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Supporting Information

Asymmetric Hydrogenation of In Situ Generated Isochromenylium Intermediates by Copper/Ruthenium Tandem Catalysis

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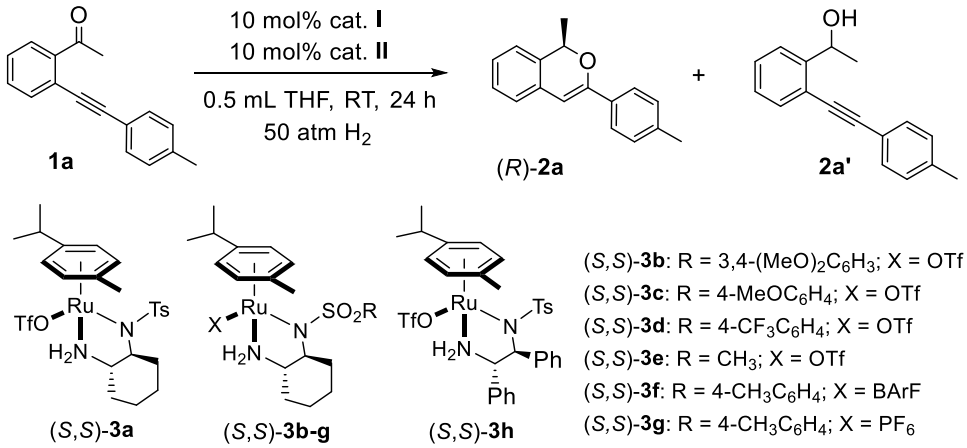
Contents

1. General information

Unless otherwise noted, all experiments were carried out under an atmosphere of nitrogen using standard Schlenk techniques or in a nitrogen-filled glovebox. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker Model Avance DMX 300 Spectrometer (^{1}H 300 MHz and ^{13}C 75 MHz, respectively), Bruker Model Avance DMX 400 Spectrometer (^{1}H 400 MHz and ^{13}C 100 MHz, respectively) and Bruker Model Avance DMX 500 Spectrometer (^{1}H 500 MHz and ^{13}C 125 MHz, respectively). Chemical shifts (δ) were given in ppm and were referenced to residual solvent or TMS peaks. Optical rotations were measured with Rudolph Autopl VI polarimeter. High resolution mass spectra (P-ESI HRMS) were obtained on Thermo Fisher Q Exactive Mass Spectrometer. HPLC analyses were performed on a Varian Prostar 210 liquid chromatograph. All organic solvents were dried using standard, published methods and were distilled before use. All other chemicals were used as received from Aldrich or Acros without further purification. The catalysts[1] and substrates[2] were synthesized according to the modified literature methods.

2. Optimization of conditions for asymmetric tandem reactions

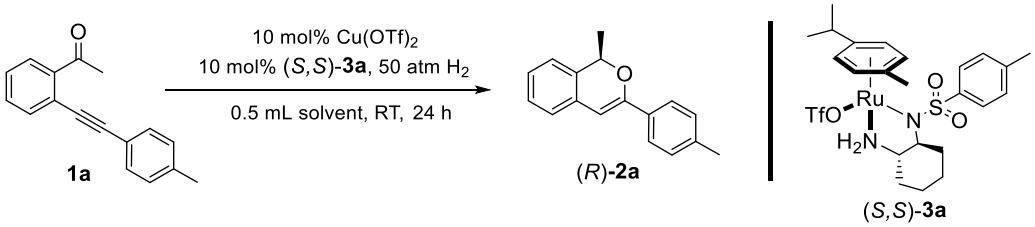
***Table S1*:** Asymmetric tandem reaction of **1a**: Screening of catalytic systems[a]



Entry	Catalyst **I**	Catalyst **II**	Conv. (%)[b]	Yield (%)[b] **2a**	**2a'**	Ee of **2a** (%)[c]	Ee of **2a'** (%)[c]
1	$Cu(OTf)_2$	$[Ru(BINAP)Cl_2]_2$[d]	72[e]	14	--[f]	30	--
2	$Cu(OTf)_2$	$[Rh(BINAP)Cl]_2$[d]	50[e]	33	--[f]	40	--
3	$Cu(OTf)_2$	$[Ir(BINAP)Cl]_2$[d]	92[e]	25	--[f]	28	--
4	$Cu(OTf)_2$	$Rh(BINAP)BF_4$[d]	<5	<5	--[f]	--[g]	--
5	$Cu(OTf)_2$	$Ir(BINAP)BF_4$[d]	85[e]	20	--[f]	11	--
6	$Cu(OTf)_2$	(*S*,*S*)-**3a**	>95	>95	--[f]	88	--
7	AgOTf	(*S*,*S*)-**3a**	>95[e]	70	--[f]	88	--
8	$Zn(OTf)_2$	(*S*,*S*)-**3a**	24	<5	24	--[g]	4
9	$Pd(OAc)_2$	(*S*,*S*)-**3a**	44[e]	<5	27	--[g]	7
10	$CuSO_4$	(*S*,*S*)-**3a**	>95[e]	30	--[f]	17	--
11	$W(CO)_6$	(*S*,*S*)-**3a**	24	<5	24	--[g]	5
12	$Ni(acac)_2$	(*S*,*S*)-**3a**	<5	<5	--[f]	--[g]	--
13	$PtCl_2$	(*S*,*S*)-**3a**	>95[e]	<5	--[f]	--[g]	--
14	TfOH[f]	(*S*,*S*)-**3a**	18	15	--[f]	81	--
15	none	(*S*,*S*)-**3a**	24	--[f]	21	--[g]	5
16	$Cu(OTf)_2$	(*S*,*S*)-**3b**	>95	92	--[f]	91	--
17	$Cu(OTf)_2$	(*S*,*S*)-**3c**	>95	92	--[f]	90	--
18	$Cu(OTf)_2$	(*S*,*S*)-**3d**	>95	>95	--[f]	50	--
19	$Cu(OTf)_2$	(*S*,*S*)-**3e**	>95[e]	50	--[f]	57	--
20	$Cu(OTf)_2$	(*S*,*S*)-**3f**	>95	95	--[f]	87	--
21	$Cu(OTf)_2$	(*S*,*S*)-**3g**	>95	88	--[f]	86	--
22	$Cu(OTf)_2$	(*S*,*S*)-**3h**	>95[e]	60	--[f]	55	--
23[h]	$Cu(OTf)_2$	**(*S*,*S*)-3b**	>95	>95	--[f]	93	--
24[h,i]	$Cu(OTf)_2$	(*S*,*S*)-**3b**	>95	>95	--[f]	91	--

[a] Reaction conditions: **1a** (0.1 mmol) in 0.5 mL THF, catalyst **I** (10 mol %), catalyst **II** (10 mol %), H_2 (50 atm), stirred at room temperature for 24 h. [b] Determined by ^1H NMR spectroscopic analysis of the crude product with 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by HPLC with a chiral OD-H column and a chiral OJ-H column. Absolute configurations of product **2a** were determined by comparison with literature data. [d] Generated *in situ* by mixing metal precursor with (*R*)-BINAP. [e] A complex mixture was obtained. [f] Product **2a** or by-product **2a'** was not observed. [g] The *ee* value was not determined. [h] Ethylene glycol dimethyl ether (GDME) was used as the solvent and reacted for 4 h. [i] 3 mol % $Cu(OTf)_2$ and 1 mol % (*S*,*S*)-**3b**, 24 h.

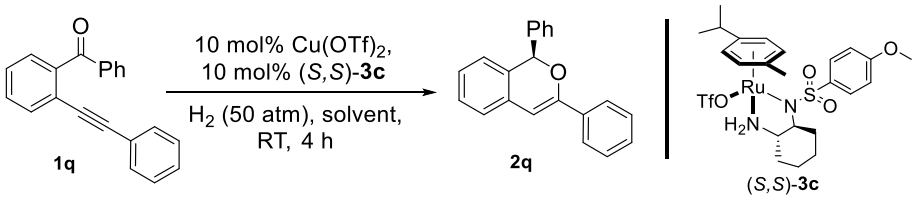
***Table S2*:** Asymmetric tandem reaction of **1a**: Screening of solvents[a]



Entry	Solvent	Conv. (%)[b]	Yield of **2a** (%)[b]	Ee of **2a** (%)[c]
1	MeOH	>95[d]	83	63
2	acetone	>95	>95	88
3	1,4-dioxane	>95	94	84
4[e]	**GDME**	**>95**	**>95**	**91**
5	THF	>95	>95	88
6	diethyl ether	>95[d]	82	88
7	EA	>95	92	88
8	DCM	>95[d]	78	84
9	DCE	>95[d]	77	83
10	toluene	>95	>95	87
11[e,f]	GDME	>95	>95	93

[a] Reaction conditions: **1a** (0.1 mmol) in solvent (0.5 mL), (*S,S*)-**3a** (10 mol %), $Cu(OTf)_2$ (10 mol %), H_2 (50 atm), stirred at room temperature for 24 h. THF = tetrahydrofuran; EA = ethyl acetate; DCM = dichloromethane; DCE = 1, 2-dichloroethane. [b] Determined by ^1H NMR spectroscopic analysis of the crude product with 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by HPLC with a chiral OD-H column. [d] A complex mixture was obtained. [e] Reacted for 4 h. [f] Catalyst (*S,S*)-**3b** was used.

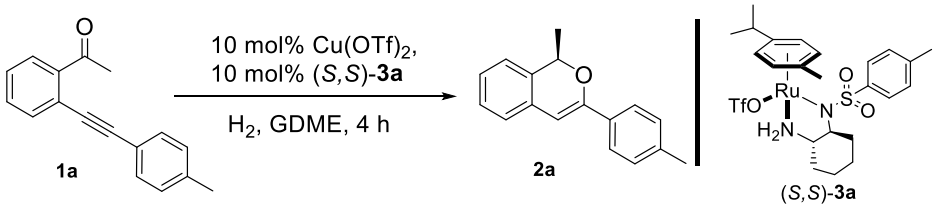
***Table S3*:** Asymmetric tandem reaction of **1q**: Screening of solvents[a]



Entry	Solvent	Conv. (%)[b]	Yield (%)[b]	Ee (%)[c]
1	MeOH	21[d]	5	-
2	acetone	41[d]	23	63
3	1,4-dioxane	50[d]	28	61
4	GDME	40	27	79
5	THF	37[d]	11	-
6	EA	90[d]	42	70
7	diethyl ether	>95[d]	40	78
8	**DCM**	**>95**	**>95**	**86**
9	DCE	>95	95	82
10	toluene	>95[d]	51	69

[a] Reaction conditions: **1q** (0.1 mmol) in solvent (0.5 mL), (*S*,*S*)-**3c** (10 mol %), $Cu(OTf)_2$ (10 mol %), H_2 (50 atm), stirred at room temperature for 4 h. Absolute configurations of products were determined by comparison with literature data. [b] The conversions were determined by ^1H NMR spectroscopy of the crude reaction mixtures, and the yields were determined by ^1H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by HPLC with a chiral OD-H column. [d] A complex mixture was obtained.

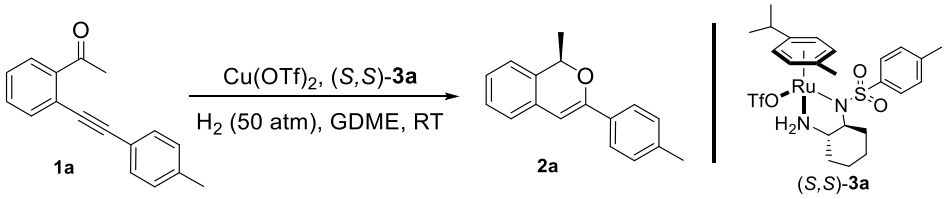
***Table S4*:** Optimization of conditions for the asymmetric tandem reaction of **1a**: the effects of temperature and H_2 pressure[a]



Entry	Temp. (℃)	H_2 (atm)	Conv. (%)[b]	Yield (%)[b]	*ee* (%)[c]
1	0	50	60[d]	32	88
2	**25**	**50**	**>95**	**>95**	**91**
3	40	50	>95	89	90
4	25	10	>95	>95	89
5	25	20	>95	>95	91
6	25	80	>95	>95	91

[a] Reaction conditions: **1a** (0.1 mmol) in GDME (0.5 mL), (*S*,*S*)-**3a** (10 mol %), $Cu(OTf)_2$ (10 mol %), stirred for 4 h. [b] The conversions were determined by ^1H NMR spectroscopy of the crude reaction mixtures, and the yields were determined by ^1H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by HPLC with a chiral OD-H column. [d] A complex mixture was obtained.

***Table S5*: Optimization of conditions for the asymmetric tandem reaction of **1a**: screening of catalytic binary systems[a]**

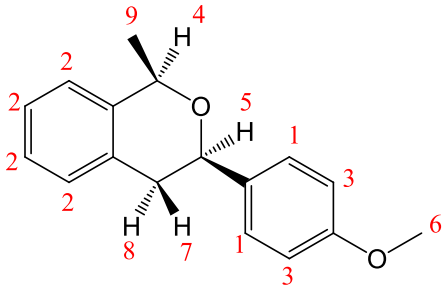


Entry	$Cu(OTf)_2$ (mol %)	(*S*,*S*)-**3a** (mol %)	Time (h)	Conv. (%)[b]	Yield (%)[b]	Ee (%)[c]
1	**10**	**10**	**4**	**>95**	**>95**	**91**
2	5	10	4	40[d]	16	83
3	10	5	4	>95	>95	87
4	15	5	4	>95	>95	91
5	5	5	4	73	60	91
6	5	5	13	>95	95	91
7	5	5	24	>95	>95	91
8	5	1	4	81[d]	40	89
9	5	1	24	>95[d]	75	90
10	3	1	4	67[d]	30	88
11[e]	**3**	**1**	**24**	**>95**	**95**	**91**
12	2	2	4	20	10	88
13	1	1	4	10	4	--

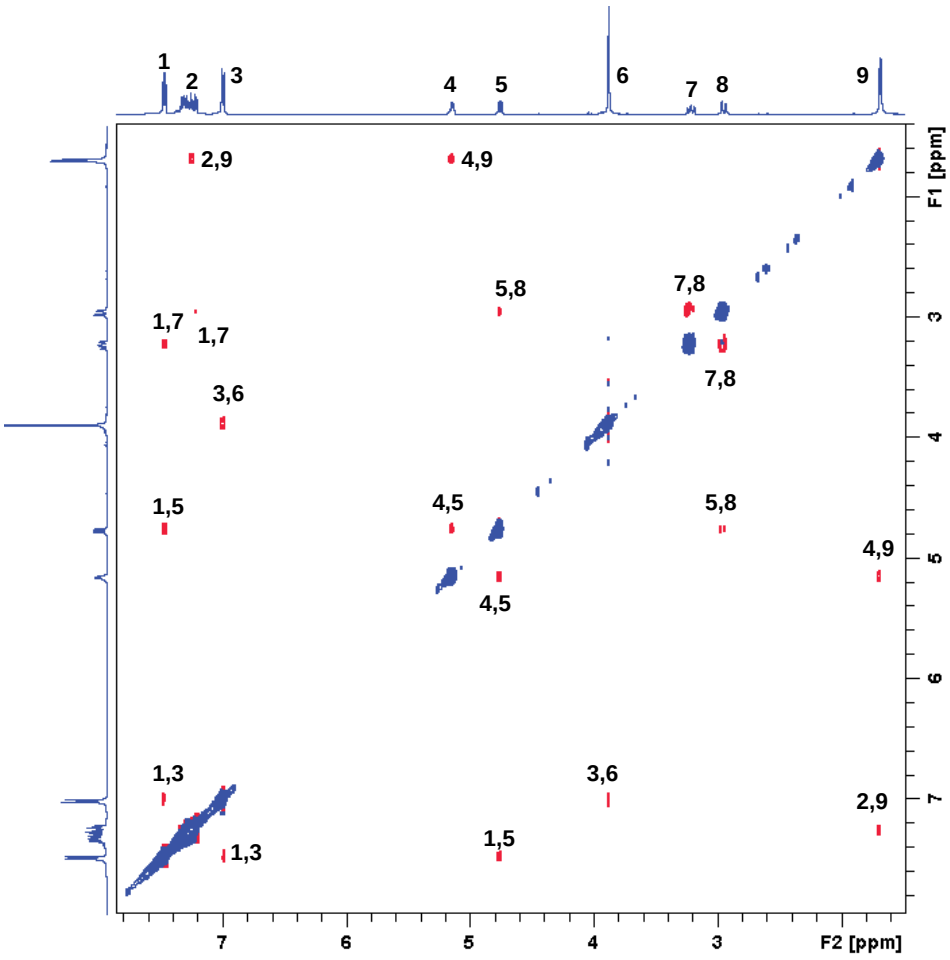
[a] Reaction conditions: **1a** (0.1 mmol) in GDME (0.5 mL), (*S*,*S*)-**3a**, $Cu(OTf)_2$, H_2 (50 atm), stirred at room temperature. [b] The conversions were determined by ^1H NMR spectroscopy of the crude reaction mixtures, and the yields were determined by ^1H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard. [c] Determined by HPLC with a chiral OD-H column. [d] A complex mixture was obtained. [e] Catalyst (*S*,*S*)-**3b** was used.

3. Determination of the absolute configuration of 4b

The absolute configuration of **4b** was determined to be *R,R* according to 2D NMR spectroscopic analysis (*Scheme S1*).



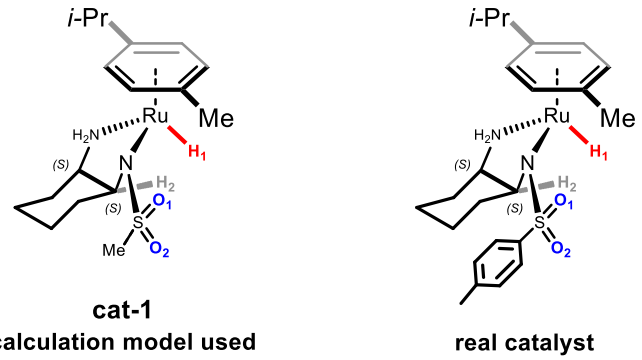
(*R,R*)-**4b**



Scheme S1. NOESY of **4b** (500 MHz, $CDCl_3$, -50 °C)

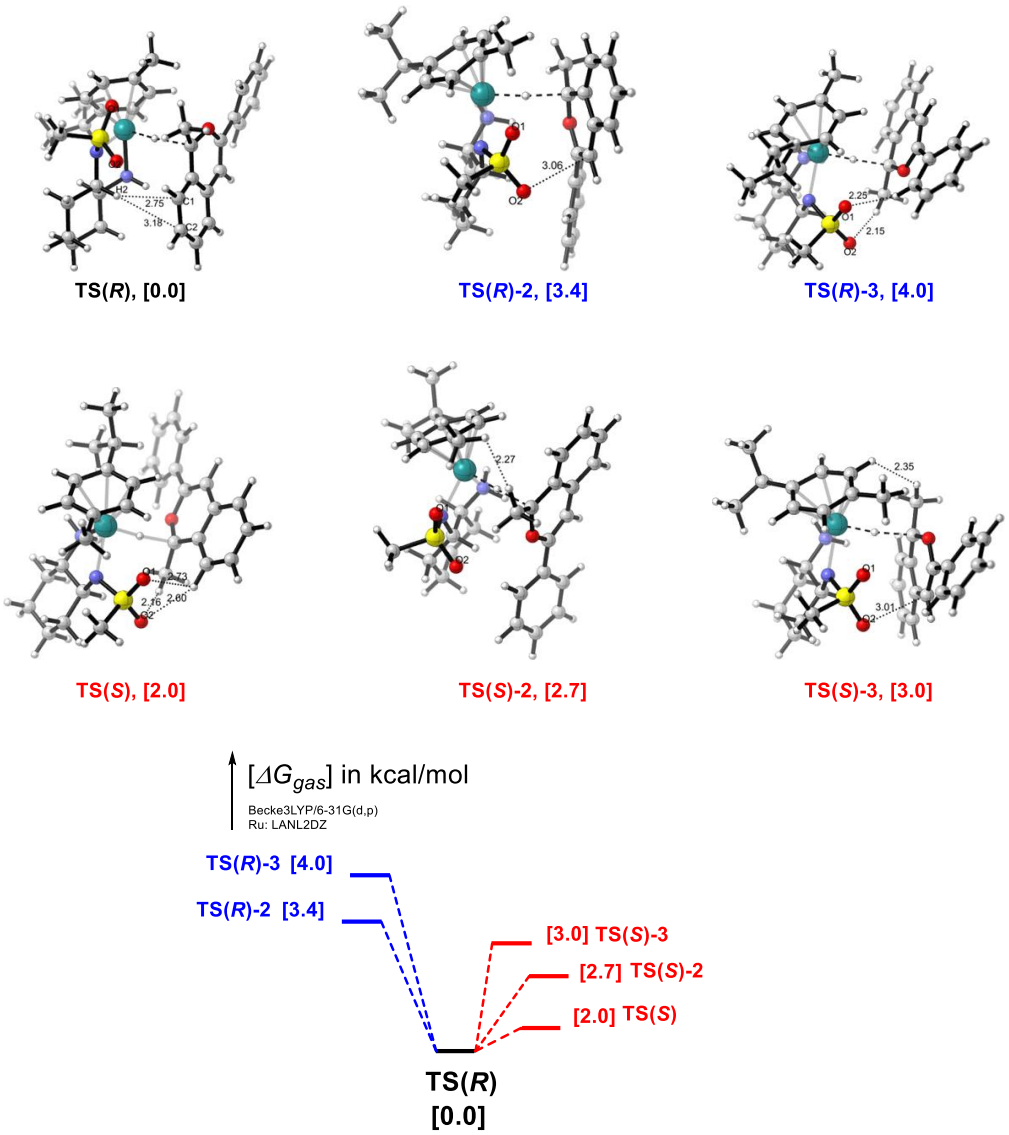
4. Theoretical calculations to elucidate the origin of chiral induction

Calculations were performed in Gaussian 09 program.[3] Becke3LYP functional[4] was used to locate all the stationary points and execute frequency analysis in the gas phase. The 6-31G(d,p) basis set is applied for all elements except for Ru, which used the LANL2DZ[4d] pseudopotential and basis set (5d keyword was used for all species). Quasiharmonic corrections were applied during the entropy calculations by setting all positive frequencies that are less than 100 cm^{-1} to 100 cm^{-1}.[5] Without sacrificing the reliability and efficiency of computations, a simplified model was used where the tosyl group in the real catalyst was replaced by a mesyl group. (Scheme S2).



Scheme S2. The simplified model catalyst for calculations

Initially, we hypothesized that the key chiral determining factors are related to the CH(sp^2)/π attraction between phenyl C-H bond on the catalyst and the π system on substrate in the hydride transfer transition states, similar to our previous report[1b] and Noyori's reaction systems.[6] But we could not locate such kinds of transition states. Instead, we found three pairs of transition states without such interaction (Scheme S3). **TS(*R*)** is the lowest transition state leading to *R* product while **TS(*S*)** is the lowest transition state leading to *S* product. The relative Gibbs free energy of **TS(*S*)** is higher than **TS(*R*)** by 2.0 kcal/mol in the gas phase. As mentioned in the main-text of this paper, the most favored **TS(*R*)** has hydrogen bondings and CH(sp^3)/π attraction. **TS(*R*)-2**, which also leads to *R* product, is 3.4 kcal/mol higher than **TS(*R*)** and experiences steric repulsion between tosyl group and substrate (the distance of O of tosyl group and the carbon of substrate is less than the sum (3.2 Å) of van der Waals

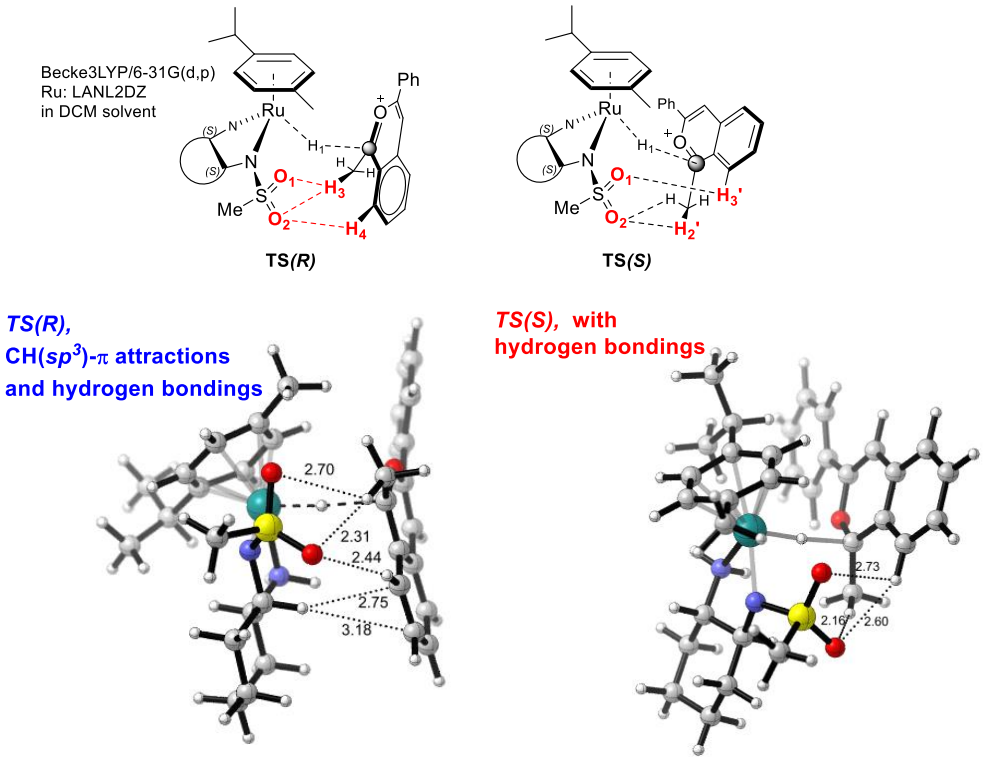


Scheme S3. The gas phase H-transfer transition states and their relative free energies computed at the B3LYP level of theory (quasiharmonic corrections applied)

radius of these two atoms, see Scheme S3). **TS(*R*)-3** is another transition state leading to *R* product with fewer hydrogen bondings, and is disfavored over **TS(*R*)** by 4.0 kcal/mol. Both **TS(*R*)-2** and **TS(*R*)-3** do not have the CH(sp^3)/π attraction. None of CH(sp^3)/π attraction exist in–**TS(*S*), TS(*S*)-2&3** that lead to *S* product. **TS(*S*)-2&3** have H...H repulsion, while such repulsion is absent in **TS(*S*)**. The steric hindrances in **TS(*S*)-2&3** make these two transition states about 2.7 and 3.0 kcal/mol is favored over **TS(*R*)**, respectively. Comparing all 6 transition states, we conclude three factors make **TS(*R*)** the most stabilized one: hydrogen bonding interaction, and CH(sp^3)/π attraction, absence of steric repulsion between catalyst and substrate. We emphasize

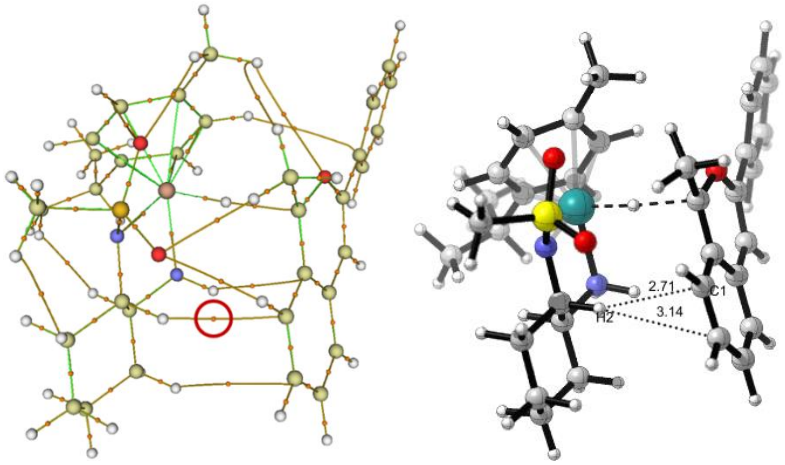
here that the benzene ring can rotate and there should have many conformations. We have considered this in search the most favored transition states by trying to locate all hydride-transfer transition states that can avoid the steric repulsion of the *i*-Pr and Me groups of the catalyst with the substrate. In Scheme S3, the relative energies of transition states in the gas phase are referred to **TS(*R*)**.

To study the solvent effect to the geometry of transition states in the gas phase, we then optimized both **TS(*R*)** and **TS(*S*)** in DCM solvent with IEFPCM using UA0[7] radii by the B3LYP method (6-31G(d,p) basis set for all elements except for Ru, which used the LANL2DZ pseudopotential and basis set). We found that **TS(*R*)** and **TS(*S*)** are close in structure with respect to their gas phase structures (Scheme S4). **TS(*R*)** is favored over **TS(*S*)** by 2.4 kcal/mol in solution (while **TS(*R*)** is favored over **TS(*S*)** by 2.0 kcal/mol in the gas phase). These are the relative energies discussed in the main text of this paper.

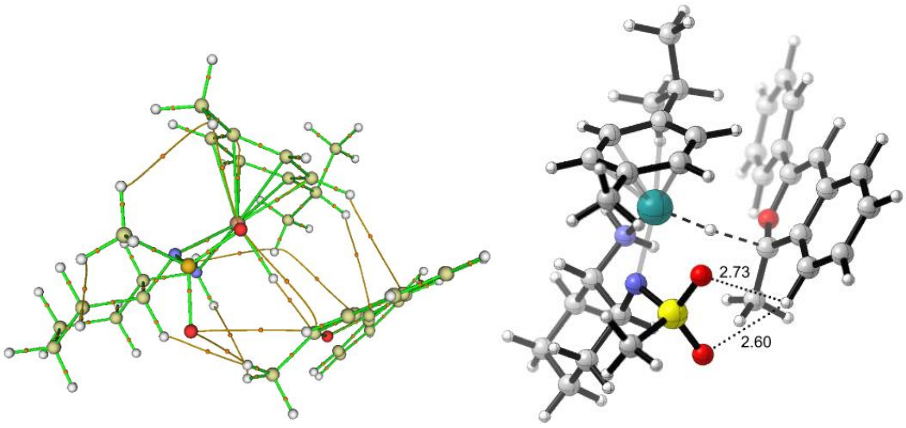


Scheme S4. The optimized transition states in DCM solvent

Atoms in molecules (AIM)[8] analysis for **TS(*R*)** and **TS(*S*)** (Scheme S5) at the bond critical point suggested a weak interaction between H_2 and C_1, where the electron density (ρ_b) was 0.0066 au and the Laplacian values ($\Delta^2\rho_b$) was 0.02005 au, indicating that a CH(sp^3)/π attraction was present.[6] The analysis also indicated that all of the hydrogen bondings such as O atom in tosyl with H in the substrate above were present. Consequently, the CH(sp^3)/π attraction and conventional hydrogen bondings are factors stabilizing **TS(*R*)**.



TS(*R*) in the gas phase



TS(*S*) in the gas phase

Scheme S5. AIM analysis of **TS(*R*)** and **TS(*S*)**

We also checked how the basis set and computational methods affect the calculation results (Table S6, electronic energies without zero-point energy corrections are used). At the B3LYP level using a larger basis set (6-311+G(d,p) for all elements and SDD pseudopotential and basis set for Ru), **TS(*R*)** is still lower in energy than **TS(*S*)** by about 2.4 kcal/mol in both the gas phase and DCM solution. Single point energy calculations using B3LYP-D3[9] with lager basis set in both gas phase and solution showed that TS(***R***) is favored by 1.9 and 1.8 kcal/mol, respectively. We also used B3LYP-D3 located both TS(***R***) and TS(***S***), finding that their geometries are similar and TS(***R***) is lower than TS(***S***) by 1.6 and 2.0 kcal/mol in the gas phase and DCM solution, respectively. M06-2X [10] calculations to consider the dispersion effects also showed that **TS(*R*)** is lower in energy than **TS(*S*)** by about 2.7 and 2.5 kcal/mol in the gas phase and DCM solution, respectively. Therefore, we think that it is reasonable to use the results in Schemes S3 and S4 to understand the origin of enantioselectivity of the present reaction.

Table S6, ΔE in kcal/mol, others in Hartree/Particle

	***ΔE*=(*S*-*R*)**	**TS(*R*) Single Point Energy**	**TS(*S*) Single Point Energy**
B3LYP/6-31G(d,p)/LANL2DZ in gas phase	2.4	-2110.467392	-2110.463604
B3LYP/6-311+G(d,p)/SDD// B3LYP/6-31G(d,p)/LANL2DZ in gas phase	2.4	-2111.922976	-2111.919096
B3LYP/6-311+G(d,p)/SDD//B3LYP/6-31G(d,p)/LANL2DZ in DCM	2.4	-2111.977634	-2111.973816
M06-2X/6-311+G(d,p)/SDD//B3LYP/6-31G(d,p)/LANL2DZ in gas phase	2.7	-2111.053151	-2111.04884
M06-2X/6-311+G(d,p)/SDD//B3LYP/6-31G(d,p)/LANL2DZ in DCM	2.5	-2111.108116	-2111.104184
B3LYP-D3/6-311+G(d,p)/SDD//B3LYP/6-31G(d,p)/LANL2DZ in gas phases	1.9	-2112.050221	-2112.047222
B3LYP-D3/6-311+G(d,p)/SDD//B3LYP/6-31G(d,p)/LANL2DZ in DCM	1.8	-2112.10488	-2112.101942
B3LYP-D3/6-31G(d,p)/LANL2DZ in gas phases	1.6	-2110.598533	-2110.595925
B3LYP-D3/6-31G(d,p)/LANL2DZ in DCM	2.0	-2110.652161	-2110.648897

5. Cartesian Coordinates and energies

For *Scheme S3*

In gas phase	*ΔG*	*ΔH*	*ΔE*	Quasiharmonic correction to Gibbs Free Energy	Energy with zero-point correction	Thermal Enthalpy	Thermal Free Energy	Zero-point correction	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
TS(*R*)	0.0	0.0	0.0	0.638689	-2109.766494	-2109.726184	-2109.837899	0.700898	0.741209	0.629494
TS(*R*)-2	3.4	3.8	3.7	0.638034	-2109.760623	-2109.720198	-2109.831357	0.700641	0.741066	0.629907
TS(*R*)-3	4.0	4.1	4.2	0.638139	-2109.759826	-2109.719681	-2109.830355	0.701055	0.7412	0.630526
TS(*S*)	2.0	2.3	2.2	0.638267	-2109.762931	-2109.722585	-2109.834772	0.700673	0.741019	0.628833
TS(*S*)-2	2.7	2.8	2.8	0.638440	-2109.762076	-2109.721773	-2109.832626	0.700814	0.741118	0.630265
TS(*S*)-3	3.0	3.4	3.3	0.637672	-2109.761257	-2109.720807	-2109.832747	0.70027	0.74072	0.62878

Becke3LYP method, 6-31G(d,p) for C,H,O,N,S; LANL2DZ for Ru

ΔG, ΔH, ΔE in kcal/mol, others in Hartree/Particle

For *Scheme S4*

	ΔG	*ΔH*	*ΔE*	Quasiharmonic correction to Gibbs Free Energy	Energy with zero-point correction	Thermal Enthalpy	Thermal Free Energy	Zero-point correction	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
In DCM solution phase										
TS(*R*)	0.0	0.0	0.0	0.638598	-2109.820231	-2109.779884	-2109.892154	0.700864	0.741211	0.628941
TS(*S*)	2.4	2.3	2.8	0.63831	-2109.816457	-2109.776222	-2109.887635	0.70058	0.740815	0.629402

Becke3LYP/6-31G(d,p), LANL2DZ

In DCM solvent

ΔG, ΔH, ΔE in kcal/mol, others in Hartree/Particle

Cartesian Coordinates

TS(*R*) in DCM solvent

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.279396	1.013288	0.171468
2	1	0	0.294248	-0.470893	0.691810
3	6	0	1.133197	-1.943048	1.149829
4	6	0	0.749145	-1.931973	2.596088
5	1	0	-0.331279	-1.907046	2.724472
6	1	0	1.185504	-1.068949	3.095426
7	1	0	1.145606	-2.845898	3.056559
8	8	0	2.392302	-1.515727	0.961757
9	6	0	3.049945	-1.614603	-0.240876
10	6	0	2.508211	-2.367354	-1.235476
11	1	0	3.050753	-2.500509	-2.163044
12	6	0	1.273808	-3.062104	-1.032046
13	6	0	0.570514	-2.858628	0.191054
14	6	0	-0.637728	-3.550024	0.435471
15	6	0	0.748988	-3.964349	-1.982269
16	1	0	1.282830	-4.124222	-2.913534
17	6	0	-1.119686	-4.442777	-0.506033
18	1	0	-0.816761	-5.349637	-2.446554
19	6	0	-0.425169	-4.648787	-1.716154
20	1	0	-2.040465	-4.983241	-0.314359
21	1	0	-1.195175	-3.366816	1.346789
22	8	0	-2.758049	-1.559505	2.464770
23	8	0	-1.510868	0.522740	3.157154
24	6	0	-2.846336	-0.622042	-0.282492
25	6	0	1.743274	1.971903	0.410012
26	6	0	1.046476	2.191283	1.646329
27	6	0	-0.732998	3.333696	0.340441
28	6	0	-0.033176	3.166003	-0.863710
29	7	0	-2.257650	0.304419	0.721817
30	1	0	-2.686777	0.855811	-1.828680
31	1	0	-2.483507	-1.646771	-0.114598
32	1	0	-0.484742	0.336878	-2.432665
33	1	0	-0.462333	-1.028001	-1.548307

34	1	0	2.689809	1.443852	0.413343
35	1	0	-1.701374	3.818508	0.347571
36	16	0	-2.537659	-0.094967	2.288718
37	6	0	1.196341	2.416268	-0.811309
38	6	0	-0.215539	2.815408	1.572246
39	6	0	-2.335946	-0.167712	-1.653140
40	7	0	-0.849932	-0.084588	-1.579265
41	6	0	-4.077230	0.723186	2.777543
42	1	0	-4.908921	0.376780	2.167173
43	1	0	-3.937672	1.797901	2.657939
44	1	0	-4.248778	0.476954	3.827133
45	6	0	-4.387811	-0.679326	-0.311270
46	1	0	-4.781045	0.340301	-0.420936
47	1	0	-4.756526	-1.077243	0.637300
48	6	0	-2.822331	-1.071035	-2.792486
49	1	0	-2.432804	-0.698278	-3.747675
50	1	0	-2.414000	-2.081379	-2.651260
51	6	0	-4.356807	-1.131685	-2.817346
52	1	0	-4.754692	-0.140004	-3.071644
53	1	0	-4.690194	-1.815547	-3.605438
54	6	0	-4.904984	-1.570216	-1.454149
55	1	0	-6.000502	-1.555044	-1.461524
56	1	0	-4.609229	-2.610706	-1.262667
57	6	0	4.337304	-0.909414	-0.252903
58	6	0	4.982971	-0.577522	0.952711
59	6	0	4.950178	-0.568887	-1.473510
60	6	0	6.217519	0.068807	0.933012
61	1	0	4.525559	-0.840786	1.899498
62	6	0	6.183523	0.076698	-1.484319
63	1	0	4.456689	-0.789610	-2.414329
64	6	0	6.822487	0.395904	-0.282554
65	1	0	6.708969	0.312281	1.869712
66	1	0	6.643024	0.337772	-2.432396
67	1	0	7.783880	0.899866	-0.294669
68	1	0	-0.812487	2.896863	2.471612
69	1	0	1.729530	2.211702	-1.734369
70	6	0	1.633462	1.770486	2.965134
71	1	0	2.144104	2.619768	3.434546
72	1	0	0.847404	1.424767	3.639096
73	1	0	2.370923	0.974826	2.834613
74	6	0	-0.493150	3.735013	-2.196259
75	1	0	-0.302265	2.965217	-2.956887
76	6	0	0.381951	4.956964	-2.554828
77	1	0	0.111099	5.335237	-3.545320

78	1	0	0.233888	5.764064	-1.829466
79	1	0	1.446079	4.702788	-2.567949
80	6	0	-1.982095	4.098251	-2.252671
81	1	0	-2.247050	4.410319	-3.266972
82	1	0	-2.620185	3.251554	-1.981691
83	1	0	-2.219061	4.932193	-1.583464

TS(*S*) in DCM solvent

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.721961	-0.142292	0.974323
2	1	0	-0.004237	0.344326	-0.482053
3	6	0	-0.859276	0.838055	-1.904571
4	8	0	3.276102	1.116099	-2.222944
5	8	0	2.611549	2.320513	-0.104943
6	6	0	2.759026	-1.456496	-0.923732
7	6	0	-0.656203	1.251370	2.087051
8	6	0	0.656159	1.763552	2.264941
9	6	0	1.346646	-0.374322	3.222375
10	6	0	0.035230	-0.873631	3.007219
11	7	0	2.605428	-0.227229	-0.100209
12	1	0	2.520081	-2.706195	0.802211
13	1	0	2.259010	-1.330158	-1.896448
14	1	0	0.193020	-2.769803	0.743470
15	1	0	0.101136	-2.110973	-0.739233
16	1	0	-1.406552	1.884168	1.625033
17	1	0	0.901406	2.756208	1.911962
18	1	0	2.111148	-1.024531	3.631985
19	1	0	-0.166648	-1.910776	3.255069
20	1	0	0.967003	2.839313	-2.248589
21	6	0	0.006312	3.175864	-1.880474
22	6	0	-0.206905	4.518355	-1.620730
23	6	0	-1.023473	2.243886	-1.632177
24	6	0	-1.440563	4.956876	-1.099094
25	1	0	0.582570	5.236636	-1.814382
26	6	0	-2.270437	2.681853	-1.102356

27	6	0	-2.458871	4.054575	-0.839823
28	1	0	-1.592984	6.012669	-0.898220
29	6	0	-3.304672	1.716324	-0.885149
30	16	0	3.249091	1.141760	-0.732364
31	1	0	-3.409999	4.392639	-0.440834
32	1	0	-4.254242	2.040428	-0.478807
33	6	0	-1.020998	-0.060347	2.503342
34	6	0	1.668592	0.957444	2.852608
35	6	0	0.120715	0.312875	-2.911319
36	1	0	0.115685	-0.777455	-2.905458
37	1	0	-0.211706	0.645184	-3.903046
38	1	0	1.133687	0.676187	-2.739438
39	6	0	2.035298	-2.578184	-0.172926
40	7	0	0.651872	-2.108019	0.119283
41	6	0	4.980195	1.227265	-0.206208
42	1	0	5.539532	0.377226	-0.591283
43	1	0	5.007487	1.240587	0.882646
44	1	0	5.383628	2.158475	-0.608562
45	6	0	4.209728	-1.895937	-1.211492
46	1	0	4.752658	-1.979953	-0.260513
47	1	0	4.708876	-1.133973	-1.814786
48	6	0	2.059795	-3.910985	-0.930446
49	1	0	1.537938	-4.676156	-0.343184
50	1	0	1.509464	-3.801039	-1.875373
51	8	0	-1.940574	0.040226	-1.824942
52	6	0	-3.129206	0.417056	-1.244712
53	6	0	3.504395	-4.342511	-1.223262
54	1	0	4.015135	-4.566625	-0.277018
55	1	0	3.504468	-5.269032	-1.807450
56	6	0	4.260616	-3.235286	-1.966324
57	1	0	3.821561	-3.103718	-2.964685
58	1	0	5.305433	-3.525684	-2.122093
59	6	0	-4.097781	-0.683784	-1.156911
60	6	0	-3.860439	-1.902103	-1.819789
61	6	0	-5.286198	-0.533970	-0.416700
62	6	0	-4.789900	-2.937867	-1.745825
63	1	0	-2.955497	-2.031360	-2.401501
64	6	0	-6.209700	-1.573125	-0.346808
65	1	0	-5.490313	0.388655	0.115906
66	6	0	-5.966508	-2.779105	-1.010869
67	1	0	-4.594962	-3.869570	-2.267841
68	1	0	-7.119859	-1.441659	0.229877
69	1	0	-6.688714	-3.587591	-0.954496
70	6	0	3.042965	1.513297	3.094801

71	1	0	3.287528	2.276136	2.354595
72	1	0	3.072197	1.976349	4.088555
73	1	0	3.801627	0.727190	3.073823
74	6	0	-2.473842	-0.507169	2.478075
75	1	0	-2.961419	0.051618	1.671819
76	6	0	-2.676573	-2.003261	2.200511
77	1	0	-3.745192	-2.220538	2.116624
78	1	0	-2.203540	-2.308423	1.262083
79	1	0	-2.281473	-2.627627	3.008932
80	6	0	-3.152840	-0.100631	3.804222
81	1	0	-3.065751	0.975264	3.985210
82	1	0	-4.216967	-0.356460	3.778810
83	1	0	-2.699402	-0.624888	4.652731

TS(*R*) in gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.300023	1.012176	0.171531
2	1	0	0.294740	-0.474281	0.659473
3	6	0	1.169446	-1.973010	1.094006
4	6	0	0.802093	-2.006419	2.542348
5	1	0	-0.275840	-2.048048	2.688665
6	1	0	1.190931	-1.129026	3.055178
7	1	0	1.259221	-2.904622	2.979305
8	8	0	2.420245	-1.519853	0.904885
9	6	0	3.076283	-1.584877	-0.300873
10	6	0	2.541348	-2.330192	-1.305613
11	1	0	3.088196	-2.445801	-2.233348
12	6	0	1.313208	-3.040211	-1.114482
13	6	0	0.607240	-2.864003	0.111929
14	6	0	-0.602112	-3.560619	0.340457
15	6	0	0.795065	-3.929372	-2.080382
16	1	0	1.334226	-4.075418	-3.011561
17	6	0	-1.077959	-4.437410	-0.619721
18	1	0	-0.761639	-5.316260	-2.571416
19	6	0	-0.377623	-4.622870	-1.829392

20	1	0	-1.998056	-4.983596	-0.439935
21	1	0	-1.168236	-3.386205	1.249021
22	8	0	-2.545055	-1.717444	2.377698
23	8	0	-1.355745	0.382991	3.139146
24	6	0	-2.872618	-0.607204	-0.261573
25	6	0	1.716084	1.996536	0.404076
26	6	0	1.038245	2.158011	1.659741
27	6	0	-0.786263	3.311783	0.429535
28	6	0	-0.106660	3.200767	-0.793068
29	7	0	-2.257262	0.287616	0.752383
30	1	0	-2.744657	0.922252	-1.759600
31	1	0	-2.505293	-1.638024	-0.139882
32	1	0	-0.562293	0.378789	-2.449720
33	1	0	-0.540298	-0.998549	-1.576822
34	1	0	2.671817	1.485892	0.371155
35	1	0	-1.765632	3.772053	0.469473
36	16	0	-2.410848	-0.236702	2.312333
37	6	0	1.138747	2.475733	-0.789260
38	6	0	-0.235301	2.762739	1.632472
39	6	0	-2.404021	-0.112070	-1.631743
40	7	0	-0.913418	-0.048726	-1.593628
41	6	0	-3.949317	0.458719	2.961617
42	1	0	-4.807731	0.095655	2.400199
43	1	0	-3.879594	1.544816	2.899401
44	1	0	-4.014873	0.140230	4.003520
45	6	0	-4.414192	-0.667975	-0.239410
46	1	0	-4.811744	0.354585	-0.286976
47	1	0	-4.745068	-1.109050	0.703809
48	6	0	-2.933898	-0.970421	-2.785846
49	1	0	-2.575075	-0.569913	-3.742978
50	1	0	-2.528879	-1.988452	-2.692296
51	6	0	-4.469347	-1.022826	-2.761789
52	1	0	-4.869328	-0.020521	-2.965935
53	1	0	-4.832807	-1.672616	-3.564773
54	6	0	-4.973390	-1.511105	-1.398520
55	1	0	-6.068013	-1.492762	-1.370006
56	1	0	-4.678655	-2.560016	-1.257703
57	6	0	4.351071	-0.858543	-0.304271
58	6	0	4.991243	-0.528462	0.904942
59	6	0	4.961180	-0.497112	-1.520319
60	6	0	6.215719	0.135991	0.892725
61	1	0	4.539525	-0.812135	1.848660
62	6	0	6.184220	0.166639	-1.524288
63	1	0	4.472737	-0.717913	-2.464187

64	6	0	6.816488	0.483761	-0.318771
65	1	0	6.704664	0.375479	1.831710
66	1	0	6.642638	0.442032	-2.468802
67	1	0	7.771073	1.000382	-0.324923
68	1	0	-0.814979	2.796410	2.546180
69	1	0	1.662459	2.321024	-1.728039
70	6	0	1.652998	1.698357	2.952457
71	1	0	2.149340	2.539932	3.450320
72	1	0	0.883478	1.305673	3.619705
73	1	0	2.408141	0.927482	2.778449
74	6	0	-0.605341	3.807985	-2.095179
75	1	0	-0.420894	3.065881	-2.886397
76	6	0	0.240716	5.055653	-2.435331
77	1	0	-0.062008	5.464548	-3.403919
78	1	0	0.100160	5.835320	-1.679523
79	1	0	1.308700	4.823241	-2.485247
80	6	0	-2.100849	4.149862	-2.104970
81	1	0	-2.399673	4.480736	-3.103526
82	1	0	-2.721424	3.290522	-1.832491
83	1	0	-2.330592	4.966964	-1.413079

TS(*R*)-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.567297	0.134874	-0.262609
2	1	0	-0.288271	1.088441	-0.813013
3	6	0	0.947500	1.853734	-1.744435
4	6	0	0.221816	1.876725	-3.061720
5	1	0	-0.739813	2.379343	-2.978264
6	1	0	0.055935	0.861046	-3.421486
7	1	0	0.836288	2.408837	-3.798081
8	8	0	1.874527	0.875028	-1.723392
9	6	0	2.836770	0.778052	-0.739054
10	6	0	2.967337	1.785519	0.162671
11	1	0	3.726866	1.714000	0.929043
12	6	0	2.174020	2.966283	0.059096

13	6	0	1.174824	3.029682	-0.954054
14	6	0	0.449816	4.227590	-1.149107
15	6	0	2.397035	4.094330	0.876048
16	1	0	3.148431	4.040373	1.657045
17	6	0	0.705429	5.327111	-0.352353
18	1	0	1.853810	6.120614	1.300537
19	6	0	1.672853	5.253825	0.672732
20	1	0	0.160872	6.251704	-0.513665
21	1	0	-0.293957	4.293696	-1.935053
22	8	0	1.869121	0.067370	2.445964
23	8	0	-0.112920	1.638229	2.228027
24	6	0	0.526328	-1.865636	0.809144
25	6	0	-3.480534	0.321893	-1.477758
26	6	0	-3.067595	1.610469	-1.080457
27	6	0	-3.094086	0.896095	1.234545
28	6	0	-3.593954	-0.388121	0.842926
29	7	0	-0.289553	-0.709849	1.247408
30	1	0	-1.173496	-2.886901	-0.006532
31	1	0	1.507657	-1.529757	0.443492
32	1	0	-1.080614	-1.803014	-2.114729
33	1	0	0.326637	-1.060007	-1.732827
34	1	0	-3.595712	0.103301	-2.534957
35	1	0	-2.880304	2.368088	-1.833856
36	1	0	-2.874133	1.085643	2.278365
37	1	0	-3.749259	-1.142383	1.603910
38	16	0	0.399609	0.261546	2.384642
39	6	0	-3.809985	-0.692987	-0.510017
40	6	0	-2.894091	1.938374	0.305918
41	6	0	-0.209842	-2.509658	-0.367363
42	7	0	-0.542036	-1.423254	-1.337081
43	6	0	-0.241901	-0.302662	3.980543
44	1	0	0.053841	-1.337140	4.151615
45	1	0	-1.328626	-0.213743	3.971418
46	1	0	0.185822	0.345572	4.747686
47	6	0	0.786488	-2.943605	1.881883
48	1	0	-0.176774	-3.279342	2.290008
49	1	0	1.361433	-2.506035	2.701732
50	6	0	0.583170	-3.663944	-0.988658
51	1	0	0.023825	-4.091980	-1.830961
52	1	0	1.531159	-3.280685	-1.391202
53	6	0	0.866283	-4.740888	0.072411
54	1	0	-0.082482	-5.202727	0.378018
55	1	0	1.475083	-5.540241	-0.362859
56	6	0	1.564142	-4.137718	1.298896

57	1	0	1.696272	-4.903313	2.071121
58	1	0	2.571083	-3.805271	1.014443
59	6	0	3.663780	-0.427340	-0.850158
60	6	0	3.857445	-1.055000	-2.094314
61	6	0	4.295226	-0.950817	0.293622
62	6	0	4.680194	-2.175449	-2.192949
63	1	0	3.387138	-0.649145	-2.983956
64	6	0	5.118183	-2.069246	0.183643
65	1	0	4.094685	-0.513401	1.265835
66	6	0	5.315606	-2.682755	-1.056773
67	1	0	4.836273	-2.644574	-3.159505
68	1	0	5.599726	-2.468322	1.070960
69	1	0	5.960615	-3.552261	-1.137432
70	6	0	-2.515034	3.318237	0.763842
71	1	0	-2.075966	3.902404	-0.046842
72	1	0	-3.406555	3.851141	1.115639
73	1	0	-1.793106	3.259926	1.580233
74	6	0	-4.389909	-2.013108	-0.995839
75	1	0	-3.798124	-2.320890	-1.870552
76	6	0	-4.345288	-3.148473	0.034773
77	1	0	-5.008047	-2.946493	0.882837
78	1	0	-4.686277	-4.079961	-0.425361
79	1	0	-3.336931	-3.316310	0.425209
80	6	0	-5.838840	-1.783453	-1.483419
81	1	0	-5.892805	-1.014274	-2.259343
82	1	0	-6.247920	-2.709716	-1.897587
83	1	0	-6.480795	-1.471080	-0.653277

TS(*R*)-3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.773862	0.261823	0.949627
2	1	0	0.264999	0.897247	-0.247764
3	6	0	1.421840	1.456635	-1.399001
4	6	0	0.495781	1.566878	-2.574514
5	1	0	-0.319359	2.264726	-2.384634

6	1	0	0.082556	0.591656	-2.839587
7	1	0	1.077628	1.949623	-3.423096
8	8	0	2.203532	0.368826	-1.509183
9	6	0	3.340168	0.163581	-0.766921
10	6	0	3.815406	1.179250	0.007745
11	1	0	4.711550	1.025827	0.596351
12	6	0	3.173015	2.456550	0.011446
13	6	0	1.958652	2.612156	-0.714374
14	6	0	1.328410	3.875492	-0.757558
15	6	0	3.715157	3.572435	0.688458
16	1	0	4.644969	3.457189	1.237444
17	6	0	1.881839	4.955172	-0.092986
18	1	0	3.508313	5.653054	1.151717
19	6	0	3.078853	4.799653	0.636216
20	1	0	1.401617	5.927006	-0.141254
21	1	0	0.418826	4.009792	-1.332556
22	8	0	-1.142287	-1.166573	-3.014009
23	8	0	-0.106730	-2.270858	-0.976302
24	6	0	-2.869223	0.403812	-1.292037
25	6	0	1.050728	-0.221361	2.195289
26	6	0	0.414535	-1.456227	1.913735
27	6	0	-1.636697	-0.640507	2.945249
28	6	0	-0.994989	0.611299	3.166316
29	7	0	-1.985762	-0.587909	-0.627492
30	1	0	-3.831236	0.847410	0.569407
31	1	0	-2.314633	0.962091	-2.064105
32	1	0	-2.291236	2.483529	1.245751
33	1	0	-1.572066	2.537987	-0.212845
34	1	0	2.075985	-0.074063	1.876544
35	1	0	0.943743	-2.215340	1.353021
36	1	0	-2.675300	-0.761863	3.224646
37	1	0	-1.568729	1.419017	3.614583
38	16	0	-1.300108	-1.702502	-1.640826
39	6	0	0.378258	0.833343	2.876054
40	6	0	-0.932472	-1.695029	2.317111
41	6	0	-3.295808	1.400922	-0.211453
42	7	0	-2.052065	1.914141	0.435017
43	6	0	-2.443700	-3.099800	-1.779022
44	1	0	-3.383334	-2.783140	-2.226610
45	1	0	-2.611609	-3.516352	-0.787048
46	1	0	-1.948994	-3.830346	-2.421729
47	6	0	-4.128349	-0.171578	-1.974275
48	1	0	-4.674485	-0.790142	-1.249454
49	1	0	-3.825804	-0.814240	-2.803923

