Supporting Information

Copper-Catalyzed Intramolecular Annulation of Conjugated Enynones to Substituted 1*H*-Indenes and Mechanistic Studies

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CONTENTS

1. DFT Calculations

Computational Details and Discussion

All of the calculations were performed with the Gaussian 09 program.[1] Geometry optimizations of all the minima and transition states involved were carried out at the B3LYP level of theory[2] in the gas phase. The SDD basis set[3] and pseudopotential were used for Cu and the 6-31G(d) basis set[4] for the other atoms. The key word "5D" was used to specify that five d-type orbitals were used for all elements in the calculations. For open-shell species, (U)B3LYP method was used. Frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and the thermal corrections at 298 K. Key transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.[5] Solvation energies in dichloroethane (ε = 10.125) were evaluated by IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model[6] using the gas-phase optimized structures. Standard state concentrations of 1.0 mol/L were used for all species in calculations. To improve the calculation accuracy, single-point energies calculations were computed at the B3LYP level of theory with the SDD basis set and pseudopotential for Cu and the 6-311+G(d,p) basis set[7] for the other atoms. The given Gibbs free energies in dichloroethane were calculated according to the formula: G_{sol} = TCG + ΔG_{sol} + SPE + 1.89 kcal/mol. The CYL View software was employed to show the 3D structures of the studied species.[8]

A competitive pathway of carbene formation has also been considered in this study (Figure S1). From copper complex **INT1**, the *5-exo-dig* nucleophilic attack in a *cis*-addition fashion occurs *via* transition state **TS1-10**, affording the Cu carbene intermediate **INT10**.[9] However, the corresponding activation free energy of **TS1-10** is 18.2 kcal/mol, which is higher than that of *trans*-addition by 8.1 kcal/mol. So this carbene formation *via* **TS1-10** can be ruled out because of its relatively high energy barrier.

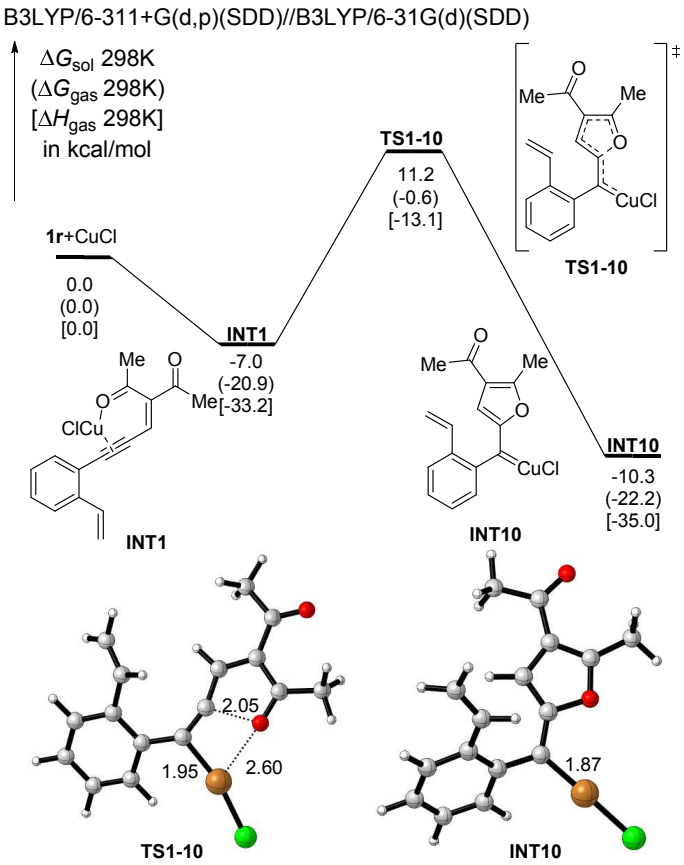

Figure S1. Potential energy surface and 3D structures of key species of competitive pathway of carbene formation. The bond lengths in the structures at the bottom are given in Å.

The metal-free 1,5-hydrogen shift was also calculated (Figure S2). This alternative pathway for indene formation starts from **INT11** involving an intermolecular ligand exchange of **INT4**, which found to be less favorable than the intramolecular pathway. Calculations indicate the metal-free hydrogen shift occurs *via* **TS11-2r** with a similar energy barrier of 17.2 kcal/mol and the activation free energy difference of the two 1,5-hydrogen shift transition states is 2.6 kcal/mol.

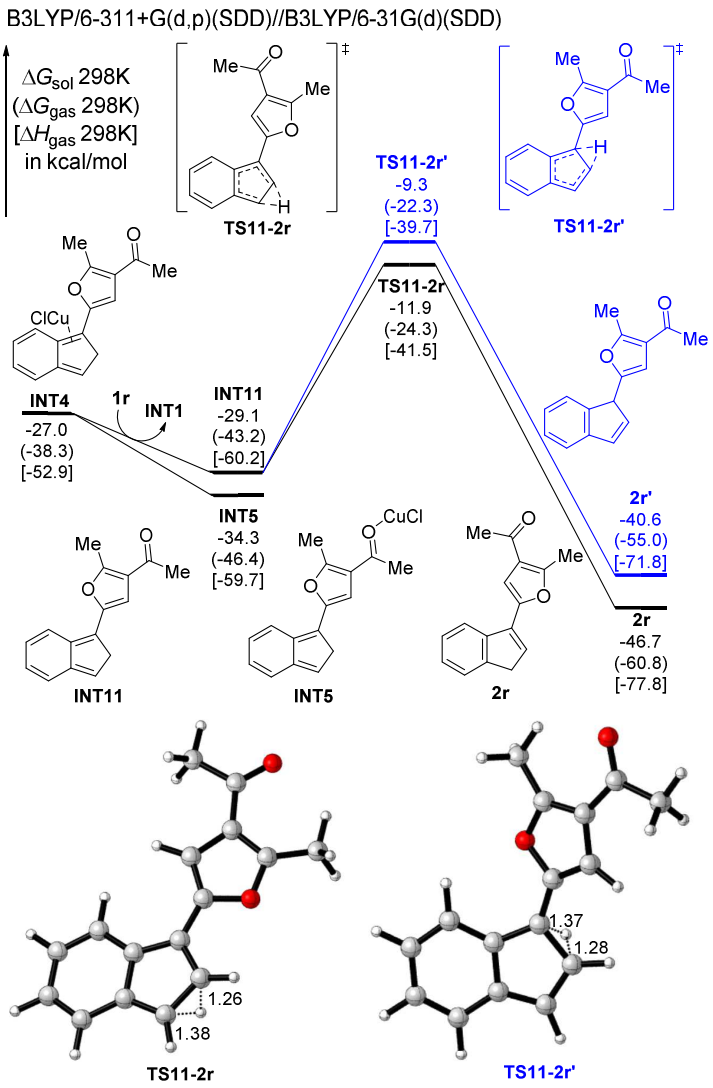

Figure S2. Free energy profiles for metal-free 1,5-H shift. The bond lengths in the structures at the bottom are given in Å.

DFT calculated free energy surface of $CuCl_2$ catalyzed cascade annulation of **1r** is shown in Figure S3. This similar cascade process catalyzed by $CuCl_2$ involves carbene formation, nucleophilic attack of alkene and 1,5-hydrogen shift. Calculations indicate that **TS16-2r** is favored over **TS16-2r'** by 3.1 kcal/mol, therefore **2r** should be generated predominantly, which agrees with experimental observations.

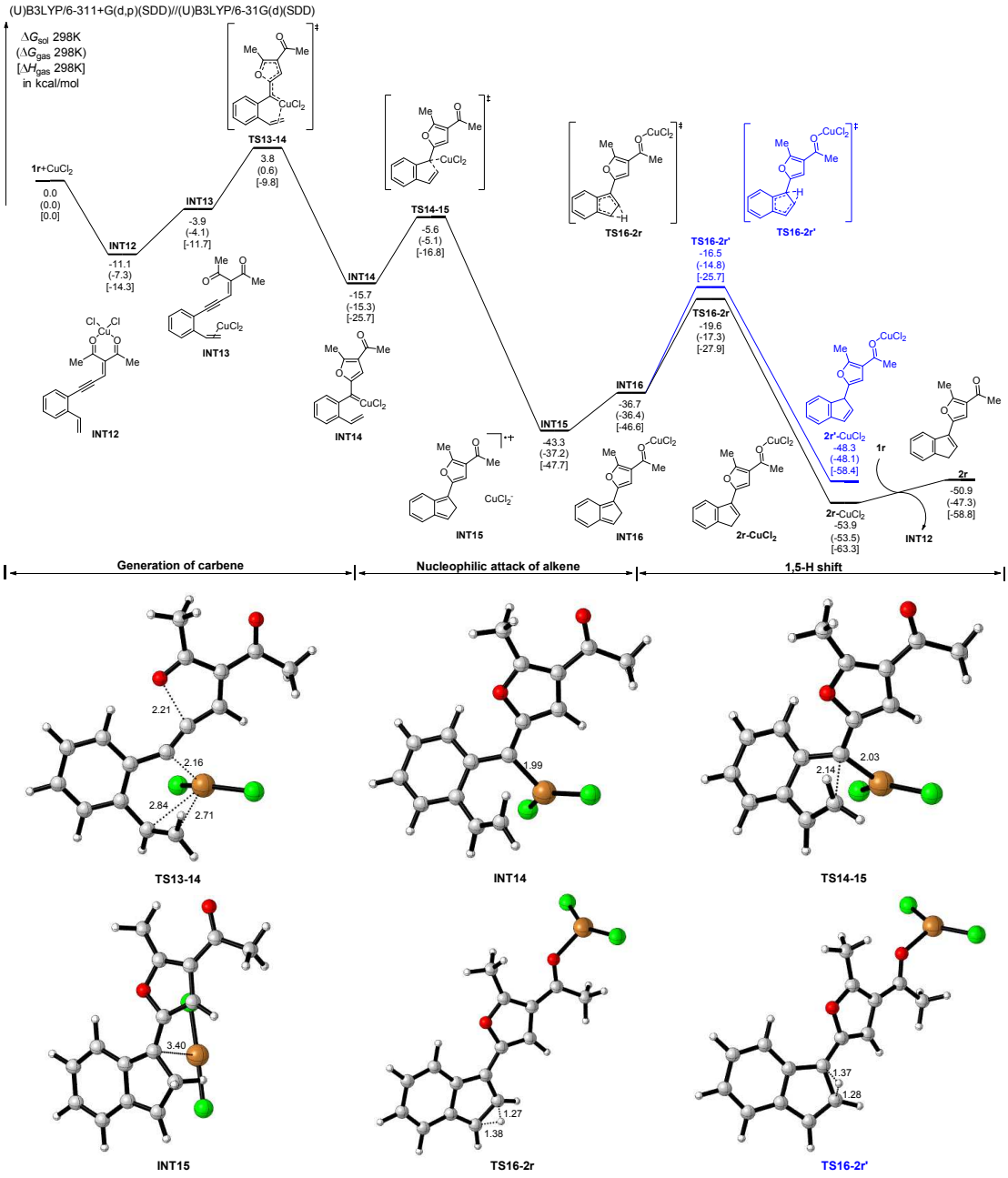

Figure S3. Potential energy surface and 3D structures of key species of $CuCl_2$ catalyzed cascade annulation of **1r**. The bond lengths in the structures at the bottom are given in Å.

In the present case, spin density plots of the key intermediates **INT14** and **INT15** are presented in Figure S4. For intermediate **INT14**, the highest spin polpulation is found on the copper atom, in agreement with a Cu(II)-stabilized carbenoid species rather than a radical electronic structure like Co(II)-catalyzed system.[10] However, in intermediate **INT15**, most spin population is found delocalizing over the whole isoindene moiety and less than 10% spin population at $CuCl_2$, thus confirming the

formation of a charge-transfer complex.

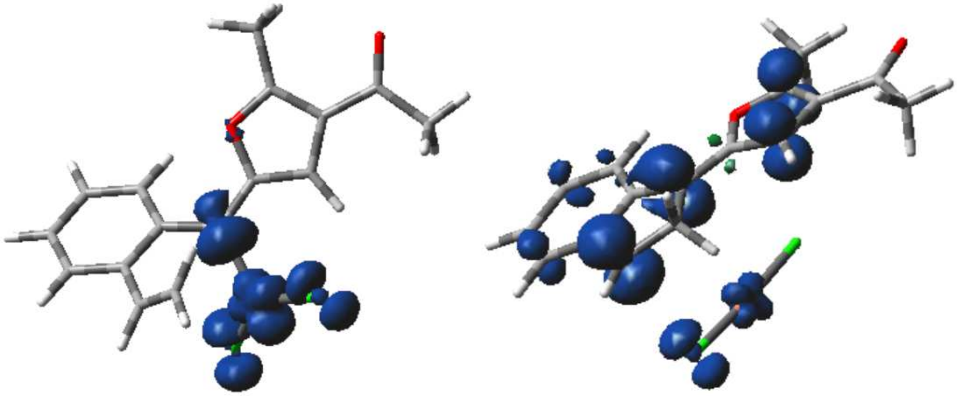

Figure S4. Spin density plots of the DFT optimized Cu(II)-carbene species **INT14** (left) and cyclized charge-transfer complex **INT15** (right).

We also checked the calculation results with other DFT functional (Figure S5). Single point energy calculations using B3LYP-D3[11] with the above mentioned lager basis set in gas phase showed the similar energy surfaces, and the same conclusions were found. This suggested that dispersion effects would not be critical in affecting the calculation results.

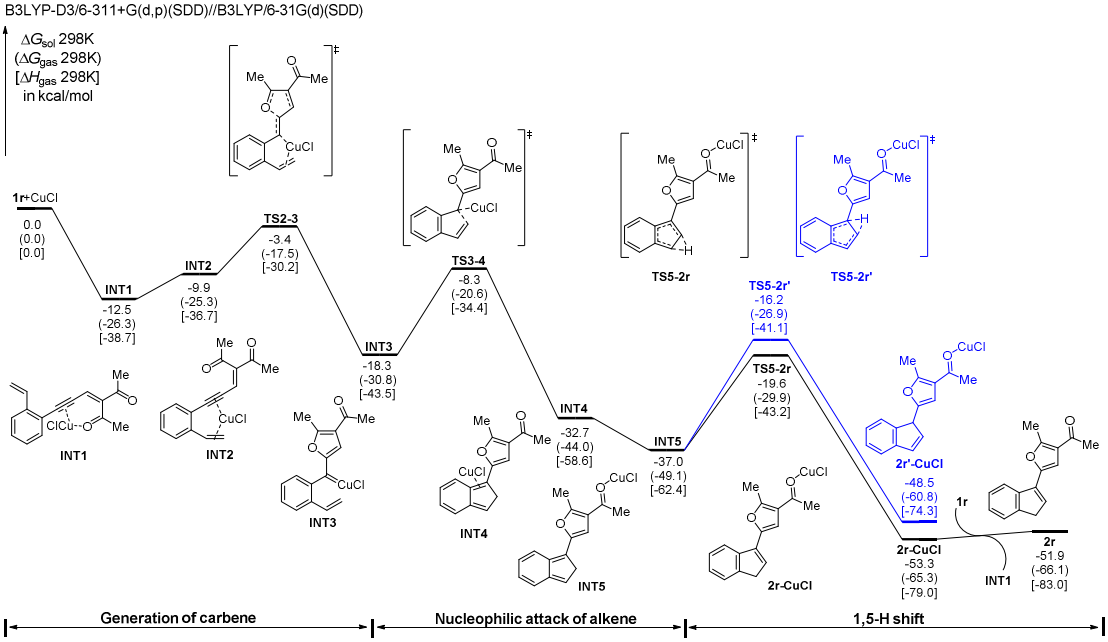

Figure S5. Potential energy surface of CuCl catalyzed cascade annulation of **1r** at B3LYP-D3/6-311+G(d,p)(SDD)//B3LYP/6-31G(d)(SDD).

IRC Calculations for TS3-4:

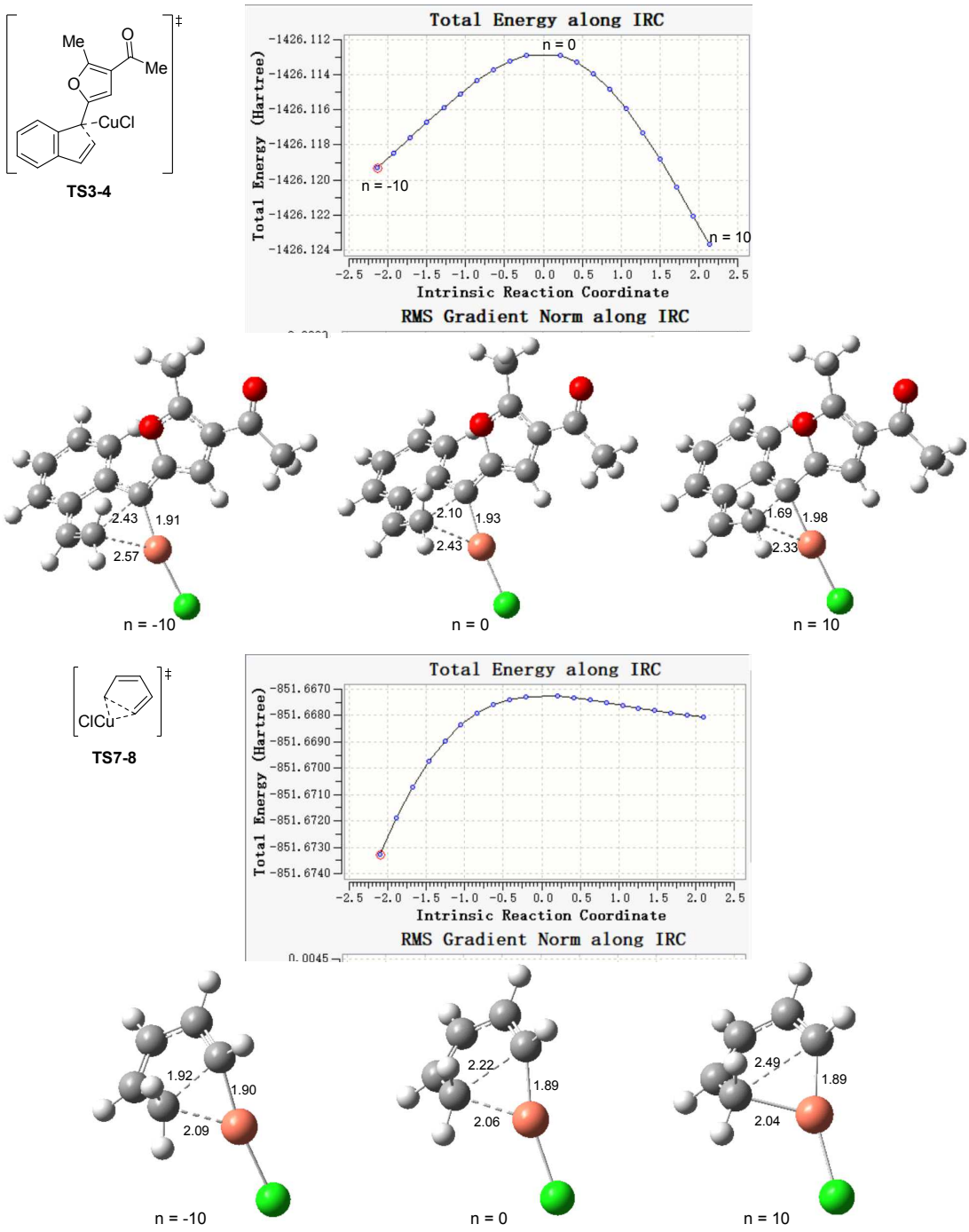

Figure S6. IRC calculations of transition states of **TS3-4** and **TS7-8**. The bond lengths in the structures at the bottom are given in Å.

Computed Energies of All Stationary Points

Table S1. Thermal correction to Gibbs free energies (***TCG***, in Hartree), sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), solvation Gibbs free energies in dichloroethane (ΔG_{sol}, in Hartree), and single point energies computed at the B3LYP/6-311+G(d,p)(SDD)//B3LYP/6-31G(d)(SDD) level (***SPE***, in Hartree).

Name	*TCG*/a.u.	*H*/a.u.	*G*/a.u.	ΔG_{sol}/a.u.	*SPE*/a.u.
CuCl	-0.022408	-657.573792	-657.600727	-0.041698	-657.612026
1r	0.203581	-768.204714	-768.272701	-0.020286	-768.699126
INT1	0.202070	-1425.839805	-1425.914968	-0.036831	-1426.365276
INT2	0.200153	-1425.832554	-1425.909322	-0.034469	-1426.359476
TS2-3	0.200868	-1425.825475	-1425.900065	-0.036452	-1426.348350
INT3	0.203358	-1425.851126	-1425.925823	-0.039128	-1426.372974
TS3-4	0.203488	-1425.836342	-1425.909297	-0.039399	-1426.356981
INT4	0.207067	-1425.876552	-1425.948261	-0.040961	-1426.398129
INT5	0.205333	-1425.889514	-1425.963230	-0.039619	-1426.409288
TS5-2r	0.201803	-1425.858002	-1425.931721	-0.042549	-1426.375867
2r-CuCl	0.206659	-1425.916659	-1425.989861	-0.039713	-1426.436775
2r	0.212996	-768.285245	-768.345957	-0.019883	-768.772258
TS5-2r'	0.203115	-1425.853460	-1425.925766	-0.041865	-1426.372402
2r'-CuCl	0.206592	-1425.906688	-1425.980117	-0.039348	-1426.428994
2r'	0.212687	-768.273885	-768.334893	-0.019546	-768.762620
INT6	0.057716	-851.558131	-851.603545		
TS6-7	0.056655	-851.542543	-851.587109		
INT7	0.059747	-851.566070	-851.608712		
TS7-8	0.059738	-851.565930	-851.607508		
INT8	0.061742	-851.626639	-851.669094		
TS3-9	0.204733	-1425.802578	-1425.874564	-0.042917	-1426.322100
INT9	0.205142	-1425.811798	-1425.884860	-0.042528	-1426.331735
TS1-10	0.200255	-1425.808757	-1425.883892	-0.040124	-1426.331261
INT10	0.203614	-1425.846546	-1425.921132	-0.039918	-1426.368993
INT11	0.212044	-768.256983	-768.317711	-0.019959	-768.743263
TS11-2r	0.208898	-768.225164	-768.285546	-0.022664	-768.709995

TS11-2r'	0.209166	-768.221654	-768.281639	-0.021740	-768.707033
$CuCl_2$	-0.020764	-1117.794043	-1117.822018	-0.022455	-1117.867182
INT12	0.195784	-1886.028891	-1886.113765	-0.045778	-1886.590968
INT13	0.197034	-1886.021687	-1886.105476	-0.039473	-1886.587075
TS13-14	0.199462	-1886.021544	-1886.100981	-0.034492	-1886.582069
INT14	0.201828	-1886.050656	-1886.130088	-0.040371	-1886.609745
TS14-15	0.202496	-1886.036305	-1886.113678	-0.040511	-1886.594124
INT15	0.202994	-1886.086937	-1886.166283	-0.049384	-1886.645846
INT16	0.202528	-1886.087815	-1886.167514	-0.040169	-1886.644032
TS16-2r	0.199566	-1886.056330	-1886.135499	-0.043343	-1886.610675
2r-$CuCl_2$	0.202720	-1886.114798	-1886.195147	-0.040355	-1886.671439
TS16-2r'	0.200126	-1886.051671	-1886.130186	-0.042523	-1886.607134
2r'-$CuCl_2$	0.203578	-1886.105008	-1886.184644	-0.039990	-1886.663790

Coordinates of All Stationary Points

CuCl

Cu	0.00000000	0.00000000	0.77060400
Cl	0.00000000	0.00000000	-1.31456000

1r

C	4.47795200	-1.89022800	0.05753200
C	5.11059400	-0.64052700	0.04152700
C	4.35973100	0.52958300	0.00803200
C	2.95491700	0.50758700	-0.01295200
C	2.31680200	-0.76945300	0.00817300
C	3.09243300	-1.95001900	0.04142500
C	0.90435000	-0.88368600	-0.00348400
C	-0.31761900	-0.91931800	-0.01078200
C	-1.69637300	-1.15338800	-0.02525400
C	-2.73260900	-0.25337700	-0.00524600
C	-2.43345400	1.22134100	0.05454300
C	-4.13169900	-0.77341000	-0.05132800
O	-5.09625100	-0.02121000	-0.11479700
C	-4.37940700	-2.28110200	-0.02792100
C	-3.54115900	2.24162600	0.21830500
O	-1.27085400	1.60123200	-0.01412000
C	2.14056900	1.73132700	-0.05407000
C	2.60153000	2.98724400	-0.14256400
H	5.06463700	-2.80375800	0.08422400
H	6.19558000	-0.58109400	0.05691200
H	4.87478100	1.48496900	0.00130500
H	2.58030000	-2.90713100	0.05527900
H	-1.95481600	-2.20980100	-0.05544500
H	-5.45951900	-2.43654100	-0.02896900
H	-3.95090700	-2.77546800	-0.90782900
H	-3.94937100	-2.75310500	0.86297300
H	-3.07362700	3.22292000	0.32729400

H	-4.21180600	2.23341900	-0.64555000
H	-4.16874900	2.01782600	1.08609600
H	1.06484900	1.58059900	-0.01568600
H	1.90860900	3.82266700	-0.16621100
H	3.65752900	3.23912600	-0.19867300

INT1

C	4.57343800	-0.78988200	0.17058400
C	5.15938400	0.47672400	0.08001900
C	4.36679200	1.61313300	-0.07667000
C	2.96945400	1.52696000	-0.12982500
C	2.37857900	0.22883400	-0.03195600
C	3.19162200	-0.91633100	0.11031800
C	0.95775400	0.09262900	-0.03622100
C	2.14109800	2.72968500	-0.31346800
C	-0.26890400	0.40577300	-0.03791400
C	-1.44903200	1.16242100	0.00181700
C	-2.75837500	0.73603200	0.01329600
C	-3.83498800	1.77702200	0.11402600
O	-5.00658300	1.47226000	0.28327200
C	-3.10705000	-0.71063300	-0.05767700
O	-2.23196900	-1.59361900	-0.04203800
C	-4.53460800	-1.18212000	-0.17495000
C	-3.46343200	3.25413400	0.01549900
C	2.45477700	3.96182600	0.10803400
H	5.19193500	-1.67541500	0.27957900
H	6.24056900	0.57984800	0.11461800
H	4.83746600	2.58500600	-0.18885900
H	2.71217700	-1.88961500	0.17372800
H	1.20095900	2.58332800	-0.84190900
H	-1.27601100	2.23612800	0.03667000
H	-5.09400000	-0.94315800	0.73402400
H	-5.05909300	-0.67578200	-0.99008800
H	-4.51671200	-2.26139500	-0.33753100
H	-2.84609300	3.57208100	0.86431600
H	-4.39245300	3.82613200	0.02899000
H	-2.91334900	3.48084700	-0.90488400
H	3.35899300	4.17035300	0.67370900
Cu	-0.18634900	-1.55522100	-0.01725800
Cl	0.67103700	-3.55997200	0.02876300
H	1.80146700	4.80621000	-0.09020700

INT2

C	3.16382100	-3.24555700	0.22690500
C	4.36857600	-2.54626600	0.09526000
C	4.36891700	-1.16604900	-0.12431100
C	3.16239900	-0.46710400	-0.20342600
C	1.94898000	-1.17668500	-0.06481000
C	1.95121300	-2.56849100	0.14773700
C	0.71849800	-0.44800700	-0.12284400
C	-0.49663800	-0.21106900	-0.11828900
C	-1.82871300	0.23205200	-0.10326800
C	-2.94785600	-0.55045700	-0.04241800
C	-2.77987700	-2.04767700	0.00601000
C	-4.29205200	0.11202300	-0.01789000
O	-5.31854800	-0.54916400	0.06519400
C	-4.37490200	1.62980800	-0.09744800
C	-3.97168900	-2.97679900	0.02874000

O	-1.64412000	-2.51120400	0.02207600
C	3.11735700	0.99691100	-0.50604500
C	3.18426900	2.00766300	0.41617900
H	3.17302100	-4.31879500	0.39272700
H	5.31358200	-3.07798800	0.16199700
H	5.30838000	-0.63180000	-0.23429000
H	1.00138200	-3.08404300	0.24857900
H	-1.91864200	1.31811300	-0.12663600
H	-5.42942300	1.90864500	-0.06356600
H	-3.84691600	2.11106300	0.73356200
H	-3.93107200	2.00976600	-1.02481400
H	-3.59795600	-4.00314400	0.03225000
H	-4.59470200	-2.79247400	0.90868300
H	-4.62099300	-2.80726600	-0.83519800
H	3.20041600	1.26362300	-1.56274800
H	3.33557600	3.03862200	0.10966000
H	3.25097200	1.79804600	1.48191300
Cu	1.11764200	1.70266100	-0.05076500
Cl	-0.30045400	3.34868400	0.20184900

TS2-3

C	-2.73376700	3.34916300	-0.57470600
C	-4.03606500	2.84974600	-0.44105800
C	-4.24044400	1.50959000	-0.12985800
C	-3.15890600	0.63647600	0.06941700
C	-1.83402600	1.13214500	-0.11734700
C	-1.64654500	2.50201700	-0.41666500
C	-0.70960900	0.22998800	-0.11608700
C	0.58283000	0.28740100	-0.08630800
C	1.85166900	-0.28665700	-0.21945400
C	2.97846600	0.47824500	-0.01517600
C	2.61885500	1.85545700	0.32018600
C	4.36678000	-0.02771700	-0.12132800
O	5.32102300	0.71595000	0.07447600
C	4.57685500	-1.48955000	-0.47844600
C	3.60588000	2.94501700	0.61869000
O	1.39214200	2.09859500	0.35142600
C	-3.42993600	-0.75119400	0.46010200
C	-2.76043800	-1.44867500	1.40948100
H	-2.57254800	4.39558000	-0.81710600
H	-4.88923900	3.50854400	-0.57647200
H	-5.25165400	1.13012100	-0.00937200
H	-0.63578900	2.87217900	-0.53895000
H	1.89754100	-1.33845400	-0.48458100
H	5.64940400	-1.68911600	-0.50462900
H	4.10317700	-2.15161100	0.25625600
H	4.14260300	-1.72518100	-1.45762500
H	3.06833200	3.86808100	0.84456100
H	4.24755900	2.65711400	1.45718200
H	4.27949100	3.08909500	-0.23186300
H	-4.26092600	-1.23834800	-0.04988200
H	-3.04265400	-2.46796700	1.65351100
H	-2.04246800	-0.96925000	2.07179700
Cu	-0.94623400	-1.73261900	-0.05457800
Cl	-0.42040900	-3.81411200	-0.25917200

INT3

C	2.24976800	-3.28241800	-1.17334400

C	3.52858500	-3.13135000	-0.62123300	H	2.73748400	1.60211400	2.69294400
C	3.81576600	-2.02030400	0.16161800	H	1.35665500	0.44544400	2.28481900
C	2.84947800	-1.03353800	0.42295100	Cu	1.11663300	1.74315000	-0.23067500
C	1.54879000	-1.16295300	-0.16505000	Cl	1.49841400	3.82924900	-0.48986900
C	1.27714800	-2.32364100	-0.93665100				
C	0.59089600	-0.07050500	-0.14080600	**TS3-4**			
C	-0.78730000	-0.32206400	-0.06132600	C	-3.02968600	-0.20790700	0.01123200
C	-1.87767700	0.53593300	-0.19207500	C	-1.83659600	0.56059300	-0.09533900
C	-3.05690300	-0.20462900	0.02265600	C	-0.76817100	-0.29013700	0.08460000
C	-2.64012500	-1.51297400	0.29512800	O	-1.28083900	-1.57568300	0.31025000
C	-4.47134300	0.23831300	-0.00475100	C	-2.62235000	-1.51306200	0.25990300
O	-5.37123800	-0.56070700	0.21631800	C	-3.37615800	-2.77819300	0.46440600
C	-4.74576600	1.69601400	-0.31288400	C	-4.43969900	0.22069400	-0.11288500
C	-3.39944900	-2.74646600	0.62211700	C	-4.70719200	1.68702800	-0.39314700
O	-1.31069700	-1.59906000	0.24471200	O	-5.34993700	-0.58977300	0.00714200
C	3.21263200	0.07911600	1.29602500	H	-1.75192100	1.61975300	-0.29782500
C	2.38300900	0.75483300	2.11404300	H	-3.96988400	-3.02018700	-0.42376400
H	2.02030300	-4.14332200	-1.79476900	H	-2.68508400	-3.59752400	0.67745500
H	4.29461800	-3.87984600	-0.80322700	H	-4.09037000	-2.67067900	1.28673400
H	4.80392900	-1.90986100	0.60067900	H	-4.28829800	2.31860500	0.40016700
H	0.30297300	-2.42930700	-1.39951700	H	-4.23482900	1.99550900	-1.33408500
H	-1.78948200	1.58853600	-0.42558000	H	-5.78447000	1.84982100	-0.45675000
H	-5.82329700	1.86824100	-0.30259300	C	0.64780000	-0.07913100	0.10610800
H	-4.26446600	2.34747000	0.42715100	C	1.57210500	-1.14136000	-0.14350600
H	-4.34101500	1.96930400	-1.29521300	C	1.38690200	-2.16897700	-1.11120300
H	-2.71340200	-3.58175500	0.77954300	C	2.81097200	-1.10520700	0.59460400
H	-4.01056500	-2.59098000	1.51738300	C	2.42721200	-3.02032900	-1.40672700
H	-4.10159300	-2.98490800	-0.18368700	H	0.44809000	-2.23834000	-1.64981600
H	4.26291200	0.36819700	1.27265400	C	3.87446100	-1.98441800	0.24595200

C	3.67913400	-2.92520300	-0.73472500
H	2.29929200	-3.77369500	-2.17910800
H	4.81779800	-1.91920500	0.78114600
H	4.47684600	-3.61364300	-0.99800900
Cu	1.18420400	1.76340200	-0.10192000
Cl	1.62622700	3.79231600	-0.56505800
C	2.80700000	-0.14095800	1.61006000
H	3.72666800	0.26031300	2.02890500
C	1.54928800	0.44087900	1.88677700
H	1.49711100	1.40560400	2.39065800
H	0.74733900	-0.22660000	2.20015100

INT4

C	-3.16098700	-0.31749700	0.10030500
C	-2.09976800	-0.24646100	1.06508900
C	-0.92679300	-0.46044800	0.39119000
O	-1.21182800	-0.66013800	-0.94606000
C	-2.55759000	-0.56983400	-1.11652200
C	-3.06871900	-0.74976700	-2.49894900
C	-4.61377800	-0.15392500	0.33590900
C	-5.05218500	0.15852000	1.75670500
O	-5.43424400	-0.26225600	-0.56621300
H	-2.19649400	-0.05296300	2.12374800
H	-4.15509800	-0.66270300	-2.48962400
H	-2.64714000	0.00928800	-3.16977300
H	-2.78532100	-1.73345100	-2.89435800
H	-4.73900800	-0.63610400	2.44541400
H	-4.59641200	1.09287200	2.10708000
H	-6.13918000	0.25260000	1.78179400
C	0.45414100	-0.49295900	0.81067900
C	1.60107400	-0.88677900	0.07889200
C	1.79748000	-1.23966100	-1.31041700
C	2.72365300	-1.08704100	1.03243000
C	3.03432000	-1.64874600	-1.71507900
H	0.96966900	-1.17089000	-2.00591600
C	4.01430500	-1.48221700	0.52445900
C	4.15246100	-1.75024200	-0.80181200
H	3.19579700	-1.90617700	-2.75798200
H	4.85139400	-1.57654000	1.21029700
H	5.11582800	-2.05846700	-1.19760400
Cu	1.33178500	1.22872900	-0.07465100
Cl	1.61210000	3.27172900	-0.53890100
C	2.28646100	-0.86875900	2.30277100
H	2.88446700	-0.90878800	3.20558400
C	0.83356100	-0.49646300	2.28678100
H	0.64880500	0.46871400	2.78029300
H	0.22802700	-1.23709600	2.83087500

INT5

C	-0.62200300	0.34973100	-0.00092200
C	0.50843100	1.23961400	-0.00064700
C	1.63543400	0.45924600	-0.00048000
O	1.24148300	-0.87648600	-0.00065900
C	-0.10423800	-0.93915200	-0.00085600
C	-0.72259400	-2.29040600	-0.00097900
C	-2.02937900	0.68178500	-0.00094200
C	-2.43895100	2.13149800	-0.00040700
O	-2.87969600	-0.24013200	-0.00048100

H	0.48576600	2.31952100	-0.00040700
H	-1.36454700	-2.42657200	-0.87836300
H	0.05634500	-3.05676700	-0.00113700
H	-1.36439000	-2.42678100	0.87649000
H	-2.04255300	2.63617500	0.88919400
H	-2.02415400	2.64361400	-0.87708200
H	-3.52746100	2.22175700	-0.01073400
C	3.03286000	0.75821100	-0.00021000
C	4.12487000	-0.09090600	0.00010900
C	4.23673600	-1.52397800	0.00012600
C	5.36104600	0.71930600	0.00041500
C	5.47642100	-2.09329900	0.00045700
H	3.34311500	-2.13671100	-0.00015500
C	6.64258600	0.05903500	0.00077300
C	6.68709200	-1.30048100	0.00079900
H	5.57043400	-3.17598000	0.00044700
H	7.55209700	0.65371400	0.00100000
H	7.64367200	-1.81582400	0.00107900
Cu	4.77982700	-0.20791700	0.00030000
Cl	-6.87764800	-0.18533300	0.00087400
C	5.03642100	2.04303700	0.00028700
H	5.72220100	2.88183900	0.00047000
C	3.54355200	2.18157300	-0.00003800
H	3.19039600	2.74322700	-0.87849600
H	3.19008200	2.74310600	0.87835500

TS5-2r

C	-0.62990300	0.37458000	-0.03631500
C	0.49433200	1.27493800	0.00826000
C	1.62375800	0.50765800	-0.06263100
O	1.24433400	-0.82603100	-0.14677300
C	-0.10209100	-0.90511700	-0.13100900
C	-0.70506200	-2.26098100	-0.21395000
C	-2.03891900	0.69226300	0.01151500
C	-2.46045300	2.13522100	0.11467700
O	-2.88263100	-0.23507800	-0.03203400
H	0.45923600	2.35134900	0.09169000
H	-1.36915900	-2.34145100	-1.08153600
H	0.08254200	-3.01450700	-0.29205500
H	-1.32020700	-2.47136900	0.66813800
H	-2.05561400	2.58248100	1.03084700
H	-2.06224300	2.70864800	-0.73109200
H	-3.54970800	2.21624300	0.12565600
C	3.03354700	0.80179800	-0.08215900
C	4.14212400	-0.09420200	-0.01252100
C	4.22064700	-1.50833600	0.09779900
C	5.36418400	0.67028500	-0.01983500
C	5.46028700	-2.10707400	0.16644600
H	3.31730900	-2.10623900	0.11716000
C	6.62277900	0.02763700	0.06925500
C	6.66204000	-1.34627700	0.14809500
H	5.52616800	-3.18956100	0.23851700
H	7.53755300	0.61463900	0.06231400
H	7.61722700	-1.86095700	0.20153200
Cu	-4.78211900	-0.21731700	0.01666400
Cl	-6.87979300	-0.20911200	0.07343300
C	5.03335900	2.04301000	-0.10989000
H	5.69283500	2.89173800	-0.23820200

C	3.55618100	2.12463100	-0.12485500
H	3.00942800	3.02727600	-0.37295600
H	4.19807900	2.35746600	0.94152800

2r-CuCl

C	-0.62769200	0.39716800	-0.04928600
C	0.49807800	1.28500500	0.08309000
C	1.62062400	0.53804000	-0.11825400
O	1.24154900	-0.77542800	-0.36064700
C	-0.10163400	-0.85908600	-0.32099900
C	-0.70821300	-2.19498400	-0.55857100
C	-2.03607200	0.70403900	0.07834400
C	-2.45425400	2.12040000	0.37561500
O	-2.87831900	-0.21307900	-0.06227200
H	0.47271000	2.33975900	0.31524200
H	-1.40996400	-2.16031800	-1.39871300
H	0.07491600	-2.92678300	-0.77111600
H	-1.28374300	-2.52418300	0.31394800
H	-1.99327700	2.46528800	1.30894700
H	-2.11339700	2.79043000	-0.42319800
H	-3.54098800	2.18784600	0.46244600
C	3.03907400	0.84780000	-0.13790700
C	4.15169700	-0.11257000	0.04587400
C	4.16686500	-1.49376400	0.25890900
C	5.36095500	0.61285100	-0.00917800
C	5.39966500	-2.13489100	0.41038800
H	3.24512500	-2.06243000	0.30333800
C	6.58268900	-0.03055200	0.14344200
C	6.59687600	-1.41455900	0.35316100
H	5.42619200	-3.20865800	0.57533300
H	7.51467300	0.52821300	0.10257900
H	7.54468200	-1.93214700	0.47279500
Cu	-4.77680900	-0.21831500	0.02958100
Cl	-6.87165500	-0.23648400	0.13134200
C	5.05537900	2.07501000	-0.23431700
H	5.51020000	2.46283500	-1.15808800
C	3.55275700	2.09270600	-0.30464800
H	2.97591400	2.99315100	-0.48427700
H	5.43595600	2.71076300	0.57947800

2r

C	3.36464000	2.19406700	-0.24324800
C	4.56233500	1.48444700	-0.11913000
C	4.54656800	0.09382400	0.04390200
C	3.32479900	-0.56515900	0.08963500
C	2.11209400	0.14928400	-0.02064800
C	2.13220200	1.53501900	-0.19809500
C	3.02176300	-2.03818700	0.23094900
C	1.51824900	-2.07228500	0.19466700
C	0.99941900	-0.82475000	0.06060000
C	-0.41423800	-0.51005400	0.01215000
C	-1.15690600	0.63141900	0.11523800
C	-2.54257000	0.24971600	0.02585100
C	-2.54797500	-1.12212200	-0.12755000
O	-1.27395000	-1.58407300	-0.13600300
C	-3.62751800	-2.13169000	-0.28350600
C	-3.73026100	1.12555500	0.08486900
C	-3.48243200	2.61609500	0.25812500

O	-4.87256100	0.68885900	0.00046600
H	3.38936300	3.27189700	-0.38049100
H	5.51063700	2.01371900	-0.15559700
H	5.47922300	-0.45913200	0.12894900
H	1.21594000	2.10262000	-0.31999400
H	3.46957900	-2.63202600	-0.58041800
H	3.41726100	-2.46091900	1.16706500
H	0.93652400	-2.98202800	0.27938300
H	-0.77592400	1.62905900	0.26903600
H	-4.59292300	-1.62721200	-0.24603600
H	-3.53035000	-2.66219100	-1.23919400
H	-3.57616700	-2.88313200	0.51436100
H	-2.93551500	2.81477400	1.18821200
H	-4.44167500	3.13631800	0.28278300
H	-2.87490000	3.00889600	-0.56660800

TS5-2r'

C	-0.61759500	0.34774900	0.11738300
C	0.52890100	1.21110400	-0.01583600
C	1.62908700	0.45252100	0.25485800
O	1.21865700	-0.84331100	0.54724800
C	-0.12388400	-0.90497800	0.45590400
C	-0.76268200	-2.22166300	0.71501900
C	-2.01500000	0.67165000	-0.07159300
C	-2.39673800	2.08066100	-0.44358400
O	-2.87784900	-0.22557100	0.07450600
H	0.53122100	2.25301100	-0.30111700
H	-1.31497000	-2.56843800	-0.16562000
H	-0.00069200	-2.95961600	0.97720000
H	-1.49151300	-2.14729400	1.52913900
H	-2.02566300	2.78753500	0.30819100
H	-1.93917800	2.35443200	-1.40230000
H	-3.48202600	2.17435000	-0.52387200
C	3.04601000	0.73080800	0.31028500
C	4.15730000	-0.11484200	-0.01118400
C	4.24150900	-1.50972100	-0.22774300
C	5.33666300	0.70611800	-0.09211600
C	5.47049700	-2.06156900	-0.52535800
H	3.35305100	-2.12962900	-0.16810400
C	6.59011000	0.09994400	-0.37024900
C	6.64207800	-1.25868000	-0.59057000
H	5.55054600	-3.12932900	-0.70967300
H	7.48999700	0.70748900	-0.41832500
H	7.59351500	-1.73264400	-0.81690300
Cu	-4.77204200	-0.19682400	-0.07775200
Cl	-6.86305300	-0.17401400	-0.23930400
C	4.99381700	2.05015000	0.17620000
H	5.67689600	2.88762200	0.23523500
C	3.61577300	2.11085700	0.44912300
H	3.00314200	2.99924100	0.55316300
H	3.37526100	1.37980600	1.46871800

2r'-CuCl

C	-0.46136700	0.24670300	0.50422000
C	0.75259600	1.03026000	0.45729300
C	1.73464600	0.26016200	0.98586600
O	1.20172300	-0.96260800	1.36374300
C	-0.11588300	-0.97023200	1.07279100

C	-0.87917300	-2.20134700	1.40685600	**2r'**			
C	-1.78754300	0.61478700	0.06114200	C	2.44473400	-0.13359400	0.06535000
C	-2.00694400	1.97653000	-0.54506600	C	1.26757100	-0.95033700	-0.12465000
O	-2.72627100	-0.20705900	0.18377300	C	0.35446900	-0.18252200	-0.77139400
H	0.87247700	2.03233100	0.07265900	O	0.88904400	1.06864900	-1.00017500
H	-1.34380800	-2.62760000	0.51102800	C	2.15045700	1.09288500	-0.49096300
H	-0.21236700	-2.94169300	1.85560900	C	2.90860400	2.36323000	-0.63772700
H	-1.69455200	-1.97890400	2.10388300	C	3.71491600	-0.51305500	0.71569300
H	-1.67643000	2.76132000	0.14549400	C	3.81509800	-1.93020400	1.25920600
H	-1.41332000	2.07867100	-1.46200900	O	4.65776300	0.26340600	0.82225200
H	-3.06280400	2.12332100	-0.78324600	H	1.12454800	-1.97443700	0.18814700
C	3.20585400	0.42945600	1.20195100	H	3.89484200	2.23900200	-0.19030200
C	4.07883700	-0.23527900	0.13799600	H	3.01984000	2.63358500	-1.69544100
C	4.13119500	-1.55601300	-0.28388200	H	2.38583100	3.19078300	-0.14160400
C	4.92604400	0.74106700	-0.42564000	H	3.04214300	-2.11176100	2.01628300
C	5.04831700	-1.90296600	-1.28624400	H	3.66475700	-2.66596000	0.45944100
H	3.47654200	-2.30823100	0.14824600	H	4.80135700	-2.07299800	1.70461200
C	5.84093900	0.39270300	-1.42003300	C	-1.05426900	-0.38825400	-1.23621200
C	5.89275400	-0.93878100	-1.84567600	C	-2.12233300	0.21218000	-0.32403200
H	5.10342800	-2.93188200	-1.63073100	C	-2.28603200	1.51307300	0.12970700
H	6.50067000	1.13791100	-1.85691000	C	-3.03028700	-0.80322400	0.04169500
H	6.59843600	-1.22780300	-2.61974700	C	-3.37851300	1.80107100	0.96020000
Cu	-4.56794100	-0.10478800	-0.27364100	H	-1.58064100	2.29201700	-0.14700900
Cl	-6.60388300	-0.00482100	-0.77040500	C	-4.11968300	-0.51354600	0.86456400
C	4.63571300	2.02768200	0.21682900	C	-4.28444700	0.79847600	1.32090300
H	5.14954700	2.95482600	-0.01580900	H	-3.52209400	2.81369400	1.32727400
C	3.66117000	1.87653800	1.13256500	H	-4.82678000	-1.28910900	1.14807600
H	3.24332200	2.65000000	1.76705200	H	-5.12637300	1.04171300	1.96365400
H	3.44861300	0.00825500	2.19101300	C	-2.59014400	-2.05704600	-0.58026800

H	-3.10853600	-3.00476600	-0.47491400	H	2.97535100	-1.92901800	0.03794900
C	-1.47036800	-1.84652900	-1.29686300	C	0.82585800	-1.55231100	0.19141200
H	-1.14256500	0.06211700	-2.23889300	H	0.74739700	-2.62027900	0.43300000
H	-0.91942400	-2.58594300	-1.86718300	Cu	-0.71382000	-0.55576200	0.07317600
				Cl	-2.52433800	0.53298200	-0.13241100

INT6

				INT7			
C	2.78023800	2.07189700	-0.00011600				
H	3.86391600	1.97463900	0.00001700	C	0.58027000	1.12422700	0.84186300
H	2.37872300	3.08064000	-0.00027100	H	0.90712800	0.63645600	1.76136700
C	1.97103500	0.99110200	0.00006800	H	-0.22033200	1.84588100	0.99276100
H	0.89172100	1.11937600	0.00012100	C	1.61200000	1.45754400	-0.10096200
C	2.51426100	-0.33727800	0.00014900	H	1.62654100	2.46340800	-0.51686400
H	3.60416600	-0.38998500	0.00012800	C	2.51809100	0.52499100	-0.53277200
C	1.83505200	-1.54632400	0.00001600	H	3.38098000	0.81785300	-1.12501500
H	2.46808600	-2.43532600	-0.00006600	C	2.30778500	-0.85594200	-0.20925600
C	0.42961900	-1.69455400	-0.00005800	H	3.15191900	-1.53926100	-0.32274700
H	0.15697500	-2.75780600	-0.00013300	C	1.10472900	-1.33509700	0.21600200
Cu	-0.96104100	-0.48153600	-0.00002900	H	1.07821700	-2.29193100	0.74714400
Cl	-2.51027200	0.96846700	0.00004100	Cu	-0.53273400	-0.40743700	0.06615300
				Cl	-2.54190700	0.25817200	-0.27907800

TS6-7

				TS7-8			
C	1.43757300	2.15121400	0.53474900				
H	1.82689700	2.01991700	1.54091500	C	1.05685800	-1.21691200	0.31324400
H	0.79872100	3.01087200	0.36011500	C	2.22279800	-0.94221500	-0.33164400
C	1.69950000	1.28425700	-0.44642600	C	2.53490200	0.40949500	-0.70486900
H	1.29255100	1.45586600	-1.44513100	Cu	-0.57981000	-0.29690200	0.11262200
C	2.57400800	0.10293300	-0.31172200	Cl	-2.60143700	0.23362400	-0.33496400
H	3.63955400	0.27196100	-0.48745500	C	1.77847800	1.36274100	-0.09216600
C	2.18540400	-1.17824700	-0.01976300	H	1.81108100	2.40829300	-0.38860400

