Supporting Information

Reaction of Aldehydes/Ketones with Electron Deficient 1,3,5-Triazines Leading to Functionalized Pyrimidines as Diels-Alder/Retro-Diels-Alder Reaction Products: Reaction Development and Mechanistic Studies

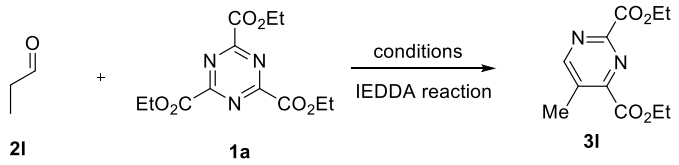
Kai Yang,[†] Qun Dang,[†] Pei-Jun Cai,[‡] Yang Gao,[‡] Zhi-Xiang Yu,*[,‡] and Xu Bai*[,†]

[†] The Center for Combinatorial Chemistry and Drug Discovery of Jilin University, The College of Chemistry and The School of Pharmaceutical Sciences, Jilin University, 1266 Fujin Lu, Changchun, Jilin 130021, P. R. China

[‡] Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China

Table of Contents:

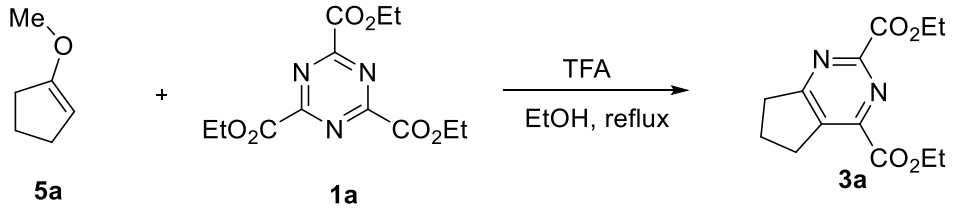
Table S1. Optimization of IEDDA Reaction of **1a** with **2l**.[a]



entry	conditions	time (d)	yield (%)[b]
1	TFA (0.1 equiv.), EtOH, reflux	7	35
2	TFA (1.0 equiv.), EtOH, reflux	1.5	28
3	TFA (2.0 equiv.), EtOH, reflux	1	27
4	TFA (1.0 equiv.), 1,4-dioxane, reflux	14	8
5	TFA (1.0 equiv.), EtOH, reflux	1	20[c]
6	EtOH, reflux	3	39
7	EtOH, reflux	3	42[d]
8	EtOH, reflux	1.5	48[e]

[a] Reaction conditions: **1a** (0.5 mmol), **2l** (1.0 mmol), additive and solvent (1 mL) was stirred at the indicated temperature under nitrogen atmosphere, and monitored by LC-MS until all **1a** was consumed. [b] Yield of isolated product. [c] 5.0 equiv. **2l** (2.5 mmol) was used. [d] **1a** (0.5 mmol) and **2l** (0.5 mmol) in EtOH (1 mL) at reflux under nitrogen atmosphere. After 24 h, additional 0.5 mmol **2l** was added**.** [e] **1a** (0.5 mmol) and **2l** (1.0 mmol) in EtOH (1 mL) at reflux under nitrogen atmosphere. After 24 h, additional 1.0 mmol **2l** was added**.**

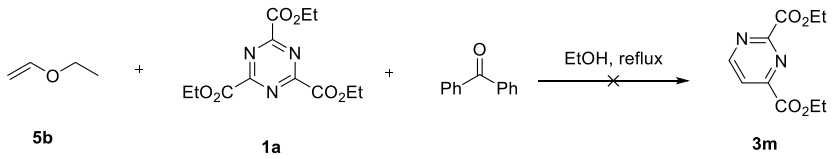
Table S2. Reactions of Vinyl Ether **5a** with **1a** Under Acidic Conditions.[a]



entry	TFA (equiv.)	time	yield (%)[b]	remarks
1	0.1	10 d	43	Trace **5a** was detected in an hour, monitored by TLC.
2	1.0	18 h	61	**5a** ran out in an hour, monitored by TLC

[a] Reaction conditions: **1a** (0.5 mmol), **5a** (1.0 mmol), TFA in EtOH (2 mL) at reflux under nitrogen atmosphere. **1a** ran out in all reactions, monitored by LC-MS. [b] Yield of isolated product.

Scheme S1. Reaction of **1a** with **5b** and Diphenyl Ketone.



Crystallographic data for **4b**

The crystallographic data collection for **4b** was gathered on a Bruker Smart Apex CCD single-crystal X-ray diffractometer with a graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 293 K. Absorption corrections were applied using the multi-scan program SADABS[1]. The structure was solved by direct methods using the SHELXS-97 program of the SHELXTL package and refined by the full-matrix least-squares method using SHELXL-97[2,3]. All non-hydrogen atoms in structure were refined on F^2 with anisotropic displacement parameters and the hydrogen atoms were generated geometrically. The F1-F6 atoms in **1** are disordered in two positions, each with site occupancies of 0.50. The details of the crystal parameters, data collection and refinements for **4b** is summarized in Table S3.

Table S3. Crystal data and structure refinements for **4b**.

Compound	**4b**
Formula	$C_{15}H_8F_9N_3O$
Mr	417.24
Crystal system	Triclinic
Space group	*P*-1
a (Å)	8.9500(10)
b (Å)	9.4770(10)
c (Å)	17.4982(17)
α(°)	83.849(2)
β (°)	87.952(2)
γ(°)	64.7730(10)
V (Å^3)	2454.7(4)
Z	6

Dc (g cm^{-3})	1.694
M (mm^{-1})	0.179
F (000)	1248
Data collected	12757
Unique reflections	9386
Goodness-of-fit	1.175
Final R indices	R_1 = 0.0686
[I> 2σ(I)]^{a,b}	wR_2= 0.1757
R indices	R_1 = 0.1039
(all data)	wR_2= 0.2111

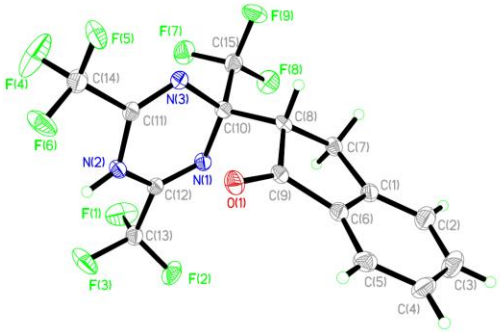
$^{a}R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.

[1] G. M. Sheldrick, SADABS, Program for Bruker Area Detector. Absorption Correction; University of Göttingen: Göttingen, Germany, 1997.

[2] G.M. Sheldrick, SHELXS-97, Program for Crystal Structure Solution, University of Götingen, Germany, 1997.

[3] G.M. Sheldrick, SHELXL-97, Program for Crystal Structure Refinement, University of Götingen, Germany, 1997.

Figure S1 ORTEP drawing of **4b** (Thermal ellipsoids of **4b** are drawn at the 30% probability level).



Computational study

(1) Computational Methods

All calculations were performed with the Gaussian 09 software package.[1] Geometry optimization and frequency calculations were carried out using the B3LYP functional[2] with 6-31G(d) basis set in conjunction with IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model[3] in ethanol. Solvation energies in ethanol using B3LYP, M06-2X,[4] PBE0[5] functionals and MP2 perturbation method[6] with 6-311+G(d,p) basis set were evaluated by IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model[3] using the solution-phase B3LYP-optimized structures. All discussed energies are based on SMD/MP2/6-311+G(d,p)//B3LYP/6-31G(d) calculations. We found that MP2 single point energies gave results consistent with experimental observation. If not specifically mentioned, all discussed energies in the paper and here are based on MP2/6-311+G(d,p)-SMD//B3LYP/6-31G(d)-SMD calculations. In all calculations of solvent effects, we only considered this by using implicit PCM model. We expected that using explicit ethanol solvent model could only modify slightly the energy surface in Figure 1 (as can be seen in Figures S8 and S9 below). All 3D structures in the Figures were prepared with CYLview.[7]

(2) Energy Profiles of Concerted and Stepwise Pathways of IEDDA Reaction between Neutral Triazine and Acetone

The direct IEDDA reaction between neutral triazine **A** and enol was also considered. Our quantum chemical calculations found that the activation enthalpies for concerted and stepwise pathway via neutral triazine **A** are 36.8 and 34.8 kcal/mol respectively at the B3LYP/6-31G(d)-SMD(EtOH) level of theory (Figure S2). These pathways are not favored both kinetically and thermodynamically compared with pathways in Figure S6 (The barrier of **TS1** is 15.6 kcal/mol relative to **Acetone** and **H-A** at the B3LYP/6-31G(d)-SMD(EtOH) level of theory). Therefore, we can rule out the stepwise and concerted pathways involving neutral triazine as the diene and propose that the protonated triazine is the real active reactant (it is more electronically deficient compared to its neutral one).

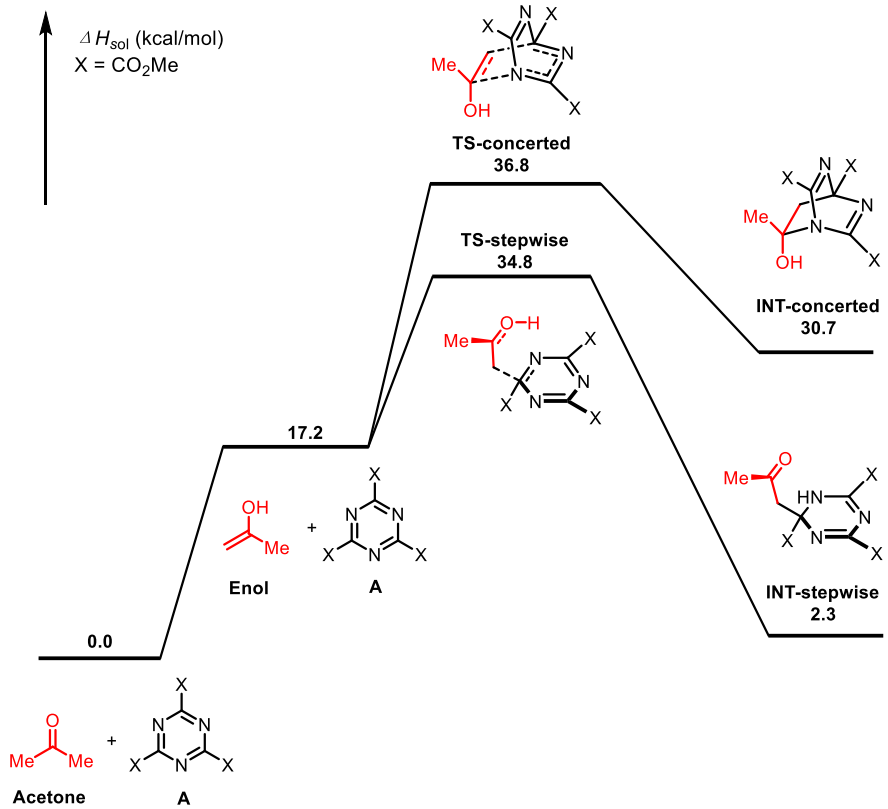


Figure S2. Energy profiles of the IEDDA reaction between A and acetone (Geometries were optimized at the B3LYP/6-31G(d)-SMD(EtOH) level of theory, and energies were calculated at the B3LYP/6-31G(d)-SMD(EtOH) level of theory).

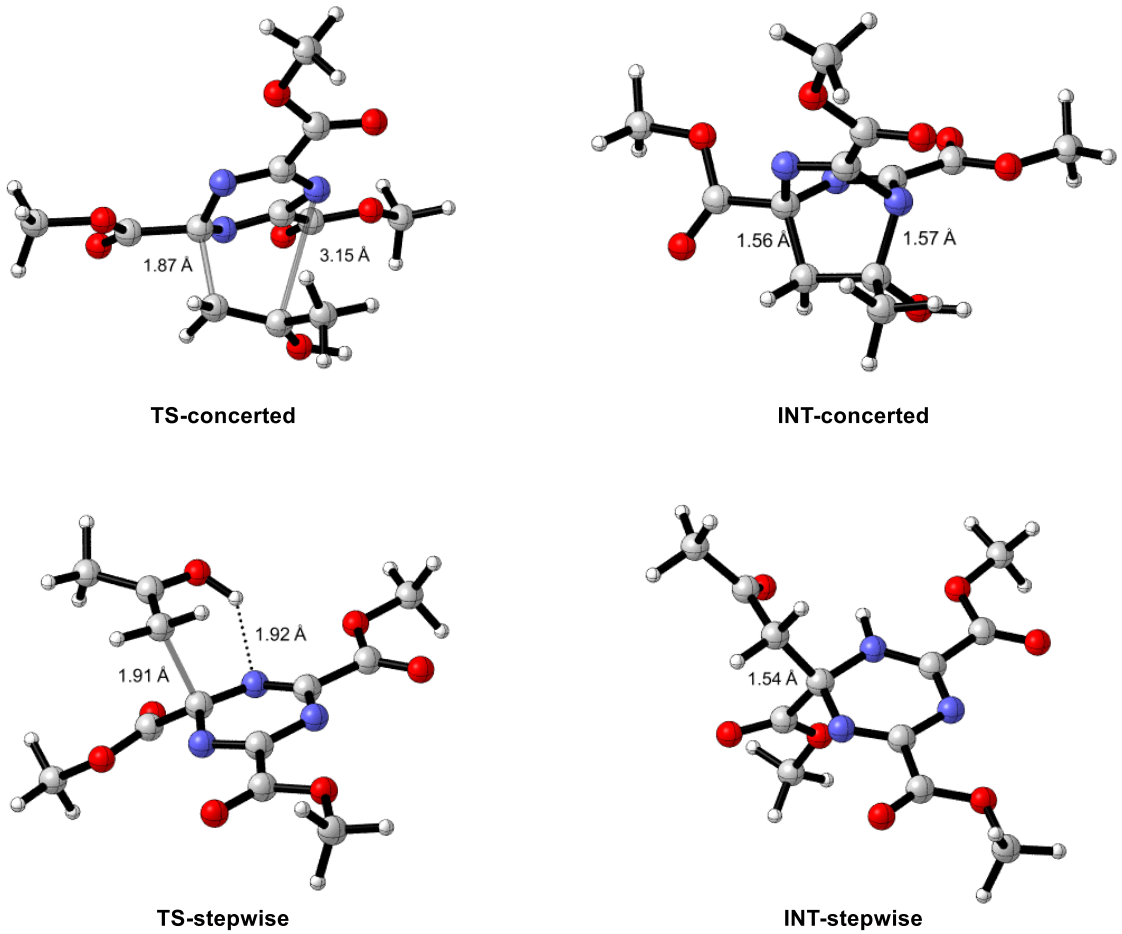


Figure S3. Computed key structures in Figure S2 (Geometries were optimized at the B3LYP/6-31G(d)-SMD(EtOH) level of theory).

(3) Energy Profiles of *[3,3]-Sigmatropic Rearrangement* Pathway

We also calculated the *[3,3]-sigmatropic rearrangement* pathway at the B3LYP/6-31G(d)-SMD(EtOH) level of theory. This route also starts from neutral triazine **A** and actone. Then the direct attack of oxygen on acetone to the imine carbon, concerted with a proton transfer from methyl to nitrogen via **TS6** furnishes **INT6**. The *[3,3]-sigmatropic rearrangement* of **INT6** via **TS7** then gives **INT7** with the newly formed C-C bond. The activation enthalpy for the first two steps is 43.1 kcal/mol, suggesting that this pathway is difficult to occur.

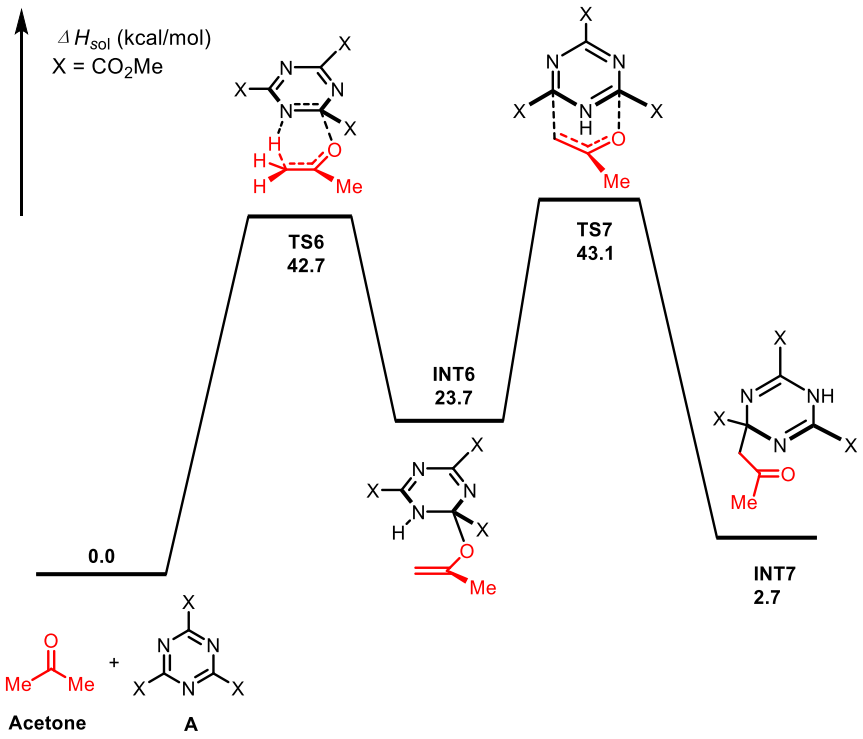


Figure S4. Energy profiles of the IEDDA reaction between A and acetone by *[3,3]-Sigmatropic Rearrangement* pathway (Geometries were optimized at B3LYP/6-31G(d)-SMD(EtOH) level of theory, and energies were calculated at the B3LYP/6-31G(d)-SMD(EtOH) level of theory).

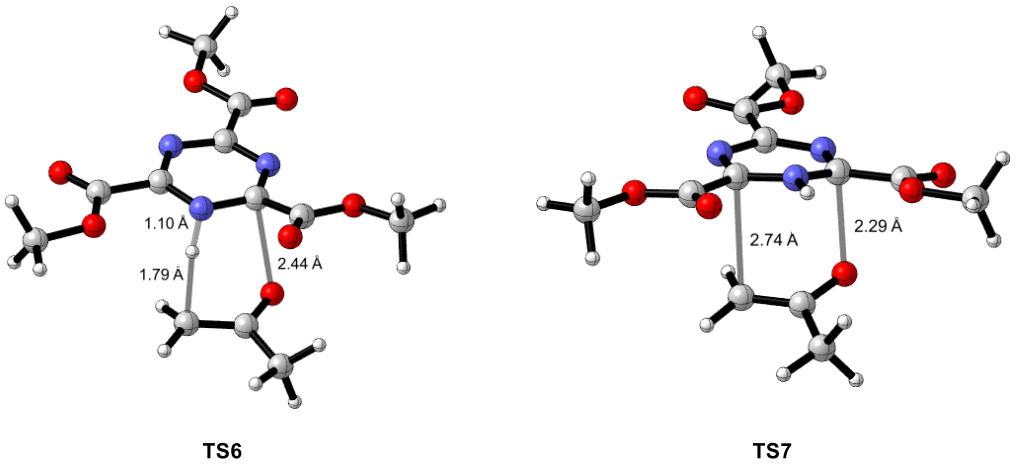


Figure S5. Computed Structures in Figure S4 (Geometries were optimized at B3LYP/6-31G(d)-SMD(EtOH) level of theory).

(4) Energy Profiles of Stepwise Pathways of IEDDA Reaction between Protonated Triazine and Acetone

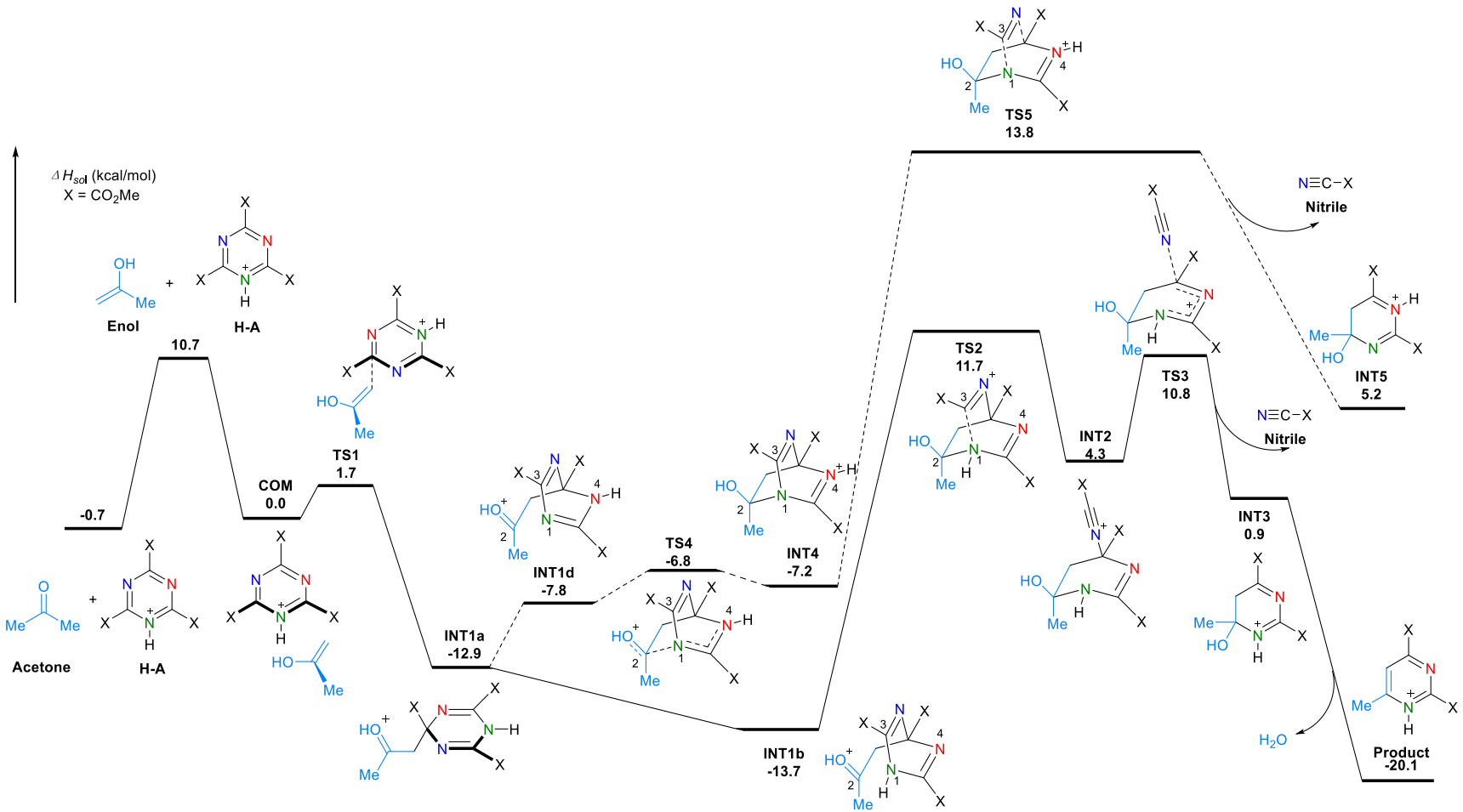


Figure S6. Energy profiles of the IEDDA reaction between H-A and acetone (Geometries were optimized at the B3LYP/6-31G(d)-SMD(EtOH) level of theory, and energies were calculated at the MP2/6-311+G(d,p)-SMD(EtOH)//B3LYP/6-31G(d)-SMD(EtOH) level of theory).

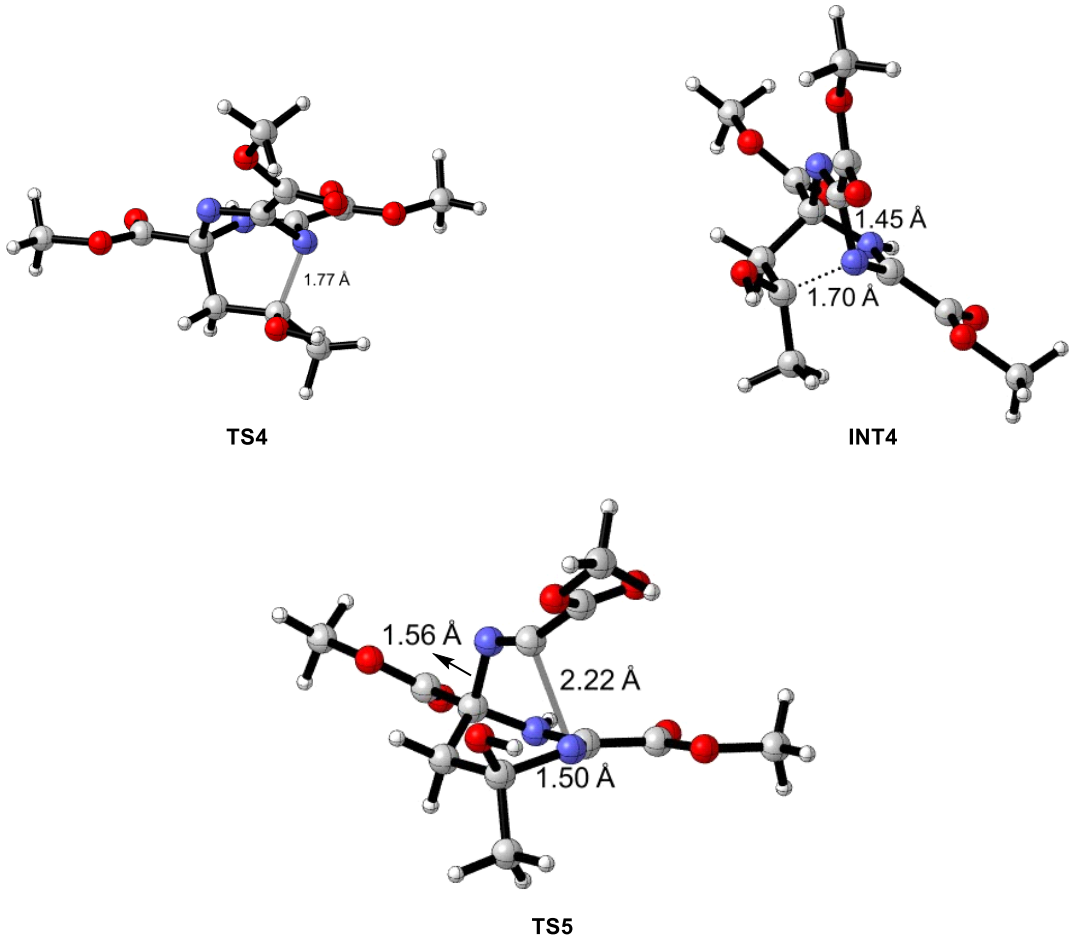


Figure S7. Computed structures in **Figure S6** (Geometries were optimized at the B3LYP/6-31G(d)-SMD(EtOH) level of theory).

