Electronic Supplementary Information

Allenoate-Derived 1,5-, 1,7-, and 1,9-Zwitterion as Highly Versatile Coupling Partners for Phosphine-Triggered Cycloaddition Reactions

Wei Meng,[a] Hai-Tao Zhao,[a] Jing Nie,[a] Yan Zheng,[a] Aiping Fu,[c] Jun-An Ma [a,b]*

[a]*Department of Chemistry, Tianjin University, Tianjin 30072, China*

[b]*Key Laboratory of Organofluorine Chemistry, CAS, Shanghai 200032, China*

[c]*Laboratory of New Fiber Materials and Modern Textile, Growing Base for State Key Laboratory, Qingdao University, Qingdao 266071, China*

Email: majun_an68@tju.edu.cn

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1. General information:

All reactions were performed under an Ar atmosphere in oven-dried glassware with magnetic stirring. Reactions were monitored through thin-layer chromatography (TLC). Chromatograms were visualized by fluorescence quenching under UV light at 254 nm. ^{1}H and ^{13}C NMR were recorded on Varian Mercury Plus 400 and 500 instruments at 400 / 500 MHz (^{1}H NMR) and 100 /125 MHz (^{13}C NMR). Chemical shifts were reported in ppm down field from internal Me_4Si. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), br (broad). Coupling constants were reported in Hertz (Hz). HRMS were recorded on an IonSpec FT-ICR mass spectrometer with MALDI resource. IR spectra were recorded on an AVATAR 360 FT-IR spectrometer. Crystal data were collected on a Bruker Nonius Kappa CCD with a Morotating anode generator, standard procedures were followed.

Materials:

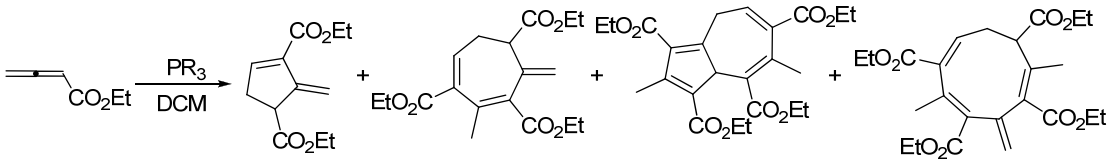
Unless otherwise stated, all solvents and reagents were purchased from commercial suppliers and used without further purification. Dichloromethane employed in the reactions was freshly distilled from CaH_2. Analytical thin layer chromatography was performed on 0.20 mm Qingdao Haiyang silica gel plates. Silica gel (200-300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography. Ethyl 2,3−butadienoate (**1**),[1] *N*,*N*′-cyclic azomethine imines[2] were prepared according to literature procedures. All reactions were performed under argon.

2. Experimental Details and Spectroscopic Data

General procedure for the self-cycloaddition reaction of ethyl allenoate

Into an oven-dried Schlenk was added ethyl 2,3-butadienoate (**1**), nucleophilic phosphine and dichloromethane (4 ml CH_2Cl_2) under an argon atmosphere. The mixture was stirred at –10 ^{o}C for 0.5 h. After recovering to room temperature, the reaction tube was sealed and the reaction mixture was stirred at 40 ^{o}C for stated time. Then, the reaction mixture was concentrated, and the residue purified through flash column chromatography (pre-treated with 0.1% NEt_3 in hexane, Hexane/EtOAc = 80/1 to 20/1 as eluent) to afford the corresponding product. The results are listed in Table-SI-1.

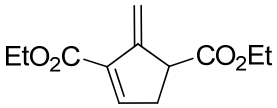
Table-SI-1. Phosphine-mediated self-cycloaddition of ethyl allenoate (1).



1 **2** **3** **4** **5**

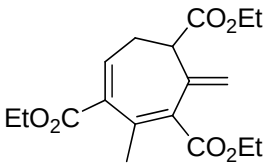
entry	**1** (equiv.)	PR_3 (mol%)	Temp (^oC)	Time (h)	yield (%)[a]			
					2	**3**	**4**	**5**
1	2.0	PPh_3 (10)	25	2	18	-	-	-
2	2.0	PPh_3 (100)	25	2	14	-	-	-
3	2.2	PPh_3 (100)	40	12	20	-	-	-
4	2.2	P(*n*-Bu)$_3$ (100)	40	12	15	-	-	-
5	2.2	$P(NMe_2)_3$ (100)	40	12	22	8	-	-
6	2.2	$P(NEt_2)_3$ (100)	40	48	36	10	5	-
7[b]	3.0	$P(NEt_2)_3$ (100)	40	240	-	73	8	-
8[b]	4.0	$P(NEt_2)_3$ (100)	40	240	-	52	5	30
9[b]	5.0	$P(NEt_2)_3$ (100)	40	240	-	44	10	28
10[b]	6.0	$P(NEt_2)_3$ (100)	40	240	-	48	12	25

[a] Isolated yield. [b] The reaction tube was sealed.



2

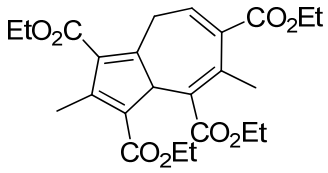
Diethyl 2-methylenecyclopent-3-ene-1,3-dicarboxylate (2):[3] colorless oil, **^{1}H NMR** ($CDC1_3$, 400 MHz) δ (ppm): 7.06 (t, *J* = 1.2 Hz, 1H), 5.87 (d, *J* = 2.4 Hz, 1H), 5.31 (s, 1H), 4.13-4.26 (m, 4H), 3.71-3.75 (m, 1H), 2.98 (dt, *J* = 3.2, 19.6 Hz, 1H), 2.72 (ddd, *J* = 2.4, 8.4, 19.6 Hz, 1H), 1.26-1.33 (m, 6H); **IR** (film) ν: 1718, 1624, 1259, 1225, 1042, 765 cm^{-1}.



3

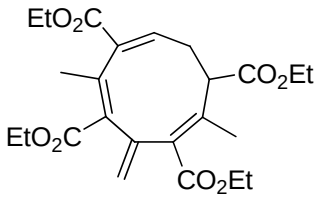
Triethyl 2-methyl-4-methylenecyclohepta-2,7-diene-1,3,5-tricarboxylate (3): colorless viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.23-1.31 (m, 9H), 2.13 (s, 3H), 2.33-2.37 (m, 1H), 2.62-2.65 (m, 1H), 3.75 (dd, *J* = 4.0, 9.6 Hz, 1H), 4.11-4.24 (m, 6H), 5.08 (s, 1H), 5.22 (s, 1H), 7.18 (t, *J* = 6.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.0, 14.1, 19.2, 27.6, 29.9, 60.6, 60.8, 60.9, 118.2, 132.4, 137.8,

140.4, 140.9, 142.3, 164.8, 166.9, 171.2; **IR** (film) ν: 2981, 1718, 1624, 1446, 1367, 1302, 1259, 1225, 1042, 916, 893, 765 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{18}H_{24}O_6Na^+$ $[M+Na]^+$. 359.1471, found 359.1465.



4

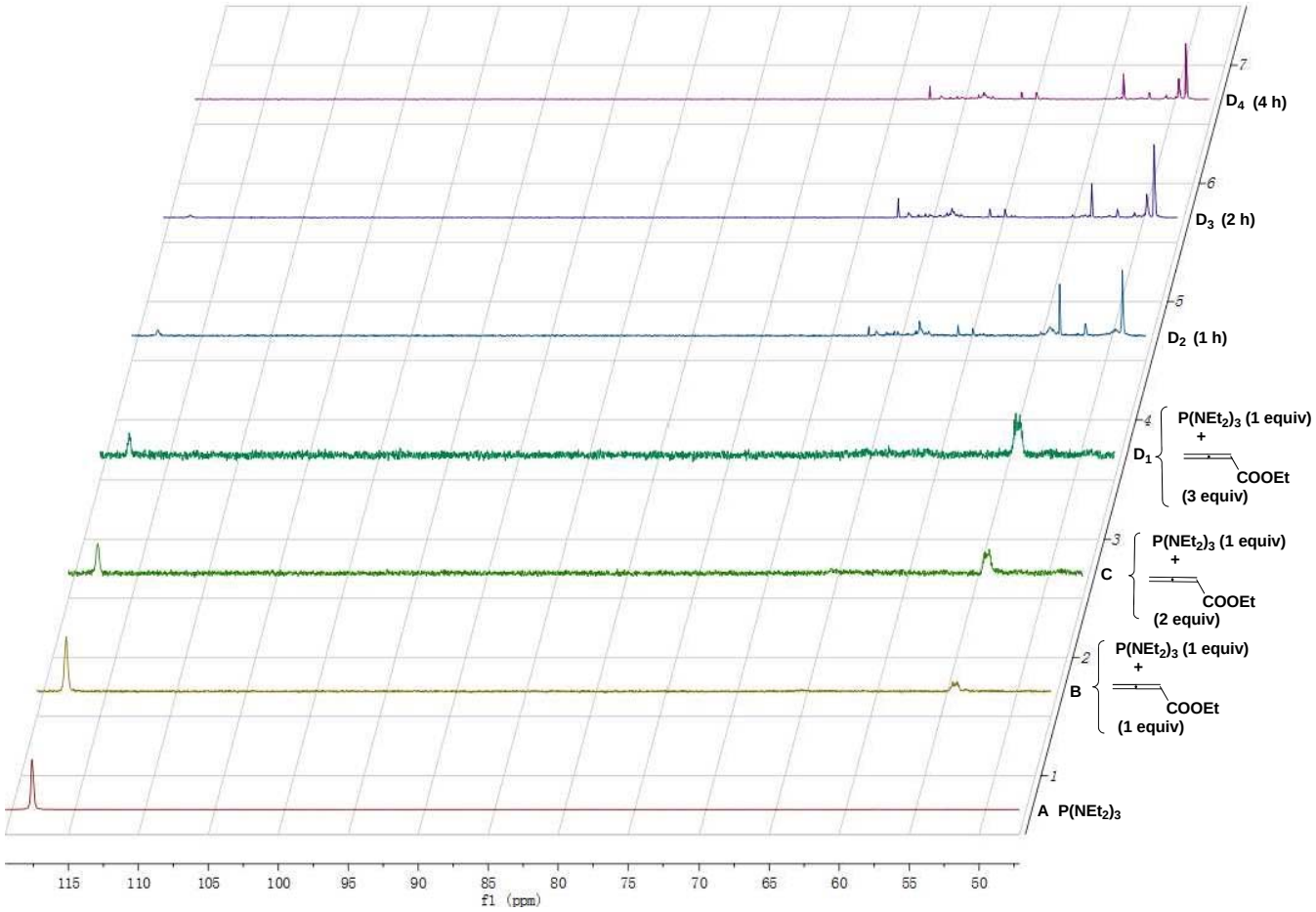
Tetraethyl 2,5-dimethyl-8,8a-dihydroazulene-1,3,4,6-tetracarboxylate (4): colorless viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.27-1.33 (m, 12H), 1.99 (d, *J* = 3.2 Hz, 1H), 2.05 (s, 1H), 2.08 (s, 3H), 2.18 (s, 3H), 3.34 (d, *J* = 7.6 Hz, 1H), 4.16-4.35 (m, 8H), 6.85 (t, *J* = 6.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.1, 14.2, 17.8, 20.7, 28.7, 60.7, 60.8, 61.1, 125.8, 132.5, 138.8, 139.2, 140.2, 165.6, 166.4, 168.2; **IR** (film) ν: 2981, 1718, 1624, 1446, 1367, 1302, 1259, 1225, 1195, 1042, 916, 893, 765 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{24}H_{30}O_8Na^+$ $[M+Na]^+$. 469.1838, found 469.1835.



5

(2*E*,5*E*,7*E*)-Tetraethyl 2,6-dimethyl-4-methylenecyclonona-2,5,7-triene-1,3,5,7- tetracarboxylate (5): colorless viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.24-1.35 (m, 12H), 1.56 (s, 3H), 2.14 (s, 3H), 2.32-2.37 (m, 1H), 2.61-2.68 (m, 1H), 3.76 (dd, *J* = 5.2, 11.6 Hz, 1H), 4.10-4.33 (m, 8H), 5.09 (s, 1H), 5.23 (s, 1H), 7.20 (t, *J* = 7.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.3, 14.4, 14.5, 19.5, 27.9, 29.9, 60.8, 61.1, 61.2, 118.5, 132.6, 138.0, 140.6, 141.2, 142.5, 165.4, 167.3, 171.7; **IR** (film) ν: 2981, 1718, 1624, 1446, 1367, 1302, 1259, 1225, 1042, 916, 893, 766 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{24}H_{33}O_8^+$ $[M+H]^+$. 449.2175, found 449.2174.

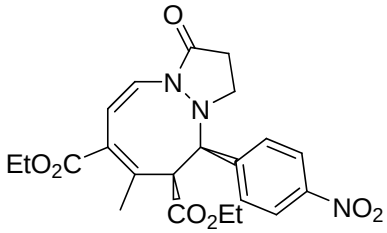
^{31}P NMR Control Experiments (CD_2Cl_2):



Bottom to top: A) $P(NEt_2)_3$; **B**) $P(NEt_2)_3$ + ethyl allenoate (1.0 equiv); **C**) $P(NEt_2)_3$ + ethyl allenoate (2.0 equiv); **D_1**) $P(NEt_2)_3$ + ethyl allenoate (3.0 equiv); **D_2**) $P(NEt_2)_3$ + ethyl allenoate (3.0 equiv): at 40 ^oC for 1 h; **D_3**) $P(NEt_2)_3$ + ethyl allenoate (3.0 equiv): at 40 ^oC for 2 h; **D_4**) $P(NEt_2)_3$ + ethyl allenoate (3.0 equiv): at 40 ^oC for 4 h.

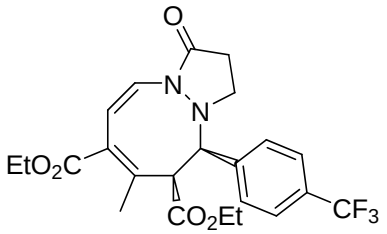
General Procedure for the Intermolecular Cycloaddition of Ethyl Allenoate with Electrophilic-coupling Reagents.

Into an oven-dried Schlenk was added ethyl 2,3-butadienoate (**1**) (247 mg, 2.2 mmol) and $P(NEt_2)_3$ (247 mg, 1.0 mmol) in dichloromethane (1.0 mL) under an argon atmosphere. After the mixture was stirred at –10 ^oC for 0.5 h, a solution of electrophilic-coupling reagent (1.0 mmol) in dichloromethane (2.0 mL) was transferred slowly into the Schlenk during 2 h. After recovering to room temperature, the reaction tube was sealed and the reaction mixture was stirred at 40 ^oC for the stated time. The reaction mixture was concentrated and the residue purified through flash column chromatography (pre-treated with 1% NEt_3 in hexane, Hexane/EtOAc = 20/1 to 4/1 as eluent) to afford the corresponding cycloadduct.



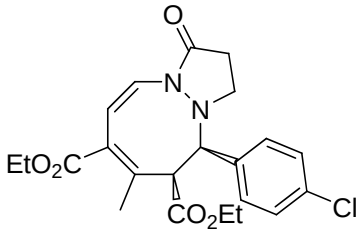
7a

(7E,9Z)-Diethyl 7-methyl-5-(4-nitrophenyl)-1-oxo-2,3,5,6-tetrahydro-1H-pyra- zolo[1,2-a][1,2]diazocine-6,8-dicarboxylate (7a): 80%; yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.21 (t, *J* = 5.6 Hz, 3H), 1.37 (t, *J* = 6.0 Hz, 3H), 1.39 (s, 3H), 2.29-2.35 (m, 1H), 2.83-2.94 (m, 2H), 3.37-3.44 (m, 1H), 4.09-4.19 (m, 3H), 4.27-4.31 (m, 2H), 4.52 (d, *J* = 2.8 Hz, 1H), 5.49 (dd, *J* = 0.8, 8.4 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 7.61-7.63 (m, 1H), 7.88-7.90 (m, 1H), 8.16-8.18 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.4, 14.5, 21.4, 28.2, 48.9, 53.9, 60.3, 61.3, 61.6, 105.1, 122.5, 123.1, 123.6, 130.2, 131.2, 132.3, 137.6, 145.0, 148.1, 167.6, 170.2, 172.5; **IR** (film) ν: 2981, 2351, 2340, 1710, 1649, 1603, 1526, 1413, 1336, 1290, 1208, 1096, 1065, 1034, 855, 722, 666 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{22}H_{25}N_3O_7^+$ $[M+Na]^+$. 466.1590, found 466.1585.



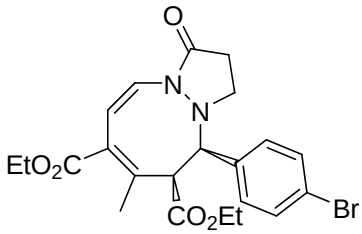
7b

(7E,9Z)-Diethyl 7-methyl-1-oxo-5-(4-(trifluoromethyl)phenyl)-2,3,5,6-tetrahydro- 1H-pyrazolo[1,2-a][1,2]diazocine-6,8-dicarboxylate (7b): 62%; yellow viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.22 (t, *J* = 7.2 Hz, 3H), 1.37 (t, *J* = 6.8 Hz, 3H), 1.42 (s, 3H), 2.27-2.33 (m, 1H), 2.82-3.00 (m, 2H), 3.35-3.44 (m, 1H), 4.12-4.20 (m, 3H), 4.27-4.33 (m, 2H), 4.49 (d, *J* = 3.2 Hz, 1H), 5.49 (d, *J* = 10.4 Hz, 1H), 6.91 (d, *J* = 10.4 Hz, 1H), 7.55-7.59 (m, 2H), 7.63-7.68 (m, 1H), 7.80 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.1, 14.3, 21.2, 22.7, 29.7, 31.9, 48.6, 53.7, 60.3, 61.0, 61.2, 104.8, 122.3, 124.7, 125.2, 129.3, 130.7, 131.4, 138.2, 141.4, 167.4, 170.0, 172.5; **IR** (film) ν: 2919, 2853, 1721, 1649, 1454, 1418, 1321, 1290, 1203, 1116, 1059 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{23}H_{25}F_3N_2O_5^+$ $[M+Na]^+$. 489.1613, found 489.1608.



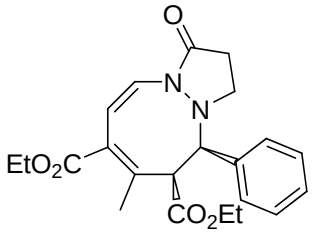
7c

(7E,9Z)-Diethyl 5-(4-chlorophenyl)-7-methyl-1-oxo-2,3,5,6-tetrahydro-1H-pyra- zolo[1,2-a][1,2]diazocine-6,8-dicarboxylate (7c): 50%; yellow viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.21 (t, *J* = 7.2 Hz, 3H), 1.36 (t, *J* = 6.8 Hz, 3H), 1.45 (s, 3H), 2.25-2.31 (m, 1H), 2.80-2.90 (m, 1H), 2.99-3.04 (m, 1H), 3.32-3.41 (m, 1H), 4.08 (d, *J* = 3.6 Hz, 1H), 4.10-4.18 (m, 2H), 4.25-4.30 (m, 2H), 4.40 (d, *J* = 3.6 Hz, 1H), 5.46 (dd, *J* = 0.8, 10.4 Hz, 1H), 6.89 (d, *J* = 10.4 Hz, 1H), 7.27 (s, 1H), 7.29 (s, 1H), 7.33-7.36 (m, 1H), 7.57-7.59 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.1, 14.2, 21.3, 28.1, 29.7, 48.4, 53.6 (d, *J* = 4.7 Hz), 60.0 (d, *J* = 3.7 Hz), 60.9, 61.1, 104.8, 122.2 (d, *J* = 10.4 Hz), 127.9, 128.6, 130.2, 130.5, 132.2, 134.2, 135.8, 138.6, 167.5, 170.1, 172.6; **IR** (film) ν: 2924, 2847, 1721, 1644, 1418, 1336, 1280, 1214, 1091, 1075, 1024, 1019 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{22}H_{26}ClN_2O_5^+$ $[M+H]^+$. 433.1530, found 433.1525.



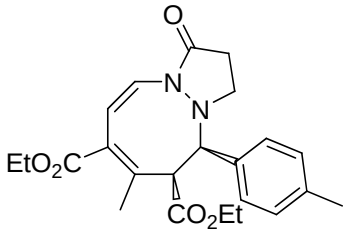
7d

(7E,9Z)-Diethyl 5-(4-bromophenyl)-7-methyl-1-oxo-2,3,5,6-tetrahydro-1H-pyra- zolo[1,2-a][1,2]diazocine-6,8-dicarboxylate (7d): 53%; yellow viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.21 (t, *J* = 7.2 Hz, 3H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.46 (s, 3H), 2.25-2.31 (m, 1H), 2.75-2.90 (m, 1H), 2.99-3.04 (m, 1H), 3.32-3.41 (m, 1H), 4.08 (d, *J* = 3.6 Hz, 1H), 4.10-4.18 (m, 2H), 4.25-4.31 (m, 2H), 4.39 (d, *J* = 3.2 Hz, 1H), 5.46 (d, *J* = 10.4 Hz, 1H), 6.89 (d, *J* = 10.4 Hz, 1H), 7.28-7.30 (m, 1H), 7.43-7.45 (m, 2H), 7.51-7.53 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.1, 14.3, 21.3, 28.1, 48.4, 53.6 , 60.1, 60.9, 61.1, 104.8, 122.2, 122.4, 130.5, 130.6, 130.9, 131.6, 132.6, 136.3, 138.5, 167.5, 170.0, 172.5; **IR** (film) ν: 2975, 2924, 2842, 1716, 1644, 1495, 1413, 1331, 1290, 1214, 1070, 1034, 1014, 814, 747 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{22}H_{26}BrN_2O_5^+$ $[M+H]^+$. 477.1025, found 477.1020.



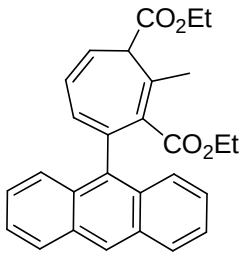
7e

(7E,9Z)-Diethyl 7-methyl-1-oxo-5-phenyl-2,3,5,6-tetrahydro-1H-pyrazolo[1,2-a]- [1,2]diazocine-6,8-dicarboxylate (7e): 30%; light yellow viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.22 (t, *J* = 7.2 Hz, 3H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.46 (s, 3H), 2.24-2.30 (m, 1H), 2.80-2.92 (m, 1H), 3.04-3.09 (m, 1H), 3.33-3.41 (m, 1H), 4.11-4.18 (m, 3H), 4.24-4.34 (m, 2H), 4.45 (d, *J* = 3.6 Hz , 1H), 5.47 (dd, *J* = 0.8, 10.4 Hz, 1H), 6.90 (d, *J* = 10.4 Hz, 1H), 7.29-7.33 (m, 3H), 7.38-7.39 (m, 1H), 7.59-7.61 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.1, 14.3, 21.4, 29.7, 30.0, 48.4, 53.4, 60.8, 61.0, 104.8, 122.2, 127.7, 128.3, 128.4, 128.8, 130.2, 130.8, 137.2, 139.4, 167.6, 170.1 , 172.7; **IR** (film) ν: 2940, 2858, 1721, 1669, 1613, 1598, 1459, 1418, 1116, 671, 609, 548 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{22}H_{26}N_2O_5Na^+$ $[M+Na]^+$. 421.1739, found 421.1734.



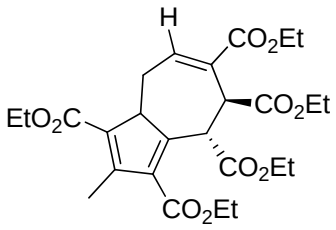
7f

(7E,9Z)-Diethyl 7-methyl-1-oxo-5-p-tolyl-2,3,5,6-tetrahydro-1H-pyrazolo[1,2-a] -[1,2]diazocine-6,8-dicarboxylate (7f): 26%; light yellow viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.22 (t, *J* = 7.2 Hz, 3H), 1.36 (t, *J* = 6.8 Hz, 3H), 1.49 (s, 3H), 2.22-2.28 (m, 1H), 2.33 (s, 3H), 2.74-2.91 (m, 1H), 3.05-3.10 (m, 1H), 3.31-3.40 (m, 1H), 4.09-4.19 (m, 3H), 4.25-4.33 (m, 2H), 4.40 (d, *J* = 3.6 Hz, 1H), 5.46 (dd, *J* = 0.8, 10.4 Hz, 1H), 6.89 (d, *J* = 10.4 Hz, 1H), 7.10 (d, *J* = 8 Hz, 2H), 7.24-7.27 (m, 1H), 7.45-7.47 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm):14.2, 14.3, 21.5, 29.7, 48.3, 53.8, 60.6, 60.8, 60.9, 104.8, 122.2, 128.3, 128.6, 129.1, 130.0, 130.7, 134.2, 138.0, 139.7, 167.6, 170.1, 172.8; **IR** (film) ν: 2919, 2858, 1721, 1644, 1424, 1331, 1290, 1219, 1060, 824, 742 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{23}H_{28}N_2O_5^+$ $[M+Na]^+$. 435.1896, found 435.1890.



9

Diethyl 4-(anthracen-9-yl)-2-methylcyclohepta-4,6-diene-1,3-dicarboxylate (9): 77%; colorless solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 0.18 (t, *J* = 7.2 Hz, 3H), 1.44 (t, *J* = 7.2 Hz, 3H), 2.07 (s, 3H), 3.25-3.45 (m, 2H), 2.18 (s, 3H), 4.36-4.48 (m, 2H), 6.02-6.06 (m, 1H), 6.55 (dd, *J* = 5.6, 8.8 Hz, 1H), 6.84 (d, *J* = 5.6 Hz, 1H), 7.43-7.49 (m, 4H), 7.86 (d, *J* = 8 Hz, 1H), 7.98-8.0 (m, 2H), 8.35-8.38 (m, 1H), 8.44 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 12.8, 14.4, 17.9, 49.6, 60.4, 61.4, 121.1, 125.0, 125.4, 125.7, 125.9, 126.0, 127.3, 127.5, 128.2, 128.4, 129.9, 130.3, 131.0, 131.6, 132.2, 135.2, 135.5, 137.3, 167.9, 171.6; **IR** (film) ν: 3051, 2982, 2034, 1731, 1600, 1445, 1369, 1316, 1261, 1224, 1170, 1055, 1026, 736 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{28}H_{27}O_4^+$ $[M+H]^+$. 427.1909, found 427.1904.



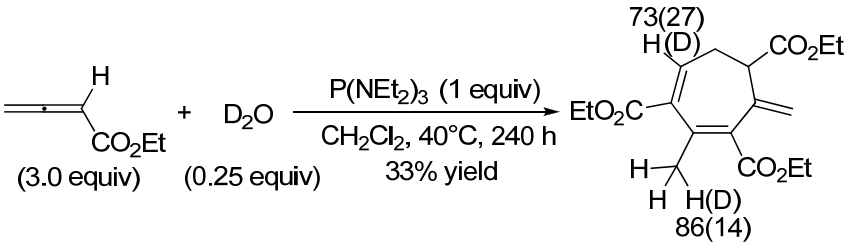
11

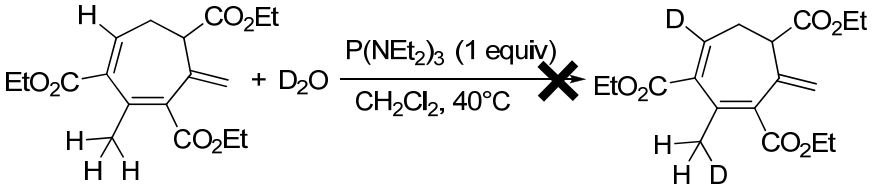
(4S,5S)-Pentaethyl 2-methyl-4,5,8,8a-tetrahydroazulene-1,3,4,5,6-pentacarboxyl- ate (11): 63%; colorless viscous liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 1.18 (t, *J* = 7.2 Hz, 3H), 1.25-1.26 (m, 3H), 1.29-1.37 (m, 9H), 2.18 (s, 3H), 2.35 (t, *J* = 6.8 Hz, 2H), 3.84 (dd, *J* = 6.8, 13.2 Hz, 1H), 3.96-4.03 (m, 2H), 4.04-4.13 (m, 2H), 4.15-4.27 (m, 8H), 7.22 (t, *J* = 7.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 14.2, 14.4, 19.7, 27.9, 29.9, 46.9, 55.0, 61.0, 61.1, 61.2, 61.3, 61.5, 129.8, 137.9, 142.7, 145.0, 164.6, 167.1, 171.9, 173.4; **IR** (film) ν: 2981, 1718, 1624, 1446, 1367, 1302, 1259, 1225, 1195 cm^{-1}; **IR** (film) ν: 2981, 1718, 1624, 1446, 1367, 1302, 1259, 1225, 1195 cm^{-1}; **HRMS (MALDI)**: calcd for $C_{26}H_{34}O_{10}Na^+$ $[M+Na]^+$. 529.2050, found 529.2044.