C	0.84463400	0.93546200	0.93786100
H	0.06395600	1.64376100	1.22476200
H	1.30771200	0.48182100	1.81766300
H	0.95767700	-2.08922000	0.96442800
H	3.32865200	0.64110900	-1.40789500
H	2.94381600	-1.73863900	-0.51656000

INT8

C	1.21632500	0.69768900	0.84864800
C	1.23579600	-0.68950000	0.89089300
C	1.95105100	-1.19502000	-0.29522700
Cu	-0.65590700	0.00020700	0.24937100
Cl	-2.65206400	0.00020800	-0.43633500
C	2.39709500	-0.14965600	-1.02276700
H	2.93984500	-0.20403200	-1.95947800
C	2.00315200	1.14664700	-0.36662100
H	1.44168600	1.81044600	-1.03927900
H	2.88660500	1.72152900	-0.04556800
H	0.98320600	1.35300600	1.68221800
H	2.07657800	-2.24689500	-0.52419600
H	0.95796300	-1.30455800	1.74267200

TS3-9

C	-2.70971600	0.56386300	-0.13656600
C	-1.33658900	0.86966000	-0.43017500
C	-0.56779400	0.11914000	0.42118900
O	-1.39930900	-0.63219200	1.23094800
C	-2.68901800	-0.35607400	0.89409000
C	-3.74432600	-1.07125600	1.65501800
C	-3.92038400	1.10797000	-0.79220900
C	-3.70575100	2.05631000	-1.95980400
O	-5.04954000	0.81449600	-0.42003900
H	-0.96221900	1.54843300	-1.18203900
H	-3.67136400	-0.84855900	2.72729700
H	-4.72117200	-0.75799500	1.28691200
H	-3.63825300	-2.15699700	1.53778800
H	-3.13358700	2.93852600	-1.64633600
H	-3.13600500	1.56569400	-2.75861200
H	-4.67651000	2.37207600	-2.34587500
C	0.86994500	-0.08767700	0.55207500
C	1.75352400	1.00868400	-0.05420500
C	2.15953700	1.29450300	-1.34439700
C	2.11500700	1.83197500	1.02082300
C	2.93359500	2.45633000	-1.53627500
H	1.88176300	0.66271700	-2.18379500
C	2.84383600	3.00190400	0.83797500
C	3.26335500	3.29602400	-0.46897600
H	3.26987500	2.71060300	-2.53742500
H	3.09131400	3.66048000	1.66588000
H	3.85247000	4.18958400	-0.65329200
Cu	1.11761000	-1.92713900	-0.15527000
Cl	1.48835900	-3.72330700	-1.21759800
C	1.49290100	1.15527500	2.16842600
H	0.76074900	1.65482700	2.80235100
C	1.51116600	-0.28552700	2.05707300
H	2.48905100	-0.75256900	1.96181100
H	0.85614200	-0.82860900	2.73568700

INT9

C	2.75903200	-0.72175200	-0.19162700
C	1.39500600	-0.71032400	-0.66043300
C	0.61726400	-0.40151100	0.41309300
O	1.41019100	-0.22003600	1.52442400
C	2.70946500	-0.41055300	1.14978200
C	3.73869800	-0.24265500	2.20728800
C	3.98346500	-0.99794200	-0.97765300
C	3.80546400	-1.26249300	-2.46279900
O	5.09474800	-1.01231900	-0.46394600
H	1.04569800	-0.89978000	-1.66472300
H	3.55867500	-0.93161400	3.04211200
H	4.72026700	-0.44331600	1.77783200
H	3.72017800	0.77746500	2.61094700
H	3.15121600	-2.12718700	-2.63042900
H	3.34015100	-0.40033000	-2.95653900
H	4.78224400	-1.45412500	-2.91029500
C	-0.83429100	-0.28909800	0.60974800
C	-1.92679700	-0.89282700	-0.26904300
C	-2.38287800	-1.00522700	-1.56954400
C	-2.59972400	-1.44539400	0.82571600
C	-3.57210300	-1.74477800	-1.72586100
H	-1.87111700	-0.57316200	-2.42431300
C	-3.77461400	-2.15976200	0.68707200
C	-4.24537100	-2.30374200	-0.63375100
H	-3.97893900	-1.88493800	-2.72332200
H	-4.30404400	-2.60709800	1.52334600
H	-5.15754400	-2.86667200	-0.81133400
Cu	-0.85597300	1.77069200	0.09123900
Cl	-0.64065000	3.56084600	-1.00441800
C	-1.59362200	-0.89710600	1.81704100
H	-1.08990100	-1.45630000	2.59911800
C	-1.55845800	0.59653600	1.83030500
H	-2.49070200	1.13667100	1.66341800
H	-0.87464500	1.03655300	2.55355600

TS1-10

C	-4.45947800	0.50785700	-0.51196600
C	-4.58723400	1.87976800	-0.28359900
C	-3.48431100	2.62307300	0.13418300
C	-2.22180400	2.03646900	0.29993100
C	-2.08687500	0.63509700	0.05656300
C	-3.22707000	-0.10607900	-0.32332900
C	-0.80988300	-0.05848300	0.14300600
C	-1.09633400	2.85661800	0.78259700
C	0.44090600	0.26703900	0.13494900
C	1.55257200	1.06157100	-0.15408500
C	2.83562300	0.57225900	-0.09860900
C	4.05622600	1.35064500	-0.41106000
O	5.16748000	0.85245500	-0.28467300
C	2.83057500	-0.82410000	0.35138900
O	1.69392700	-1.29280300	0.56699400
C	4.05292000	-1.66266800	0.56788200
C	3.89570900	2.78296800	-0.89590000
C	-0.87653900	4.13782600	0.45768100
H	-5.31716900	-0.08381300	-0.81696800
H	-5.54988400	2.36818700	-0.40687900
H	-3.60197700	3.67787600	0.36311900

H	-3.12093100	-1.17476600	-0.48531600
H	-0.41067200	2.36839600	1.47368800
H	1.32756800	2.08778800	-0.43164600
H	4.62317600	-1.73900300	-0.36365200
H	4.72204500	-1.18150500	1.28776500
H	3.75473200	-2.65305600	0.91603000
H	3.31058200	2.82415500	-1.82248700
H	4.88749900	3.19993700	-1.07831100
H	3.37889900	3.39920600	-0.15007000
H	-1.50417900	4.67113000	-0.25177000
Cu	-0.75169600	-2.00610000	0.04213100
Cl	-1.20170000	-4.06586800	-0.24151400
H	-0.05288000	4.69573800	0.89407000

INT10

C	-2.82563700	-2.69184800	1.49599600
C	-2.38676500	-3.79564200	0.75965900
C	-1.46204800	-3.62154600	-0.26667300
C	-0.89964100	-2.36720100	-0.55541500
C	-1.33215800	-1.24151700	0.21211500
C	-2.33253400	-1.42888200	1.19319700
C	-0.82290000	0.12577400	0.06115600
C	0.01693500	-2.22299300	-1.70590500
C	0.55851000	0.32279700	0.05357900
C	1.67857300	-0.45933700	0.35152100
C	2.81878900	0.35786300	0.28189100
C	4.24283700	0.01538300	0.51082000
O	5.11022100	0.86861700	0.38938700
C	2.35091200	1.63754200	-0.06485600
O	1.02997600	1.62602700	-0.18786000
C	3.05652500	2.92109500	-0.29834400
C	4.56913900	-1.41496300	0.89239700
C	0.80742900	-3.18253600	-2.20571800
H	-3.57265100	-2.80954400	2.27535600
H	-2.79474900	-4.78318200	0.95622600
H	-1.19038200	-4.46959200	-0.88780200
H	-2.69434600	-0.55883500	1.73288800
H	0.02361400	-1.24838000	-2.18920600
H	1.63974200	-1.51023600	0.59825400
H	3.64339900	3.19464500	0.58474300
H	3.77557300	2.81608300	-1.11789200
H	2.33713000	3.70941700	-0.52980600
H	4.07713200	-1.68646000	1.83477000
H	5.64960600	-1.51766400	1.00577900
H	4.21305300	-2.11371500	0.12534100
H	0.88104400	-4.17214300	-1.76166300
Cu	-1.99453900	1.58206100	-0.06795600
Cl	-3.34782200	3.21115100	-0.20443100
H	1.41708800	-3.00081700	-3.08566800

INT11

C	-2.66425800	-0.05830300	0.00000600
C	-1.60233400	-1.02610300	-0.00009000
C	-0.41727400	-0.33338000	-0.00007000
O	-0.70423700	1.02229500	-0.00015200
C	-2.05265000	1.18041100	-0.00007700
C	-2.56167500	2.57619000	-0.00015600
C	-4.11998100	-0.31020900	0.00017400

C	-4.56841100	-1.76338000	0.00010200	C	-0.40794400	-0.45981000	-0.03447100
O	-4.94411300	0.59720500	0.00014600	O	-1.24673400	-1.55458900	0.09921500
H	-1.70499000	-2.10176700	-0.00007200	C	-2.53336500	-1.11754700	0.10557700
H	-3.65154400	2.55694400	0.00048900	C	-3.59082800	-2.15230200	0.24592800
H	-2.20634000	3.12168100	0.88349800	C	-3.75890200	1.10699500	-0.06039300
H	-2.20747100	3.12118500	-0.88458100	C	-3.54147300	2.60489600	-0.21124400
H	-4.18421500	-2.28917000	-0.88278400	O	-4.89302300	0.64794900	0.02387200
H	-4.18493700	-2.28891000	0.88346800	H	-0.81625200	1.67706300	-0.25322800
H	-5.65929900	-1.80052300	-0.00030300	H	-3.48016800	-2.70148600	1.18988900
C	0.95223600	-0.74436500	-0.00005600	H	-4.56610700	-1.66592300	0.22403700
C	2.10874500	0.01409700	0.00000300	H	-3.53148200	-2.88637200	-0.56787900
C	2.33124800	1.43449600	0.00005800	H	-2.93424400	2.99558500	0.61468700
C	3.27713800	-0.89191300	-0.00001100	H	-3.00560900	2.82861300	-1.14208200
C	3.61072700	1.90754000	0.00008200	H	-4.51056700	3.10719700	-0.22001800
H	1.48523700	2.11190200	0.00007000	C	1.00262000	-0.75082900	-0.08641300
C	4.60576700	-0.33087000	0.00001900	C	2.10517200	0.14860600	-0.01628600
C	4.75515600	1.02132600	0.00006000	C	2.17595900	1.55529200	0.16417300
H	3.78895000	2.97968900	0.00011700	C	3.33433700	-0.60208700	-0.09814200
H	5.46752600	-0.99330000	0.00000300	C	3.40935400	2.16851000	0.21457700
H	5.74966000	1.45989800	0.00007500	H	1.27187500	2.14576900	0.27044400
C	2.85008400	-2.18616700	-0.00004800	C	4.58753800	0.05352300	-0.02797600
H	3.46736800	-3.07663600	-0.00009000	C	4.61664400	1.42343600	0.10958600
C	1.34982800	-2.20416500	-0.00000700	H	3.46638800	3.24629000	0.34365800
H	0.95045600	-2.73398500	0.87832700	H	5.50825300	-0.52091900	-0.09311600
H	0.95031500	-2.73423000	-0.87811300	H	5.56823400	1.94629400	0.14921500
				C	3.01238200	-1.97335700	-0.22654100
TS11-2r				H	3.67441500	-2.81184800	-0.39982200
C	-2.55367400	0.25536100	-0.02268300	C	1.53387500	-2.06689200	-0.19143600
C	-1.17610000	0.66911200	-0.11458200	H	2.20595500	-2.32483500	0.84288400

H	0.97379500	-2.95974400	-0.44139400

TS11-2r'

C	-2.65729000	-0.07533600	-0.03659300
C	-1.56871200	-1.01585800	-0.10279900
C	-0.42730900	-0.32999500	0.19758800
O	-0.75044500	0.99206300	0.44578700
C	-2.09158100	1.13969400	0.29480700
C	-2.64095800	2.50546700	0.49912300
C	-4.09187300	-0.33106300	-0.28224700
C	-4.48716900	-1.75430400	-0.64350500
O	-4.93849000	0.55138000	-0.20285500
H	-1.62733900	-2.06271600	-0.36406400
H	-3.72321900	2.47508300	0.37318800
H	-2.39875100	2.87789000	1.50228900
H	-2.21160100	3.21046500	-0.22416600
H	-3.97783100	-2.07895900	-1.55931500
H	-4.20072800	-2.45235800	0.15291300
H	-5.56740700	-1.79741800	-0.79359400
C	0.96280000	-0.71320200	0.31390600
C	2.14685400	0.04086600	0.02652500
C	2.33913500	1.42059200	-0.21526600
C	3.26605100	-0.86454000	0.01283900
C	3.61557000	1.87839100	-0.47019200
H	1.49311000	2.09986900	-0.20519600
C	4.57009600	-0.35351100	-0.22253400
C	4.72815000	0.99280700	-0.46764100
H	3.77964500	2.93341800	-0.67226000
H	5.42622200	-1.02342200	-0.21905400
H	5.72016900	1.39276600	-0.66166100
C	2.81509700	-2.17369800	0.29170100
H	3.43175200	-3.05660900	0.40006100
C	1.42533700	-2.12478000	0.50777600
H	1.19888800	-1.35265500	1.50062600
H	0.74337500	-2.96207000	0.60585100

$CuCl_2$

Cu	0.00000000	0.00000000	-0.00036700
Cl	0.00000000	2.08590200	0.00031300
Cl	0.00000000	-2.08590200	0.00031300

INT12

C	-6.42569900	-0.50098300	-0.44645400
C	-6.48419600	-1.87275500	-0.22099100
C	-5.33101600	-2.58570300	0.13054400
C	-4.12495600	-1.91241100	0.25189300
C	-4.05196600	-0.51846200	0.02862400
C	-5.22433800	0.21475100	-0.32367200
C	-2.79745800	0.12248000	0.17138600
C	-1.69049600	0.62263500	0.31521600
C	-0.48333300	1.31823500	0.41709500
C	0.77122300	0.87920200	0.76423100
C	1.87455700	1.87331700	0.68226700
C	1.08914200	-0.51391900	1.20824800
O	2.24903900	-0.91969600	1.24858700
C	-0.01686700	-1.44089800	1.65978600
C	1.58244600	3.34942700	0.86632900
O	3.05161000	1.55636800	0.47467100

C	-5.15059200	1.66416500	-0.55553100
C	-6.18547100	2.51396500	-0.60115100
H	-7.32691800	0.02584800	-0.74305000
H	-7.43133000	-2.39352800	-0.32990300
H	-5.37645700	-3.65726200	0.29852800
H	-3.21924100	-2.44826400	0.51708800
H	-0.56764600	2.36283900	0.12033400
H	0.44419300	-2.27423800	2.19349600
H	-0.75588000	-0.94185100	2.29277200
H	-0.54257800	-1.83259400	0.78107000
H	2.51959000	3.85441100	1.10769700
H	1.21129000	3.77337200	-0.07594100
H	0.84052000	3.53927900	1.64664000
H	-4.14735400	2.06354600	-0.68400600
H	-6.02673100	3.57174700	-0.78610200
H	-7.21510000	2.20277800	-0.44774800
Cu	3.80266900	-0.20345900	-0.24991000
Cl	2.70652100	-0.14494800	-2.16892100
Cl	5.57613600	-1.40313400	-0.09675300

INT13

C	2.22702300	4.04787400	0.19259800
C	3.51809600	3.56713600	-0.05563600
C	3.69895000	2.24289100	-0.43480100
C	2.60709700	1.36672900	-0.60277000
C	1.29554200	1.85431500	-0.31317600
C	1.13099800	3.19949100	0.07431400
C	0.13797900	1.03910000	-0.32647300
C	-0.97143700	0.53015800	-0.26713100
C	-2.15911700	-0.21861000	-0.22373000
C	-3.42469600	0.25187800	-0.01450300
C	-3.63739100	1.72879100	0.22919500
C	-4.57193700	-0.71222000	-0.04449300
O	-5.72751100	-0.31134100	-0.01098700
C	-4.29345400	-2.20615300	-0.13844200
C	-4.92771200	2.23132100	0.84003000
O	-2.73694200	2.51299600	-0.03824000
C	2.91526900	0.03180600	-1.08146000
C	2.08733600	-0.89700800	-1.67211300
H	2.07716500	5.08115000	0.49151000
H	4.37721900	4.22191000	0.05325500
H	4.70137300	1.86903600	-0.62398400
H	0.12579800	3.54920600	0.28627700
H	-2.00316700	-1.28610000	-0.36608900
H	-5.25001800	-2.72829600	-0.08125300
H	-3.80632200	-2.46405000	-1.08620200
H	-3.63911000	-2.55237700	0.66933200
H	-4.78310800	3.27773200	1.11798600
H	-5.74907400	2.14009000	0.12383500
H	-5.22010800	1.63955000	1.71322700
H	3.96654700	-0.23720900	-0.99883200
H	2.53470500	-1.76548700	-2.15074700
H	1.06419600	-0.66702900	-1.94387700
Cu	1.71918400	-1.96547000	0.22048300
Cl	3.21597000	-1.52534900	1.71049100
Cl	0.05861300	-3.12392900	-0.54420200

TS13-14

C	2.48826800	3.54022500	0.21037000	H	4.16357400	-0.95665500	-0.55486700
C	3.78476900	3.10474900	-0.08403800	H	2.85833200	-2.21589600	-2.17667200
C	4.01164400	1.77885900	-0.44401000	H	1.69243700	-0.80222000	-2.39449200
C	2.95968000	0.85700000	-0.53260900	Cu	1.00603800	-1.68347700	0.28880300
C	1.64879300	1.29199900	-0.19282200	Cl	2.04683300	-1.47141300	2.17853400
C	1.43035500	2.64317100	0.16234500	Cl	-0.16872800	-3.01452500	-0.99531300
C	0.53504500	0.38562400	-0.11875500				
C	-0.72982800	0.30509100	-0.06396300	**INT14**			
C	-1.99803300	-0.28245200	-0.01047000	C	2.35845700	3.36533800	0.75188400
C	-3.15310600	0.45214900	-0.00253100	C	3.59993600	3.09501700	0.16223100
C	-2.91603200	1.91310000	-0.05951300	C	3.78995900	1.91650800	-0.55072600
C	-4.50213600	-0.17451800	0.05052700	C	2.75786700	0.97933700	-0.70344800
O	-5.51102800	0.51863300	0.05926300	C	1.49422900	1.23224500	-0.07875500
C	-4.59835500	-1.69007800	0.09489300	C	1.32204500	2.45485200	0.62454100
C	-4.01825000	2.93343300	-0.00437100	C	0.48088400	0.20696700	-0.00398600
O	-1.73523000	2.27595800	-0.15467100	C	-0.88126200	0.47410000	0.02190400
C	3.26218200	-0.51439700	-0.97652000	C	-1.98397000	-0.36868700	0.20272000
C	2.55707300	-1.21514100	-1.88350800	C	-3.15140300	0.40117100	0.08934000
H	2.30710600	4.57318300	0.49212500	C	-2.72483400	1.71100100	-0.17746300
H	4.61853400	3.79927100	-0.03310900	C	-4.57228000	-0.01921300	0.18800000
H	5.01886600	1.44830200	-0.68206000	O	-5.46406800	0.80693500	0.05388400
H	0.42404300	2.95939100	0.40873800	C	-4.85329500	-1.48206500	0.45484300
H	-2.00363100	-1.36965700	-0.00824600	C	-3.48104600	2.96428400	-0.41882400
H	-5.65383100	-1.96649300	0.11273600	O	-1.39670100	1.77196300	-0.21890100
H	-4.11816400	-2.14876100	-0.77745400	C	3.00817000	-0.20852200	-1.52160400
H	-4.10604300	-2.09249600	0.98838800	C	2.11421400	-0.81390500	-2.32266600
H	-3.57965000	3.93233300	-0.04461600	H	2.21065000	4.27661200	1.32378800
H	-4.71572200	2.78409900	-0.83419600	H	4.41711600	3.80369300	0.26301000
H	-4.61110100	2.80775300	0.90681000	H	4.75147600	1.71449200	-1.01464400

H	0.38025200	2.64711000	1.12324800
H	-1.90237400	-1.43528800	0.36119600
H	-5.93252600	-1.64066300	0.48435800
H	-4.40879600	-2.11325900	-0.32448500
H	-4.41214000	-1.79280300	1.41014400
H	-2.79509100	3.78852000	-0.62571600
H	-4.17430300	2.83113700	-1.25578500
H	-4.10343800	3.20244300	0.45049000
H	4.02540600	-0.59560900	-1.48386200
H	2.37352800	-1.70925100	-2.87872900
H	1.11133400	-0.42815000	-2.47594000
Cu	1.03152400	-1.68706100	0.28219400
Cl	2.44535400	-1.63760500	1.94226000
Cl	-0.22389200	-3.05098200	-0.91452400

TS14-15

C	-2.55059700	3.02488500	-1.05140500
C	-3.72173800	2.87880800	-0.27170000
C	-3.78955800	1.91498500	0.71421000
C	-2.66962500	1.08631600	0.94681900
C	-1.51043000	1.18088300	0.11163800
C	-1.45212300	2.20622100	-0.86074900
C	-0.52457800	0.13159400	0.26178700
C	0.86326000	0.40558100	0.12883700
C	1.97159600	-0.39438800	-0.08185800
C	3.11597000	0.44221700	-0.08474200
C	2.65023200	1.73509200	0.13921900
C	4.54062000	0.08235900	-0.27170000
O	5.40645600	0.94722900	-0.24022000
C	4.87133900	-1.37847200	-0.50095900
C	3.34373500	3.04462300	0.24832900
O	1.31544600	1.72856400	0.27152700
C	-2.53730200	0.08412200	1.94184700
C	-1.24464800	-0.34847400	2.21483600
H	-2.52447500	3.77937400	-1.83254600
H	-4.56821400	3.53507200	-0.45084600
H	-4.67757500	1.80674200	1.33040900
H	-0.57813700	2.30530100	-1.49424100
H	1.93368800	-1.46858500	-0.19817900
H	5.95187000	-1.48997600	-0.60605500
H	4.51705200	-1.99540500	0.33396900
H	4.37583200	-1.74979000	-1.40668100
H	2.62989800	3.82960400	0.50949900
H	4.13784500	2.99367200	0.99932400
H	3.83644900	3.29729900	-0.69723600
H	-3.40825200	-0.44026200	2.33034300
H	-0.46690400	0.38691500	2.39858700
H	-1.05319300	-1.32087200	2.66048700
Cu	-1.05645100	-1.74978900	-0.28876100
Cl	-2.61971800	-1.51909400	-1.77571800
Cl	0.18554500	-3.22853500	0.76044300

INT15

C	-2.77217500	2.78636600	-1.09434100
C	-3.99770200	2.38853700	-0.48190200
C	-4.01145500	1.50989000	0.57584300
C	-2.77251100	1.00799000	1.05816900
C	-1.52637100	1.41526000	0.43716000

C	-1.55159900	2.31468400	-0.65730000	Cl	-2.63878300	-2.36674800	0.52551800
C	-0.45535300	0.76270800	1.09328400				
C	0.91123900	0.77840500	0.78491500	**INT16**			
C	1.99855200	0.10507100	1.32829100	C	5.83515700	-2.02260700	0.45864100
C	3.12747600	0.41767000	0.53501700	C	7.04255100	-1.24767400	0.26956400
C	2.66825000	1.27506100	-0.46566600	C	6.99202800	0.07620600	-0.03857800
C	4.52154200	-0.07082100	0.69296900	C	5.70766900	0.71539900	-0.17943100
O	5.42765000	0.34832200	-0.01212900	C	4.47452500	-0.07651300	0.01359400
C	4.77110200	-1.11557200	1.76416600	C	4.59291300	-1.47183600	0.33885000
C	3.31783400	1.90660400	-1.63736000	C	3.37976500	0.74809000	-0.17389300
O	1.35250200	1.50896900	-0.30065900	C	1.98341000	0.45433100	-0.09839700
C	-2.50570100	0.09406500	2.06913500	C	0.85352500	1.20751000	-0.27843300
C	-1.02591800	-0.04504000	2.23884000	C	-0.27355100	0.33741000	-0.06432200
H	-2.80813600	3.47309400	-1.93501300	C	0.25356300	-0.91550100	0.23836200
H	-4.93126000	2.78390300	-0.87113700	C	-1.68248500	0.62957600	-0.14136800
H	-4.94335400	1.19033600	1.03192000	O	-2.50339200	-0.29840900	0.08186600
H	-0.63200000	2.61184900	-1.14499000	C	-2.17799200	2.00559200	-0.48821400
H	1.96329900	-0.55652200	2.18196100	C	-0.35769800	-2.23098700	0.55724600
H	5.83340000	-1.36479300	1.77707600	O	1.59501000	-0.84714900	0.21867500
H	4.47186100	-0.74576900	2.75284300	C	5.37786600	2.00339300	-0.47939900
H	4.18617900	-2.02104200	1.56031300	C	3.88485000	2.13483300	-0.50176800
H	3.09383300	2.97924100	-1.67307600	H	5.93364100	-3.07675600	0.70381500
H	4.39443900	1.74872200	-1.58621700	H	8.00118700	-1.74716100	0.37941500
H	2.92498800	1.45241000	-2.55649400	H	7.89880100	0.65795900	-0.18046100
H	-3.23329300	-0.37190600	2.71994100	H	3.70268500	-2.07191700	0.48506700
H	-0.71463300	0.37726500	3.20860000	H	0.82995600	2.25611400	-0.53443600
H	-0.71165300	-1.09301000	2.22620200	H	-2.86396900	2.34028200	0.29942700
Cu	-1.08050400	-1.91200100	-0.90256600	H	-1.37576800	2.73409800	-0.60930400
Cl	0.52210400	-1.34262600	-2.19978500	H	-2.75278900	1.94963000	-1.42144900

H	-0.99356800	-2.15849600	1.44673400
H	-1.00571400	-2.56706600	-0.25989300
H	0.42493600	-2.97349400	0.73035400
H	6.06059600	2.82139800	-0.67588700
H	3.53475700	2.88106000	0.22791600
H	3.52576500	2.48104900	-1.48317700
Cu	-4.46149900	-0.17308700	0.04125900
Cl	-4.94253800	0.89558300	1.86073700
Cl	-5.03314200	-1.09711400	-1.81977700

TS16-2r

C	5.81577800	2.00861100	-0.60583200
C	7.01609400	1.27110300	-0.40985900
C	6.97364100	-0.05167900	-0.03075300
C	5.71325000	-0.65889700	0.18734500
C	4.49239000	0.08486700	0.00203900
C	4.57451800	1.43969000	-0.41723600
C	3.38254200	-0.77450300	0.26022000
C	1.97354900	-0.49277600	0.16645700
C	0.84309600	-1.25552700	0.24967000
C	-0.27951500	-0.36366000	0.09394200
C	0.25491100	0.90911600	-0.07917000
C	-1.68933700	-0.65721000	0.11055600
O	-2.50443100	0.28785700	-0.05783600
C	-2.19459800	-2.05539000	0.33359500
C	-0.34357000	2.25254900	-0.28718000
O	1.59678100	0.83123400	-0.03558500
C	5.37997000	-1.97782500	0.57638400
C	3.90314700	-2.05489500	0.59854400
H	5.88376400	3.04847100	-0.91459400
H	7.97253200	1.76159800	-0.56702600
H	7.88719500	-0.62269000	0.11332700
H	3.67307900	2.01938600	-0.57628400
H	0.80997100	-2.32504700	0.39376100
H	-2.87137800	-2.31998100	-0.48771800
H	-1.39635600	-2.79480400	0.40467300
H	-2.78124000	-2.07530800	1.26100100
H	-0.92812300	2.27980400	-1.21400900
H	-1.03721200	2.49918200	0.52395300
H	0.44462200	3.00781600	-0.33504300
H	6.03758800	-2.77675600	0.89412800
H	4.55197500	-2.51837900	-0.38527200
H	3.35388800	-2.88014200	1.03733600
Cu	-4.46273600	0.17760700	-0.06472200
Cl	-4.92412500	-0.79298100	-1.94427100
Cl	-5.06499100	1.01957200	1.82566600

2r-$CuCl_2$

C	5.76809000	-2.06527900	0.56693100
C	6.95889600	-1.34192800	0.44740600
C	6.93252000	0.01973200	0.12378700
C	5.70508700	0.63783300	-0.07922600
C	4.50234700	-0.09097800	0.03861900
C	4.52957800	-1.44946300	0.36539100
C	3.38160100	0.84130900	-0.22259600
C	1.96574700	0.52313000	-0.17441900
C	0.83846200	1.27338600	-0.02716500
C	-0.28110500	0.36832000	-0.08851900

C	0.25770900	-0.90306500	-0.26666600	C	-6.94013300	-0.01720500	-0.37148700
C	-1.69114000	0.65393700	0.01062900	C	-5.68108300	-0.67046900	-0.30877600
O	-2.50446500	-0.30370000	-0.04693500	C	-4.50686700	0.08939500	0.03016200
C	-2.19350500	2.06115900	0.17458100	C	-4.60158700	1.47824000	0.27817200
C	-0.33771000	-2.25695800	-0.40454300	C	-3.38854700	-0.80619800	0.05752700
O	1.59641000	-0.80979200	-0.31657400	C	-1.97427700	-0.51293100	0.09260900
C	5.38635600	2.07347700	-0.42472300	C	-0.86946500	-1.12862200	-0.41395400
C	3.88361000	2.07237500	-0.49391800	C	0.27085200	-0.34595700	-0.00451800
H	5.80414500	-3.12134800	0.82039200	C	-0.23534700	0.72352300	0.72864100
H	7.91132000	-1.83972600	0.60739000	C	1.67044300	-0.55875000	-0.27805000
H	7.85957800	0.58104300	0.03478500	O	2.50369200	0.26906400	0.17229900
H	3.61296900	-2.02055400	0.45876100	C	2.14000000	-1.73655400	-1.08505300
H	0.81011200	2.34171900	0.12687000	C	0.39245500	1.88754900	1.40479000
H	-2.79368300	2.11440200	1.09129500	O	-1.57307800	0.62086100	0.79484700
H	-1.39493700	2.80227200	0.21687400	C	-5.32772100	-2.02616800	-0.49132800
H	-2.85781200	2.29988800	-0.66543100	C	-3.94796000	-2.16147100	-0.25726100
H	-0.88357900	-2.53661600	0.50395800	H	-5.92395400	3.15592700	0.35129400
H	-1.06481100	-2.27876800	-1.22316200	H	-7.95813500	1.85315400	-0.19693200
H	0.44855300	-2.99154900	-0.59414200	H	-7.83608600	-0.58386700	-0.61091700
H	5.83669700	2.38723400	-1.37827400	H	-3.71740900	2.05284200	0.53349600
H	5.76154500	2.77826600	0.33272300	H	-0.86855200	-2.01796700	-1.02624100
H	3.29852300	2.94940600	-0.74759500	H	2.86447600	-2.30328800	-0.48719200
Cu	-4.46100800	-0.18410100	0.07605500	H	1.33024400	-2.39579500	-1.39922800
Cl	-4.80966800	0.19460200	2.17747900	H	2.66628200	-1.36834700	-1.97473000
Cl	-5.15234400	-0.41346800	-1.95132500	H	-0.37709300	2.50329400	1.87626400
				H	1.10836900	1.55442000	2.16419700

TS16-2r'

C	-5.83584600	2.08679400	0.17909100	H	0.95887000	2.49387200	0.68914700
C	-7.00240500	1.33902300	-0.13941300	H	-6.00480400	-2.84288200	-0.70577300
				H	-3.70692000	-1.79873300	0.94338400

H	-3.32908400	-3.03078600	-0.44863200
Cu	4.45634700	0.18732100	-0.02439700
Cl	5.02278600	-1.38284300	1.35314100
Cl	4.92661000	1.63785800	-1.54518200

2r'-$CuCl_2$

C	-5.41703100	-2.21792000	-0.09835500
C	-6.25245000	-1.75266600	0.92209700
C	-6.17769500	-0.42642800	1.36047400
C	-5.24892300	0.42423200	0.75975400
C	-4.41097700	-0.04847300	-0.27132800
C	-4.48612100	-1.36373800	-0.70655200
C	-3.51913800	1.10009700	-0.74176200
C	-2.05298000	0.81032500	-0.66669300
C	-1.06441300	1.11077500	0.20877900
C	0.13849100	0.47975800	-0.28848800
C	-0.22351400	-0.17372400	-1.46127400
C	1.46795100	0.48685800	0.26693200
O	2.37744800	-0.13734100	-0.33849400
C	1.77695700	1.21449900	1.54537200
C	0.52326200	-0.99382200	-2.44978700
O	-1.53467900	0.02569300	-1.68836900
C	-4.93423600	1.83755000	0.99638900
C	-3.95353100	2.23747900	0.16606900
H	-5.48984600	-3.25174400	-0.42427500
H	-6.96883500	-2.42965300	1.37942100
H	-6.83015200	-0.06918100	2.15296300
H	-3.83899500	-1.72965300	-1.49929400
H	-1.17636400	1.70405500	1.10377600
H	2.59521500	1.92035700	1.35757700
H	0.91928000	1.74879000	1.95495800
H	2.13321600	0.48885000	2.28752400
H	-0.15269200	-1.33182800	-3.23890700
H	1.34152200	-0.41645500	-2.89438600
H	0.98318700	-1.86222300	-1.96556900
H	-5.43695500	2.45937900	1.73007700
H	-3.75797200	1.34567800	-1.78925600
H	-3.51949200	3.22916600	0.10657400
Cu	4.26152300	-0.26864300	0.19885500
Cl	5.06872800	1.67508400	-0.30413200
Cl	4.45354700	-2.23217500	1.06514100