It is possible that the proton in **INT1a** could be transferred to another nitrogen atom to form **INT1d**, which then undergoes C-N bond formation via **TS4** to give **INT4** (Figure S6). This intermediate can then liberate nitrile via **TS5** to give **INT5**. However, **TS5** is disfavored by 2.1 kcal/mol kinetically compared with **TS2** and this pathway was ruled out for further consideration.

Table S4. Comparison of Relative Energies of Species Shown in Fig. S6. Calculated at the B3LYP/6-31G(d)-SMD(EtOH), and Method/6-311+G(d,p)-SMD(EtOH)//B3LYP/6-31G(d)-SMD(EtOH) level of theory respectively.

	B3LYP	MP2/B3LYP	B3LYP/B3LYP	M06-2X/B3LYP	PBE0/B3LYP
Acetone + H-A	-14.6	-0.7	-13.7	-4.9	-10.8
Enol + H-A	2.6	10.7	-0.4	6.5	2.1
COM	0.0	0.0	0.0	0.0	0.0
TS1	1.0	1.7	1.9	2.0	-0.2
INT1a	-9.4	-12.9	-9.0	-15.0	-15.2
INT1b	-10.2	-13.7	-9.8	-15.3	-16.0
INT1d	-6.5	-7.8	-6.6	-11.2	-12.6
TS2	27.9	11.7	28.5	20.8	22.5
INT2	18.2	4.3	16.3	10.5	12.1
TS3	21.2	10.8	19.1	16.1	17.2
INT3 + Nitrile	5.1	0.9	1.2	4.5	4.4
Product + H_2O	-9.7	-20.1	-22.8	-11.4	-14.0
TS4	7.6	-6.8	9.5	-2.1	-1.8
INT4	8.2	-7.2	10.1	-2.1	-1.7
TS5	32.0	13.8	33.1	26.1	26.5
INT5 + Nitrile	9.0	5.2	5.0	8.5	8.5

We investigated how computational methods affect the calculations. **Table S4** gives the energies obtained by solvation energy calculations with different methods. Here we can see only MP2 method gives the reasonable activation energy (24.6 kcal/mol) whereas the activation energies obtained by other methods are too high (>30 kcal/mol). Besides, MP2 is the only method here that makes the energy of **INT4** to be lower than **TS4** (the single point energy of **INT4** is lower than **TS4** by 0.02 kcal/mol at B3LYP/6-31G(d)-SMD(EtOH) level of theory). We can conclude that for the present reaction, MP2 method is reasonable to study the reaction mechanism.

(5) Effect of Solvents to the IEDDA Reaction between Protonated Triazine and Acetone

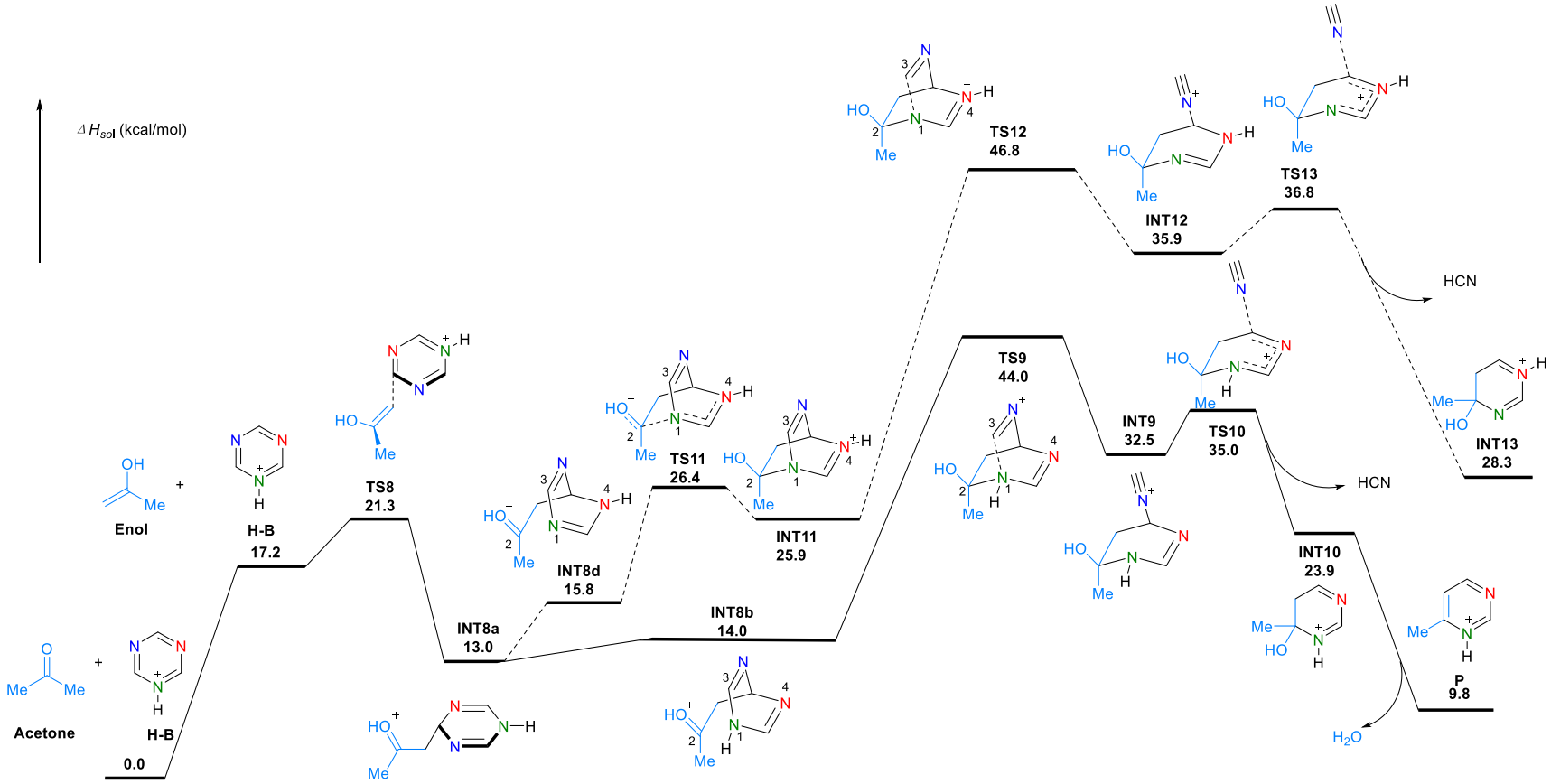


Figure S8. Energy profiles of the IEDDA reaction between H-B and acetone (Geometries were optimized at the B3LYP/6-31G(d)-SMD(EtOH) level of theory, and energies were calculated at the B3LYP/6-31G(d)-SMD(EtOH) level of theory).

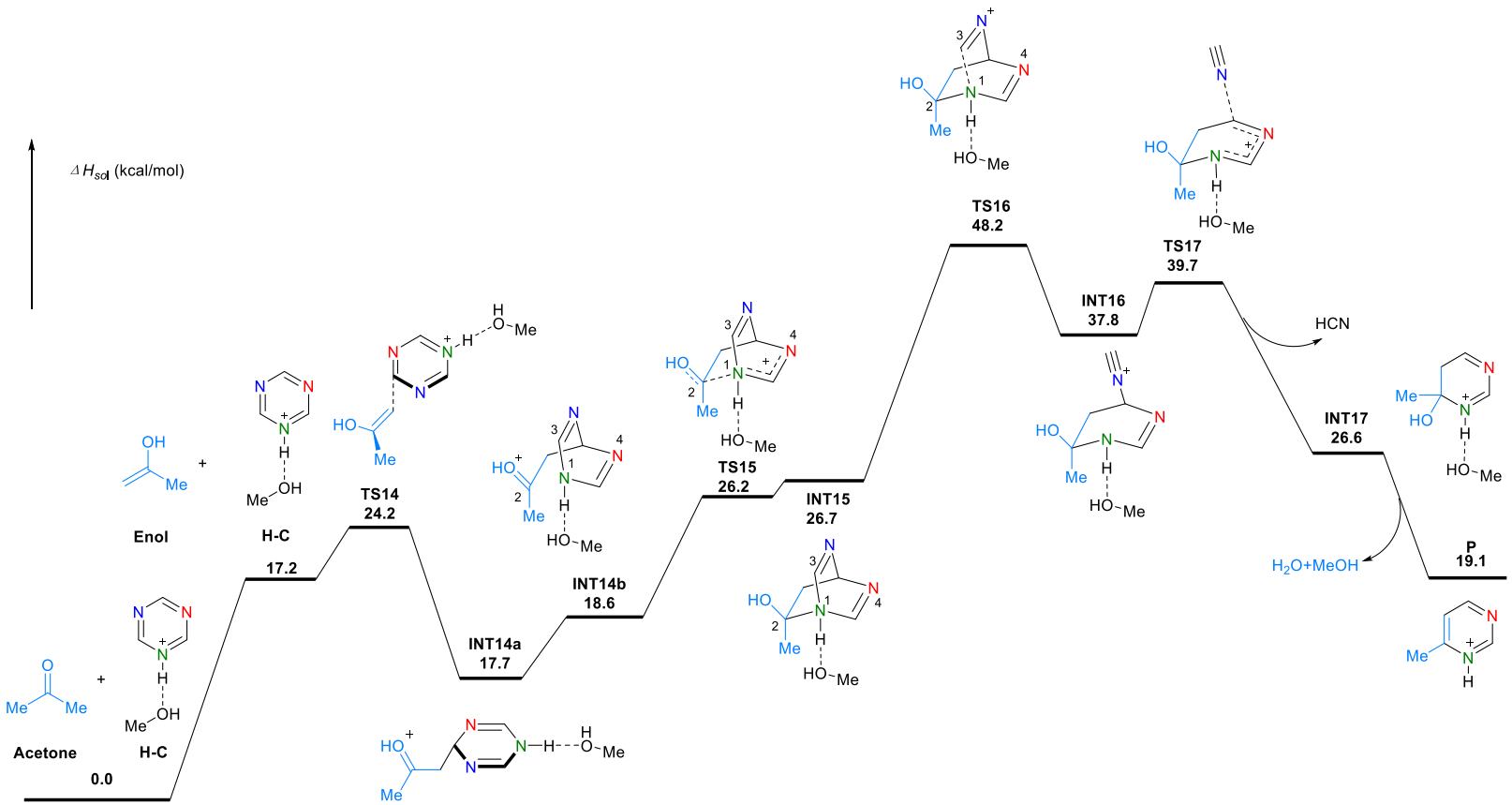


Figure S9. Energy profiles of the IEDDA reaction between H-C and acetone (Geometries were optimized at the B3LYP/6-31G(d)-SMD(EtOH) level of theory, and energies were calculated at the B3LYP/6-31G(d)-SMD(EtOH) level of theory).

To test whether the solvent (ethanol) can accelerate the IEDDA reaction, the IEDDA reaction of the simplest triazine **H-B** was calculated (**Figure S8**). The reaction mechanism for **H-B** is similar to that for **H-A** and the cleavage of N1-C3 bond via **TS9** is still the rate-determining step, with an activation enthalpy of 44.0 kcal/mol. We then investigated whether alcohol could affect the reaction significantly or not (**Figure S9**). We speculated that alcohol could stabilize the protonated triazine via hydrogen bonding interaction. With this model, we calculated the IEDDA reaction with an alcohol stabilizing triazine, **H-C**. In this model, intermediate **INT15** could be located (whereas in Figure 1, its counterpart **INTc** was not a stationary point), showing the hydrogen bonding can stabilize this intermediate. In this model system, the cleavage of N1-C3 bond via **TS16** is the rate-determining step, with an activation enthalpy of 48.2 kcal/mol, which is slightly higher than that in **Figure S8** for the model system without the participation of alcohol. This suggests that the alcohol does not participate in the reaction pathway in Figure 1 and using an implicit solvent model to investigate the solvent effects on the present reaction is reasonable.

(6) Computed Energy of All Species

Table S5. Sum of electronic and thermal enthalpies *H*, sum of electronic and thermal free energies *G*, thermal correction to enthalpy *TCH*, total free energy in EtOH with non-electrostatic terms $E_{\mathrm{Method,sol}}$, reported in Hartree.

	H	*G*	*TCH*	$E_{\mathrm{MP2,sol}}$	$E_{\mathrm{B3LYP,sol}}$	$E_{\mathrm{M06\text{-}2X,sol}}$	$E_{\mathrm{PBE0,sol}}$
A	-963.780988	-963.847537	0.211691				
TS-stepwise	-1156.799649	-1156.876187	0.302949				
INT-stepwise	-1156.851439	-1156.930428	0.30574				
TS-concerted	-1156.796453	-1156.873755	0.303483				
INT-concerted	-1156.806167	-1156.879433	0.305968				
Acetone	-193.074125	-193.107709	0.090346	-192.660875	-193.229212	-193.130152	-192.993831
H-A	-964.191387	-964.259973	0.22456	-962.190556	-964.692975	-964.319806	-963.622731
Enol	-193.046639	-193.079259	0.090386	-192.642643	-193.207947	-193.111996	-192.973224
COM	-1157.242224	-1157.323538	0.317174	-1154.852509	-1157.90257	-1157.44441	-1156.601593
TS1	-1157.240617	-1157.320369	0.316301	-1154.848986	-1157.898652	-1157.440404	-1156.600989
INT1a	-1157.257185	-1157.335585	0.31905	-1154.874886	-1157.91879	-1157.470252	-1156.627653
INT1b	-1157.258551	-1157.337942	0.318962	-1154.876151	-1157.919909	-1157.470523	-1156.628903
INT1d	-1157.252596	-1157.332267	0.318994	-1154.866725	-1157.914844	-1157.46414	-1156.623524
TS2	-1157.197837	-1157.27326	0.316434	-1154.833197	-1157.856419	-1157.410546	-1156.564991
INT2	-1157.213178	-1157.292696	0.318068	-1154.846594	-1157.877546	-1157.428594	-1156.583216
TS3	-1157.208481	-1157.287491	0.316476	-1154.834632	-1157.871402	-1157.418035	-1156.573456
Nitrile	-321.2292	-321.266294	0.06787	-320.566255	-321.397013	-321.26773	-321.028535
INT3	-836.004881	-836.066851	0.247483	-834.282967	-836.50184	-836.167628	-835.564208
H_2O	-76.396875	-76.418331	0.024785	-76.287456	-76.471843	-76.434398	-76.385361

Product	-759.631618	-759.689751	0.219643	-758.025938	-760.06516	-759.755554	-759.205127
TS4	-1157.230099	-1157.303514	0.317692	-1154.863935	-1157.887932	-1157.448339	-1156.605026
INT4	-1157.229219	-1157.303378	0.318608	-1154.865377	-1157.887971	-1157.449261	-1156.605674
TS5	-1157.191195	-1157.267025	0.316317	-1154.829598	-1157.848939	-1157.401911	-1156.558467
INT5	-835.998649	-836.060226	0.247446	-834.276177	-836.4958	-836.161315	-835.557642
TS6	-1156.787141	-1156.866101	0.300004				
INT6	-1156.817357	-1156.895189	0.305318				
TS7	-1156.786451	-1156.864999	0.302145				
INT7	-1156.850735	-1156.928133	0.306152				
H-B	-280.73	-280.763	0.084095				
TS8	-473.771	-473.818	0.175987				
INT8a	-473.784	-473.83	0.178132				
INT8b	-473.782	-473.828	0.178164				
INT8d	-473.779	-473.825	0.177972				
TS9	-473.734	-473.776	0.175179				
INT9	-473.753	-473.798	0.176032				
TS10	-473.749	-473.795	0.174528				
INT10	-380.359	-380.399	0.153352				
TS11	-473.763	-473.803	0.176942				
INT11	-473.763	-473.804	0.177867				
TS12	-473.73	-473.772	0.17477				
INT12	-473.747	-473.793	0.175932				
TS13	-473.746	-473.793	0.174431				
INT13	-380.352	-380.392	0.153087				
HCN	-93.4071	-93.4299	0.020047				
P	-303.985	-304.022	0.125643				
H-C	-396.412	-396.458	0.141361				
TS14	-589.447	-589.505	0.233843				
INT14a	-589.458	-589.516	0.236047				
INT14b	-589.456	-589.514	0.23588				
TS15	-589.444	-589.496	0.23486				
INT15	-589.443	-589.496	0.235742				
TS16	-589.409	-589.463	0.232691				
INT16	-589.426	-589.484	0.233909				
TS17	-589.423	-589.482	0.232365				
INT17	-496.036	-496.088	0.211066				
MeOH	-115.666596	-115.693527	0.055698				

(7) Computed Coordinates of All Species

A

C	0.87900000	-0.95508400	-0.00925200
N	-0.40680900	-1.30802700	-0.00055400
C	-1.26390800	-0.28325600	0.00740400
C	0.38977600	1.23661700	0.00683600
N	1.33761500	0.29947900	-0.00890600
N	-0.92613500	1.00629500	0.01464300
C	-2.73763300	-0.65450200	0.00733900
C	1.93913300	-2.04425400	-0.02474000
C	0.80309900	2.69898800	0.01973300
O	-3.11901700	-1.80726700	0.00997500
O	3.12638100	-1.79633900	-0.08278800
O	-0.00545000	3.60347600	0.07069600
O	1.40268900	-3.25721600	0.03249200
O	-3.51755300	0.41998500	0.00249900
O	2.12220600	2.84021100	-0.02913900

C	-4.94323300	0.16612600	-0.00132200
H	-5.40883800	1.15092200	-0.00742900
H	-5.22088700	-0.39648100	-0.89590300
H	-5.22699300	-0.38877800	0.89612800
C	2.33760800	-4.36348200	0.02450500
H	2.90310300	-4.36719600	-0.91046100
H	3.01866900	-4.28480100	0.87505700
H	1.72229200	-5.25885900	0.10493600
C	2.61405200	4.20256000	-0.01580300
H	3.69973700	4.11445100	-0.03587100
H	2.25371400	4.73749700	-0.89778000
H	2.28391600	4.71004400	0.89361100

TS-concerted

C	1.31214400	-0.38407000	-0.53018300
N	1.08860000	0.90657100	-0.19468700
C	-0.22228000	1.23384900	-0.27716600
N	-1.23515300	0.40732200	-0.35323500
C	-0.85161600	-0.93756400	-0.18541300
N	0.41497500	-1.33556800	-0.63413600
C	-0.91348200	-1.32983300	1.63823500
C	0.12791500	-0.68137500	2.34524800
C	-1.94364300	-1.92967700	-0.62097800
O	0.31158400	3.55174800	0.09144000
O	3.04146800	-1.88885900	-1.28337000
O	-1.70828200	-3.02522600	-1.08937600
O	3.61592600	0.17687500	-0.57844800
O	-1.73700200	3.01451700	-0.69099300
O	-3.16755300	-1.44825000	-0.40310500
C	-2.08440600	4.41757000	-0.69886000
H	-3.10547100	4.45882300	-1.07802700
H	-2.03515600	4.82386200	0.31462500
H	-1.40972400	4.97257900	-1.35549300
C	5.00323800	-0.13883300	-0.83020200
H	5.15567200	-0.35506600	-1.89076600
H	5.55844400	0.75305200	-0.53934300
H	5.31316900	-0.99636200	-0.22741300
C	-4.26682000	-2.31223400	-0.77312400
H	-5.16772900	-1.76290500	-0.49982700
H	-4.24834600	-2.50499700	-1.84867700
H	-4.21135200	-3.25490500	-0.22314500
C	-0.50387000	2.72427500	-0.27092300
H	-1.91024500	-0.98873400	1.90609600
H	-0.79917100	-2.41205200	1.59552300
C	2.73959300	-0.79438000	-0.84567300
C	-0.03928300	0.60617200	3.07060100
H	-0.85131500	1.19508900	2.63769200
H	-0.31627500	0.37566700	4.11022500
H	0.88602800	1.18972100	3.08961500
O	1.28633500	-1.30676600	2.37079500
H	1.97778100	-0.77775500	2.81841200

INT-concerted

C	0.72739100	-1.00481700	-0.34537600
N	1.02451400	0.18723600	0.41802200
C	0.07088900	1.17394800	-0.02183400
N	-1.16793500	0.87997200	-0.09428200
C	-1.35298800	-0.52327500	0.33612200
N	-0.47395300	-1.41970200	-0.44093400
C	-0.89211500	-0.61334700	1.82127800
C	0.59687000	-0.20544400	1.87760300
C	-2.81254800	-0.93207500	0.13775800

O	1.76623800	2.85962800	-0.16713200
O	1.64605400	-2.77808200	-1.66449100
O	-3.54284400	-1.30727900	1.03399000
O	3.03921800	-1.26647400	-0.71997800
O	-0.33979600	3.34014800	-0.84258400
O	-3.16999500	-0.82015800	-1.14043800
C	0.08124700	4.67896000	-1.19669300
H	0.85012300	4.63793100	-1.97228900
H	-0.81558000	5.17150500	-1.57126200
H	0.46542800	5.19792600	-0.31523900
C	4.17198400	-1.95335900	-1.30330300
H	4.08685300	-1.95867600	-2.39263700
H	5.04589400	-1.38360200	-0.98877500
H	4.22468000	-2.97760100	-0.92623200
C	-4.53741500	-1.17492500	-1.45688200
H	-4.64252700	-0.99097900	-2.52582100
H	-4.71441600	-2.22906800	-1.22979700
H	-5.22936000	-0.54745300	-0.89013500
C	0.60601500	2.54513500	-0.34842100
H	-1.51637000	0.04648900	2.42611500
H	-1.01849200	-1.63826400	2.17405300
C	1.84453100	-1.78786600	-0.98769900
C	0.90121700	0.96508600	2.80042000
H	0.30771800	1.85018700	2.55301800
H	0.66076400	0.67318300	3.82793400
H	1.96365500	1.22408900	2.74352000
O	1.34406000	-1.34467600	2.21717500
H	2.27930100	-1.08118300	2.29771500

TS-stepwise

C	-1.65470900	-0.66473700	-0.07017500
N	-1.78747200	0.67996100	-0.02667100
C	-0.63471200	1.30741300	0.25162900
N	0.55114400	0.76337400	0.43759500
C	0.62018500	-0.61175100	0.15463800
N	-0.55293200	-1.36436600	0.04800300
C	1.36681800	-0.65268200	-1.60492100
C	2.63400700	-0.02574600	-1.53711100
C	1.73890400	-1.31280200	0.93034000
O	-1.81021700	3.40476700	0.44566000
O	-2.92153600	-2.70221200	-0.33902200
O	2.63403100	-0.70936600	1.49240200
O	-4.01993900	-0.73159100	-0.26447700
O	0.44782700	3.41074700	0.42435100
O	1.63062000	-2.63909900	0.88638600
C	0.43673200	4.85180600	0.54543700
H	1.48550900	5.14712500	0.56449100
H	-0.07169300	5.29817600	-0.31290900
H	-0.06323900	5.14848800	1.47077400
C	-5.27146900	-1.43640900	-0.42614500
H	-5.42911000	-2.12304900	0.40964100
H	-6.03878600	-0.66231400	-0.43364100
H	-5.27572200	-1.99000200	-1.36846900
C	2.65976300	-3.38466300	1.57873100
H	2.41086000	-4.43332700	1.41686100
H	3.64228200	-3.15635800	1.15921600
H	2.64340000	-3.14790200	2.64533500
C	-0.74734700	2.81776700	0.39089400
H	1.37416000	-1.68598400	-1.94028100
H	0.56801800	-0.05178800	-2.03457700
C	-2.92304900	-1.48975000	-0.23900300

C	3.93361100	-0.71271000	-1.74714800
H	4.45397700	-0.80113200	-0.78296300
H	3.80117000	-1.70281200	-2.18474500
H	4.56975700	-0.10005800	-2.39722200
O	2.74028900	1.22604700	-1.15433200
H	1.89321900	1.51938100	-0.71472400