50	6	0	-4.187154	2.524078	-0.751920
51	1	0	-4.468428	3.201334	0.064915
52	1	0	-3.615723	3.120543	-1.478502
53	6	0	-5.437110	1.947425	-1.433892
54	1	0	-6.066047	1.455025	-0.679940
55	1	0	-6.036696	2.759255	-1.858284
56	6	0	-5.043845	0.938334	-2.519234
57	1	0	-5.939219	0.488078	-2.960531
58	1	0	-4.529025	1.463414	-3.335271
59	6	0	3.926434	-1.164693	-0.956815
60	6	0	3.127266	-2.242827	-1.380569
61	6	0	5.298874	-1.370216	-0.716213
62	6	0	3.699272	-3.503059	-1.544523
63	1	0	2.065370	-2.102073	-1.551335
64	6	0	5.857655	-2.632575	-0.883487
65	1	0	5.935896	-0.538738	-0.431431
66	6	0	5.058852	-3.702963	-1.297486
67	1	0	3.075673	-4.331529	-1.865540
68	1	0	6.918320	-2.779502	-0.705892
69	1	0	5.498359	-4.686615	-1.432193
70	6	0	-1.540830	-3.064506	2.081275
71	1	0	-1.155554	-3.400414	1.112116
72	6	0	1.076734	2.102648	3.284624
73	1	0	0.375539	2.938612	3.359782
74	1	0	1.542700	1.977009	4.269586
75	1	0	1.862173	2.376475	2.577221
76	6	0	-1.017304	-4.039366	3.161009
77	1	0	-1.394378	-5.047877	2.966481
78	1	0	0.075671	-4.084669	3.171700
79	1	0	-1.355163	-3.740070	4.159031
80	6	0	-3.074285	-3.071922	2.033303
81	1	0	-3.452925	-2.351252	1.303094
82	1	0	-3.431743	-4.067405	1.752904
83	1	0	-3.513627	-2.843442	3.010841

TS(*S*) in gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	44	0	0.707035	-0.279582	0.965678
2	1	0	0.012490	0.343836	-0.461677
3	6	0	-0.823739	0.970911	-1.837396
4	8	0	3.140976	1.340067	-2.057757
5	8	0	2.503178	2.303963	0.192495
6	6	0	2.795825	-1.356828	-1.005450
7	6	0	-0.739145	0.972012	2.157000
8	6	0	0.553436	1.517136	2.388717
9	6	0	1.305788	-0.656309	3.204360
10	6	0	0.017397	-1.184342	2.934547
11	7	0	2.609021	-0.229912	-0.055253
12	1	0	2.570009	-2.777637	0.583561
13	1	0	2.297205	-1.142857	-1.964469
14	1	0	0.228201	-2.890676	0.461293
15	1	0	0.170467	-2.069829	-0.943591
16	1	0	-1.503794	1.609065	1.725722
17	1	0	0.770695	2.536403	2.098947
18	1	0	2.088264	-1.305015	3.581754
19	1	0	-0.152830	-2.241888	3.112842
20	1	0	1.079245	2.921684	-2.058239
21	6	0	0.131580	3.267007	-1.663988
22	6	0	-0.030704	4.596437	-1.313947
23	6	0	-0.933393	2.360905	-1.472549
24	6	0	-1.244928	5.045953	-0.760178
25	1	0	0.787322	5.293446	-1.460549
26	6	0	-2.162922	2.810340	-0.908471
27	6	0	-2.297760	4.167887	-0.556378
28	1	0	-1.357365	6.091650	-0.490545
29	6	0	-3.233573	1.871300	-0.755010
30	16	0	3.172489	1.233626	-0.574656
31	1	0	-3.235715	4.518286	-0.136102
32	1	0	-4.175399	2.204239	-0.336504
33	6	0	-1.062632	-0.376350	2.472143
34	6	0	1.585443	0.710494	2.937035
35	6	0	0.128949	0.481126	-2.888278
36	1	0	0.092183	-0.607829	-2.949585
37	1	0	-0.205408	0.880238	-3.854793
38	1	0	1.153872	0.808252	-2.707775
39	6	0	2.096519	-2.568945	-0.383493
40	7	0	0.694755	-2.159671	-0.073504
41	6	0	4.913832	1.347608	-0.093629
42	1	0	5.501077	0.572988	-0.581800
43	1	0	4.977240	1.253427	0.989912

44	1	0	5.252761	2.335315	-0.411734
45	6	0	4.258237	-1.722536	-1.334233
46	1	0	4.807152	-1.877747	-0.395716
47	1	0	4.727321	-0.890555	-1.864598
48	6	0	2.164951	-3.818714	-1.268097
49	1	0	1.659648	-4.655471	-0.768862
50	1	0	1.620069	-3.629333	-2.204499
51	8	0	-1.937645	0.209623	-1.809554
52	6	0	-3.111314	0.593425	-1.202570
53	6	0	3.623852	-4.177317	-1.588262
54	1	0	4.135129	-4.476293	-0.663343
55	1	0	3.656011	-5.043609	-2.256993
56	6	0	4.348941	-2.980757	-2.215255
57	1	0	3.911443	-2.765538	-3.199546
58	1	0	5.401354	-3.225523	-2.393262
59	6	0	-4.126506	-0.467664	-1.193945
60	6	0	-3.975379	-1.611479	-1.999066
61	6	0	-5.277523	-0.350738	-0.391828
62	6	0	-4.952143	-2.604802	-2.004343
63	1	0	-3.102698	-1.710058	-2.634005
64	6	0	-6.249063	-1.347220	-0.400827
65	1	0	-5.412564	0.512790	0.251437
66	6	0	-6.091176	-2.477947	-1.207147
67	1	0	-4.826565	-3.476348	-2.639269
68	1	0	-7.130935	-1.241789	0.223236
69	1	0	-6.851890	-3.252189	-1.214550
70	6	0	2.936055	1.292335	3.241542
71	1	0	3.168261	2.105341	2.552838
72	1	0	2.933349	1.692075	4.263008
73	1	0	3.718665	0.531613	3.185447
74	6	0	-2.492706	-0.885323	2.390576
75	1	0	-3.027720	-0.216101	1.707072
76	6	0	-2.626016	-2.311440	1.836799
77	1	0	-3.682232	-2.580788	1.749230
78	1	0	-2.181787	-2.394187	0.839946
79	1	0	-2.159392	-3.053810	2.493959
80	6	0	-3.158699	-0.770623	3.778875
81	1	0	-3.110784	0.252337	4.164495
82	1	0	-4.211794	-1.063256	3.722457
83	1	0	-2.667341	-1.426459	4.505829

TS(*S*)-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.518381	-0.155701	-0.095425
2	1	0	0.365430	0.983255	-0.603635
3	6	0	-0.736958	2.223362	-1.159364
4	8	0	-1.628768	-1.287186	-2.617743
5	8	0	0.811575	-0.872874	-3.143324
6	6	0	-0.938003	-1.971463	0.110940
7	6	0	3.313185	0.720891	0.986064
8	6	0	3.194949	1.350789	-0.268743
9	6	0	3.297831	-0.813174	-1.361372
10	6	0	3.476683	-1.453717	-0.093972
11	7	0	0.192131	-1.695285	-0.811288
12	1	0	0.425146	-2.486497	1.679887
13	1	0	-1.746750	-1.240907	-0.038198
14	1	0	0.701521	-0.296307	2.478779
15	1	0	-0.531759	0.281121	1.582056
16	1	0	3.279011	1.323050	1.888504
17	1	0	3.068343	2.426750	-0.313749
18	1	0	3.208777	-1.418275	-2.255332
19	1	0	3.539217	-2.533833	-0.058685
20	1	0	1.236509	4.075669	-1.590555
21	6	0	0.744202	4.168873	-0.629482
22	6	0	1.135845	5.160100	0.253675
23	6	0	-0.308300	3.292714	-0.289095
24	6	0	0.494198	5.290162	1.502213
25	1	0	1.934004	5.843679	-0.016670
26	6	0	-0.975168	3.439553	0.959503
27	6	0	-0.545662	4.445537	1.851305
28	1	0	0.810220	6.068921	2.189364
29	6	0	-2.090980	2.587794	1.245902
30	16	0	-0.206819	-1.658409	-2.414813
31	1	0	-1.053337	4.562301	2.804112
32	1	0	-2.598480	2.679148	2.198243
33	6	0	3.505851	-0.701893	1.093484
34	6	0	3.228770	0.590338	-1.485407
35	6	0	-0.413268	2.144586	-2.618964

36	1	0	-0.676899	1.162857	-3.010011
37	1	0	-1.006617	2.909827	-3.136366
38	1	0	0.641142	2.326421	-2.809290
39	6	0	-0.399993	-1.780345	1.530897
40	7	0	0.209599	-0.418969	1.594419
41	6	0	-0.003659	-3.341316	-3.049112
42	1	0	-0.684349	-4.028078	-2.549561
43	1	0	1.032211	-3.641472	-2.889887
44	1	0	-0.226761	-3.296287	-4.116679
45	6	0	-1.562675	-3.376513	-0.013533
46	1	0	-0.765180	-4.128130	0.058890
47	1	0	-2.026585	-3.476807	-0.997707
48	6	0	-1.466648	-2.002724	2.608751
49	1	0	-1.024513	-1.862617	3.603787
50	1	0	-2.255381	-1.245077	2.497663
51	8	0	-1.920617	1.642483	-0.903397
52	6	0	-2.587488	1.748842	0.291758
53	6	0	-2.081438	-3.404982	2.480550
54	1	0	-1.314804	-4.159125	2.704526
55	1	0	-2.872526	-3.533634	3.226676
56	6	0	-2.629597	-3.628857	1.065949
57	1	0	-3.480888	-2.956768	0.896066
58	1	0	-3.014804	-4.649419	0.966912
59	6	0	-3.812705	0.943866	0.331968
60	6	0	-4.077699	-0.000774	-0.679480
61	6	0	-4.748815	1.120862	1.370301
62	6	0	-5.252696	-0.749973	-0.639083
63	1	0	-3.364332	-0.162217	-1.480693
64	6	0	-5.913987	0.362741	1.403350
65	1	0	-4.584316	1.866614	2.141285
66	6	0	-6.170649	-0.575172	0.398175
67	1	0	-5.447892	-1.472720	-1.425021
68	1	0	-6.629806	0.512888	2.205322
69	1	0	-7.085458	-1.159329	0.421943
70	6	0	3.199779	1.246487	-2.838145
71	1	0	2.911386	2.298710	-2.766482
72	1	0	4.199048	1.216220	-3.287868
73	1	0	2.506303	0.723540	-3.499196
74	6	0	3.748750	-1.307992	2.467683
75	1	0	3.039293	-0.830226	3.160567
76	6	0	3.540641	-2.825882	2.543983
77	1	0	3.637247	-3.161184	3.580282
78	1	0	2.553047	-3.127361	2.182022
79	1	0	4.294663	-3.363412	1.959690

80	6	0	5.170356	-0.931825	2.944061
81	1	0	5.325661	0.150965	2.953236
82	1	0	5.339332	-1.306077	3.958069
83	1	0	5.926731	-1.375773	2.288616

TS(*S*)-3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.044385	0.977679	-0.384390
2	1	0	0.223092	0.206511	-1.201979
3	6	0	1.449765	-0.436248	-2.197687
4	8	0	1.086669	-1.840942	2.211829
5	8	0	1.312311	0.660233	1.871002
6	6	0	-1.515328	-1.777681	0.926030
7	6	0	-2.022980	2.693091	-1.505633
8	6	0	-0.628510	2.898002	-1.493785
9	6	0	-0.643709	2.789954	0.929534
10	6	0	-2.070235	2.656472	0.921361
11	7	0	-0.865626	-0.474269	1.195901
12	1	0	-3.398685	-0.825429	0.568440
13	1	0	-0.833198	-2.446434	0.375351
14	1	0	-2.999544	-0.375574	-1.712784
15	1	0	-1.632694	-1.272155	-1.718046
16	1	0	-2.539678	2.622386	-2.458082
17	1	0	-0.095681	2.991898	-2.433233
18	1	0	-0.108116	2.734486	1.868641
19	1	0	-2.586829	2.525421	1.863884
20	1	0	-0.193834	-2.081653	-3.662261
21	6	0	0.303505	-2.568836	-2.829528
22	6	0	0.087200	-3.914348	-2.590856
23	6	0	1.207850	-1.843281	-2.017860
24	6	0	0.753651	-4.562489	-1.527321
25	1	0	-0.586593	-4.477576	-3.228504
26	6	0	1.902299	-2.502079	-0.964799
27	6	0	1.646256	-3.871712	-0.729198
28	1	0	0.570128	-5.616685	-1.344399

29	6	0	2.866890	-1.766503	-0.215220
30	16	0	0.451648	-0.501570	2.179440
31	1	0	2.162518	-4.370202	0.084516
32	1	0	3.389235	-2.243808	0.602071
33	6	0	-2.785434	2.616595	-0.285983
34	6	0	0.097626	2.970355	-0.256789
35	6	0	1.098637	0.295323	-3.464869
36	1	0	1.314488	1.356801	-3.349782
37	1	0	1.711842	-0.095690	-4.285629
38	1	0	0.047013	0.174429	-3.722575
39	6	0	-2.713192	-1.481289	0.019273
40	7	0	-2.215651	-0.672150	-1.132401
41	6	0	-0.157735	-0.192518	3.856958
42	1	0	-0.839383	-0.987372	4.156688
43	1	0	-0.665239	0.772614	3.870430
44	1	0	0.712559	-0.172662	4.515643
45	6	0	-2.013994	-2.554788	2.163736
46	1	0	-2.680230	-1.904014	2.746742
47	1	0	-1.162079	-2.816241	2.795028
48	6	0	-3.454966	-2.749952	-0.416570
49	1	0	-4.306843	-2.484246	-1.056005
50	1	0	-2.780160	-3.370712	-1.022898
51	8	0	2.527610	0.106809	-1.608862
52	6	0	3.185433	-0.488874	-0.556496
53	6	0	-3.928084	-3.547643	0.809398
54	1	0	-4.698350	-2.971669	1.339855
55	1	0	-4.404759	-4.478624	0.485081
56	6	0	-2.759451	-3.837476	1.759005
57	1	0	-2.055645	-4.525794	1.271722
58	1	0	-3.120795	-4.350805	2.656381
59	6	0	4.234690	0.347109	0.029119
60	6	0	4.907971	1.307369	-0.746742
61	6	0	4.595645	0.170548	1.376523
62	6	0	5.934845	2.063442	-0.187069
63	1	0	4.640342	1.444345	-1.789190
64	6	0	5.622623	0.931357	1.927759
65	1	0	4.042268	-0.527202	1.995149
66	6	0	6.296736	1.875679	1.149114
67	1	0	6.458123	2.794227	-0.795876
68	1	0	5.889715	0.795592	2.971064
69	1	0	7.097925	2.465997	1.583056
70	6	0	1.580159	3.212619	-0.218224
71	1	0	2.065930	2.875979	-1.136957
72	1	0	1.780920	4.284924	-0.106003

73	1	0	2.029025	2.681355	0.622263
74	6	0	-4.301206	2.524475	-0.368277
75	1	0	-4.535293	1.819781	-1.180061
76	6	0	-4.874653	3.899817	-0.779291
77	1	0	-5.958938	3.832388	-0.908389
78	1	0	-4.671299	4.649524	-0.007654
79	1	0	-4.444900	4.258302	-1.719337
80	6	0	-4.978998	2.018526	0.911300
81	1	0	-6.049962	1.884676	0.735772
82	1	0	-4.568940	1.060122	1.244324
83	1	0	-4.874510	2.736093	1.731935

TS(*R*) optimized with B3LYP-D3 in gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.030273	0.991736	0.210912
2	1	0	0.240446	-0.547874	0.660106
3	6	0	0.828687	-2.340745	1.082920
4	6	0	0.505413	-2.377418	2.532992
5	1	0	-0.556302	-2.215151	2.709720
6	1	0	1.069803	-1.612176	3.061262
7	1	0	0.788362	-3.365393	2.920276
8	8	0	2.103777	-2.027763	0.846553
9	6	0	2.626507	-1.939440	-0.418200
10	6	0	1.907425	-2.430636	-1.465899
11	1	0	2.340877	-2.425708	-2.458429
12	6	0	0.617490	-3.006338	-1.258689
13	6	0	0.054757	-2.954187	0.053490
14	6	0	-1.238320	-3.475672	0.295347
15	6	0	-0.127347	-3.603769	-2.297804
16	1	0	0.296135	-3.652867	-3.296370
17	6	0	-1.938333	-4.065023	-0.741118
18	1	0	-1.945877	-4.596965	-2.838293
19	6	0	-1.381331	-4.131731	-2.036103
20	1	0	-2.929170	-4.467395	-0.559410
21	1	0	-1.694303	-3.368467	1.271482
22	8	0	-2.686404	-1.473327	2.299694
23	8	0	-1.122260	0.313707	3.163039

24	6	0	-2.771455	-0.234665	-0.264406
25	6	0	2.118852	1.639502	0.424746
26	6	0	1.491491	1.765004	1.710742
27	6	0	-0.172757	3.287470	0.663526
28	6	0	0.434807	3.172478	-0.595549
29	7	0	-2.051489	0.535189	0.780025
30	1	0	-2.498402	1.347134	-1.685660
31	1	0	-2.510741	-1.301133	-0.205147
32	1	0	-0.402946	0.623784	-2.438849
33	1	0	-0.531563	-0.823370	-1.696887
34	1	0	2.992413	1.009245	0.310926
35	1	0	-1.079452	3.867297	0.781629
36	16	0	-2.275703	-0.041647	2.311749
37	6	0	1.573395	2.293081	-0.698227
38	6	0	0.328089	2.561430	1.794740
39	6	0	-2.275590	0.276078	-1.617875
40	7	0	-0.788922	0.160597	-1.617068
41	6	0	-3.656652	0.899653	2.999038
42	1	0	-4.555327	0.746412	2.404334
43	1	0	-3.370217	1.951625	2.998612
44	1	0	-3.805456	0.542178	4.019456
45	6	0	-4.306733	-0.136608	-0.203437
46	1	0	-4.593864	0.923344	-0.202422
47	1	0	-4.655389	-0.580841	0.731604
48	6	0	-2.920276	-0.461472	-2.795285
49	1	0	-2.538825	-0.054949	-3.740764
50	1	0	-2.622173	-1.519167	-2.755625
51	6	0	-4.450856	-0.355377	-2.731187
52	1	0	-4.746686	0.694174	-2.862481
53	1	0	-4.900082	-0.914218	-3.558755
54	6	0	-4.967831	-0.868521	-1.381981
55	1	0	-6.055639	-0.758714	-1.323184
56	1	0	-4.757268	-1.943975	-1.299679
57	6	0	3.953334	-1.322076	-0.444789
58	6	0	4.725271	-1.235680	0.728574
59	6	0	4.456522	-0.773462	-1.638988
60	6	0	5.974698	-0.620793	0.701140
61	1	0	4.348624	-1.656310	1.653838
62	6	0	5.705595	-0.160184	-1.658222
63	1	0	3.862719	-0.801181	-2.547008
64	6	0	6.468517	-0.082033	-0.489241
65	1	0	6.564709	-0.565284	1.610317
66	1	0	6.081848	0.264076	-2.583613
67	1	0	7.441509	0.398553	-0.506590

68	1	0	-0.218102	2.588764	2.729152
69	1	0	2.037018	2.143867	-1.669716
70	6	0	2.044387	1.057716	2.916230
71	1	0	2.717112	1.722241	3.470509
72	1	0	1.230684	0.750954	3.575794
73	1	0	2.618113	0.176537	2.616244
74	6	0	-0.050099	3.894402	-1.839584
75	1	0	0.016204	3.173048	-2.668665
76	6	0	0.905524	5.061348	-2.165649
77	1	0	0.609189	5.549100	-3.099204
78	1	0	0.879662	5.810008	-1.367002
79	1	0	1.939407	4.719042	-2.273048
80	6	0	-1.501289	4.381809	-1.754138
81	1	0	-1.820820	4.777642	-2.722119
82	1	0	-2.184373	3.575733	-1.469028
83	1	0	-1.607954	5.190095	-1.023114

TS(*S*) optimized with B3LYP-D3 in gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.607897	-0.277099	0.968101
2	1	0	0.056972	0.295952	-0.490920
3	6	0	-0.700670	0.940330	-1.960218
4	8	0	3.202289	1.222095	-1.961005
5	8	0	2.480621	2.265878	0.227638
6	6	0	2.747890	-1.423330	-0.873099
7	6	0	-0.843115	1.073961	2.021443
8	6	0	0.460977	1.560062	2.305568
9	6	0	1.053483	-0.623169	3.240776
10	6	0	-0.239165	-1.096876	2.901630
11	7	0	2.552381	-0.281135	0.054092
12	1	0	2.432513	-2.815171	0.726654
13	1	0	2.286258	-1.215538	-1.850893
14	1	0	0.091808	-2.888758	0.508558
15	1	0	0.111229	-2.098330	-0.914860
16	1	0	-1.548094	1.732291	1.527325
17	1	0	0.749609	2.552695	1.987617
18	1	0	1.780252	-1.295436	3.682780

19	1	0	-0.474687	-2.139443	3.094493
20	1	0	1.319525	2.768187	-2.164434
21	6	0	0.401345	3.158288	-1.744388
22	6	0	0.334712	4.475138	-1.325989
23	6	0	-0.721656	2.320245	-1.576744
24	6	0	-0.839171	4.977561	-0.731531
25	1	0	1.199751	5.118415	-1.443158
26	6	0	-1.913144	2.823544	-0.974816
27	6	0	-1.950835	4.167028	-0.556604
28	1	0	-0.873732	6.012515	-0.405259
29	6	0	-3.028546	1.941114	-0.821659
30	16	0	3.160462	1.157993	-0.474011
31	1	0	-2.856003	4.559671	-0.103293
32	1	0	-3.935959	2.309789	-0.359982
33	6	0	-1.241478	-0.255351	2.333932
34	6	0	1.424479	0.710088	2.917003
35	6	0	0.269655	0.359716	-2.937876
36	1	0	0.173236	-0.726875	-2.958721
37	1	0	0.011967	0.740507	-3.934475
38	1	0	1.297923	0.640739	-2.708516
39	6	0	2.002942	-2.613421	-0.262225
40	7	0	0.595802	-2.179015	-0.021248
41	6	0	4.877055	1.245673	0.089592
42	1	0	5.466862	0.444058	-0.349186
43	1	0	4.878520	1.174925	1.176332
44	1	0	5.255751	2.217234	-0.232848
45	6	0	4.213102	-1.813178	-1.144793
46	1	0	4.723305	-1.960952	-0.183805
47	1	0	4.708560	-0.992889	-1.669089
48	6	0	2.087381	-3.873125	-1.128601
49	1	0	1.543105	-4.693511	-0.644033
50	1	0	1.589208	-3.680373	-2.090134
51	8	0	-1.840727	0.233313	-1.924201
52	6	0	-2.980224	0.663588	-1.284963
53	6	0	3.552135	-4.258365	-1.380426
54	1	0	4.021529	-4.537930	-0.427681
55	1	0	3.600991	-5.140585	-2.026677
56	6	0	4.314143	-3.083562	-2.004458
57	1	0	3.904987	-2.875821	-3.002620
58	1	0	5.367290	-3.345584	-2.149060
59	6	0	-4.023998	-0.364179	-1.227746
60	6	0	-3.891027	-1.561567	-1.953635
61	6	0	-5.165360	-0.180882	-0.424793
62	6	0	-4.871782	-2.547353	-1.873655

63	1	0	-3.023573	-1.714418	-2.584859
64	6	0	-6.140316	-1.170328	-0.346480
65	1	0	-5.288681	0.725600	0.158289
66	6	0	-5.997144	-2.358825	-1.068823
67	1	0	-4.758242	-3.463757	-2.444230
68	1	0	-7.012295	-1.015168	0.280864
69	1	0	-6.759069	-3.129291	-1.006442
70	6	0	2.809292	1.204966	3.220516
71	1	0	3.064124	2.049238	2.580187
72	1	0	2.861874	1.524660	4.267699
73	1	0	3.542428	0.407638	3.073770
74	6	0	-2.665888	-0.729429	2.113393
75	1	0	-3.137743	-0.002640	1.444850
76	6	0	-2.758276	-2.103534	1.434576
77	1	0	-3.802890	-2.354715	1.232232
78	1	0	-2.228950	-2.103021	0.477916
79	1	0	-2.347160	-2.898550	2.066914
80	6	0	-3.438963	-0.717287	3.446255
81	1	0	-3.409004	0.270332	3.916627
82	1	0	-4.487006	-0.986921	3.281335
83	1	0	-3.013094	-1.438773	4.152108

TS(*R*) optimized with B3LYP-D3 in DCM

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.026962	0.980770	0.210067
2	1	0	0.205903	-0.559859	0.704913
3	6	0	0.777124	-2.261932	1.136479
4	6	0	0.429807	-2.265107	2.584362
5	1	0	-0.623854	-2.040849	2.738283
6	1	0	1.032317	-1.530740	3.114250
7	1	0	0.646235	-3.263848	2.983830
8	8	0	2.064931	-1.988437	0.916456
9	6	0	2.608256	-1.956526	-0.343398
10	6	0	1.898552	-2.467522	-1.386524
11	1	0	2.341314	-2.492530	-2.374259
12	6	0	0.600566	-3.027247	-1.177719
13	6	0	0.019933	-2.925641	0.121733

14	6	0	-1.274712	-3.437661	0.365991
15	6	0	-0.131377	-3.659553	-2.205428
16	1	0	0.303648	-3.738651	-3.196308
17	6	0	-1.962735	-4.064554	-0.656767
18	1	0	-1.946612	-4.663376	-2.735323
19	6	0	-1.389788	-4.175433	-1.941890
20	1	0	-2.956347	-4.459406	-0.475014
21	1	0	-1.738441	-3.302346	1.335166
22	8	0	-2.850219	-1.284283	2.392511
23	8	0	-1.265725	0.510699	3.187260
24	6	0	-2.773480	-0.236812	-0.279779
25	6	0	2.130143	1.570387	0.458509
26	6	0	1.472893	1.793985	1.715821
27	6	0	-0.107293	3.303393	0.528820
28	6	0	0.533497	3.091936	-0.701479
29	7	0	-2.071933	0.574458	0.749702
30	1	0	-2.465418	1.288270	-1.750404
31	1	0	-2.517633	-1.298355	-0.164463
32	1	0	-0.356641	0.560957	-2.428338
33	1	0	-0.490814	-0.871901	-1.673314
34	1	0	2.983467	0.905642	0.409697
35	1	0	-0.992816	3.924098	0.585655
36	16	0	-2.386503	0.130866	2.298497
37	6	0	1.644323	2.172708	-0.719175
38	6	0	0.334733	2.629674	1.715707
39	6	0	-2.241837	0.221417	-1.639484
40	7	0	-0.757283	0.110448	-1.606296
41	6	0	-3.761446	1.174004	2.838521
42	1	0	-4.631270	1.011981	2.204587
43	1	0	-3.428883	2.210366	2.772743
44	1	0	-3.985377	0.907663	3.873167
45	6	0	-4.309650	-0.128958	-0.266466
46	1	0	-4.592396	0.930615	-0.326164
47	1	0	-4.691126	-0.525551	0.677343
48	6	0	-2.858482	-0.556374	-2.806213
49	1	0	-2.452070	-0.178095	-3.751914
50	1	0	-2.562509	-1.611391	-2.727600
51	6	0	-4.389347	-0.448768	-2.784142
52	1	0	-4.682234	0.595069	-2.960575
53	1	0	-4.817542	-1.040802	-3.600100
54	6	0	-4.939271	-0.911359	-1.429933
55	1	0	-6.028803	-0.801501	-1.401016
56	1	0	-4.726349	-1.981473	-1.300061
57	6	0	3.949278	-1.367392	-0.367725

58	6	0	4.703571	-1.261087	0.815601
59	6	0	4.479972	-0.862257	-1.568935
60	6	0	5.963981	-0.668007	0.791454
61	1	0	4.303313	-1.645401	1.746734
62	6	0	5.740164	-0.270738	-1.584118
63	1	0	3.899941	-0.905355	-2.484699
64	6	0	6.486040	-0.171475	-0.405596
65	1	0	6.538421	-0.594235	1.709307
66	1	0	6.136323	0.122602	-2.514829
67	1	0	7.466240	0.294522	-0.420171
68	1	0	-0.237160	2.735546	2.628844
69	1	0	2.126438	1.944202	-1.665173
70	6	0	1.973395	1.146065	2.976423
71	1	0	2.629713	1.834265	3.521372
72	1	0	1.132914	0.878139	3.619007
73	1	0	2.551190	0.246954	2.746466
74	6	0	0.113017	3.756584	-1.999266
75	1	0	0.192100	2.993073	-2.786381
76	6	0	1.110651	4.881771	-2.345255
77	1	0	0.860626	5.326190	-3.313649
78	1	0	1.073296	5.670824	-1.586532
79	1	0	2.137629	4.507198	-2.395941
80	6	0	-1.326624	4.282813	-1.994945
81	1	0	-1.596277	4.635748	-2.994321
82	1	0	-2.038982	3.506348	-1.701062
83	1	0	-1.441633	5.127483	-1.307427

TS(*S*) optimized with B3LYP-D3 in DCM

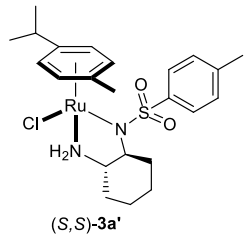
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.604218	-0.221463	0.971500
2	1	0	0.049374	0.316959	-0.495635
3	6	0	-0.697761	0.895809	-1.987646
4	8	0	3.318237	1.143972	-1.993877
5	8	0	2.567332	2.264770	0.141931
6	6	0	2.720537	-1.465733	-0.850974
7	6	0	-0.830185	1.166392	2.003935
8	6	0	0.478729	1.643731	2.280055

9	6	0	1.052485	-0.530565	3.250222
10	6	0	-0.244285	-0.998055	2.919243
11	7	0	2.545953	-0.285829	0.034790
12	1	0	2.365690	-2.813654	0.779084
13	1	0	2.277726	-1.274795	-1.839358
14	1	0	0.037839	-2.828808	0.584247
15	1	0	0.048722	-2.083935	-0.859928
16	1	0	-1.531948	1.824167	1.504052
17	1	0	0.773632	2.632102	1.954210
18	1	0	1.773150	-1.203571	3.700416
19	1	0	-0.486467	-2.035632	3.126083
20	1	0	1.308726	2.728302	-2.231051
21	6	0	0.387352	3.126493	-1.826391
22	6	0	0.309550	4.453984	-1.446189
23	6	0	-0.730516	2.286101	-1.641494
24	6	0	-0.870121	4.963318	-0.866438
25	1	0	1.167288	5.103628	-1.582025
26	6	0	-1.925328	2.794720	-1.054656
27	6	0	-1.974308	4.149004	-0.670118
28	1	0	-0.912322	6.005863	-0.567193
29	6	0	-3.032152	1.907509	-0.873752
30	16	0	3.221317	1.106554	-0.504629
31	1	0	-2.881665	4.542756	-0.223278
32	1	0	-3.936601	2.278442	-0.409078
33	6	0	-1.238346	-0.154874	2.338623
34	6	0	1.434123	0.793911	2.904511
35	6	0	0.284709	0.294430	-2.939335
36	1	0	0.188436	-0.791699	-2.939484
37	1	0	0.040086	0.656774	-3.945502
38	1	0	1.308420	0.580459	-2.701319
39	6	0	1.937650	-2.615748	-0.210958
40	7	0	0.545857	-2.141956	0.028400
41	6	0	4.923101	1.145066	0.110696
42	1	0	5.492180	0.306931	-0.285488
43	1	0	4.886950	1.102942	1.198273
44	1	0	5.355841	2.090367	-0.221894
45	6	0	4.176729	-1.909323	-1.086718
46	1	0	4.663403	-2.057533	-0.113790
47	1	0	4.714429	-1.118514	-1.614942
48	6	0	1.984988	-3.894333	-1.052944
49	1	0	1.410316	-4.683103	-0.553372
50	1	0	1.499991	-3.703833	-2.020857
51	8	0	-1.830999	0.184363	-1.938067
52	6	0	-2.972365	0.620301	-1.307878

53	6	0	3.437601	-4.334478	-1.282279
54	1	0	3.887693	-4.611118	-0.319335
55	1	0	3.462466	-5.229383	-1.913039
56	6	0	4.247640	-3.199550	-1.919382
57	1	0	3.856278	-2.998235	-2.925959
58	1	0	5.294067	-3.498490	-2.043562
59	6	0	-4.004604	-0.417448	-1.221193
60	6	0	-3.839178	-1.647735	-1.882973
61	6	0	-5.163131	-0.210800	-0.448925
62	6	0	-4.806145	-2.644261	-1.769078
63	1	0	-2.954857	-1.822097	-2.484236
64	6	0	-6.123321	-1.211832	-0.336546
65	1	0	-5.311462	0.721563	0.084580
66	6	0	-5.948834	-2.433481	-0.994263
67	1	0	-4.664833	-3.588126	-2.286211
68	1	0	-7.006841	-1.039581	0.269788
69	1	0	-6.698032	-3.213537	-0.902392
70	6	0	2.819343	1.288538	3.208163
71	1	0	3.098850	2.091016	2.525541
72	1	0	2.850728	1.672197	4.234528
73	1	0	3.547632	0.477375	3.131196
74	6	0	-2.668829	-0.613991	2.128578
75	1	0	-3.120953	0.086817	1.420814
76	6	0	-2.782939	-2.020267	1.524626
77	1	0	-3.831908	-2.257569	1.327520
78	1	0	-2.247438	-2.082222	0.573921
79	1	0	-2.391721	-2.787894	2.201000
80	6	0	-3.449517	-0.514564	3.453237
81	1	0	-3.403811	0.497890	3.866725
82	1	0	-4.501397	-0.772801	3.293398
83	1	0	-3.039575	-1.204893	4.198863

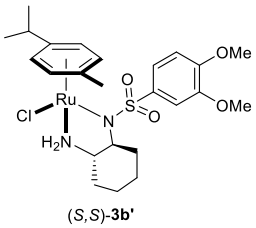
6. General procedure for the synthesis of Ru-Cl catalysts



(*S*,*S*)-**3a'**

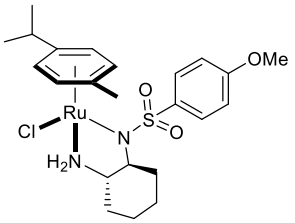
(*S*,*S*)-**3a':** (known compound, see: X. Wu, D. Vinci, T. Ikariya, J. Xiao, *Chem. Commun.* **2005**, *48*, 4447-4449). A mixture of $[RuCl_2(p\text{-cymene})]_2$ (429 mg, 0.7 mmol), (*S*,*S*)-Ts-CYDN (375 mg, 1.4 mmol) and NEt_3 (0.5 mL, 3.5 mmol) in CH_2Cl_2 (40 mL) was stirred at room temperature for 4 h under N_2 atmosphere. Then the mixture was washed with water (40 mL), dried over anhydrous Na_2SO_4 and purified by flash column chromatography using DCM/MeOH = 10/1 (v/v) as eluent on silica gel to give the crude product. The crude product was precipitated in EA and PE, giving the yellow powdery product (215 mg, 29% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.90 (d, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 6.45-6.43 (m, 1H), 5.75-5.74 (m, 1H), 5.66-5.61 (m, 3H), 3.02-2.96 (m, 1H), 2.44-2.42 (m, 1H), 2.35-2.15 (m, 10H), 1.43-1.37 (m, 2H), 1.31-1.28 (m, 6H), 0.98-0.79 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 144.2, 140.3, 128.9, 127.3, 104.2, 94.4, 84.6, 82.3, 80.4, 79.7, 65.0, 62.3, 35.5, 33.9, 30.7, 24.8, 24.7, 23.2, 22.0, 21.4, 18.8. HRMS-ESI exact mass calcd. for $C_{23}H_{33}N_2O_2RuS^+$ ($[M\text{-}Cl]^+$) requires m/z 503.13062, found m/z 503.13004.

The other catalyst precursors (*S*,*S*)-**3b',** (*S*,*S*)-**3c',** (*S*,*S*)-**3d',** (*S*,*S*)-**3e'** were prepared with the similar method described above.



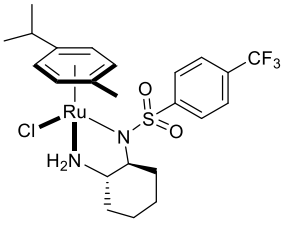
(*S*,*S*)-**3b'**

(*S*,*S*)-**3b':** (new compound). 62% yield. Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.75 (s, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 8.5 Hz, 1H), 6.32-6.31 (m, 1H), 5.61-5.58 (m, 4H), 3.91 (s, 3H), 3.86 (s, 3H), 2.99-2.93 (m, 1H), 2.41-2.34 (m, 1H), 2.23-2.21 (m, 5H), 2.10-1.97 (m, 2H), 1.44-1.36 (m, 2H), 1.26 (t, *J* = 7.8 Hz, 6H), 0.98-0.93 (m, 3H), 0.72-0.70 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 150.5, 148.5, 137.5, 120.9, 111.3, 110.0, 103.7, 94.8, 84.2, 81.6, 80.6, 79.8, 65.6, 62.3, 56.6, 56.0, 53.5, 35.4, 34.2, 30.7, 24.7, 23.2, 21.8, 18.9. HRMS-ESI exact mass calcd. for $C_{24}H_{35}N_2O_4RuS^+$ ($[M\text{-}Cl]^+$) requires m/z 549.13610, found m/z 549.13558.



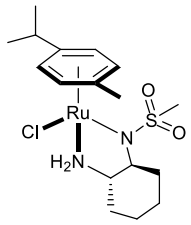
(*S*,*S*)-**3c'**

(*S*,*S*)-**3c':** (new compound). 65% yield. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.96 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 6.41-6.40 (m, 1H), 5.72-5.70 (m, 1H), 5.63-5.62 (m, 3H), 3.80 (s, 3H), 2.99-2.96 (m, 1H), 2.41-2.39 (m, 1H), 2.22-2.10 (m, 7H), 1.43-1.37 (m, 2H), 1.29 (t, *J* = 7.0 Hz, 6H), 0.98 (s, 2H), 0.86-0.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 160.9, 138.6, 129.2, 113.4, 104.0, 94.4, 84.5, 82.1, 80.5, 79.7, 65.1, 62.3, 55.4, 35.5, 34.0, 30.7, 24.8, 24.7, 23.2, 21.9, 18.8. HRMS-ESI exact mass calcd. for $C_{23}H_{33}N_2O_3RuS^+$ ($[M-Cl]^+$) requires m/z 519.12554, found m/z 519.12499.



(*S*,*S*)-**3d'**

(*S*,*S*)-**3d':** (new compound). 58% yield. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.11 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 5.95-5.93 (m, 1H), 5.70-5.55 (m, 4H), 3.00-2.96 (m, 1H), 2.59-2.57 (m, 1H), 2.25-2.04 (m, 7H), 1.45-1.39 (m, 2H), 1.31 (t, *J* = 6.8 Hz, 6H), 1.01 (s, 2H), 0.86-0.77 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 151.2, 131.8 (q, *J* = 32 Hz), 127.4, 125.4, 123.8 (q, *J* = 271 Hz), 104.3, 94.4, 84.5, 82.4, 80.5, 79.4, 64.7, 62.3, 35.5, 33.8, 30.7, 24.7, 24.5, 23.1, 21.8, 18.7. HRMS-ESI exact mass calcd. for $C_{23}H_{30}F_3N_2O_2RuS^+$ ($[M-Cl]^+$) requires m/z 557.10236, found m/z 557.10163.



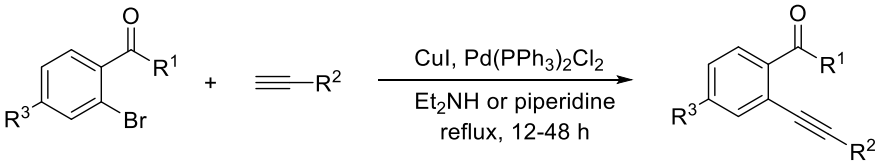
(*S*,*S*)-**3e'**

(*S*,*S*)-**3e'**: (new compound). A mixture of $[RuCl_2(p\text{-cymene})]_2$ (429 mg, 0.7 mmol), (*S*,*S*)-Ms-CYDN (269 mg, 1.4 mmol) and NEt_3 (0.5 mL, 3.5 mmol) in CH_2Cl_2 (40 mL) was stirred at room temperature for 4 h under N_2 atmosphere. Then the mixture was purified by flash column chromatography using DCM/MeOH = 10/1 (v/v) as eluent on silica gel to give the crude product. The crude product was precipitated in EA, giving the yellow powdery product (278mg, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 5.90-5.88 (m, 1H), 5.69 (d, *J* = 5.6 Hz, 1H), 5.57-5.51 (m, 2H), 5.43 (d, *J* = 5.6 Hz, 1H), 2.93-2.89 (m, 4H), 2.80-2.77 (m, 1H), 2.52 (br, s, 1H), 2.18 (s, 6H), 1.65-1.62 (m, 2H), 1.32-1.26 (m, 6H), 1.17-1.02 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm)

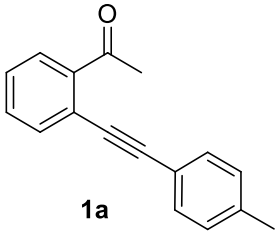
102.4, 96.5, 83.5, 81.9, 81.2, 81.1, 65.5, 62.4, 41.3, 35.9, 34.2, 30.8, 24.8, 24.8, 23.4, 21.8, 18.9. HRMS-ESI exact mass calcd. for $C_{17}H_{29}N_2O_2RuS$ ($[M-Cl]^+$) requires m/z 427.09932, found m/z 427.09879.

7. General procedure for the synthesis of substrates

7.1 General procedure for the synthesis of substrates 1a, 1c, 1e~f, 1i~1p:

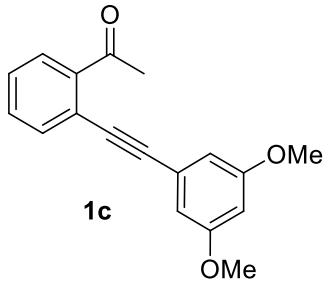


Typical procedure:[2a,2b] Using **1f** as an example. To a mixture of CuI (49 mg, 0.26 mmol) and $(PPh_3)_2PdCl_2$ (73 mg, 0.10 mmol) was added the solution of *o*-bromoacetophenone (0.35 mL, 2.6 mmol), 1-phenylethyne (0.43 mL, 3.9 mmol) in Et_2NH (20 mL) under nitrogen. Then, the mixture was refluxed at 90 °C and stirred for 12 h. The resulting mixture was concentrated under reduced pressure to give a residue, which was washed with water (100 mL) and extracted with EA. The combined organic layers were washed with brine (50 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The resulting residue was purified by silical gel column chromatography (eluent: dichloromethane/methanol = 30/1, *v*/*v*) to give **1f** as an orange oil (0.53 g, 91% yield).



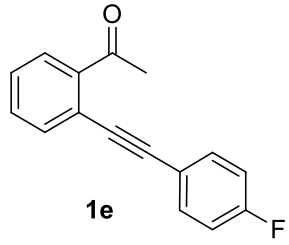
1a

1a: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2013**, *52*, 13284). White needle-like solid; 91% yield (stirred in Et_2NH for 12 h and recrystallized from $MeOH/H_2O$). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.73 (d, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.43 (d, *J* = 7.6 Hz, 3H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 2.77 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 200.4, 140.7, 139.0, 133.8, 131.4, 131.3, 129.3, 128.7, 128.1, 121.9, 119.8, 95.4, 88.0, 30.0, 21.6.



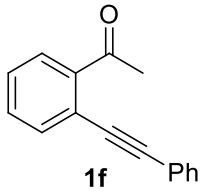
1c

1c: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Light yellow solid; 70% yield (stirred in Et_2NH for 12 h and recrystallized from MeOH). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 6.70 (s, 2H), 6.49 (s, 1H), 3.80 (s, 6H), 2.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 200.4, 160.7, 140.8, 134.0, 131.4, 128.8, 128.5, 124.2, 121.6, 109.4, 102.2, 95.0, 88.1, 55.5, 30.1.



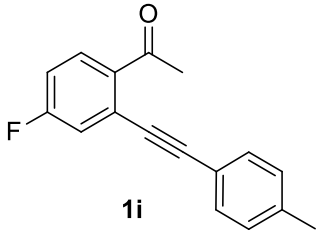
1e

1e: (known compound, see: B. Guo, L. Zheng, L. Yang, R. Hua, *J. Org. Chem.* **2014**, *79*, 4352). Yellow oil; 83% yield (stirred in Et_2NH for 12 h). ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.74 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.54-7.49 (m, 2H), 7.46-7.34 (m, 2H), 7.03 (t, *J* = 8.4 Hz, 2H), 2.74 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 199.9, 162.7 (d, *J* = 249 Hz), 140.5, 133.8, 133.5 (d, *J* = 8 Hz), 131.3, 128.8, 128.3, 121.5, 119.0 (d, *J* = 3 Hz), 115.7 (d, *J* = 22 Hz), 93.7, 88.3, 29.7.



1f

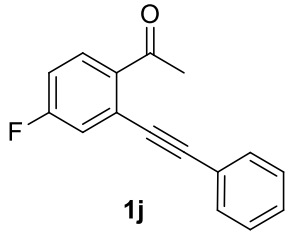
1f: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2013**, *52*, 13284). Light yellow oil; 91% yield (stirred in Et_2NH for 12 h). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.74 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.55-7.53 (m, 2H), 7.46-7.42 (m, 1H), 7.38-7.34 (m, 4H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 200.2, 140.8, 133.9, 131.5, 131.3, 128.8, 128.7, 128.5, 128.3, 122.9, 121.7, 95.1, 88.6, 30.0.



1i

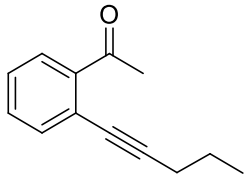
1i: (known compound, see: C. Dong, Z. Liao, X. Xu, H. Zhou, *J. Heterocycl.* **2014**, *51*, 1282). Light yellow solid; 70% yield (stirred in Et_2NH for 12 h and recrystallized

from DCM/PE). ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.82-7.77 (m, 1H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.28-7.24 (m, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.08-7.01 (m, 1H), 2.76 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 198.5, 164.0 (d, *J* = 252 Hz), 139.5, 136.7 (d, *J* = 4 Hz), 131.6 (d, *J* = 10 Hz), 131.5, 129.3, 124.8 (d, *J* = 11 Hz), 120.3 (d, *J* = 23 Hz), 119.4, 115.6 (d, *J* = 22 Hz), 96.7, 87.1 (d, *J* = 2 Hz), 30.0, 21.6.



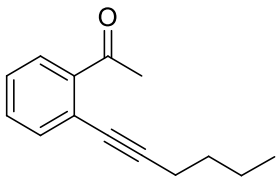
1j

1j: (known compound, see: C. Dong, Z. Liao, X. Xu, H. Zhou, *J. Heterocycl. Chem*. **2014**, *51*, 1282). Yellow oil; 85% yield (stirred in Et_2NH for 12 h). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.82-7.79 (m, 1H), 7.56-7.53 (m, 2H), 7.37-7.36 (m, 3H), 7.30-7.27 (m, 1H), 7.09-7.04 (m, 1H), 2.77 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 198.3, 164.0 (d, *J* = 253 Hz), 136.8 (d, *J* = 3 Hz), 131.6 (d, *J* = 10 Hz), 131.6, 129.2, 128.6, 124.5 (d, *J* = 11 Hz), 122.4, 120.4 (d, *J* = 23 Hz), 115.7 (d, *J* = 21 Hz), 96.3, 87.6 (d, *J* = 2 Hz), 29.9.



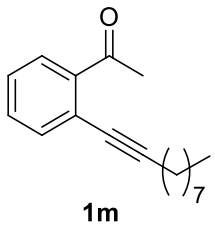
1k

1k: (new compound). Colorless oil; 76% yield (stirred in Et_2NH for 24 h). ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.67-7.64 (m, 1H), 7.50-7.47 (m, 1H), 7.42-7.30 (m, 2H), 2.72 (s, 3H), 2.44 (t, *J* = 7.1 Hz, 2H), 1.72-1.60 (m, 2H), 1.06 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 201.3, 141.2, 134.1, 131.2, 128.4, 127.7, 122.6, 96.9, 79.9, 30.2, 22.1, 21.8, 13.8. HRMS-APCI exact mass calcd. for $C_{13}H_{15}O^+$ ($[M+H]^+$) requires m/z 187.11229, found m/z 187.11174.



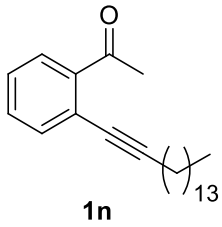
1l

1l: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed*. **2014**, *53*, 235). Colorless oil; 73% yield (stirred in Et_2NH for 24 h). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.67-7.64 (m, 1H), 7.49-7.47 (m, 1H), 7.41-7.37 (m, 1H), 7.33-7.29 (m, 1H), 2.72 (s, 3H), 2.46 (t, *J* = 7.0 Hz, 2H), 1.63-1.57 (m, 2H), 1.51-1.45 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 201.1, 141.1, 134.0, 131.1, 128.4, 127.6, 122.5, 96.9, 79.7, 30.6, 30.1, 22.1, 19.4, 13.7.



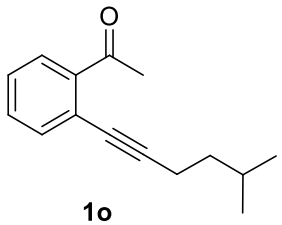
1m

1m: (known compound, see: M. Dell'Acqua, G. Abbiati, A. Arcadib, E. Rossi, *Org. Biomol. Chem*. **2011**, *9*, 7836). Colorless oil; 67% yield (stirred in Et_2NH for 48 h). ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.66 (d, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.41-7.28 (m, 2H), 2.72 (s, 3H), 2.45 (t, *J* = 6.9 Hz, 2H), 1.65-1.60 (m, 2H), 1.45 (br, s, 2H), 1.29 (br, s, 8H), 0.88-0.86 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 201.1, 141.1, 134.0, 131.1, 128.4, 127.6, 122.6, 97.0, 79.8, 31.9, 30.2, 29.3, 29.2, 29.1, 28.5, 22.7, 19.8, 14.2.



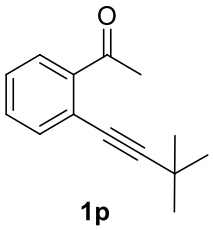
1n

1n: (new compound). Colorless oil; 60% yield (stirred in Et_2NH for 48 h). ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.66 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.41-7.28 (m, 2H), 2.72 (s, 3H), 2.45 (t, *J* = 6.9 Hz, 2H), 1.64-1.60 (m, 2H), 1.45 (br, s, 2H), 1.26 (br, s, 20H), 0.88-0.86 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 201.1, 141.1, 134.1, 131.1, 128.4, 127.6, 122.6, 97.0, 79.8, 32.0, 30.2, 29.8, 29.8, 29.6, 29.5, 29.3, 29.1, 28.6, 22.8, 19.8, 14.2. HRMS (EI) m/z calcd. for $C_{24}H_{36}O$ $(M)^+$ 340.2766, found 340.2761.



1o

1o: (new compound). Colorless oil; 83% yield (stirred in Et_2NH for 24 h). ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.65 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.41-7.28 (m, 2H), 2.72 (s, 3H), 2.46 (t, *J* = 7.4 Hz, 2H), 1.80-1.71 (m, 1H), 1.56-1.49 (m, 2H), 0.94 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 201.1, 141.1, 134.0, 131.1, 128.4, 127.6, 122.5, 97.0, 79.6, 37.4, 30.2, 27.4, 22.2, 17.8. HRMS (EI) m/z calcd. for $C_{15}H_{18}O$ $(M)^+$ 214.1358, found 214.1355.

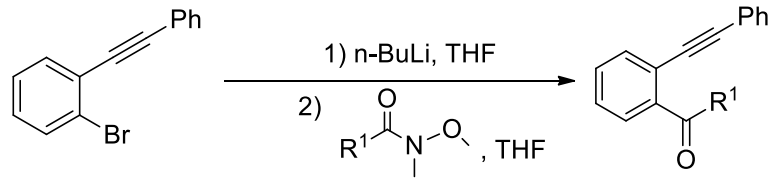


1p

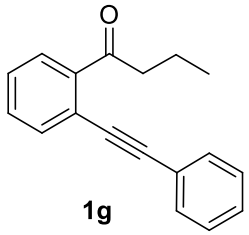
1p: (known compound, see: X. Chen, J. Jin, N. Wang, P. Lu, Y. Wang, *Eur. J. Org. Chem*. **2012**, *4*, 824). Yellow oil; 80% yield (stirred in piperidine for 48 h). ^1H NMR (400 MHz, $CDCl_3$): δ

(ppm) 7.66 (d, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.40-7.36 (m, 1H), 7.33-7.29 (m, 1H), 2.74 (s, 3H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 201.2, 141.1, 133.9, 131.1, 128.4, 127.6, 122.5, 104.7, 78.6, 30.7, 30.3, 28.3.

7.2 General procedure for the synthesis of substrates 1g, 1h, 1r:

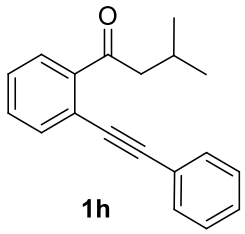


Typical procedure:[2c] Using **1g** as an example. To a stirred solution of 2-bromo-diphenylacetylene (0.38 g, 1.5 mmol) in THF (4 mL) was added *n*-BuLi (1.62 mol/L solution in hexane, 0.91 mL, 1.5 mmol) dropwise at -78 °C and stirred for 30 min. A solution of Weinreb amide (1.5 mmol) in THF (1 mL) was then added dropwise and stirred for another 1 h. The resulting mixture was quenched by saturated NH_4Cl and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The resulting residue was purified by silical gel column chromatography (eluent: dichloromethane/methanol = 30/1, *v*/*v*) to give **1g** as a colorless oil (0.22 g, 58% yield).



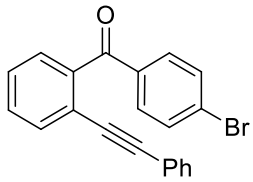
1g

1g: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Colourless oil; 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.65-7.59 (m, 2H), 7.53-7.51 (m, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.39-7.34 (m, 4H), 3.12 (t, *J* = 7.4 Hz, 2H), 1.80-1.74 (m, 3H), 0.98 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 203.8, 141.6, 133.8, 131.6, 130.9, 128.8, 128.6, 128.4, 128.2, 123.1, 121.3, 94.5, 88.4, 44.2, 18.1, 14.0.



1h

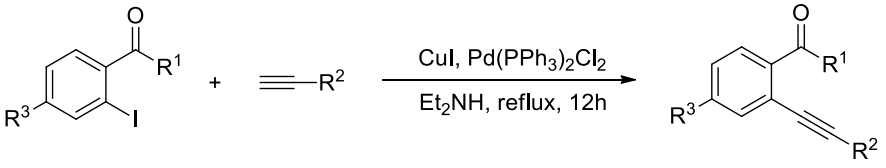
1h: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Colorless oil; 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.65-7.61 (m, 2H), 7.56-7.54 (m, 2H), 7.47-7.43 (m, 1H), 7.41-7.36 (m, 4H), 3.05 (d, *J* = 6.8 Hz, 2H), 2.34-2.25 (m, 1H), 1.00 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 203.6, 141.9, 133.8, 131.6, 130.9, 128.8, 128.6, 128.4, 128.2, 123.0, 121.2, 94.4, 88.3, 51.3, 25.3, 22.8.



1r

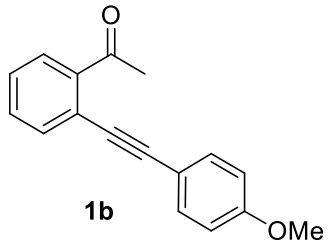
1r: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Bright yellow solid; 89% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.72 (d, *J* = 8.5 Hz, 2H), 7.60-7.57 (m, 3H), 7.51-7.46 (m, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.24-7.19 (m, 3H), 7.05 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 195.9, 140.9, 136.2, 132.7, 131.7, 131.7, 131.4, 130.7, 128.8, 128.6, 128.4, 128.3, 128.2, 122.4, 121.8, 95.6, 87.4.