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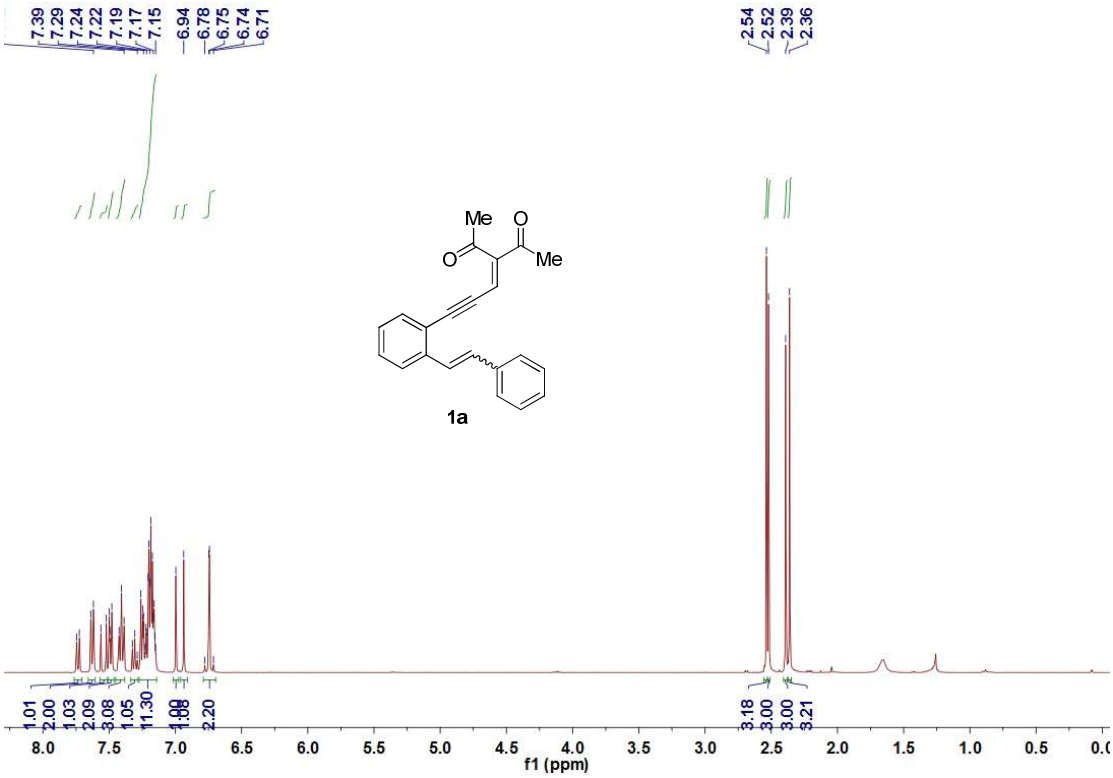
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2.52
2.39
2.36
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O
O
Me
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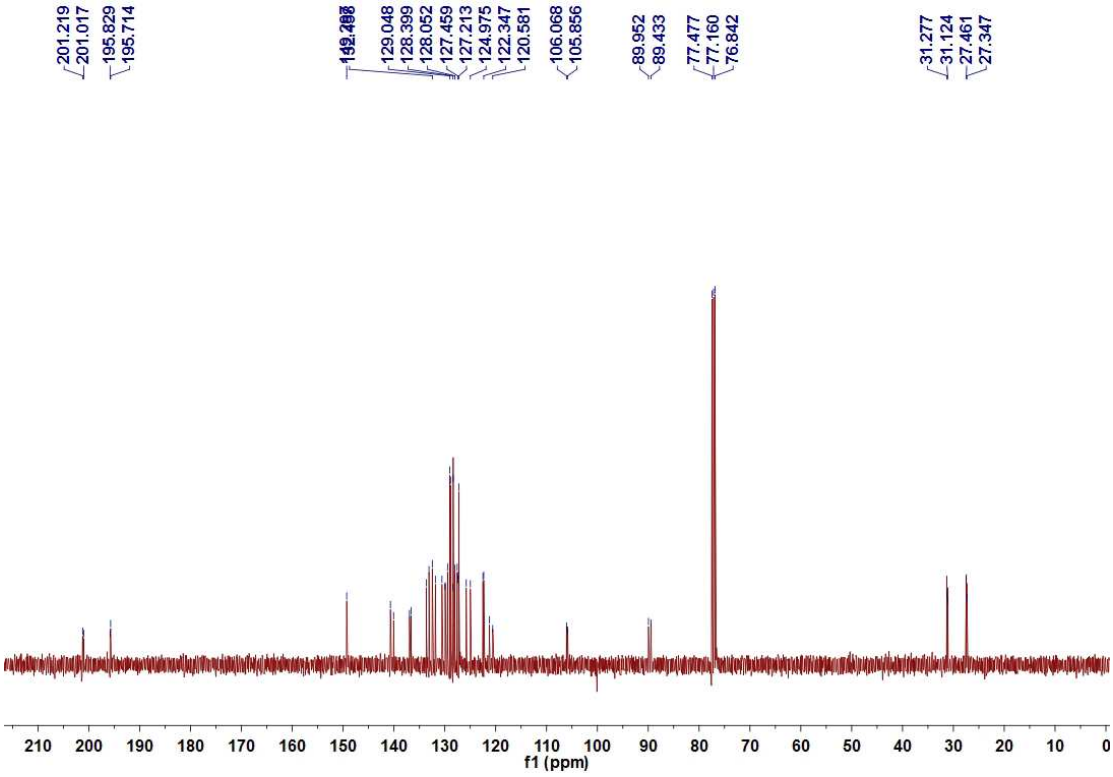
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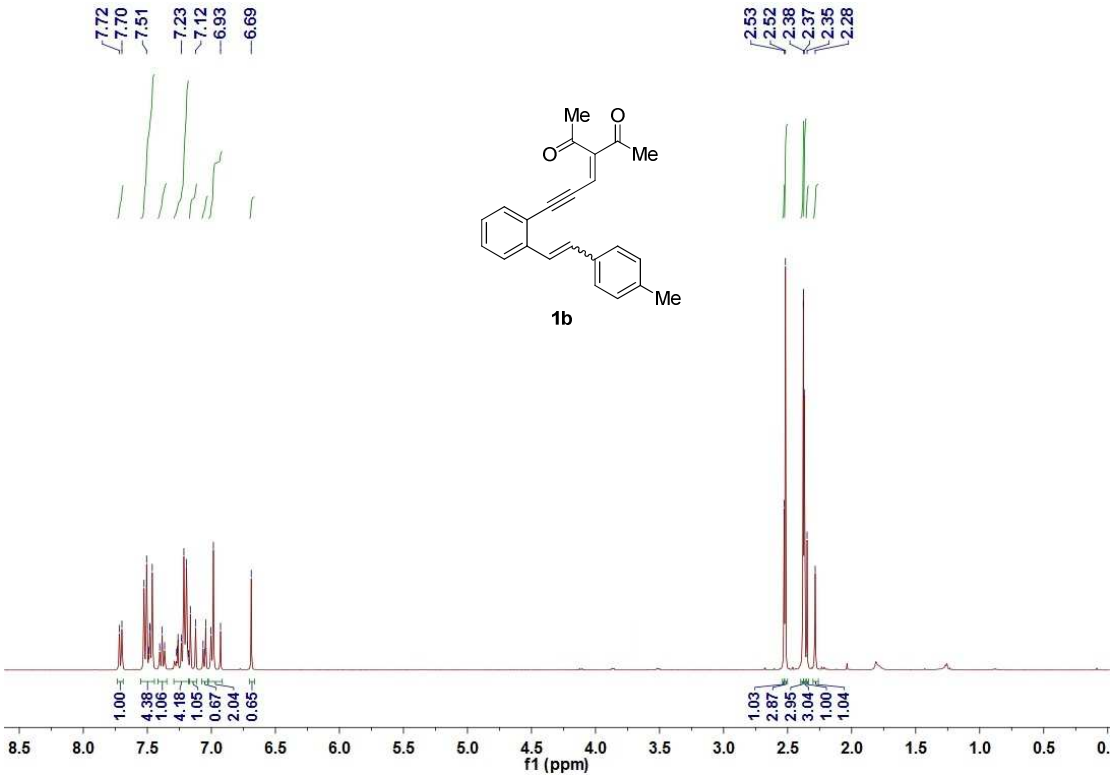
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O
O
Me
Me
1b
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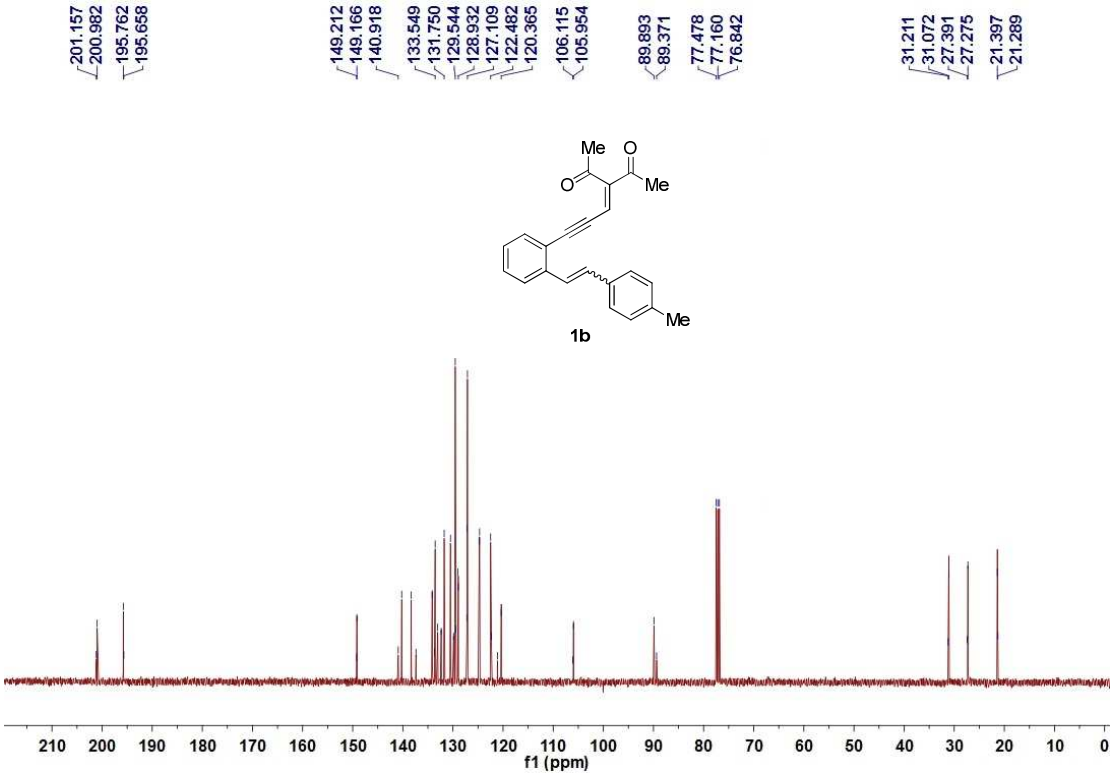
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Me
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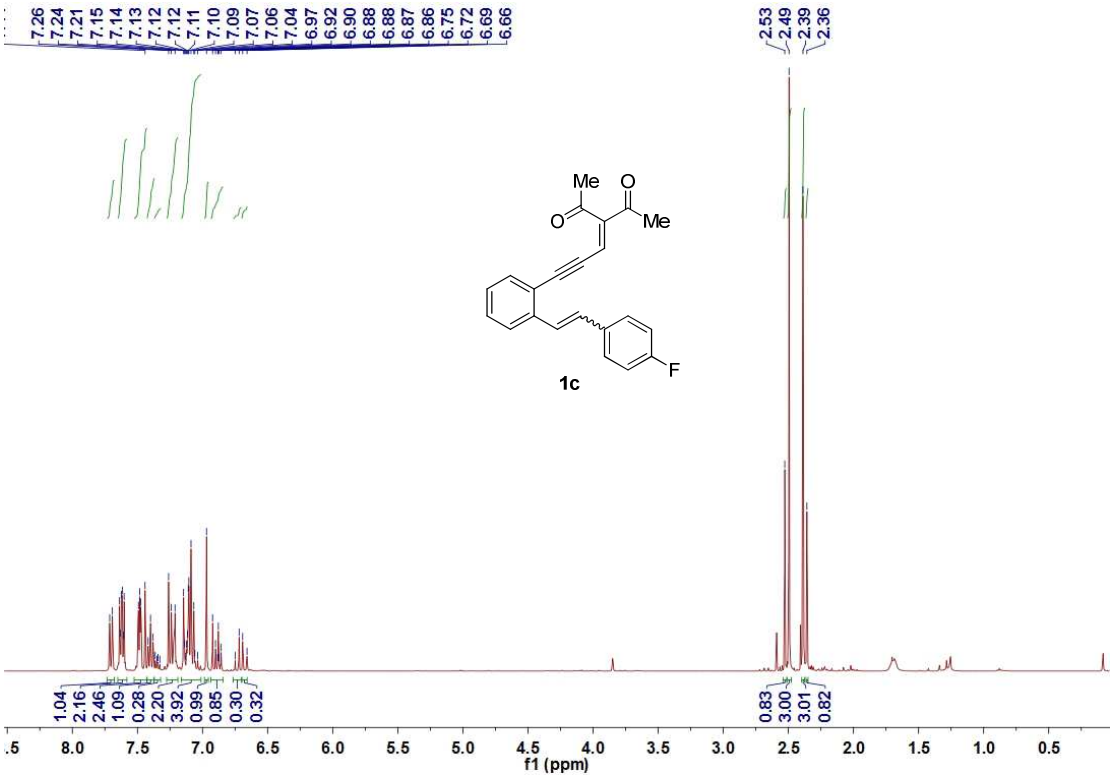
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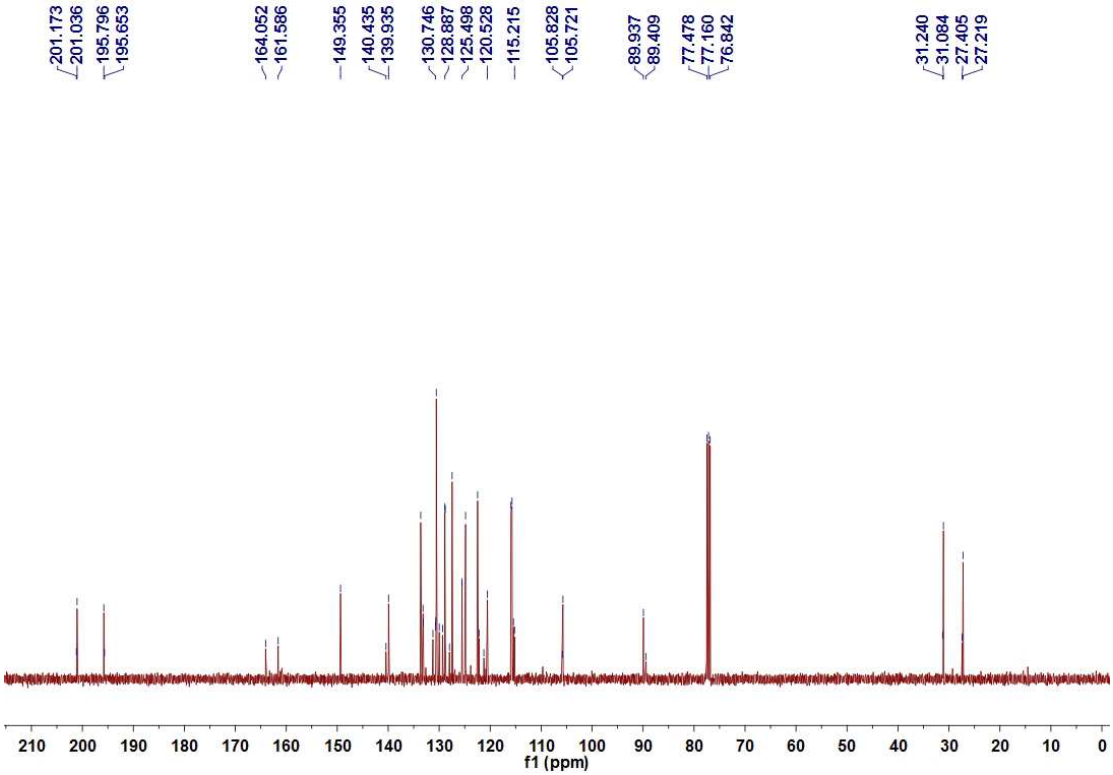
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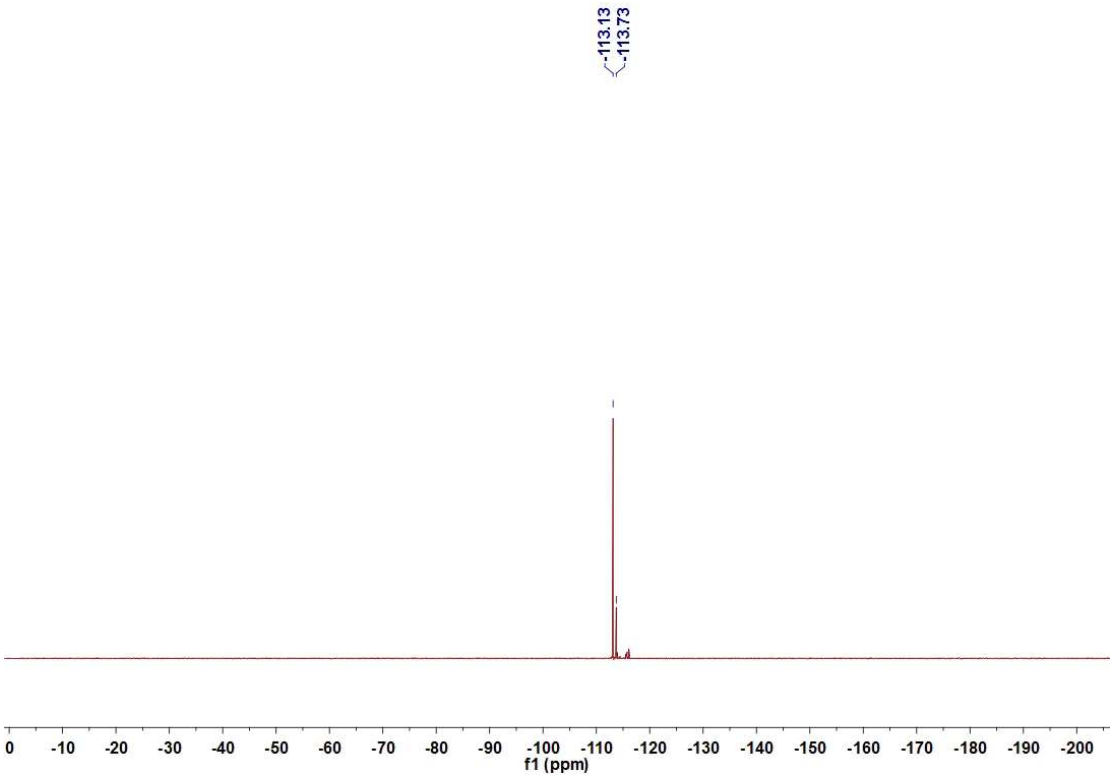
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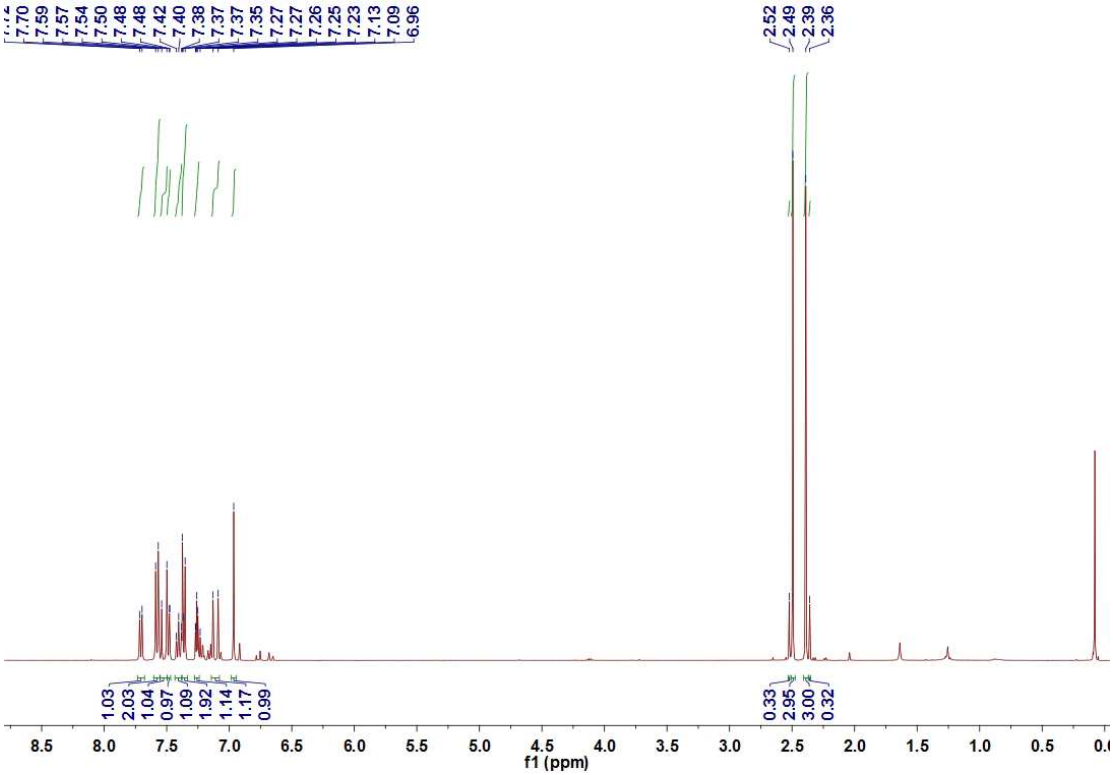
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7.09
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2.49
2.39
2.36
1.03
2.03
1.04
0.97
1.09
1.92
1.14
1.17
0.99
0.33
2.95
3.00
0.32
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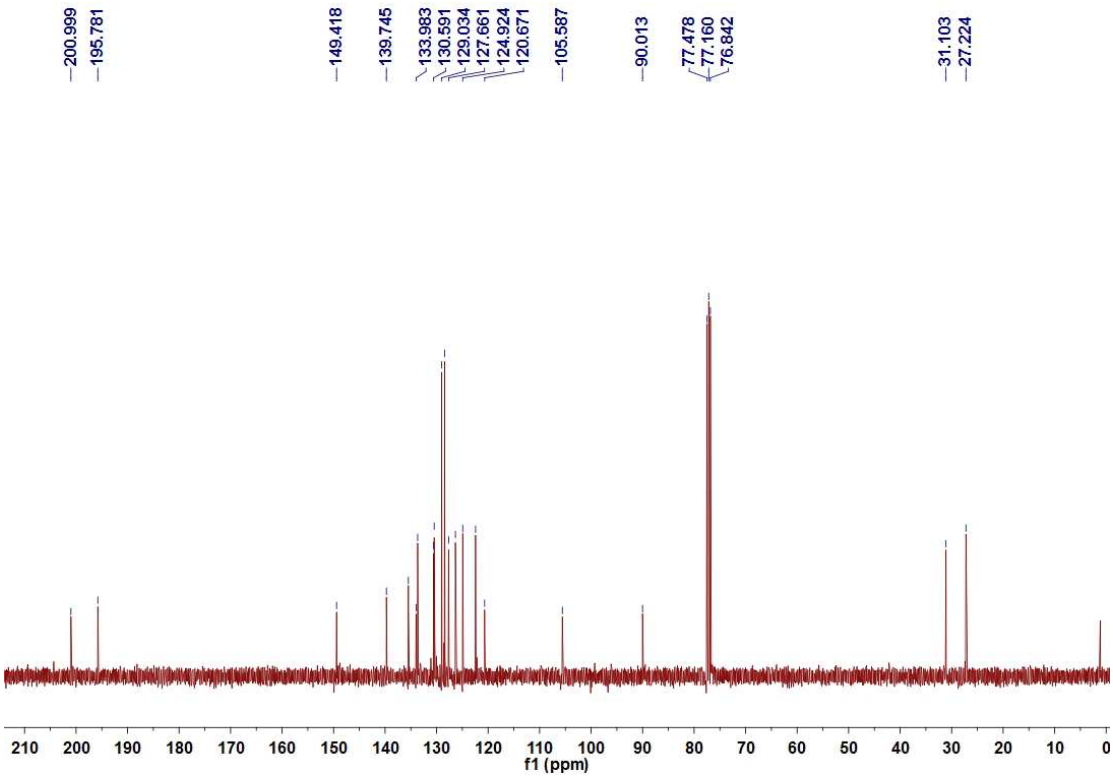
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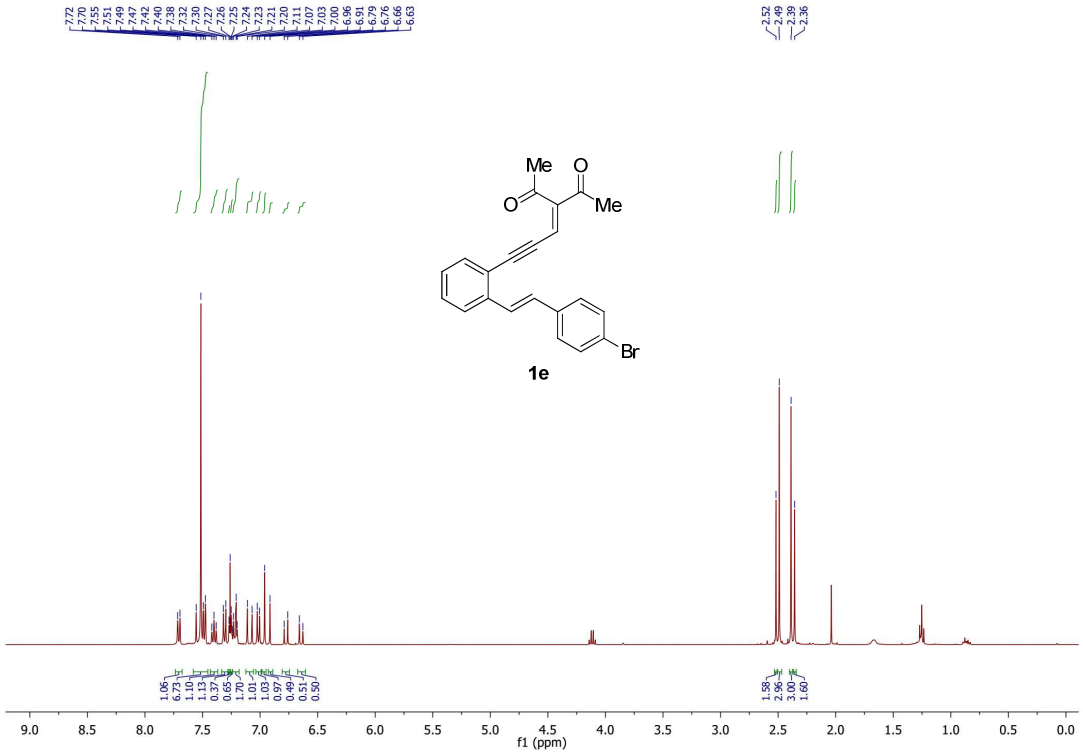
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Br
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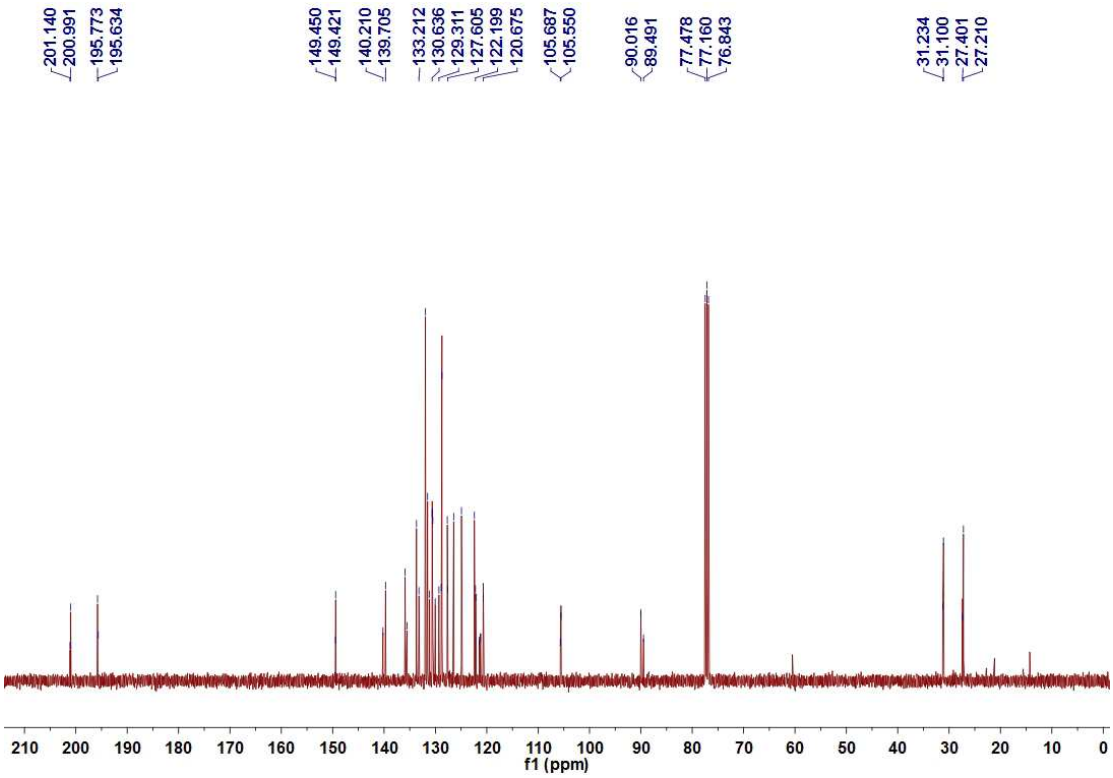
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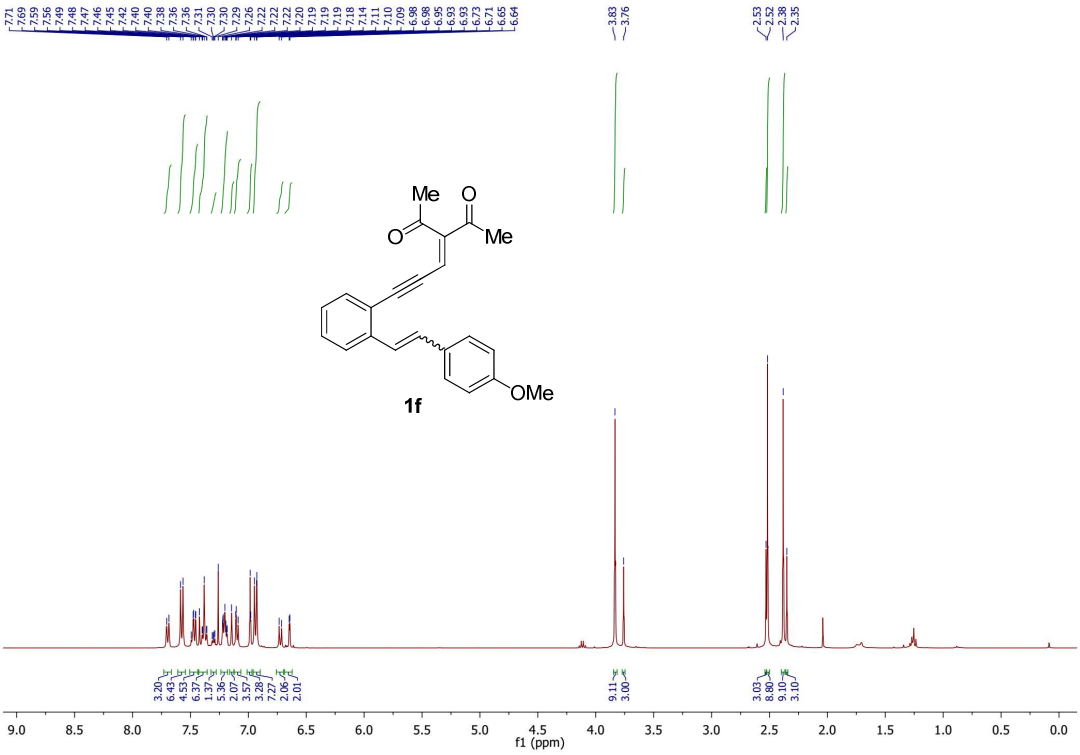
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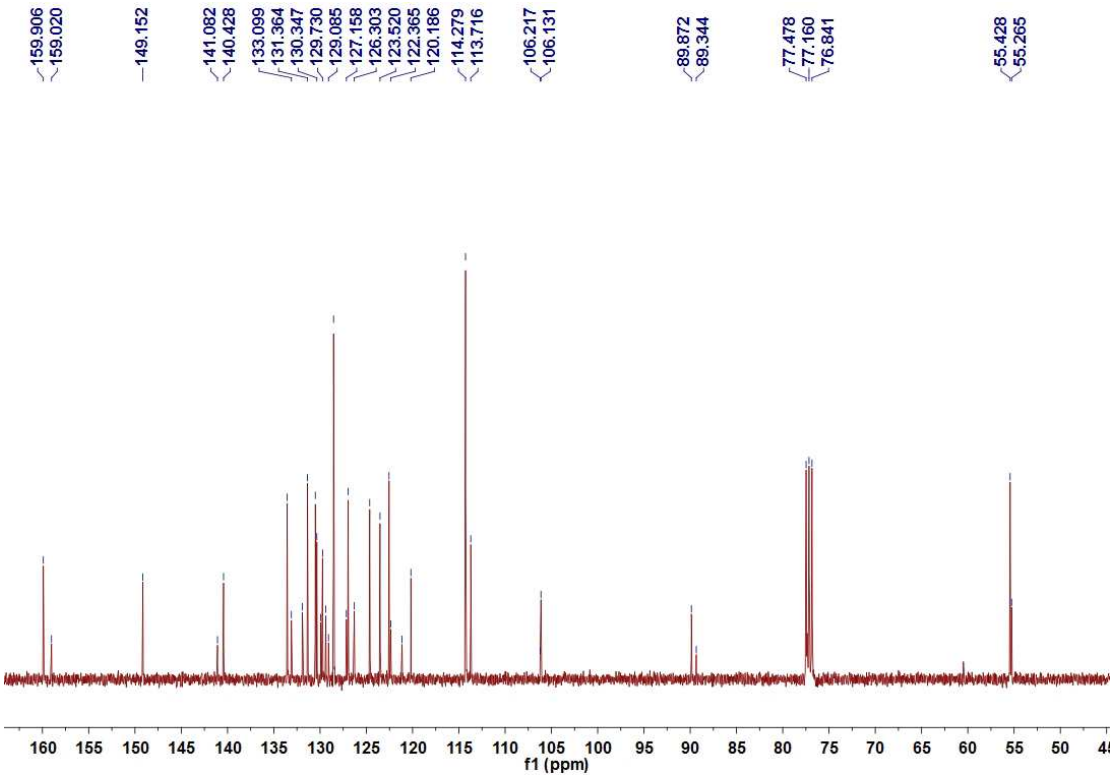
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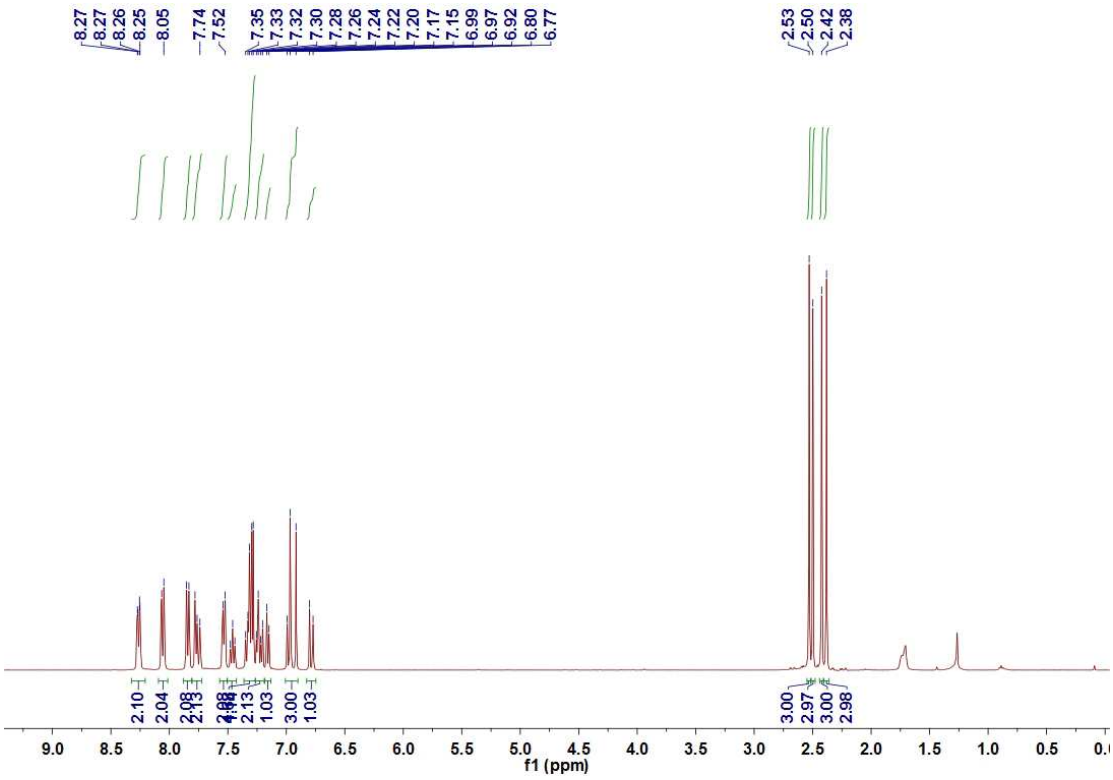
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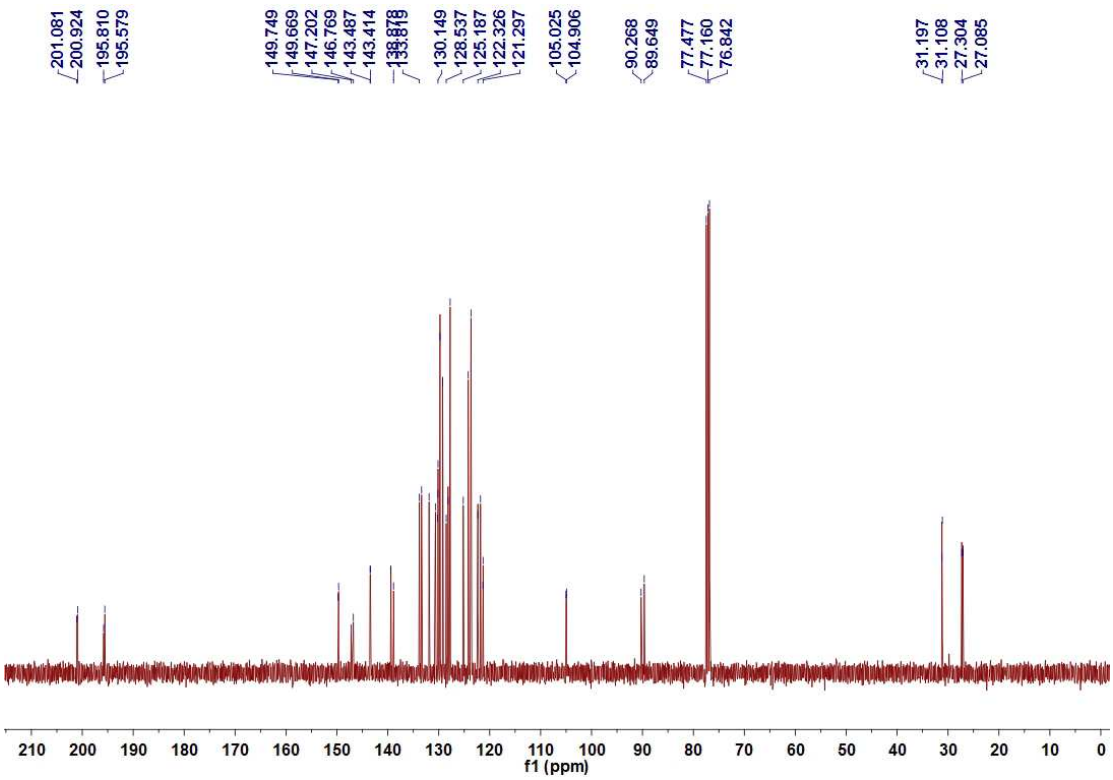
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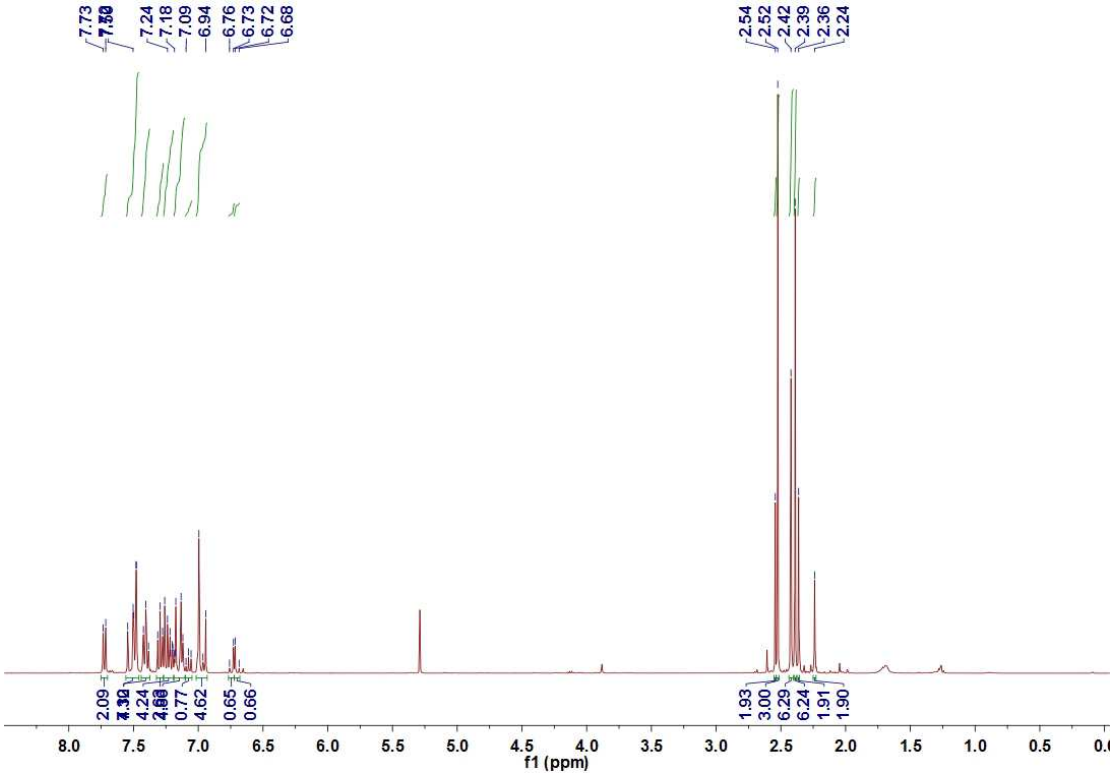
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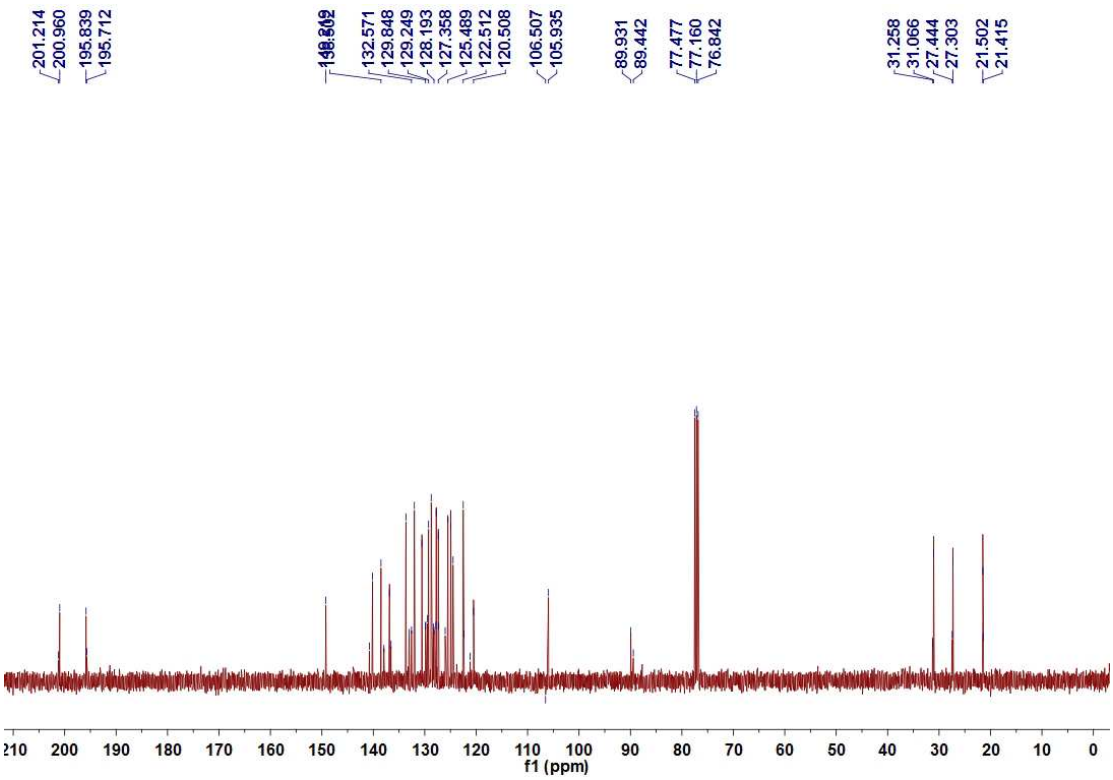
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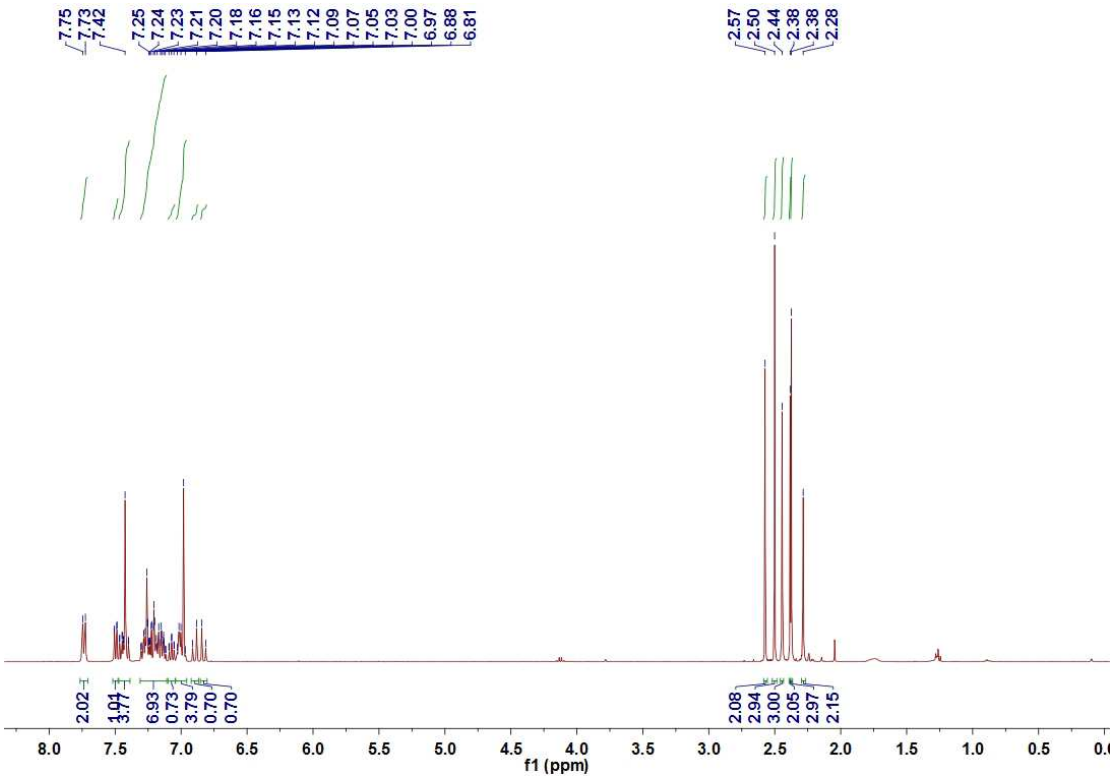
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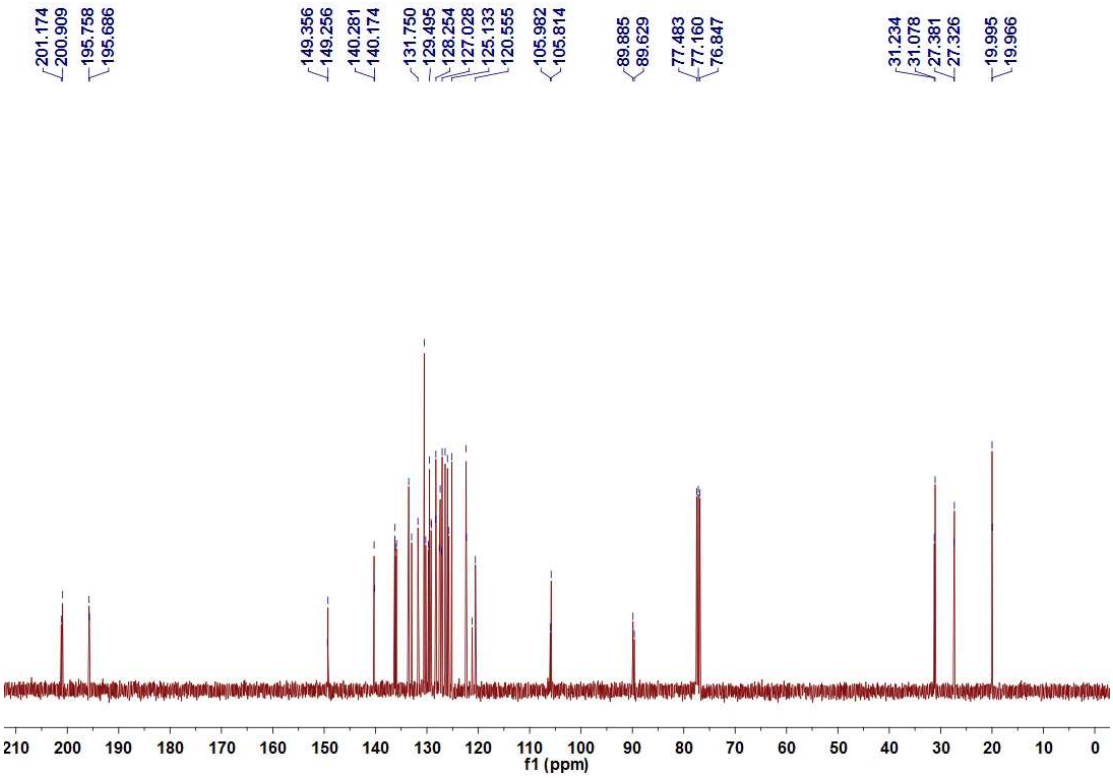
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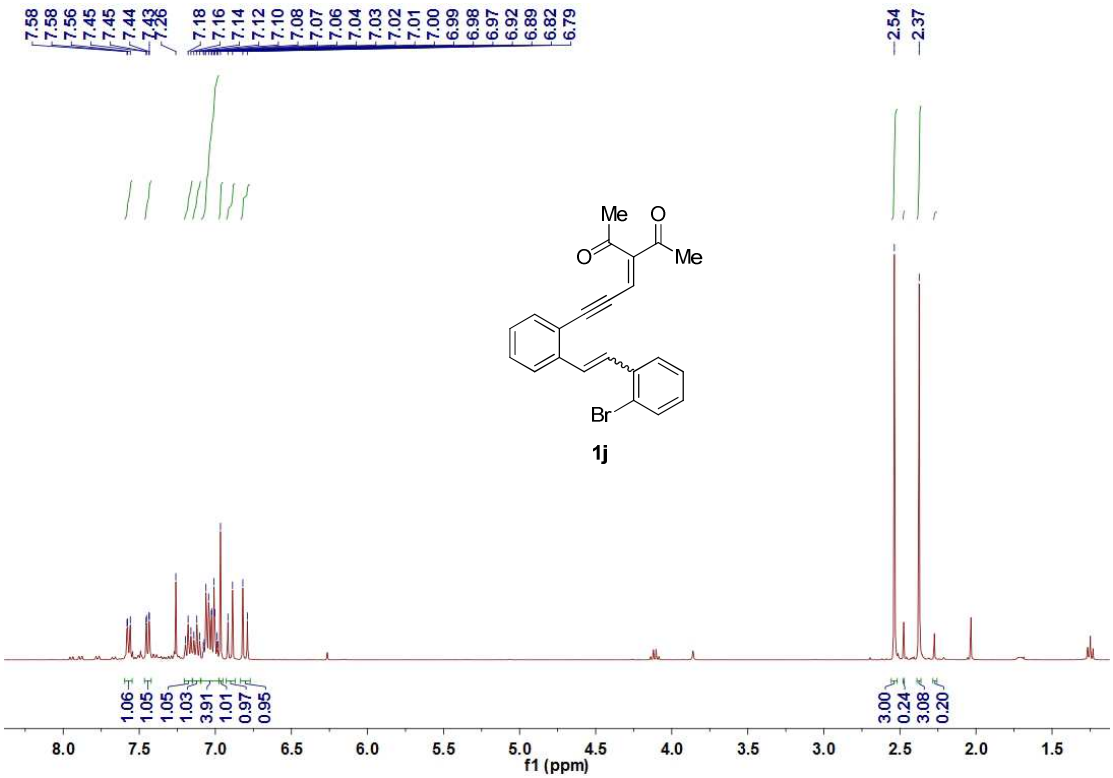
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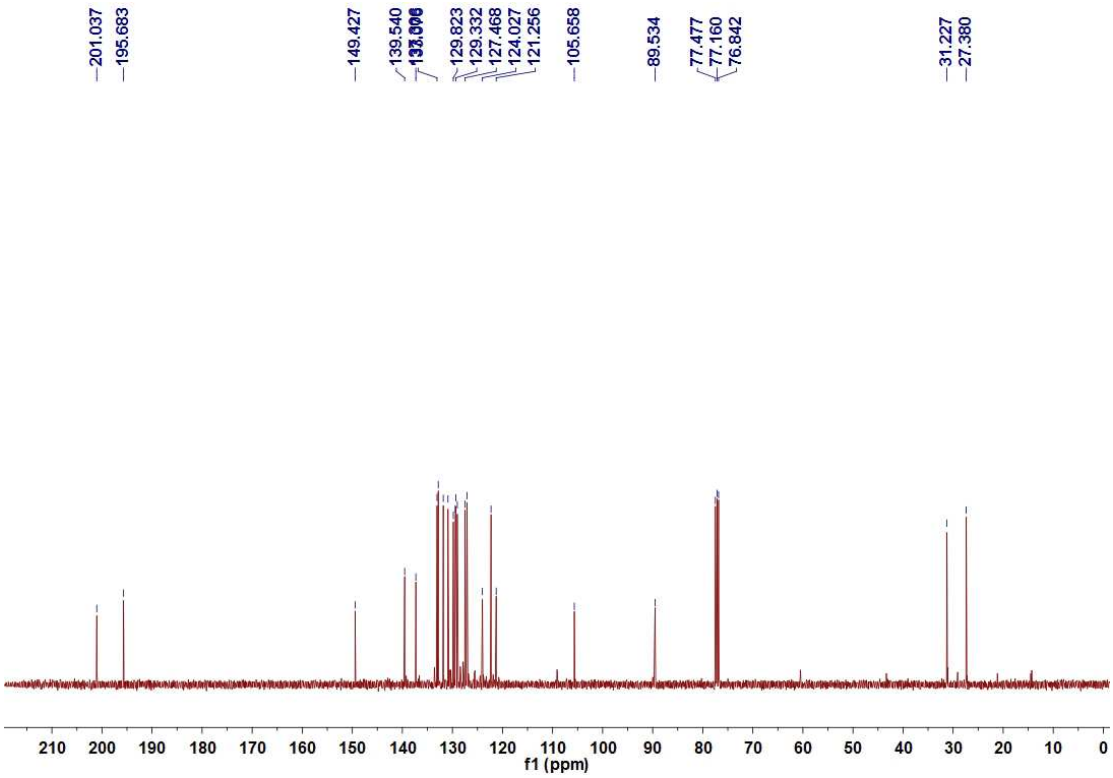
1j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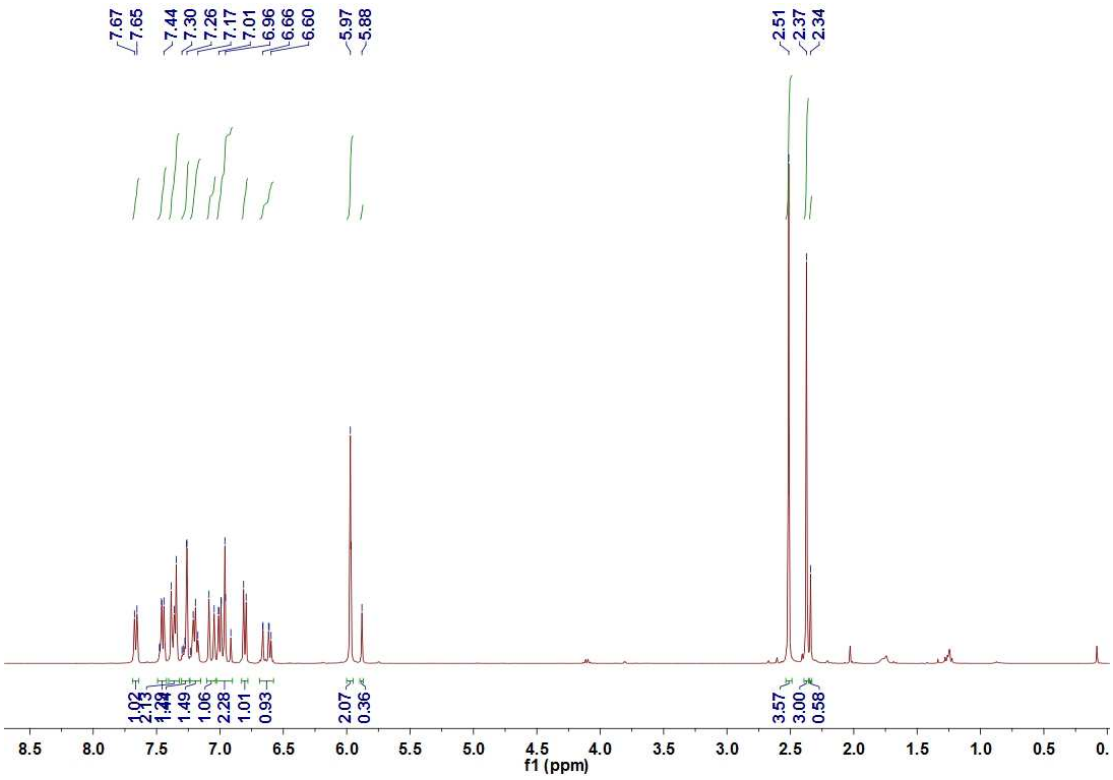
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2.34
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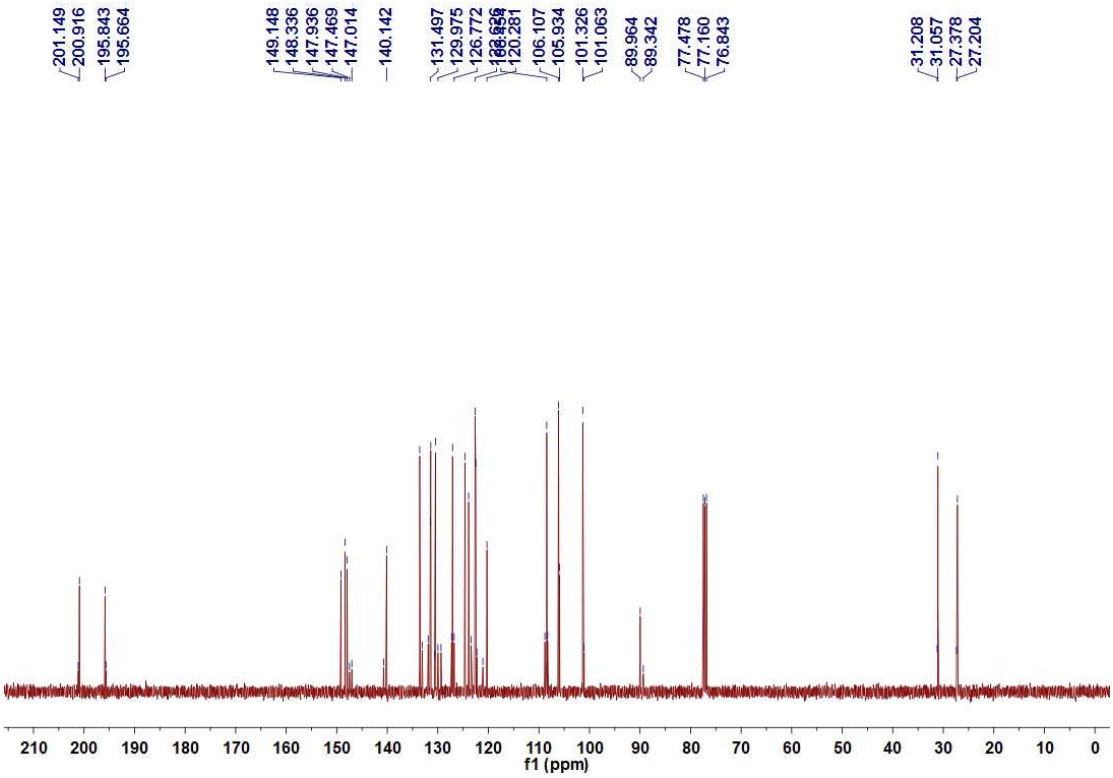
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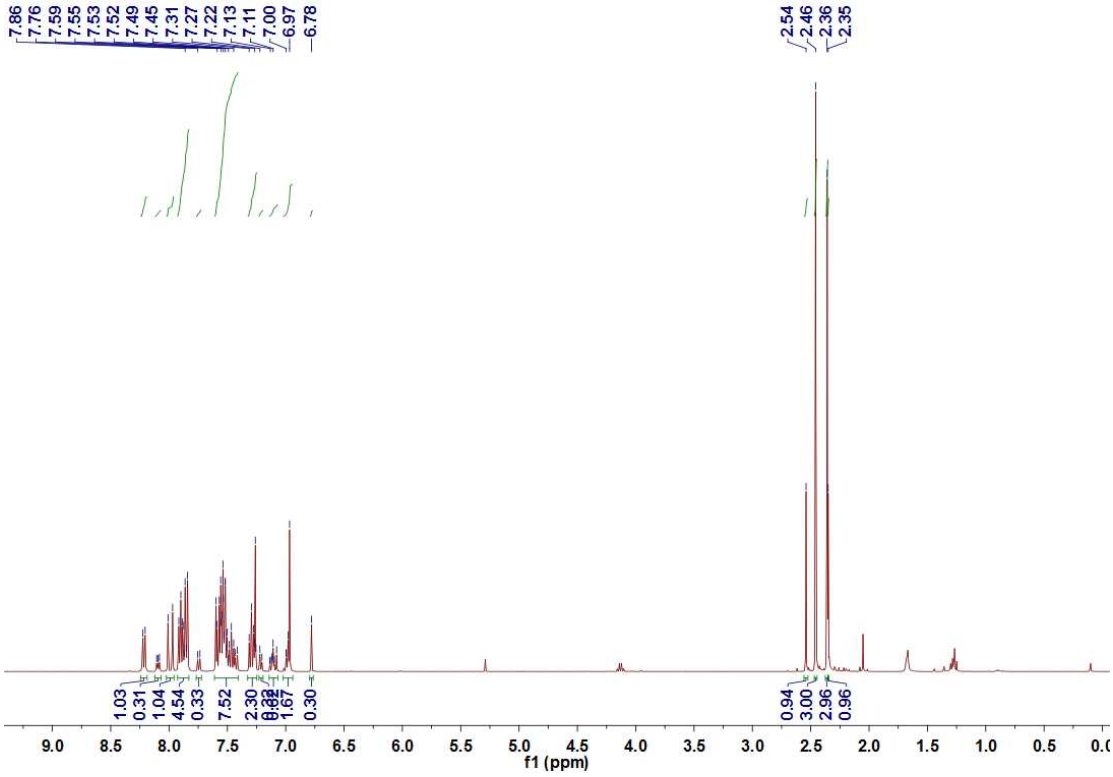
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2.46
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0.31
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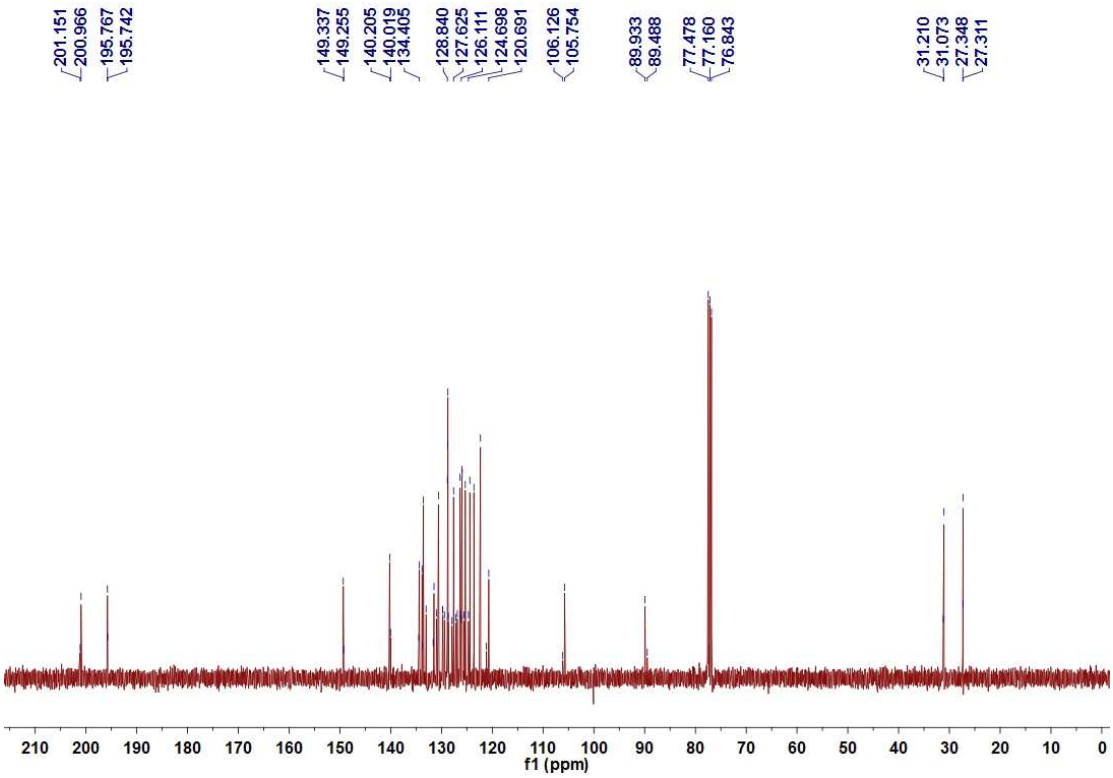
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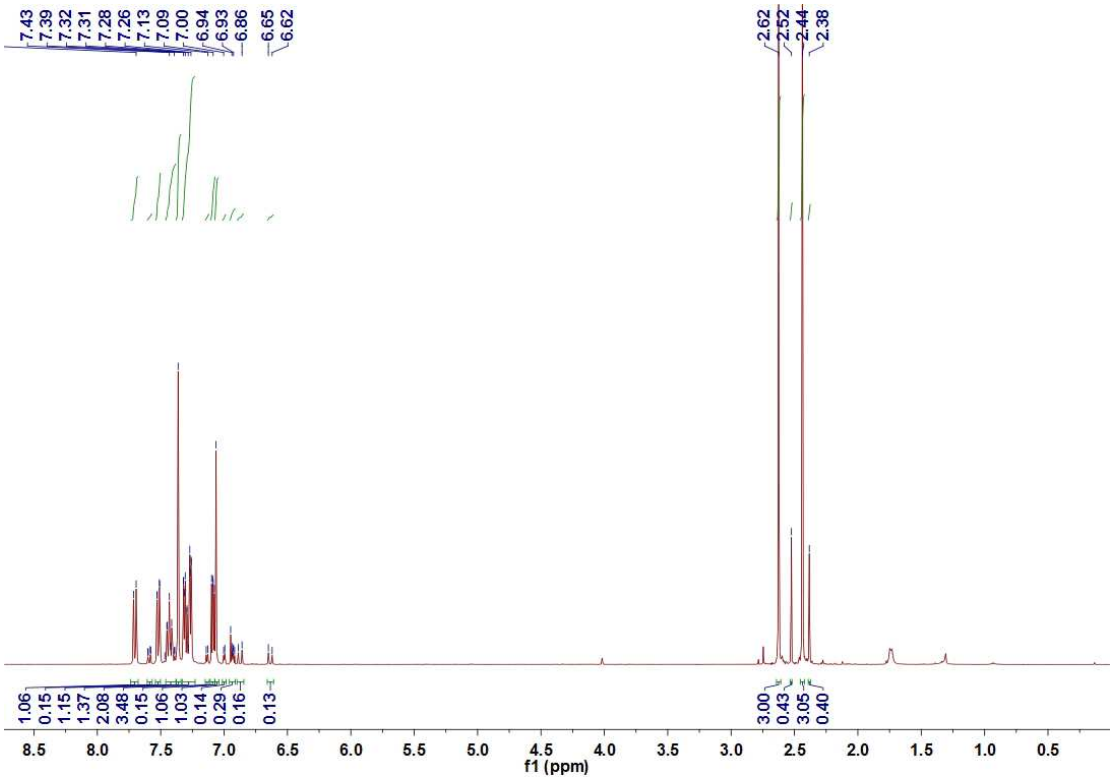
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2.38
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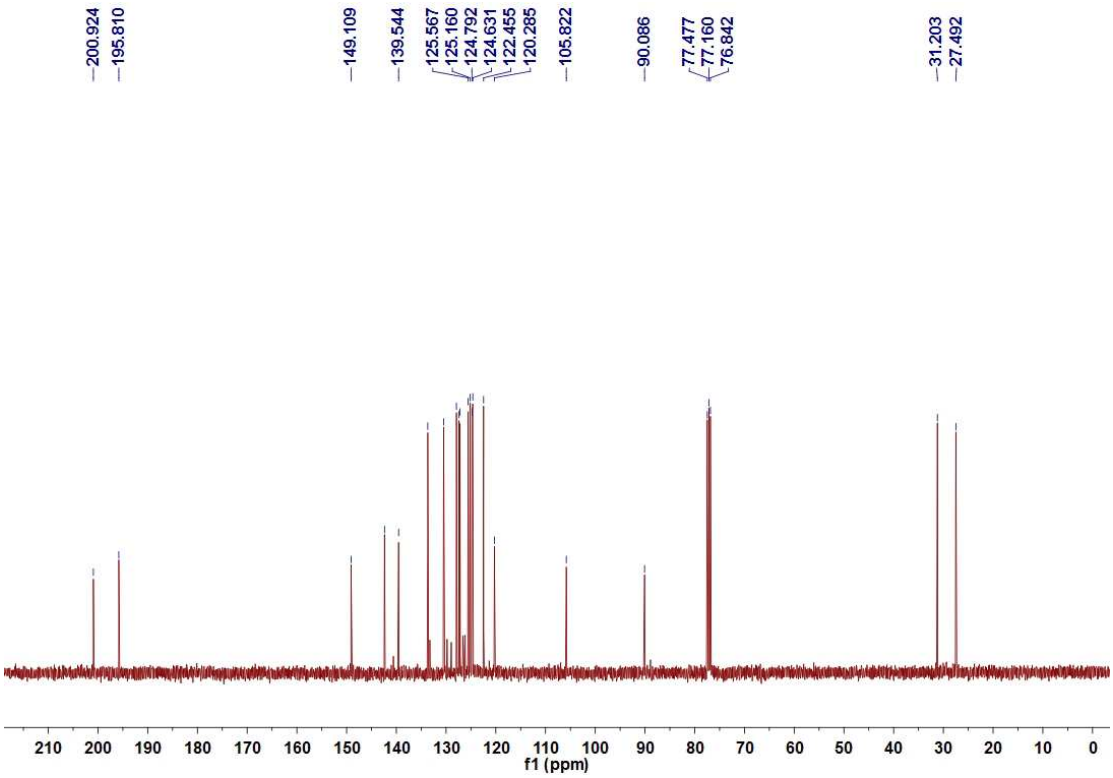
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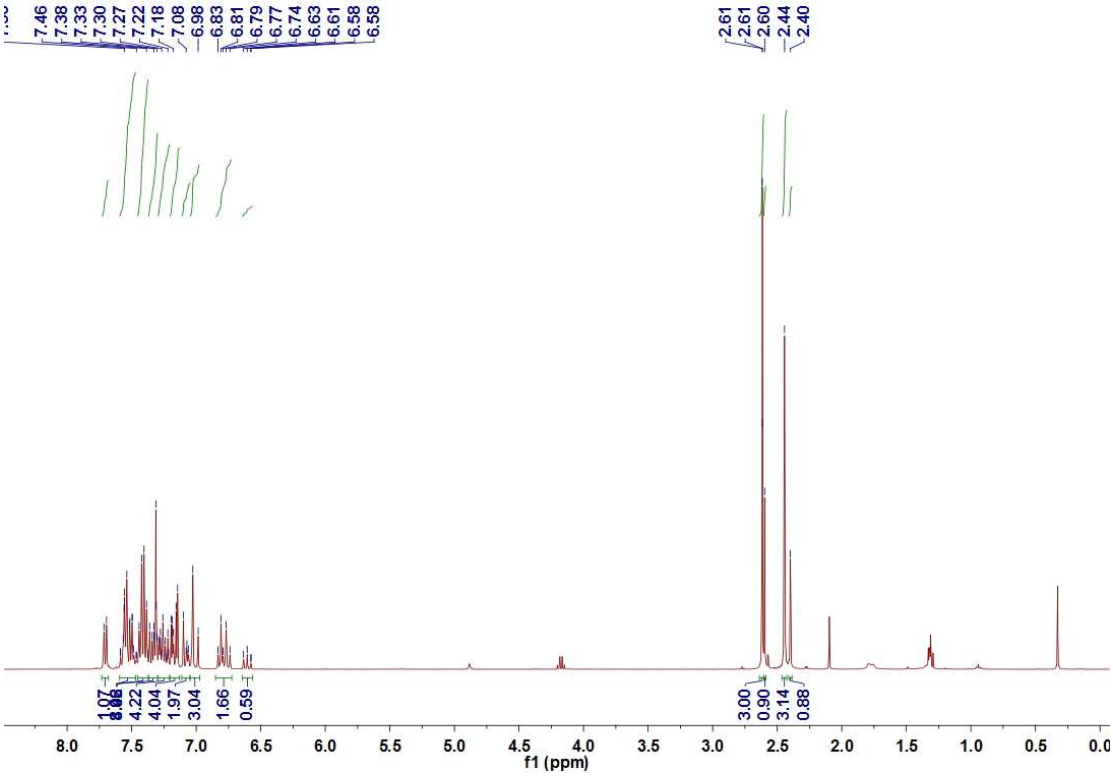
f1 (ppm)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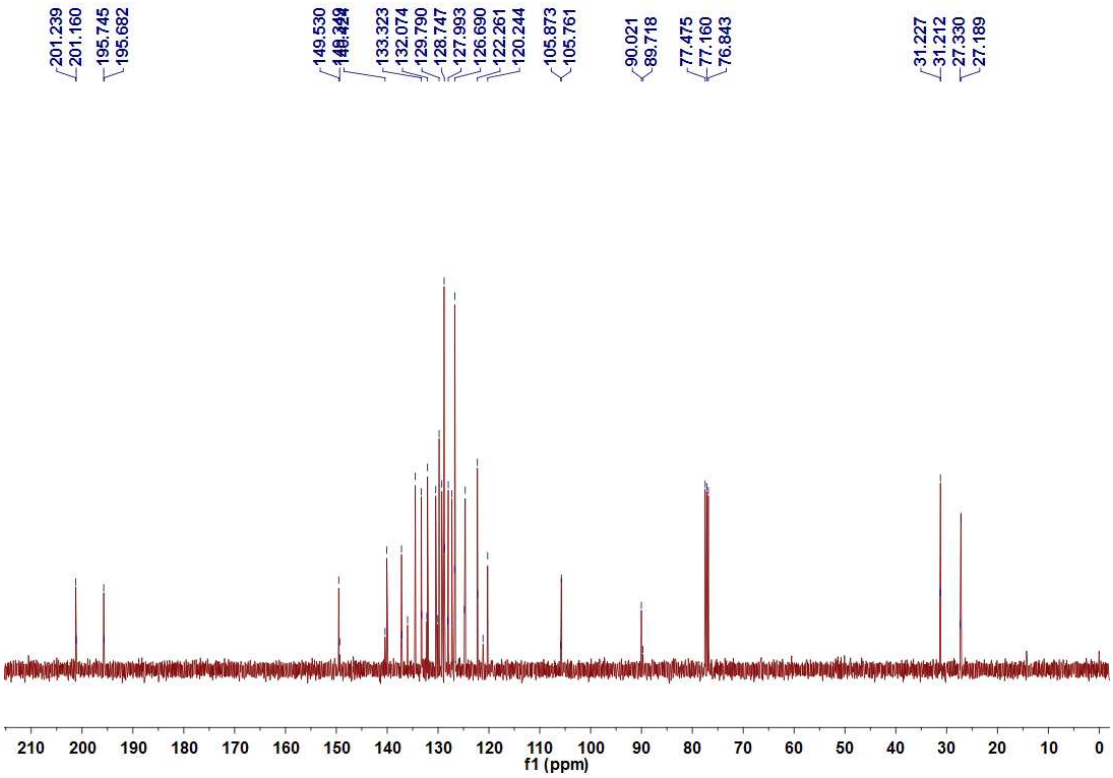
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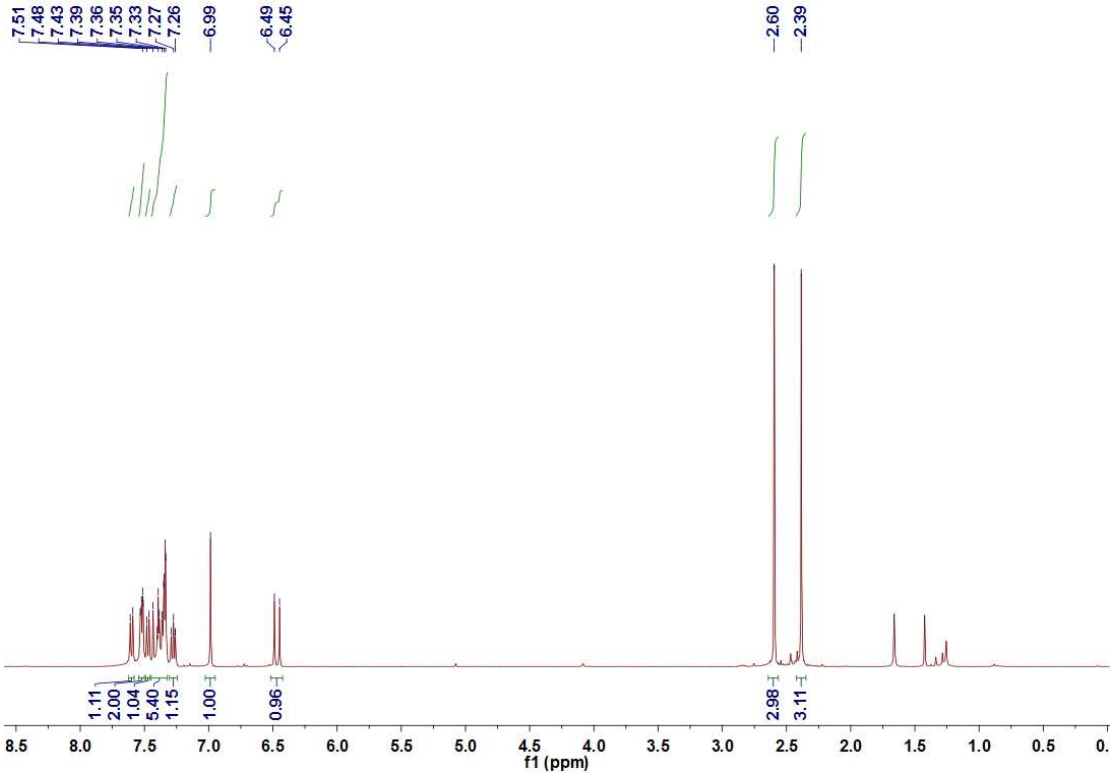
27.330
27.189
f1 (ppm)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7.48
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7.33
7.27
7.26
6.99
6.49
6.45
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2.39
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2.00
1.04
5.40
1.15
1.00
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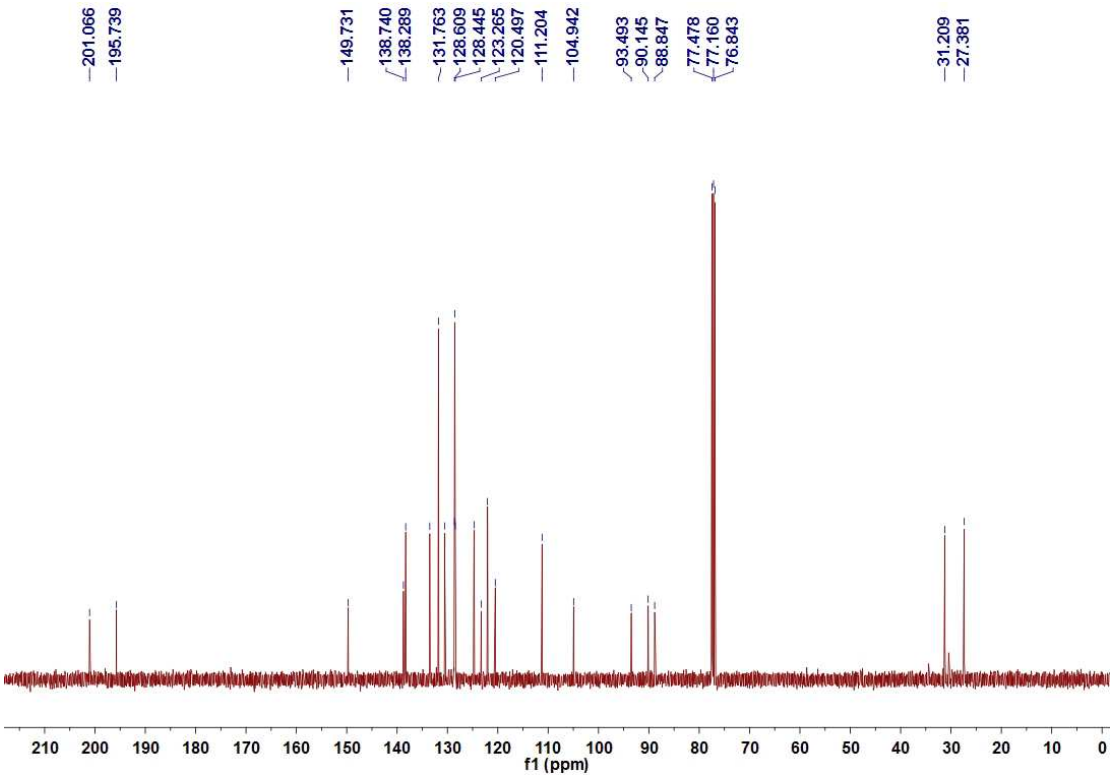
2.98
3.11
f1 (ppm)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131.763
128.609
128.445
123.265
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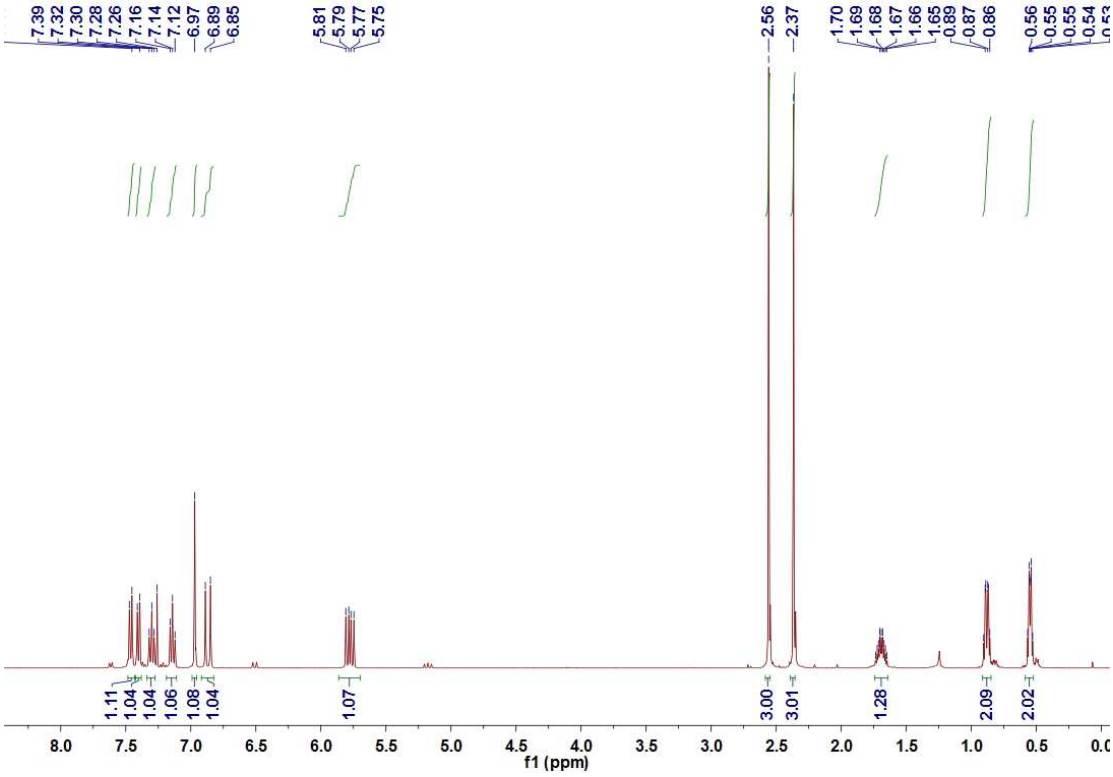
93.493
90.145
88.847
77.478
77.160
76.843
31.209
27.381
f1 (ppm)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7.16
7.14
7.12
6.97
6.89
6.85
5.81
5.79
5.77
5.75
2.56
2.37
1.70
1.69
1.68
1.67
1.66
1.65
0.89
0.87
0.86
0.56
0.55
0.55
0.54
1.11
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1.04
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1.08
1.04
1.07
3.00
3.01
1.28
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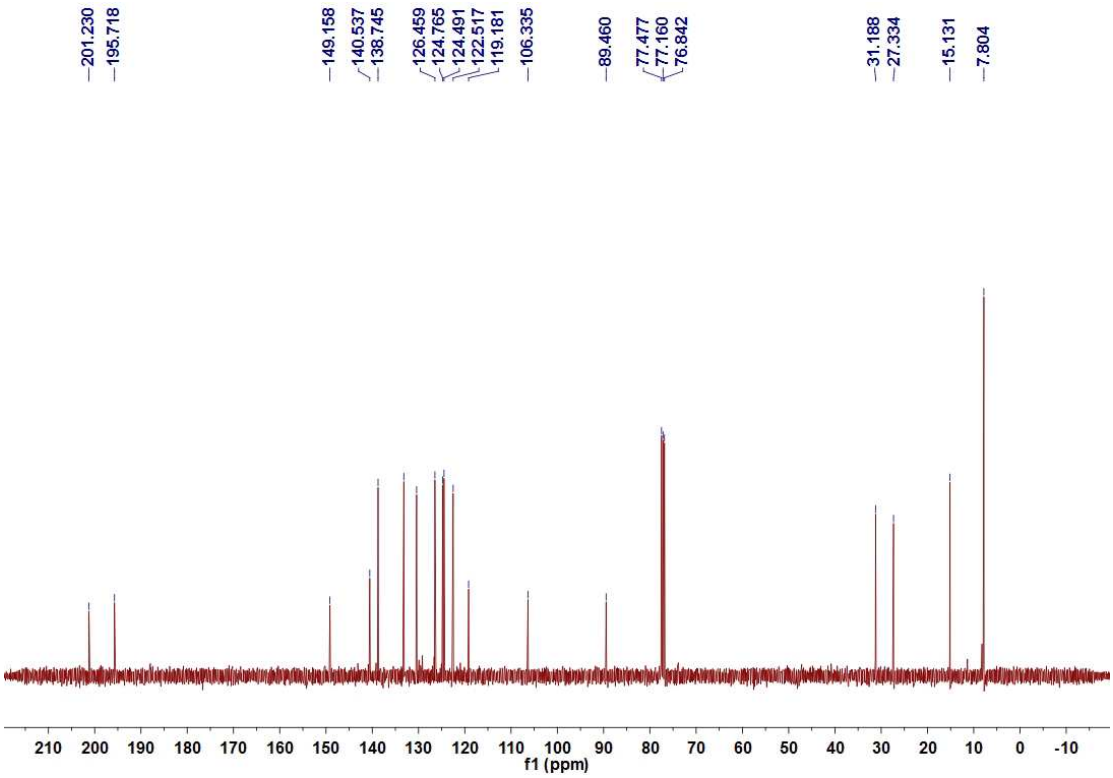
2.02
f1 (ppm)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126.459
124.765
124.491
122.517
119.181
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89.460
77.477
77.160
76.842
31.188
27.334
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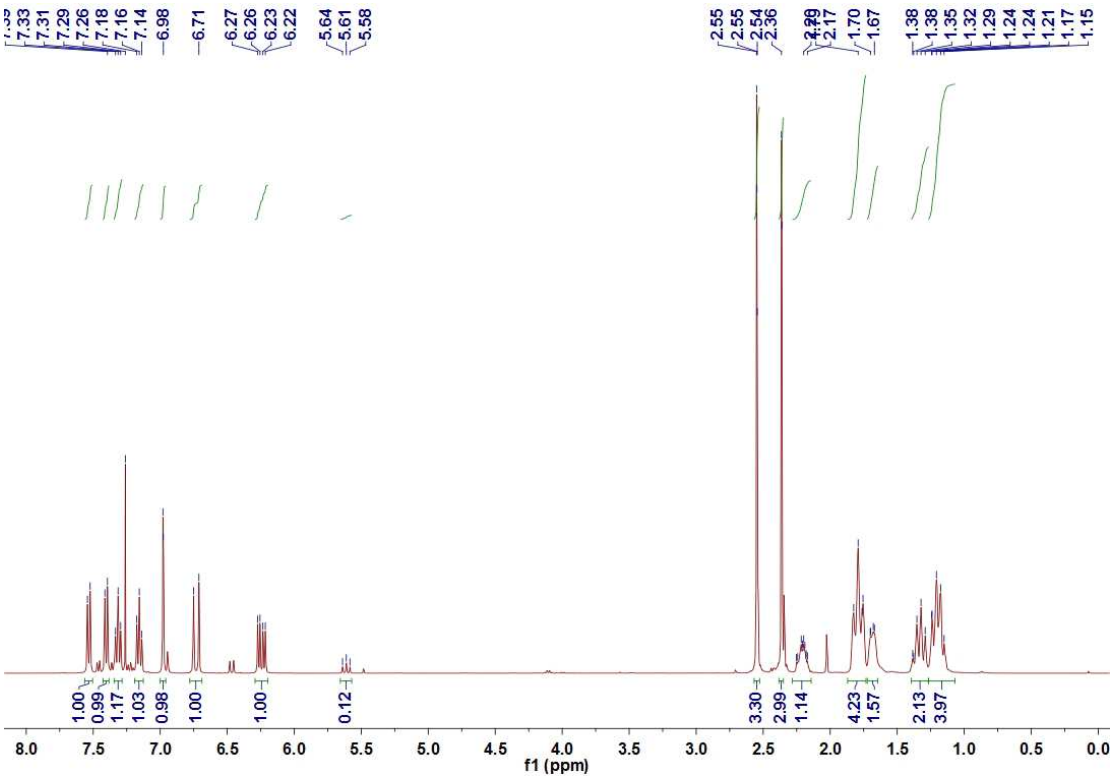
7.804
f1 (ppm)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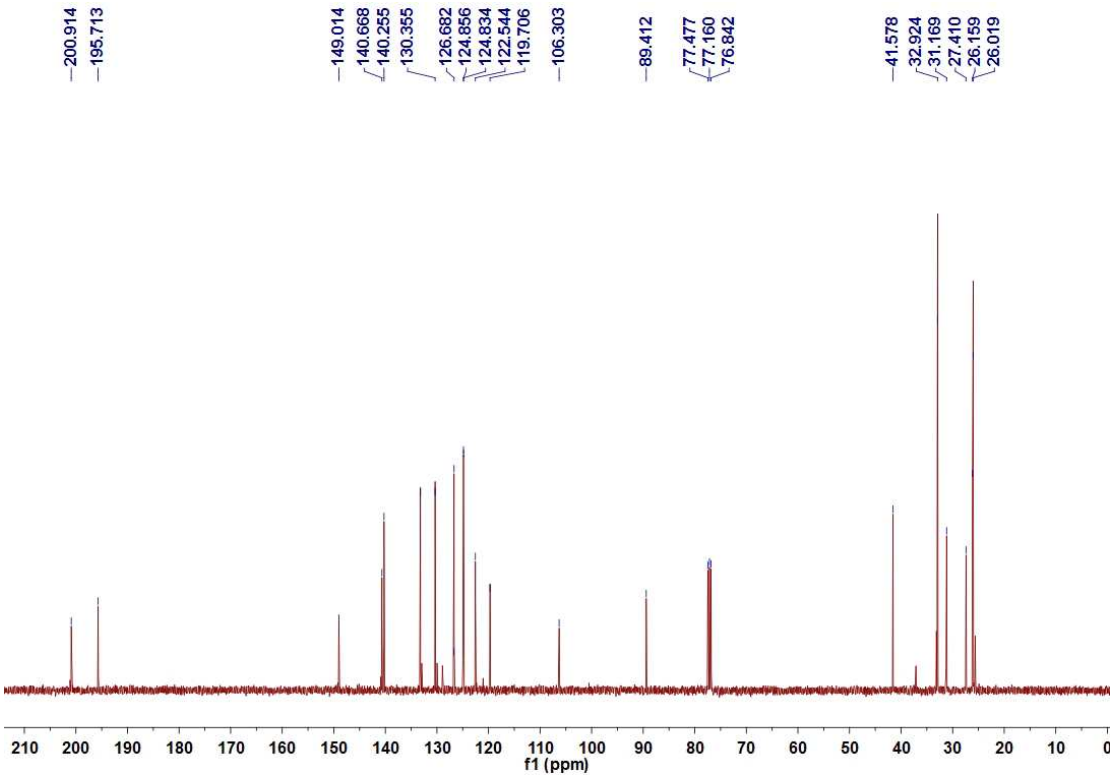
6.26
6.23
6.22
5.64
5.61
5.58
2.55
2.55
2.54
2.36
2.17
1.70
1.67
1.38
1.38
1.35
1.32
1.29
1.24
1.24
1.21
1.17
1.15
1.00
0.99
1.17
1.03
0.98
1.00
1.00
0.12
3.30
2.99
1.14
4.23
1.57
2.13
3.97
f1 (ppm)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140.255
130.355
126.682
124.856
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122.544
119.706
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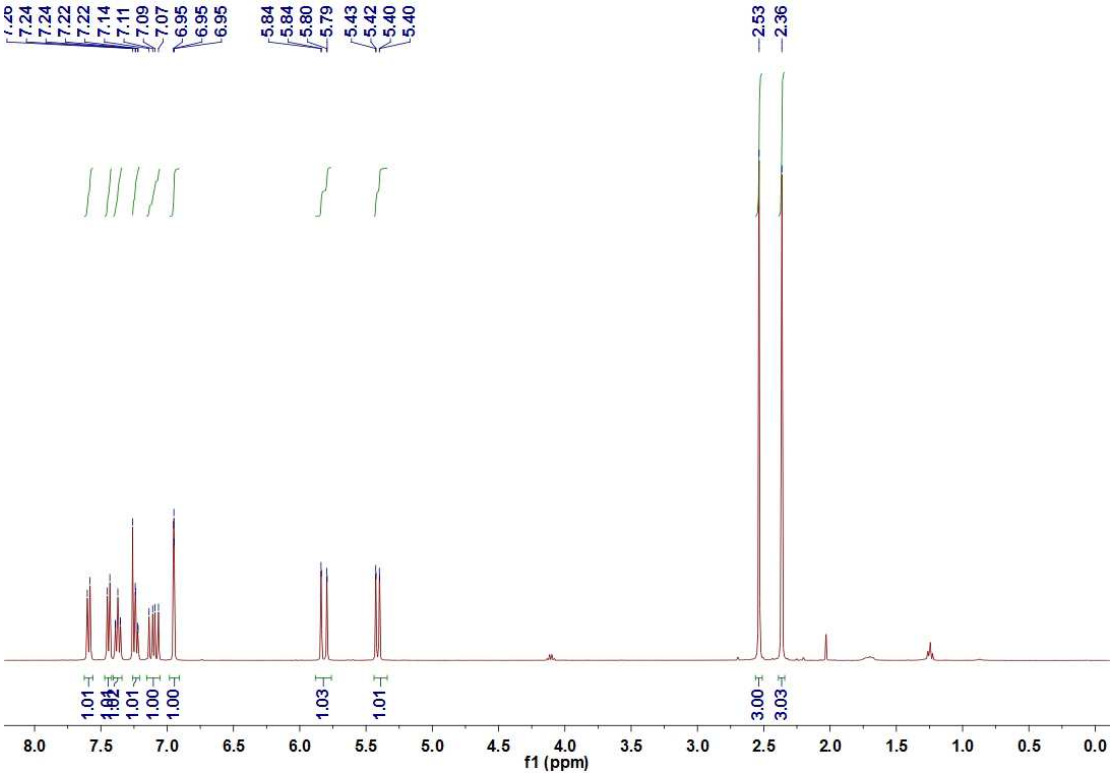
77.160
76.842
41.578
32.924
31.169
27.410
26.159
26.019
f1 (ppm)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7.22
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7.07
6.95
6.95
6.95
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5.84
5.80
5.79
5.43
5.42
5.40
5.40
2.53
2.36
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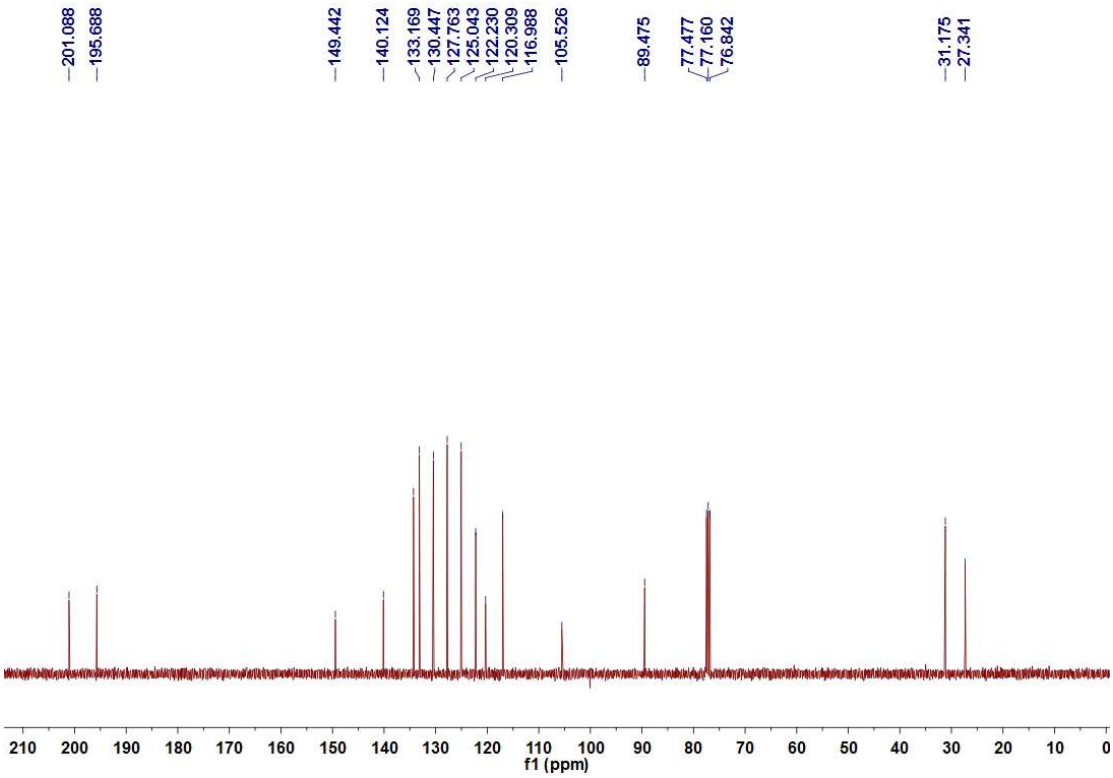
1.01
1.01
1.00
1.00
1.03
1.01
3.00
3.03
f1 (ppm)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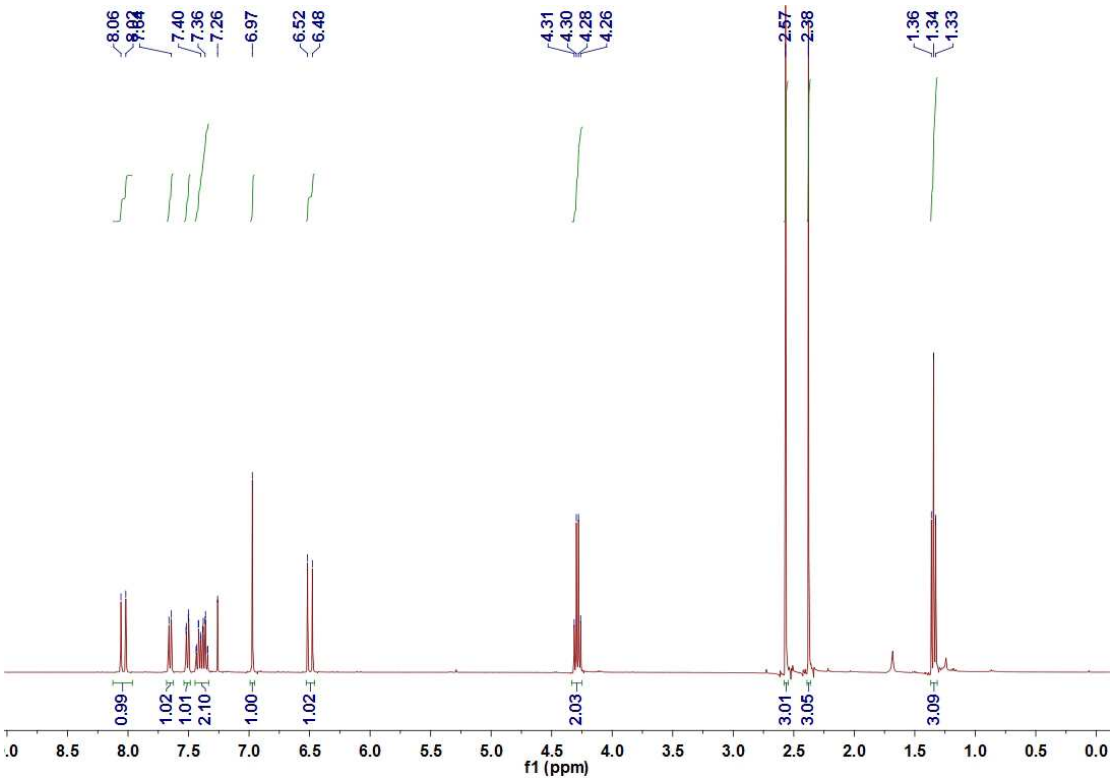
116.988
105.526
89.475
77.477
77.160
76.842
31.175
27.341
f1 (ppm)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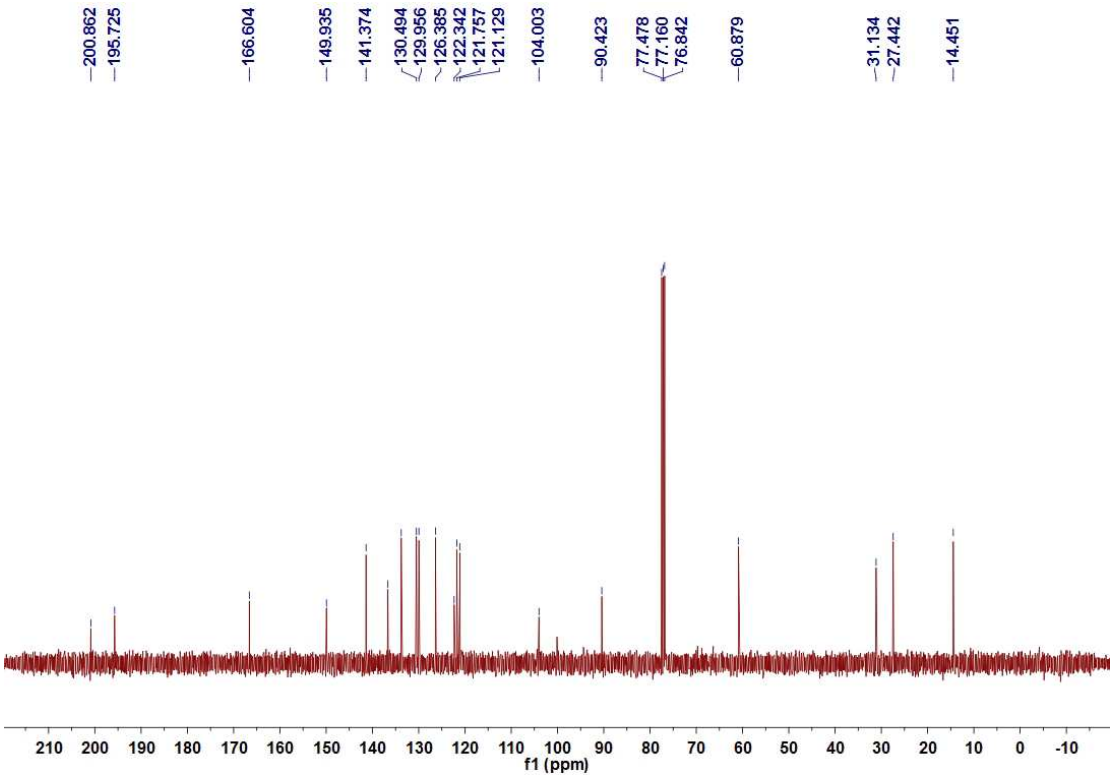
7.40
7.36
7.26
6.97
6.52
6.48
4.31
4.30
4.28
4.26
2.57
2.38
1.36
1.34
1.33
0.99
1.02
1.01
2.10
1.00
1.02
2.03
3.01
3.05
3.09
f1 (ppm)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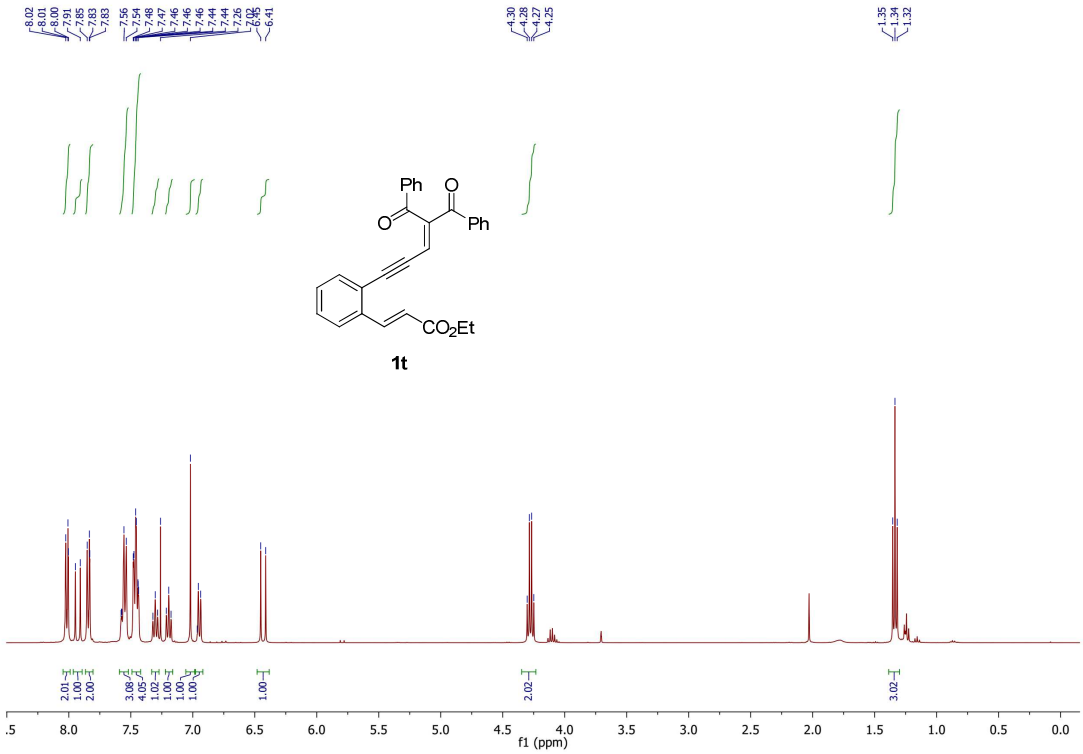
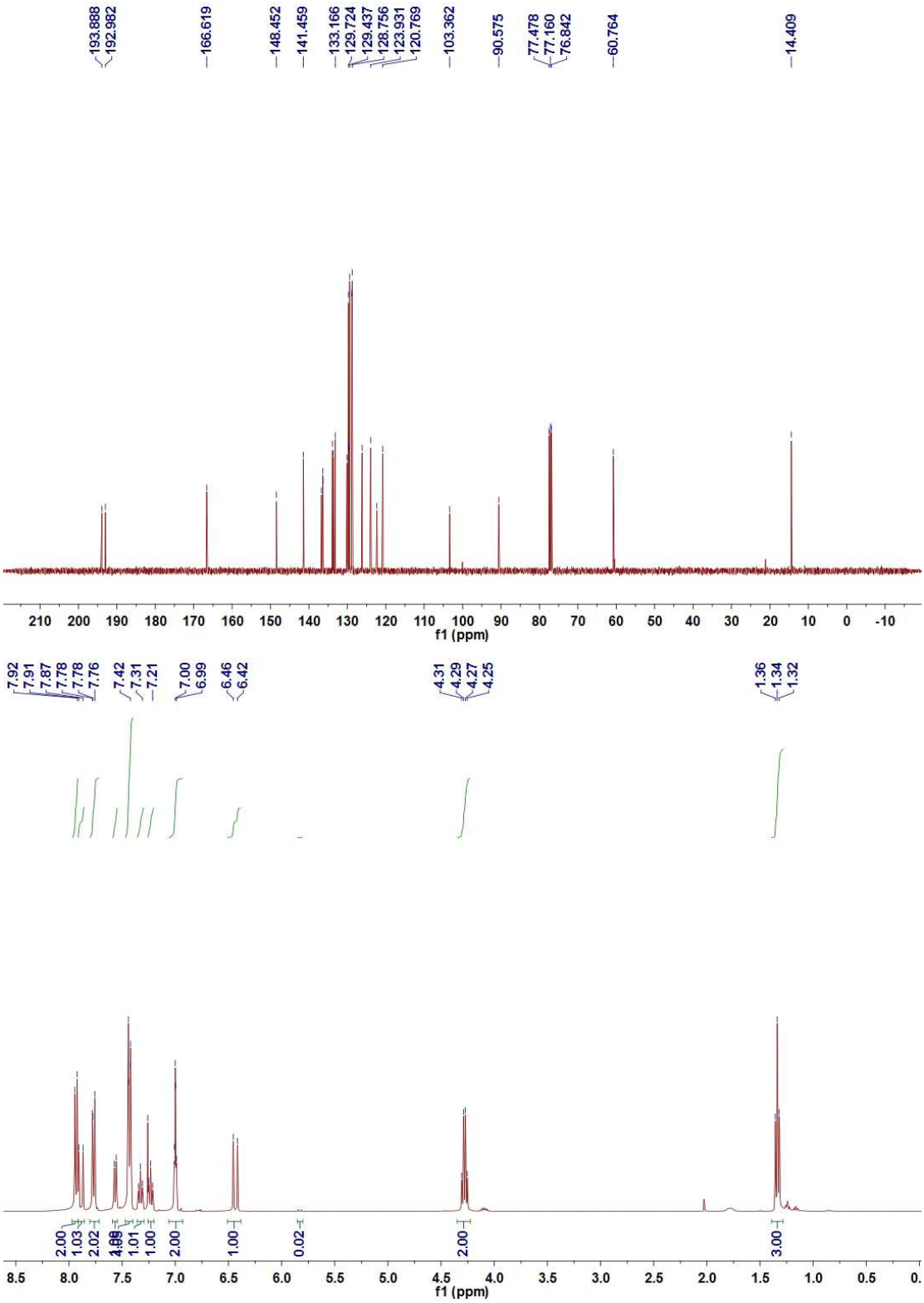
141.374
130.494
129.956
126.385
122.342
121.757
121.129
104.003
90.423
77.478
77.160
76.842
60.879
31.134
27.442
14.451
f1 (ppm)