INT-stepwise

C	-1.66838700	-0.54389100	-0.24473200
N	-1.63343800	0.83649000	-0.14409900
C	-0.42037900	1.32617400	-0.14679400
N	0.69785100	0.60320400	-0.21661300
C	0.67419500	-0.86719200	-0.20016300
N	-0.68964500	-1.38021000	-0.28337200
C	1.49101600	-1.43378000	-1.37405600
C	2.96387200	-1.06935900	-1.32147400
C	1.25156300	-1.41966900	1.13463200
O	-1.23004700	3.58890800	-0.02284500
O	-3.23659600	-2.36247200	-0.51787500
O	1.72794800	-2.53332500	1.23623200
O	-4.02528600	-0.27120800	-0.20941400
O	1.00008300	3.20748800	-0.08796100
O	1.09408100	-0.56228300	2.14021900
C	1.26202900	4.63007000	-0.01192300
H	2.34699500	4.72359100	-0.03513900
H	0.81193500	5.13778900	-0.86795100
H	0.86010700	5.03203400	0.92088300
C	-5.37422500	-0.78386800	-0.29231100
H	-5.54997400	-1.51560600	0.50037300
H	-6.01999400	0.08403600	-0.16013500
H	-5.54437600	-1.24341100	-1.26923000
C	1.53808900	-1.01469700	3.44261600
H	1.32668300	-0.18827000	4.12063600
H	0.98272600	-1.90755700	3.73974300
H	2.60930000	-1.22855600	3.42001200
C	-0.27935900	2.83884500	-0.08030700
H	1.38614700	-2.52319300	-1.39715200
H	1.06826500	-1.05782300	-2.31404900
C	-3.05210600	-1.17340600	-0.34182000
C	3.86385100	-1.72086700	-2.33483100
H	3.45312800	-1.60623300	-3.34499800
H	4.86749400	-1.29221000	-2.28479600
H	3.91624900	-2.79854000	-2.13140900
O	3.38912700	-0.27943700	-0.48343100
H	1.60649600	1.05604000	-0.20061300

Acetone

C	0.00000800	0.17808500	-0.00003700
O	0.00015700	1.40372300	0.00000600
C	1.28702200	-0.61309600	-0.00231500
H	1.38804100	-1.14846800	0.95111500
H	1.27285500	-1.37313500	-0.79280500
H	2.14527200	0.05002300	-0.13662600
C	-1.28715000	-0.61288200	0.00230900
H	-1.38819000	-1.14859800	-0.95092300
H	-1.27322300	-1.37266600	0.79307500
H	-2.14528800	0.05041900	0.13637300

H-A

C	-0.26201700	1.18152900	-0.00179200
N	-1.22874000	0.25350000	0.00426900
C	-0.82622600	-1.00042200	0.00833700
C	1.40543900	-0.33416300	0.00304000

N	1.05571900	0.93397900	-0.00458400
N	0.48264000	-1.31542800	0.01022100
C	-1.77445600	-2.18496000	0.00992100
C	-0.65358800	2.65333900	-0.01232900
C	2.84819300	-0.80502700	0.00391800
O	-1.32847600	-3.31325300	0.03680800
O	0.18191800	3.52933400	-0.06722600
O	3.09379300	-1.99353500	0.01260900
O	-1.96459300	2.80335900	0.04257700
O	-3.02776100	-1.79968000	-0.02434100
O	3.68464000	0.20487700	-0.00541600
C	-4.02723800	-2.85971400	-0.03868800
H	-4.98218300	-2.34206100	-0.10666600
H	-3.86440200	-3.50041700	-0.90746400
H	-3.95712800	-3.43593600	0.88602400
C	-2.44895400	4.17269800	0.03384700
H	-2.11581600	4.67495900	-0.87692600
H	-3.53435500	4.08905500	0.05811500
H	-2.07826500	4.69854700	0.91651400
C	5.10146800	-0.13195200	-0.00572000
H	5.61658600	0.82688200	-0.01344900
H	5.34097100	-0.69883700	0.89618000
H	5.33751400	-0.71112800	-0.90070400
H	0.77784300	-2.30221600	0.01572300

Enol

C	0.97802800	-1.04723000	-0.00004500
H	0.65175100	-2.08158600	0.00004200
H	2.04865700	-0.85388400	0.00009900
C	0.08228000	-0.05123500	-0.00001300
C	-1.40683900	-0.22115700	-0.00002800
H	-1.68368700	-1.27824600	-0.00022600
H	-1.84929300	0.25843000	0.88268500
H	-1.84926900	0.25928200	-0.88221200
O	0.42117900	1.28122500	-0.00001700
H	1.39159500	1.36393500	0.00026900

COM

C	-0.94453000	1.16118900	-0.48394200
N	-1.86695900	0.29648600	-0.13492300
C	-1.47098100	-0.99146900	-0.08303300
N	-0.23560600	-1.43411600	-0.30460600
C	0.66343600	-0.52022200	-0.64322200
N	0.31293200	0.77450200	-0.77969400
C	1.88007300	-0.30716900	2.06675600
C	2.35146300	0.90976500	1.72651300
C	2.08811100	-0.85669600	-1.02667400
O	-3.71164600	-1.65097600	0.43341800
O	-0.29038300	3.39692800	-0.91645900
O	2.35166500	-2.13384900	-0.85458000
O	-2.41300300	2.97023000	-0.21985100
O	-2.08505100	-3.22695200	0.32298100
O	2.81992100	0.00491000	-1.47446600
C	-3.05213500	-4.26827500	0.61790000
H	-2.48069100	-5.19537400	0.61166400
H	-3.49736700	-4.09297800	1.59992700
H	-3.82545700	-4.28163000	-0.15343900
C	-2.74363300	4.38809500	-0.24261600
H	-2.67170200	4.76046000	-1.26664300
H	-3.76761600	4.44235700	0.12261000
H	-2.06243100	4.93250100	0.41427500
C	-2.56206600	-1.99498700	0.25897800

H	0.82796500	-0.45998100	2.28490500
H	2.56270400	-1.13439000	2.22138200
C	-1.18693300	2.65564200	-0.56805500
C	3.79045400	1.24047400	1.48326400
H	4.11225000	2.04941500	2.15225800
H	4.42960500	0.37118300	1.65273000
H	3.93581300	1.58998300	0.45274200
O	1.45293100	1.92385400	1.55012800
H	1.00792800	1.47231600	-1.07096700
H	1.91395700	2.74353900	1.29752400
C	3.69372200	-2.56460600	-1.21261600
H	3.70284300	-3.63708400	-1.02541900
H	3.87999500	-2.35014700	-2.26692600
H	4.42227600	-2.05187300	-0.58094200

TS1

C	1.88875900	-0.15628500	-0.04050300
N	1.56744300	1.15681500	0.10743600
C	0.28362700	1.53906800	-0.12734500
N	-0.66143900	0.68613800	-0.38098100
C	-0.30946500	-0.64378100	-0.35066800
N	1.00044900	-1.06689500	-0.29673500
C	-0.90405400	-1.30922600	1.73005400
C	-2.28727600	-1.28253200	1.75106700
C	-1.24984600	-1.63113000	-1.02435200
O	0.97343400	3.79218500	0.16026000
O	4.16095100	0.43188200	0.31566400
O	-2.39709700	-1.05916400	-1.37010300
O	3.62426000	-1.74079900	-0.07473100
O	-1.18675100	3.35501900	-0.38901200
O	-0.95174700	-2.79318100	-1.21061100
C	-1.49278700	4.77578400	-0.42105400
H	-2.54243100	4.83074400	-0.70507900
H	-1.33390700	5.20881000	0.56886700
H	-0.86155100	5.27050300	-1.16211900
C	5.02026200	-2.13237000	0.02646700
H	5.39852900	-1.89120800	1.02204600
H	5.02303300	-3.20833500	-0.14089900
H	5.60325200	-1.61793700	-0.74041200
C	0.05806500	3.03620800	-0.10054300
H	-0.39328500	-2.26641100	1.66868500
H	-0.36807600	-0.48343500	2.18330600
C	3.36677000	-0.45959000	0.08717600
C	-3.10321000	-0.06600900	2.01209300
H	-2.47281700	0.79941700	2.21924700
H	-3.74344100	0.14238600	1.14594000
H	-3.76426700	-0.24546500	2.86930500
O	-3.02392900	-2.34862900	1.45122500
H	-2.46626000	-3.13900400	1.30338500
C	-3.35836900	-1.91559300	-2.03943700
H	-4.22583900	-1.28117000	-2.21698100
H	-2.94031200	-2.27036800	-2.98410000
H	-3.62142800	-2.76008200	-1.39976000
H	2.29581900	1.85338100	0.28126200

INT1a

C	0.40212700	1.47329900	-0.13567900
N	-0.94176900	1.60528600	0.12176900
C	-1.69460500	0.45828300	0.19406700
N	-1.21467100	-0.72806200	0.18218900
C	0.24541700	-0.85142300	0.10101700
N	1.01759500	0.35493400	-0.19429000

C	0.72722600	-1.40156800	1.49901200
C	2.20524900	-1.51780500	1.60274400
C	0.50712500	-1.86774300	-1.04476400
O	-3.62375200	1.85281800	0.30846400
O	0.48635500	3.84375400	-0.36811800
O	0.11330700	-3.09475300	-0.71232200
O	2.40182100	2.65226600	-0.58088000
O	-3.89633600	-0.39599700	0.29709700
O	0.97472700	-1.55104500	-2.11847100
C	-5.33547600	-0.22682400	0.35802100
H	-5.73978500	-1.23815400	0.35841600
H	-5.61156700	0.30054100	1.27399600
H	-5.68103900	0.32782700	-0.51737600
C	3.14012800	3.87241700	-0.84399100
H	3.06208000	4.54837800	0.01060700
H	4.17163400	3.55425900	-0.98996600
H	2.75306000	4.35482400	-1.74437300
C	-3.18403300	0.71811400	0.27480700
H	0.35006100	-0.71804100	2.26365100
H	0.28978600	-2.39350800	1.64697300
C	1.10293600	2.79410500	-0.37553300
C	2.99043200	-2.53918400	0.88989100
H	3.98266800	-2.65008600	1.33129400
H	2.45067100	-3.48873500	0.85658100
H	3.11400200	-2.19540600	-0.15036700
O	2.88162800	-0.70642000	2.32218300
H	2.33799900	-0.01330100	2.76366400
C	0.27189300	-4.11582900	-1.72854200
H	-0.05977100	-5.04119400	-1.25880700
H	-0.35109400	-3.88028800	-2.59453800
H	1.32006400	-4.18851300	-2.02653700
H	-1.38937000	2.51626500	0.07918700

INT1b

C	0.92335800	1.03879600	-0.25458400
N	-0.33782700	1.43750400	-0.63096100
C	-1.37566100	0.58739700	-0.31535200
N	-1.22292600	-0.63053600	0.04089100
C	0.14488900	-1.14771100	0.01718400
N	1.22223800	-0.15345700	0.10584900
C	0.31044900	-2.19586700	1.17788400
C	0.11760400	-1.57404700	2.50980600
C	0.33998300	-1.91511400	-1.32718500
O	-2.85511200	2.41012900	-0.72320300
O	1.64264600	3.28510600	-0.59677700
O	-0.44606200	-1.84544700	-2.24764800
O	3.13315200	1.75774500	0.16516100
O	-3.72267100	0.41393200	-0.09469800
O	1.47714600	-2.60365700	-1.33432900
C	-5.06256600	0.96286800	-0.17952300
H	-5.72489900	0.13338500	0.06504700
H	-5.17871000	1.77610200	0.54057800
H	-5.25205100	1.32434400	-1.19267100
C	4.16537600	2.77547000	0.21378600
H	5.05480900	2.26054000	0.57459400
H	4.33373700	3.18311500	-0.78558400
H	3.87187400	3.57055800	0.90297600
C	1.78530700	-3.31988800	-2.55717500
H	2.73454500	-3.81915000	-2.36525500
H	1.00185400	-4.05042100	-2.77070500
H	1.88213100	-2.61529400	-3.38629000

C	-2.73738900	1.24296200	-0.39695900
H	-0.43331800	-2.98301000	1.03436000
H	1.31970300	-2.60614000	1.12076900
C	1.94169700	2.15776800	-0.24837600
C	1.21939700	-0.93671400	3.24118000
H	0.88527900	-0.39631600	4.12960200
H	1.92636000	-1.73080800	3.52598700
H	1.76764300	-0.28144400	2.55128900
O	-1.07336000	-1.62202500	2.97116100
H	-1.17365800	-1.18301900	3.84758100
H	-0.52628100	2.42119300	-0.80419500

INT1c

C	0.49227906	1.25884529	0.11496679
N	-0.53255494	0.90074629	0.94977579
C	-1.37292494	-0.81224171	-0.37314521
N	-0.32290394	-1.31818471	-0.55100621
C	1.04073206	-0.94200971	0.03357579
N	1.32184306	0.39745129	-0.37880921
C	0.87393406	-1.03609171	1.56832079
C	-0.27178194	-0.11656971	2.04147279
C	2.04790206	-1.96216571	-0.51374421
O	-3.43807394	0.22520629	0.18188379
O	-0.26828294	3.51387429	0.18912579
O	1.72367006	-3.02060671	-1.00741421
O	1.48587406	2.98829029	-1.14736621
O	-3.29443194	-1.34531171	-1.46659821
O	3.28415506	-1.53063471	-0.31574421
C	-4.72639094	-1.25191671	-1.75180021
H	-4.88522494	-1.93245271	-2.58583521
H	-5.28659094	-1.56786371	-0.86995021
H	-4.97247594	-0.22446071	-2.02514421
C	1.60317206	4.37540529	-1.55920321
H	2.42218706	4.38914429	-2.27706121
H	0.67272706	4.70316829	-2.02779921
H	1.83504206	5.00049329	-0.69390521
C	4.35125206	-2.41765871	-0.74316321
H	5.27256806	-1.89963771	-0.47982321
H	4.27765606	-3.37027471	-0.21426121
H	4.29076506	-2.57583571	-1.82209321
C	-2.84888294	-0.56754271	-0.50673421
H	0.65920106	-2.06195971	1.87399179
H	1.82855206	-0.72860171	2.00073279
C	0.52744306	2.72087629	-0.27897321
C	0.04228206	0.61738329	3.34026079
H	-0.82017094	1.22115529	3.64555579
H	0.25371006	-0.11622671	4.12426279
H	0.91061506	1.27102629	3.22045179
O	-1.42042994	-0.92574771	2.16357379
H	-2.14375894	-0.40042671	2.55473579
H	-1.14807194	1.66885229	1.22393779

INT1d

C	1.49529900	-0.01125000	-0.36216900
N	1.03762300	1.20867000	-0.27239600
C	-0.33848800	1.26727000	-0.14780000
N	-1.17929700	0.29705000	-0.02343700
C	-0.67326500	-1.05355500	0.03125900
N	0.75155000	-1.11951500	-0.27019200
C	-1.01310900	-1.71721000	1.43595300
C	-0.36550900	-1.03427100	2.57939100
C	-1.41000900	-1.93745600	-1.02175200

O	-0.17369500	3.66419600	-0.05253600
O	3.40121100	-1.41832200	-0.66847000
O	-0.80912700	-2.64881600	-1.79973100
O	3.67107100	0.82989000	-0.73511000
O	-2.20810400	2.71897400	-0.32179500
O	-2.72497300	-1.81255700	-0.93608400
C	-2.80695000	4.03521000	-0.35700800
H	-3.87149500	3.86113500	-0.51219100
H	-2.63758100	4.55440400	0.58963300
H	-2.38983400	4.61624300	-1.18311700
C	5.09094400	0.66160500	-0.97980300
H	5.48510000	1.67299200	-1.06988700
H	5.55465000	0.13945000	-0.13978300
H	5.24428300	0.10288700	-1.90568800
C	-3.50707500	-2.59433800	-1.87731300
H	-4.54548800	-2.35259200	-1.65418100
H	-3.25301100	-2.30572900	-2.89951400
H	-3.31643900	-3.65887300	-1.72414500
C	-0.88612800	2.68593800	-0.16787900
H	-2.09794800	-1.65312200	1.55720900
H	-0.69827600	-2.76287600	1.40332200
C	2.96925500	-0.28196100	-0.60497000
C	0.81769000	-1.57974100	3.25739600
H	1.24126800	-0.89399300	3.99422200
H	0.51185100	-2.51742100	3.74683700
H	1.56393200	-1.86563900	2.50462400
O	-0.91053000	0.06883800	2.92962600
H	-0.44777300	0.52072100	3.67332600
H	1.18485000	-2.02008900	-0.45752700

TS2

C	0.48279200	1.24869600	0.09800800
N	-0.54204200	0.89059700	0.93281700
C	-1.38241200	-0.82239100	-0.39010400
N	-0.33239100	-1.32833400	-0.56796500
C	1.03124500	-0.95215900	0.01661700
N	1.31235600	0.38730200	-0.39576800
C	0.86444700	-1.04624100	1.55136200
C	-0.28126900	-0.12671900	2.02451400
C	2.03841500	-1.97231500	-0.53070300
O	-3.44756100	0.21505700	0.16492500
O	-0.27777000	3.50372500	0.17216700
O	1.71418300	-3.03075600	-1.02437300
O	1.47638700	2.97814100	-1.16432500
O	-3.30391900	-1.35546100	-1.48355700
O	3.27466800	-1.54078400	-0.33270300
C	-4.73587800	-1.26206700	-1.76875900
H	-4.89471200	-1.94260300	-2.60279400
H	-5.29607800	-1.57801400	-0.88690900
H	-4.98196300	-0.23461100	-2.04210300
C	1.59368400	4.36525600	-1.57616200
H	2.41269900	4.37899500	-2.29402000
H	0.66323900	4.69301900	-2.04475800
H	1.82555400	4.99034400	-0.71086400
C	4.34176500	-2.42780700	-0.76012200
H	5.26308100	-1.90978600	-0.49678200
H	4.26816900	-3.38042300	-0.23122000
H	4.28127800	-2.58598400	-1.83905200
C	-2.85837000	-0.57769200	-0.52369300
H	0.64971400	-2.07210900	1.85703300
H	1.81906500	-0.73875100	1.98377400

C	0.51795600	2.71072700	-0.29593200
C	0.03279500	0.60723400	3.32330200
H	-0.82965800	1.21100600	3.62859700
H	0.24422300	-0.12637600	4.10730400
H	0.90112800	1.26087700	3.20349300
O	-1.42991700	-0.93589700	2.14661500
H	-2.15324600	-0.41057600	2.53777700
H	-1.15755900	1.65870300	1.20697900

INT2

C	-1.70288200	-0.69423400	-0.05838100
N	-1.64459100	-1.16020000	1.19790500
C	2.26011700	-0.12758500	-0.25554100
N	1.26026900	0.36880800	0.00198600
C	-0.07251400	0.92895700	0.28620400
N	-1.00542300	0.26572700	-0.59314900
C	-0.35182800	0.78322000	1.79975500
C	-0.67275800	-0.66740100	2.17492900
C	0.05100100	2.43141000	-0.09176200
O	3.58936300	-1.99575600	0.12347400
O	-3.41806700	-2.31696200	-0.45872900
O	1.10748800	2.98106300	-0.31637700
O	-2.85858100	-0.88961300	-2.12184000
O	4.34184000	-0.29476600	-1.21030200
O	-1.14677400	2.99005400	-0.09674900
C	5.62571200	-0.95486700	-1.45661100
H	6.16299600	-0.27110300	-2.11019900
H	6.14545200	-1.08693300	-0.50619100
H	5.44766400	-1.91414800	-1.94541100
C	-3.86201200	-1.48990700	-2.97928600
H	-3.79132900	-0.94756400	-3.92131100
H	-3.64352900	-2.55000200	-3.12663500
H	-4.85254800	-1.36518100	-2.53555900
C	-1.19192500	4.40861300	-0.40759500
H	-2.25009100	4.66649000	-0.39866900
H	-0.64986800	4.97201900	0.35508900
H	-0.75836700	4.58524300	-1.39409400
C	3.50606700	-0.93121700	-0.43490900
H	0.49630400	1.14673600	2.38420900
H	-1.21907500	1.41348000	2.01217600
C	-2.75757700	-1.39632800	-0.90433800
H	-2.26478500	-1.92623000	1.44502900
C	-1.26458800	-0.78643500	3.57501500
H	-1.48902900	-1.83791500	3.79217500
H	-0.54052900	-0.42593200	4.31122500
H	-2.18743800	-0.20567500	3.66522900
O	0.55099700	-1.38549500	2.06810500
H	0.39138100	-2.30718800	2.34019400

TS3

C	-1.76758600	-0.58647700	-0.05386700
N	-1.88068200	-0.94181200	1.21559800
C	2.25777600	-0.30216100	0.05402300
N	1.34624100	0.34214300	0.33875700
C	-0.27156100	1.08704500	0.35421700
N	-1.00221800	0.37048200	-0.55158800
C	-0.66422500	1.06101500	1.82087500
C	-1.07779600	-0.33418000	2.29860000
C	0.18009600	2.49430400	-0.09475100
O	3.29851900	-2.39133600	0.11794600
O	-3.39353900	-2.26362600	-0.56804500
O	1.07639200	3.09171100	0.46355200

O	-2.52838500	-1.02388000	-2.25345300
O	4.35295400	-0.60106200	-0.83080800
O	-0.56872800	2.95101100	-1.08348900
C	5.53168800	-1.39995700	-1.15863900
H	6.20666300	-0.70424600	-1.65297500
H	5.97099300	-1.78777600	-0.23787500
H	5.24246100	-2.21321900	-1.82675300
C	-3.34571300	-1.74358400	-3.21315200
H	-3.07590500	-1.32764500	-4.18285300
H	-3.11702600	-2.81072000	-3.17095200
H	-4.40299000	-1.57231200	-2.99823500
C	-0.27563300	4.30280600	-1.52653600
H	-0.98016200	4.49443600	-2.33481300
H	-0.42951700	5.00357100	-0.70311400
H	0.75344900	4.35962100	-1.88762200
C	3.38066600	-1.23576700	-0.22084500
H	0.13233600	1.45571700	2.45256000
H	-1.52318900	1.74003900	1.89779500
C	-2.66047000	-1.39022500	-0.99234500
H	-2.50918700	-1.71382100	1.43387200
C	-1.92006400	-0.28891100	3.56788700
H	-2.19601300	-1.30712900	3.86739900
H	-1.33604700	0.16652100	4.37274700
H	-2.83400800	0.29208000	3.41467600
O	0.10826900	-1.07978000	2.47928100
H	-0.11218500	-1.91854700	2.92409800

Nitrile

C	1.48870500	-0.17426500	0.00001200
N	2.60737400	-0.47889000	-0.00002800
O	-0.17856600	1.47859000	-0.00000400
O	-0.73884100	-0.72782000	0.00003500
C	-2.15602000	-0.39786300	-0.00002900
H	-2.66691200	-1.35935400	-0.00070300
H	-2.40123600	0.17272000	0.89815500
H	-2.40094000	0.17384900	-0.89757100
C	0.09343600	0.29860300	0.00002900

INT3

C	1.13494100	0.05139200	-0.01820400
N	1.26103400	1.33938100	-0.04459300
C	-1.12198900	0.10729800	0.21069200
N	-0.07026300	-0.60026300	-0.05179800
C	-1.07650600	1.54777200	0.60341000
C	0.08063100	2.27823200	-0.08172400
C	-2.48104200	-0.56522400	0.14853100
O	3.50451800	-0.18088300	-0.00725700
O	-3.50095700	0.05307000	0.38693100
O	2.20482000	-2.04166600	0.06303000
O	-2.40233000	-1.84670700	-0.17332100
C	3.38278400	-2.89409500	0.09737400
H	2.99388700	-3.91006200	0.13891600
H	3.97285800	-2.73702200	-0.80787700
H	3.97465800	-2.66520200	0.98614700
C	-3.66269500	-2.56073100	-0.24885600
H	-3.39433600	-3.58598400	-0.50020500
H	-4.17238600	-2.51756000	0.71624900
H	-4.29034900	-2.12196900	-1.02807400
H	-2.01651500	2.04433900	0.35447200
H	-0.96327200	1.59549400	1.69661000
C	2.43048900	-0.74698800	0.01081500
H	2.20920000	1.72413600	-0.10449600

C	0.48119100	3.57082200	0.61011600
H	1.30731500	4.04513900	0.06738900
H	-0.37601400	4.25006300	0.61033700
H	0.79257500	3.38664800	1.64196500
O	-0.27115400	2.45331500	-1.42571700
H	0.34097900	3.09024000	-1.83896100

H_2O

O	0.00000000	0.00000000	0.12134200
H	0.00000000	0.75813300	-0.48537000
H	0.00000000	-0.75813300	-0.48537000

Product

C	-1.15044500	0.05847200	-0.00018800
N	-1.24073700	1.36907600	-0.00136600
C	1.19611100	0.08025300	-0.00009600
N	0.02738000	-0.59190600	0.00033100
C	1.15986700	1.45885700	-0.00125600
C	-0.09907500	2.09337000	-0.00187000
C	2.42196900	-0.79333100	0.00014600
O	-2.22902000	-2.05586700	0.00117200
O	2.32526000	-2.00502100	0.00077100
O	-3.48920000	-0.16663700	-0.00054400
O	3.53113500	-0.08004700	-0.00034700
C	-4.71164200	-0.95314400	-0.00037700
H	-5.51625000	-0.21942800	-0.00078000
H	-4.75030700	-1.57372500	-0.89809700
H	-4.75056000	-1.57302100	0.89781600
C	4.77847900	-0.82696900	-0.00021000
H	4.83575500	-1.44574600	-0.89812600
H	5.55985100	-0.06863300	-0.00033200
H	4.83575700	-1.44547200	0.89789100
H	2.07725700	2.03298200	-0.00192000
C	-2.36225100	-0.84722300	0.00021400
C	-0.24034900	3.57611400	0.00111500
H	0.72868800	4.07553300	-0.05113000
H	-0.86230200	3.88831300	-0.84613500
H	-0.76210600	3.88979500	0.91415500
H	0.03633600	-1.61859200	0.00062000