7.3 General procedure for the synthesis of substrates 1b, 1d, 1q, 1s:



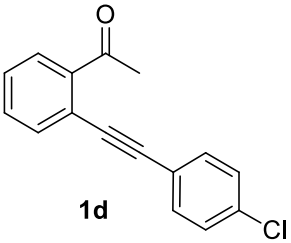
Typical procedure:[2a,2b] Using **1b** as an example. To a mixture of CuI (49 mg, 0.26 mmol) and $(PPh_3)_2PdCl_2$ (73 mg, 0.10 mmol) was added the solution of *o*-iodoacetophenone (0.40 mL, 2.8 mmol), 4-methoxyphenylacetylene (0.54 mL, 4.2 mmol) in Et_2NH (20 mL) under nitrogen. Then the mixture was refluxed at 90 °C and stirred for 12 h. The resulting mixture was concentrated under reduced pressure to give a residue, which was washed with water and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The resulting residue was purified by silical gel

column chromatography (eluent: dichloromethane/methanol = 30/1, *v*/*v*) to give **1b** as an orange oil. The crude product was recrystallized from DCM/PE, giving the light yellow solid (0.60 g, 91% yield).



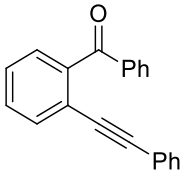
1b

1b: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Light yellow solid; 91% yield (recrystallized from DCM/PE). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.76-7.74 (m, 1H), 7.62-7.60 (m, 1H), 7.51-7.44 (m, 3H), 7.40-7.36 (m, 1H), 6.92-6.88 (m, 2H), 3.84 (s, 3H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 200.5, 160.2, 140.7, 133.8, 133.1, 131.3, 128.8, 128.0, 122.2, 115.1, 114.3, 95.4, 87.5, 55.4, 30.1.



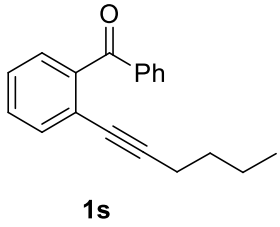
1d

1d: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2013**, *52*, 13284). Orange needle-like solid; 72% yield (recrystallized from DCM/PE). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.74 (d, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.47-7.45 (m, 3H), 7.40-7.37 (m, 1H), 7.33-7.30 (m, 2H), 2.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 199.9, 140.6, 134.8, 134.0, 132.8, 131.4, 128.9, 128.5, 121.5, 121.4, 93.7, 89.6, 29.8.



1q

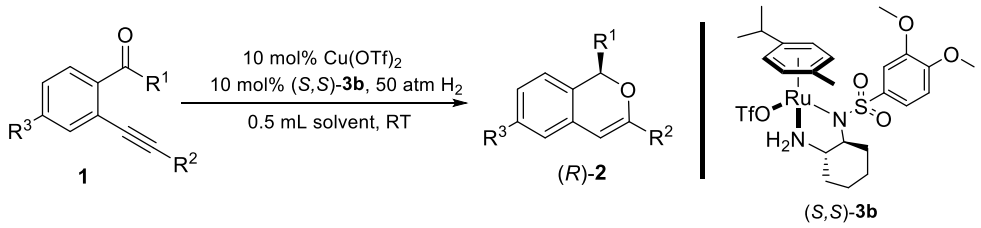
1q: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White powdery solid; 82% yield (recrystallized from MeOH/H_2O). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.89-7.87 (m, 2H), 7.62-7.41 (m, 7H), 7.24-7.16 (m, 3H), 7.05-7.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 197.1, 141.6, 137.5, 133.3, 132.7, 131.5, 130.4, 130.3, 128.8, 128.5, 128.3, 128.2, 122.7, 121.9, 95.2, 87.6.



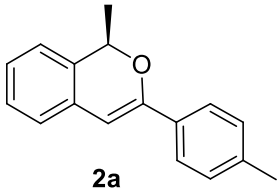
1s

1s: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Light yellow oil; 70% yield (stirred in Et_2NH for 24 h). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.81 (d, *J* = 7.6 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.48-7.33 (m, 6H), 2.10 (t, *J* = 6.2 Hz, 2H), 1.17-1.13 (m, 4H), 0.77 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 197.4, 141.8, 137.4, 133.0, 132.6, 130.2, 130.0, 128.3, 128.1, 127.4, 122.5, 96.7, 78.7, 30.3, 21.8, 19.0, 13.6.

8. General procedure for asymmetric tandem reactions



A 15 mL glass-lined stainless-steel reactor equipped with a magnetic stirrer bar was charged with substrate **1a** (0.1 mmol), $Cu(OTf)_2$ (0.01 mmol) and Ru-catalyst (*S*,*S*)-**3b** (0.01 mmol) in DCM or GDME (0.5 mL) under N_2 atmosphere in a glove box. The autoclave was closed, and the final pressure of the hydrogen gas was adjusted to 50 atm after purging the autoclave with hydrogen gas several times. The reaction mixture was stirred at room temperature for a certain time. Then the hydrogen gas was carefully released. The reaction mixture was filtered through a short pad of silica eluted with CH_2Cl_2 and PE to give the isolated pure products. The enantiomeric excess of the product was determined by HPLC with a chiral column.

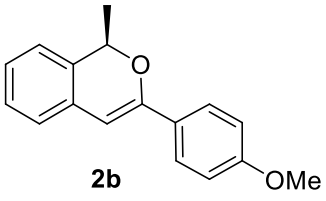


2a

R-**2a**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 23 mg; isolated yield 97%, 93% ee; $[\alpha]^{24}_D$ = -44.7(*c* 1.17, CH_2Cl_2); ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.63 (d, *J* = 8.1 Hz, 2H), 7.25-7.13 (m,

4H), 7.07 (t, *J* = 6.3 Hz, 2H), 6.37 (s, 1H), 5.35 (q, *J* = 6.5 Hz, 1H), 2.37 (s, 3H), 1.66 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 152.6, 138.9, 132.6, 132.1, 131.5, 129.2, 128.0, 126.5, 125.2, 123.8, 123.3, 100.0, 74.4, 21.5, 19.6.

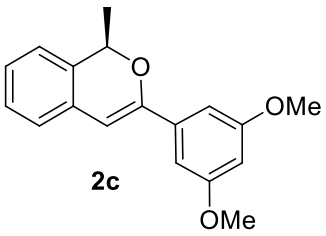
The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column (Hexane/IPA = 99.6 : 0.4, 1.0 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 11.13 min; major enantiomer: t_2 = 12.63 min.



2b

R-**2b**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 24 mg; isolated yield 94%, 93% ee; $[\alpha]^{24}_D$ = -39.2 (*c* 0.89, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.68 (d, *J* = 8.8 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.07 (t, *J* = 6.0 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.31 (s, 1H), 5.34 (q, *J* = 6.5 Hz, 1H), 3.83 (s, 3H), 1.67 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 160.3, 152.4, 132.4, 131.7, 128.0, 127.5, 126.7, 126.3, 123.6, 123.3, 113.9, 99.2, 74.4, 55.5, 19.6.

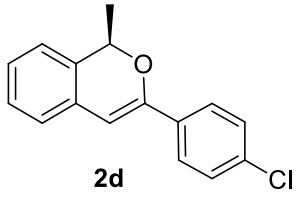
The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column (Hexane/IPA = 99.0 : 1.0, 1.0 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 10.23 min; major enantiomer: t_2 = 10.87 min.



2c

R-**2c**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2013**, *52*, 13284). Yellow solid; 26 mg; isolated yield 93%, 92% ee; $[\alpha]^{24}_D$ = -34.0 (*c* 1.11, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.17-7.08 (m, 2H), 7.02-6.98 (m, 2H), 6.82 (s, 2H), 6.39 (s, 1H), 6.32 (s, 1H), 5.28 (q, *J* = 6.4 Hz, 1H), 3.76 (s, 6H), 1.58 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 160.9, 152.1, 137.0, 132.7, 131.1, 128.0, 126.8, 124.0, 123.3, 103.4, 101.2, 74.5, 55.6, 19.7.

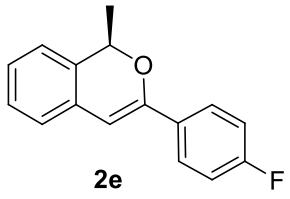
The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column (Hexane/IPA = 99.6 : 0.4, 1.0 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 22.56 min; major enantiomer: t_2 = 24.68 min.



2d

R-**2d**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2013**, *52*, 13284). Yellow solid; 24 mg; isolated yield 93%, 92% ee; $[\alpha]^{24}_{D}$ = -24.5 (*c* 0.89, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.66 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.25-7.17 (m, 2H), 7.09-7.06 (m, 2H), 6.39 (s, 1H), 5.36 (q, *J* = 6.4 Hz, 1H), 1.66 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 151.3, 134.6, 133.4, 132.6, 131.0, 128.6, 128.1, 127.0, 126.4, 124.0, 123.4, 101.1, 74.5, 19.7.

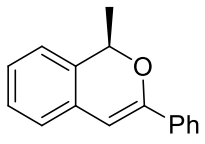
The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column (Hexane/IPA = 99.6 : 0.4, 1.0 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 9.07 min; major enantiomer: t_2 = 10.39 min.



2e

R-**2e**: (new compound). Colorless oil; 21 mg; isolated yield 89%, 90% ee; $[\alpha]^{24}_{D}$ = - 28.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.65-7.60 (m, 2H), 7.17-7.07 (m, 2H), 7.01-6.95 (m, 4H), 6.26 (s, 1H), 5.27 (q, *J* = 6.5 Hz, 1H), 1.58 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 163.2 (d, *J* = 247 Hz), 151.6, 132.4, 131.2, 131.0 (d, *J* = 3 Hz), 128.1, 127.1 (d, *J* = 8 Hz), 126.8, 123.9，123.3, 115.4 (d, *J* = 21 Hz), 100.4 (d, *J* = 2 Hz), 74.5, 19.6. HRMS (EI) m/z calcd. for $C_{16}H_{13}FO$ $(M)^+$ 240.0950, found 240.0954.

The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column (Hexane/IPA = 99.8 : 0.2, 0.6 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 10.41 min; major enantiomer: t_2 = 11.68 min.

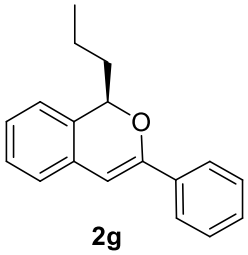


2f

R-**2f**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 21 mg; isolated yield 96%, 92% ee; $[\alpha]^{24}_{D}$ = -38.7 (*c* 0.62, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (d, *J* = 7.2 Hz, 2H), 7.40-7.32 (m, *3*H), 7.25-7.17 (m, *2*H), 7.09 (t, *J* = 8.4 Hz, 2H), 6.43 (s, 1H), 5.38 (q, *J* = 6.4 Hz, 1H), 1.68 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 152.4, 134.9, 132.7, 131.3, 128.9, 128.5,

128.0, 126.7, 125.2, 123.9, 123.3, 100.7, 74.4, 19.7.

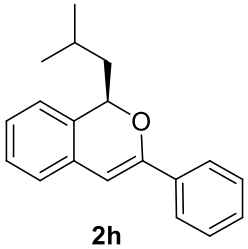
The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column (Hexane/IPA = 99.6 : 0.4, 1.0 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 10.43 min; major enantiomer: t_2 = 12.13 min.



2g

R-**2g**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 24 mg; isolated yield 95%, 92% ee; $[\alpha]^{24}_D$ = -84.6 (*c* 1.07, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (d, *J* = 7.2 Hz, 2H), 7.40-7.30 (m, 3H), 7.23-7.13 (m, 2H), 7.08 (d, *J* = 7.2 Hz, 1H), 7.03 (d, *J* = 7.2 Hz, 1H), 6.41 (s, 1H), 5.26 (q, *J* = 4.4 Hz, 1H), 2.10-2.05 (m, 1H), 1.78-1.64 (m, 2H), 1.56-1.50 (m, 1H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 151.8, 134.9, 131.9, 131.2, 128.8, 128.5, 127.9, 126.5, 125.1, 124.0, 123.9, 100.4, 78.0, 36.1, 18.8, 14.1.

The enantiomeric excess was determined by HPLC on the connection of two Chiralcel AD-H columns (Hexane/IPA = 98.0 : 2.0, 0.6 mL/min, 254 nm, 25 °C), major enantiomer: t_1 = 17.65 min; minor enantiomer: t_2 = 19.15 min.

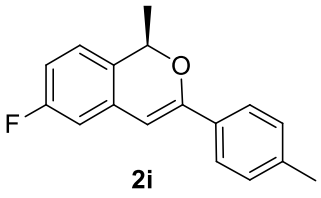


2h

R-**2h**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 25 mg; isolated yield 94%, 92% ee; $[\alpha]^{24}_D$ = -59.4(*c* 0.32, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.68-7.66 (m, 2H), 7.33-7.25 (m, 3H), 7.16-7.06 (m, 2H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.35 (s, 1H), 5.27 (q, *J* = 4.8 Hz, 1H), 2.08-1.92 (m, 2H), 1.44-1.37 (m, 1H), 0.98 (d, *J* = 6.4 Hz, 3H), 0.91 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 151.7, 134.9, 132.2, 131.2, 128.8, 128.5, 127.9, 126.5, 125.1, 124.0, 123.7, 100.5, 76.2, 42.9, 24.3, 23.7, 21.8.

The enantiomeric excess was determined by HPLC on the connection of two Chiralcel AD-H columns (Hexane/IPA = 98.0 : 2.0, 0.5 mL/min, 254 nm, 25 °C), major

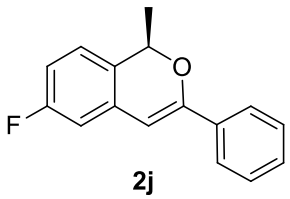
enantiomer: t_1 = 20.25 min; minor enantiomer: t_2 = 21.31 min.



2i

R-**2i**: (new compound). Yellow oil; 24 mg; isolated yield 95%, 86% ee; $[\alpha]^{24}_D$ = -30.0 (*c* 0.36, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.54 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.93-6.90 (m, 1H), 6.77-6.67 (m, 2H), 6.23 (s, 1H), 5.24 (q, *J* = 6.4 Hz, 1H), 2.29 (s, 3H), 1.57 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.8 (d, *J* = 243 Hz), 153.7, 139.4, 133.8 (d, *J* = 9 Hz), 131.6, 129.2, 128.1 (d, *J* = 3 Hz), 125.3, 124.8 (d, *J* =8 Hz), 112.7 (d, *J* = 22 Hz), 110.2 (d, *J* = 23 Hz), 99.3 (d, *J* = 2 Hz), 74.2, 21.5, 19.6. HRMS (EI) m/z calcd. for $C_{17}H_{15}FO$ $(M)^+$ 254.1107, found 254.1110.

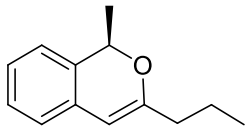
The enantiomeric excess was determined by HPLC on a Chiralcel AD-H column (Hexane/IPA = 98.0 : 2.0, 0.5 mL/min, 254 nm, 25 °C), major enantiomer: t_1 = 12.73 min; minor enantiomer: t_2 = 14.44 min.



2j

R-**2j**: (new compound). Yellow oil; 21 mg; isolated yield 89%, 87% ee; $[\alpha]^{24}_D$ = -27.3 (*c* 0.62, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.65 (d, *J* = 6.8 Hz, 2H), 7.32-7.24 (m, 3H), 6.94-6.90 (m, 1H), 6.78-6.69 (m, 2H), 6.27 (s, 1H), 5.25 (q, *J* = 6.5 Hz, 1H), 1.57 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.8 (d, *J* = 243 Hz), 153.6, 134.4, 133.6 (d, *J* = 9 Hz), 129.2, 128.5, 128.2 (d, *J* = 3 Hz), 125.4, 124.8 (d, *J* = 9 Hz), 112.9 (d, *J* = 22 Hz), 110.4 (d, *J* = 22 Hz), 100.1 (d, *J* = 3 Hz), 74.2, 19.7. HRMS (EI) m/z calcd. for $C_{16}H_{13}FO$ $(M)^+$ 240.0950, found 240.0953.

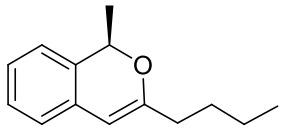
The enantiomeric excess was determined by HPLC on a Chiralcel AD-H column (Hexane/IPA = 98.0 : 2.0, 0.5 mL/min, 254 nm, 25 °C), major enantiomer: t_1 = 11.81 min; minor enantiomer: t_2 = 13.07 min.



2k

R-**2k**: (new compound). Colourless oil; 16 mg; isolated yield 86%, 90% ee; $[\alpha]^{24}_{D}$ = +8.1 (*c* 1.00, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.12-7.00 (m, 2H), 6.91 (d, *J* =7.5 Hz, 1H), 6.84 (d, *J* = 7.2 Hz, 1H), 5.53 (s, 1H), 5.11 (q, *J* = 6.5 Hz, 1H), 2.08 (t, *J* = 7.4 Hz, 2H), 1.58-1.48 (m, 5H), 0.89 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 156.9, 131.8, 131.4, 127.9, 125.9, 123.3, 122.7, 100.5, 74.1, 36.0, 20.3, 19.9, 13.9. HRMS (EI) m/z calcd. for $C_{13}H_{16}O$ $(M)^+$ 188.1201, found 188.1203.

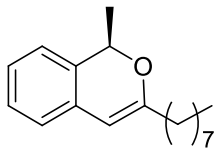
The enantiomeric excess was determined by HPLC on the connection of two Chiralcel OD-H columns (Hexane/IPA = 98.0 : 2.0, 0.25 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 30.97 min; major enantiomer: t_2 = 33.39 min.



2l

R-**2l**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Colorless oil; 18 mg; isolated yield 87%, 90% ee; $[\alpha]^{24}_{D}$ = +13.3 (*c* 0.6, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.09 (t, *J* = 7.4 Hz, 1H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 5.53 (s, 1H), 5.11 (q, *J* = 6.5 Hz, 1H), 2.10 (t, *J* = 7.6 Hz, 2H), 1.50-1.46 (m, 5H), 1.34-1.28 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 157.2, 131.8, 131.4, 127.9, 125.8, 123.3, 122.7, 100.3, 74.1, 33.7, 29.2, 22.5, 19.9, 14.1.

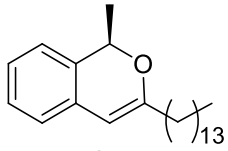
The enantiomeric excess was determined by HPLC on the connection of two Chiralcel OD-H columns (Hexane/IPA = 98.0 : 2.0, 0.25 mL/min, 254 nm, 25 °C), minor enantiomer: t_1 = 31.71 min; major enantiomer: t_2 = 34.12 min.



2m

R-**2m:** (new compound). Colorless oil; 22 mg; isolated yield 87%, 88% ee; $[\alpha]^{24}_{D}$ = +8.3 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.10-6.98 (m, 2H), 6.89 (d, *J* = 6.9 Hz, 1H), 6.82 (d, *J* = 6.6 Hz, 1H), 5.52 (s, 1H), 5.11-5.09 (m, 1H), 2.08 (t, *J* = 7.7 Hz, 3H), 1.49-1.46 (m, 5H), 1.20 (br, s, 10H), 0.80 (br, s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 157.2, 131.8, 131.4, 127.8, 125.8, 123.3, 122.7, 100.3, 74.1, 34.0, 32.0, 29.6, 29.4, 29.4, 27.0,

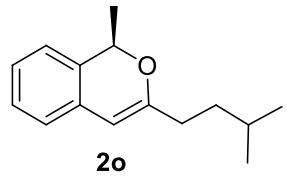
22.8, 19.9, 14.3. HRMS (EI) m/z calcd. for $C_{18}H_{26}O$ $(M)^+$ 258.1984, found 258.1981. The enantiomeric excess was determined by HPLC on the connection of two Chiralcel OD-H columns (Hexane/IPA = 98.0 : 2.0, 0.25 mL/min, 254 nm, 25 °C), minor enantiomer: t_1 = 29.61 min; major enantiomer: t_2 = 31.94 min.



2n

R-**2n:** (new compound). Colorless oil; 28 mg; isolated yield 81%, 89% ee; $[\alpha]^{24}_D$ = +6.4 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.24-7.07 (m, 2H), 6.97 (d, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.2 Hz, 1H), 5.60 (s, 1H), 5.18 (q, *J* = 6.4 Hz, 1H), 2.16 (t, *J* = 7.5 Hz, 2H), 1.57-1.55 (m, 5H), 1.30-1.26 (m, 22H), 0.90-0.86 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 157.2, 131.8, 131.5, 127.9, 125.8, 123.3, 122.7, 100.3, 74.1, 34.0, 32.1, 29.8, 29.8, 29.6, 29.5, 29.4, 27.0, 22.9, 19.9, 14.3. HRMS (EI) m/z calcd. for $C_{24}H_{38}O$ $(M)^+$ 342.2923, found 342.2927.

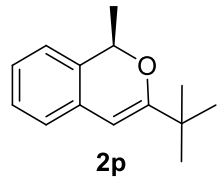
The enantiomeric excess was determined by HPLC on the connection of two Chiralcel OD-H columns (Hexane/IPA = 98.0 : 2.0, 0.25 mL/min, 254 nm, 25 °C), minor enantiomer: t_1 = 27.84 min; major enantiomer: t_2 = 29.94 min.



2o

R-**2o**: (new compound). Colorless oil; 19 mg; isolated yield 86%, 89% ee; $[\alpha]^{24}_D$ = +4.1 (*c* 1.00, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.24-7.07 (m, 2H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.90 (d, *J* = 7.2 Hz, 1H), 5.60 (s, 1H), 5.19-5.15 (m, 1H), 2.17 (t, *J* = 7.8 Hz, 2H), 1.64-1.55 (m, 4H), 1.49-1.42 (m, 2H), 0.92 (d, *J* = 6.3 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 157.4, 131.7, 131.4, 127.9, 125.8, 123.3, 122.7, 100.1, 74.1, 36.1, 32.0, 27.8, 22.7, 22.6, 19.9. HRMS (EI) m/z calcd. for $C_{15}H_{20}O$ $(M)^+$ 216.1514, found 216.1512.

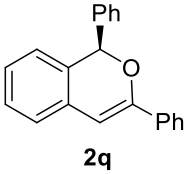
The enantiomeric excess was determined by HPLC on the connection of two Chiralcel OD-H columns (Hexane/IPA = 98.0 : 2.0, 0.25 mL/min, 254 nm, 25 °C), minor enantiomer: t_1 = 30.30 min; major enantiomer: t_2 = 32.14 min.



2p

R-**2p**: (new compound). Colorless oil; 17 mg; isolated yield 86%, 67% ee; $[\alpha]^{24}_D$ = +6.6 (*c* 1.00, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.13 (t, *J* = 7.4 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 2H), 5.65 (s, 1H), 5.15 (q, *J* = 6.5 Hz, 1H), 1.48 (d, *J* = 6.4 Hz, 3H), 1.16 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.7, 132.0, 131.4, 127.8, 125.9, 123.3, 123.2, 97.1, 73.9, 35.1, 27.9, 19.7. HRMS (EI) m/z calcd. for $C_{14}H_{18}O$ $(M)^+$ 202.1358, found 202.1361.

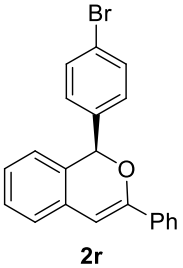
The enantiomeric excess was determined by HPLC on a Chiralcel OJ-H column (Hexane/IPA = 99.6 : 0.4, 0.6 mL/min, 254 nm, 25 °C), major enantiomer: t_1 = 7.23 min; minor enantiomer: t_2 = 8.03min.



2q

R-**2q**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 26 mg; isolated yield 90%, 86% ee; $[\alpha]^{24}_D$ = -58.2(*c* 0.94, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.65-7.63 (m, 2H), 7.33-7.15 (m, 9H), 7.07-7.03 (m, 2H), 6.70 (d, *J* = 7.2 Hz, 1H), 6.40 (s, 1H), 6.17 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 152.6, 139.9, 134.5, 131.9, 130.6, 128.9, 128.5, 128.4, 128.0, 126.6, 125.5, 125.3, 123.9, 101.2, 80.2.

The enantiomeric excess was determined by HPLC on a Chiralcel OD-H columns (Hexane/IPA = 99.6 : 0.4, 1.0 mL/min, 338 nm, 25 °C), minor enantiomer: t_1 = 13.87 min; major enantiomer: t_2 = 19.29 min.

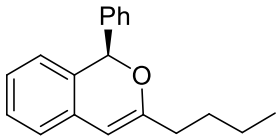


2r

R-**2r**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). White solid; 30 mg; isolated yield 83%, 87% ee; $[\alpha]^{24}_D$ = -70.0 (*c* 0.91, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.64-7.62 (m, 2H), 7.41-7.39 (m, 2H), 7.30-7.18 (m, 6H), 7.09-7.05 (m, 2H), 6.73 (d, *J* = 7.6 Hz, 1H), 6.41 (s, 1H), 6.14 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 152.4, 139.0, 134.3, 131.7, 131.7, 129.9, 129.7, 129.1, 128.7, 128.5, 126.8, 125.4, 125.2, 124.1, 122.5, 101.3, 79.5.

The enantiomeric excess was determined by HPLC on a Chiralcel OD-H column

(Hexane/IPA = 99.6 : 0.4, 1.0 mL/min, 254 nm, 25 °C), minor enantiomer: t_1 = 13.77 min; major enantiomer: t_2 = 15.83 min.

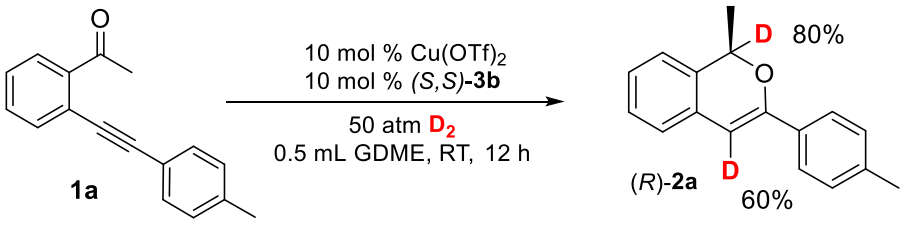


2s

R-**2s**: (known compound, see: K. Saito, Y. Kajiwara, T. Akiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 235). Colourless oil; 24 mg; isolated yield 90%, 72% ee; $[\alpha]^{24}_D$ = +70.6 (*c* 1.03, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.27 (br, s, 5H), 7.16-7.11 (m, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.62 (d, *J* = 7.6 Hz, 1H), 6.00 (s, 1H), 5.60 (s, 1H), 2.17-2.05 (m, 2H), 1.40-1.35 (m, 2H), 1.25-1.13 (m, 2H), 0.78 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 157.5, 140.3, 132.0, 129.6, 128.4, 128.3, 128.3, 128.2, 125.8, 125.4, 122.7, 101.0, 80.0, 33.7, 28.9, 22.3, 14.0.

The enantiomeric excess was determined by HPLC on the connection of two Chiralcel OD-H columns (Hexane/IPA = 98.0 : 2.0, 0.3 mL/min, 254 nm, 25 °C), minor enantiomer: t_1 = 29.64 min; major enantiomer: t_2 = 31.76 min.

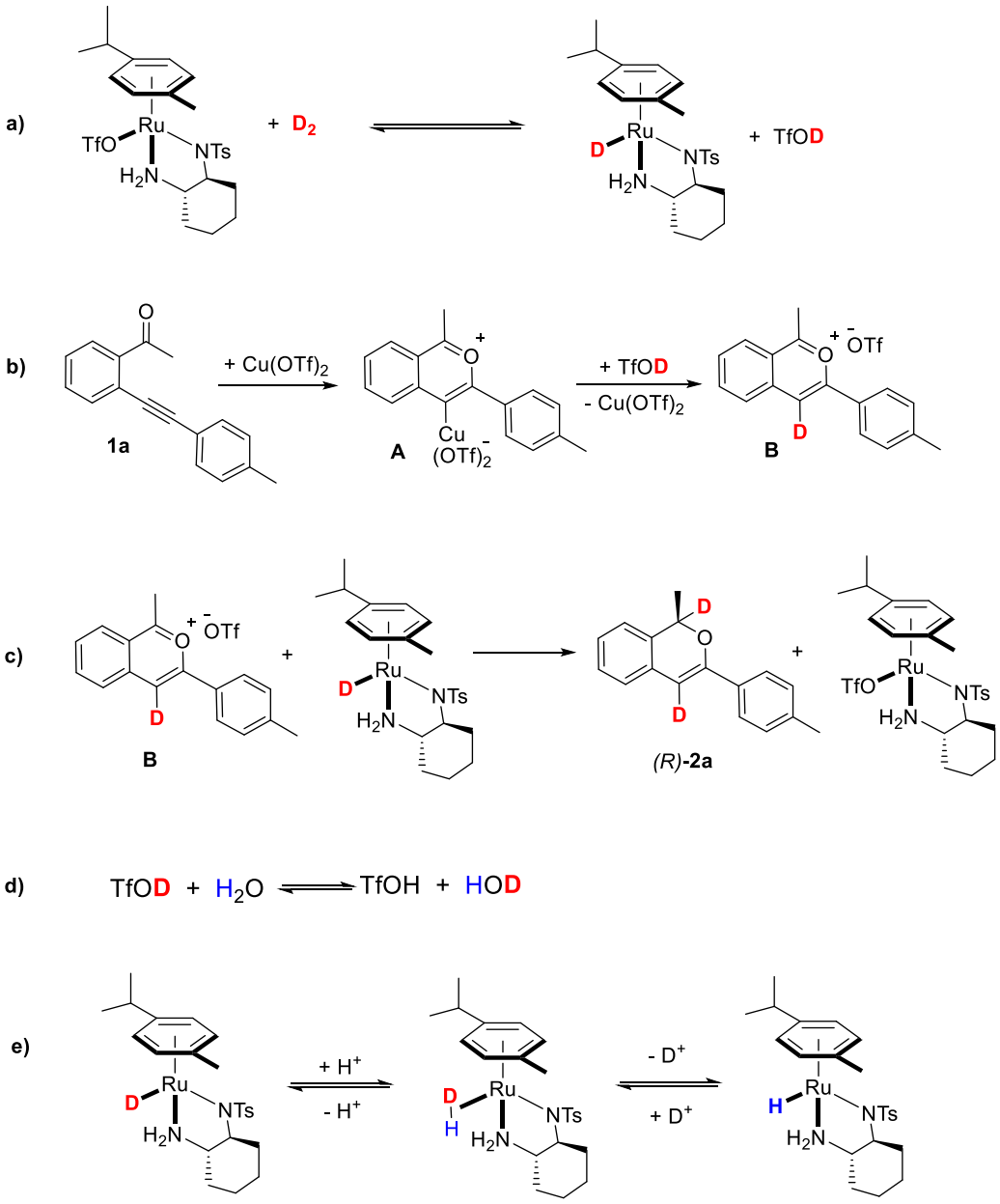
9. Deuteration study



To further understand the tandem reaction process, isotope labeling experiments using deuterated gas was carried out at room temperature under the hydrogenation conditions as described above and monitored by ^{1}H NMR spectroscopy to identify the concentration of deuterium in the various positions of the hydrogenated product. It was found that 80% and 60% deuterium incorporation at C1 and C4 positions were observed, respectively. This deuterium distribution can be explained as follows.

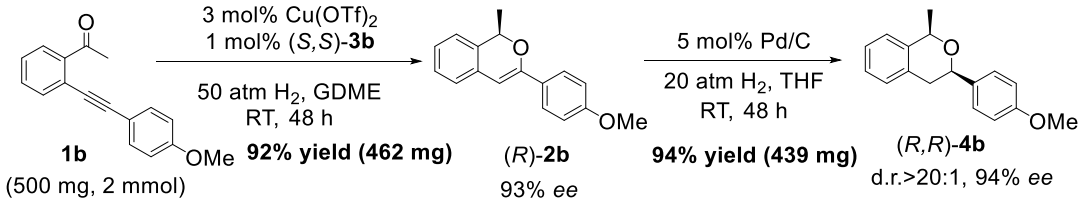
In addition, the unavoidably existed moisture (H2O) in the reaction system is the

main reason why the deuteration is not 100% at C1 and C4-positions.



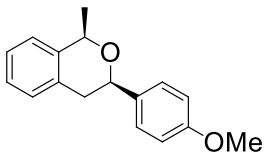
Scheme S7 Deuterium-Labeling Studies

10. Synthesis of compound (*R,R*)-4b



A 30 mL glass-lined stainless-steel reactor equipped with a magnetic stirrer bar was charged with substrate **1b** (500 mg, 2 mmol), $Cu(OTf)_2$ (0.06 mmol) and (*S,S*)-**3b** (0.02 mmol) in GDME (5 mL) under N_2 atmosphere in a glove box. The autoclave was closed, and the final pressure of the hydrogen gas was adjusted to 50 atm after purging the autoclave with hydrogen gas several times. The reaction mixture was stirred at room temperature for 48 h. Then the hydrogen gas was carefully released. The reaction mixture was filtered through a short pad of silica eluted with CH_2Cl_2 and PE to give the isolated pure product (*R*)-**2b**. The enantiomeric excess of the **2b** was determined by HPLC with a chiral column.

A 30 mL glass-lined stainless-steel reactor equipped with a magnetic stirrer bar was charged with substrate **2b** (462 mg, 1.86 mmol), 5 mol% Pd/C in THF (5 mL). The autoclave was closed, and the final pressure of the hydrogen gas was adjusted to 20 atm after purging the autoclave with hydrogen gas several times. The reaction mixture was stirred at room temperature for 48 h. Then the hydrogen gas was carefully released. The reaction mixture was filtered through a short pad of silica eluted with CH_2Cl_2 and PE to give the isolated pure product as a colorless oil.



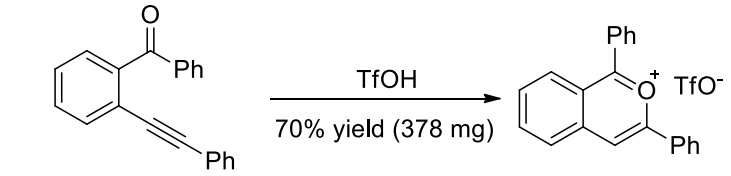
(*R,R*)-**4b**

(*R,R*)-**4b**: (new compound). Colourless oil; 439 mg; isolated yield 94%, 94% ee; $[\alpha]^{24}_D$ = +12.1 (*c* 1.03, CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.40 (d, *J* = 8.5 Hz, 2H), 7.25-7.12 (m, 4H), 6.93 (d, *J* = 8.5 Hz, 2H), 5.07 (q, *J* = 6.3 Hz, 1H), 4.72-4.69 (m, 1H), 3.83 (s, 3H), 3.14-3.08 (m, 1H), 2.93-2.89 (m, 1H), 1.63 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (125

MHz, $CDCl_3$): δ (ppm) 159.3, 139.5, 134.8, 134.1, 128.8, 127.4, 126.5, 126.5, 124.6, 114.0, 76.2, 74.1, 55.5, 37.0, 22.2. HRMS (EI) m/z calcd. for $C_{17}H_{18}O_2^+$ $(M)^+$ 254.1307, found 254.1303.

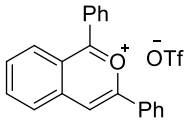
The enantiomeric excess was determined by HPLC on a Chiralcel AD-H columns (Hexane/IPA = 99.0 : 1.0, 1.0 mL/min, 220 nm, 25 °C), minor enantiomer: t_1 = 7.57 min; major enantiomer: t_2 = 8.26 min.

11. Synthesis of 1,3-diphenylisobenzopyrylium 5q



1q (353 mg, 1.25 mmol) **5q**

To a mixture of **1q** (353 mg, 1.25 mmol) in DCM was added TfOH (20 equiv.) dropwise under N_2 atmosphere and stirred for 1.5 h. The solvent was removed about 90%, and anhydrous diethyl ether was added to precipitate the crude product as an orange solid. Then the solid was washed with cold diethyl ether, giving the desired pure product **5q**.



5q

5q: (known compound, see: J.- D. Tovar, T.- M. Swager, *J. Org. Chem*. **1999**, *64*, 6499). Orange solid, isolated yield 70%; ^{1}H NMR (500 MHz, CD_3CN): δ (ppm) 8.84 (br, s, 1H), 8.67 (br, s, 1H), 8.45 (br, s, 1H), 8.37 (br, s, 1H), 8.23 (br, s, 4H), 8.09 (br, s, 1H), 7.98 (br, s, 1H), 7.87 (br, s, 2H), 7.70 (br, s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 182.1, 161.7, 145.1, 144.0, 136.5, 134.1, 134.0, 133.9, 133.6, 130.9, 130.9, 130.4, 130.3, 129.4, 127.9, 124.2, 116.4.

12. References

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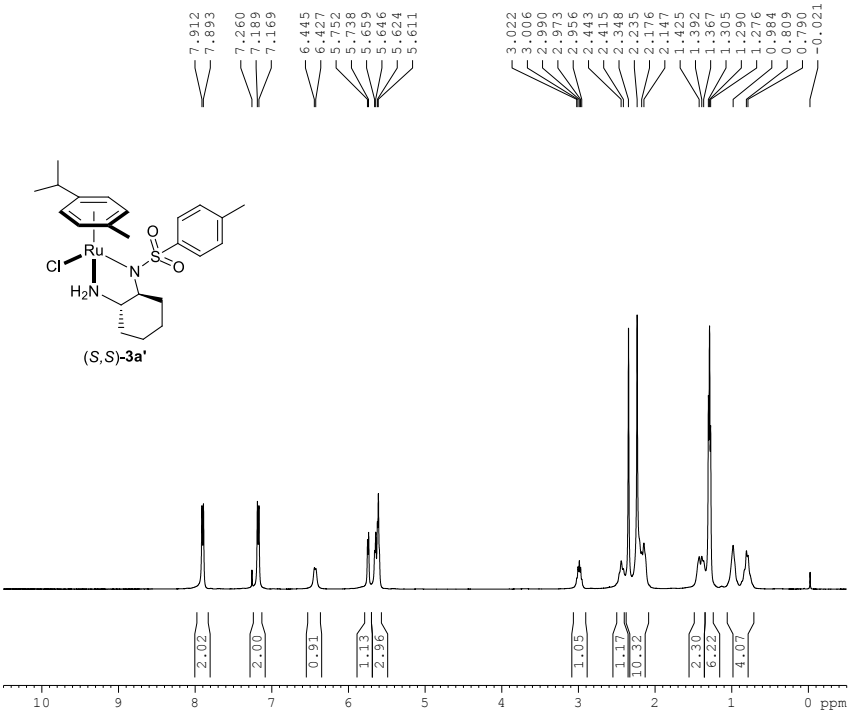
13. Copy of NMR and HRMS spectra

13.1 Catalyst precursors:

Compound 3a'

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PROCNO               1

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FIDRES          0.244532 Hz
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DW                62.400 usec
DE                 6.50 usec
TE                297.6 K
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TD0                    1

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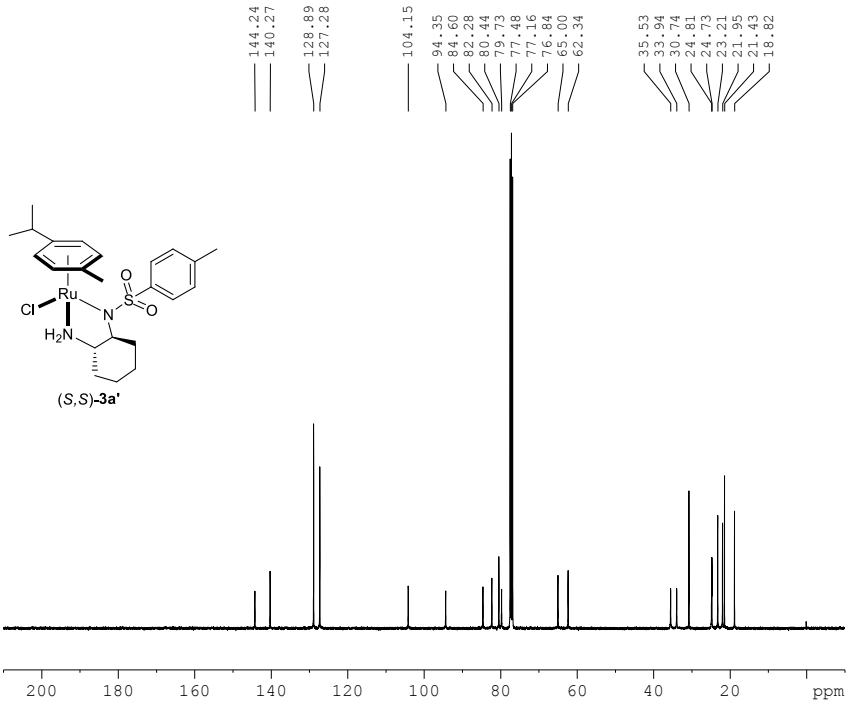


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SOLVENT            CDCl3
NS                  3247
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

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NUC1                  13C
P1                 10.00 usec

F2 - Processing parameters
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WDW                   EM
SSB                    0
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GB                     0
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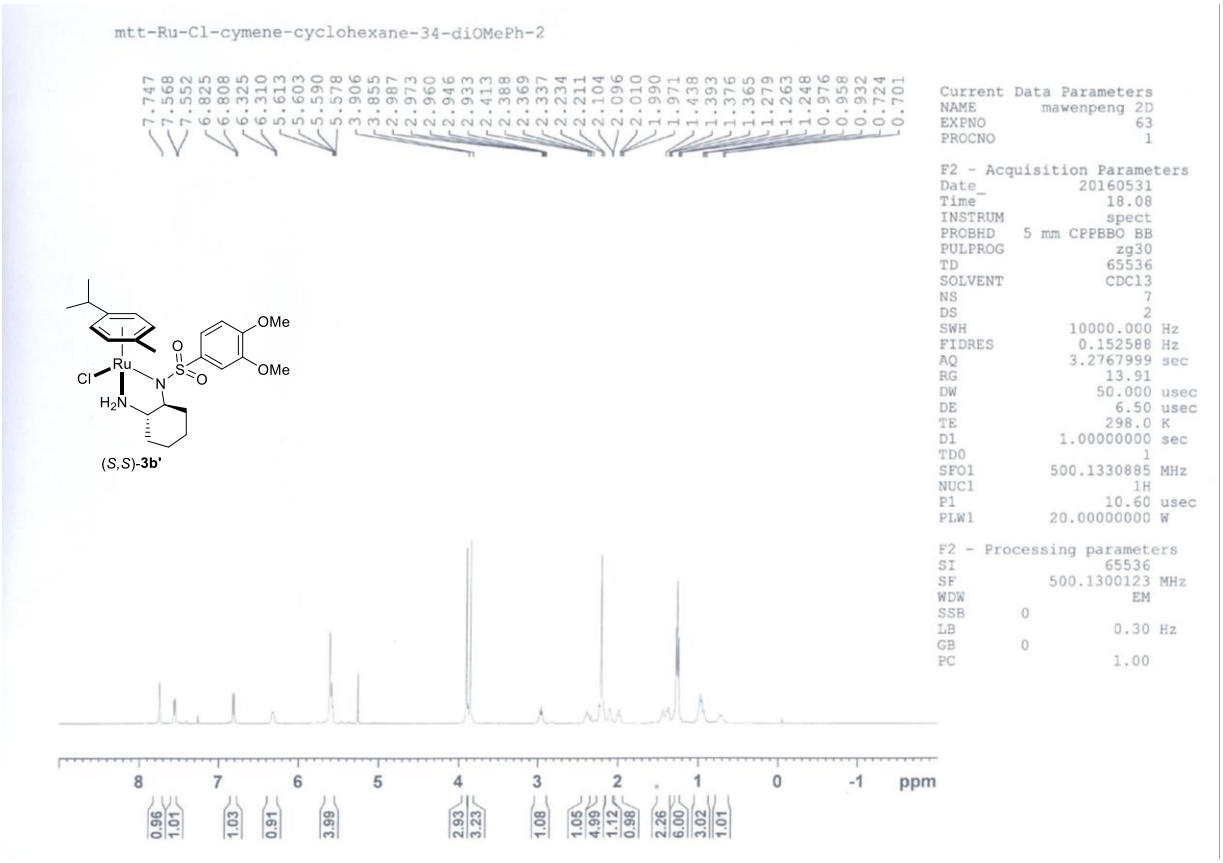
Compound 3b’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6.808
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5.603
5.590
5.578
3.906
3.855
2.987
2.973
2.960
2.946
2.933
2.413
2.388
2.369
2.337
2.234
2.211
2.104
2.096
2.010
1.990
1.971
1.438
1.393
1.376
1.365
1.279
1.263
1.248
0.976
0.958
0.932
0.724
0.701
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PROCNO 1
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FIDRES 0.152588 Hz
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RG 13.91
DW 50.000 usec
DE 6.50 usec
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TD0 1
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NUC1 1H
P1 10.60 usec
PLW1 20.00000000 W
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SF 500.1300123 MHz
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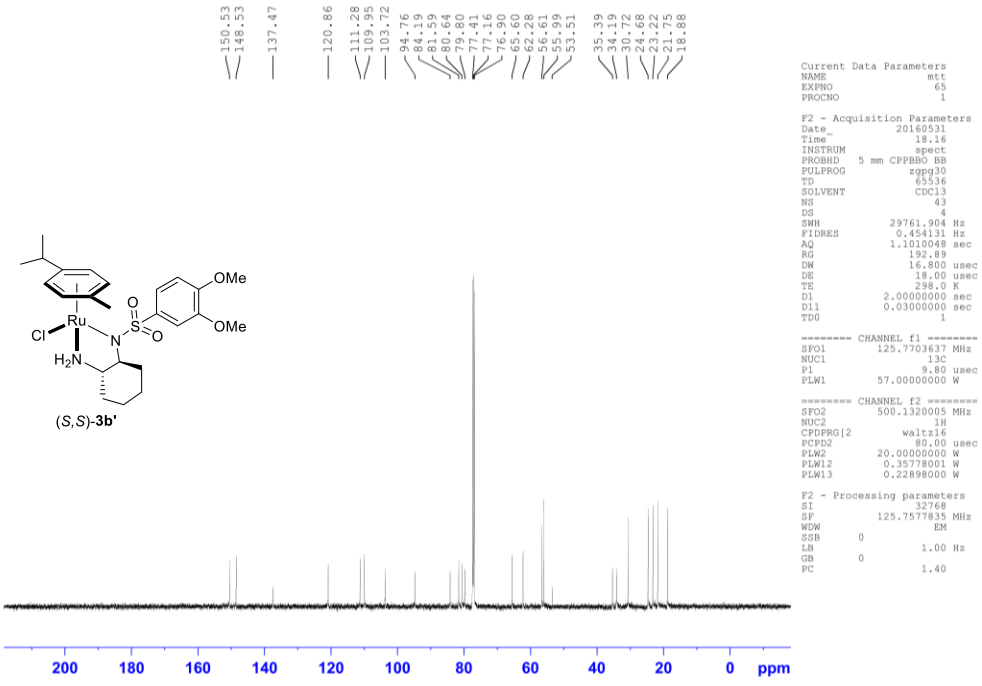
LB 0.30 Hz
GB 0
PC 1.00
OMe
OMe
Ru
Cl
H2N
(S,S)-3b'
8
7
6
5
4
3
2
1
0
-1
ppm
0.96
1.01
1.03
0.91
3.99
2.93
3.23
1.08
1.05
4.99
1.12
0.98
2.26
6.00
3.02
1.01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81.59
80.64
79.80
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77.16
76.90
65.60
62.28
56.61
55.99
53.51
35.39
34.19
30.72
24.68
23.22
21.75
18.88
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SOLVENT CDCl3
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DS 4
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FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W
======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OMe
OMe
Ru
Cl
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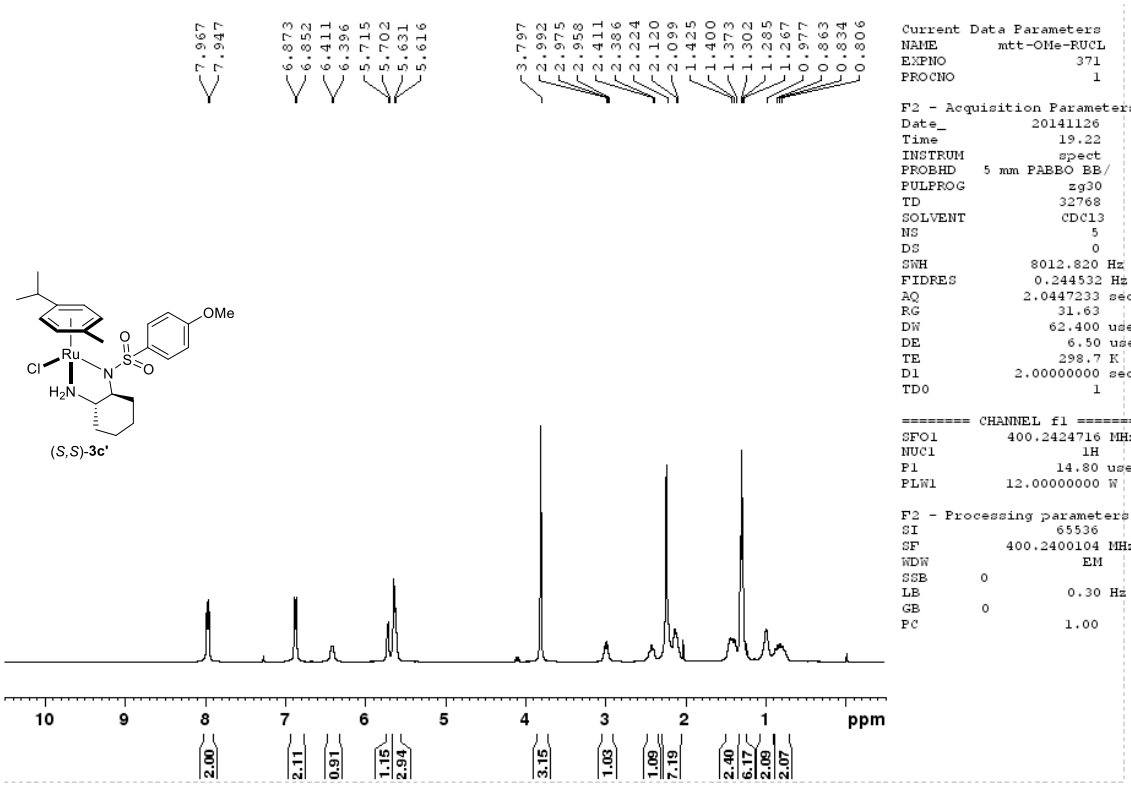
160
140
120
100
80
60
40
20
0
ppm

Compound 3c’

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PROCNO                  1

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PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
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DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
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RG                 31.63
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TE                298.7 K
D1              2.00000000 sec
TD0                    1

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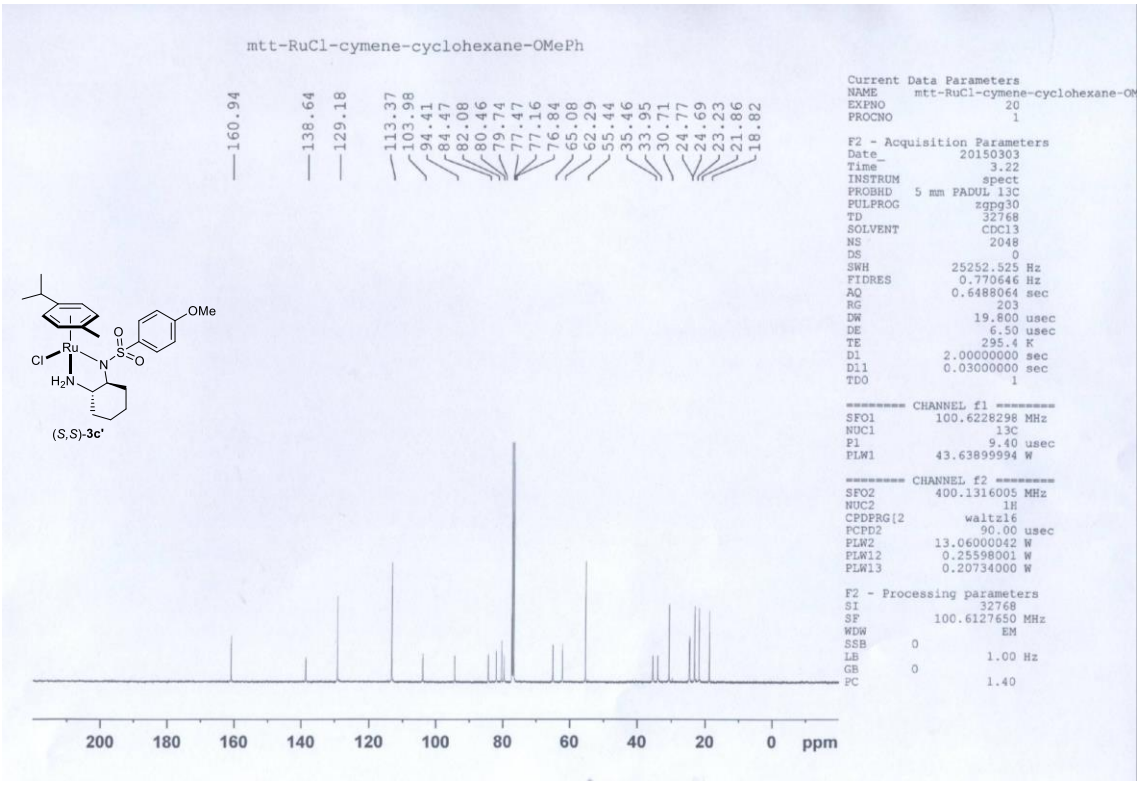


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SOLVENT           CDCl3
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DS                    0
SWH            25252.525 Hz
FIDRES             0.770646 Hz
AQ              0.6488064 sec
RG                  203
DW                 19.800 usec
DE                  6.50 usec
TE                295.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
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NUC1                  13C
P1                  9.40 usec
PLW1           43.63899994 W

======== CHANNEL f2 ========
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NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2           13.06000042 W
PLW12           0.25598001 W
PLW13           0.20734000 W