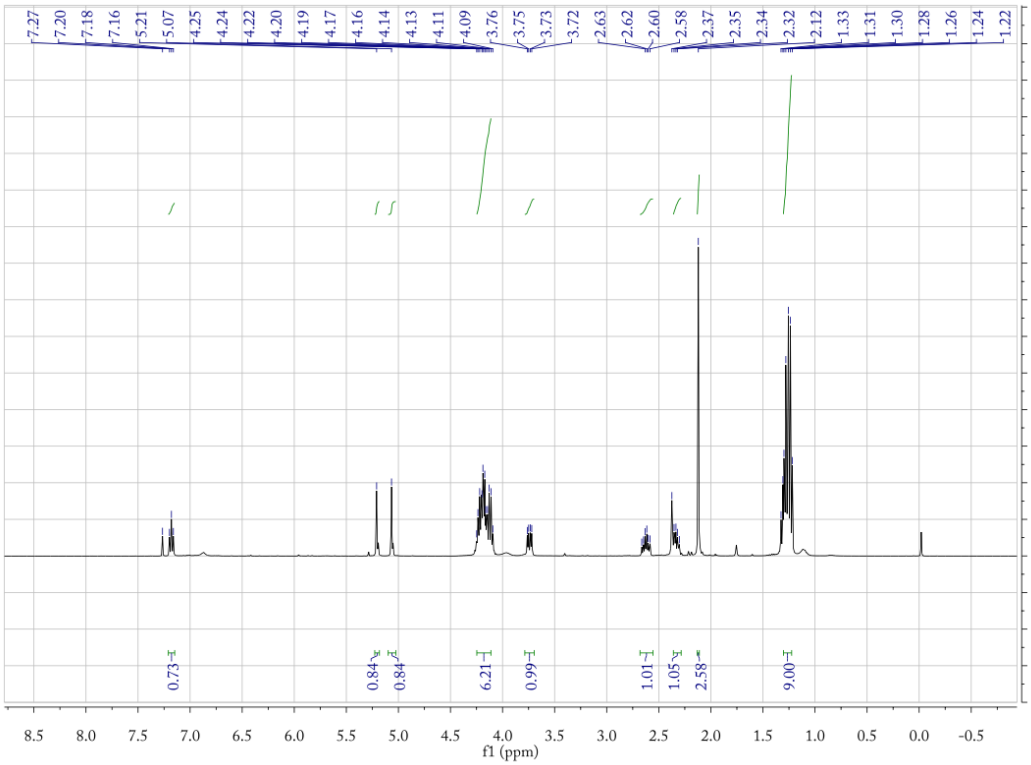
General procedure for the isotopic labeling experiments of the self-cycloaddition reaction of ethyl allenoate.

Into an oven-dried Schlenk was added ethyl 2,3-butadienoate **1** (336 mg, 3.0 equiv), $P(NEt_2)_3$ (247 mg, 1.0 equiv), D_2O (5 mg, 0.25 equiv), and dichloromethane (4 ml CH_2Cl_2) under an argon atmosphere. The mixture was stirred at –10 ^oC for 0.5 h. After recovering to room temperature, the reaction tube was sealed and the reaction mixture was stirred at 40 ^oC for 240 h. Then, the reaction mixture was concentrated, and the residue purified through flash column chromatography (pre-treated with 0.1% NEt_3 in hexane, Hexane/EtOAc = 80/1 to 20/1 as eluent) to afford the corresponding product (111 mg, 33%). The ratio of D over H in the product was measured based on the integrations of olefinic protons and methylic protons on the seven-member-ring versus the methylic protons in ethoxyl groups.

A control experiment was performed with D-labeled cycloadduct **3** in D_2O (1.0 equiv). The analysis of ^{1}H NMR spectra indicated no deuterium and hydrogen exchange occurred.





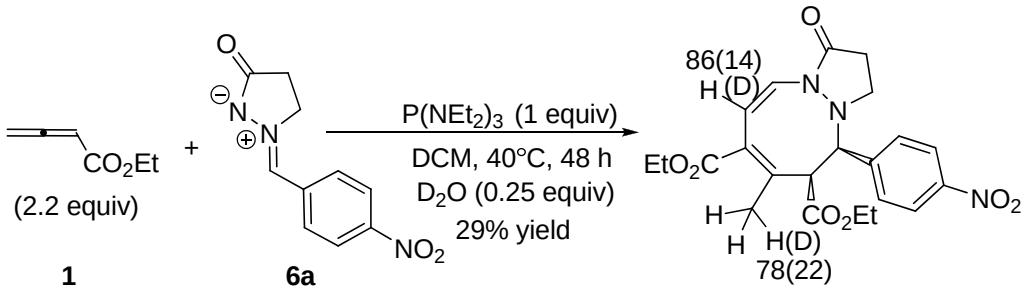


General procedure for the isotopic labeling experiments of the Intermolecular Cycloaddition of Ethyl Allenoate with Azomethine Imines 6.

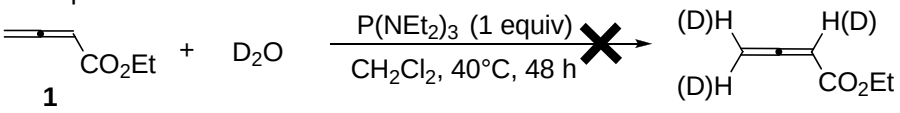
Into an oven-dried Schlenk was added ethyl 2,3-butadienoate **1** (247 mg, 2.2 mmol), D_2O (5 mg, 0.25 equiv), and $P(NEt_2)_3$ (247 mg, 1.0 mmol) in dichloromethane (1.0 mL) under an argon atmosphere. After the mixture was stirred at –10 ^oC for 0.5 h, a solution of Azomethine Imines **6** (219 mg, 1.0 mmol) in dichloromethane (6.0 mL) was transferred slowly into the Schlenk during 2 h. After recovering to room temperature, the reaction tube was sealed and the reaction mixture was stirred at 40 ^oC for 48 h. The reaction mixture was concentrated and the residue purified through flash column chromatography (pre-treated with 1% NEt_3 in hexane, Hexane/EtOAc = 20/1 to 4/1 as eluent) to afford the corresponding cycloadduct **7a** (128 mg, 29%). The ratio of D or H in the product was measured based on the integrations

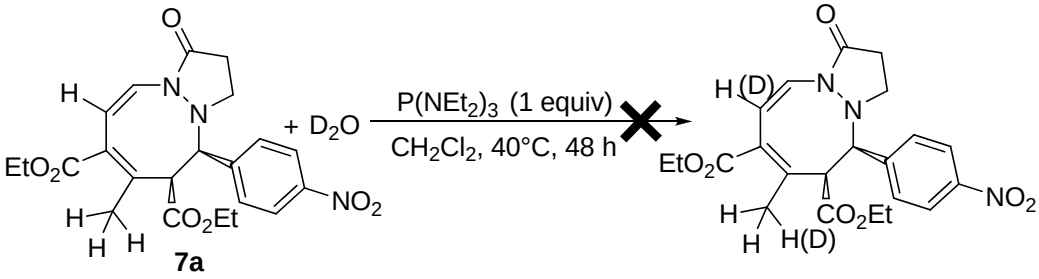
of olefinic protons and methylic protons on the eight-member-ring versus the methylic protons in ethoxyl groups.

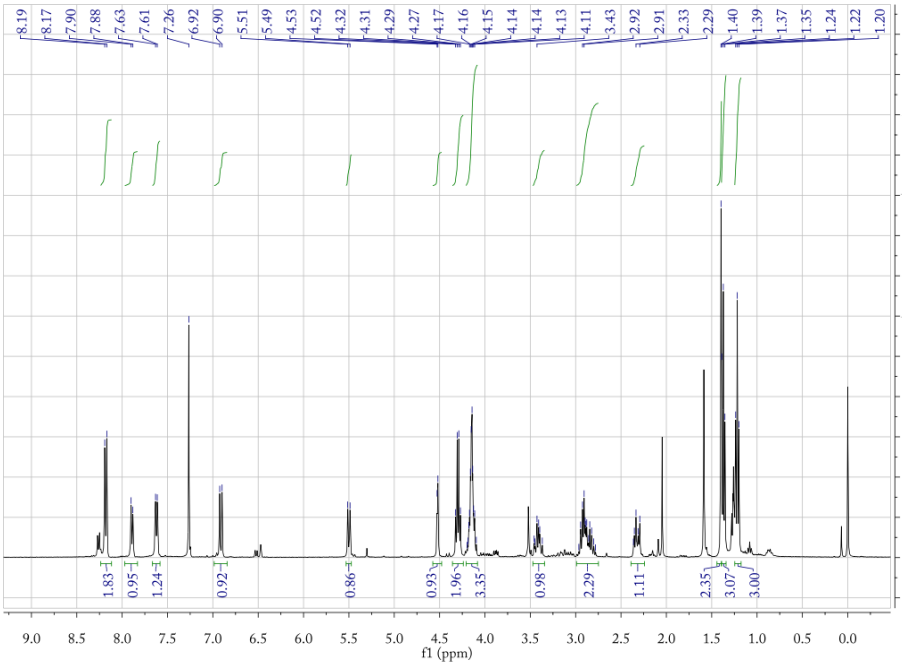
Two control experiments were performed with ethyl allenoate and cycloadduct **7a** in D_2O (1.0 equiv). The analysis of ^1H NMR spectra indicated no deuterium and hydrogen exchange occurred.



Control experiments:



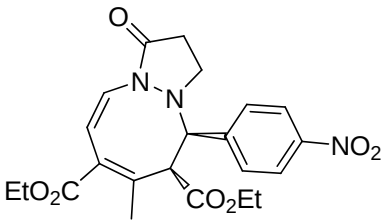




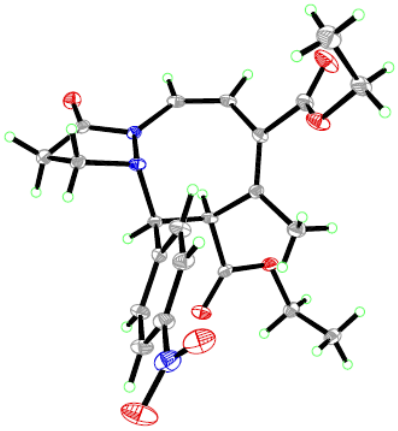
3. Crystallographic Data for 7a and 9

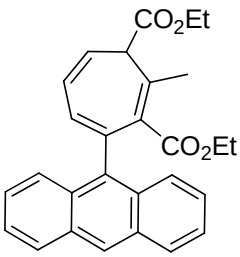
Crystallographic data for **7a** and **9** have been deposited with the Cambridge Crystallographic Data Centre as supplementary numbers CCDC 839605 and 839553, respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk/ data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

ORTEP Representations of 7a and 9



7a





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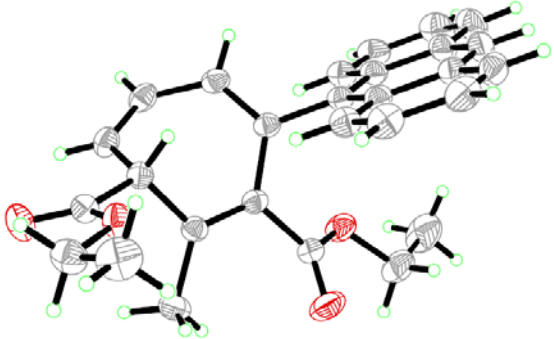


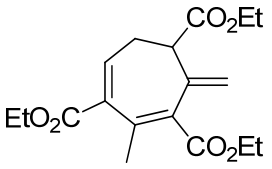
References:

[1] R. W. Lang, H. Hansen, *Org. Synth.* **1990**, *7*, 232.

[2] a) R. Shintani, G. C. Fu, *J. Am. Chem. Soc.* **2003**, *125*, 10778; b) A. Suárez, C. W. Downey, G. C. Fu, *J. Am. Chem. Soc.* **2005**, *127*, 11244; c) R. Shintani, T. Hayashi, *J. Am. Chem. Soc.* **2006**, *128*, 6330.

[3] C. Zhang, X. Lu, *J. Org. Chem.* **1995**, *60*, 2906.

4. Copies of ^{1}H, ^{13}C NMR Spectra



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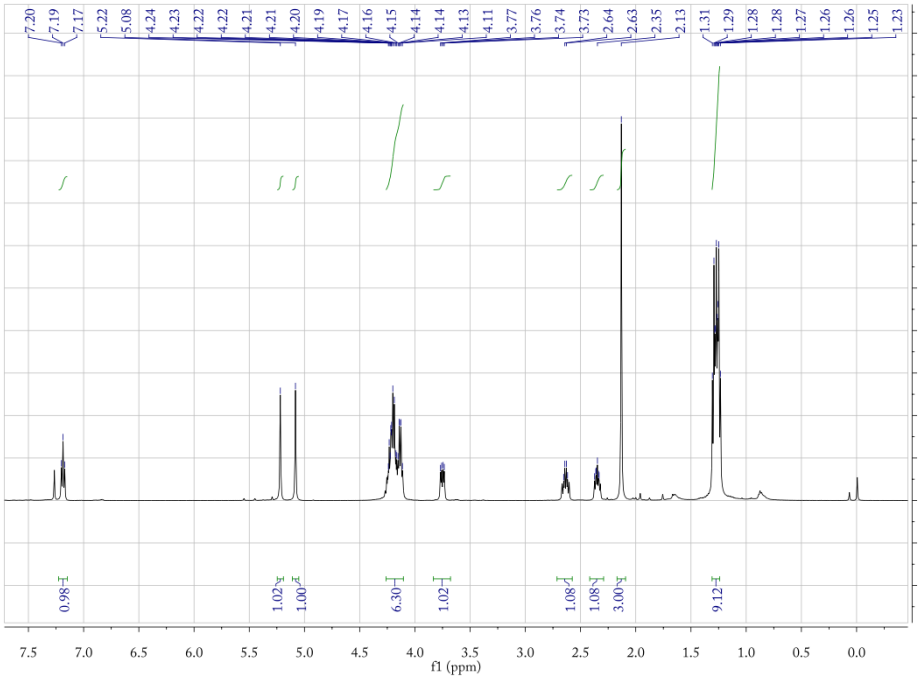
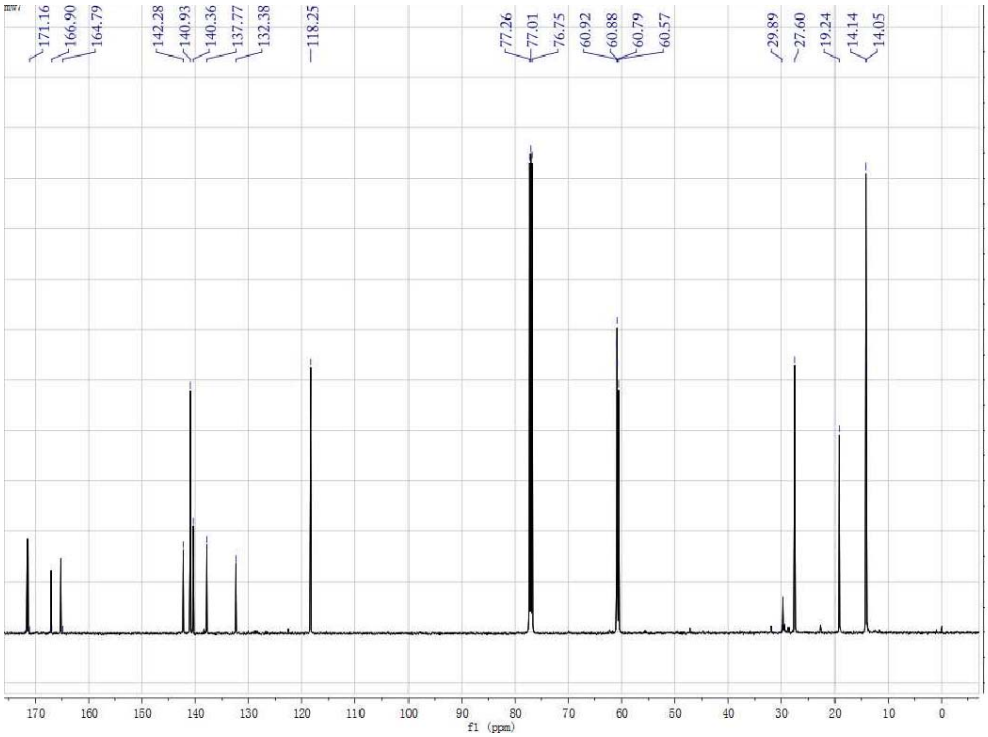
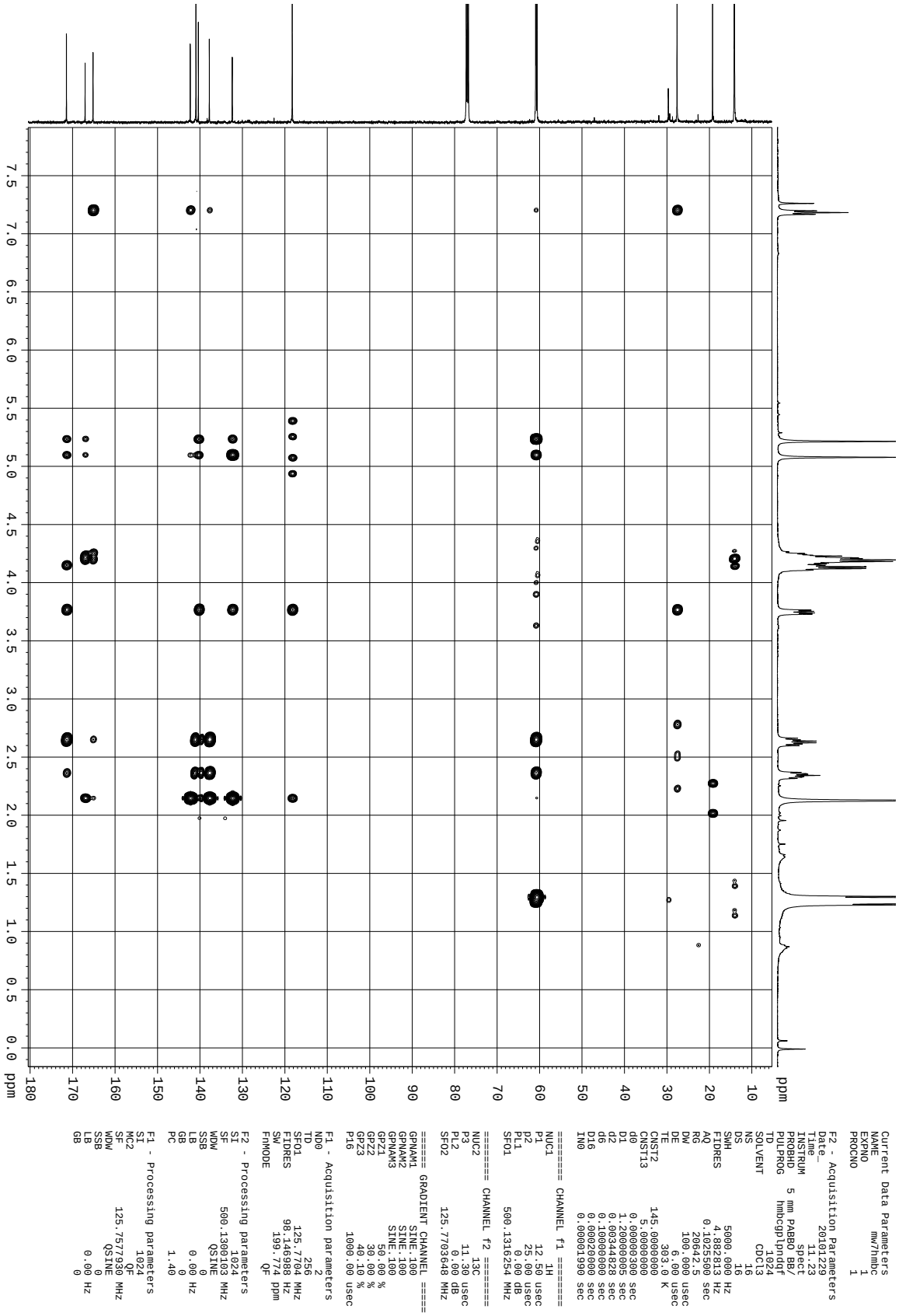




2D NMR HMBC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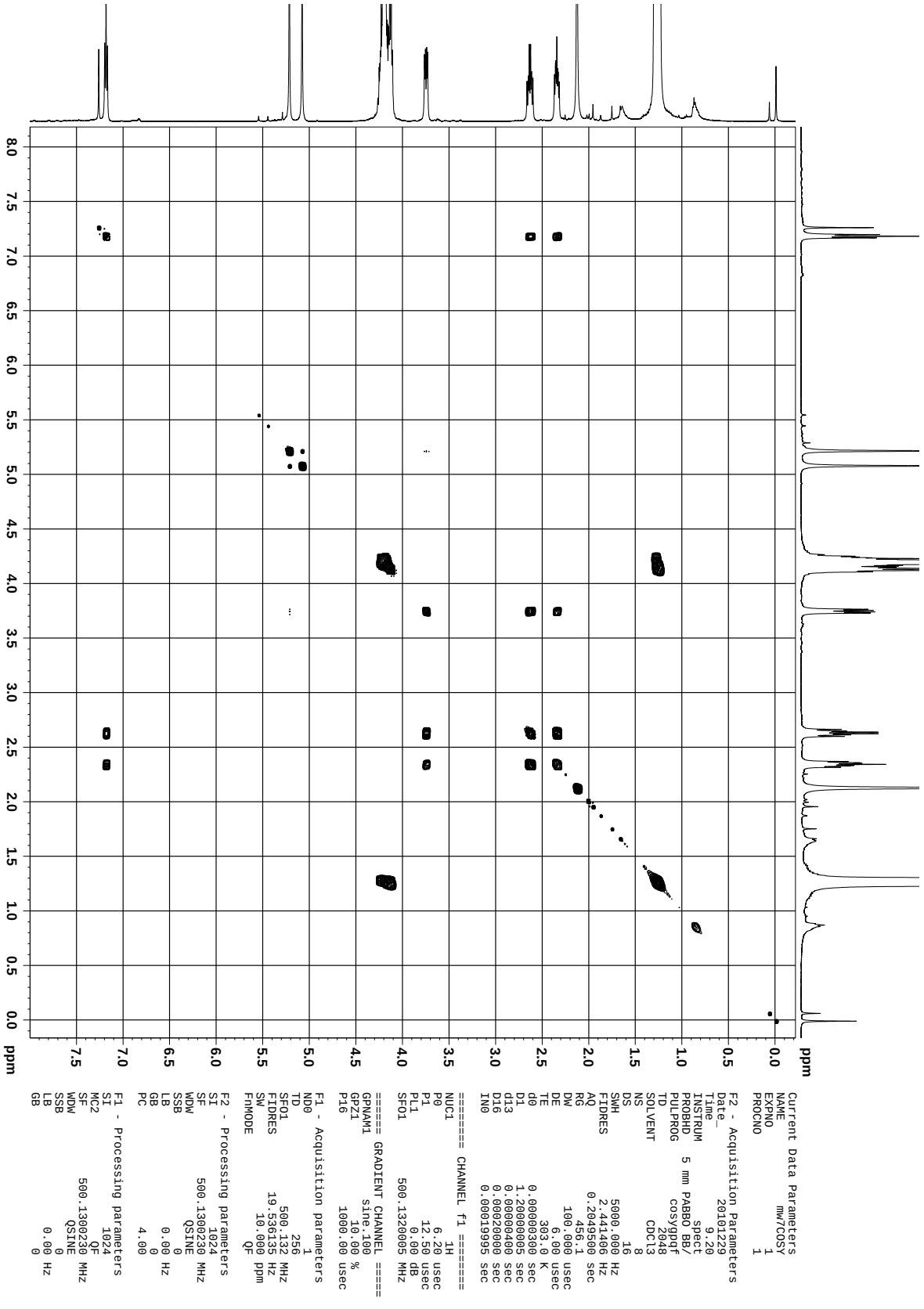
2D NMR COSY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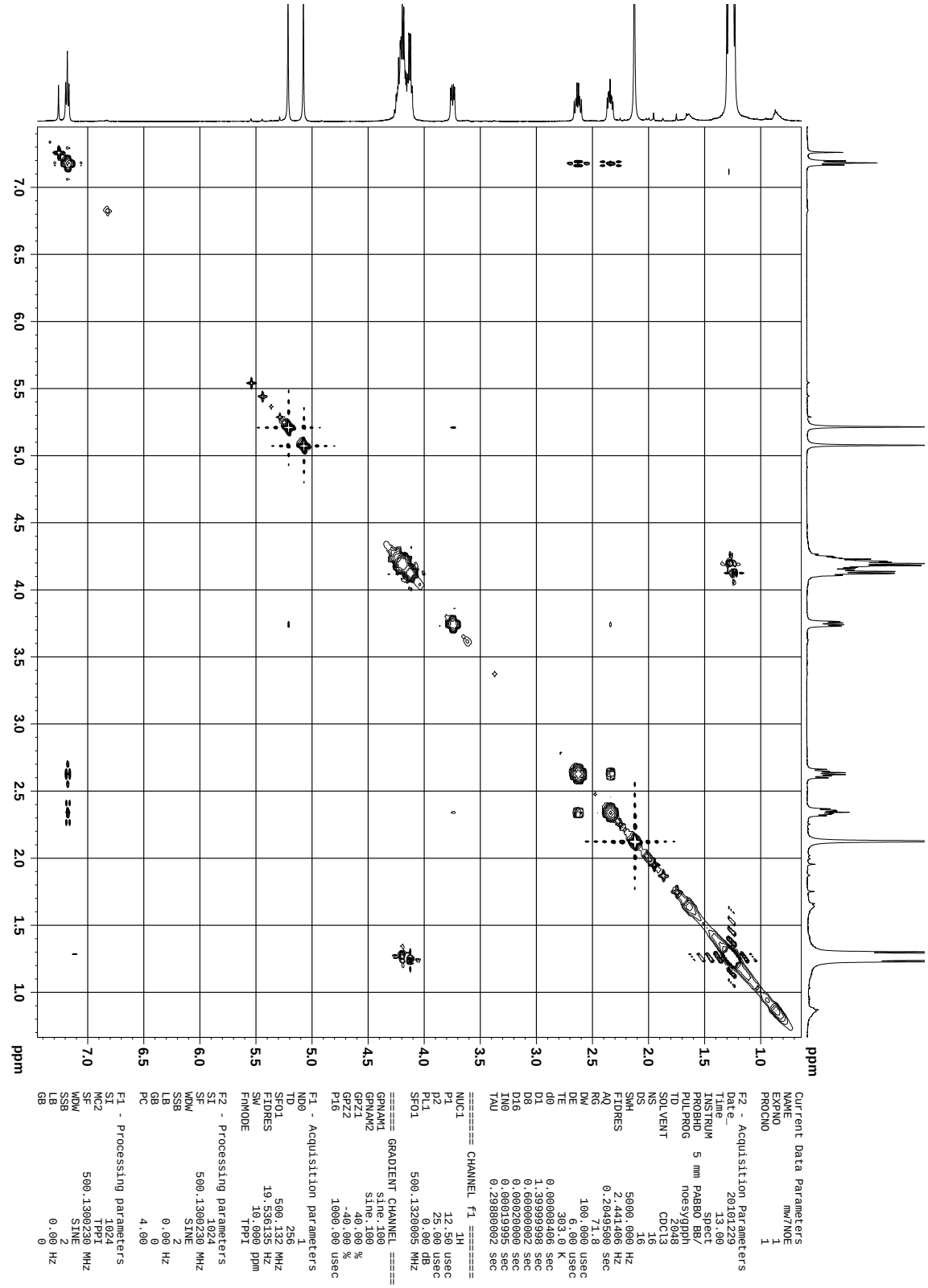
2D NMR NOESY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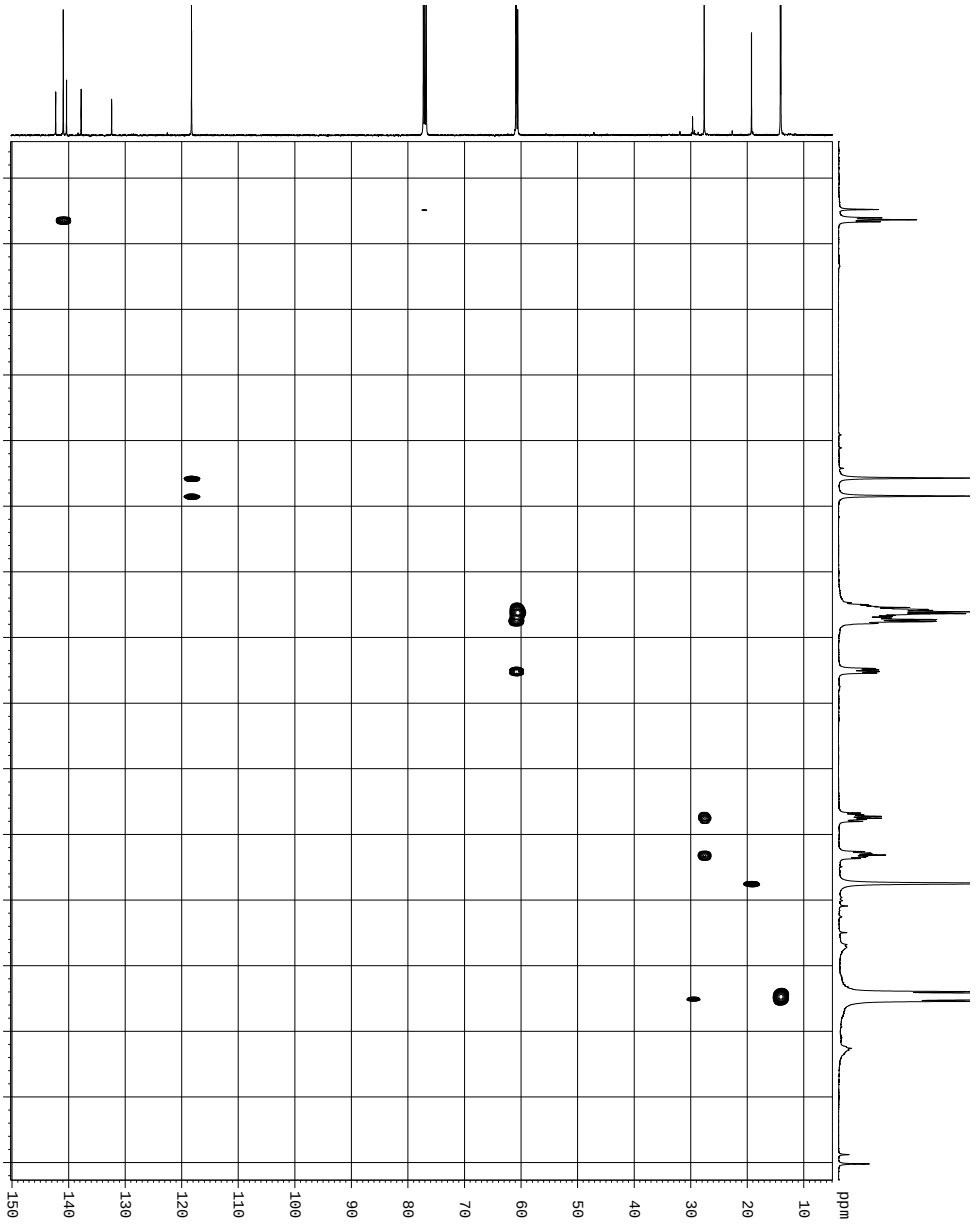
2D NMR HMQC