Ph
O
O
Ph
CO2Et
f1 (ppm)

1t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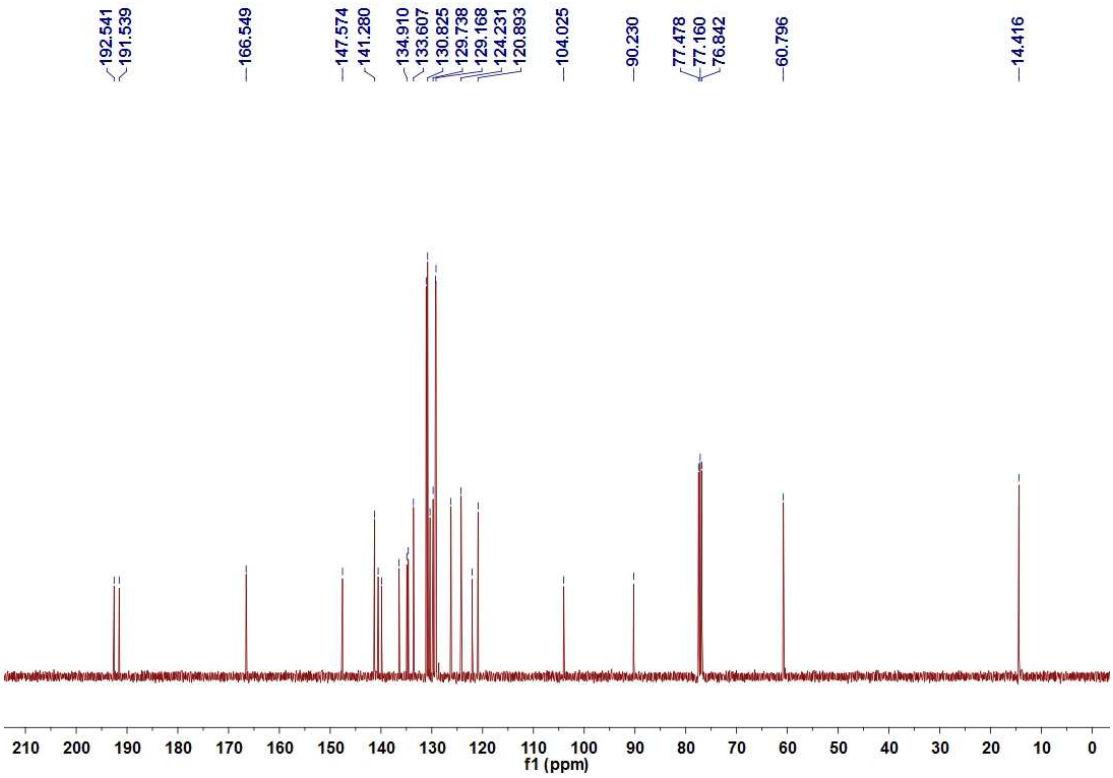
148.452
141.459
133.166
129.724
129.437
128.756
123.931
120.769
103.362
90.575
77.478
77.160
76.842
60.764
14.409
f1 (ppm)
7.92
7.91
7.87
7.78
7.78
7.76
7.42
7.31
7.21
7.00
6.99
6.46
6.42
4.31
4.29
4.27
4.25
1.36
1.34
1.32
2.00
1.03
2.02
1.01
1.00
2.00
1.00
0.02
2.00
3.00
f1 (ppm)