F2 - Processing parameters
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GB        0
PC                 1.40
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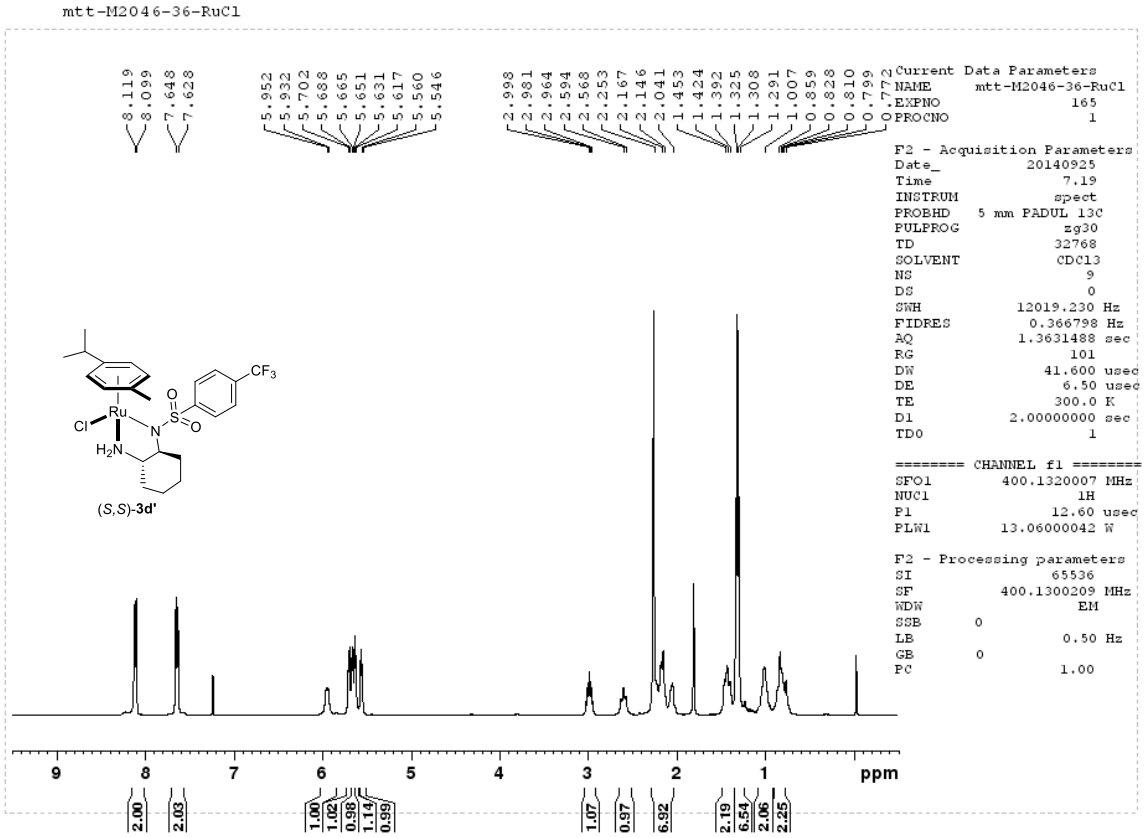
Compound 3d'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5.546
2.998
2.981
2.964
2.594
2.568
2.253
2.167
2.146
2.041
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1.325
1.308
1.291
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0.810
0.799
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DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
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(S,S)-3d'
9
8
7
6
5
4
3
2
1
ppm
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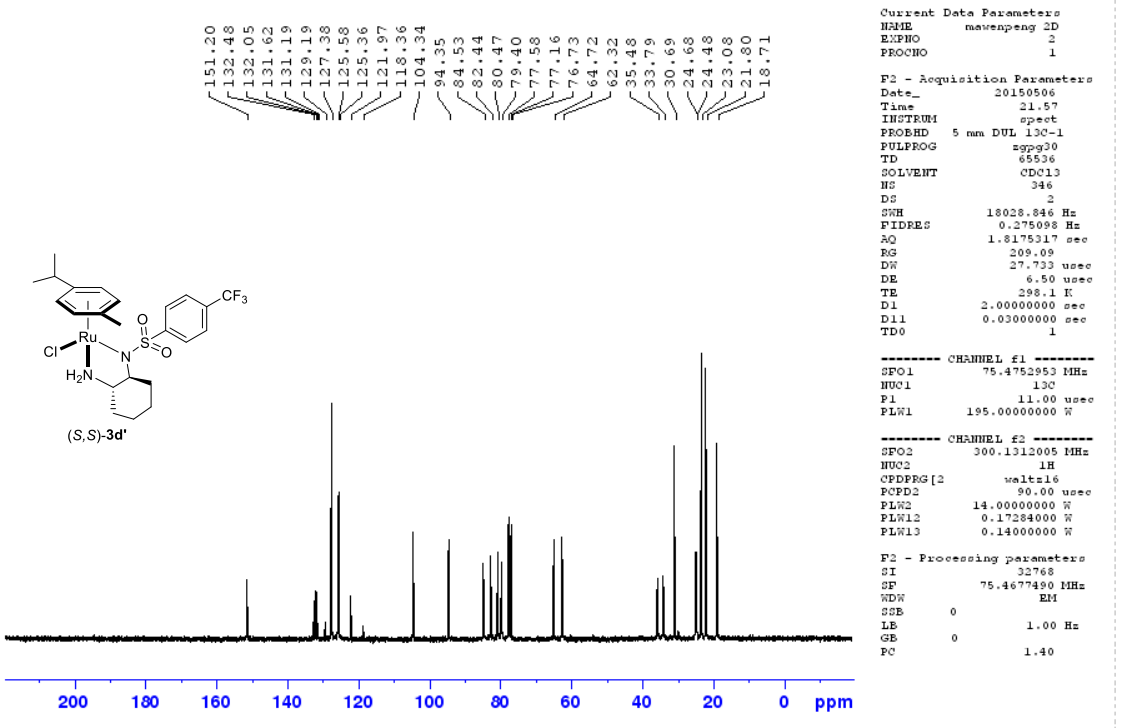
2.06
2.25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30.69
24.68
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23.08
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18.71
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SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 209.09
DW 27.733 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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NUC1 13C
P1 11.00 usec
PLW1 195.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
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PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W
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LB 1.00 Hz
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120
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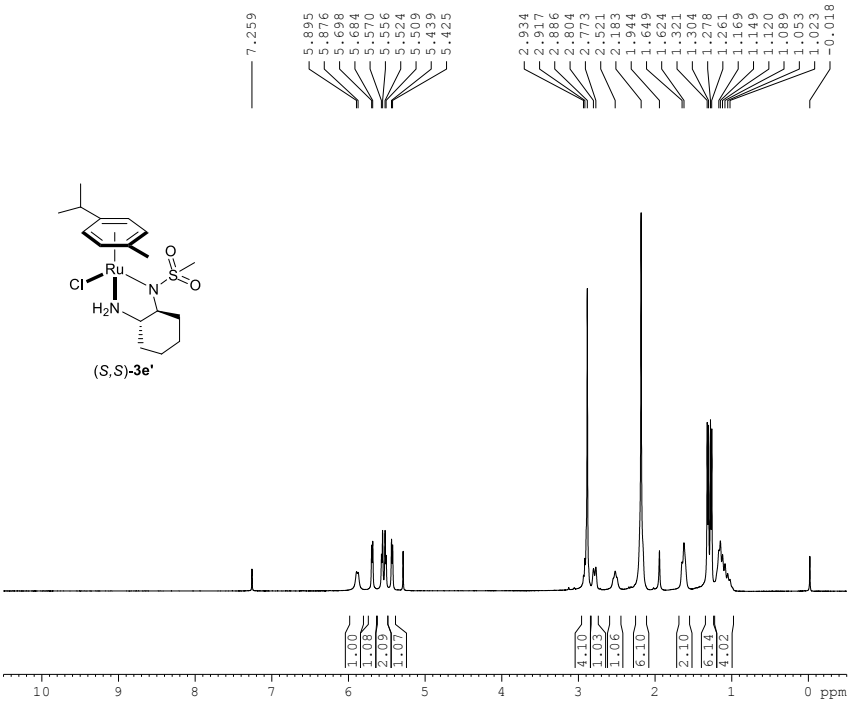
80
60
40
20
0
ppm

Compound 3e’



(*S*,*S*)-**3e'**

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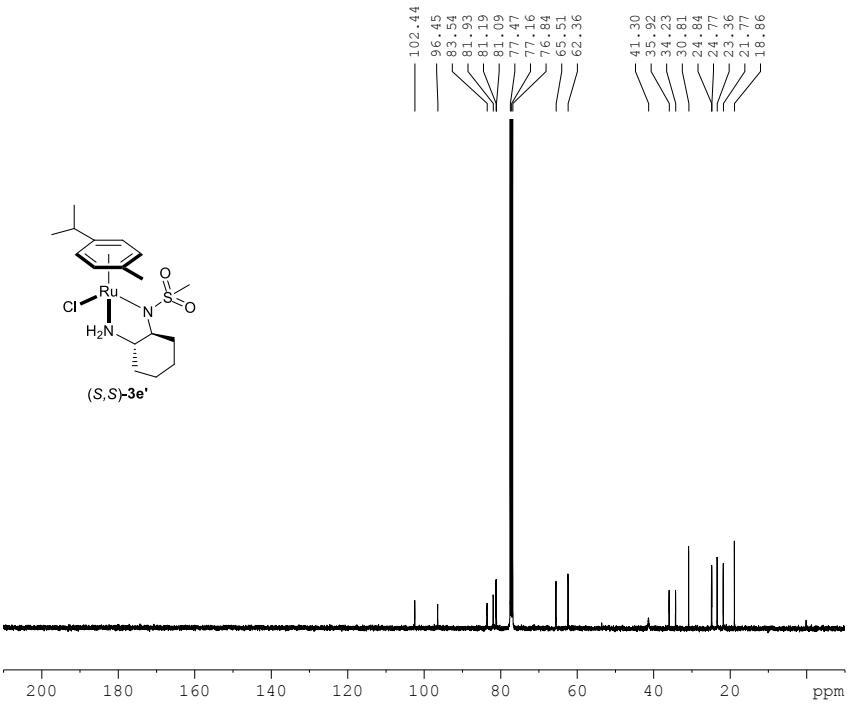
F2 - Acquisition Parameters
Date_           20141124
Time              11.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   12
DS                    0
SWH            8012.820 Hz
FIDRES            0.244532 Hz
AQ             2.0447731 sec
RG                102.73
DW                62.400 usec
DE                 6.50 usec
TE                298.5 K
D1             2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec

F2 - Processing parameters
SI                65536
SF           400.2400104 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



(*S*,*S*)-**3e'**

```
Current Data Parameters
NAME      mtt-M2051-41 400
EXPNO                 91
PROCNO                 1

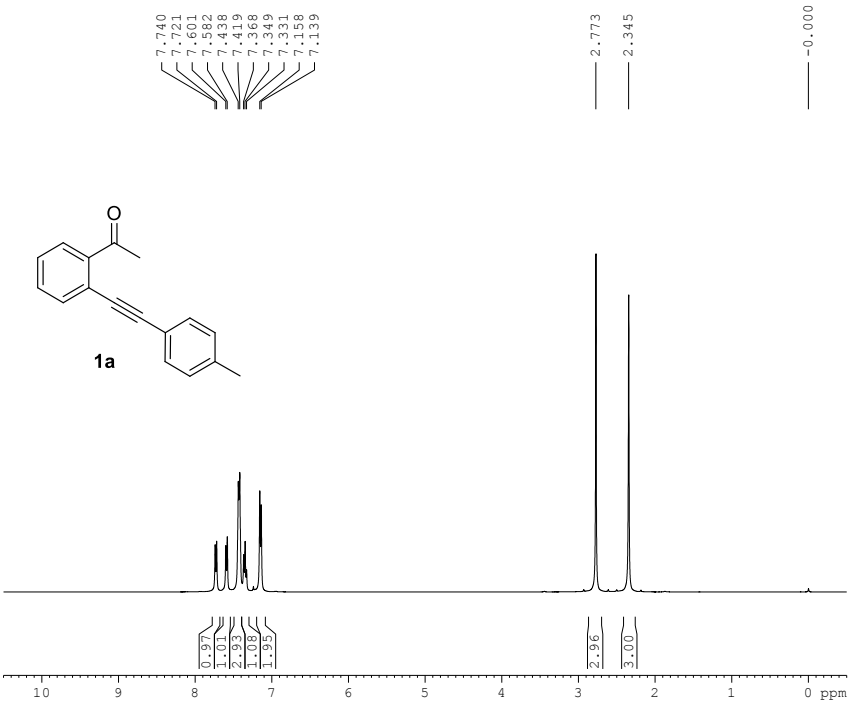
F2 - Acquisition Parameters
Date_           20141124
Time              11.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES            0.366798 Hz
AQ             1.3631988 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                299.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec

F2 - Processing parameters
SI                32768
SF           100.6404165 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

13.2 Substrates:

Compound 1a

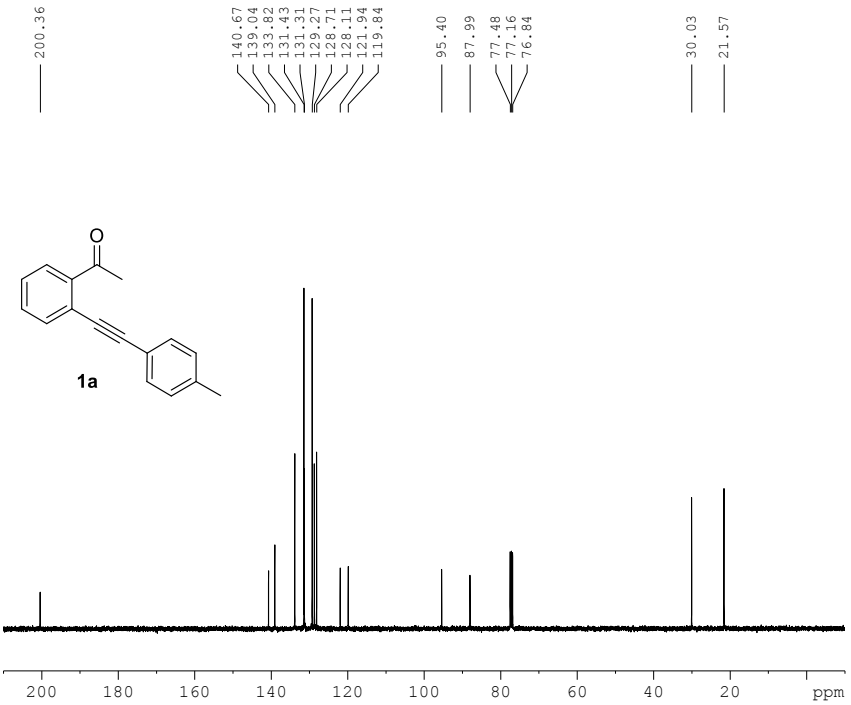



```
Current Data Parameters
NAME      mtt-subs-Me-H-MePh
EXPNO                  110
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141212
Time              21.13
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    5
DS                    0
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             2.0447731 sec
RG                25.38
DW               62.400 usec
DE                6.50 usec
TE                297.2 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec

F2 - Processing parameters
SI                65536
SF           400.2400172 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



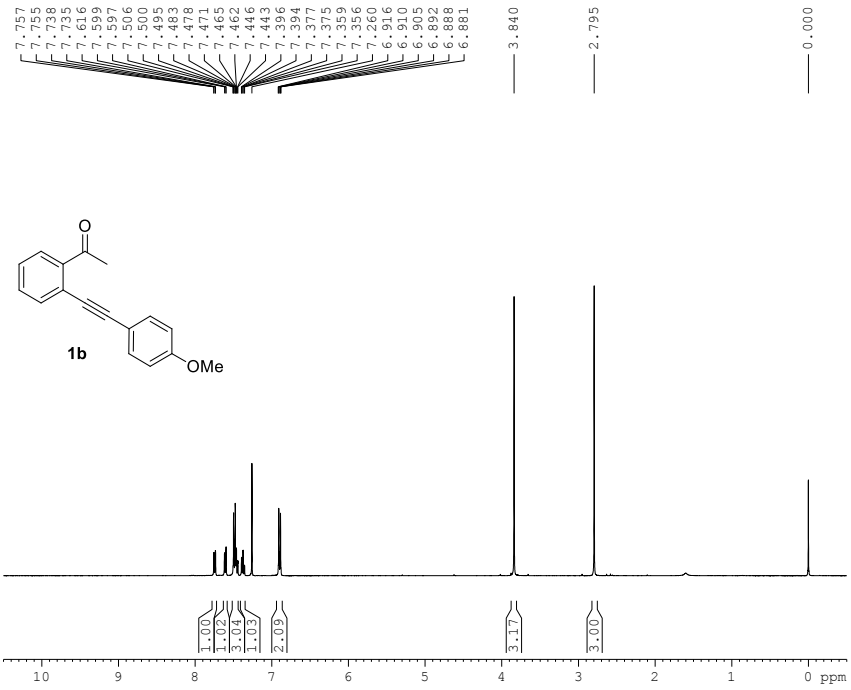

```
Current Data Parameters
NAME      mtt-subs-Me-H-MePh
EXPNO                   28
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141212
Time              21.15
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   36
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                206.33
DW               20.800 usec
DE                6.50 usec
TE                297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec

F2 - Processing parameters
SI                32768
SF           100.6404296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 1b

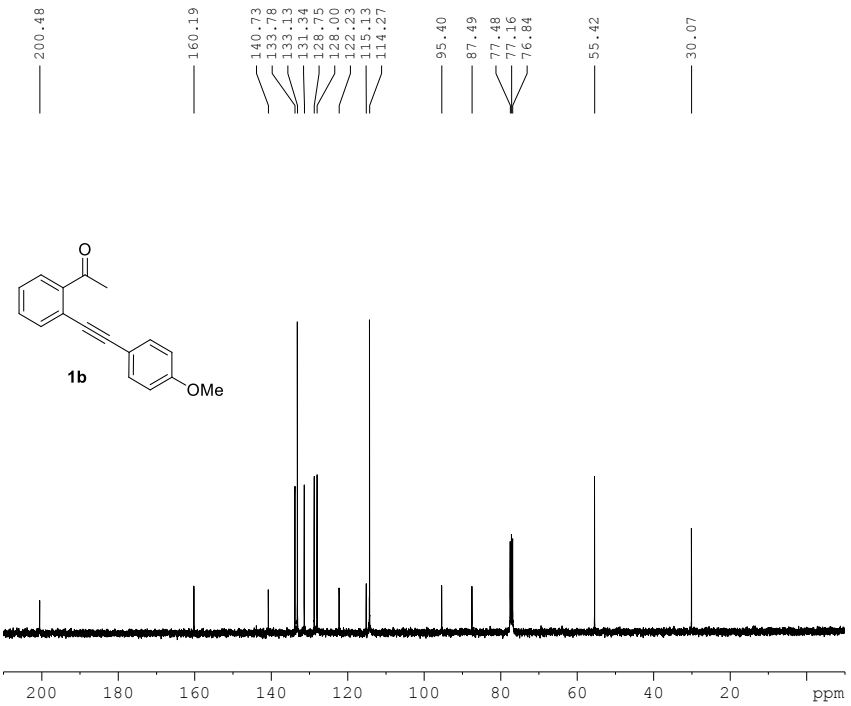



```
Current Data Parameters
NAME        mtt-M2019-13
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140527
Time                2.27
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                   203
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF           400.1300098 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



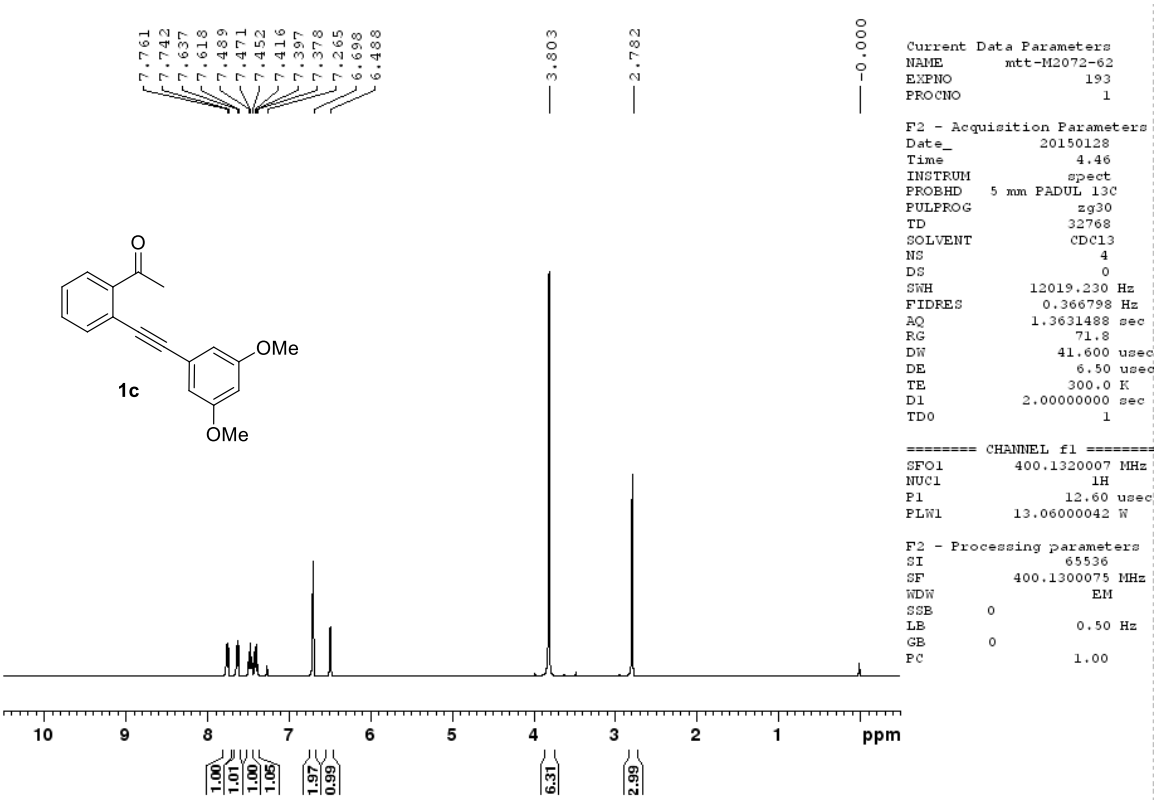

```
Current Data Parameters
NAME        mtt-M2019-13
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140524
Time                5.39
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   124
DS                     0
SWH            25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127588 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1c

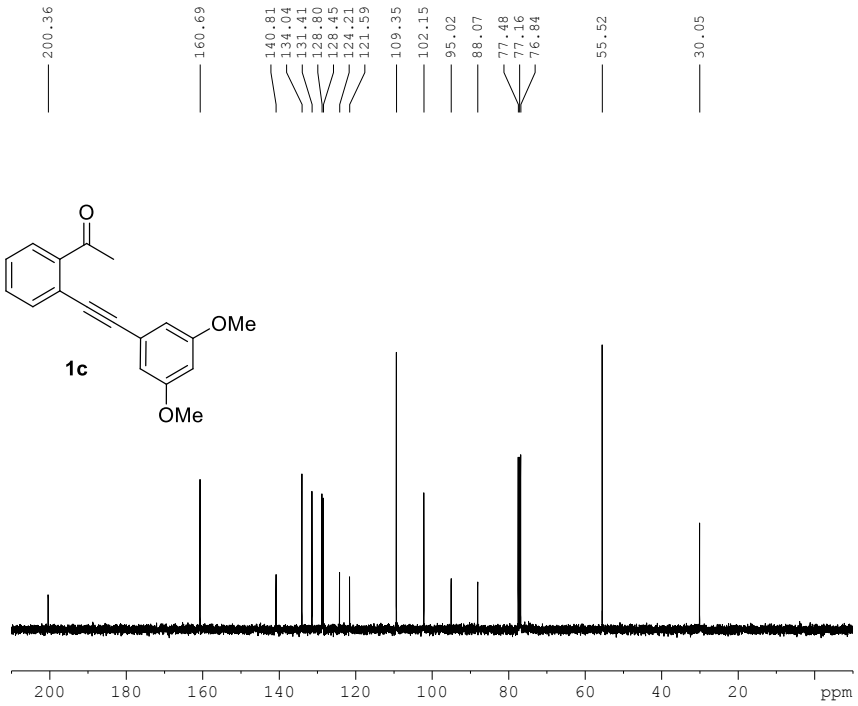



```
Current Data Parameters
NAME        mtt-M2072-62
EXPNO                193
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150128
Time                4.46
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     4
DS                     0
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                  71.8
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                1H
P1                12.60 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300075 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
```



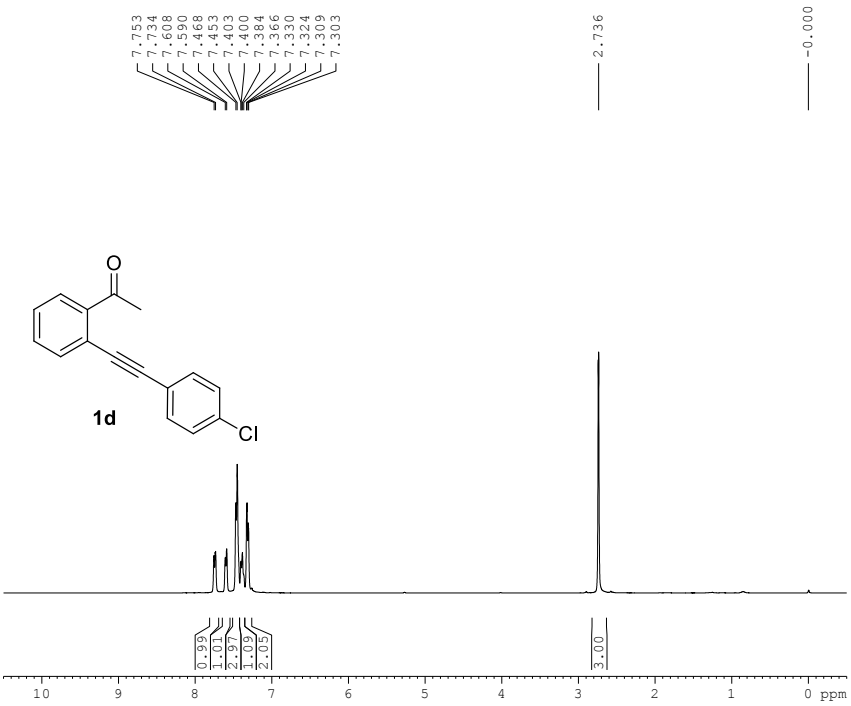

```
Current Data Parameters
NAME      mtt-M2072-62 again
EXPNO                    59
PROCNO                    1

F2 - Acquisition Parameters
Date_           20150128
Time                4.48
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    35
DS                     0
SWH            25252.525 Hz
FIDRES          0.770646 Hz
AQ              0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127634 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

Compound 1d

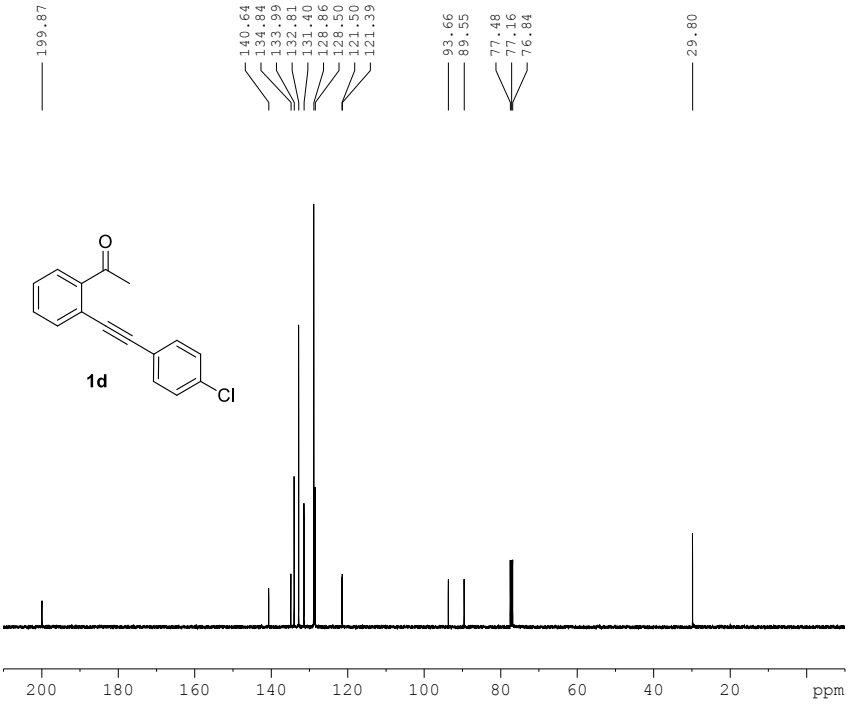



```
Current Data Parameters
NAME      mtt-subs-Me-H-ClPh
EXPNO                  131
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150114
Time               12.58
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  40.3
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF           400.1300096 MHz
WDW                  EM
SSB                   0
LB                 0.50 Hz
GB                    0
PC                 1.00
```



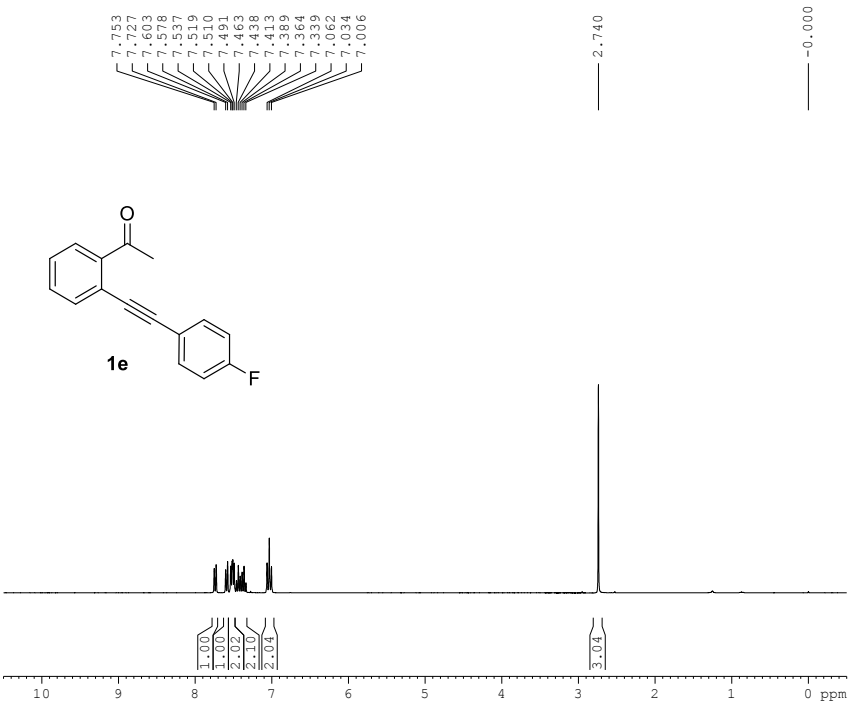

```
Current Data Parameters
NAME      mtt-subs-Me-H-ClPh
EXPNO                   44
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150114
Time               13.01
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   152
DS                     0
SWH            25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127657 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 1e

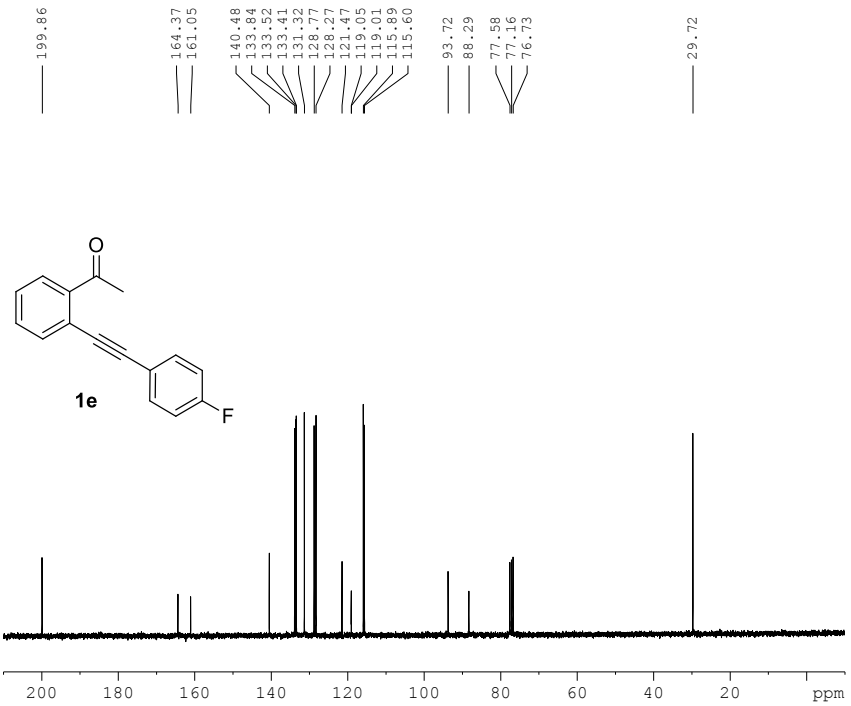



```
Current Data Parameters
NAME      mtt-subs-Me-H-4FPh
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150203
Time                 20.10
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      7
DS                      0
SWH              8992.806 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                   40.3
DW                 55.600 usec
DE                  6.50 usec
TE                 295.9 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.30 usec
PL1                  3.00 dB
SFO1          300.1315007 MHz

F2 - Processing parameters
SI                    65536
SF            300.1300004 MHz
WDW                     EM
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    4.00
```




```
Current Data Parameters
NAME      mtt-subs-Me-H-4FPh
EXPNO                    2
PROCNO                   1

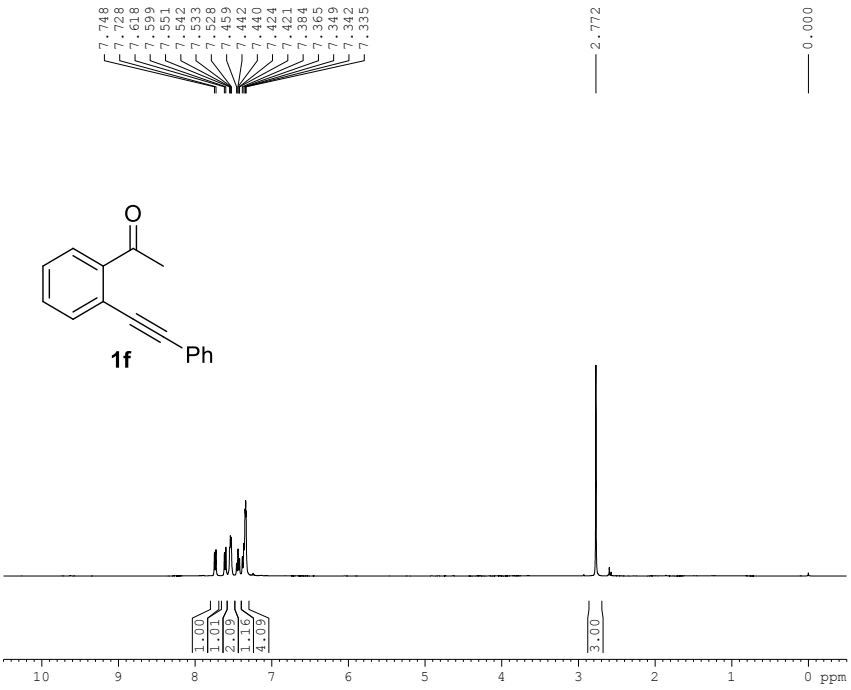
F2 - Acquisition Parameters
Date_             20150203
Time                 20.12
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                     37
DS                      0
SWH             18832.393 Hz
FIDRES           0.574719 Hz
AQ               0.8700404 sec
RG                   574.7
DW                 26.550 usec
DE                  6.50 usec
TE                 296.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  12.50 usec
PL1                  2.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  3.00 dB
PL12                22.74 dB
PL13                23.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
```

Compound 1f

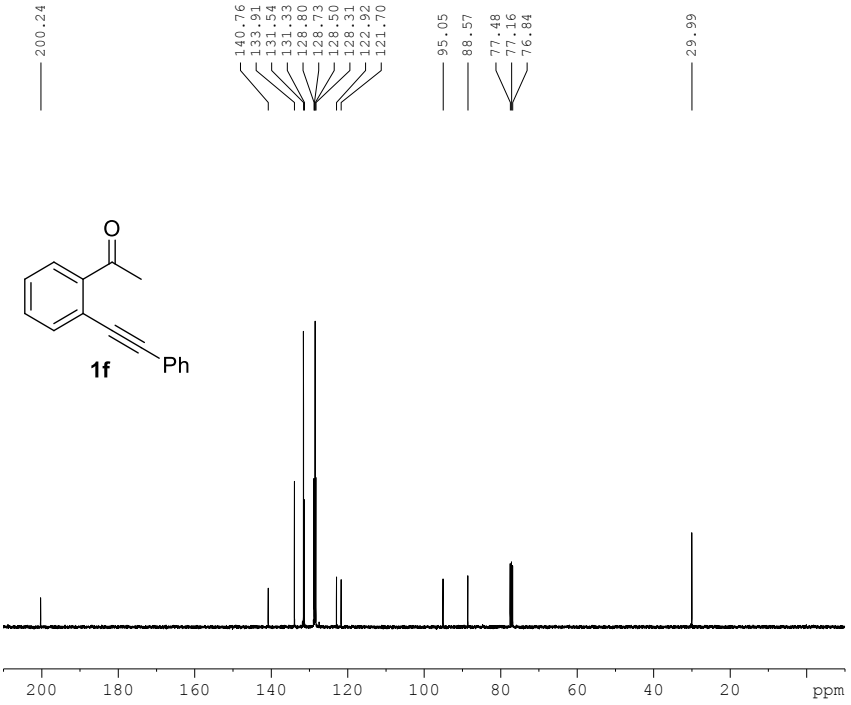



```
Current Data Parameters
NAME      mtt-pro-Me-H-Ph
EXPNO                 110
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141226
Time                18.26
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               2.0447731 sec
RG                  25.38
DW                 62.400 usec
DE                  6.50 usec
TE                 298.0 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                   1H
P1                  14.80 usec

F2 - Processing parameters
SI                  65536
SF           400.2400152 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



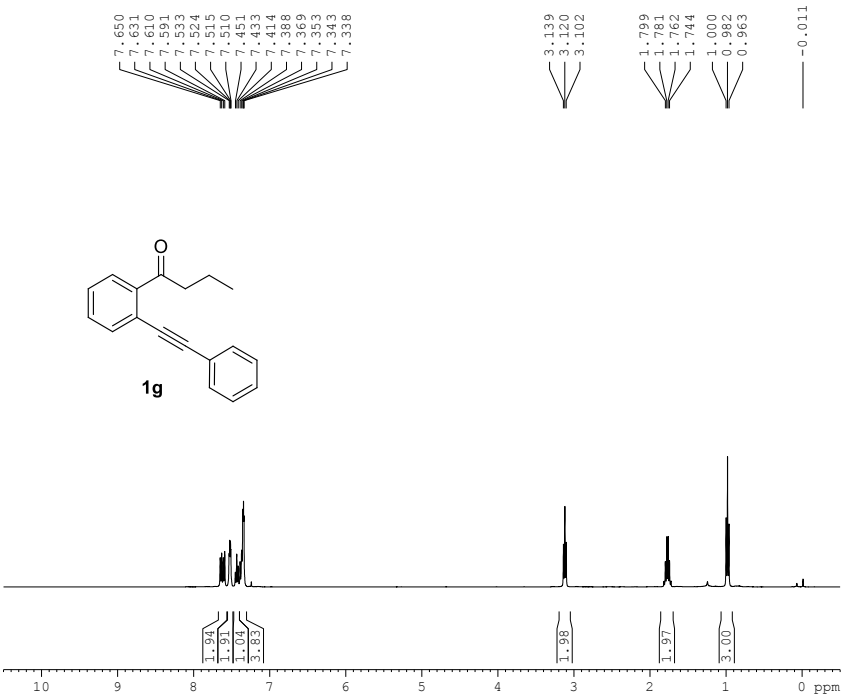

```
Current Data Parameters
NAME      mtt-pro-Me-H-Ph
EXPNO                 438
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141226
Time                18.29
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     54
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                 206.33
DW                 20.800 usec
DE                  6.50 usec
TE                 298.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        100.6504916 MHz
NUC1                   13C
P1                  10.00 usec

F2 - Processing parameters
SI                  32768
SF           100.6404289 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Compound 1g

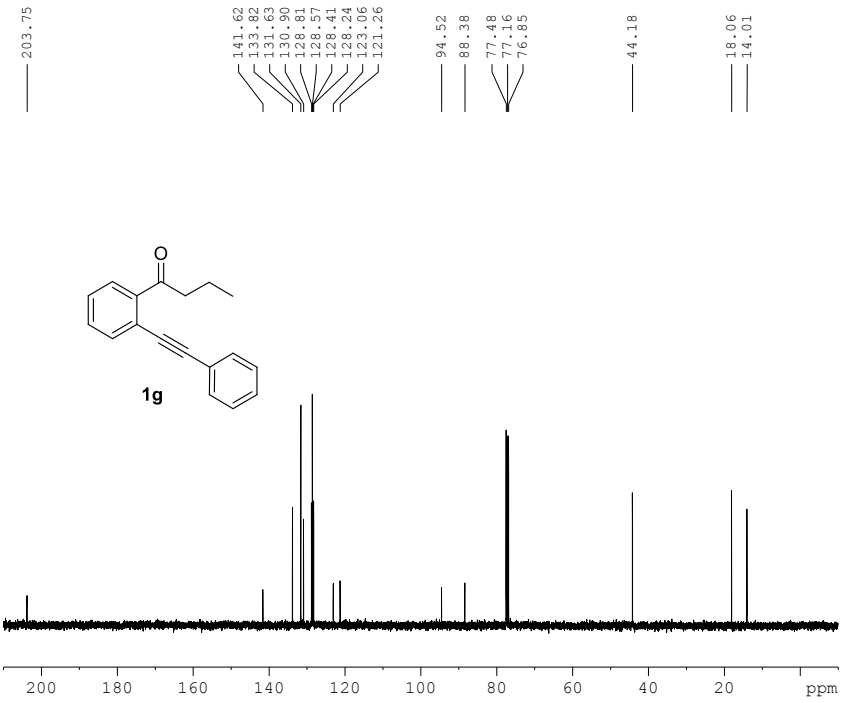



```
Current Data Parameters
NAME      mtt-M2067-57-1 again
EXPNO              463003
PROCNO                  3

F2 - Acquisition Parameters
Date_           20141230
Time               11.38
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    13
DS                     0
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                   101
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1320007 MHz
NUC1                 1H
P1                12.60 usec

F2 - Processing parameters
SI                 65536
SF            400.1300175 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



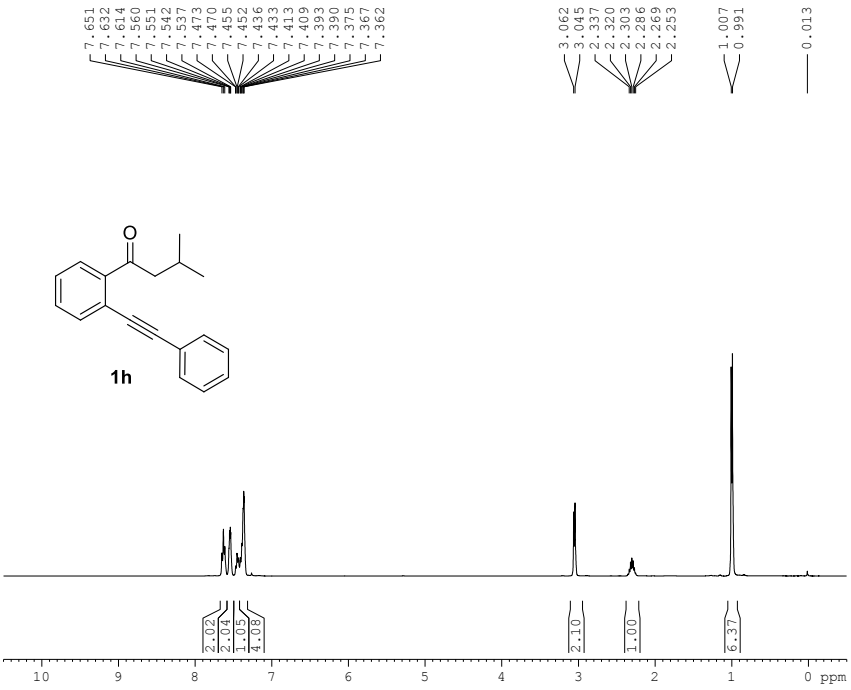

```
Current Data Parameters
NAME      mtt-M2067-57-1 again
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141230
Time               11.41
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    63
DS                     0
SWH            25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                 13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF            100.6127588 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1h

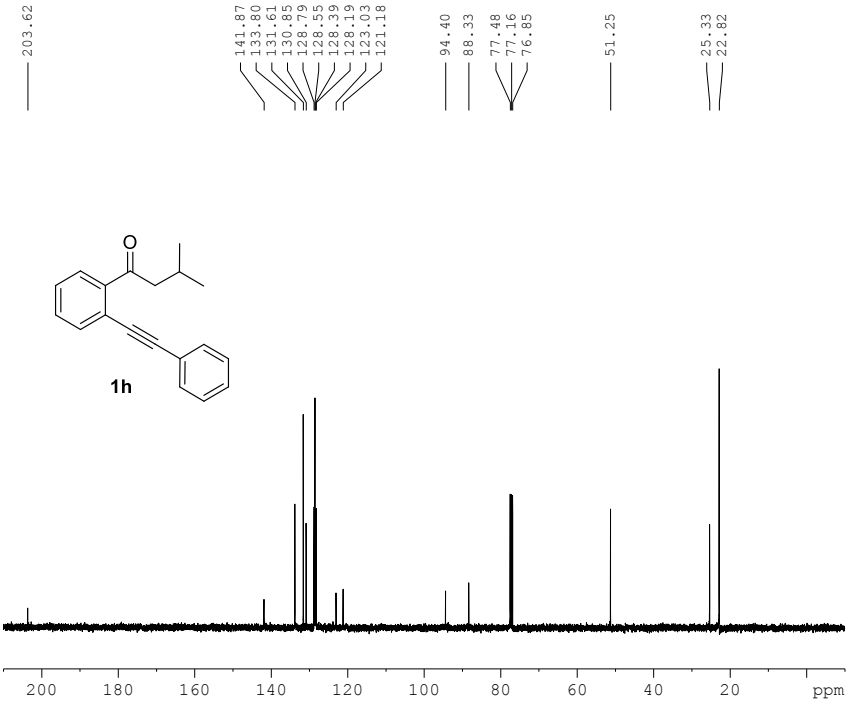



```
Current Data Parameters
NAME      mtt-T2082-71-1 subs
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150101
Time                8.23
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                    64
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF           400.1300080 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



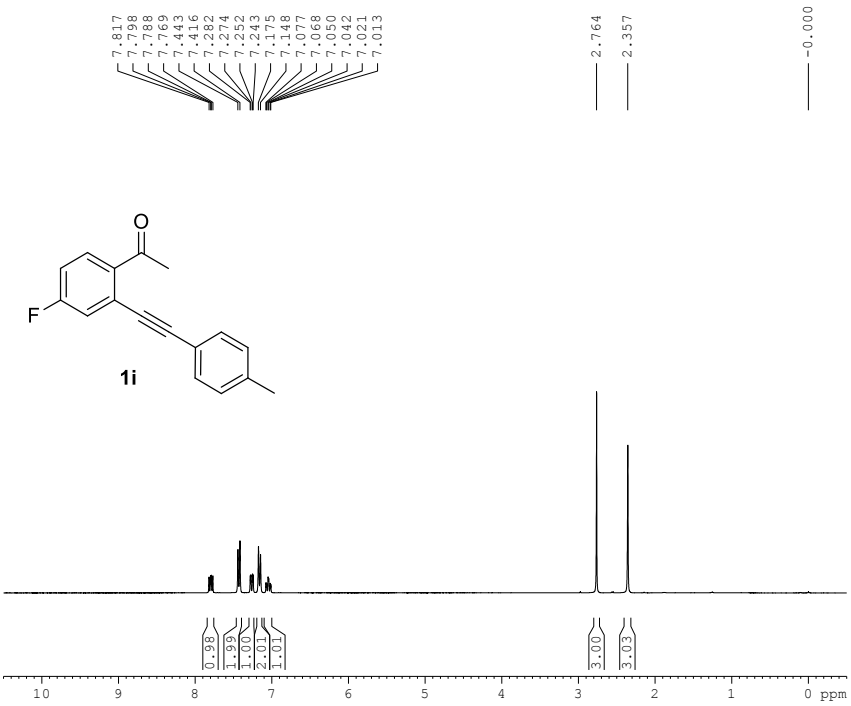

```
Current Data Parameters
NAME      mtt-T2082-71-1 subs
EXPNO                  36
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150101
Time                8.24
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    53
DS                     0
SWH            25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127611 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1i

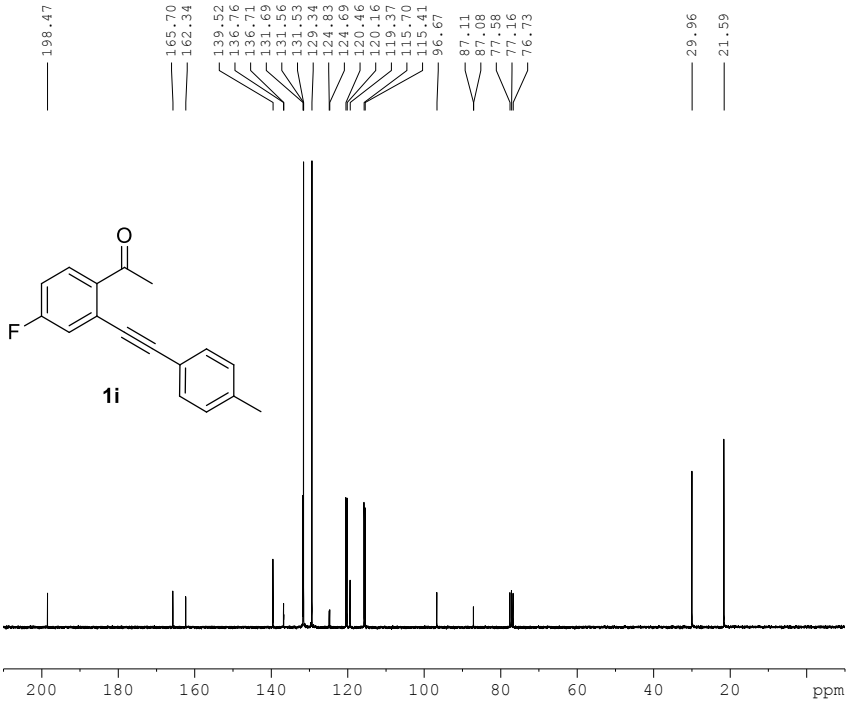



```
Current Data Parameters
NAME        mtt-300M new
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150507
Time               21.18
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ             5.4526453 sec
RG                 50.48
DW                83.200 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                  1H
P1                10.00 usec

F2 - Processing parameters
SI                 65536
SF          300.1300088 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



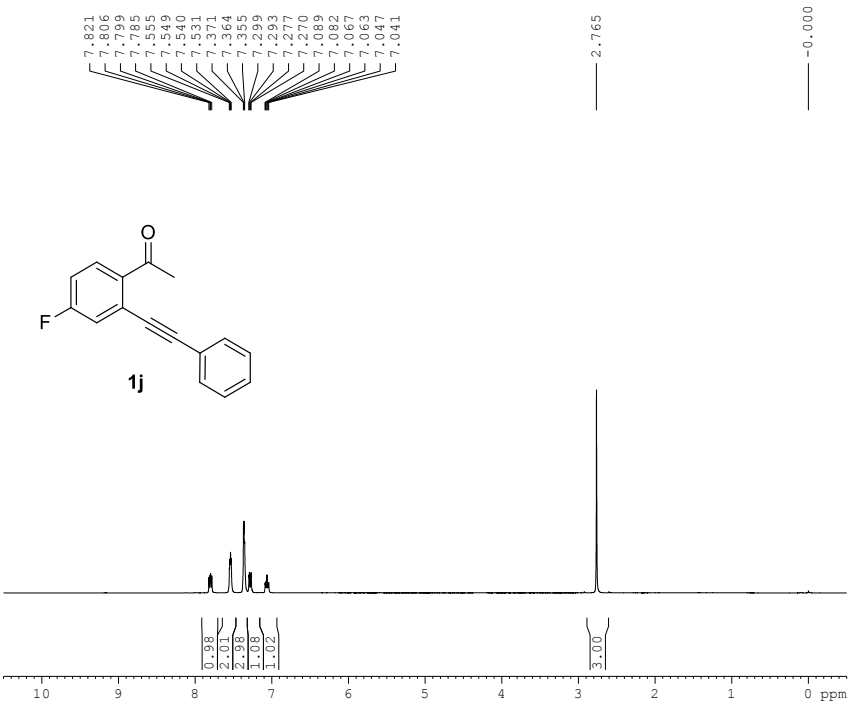

```
Current Data Parameters
NAME        mtt-300M new
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150507
Time               21.21
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   131
DS                     2
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ             1.8175818 sec
RG                 209.09
DW                27.733 usec
DE                 6.50 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         75.4752953 MHz
NUC1                 13C
P1                11.00 usec

F2 - Processing parameters
SI                 32768
SF          75.4677472 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1j

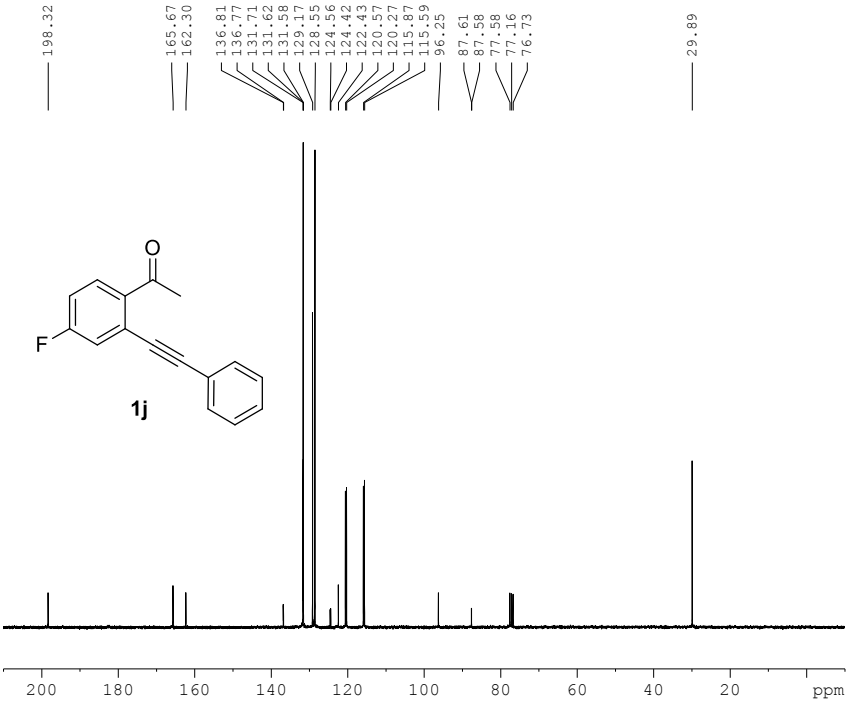



```
Current Data Parameters
NAME      mtt-T2082-72-2 subs
EXPNO                  28
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150105
Time              19.11
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     7
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             2.0447731 sec
RG                 27.92
DW                62.400 usec
DE                 6.50 usec
TE                295.8 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                1H
P1                14.80 usec

F2 - Processing parameters
SI                 65536
SF          400.2400109 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



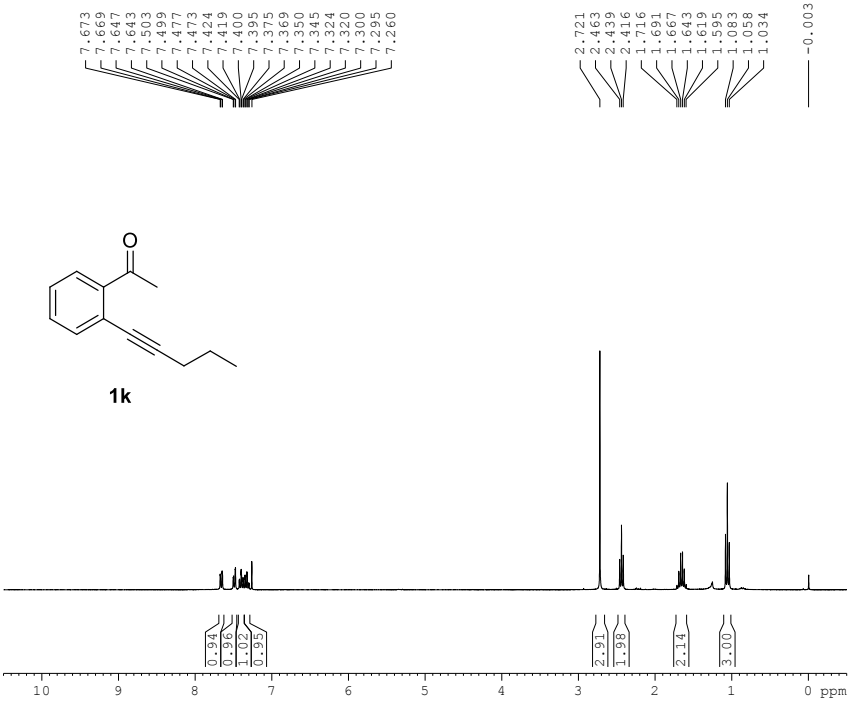

```
Current Data Parameters
NAME        mtt-300M new
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150507
Time              21.07
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   108
DS                     2
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ             1.8175818 sec
RG                 209.09
DW                27.733 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         75.4752953 MHz
NUC1                13C
P1                11.00 usec

F2 - Processing parameters
SI                 32768
SF          75.4677484 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1k

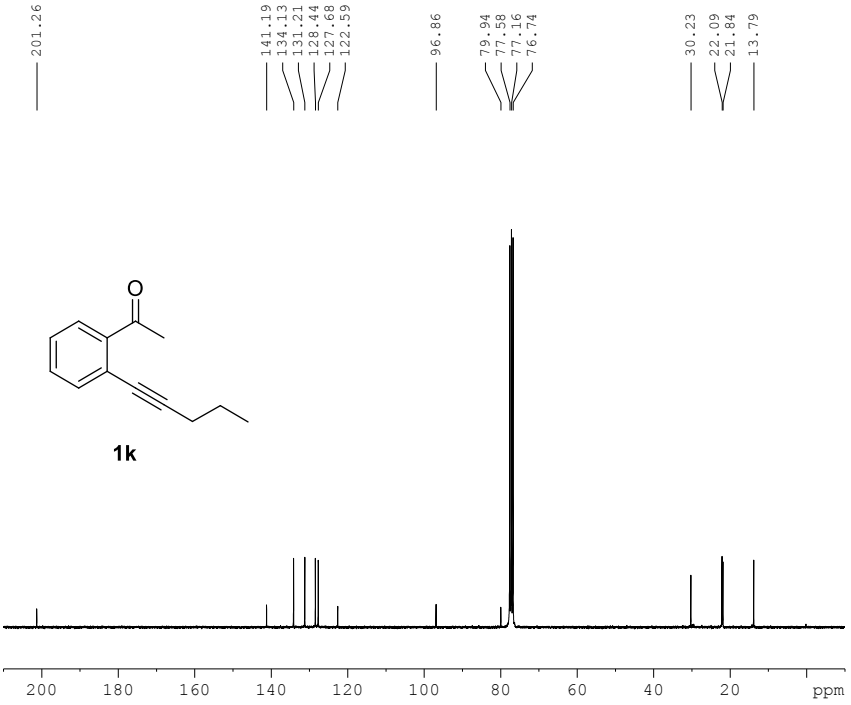