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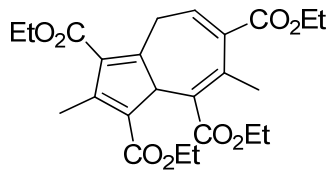
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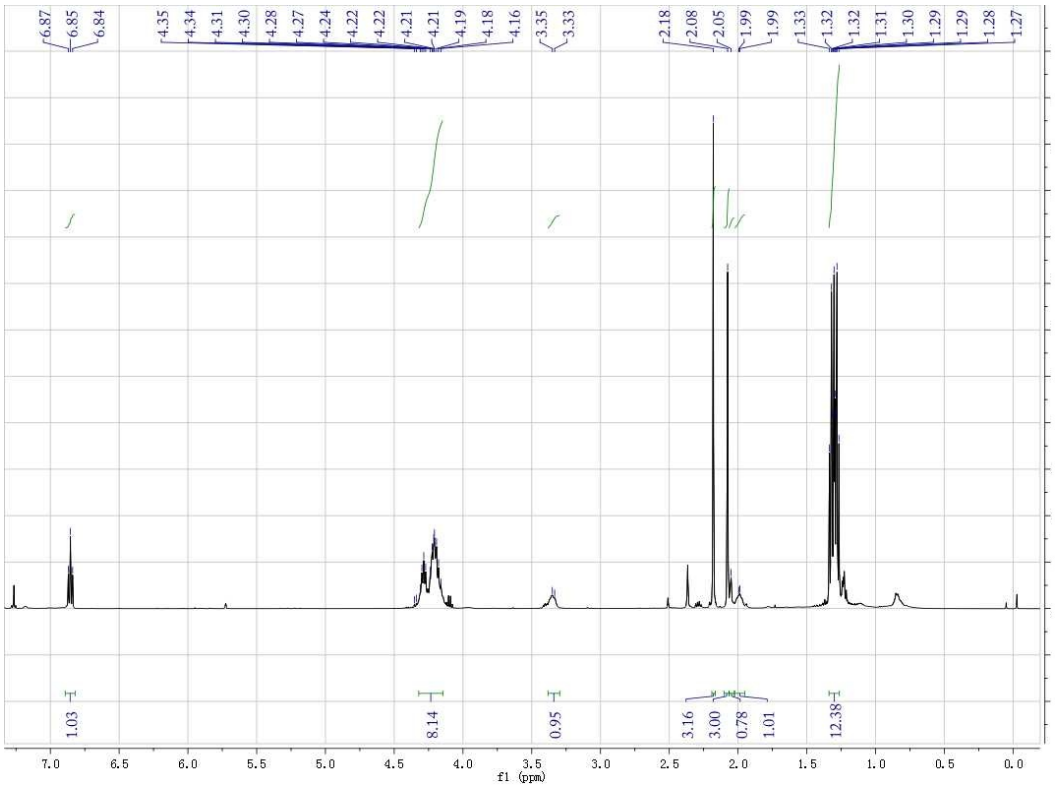
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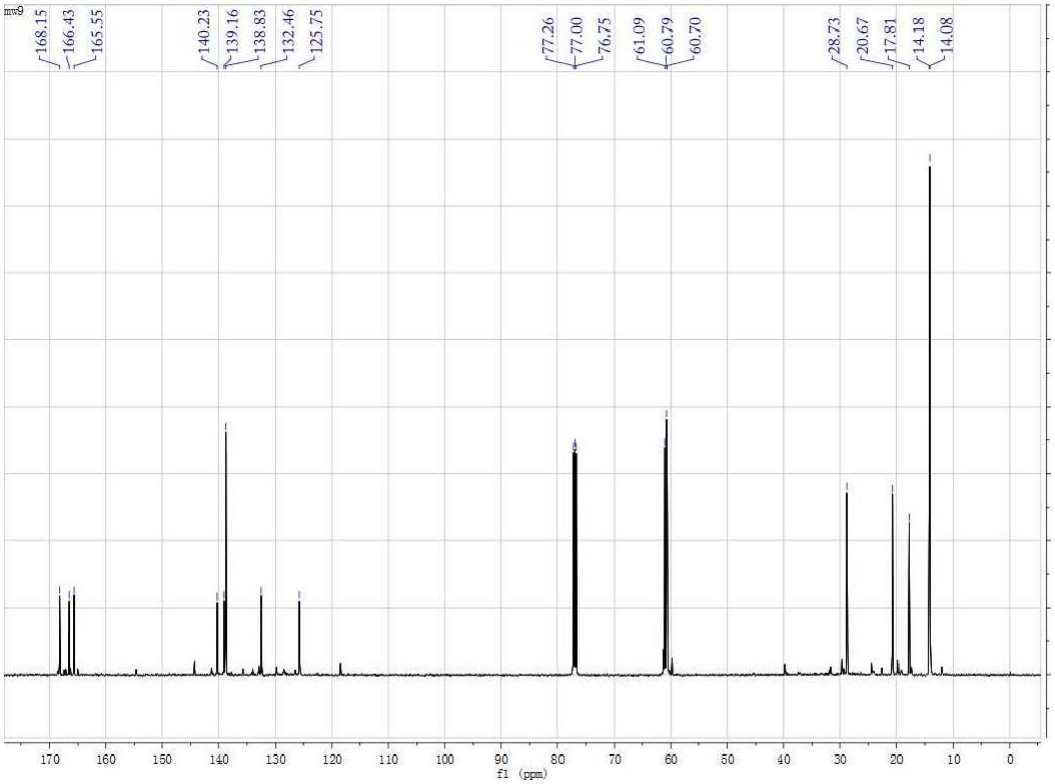
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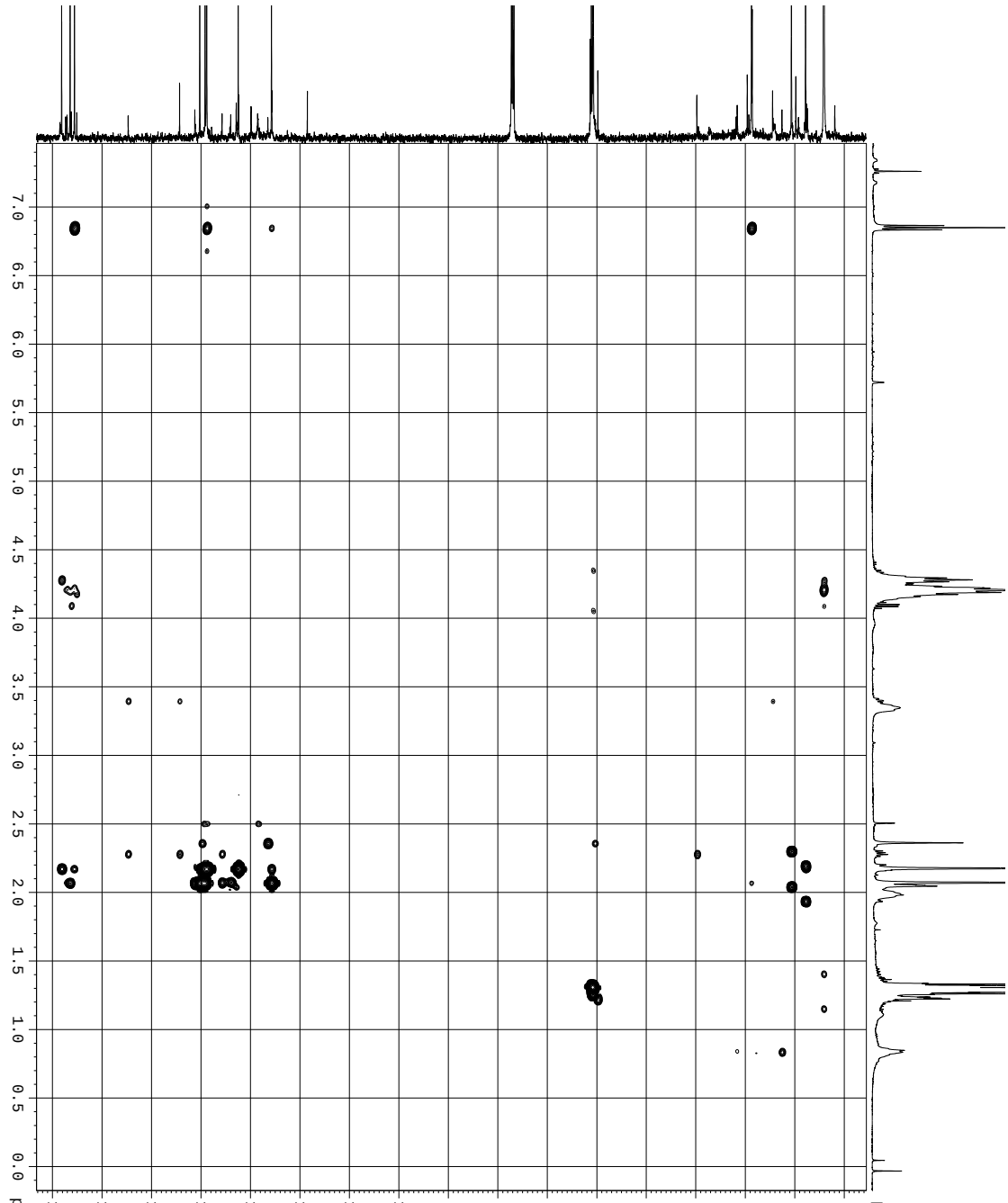
2D NMR HMBC

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NUC1                 1H
P1                12.50 usec
p2                25.00 usec
PL1                0.00 dB
SFO1         500.1314004 MHz

======== CHANNEL f2 ========
NUC2                 13C
P3                11.30 usec
PL2                0.00 dB
SFO2         125.7691072 MHz

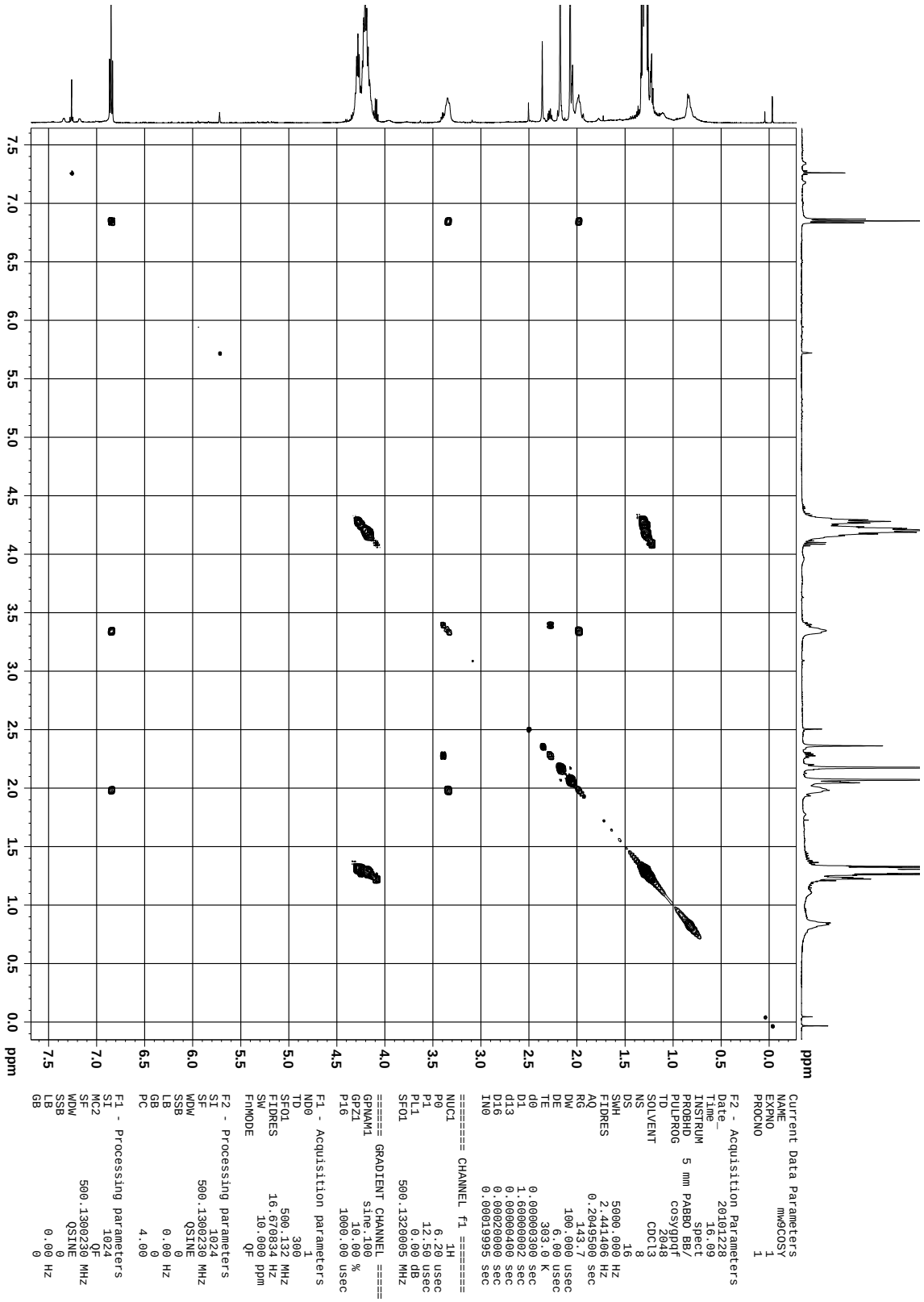
====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1              50.00 %
GPZ2              30.00 %
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
ND0                   2
TD                  300
SFO1         125.7691 MHz
FIDRES        75.414780 Hz
SW           179.889 ppm
FnMODE                QF

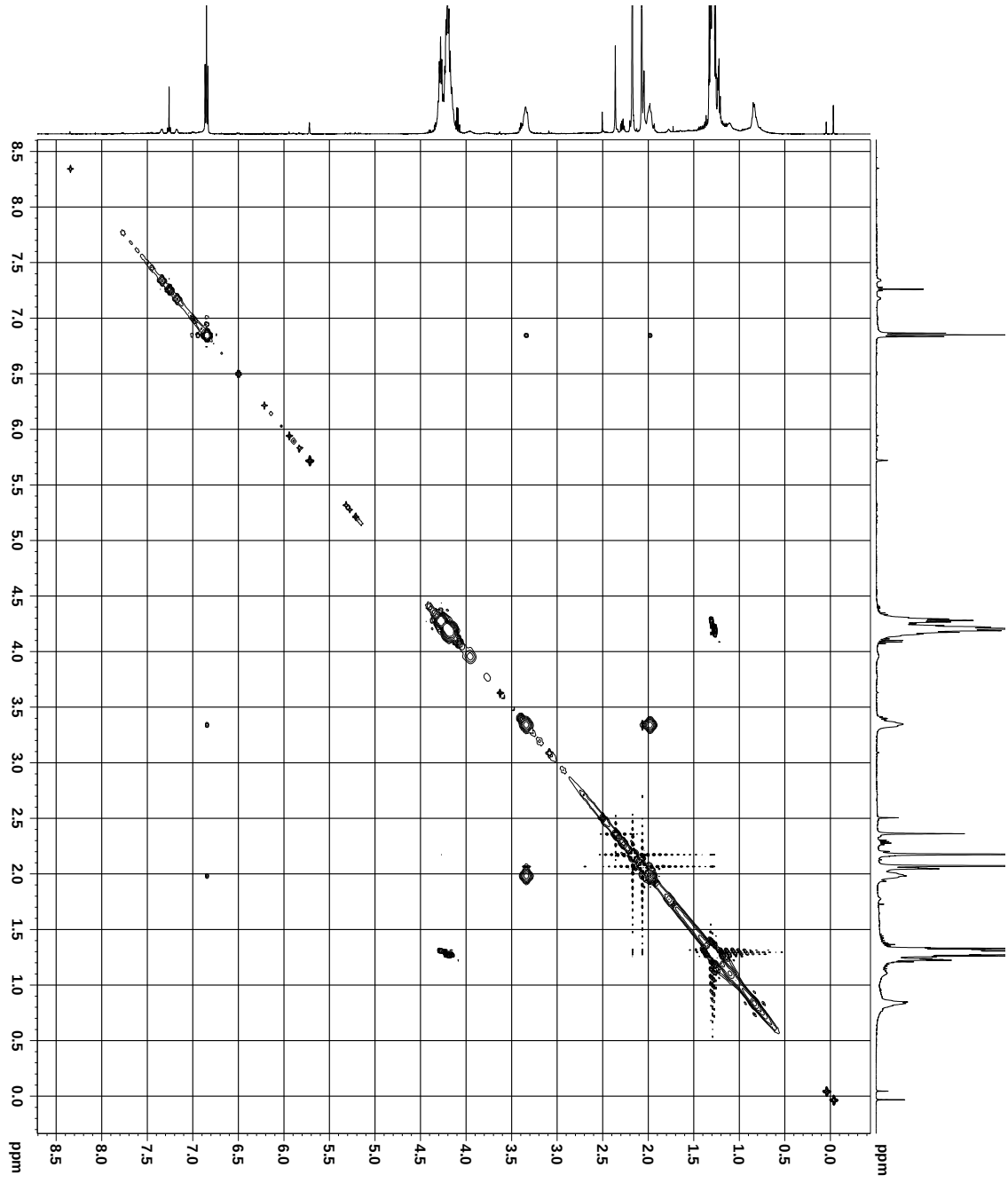
F2 - Processing parameters
SI                  1024
SF           500.1300230 MHz
WDW                QSINE
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40

F1 - Processing parameters
SI                  1024
SF                    QF
MC2                QSINE
SF           125.7577985 MHz
WDW                   0
SSB                   0
LB                 0.00 Hz
GB                    0
```

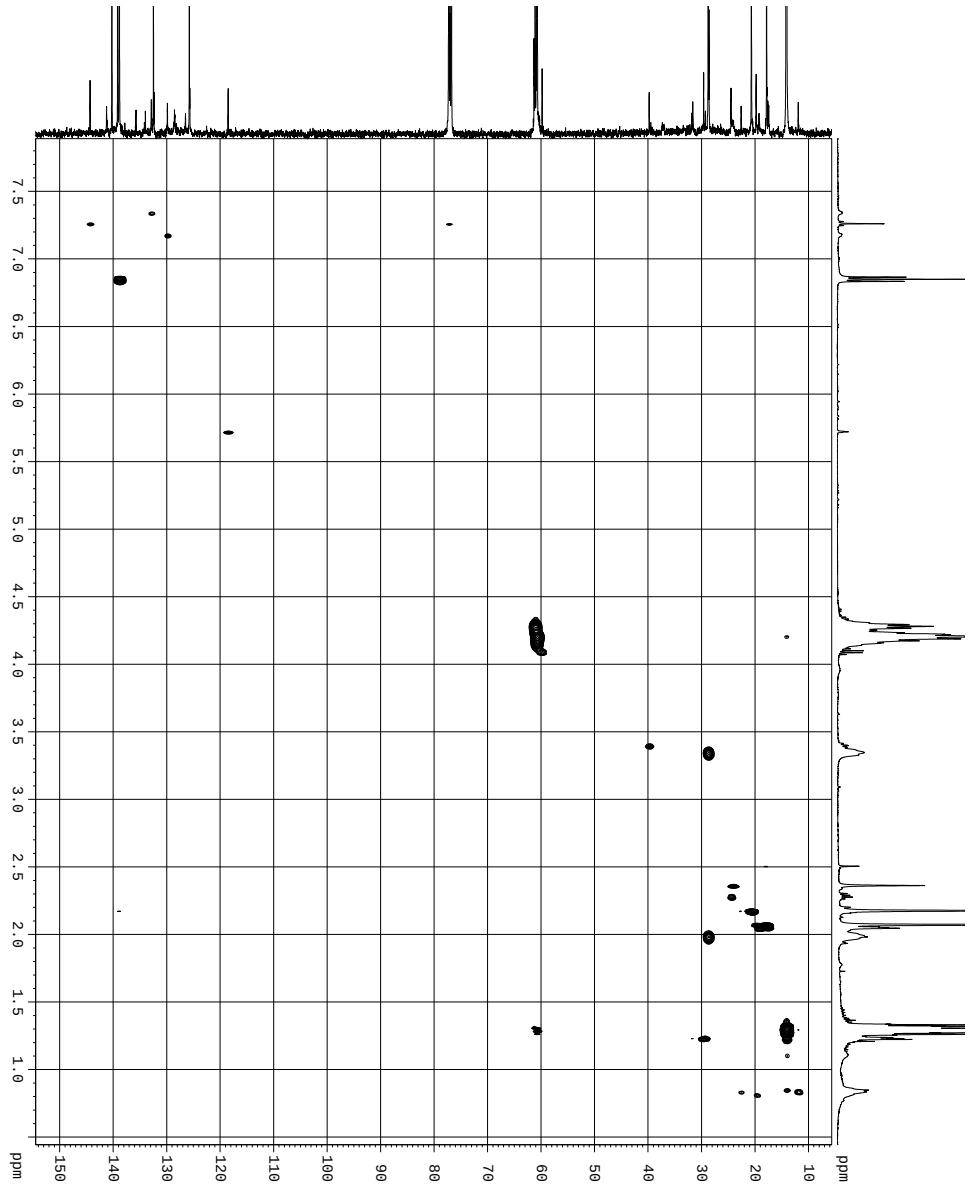
2D NMR COSY


ppm
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 0.0
Current Data Parameters
NAME mw6COSY
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101228
Time 16.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2049500 sec
RG 143.7
DW 100.000 usec
DE 6.00 usec
TE 303.0 K
d0 0.00000300 sec
D1 1.60000002 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019995 sec
======== CHANNEL f1 ========
NUC1 1H
P0 6.20 usec
P1 12.50 usec
PL1 0.00 dB
SFO1 500.1320005 MHz
====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPZ1 10.00 %
P16 1000.00 usec
F1 - Acquisition parameters
ND0 1
TD 300
SFO1 500.132 MHz
FIDRES 16.670834 Hz
SW 10.000 ppm
FnMODE QF
F2 - Processing parameters
SI 1024
SF 500.1300230 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 4.00
F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300230 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR NOESY


8.5 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 0.0
ppm
Current Data Parameters
NAME mw9NOE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101228
Time 21.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG noesygpph
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2049500 sec
RG 16
DW 100.000 usec
DE 6.00 usec
TE 303.0 K
d0 0.000008406 sec
D1 1.600000002 sec
D8 0.600000002 sec
D16 0.000200000 sec
IN0 0.000119995 sec
TAU 0.298800002 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
p2 25.00 usec
PL1 0.00 dB
SFO1 500.1320005 MHz
====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
F1 - Acquisition parameters
ND0 1
TD 300
SFO1 500.132 MHz
FIDRES 16.670834 Hz
SW 10.0000 ppm
FnMODE TPPI
F2 - Processing parameters
SI 1024
SF 500.1300230 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0
PC 4.00
F1 - Processing parameters
SI 1024
MC2 TPPI
SF 500.1300230 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR HMQC




```
Current Data Parameters
NAME                  mw9hsqc
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20101228
Time                   17.24
INSTRUM                 spect
PROBHD     5 mm PABBO BB/ 
PULPROG          hsqcetgpsisp2
TD                      2048
SOLVENT                 CDCl3
NS                        12
DS                        12
SWH                 5482.456 Hz
FIDRES              0.1869188 Hz
AQ                  0.2298.8 sec
RG                        512
DW                    91.200 usec
DE                     6.00 usec
TE                     303.1 K
CNST2               145.0000000
D0                  0.00000300 sec
D1                  1.00000000 sec
d4                  0.00172414 sec
d11                 0.03000000 sec
d16                 0.00020000 sec
D24                 0.00098207 sec
DELTA               0.00120800 sec
DELTA1              0.00120800 sec
DELTA2              0.00147414 sec
DELTA3              0.00016207 sec
DELTA4              0.00027414 sec
IN0                 0.00002128 sec
ST1CNT                   128
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                      12.40 usec
P2                      24.80 usec
P28                   600.00 usec
PL1                     0.00 dB
SFO1                500.1314004 MHz

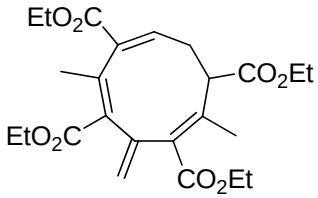
======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                      13C
P3                      11.30 usec
P4                      22.60 usec
P14                   500.00 usec
PCPD2                 60.00 usec
PL0                   120.00 dB
PL2                     0.00 dB
PL12                   14.50 dB
SFO2                125.7691072 MHz
SP3                     7.10 dB
SPNAM3             Crp60,0.5,20.1
SPOAL3                  0.500
SPOFFS3                 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINE.100
GPNAM4             SINE.100
GPZ1                80.00 %
GPZ22               20.10 %
GPZ23               11.00 %
GPZ24               -1.00 %
P16                1000.00 usec
P19                 500.00 usec

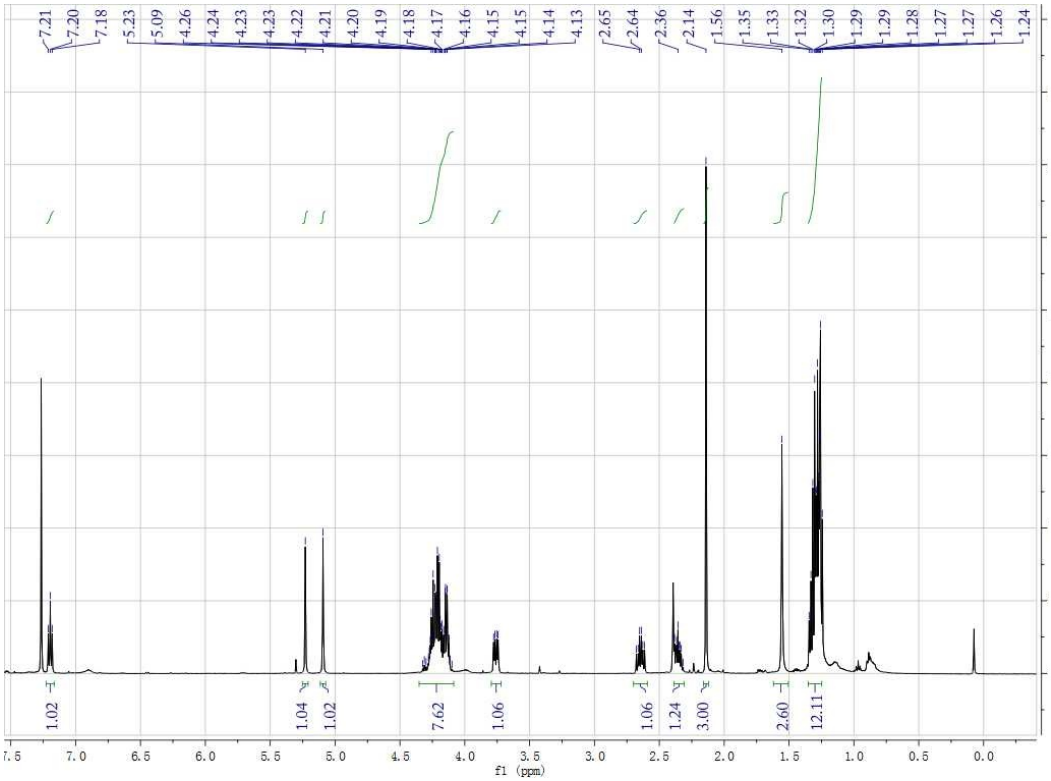
F1 - Acquisition parameters
ND0                       300
TD                      256
SFO1                125.7691 MHz
FIDRES               79.744820 Hz
SW                   190.217 ppm
FnMODE             Echo-AntiEcho

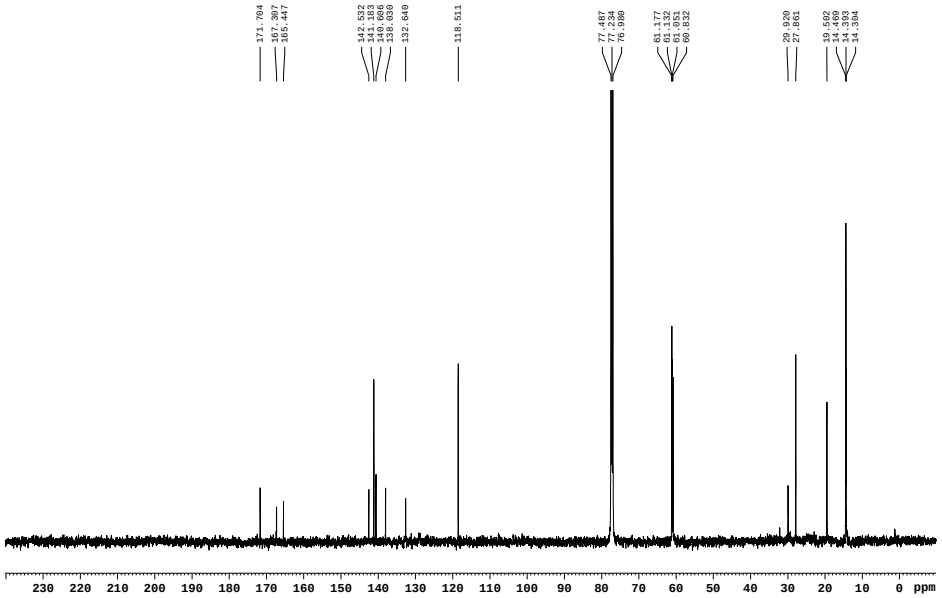
F2 - Processing parameters
SI                      1024
SF                 500.1300230 MHz
WDW                       QSIN
SSB                          2
LB                        0.00 Hz
GB                           0
PC                        1.40