192.541
191.539
166.549
147.574
141.280
134.910
133.607
130.825
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129.168
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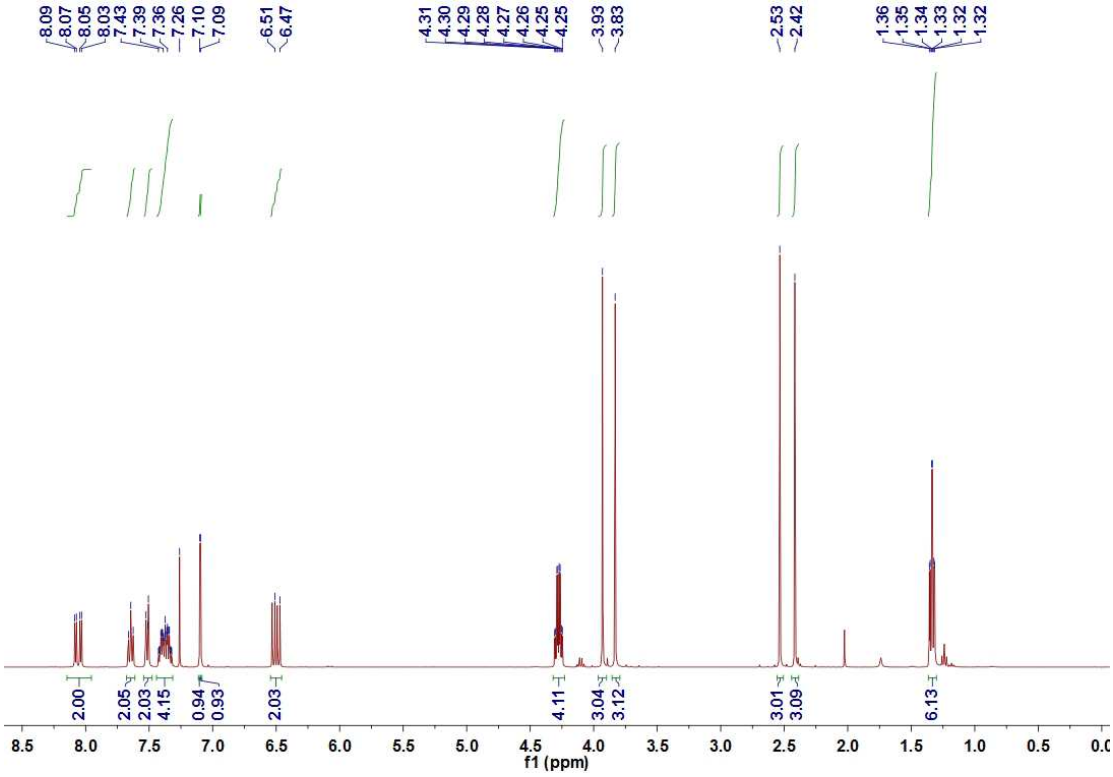
120.893
104.025
90.230
77.478
77.160
76.842
60.796
14.416
f1 (ppm)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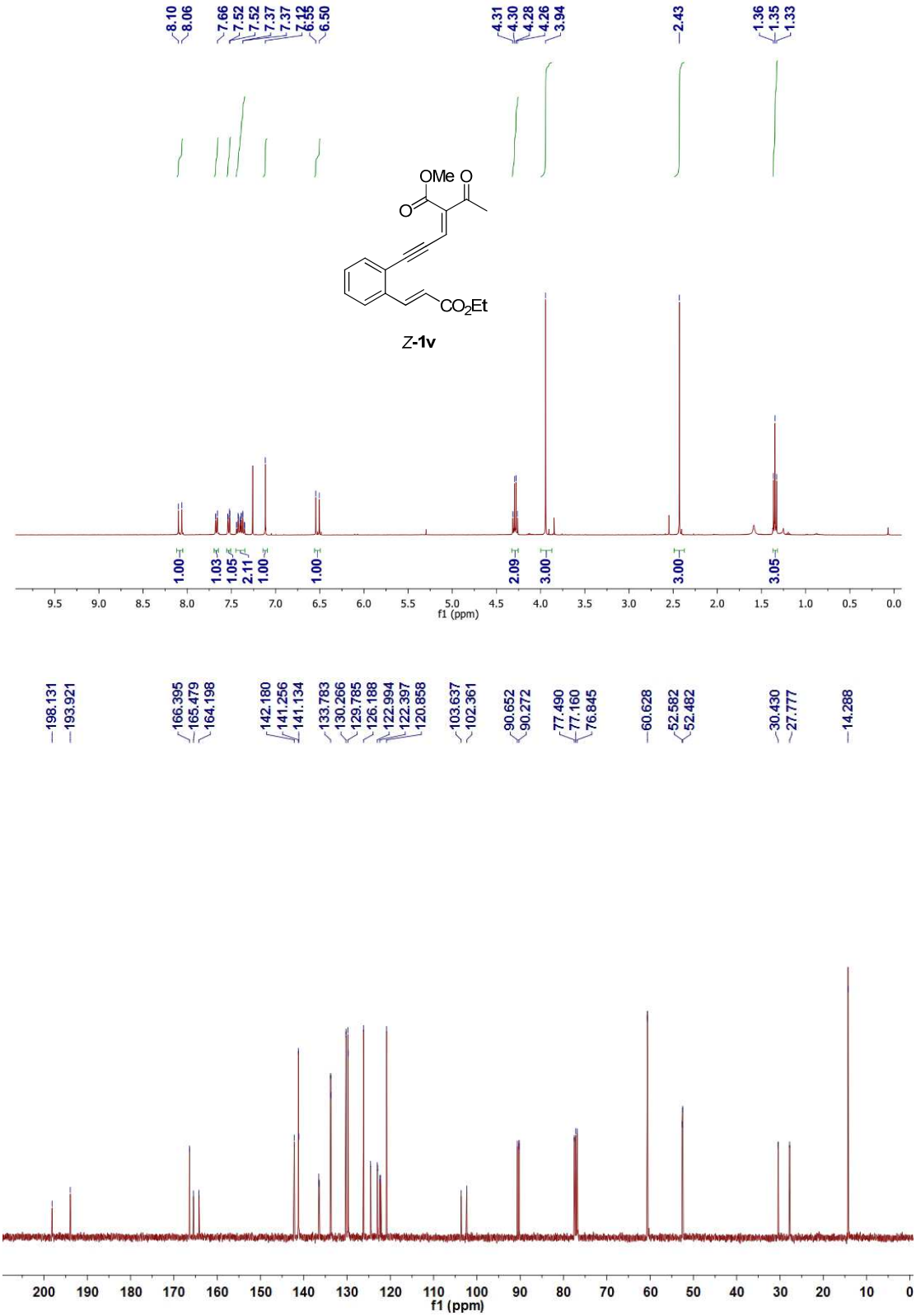
8.07
8.05
8.03
7.43
7.39
7.36
7.26
7.10
7.09
6.51
6.47
4.31
4.30
4.29
4.28
4.27
4.26
4.25
4.25
3.93
3.83
2.53
2.42
1.36
1.35
1.34
1.33
1.32
1.32
2.00
2.05
2.03
4.15
0.94
0.93
2.03
4.11
3.04
3.12
3.01
3.09
6.13
f1 (ppm)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8.06
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7.52
7.37
7.37
7.12
6.55
6.50
4.31
4.30
4.28
4.26
3.94
2.43
1.36
1.35
1.33
OMe
O
O
CO2Et
Z-1v
1.00
1.03
1.05
2.11
1.00
1.00
2.09
3.00
3.00
3.05
f1 (ppm)
198.131
193.921
166.395
165.479
164.198
142.180
141.256
141.134
133.783
130.266
129.785
126.188
122.994
122.397
120.858
103.637
102.361
90.652
90.272
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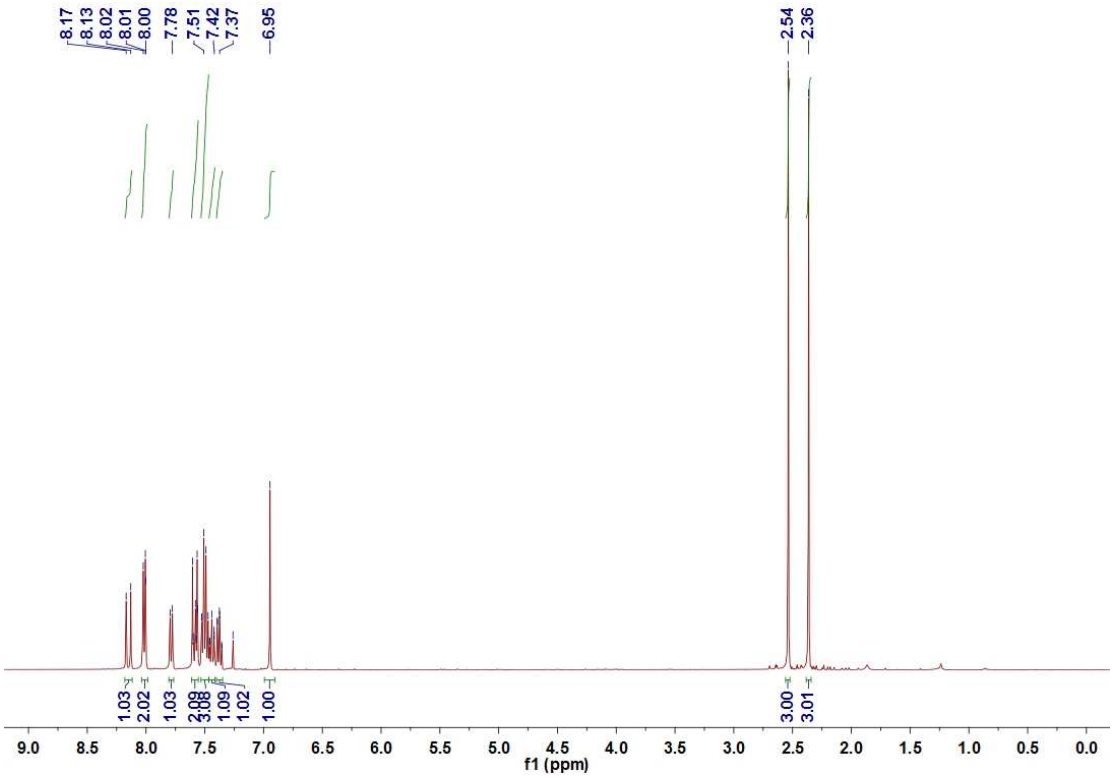
77.160
76.845
60.628
52.582
52.482
30.430
27.777
14.288
f1 (ppm)


8.17
8.13
8.02
8.01
8.00
7.78
7.51
7.42
7.37
6.95
2.54
2.36
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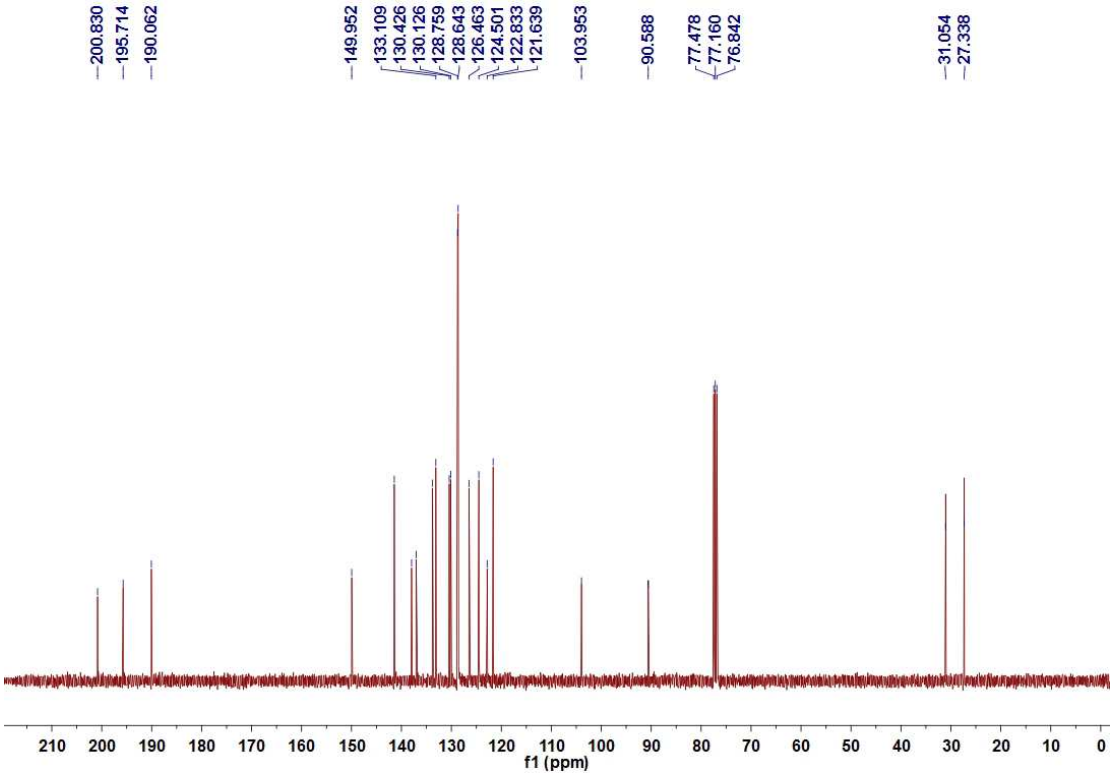
1.02
1.00
3.00
3.01
f1 (ppm)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130.126
128.759
128.643
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124.501
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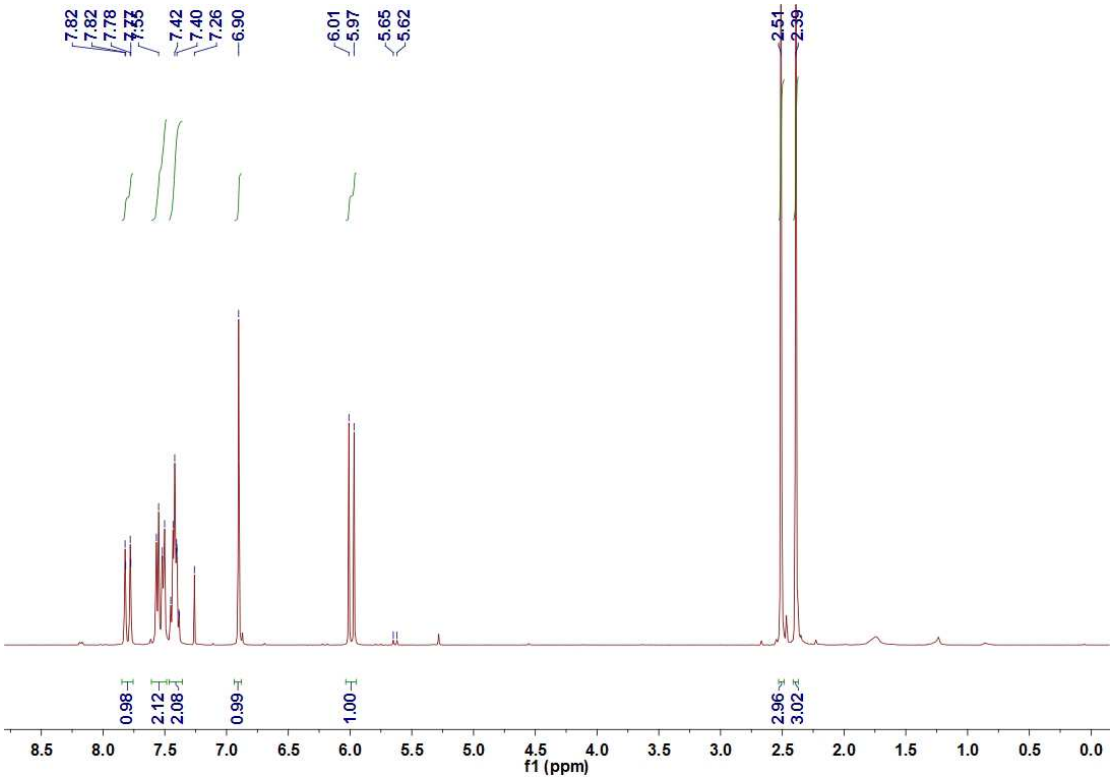
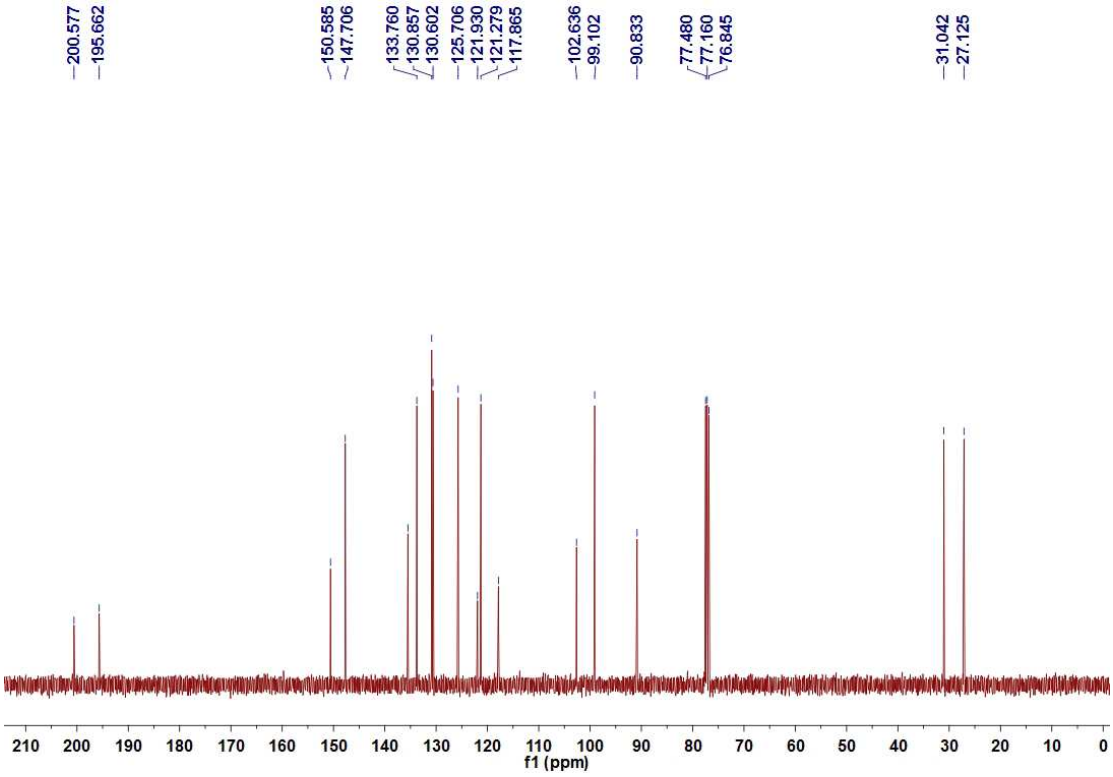
103.953
90.588
77.478
77.160
76.842
31.054
27.338
f1 (ppm)