```
Current Data Parameters
NAME        mtt-M2076-66
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150302
Time               22.01
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8992.806 Hz
FIDRES          0.274439 Hz
AQ             1.8219508 sec
RG                   362
DW                55.600 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1                3.00 dB
SFO1         300.1315007 MHz

F2 - Processing parameters
SI                 65536
SF          300.1300062 MHz
WDW                   EM
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 4.00
```




```
Current Data Parameters
NAME        mtt-M2076-66
EXPNO                  3
PROCNO                 1

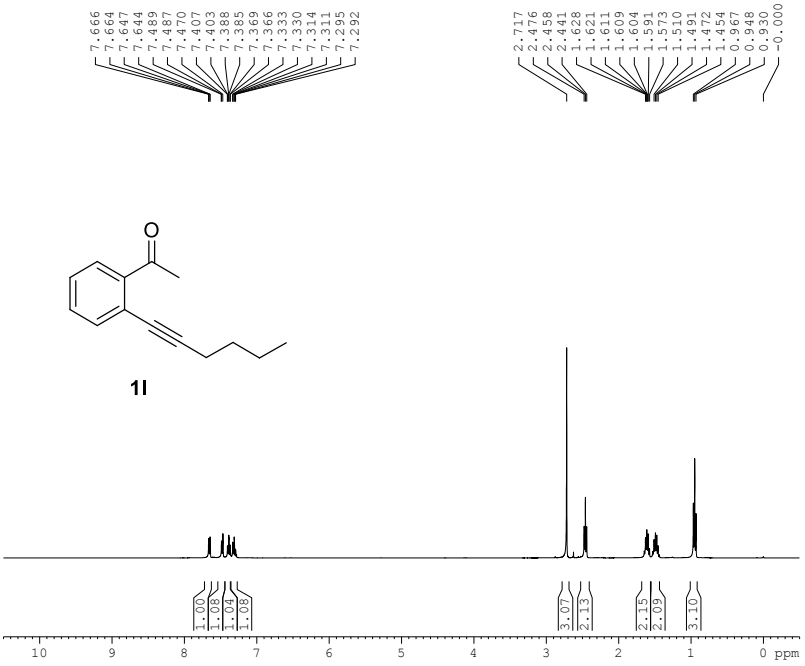
F2 - Acquisition Parameters
Date_           20150302
Time               22.03
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 13352
DS                     0
SWH            18832.393 Hz
FIDRES          0.574719 Hz
AQ             0.8700404 sec
RG                 645.1
DW                26.550 usec
DE                 6.50 usec
TE                296.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
```

Compound 1l

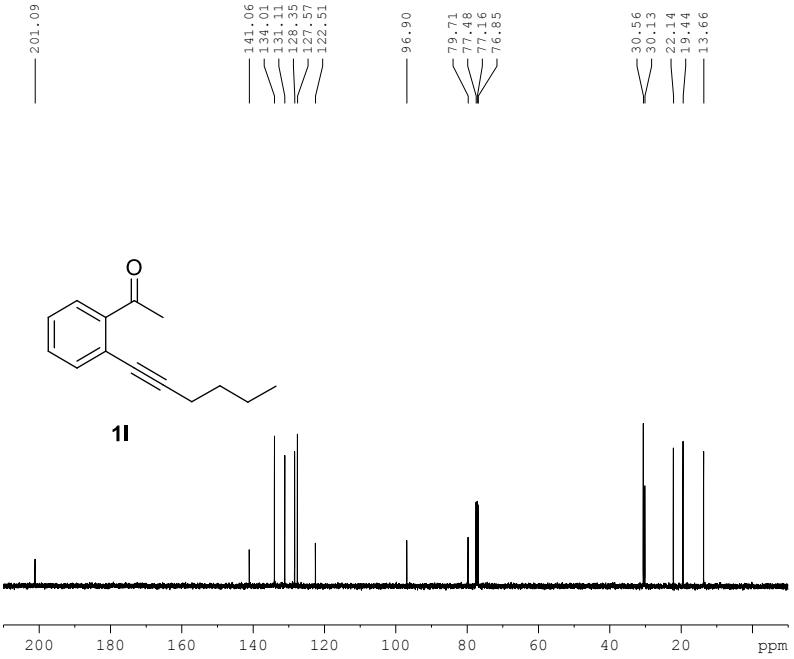



```
Current Data Parameters
NAME      mtt-subs-Me-H-nBu(M2073-63)
EXPNO                131
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150130
Time                1.55
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                  45.2
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF          400.1300013 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



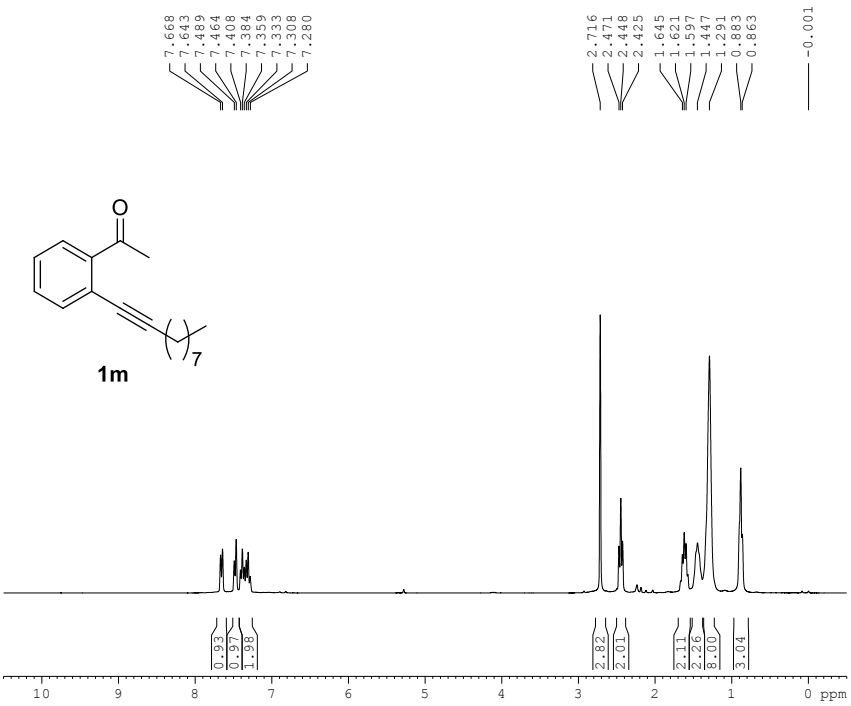

```
Current Data Parameters
NAME      mtt-subs-Me-H-nBu(M2073-63)4
EXPNO                 27
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150130
Time                1.57
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    34
DS                     0
SWH            25252.525 Hz
FIDRES          0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF          100.6127642 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1m

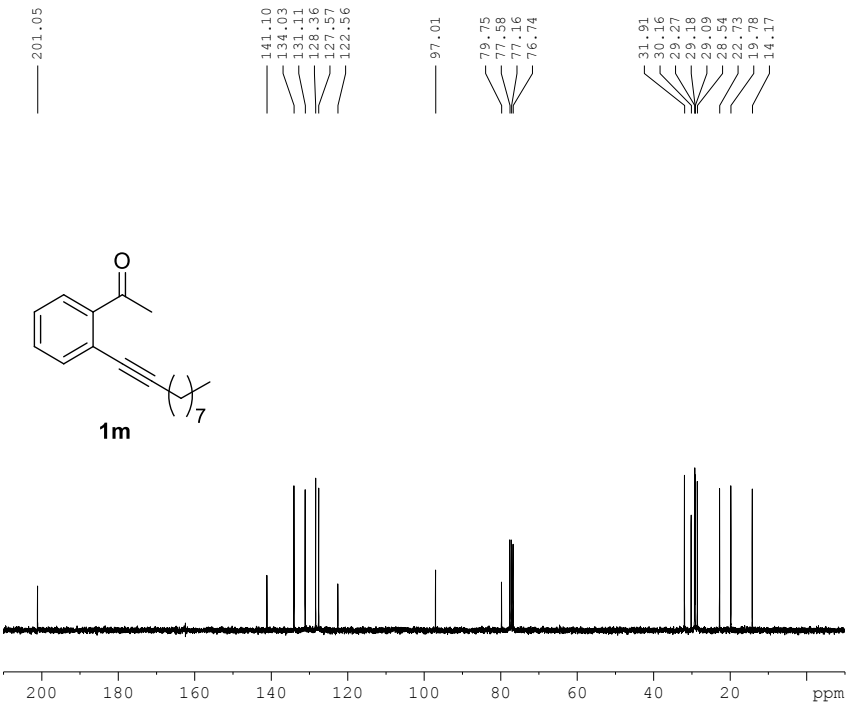



```
Current Data Parameters
NAME        mtt-M2077-67
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150305
Time               16.46
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8992.806 Hz
FIDRES          0.274439 Hz
AQ             1.8219508 sec
RG                  35.9
DW                55.600 usec
DE                 6.50 usec
TE                297.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1                3.00 dB
SFO1         300.1315007 MHz

F2 - Processing parameters
SI                 65536
SF          300.1300024 MHz
WDW                   EM
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 4.00
```




```
Current Data Parameters
NAME        mtt-M2077-67
EXPNO                  8
PROCNO                 1

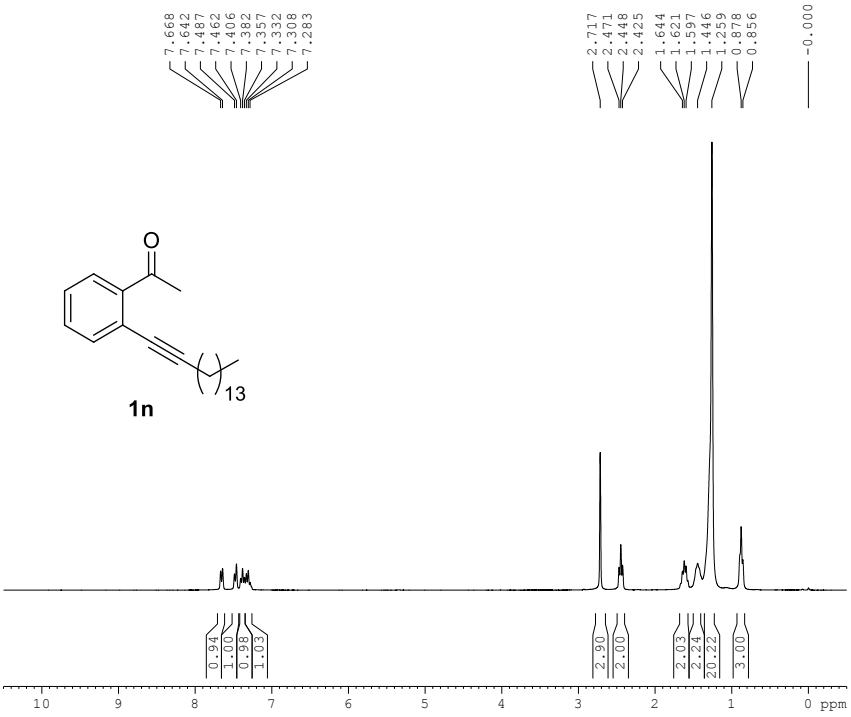
F2 - Acquisition Parameters
Date_           20150305
Time               16.42
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    78
DS                     0
SWH            18832.393 Hz
FIDRES          0.574719 Hz
AQ             0.8700404 sec
RG                   512
DW                26.550 usec
DE                 6.50 usec
TE                297.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
```

Compound 1n

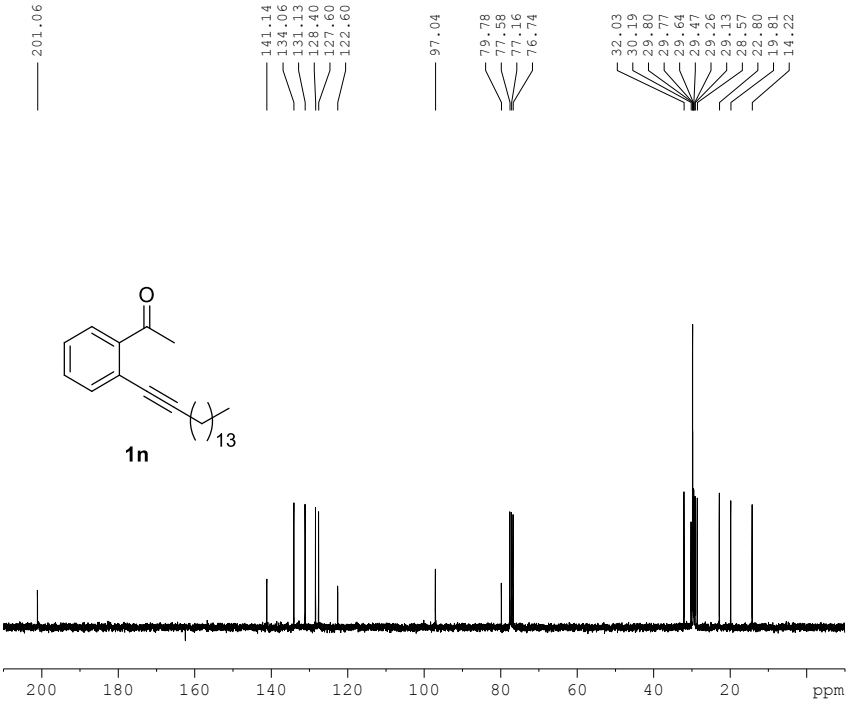



```
Current Data Parameters
NAME       mtt-M2078-68
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20150310
Time              17.22
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    9
DS                    0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ            1.8219508 sec
RG                 35.9
DW               55.600 usec
DE                6.50 usec
TE                297.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1                3.00 dB
SFO1        300.1315007 MHz

F2 - Processing parameters
SI                65536
SF          300.1300043 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 4.00
```




```
Current Data Parameters
NAME       mtt-M2078-68
EXPNO                 3
PROCNO                1

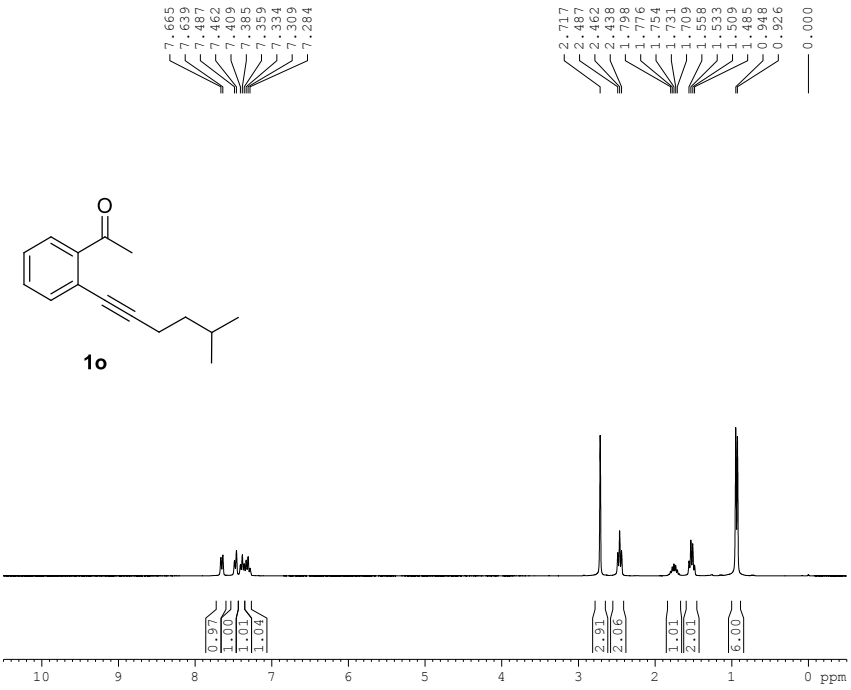
F2 - Acquisition Parameters
Date_           20150310
Time              17.25
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                   61
DS                    0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ            0.8700404 sec
RG                645.1
DW               26.550 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.50 usec
PL1                2.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
```

Compound 1o

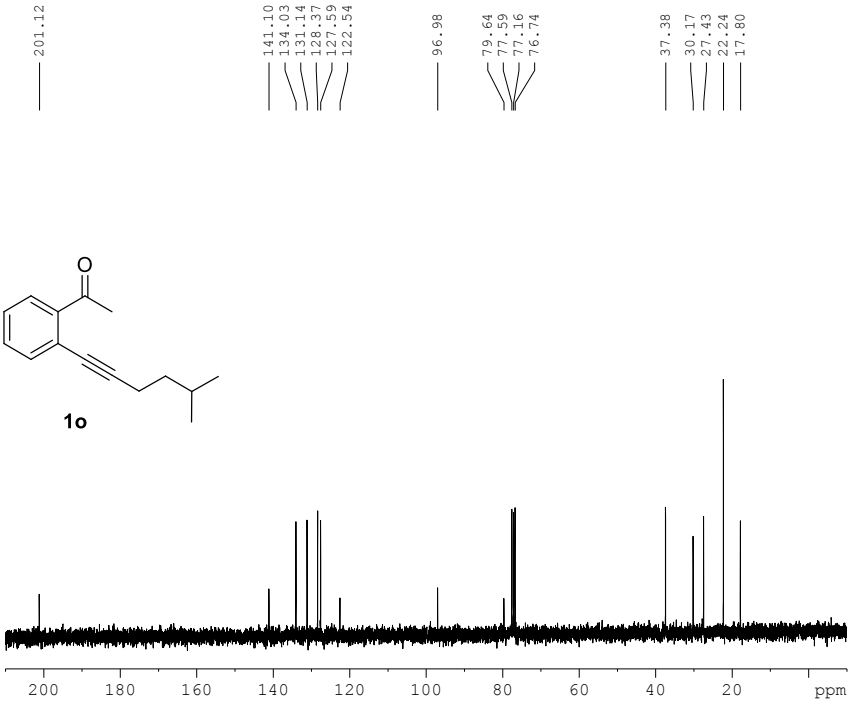



```
Current Data Parameters
NAME        mtt-M2079-69
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150309
Time              21.13
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                 45.3
DW                55.600 usec
DE                 6.50 usec
TE                296.5 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1                3.00 dB
SFO1        300.1315007 MHz

F2 - Processing parameters
SI                 65536
SF          300.1300018 MHz
WDW                   EM
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 4.00
```




```
Current Data Parameters
NAME        mtt-M2079-69
EXPNO                  3
PROCNO                 1

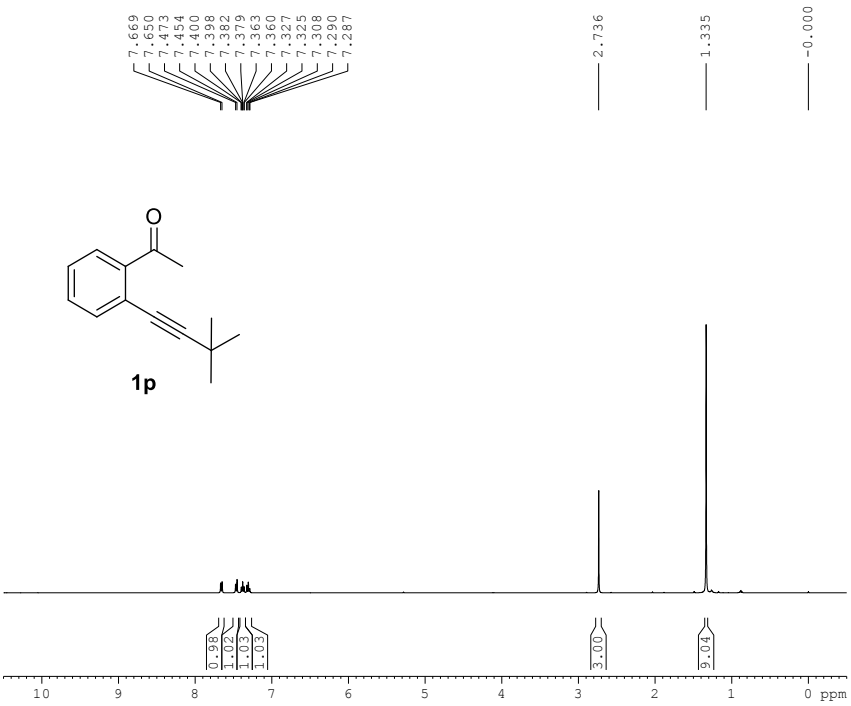
F2 - Acquisition Parameters
Date_           20150309
Time              21.26
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ             0.8700404 sec
RG                 456.1
DW                26.550 usec
DE                 6.50 usec
TE                295.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
```

Compound 1p

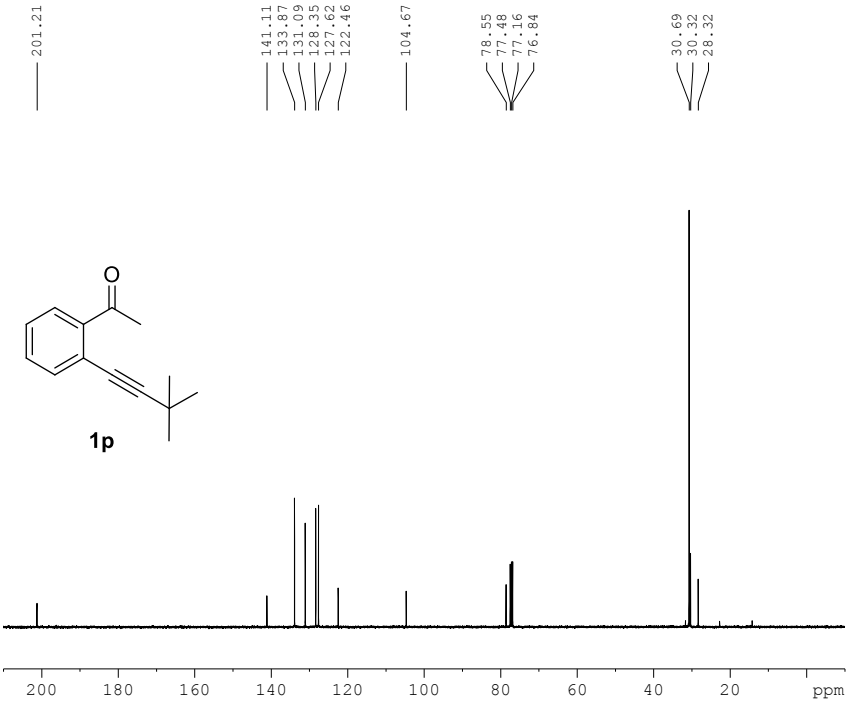



```
Current Data Parameters
NAME      mtt-subs-Me-H-tBu 2
EXPNO                  110
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150113
Time              11.11
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ           2.0447731 sec
RG                25.38
DW              62.400 usec
DE               6.50 usec
TE               296.0 K
D1          2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.2424716 MHz
NUC1                  1H
P1               14.80 usec

F2 - Processing parameters
SI                65536
SF          400.2400016 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



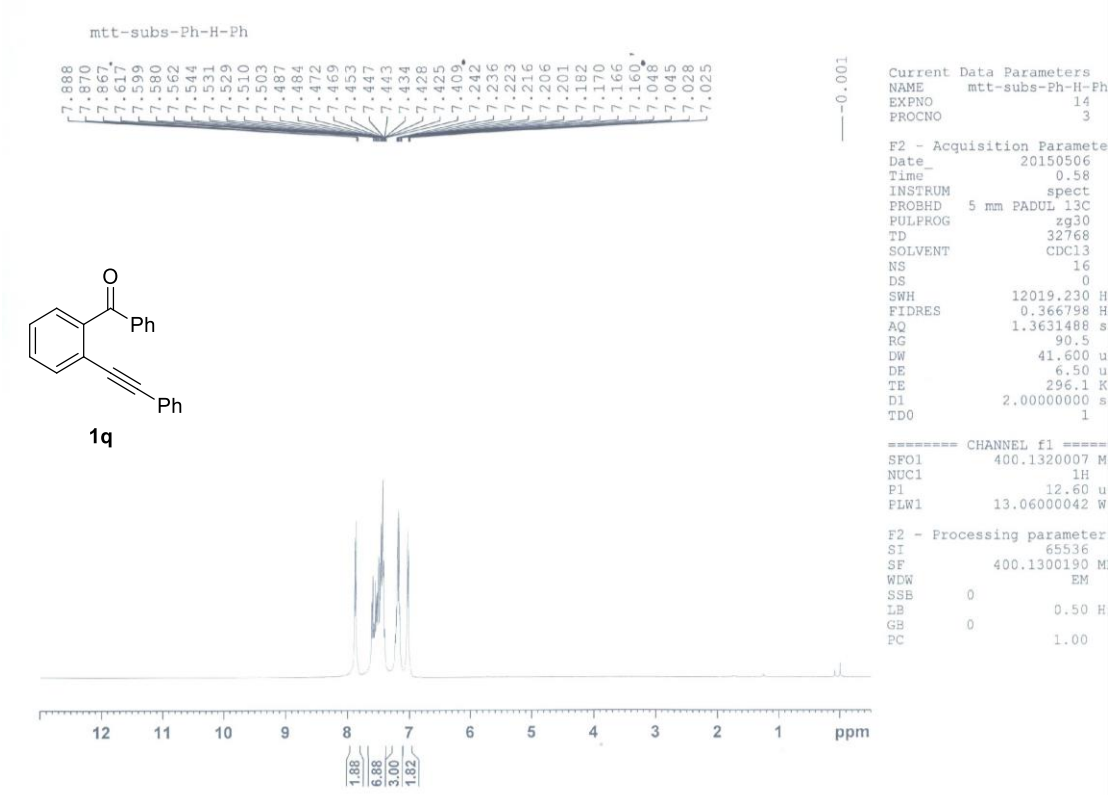

```
Current Data Parameters
NAME      mtt-subs-Me-H-tBu 2
EXPNO                  324
PROCNO                   1

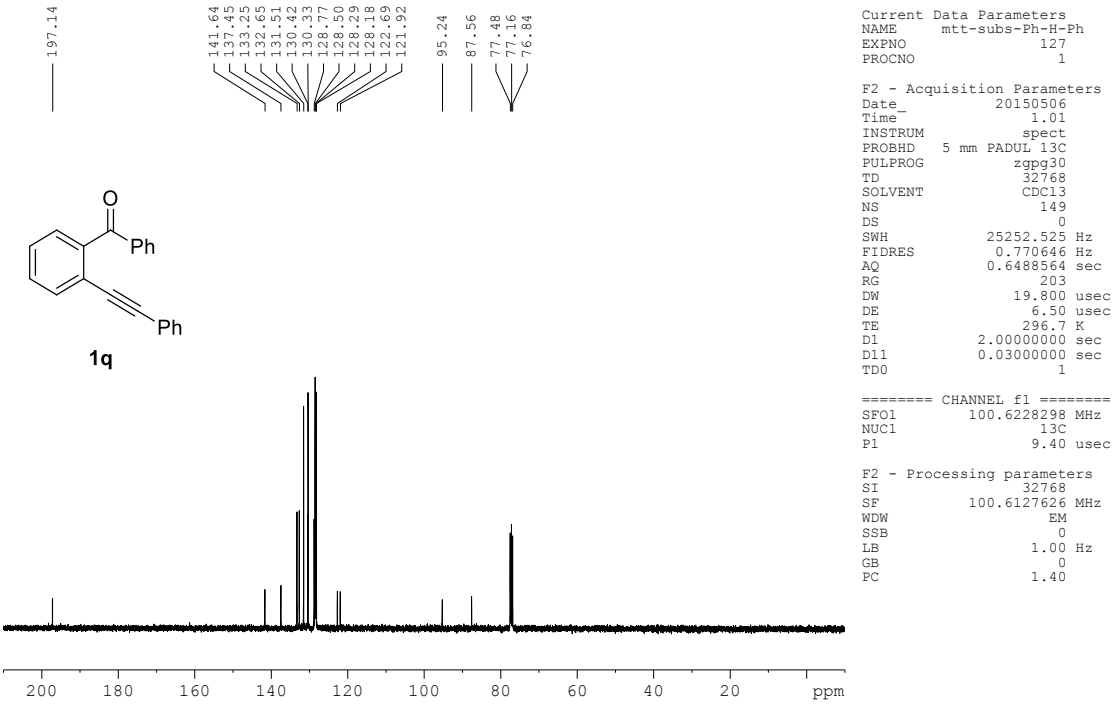
F2 - Acquisition Parameters
Date_           20150113
Time              11.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   67
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ           1.3631988 sec
RG                206.33
DW              20.800 usec
DE               6.50 usec
TE               296.7 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6504916 MHz
NUC1                 13C
P1               10.00 usec

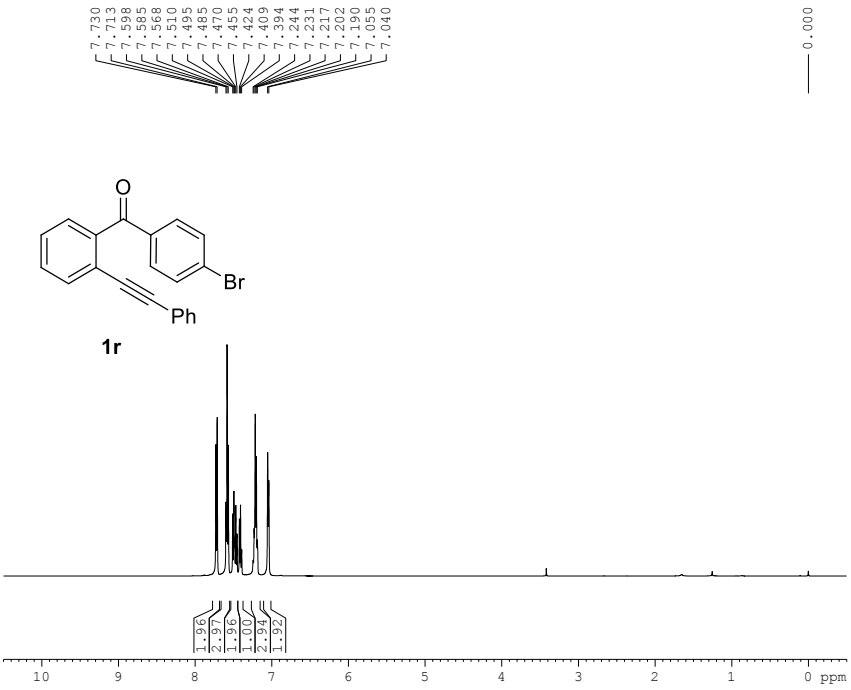
F2 - Processing parameters
SI                32768
SF          100.6404220 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 1q


mtt-subs-Ph-H-Ph
7.888
7.870
7.867
7.617
7.599
7.580
7.562
7.544
7.531
7.529
7.510
7.503
7.487
7.484
7.472
7.469
7.453
7.447
7.443
7.434
7.428
7.425
7.409
7.242
7.236
7.223
7.216
7.206
7.201
7.182
7.170
7.166
7.160
7.048
7.045
7.028
7.025
-0.001
O
Ph
Ph
1q
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.88
6.88
3.00
1.82
Current Data Parameters
NAME mtt-subs-Ph-H-Ph
EXPNO 14
PROCNO 3
F2 - Acquisition Parameters
Date_ 20150506
Time 0.58
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 90.5
DW 41.600 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1320007 MHz
NUC1 1H
P1 12.60 usec
PLW1 13.06000042 W
F2 - Processing parameters
SI 65536
SF 400.1300190 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00


197.14
141.64
137.45
133.25
132.65
131.51
130.42
130.33
128.77
128.50
128.29
128.18
122.69
121.92
95.24
87.56
77.48
77.16
76.84
O
Ph
Ph
1q
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME mtt-subs-Ph-H-Ph
EXPNO 127
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150506
Time 1.01
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 149
DS 0
SWH 25252.525 Hz
FIDRES 0.770646 Hz
AQ 0.6488564 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.40 usec
F2 - Processing parameters
SI 32768
SF 100.6127626 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 1r

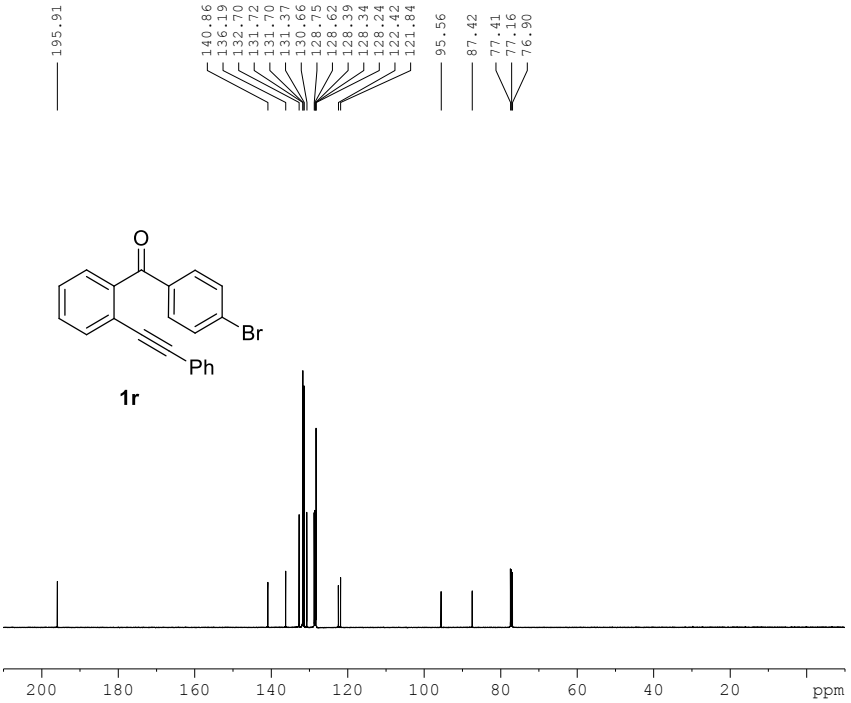



```
Current Data Parameters
NAME            mtt 500m
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150505
Time               22.09
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     2
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2768500 sec
RG                 27.92
DW                50.000 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                   1H
P1                 10.60 usec

F2 - Processing parameters
SI                 65536
SF           500.1300311 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



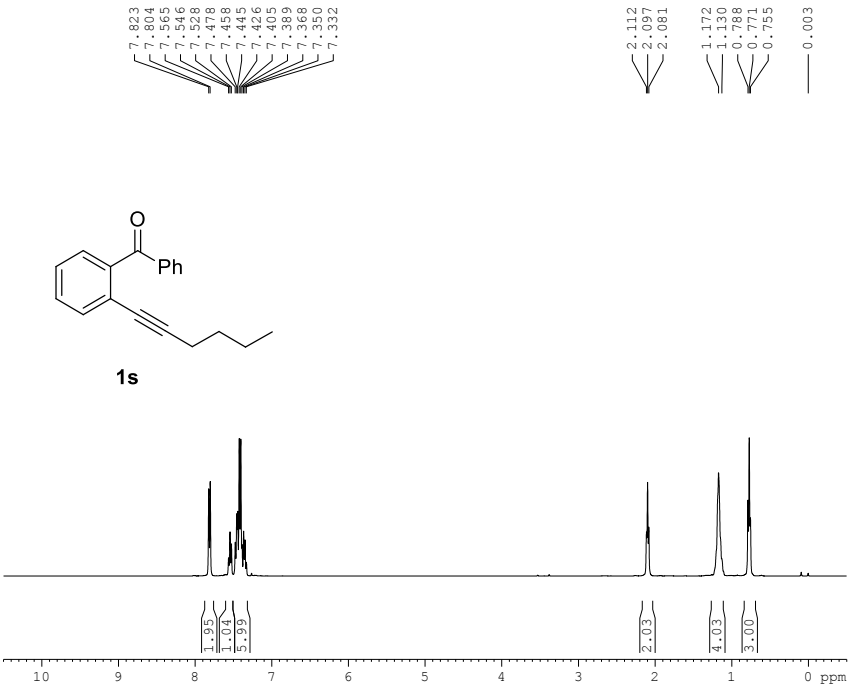

```
Current Data Parameters
NAME            mtt 500m
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150505
Time               22.13
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   100
DS                     4
SWH            29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                192.89
DW                16.800 usec
DE                18.00 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7703637 MHz
NUC1                   13C
P1                  9.80 usec

F2 - Processing parameters
SI                 32768
SF           125.7577945 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 1s

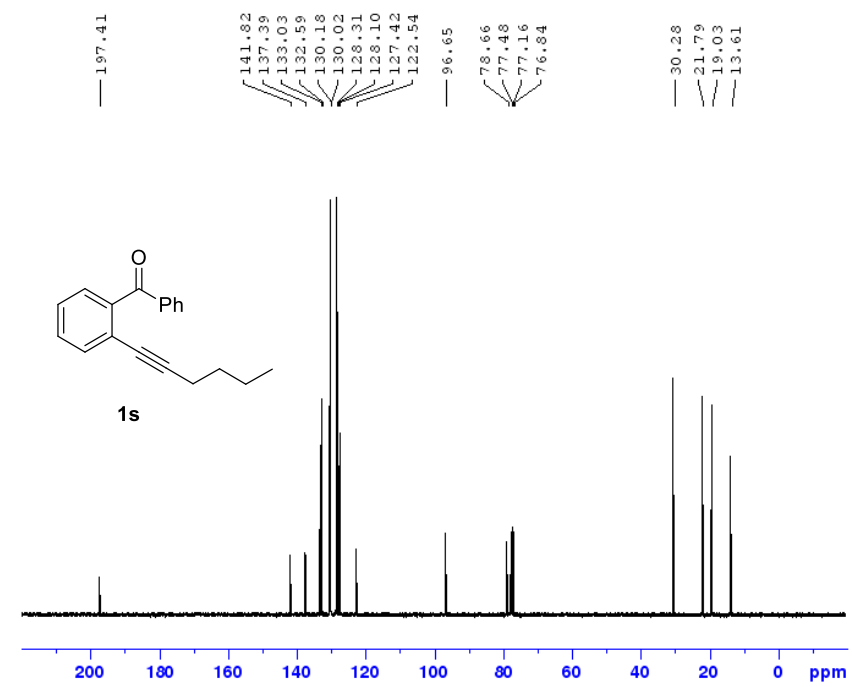



```
Current Data Parameters
NAME      mtt-subs-Ph-H-nBu
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150121
Time              12.56
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                32768
SOLVENT           CDCl3
NS                    6
DS                    0
SWH           12019.230 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   36
DW               41.600 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                1H
P1                12.60 usec

F2 - Processing parameters
SI                65536
SF           400.1300080 MHz
WDW                  EM
SSB                   0
LB                 0.50 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME      mtt-subs-Ph-H-nBu
EXPNO                   36
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150121
Time              13.04
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  189
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ            0.6488064 sec
RG                  203
DW               19.800 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

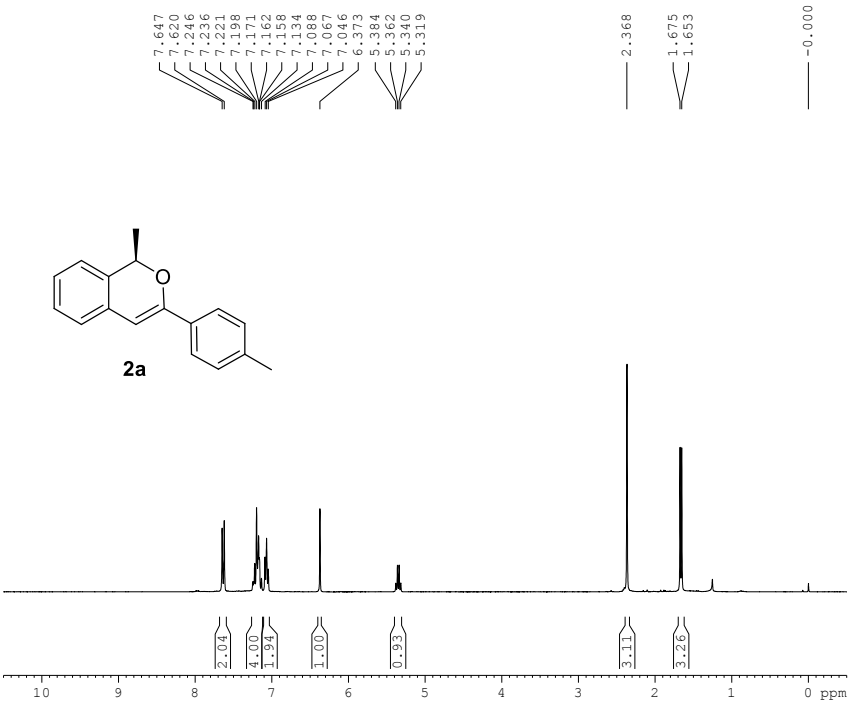
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                32768
SF           100.6127647 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

13.3 Products:

Compound 2a

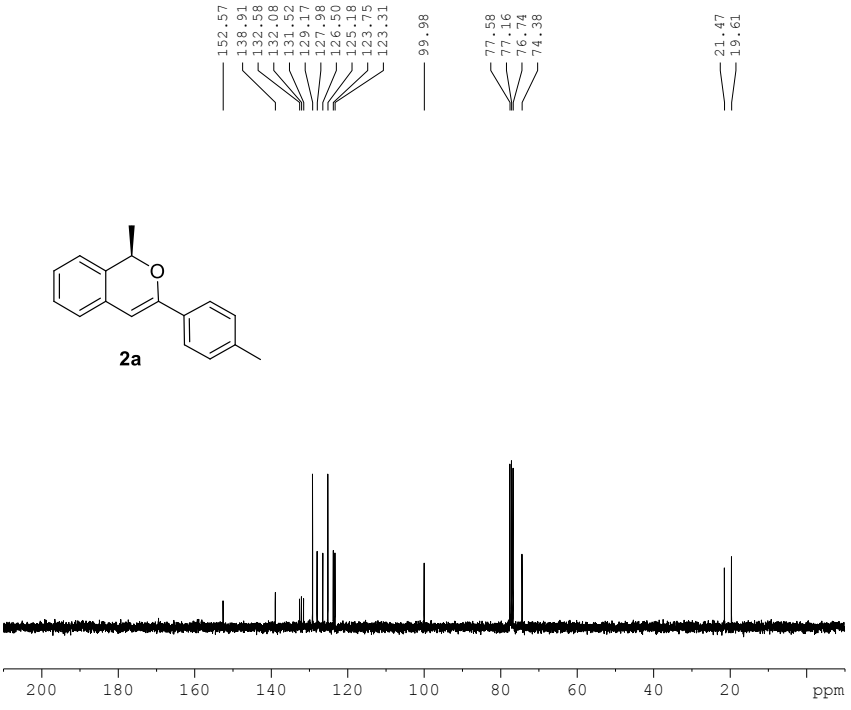



```
Current Data Parameters
NAME      mtt-T2027-21-2 race
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140514
Time              22.31
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ            1.8219508 sec
RG                  181
DW               55.600 usec
DE                6.50 usec
TE                297.5 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1                3.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300142 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME      mtt-T2027-21-2 race
EXPNO                  11
PROCNO                  1

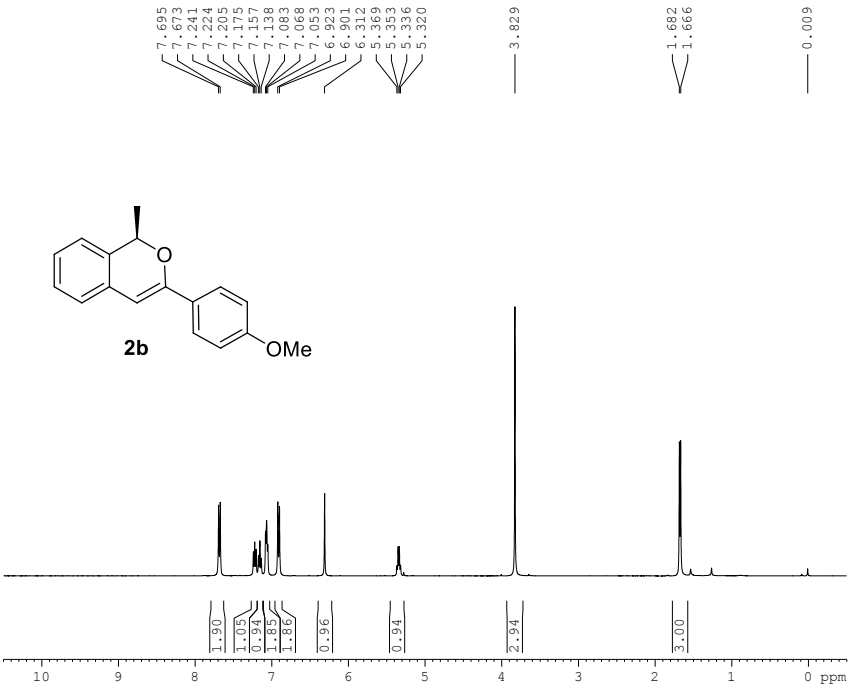
F2 - Acquisition Parameters
Date_           20140514
Time              22.34
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                   62
DS                    0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ            0.8700404 sec
RG                574.7
DW               26.550 usec
DE                6.50 usec
TE                297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
```

Compound 2b

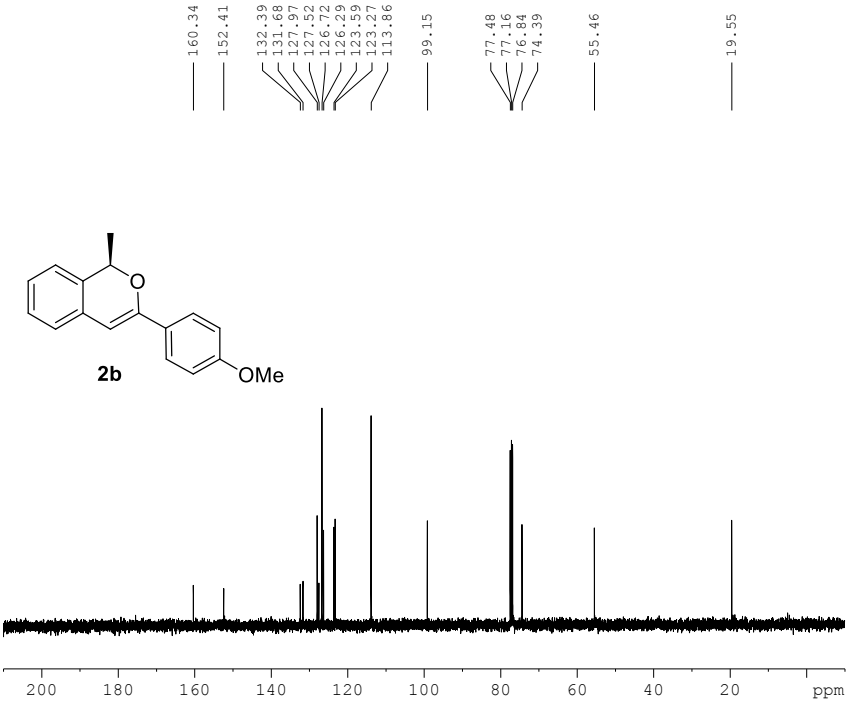



```
Current Data Parameters
NAME      mtt-T2033-27-1 race
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140530
Time                4.18
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     6
DS                     0
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                  90.5
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF           400.1300175 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



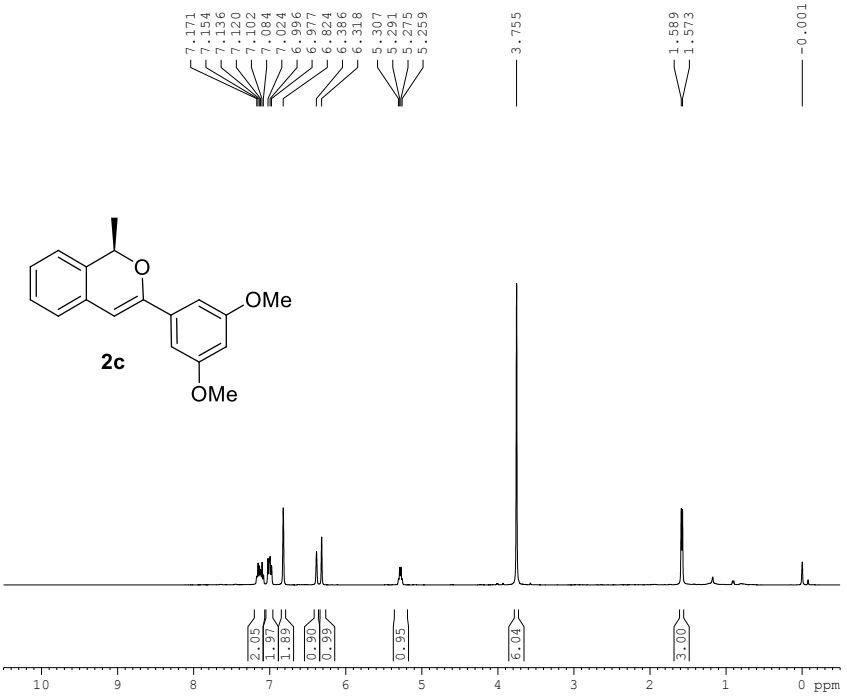

```
Current Data Parameters
NAME      mtt-T2033-27-1 race
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140530
Time                4.20
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    45
DS                     0
SWH            25252.525 Hz
FIDRES          0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127572 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 2c

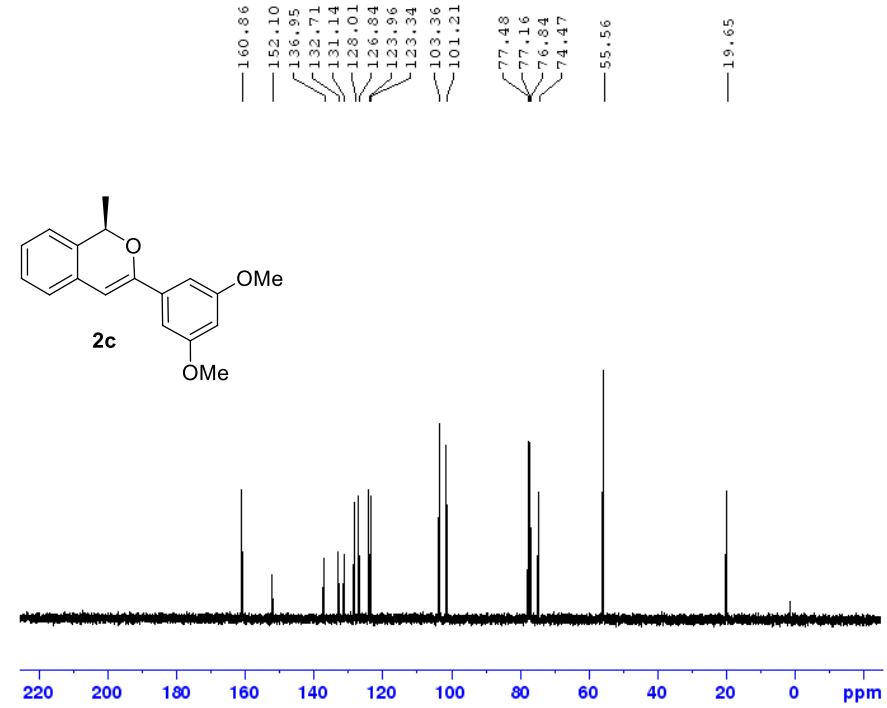



```
Current Data Parameters
NAME      mtt-product-T2086-76
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150128
Time                13.38
INSTRUM             spect
PROBHD    5 mm PADUL 13C
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      7
DS                      0
SWH             12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   90.5
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                  65536
SF            400.1300484 MHz
WDW                    EM
SSB                     0
LB                   0.50 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME      mtt-product-T2086-76
EXPNO                   10
PROCNO                   1

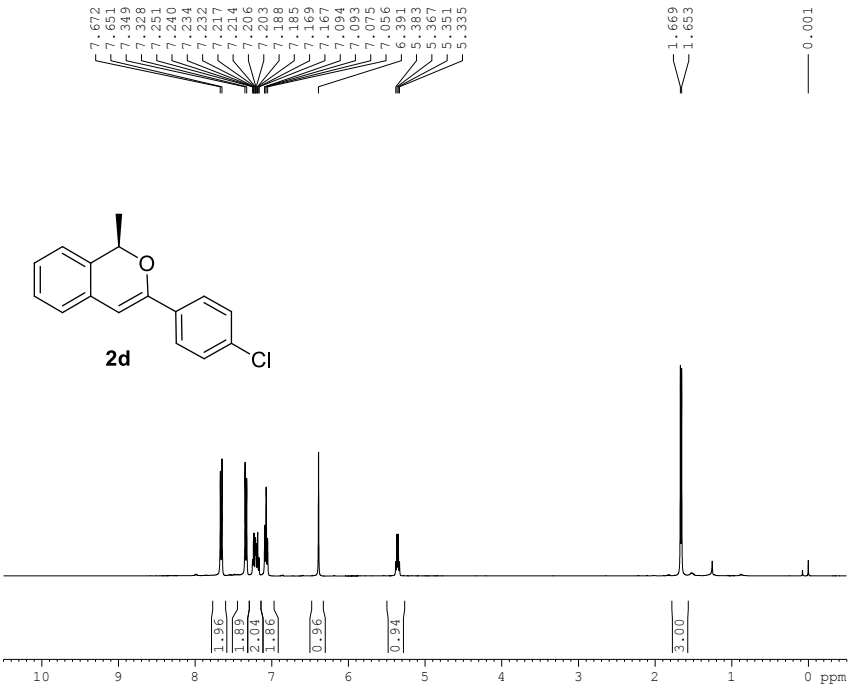
F2 - Acquisition Parameters
Date_             20150128
Time                13.41
INSTRUM             spect
PROBHD    5 mm PADUL 13C
PULPROG          zgpg30
TD                  32768
SOLVENT             CDCl3
NS                    135
DS                      0
SWH             25252.525 Hz
FIDRES          0.770646 Hz
AQ              0.6488064 sec
RG                    203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                   13C
P1                 9.40 usec
PLW1          43.63899994 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          13.06000042 W
PLW12          0.25598001 W
PLW13          0.20734000 W

F2 - Processing parameters
SI                  32768
SF            100.6127581 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Compound 2d

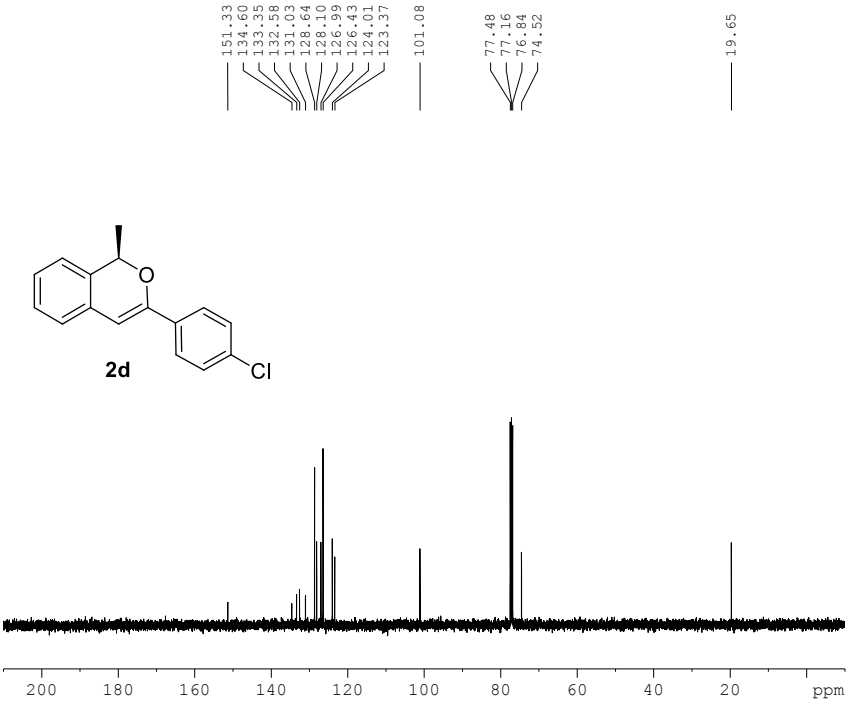



```
Current Data Parameters
NAME      mtt-T2033-27-2 race
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_           20140530
Time                4.24
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  90.5
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF           400.1300175 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