F1 - Processing parameters
SI                      1024
MC2                echo-antiecho
SF                 125.7577985 MHz
WDW                       QSIN
SSB                          2
LB                        0.00 Hz
GB                           0
```



5






```
Current Data Parameters
NAME                  mw-169-045
EXPNO                          2
PROCNO                         1

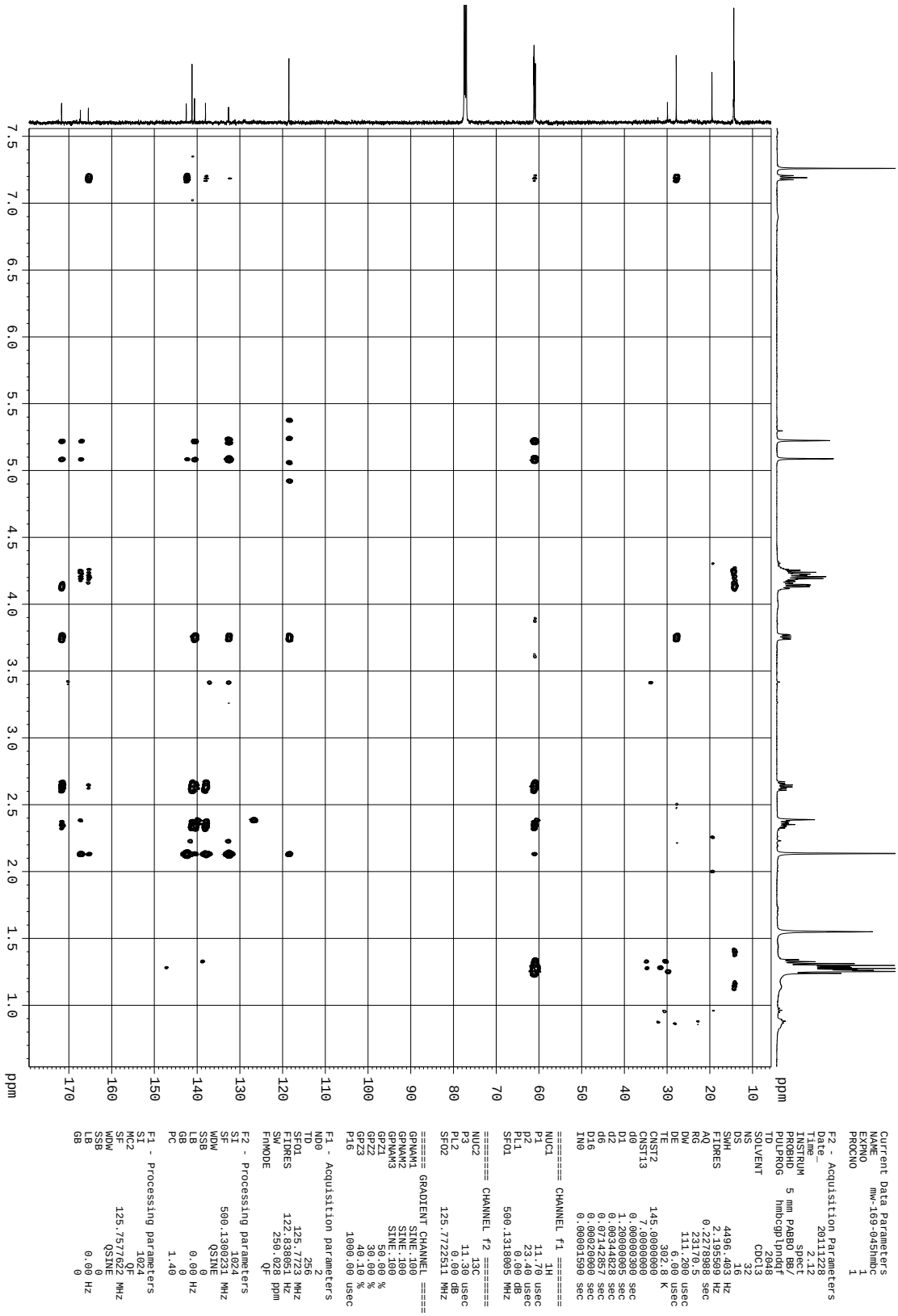
F2 - Acquisition Parameters
Date_              20111228
Time                      12.42
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                    zgdc
TD                        65536
SOLVENT                   CDCl3
NS                         3248
DS                            0
SWH                  31446.541 Hz
FIDRES                0.479836 Hz
AQ                    1.0420883 sec
RG                        32768
DW                       15.900 usec
DE                        6.00 usec
TE                       303.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                          7.00 usec
PL1                         0.00 dB
SFO1                125.7722511 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                      83.00 usec
PL2                        120.00 dB
PL12                        18.00 dB
SFO2                500.1327310 MHz

F2 - Processing parameters
SI                        32768
SF                  125.7577622 MHz
WDW                          EM
SSB                           0
LB                         3.00 Hz
GB                            0
PC                         1.00
```

2D NMR HMBC




```
Current Data Parameters
NAME                 mw-169-045hmbc
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20111228
Time                           2.12
INSTRUM                       spect
PROBHD     5 mm PABBO BB/
PULPROG             hmbcgplpndqf
TD                             2048
SOLVENT                     CDCl3
NS                               16
DS                               16
SWH                      4496.403 Hz
FIDRES                   2.195509 Hz
AQ                       0.2278988 sec
RG                          231170.5
DW                          111.200 usec
DE                             6.00 usec
TE                          302.8 K
CNST2                    145.0000000
CNST13                     7.0000000
d0                       0.0000030000 sec
D1                       1.2000000000 sec
D2                       0.0034482759 sec
d6                       0.0142857143 sec
D16                      0.0002000000 sec
IN0                      0.0000031500 sec

======== CHANNEL f1 ========
NUC1                            1H
P1                           11.70 usec
p2                           23.40 usec
PL1                           0.00 dB
SFO1                    500.1318005 MHz

======== CHANNEL f2 ========
NUC2                           13C
PL2                           0.00 dB
PL12                          0.00 dB
SFO2                    125.7722511 MHz

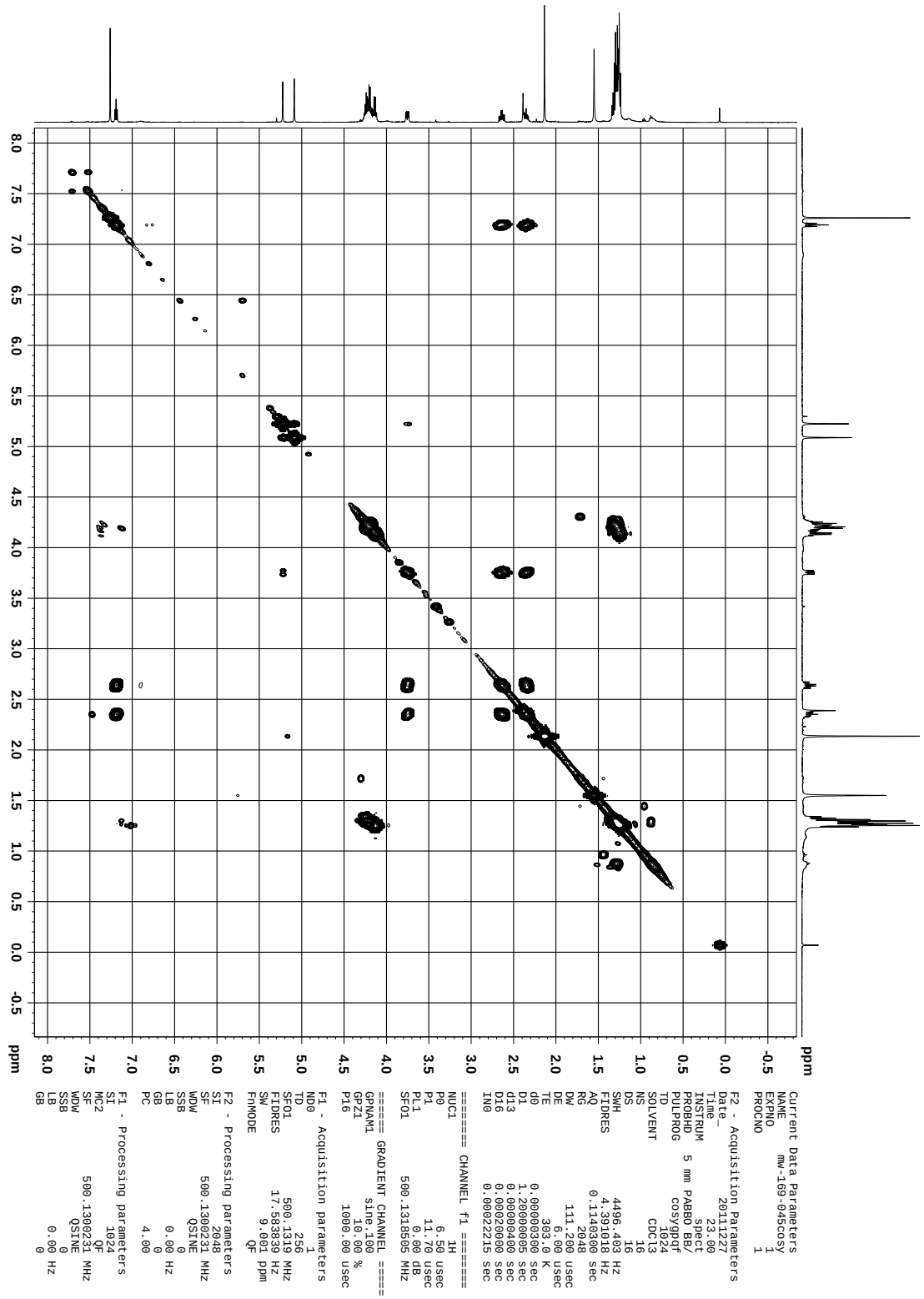
====== GRADIENT CHANNEL =====
GPNAM1                   SINE.100
GPNAM2                   SINE.100
GPNAM3                   SINE.100
GPZ1                         50.00 %
GPZ2                         30.00 %
GPZ3                         40.10 %
P16                       1000.00 usec

F1 - Acquisition parameters
ND0                               2
TD                              256
SFO1                    125.7723 MHz
FIDRES                  122.838051 Hz
SW                      250.028 ppm
FnMODE                         QF

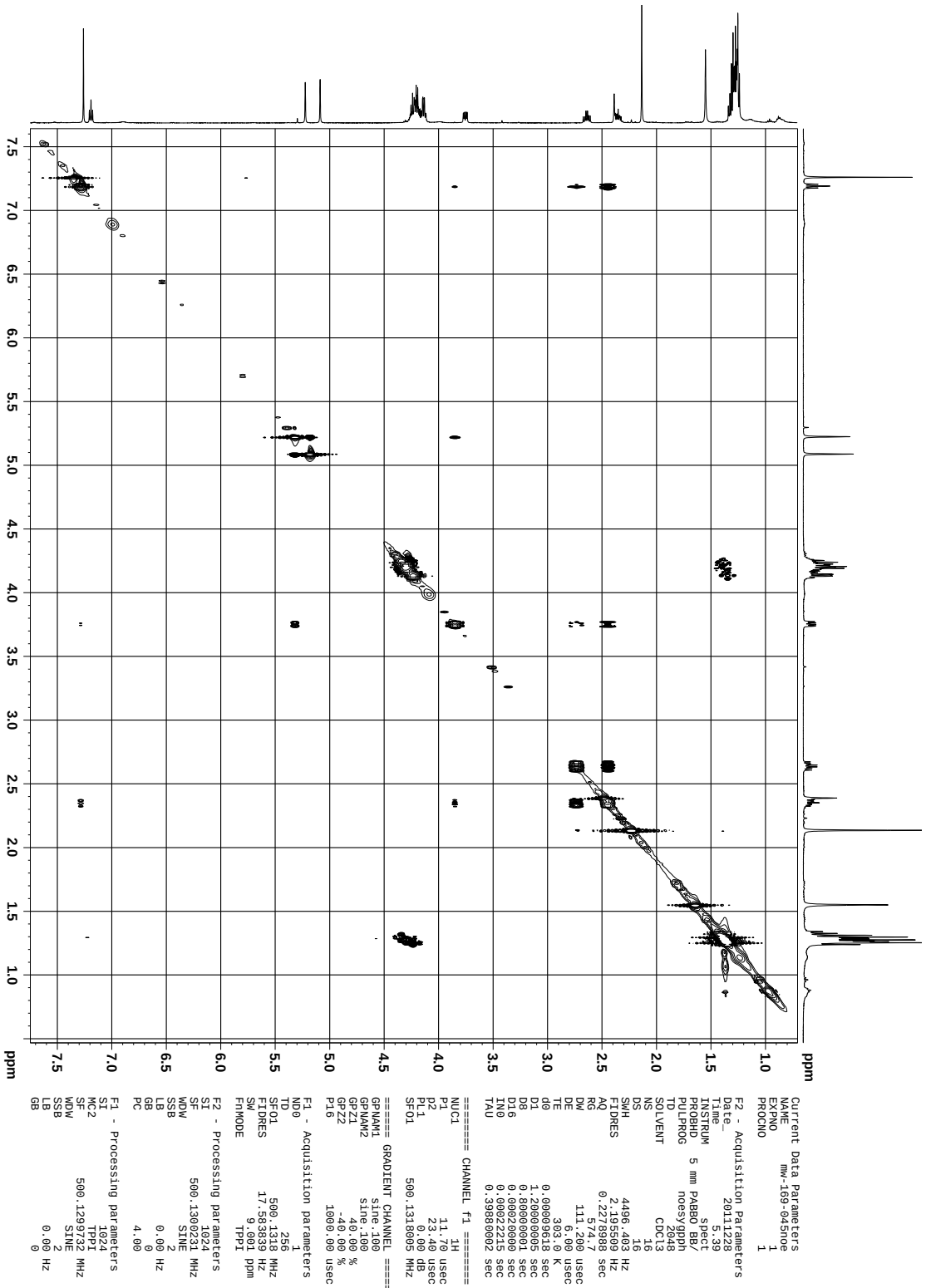
F2 - Processing parameters
SI                              1024
SF                      500.1300231 MHz
WDW                          QSINE
SSB                              0
LB                            0.00 Hz
GB                               0
PC                            1.40

F1 - Processing parameters
SI                              1024
SF                      125.7577622 MHz
WDW                          QSINE
SSB                              0
LB                            0.00 Hz
GB                               0
```

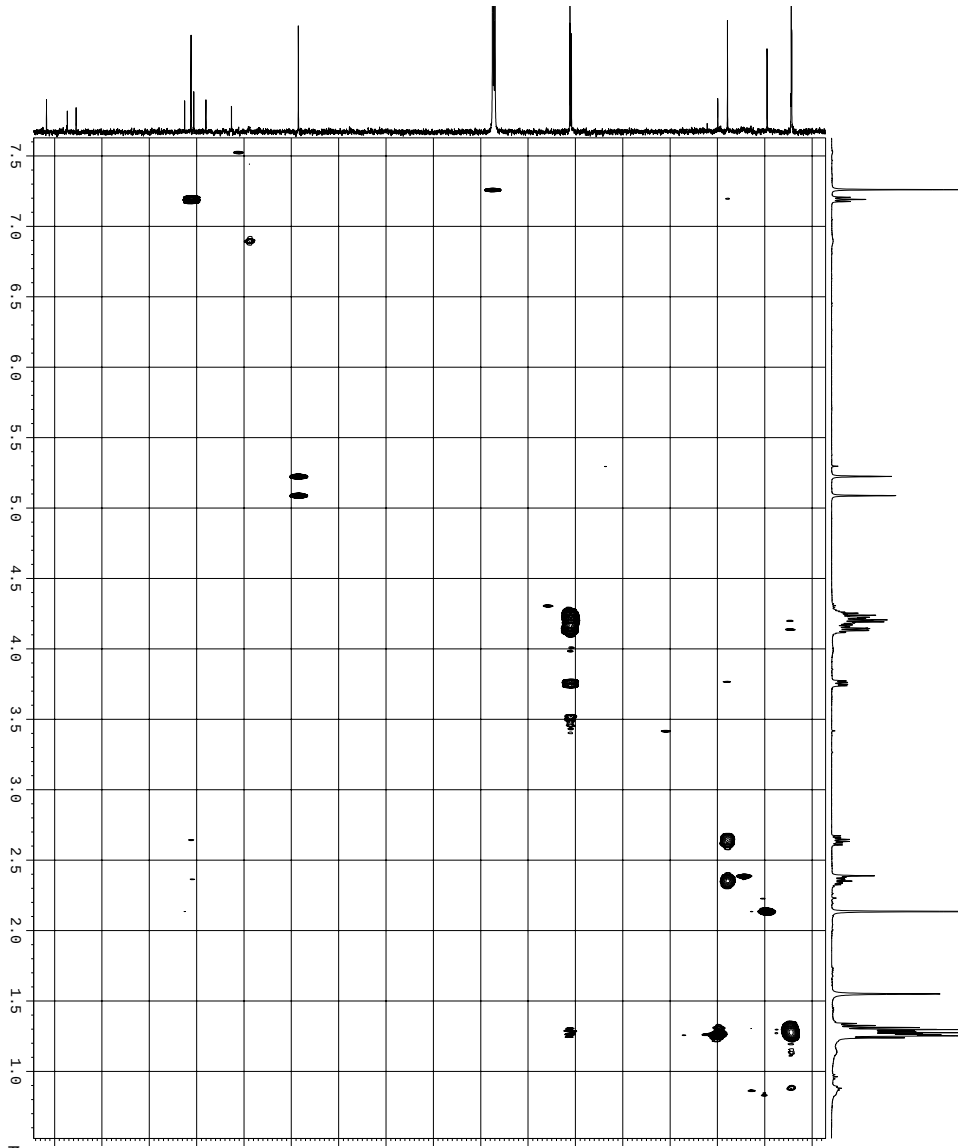
2D NMR COSY


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 0.0 -0.5 ppm
Current Data Parameters
NAME mw-169-045cosy
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111227
Time 23.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpqf
TD 1024
SOLVENT CDCl3
NS 16
DS 16
SWH 4496.403 Hz
FIDRES 4.391018 Hz
AQ 0.1140300 sec
RG 2048
DW 111.200 usec
DE 6.00 usec
TE 303.0 K
d0 0.00000300 sec
D1 1.20000005 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00022215 sec
======== CHANNEL f1 ========
NUC1 1H
P0 6.50 usec
P1 11.70 usec
PL1 0.00 dB
SFO1 500.1318505 MHz
====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPZ1 16.00 %
P16 1000.00 usec
F1 - Acquisition parameters
TD 256
SFO1 500.1319 MHz
FIDRES 17.583839 Hz
SW 9.0061 ppm
FnMODE QF
F2 - Processing parameters
SI 2048
SF 500.1300231 MHz
WDW QSINE
SSB 0
GB 0.00 Hz
PC 4.00
F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300231 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR NOESY



2D NMR HMQC




```
Current Data Parameters
NAME                 mw-169-045hsqc
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_              20111222
Time_                  0:22
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG            hsqcetgpsisp2
TD                      2048
SOLVENT                 CDCl3
NS                        16
DS                        16
SWH                 4496.403 Hz
FIDRES              0.2278988 Hz
AQ                  2.2749119 sec
RG                      16384
DW                    111.200 usec
DE                      6.00 usec
TE                     305.0 K
CNST2               145.0000000
d0                  0.00000300 sec
D1                  1.20000005 sec
d11                 0.03000000 sec
d1                  0.00372444 sec
D16                 0.00020000 sec
D24                 0.00086207 sec
DELTA               0.00127980 sec
DELTA1              0.00127980 sec
DELTA3              0.00016207 sec
DELTA4              0.00027414 sec
IN0                 0.00001590 sec
SILCNT                     256
ZGOPTNS                    128

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.10 usec
P2                     23.10 usec
P28                   600.00 usec
PL1                     0.00 dB
SFO1             500.1318005 MHz

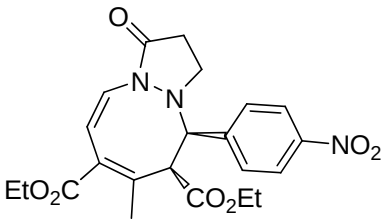
======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                       13C
P3                     11.30 usec
P4                     22.60 usec
P14                   500.00 usec
PCPD2                  60.00 usec
PL0                   120.00 dB
PL2                     0.00 dB
PL12                   17.00 dB
SFO2             125.7725519 MHz
SP3                    7.10 dB
SPNAM3          Crp60,0.5,20.1
SPOAL3                  0.500
SPOFFS3                 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPNAM4          SINE.100
GPZ1                   80.00 %
GPZ2                   20.10 %
GPZ3                   11.00 %
GPZ4                   50.00 %
P16                  1000.00 usec
P19                   500.00 usec

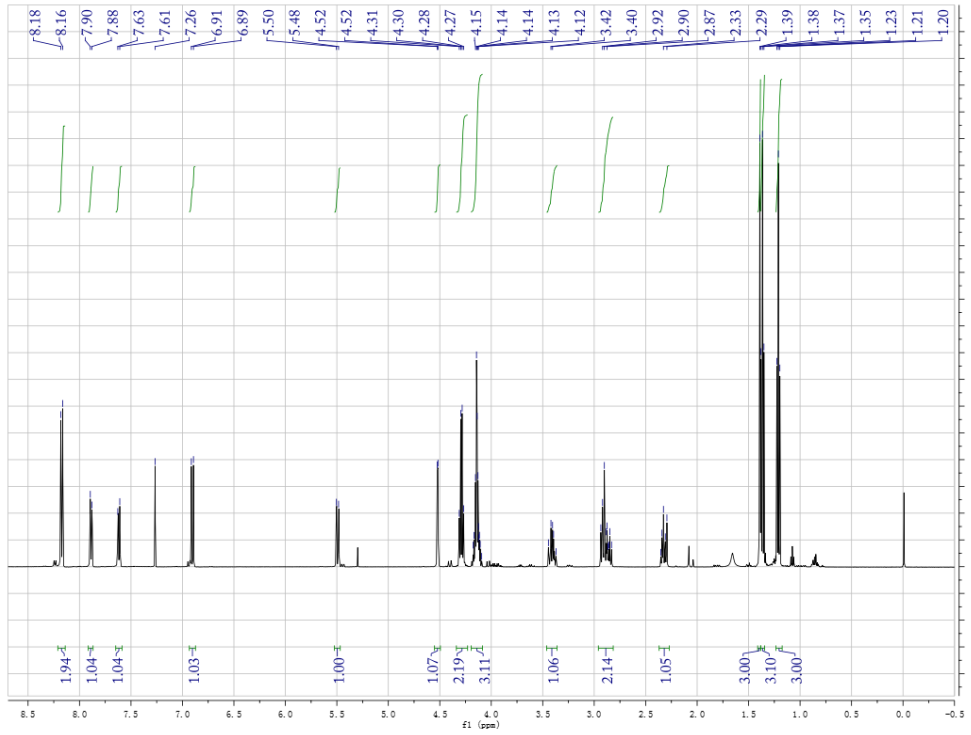
F1 - Acquisition parameters
ND0                       256
TD                       1024
SFO1             125.7723 MHz
FIDRES           122.838051 Hz
SW               250.028 ppm
FnMODE           Echo-AntiEcho

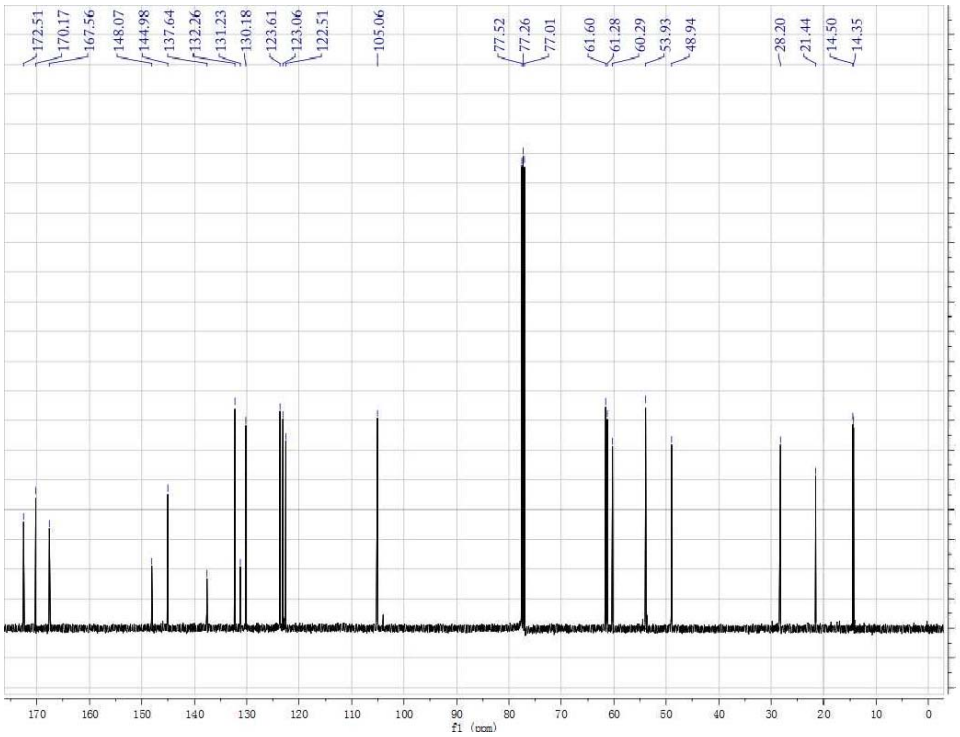
F2 - Processing parameters
SI                       2048
SF               500.1302231 MHz
WDW                      QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
PC                       1.40