TS4

C	1.04973900	-0.83545000	-0.34981000
N	1.01412500	0.34551700	0.36168100
C	-0.05270000	1.16176100	-0.17408500
N	-1.20785700	0.67939800	-0.40800400
C	-1.23648900	-0.72737100	0.00415900
N	-0.08775100	-1.40854400	-0.59407400
C	-1.01201700	-0.75458300	1.56045700
C	0.31196000	-0.07618900	1.92735400
C	-2.51171500	-1.45781700	-0.42295000
O	1.28744400	3.12100600	0.11781200
O	2.26686500	-2.55724900	-1.44241100
O	-2.47586700	-2.53969800	-0.97488400
O	3.38893100	-0.83377900	-0.47093800
O	-0.67932300	3.26743800	-0.99814200
O	-3.58903500	-0.77633700	-0.08429700
C	-0.47015500	4.68885400	-1.19672300
H	-1.35142100	5.03273900	-1.73672900
H	-0.38630100	5.19289700	-0.23127500
H	0.43374400	4.85144900	-1.78850400
C	4.66838500	-1.39494700	-0.87673600
H	5.41425800	-0.70922700	-0.47836900
H	4.78412400	-2.39255800	-0.44803000

H	4.71783700	-1.43654500	-1.96679400
C	-4.86838600	-1.39383500	-0.39423900
H	-5.61589900	-0.68321000	-0.04487700
H	-4.95228700	-1.54887200	-1.47169300
H	-4.95640800	-2.34318400	0.13813000
C	0.27395400	2.62881600	-0.33287600
H	-1.84024600	-0.21532900	2.02222300
H	-1.02123100	-1.79481700	1.89013800
C	2.31996100	-1.51667900	-0.82063500
C	1.36720900	-0.91734100	2.60675700
H	2.30652800	-0.36202300	2.68080100
H	1.00836800	-1.14606900	3.61671100
H	1.54141900	-1.86272400	2.08621800
O	0.06945800	1.12460900	2.51471200
H	0.90080400	1.49934900	2.86480200
H	-0.19918800	-2.27570000	-1.12883100

INT4

C	1.02728500	-0.86602700	-0.33372500
N	1.00372400	0.30975100	0.40151600
C	-0.03316500	1.16006600	-0.16024400
N	-1.19417800	0.70224200	-0.40519700
C	-1.25886400	-0.70485400	0.00923900
N	-0.11919800	-1.41219200	-0.58259700
C	-1.03465800	-0.72963300	1.56279200
C	0.32014700	-0.08422400	1.90180900
C	-2.54602800	-1.40819600	-0.42573600
O	1.37599300	3.07481700	0.09985200
O	2.21857200	-2.58797100	-1.45208400
O	-2.52915100	-2.49009200	-0.97851800
O	3.36373200	-0.88533200	-0.46937200
O	-0.60530500	3.27973400	-0.98191700
O	-3.61023500	-0.70478600	-0.09150400
C	-0.35719700	4.69338000	-1.19089200
H	-1.23071800	5.05752100	-1.73017900
H	-0.25701700	5.20064900	-0.22863500
H	0.54875800	4.82741400	-1.78649100
C	4.63601900	-1.45124700	-0.89161000
H	5.38979700	-0.77461200	-0.49269600
H	4.74791900	-2.45376500	-0.47350500
H	4.67545500	-1.48234000	-1.98242200
C	-4.90057400	-1.29310900	-0.41303800
H	-5.63526900	-0.57344500	-0.05512000
H	-4.98422700	-1.43051900	-1.49290700
H	-5.00786800	-2.24840100	0.10487200
C	0.33869900	2.61490000	-0.32990600
H	-1.84242900	-0.16036200	2.02461600
H	-1.07551900	-1.76598500	1.90209700
C	2.28721000	-1.55478000	-0.82005900
C	1.33276400	-0.96419000	2.60409100
H	2.29040800	-0.44288200	2.69197800
H	0.95068500	-1.18012700	3.60764200
H	1.48344000	-1.91587300	2.08644600
O	0.10406200	1.12201500	2.51508300
H	0.95126600	1.47618800	2.84656500
H	-0.24828900	-2.27166100	-1.12694400

TS5

C	0.49063700	-1.24196100	0.34181800
N	0.90856700	-0.19458500	1.01215000
C	0.26038000	1.15044400	-0.63505400
N	-0.88047300	0.85299900	-0.79762200

C	-1.59953900	-0.23318800	0.06823100
N	-0.80122700	-1.39449500	-0.01380700
C	-1.55133100	0.32817400	1.49261100
C	-0.06771500	0.49451400	1.92090300
C	-2.99536800	-0.48541600	-0.51430500
O	2.25288300	1.11220600	-1.83966500
O	1.01821600	-3.20431800	-0.89988500
O	-3.35171800	-1.58925600	-0.86721700
O	2.69736400	-2.01515700	0.05744900
O	1.75547900	2.92188200	-0.54251100
O	-3.69795700	0.63013600	-0.54913700
C	2.99939300	3.59111200	-0.91557300
H	2.99051800	4.52311000	-0.35405600
H	3.84615100	2.96491000	-0.62847000
H	3.00055300	3.77892600	-1.99074900
C	3.68178100	-2.94245900	-0.47190400
H	4.64125600	-2.56951300	-0.11665800
H	3.48861000	-3.94611800	-0.08720500
H	3.64411000	-2.93838600	-1.56357700
C	-5.04051100	0.53264800	-1.10058100
H	-5.42943800	1.54924700	-1.07390600
H	-4.99003400	0.16205500	-2.12629600
H	-5.64546800	-0.13162400	-0.48004100
C	1.55992700	1.74247700	-1.07666300
H	-2.06780600	1.28757700	1.54097500
H	-2.06775200	-0.38947500	2.13494500
C	1.43876800	-2.27058500	-0.24417600
C	0.18213500	-0.05732400	3.32472300
H	1.22237600	0.11886300	3.61653500
H	-0.47868700	0.45961700	4.02853400
H	-0.02305300	-1.13085400	3.37015100
O	0.20848900	1.88049400	1.85367600
H	1.13221700	2.02236200	2.13522200
H	-1.06501800	-2.14664800	-0.65230900

INT5

C	-1.20254700	-0.05400800	-0.03309500
N	-1.30950200	1.20366800	-0.06995600
C	1.17907400	-0.13152000	-0.08983300
N	0.04931600	-0.74306800	0.04683800
C	1.19366000	1.31143600	-0.39860000
C	-0.08228500	2.04053800	0.05844600
C	2.40859800	-1.01689700	0.02265200
O	-2.17251100	-2.21890000	0.06167700
O	2.30241500	-2.20019200	0.27044700
O	-3.52682100	-0.40762500	-0.12749100
O	3.50936300	-0.32889300	-0.18806600
C	-4.69999000	-1.26467500	-0.12006600
H	-5.54386800	-0.58936000	-0.25200700
H	-4.76679300	-1.78849900	0.83601400
H	-4.64253800	-1.98095000	-0.94239700
C	4.75811000	-1.07449000	-0.13112200
H	4.88546500	-1.49129900	0.87010200
H	5.53308700	-0.34286000	-0.35197200
H	4.74108300	-1.86830600	-0.88075700
H	1.31340700	1.38029100	-1.49252900
H	2.07585700	1.78642400	0.03823900
C	-2.36380000	-1.01942000	-0.02920500
C	-0.29936200	3.33204000	-0.71427000
H	0.58182100	3.97373000	-0.61671100
H	-1.17166700	3.85707800	-0.31079100

H	-0.47602900	3.12782900	-1.77472900
O	0.07830200	2.26166400	1.44557800
H	-0.61244400	2.88292600	1.74124200
H	0.02919100	-1.75766100	0.21151800

TS6

C	2.31165700	1.34534600	1.47787600
H	1.47044700	1.04993300	-0.07010500
N	0.54098000	0.60421600	-0.46199300
C	0.44777000	-0.76041900	-0.39521100
O	1.71847100	-0.91305900	1.67644700
N	-0.70870200	-1.37322300	-0.15582700
C	1.64375400	-1.52236700	-0.88110100
C	-0.55178800	2.82304700	-0.37883000
C	-3.08492500	-1.31172300	0.22775200
O	2.60068800	-0.94778900	-1.37031300
O	-1.52680200	3.51466900	-0.18168000
O	-3.14878300	-2.51448700	0.38472400
O	0.67443100	3.24225500	-0.65851400
O	1.48717200	-2.83446200	-0.76471200
O	-4.11007300	-0.46832100	0.26820400
C	2.58424300	-3.65047400	-1.24065900
H	2.23722700	-4.67852600	-1.14208900
H	2.80424200	-3.41597100	-2.28464700
H	3.46867500	-3.48318100	-0.62087400
C	0.86534000	4.68041700	-0.70867800
H	0.59859600	5.12110800	0.25418800
H	1.92439600	4.81982100	-0.92007000
H	0.25055700	5.10462100	-1.50542000
C	-5.40621800	-1.06487200	0.51606000
H	-6.10832500	-0.23189000	0.52284300
H	-5.65070200	-1.76975800	-0.28220900
H	-5.40328000	-1.57679500	1.48117500
C	2.62802000	-0.01809200	1.56138300
N	-1.78604700	0.74812300	-0.16444200
C	-0.61100200	1.30809700	-0.32478300
H	1.36003300	1.68984100	1.87617100
H	3.09421500	2.09025800	1.36253800
C	-1.77654900	-0.59828000	-0.04106400
C	4.07402300	-0.46744100	1.45602400
H	4.16991200	-1.33862800	0.80126800
H	4.73708800	0.32817600	1.10277400
H	4.41653000	-0.77271000	2.45442400

INT6

C	0.82628300	1.26799200	0.09370200
N	1.77156800	0.40480700	-0.16600500
C	1.33915800	-0.90273600	-0.12038400
N	0.13186600	-1.34901800	-0.00534700
C	-0.93826300	-0.37685100	-0.04655100
N	-0.45935900	0.94626300	0.29059800
C	-2.57958900	0.17722500	-1.81271800
C	-2.03442300	-0.89020100	0.93151800
O	3.58792100	-1.62202500	-0.58112100
O	0.24952000	3.54225300	0.53127000
O	-2.68781200	-1.88182200	0.69089600
O	2.40303000	3.02591900	0.05322300
O	2.08584800	-3.13859800	0.15811100
O	-2.09479300	-0.16626400	2.04345300
C	3.09426400	-4.17080700	0.06381200
H	2.59919000	-5.08542300	0.38942000
H	3.43921900	-4.26721000	-0.96854700

H	3.93702700	-3.93745400	0.71935400
C	2.77543200	4.42166200	0.18087800
H	2.54784300	4.77726700	1.18823200
H	3.84854900	4.44688200	-0.00428900
H	2.24136400	5.01839200	-0.56220300
C	-3.03232200	-0.62069400	3.05296800
H	-2.96878000	0.11608900	3.85306300
H	-4.04213400	-0.65463300	2.63846400
H	-2.73595900	-1.60866900	3.41265400
C	2.46949000	-1.91726700	-0.20717500
C	1.12627500	2.74559000	0.25016400
C	-2.81702900	-0.17366800	-3.25064100
H	-1.96386200	0.13484200	-3.86778300
H	-2.92763700	-1.25873900	-3.36941000
H	-3.71836600	0.31686800	-3.62570200
H	-1.09876200	1.68432400	0.57178000
O	-1.41090600	-0.44245600	-1.39083400
C	-3.37277900	0.96583800	-1.07996900
H	-3.20334700	1.23234200	-0.04310700
H	-4.26432900	1.37819700	-1.54025600

TS7

C	1.15115700	1.09195100	2.04789000
C	0.18408700	1.16421400	-0.51605200
C	0.10782200	-1.15722100	-0.42479000
O	1.12084100	-1.22965700	1.62488300
C	-1.75768200	0.08312600	-0.15805300
N	0.75861800	-0.03125800	-0.76578500
C	1.76171800	-0.14404000	1.92025100
C	0.80609900	-2.48402000	-0.57814200
O	-3.85556300	1.24456100	-0.01557900
O	2.21224400	2.22478100	-1.15532500
O	0.27868400	-3.53058000	-0.27281600
O	0.46409900	3.48885300	-0.43833800
O	-3.82178700	-1.00577100	0.21401600
O	2.01819500	-2.32815100	-1.10298300
C	-5.25927200	-1.01369700	0.38756100
H	-5.52272100	-2.06081000	0.53285900
H	-5.53396400	-0.42242100	1.26441500
H	-5.74607000	-0.61346000	-0.50500600
C	1.24864600	4.69705000	-0.60516800
H	1.60899000	4.76967400	-1.63344500
H	0.56484900	5.51323700	-0.37600600
H	2.08851300	4.68960100	0.09388500
C	2.79843900	-3.53662400	-1.28457400
H	3.72640000	-3.20934300	-1.75130300
H	2.99415700	-3.99744100	-0.31367100
H	2.26063900	-4.23001600	-1.93463700
C	-3.26576900	0.18376600	0.02150700
C	1.07841800	2.35436400	-0.72832800
C	3.27139500	-0.26381600	2.03842700
H	3.75283800	0.67679500	2.32261800
H	3.52646100	-1.02806900	2.78347500
H	3.69187600	-0.60112300	1.08137900
H	1.74955200	-0.05606100	-1.02152200
N	-1.20799800	-1.13044800	-0.16518200
N	-1.12791100	1.25737900	-0.28672100
H	0.07004200	1.16663000	2.10018100
H	1.72542300	1.97047100	2.32654200

INT7

C	0.41889300	1.45747200	-0.09858400

N	-0.91018500	1.57502500	0.25338200
C	-1.67360800	0.42870300	0.19705400
N	-1.19750300	-0.75280400	0.09039300
C	0.27498300	-0.87125100	0.08715100
N	1.02850900	0.34573600	-0.24212500
C	0.70876100	-1.34952000	1.50010900
C	2.21638800	-1.39847900	1.74392000
C	0.57214700	-1.90708800	-1.02732400
O	-3.60212000	1.82670900	0.31125800
O	0.49596800	3.83869300	-0.20829000
O	0.20082700	-3.13725100	-0.66808000
O	2.36671300	2.65913100	-0.69413800
O	-3.88193700	-0.41829800	0.21955400
O	1.03779000	-1.61947000	-2.11182200
C	-5.31951000	-0.24046400	0.26103900
H	-5.73112200	-1.24883100	0.24257300
H	-5.60660700	0.27759100	1.17902100
H	-5.65027300	0.32679200	-0.61220400
C	3.07697800	3.89362800	-0.95971700
H	3.11838100	4.50328900	-0.05397100
H	4.07812000	3.58718400	-1.26102200
H	2.58378600	4.44408100	-1.76411800
C	-3.16157100	0.69272600	0.24780100
H	0.28488600	-0.65169200	2.22719500
H	0.28145000	-2.34214900	1.67915400
C	1.09728200	2.78745100	-0.33956100
C	3.06190500	-2.33689800	0.91819200
H	4.08368300	-2.35034000	1.30536600
H	2.64339600	-3.34977500	0.93096400
H	3.08708900	-2.00738500	-0.12824100
O	2.70811200	-0.70587600	2.62453000
C	0.37732400	-4.17287800	-1.66305000
H	0.04429700	-5.09267100	-1.18263200
H	-0.23374200	-3.95809400	-2.54309700
H	1.42985000	-4.24765600	-1.94602600
H	-1.36160000	2.48443400	0.22921000

H-B

N	0.72740200	-1.19433600	-0.00000100
N	0.72427500	1.19597100	-0.00000300
N	-1.26492400	-0.00158900	0.00000300
H	-2.28815800	-0.00258000	0.00000400
C	1.33491500	0.00178100	0.00000200
H	2.42047600	0.00303700	0.00000800
C	-0.59001900	-1.16877300	0.00000100
H	-1.17274500	-2.08344500	-0.00001500
C	-0.59300900	1.16735900	-0.00000200
H	-1.17817100	2.08046700	0.00000400

TS8

N	2.59512400	0.54090500	0.38772000
N	0.65814200	0.82133500	-0.87835300
N	1.41332900	-1.38358000	-0.19146200
C	-1.01064100	-0.69173900	0.86824000
C	-2.11027500	-0.07905700	0.30038600
H	-0.97766500	-1.77769800	0.90644600
H	-0.46477800	-0.15612800	1.63707800
C	-2.41028500	1.37562600	0.39880700
H	-1.67343300	1.89265800	1.01459200
H	-2.43305700	1.82351500	-0.60236900
H	-3.40605200	1.51536000	0.83857900
O	-2.95857600	-0.73056000	-0.49340600

H	-2.75268400	-1.68619500	-0.52024100
H	3.42442400	0.95606100	0.80720500
C	2.43903300	-0.81282400	0.36270400
H	3.23635400	-1.40100200	0.80670900
C	0.43969300	-0.53364100	-0.69266100
H	-0.24426500	-0.99047900	-1.39800600
C	1.71062300	1.31567100	-0.30333700
H	1.94472000	2.37355000	-0.37291600

INT8a

N	2.54952700	0.64931000	0.31886300
N	0.54192600	0.75796200	-0.89135800
N	1.44274800	-1.39794600	-0.00305400
C	-0.79022400	-0.64196200	0.68240400
C	-2.06351400	-0.06783800	0.21596000
H	-0.93730800	-1.69343100	0.95257600
H	-0.41225000	-0.08025600	1.53872000
C	-2.49587200	1.29615300	0.54928000
H	-2.63283100	1.35757100	1.63826700
H	-1.67587300	1.98489800	0.30619100
H	-3.41454100	1.57520300	0.03184500
O	-2.84415100	-0.73576400	-0.55492800
H	-2.52268300	-1.64749300	-0.74367500
H	3.43052300	1.10423600	0.52914700
C	2.46076500	-0.72769600	0.38755400
H	3.34286200	-1.23292600	0.77540100
C	0.29915500	-0.62039500	-0.47460400
H	-0.14702400	-1.15651700	-1.31799200
C	1.61209700	1.30664400	-0.45166400
H	1.84848300	2.34010900	-0.69579900

INT8b

N	-1.89459900	-0.20323200	-1.04445900
C	-1.65809200	1.06344000	-0.55012300
N	-1.00876300	1.30105100	0.52704700
C	-0.46023300	0.15124600	1.23770200
N	-0.91323300	-1.18311000	0.85177300
C	1.13618500	0.22650100	1.24249100
C	1.71647400	0.10053000	-0.09937800
H	1.39420400	1.19967100	1.66712500
H	1.49344200	-0.58350100	1.88106500
C	2.16725900	-1.18589000	-0.64966400
H	2.39429800	-1.13613100	-1.71703000
H	3.06398000	-1.49265100	-0.09063700
H	1.40550800	-1.94766500	-0.43936900
O	1.76071100	1.18347800	-0.78925400
H	2.10754800	1.04460700	-1.69930600
H	-2.50807900	-0.33112500	-1.84075900
C	-1.57213500	-1.27865400	-0.24208000
H	-1.93228000	-2.24436700	-0.59044800
H	-2.08332100	1.87797200	-1.13289700
H	-0.68158500	0.27936700	2.30207900

INT8d

C	1.60812800	1.11936400	-0.63021000
C	1.61299700	-1.13051700	-0.48352100
C	0.53113400	0.00901800	1.24499500
C	-1.07362400	-0.01111800	1.27275400
C	-1.70094100	-0.11385000	-0.05012100
H	-1.33393800	-0.89010800	1.86928800
H	-1.40295400	0.90121600	1.77454200
C	-2.24909500	1.05264100	-0.76306200
H	-2.49135000	0.83840500	-1.80655400

H	-3.16021200	1.36339200	-0.22882000
H	-1.54941500	1.89325900	-0.68384200
O	-1.72507900	-1.29416100	-0.55810500
H	-2.11132500	-1.32277400	-1.46252600
H	0.77270800	0.05931300	2.30995000
H	1.87197400	2.06734000	-1.09446500
H	1.97805800	-2.06122900	-0.91750500
N	1.05544000	-1.20982400	0.67909300
N	1.85511600	-0.00554700	-1.25736000
N	1.07264100	1.19446300	0.59446600
H	0.97310800	2.09759900	1.04635900

TS9

N	0.22062600	-0.30581300	-1.09963100
C	-1.12194600	1.47818300	-0.74438200
N	-1.64315000	1.07229400	0.23164300
C	-1.30936000	-0.25036900	0.97404800
N	-1.53859100	-1.31882600	0.05416600
C	0.16701800	-0.12358500	1.36756100
C	1.05291200	0.06464600	0.11559900
H	0.32356200	0.71884400	2.04462100
H	0.43144200	-1.04397900	1.89442900
C	2.31390400	-0.79190400	0.13349100
H	2.91533300	-0.59898600	-0.76298700
H	2.90947100	-0.53767000	1.01616100
H	2.06406700	-1.85624300	0.17000000
O	1.36211500	1.43868900	0.02689700
H	2.02176100	1.57015600	-0.67952300
H	0.76376100	-0.34632100	-1.96222700
C	-0.74337000	-1.28116000	-0.96431900
H	-0.86712100	-1.97685400	-1.79068500
H	-0.90370200	2.14430900	-1.56441300
H	-1.98265300	-0.29121100	1.82422500

INT9

N	-1.15002500	0.97167100	-0.61288500
C	2.70993200	-1.17435300	-0.50641100
N	1.99716600	-0.51280500	0.09348200
C	1.12401700	0.41850800	0.85162400
N	1.02429300	1.63967800	0.08941100
C	-0.19283200	-0.28508700	1.20368500
C	-1.13940000	-0.35336000	0.00154700
H	-0.01170900	-1.28772900	1.59876000
H	-0.65174600	0.31560200	1.99445700
H	-1.95234400	1.24509500	-1.16897000
C	-2.55976100	-0.74691200	0.38992500
H	-3.19703200	-0.77840100	-0.50264600
H	-2.55470800	-1.74178600	0.84489500
H	-2.99039900	-0.03317900	1.09900500
O	-0.56869600	-1.31657100	-0.88575500
H	-1.14786400	-1.38811100	-1.66534700
C	-0.09308600	1.80565700	-0.55530100
H	-0.22195700	2.73681000	-1.10505600
H	1.70344900	0.59355500	1.76249700
H	3.38062100	-1.80582300	-1.07202800

TS10

N	-1.12761000	0.88763900	-0.73830200
C	2.92671100	-1.09456800	-0.49695900
N	2.08257200	-0.60001700	0.10568700
C	0.99647400	0.58380800	0.93746000
N	0.94013600	1.67921400	0.11849000
C	-0.25429700	-0.20743000	1.23266700

C	-1.14903000	-0.38944400	0.00210600
H	-0.02374800	-1.17809400	1.67583500
H	-0.78957500	0.38412000	1.98664900
H	-1.88697000	1.08055300	-1.38555300
C	-2.59023900	-0.72971200	0.36424600
H	-3.18466100	-0.86006500	-0.54851700
H	-2.61301500	-1.66667700	0.92865600
H	-3.04523100	0.06116900	0.96784200
O	-0.55999400	-1.41009800	-0.78525100
H	-1.16858600	-1.62451600	-1.51513200
C	-0.13281000	1.76217400	-0.65237900
H	-0.23855900	2.64936500	-1.27301600
H	1.67172400	0.69030200	1.78329500
H	3.71203000	-1.57218400	-1.06203000

INT10

N	-0.00195200	1.18526000	-0.13344200
C	-1.49176800	-1.05963800	-0.06819900
N	-2.08312000	0.08610700	0.07032900
C	-0.05850100	-1.23047800	-0.43997000
C	0.81324100	-0.06676100	0.03939000
H	0.33209400	-2.16616700	-0.03024600
H	-0.01461300	-1.32092800	-1.53631800
H	0.49465900	2.07481600	-0.20428400
C	2.10790200	0.08970100	-0.74289200
H	2.69074500	0.92681300	-0.34068600
H	2.69446200	-0.82771500	-0.64095300
H	1.91118300	0.27235300	-1.80306400
O	1.02818300	-0.25213100	1.41546700
H	1.72477300	0.36165900	1.71274800
C	-1.29786800	1.19881000	-0.10544200
H	-1.79837100	2.15687500	-0.21141600
H	-2.10291800	-1.95003900	0.07494900

TS11

C	0.80059500	1.19001500	-0.88723100
C	0.84119800	-1.09313600	-0.98005300
C	1.27855900	-0.10979800	0.97706800
C	-0.22888400	-0.13252400	1.39984900
C	-1.16465600	-0.07044900	0.20612400
H	-0.40284300	-1.06497900	1.94077900
H	-0.41509800	0.71098300	2.06736600
C	-2.03915300	1.13991300	0.01647800
H	-2.51582700	1.12424500	-0.96771100
H	-2.81956800	1.10369100	0.78709200
H	-1.48392300	2.07265400	0.13972400
O	-1.74604200	-1.25751900	-0.02816300
H	-2.43392700	-1.17176500	-0.71719800
H	1.93442100	-0.12169800	1.84247900
H	0.78491600	2.10519300	-1.47254900
H	0.79967800	-1.86058400	-1.74839900
N	1.51105600	-1.25210800	0.09284300
N	0.07037600	0.09126700	-1.24941100
N	1.49070800	1.12376400	0.21543600
H	2.08958300	1.87783000	0.54824300

INT11

C	0.73915700	1.16073700	-0.93844600
C	0.78589700	-1.14257900	-0.93865100
C	1.31780200	-0.06602200	0.94906300
C	-0.17106600	-0.07815300	1.39807900
C	-1.07355300	-0.04778300	0.14779800
H	-0.35143800	-0.99519500	1.96204100

H	-0.35942100	0.78077400	2.04465500
C	-2.01916300	1.13623500	0.04944800
H	-2.55995100	1.11045600	-0.90190900
H	-2.74093300	1.07151600	0.87039700
H	-1.49330300	2.09240400	0.13352200
O	-1.72277900	-1.26632100	0.03645000
H	-2.37203600	-1.21336100	-0.68981200
H	2.02207200	-0.03605300	1.77445200
H	0.73226000	2.00899100	-1.61672200
H	0.71521700	-1.91361700	-1.69947800
N	1.52393700	-1.24142500	0.08748700
N	-0.06534400	0.03666700	-1.13874900
N	1.48241000	1.14148700	0.11743200
H	2.12831200	1.89294900	0.36431500