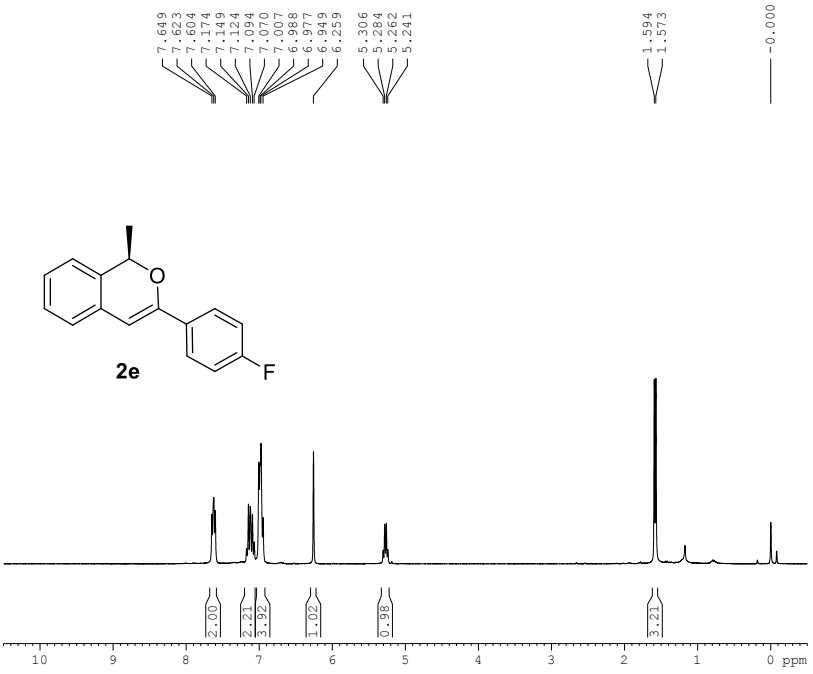

```
Current Data Parameters
NAME      mtt-T2033-27-2 race
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_           20140530
Time                4.26
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                    39
DS                     0
SWH            25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127557 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 2e

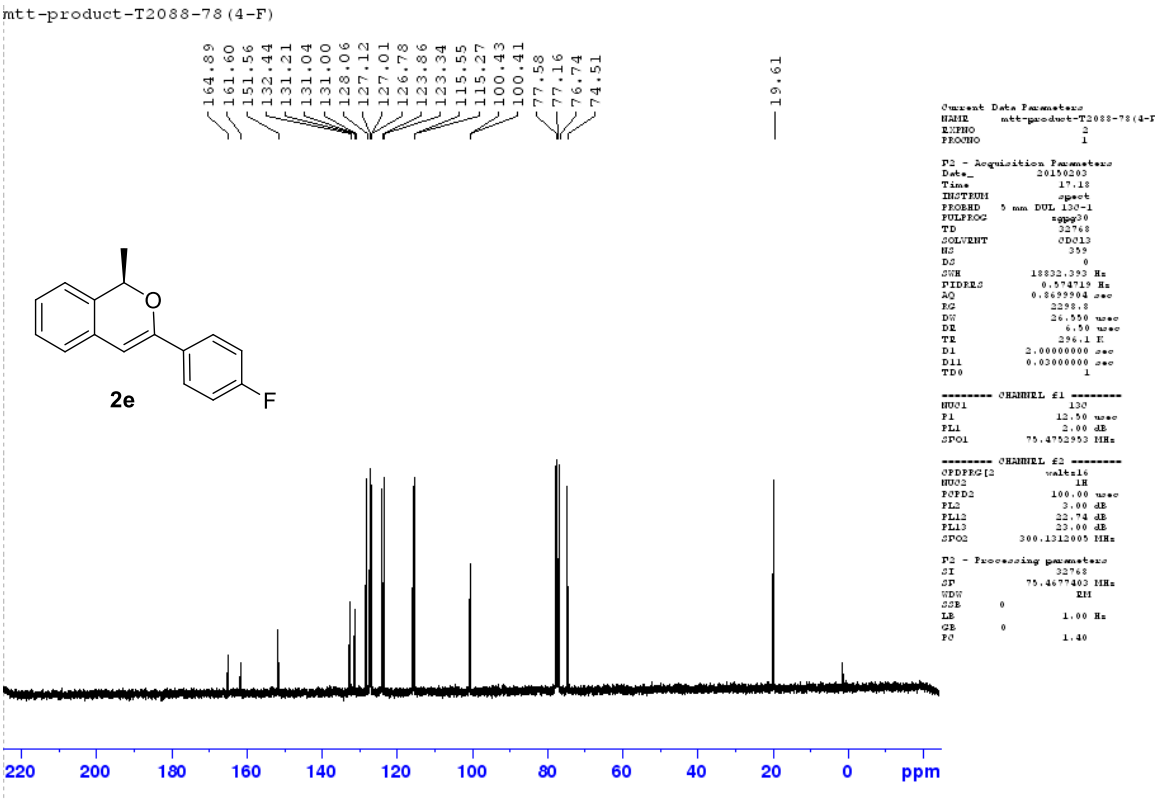



```
Current Data Parameters
NAME      mtt-product-T2088-78(4-F)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20150203
Time              17.15
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                32768
SOLVENT           CDCl3
NS                   10
DS                    0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                  181
DW                55.600 usec
DE                 6.50 usec
TE                296.3 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.30 usec
PL1                3.00 dB
SFO1         300.1315007 MHz

F2 - Processing parameters
SI                65536
SF           300.1300399 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 4.00
```




```
Current Data Parameters
NAME      mtt-product-T2088-78(4-F
EXPNO                 2
PROCNO                1

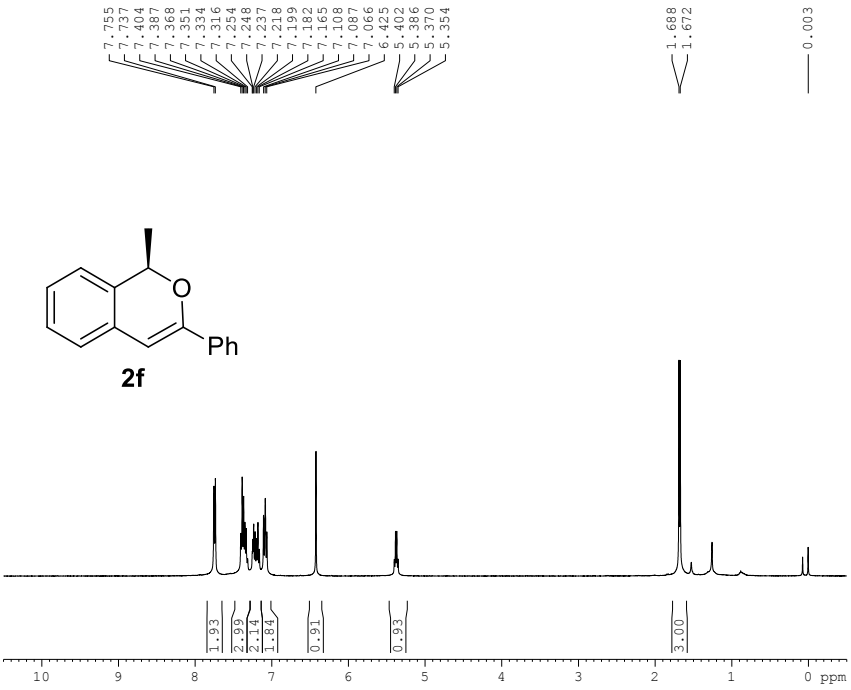
F2 - Acquisition Parameters
Date_           20150203
Time              17.18
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  359
DS                    0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ             0.8699904 sec
RG                 2298.8
DW                26.550 usec
DE                 6.50 usec
TE                296.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                32768
SF            75.4677403 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 2f

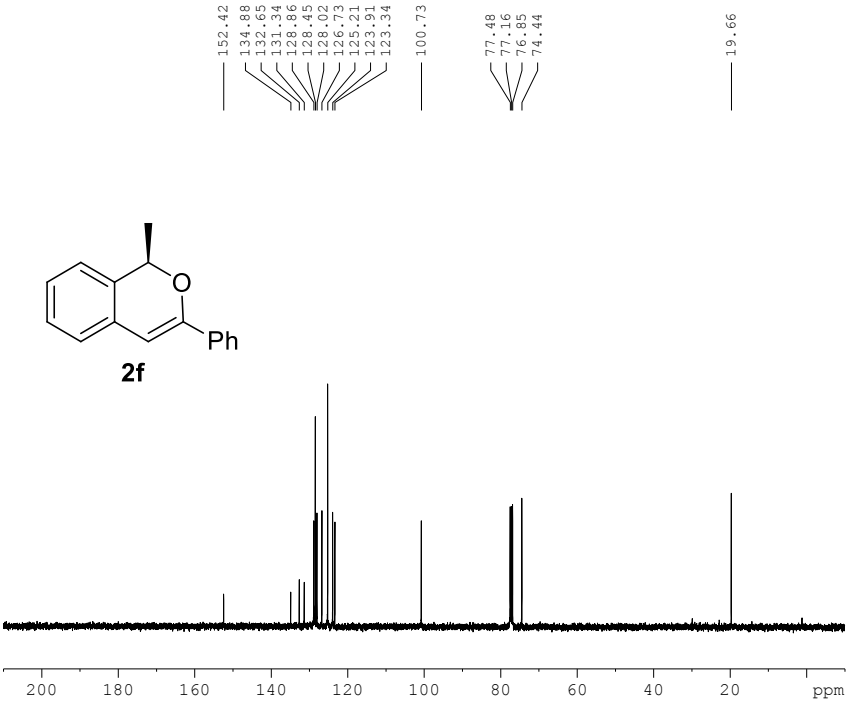



```
Current Data Parameters
NAME      mtt-subs-Me-H-Ph
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141219
Time                9.30
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                   203
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                 65536
SF           400.1300148 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



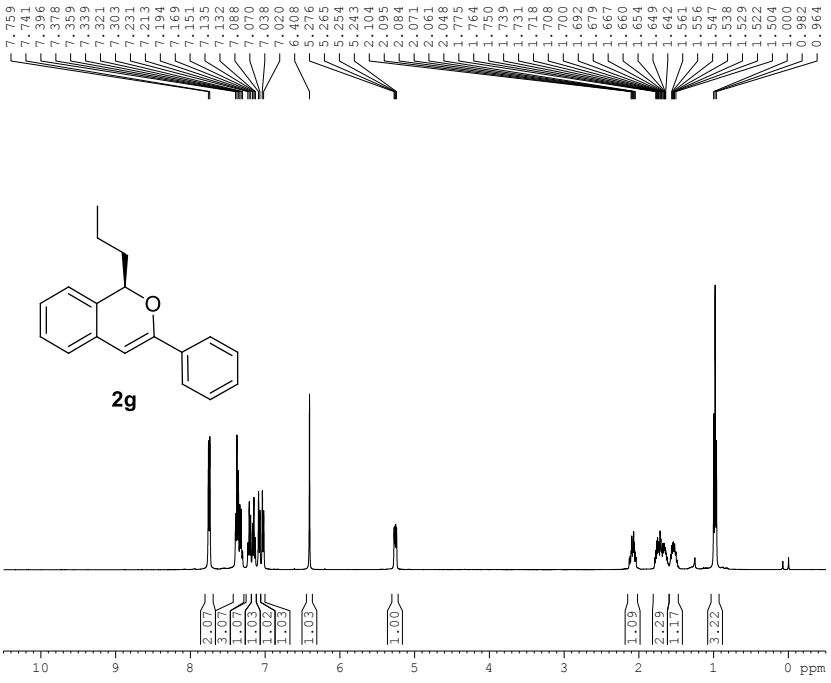

```
Current Data Parameters
NAME      mtt-subs-Me-H-Ph
EXPNO                  115
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141219
Time               10.52
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   239
DS                     0
SWH            25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488564 sec
RG                   203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 9.40 usec

F2 - Processing parameters
SI                 32768
SF           100.6127573 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 2g

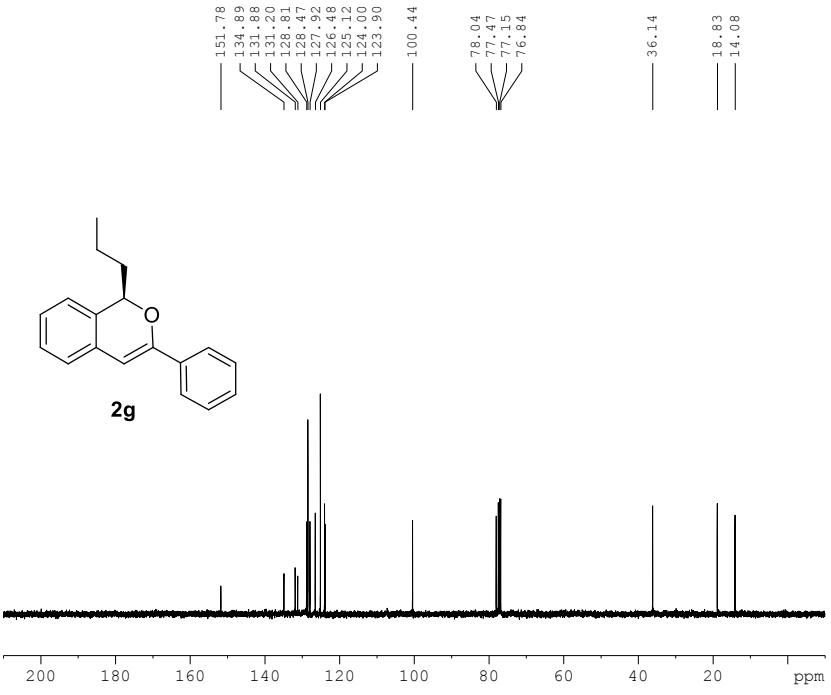



```
Current Data Parameters
NAME      mtt-T2081-71-2 product
EXPNO                 361
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141230
Time              20.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             2.0447731 sec
RG                80.72
DW               62.400 usec
DE                6.50 usec
TE               297.5 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                1H
P1                14.80 usec

F2 - Processing parameters
SI                65536
SF           400.2400247 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



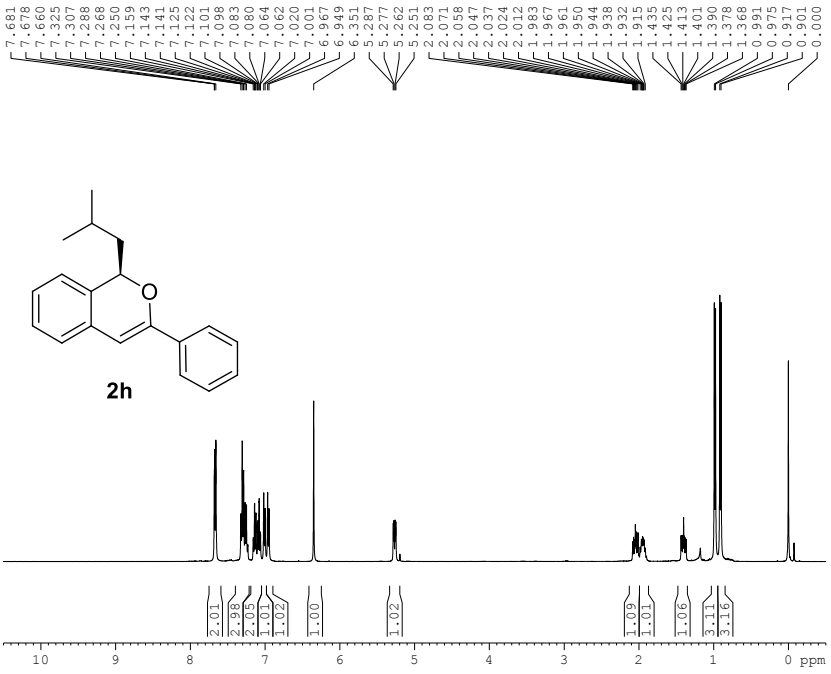

```
Current Data Parameters
NAME      mtt-T2081-71-2 product
EXPNO                 140
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141230
Time              20.44
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   57
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                206.33
DW               20.800 usec
DE                6.50 usec
TE               298.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6504916 MHz
NUC1                13C
P1                10.00 usec

F2 - Processing parameters
SI                32768
SF           100.6404176 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 2h

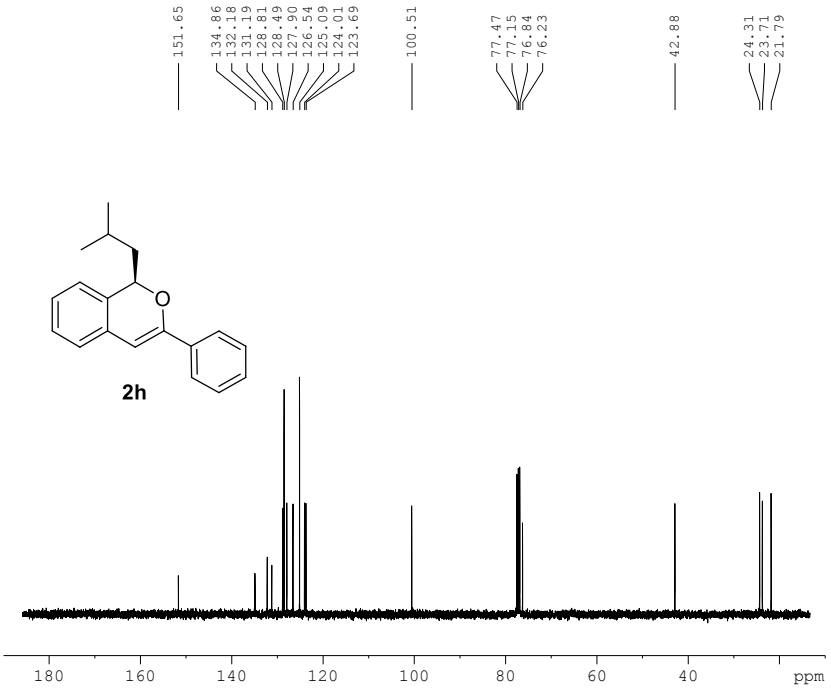



```
Current Data Parameters
NAME      mtt-T2082-72-1 product
EXPNO                  28
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141231
Time_               17.34
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                  80.72
DW                 62.400 usec
DE                  6.50 usec
TE                296.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.2424716 MHz
NUC1                  1H
P1                 14.80 usec

F2 - Processing parameters
SI                 65536
SF            400.2400512 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



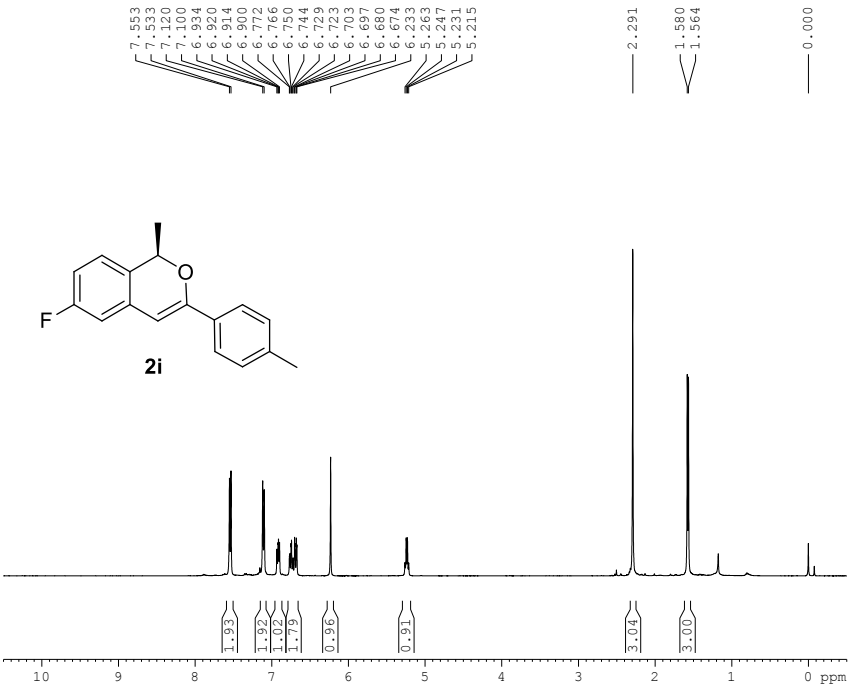

```
Current Data Parameters
NAME      mtt-T2082-72-1 product
EXPNO                 353
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141231
Time               17.35
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    54
DS                     4
SWH            17361.111 Hz
FIDRES             0.264910 Hz
AQ              1.8874868 sec
RG                 206.33
DW                 28.800 usec
DE                  6.50 usec
TE                296.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6504304 MHz
NUC1                  13C
P1                 10.00 usec

F2 - Processing parameters
SI                 32768
SF            100.6404170 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 2i

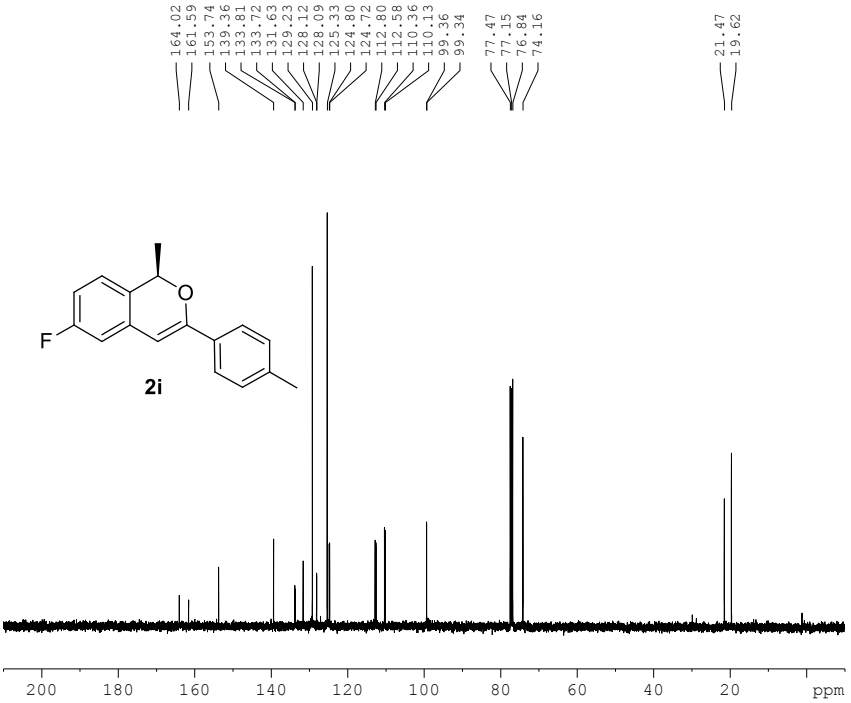



```
Current Data Parameters
NAME      mtt-pro-Me-F-MePh
EXPNO                  110
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141224
Time              21.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    6
DS                    0
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             2.0447731 sec
RG                92.09
DW               62.400 usec
DE                6.50 usec
TE                297.8 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                1H
P1                14.80 usec

F2 - Processing parameters
SI                65536
SF           400.2400509 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



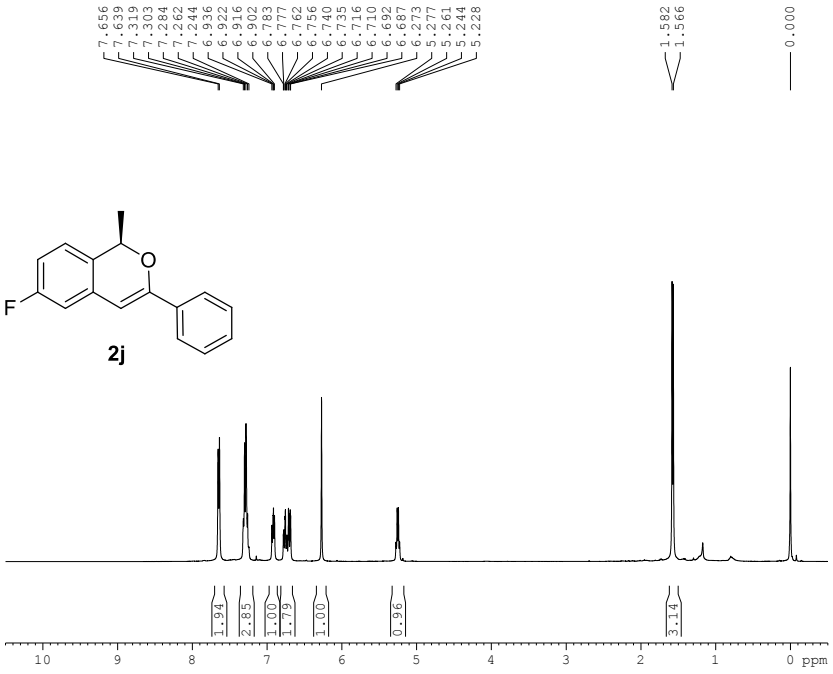

```
Current Data Parameters
NAME      mtt-pro-Me-F-MePh
EXPNO                  324
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141224
Time              21.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  117
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                206.33
DW               20.800 usec
DE                6.50 usec
TE                298.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6504916 MHz
NUC1                13C
P1                10.00 usec

F2 - Processing parameters
SI                32768
SF           100.6404161 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 2j

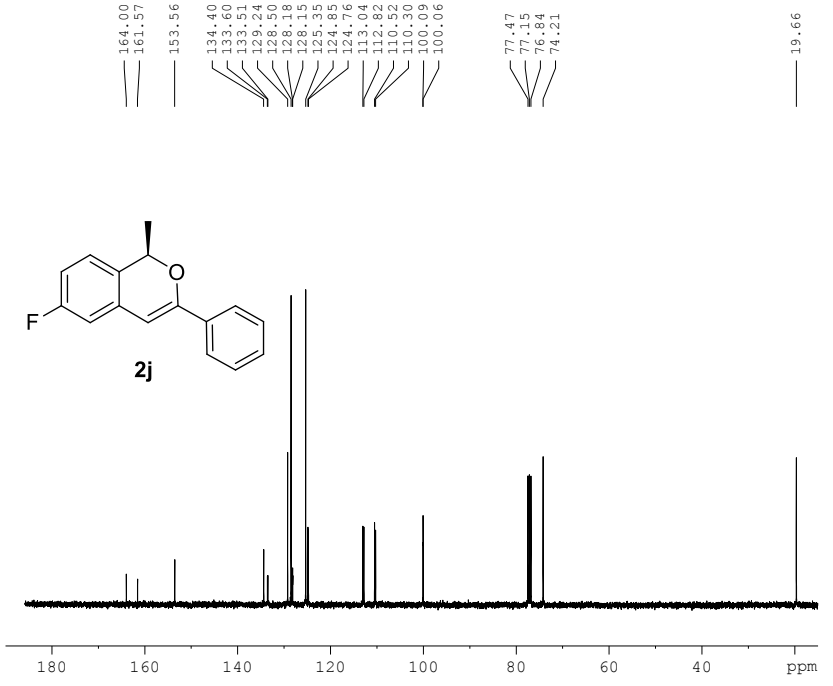



```
Current Data Parameters
NAME      mtt-T2082-72-2 product
EXPNO                  28
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150105
Time                19.20
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    11
DS                     0
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ              2.0447731 sec
RG                  73.9
DW                62.400 usec
DE                 6.50 usec
TE                296.1 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.2424716 MHz
NUC1                  1H
P1                 14.80 usec

F2 - Processing parameters
SI                 65536
SF            400.2400555 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



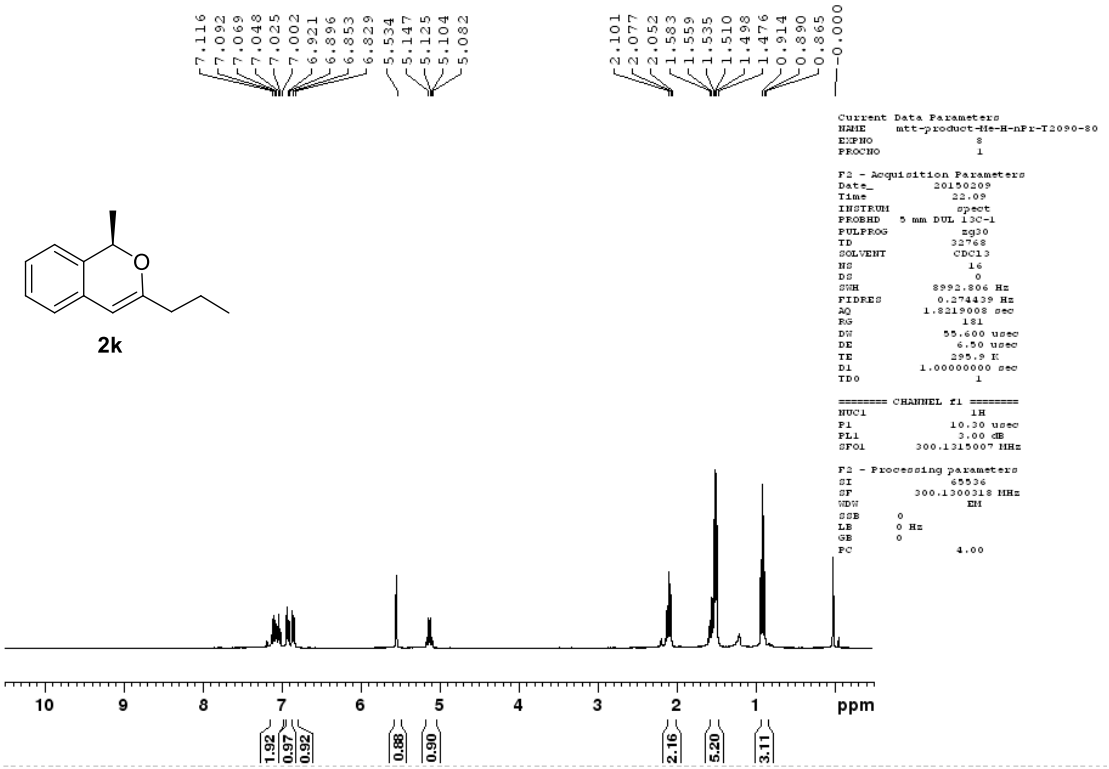

```
Current Data Parameters
NAME      mtt-T2082-72-2 product
EXPNO                 353
PROCNO                  1

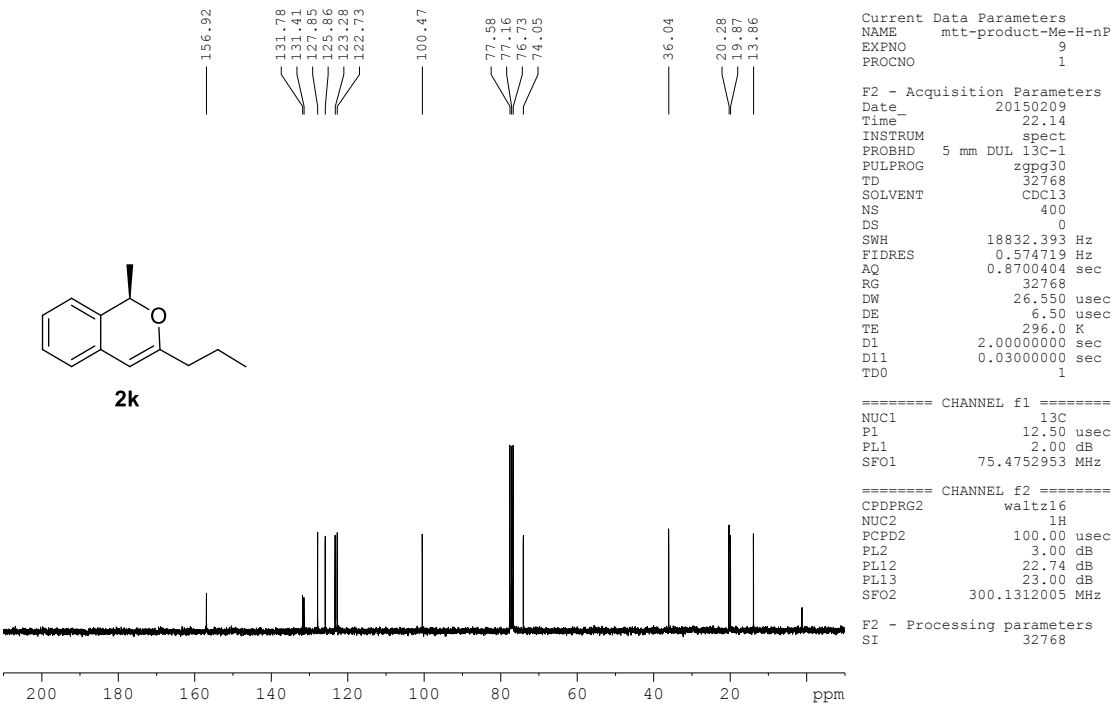
F2 - Acquisition Parameters
Date_            20150105
Time                19.23
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   105
DS                     4
SWH             17361.111 Hz
FIDRES           0.264910 Hz
AQ              1.8874868 sec
RG                206.33
DW                28.800 usec
DE                 6.50 usec
TE                296.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6504304 MHz
NUC1                  13C
P1                 10.00 usec

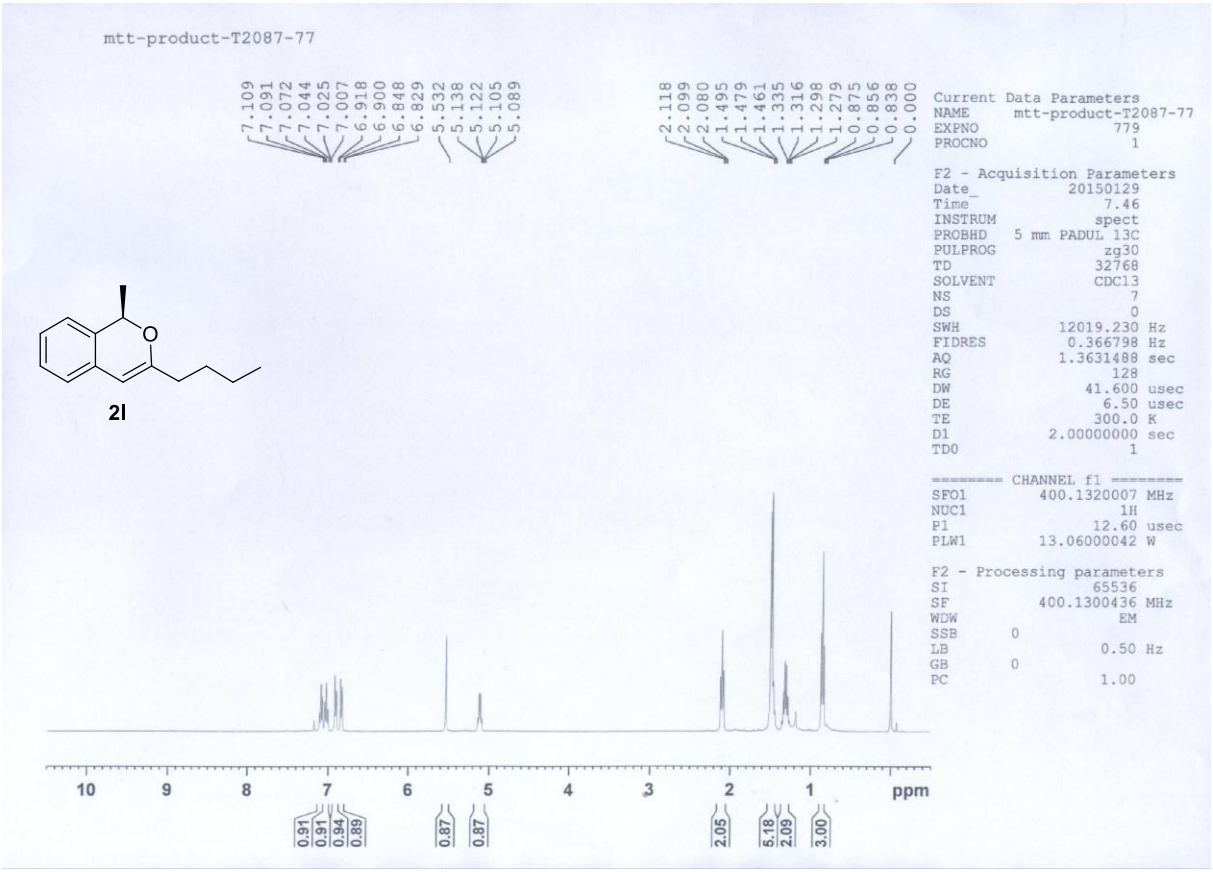
F2 - Processing parameters
SI                 32768
SF            100.6404180 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

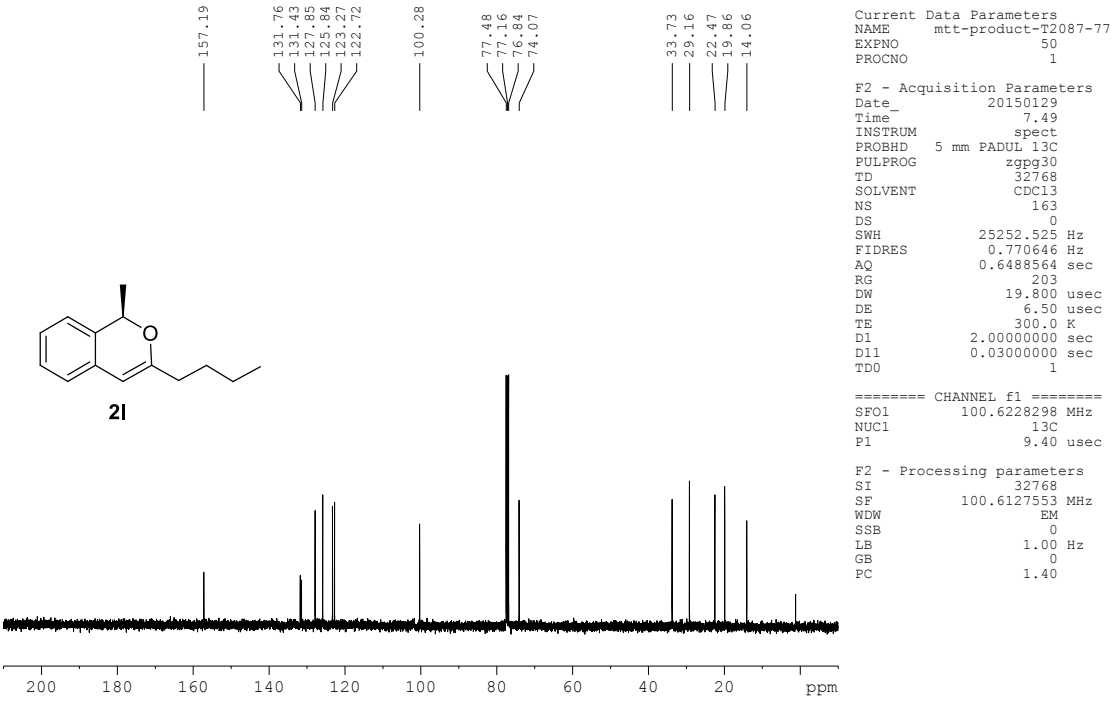
Compound 2k


7.116
7.092
7.069
7.048
7.025
7.002
6.921
6.896
6.853
6.829
5.534
5.147
5.125
5.104
5.082
2.101
2.077
2.052
1.583
1.559
1.535
1.510
1.498
1.476
0.914
0.890
0.865
-0.000
2k
Current Data Parameters
NAME mtt-product-Me-H-nPr-T2090-80
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150209
Time 22.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.274439 Hz
AQ 1.8219008 sec
RG 181
DW 55.600 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.30 usec
PL1 3.00 dB
SFO1 300.1315007 MHz
F2 - Processing parameters
SI 65536
SF 300.1300218 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 4.00
10 9 8 7 6 5 4 3 2 1 ppm
1.92 0.97 0.92 0.88 0.90 2.16 5.20 3.11

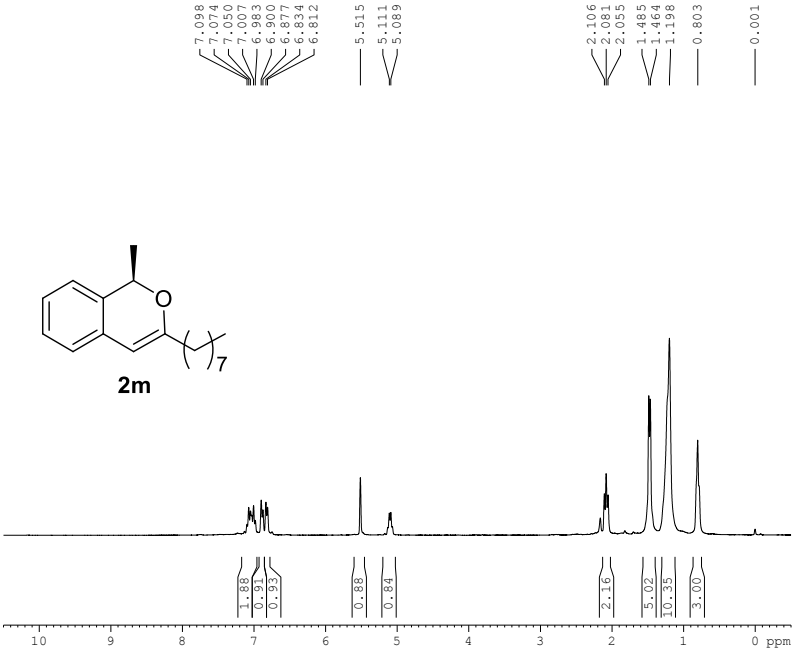

156.92
131.78
131.41
127.85
125.86
123.28
122.73
100.47
77.58
77.16
76.73
74.05
36.04
20.28
19.87
13.86
2k
Current Data Parameters
NAME mtt-product-Me-H-nP
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150209
Time 22.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 32768
DW 26.550 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.74 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
200 180 160 140 120 100 80 60 40 20 ppm

Compound 2l


mtt-product-T2087-77
7.109
7.091
7.072
7.044
7.025
7.007
6.918
6.900
6.848
6.829
5.532
5.138
5.122
5.105
5.089
2.118
2.099
2.080
1.495
1.479
1.461
1.335
1.316
1.298
1.279
0.875
0.856
0.838
0.000
2l
Current Data Parameters
NAME mtt-product-T2087-77
EXPNO 779
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150129
Time 7.46
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1320007 MHz
NUC1 1H
P1 12.60 usec
PLW1 13.06000042 W
F2 - Processing parameters
SI 65536
SF 400.1300436 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
0.91 0.91 0.94 0.89 0.87 0.87 2.05 5.18 2.09 3.00


157.19
131.76
131.43
127.85
125.84
123.27
122.72
100.28
77.48
77.16
76.84
74.07
33.73
29.16
22.47
19.86
14.06
2l
Current Data Parameters
NAME mtt-product-T2087-77
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150129
Time 7.49
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 163
DS 0
SWH 25252.525 Hz
FIDRES 0.770646 Hz
AQ 0.6488564 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.40 usec
F2 - Processing parameters
SI 32768
SF 100.6127553 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

Compound 2m

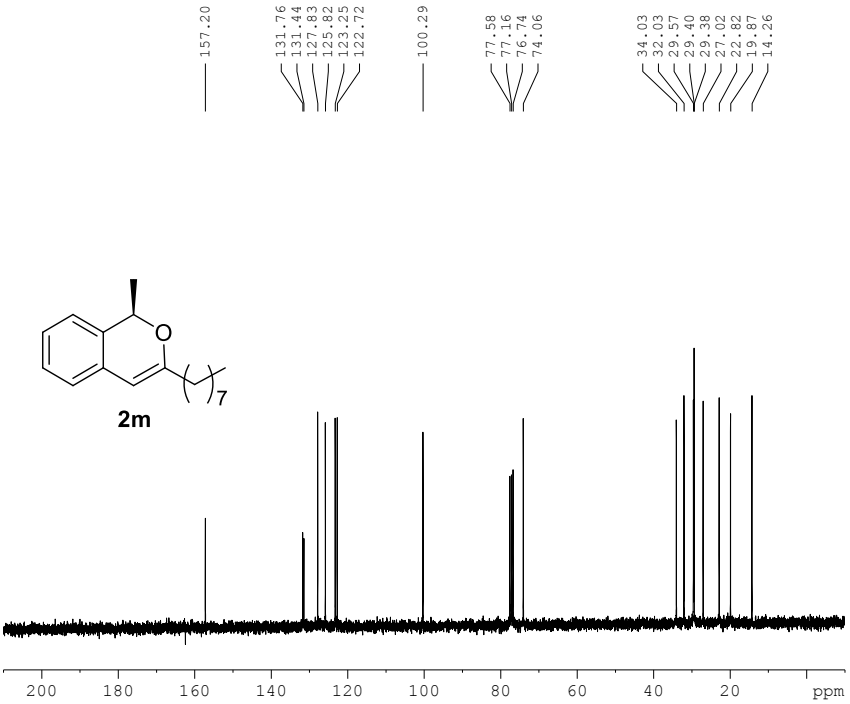



```
Current Data Parameters
NAME     mtt-product-T2091-81(kuique)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20150306
Time              12.53
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                 40.3
DW                55.600 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.30 usec
PL1                3.00 dB
SFO1        300.1315007 MHz

F2 - Processing parameters
SI                65536
SF          300.1300441 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 4.00
```




```
Current Data Parameters
NAME     mtt-product-T2091-8
EXPNO                 2
PROCNO                1

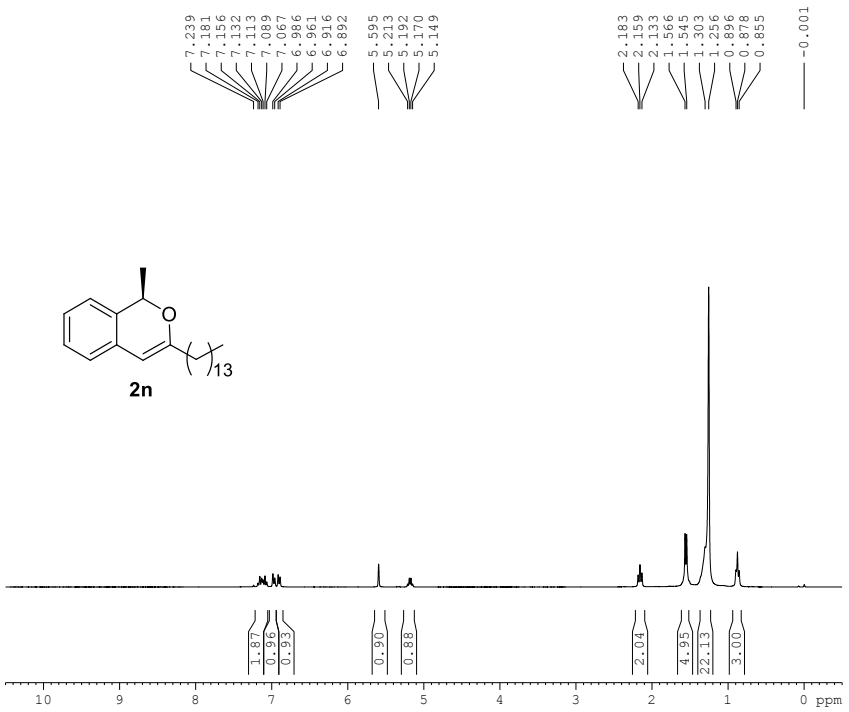
F2 - Acquisition Parameters
Date_           20150306
Time              12.58
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD               32768
SOLVENT           CDCl3
NS                   98
DS                    0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ             0.8700404 sec
RG                1625.5
DW                26.550 usec
DE                 6.50 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
```

Compound 2n

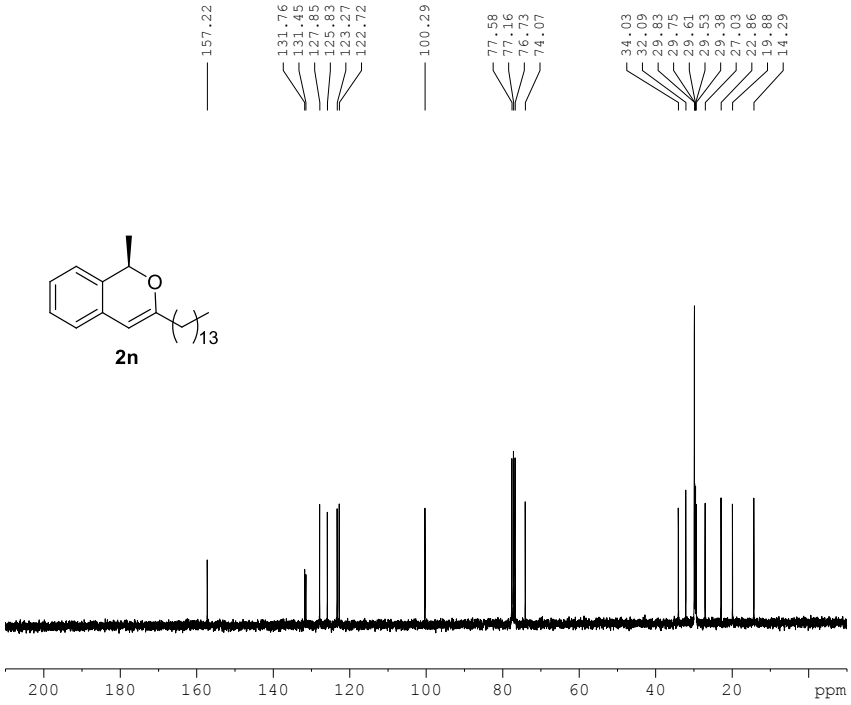



```
Current Data Parameters
NAME      mtt-T2093-83-product
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150311
Time               10.40
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                   64
DW                55.600 usec
DE                 6.50 usec
TE                296.6 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.30 usec
PL1                3.00 dB
SFO1         300.1315007 MHz

F2 - Processing parameters
SI                65536
SF           300.1300126 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 4.00
```




```
Current Data Parameters
NAME      mtt-T2093-83-produc
EXPNO                    2
PROCNO                   1

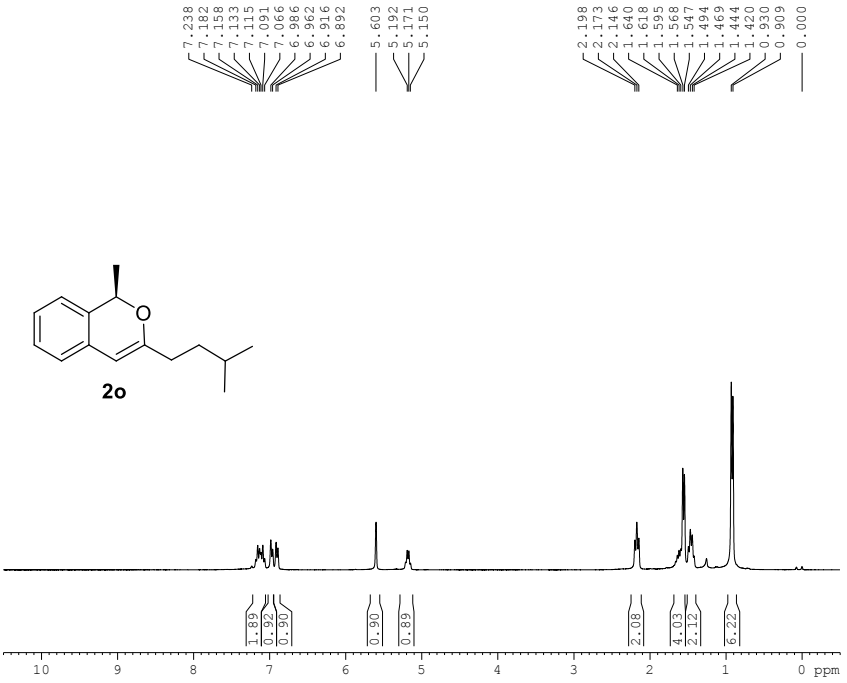
F2 - Acquisition Parameters
Date_           20150311
Time               10.44
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  151
DS                    0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ             0.8700404 sec
RG                2580.3
DW                26.550 usec
DE                 6.50 usec
TE                296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

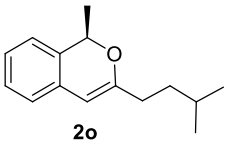
======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                32768
```

Compound 2o





2o

```
Current Data Parameters
NAME      mtt-T2092-82-product
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150310
Time              13.12
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                  16
DS                   0
SWH            8992.806 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                71.8
DW              55.600 usec
DE               6.50 usec
TE              296.4 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.30 usec
PL1                3.00 dB
SFO1        300.1315007 MHz

F2 - Processing parameters
SI                65536
SF           300.1300131 MHz
WDW                  EM
SSB                  0
LB                0.00 Hz
GB                   0
PC                4.00
```


2o

```
Current Data Parameters
NAME      mtt-T2092-82-produc
EXPNO                    2
PROCNO                   1

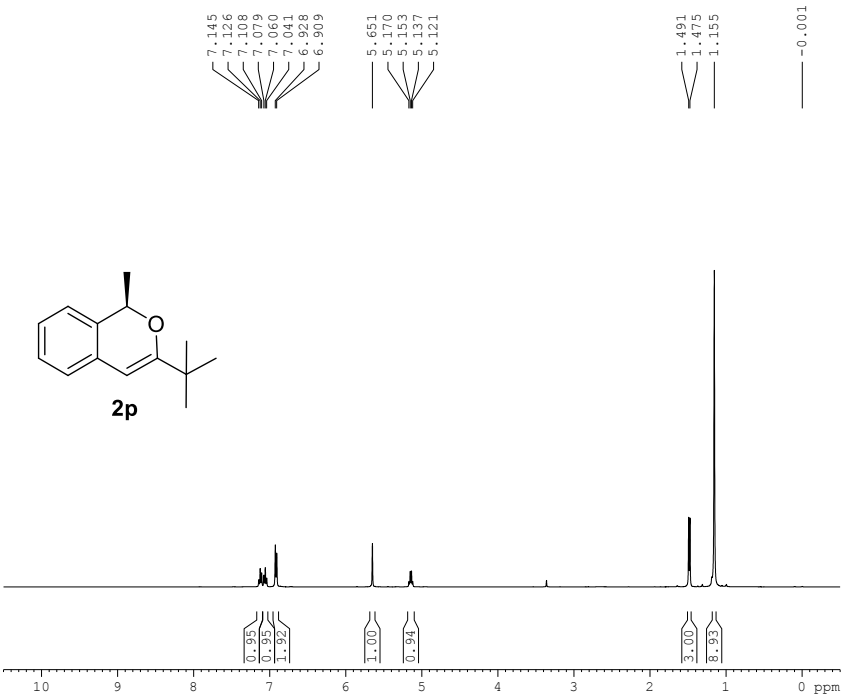
F2 - Acquisition Parameters
Date_           20150310
Time              13.16
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                  74
DS                   0
SWH           18832.393 Hz
FIDRES         0.574719 Hz
AQ             0.8700404 sec
RG                574.7
DW              26.550 usec
DE               6.50 usec
TE              296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.74 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
```