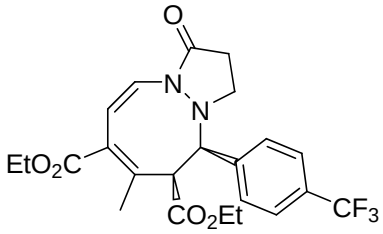
F1 - Processing parameters
SI                       2048
MC2              echo-antiecho
SF               125.7577022 MHz
WDW                      QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
```


O
N
N
NO2
EtO2C
CO2Et

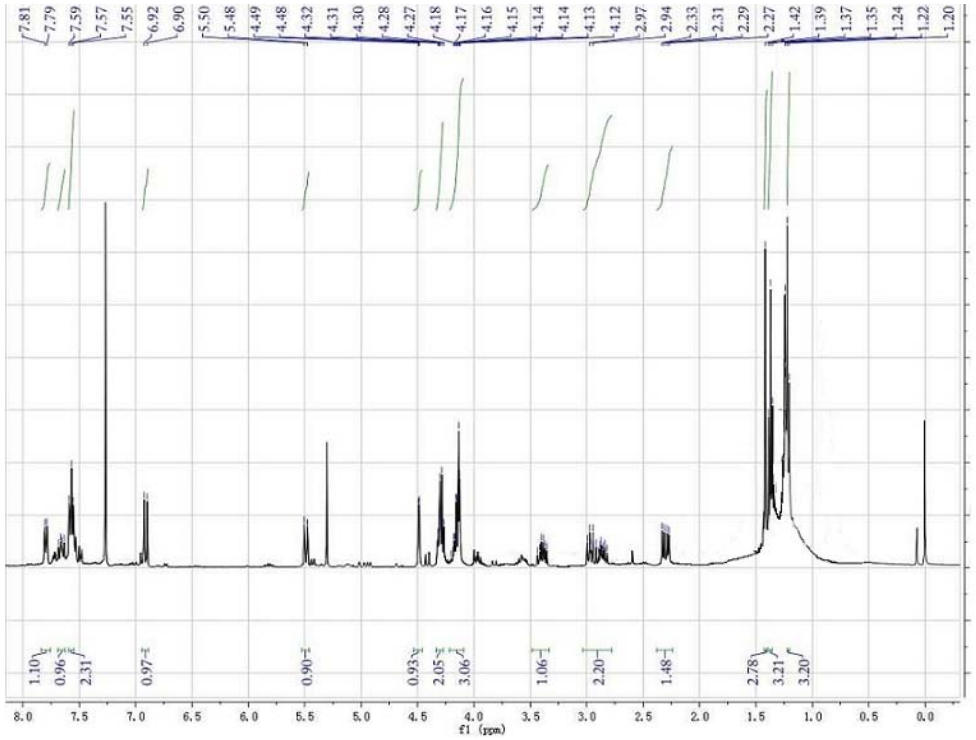
7a

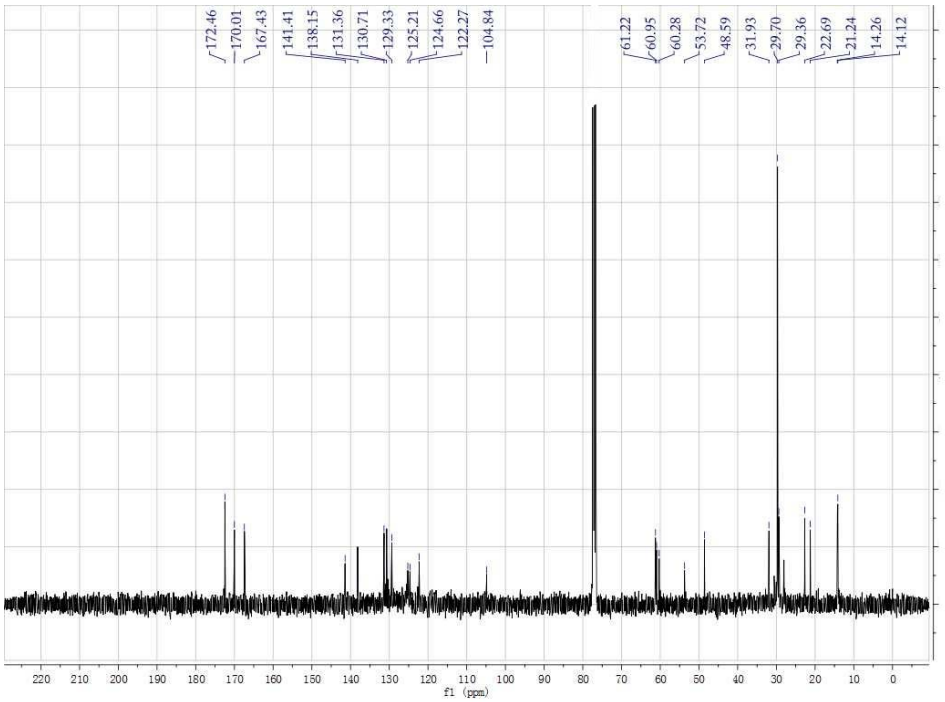

8.18
8.16
7.90
7.88
7.63
7.61
7.26
6.91
6.89
5.50
5.48
4.52
4.52
4.31
4.30
4.28
4.27
4.15
4.14
4.14
4.13
4.12
3.42
3.40
2.92
2.90
2.87
2.33
2.29
1.39
1.38
1.37
1.35
1.23
1.21
1.20
1.94
1.04
1.04
1.03
1.00
1.07
2.19
3.11
1.06
2.14
1.05
3.00
3.10
3.00
f1 (ppm)

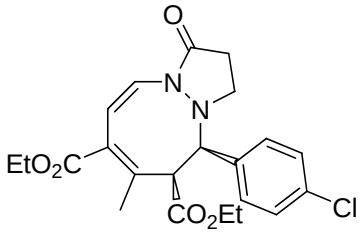

172.51
170.17
167.56
148.07
144.98
137.64
132.26
131.23
130.18
123.61
123.06
122.51
105.06
77.52
77.26
77.01
61.60
61.28
60.29
53.93
48.94
28.20
21.44
14.50
14.35
f1 (ppm)


O
N
N
EtO2C
CO2Et
CF3

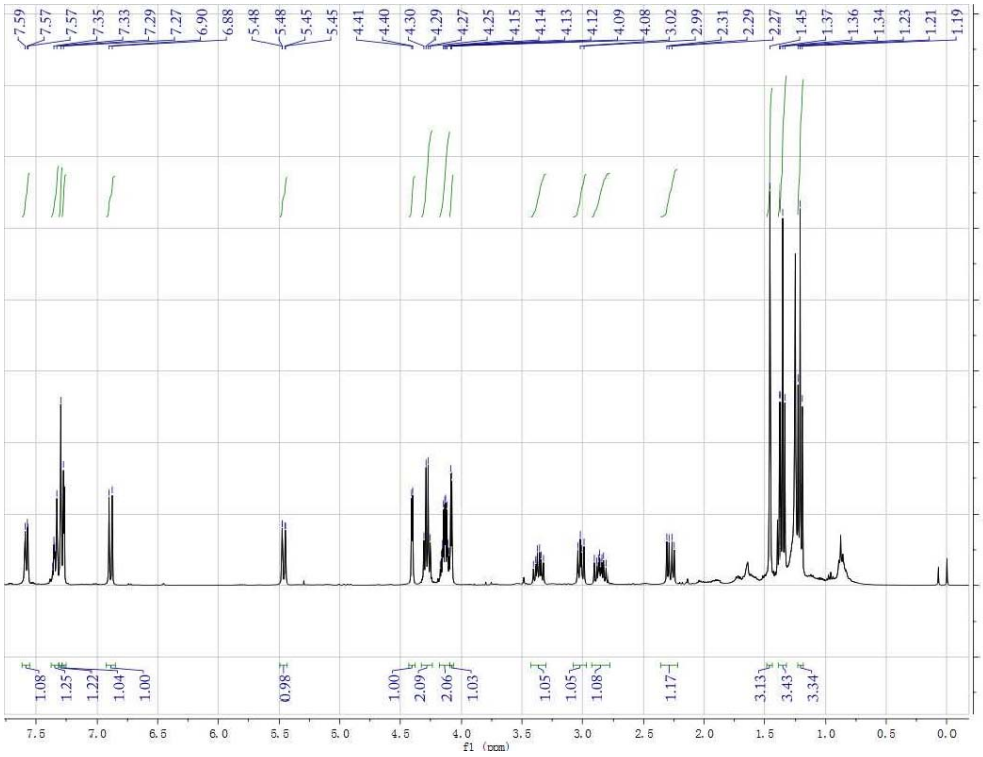
7b

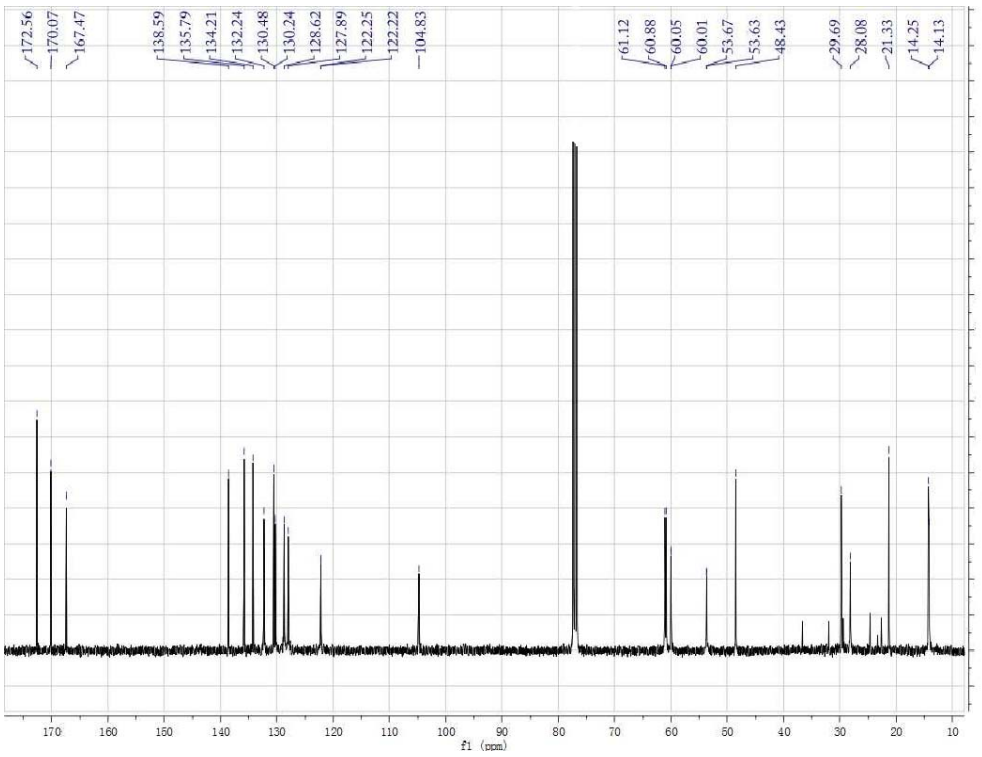

7.81 7.79 7.59 7.57 7.55 6.92 6.90 5.50 5.48 4.49 4.48 4.32 4.31 4.30 4.28 4.27 4.18 4.17 4.16 4.15 4.14 4.14 4.13 4.12 2.97 2.94 2.33 2.31 2.29 2.27 1.42 1.39 1.37 1.35 1.24 1.22 1.20
1.10 0.96 2.31 0.97 0.90 0.93 2.05 3.06 1.06 2.20 1.48 2.78 3.21 3.20
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

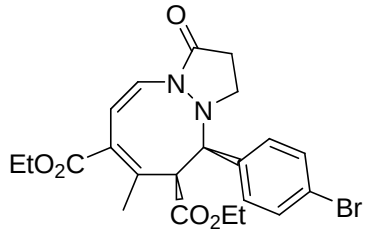

172.46 170.01 167.43 141.41 138.15 131.36 130.71 129.33 125.21 124.66 122.27 104.84
61.22 60.95 60.28 53.72 48.59 31.93 29.70 29.36 22.69 21.24 14.26 14.12
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
N
EtO2C
CO2Et
Cl

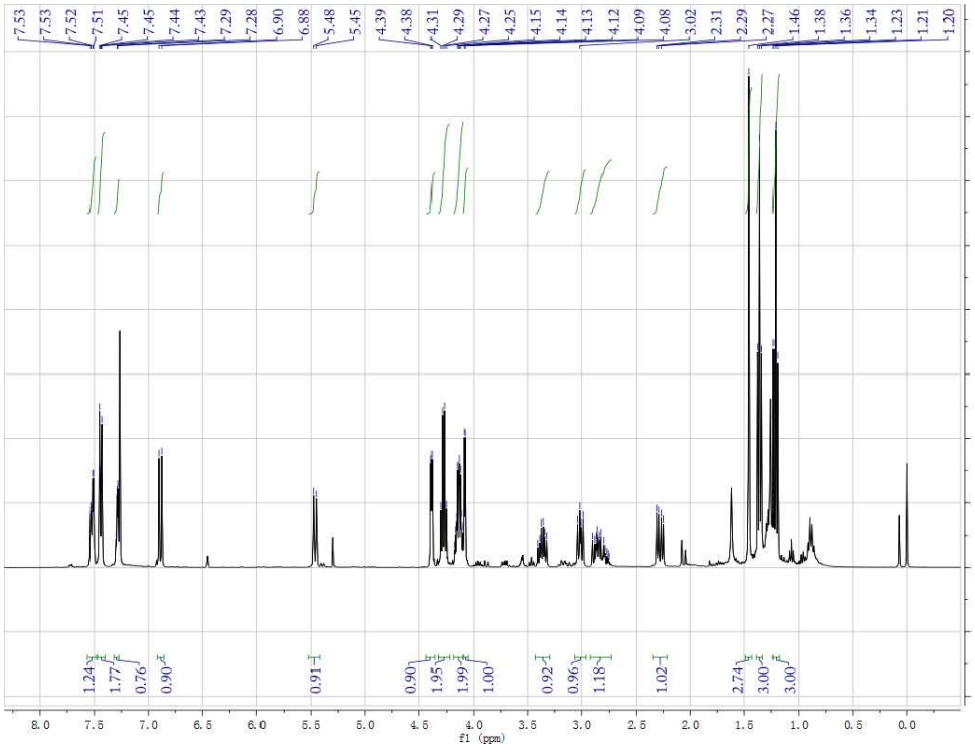
7c

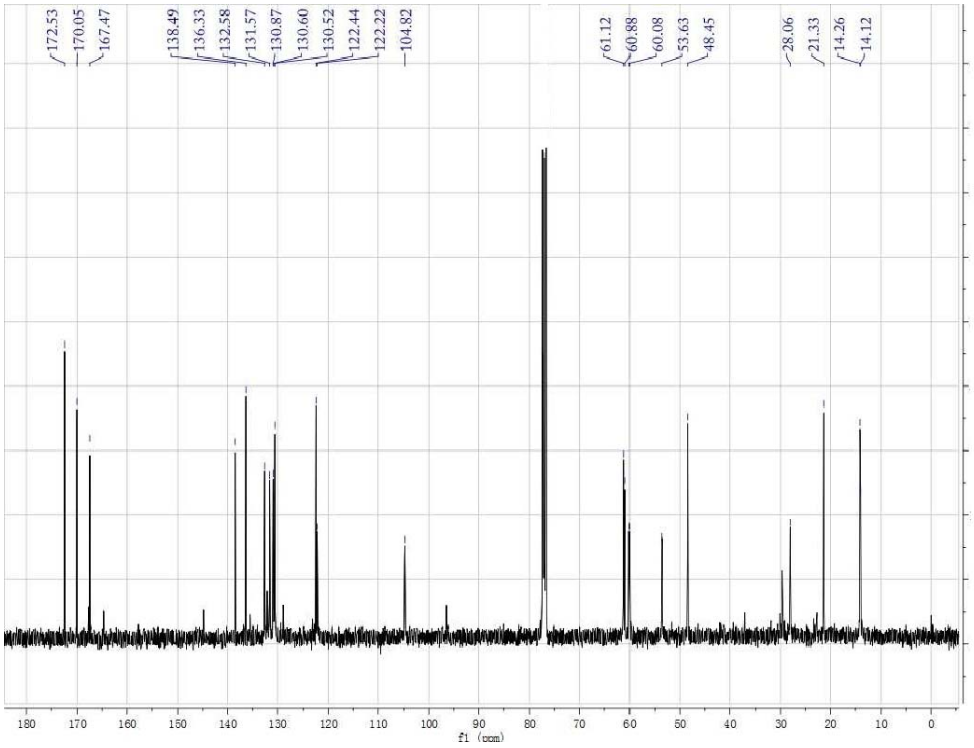

7.59 7.57 7.57 7.35 7.33 7.29 7.27 6.90 6.88 5.48 5.48 5.45 5.45 4.41 4.40 4.30 4.29 4.27 4.25 4.15 4.14 4.13 4.12 4.09 4.08 3.02 2.99 2.31 2.29 2.27 1.45 1.37 1.36 1.34 1.23 1.21 1.19
1.08 1.25 1.22 1.04 1.00 0.98 1.00 2.09 2.06 1.03 1.05 1.05 1.08 1.17 3.13 3.43 3.34
f1 (ppm)

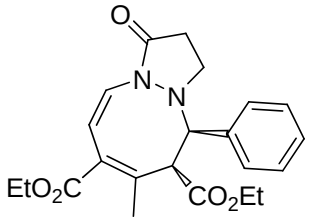

172.56 170.07 167.47 138.59 135.79 134.21 132.24 130.48 130.24 128.62 127.89 122.25 122.22 104.83 61.12 60.88 60.05 60.01 53.67 53.63 48.43 29.69 28.08 21.33 14.25 14.13
f1 (ppm)


O
N
N
EtO2C
CO2Et
Br

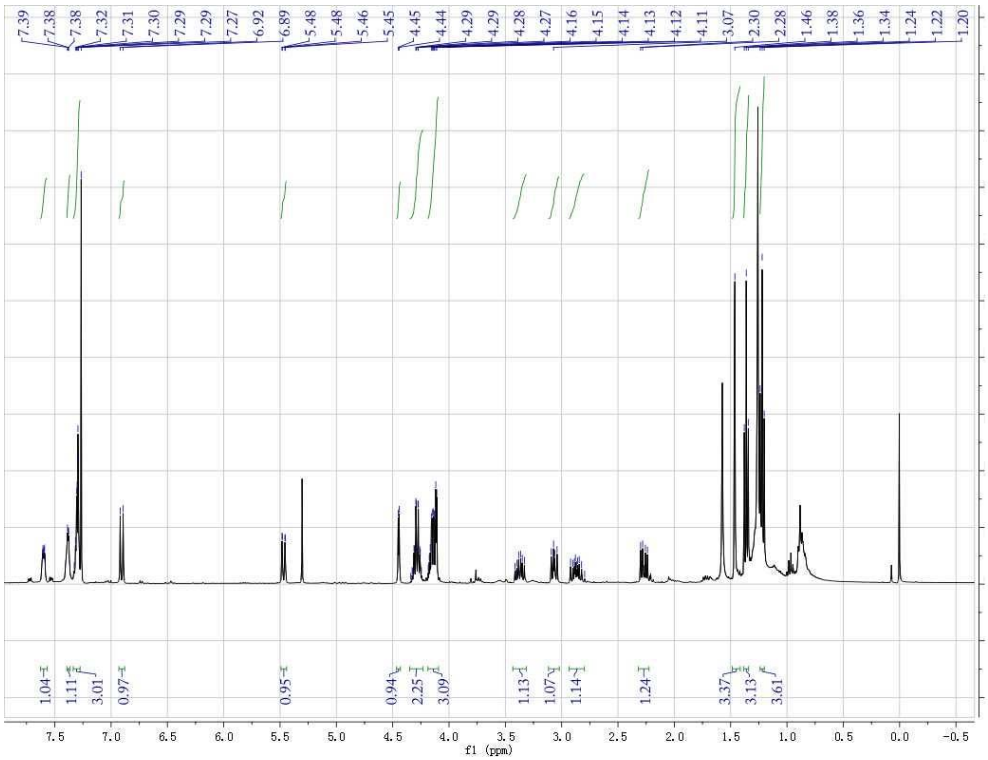
7d

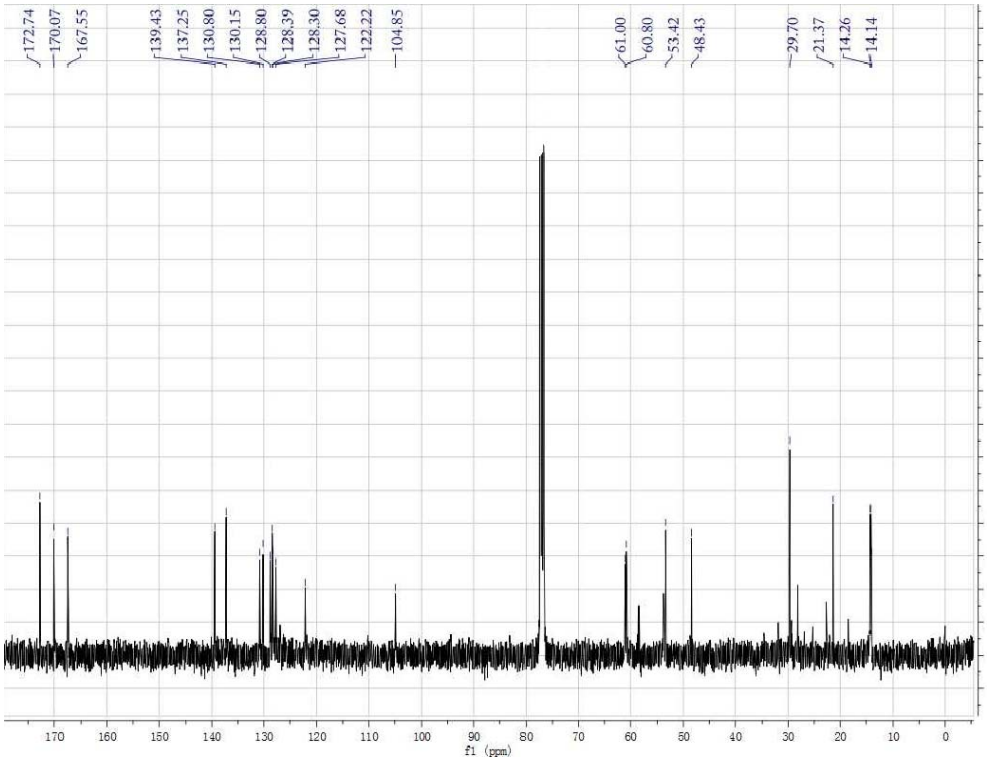

7.53 7.53 7.52 7.51 7.45 7.45 7.44 7.43 7.29 7.28 6.90 6.88 5.48 5.45 4.39 4.38 4.31 4.29 4.27 4.25 4.15 4.14 4.13 4.12 4.09 4.08 3.02 2.31 2.29 2.27 1.46 1.38 1.36 1.34 1.23 1.21 1.20
1.24 1.77 0.76 0.90 0.91 0.90 1.95 1.99 1.00 0.92 0.96 1.18 1.02 2.74 3.00 3.00
f1 (ppm)

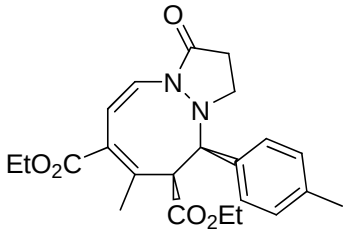

172.53 170.05 167.47 138.49 136.33 132.58 131.57 130.87 130.60 130.52 122.44 122.22 104.82 61.12 60.88 60.08 53.63 48.45 28.06 21.33 14.26 14.12
f1 (ppm)


O
N
N
EtO2C
CO2Et

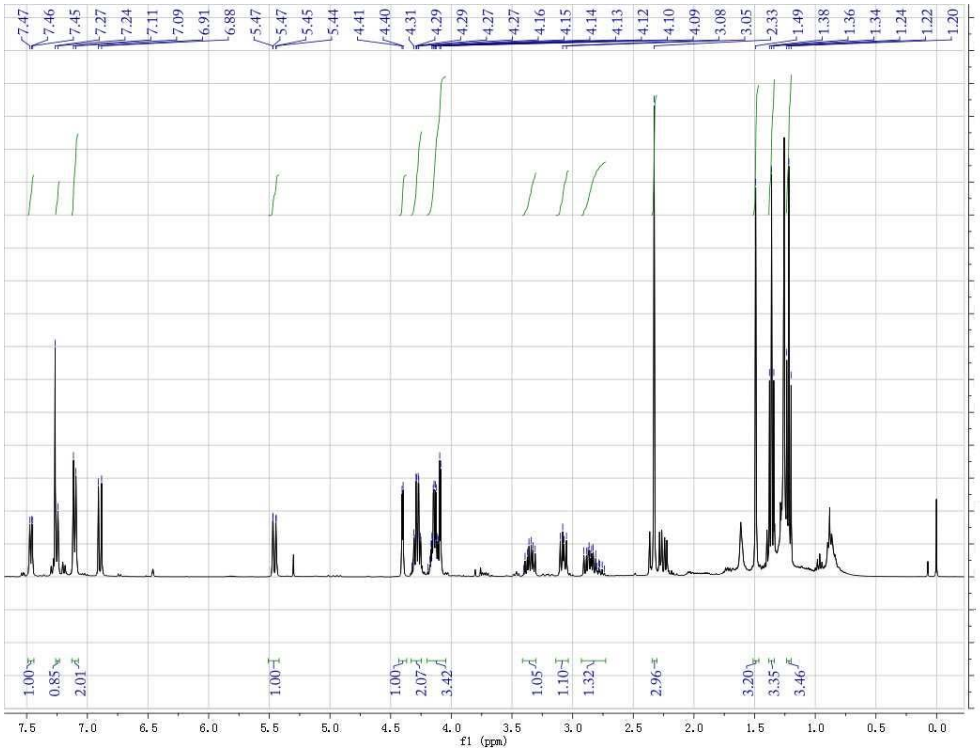
7e

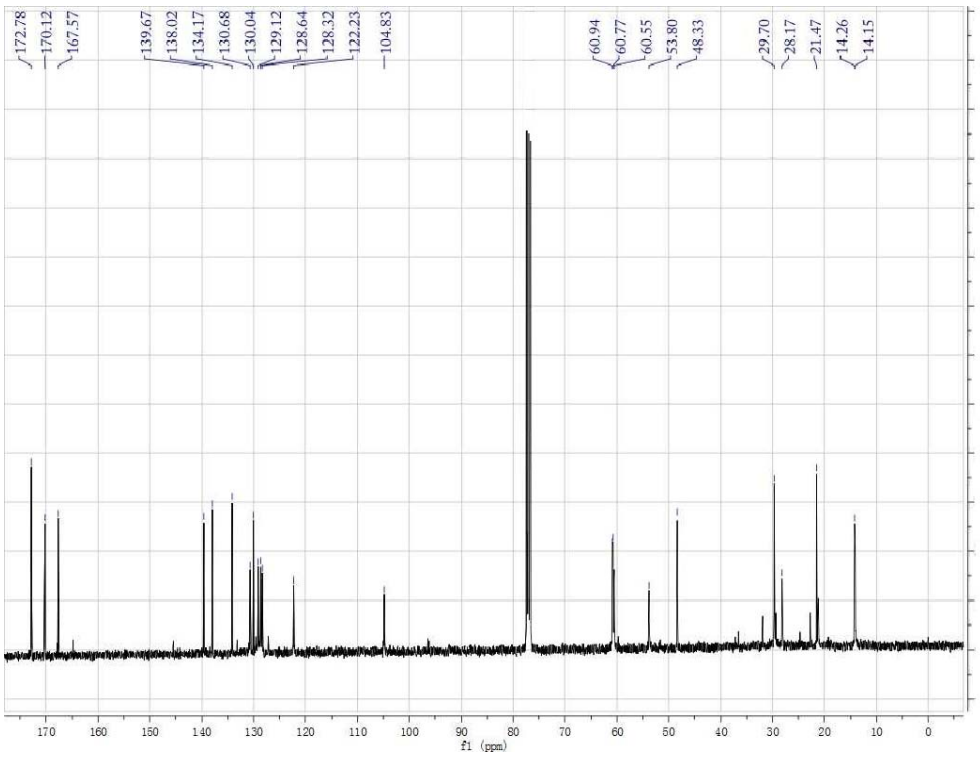

7.39 7.38 7.38 7.32 7.31 7.30 7.29 7.29 7.27 6.92 6.89 5.48 5.48 5.46 5.45 4.45 4.44 4.29 4.29 4.28 4.27 4.16 4.15 4.14 4.13 4.12 4.11 3.07 2.30 2.28 1.46 1.38 1.36 1.34 1.24 1.22 1.20
1.04 1.11 3.01 0.97 0.95 0.94 2.25 3.09 1.13 1.07 1.14 1.24 3.37 3.13 3.61
f1 (ppm)

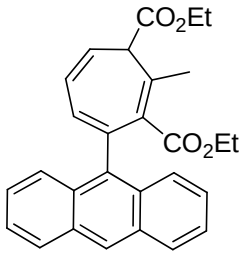

172.74 170.07 167.55 139.43 137.25 130.80 130.15 128.80 128.39 128.30 127.68 122.22 104.85 61.00 60.80 53.42 48.43 29.70 21.37 14.26 14.14
f1 (ppm)


O
N
N
EtO2C
CO2Et

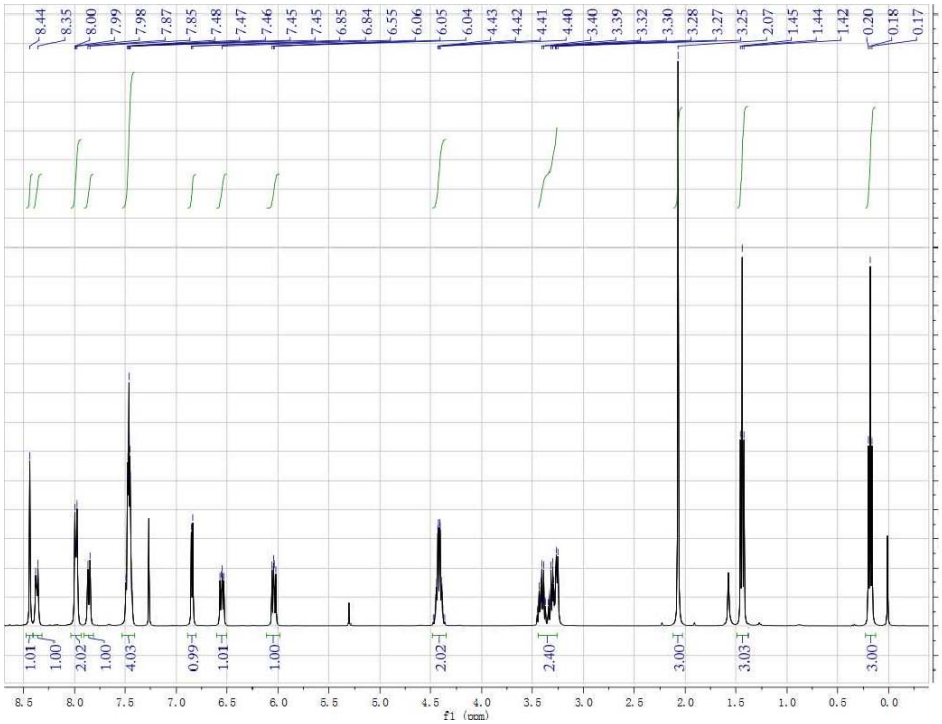
7f

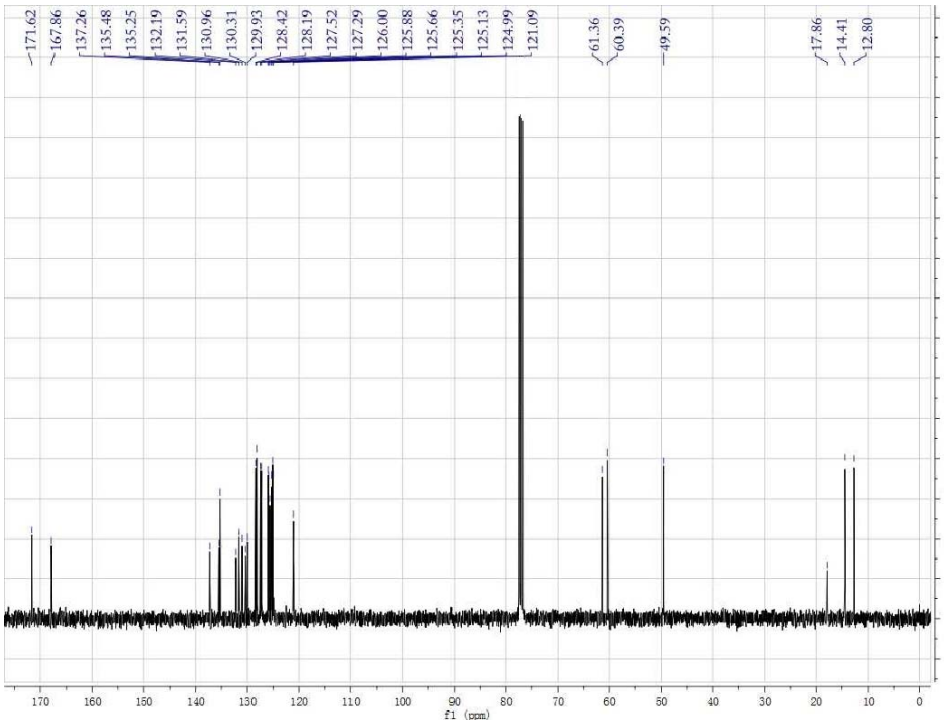

7.47 7.46 7.45 7.27 7.24 7.11 7.09 6.91 6.88 5.47 5.47 5.45 5.44 4.41 4.40 4.31 4.29 4.29 4.27 4.27 4.16 4.15 4.14 4.13 4.12 4.10 4.09 3.08 3.05 2.33 1.49 1.38 1.36 1.34 1.24 1.22 1.20
1.00 0.85 2.01 1.00 1.00 2.07 3.42 1.05 1.10 1.32 2.96 3.20 3.35 3.46
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

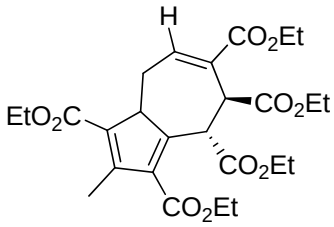

172.78 170.12 167.57 139.67 138.02 134.17 130.68 130.04 129.12 128.64 128.32 122.23 104.83 60.94 60.77 60.55 53.80 48.33 29.70 28.17 21.47 14.26 14.15
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CO2Et
CO2Et

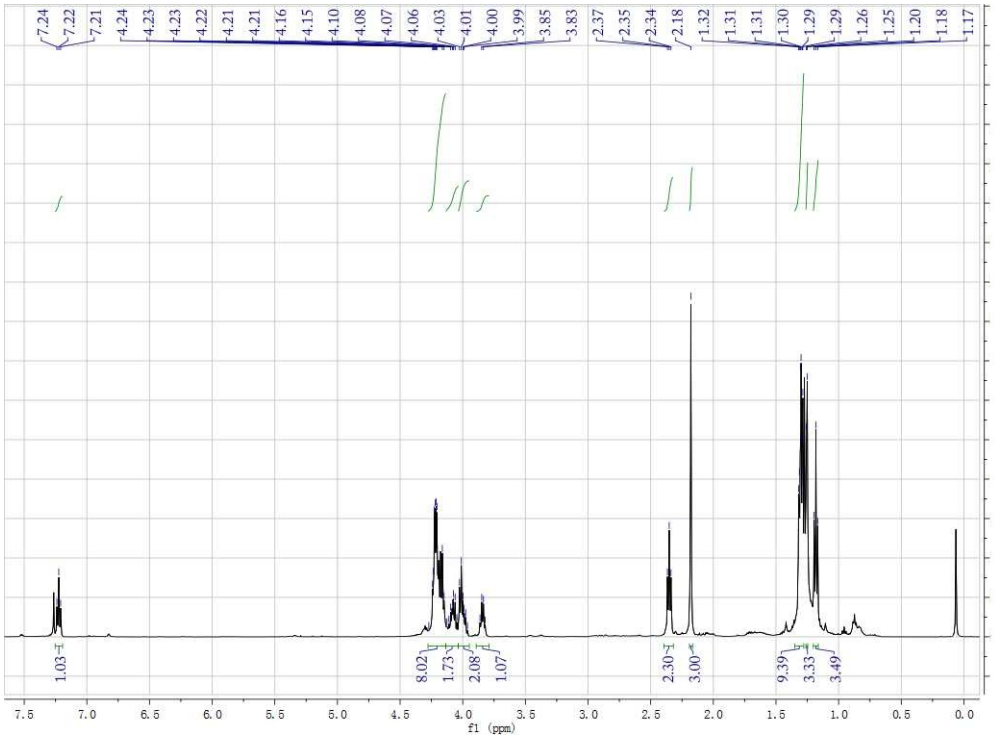
9

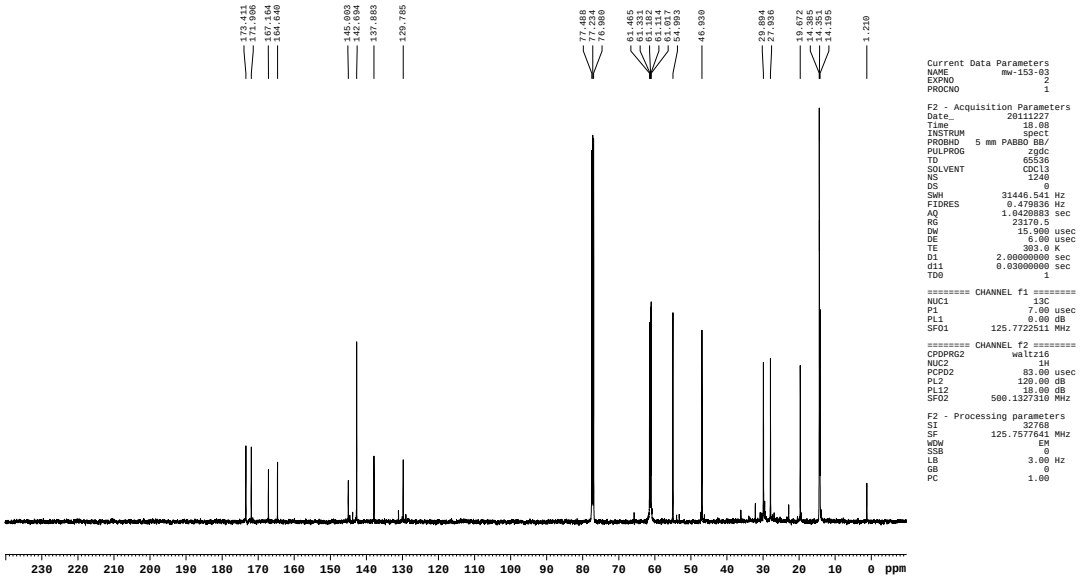

8.44
8.35
8.00
7.99
7.98
7.87
7.85
7.48
7.47
7.46
7.45
7.45
6.85
6.84
6.55
6.06
6.05
6.04
4.43
4.42
4.41
4.40
3.40
3.39
3.32
3.30
3.28
3.27
3.25
2.07
1.45
1.44
1.42
0.20
0.18
0.17
1.01
1.00
2.02
1.00
4.03
0.99
1.01
1.00
2.02
2.40
3.00
3.03
3.00
f1 (ppm)


171.62
167.86
137.26
135.48
135.25
132.19
131.59
130.96
130.31
129.93
128.42
128.19
127.52
127.29
126.00
125.88
125.66
125.35
125.13
124.99
121.09
61.36
60.39
49.59
17.86
14.41
12.80
f1 (ppm)



11



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Current Data Parameters
NAME                  mw-153-03
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_              20111227
Time                   10.08
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgdc
TD                    65536
SOLVENT               CDCl3
NS                     1240
DS                        0
SWH               31446.541 Hz
FIDRES             0.479836 Hz
AQ                1.0420883 sec
RG                   23170.5
DW                  15.900 usec
DE                   6.00 usec
TE                   303.0 K
D1                2.00000000 sec
d11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                     7.00 usec
PL1                    0.00 dB
SFO1            125.7722511 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                 83.00 usec
PL2                   120.00 dB
PL12                   18.00 dB
SFO2            500.1327310 MHz

F2 - Processing parameters
SI                     32768
SF              125.7577641 MHz
WDW                       EM
SSB                        0
LB                    3.00 Hz
GB                         0
PC                      1.00
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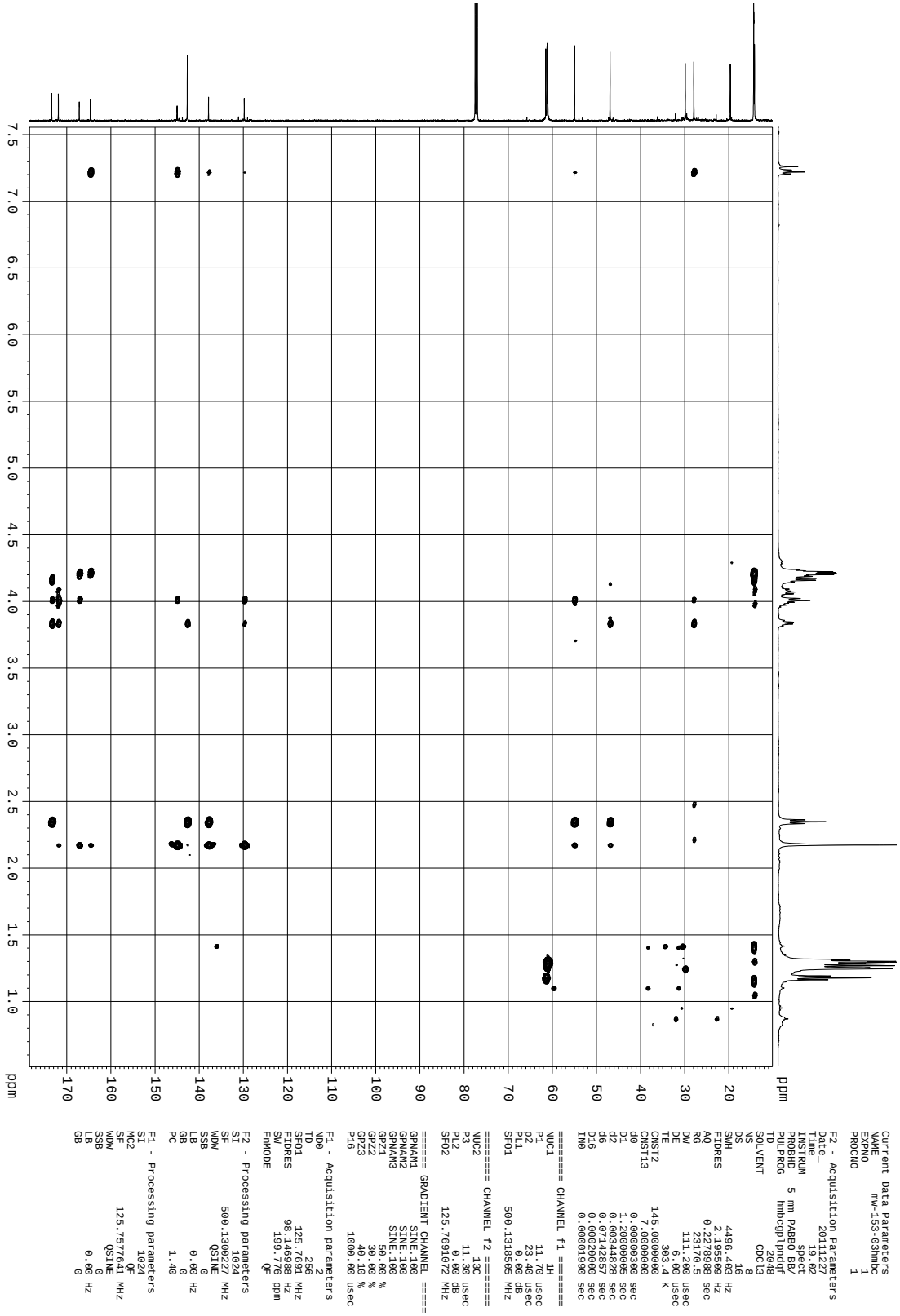
2D NMR HMBC

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Current Data Parameters
NAME                   mw-153-03hmbc
EXPNO                              1
PROCNO                             1

F2 - Acquisition Parameters
Date_                       20111227
Time                           19.02
INSTRUM                      spect
PROBHD     5 mm PABBO BB/
PULPROG                hmbcgplpndqf
TD                             2048
SOLVENT                       CDCl3
NS                                8
DS                               16
SWH                        4496.403 Hz
FIDRES                     2.195509 Hz
AQ                         0.2278988 sec
RG                            23170.5
DW                           111.200 usec
DE                             6.00 usec
TE                            303.4 K
CNST2                      145.0000000
CNST13                     7.0000000
d0                         0.00000300 sec
D1                         1.20000005 sec
d2                         0.00344828 sec
d6                         0.07142857 sec
D16                        0.00020000 sec
IN0                        0.00001990 sec

======== CHANNEL f1 ========
NUC1                             1H
P1                            11.70 usec
P2                            23.40 usec
PL1                            0.00 dB
SFO1                    500.1318505 MHz

======== CHANNEL f2 ========
NUC2                             13C
P3                            11.30 usec
PL2                            0.00 dB
SFO2                    125.7691072 MHz

====== GRADIENT CHANNEL =====
GPNAM1                    SINE.100
GPNAM2                    SINE.100
GPNAM3                    SINE.100
GPZ1                          50.00 %
GPZ2                          30.00 %
GPZ3                          40.10 %
P16                         1000.00 usec

F1 - Acquisition parameters
ND0                               2
TD                              256
SFO1                    125.7601693 MHz
FIDRES                   98.146993 Hz
SW                       199.7778 ppm
FnMODE                         QF

F2 - Processing parameters
SI                             1024
SF                      500.1300227 MHz
WDW                          QSINE
SSB                               0
LB                             0.00 Hz
GB                                0
PC                             1.40

F1 - Processing parameters
SI                             1024
MC2                              QF
SF                      125.7577641 MHz
WDW                          QSINE
SSB                               0
LB                             0.00 Hz
GB                                0
```
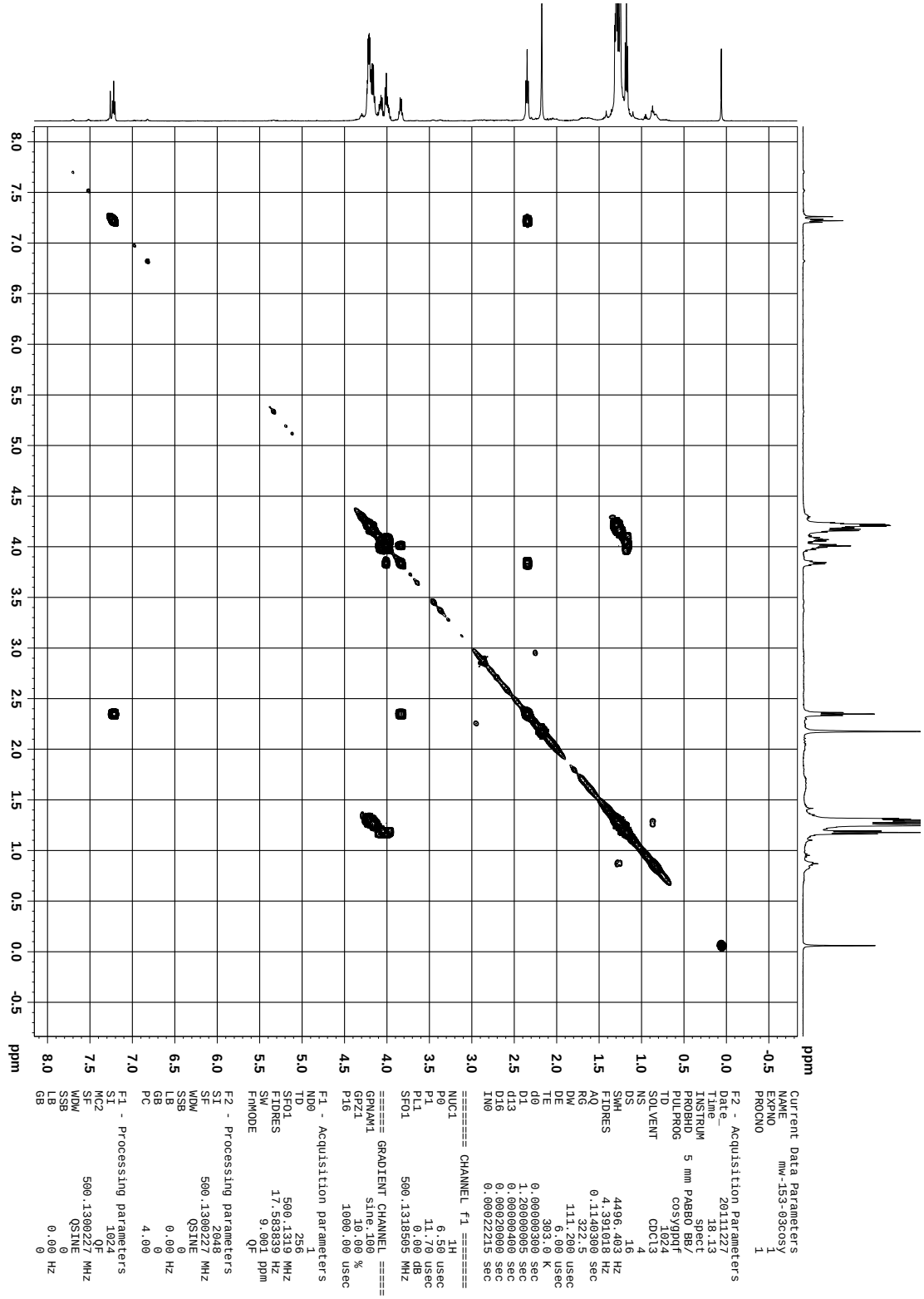
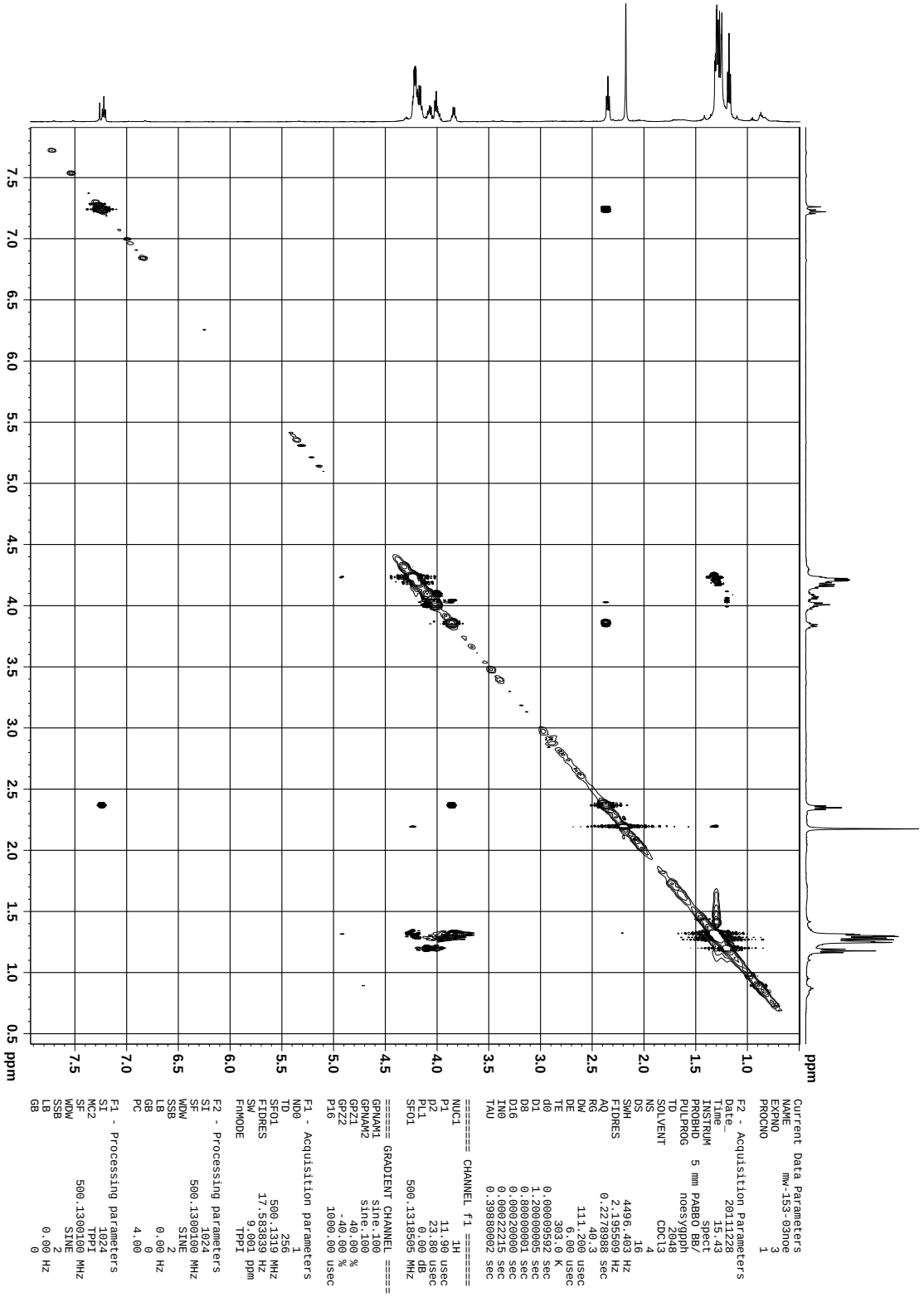
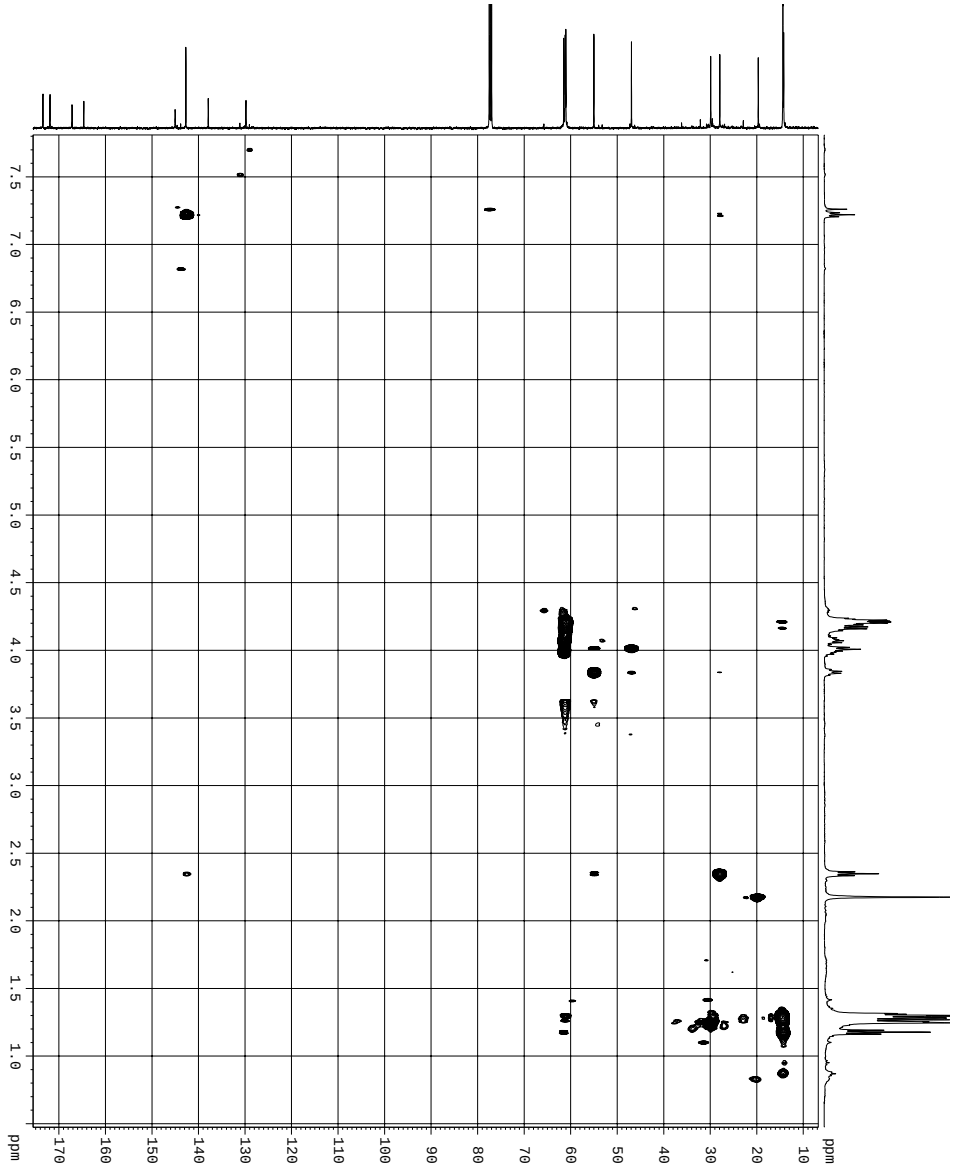