TS12

N	0.29360600	-0.27301500	-1.18184700
C	-1.01681500	1.46982500	-0.72068400
N	-1.56827000	1.14376000	0.27852200
C	-1.26767000	-0.20215600	0.99901500
C	0.20740000	-0.11214800	1.37185000
C	1.05359700	0.02293300	0.07721600
H	0.38616400	0.74182800	2.02869500
H	0.45993400	-1.02761200	1.91300800
C	2.26418400	-0.91074900	0.08740900
H	2.86319900	-0.75620600	-0.81621700
H	2.88114000	-0.69069000	0.96523800
H	1.95326000	-1.95930000	0.12935500
O	1.46485100	1.38158000	0.01303800
H	1.99738600	1.49299800	-0.79631100
C	-0.73234400	-1.08761700	-1.10186300
H	-1.10973900	-1.59392900	-1.98805300
H	-0.79391500	2.14320300	-1.53351600
H	-1.95857800	-0.29600400	1.82905800
N	-1.45470800	-1.22340200	0.03096600
H	-2.34215500	-1.71885200	-0.00671000

INT12

N	1.24970300	-0.95743500	-0.73149100
C	-2.68393100	1.24060900	-0.48664400
N	-1.97702800	0.55407000	0.09191500
C	-1.10551600	-0.40980500	0.86142600
C	0.22108900	0.26726100	1.20169400
C	1.16108400	0.32238200	-0.01170300
H	0.04604000	1.26817800	1.60354900
H	0.67196800	-0.34237200	1.99067600
C	2.56835400	0.74098700	0.40455700
H	3.20251400	0.81842800	-0.48587100
H	2.54538400	1.71400100	0.90664100
H	3.01624300	0.00520800	1.08126500
O	0.59215100	1.30295900	-0.89100000
H	1.08470400	1.24890600	-1.72974800
C	0.25172400	-1.75545000	-0.64311900
H	0.26946800	-2.70554100	-1.17584700
H	-3.34917100	1.89413200	-1.03452900
H	-1.70690800	-0.60811600	1.74992800
N	-0.89762300	-1.57740300	0.09607500
H	-1.61964100	-2.28702800	0.06917900

TS13

N	-1.23982800	0.86708500	-0.83225400
C	2.87784600	-1.18277400	-0.46449700
N	2.06541400	-0.59284500	0.09156200

C	0.99787600	0.56142900	0.92707400
C	-0.25494500	-0.22025600	1.21579400
C	-1.16778300	-0.36064800	-0.01378700
H	-0.01670600	-1.19974100	1.63503900
H	-0.77247000	0.35716000	1.99212900
C	-2.58665400	-0.74037800	0.40030300
H	-3.19982200	-0.89045800	-0.49532000
H	-2.57711000	-1.66885600	0.98089100
H	-3.04659900	0.04958800	1.00339700
O	-0.58639900	-1.38676700	-0.81765400
H	-1.12693200	-1.46363000	-1.62492600
C	-0.29414300	1.71389300	-0.73950500
H	-0.29496800	2.61767300	-1.34571400
H	1.68173300	0.72504500	1.75368800
H	3.63555400	-1.74646200	-0.98759300
N	0.81029500	1.63096400	0.11545600
H	1.52416400	2.34979300	0.05399700

INT13

N	-0.09666400	-1.26281700	-0.22051500
C	1.44844800	1.09546700	-0.02605100
C	0.01065100	1.25998100	-0.29762700
C	-0.82542200	0.01054100	0.02640400
H	-0.37277900	2.13041800	0.24446600
H	-0.05558500	1.51541700	-1.36871300
C	-2.12220300	-0.01821400	-0.76976400
H	-2.72455900	-0.87876400	-0.45860200
H	-2.69160300	0.89917700	-0.58881700
H	-1.92166400	-0.10566400	-1.84226500
O	-1.06423400	0.06714700	1.42377000
H	-1.68254300	-0.65037800	1.65469300
C	1.16476500	-1.26983700	-0.18298200
H	1.75801500	-2.17414800	-0.28468300
H	2.11532900	1.94316500	0.10560100
N	1.96302500	-0.09034000	0.00593400
H	2.96729500	-0.21192700	0.15034400

HCN

C	0.00000000	0.00000000	0.50155400
N	0.00000000	0.00000000	-0.65522600
H	0.00000000	0.00000000	1.57725800

P

C	1.15043100	-1.14150500	-0.00000600
C	1.26343500	1.12043500	0.00006000
N	1.90546800	-0.06469400	0.00003100
C	-0.12241100	1.24070700	-0.00007300
C	-0.88995300	0.08076200	-0.00008500
H	-0.60224600	2.21166000	-0.00018800
C	-2.37756000	0.02311000	0.00004800
H	-2.79580400	1.03082900	-0.00093200
H	-2.73484700	-0.51718900	-0.88490500
H	-2.73462800	-0.51529800	0.88625400
H	1.59280900	-2.13136100	-0.00006700
H	1.89151400	2.00685600	0.00010100
N	-0.19782400	-1.08641400	-0.00001300
H	-0.71395800	-1.96879300	-0.00005000

H-C

N	-1.90271400	-1.26084500	0.01914600
N	-2.09103000	1.11258400	-0.17968700
N	-0.02243600	0.10471700	0.18737100
H	1.03882400	0.20322400	0.31433600
C	-2.59728500	-0.12880500	-0.16413900

H	-3.66840300	-0.22654500	-0.31248000
C	-0.60258700	-1.10880600	0.19481800
H	0.04025800	-1.96864400	0.35068800
C	-0.78503100	1.19657400	-0.00167600
H	-0.28502100	2.15921000	-0.00304800
O	2.62108800	0.42383500	0.45072800
H	2.88624300	0.10200700	1.33012900
C	3.38621700	-0.28926600	-0.53967200
H	3.06195500	0.08098200	-1.51468700
H	4.45450100	-0.08501300	-0.41130900
H	3.20832400	-1.36927000	-0.48325200

TS14

N	-1.55941900	-0.05832900	-0.00923000
N	0.43775800	0.37544300	1.12584600
N	0.02466500	-1.77631700	0.07117600
C	2.13319200	-0.44674400	-0.97151300
C	3.15165700	0.29951600	-0.40337200
H	2.32602400	-1.49145600	-1.20346600
H	1.42246200	0.07001100	-1.60727200
C	3.14451500	1.78232700	-0.27956000
H	2.27796900	2.21899900	-0.77725600
H	3.14207900	2.06752700	0.78003600
H	4.06011900	2.19282300	-0.72340900
O	4.19022100	-0.26657100	0.20423200
H	4.17291700	-1.23847800	0.09779200
H	-2.52301900	0.25410200	-0.27126900
C	-1.14681700	-1.32857200	-0.26900700
H	-1.86747900	-1.97941700	-0.75583200
C	0.88415600	-0.84943400	0.64820300
H	1.70214300	-1.28494400	1.21159100
C	-0.75174900	0.73426100	0.74846800
H	-1.16503000	1.69117600	1.05401900
C	-5.10935500	0.26139300	0.19686900
H	-4.87856300	0.63809000	1.19614600
H	-6.10599800	0.61116700	-0.09720400
H	-5.10142200	-0.83544200	0.21513200
O	-4.10633000	0.78420600	-0.68838900
H	-4.28796200	0.44270600	-1.58082600

INT14a

N	1.51171100	-0.01610400	0.18461500
N	-0.47074800	0.42148700	-0.99975800
N	-0.02386000	-1.79517300	0.06290200
C	-2.01331800	-0.51760000	0.72188600
C	-3.14103100	0.29515000	0.24352400
H	-2.38014900	-1.48724500	1.07572100
H	-1.48129000	0.00199600	1.52058000
C	-3.23461900	1.74545100	0.46098700
H	-2.29900200	2.20310700	0.11180900
H	-4.09813700	2.18221200	-0.04207400
H	-3.28078000	1.93290300	1.54290000
O	-4.08827300	-0.23580400	-0.44383400
H	-3.98599600	-1.20850900	-0.55387700
H	2.48772200	0.26618400	0.36470400
C	1.12561300	-1.32403600	0.38076400
H	1.88845000	-1.97525700	0.80362800
C	-0.98846600	-0.83063800	-0.45844100
H	-1.57534400	-1.32540500	-1.23892500
C	0.70714600	0.75880400	-0.61960200
H	1.14693700	1.69590400	-0.95576100
C	5.05671200	0.29154700	-0.43330900

H	4.75369800	0.84475200	-1.32601300
H	6.11469600	0.49749700	-0.22856700
H	4.92850400	-0.78246100	-0.61950800
O	4.22594800	0.74905600	0.64280600
H	4.48735700	0.26477000	1.44444900

INT14b

C	0.44236200	-0.96634200	1.21520300
C	0.55266200	-0.93454800	-1.13504800
N	-0.66812700	-1.30143400	-1.27407100
C	-1.46949500	-1.39235900	-0.05994900
N	-0.78666500	-1.33335700	1.22933200
C	-2.66250200	-0.32315500	-0.11718100
C	-2.18340900	1.06078400	-0.08019700
H	-3.19131900	-0.50951700	-1.05510800
H	-3.30702500	-0.51909100	0.74146800
C	-2.07250000	1.82390800	1.17304600
H	-1.51043200	2.75380200	1.05804800
H	-3.09250300	2.04534800	1.52084900
H	-1.62341800	1.18009900	1.94026300
O	-1.81675100	1.55420100	-1.20952600
H	-1.45343200	2.46514900	-1.13217100
H	-2.03186900	-2.33125900	-0.09644600
H	1.00275000	-0.89074800	2.14532100
H	1.19803200	-0.83572500	-2.00595000
N	1.15350000	-0.66934300	0.07486300
H	2.16454900	-0.46956900	0.12240500
C	4.10576700	1.31859800	-0.18125300
H	3.79065800	1.44360500	-1.22041000
H	3.48589900	1.96045500	0.45812800
H	5.15481300	1.62640500	-0.08953600
O	3.94440100	-0.06912300	0.14080500
H	4.22383500	-0.19195000	1.06430600

TS15

C	-0.80082100	-1.01436600	1.29118800
C	-0.43370800	-1.20990000	-1.03078700
N	-1.66979600	-1.08604900	-1.27670400
C	-2.33796100	-0.32274900	-0.21057800
N	-2.04903400	-0.87988100	1.12155500
C	-1.77461300	1.13555200	-0.25435400
C	-0.26827600	1.17181000	-0.05897400
H	-2.01391200	1.56865800	-1.22746800
H	-2.26652500	1.71850400	0.52650200
C	0.29270900	1.80504100	1.18761100
H	1.36715900	1.61490300	1.27348700
H	0.13089400	2.88638900	1.10541100
H	-0.21532400	1.45238900	2.08772500
O	0.37594700	1.46297800	-1.20571500
H	1.31920200	1.64778600	-1.02907000
H	-3.41118300	-0.31305000	-0.38061300
H	-0.32528400	-1.37988800	2.19552900
H	0.28915000	-1.69982000	-1.67439200
N	0.06369300	-0.62633700	0.19885500
H	1.09389900	-0.75915800	0.35898500
C	3.59304300	-0.18548300	-0.43213700
H	3.20868700	-0.38117000	-1.43584800
H	3.51132500	0.88692600	-0.21507200
H	4.64896800	-0.47874200	-0.39252000
O	2.81272100	-0.97668600	0.47681800
H	3.11730800	-0.78761900	1.38078200

INT15

C	-0.79209400	-0.97291900	1.30652100
C	-0.43236800	-1.20486000	-1.02147400
N	-1.66967400	-1.10934600	-1.25705700
C	-2.34422200	-0.32807800	-0.20318900
N	-2.04012400	-0.86684100	1.13685000
C	-1.77437400	1.11995900	-0.26652300
C	-0.25730100	1.11104900	-0.06463600
H	-1.99956100	1.54681400	-1.24561500
H	-2.25836900	1.72358700	0.50333200
C	0.28685800	1.82382500	1.15425000
H	1.36369200	1.65219300	1.25457500
H	0.11018900	2.89605900	1.01797400
H	-0.21647400	1.50818500	2.07137200
O	0.38292400	1.42163300	-1.23193500
H	1.32644200	1.59885900	-1.05455600
H	-3.41783600	-0.33514500	-0.36825400
H	-0.29732600	-1.32948600	2.20370600
H	0.30059000	-1.70596900	-1.64399700
N	0.06230800	-0.55532600	0.19637000
H	1.09732300	-0.69390200	0.35579700
C	3.59940700	-0.19864000	-0.41125500
H	3.22147200	-0.37175600	-1.42144200
H	3.54979900	0.87329000	-0.18362400
H	4.64362000	-0.52878300	-0.36004500
O	2.78124600	-0.97302200	0.48010500
H	3.08008400	-0.80426500	1.39011400

TS16

N	-0.16299000	-0.29232000	-0.48664700
C	0.75538300	-1.42774600	1.29150800
N	1.87968600	-1.18813600	1.03702400
C	2.40025200	-0.26731700	-0.11441700
N	1.94788500	-0.83942400	-1.33728800
C	1.77578000	1.10240100	0.17092300
C	0.23352000	1.00993300	0.16625100
H	2.10836600	1.49815600	1.13309200
H	2.12505000	1.77482600	-0.61699000
C	-0.43104500	2.16297800	-0.58206500
H	-1.52147200	2.06040500	-0.54470400
H	-0.14952800	3.11004600	-0.11071400
H	-0.11496300	2.18153700	-1.62923600
O	-0.18465300	0.96793200	1.51793900
H	-1.15929200	0.99472800	1.54593000
H	-1.18378400	-0.38240700	-0.65014700
C	0.65551100	-0.82879100	-1.44538200
H	0.17362700	-1.33258100	-2.28034800
H	-0.09609100	-1.84890600	1.80176000
H	3.48219600	-0.27945800	-0.02881600
C	-3.60651400	-0.60379800	0.49523600
H	-3.16413800	-1.44748800	1.03106600
H	-3.42945700	0.31606400	1.06761900
H	-4.68809500	-0.76705800	0.40900300
O	-2.98809800	-0.55929300	-0.79746000
H	-3.34981000	0.20622100	-1.27530300

INT16

N	-0.60925900	-0.34579300	-0.40469300
C	3.32096500	-0.39384900	1.61197000
N	2.79992500	-0.34633700	0.59595900
C	2.13727100	-0.38516000	-0.73630800
N	1.37570800	-1.60577800	-0.81064600
C	1.36772700	0.92259900	-0.95973300

C	0.04435400	0.94027600	-0.18942400
H	1.97587700	1.78978200	-0.69056700
H	1.16380200	0.97046000	-2.03357500
H	-1.63202700	-0.41511500	-0.31915400
C	-0.88089600	2.06670700	-0.63877600
H	-1.81124300	2.04194800	-0.05868200
H	-0.39592100	3.03309700	-0.47084300
H	-1.13127300	1.97517700	-1.70040400
O	0.40233100	1.10044000	1.18704300
H	-0.41886100	1.09251700	1.71010800
C	0.08900300	-1.46756500	-0.65085500
H	-0.52229100	-2.36419200	-0.74826000
H	2.99177600	-0.43128700	-1.41744200
H	3.80878500	-0.43231600	2.57524500
C	-4.07001200	-0.49505900	1.02808800
H	-3.60235700	-1.20006500	1.72044200
H	-5.14908600	-0.69321700	0.99650600
H	-3.90545800	0.52596500	1.39597600
O	-3.46774000	-0.70787500	-0.25407700
H	-3.86353600	-0.07561000	-0.87719500

TS17

N	-0.60312800	-0.40837400	-0.35918400
C	3.44299300	-0.38132400	1.69768800
N	2.87631000	-0.19653400	0.71571700
C	2.08108500	-0.36660400	-0.86957400
N	1.41894600	-1.56784100	-0.84128800
C	1.30293000	0.91765700	-1.04195600
C	0.00101200	0.92868800	-0.23547300
H	1.90741800	1.79360000	-0.79821800
H	1.06708500	0.96341000	-2.11279100
H	-1.62022400	-0.52133900	-0.21137600
C	-0.99174500	1.97473100	-0.73012300
H	-1.90064900	1.94836800	-0.11670400
H	-0.54664200	2.97073700	-0.64658100
H	-1.27027900	1.79557400	-1.77299600
O	0.36542000	1.17002100	1.11687000
H	-0.45116000	1.28178500	1.63568900
C	0.11637400	-1.49360800	-0.60743100
H	-0.44932400	-2.42271900	-0.64470600
H	3.02360900	-0.39118000	-1.41228700
H	3.97171900	-0.53979500	2.62508800
C	-4.09874400	-0.27132600	0.98869800
H	-3.55423100	-0.41440300	1.92566700
H	-5.11181800	-0.67861100	1.10015700
H	-4.16745500	0.80310600	0.77665100
O	-3.37214300	-0.97288800	-0.02778500
H	-3.81258800	-0.80564400	-0.87796300

INT17

N	-0.03804100	-0.51855800	-0.21699100
C	2.64894300	-0.54805300	0.08783000
N	2.00126900	-1.66717500	0.16331300
C	2.04750200	0.75101100	-0.32941200
C	0.55397300	0.84080500	-0.00447500
H	2.57203200	1.58304600	0.14918500
H	2.21472000	0.85263300	-1.41267000
H	-1.07666700	-0.59488000	-0.35767300
C	-0.19412000	1.83850200	-0.87739700
H	-1.24883600	1.88109500	-0.58327900
H	0.24842300	2.82988700	-0.74319000
H	-0.13402300	1.56168400	-1.93393400

O	0.44771300	1.14228400	1.36787100
H	-0.47758300	1.37727000	1.56489500
C	0.65459600	-1.60668700	-0.12376700
H	0.13276600	-2.54941300	-0.26327200
H	3.71287000	-0.57609100	0.32176100
C	-3.52885200	-0.11584600	0.50165100
H	-3.10761900	-0.35717900	1.48049200
H	-4.58033000	-0.42629600	0.47904800
H	-3.46981400	0.96699100	0.33924200
O	-2.76558300	-0.84473900	-0.47224400
H	-3.07782700	-0.58735800	-1.35645500

MeOH

O	0.75272700	0.12385800	0.00001300
H	1.12988500	-0.77108800	-0.00003500
C	-0.66662200	-0.01883900	0.00000600
H	-1.09103200	0.98988300	-0.00138600
H	-1.03035300	-0.54945300	-0.89199600
H	-1.03058000	-0.54717300	0.89327800

Reference：

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, **2013**.

(2) (a) Becke, A. D. *J. Chem. Phys.***1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785.

(3) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

(4) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

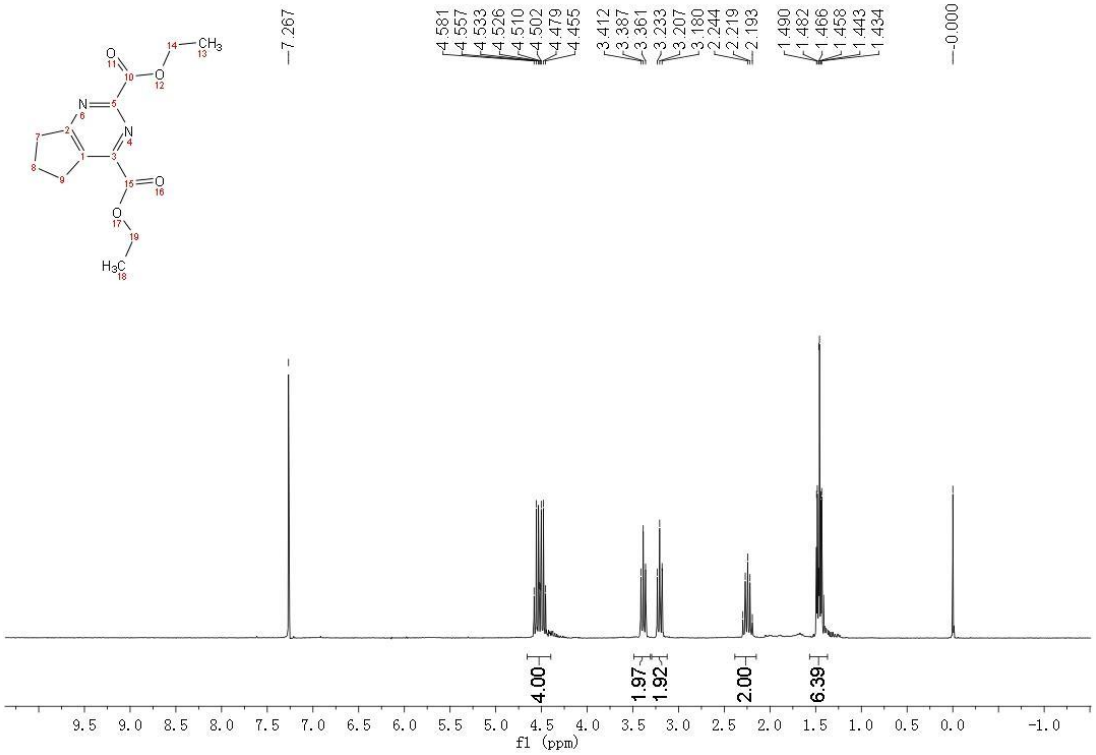
(5) Adamo, C.; Barone, V. *J. Chem. Phys*. **1999**, *110*, 615.

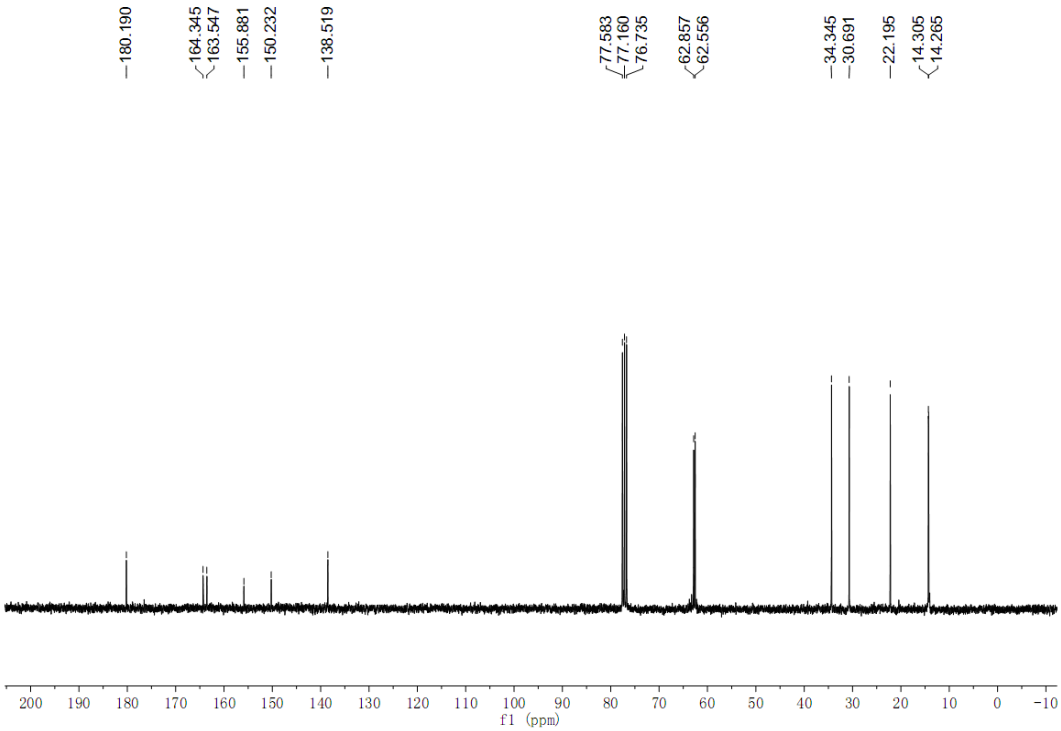
(6) Møller, C.; Plesset, M. S. *Phys. Rev.* **1934**, *46*, 618.

(7) Legault, C. Y. CYL view, 1.0 b; Université de Sherbrooke, **2009**. http://www.cylview.org.