Compound 2p

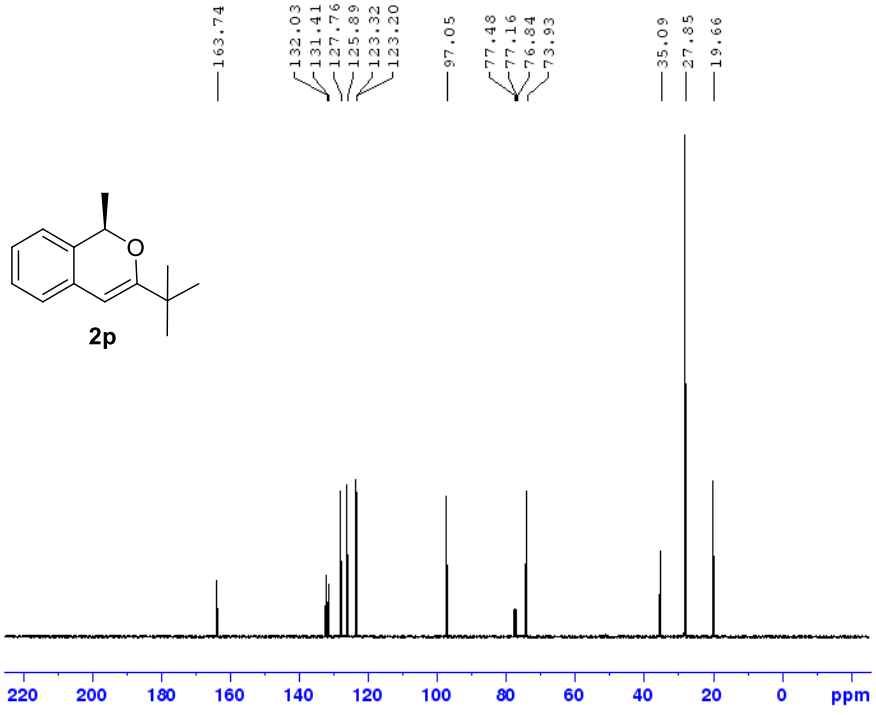



```
Current Data Parameters
NAME      mtt-product-Me-H-tBu
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150117
Time                 5.08
INSTRUM             spect
PROBHD    5 mm PADUL 13C
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      6
DS                      0
SWH             12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                     10
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1320007 MHz
NUC1                   1H
P1                 12.60 usec

F2 - Processing parameters
SI                  65536
SF            400.1300799 MHz
WDW                    EM
SSB                     0
LB                   0.50 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME      mtt-product-Me-H-tBu
EXPNO                   36
PROCNO                   1

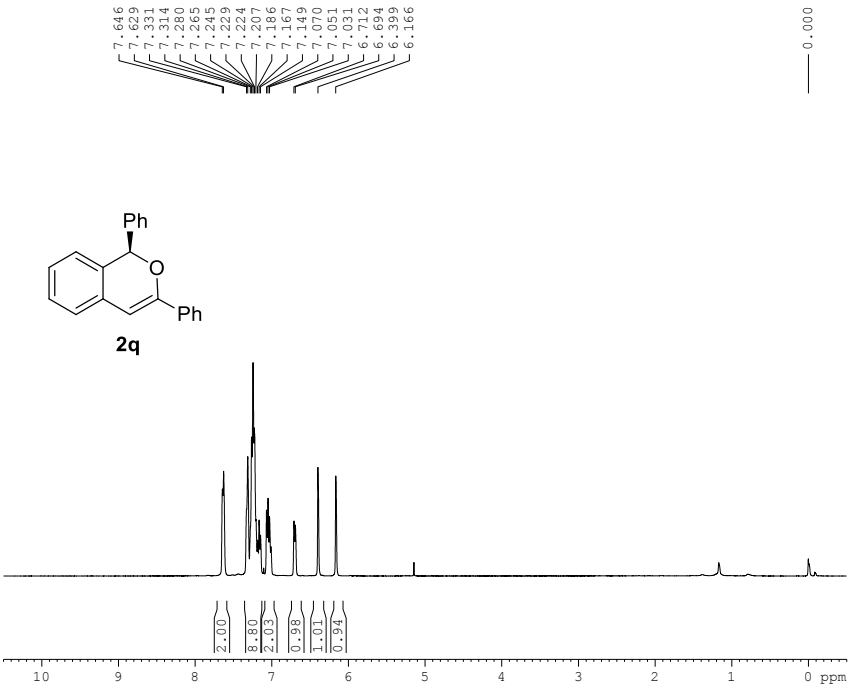
F2 - Acquisition Parameters
Date_             20150117
Time                 5.11
INSTRUM             spect
PROBHD    5 mm PADUL 13C
PULPROG           zgpg30
TD                  32768
SOLVENT             CDCl3
NS                     61
DS                      0
SWH             25252.525 Hz
FIDRES          0.770646 Hz
AQ              0.6488064 sec
RG                    203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                 9.40 usec
PLW1          43.63899994 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          13.06000042 W
PLW12          0.25598001 W
PLW13          0.20734000 W

F2 - Processing parameters
SI                  32768
SF            100.6127736 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Compound 2q

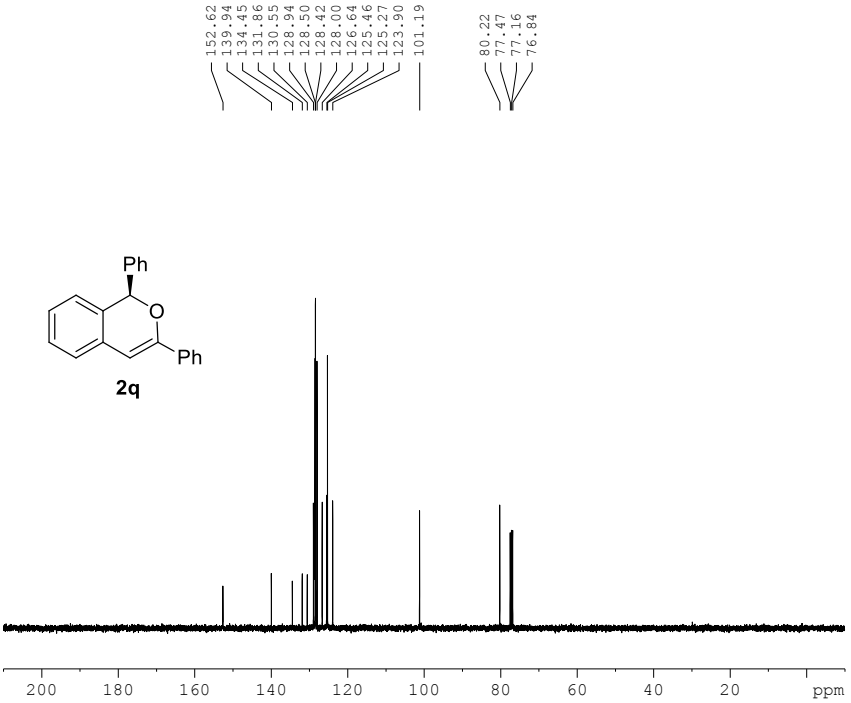



```
Current Data Parameters
NAME      mtt-product-Ph-H-Ph
EXPNO                  110
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150113
Time               11.18
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     7
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              2.0447731 sec
RG                 65.71
DW                62.400 usec
DE                 6.50 usec
TE                296.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                1H
P1                 14.80 usec

F2 - Processing parameters
SI                 65536
SF           400.2400709 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



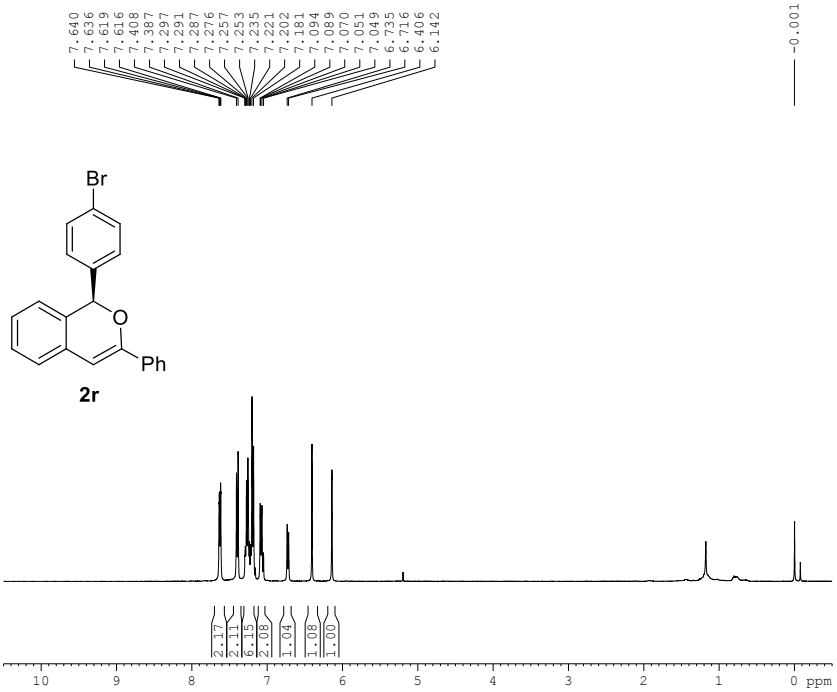

```
Current Data Parameters
NAME      mtt-product-Ph-H-Ph
EXPNO                  324
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150113
Time               11.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    83
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                296.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6504916 MHz
NUC1                13C
P1                 10.00 usec

F2 - Processing parameters
SI                 32768
SF           100.6404218 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 2r

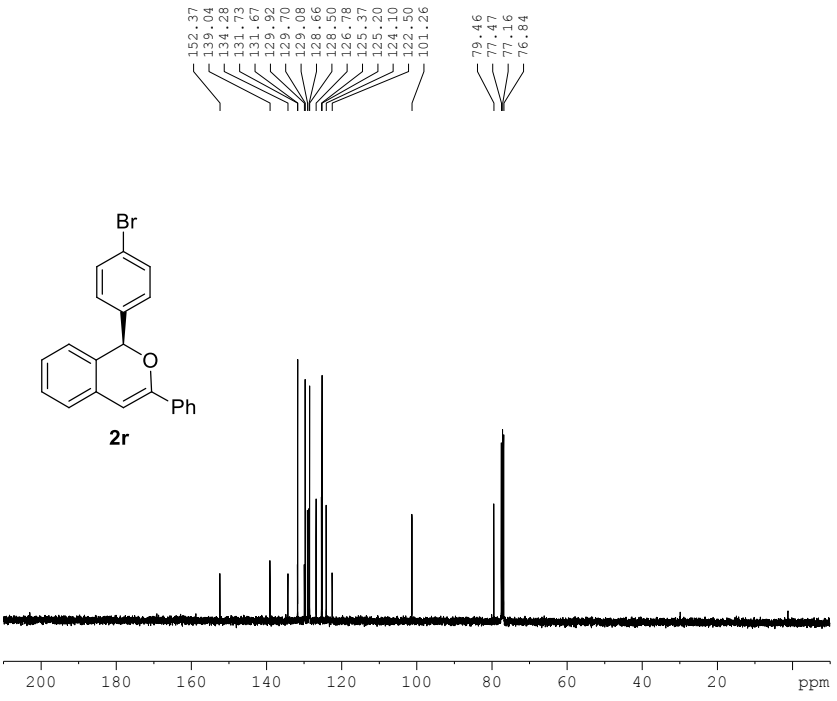



```
Current Data Parameters
NAME      mtt-product-BrPh-H-Ph
EXPNO                  122
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141222
Time               22.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                 116.67
DW                 62.400 usec
DE                  6.50 usec
TE                 298.8 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.2424716 MHz
NUC1                   1H
P1                  14.80 usec

F2 - Processing parameters
SI                 65536
SF            400.2400509 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



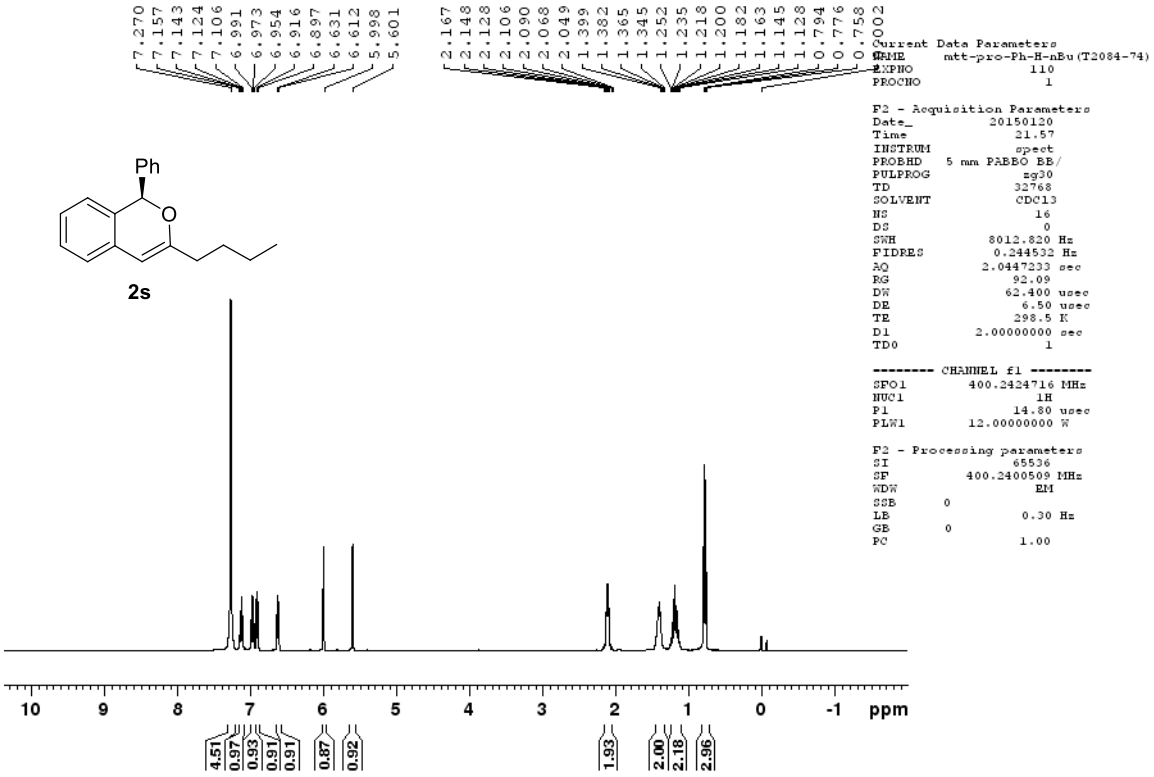

```
Current Data Parameters
NAME      mtt-product-BrPh-H-Ph
EXPNO                  123
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141222
Time               22.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   102
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                 206.33
DW                 20.800 usec
DE                  6.50 usec
TE                 299.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6504916 MHz
NUC1                   13C
P1                 10.00 usec

F2 - Processing parameters
SI                 32768
SF            100.6404161 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 2s

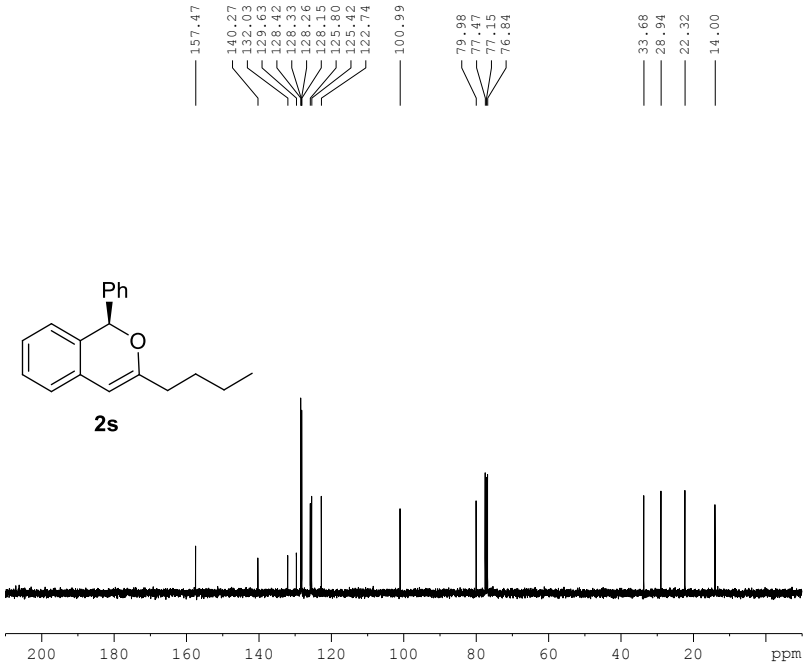


Current Data Parameters
NAME mtt-pro-Ph-H-nBu(T2084-74)
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150120
Time 21.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 92.09
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400509 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME mtt-pro-Ph-H-nBu(T2084-74)
EXPNO 324
PROCNO 1

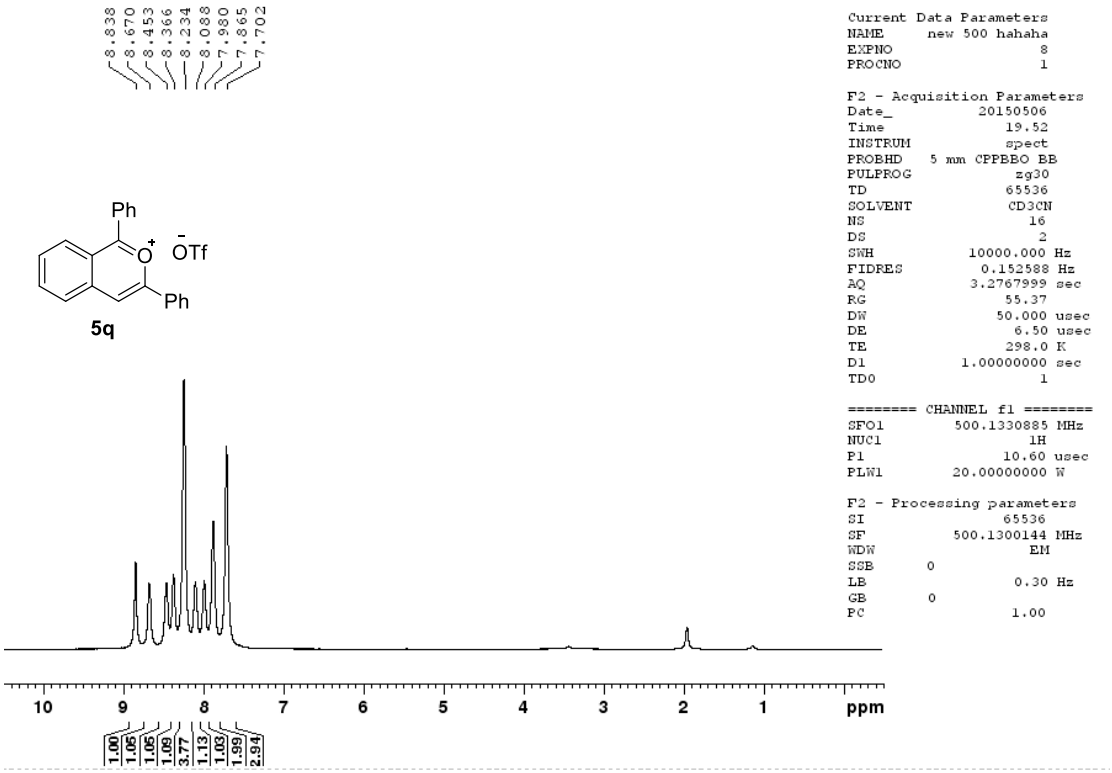
F2 - Acquisition Parameters
Date_ 20150120
Time 21.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

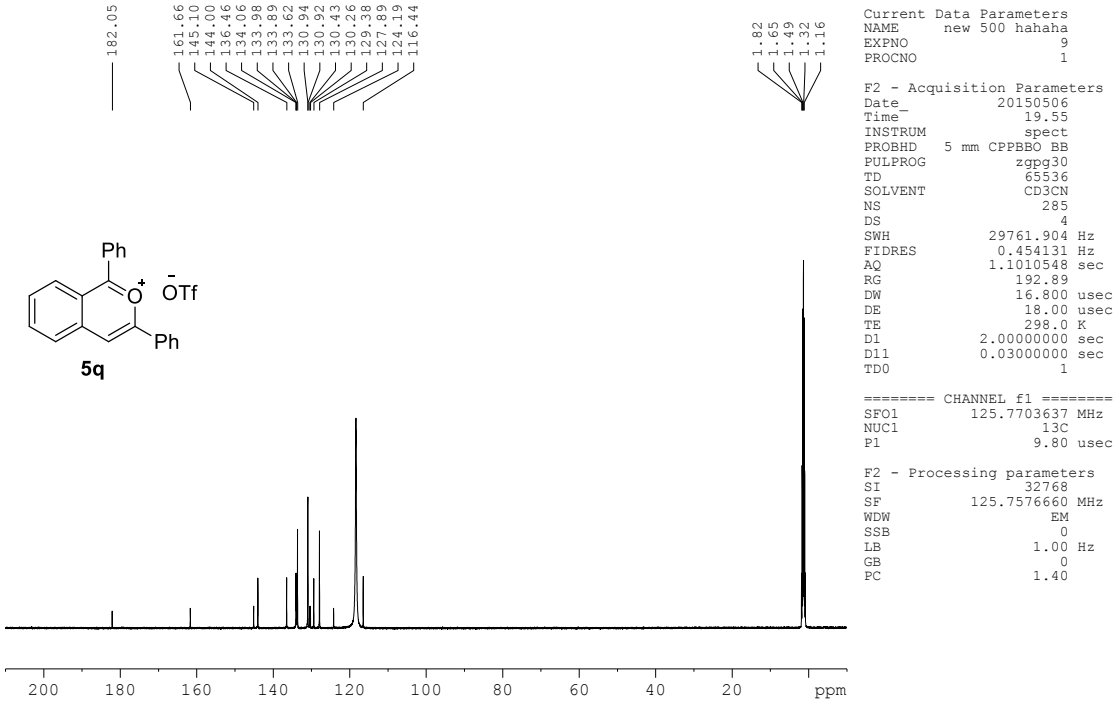
======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec

F2 - Processing parameters
SI 32768
SF 100.6404168 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

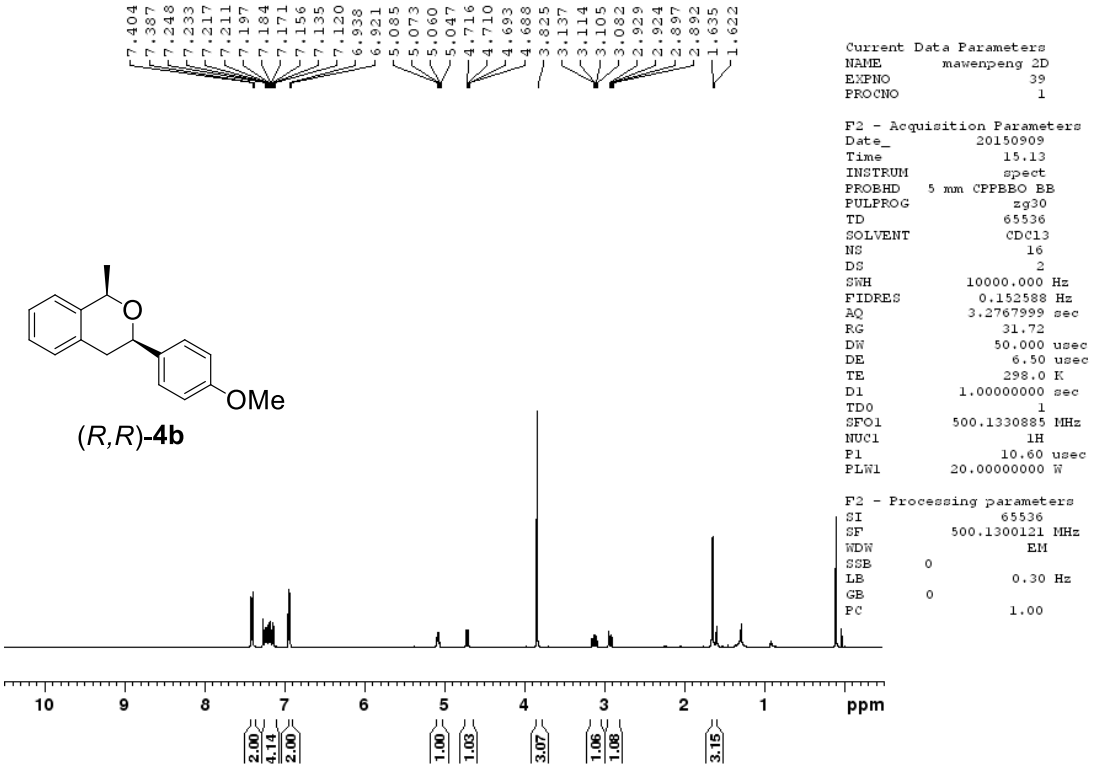
13.4 Other products:

Compound 3q





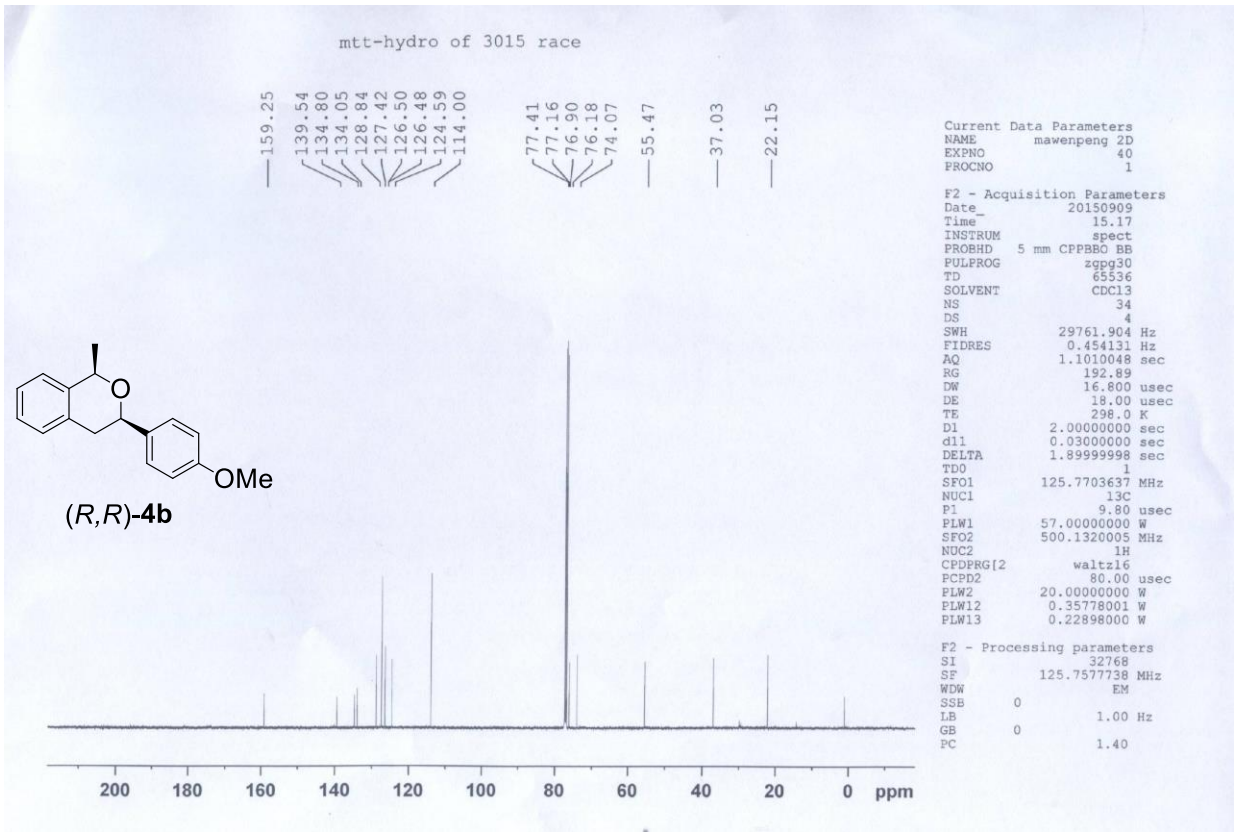
Compound (*R,R*)-4b




```
Current Data Parameters
NAME        mawenpeng 2D
EXPNO                 39
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150909
Time               15.13
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                31.72
DW               50.000 usec
DE                6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1
SFO1         500.1330885 MHz
NUC1                 1H
P1                10.60 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                65536
SF          500.1300121 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