2D NMR COSY


ppm
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 0.0 -0.5
Current Data Parameters
NAME mv-153-03cosy
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111227
Time 18.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpqf
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4496.403 Hz
FIDRES 4.391018 Hz
AQ 0.1140300 sec
RG 322.5
DW 111.200 usec
DE 6.00 usec
TE 303.0 K
d0 0.00000300 sec
D1 1.20000005 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00022215 sec
======== CHANNEL f1 ========
NUC1 1H
P0 6.50 usec
P1 11.70 usec
PL1 0.00 dB
SFO1 500.1318505 MHz
====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPZ1 10.00 %
P16 1000.00 usec
F1 - Acquisition parameters
ND0 1
TD 256
SFO1 500.1319 MHz
FIDRES 17.583839 Hz
SW 9.001 ppm
FnMODE QF
F2 - Processing parameters
SI 2048
SF 500.1300227 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 4.00
F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300227 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR NOESY


ppm
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
Current Data Parameters
NAME mw-153-03noe
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111228
Time 15.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG noesygpph
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2278988 sec
RG 40.3
DW 111.200 usec
DE 6.00 usec
TE 303.0 K
d0 0.00000592 sec
D1 1.20000005 sec
D8 0.80000001 sec
D16 0.00022213 sec
TAU 0.39880002 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.00 dB
SFO1 500.1318505 MHz
====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
F1 - Acquisition parameters
ND0 1
TD 256
SFO1 500.1319 MHz
FIDRES 17.583839 Hz
SW 9.001 ppm
FnMODE TPPI
F2 - Processing parameters
SI 1024
SF 500.1300100 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0
PC 4.00
F1 - Processing parameters
SI 1024
MC2 TPPI
SF 500.1300100 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR HMQC




```
Current Data Parameters
NAME                   mw-153-03hsqc
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20111227
Time                         18.37
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                   hsqcetgpsi2
TD                        2048
SOLVENT                   CDCl3
NS                        16
DS                        4
SWH                       4496.403 Hz
FIDRES                    2.195509 Hz
AQ                        0.2278988 sec
RG                        64
DW                        111.200 usec
DE                        6.00 usec
TE                        303.8 K
CNST2                     145.0000000
D0                        0.00000300 sec
D1                        1.20000000 sec
d4                        0.00172414 sec
d11                       0.03000000 sec
D16                       0.00020000 sec
DELTA                     0.00127940 sec
DELTA1                    0.00120800 sec
DELTA2                    0.00147414 sec
DELTA3                    0.00016207 sec
DELTA4                    0.00027027 sec
IN0                       0.00001990 sec
ST1CNT                    128
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                        11.70 usec
p2                        23.40 usec
PL1                       60.00 dB
PL18                      60.00 dBm
SFO1                      500.1318905 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz
NUC2                      13C
P3                        11.30 usec
p4                        22.60 usec
P14                       500.00 usec
PCPD2                     [80 usec]
PL2                       0.00 dB
PL12                      14.50 dB
SFO2                      125.7691072 MHz
SPNAM3                    Crp60,0.5,20.1
SPNAM4                    Crp60,0.5,20.1
SPOAL3                    0.500
SPOFFS3                   0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1                    SINE.100
GPNAM2                    SINE.100
GPNAM3                    SINE.100
GPNAM4                    SINE.100
GPZ1                      80.00 %
GPZ2                      20.10 %
GPZ3                      11.00 %
GPZ4                      100.00 %
P19                       500.00 usec

F1 - Acquisition parameters
ND0                       256
TD                        256
SFO1                      125.7691 MHz
FIDRES                    98.146988 Hz
SW                        199.776 ppm
FnMODE                    Echo-AntiEcho

F2 - Processing parameters
SI                        2048
SF                        500.1300227 MHz
WDW                       QSINE
SSB                       0
LB                        0.00 Hz
GB                        0
PC                        1.40

F1 - Processing parameters
SI                        2048
MC2                       echo-antiecho
SF                        125.7577641 MHz
WDW                       QSINE
SSB                       0
LB                        0.00 Hz
GB                        0
```

5. Computational Details

All of the DFT calculations were performed with the Gaussian 03 program package.[4] The geometry optimization of all the minima and transition states involved were performed at the B3LYP[5] levels of theory with the hybrid 6-31G* basis set[6] used. The vibrational frequencies were computed at the same level of theory to check whether the optimized geometrical structure is at an energy minimum or a transition state and to evaluate the zero-point vibration energy (ZPE). IRC calculations[7] were used to confirm that each transition state is connected with its related reactant(s) and product(s). Solvent effects were computed by the CPCM[8] method at the B3LYP/6-31G* level using the gas phase optimized structures. These methods have been shown to give very good solvation energies that are comparable with the experimentally measured ones.[8e,9] This solvation method has also been widely applied in studying organic and organometallic reaction mechanisms.[10] Even though the calculated relative free energies for bi- and tri-molecular reactions in solution are somehow overestimated, it is still important to carry out such calculations in order to know how solvent affects reactions like the phosphine-triggered cycloaddition reactions.[10] E_0 is the ZPE corrected relative electronic energy in the gas phase. The G_{sol} values in dichloromethane were calculated by adding the solvation energies to the computed gas phase relative free energies (G_{298}).

4 Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

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6 W. J. Hehre, L. Radom, P. v. R. Schleyer and J. A. Pople, *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

7 (*a*) K. Fukui, *J. Phys. Chem.*, 1970, **74**, 4161; (*b*) C. Gonzalez and H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154; (*c*) C. Gonzalez and H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523.