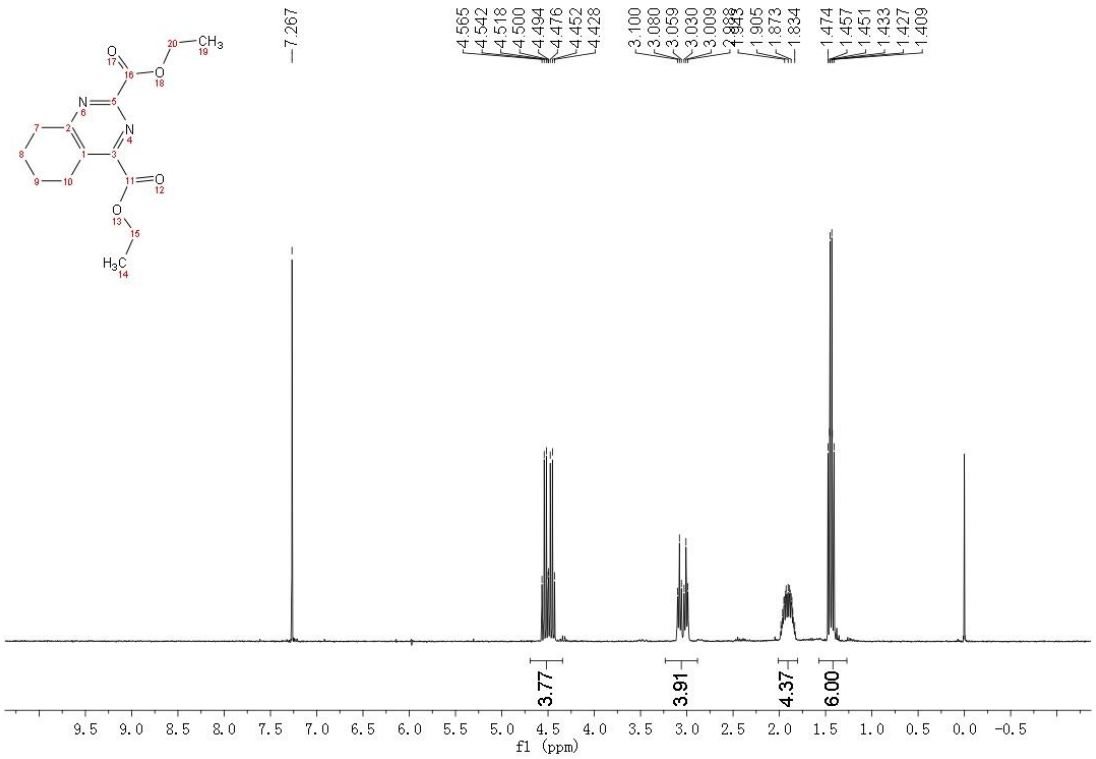
NMR Spectra：

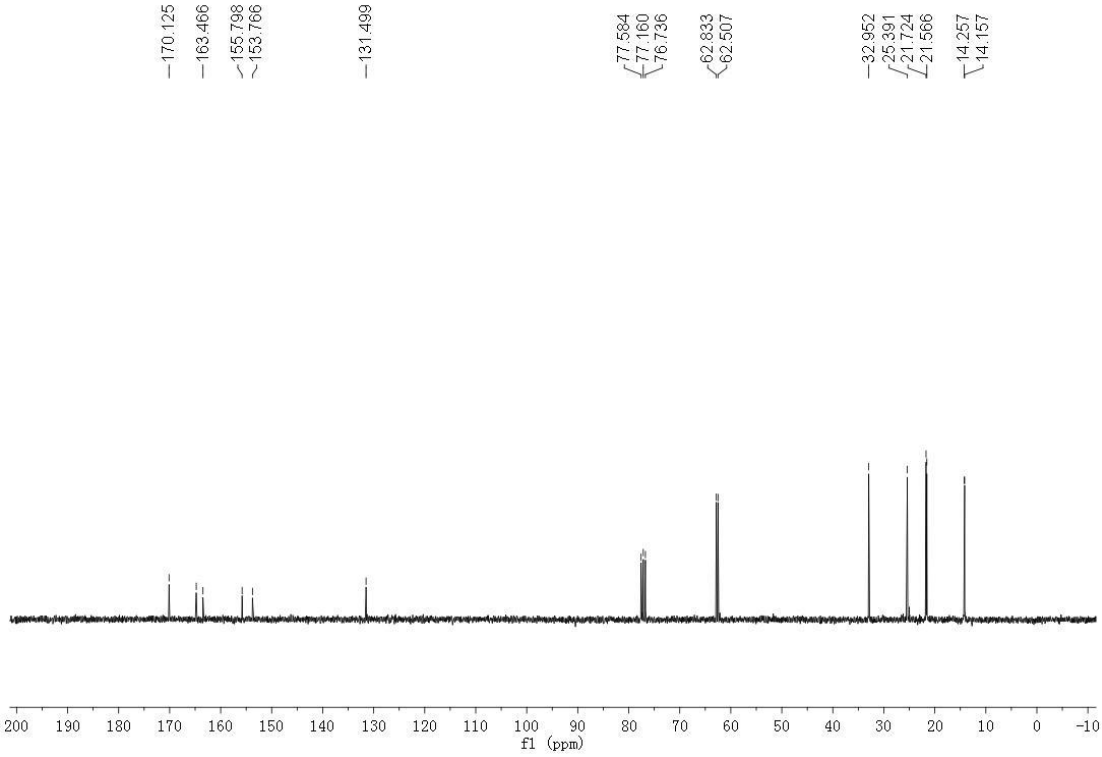
NMR Spectra of Compound **3a**



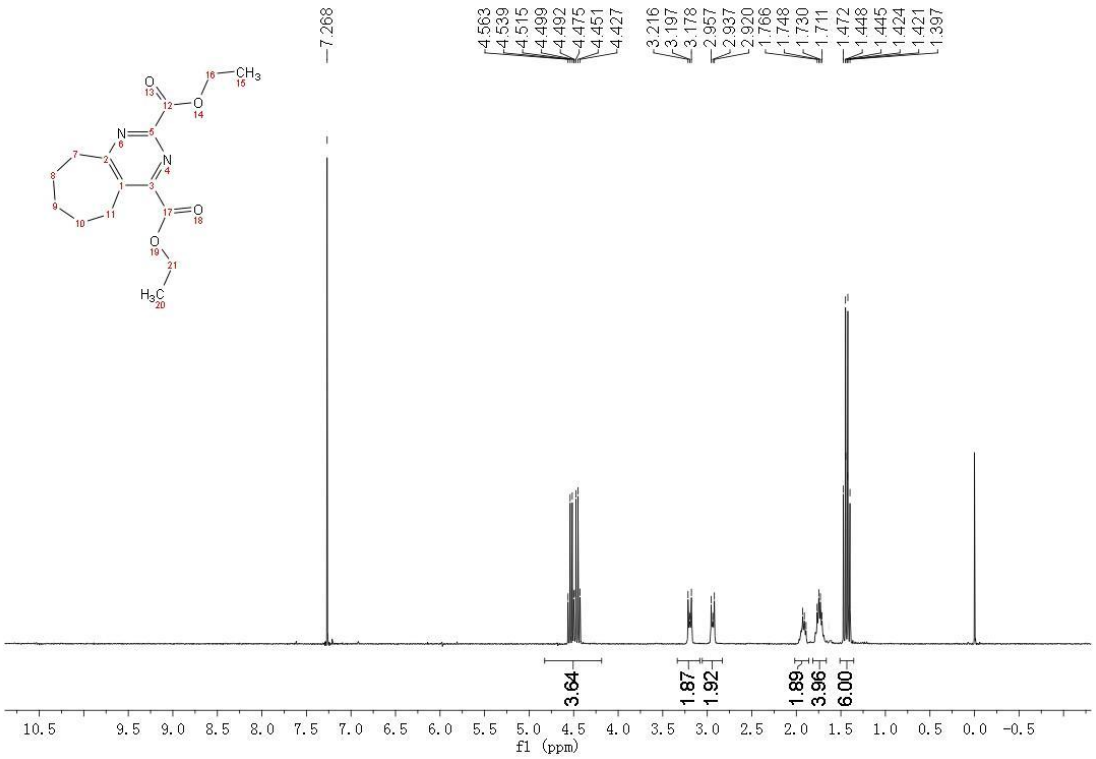


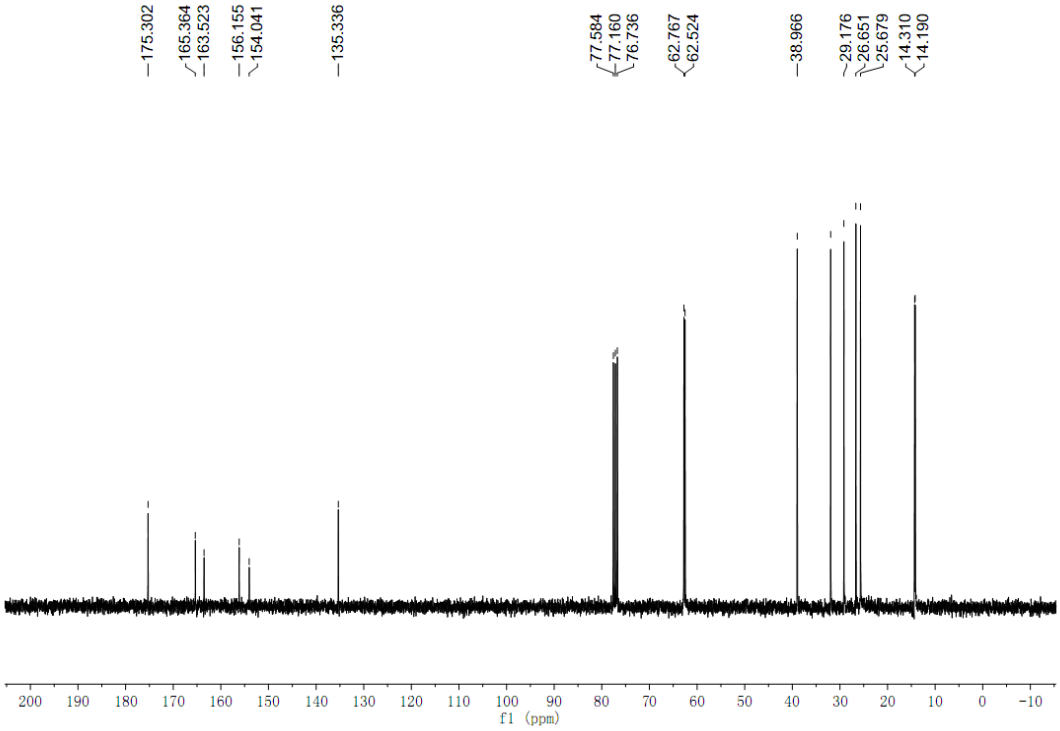
NMR Spectra of Compound **3b**



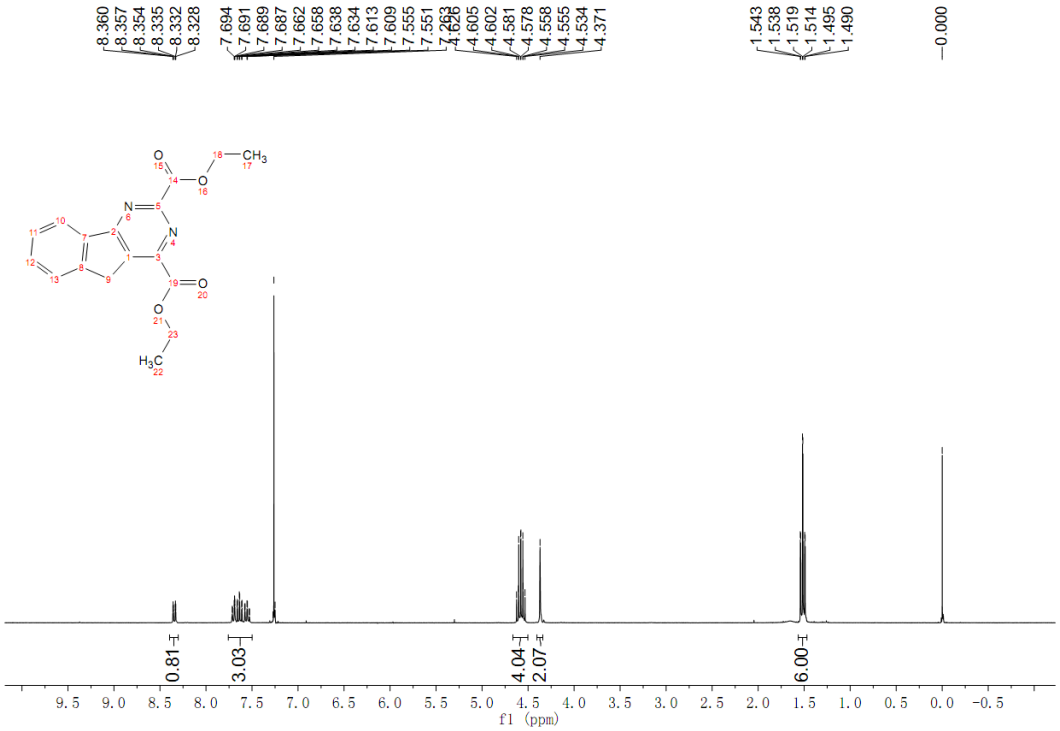


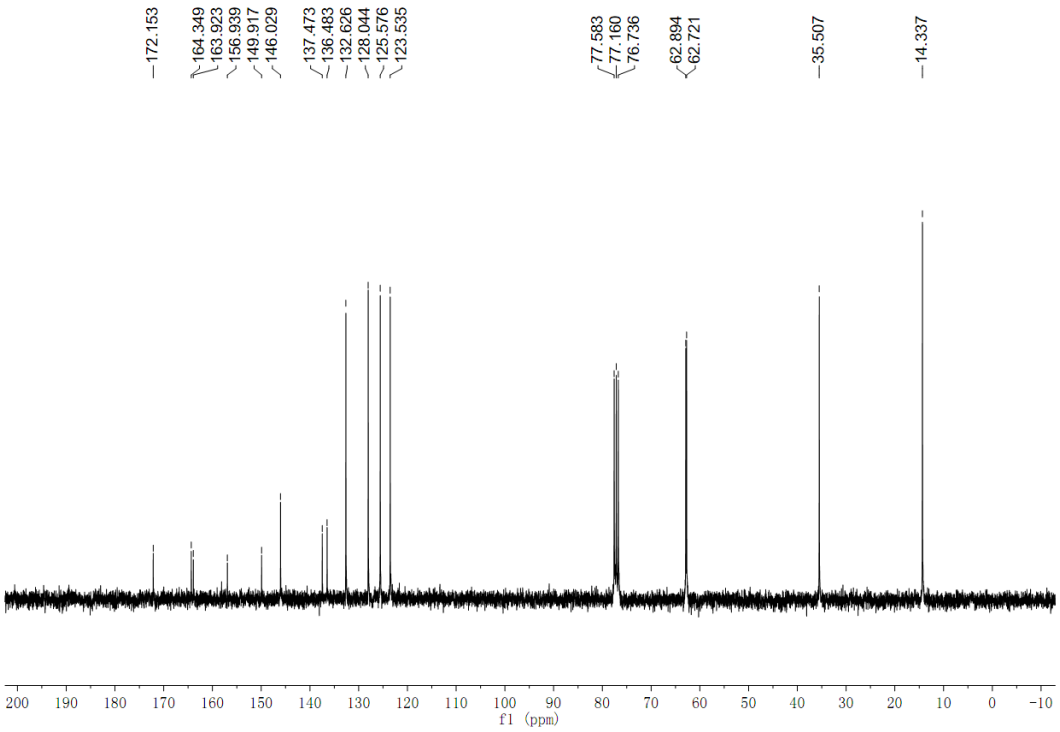
NMR Spectra of Compound **3c**



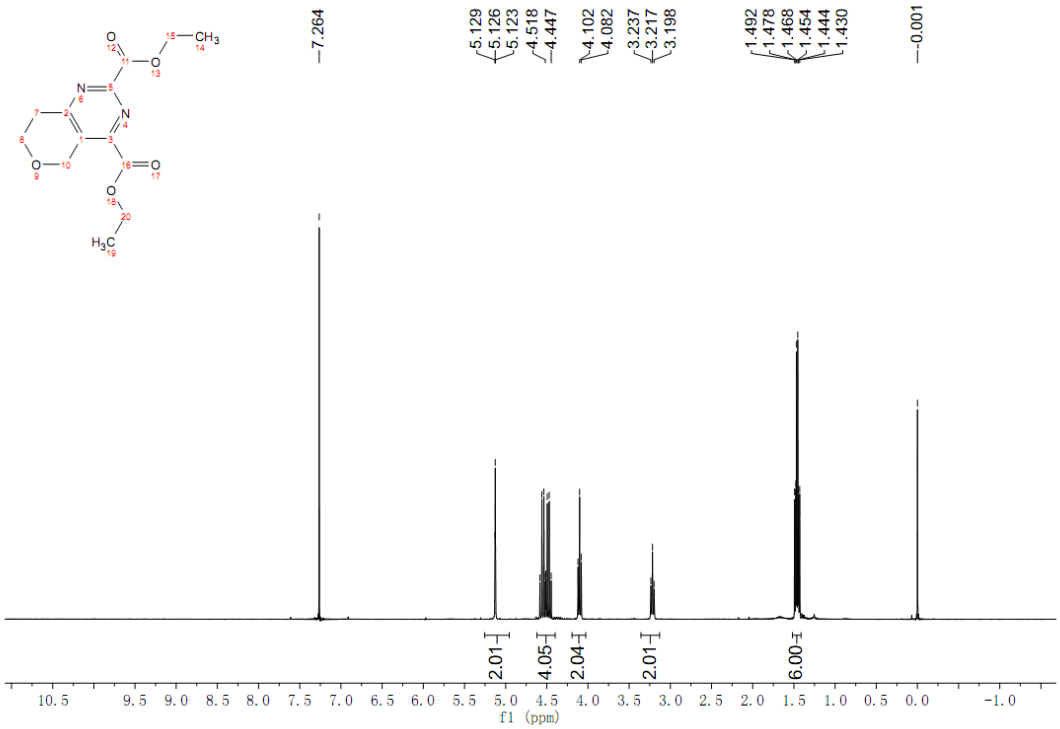


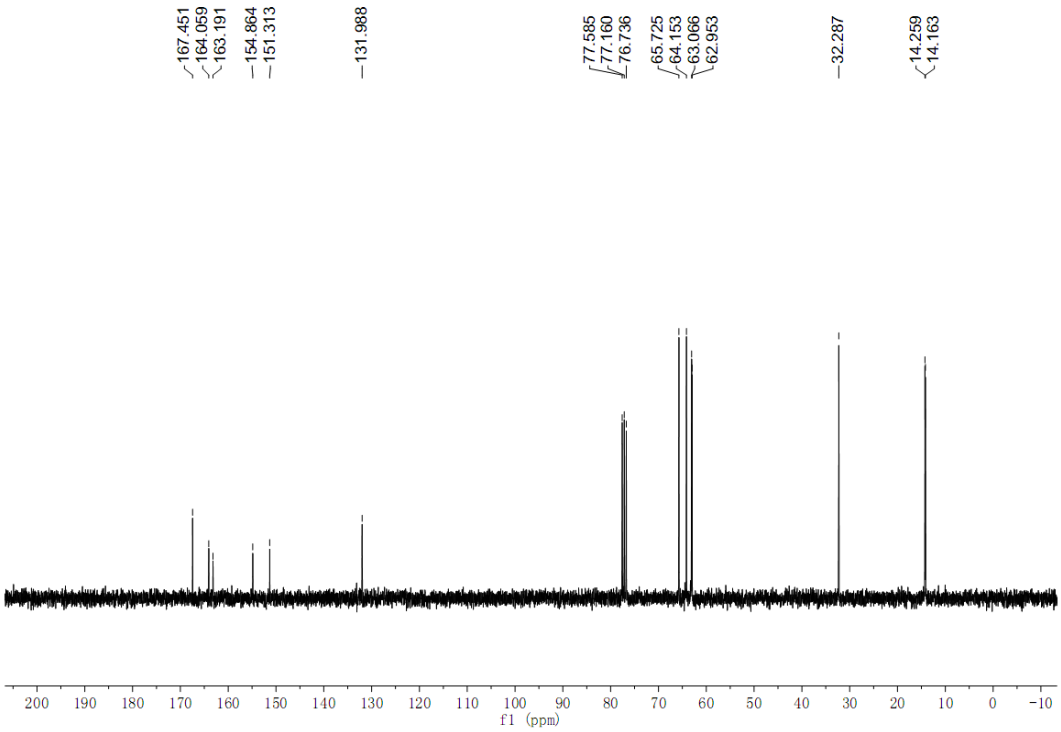
NMR Spectra of Compound **3d**



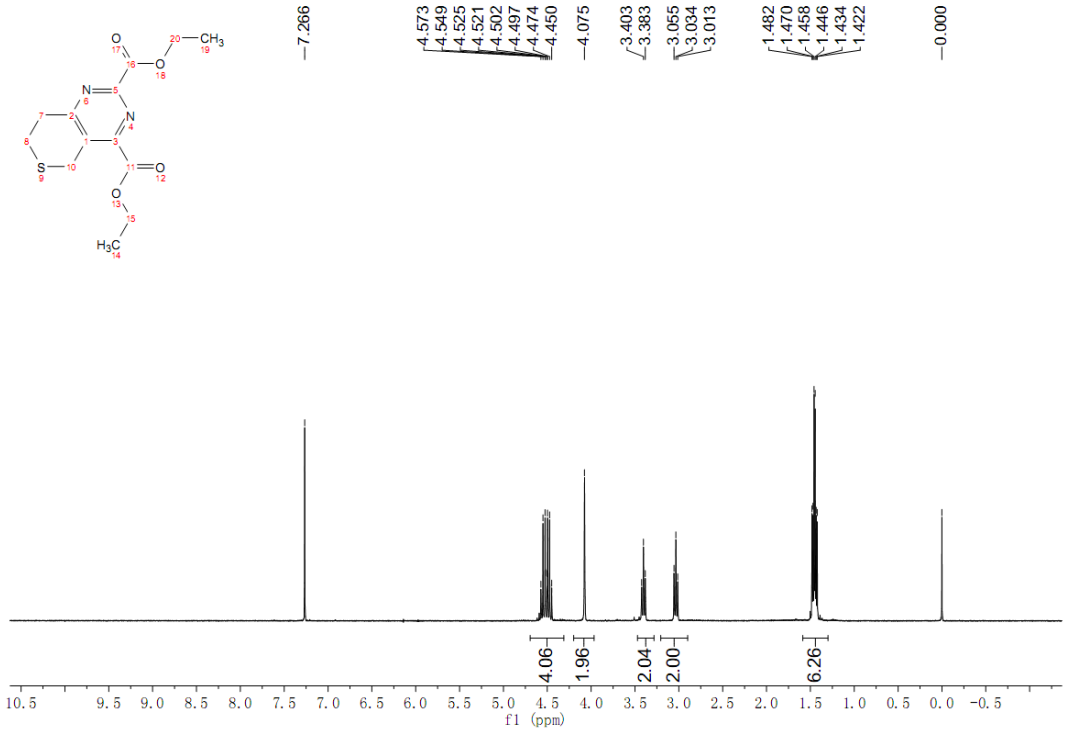


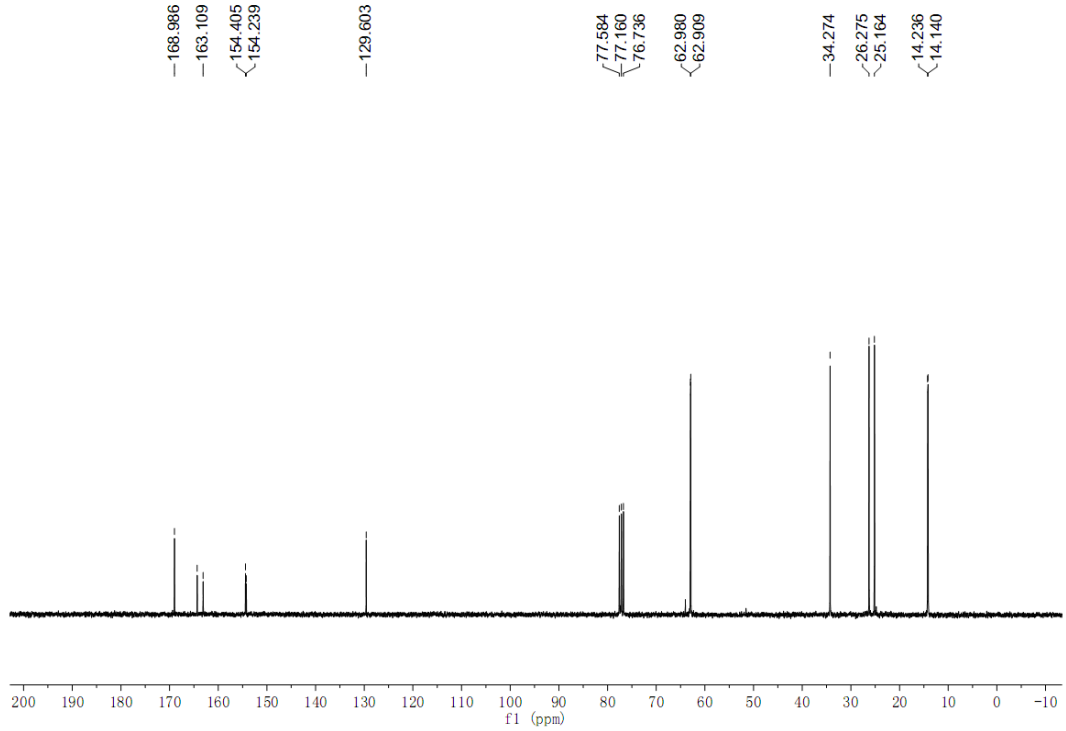
NMR Spectra of Compound **3e**