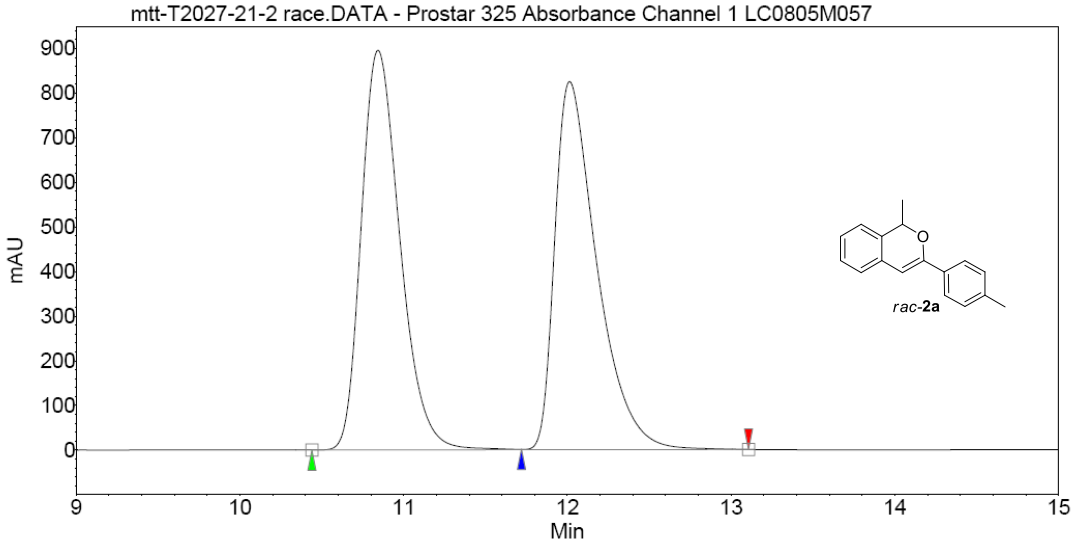



```
Current Data Parameters
NAME        mawenpeng 2D
EXPNO                 40
PROCNO                 1

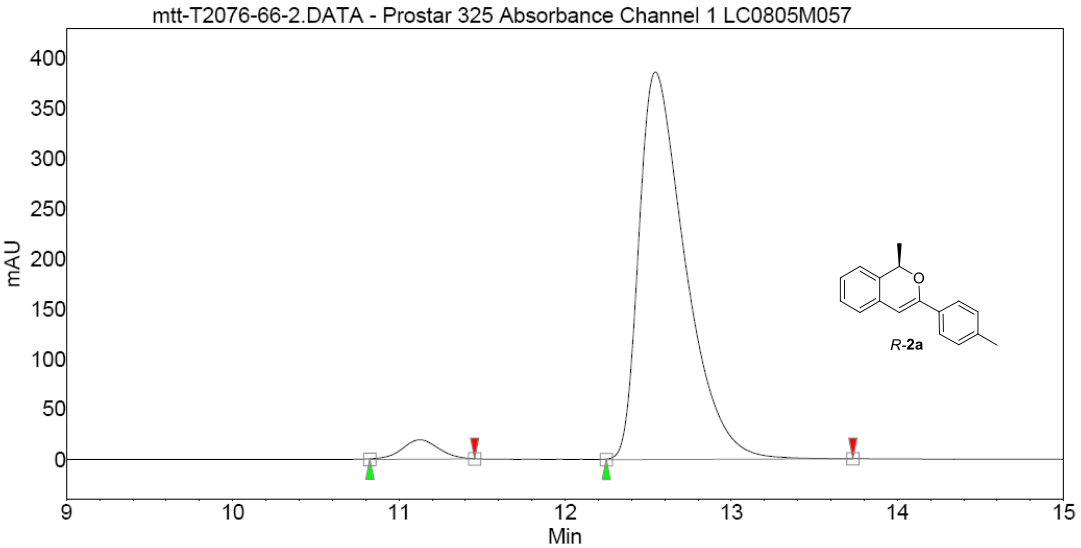
F2 - Acquisition Parameters
Date_           20150909
Time               15.17
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   34
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                192.89
DW               16.800 usec
DE                18.00 usec
TE                298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1
SFO1         125.7703637 MHz
NUC1                 13C
P1                 9.80 usec
PLW1         57.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         20.00000000 W
PLW12         0.35778001 W
PLW13         0.22898000 W

F2 - Processing parameters
SI                32768
SF          125.7577738 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

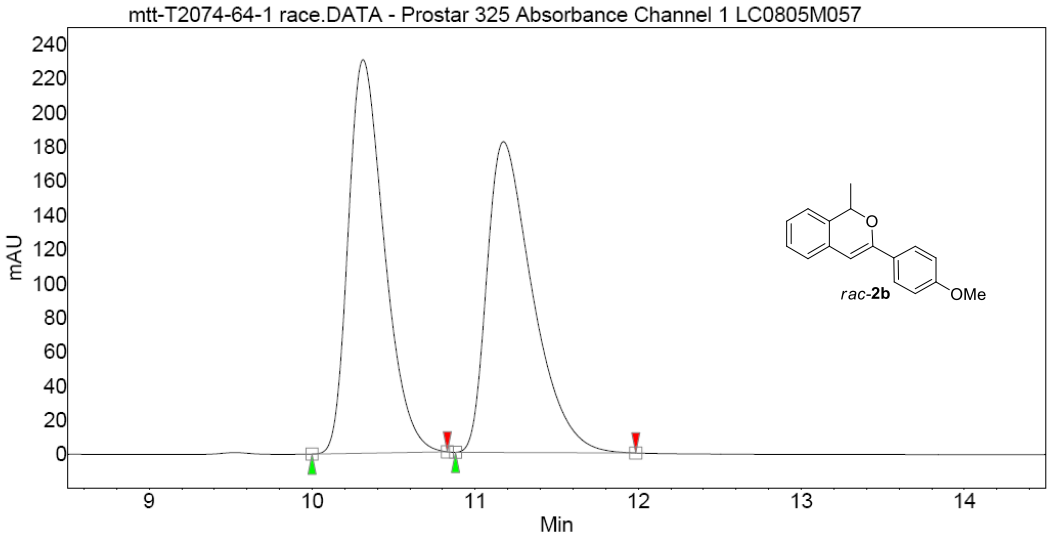
14. Copy of HPLC spectra of the racemic and chiral products



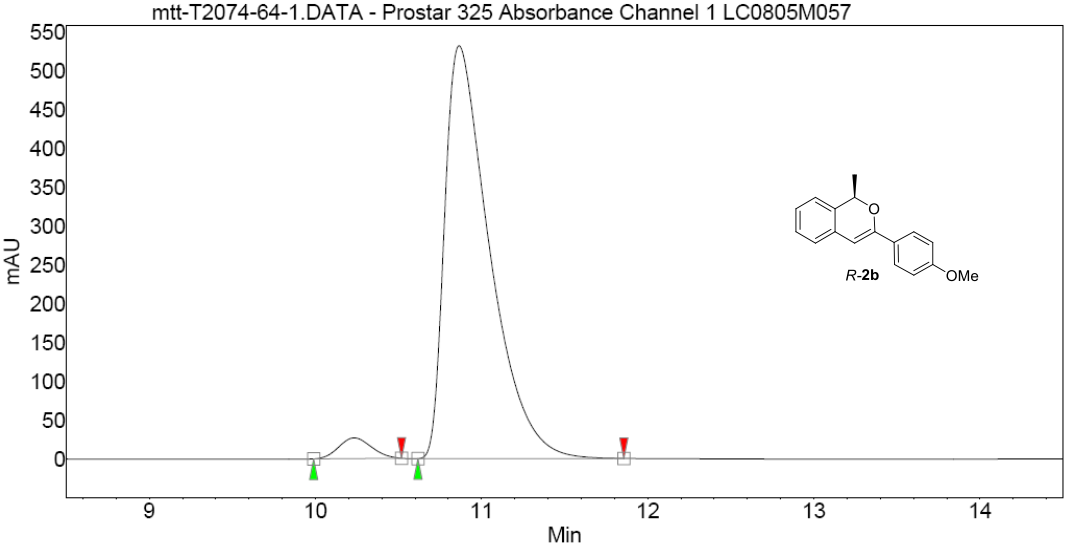
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.84	50.00	895.9	245.3	50.003
2	未知	12.01	50.00	825.5	245.3	49.997
Total			100.00	1721.4	490.6	100.000



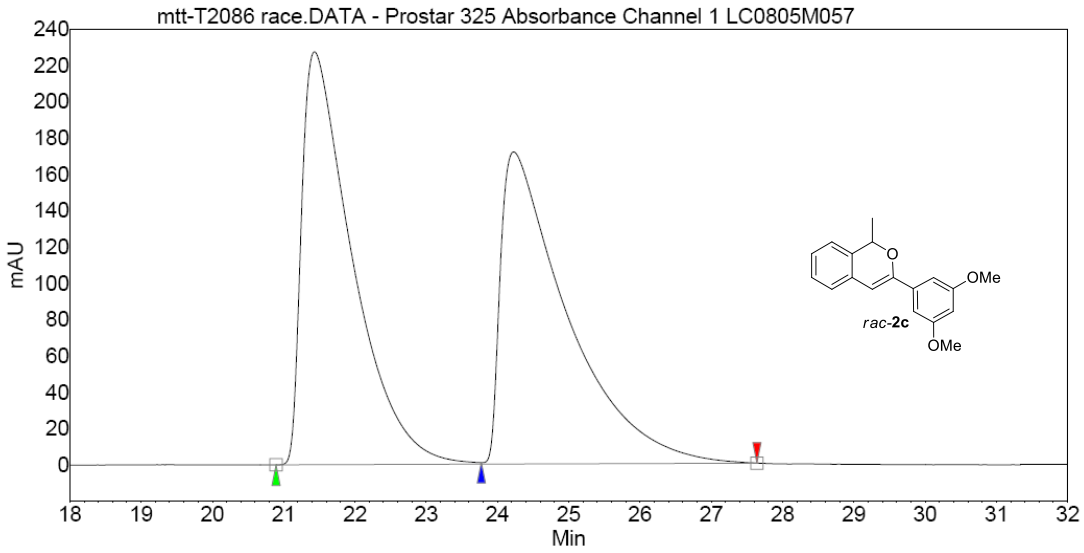
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	11.13	3.54	17.1	4.4	3.538
2	未知	12.63	96.46	362.4	121.1	96.462
Total			100.00	379.5	125.6	100.000



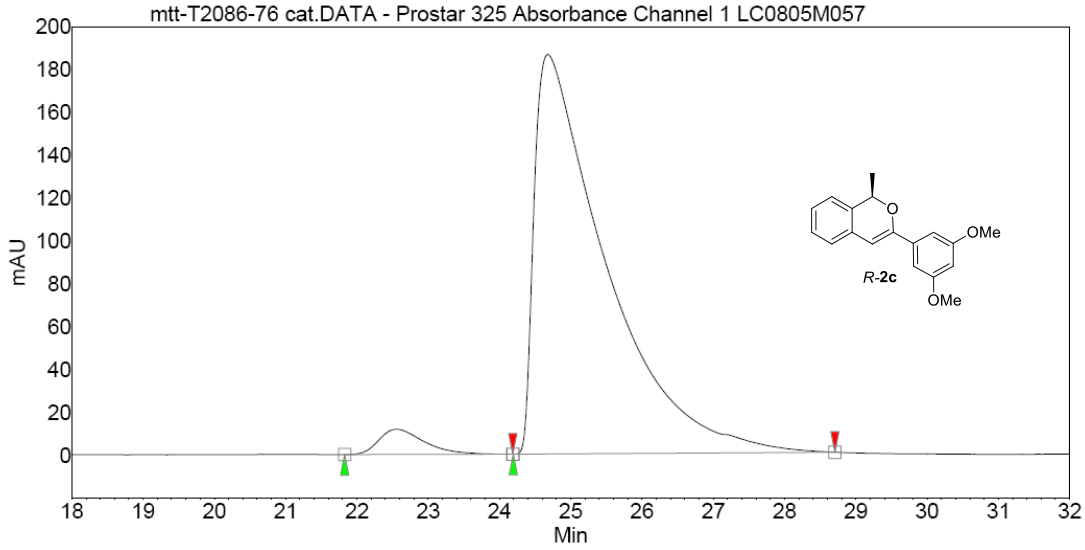
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.31	50.09	230.4	59.0	50.090
2	未知	11.17	49.91	181.9	58.8	49.910
Total			100.00	412.2	117.8	100.000



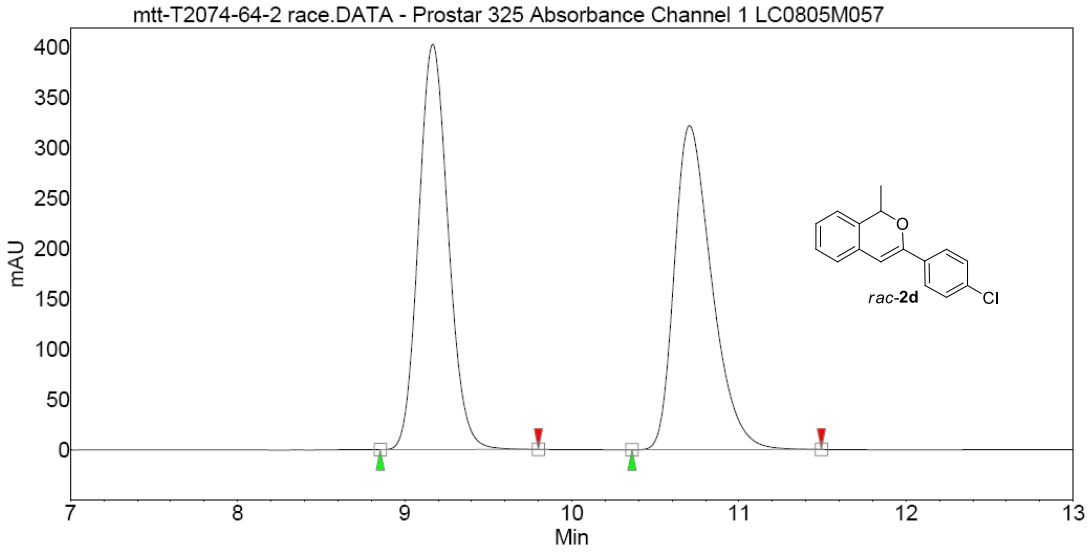
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.23	3.51	26.7	6.1	3.511
2	未知	10.87	96.49	532.5	166.7	96.489
Total			100.00	559.2	172.8	100.000



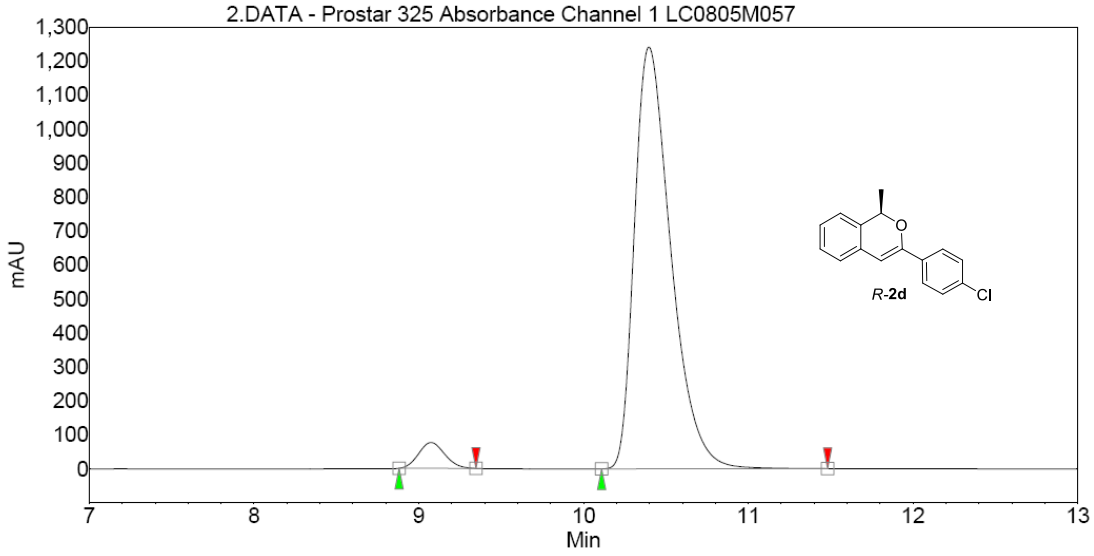
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	21.43	50.13	227.2	186.8	50.130
2	未知	24.23	49.87	171.7	185.8	49.870
Total			100.00	398.9	372.6	100.000



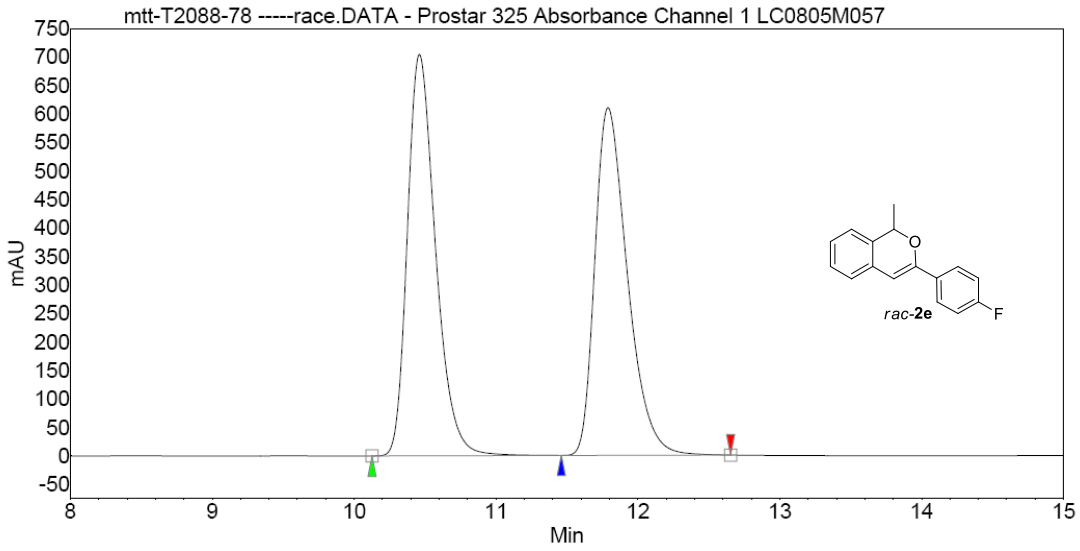
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	22.56	3.85	11.8	8.7	3.847
2	未知	24.68	96.15	186.2	216.6	96.153
Total			100.00	198.0	225.3	100.000



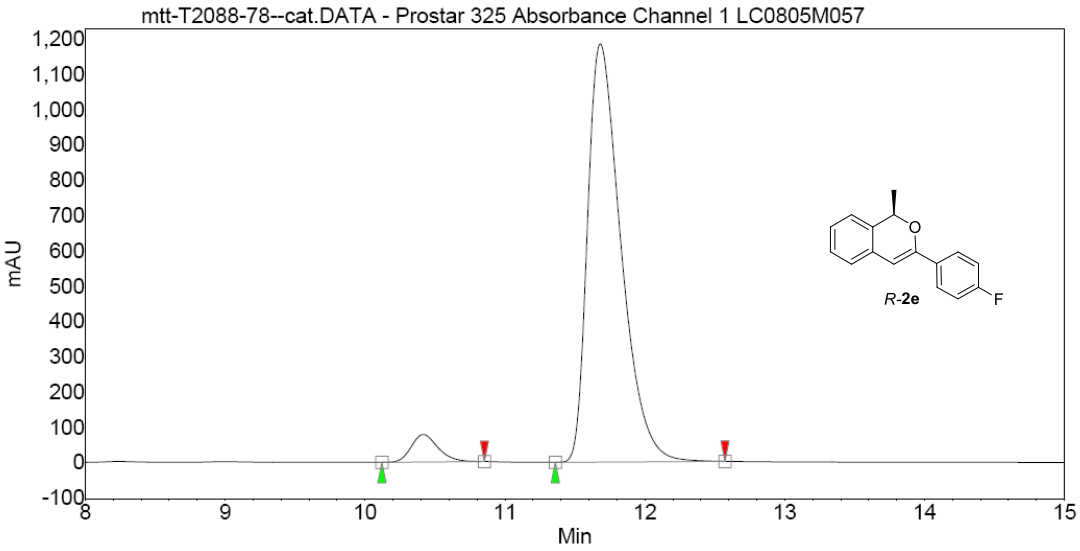
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	9.17	49.81	403.0	82.9	49.809
2	未知	10.71	50.19	322.2	83.5	50.191
Total			100.00	725.2	166.4	100.000



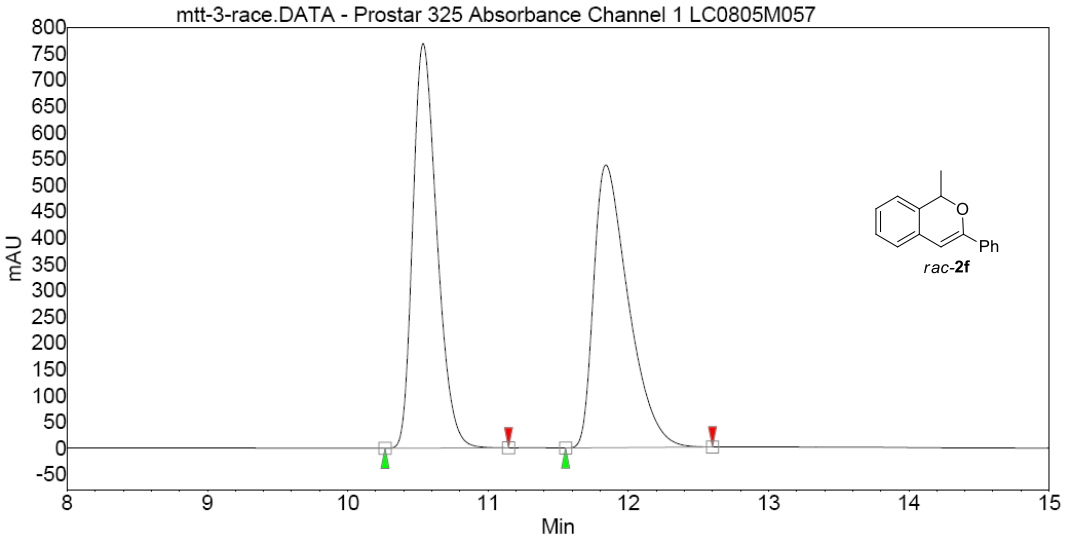
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	9.07	4.20	75.9	13.9	4.199
2	未知	10.39	95.80	1240.5	318.2	95.801
Total			100.00	1316.4	332.1	100.000



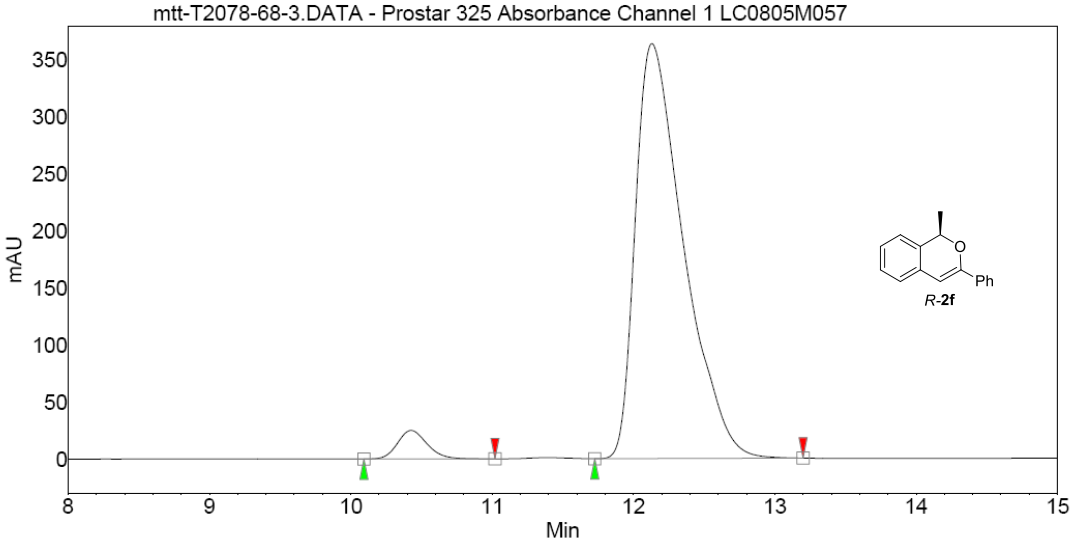
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.46	50.01	704.5	162.1	50.013
2	未知	11.79	49.99	610.0	162.0	49.987
Total			100.00	1314.5	324.1	100.000



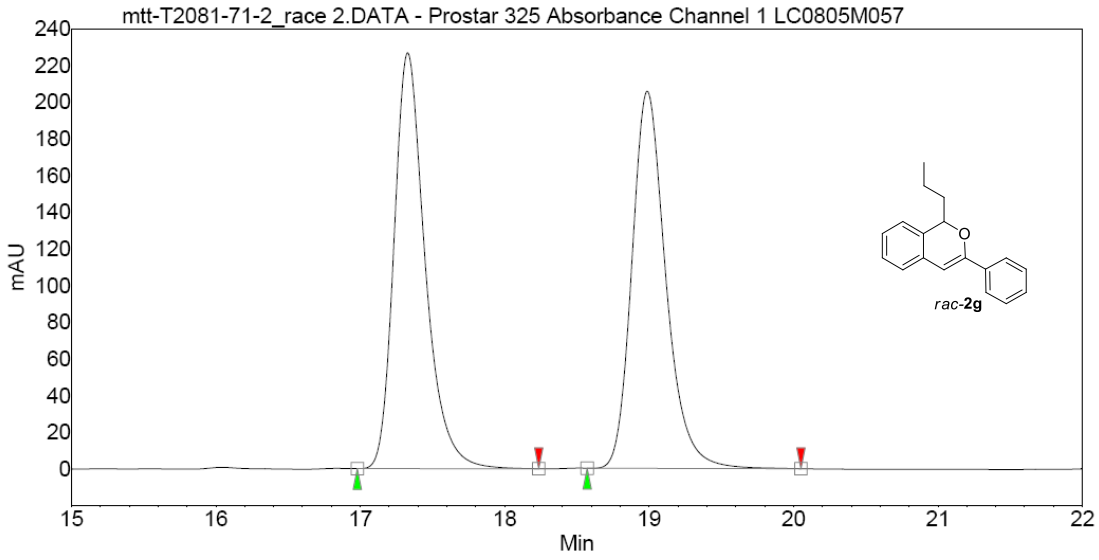
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.41	5.01	78.0	17.3	5.012
2	未知	11.68	94.99	1185.4	327.6	94.988
Total			100.00	1263.4	344.9	100.000



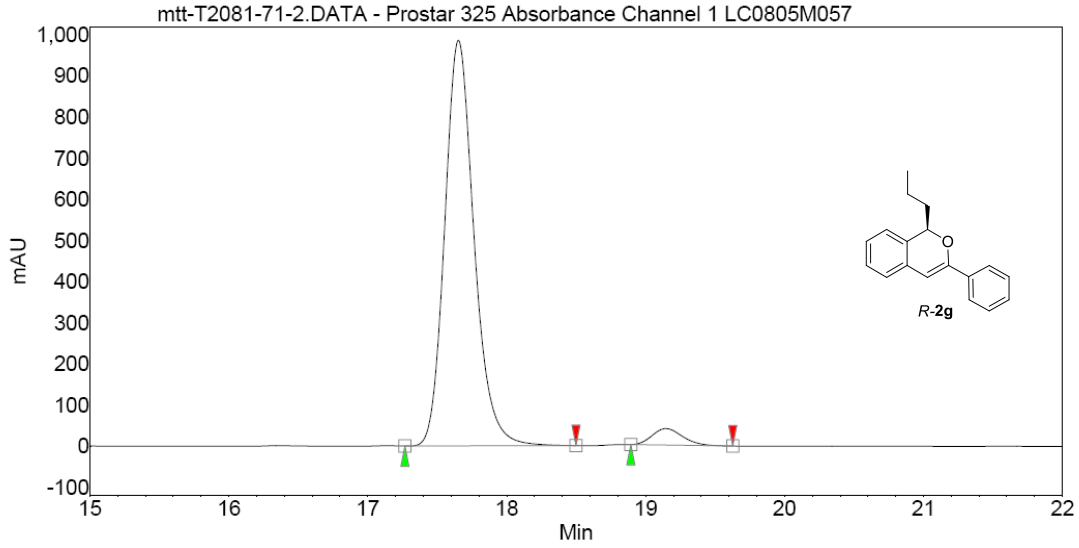
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.54	49.89	768.3	152.9	49.893
2	未知	11.84	50.11	537.4	153.5	50.107
Total			100.00	1305.6	306.4	100.000



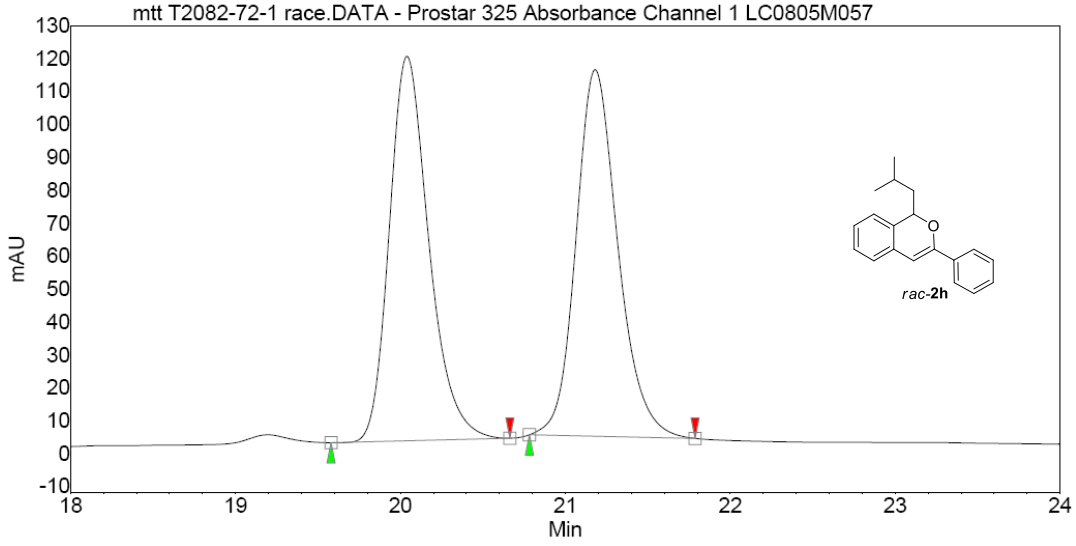
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	10.43	4.04	25.0	6.0	4.042
2	未知	12.13	95.96	363.5	143.3	95.958
Total			100.00	388.5	149.4	100.000



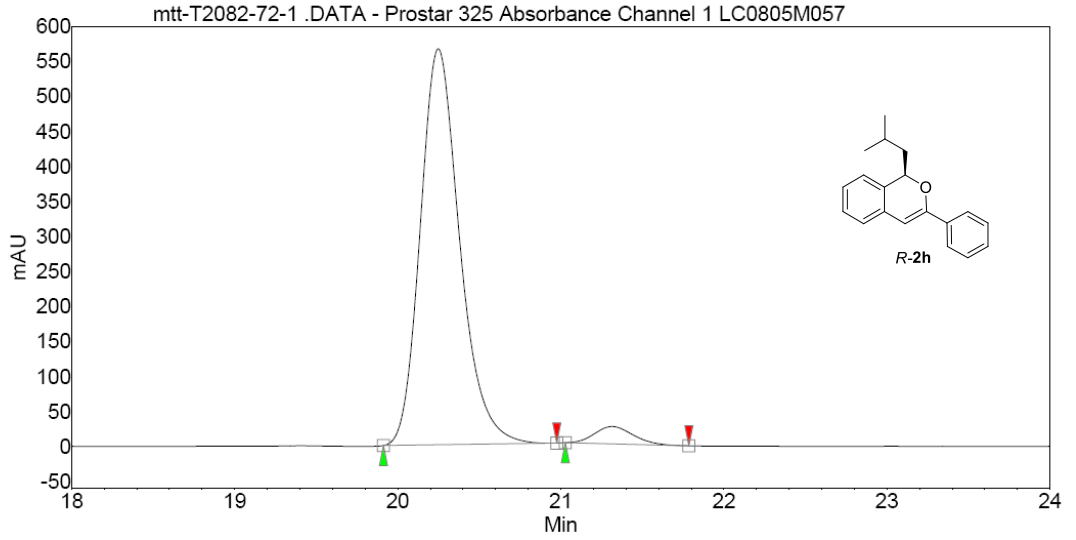
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	17.33	50.24	226.6	56.6	50.243
2	未知	18.99	49.76	205.5	56.0	49.757
Total			100.00	432.1	112.6	100.000



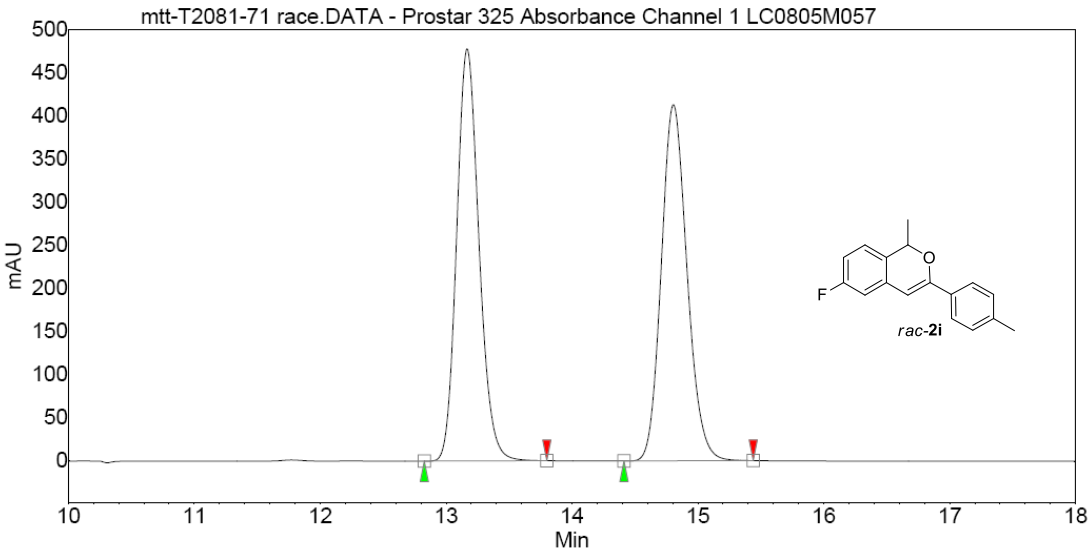
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	17.65	95.97	985.8	241.2	95.970
2	未知	19.15	4.03	40.1	10.1	4.030
Total			100.00	1025.9	251.3	100.000



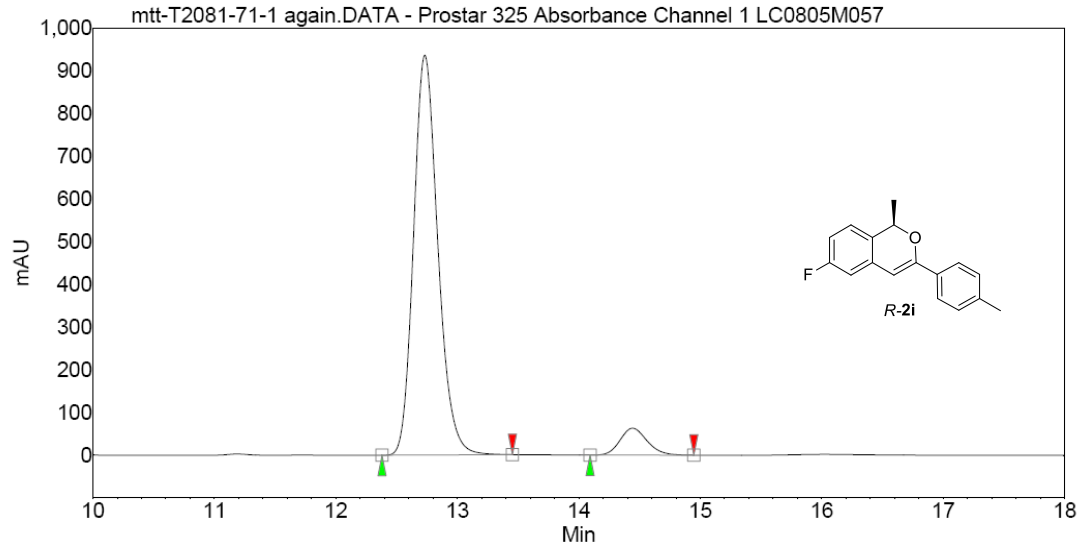
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	20.04	49.76	116.8	32.5	49.757
2	未知	21.18	50.24	111.4	32.8	50.243
Total			100.00	228.2	65.2	100.000



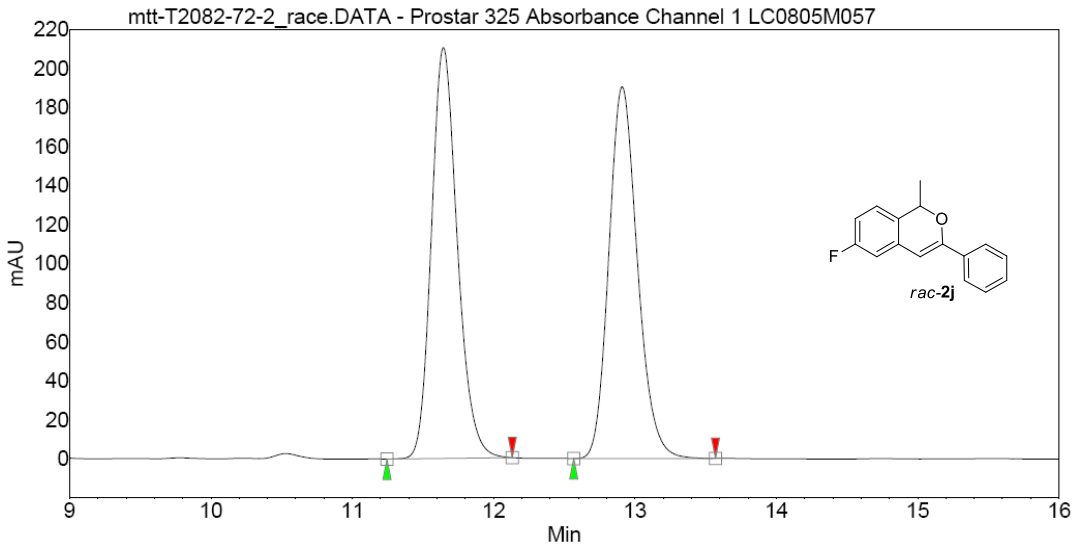
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	20.25	95.88	565.4	158.1	95.880
2	未知	21.31	4.12	24.7	6.8	4.120
Total			100.00	590.1	164.9	100.000



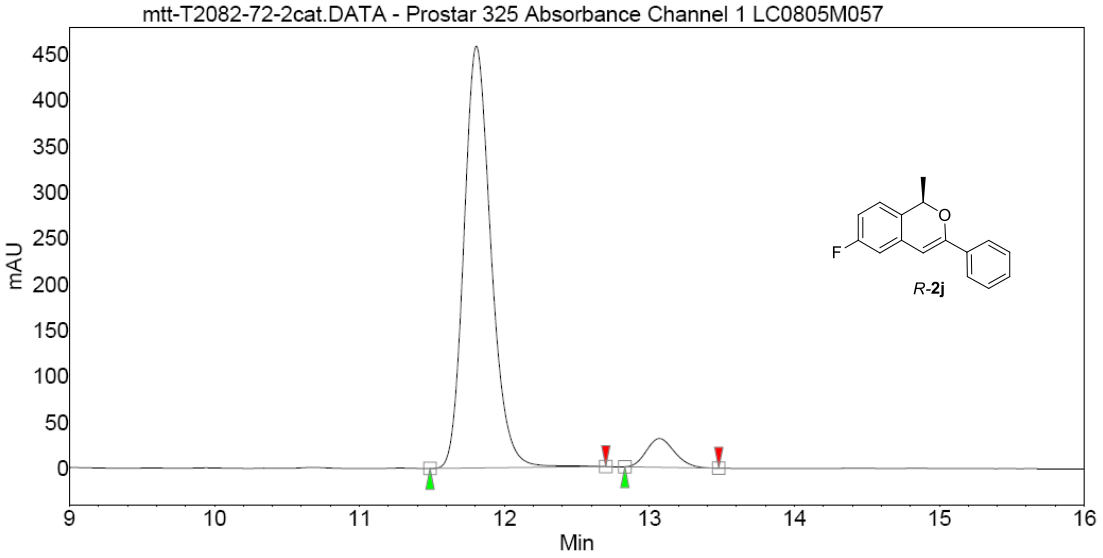
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	13.17	50.05	478.5	98.2	50.050
2	未知	14.81	49.95	413.4	98.0	49.950
Total			100.00	891.9	196.2	100.000



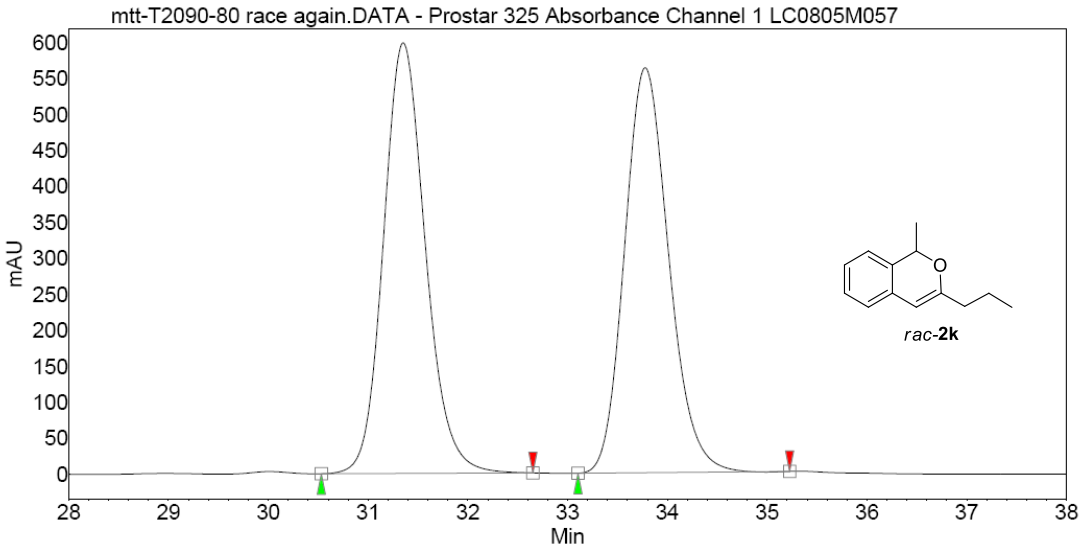
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	12.73	93.04	935.9	216.7	93.043
2	未知	14.44	6.96	63.0	16.2	6.957
Total			100.00	998.9	232.9	100.000



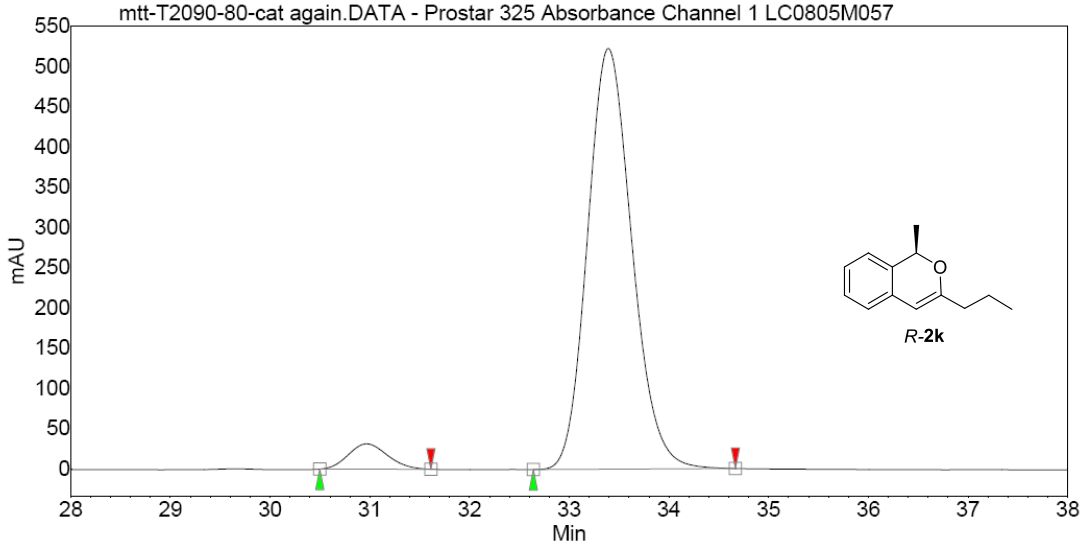
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	11.65	50.06	210.4	44.8	50.059
2	未知	12.91	49.94	190.3	44.7	49.941
Total			100.00	400.7	89.5	100.000



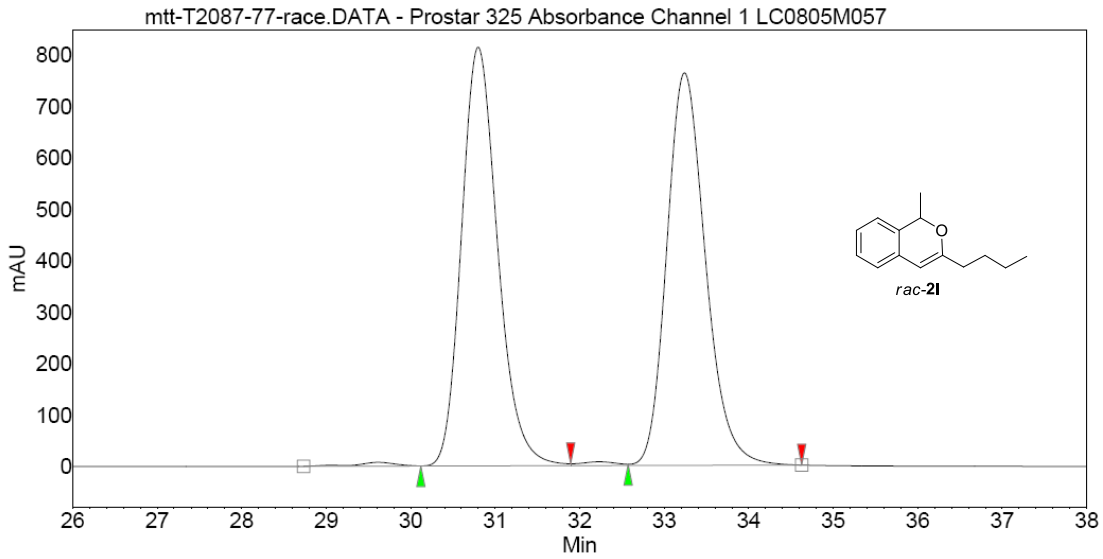
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	11.81	93.32	458.7	99.2	93.319
2	未知	13.07	6.68	31.4	7.1	6.681
Total			100.00	490.1	106.3	100.000



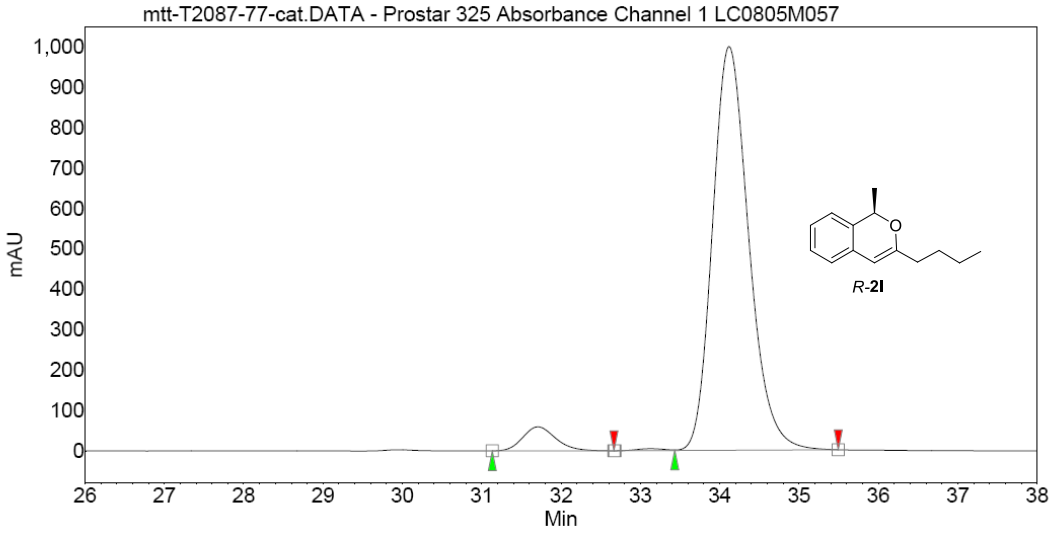
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	31.35	50.24	598.6	291.6	50.242
2	未知	33.78	49.76	562.9	288.8	49.758
Total			100.00	1161.4	580.4	100.000



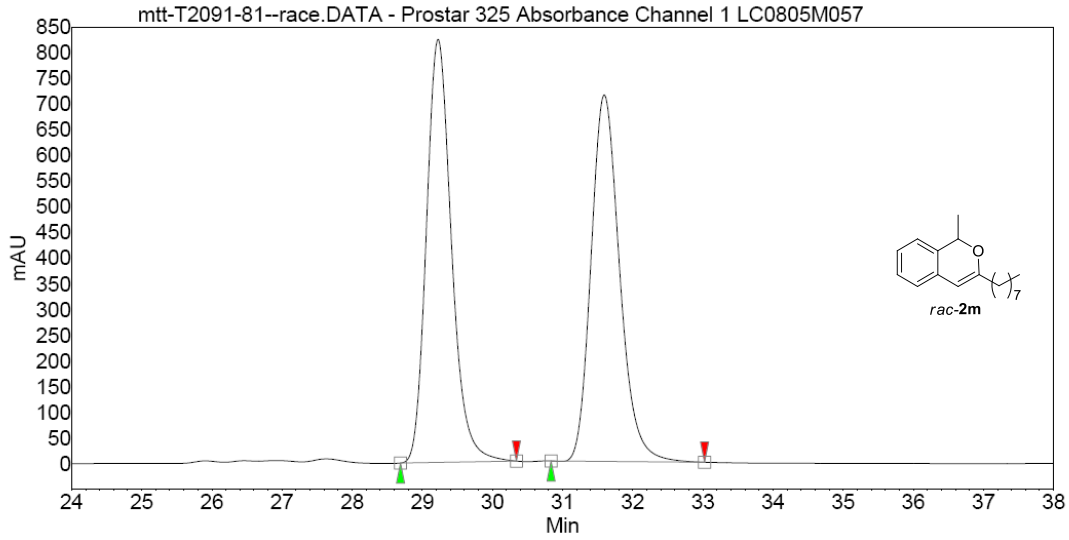
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
2	未知	30.97	5.04	31.4	14.3	5.040
1	未知	33.39	94.96	522.5	269.6	94.960
Total			100.00	553.9	283.9	100.000



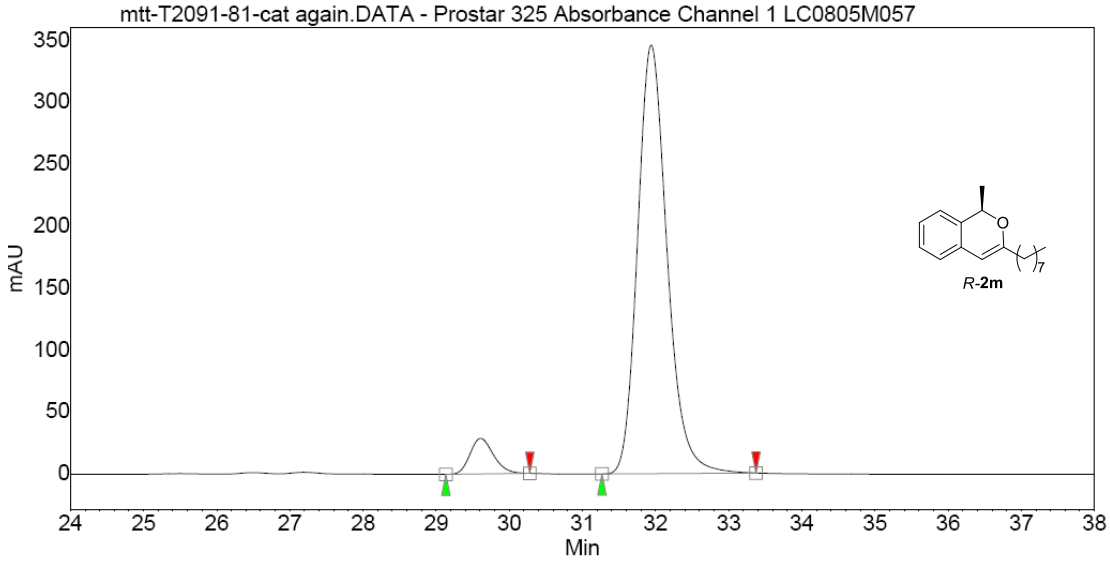
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	30.80	49.93	814.4	403.9	49.928
2	未知	33.24	50.07	763.5	405.1	50.072
Total			100.00	1578.0	809.0	100.000



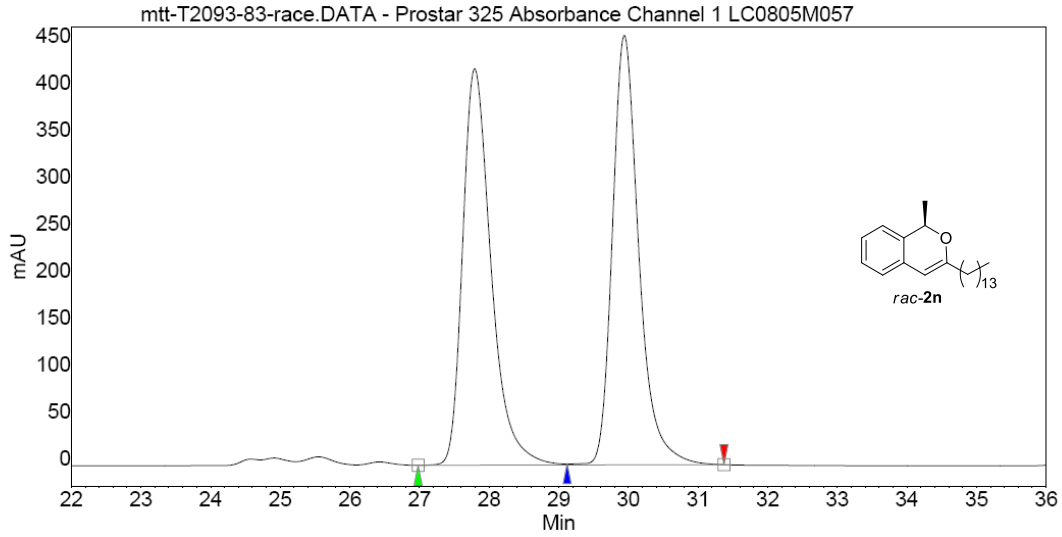
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	31.71	5.11	59.4	28.4	5.108
2	未知	34.12	94.89	998.9	528.2	94.892
Total			100.00	1058.3	556.7	100.000



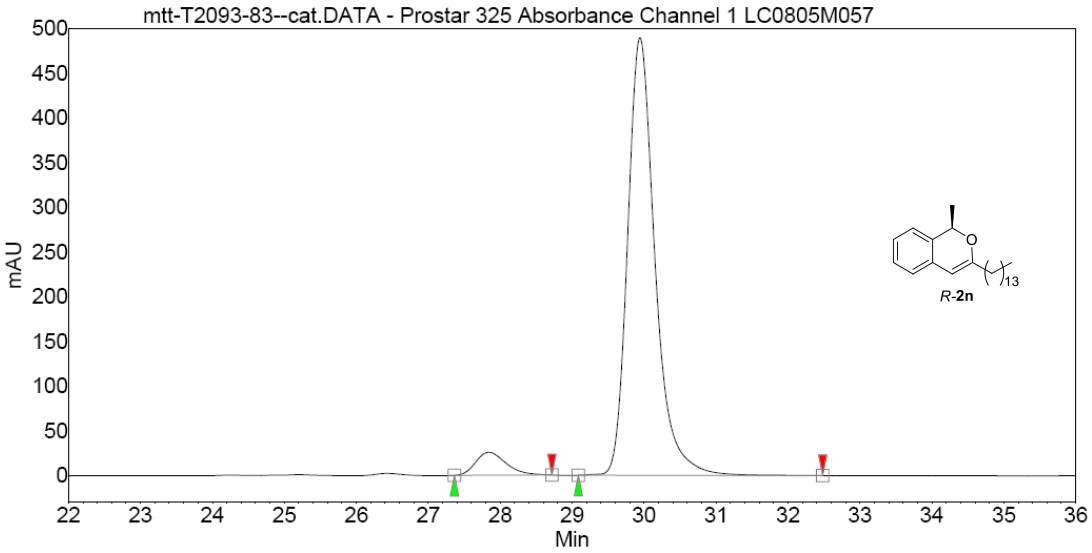
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	29.23	50.30	823.2	341.0	50.302
2	未知	31.59	49.70	713.3	336.9	49.698
Total			100.00	1536.4	677.9	100.000



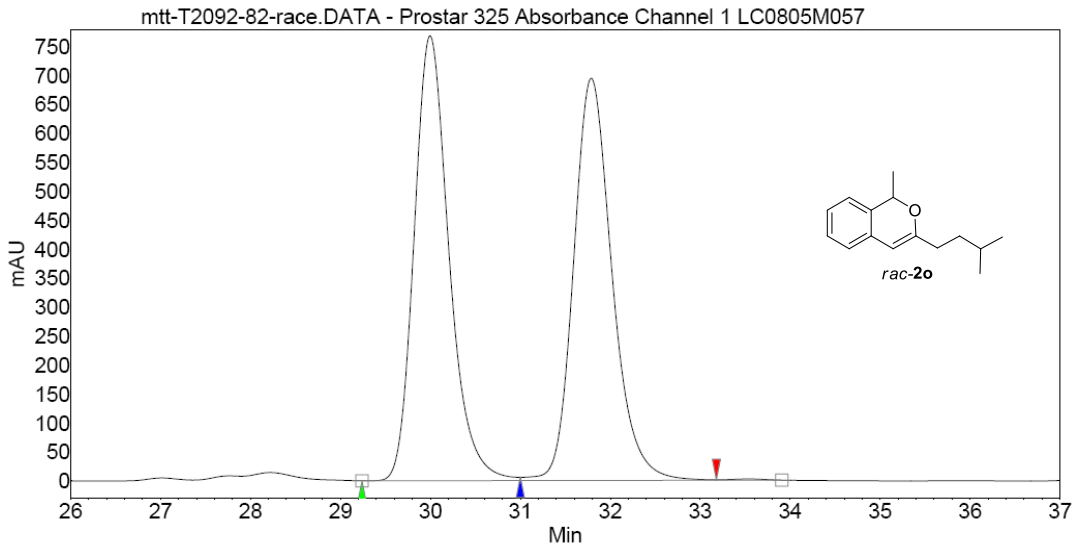
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	29.61	6.21	28.7	10.7	6.211
2	未知	31.94	93.79	346.1	161.6	93.789
Total			100.00	374.8	172.3	100.000



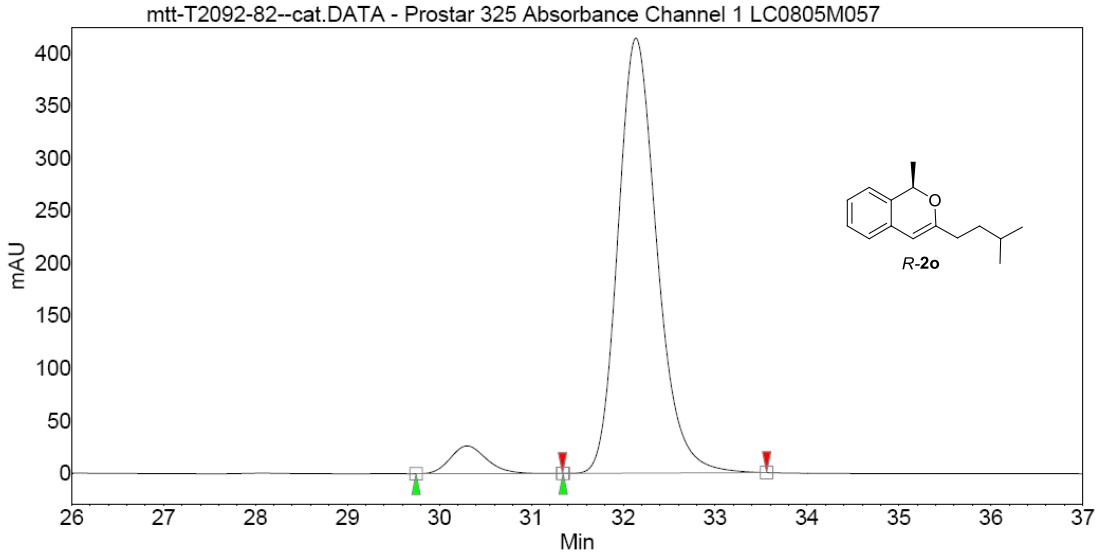
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	27.79	49.83	422.1	199.8	49.833
2	未知	29.94	50.17	457.2	201.1	50.167
Total			100.00	879.3	400.9	100.000



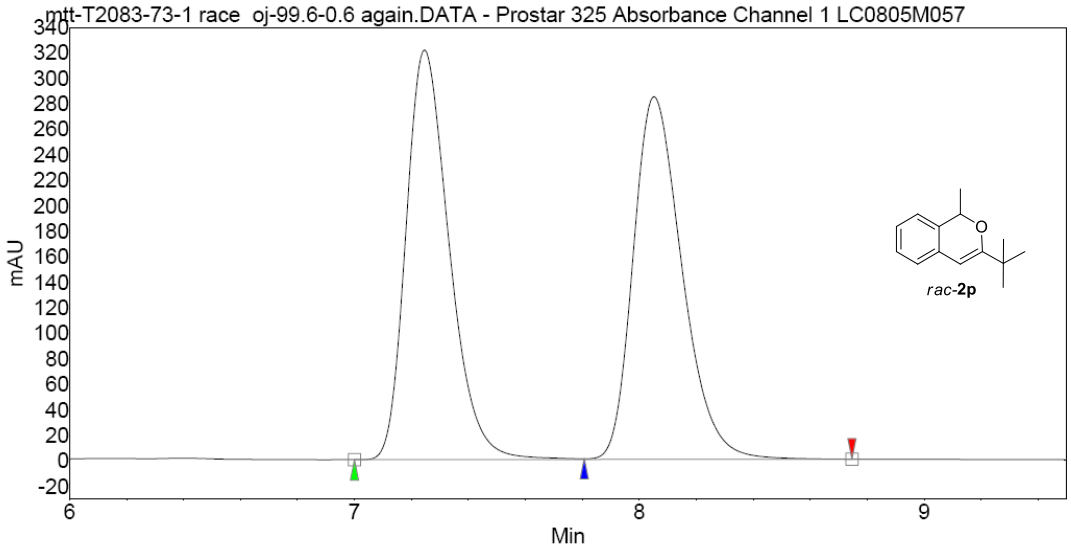
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	27.84	5.52	25.7	12.6	5.516
2	未知	29.94	94.48	489.0	215.6	94.484
Total			100.00	514.7	228.1	100.000



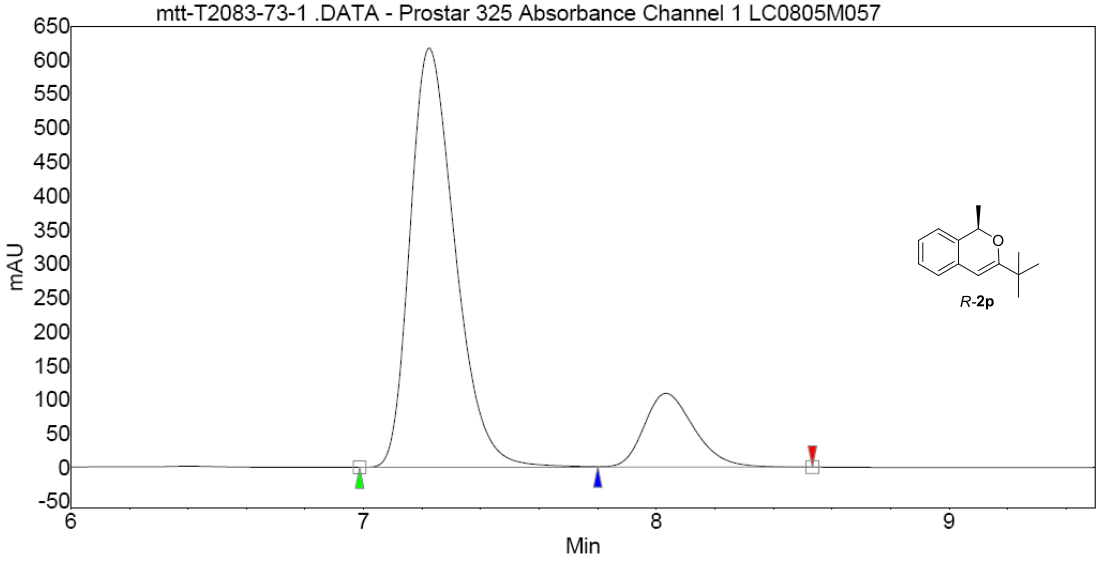
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	29.99	50.10	767.9	345.1	50.101
2	未知	31.79	49.90	694.3	343.7	49.899
Total			100.00	1462.2	688.8	100.000



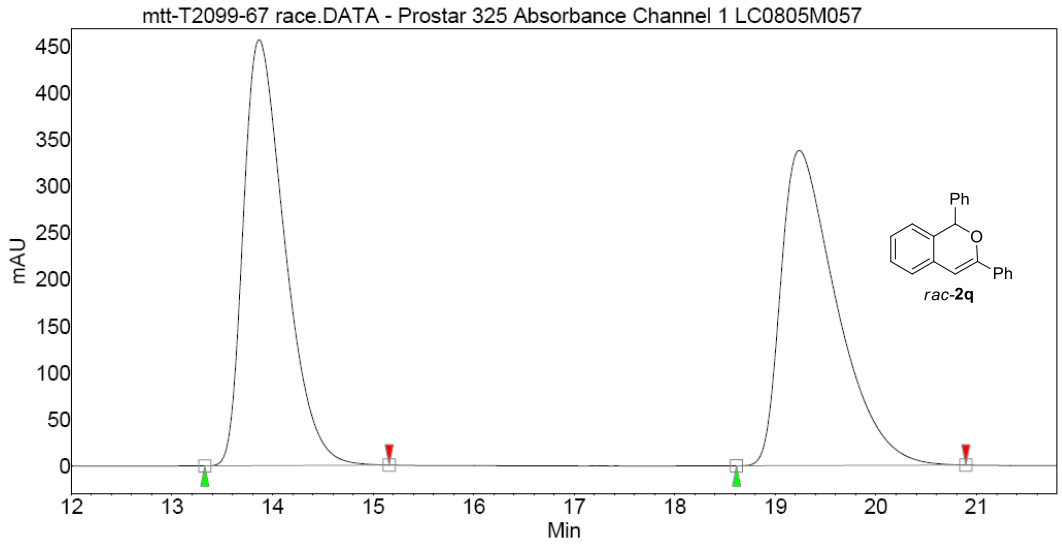
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	30.30	5.60	26.4	12.1	5.602
2	未知	32.14	94.40	414.6	203.9	94.398
Total			100.00	441.0	216.0	100.000



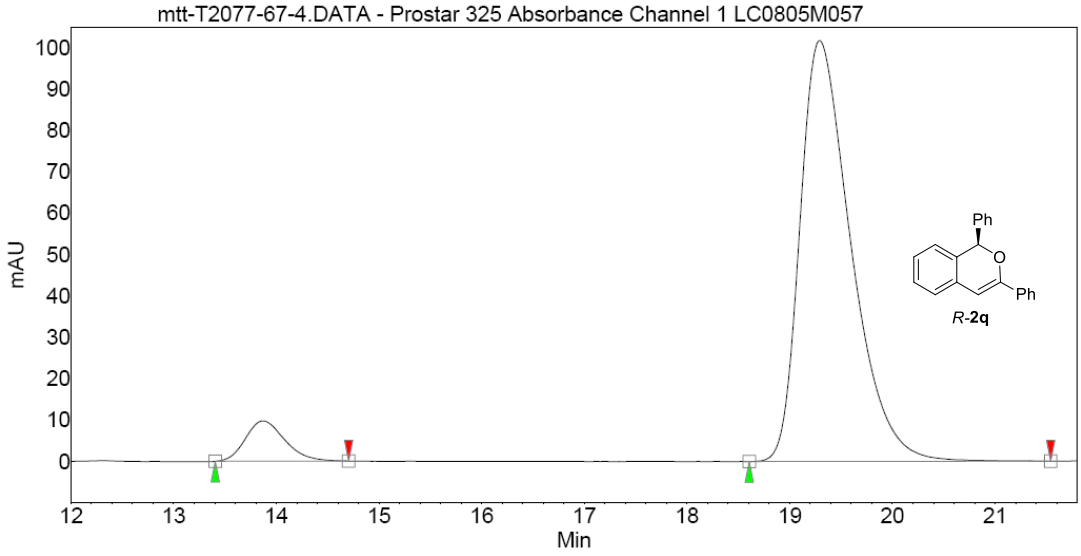
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	7.25	49.92	321.4	56.5	49.924
2	未知	8.05	50.08	284.6	56.7	50.076
Total			100.00	606.0	113.1	100.000



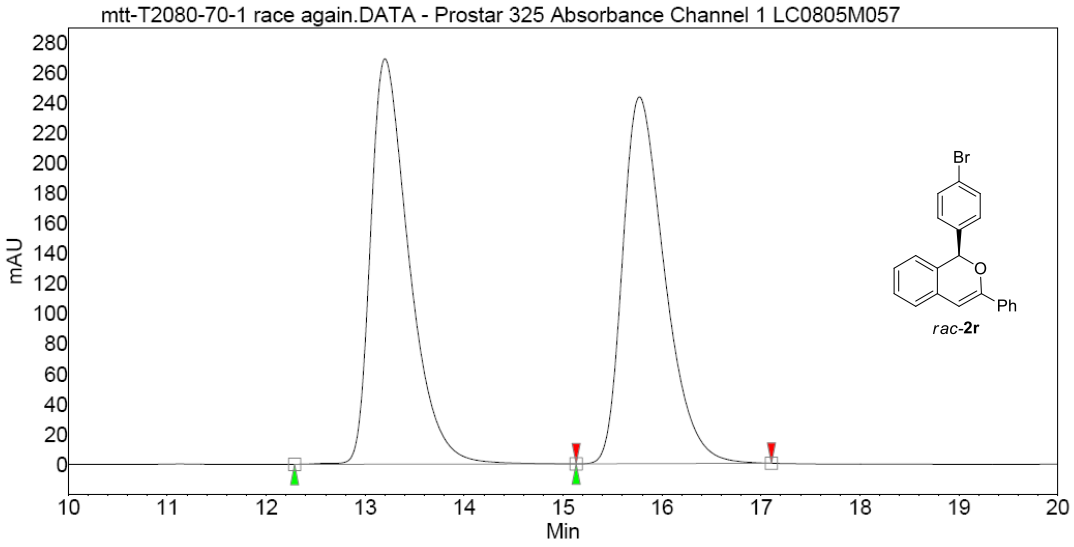
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	7.23	83.67	617.1	110.0	83.667
2	未知	8.03	16.33	108.7	21.5	16.333
Total			100.00	725.9	131.5	100.000



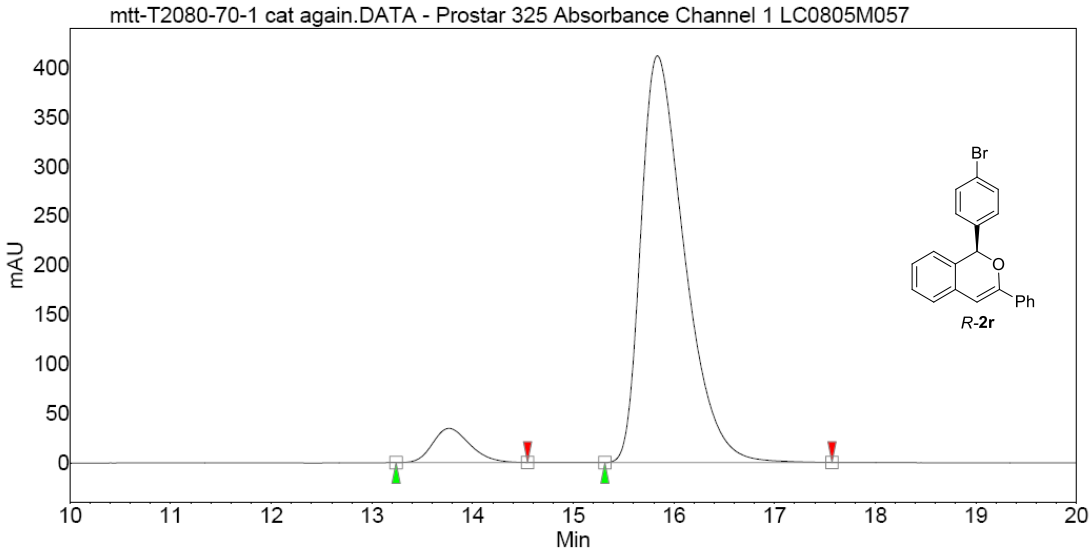
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	13.87	50.09	457.2	217.8	50.087
2	未知	19.24	49.91	338.2	217.1	49.913
Total			100.00	795.4	434.9	100.000



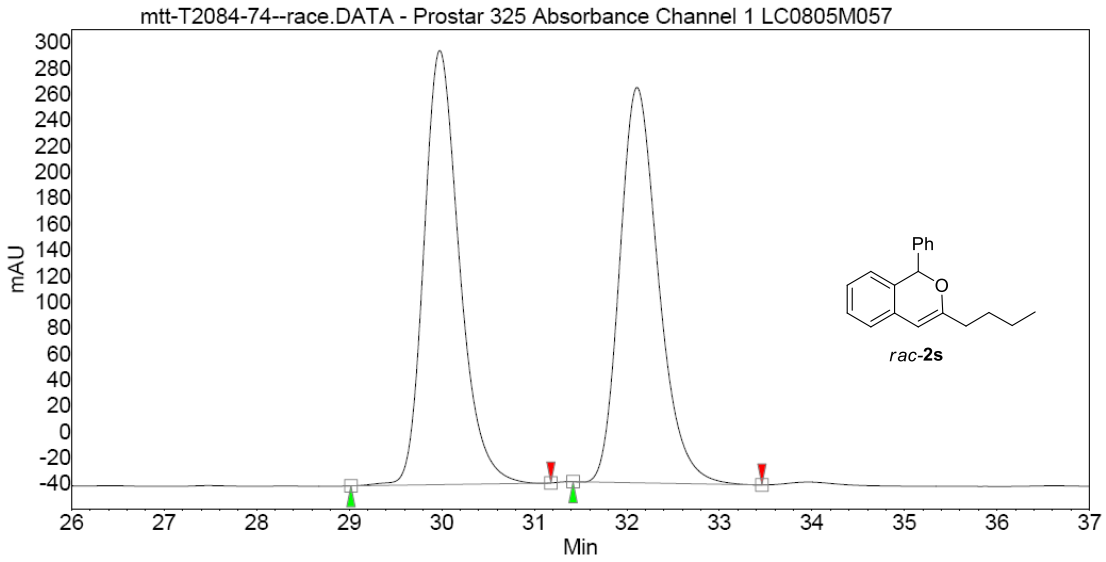
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	13.87	6.89	9.7	4.3	6.891
2	未知	19.29	93.11	101.7	58.4	93.109
Total			100.00	111.4	62.7	100.000



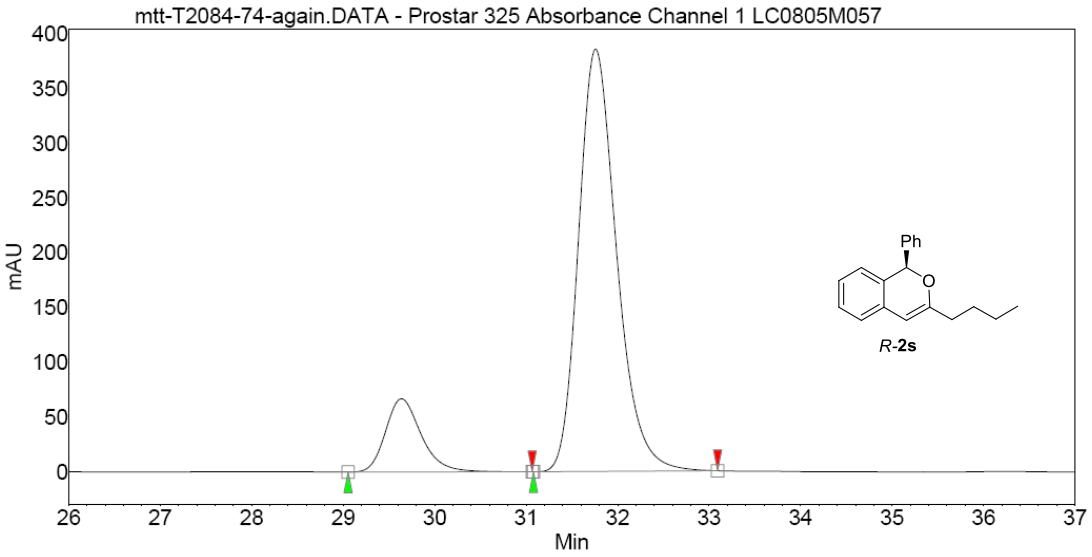
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	13.20	50.26	269.0	121.1	50.261
2	未知	15.77	49.74	243.3	119.8	49.739
Total			100.00	512.3	240.9	100.000



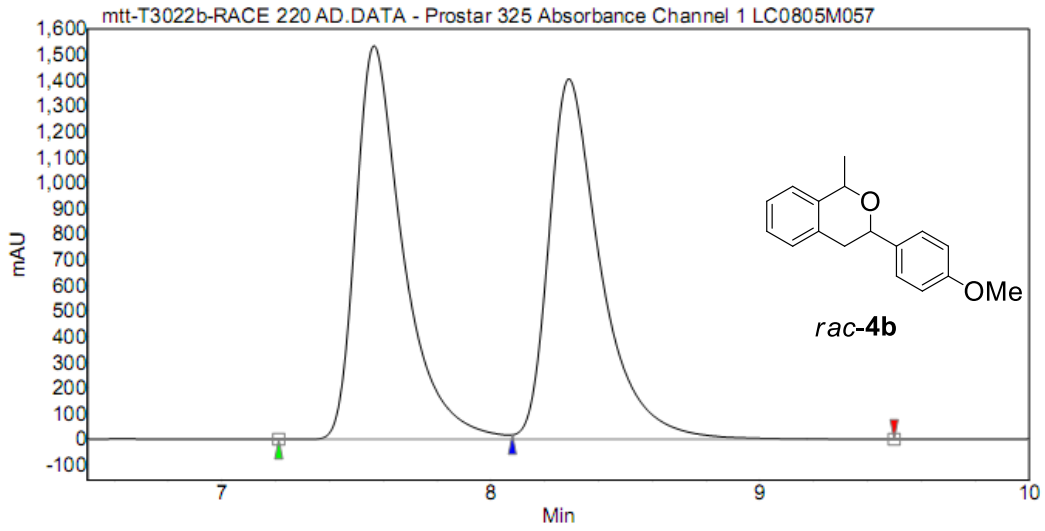
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	13.77	6.68	34.5	14.7	6.678
2	未知	15.83	93.32	411.3	205.8	93.322
Total			100.00	445.8	220.5	100.000



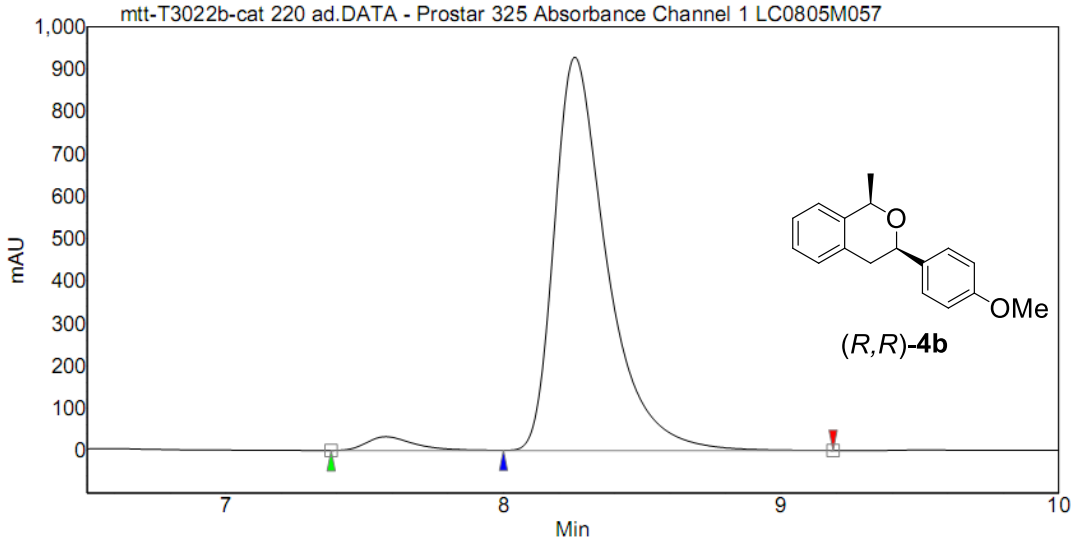
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	29.98	50.19	334.3	148.7	50.191
2	未知	32.11	49.81	304.5	147.6	49.809
Total			100.00	638.8	296.4	100.000



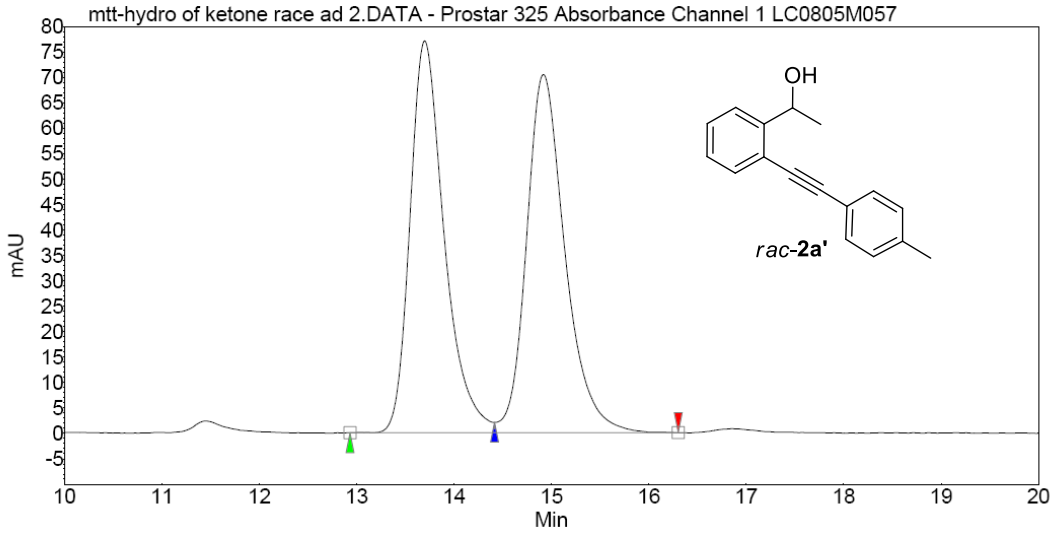
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	29.64	13.97	66.9	30.2	13.972
2	未知	31.76	86.03	385.8	186.1	86.028
Total			100.00	452.7	216.3	100.000



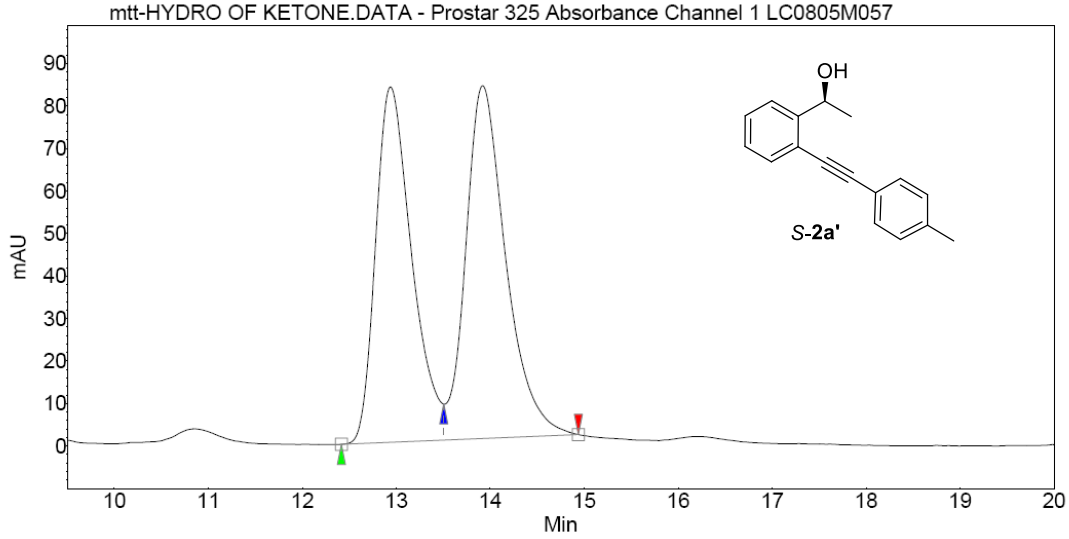
Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	7.57	49.92	1535.1	313.7	49.924
2	未知	8.29	50.08	1404.7	314.7	50.076
Total			100.00	2939.8	628.4	100.000



Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	7.57	3.10	32.5	6.5	3.104
2	未知	8.26	96.90	927.6	203.8	96.896
Total			100.00	960.1	210.3	100.000



Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
1	未知	13.70	49.29	77.0	31.4	49.289
2	未知	14.92	50.71	70.4	32.3	50.711
Total			100.00	147.5	63.7	100.000



Index	文件名	时间 [Min]	数量 [% 面积]	高度 [mAU]	Area [mAU.Min]	Area % [%]
2	未知	12.94	47.49	83.6	37.1	47.493
1	未知	13.92	52.51	83.0	41.1	52.507
Total			100.00	166.6	78.2	100.000