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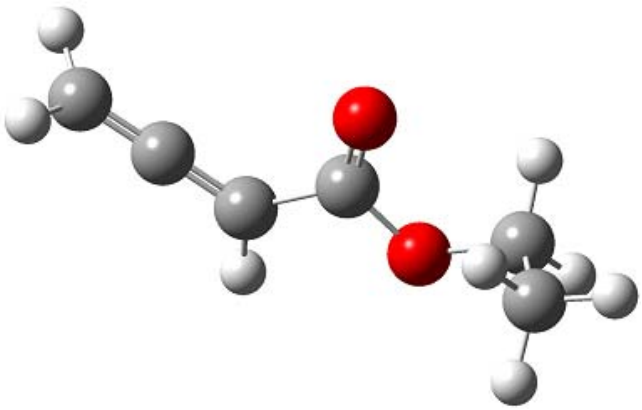
Coordinates and Geometries of All Stationary Points (Distances are in angstrom)

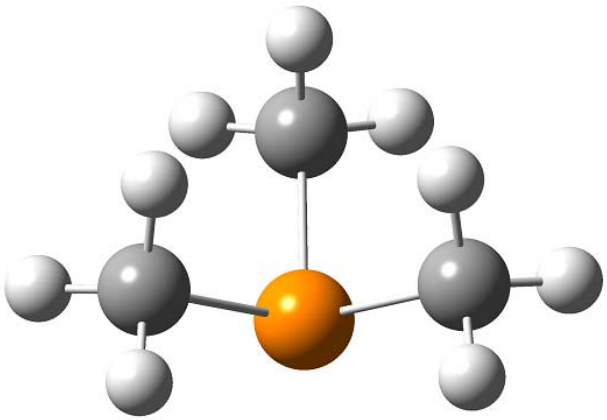
Standard coordinate and geometry of 1:



6	−3. 640974	0. 325793	0. 191556
1	−4. 032719	0. 786005	1. 096406
1	−4. 272172	0. 356316	−0. 694262
6	−2. 460010	−0. 222555	0. 164973
6	−1. 272925	−0. 785402	0. 140075
1	−1. 147705	−1. 839343	0. 377262
6	−0. 048522	−0. 017798	−0. 208893
8	1. 030864	−0. 837688	−0. 155855

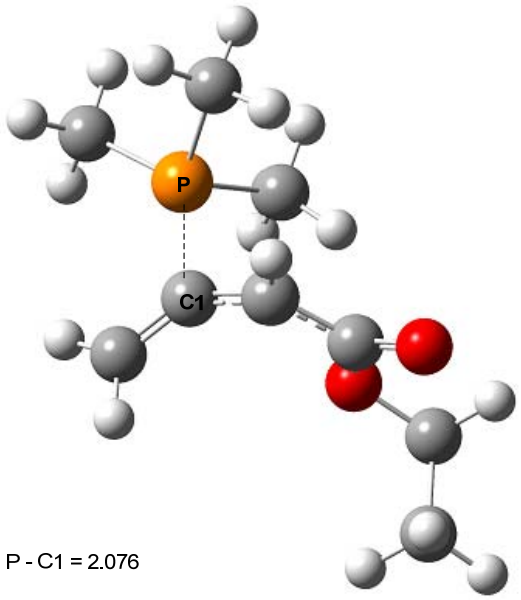
8	-0.001207	1.158705	-0.502862
6	2.307817	-0.236571	-0.469875
1	2.918921	-1.070164	-0.825409
1	2.168659	0.483768	-1.279857
6	2.925968	0.425506	0.753350
1	3.924224	0.805207	0.506184
1	2.311391	1.266647	1.086123
1	3.024012	-0.290411	1.576173

Standard coordinate and geometry of phosphine $P(CH_3)_3$:



15	-0.000720	-0.000776	-0.617982
6	1.132910	-1.196762	0.286675
1	0.885427	-2.224305	0.000129
1	2.171183	-1.008799	-0.006246
1	1.050837	-1.103927	1.376395
6	-1.604153	-0.380709	0.287048
1	-2.369613	0.346188	-0.003986
1	-1.960556	-1.375287	-0.000682
1	-1.483489	-0.349686	1.376694
6	0.472140	1.578484	0.285991
1	1.486894	1.874637	0.000395
1	-0.207002	2.386057	-0.006888
1	0.431735	1.460685	1.375630

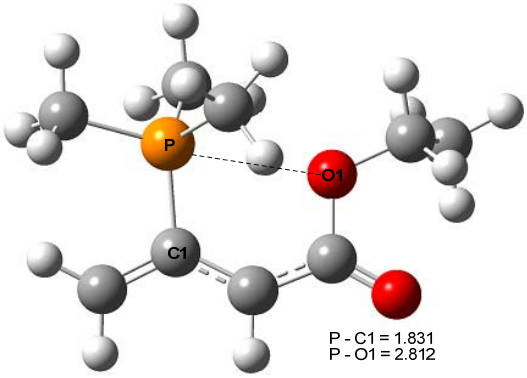
Standard coordinate and geometry of $TS_{1,3\text{-zwitterion}}$:



6	−0.618256	−0.674962	2.276219
1	−1.419257	−1.403440	2.378937
1	0.135543	−0.646538	3.060372
6	−0.515926	0.153844	1.238089
6	0.365460	1.144598	0.786020
6	1.585602	0.905479	0.071364
8	1.772342	−0.439931	−0.241662
8	2.404769	1.756019	−0.260915
6	3.025368	−0.763232	−0.861272
1	2.836926	−1.692820	−1.408977
1	3.293196	0.025111	−1.570283
6	4.132469	−0.952488	0.169164
1	5.060256	−1.271258	−0.321936
1	4.323590	−0.010204	0.690124
1	3.852264	−1.713620	0.905791
15	−2.061645	−0.132161	−0.118749
1	0.134584	2.191041	0.964759
6	−2.604359	1.570934	−0.584955
1	−3.270755	1.970528	0.185595
1	−1.716606	2.204569	−0.656808
1	−3.126596	1.565015	−1.546325

6	-3.672953	-1.082358	0.005767
1	-3.457565	-2.137958	0.195424
1	-4.263156	-0.691026	0.839663
1	-4.259222	-0.999207	-0.917130
6	-1.256908	-0.813100	-1.636312
1	-0.243729	-0.410400	-1.698601
1	-1.189328	-1.901376	-1.547163
1	-1.825335	-0.556995	-2.536095

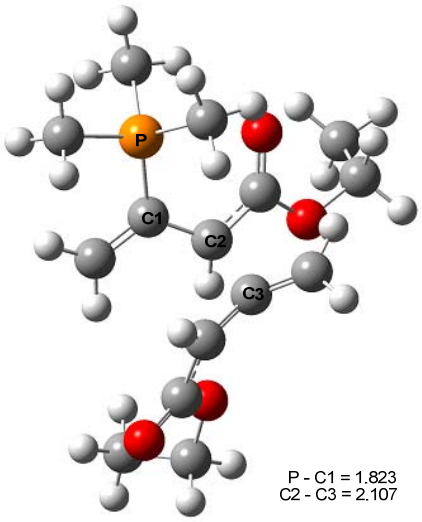
Standard coordinate and geometry of $IN_{1,3\text{-zwitterion}}$:



6	2.200930	1.988763	-0.699190
1	3.200627	1.583535	-0.773552
1	2.088823	3.038887	-0.953922
6	1.108683	1.287969	-0.250833
6	-0.178962	1.820340	0.032947
6	-1.423155	1.176826	0.208454
8	-1.339477	-0.241803	0.079460
8	-2.511529	1.689637	0.457436
6	-2.551713	-0.954613	0.364152
1	-2.233853	-1.950724	0.697485
1	-3.075665	-0.453553	1.182099
6	-3.456636	-1.052054	-0.858268
1	-4.349875	-1.644937	-0.624980
1	-3.771773	-0.050658	-1.161424
1	-2.939490	-1.530587	-1.698732
15	1.462795	-0.480371	0.064672
1	-0.243183	2.904300	0.036305

6	3.285301	−0.767764	0.134526
1	3.749849	−0.546891	−0.828452
1	3.736439	−0.139565	0.905869
1	3.457126	−1.821344	0.377090
6	0.921170	−1.601685	−1.290108
1	1.454618	−1.311354	−2.200053
1	1.165131	−2.638971	−1.039774
1	−0.151187	−1.481474	−1.434208
6	0.856916	−1.046941	1.714223
1	0.281554	−0.229266	2.150783
1	0.211388	−1.920430	1.611006
1	1.710381	−1.289112	2.353793

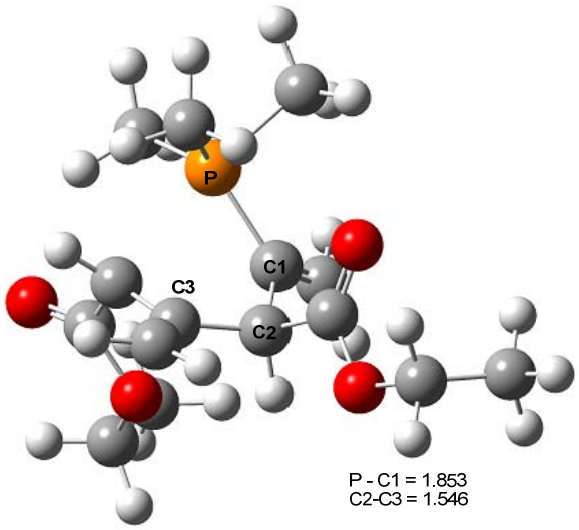
Standard coordinate and geometry of $TS_{1,5\text{-zwitterion}}$:



6	1.889921	−0.832938	1.449438
1	1.840055	−1.827882	1.882754
6	3.096926	−0.564920	0.708378
8	3.063724	0.665417	0.071010
8	4.070250	−1.305427	0.622984
6	4.266188	1.052756	−0.609951
1	4.241061	2.147048	−0.620220
1	5.130136	0.717229	−0.029867
6	0.844526	0.042439	1.634651
6	−0.155532	0.370786	−0.190712
1	0.743235	0.826960	−0.594436

6	0.212258	0.709996	2.591297
1	-0.740324	1.212559	2.456836
1	0.671543	0.801803	3.575201
6	-1.257264	1.283718	-0.008794
8	-2.447132	0.957464	0.148726
8	-0.862719	2.578661	0.043520
6	-1.876231	3.569067	0.300393
1	-1.337350	4.393474	0.775070
1	-2.607690	3.163572	1.004189
6	-0.410337	-0.975326	-0.663928
6	0.576713	-1.750706	-1.189038
1	0.470457	-2.802097	-1.423587
1	1.532660	-1.303382	-1.436657
15	-1.977349	-1.819513	-0.270627
6	-2.552149	4.021899	-0.987245
1	-3.108983	3.195408	-1.438497
1	-3.254505	4.837308	-0.777137
1	-1.810853	4.382715	-1.707931
6	4.329331	0.494766	-2.027191
1	3.449817	0.798681	-2.606721
1	5.223027	0.867711	-2.542841
1	4.378813	-0.597393	-1.998412
6	-2.490966	-1.685471	1.489238
1	-1.604249	-1.812238	2.115671
1	-2.907132	-0.693015	1.654821
1	-3.226939	-2.463484	1.714096
6	-3.380949	-1.397664	-1.382408
1	-4.245975	-2.018610	-1.128548
1	-3.616815	-0.342062	-1.254805
1	-3.081019	-1.598488	-2.415097
6	-1.748118	-3.632714	-0.530624
1	-0.946403	-4.007076	0.110129
1	-2.683111	-4.138687	-0.271779
1	-1.508110	-3.850404	-1.573788

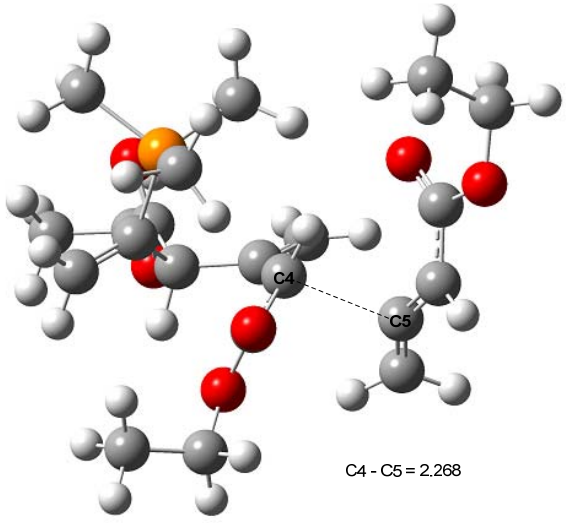
Standard coordinate and geometry of $IN_{1,5\text{-zwitterion}}$:



6	-1.215075	0.026232	1.417253
1	-1.534557	0.537153	2.325682
6	-2.324087	-0.753912	0.887622
8	-1.934921	-1.865090	0.175857
8	-3.512384	-0.463107	1.015316
6	-2.991046	-2.667479	-0.380634
1	-2.555565	-3.666690	-0.477604
1	-3.821407	-2.704297	0.329073
6	0.153283	-0.522607	1.451216
6	0.774044	-0.625833	0.039439
1	0.658238	-1.651470	-0.324702
6	0.864481	-0.766660	2.562213
1	1.909734	-1.061529	2.537945
1	0.403892	-0.689472	3.543390
6	2.255328	-0.268418	0.043234
8	2.697406	0.864169	-0.025444
8	3.027443	-1.367413	0.148073
6	4.461360	-1.155887	0.204173
1	4.840174	-2.033843	0.732617
1	4.661169	-0.259401	0.795911
6	0.039166	0.317939	-0.896145
6	-0.228849	0.018565	-2.170040
1	-0.754655	0.690310	-2.842231

1	0.058493	-0.944294	-2.588613
15	-0.674481	1.843214	-0.122501
6	5.057788	-1.041436	-1.190728
1	4.678718	-0.150403	-1.698815
1	6.148831	-0.960769	-1.122138
1	4.815621	-1.924139	-1.791706
6	-3.464724	-2.142238	-1.730154
1	-2.631477	-2.073103	-2.438016
1	-4.220366	-2.815903	-2.152408
1	-3.913207	-1.151973	-1.612607
6	0.196886	2.628625	1.313782
1	-0.197863	2.292814	2.269961
1	1.253834	2.364251	1.233252
1	0.089738	3.713033	1.216065
6	-2.477706	2.256302	-0.250901
1	-2.804657	2.065559	-1.278149
1	-3.085596	1.666121	0.435491
1	-2.583352	3.328340	-0.054123
6	-0.057353	3.096000	-1.415939
1	-0.451642	2.875780	-2.412296
1	-0.363350	4.112801	-1.146926
1	1.035156	3.049268	-1.458300

Standard coordinate and geometry of $TS_{1,7\text{-zwitterion}}$:

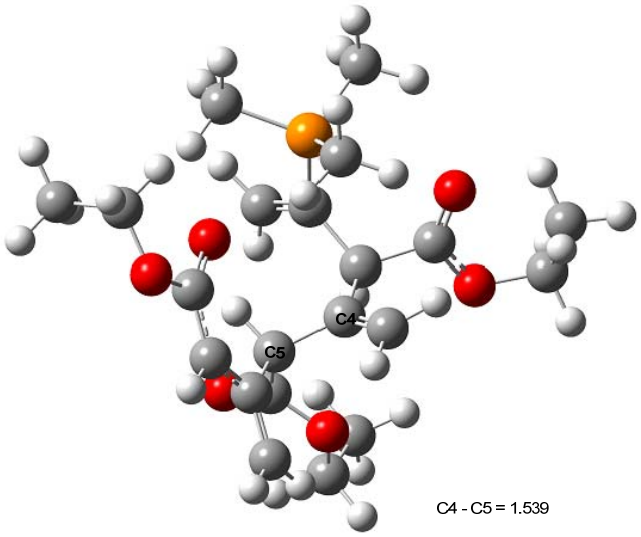


6	-0.575613	0.698632	-0.416873

1	-1.349615	-0.011372	-0.165783
6	-0.593107	1.889309	0.381702
8	0.389261	2.806062	0.032026
8	-1.412834	2.147804	1.269900
6	0.255771	4.117264	0.604372
1	0.713339	4.790181	-0.127967
1	-0.806580	4.356557	0.696346
6	0.615382	0.144180	-1.088750
6	1.923944	0.231832	-0.269256
1	2.339712	1.238177	-0.384900
6	0.565425	-0.534794	-2.246609
1	1.430904	-1.036797	-2.669688
1	-0.362816	-0.607834	-2.799499
6	2.967498	-0.789224	-0.695958
8	3.063190	-1.909569	-0.218041
8	3.761862	-0.319813	-1.668926
6	4.767614	-1.221875	-2.199498
1	4.930885	-0.867398	-3.219648
1	4.354118	-2.232650	-2.226235
6	1.635221	0.029512	1.212075
6	2.189198	0.793081	2.163053
1	2.010241	0.657107	3.226503
1	2.832603	1.625894	1.894084
15	0.526776	-1.314608	1.790252
6	6.044860	-1.165830	-1.375404
1	5.867426	-1.537961	-0.362279
1	6.814307	-1.791840	-1.841657
1	6.425490	-0.140963	-1.316149
6	0.942148	4.242365	1.959183
1	2.009761	4.004877	1.884985
1	0.849538	5.269100	2.334545
1	0.474492	3.566944	2.680571
6	-2.101430	1.386954	-1.947950
6	-1.391371	2.085808	-2.816728

1	-0.394936	2.456355	-2.604248
1	-1.799792	2.284205	-3.807903
6	-3.335886	0.963982	-1.558907
1	-4.119412	1.698325	-1.392995
6	-3.634585	-0.398166	-1.209056
8	-2.848705	-1.351660	-1.156338
8	-4.965117	-0.552487	-0.901196
6	-5.390117	-1.870738	-0.534924
1	-6.448843	-1.911519	-0.809476
1	-4.837360	-2.607941	-1.123822
6	-5.206231	-2.126556	0.956940
1	-5.610672	-3.109590	1.228368
1	-4.142696	-2.106038	1.213324
1	-5.723533	-1.363632	1.548397
6	-0.832763	-0.624564	2.815990
1	-0.430387	-0.309185	3.783380
1	-1.279008	0.242789	2.311220
1	-1.584212	-1.403144	2.979569
6	1.554238	-2.375587	2.897265
1	2.364146	-2.798217	2.297147
1	1.979813	-1.781126	3.709490
1	0.941815	-3.177816	3.320068
6	-0.142889	-2.482673	0.546696
1	0.676197	-2.800912	-0.099642
1	-0.517814	-3.342560	1.113399
1	-0.953830	-2.053062	-0.046860

Standard coordinate and geometry of $IN_{1,7\text{-zwitterion}}$:

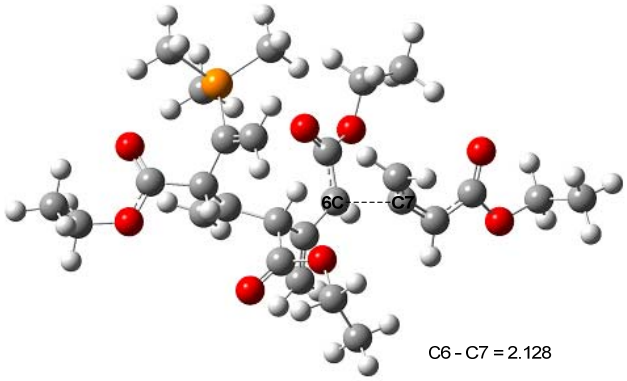


6	−0.263338	1.642174	−0.087698
1	−0.910631	1.135718	0.630730
6	0.631655	2.536531	0.767359
8	1.760232	2.925191	0.119428
8	0.397571	2.836997	1.921924
6	2.651323	3.807497	0.835987
1	3.168413	4.366957	0.052152
1	2.058019	4.495656	1.442654
6	0.548373	0.560359	−0.794781
6	1.300057	−0.370144	0.178926
1	1.885811	0.280532	0.838155
6	0.626574	0.434358	−2.119973
1	1.196839	−0.354163	−2.603798
1	0.113076	1.142962	−2.760822
6	2.305975	−1.261327	−0.529638
8	2.062036	−2.380818	−0.953150
8	3.493913	−0.660308	−0.645707
6	4.536500	−1.368929	−1.367933
1	5.160851	−0.572832	−1.778601
1	4.077457	−1.930411	−2.184613
6	0.366684	−1.161845	1.095035
6	0.229093	−0.814738	2.380748
1	−0.462623	−1.297489	3.063086

1	0.785126	0.025031	2.790278
15	-0.660380	-2.568783	0.500025
6	5.324427	-2.278640	-0.438131
1	4.689194	-3.078887	-0.047140
1	6.154564	-2.737669	-0.986842
1	5.739454	-1.712534	0.401913
6	3.634192	3.024060	1.695550
1	4.170323	2.283028	1.092206
1	4.369876	3.703430	2.142092
1	3.108048	2.511020	2.506114
6	-1.193618	2.448607	-1.011177
6	-0.723523	3.565450	-1.629804
1	0.292986	3.916606	-1.506374
1	-1.373390	4.148789	-2.277132
6	-2.545225	1.978395	-1.161188
1	-3.211120	2.611055	-1.740338
6	-3.109880	0.813264	-0.665540
8	-2.582801	-0.138336	-0.000773
8	-4.468261	0.709729	-1.005593
6	-5.213426	-0.344173	-0.421003
1	-6.065655	-0.502836	-1.092467
1	-4.619315	-1.265297	-0.396772
6	-5.704888	0.006150	0.983065
1	-6.333612	-0.797236	1.389648
1	-4.853888	0.159033	1.654049
1	-6.294215	0.929182	0.962536
6	0.233755	-4.146293	0.824674
1	1.138056	-4.182008	0.216798
1	0.496487	-4.201653	1.885011
1	-0.422356	-4.985659	0.573429
6	-2.204313	-2.642324	1.480619
1	-1.994313	-2.812242	2.539222
1	-2.722597	-1.691252	1.306799
1	-2.804914	-3.475990	1.103119

6	−1.134115	−2.502303	−1.260468
1	−0.242143	−2.488323	−1.885054
1	−1.733554	−3.393258	−1.475487
1	−1.733765	−1.593935	−1.371725

Standard coordinate and geometry of $TS_{1,9\text{-zwitterion}}$:

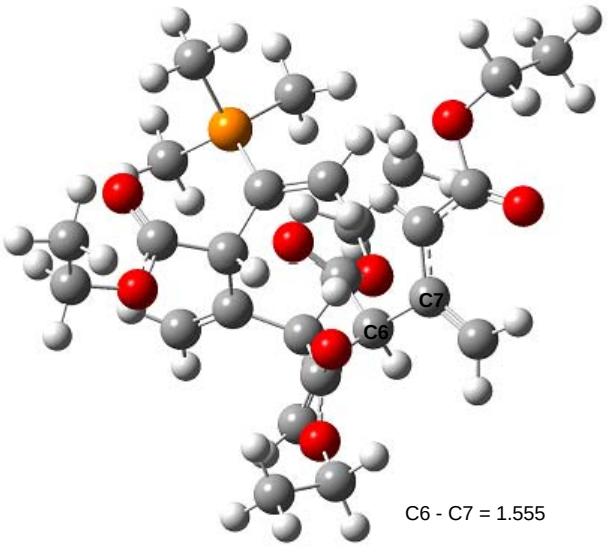


6	0.638116	1.190280	−0.280859
1	0.342021	0.572659	0.568245
6	0.901503	2.594131	0.266307
8	0.064809	2.866851	1.287217
8	1.752674	3.362165	−0.140954
6	0.061430	4.220284	1.798140
1	−0.242183	4.115132	2.842919
1	1.077404	4.620781	1.750623
6	1.916731	0.599861	−0.867869
6	3.025908	0.378127	0.178585
1	3.132784	1.329803	0.711396
6	2.091529	0.330291	−2.162125
1	3.014007	−0.089711	−2.553310
1	1.303740	0.539013	−2.877082
6	4.380242	0.093954	−0.454373
8	4.820359	−1.028577	−0.659415
8	5.020598	1.218921	−0.763663
6	6.305125	1.104633	−1.435377
1	6.378612	2.025438	−2.017004
1	6.271917	0.246666	−2.110582
6	2.660828	−0.671244	1.228039

6	2.350146	-0.305653	2.477859
1	2.038186	-1.000231	3.251221
1	2.373662	0.741816	2.769045
15	2.613245	-2.479323	0.862625
6	7.438156	0.982077	-0.428903
1	7.358457	0.048168	0.135309
1	8.399419	0.983251	-0.954961
1	7.429179	1.823069	0.271616
6	-0.918404	5.085129	1.019497
1	-1.918693	4.642144	1.034873
1	-0.969793	6.085308	1.465651
1	-0.599044	5.188185	-0.021784
6	-0.553525	1.217630	-1.249592
6	-0.669170	2.237542	-2.129338
1	0.052096	3.047591	-2.169582
1	-1.502396	2.283256	-2.825118
6	-1.561255	0.160048	-1.160938
1	-2.318053	0.214748	-1.934031
6	-1.291365	-1.183823	-0.747149
8	-0.344930	-1.593197	-0.029800
8	-2.267359	-2.040050	-1.161875
6	-2.451861	-3.249536	-0.415373
1	-1.676254	-3.978133	-0.691830
1	-2.347049	-3.031369	0.653199
6	-3.849362	-3.758791	-0.725967
1	-4.035693	-4.697965	-0.190705
1	-4.587127	-3.015296	-0.408466
1	-3.966446	-3.944813	-1.799423
8	-5.449945	-0.905936	0.596913
6	-5.316713	0.144578	-0.030998
6	-4.147352	0.970020	-0.168848
8	-6.380854	0.701454	-0.729080
6	-2.948711	0.605242	0.389783
1	-4.210388	1.810144	-0.854803

6	-7.622527	-0.000718	-0.640222
6	-2.370386	0.362776	1.557972
1	-8.171969	0.277927	-1.546262
1	-7.434903	-1.078473	-0.651624
6	-8.405760	0.386754	0.610349
1	-2.858193	0.702180	2.470424
1	-1.437923	-0.180460	1.667021
1	-9.386858	-0.105238	0.616668
1	-7.856680	0.078049	1.504329
1	-8.562668	1.470601	0.649331
6	1.284364	-3.266502	1.847915
1	1.426873	-3.104387	2.918452
1	0.337759	-2.841503	1.497867
1	1.311018	-4.342738	1.649278
6	4.196766	-3.237414	1.412637
1	5.011714	-2.832717	0.812131
1	4.361551	-3.006642	2.468868
1	4.136640	-4.322875	1.286406
6	2.304349	-2.931646	-0.878702
1	3.092041	-2.528000	-1.512549
1	2.297606	-4.025365	-0.934236
1	1.321304	-2.531397	-1.138351

Standard coordinate and geometry of $IN_{1,9\text{-zwitterion}}$:

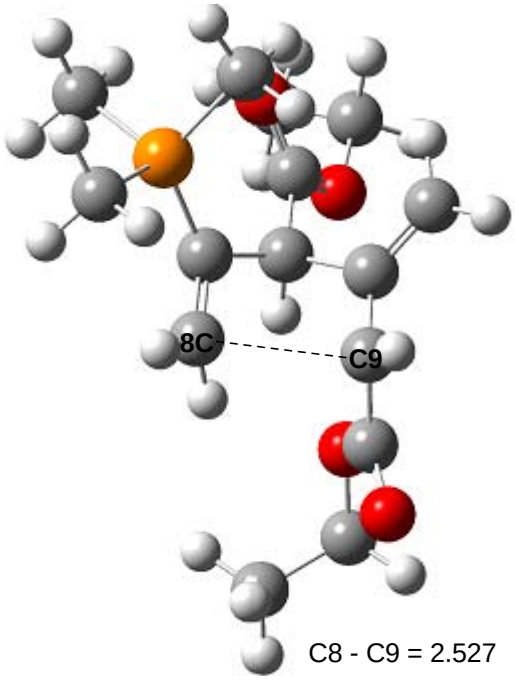


6	-0.777889	1.491499	0.279727
1	-0.051198	0.995227	-0.371305
6	-1.591573	2.332188	-0.720456
8	-1.988575	3.526170	-0.260392
8	-1.877453	1.915370	-1.831264
6	-2.754483	4.353434	-1.170812
1	-2.565136	5.373015	-0.826935
1	-2.353529	4.228388	-2.178930
6	-1.700314	0.379498	0.809872
6	-2.002918	-0.690040	-0.257430
1	-2.272060	-0.138804	-1.165096
6	-2.183043	0.321445	2.053064
1	-2.837504	-0.482446	2.379233
1	-1.923362	1.067415	2.795040
6	-3.206516	-1.552347	0.078851
8	-3.155393	-2.698777	0.499209
8	-4.350909	-0.897555	-0.150003
6	-5.591483	-1.592538	0.140250
1	-6.300164	-0.790122	0.356269
1	-5.450990	-2.205086	1.033957
6	-0.747733	-1.487400	-0.614956
6	0.009973	-1.098157	-1.664995
1	0.955710	-1.544371	-1.949228
1	-0.339275	-0.295216	-2.309736
15	-0.097241	-2.848851	0.400681
6	-6.039965	-2.432469	-1.045881
1	-5.326952	-3.238581	-1.240962
1	-7.016631	-2.881736	-0.832672
1	-6.133577	-1.816389	-1.945808
6	-4.235486	4.008811	-1.115263
1	-4.618577	4.097935	-0.093133
1	-4.800888	4.695615	-1.755887
1	-4.404961	2.988258	-1.469749
6	0.040014	2.265620	1.301637