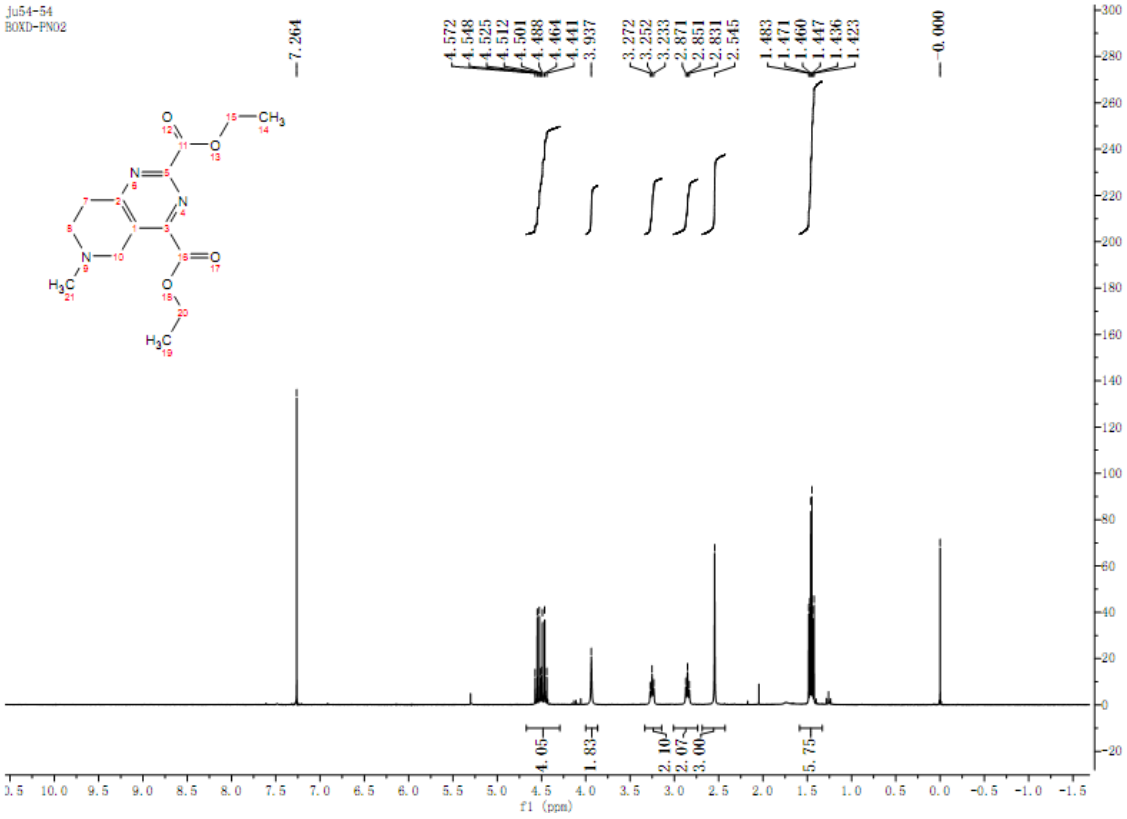


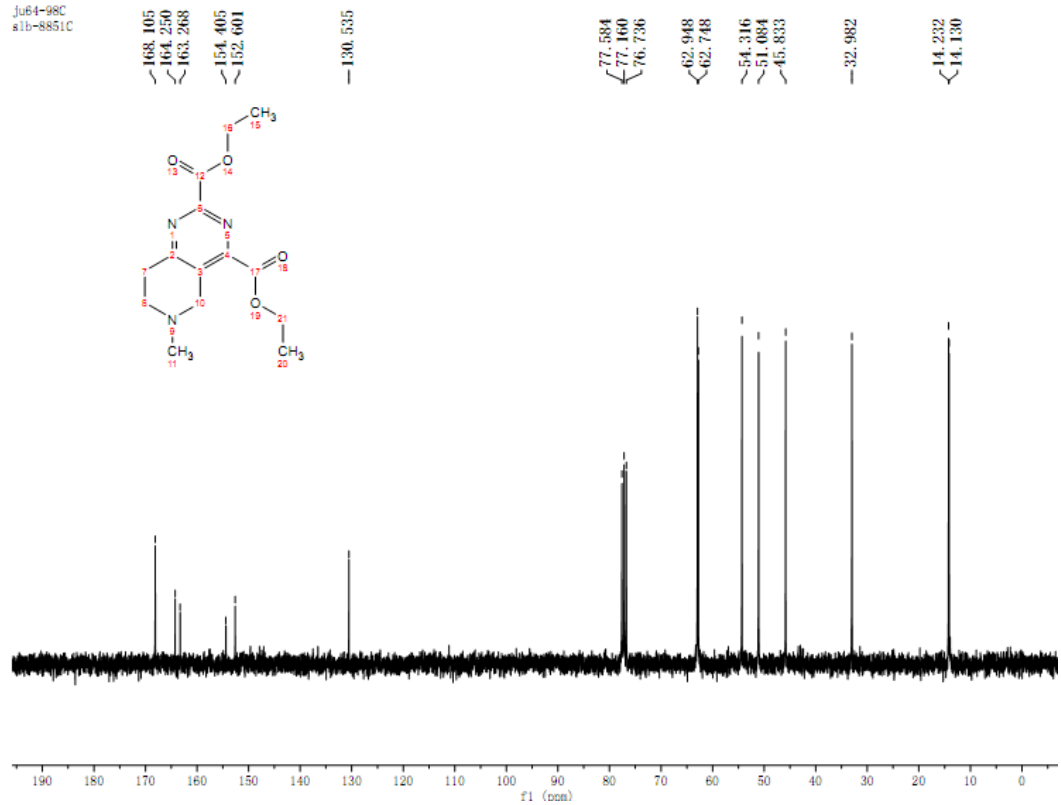
NMR Spectra of Compound **3f**



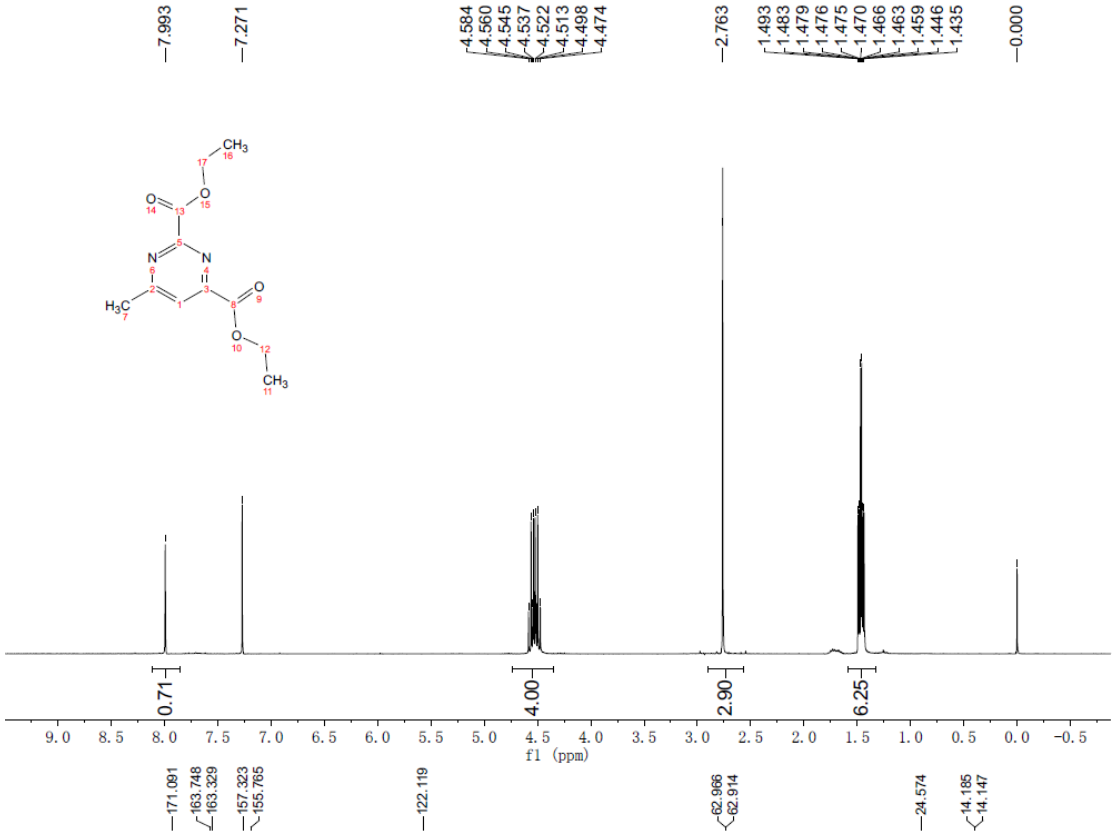


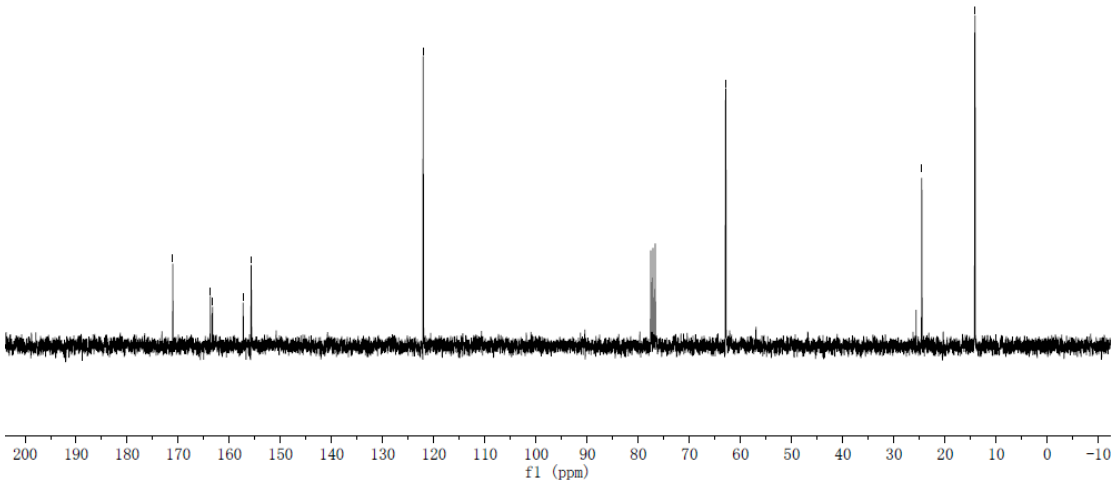
NMR Spectra of Compound **3g**



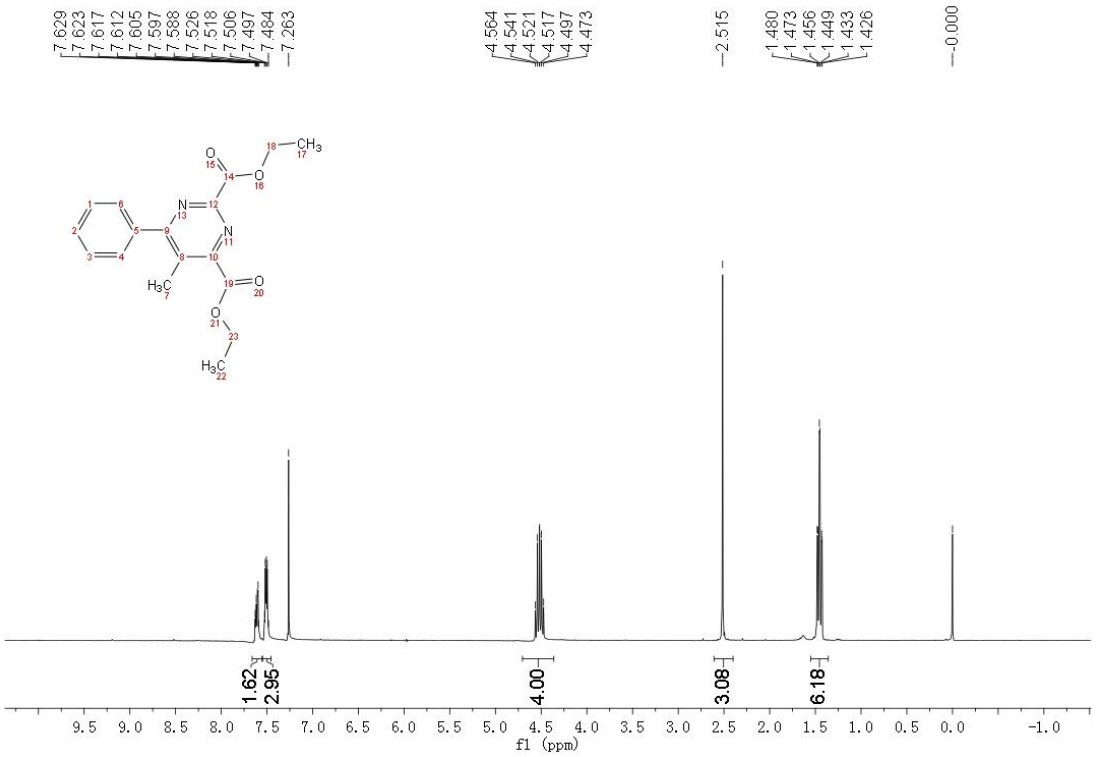


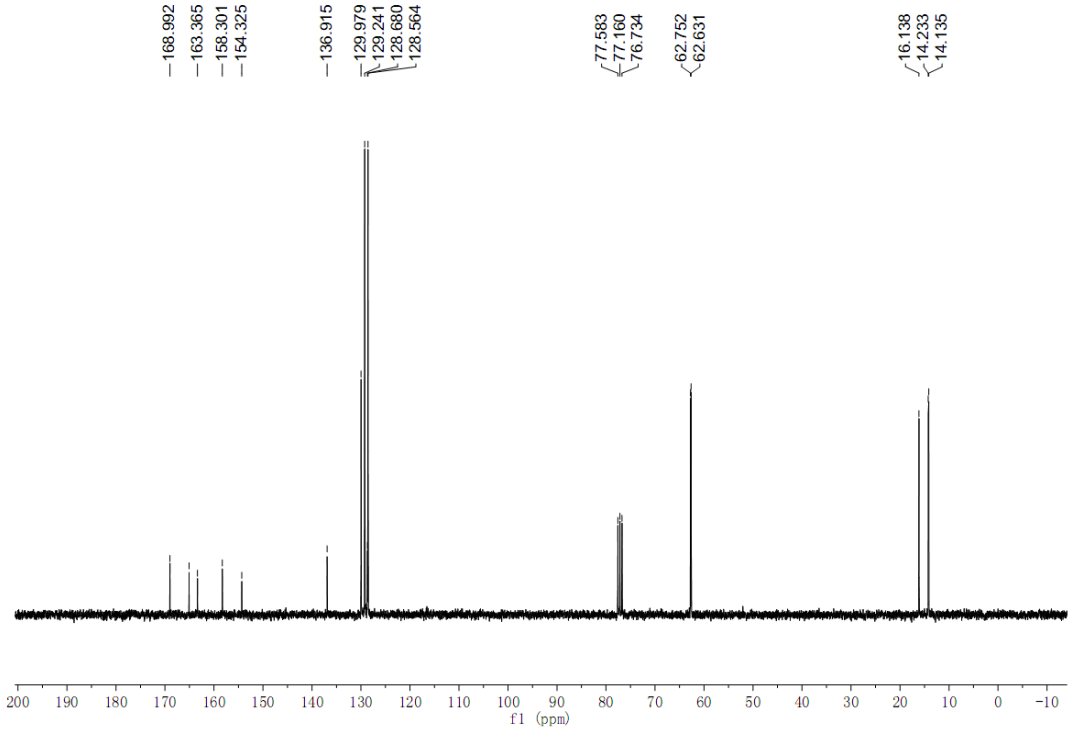
NMR Spectra of Compound **3h**



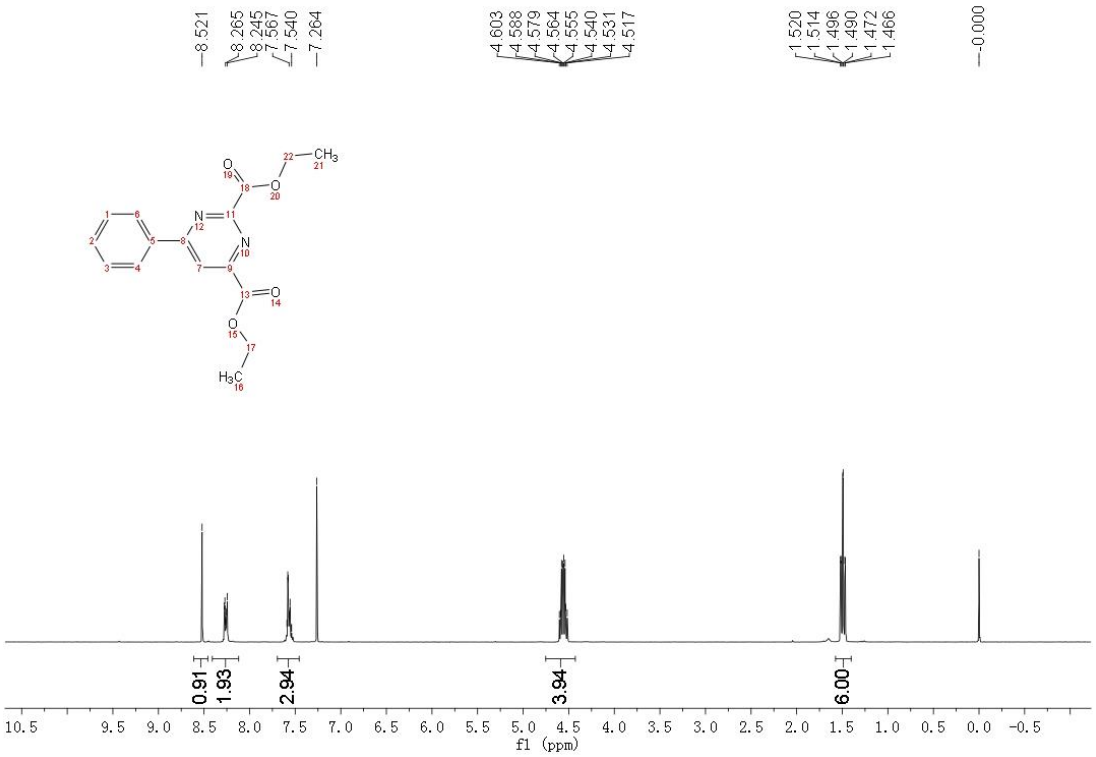


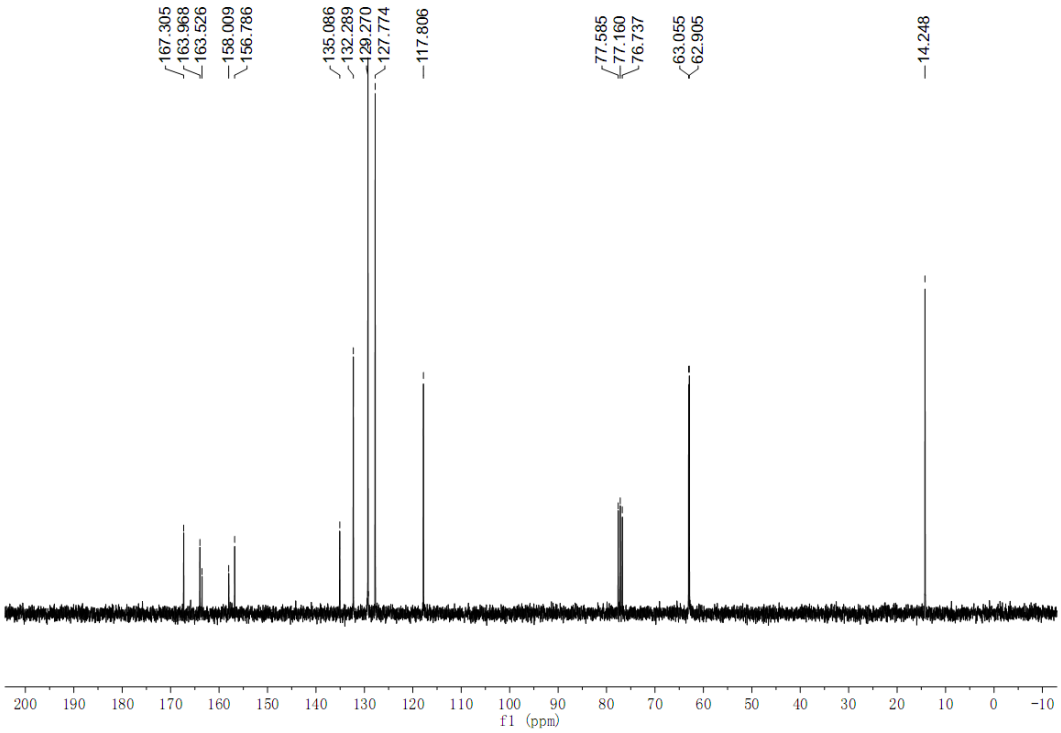
NMR Spectra of Compound **3i**



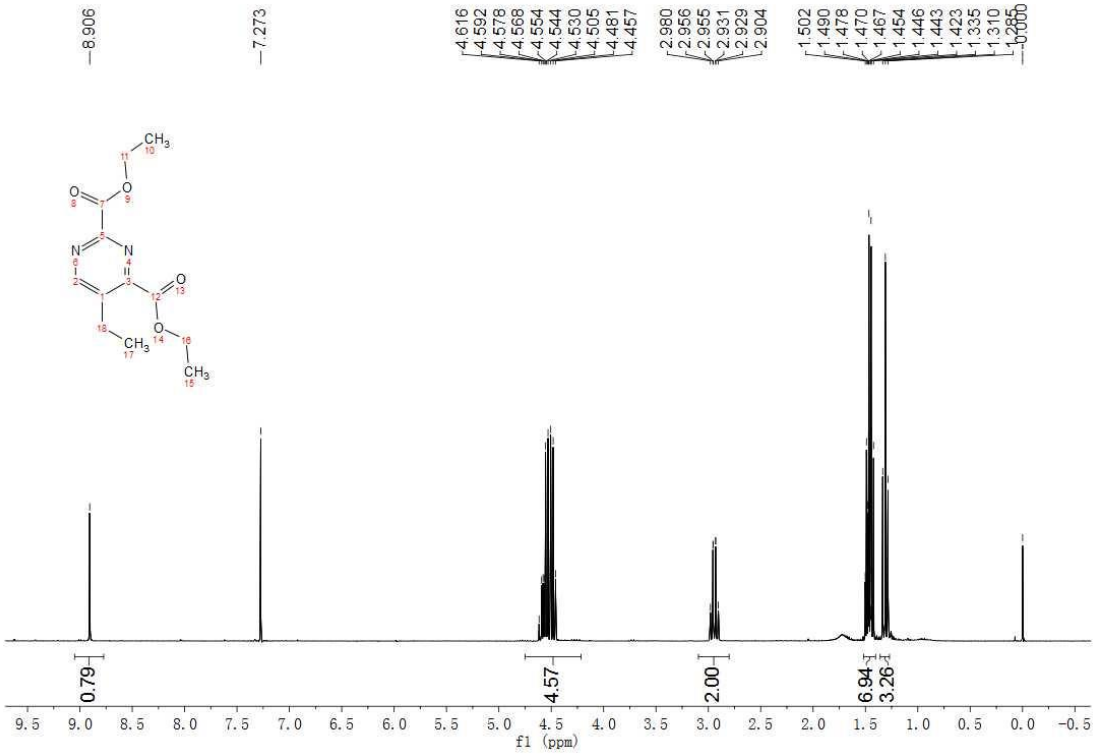


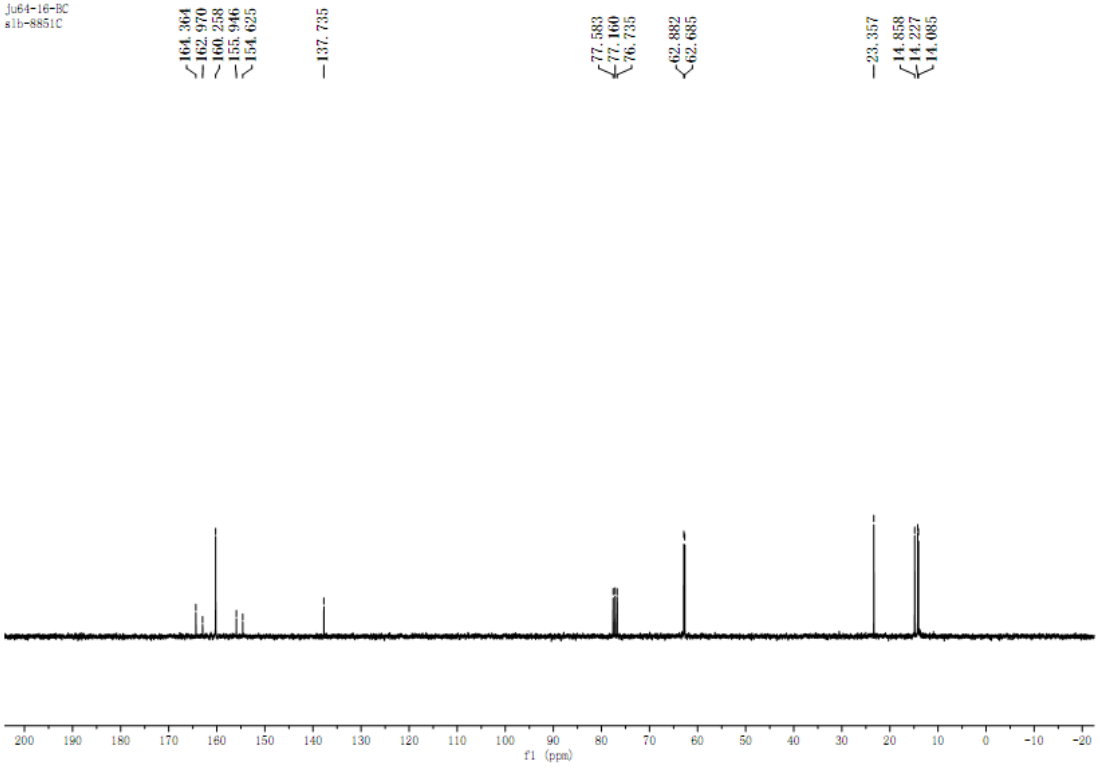
NMR Spectra of Compound **3j**



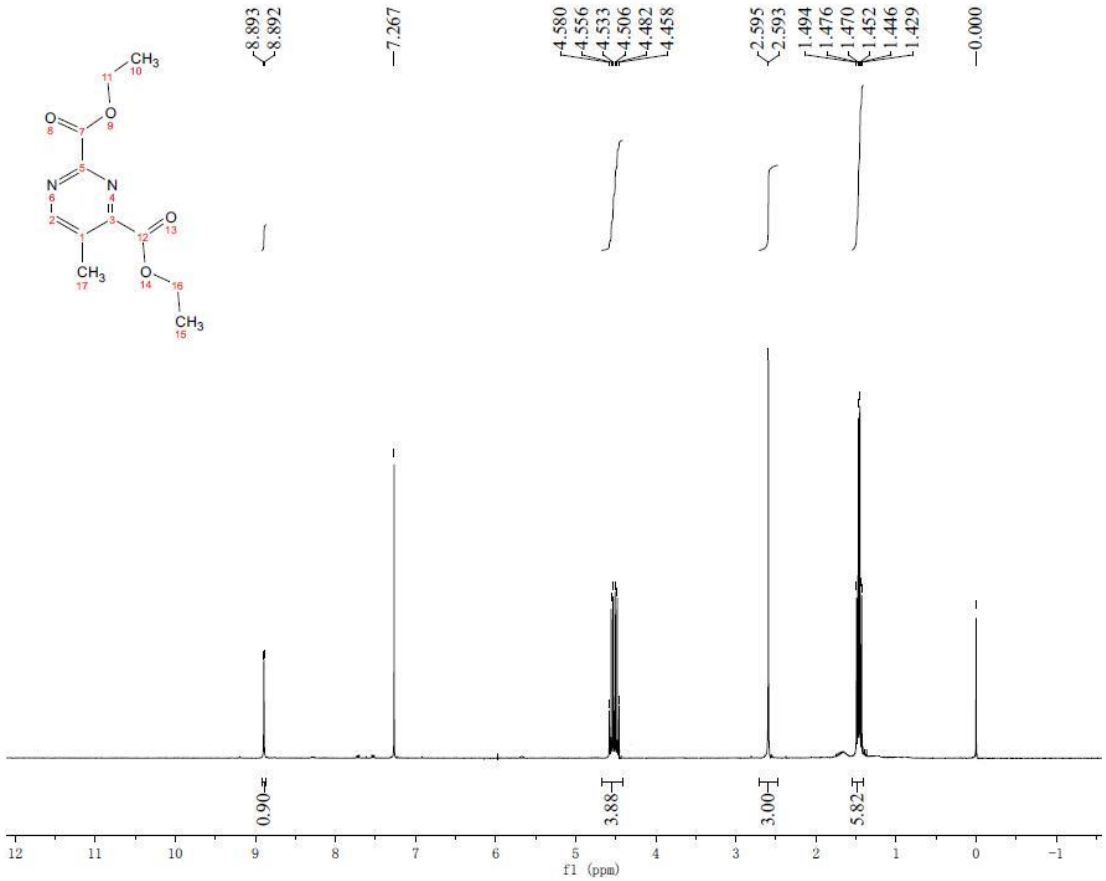