7.82
7.82
7.78
7.42
7.40
7.26
6.90
6.01
5.97
5.65
5.62
2.51
2.39
0.98
2.12
2.08
0.99
1.00
2.96
3.02
f1 (ppm)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125.706
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99.102
90.833
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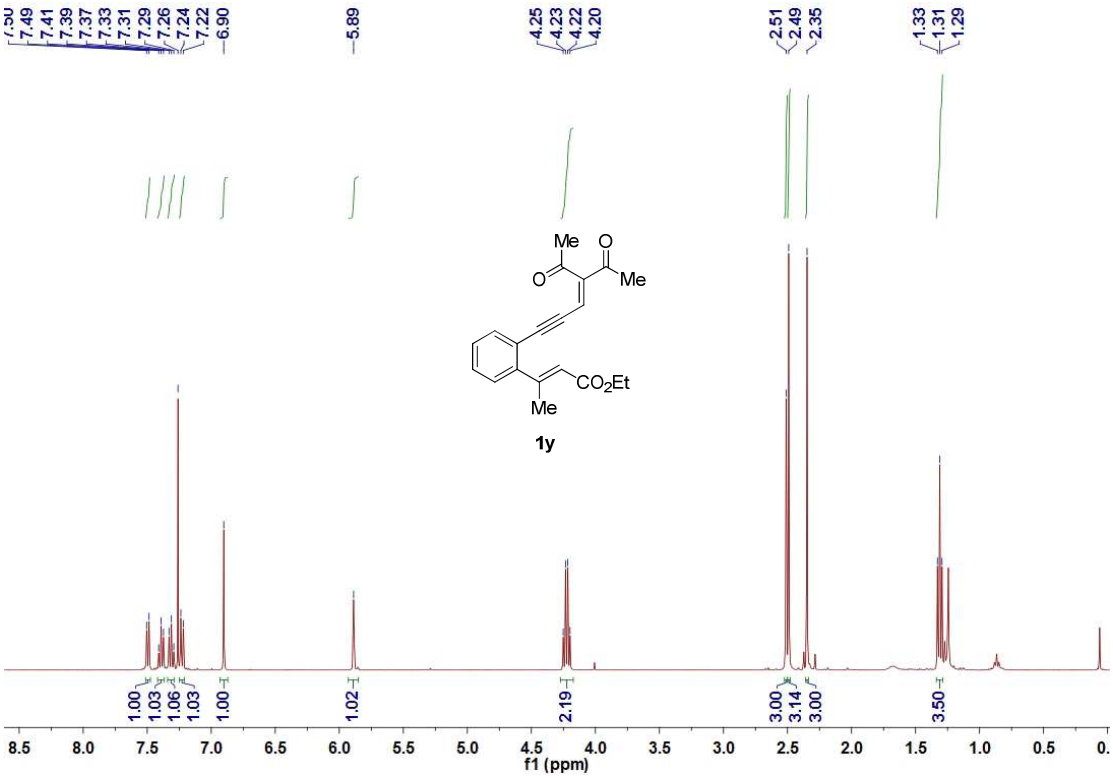
76.845
31.042
27.125
f1 (ppm)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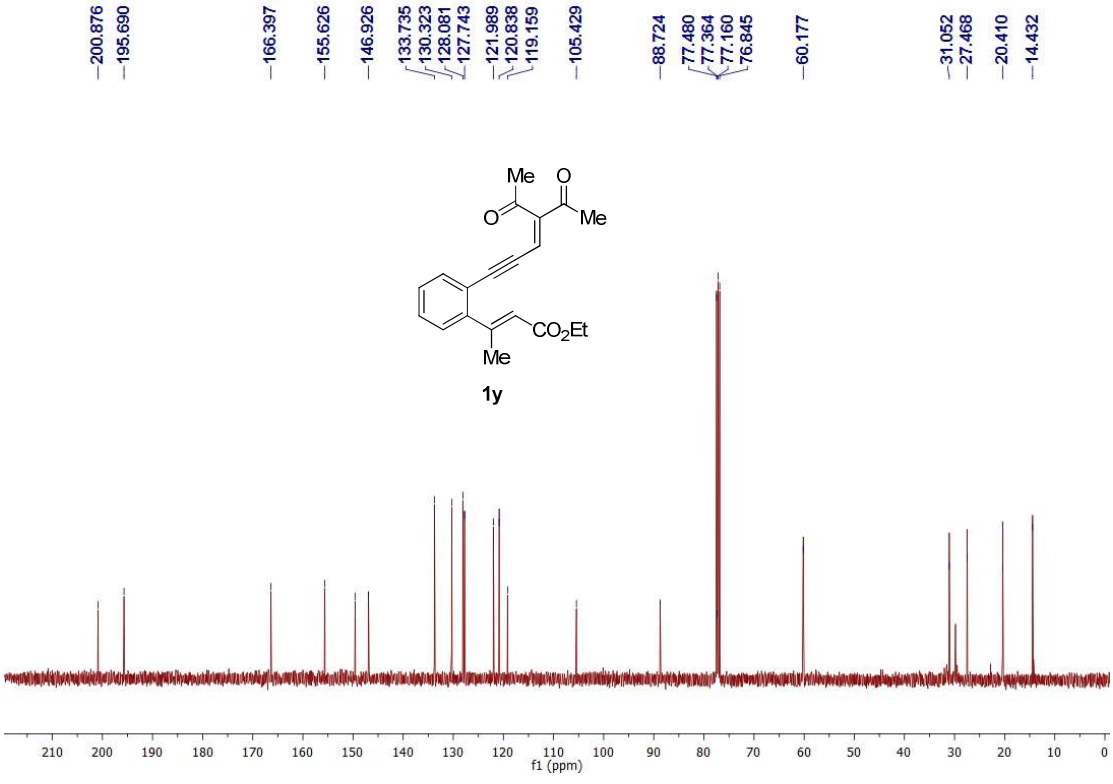
7.33
7.31
7.29
7.26
7.24
7.22
6.90
5.89
4.25
4.23
4.22
4.20
2.51
2.49
2.35
1.33
1.31
1.29
Me
O
O
Me
CO2Et
Me
1y
1.00
1.03
1.06
1.03
1.00
1.02
2.19
3.00
3.14
3.00
3.50
f1 (ppm)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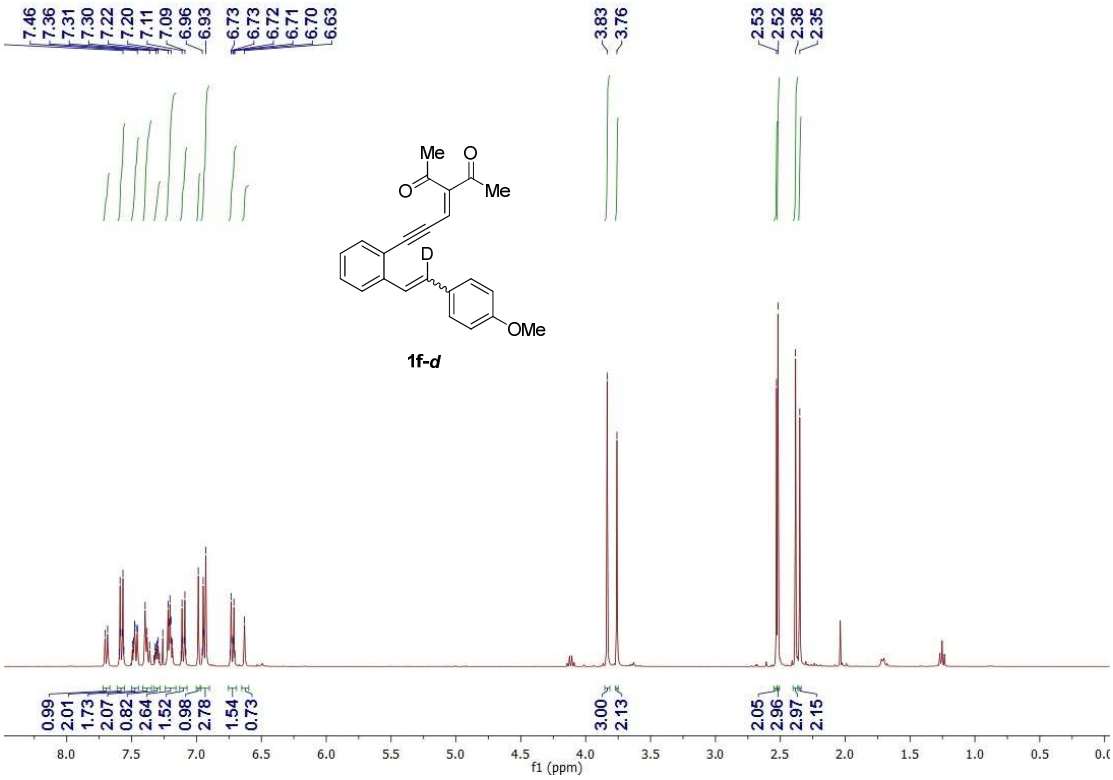
128.081
127.743
121.989
120.838
119.159
105.429
88.724
77.480
77.364
77.160
76.845
60.177
31.052
27.468
20.410
14.432
Me
O
O
Me
CO2Et
Me
1y
f1 (ppm)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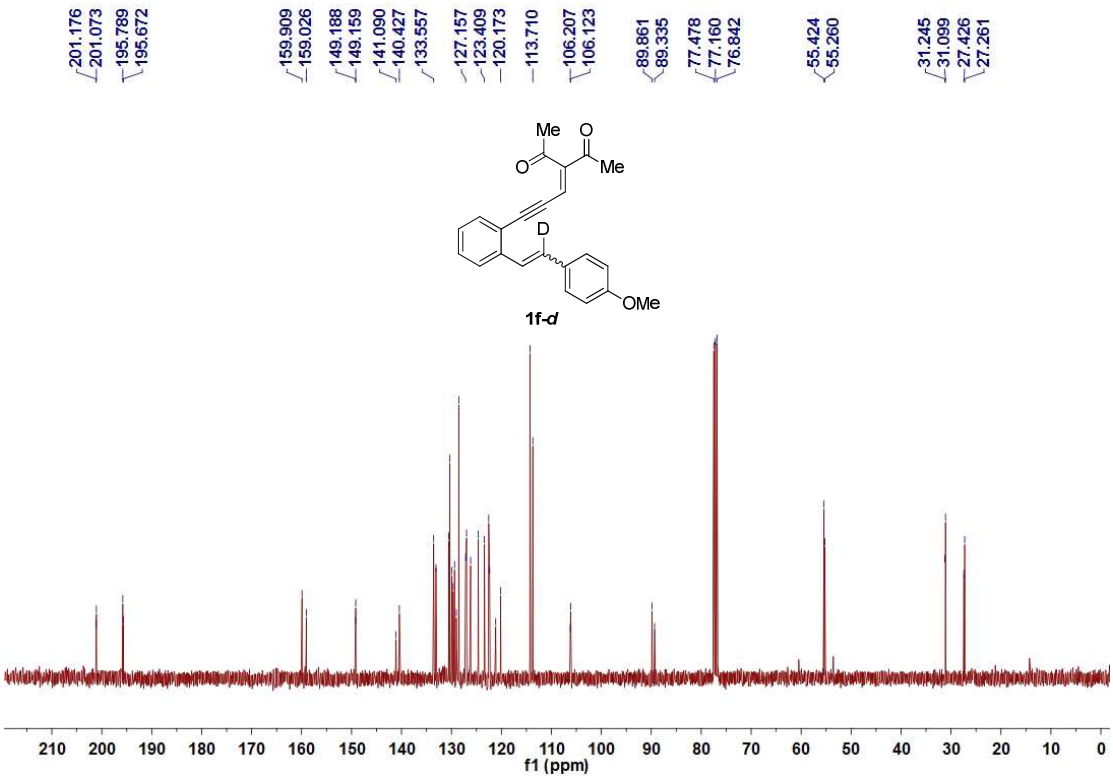
6.93
6.73
6.73
6.72
6.71
6.70
6.63
3.83
3.76
2.53
2.52
2.38
2.35
Me
O
O
Me
D
OMe
1f-d
0.99
2.01
1.73
2.07
0.82
2.64
1.52
0.98
2.78
1.54
0.73
3.00
2.13
2.05
2.96
2.97
2.15
f1 (ppm)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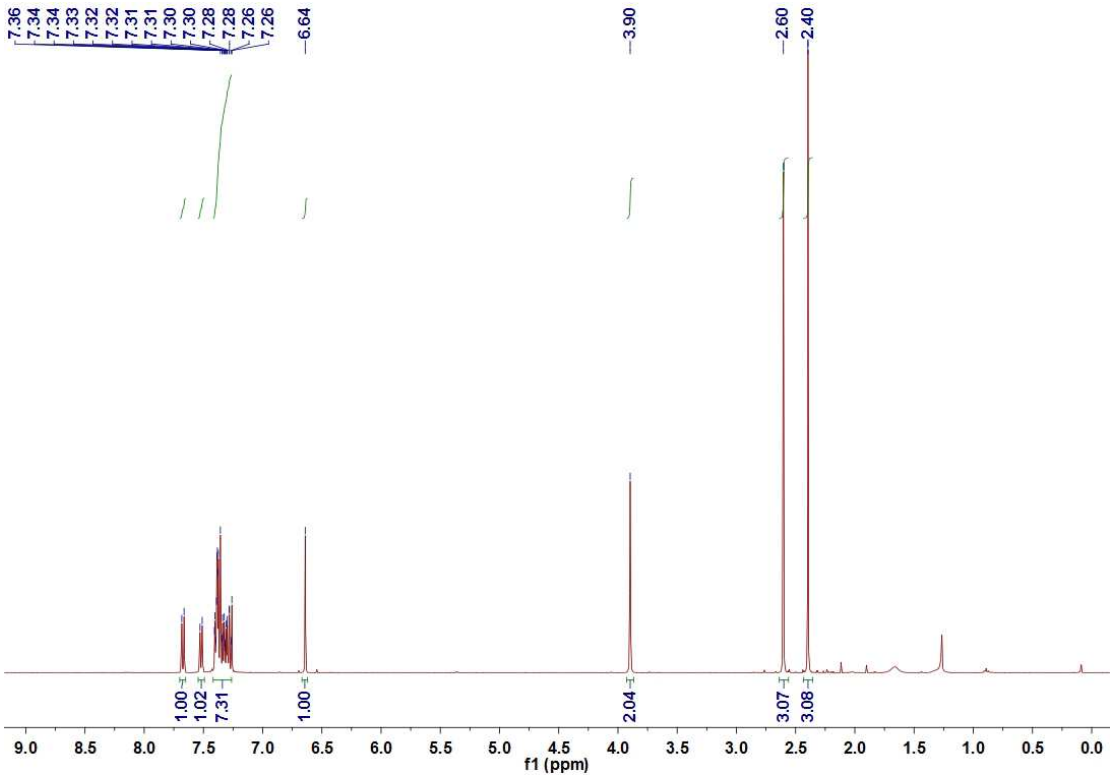
127.157
123.409
120.173
113.710
106.207
106.123
89.861
89.335
77.478
77.160
76.842
55.424
55.260
31.245
31.099
27.426
27.261
Me
O
O
Me
D
OMe
1f-d
f1 (ppm)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7.30
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7.26
7.26
6.64
3.90
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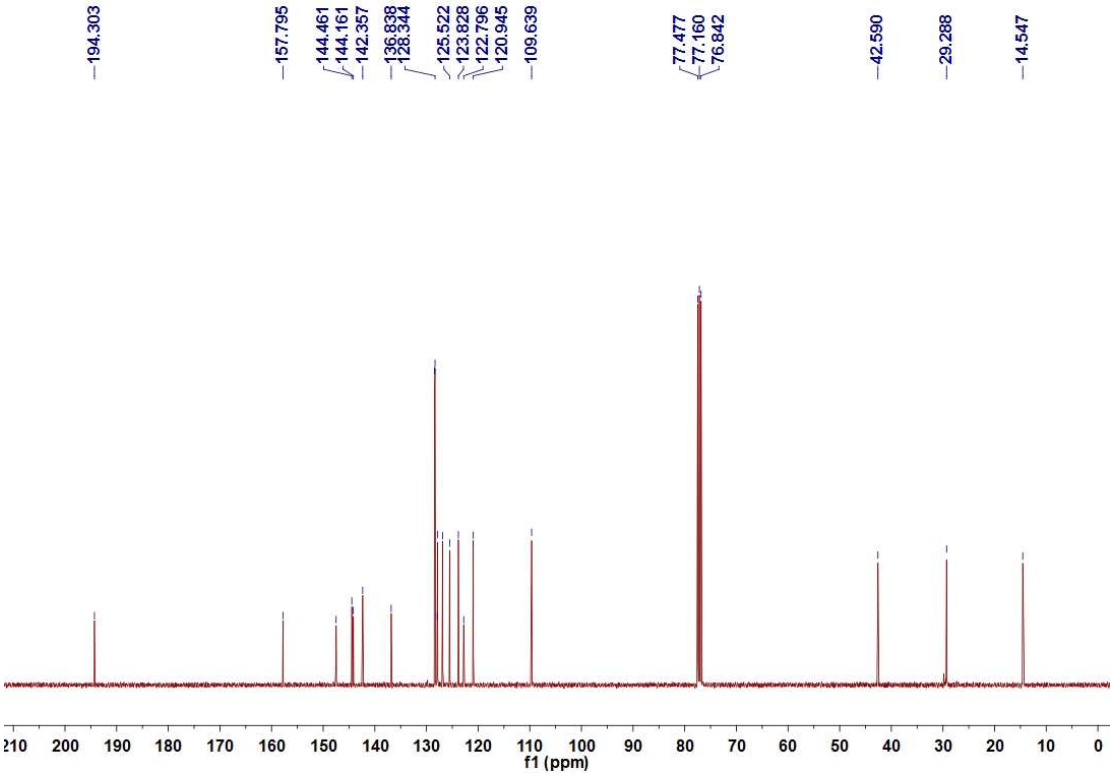
2.40
1.00
1.02
7.31
1.00
2.04
3.07
3.08
f1 (ppm)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125.522
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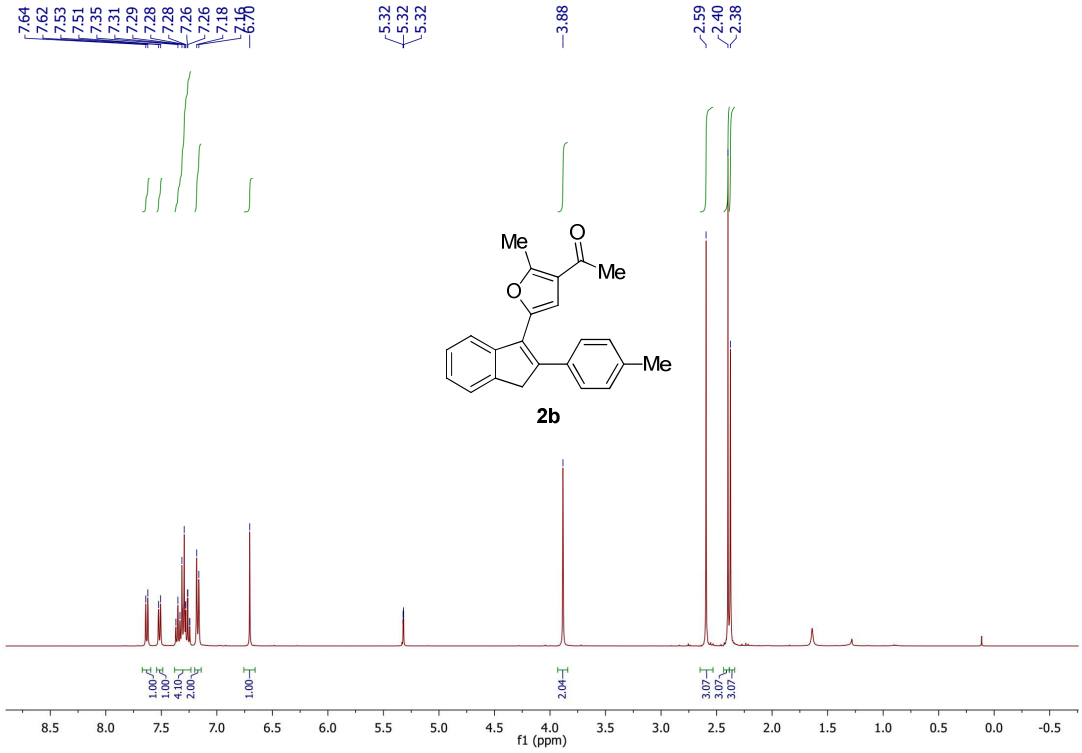
77.160
76.842
42.590
29.288
14.547
f1 (ppm)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7.16
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5.32
5.32
5.32
3.88
2.59
2.40
2.38
Me
O
Me
O
Me
2b
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1.00
4.10
2.00
1.00
2.04
3.07
3.07
3.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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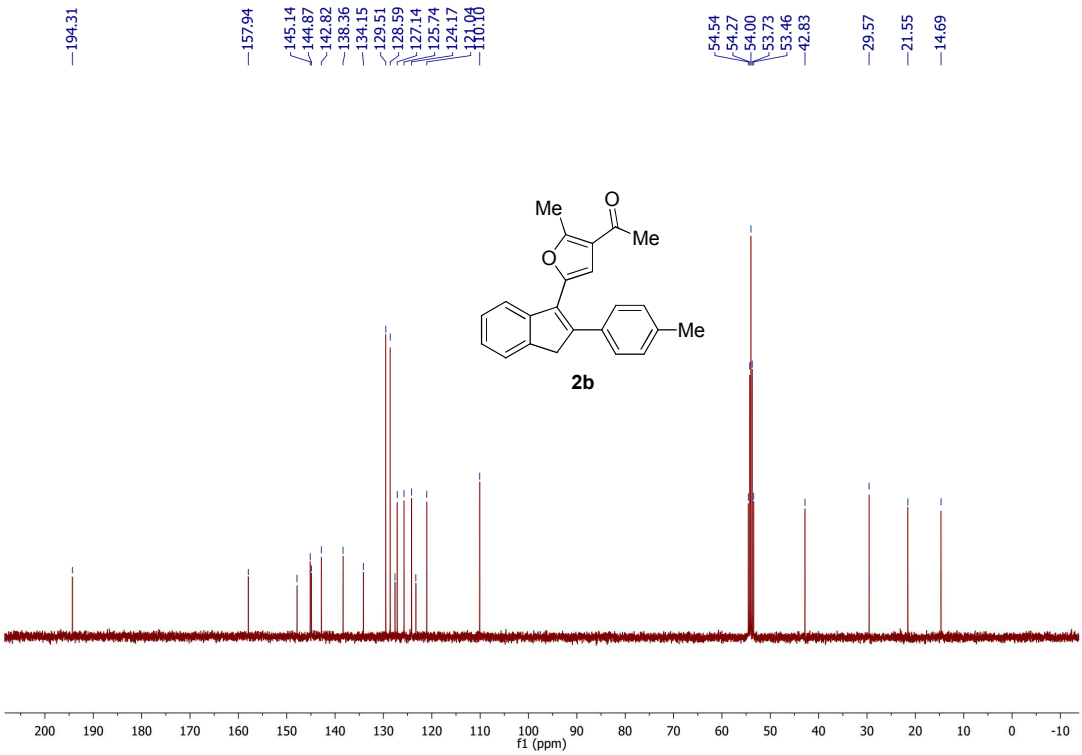
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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138.36
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128.59
127.14
125.74
124.17
121.04
110.10
54.54
54.27
54.00
53.73
53.46
42.83
29.57
21.55
14.69
Me
O
Me
O
Me
2b
200
190
180
170
160
150
140
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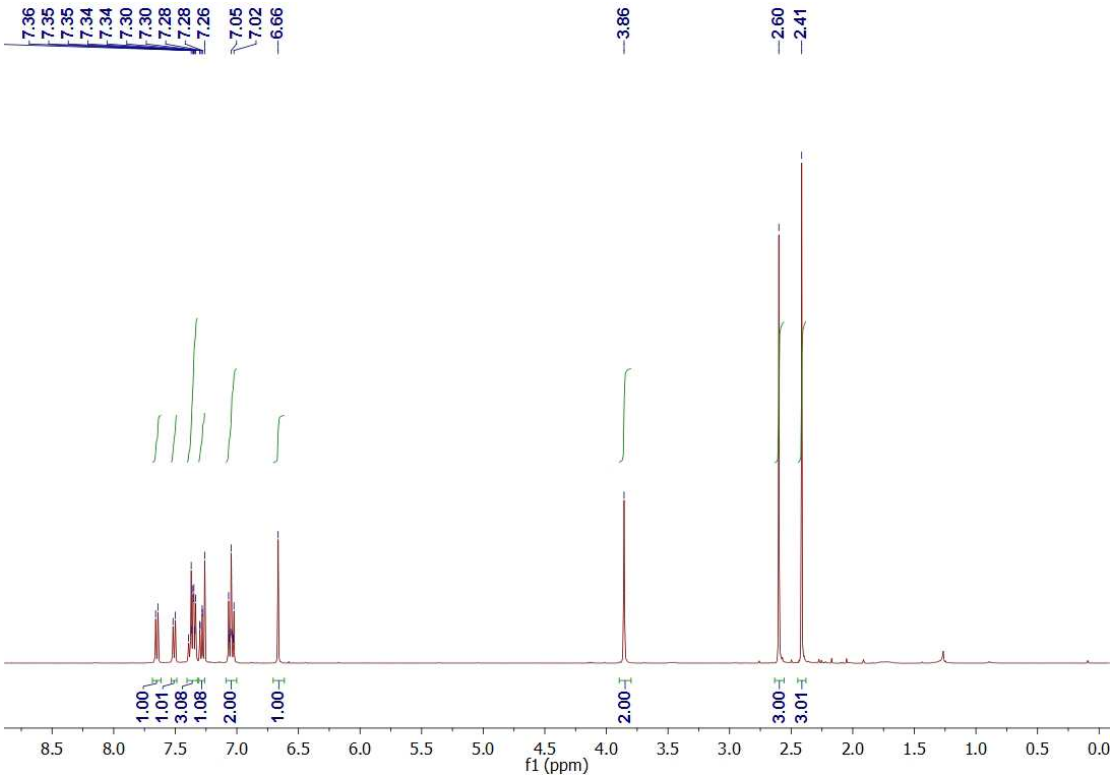
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.34
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7.28
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7.26
7.05
7.02
6.66
3.86
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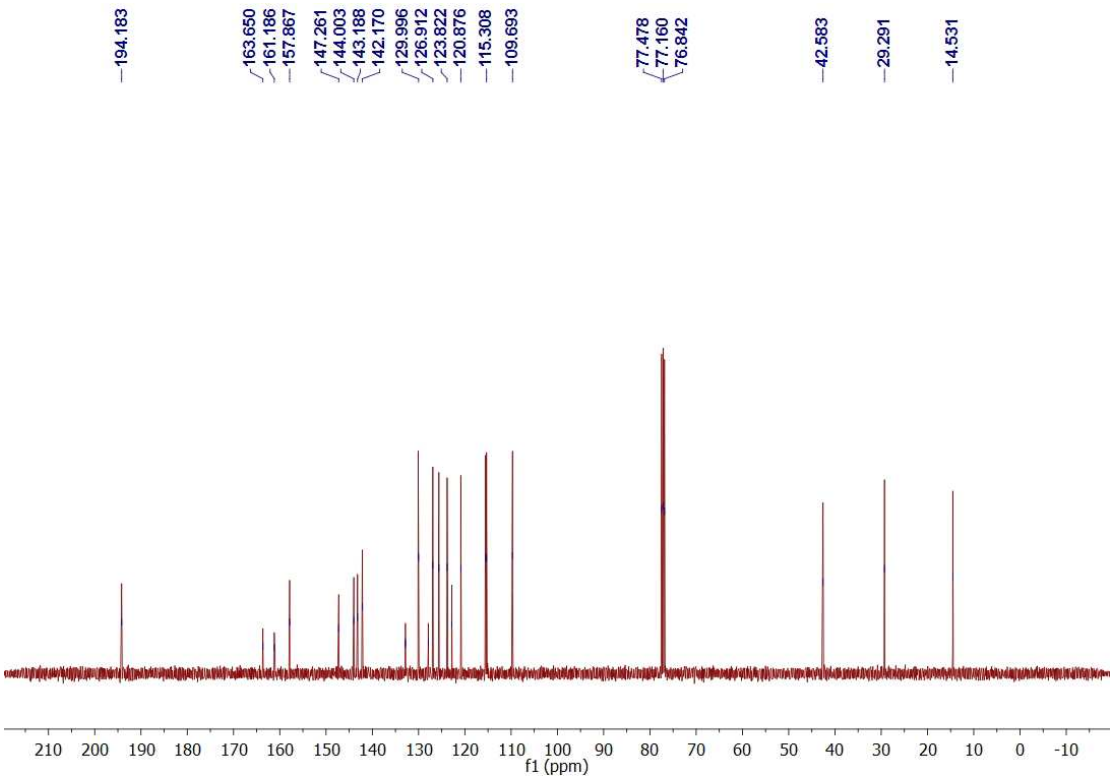
1.01
3.08
1.08
2.00
1.00
2.00
3.00
3.01
f1 (ppm)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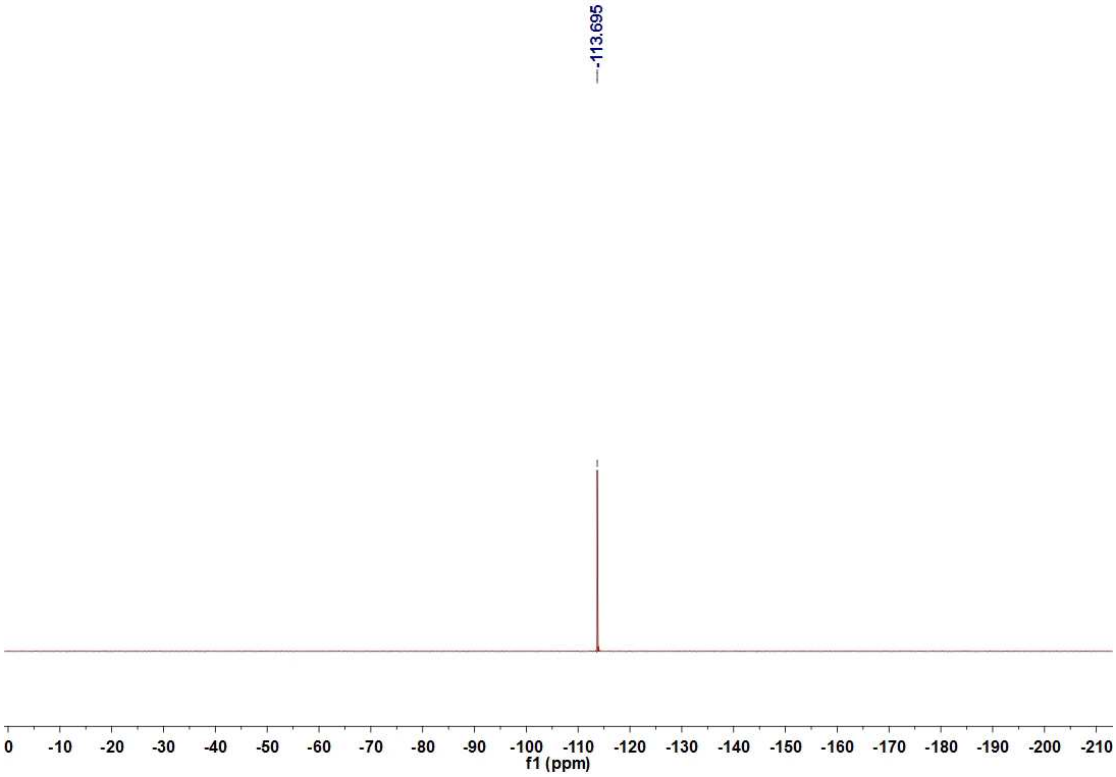
143.188
142.170
129.996
126.912
123.822
120.876
115.308
109.693
77.478
77.160
76.842
42.583
29.291
14.531
f1 (ppm)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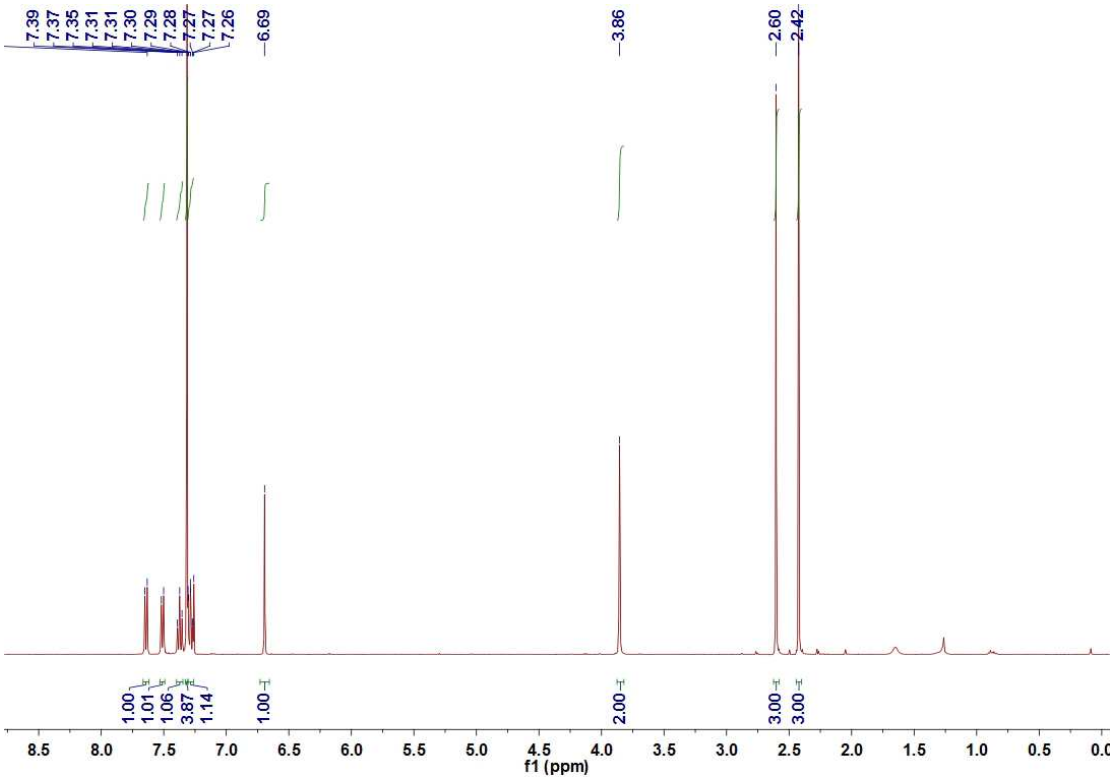
f1 (ppm)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7.27
7.26
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3.86
2.60
2.42
1.00
1.01
1.06
3.87
1.14
1.00
2.00
3.00
3.00
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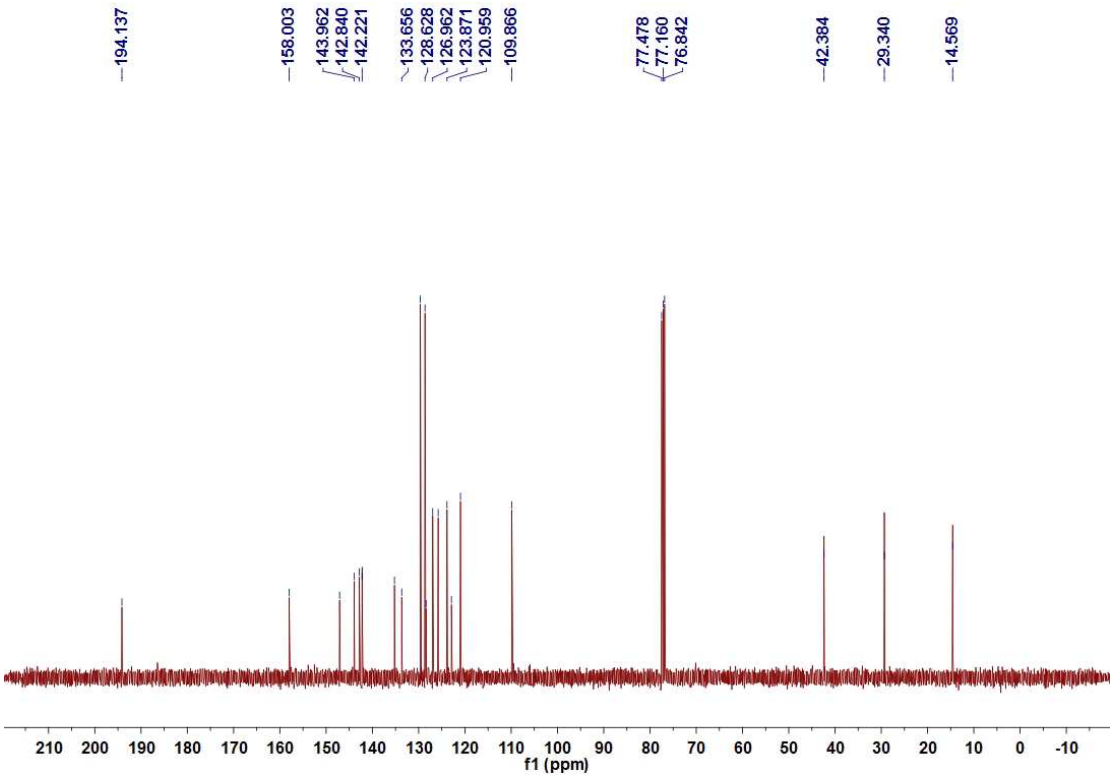
f1 (ppm)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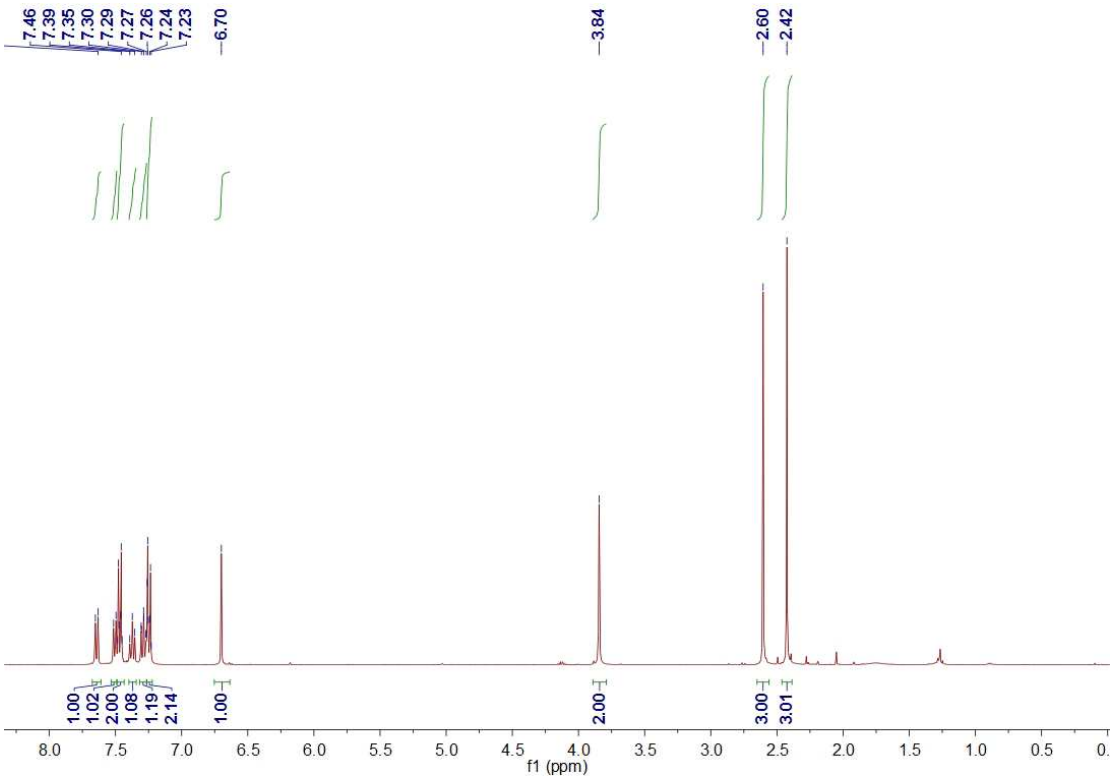
143.962
142.840
142.221
133.656
128.628
126.962
123.871
120.959
109.866
77.478
77.160
76.842
42.384
29.340
14.569
f1 (ppm)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7.27
7.26
7.24
7.23
6.70
3.84
2.60
2.42
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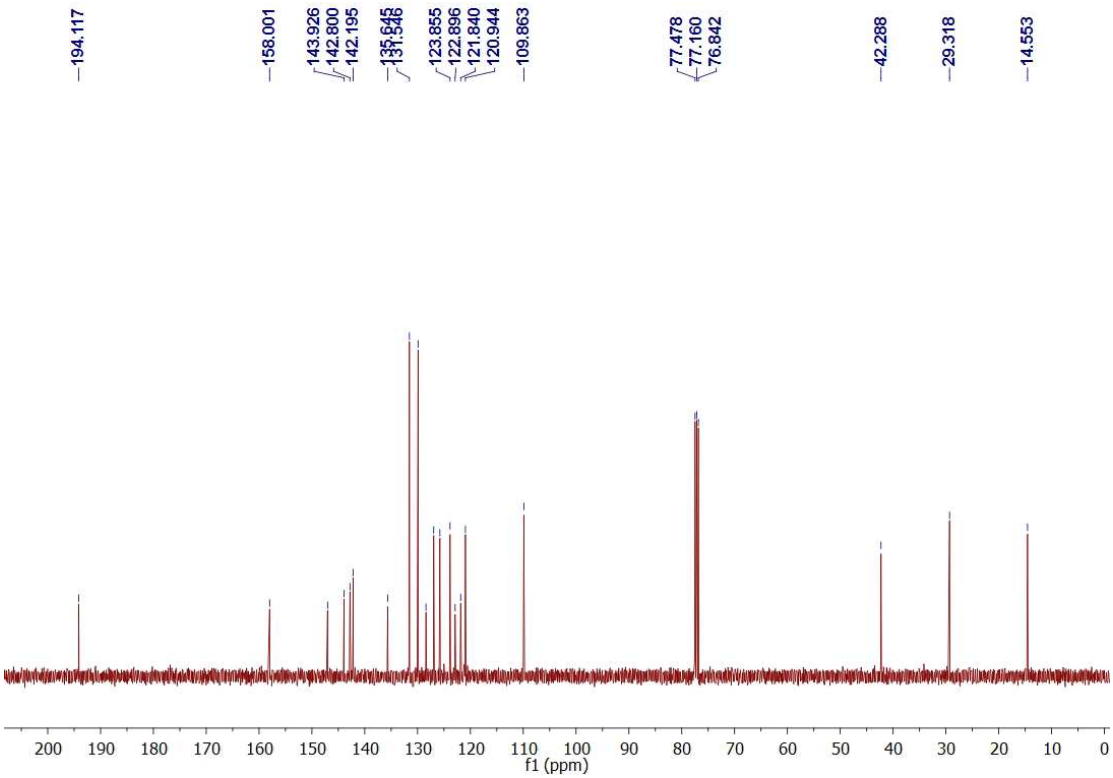
2.00
1.08
1.19
2.14
1.00
2.00
3.00
3.01
f1 (ppm)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131.546
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121.840
120.944
109.863
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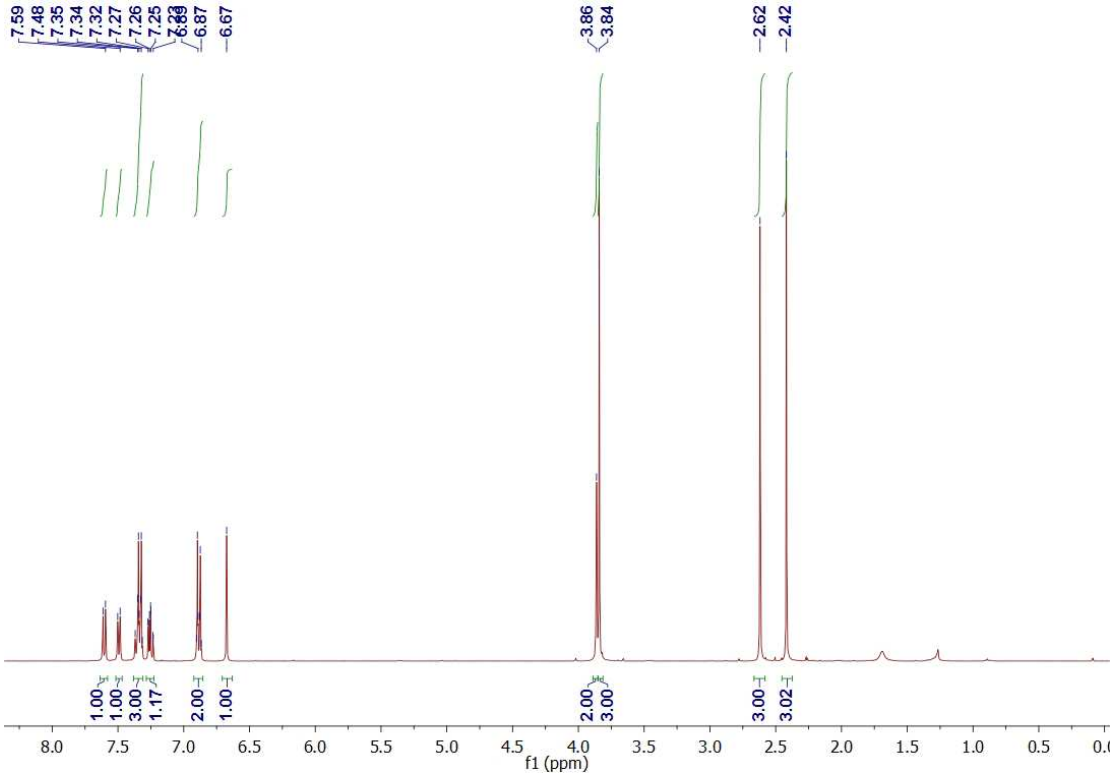
76.842
42.288
29.318
14.553
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.25
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6.67
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3.84
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2.42
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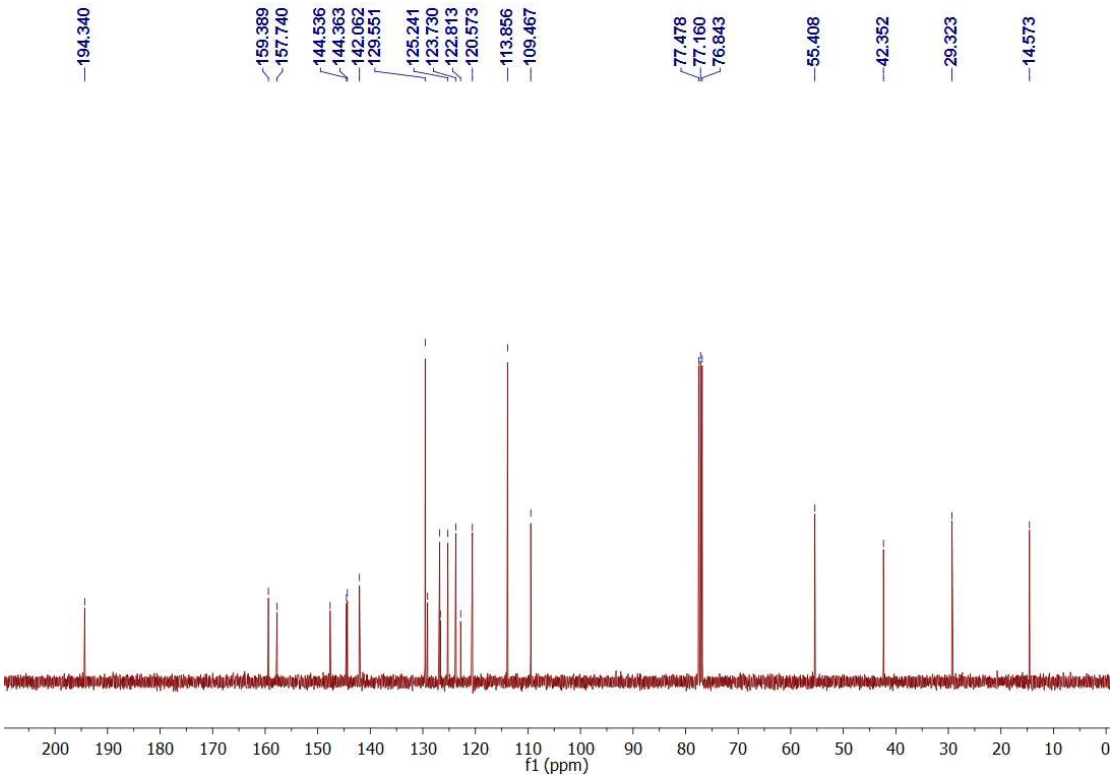
1.00
3.00
1.17
2.00
1.00
2.00
3.00
3.00
3.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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125.241
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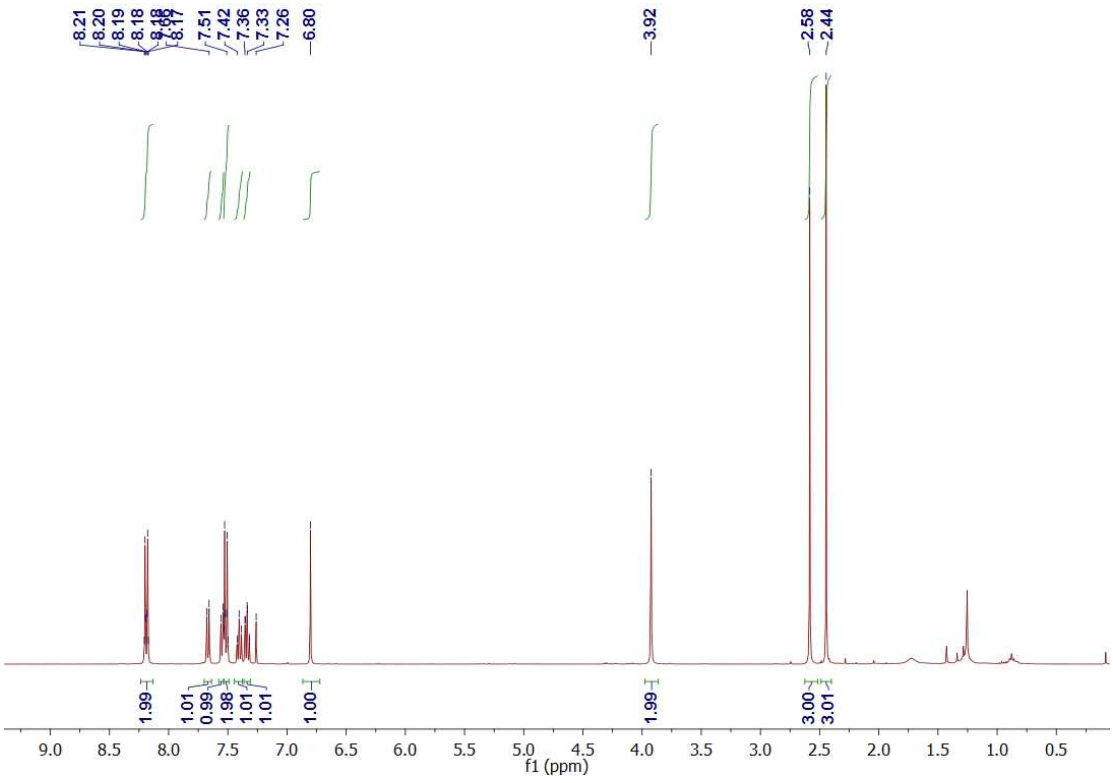
42.352
29.323
14.573
f1 (ppm)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8.18
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7.42
7.36
7.33
7.26
6.80
3.92
2.58
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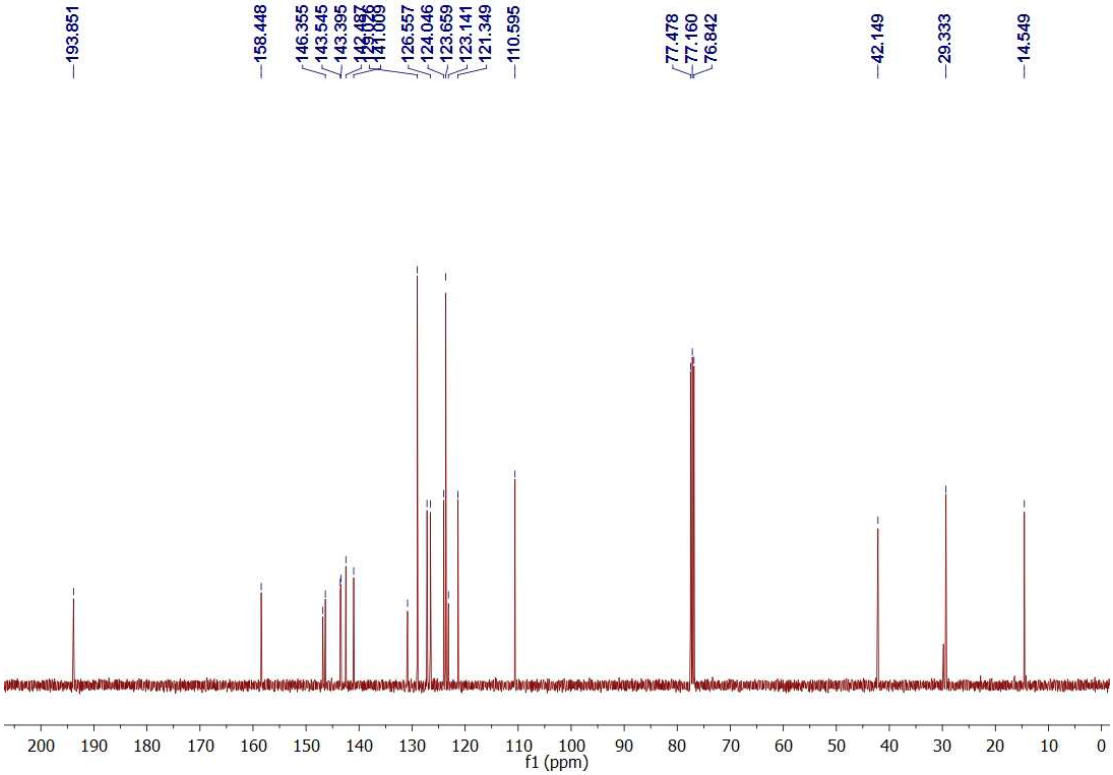
0.99
1.98
1.01
1.01
1.00
1.99
3.00
3.01
f1 (ppm)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143.395
126.557
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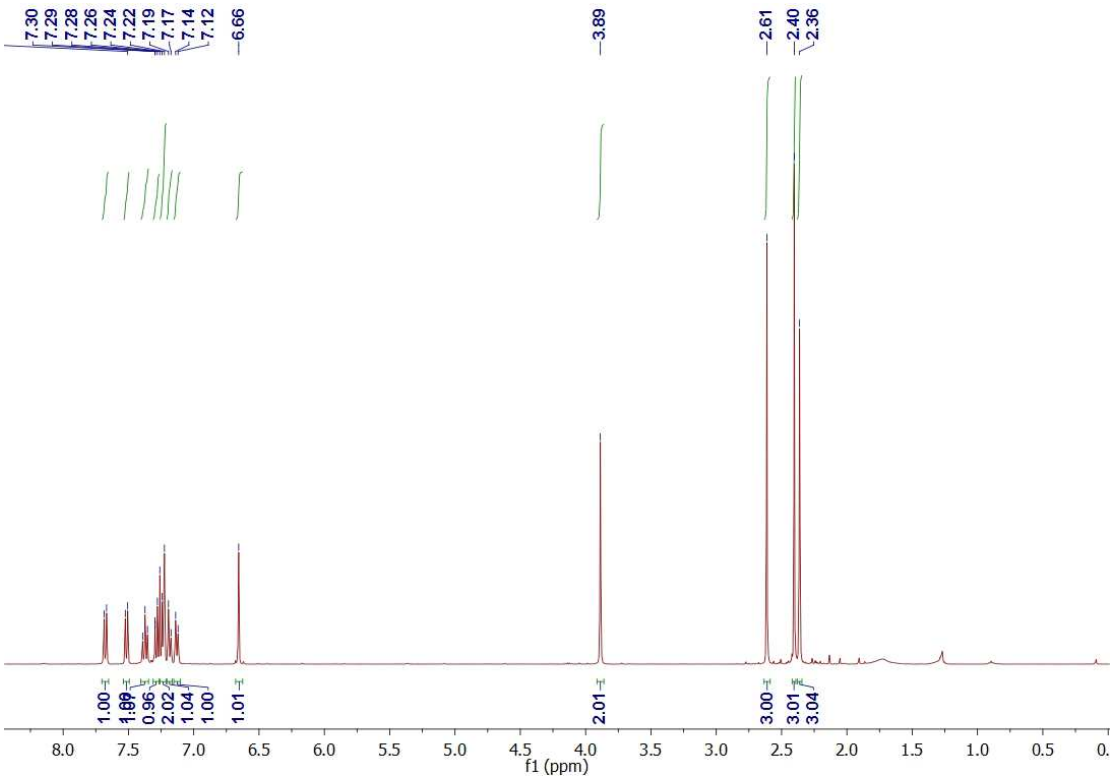
123.659
123.141
121.349
110.595
77.478
77.160
76.842
42.149
29.333
14.549
f1 (ppm)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7.28
7.26
7.24
7.22
7.19
7.17
7.14
7.12
6.66
3.89
2.61
2.40
2.36
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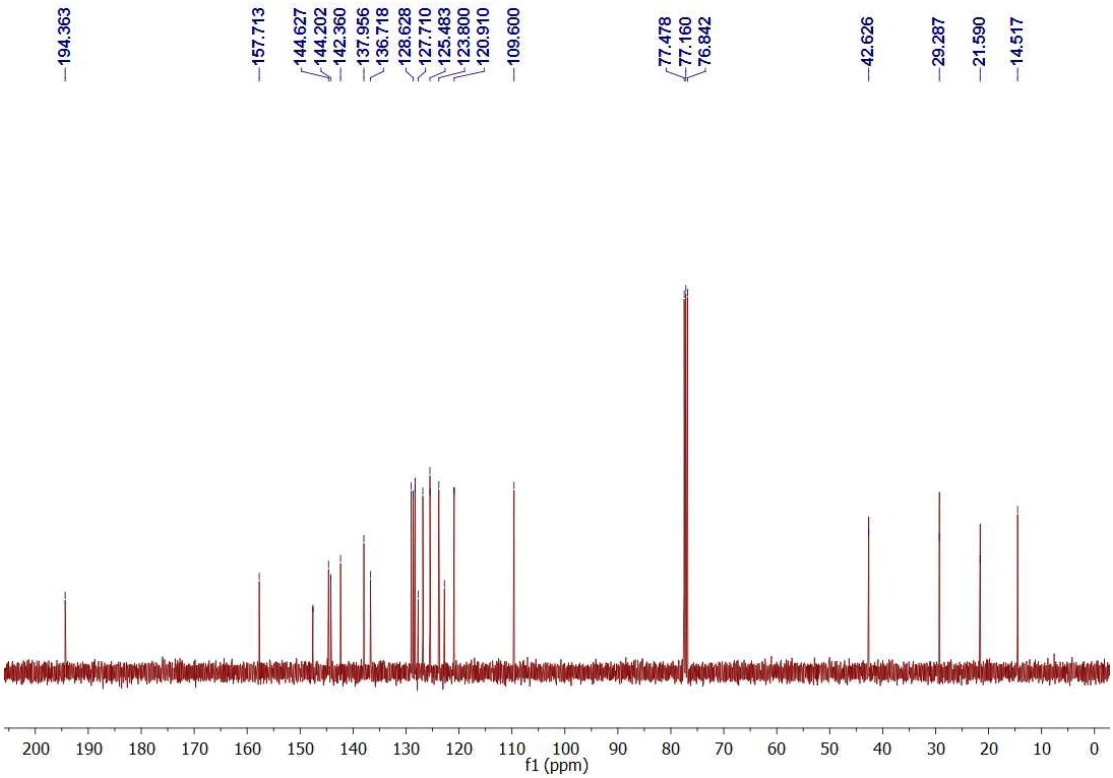
2.02
1.04
1.00
1.01
2.01
3.00
3.01
3.04
f1 (ppm)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142.360
137.956
136.718
128.628
127.710
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77.160
76.842
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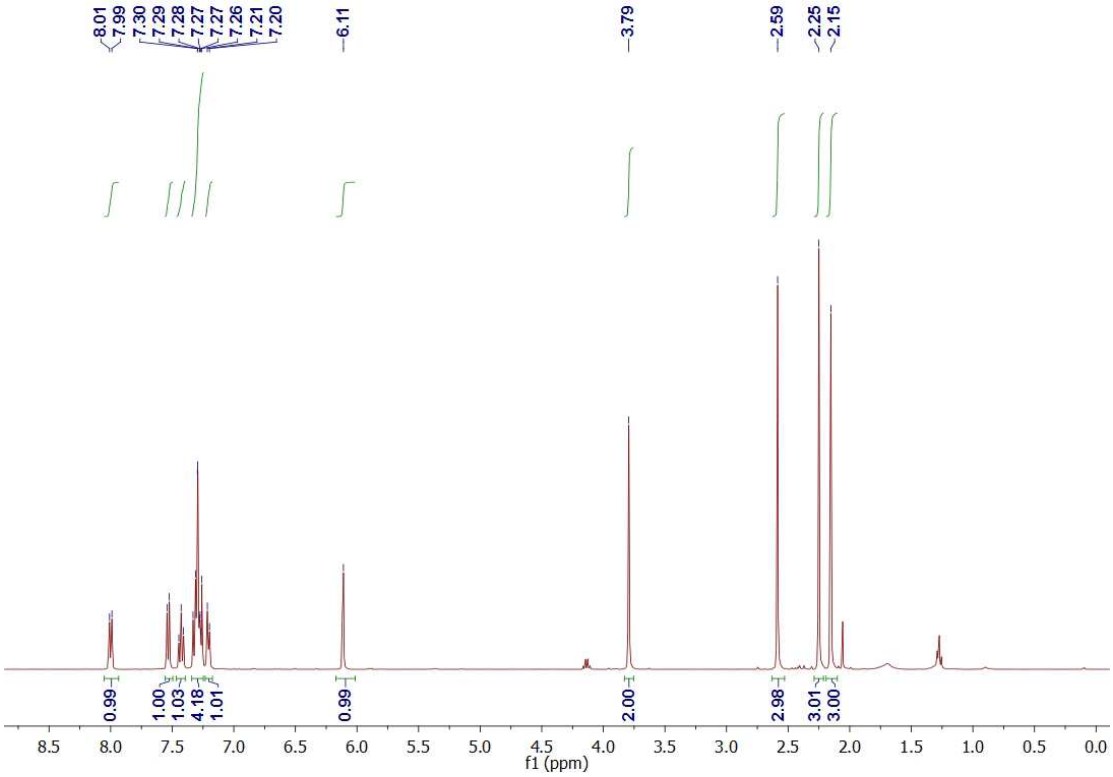
21.590
14.517
f1 (ppm)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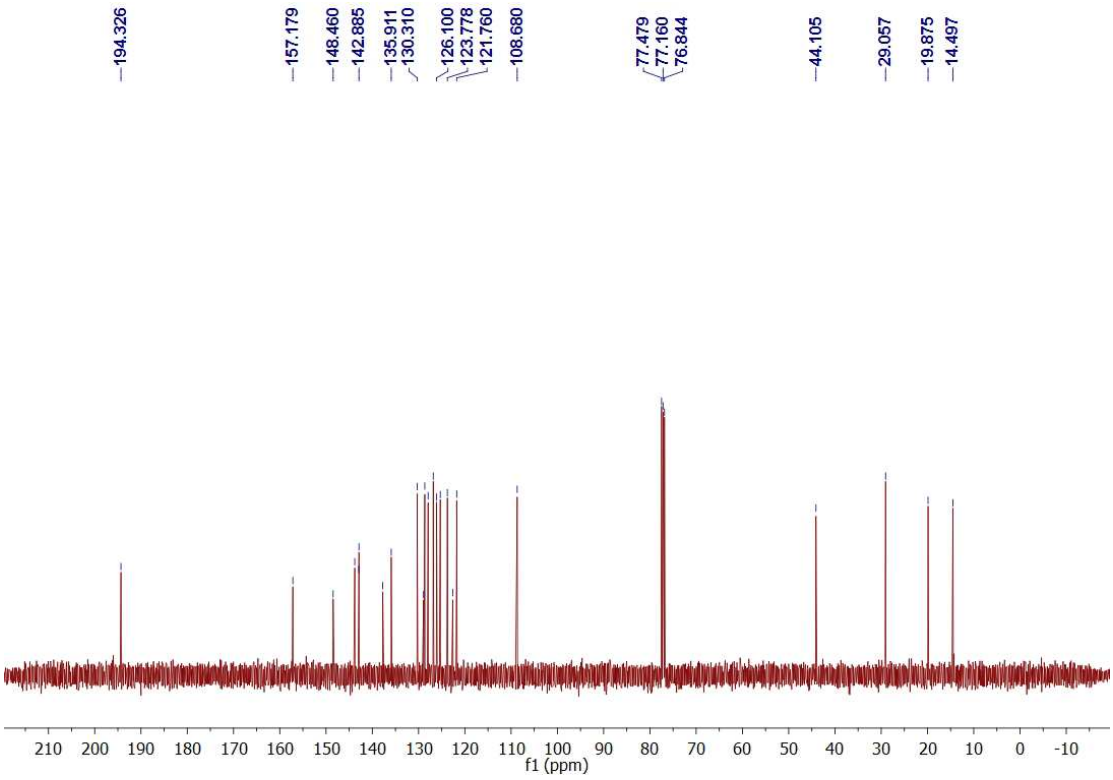
7.27
7.27
7.26
7.21
7.20
6.11
3.79
2.59
2.25
2.15
0.99
1.00
1.03
4.18
1.01
0.99
2.00
2.98
3.01
3.00
f1 (ppm)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135.911
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77.160
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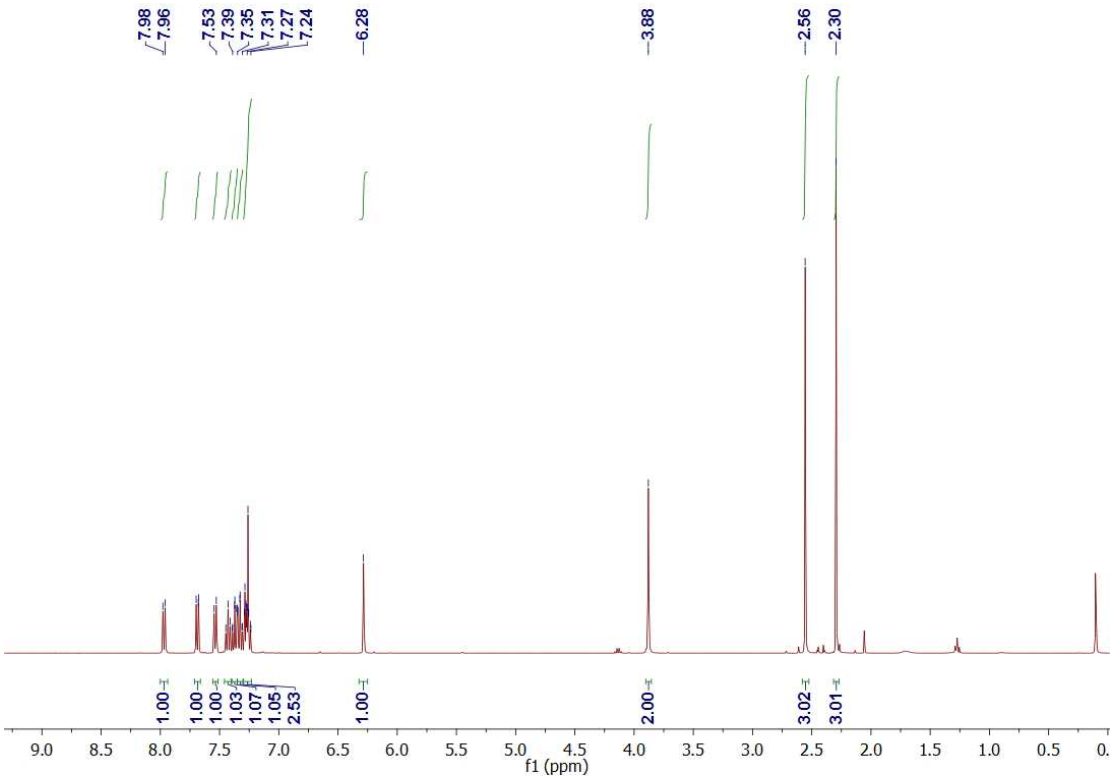
44.105
29.057
19.875
14.497
f1 (ppm)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7.27
7.24
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3.88
2.56
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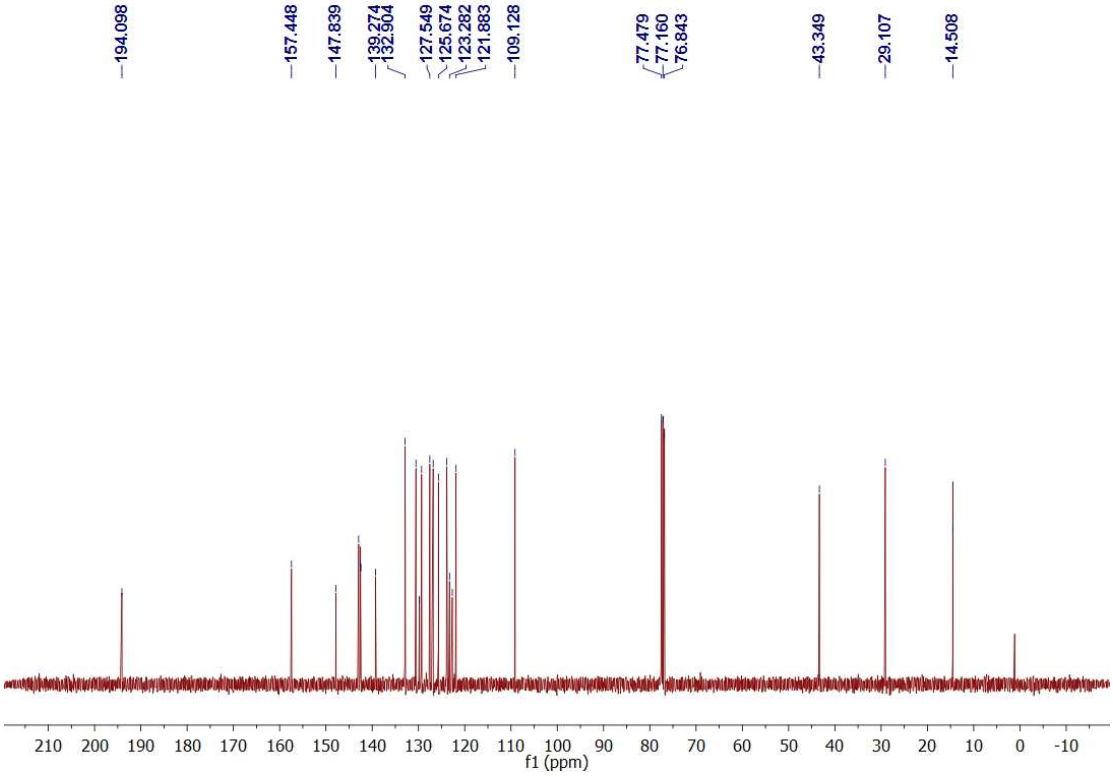
1.00
2.00
3.02
3.01
f1 (ppm)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139.274
132.904
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121.883
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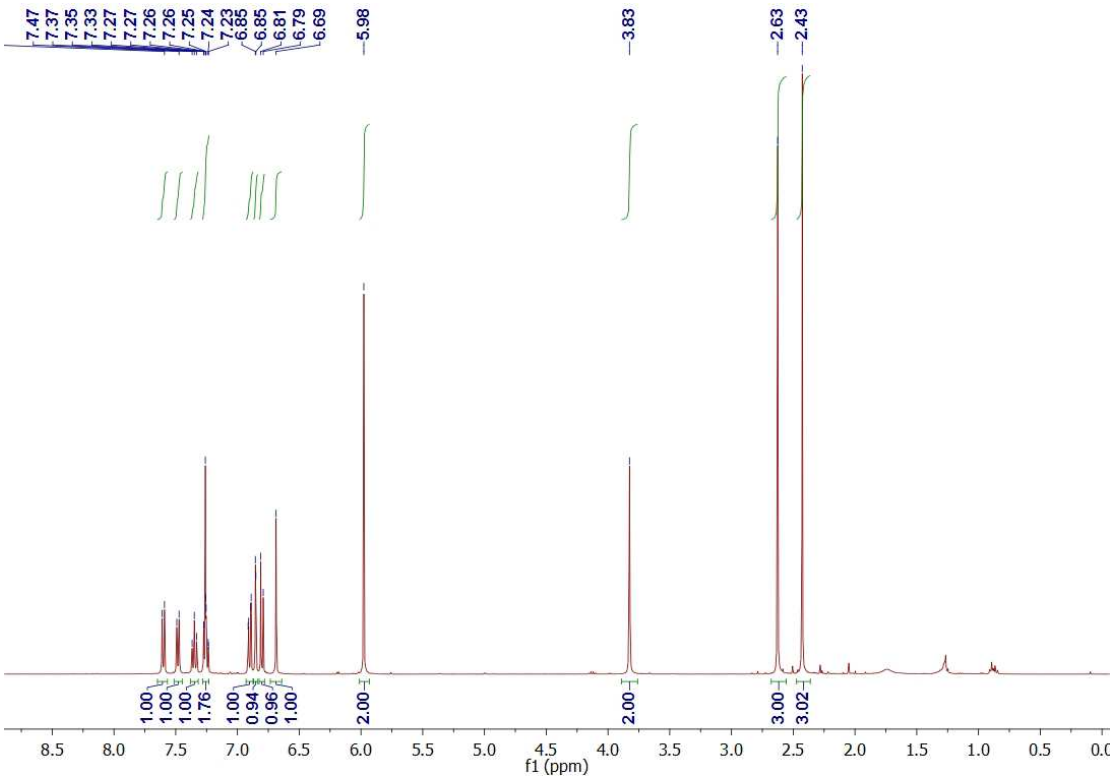
77.479
77.160
76.843
43.349
29.107
14.508
f1 (ppm)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7.26
7.26
7.25
7.24
7.23
6.85
6.81
6.79
6.69
5.98
3.83
2.63
2.43
1.00
1.00
1.00
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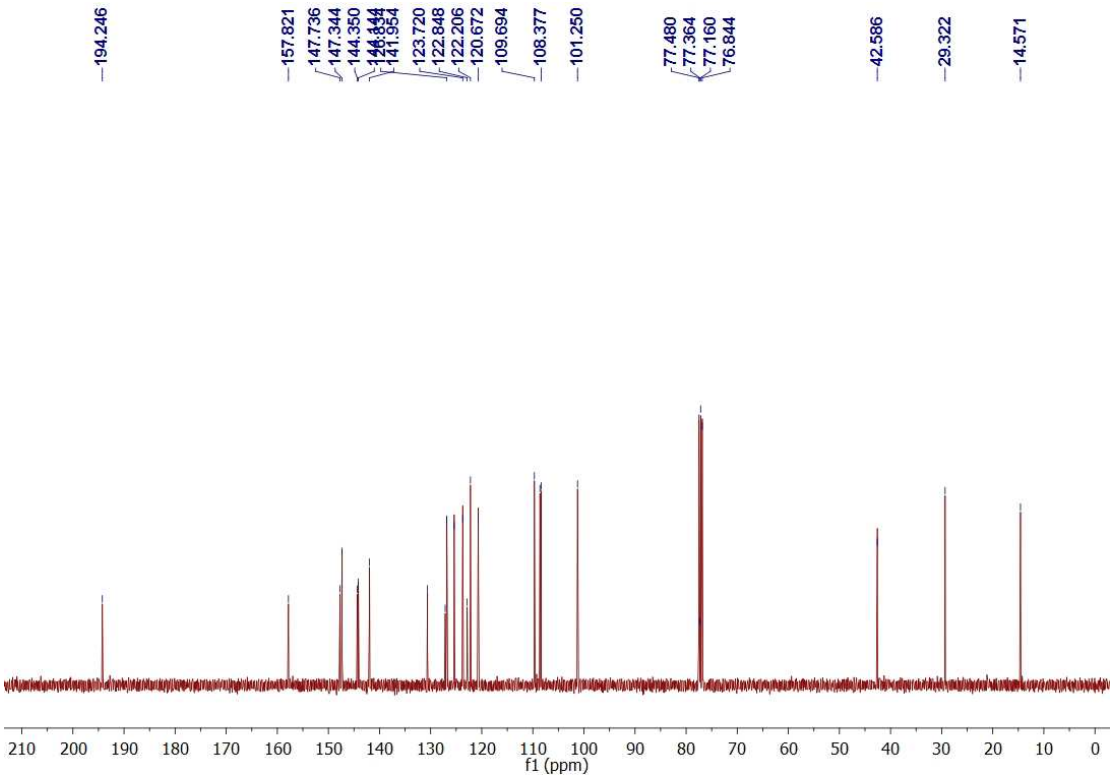
1.00
0.94
0.96
1.00
2.00
2.00
3.00
3.02
f1 (ppm)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122.848
122.206
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101.250
77.480
77.364
77.160
76.844
42.586
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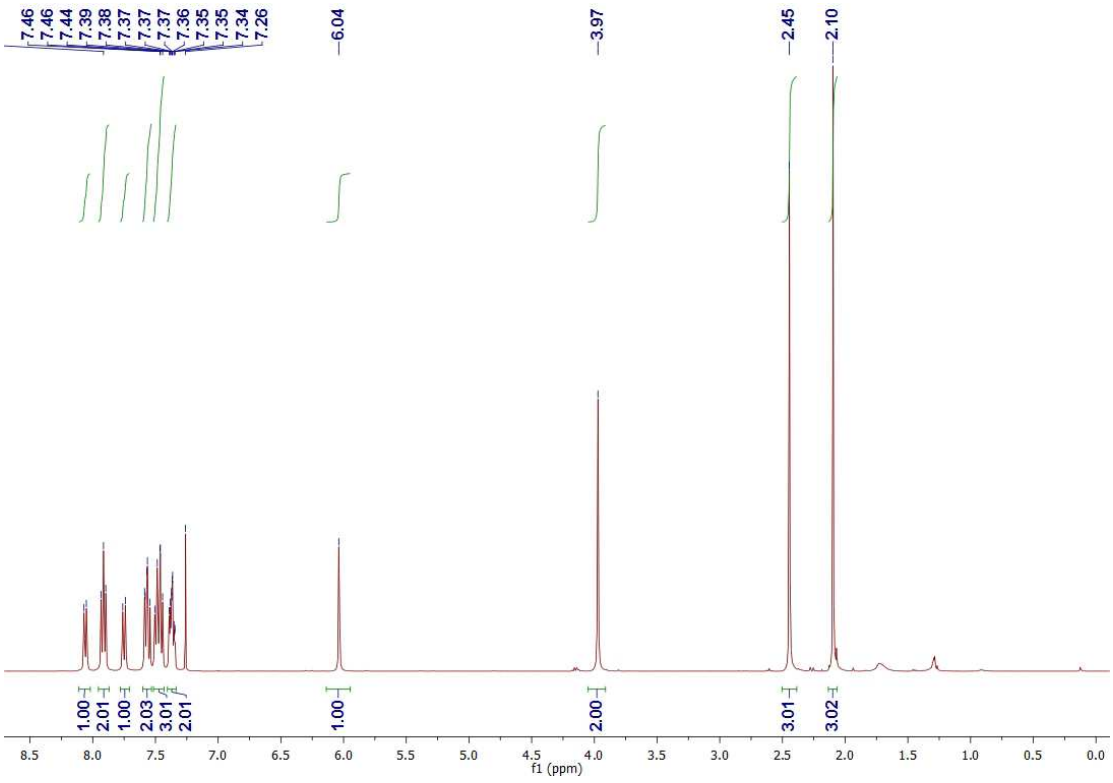
14.571
f1 (ppm)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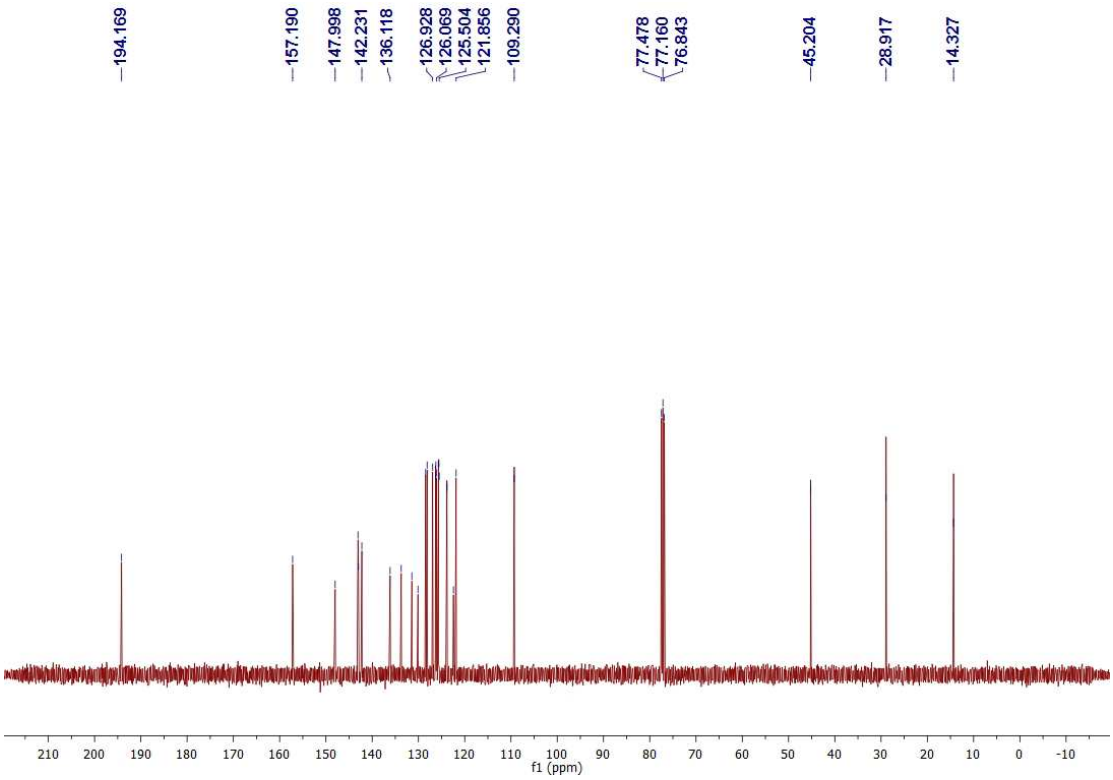
7.39
7.38
7.37
7.37
7.37
7.36
7.35
7.35
7.34
7.26
6.04
3.97
2.45
2.10
1.00
2.01
1.00
2.03
3.01
2.01
1.00
2.00
3.01
3.02
f1 (ppm)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109.290
77.478
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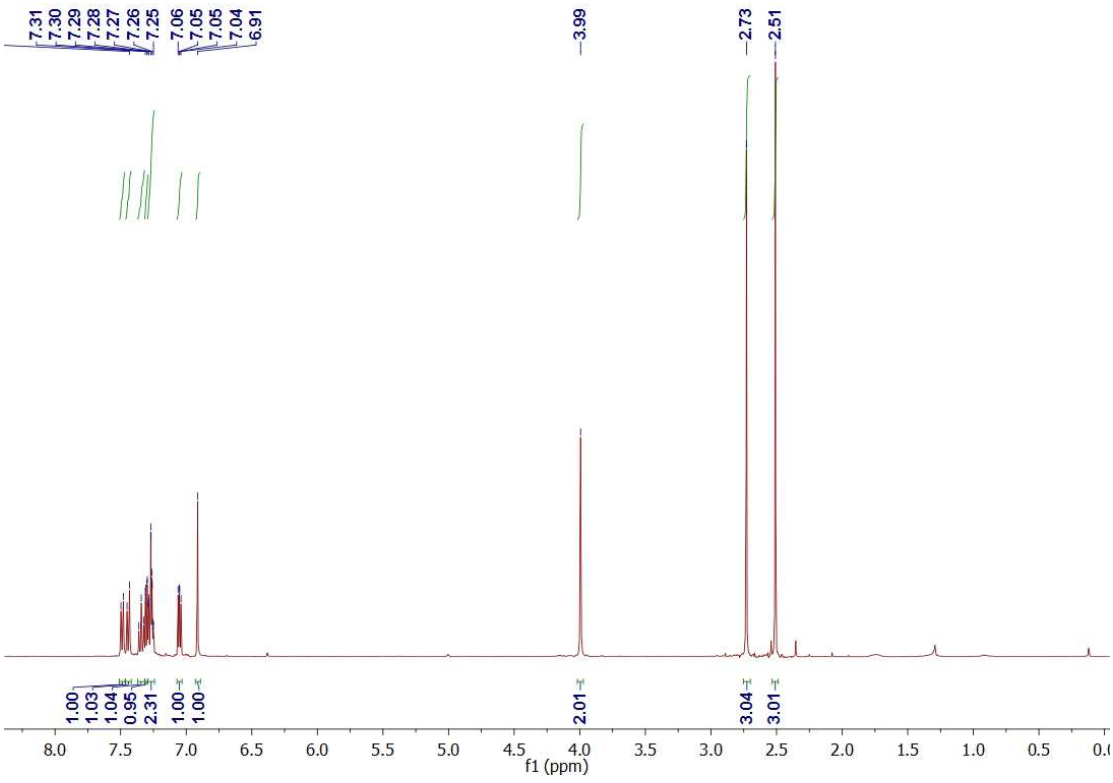
76.843
45.204
28.917
14.327
f1 (ppm)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7.06
7.05
7.05
7.04
6.91
3.99
2.73
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1.04
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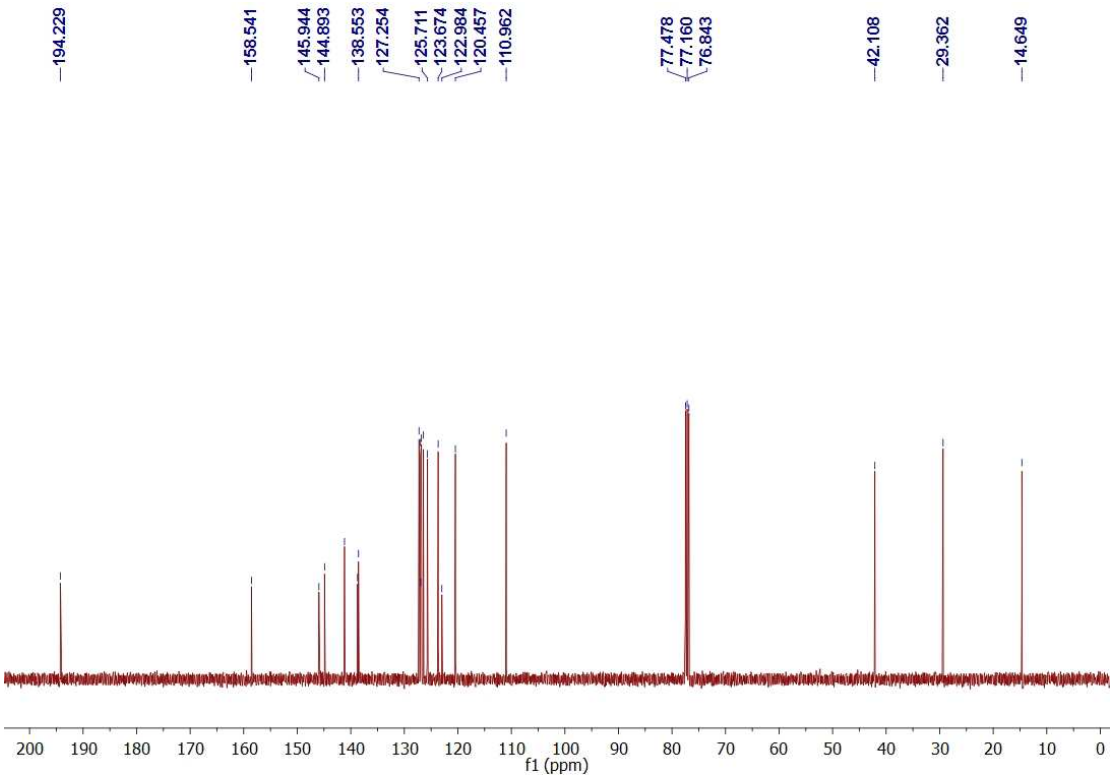
2.31
1.00
1.00
2.01
3.04
3.01
f1 (ppm)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110.962
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77.160
76.843
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14.649
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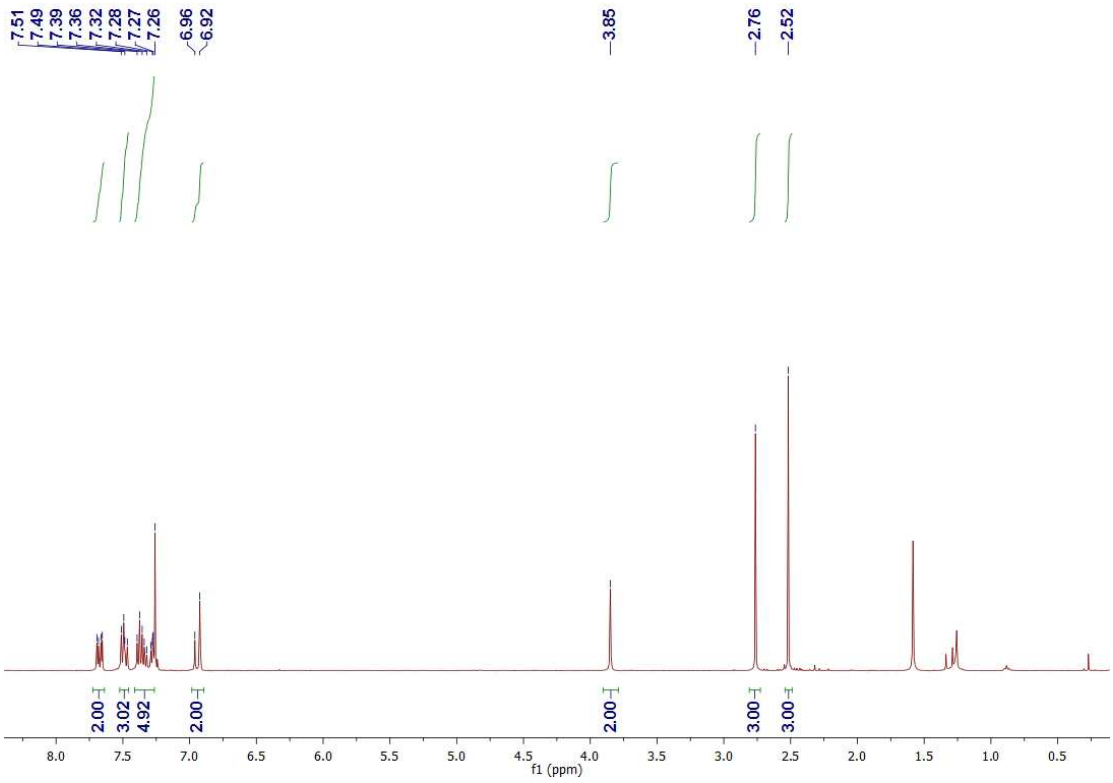
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7.27
7.26
6.96
6.92
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4.92
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2.00
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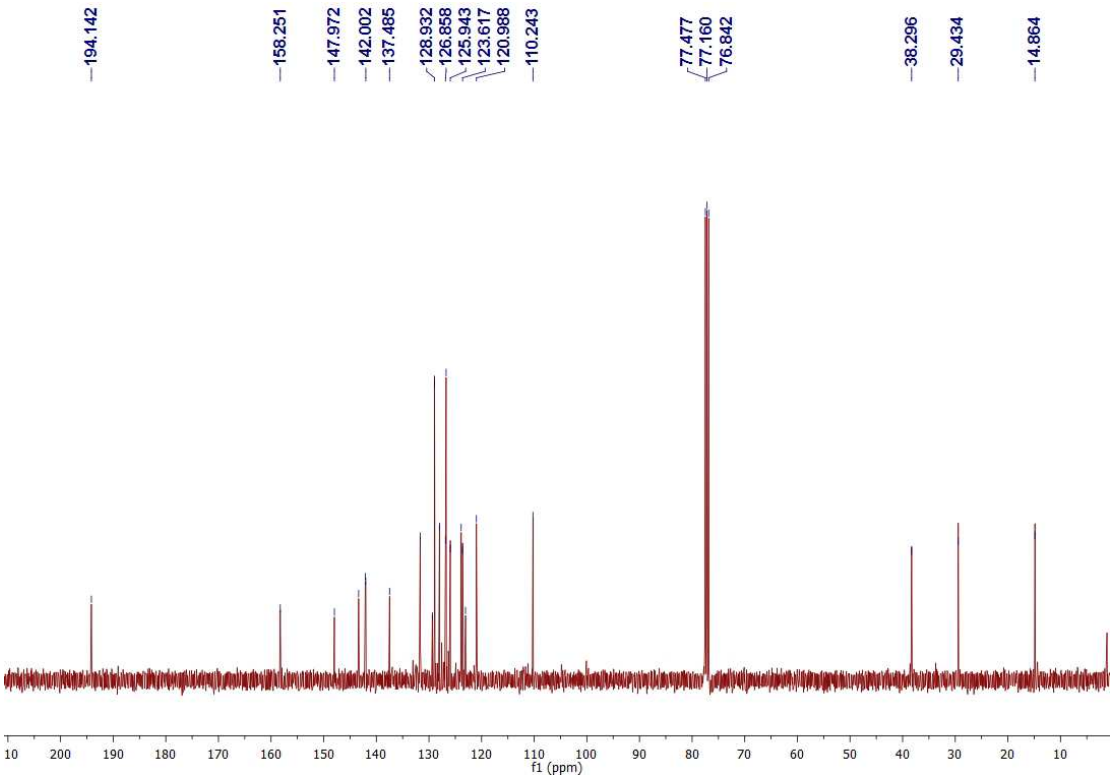
f1 (ppm)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38.296
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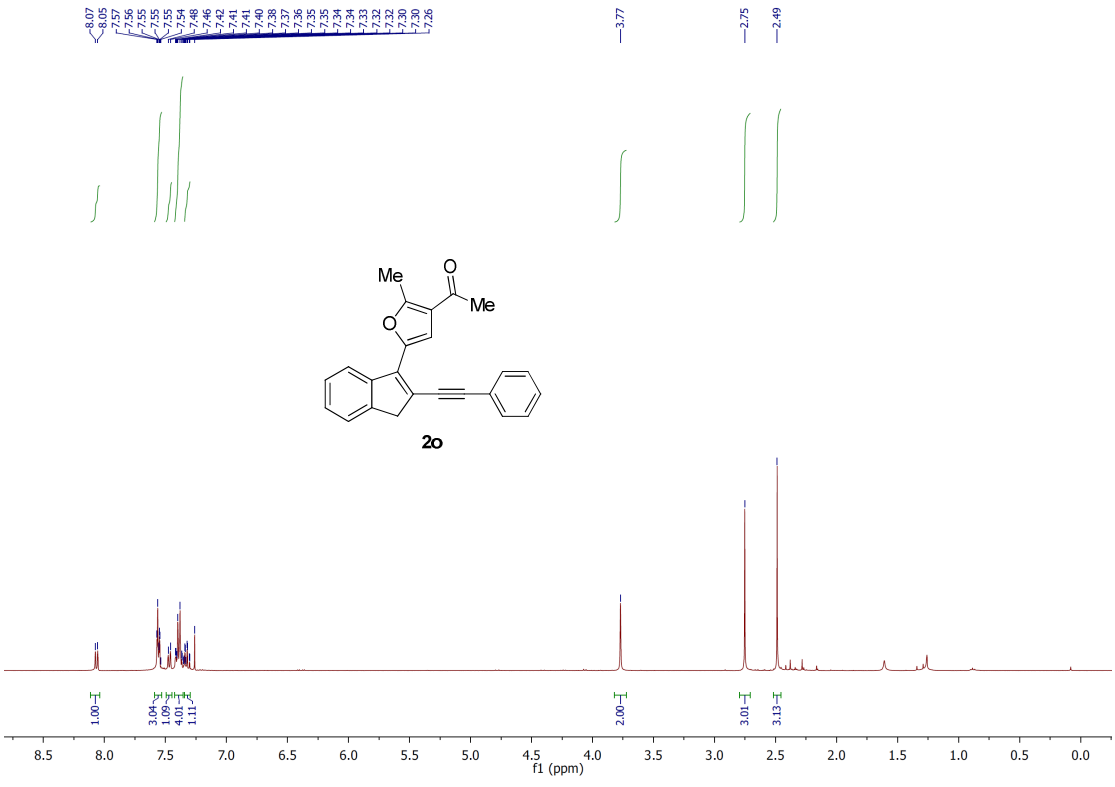
14.864
f1 (ppm)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7.55
7.55
7.54
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7.42
7.41
7.40
7.38
7.37
7.36
7.35
7.35
7.34
7.33
7.32
7.30
7.30
7.26
3.77
2.75
2.49
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Me
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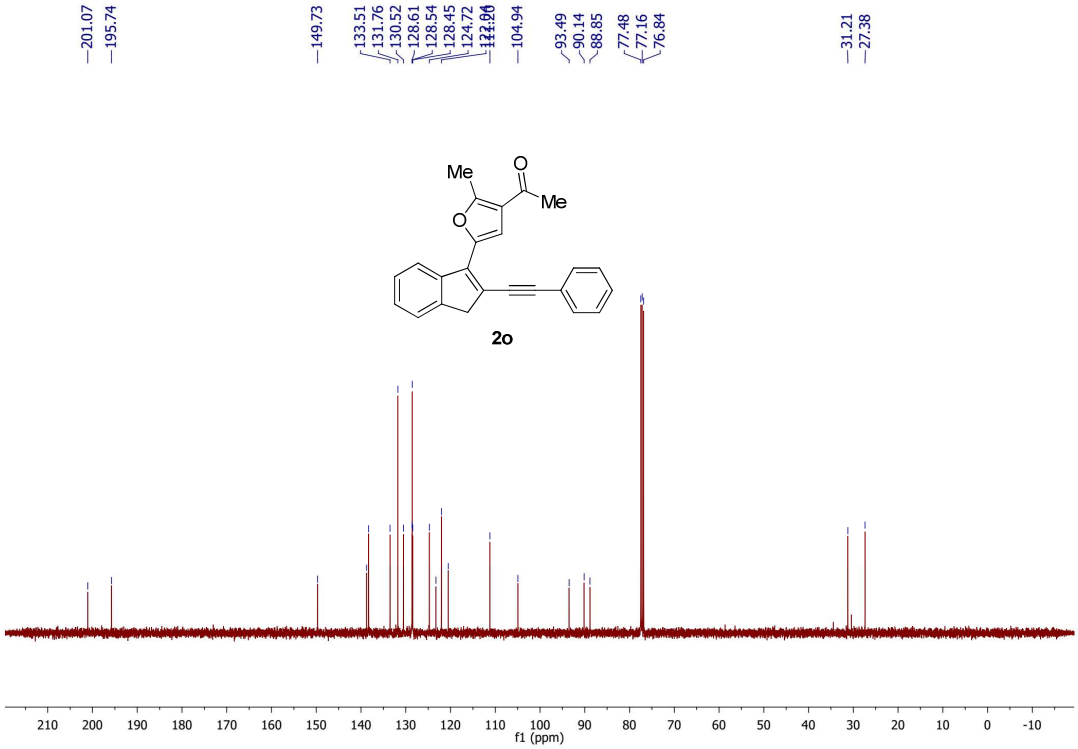
3.04
1.09
4.01
1.11
2.00
3.01
3.13
f1 (ppm)