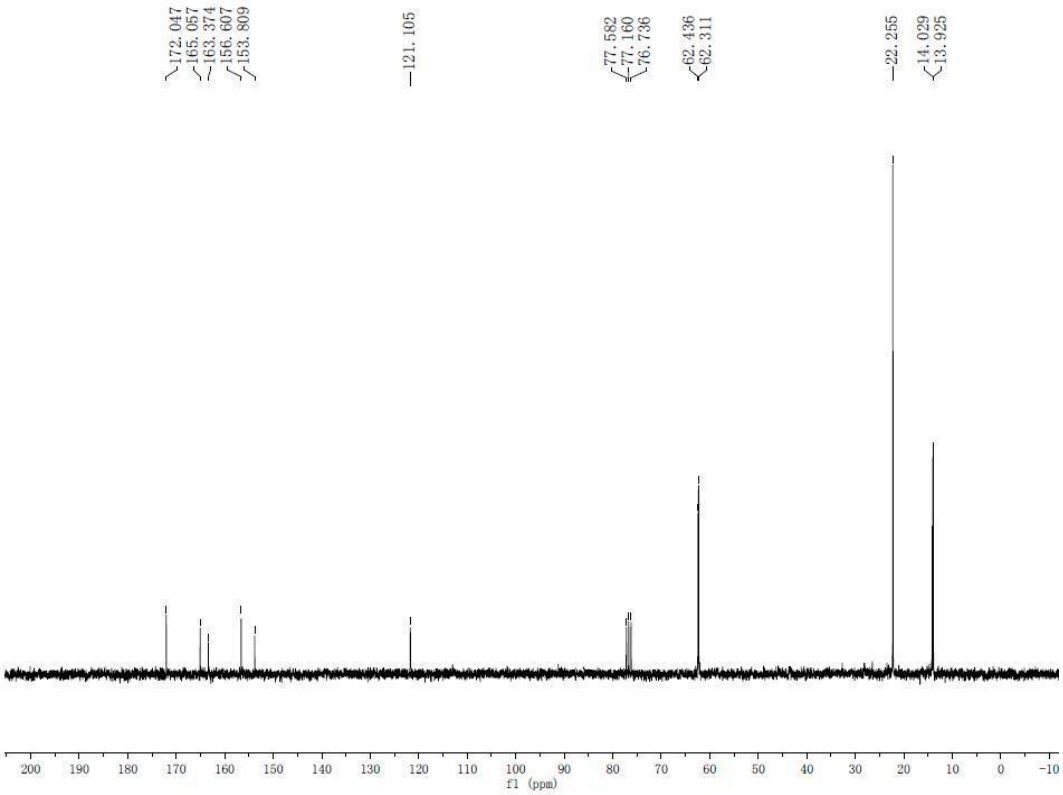
NMR Spectra of Compound **3k**



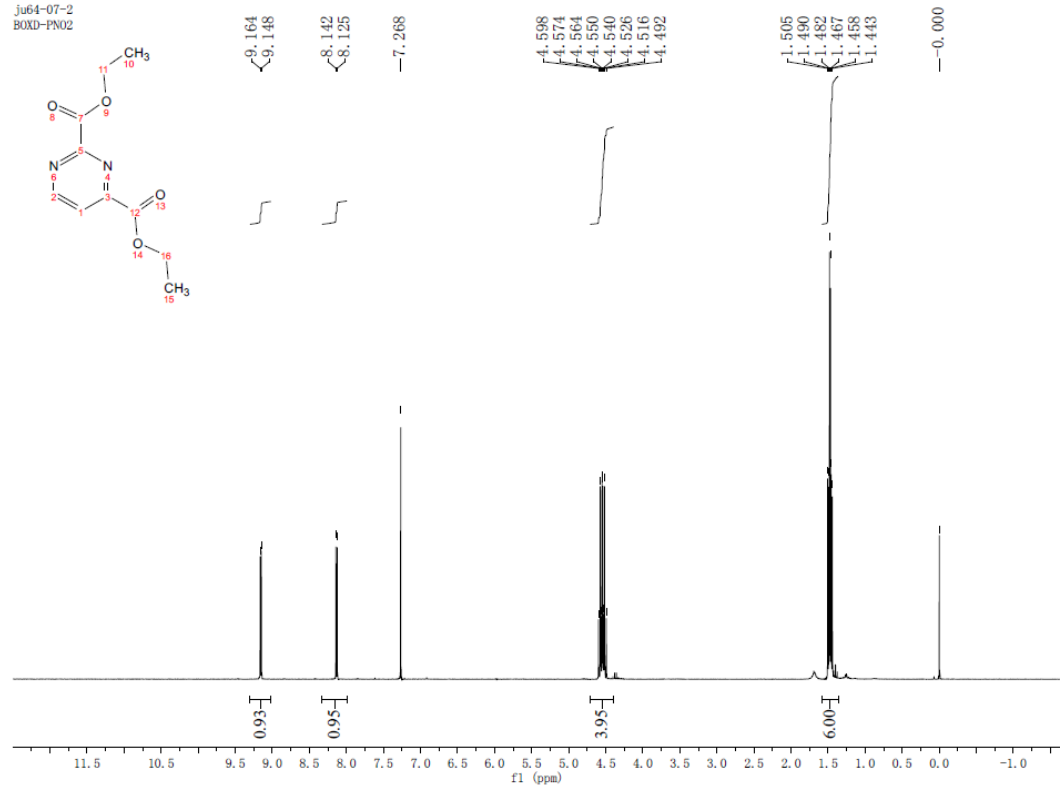


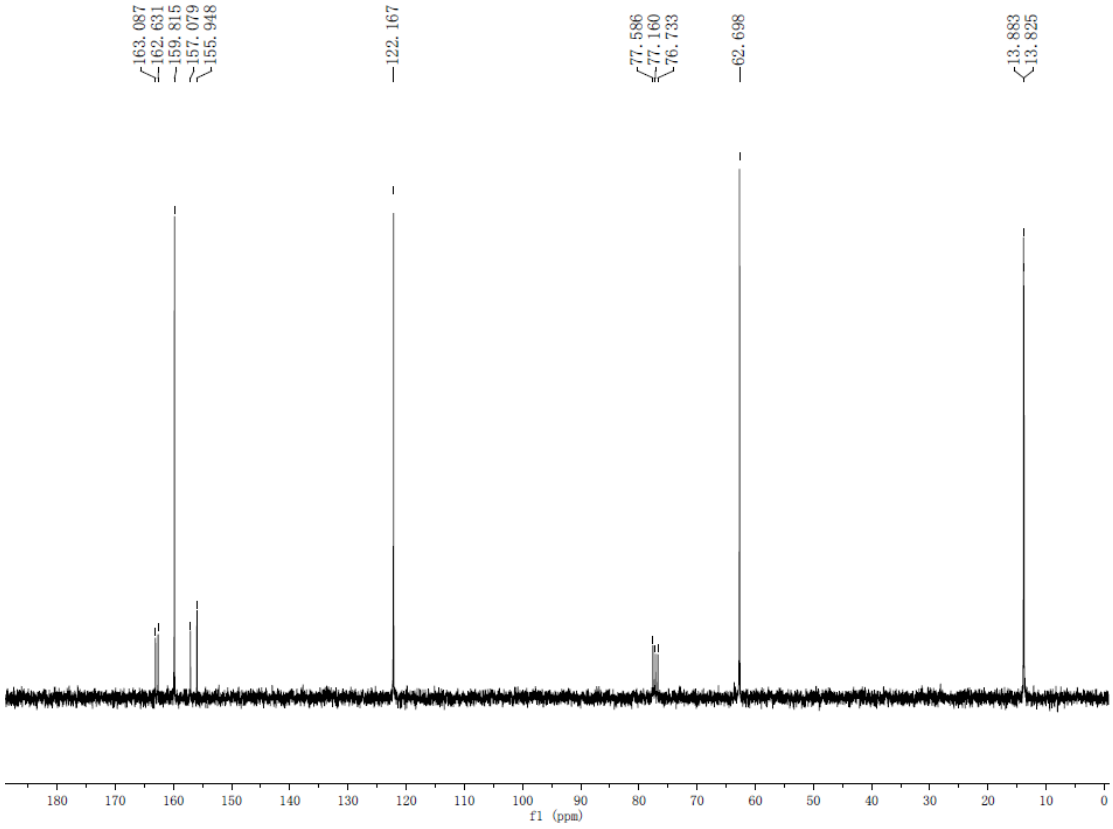
NMR Spectra of Compound **3l**



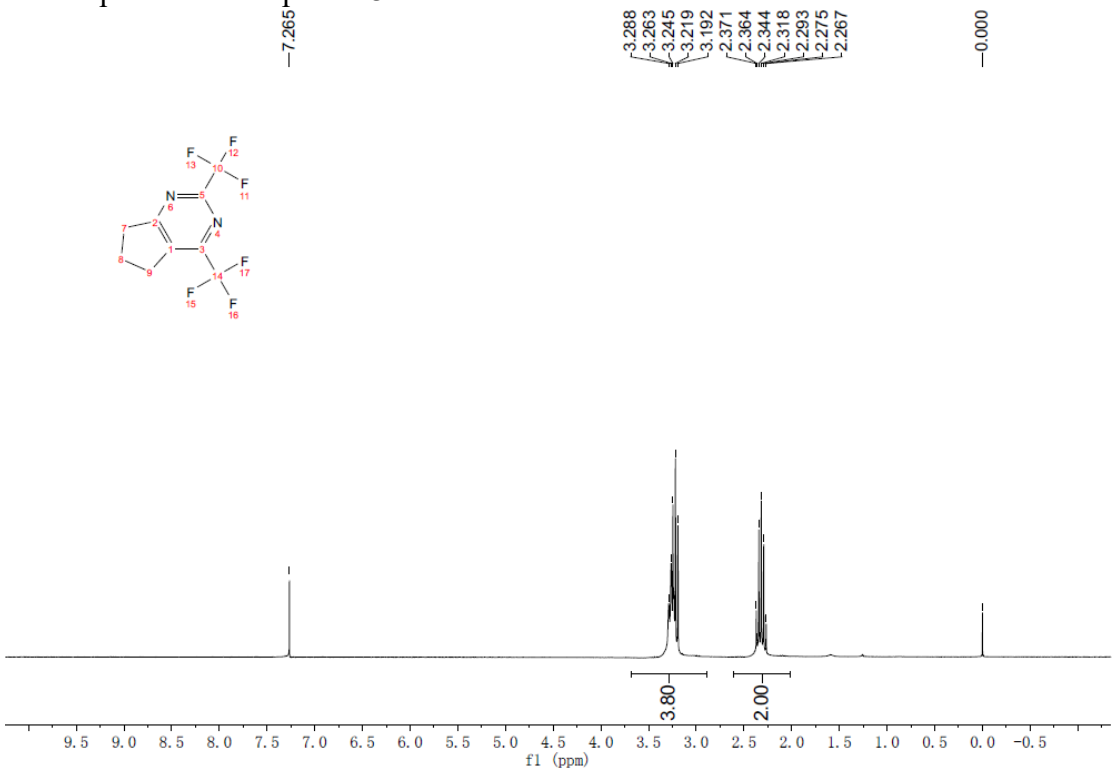


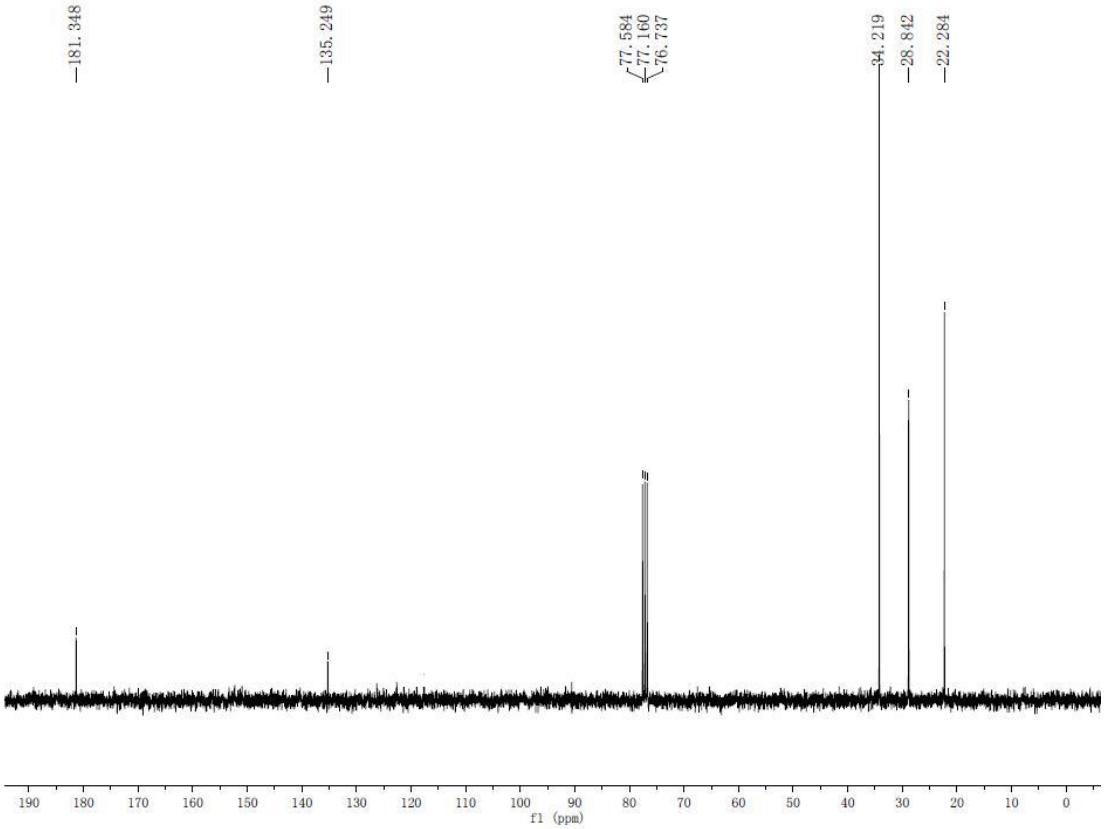
NMR Spectra of Compound **3m**



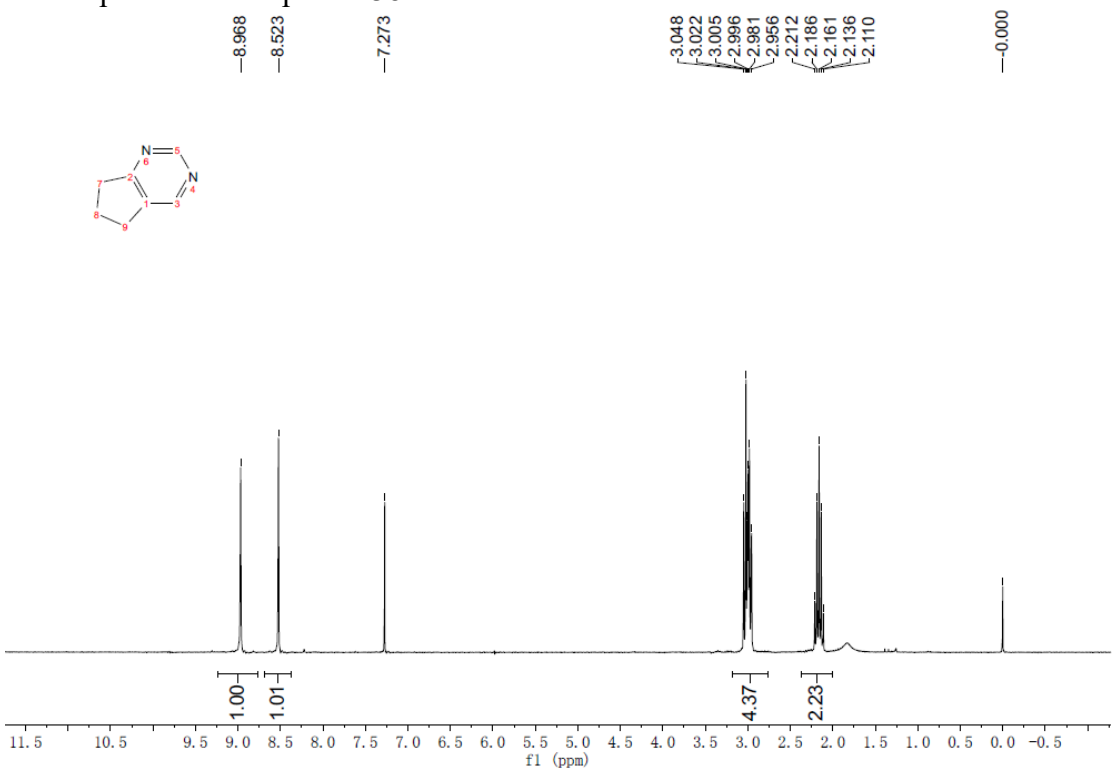


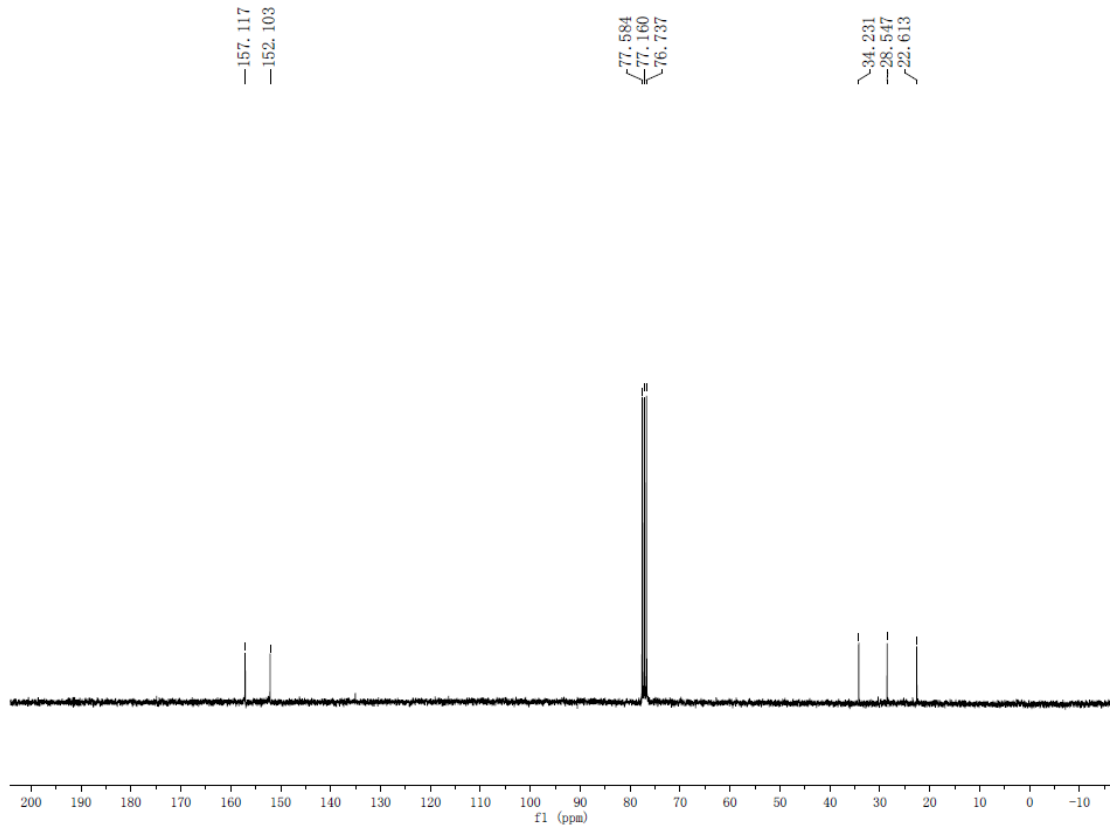
NMR Spectra of Compound **3n**



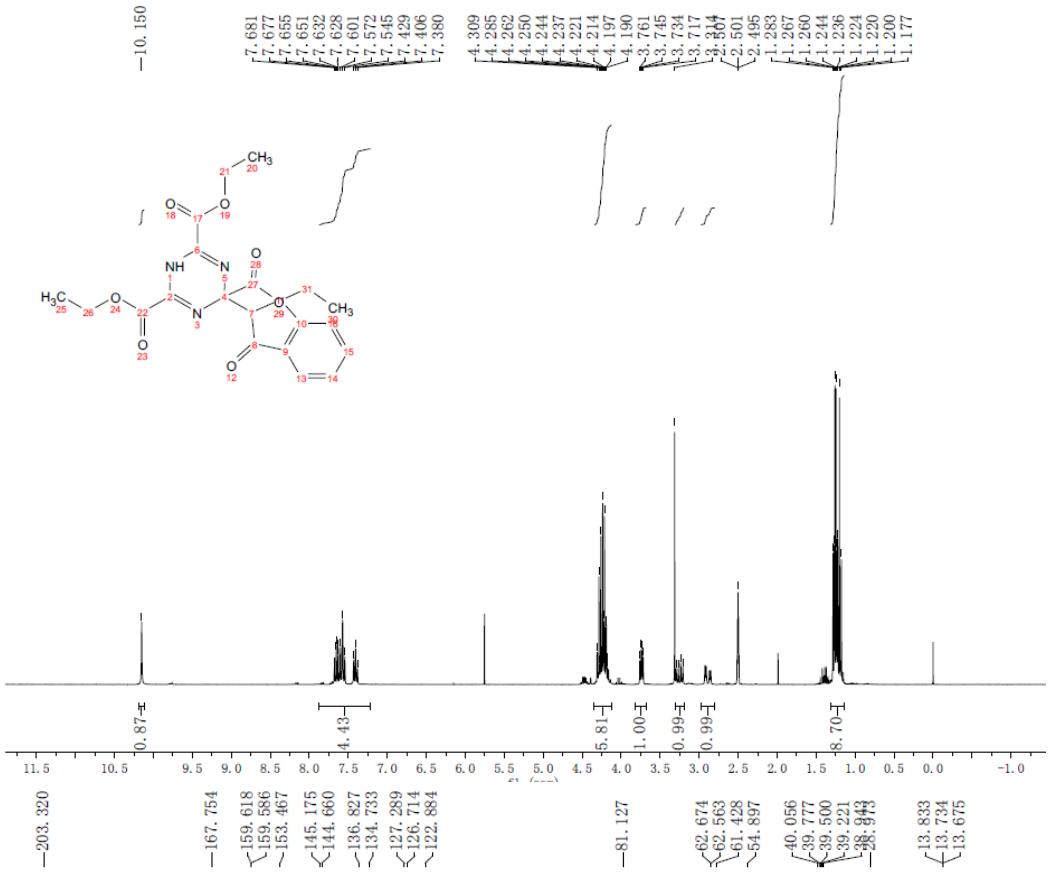


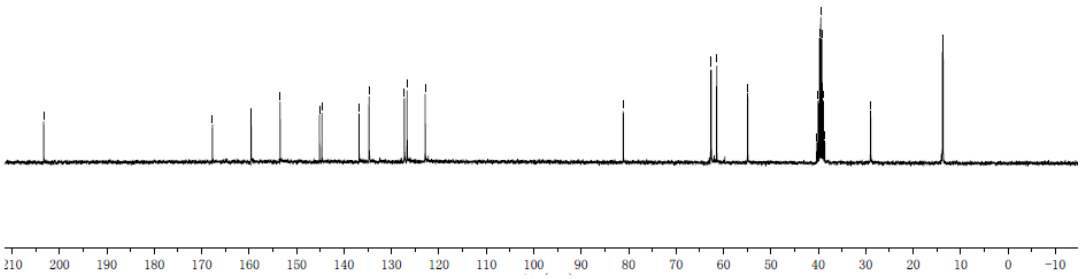
NMR Spectra of Compound **3o**





NMR Spectra of Compound **4a**





NMR Spectra of Compound **4b**