2o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128.54
128.45
124.72
104.94
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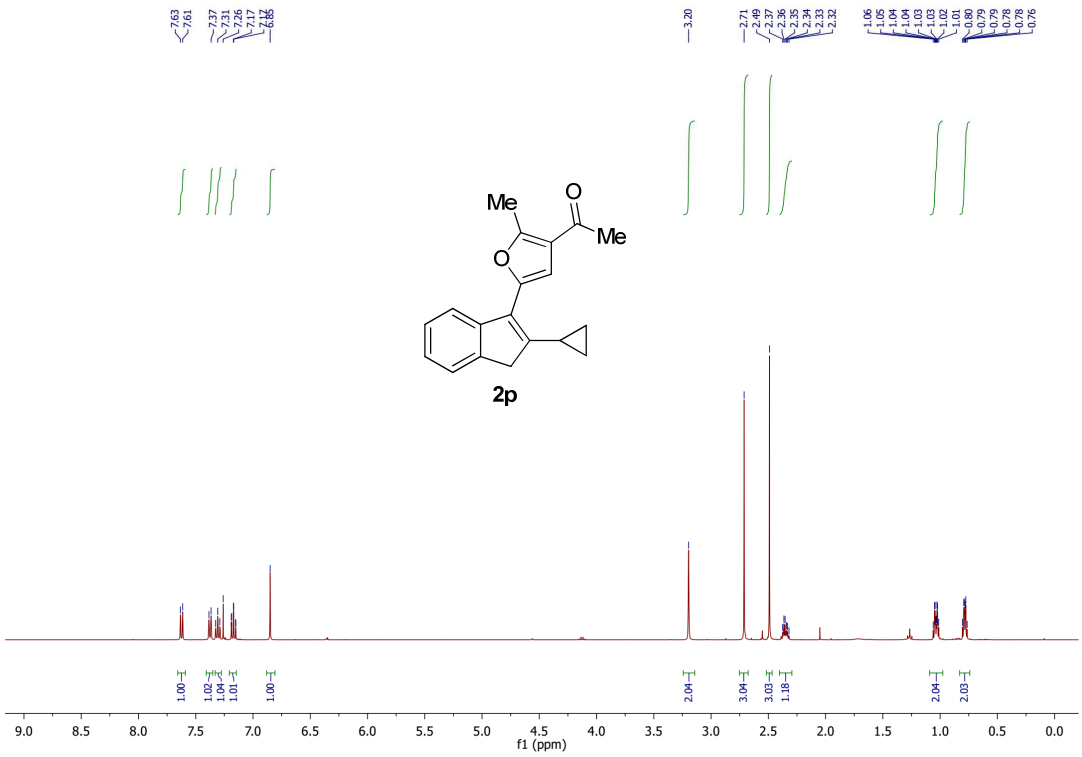
77.48
77.16
76.84
31.21
27.38
Me
O
Me
O
2o
f1 (ppm)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3.20
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2.49
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2.35
2.34
2.33
2.32
1.06
1.05
1.04
1.03
1.02
1.01
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0.79
0.79
0.78
0.78
0.76
Me
O
Me
O
2p
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1.01
1.00
2.04
3.04
3.03
1.18
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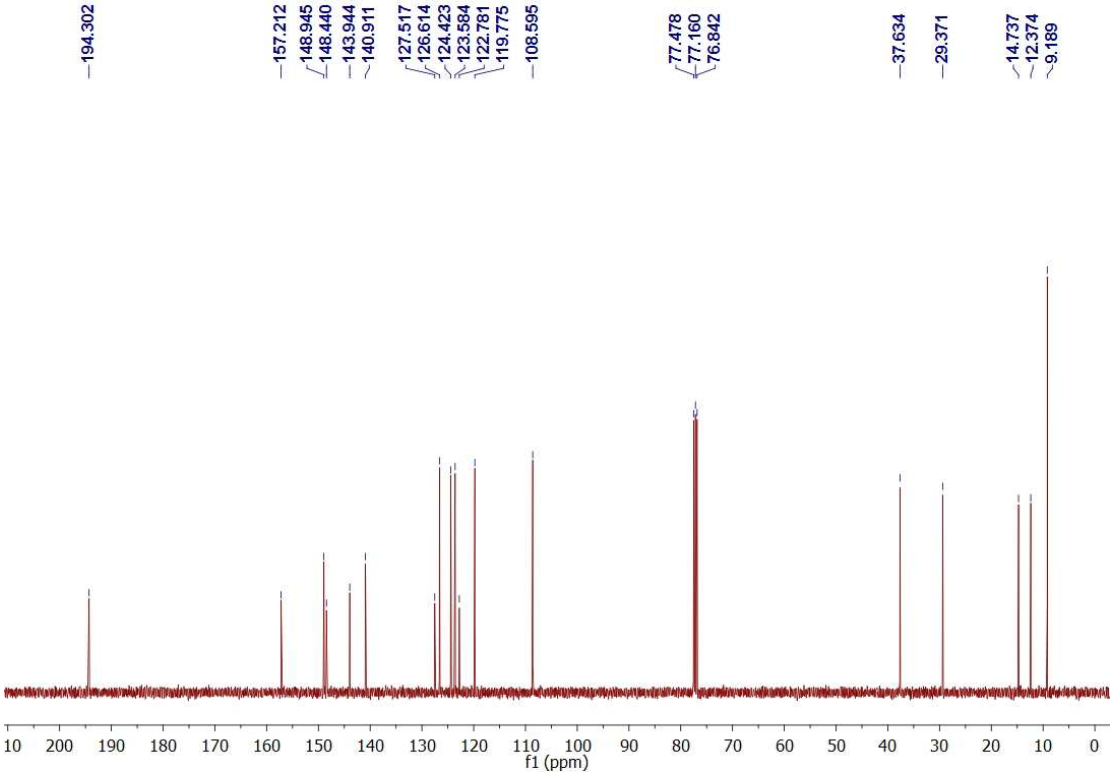
2.03
f1 (ppm)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77.160
76.842
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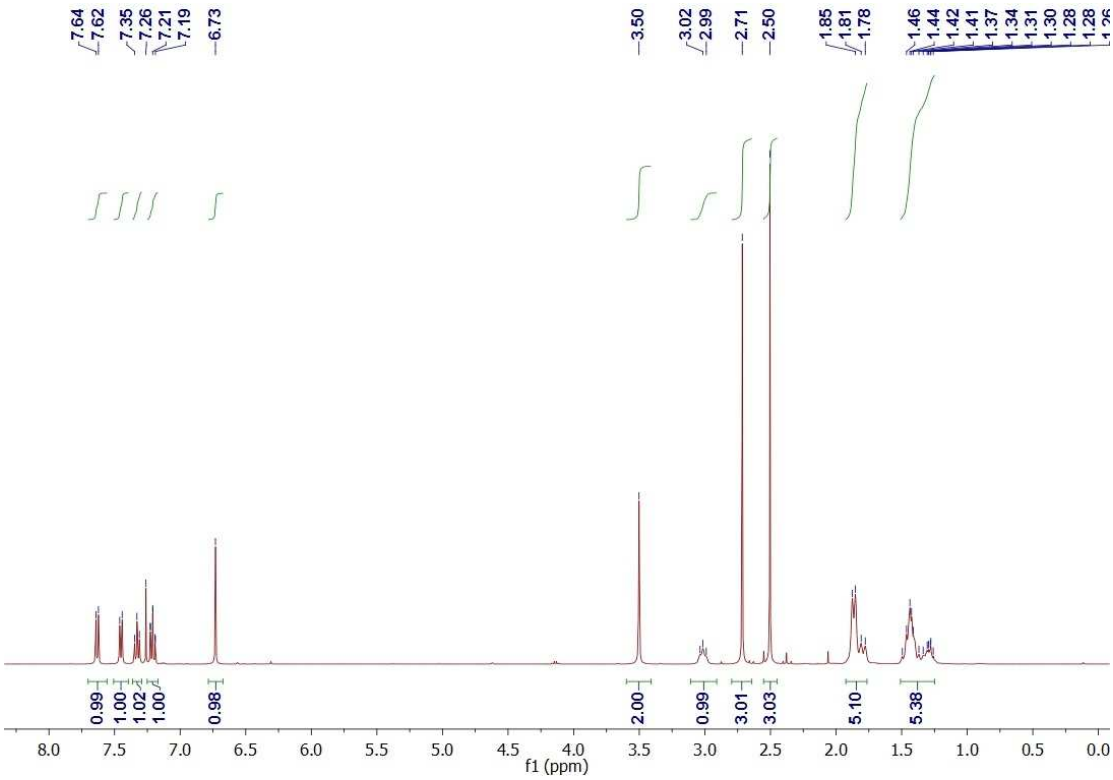
9.189
f1 (ppm)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6.73
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2.71
2.50
1.85
1.81
1.78
1.46
1.44
1.42
1.41
1.37
1.34
1.31
1.30
1.28
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0.98
2.00
0.99
3.01
3.03
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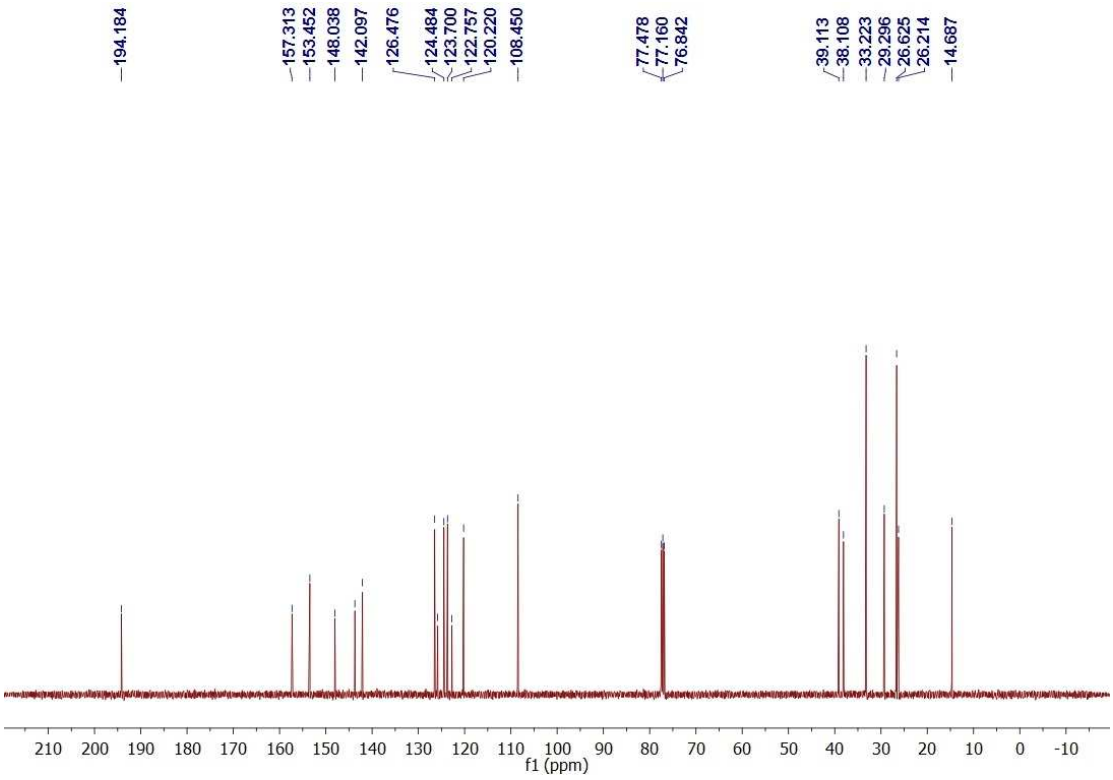
5.38
f1 (ppm)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77.478
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76.842
39.113
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33.223
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26.214
14.687
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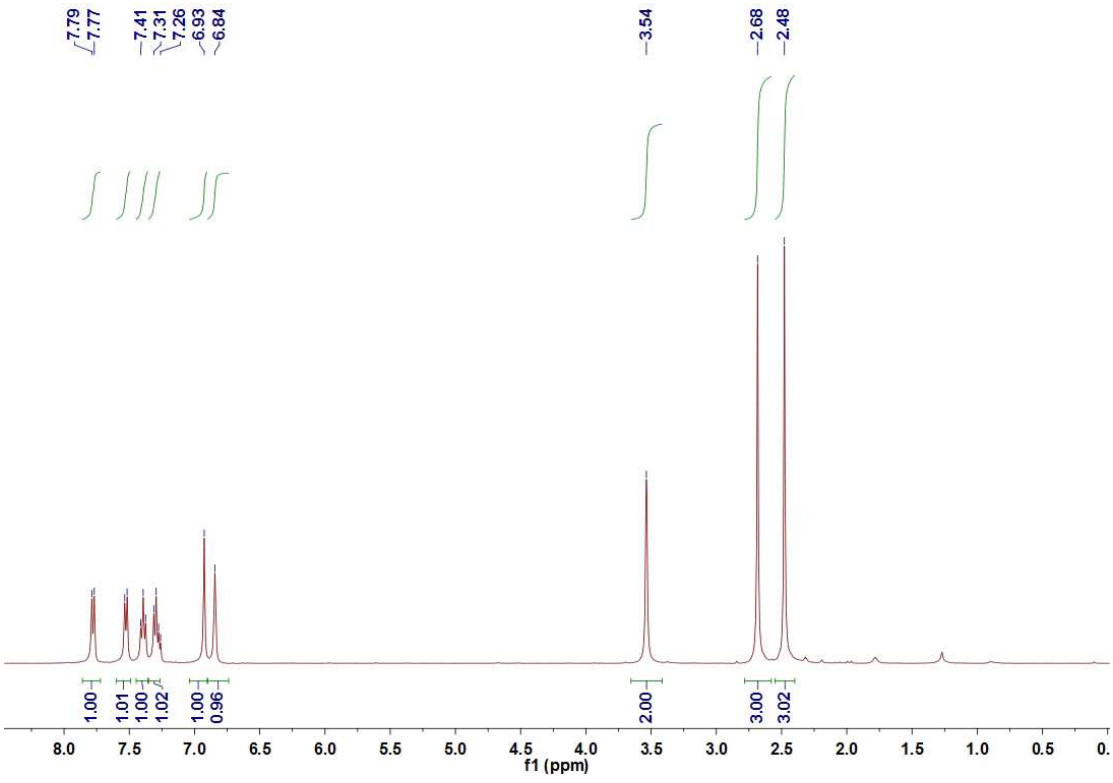
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1.02
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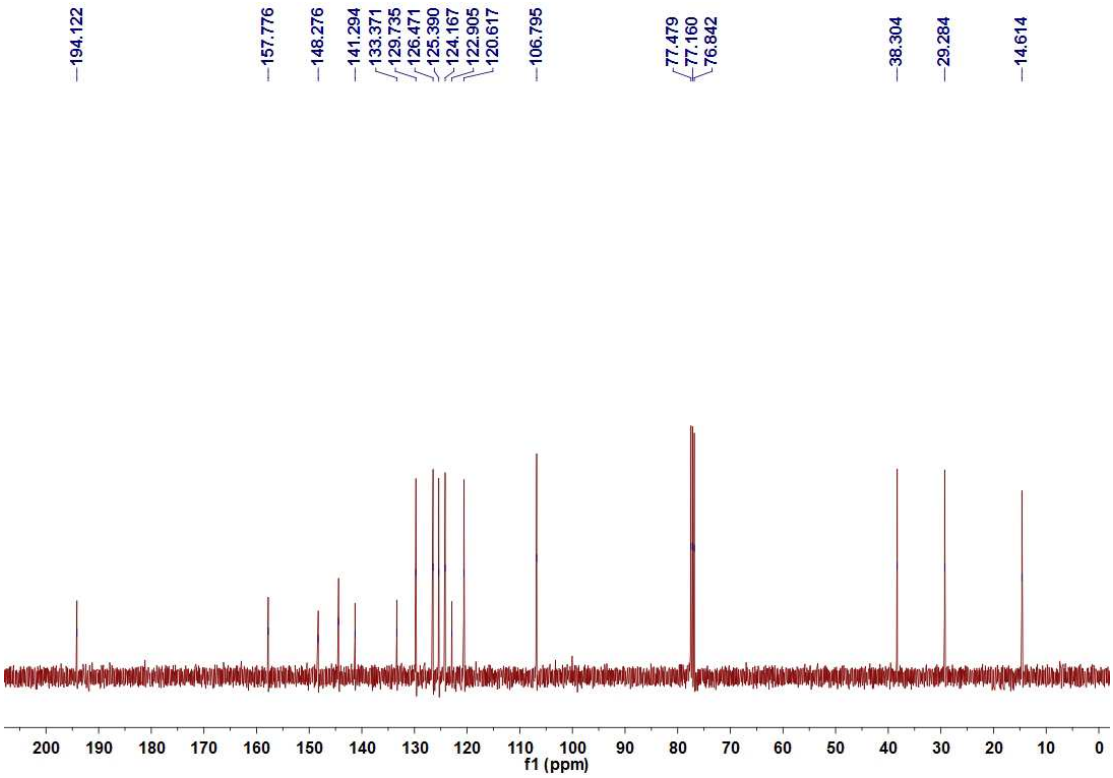
f1 (ppm)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77.160
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38.304
29.284
14.614
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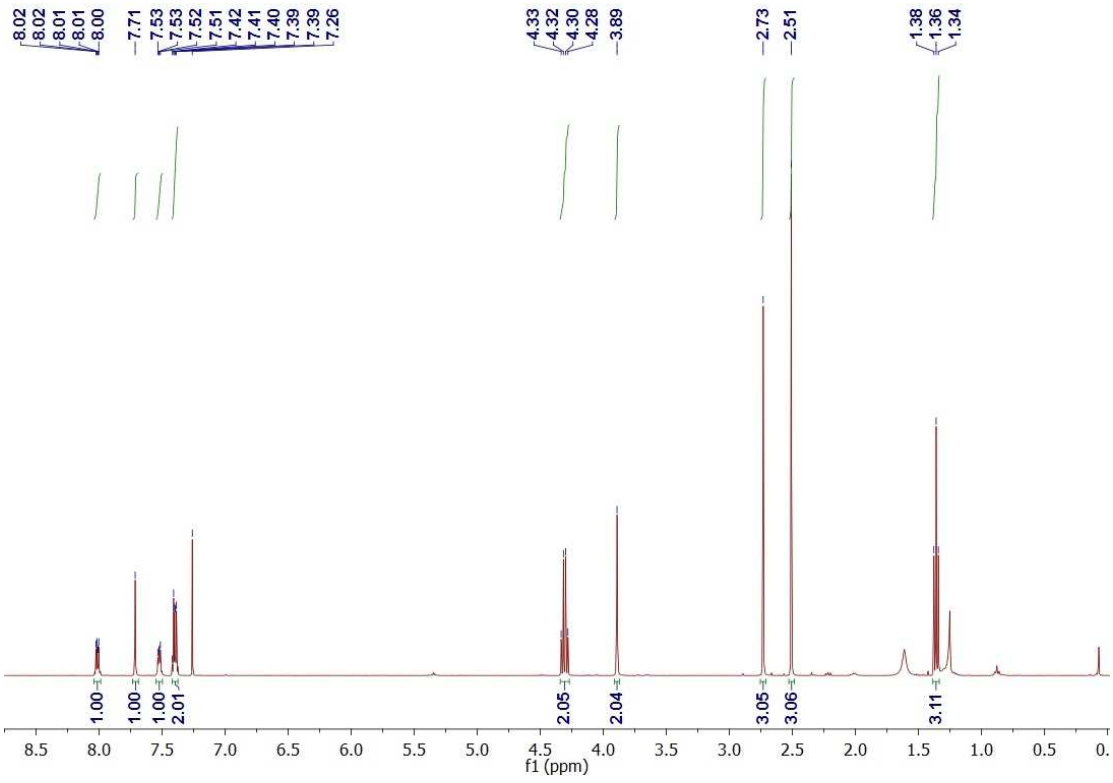
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8.02
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8.01
8.00
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7.53
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7.40
7.39
7.39
7.26
4.33
4.32
4.30
4.28
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2.51
1.38
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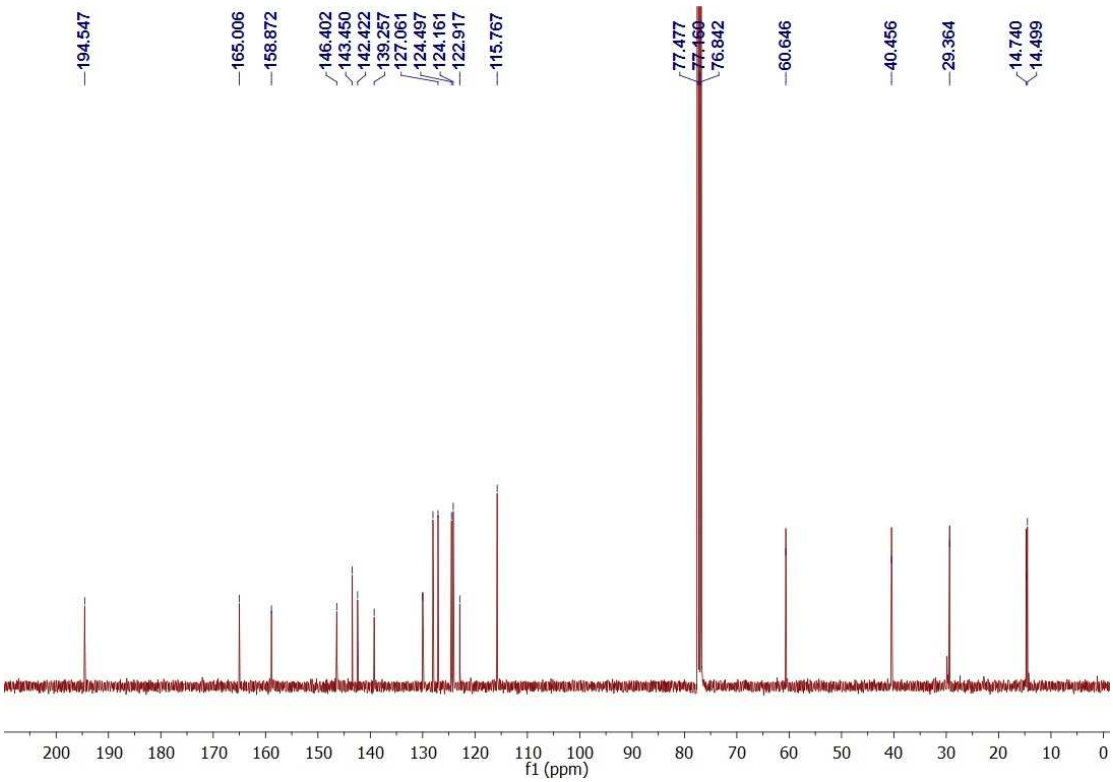
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127.061
124.497
124.161
122.917
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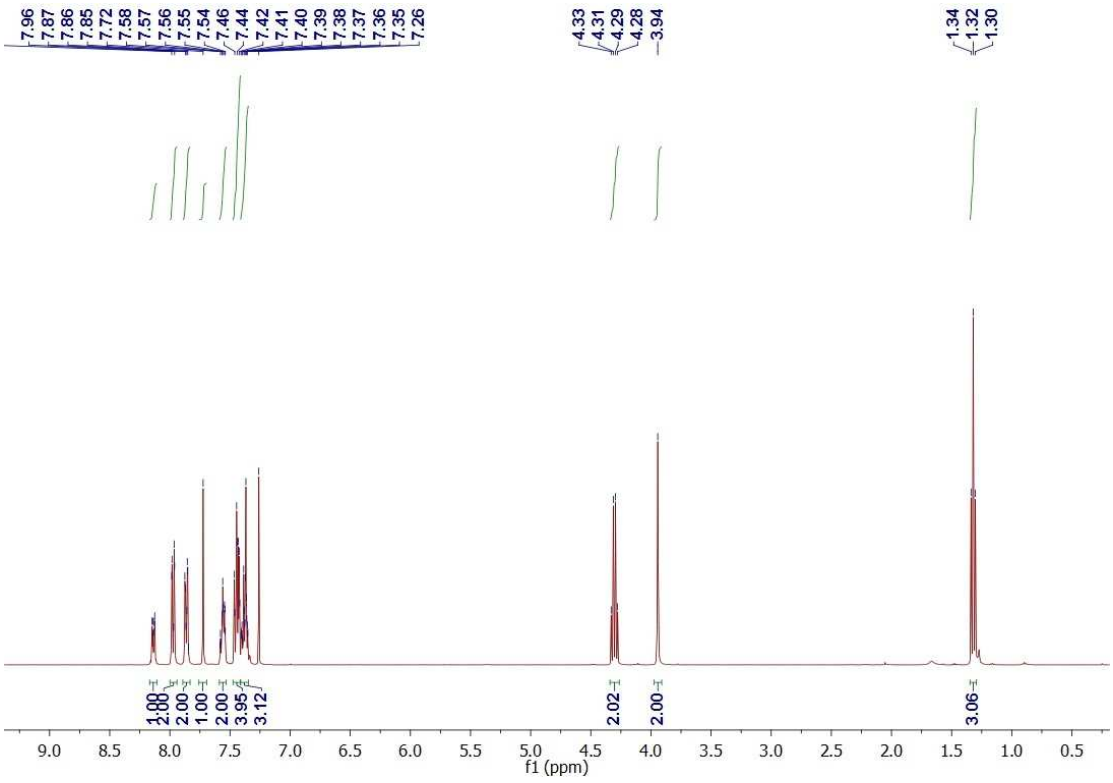
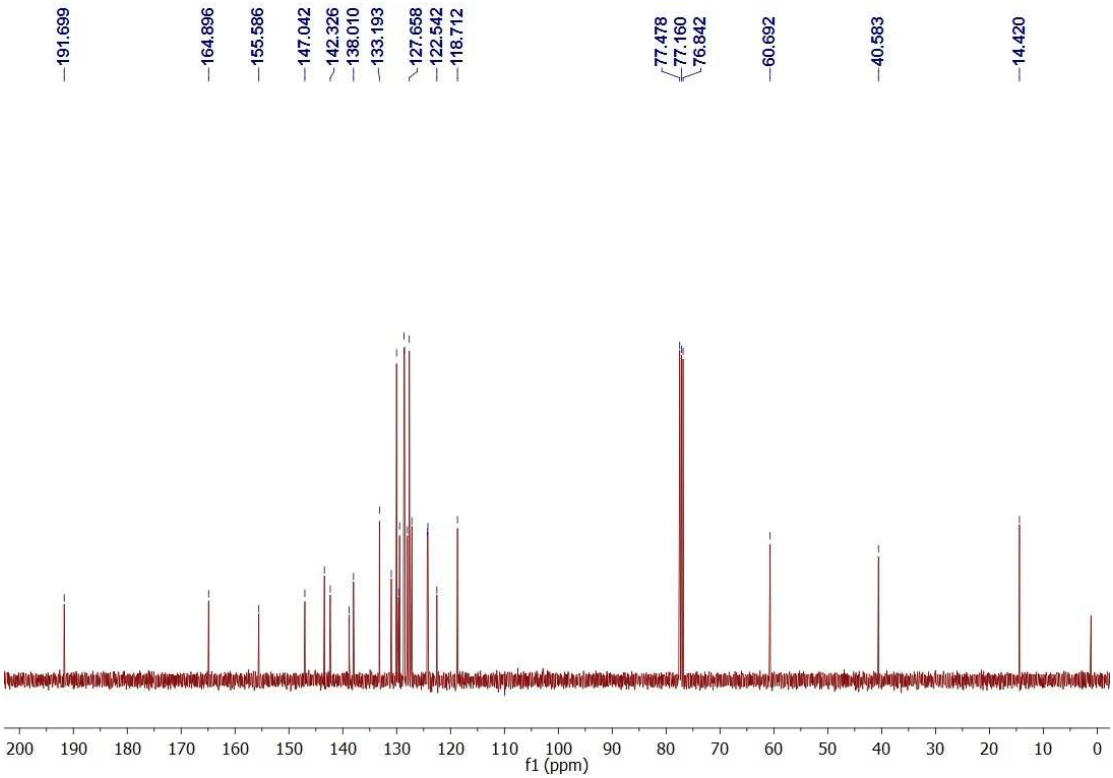
77.477
77.160
76.842
60.646
40.456
29.364
14.740
14.499
f1 (ppm)


7.96
7.87
7.86
7.85
7.72
7.58
7.57
7.56
7.55
7.54
7.46
7.44
7.42
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.26
4.33
4.31
4.29
4.28
3.94
1.34
1.32
1.30
1.00
2.08
2.00
1.00
2.00
3.95
3.12
2.02
2.00
3.06
f1 (ppm)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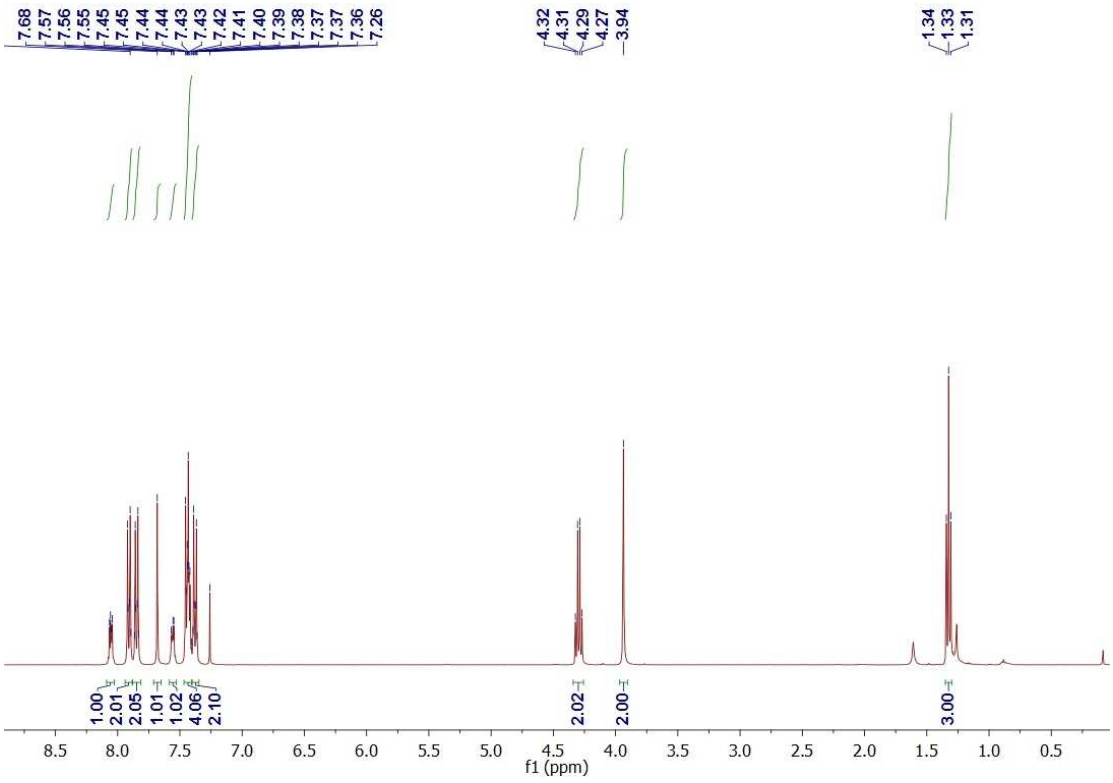
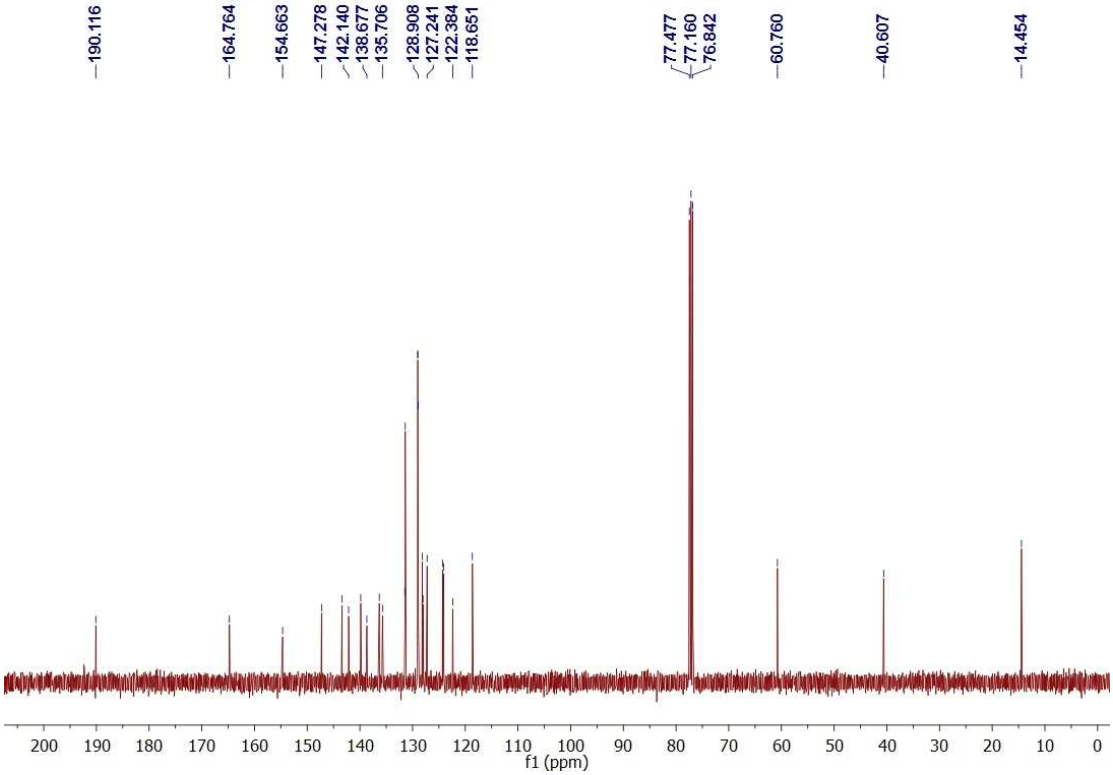
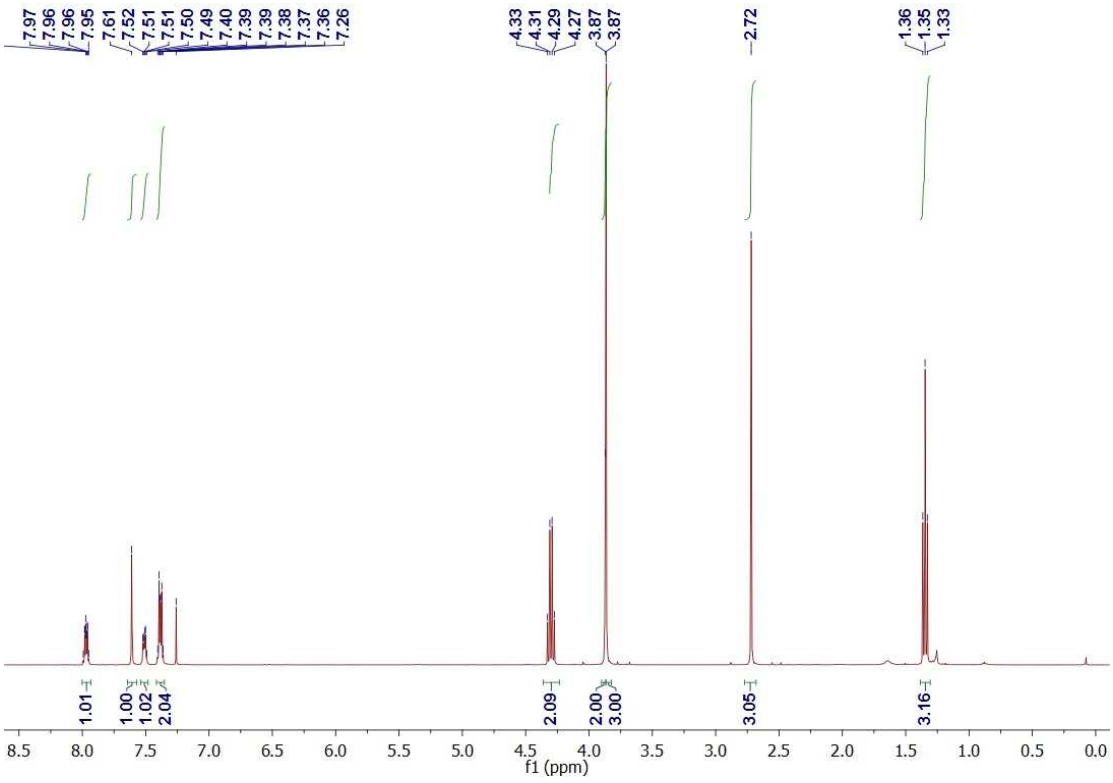
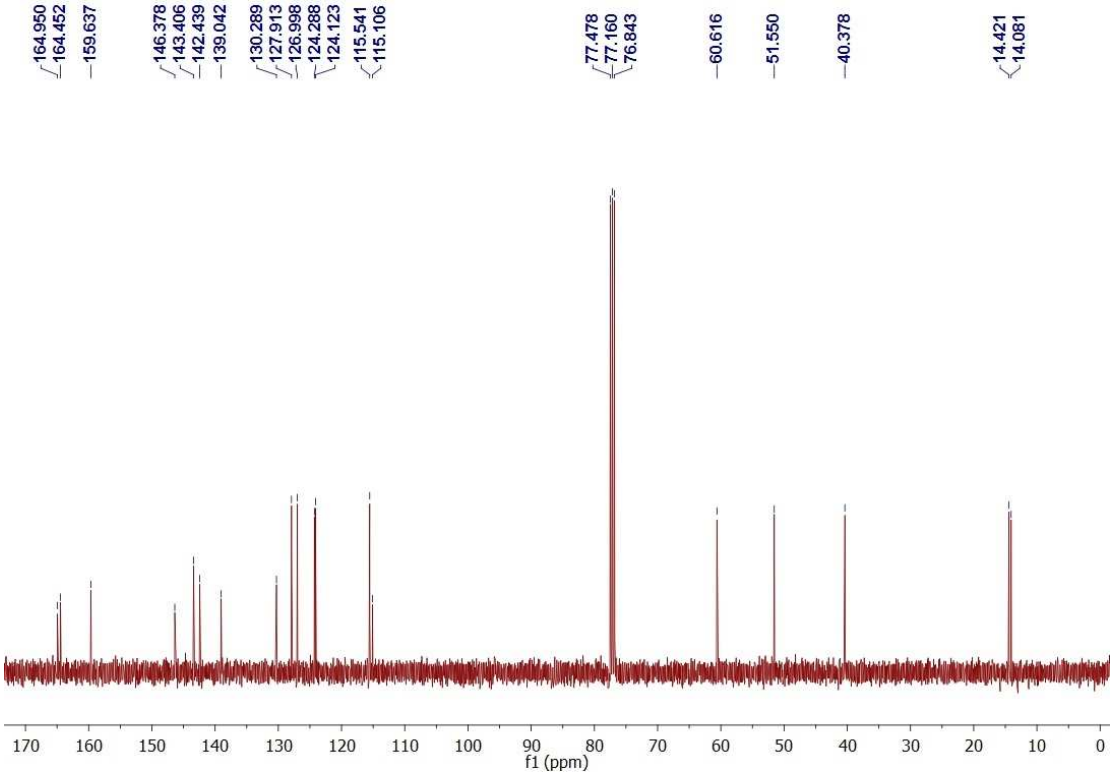
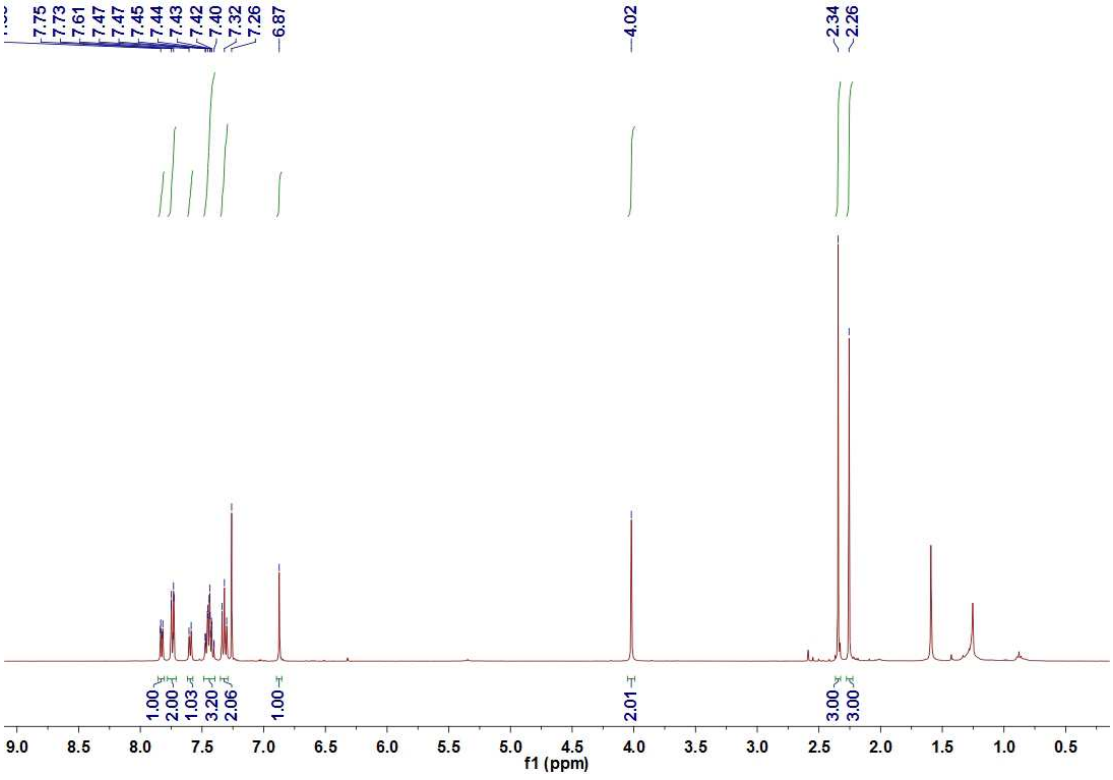
164.896
155.586
147.042
142.326
138.010
133.193
127.658
122.542
118.712
77.478
77.160
76.842
60.692
40.583
14.420
f1 (ppm)

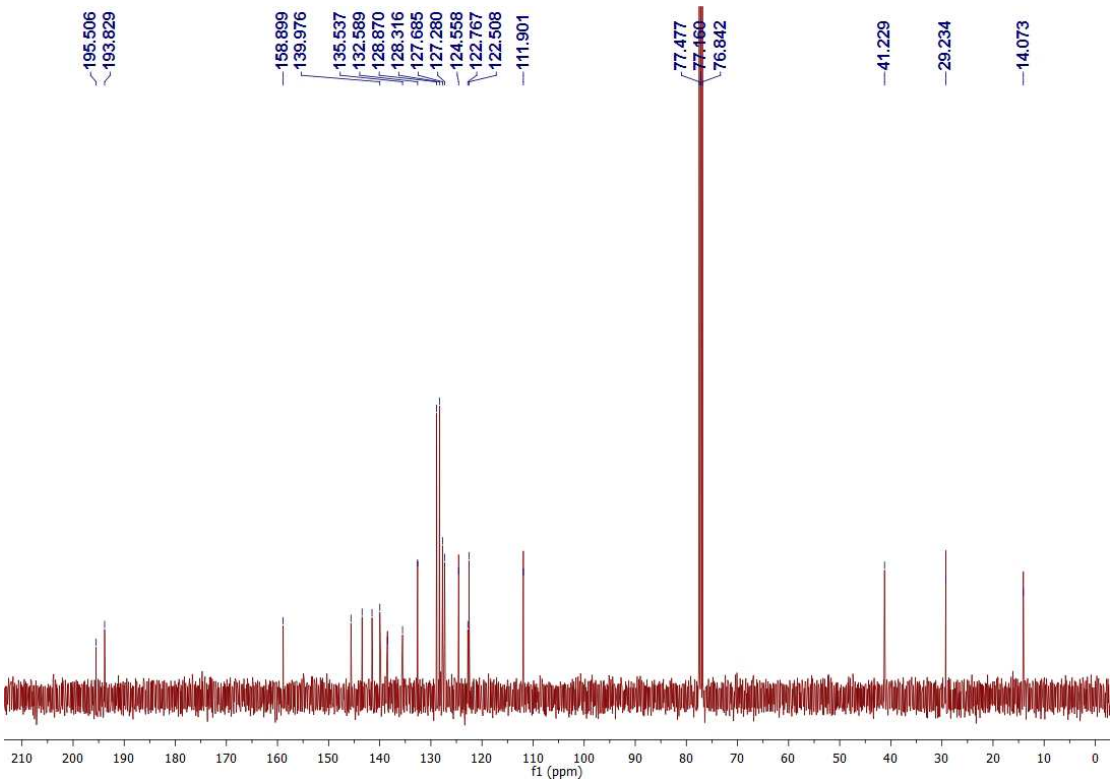

7.68
7.57
7.56
7.55
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.37
7.36
7.26
4.32
4.31
4.29
4.27
3.94
1.34
1.33
1.31
1.00
2.01
2.05
1.01
1.02
4.06
2.10
2.02
2.00
3.00
f1 (ppm)

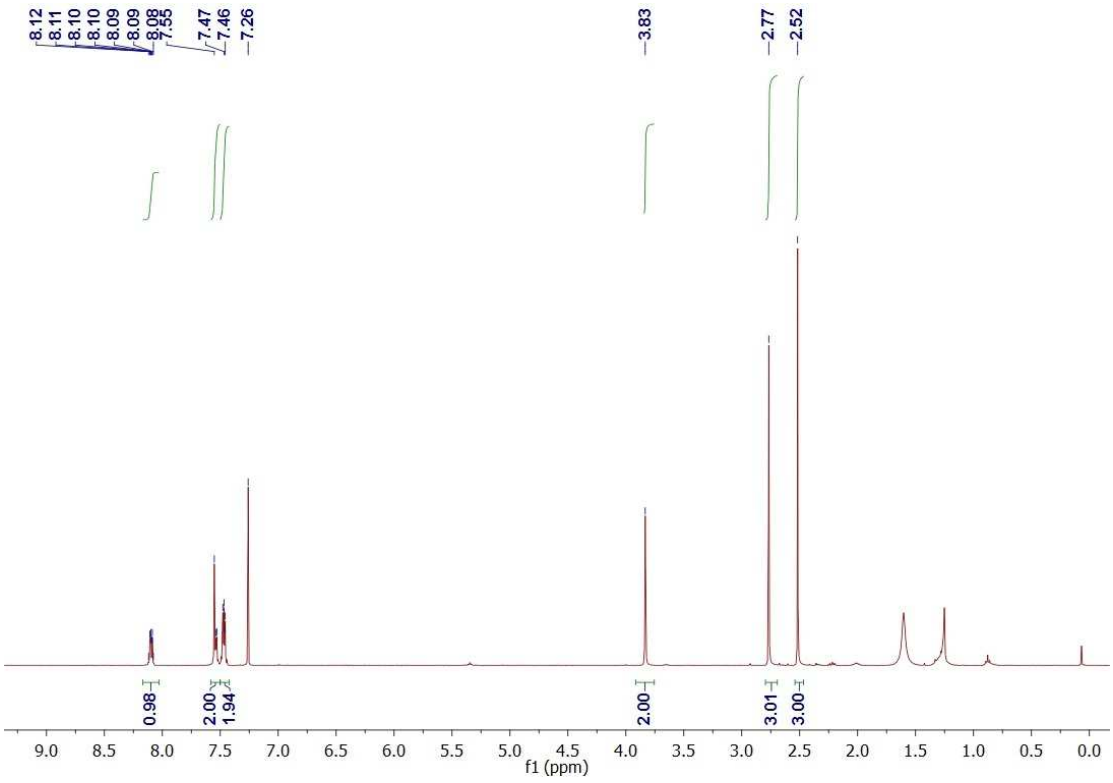

190.116
164.764
154.663
147.278
142.140
138.677
135.706
128.908
127.241
122.384
118.651
77.477
77.160
76.842
60.760
40.607
14.454
f1 (ppm)

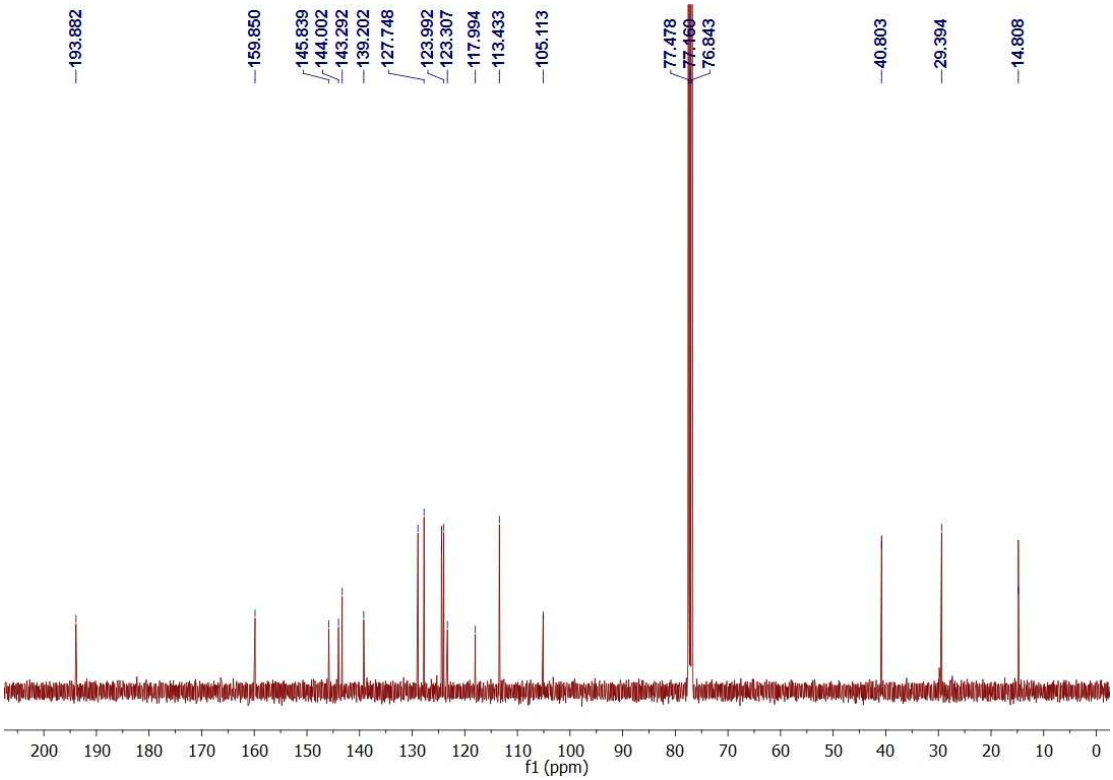

7.97
7.96
7.96
7.95
7.61
7.52
7.51
7.51
7.50
7.49
7.40
7.39
7.39
7.38
7.37
7.36
7.26
4.33
4.31
4.29
4.27
3.87
3.87
2.72
1.36
1.35
1.33
1.01
1.00
1.02
2.04
2.09
2.00
3.00
3.05
3.16
f1 (ppm)

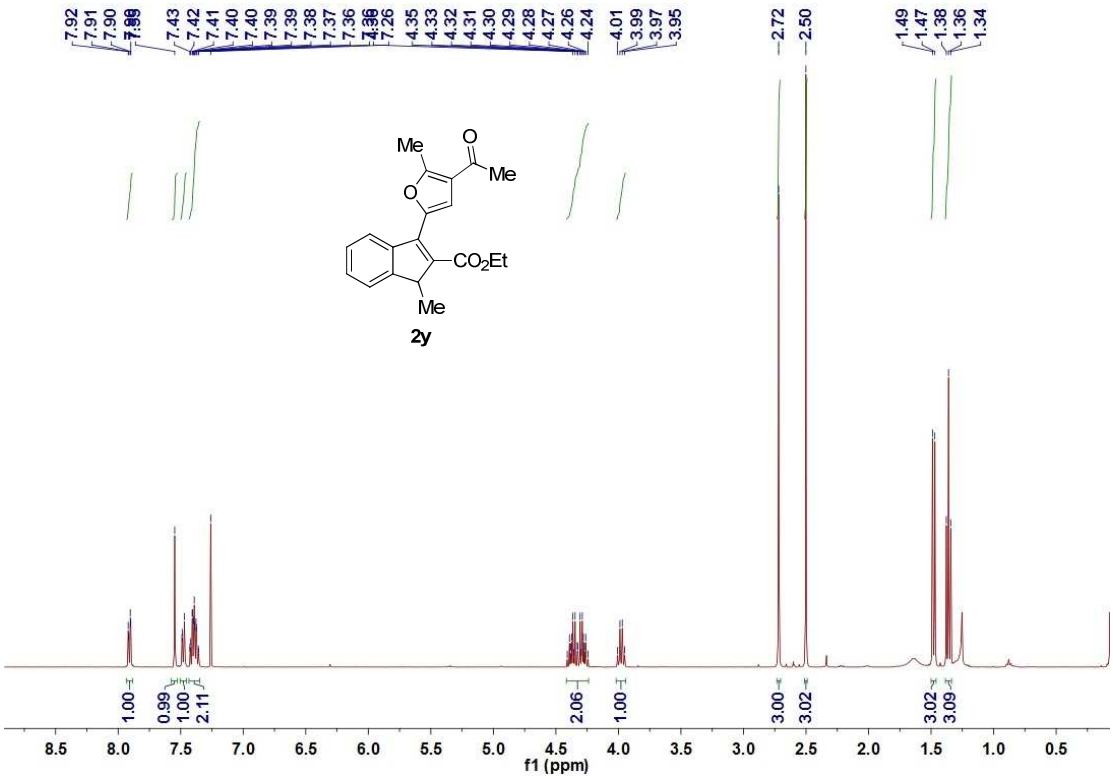

164.950
164.452
159.637
146.378
143.406
142.439
139.042
130.289
127.913
126.998
124.288
124.123
115.541
115.106
77.478
77.160
76.843
60.616
51.550
40.378
14.421
14.081
f1 (ppm)

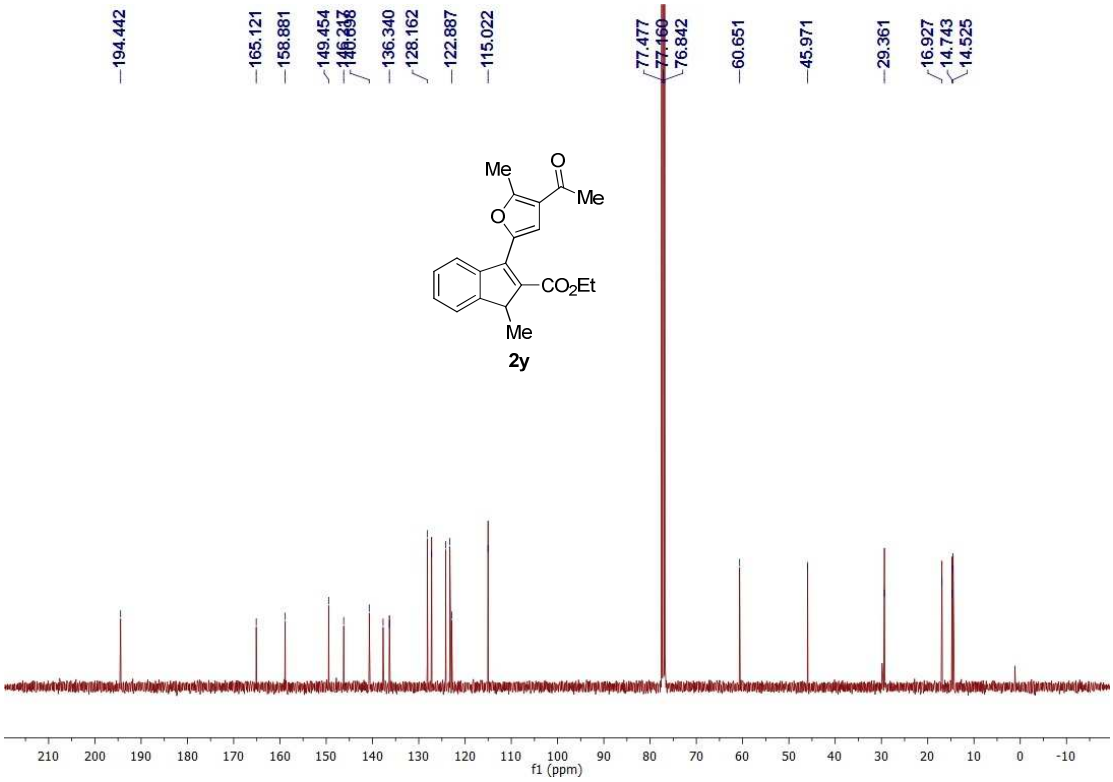

7.75
7.73
7.61
7.47
7.47
7.45
7.44
7.43
7.42
7.40
7.32
7.26
6.87
4.02
2.34
2.26
1.00
2.00
1.03
3.20
2.06
1.00
2.01
3.00
3.00
f1 (ppm)


195.506
193.829
158.899
139.976
135.537
132.589
128.870
128.316
127.685
127.280
124.558
122.767
122.508
111.901
77.477
77.160
76.842
41.229
29.234
14.073
f1 (ppm)


8.12
8.11
8.10
8.10
8.09
8.09
8.08
7.55
7.47
7.46
7.26
3.83
2.77
2.52
0.98
2.00
1.94
2.00
3.01
3.00
f1 (ppm)


193.882
159.850
145.839
144.002
143.292
139.202
127.748
123.992
123.307
117.994
113.433
105.113
77.478
77.160
76.843
40.803
29.394
14.808
f1 (ppm)


7.92
7.91
7.90
7.43
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.36
4.35
4.33
4.32
4.31
4.30
4.29
4.28
4.27
4.26
4.24
4.01
3.99
3.97
3.95
2.72
2.50
1.49
1.47
1.38
1.36
1.34
Me
O
Me
O
CO2Et
Me
2y
1.00
0.99
1.00
2.11
2.06
1.00
3.00
3.02
3.02
3.09
f1 (ppm)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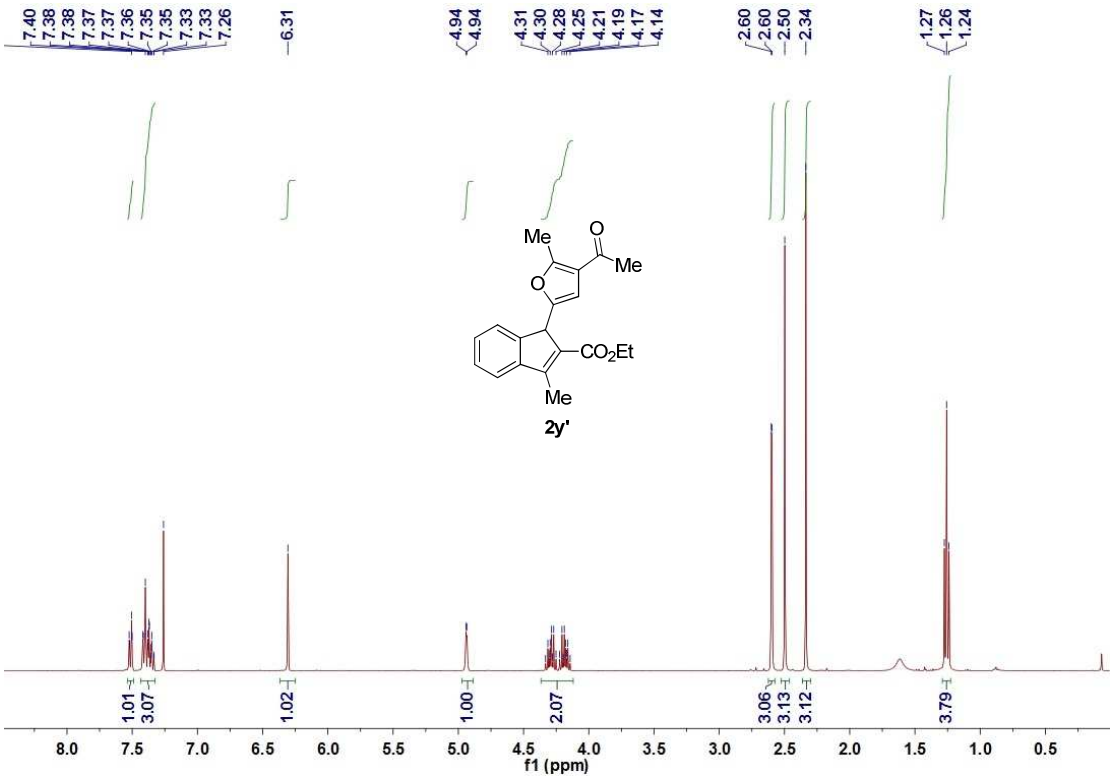
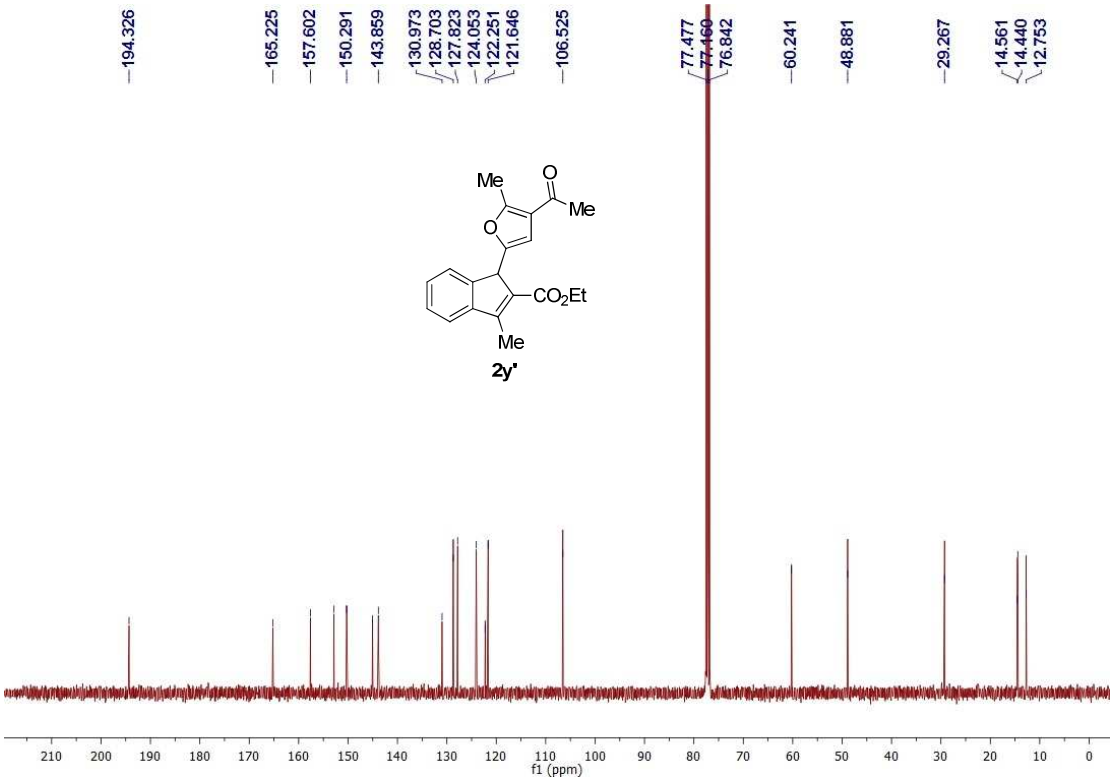
165.121
158.881
149.454
136.340
128.162
122.887
115.022
77.477
77.160
76.842
60.651
45.971
29.361
16.927
14.743
14.525
Me
O
Me
O
CO2Et
Me
2y
f1 (ppm)


7.40
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.33
7.33
7.26
6.31
4.94
4.94
4.31
4.30
4.28
4.25
4.21
4.19
4.17
4.14
2.60
2.60
2.50
2.34
1.27
1.26
1.24
Me
O
Me
O
CO2Et
Me
2y'
1.01
3.07
1.02
1.00
2.07
3.06
3.13
3.12
3.79
f1 (ppm)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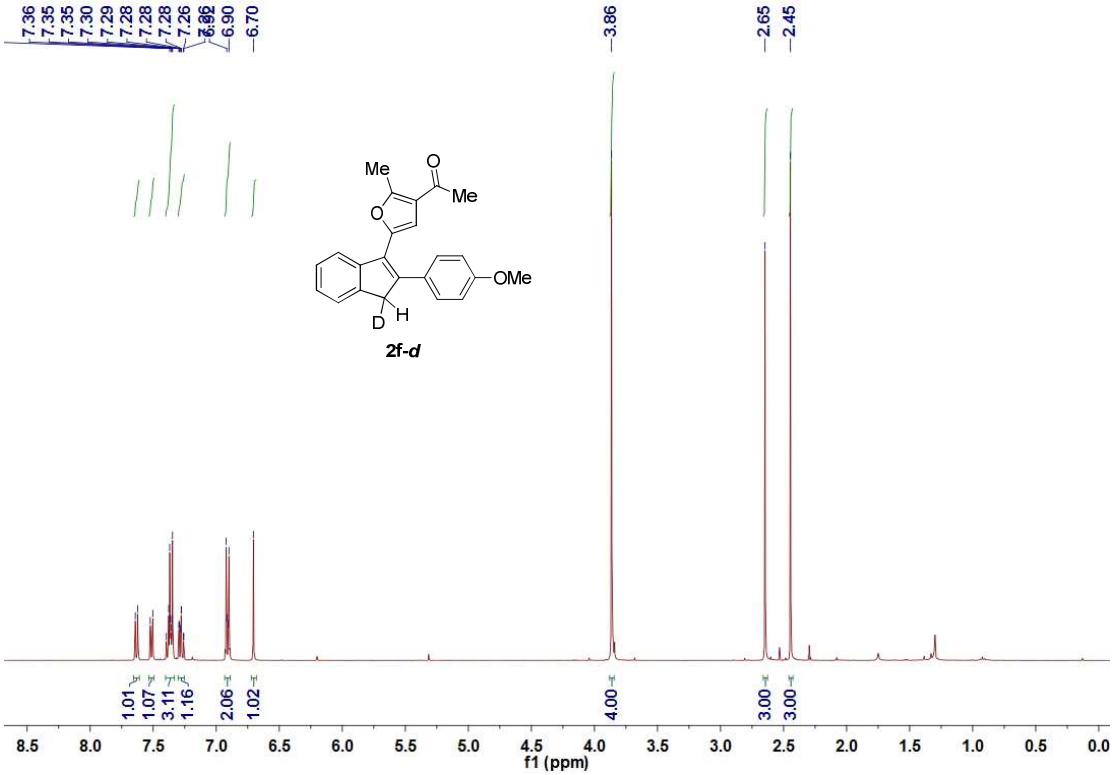
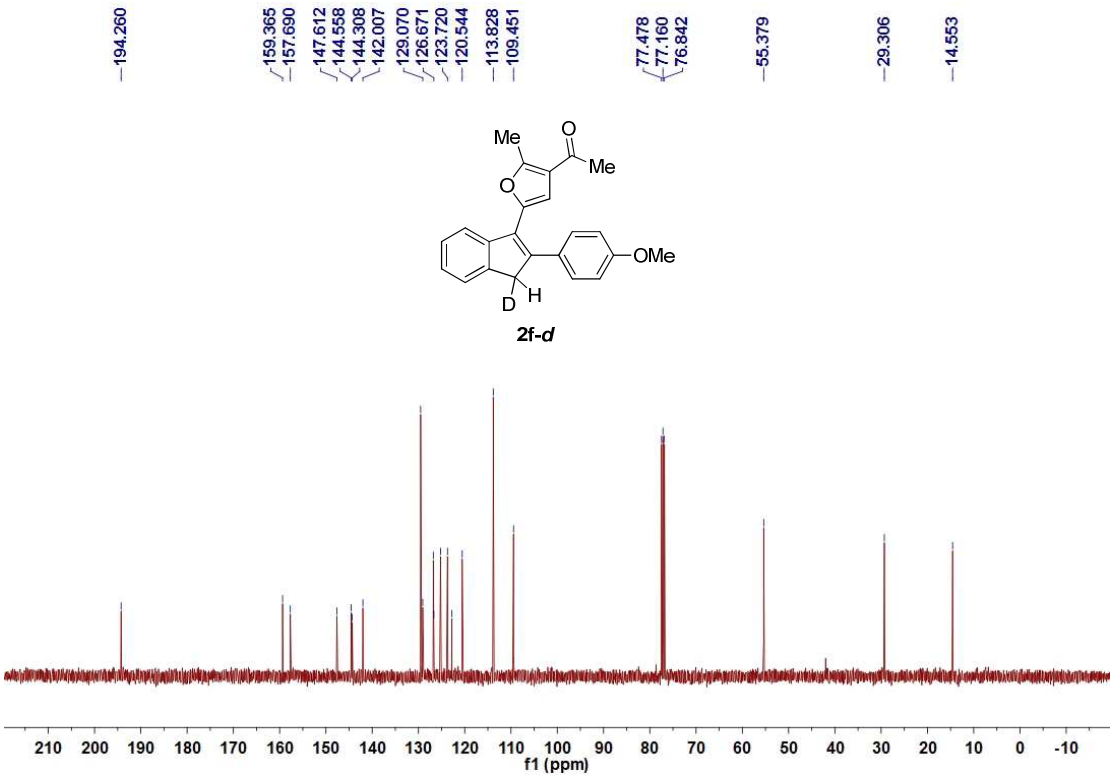
165.225
157.602
150.291
143.859
130.973
128.703
127.823
124.053
122.251
121.646
106.525
77.477
77.160
76.842
60.241
48.881
29.267
14.561
14.440
12.753
Me
O
Me
O
CO2Et
Me
2y'
f1 (ppm)


7.36
7.35
7.35
7.30
7.29
7.28
7.28
7.26
6.90
6.70
3.86
2.65
2.45
Me
O
Me
O
OMe
D
H
2f-d
1.01
1.07
3.11
1.16
2.06
1.02
4.00
3.00
3.00
f1 (ppm)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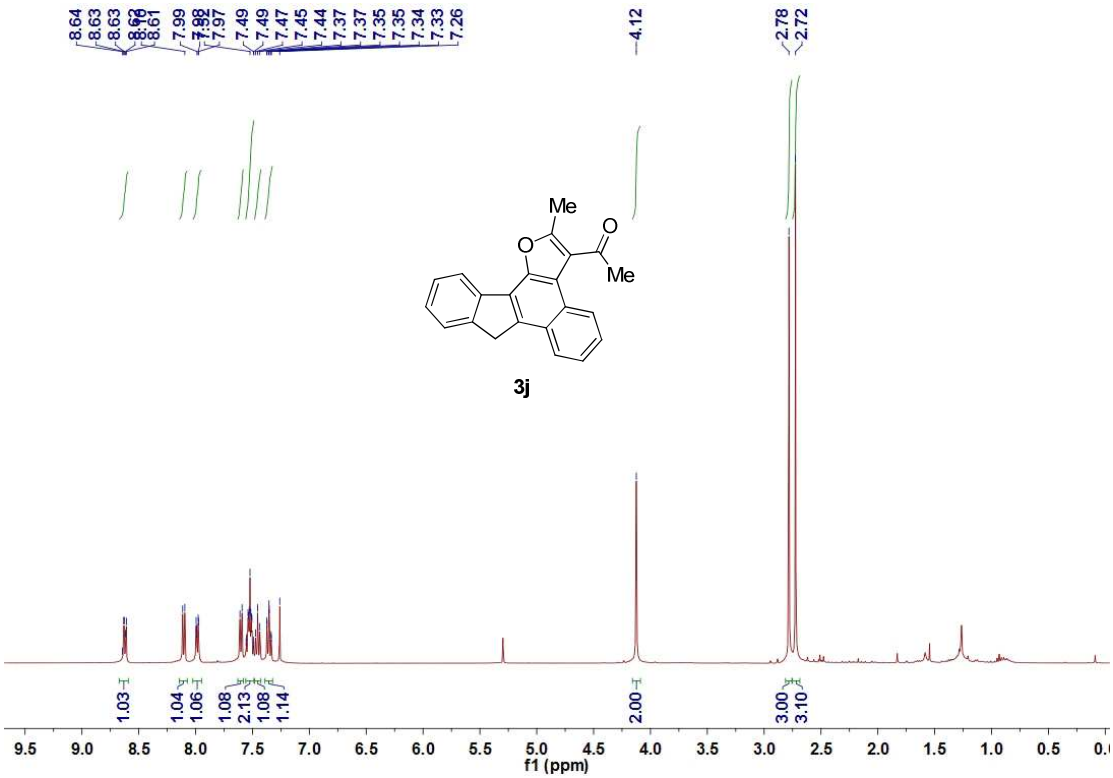
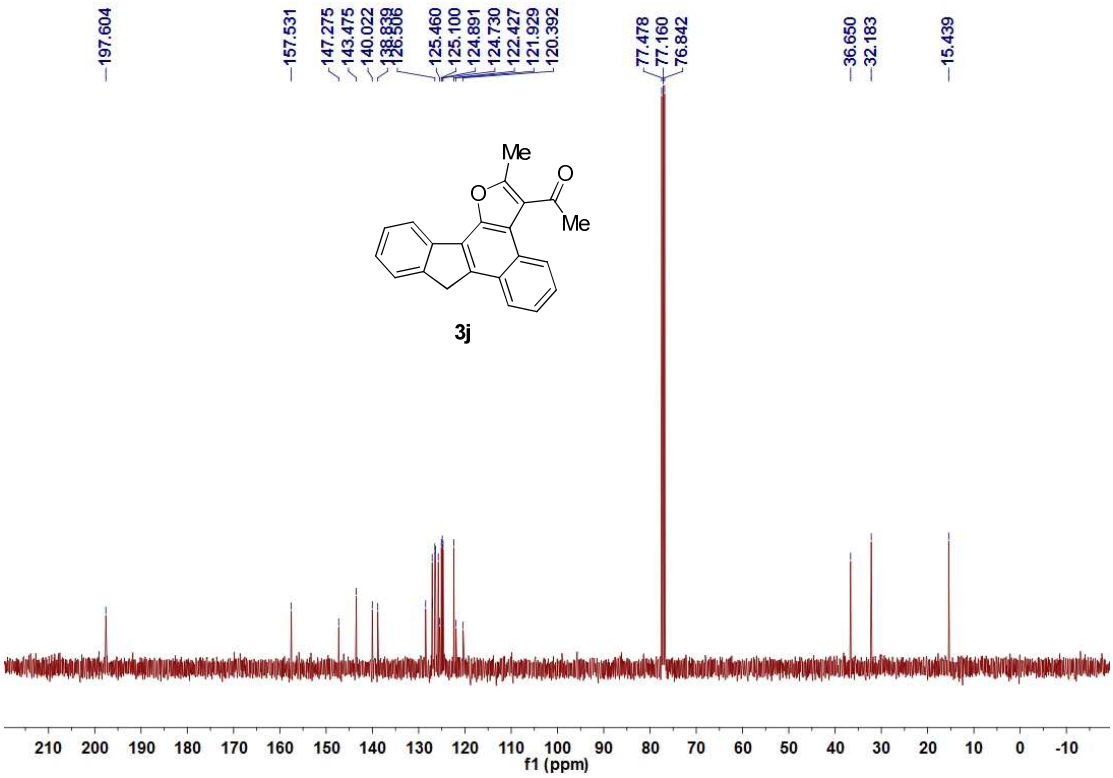
159.365
157.690
147.612
144.558
144.308
142.007
129.070
126.671
123.720
120.544
113.828
109.451
77.478
77.160
76.842
55.379
29.306
14.553
Me
O
Me
O
OMe
D
H
2f-d
f1 (ppm)


8.64
8.63
8.63
8.61
7.99
7.97
7.49
7.49
7.47
7.45
7.44
7.37
7.37
7.35
7.35
7.34
7.33
7.26
4.12
2.78
2.72
Me
O
Me
3j
1.03
1.04
1.06
1.08
2.13
1.08
1.14
2.00
3.00
3.10
f1 (ppm)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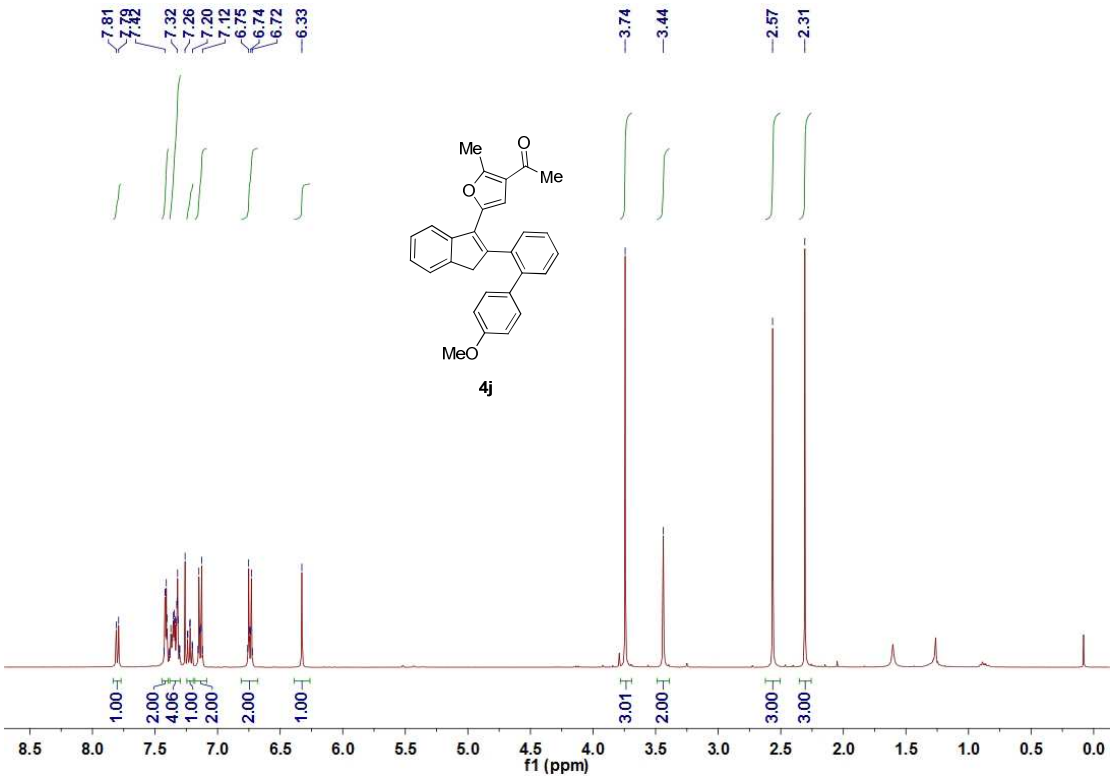
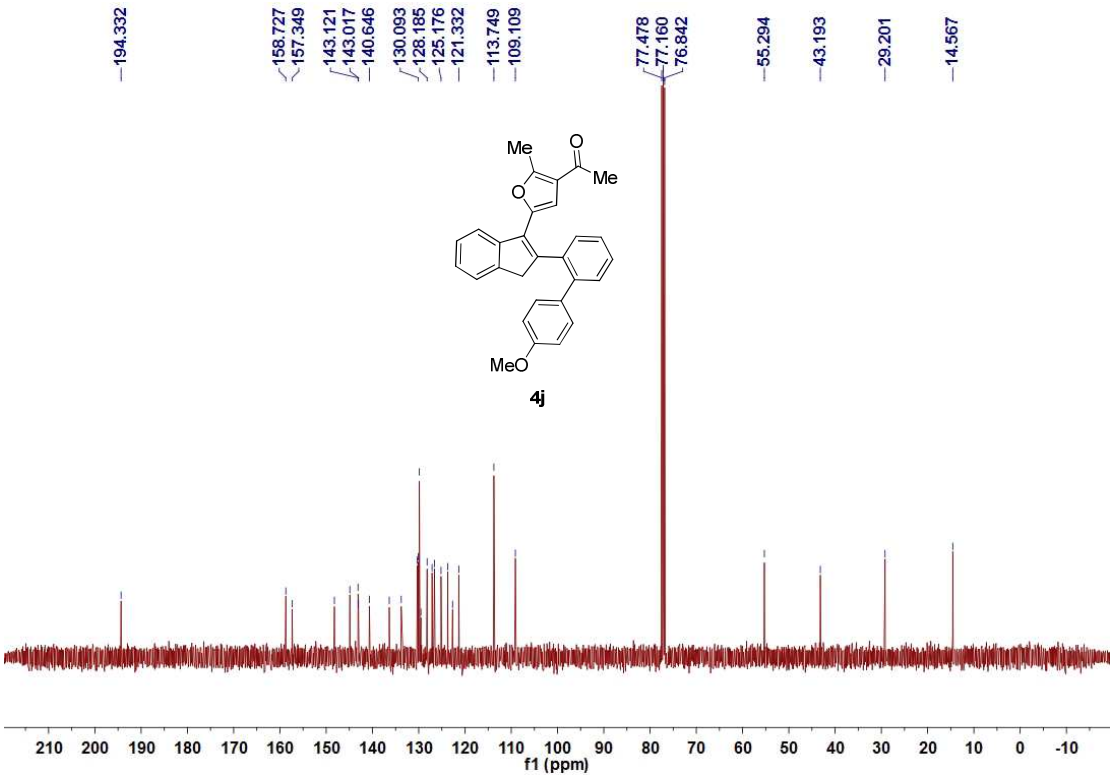
147.275
143.475
140.022
125.460
125.100
124.891
124.730
122.427
121.929
120.392
77.478
77.160
76.842
36.650
32.183
15.439
Me
O
O
Me
3j
f1 (ppm)


7.81
7.79
7.42
7.32
7.26
7.20
7.12
6.75
6.74
6.72
6.33
3.74
3.44
2.57
2.31
Me
O
O
Me
MeO
4j
1.00
2.00
4.06
1.00
2.00
2.00
1.00
3.01
2.00
3.00
3.00
f1 (ppm)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157.349
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143.017
140.646
130.093
128.185
125.176
121.332
113.749
109.109
77.478
77.160
76.842
55.294
43.193
29.201
14.567
Me
O
Me
O
MeO
4j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)