6	-0.477412	3.126901	2.185382
1	-1.538356	3.346230	2.232370
1	0.162443	3.673688	2.874548
6	1.560723	2.074899	1.236487
1	2.018729	2.965084	1.674526
6	2.026937	0.910341	2.095588
8	1.444843	-0.154139	2.247476
8	3.204817	1.199082	2.683519
6	3.881828	0.150777	3.410871
1	4.302453	0.641993	4.292736
1	3.147241	-0.592256	3.728962
6	4.972619	-0.460632	2.542750
1	5.512130	-1.233038	3.103803
1	4.546313	-0.914195	1.642264
1	5.689035	0.303688	2.226702
8	3.207302	1.121150	-2.923782
6	2.908291	0.366446	-1.998533
6	2.335307	0.642852	-0.736291
8	3.126057	-1.046218	-2.156406
6	2.103518	1.968395	-0.216403
1	2.260389	-0.193642	-0.059858
6	3.823026	-1.420101	-3.347710
6	2.247832	3.149252	-0.871678
1	3.522474	-2.455288	-3.551434
1	3.495311	-0.783422	-4.174327
6	5.335421	-1.320077	-3.175435
1	2.581011	3.172409	-1.901539
1	2.041489	4.092958	-0.373286
1	5.850475	-1.676273	-4.076731
1	5.620209	-0.278267	-3.003555
1	5.672991	-1.922415	-2.323880
6	-0.647278	-4.466595	-0.285360
1	-1.736781	-4.507234	-0.252979
1	-0.304225	-4.546424	-1.320931

1	-0.220602	-5.285537	0.302378
6	1.740534	-2.875071	0.389115
1	2.167717	-2.632885	-0.587296
1	2.075235	-2.123804	1.108643
1	2.070112	-3.869265	0.707977
6	-0.543621	-2.791804	2.177049
1	-1.621487	-2.890537	2.294805
1	-0.032673	-3.621769	2.676099
1	-0.187300	-1.841536	2.581218

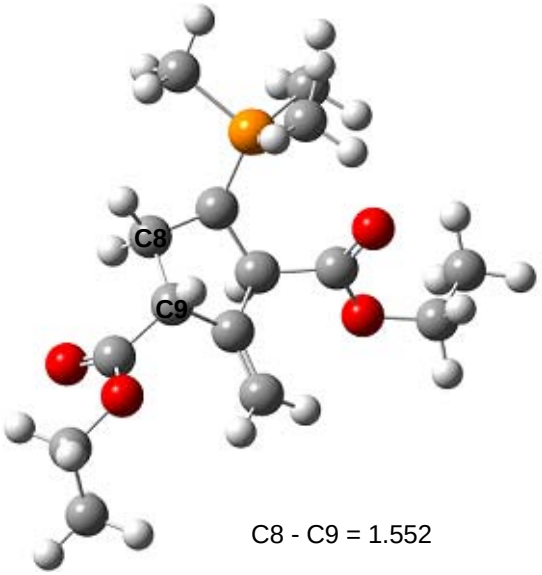
Standard coordinate and geometry of TS_{RC}-1:



6	1.737428	-0.846817	1.346653
1	1.827442	-1.609140	2.115439
6	3.003466	-0.502958	0.771305
8	2.928950	0.585713	-0.106643
8	4.070414	-1.085208	0.947743
6	4.170148	1.001238	-0.691839
1	4.032336	2.062924	-0.922989
1	4.967358	0.894150	0.048478
6	0.565828	0.008942	1.426675
6	-0.082458	0.374870	0.037703
1	0.722094	0.841286	-0.540021

6	-0.088016	0.300131	2.567200
1	-1.044121	0.818209	2.587354
1	0.336098	0.040737	3.533545
6	-1.208009	1.370825	0.128443
8	-2.398631	1.085198	0.182557
8	-0.755585	2.631164	0.163512
6	-1.730397	3.690493	0.319517
1	-1.181091	4.486507	0.827416
1	-2.537698	3.336468	0.964938
6	-0.418221	-0.964769	-0.587072
6	0.728070	-1.712219	-0.802376
1	0.725593	-2.789053	-0.939782
1	1.618659	-1.211729	-1.157791
15	-1.965854	-1.805990	-0.364262
6	-2.260906	4.151960	-1.029824
1	-2.822881	3.351121	-1.519424
1	-2.931625	5.008006	-0.892506
1	-1.440201	4.459741	-1.685758
6	4.506566	0.207407	-1.949112
1	3.698246	0.281834	-2.686343
1	5.425633	0.591248	-2.409604
1	4.660067	-0.844562	-1.693453
6	-1.721716	-3.594626	-0.741062
1	-1.308942	-3.723235	-1.744176
1	-1.043052	-4.043334	-0.011379
1	-2.690576	-4.099357	-0.685635
6	-2.760016	-1.801530	1.304567
1	-2.036597	-2.159550	2.040577
1	-3.047852	-0.779622	1.549575
1	-3.641959	-2.451278	1.294591
6	-3.273251	-1.279443	-1.556292
1	-3.514044	-0.232583	-1.371875
1	-2.889654	-1.396990	-2.573629
1	-4.167714	-1.897899	-1.427898

Standard coordinate and geometry of IN_{RC}-1:

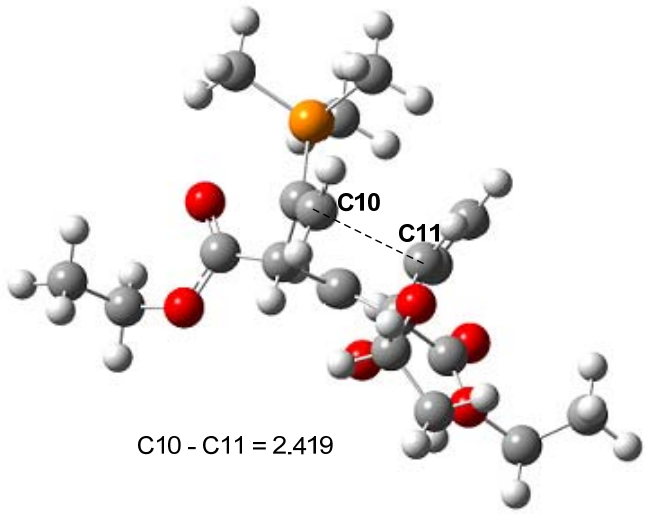


C8 - C9 = 1.552

6	1.581794	-0.549743	0.111796
1	1.539945	-0.892070	1.153111
6	3.039994	-0.416306	-0.285373
8	3.819985	-0.161163	0.797065
8	3.475793	-0.524423	-1.412622
6	5.236892	-0.006795	0.549228
1	5.708155	-0.268860	1.500195
1	5.539768	-0.725360	-0.216578
6	0.826287	0.777325	0.005305
6	-0.554227	0.490343	-0.650383
1	-0.502780	0.905617	-1.671612
6	1.279592	1.964815	0.407787
1	0.689617	2.868960	0.294372
1	2.260766	2.070277	0.862439
6	-1.650650	1.266321	0.053367
8	-2.394174	0.834347	0.916886
8	-1.707096	2.541374	-0.389673
6	-2.672880	3.418127	0.238981
1	-2.231008	4.413877	0.151821
1	-2.760714	3.150467	1.294419
6	-0.665643	-1.027865	-0.684424
6	0.770940	-1.515078	-0.793555

1	0.933087	-2.558952	-0.505057
1	1.160217	-1.411803	-1.817831
15	-1.865854	-2.000296	0.056317
6	-4.019762	3.346108	-0.465169
1	-4.460793	2.351097	-0.355300
1	-4.709173	4.076950	-0.026657
1	-3.913792	3.569438	-1.531786
6	5.582090	1.415255	0.130718
1	5.252119	2.135837	0.886716
1	6.667396	1.515823	0.011674
1	5.107174	1.659727	-0.823404
6	-1.555252	-3.757410	-0.436300
1	-1.460360	-3.825661	-1.522184
1	-0.635517	-4.126519	0.025330
1	-2.386704	-4.382635	-0.097009
6	-2.128637	-2.190678	1.914597
1	-1.195005	-2.540004	2.368055
1	-2.377095	-1.210161	2.324275
1	-2.927875	-2.904861	2.146796
6	-3.586361	-1.653554	-0.535921
1	-3.911167	-0.684883	-0.153364
1	-3.591520	-1.638904	-1.628789
1	-4.268055	-2.429223	-0.171555

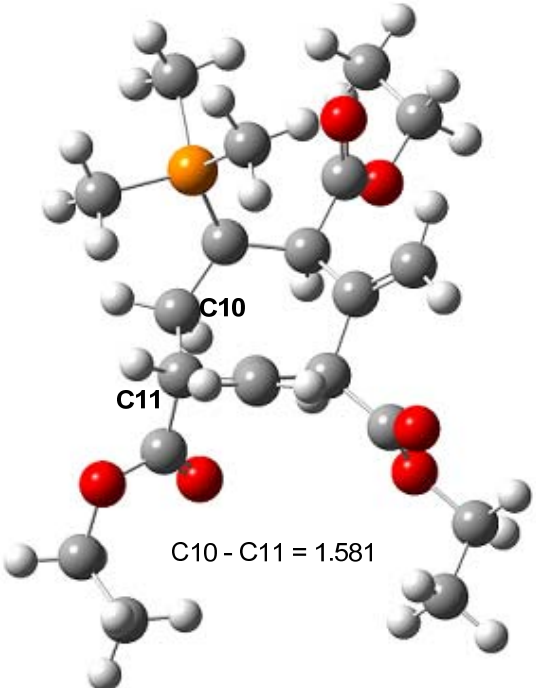
Standard coordinate and geometry of TS_{RC}-2:



6	0.995125	-1.040266	0.083618
1	1.316119	-0.532651	0.997492
6	1.901740	-2.255549	-0.077028
8	3.064615	-2.037352	0.575844
8	1.678043	-3.268521	-0.712984
6	4.093842	-3.040287	0.427591
1	4.701210	-2.939268	1.330636
1	3.627414	-4.028479	0.411509
6	-0.496778	-1.342524	0.212155
6	-1.325340	-0.109164	0.633696
1	-0.792966	0.337929	1.482055
6	-1.055445	-2.547054	0.047641
1	-2.120980	-2.704098	0.191204
1	-0.466381	-3.405914	-0.246379
6	-2.699093	-0.505266	1.150235
8	-3.703770	-0.599079	0.460052
8	-2.680176	-0.753435	2.466766
6	-3.916905	-1.191191	3.083993
1	-3.591309	-1.795532	3.933691
1	-4.460495	-1.820977	2.375903
6	-1.387768	0.984371	-0.434325
6	-0.530419	2.055920	-0.300713
1	-0.493181	2.870084	-1.016201
1	-0.135616	2.283639	0.682877
15	-2.355876	0.849665	-1.919257
6	-4.756977	-0.004568	3.531569
1	-5.089137	0.581997	2.669984
1	-5.644447	-0.359865	4.067824
1	-4.186183	0.644886	4.203007
6	4.918843	-2.798681	-0.828602
1	5.349413	-1.792174	-0.821428
1	5.737320	-3.526253	-0.884591
1	4.298008	-2.908259	-1.722390
6	1.312231	-0.071111	-1.088692

6	1.120998	-0.531918	-2.353350
1	0.833487	-1.560716	-2.544575
1	1.382657	0.077585	-3.216170
6	1.703586	1.282395	-0.811291
1	1.993454	1.871946	-1.677840
6	2.199436	1.786980	0.437308
8	2.013596	1.346016	1.578753
8	2.872287	2.979602	0.248472
6	3.355564	3.630701	1.431091
1	3.420320	4.690025	1.161071
1	2.627756	3.508490	2.238347
6	4.716674	3.091442	1.855719
1	5.099950	3.657826	2.713605
1	4.630034	2.040352	2.144746
1	5.439477	3.174309	1.036576
6	-4.033349	1.616139	-1.758615
1	-4.592781	1.064403	-1.001885
1	-3.917492	2.655990	-1.439334
1	-4.564100	1.586679	-2.716084
6	-2.654173	-0.840878	-2.572913
1	-1.694558	-1.330247	-2.744235
1	-3.235791	-1.404939	-1.843767
1	-3.212982	-0.756589	-3.510656
6	-1.567483	1.796733	-3.288308
1	-2.174160	1.685955	-4.192337
1	-1.502369	2.858335	-3.037451
1	-0.566155	1.395353	-3.456232

Standard coordinate and geometry of IN_{RC}-2:

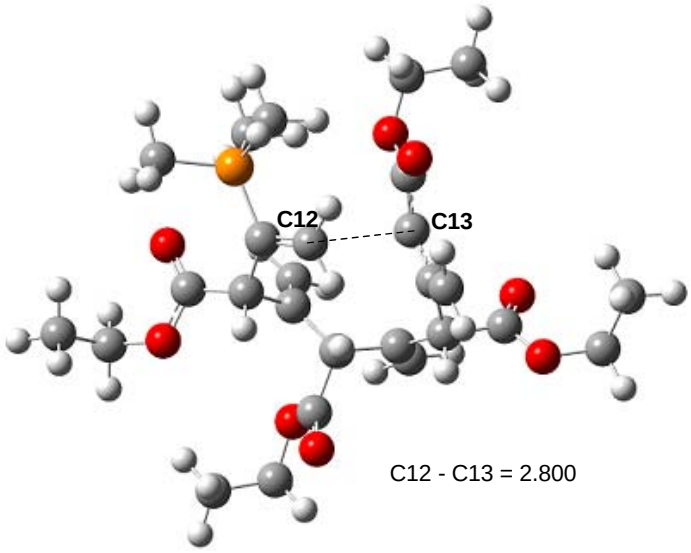


6	0.922942	0.947757	0.309656
1	1.102405	0.904632	-0.768114
6	1.811201	2.074665	0.824400
8	2.321047	2.772921	-0.213019
8	2.031544	2.351852	1.987605
6	3.170735	3.897451	0.112731
1	3.079269	4.562258	-0.749864
1	2.773657	4.395574	1.000672
6	-0.569903	1.261725	0.521942
6	-1.455684	0.490428	-0.469584
1	-1.061170	0.721450	-1.469246
6	-1.022520	2.075548	1.480687
1	-2.084317	2.260033	1.611521
1	-0.352365	2.560206	2.182625
6	-2.878105	1.017565	-0.473949
8	-3.734338	0.751227	0.355374
8	-3.098040	1.844245	-1.514462
6	-4.413523	2.439158	-1.622500
1	-4.238216	3.390999	-2.130013
1	-4.800159	2.627922	-0.618301

6	-1.364036	-1.029553	-0.306070
6	-0.128843	-1.639643	-0.931779
1	-0.272926	-2.684454	-1.235759
1	0.079551	-1.097677	-1.864515
15	-2.318929	-1.931627	0.804313
6	-5.355126	1.549312	-2.420625
1	-5.534309	0.606256	-1.895969
1	-6.318473	2.054265	-2.557598
1	-4.937998	1.328591	-3.408547
6	4.611363	3.455420	0.325583
1	4.984664	2.916299	-0.551271
1	5.249896	4.331121	0.491156
1	4.687151	2.803844	1.200698
6	1.287764	-0.428741	0.885019
6	1.657445	-0.616994	2.156273
1	1.742278	0.207767	2.854553
1	1.904524	-1.611081	2.522435
6	1.200147	-1.610576	-0.075183
1	1.255704	-2.521293	0.526994
6	2.407386	-1.612076	-1.001463
8	2.629026	-0.770799	-1.852009
8	3.205881	-2.683860	-0.784835
6	4.388757	-2.787848	-1.612809
1	4.610438	-3.858055	-1.634502
1	4.144021	-2.446130	-2.621585
6	5.545599	-1.990705	-1.027861
1	6.448452	-2.147116	-1.629825
1	5.313189	-0.922097	-1.027830
1	5.756769	-2.306928	-0.001007
6	-4.076677	-2.341049	0.320588
1	-4.063268	-2.853904	-0.645913
1	-4.549442	-2.984610	1.071344
1	-4.642407	-1.412976	0.229331
6	-2.529414	-1.301733	2.542004

1	-1.541326	-1.153156	2.985411
1	-3.051090	-0.344504	2.499236
1	-3.110258	-2.010184	3.142755
6	-1.589914	-3.615919	1.025379
1	-1.499411	-4.123642	0.061955
1	-0.603310	-3.543494	1.488160
1	-2.246116	-4.205351	1.672447

Standard coordinate and geometry of TS_{RC}-3:

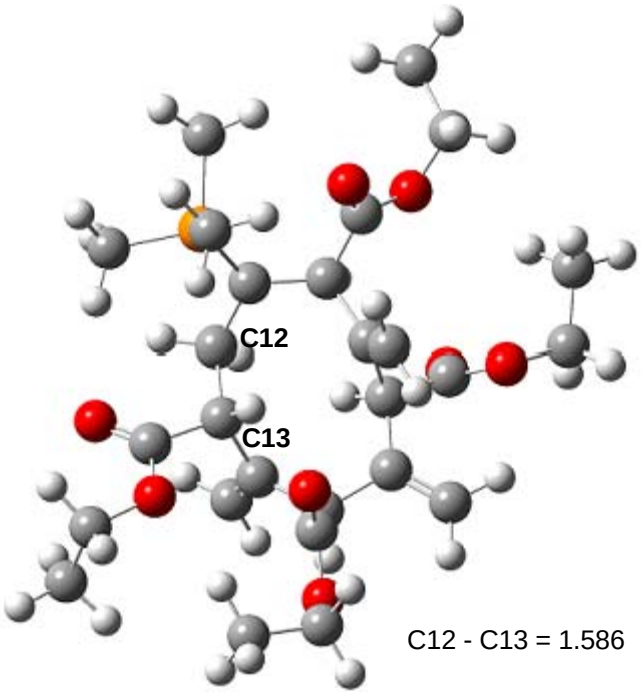


6	0.212613	-1.721629	-0.184515
1	0.002444	-1.380046	-1.199735
6	0.965814	-3.040095	-0.422239
8	1.604629	-3.486487	0.680061
8	0.960714	-3.626537	-1.484350
6	2.240671	-4.782793	0.574530
1	2.240314	-5.168022	1.597251
1	1.624589	-5.426771	-0.057395
6	1.101426	-0.673612	0.495897
6	2.032322	0.097456	-0.480748
1	2.146074	-0.519699	-1.378460
6	1.104825	-0.417039	1.803753
1	1.778453	0.313180	2.240181
1	0.420613	-0.915236	2.479471
6	3.408270	0.209744	0.138786

8	3.773638	1.131874	0.853387
8	4.169449	-0.851389	-0.155160
6	5.485951	-0.919485	0.454358
1	5.682642	-1.989880	0.542585
1	5.434983	-0.474363	1.450279
6	1.392363	1.424340	-0.922812
6	0.243612	1.355733	-1.637426
1	-0.356357	2.204878	-1.935506
1	-0.112885	0.419107	-2.051820
15	1.798799	3.076707	-0.309572
6	6.527061	-0.231649	-0.414925
1	6.332522	0.843030	-0.480329
1	7.522951	-0.372169	0.020327
1	6.531044	-0.652642	-1.425376
6	3.654094	-4.664522	0.024269
1	4.256461	-3.994908	0.647152
1	4.133236	-5.650486	0.014020
1	3.636287	-4.277800	-0.998232
6	-1.149020	-2.009946	0.469835
6	-1.245446	-2.658299	1.636383
1	-0.363365	-3.016660	2.156502
1	-2.204295	-2.844349	2.104665
6	-2.348650	-1.634567	-0.403068
1	-2.317973	-2.307455	-1.268400
6	-3.699009	-1.862962	0.271641
8	-4.016112	-1.500587	1.385644
8	-4.541135	-2.503722	-0.574270
6	-5.907806	-2.656396	-0.130253
1	-6.276897	-3.523959	-0.683798
1	-5.910161	-2.880394	0.939695
6	-6.726606	-1.409830	-0.434255
1	-7.775704	-1.575611	-0.161431
1	-6.350980	-0.556659	0.137364
1	-6.678486	-1.164991	-1.500081

8	-2.462877	2.882503	-1.235084
6	-2.156147	2.227558	-0.222964
6	-1.995695	0.843107	-0.035862
8	-1.805990	2.942370	0.965260
6	-2.367249	-0.191531	-0.967219
1	-1.757942	0.536129	0.975173
6	-2.403753	4.233525	1.101089
6	-2.750429	-0.042470	-2.262725
1	-1.757394	4.787547	1.792941
1	-2.407872	4.744567	0.132657
6	-3.823285	4.138370	1.651752
1	-2.856521	0.944777	-2.697692
1	-3.032077	-0.900545	-2.866351
1	-4.242248	5.139824	1.812368
1	-4.466915	3.606583	0.944039
1	-3.835084	3.597390	2.603911
6	0.721371	4.299335	-1.162272
1	0.933010	4.293323	-2.234900
1	-0.338909	4.085222	-1.002581
1	0.963312	5.286786	-0.756869
6	1.506838	3.316306	1.486301
1	1.690642	4.364697	1.743052
1	0.458644	3.060037	1.675920
1	2.179045	2.671776	2.052504
6	3.500454	3.655808	-0.722587
1	4.238500	3.093541	-0.153134
1	3.671410	3.517197	-1.794244
1	3.576826	4.721492	-0.484384

Standard coordinate and geometry of IN_{RC}-3:

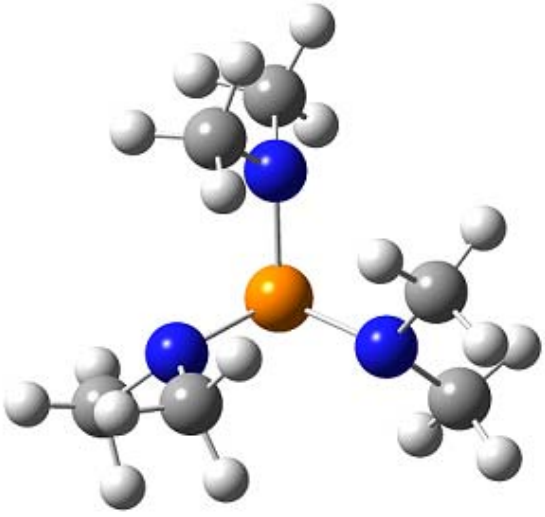


6	0.747918	-1.738270	-0.655911
1	0.498575	-1.234391	-1.594405
6	1.946206	-2.606915	-1.063610
8	2.533744	-3.225741	-0.015779
8	2.324911	-2.721068	-2.210235
6	3.653455	-4.090639	-0.323862
1	3.643048	-4.842018	0.469926
1	3.471246	-4.573728	-1.286667
6	1.151880	-0.658423	0.355219
6	1.809930	0.599645	-0.283019
1	2.178571	0.264287	-1.265331
6	0.950676	-0.786387	1.667421
1	1.255002	-0.006503	2.359471
1	0.459000	-1.655696	2.089324
6	3.053177	0.910808	0.525966
8	3.098780	1.630726	1.510200
8	4.132445	0.255346	0.049032
6	5.376745	0.424109	0.769321
1	5.911510	-0.515257	0.612165
1	5.157210	0.545185	1.832450

6	0.858631	1.772557	-0.507685
6	-0.315088	1.447014	-1.406999
1	-0.719500	2.339651	-1.889088
1	0.039419	0.817411	-2.236895
15	0.934497	3.303572	0.264952
6	6.167750	1.605496	0.226809
1	5.635850	2.544881	0.404096
1	7.141161	1.663686	0.727746
1	6.339724	1.497156	-0.849031
6	4.960835	-3.313723	-0.336640
1	5.129623	-2.827838	0.629640
1	5.796707	-3.995431	-0.533327
1	4.942993	-2.549226	-1.118146
6	-0.478569	-2.550063	-0.262281
6	-0.431505	-3.775819	0.270610
1	0.505307	-4.271283	0.494072
1	-1.344262	-4.317605	0.507799
6	-1.874896	-1.932376	-0.550577
1	-2.423027	-2.680279	-1.128742
6	-2.624971	-1.800455	0.781147
8	-2.324649	-1.075038	1.704230
8	-3.666442	-2.665659	0.816995
6	-4.431443	-2.703077	2.046097
1	-4.877143	-3.700971	2.054154
1	-3.744038	-2.604416	2.890061
6	-5.495009	-1.615829	2.075474
1	-6.099956	-1.711741	2.984746
1	-5.026496	-0.628361	2.071281
1	-6.159892	-1.698373	1.209080
8	-2.935573	2.602114	-1.455389
6	-2.808742	1.575600	-0.813760
6	-1.551945	0.703396	-0.748576
8	-3.806276	1.062526	-0.058277
6	-1.901370	-0.647923	-1.381082

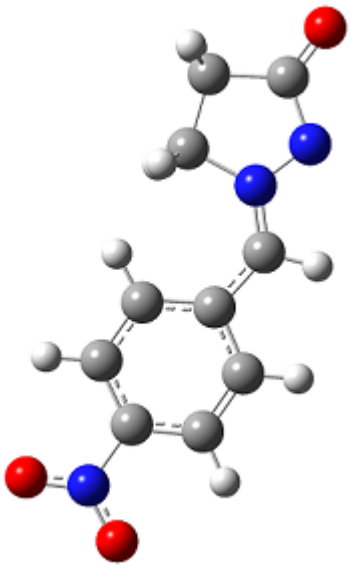
1	-1.346999	0.543577	0.311697
6	-5.070451	1.766198	-0.084176
6	-2.233581	-0.725765	-2.676811
1	-5.544873	1.503509	0.864426
1	-4.876689	2.841181	-0.107144
6	-5.921207	1.334214	-1.269612
1	-2.263778	0.157522	-3.310048
1	-2.480210	-1.671538	-3.152369
1	-6.902487	1.820749	-1.221166
1	-5.442804	1.618985	-2.210851
1	-6.072466	0.249746	-1.264762
6	2.521300	4.280922	0.139797
1	2.845790	4.294899	-0.904686
1	2.347486	5.307304	0.481445
1	3.294136	3.824358	0.757976
6	-0.270820	4.460995	-0.525001
1	0.002482	4.620311	-1.571458
1	-1.291576	4.078559	-0.488737
1	-0.221296	5.416713	0.005451
6	0.541047	3.488320	2.088124
1	-0.473190	3.120006	2.270474
1	1.249585	2.880824	2.654187
1	0.613549	4.533277	2.412395

Standard coordinate and geometry of phosphine $P(NEt_2)_3$:



15	0.000438	-0.001934	-0.719925
7	0.408284	1.533099	0.049407
7	-1.534772	-0.414723	0.042752
7	1.125388	-1.123303	0.048633
6	-0.294824	2.025068	1.225622
1	-0.427951	1.235500	1.967910
1	0.297252	2.824884	1.692136
1	-1.292280	2.432727	0.991973
6	0.735548	2.605025	-0.886705
1	1.452454	3.299479	-0.426351
1	1.199330	2.190973	-1.786812
1	-0.147100	3.192271	-1.197973
6	-1.614044	-1.260858	1.224908
1	-2.600587	-1.136919	1.693263
1	-1.476876	-2.331147	0.997970
1	-0.859649	-0.981436	1.962913
6	1.906661	-1.924970	-0.889579
1	2.165605	-2.890370	-0.432304
1	1.322388	-2.126263	-1.792213
1	2.849058	-1.436455	-1.196236
6	1.889690	-0.765772	1.235469
1	2.735734	-0.093198	1.017399
1	1.260498	-0.272380	1.978951
1	2.292036	-1.679931	1.693926
6	-2.623276	-0.672675	-0.895196
1	-3.584360	-0.391721	-0.441712
1	-2.490868	-0.073762	-1.800994
1	-2.692084	-1.733664	-1.195628

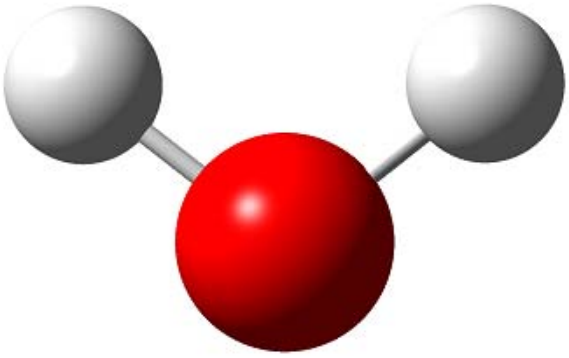
Standard coordinate and geometry of Azomethine imines:



6	0.184212	-0.549805	-0.030875
6	1.149948	-1.589712	0.016052
6	2.509555	-1.327776	0.032433
6	2.938269	-0.000195	-0.001266
6	2.027554	1.053495	-0.053555
6	0.665612	0.782840	-0.068827
1	0.810533	-2.620997	0.042188
1	3.240472	-2.125988	0.070626
1	2.396032	2.071540	-0.083871
1	-0.009514	1.624575	-0.118102
7	4.373934	0.292757	0.015861
8	4.715394	1.475900	-0.013947
8	5.149547	-0.662644	0.059258
6	-1.189197	-1.001513	-0.041248
7	-2.323605	-0.325880	-0.024690
6	-2.450511	1.179861	0.020956
6	-3.951988	1.386771	0.090739
1	-1.990862	1.581388	-0.884636
6	-4.517095	-0.047736	0.009946
1	-4.344611	1.983175	-0.736462
7	-3.490015	-0.973850	-0.044834
8	-5.700630	-0.325750	0.002085

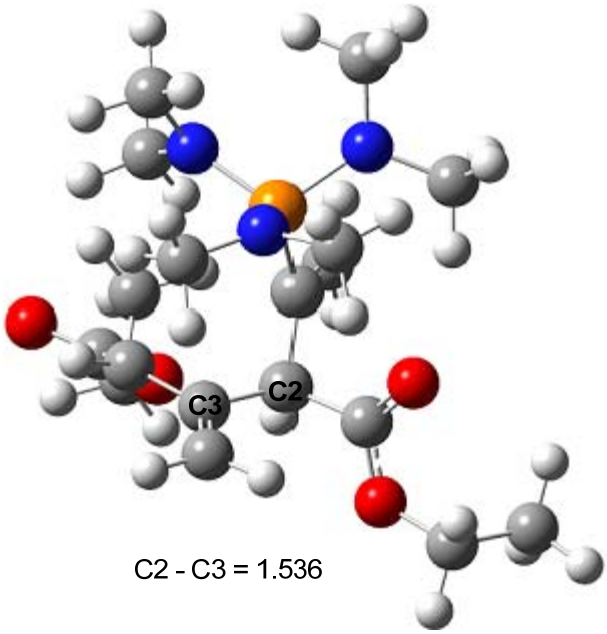
1	−4.277315	1.851791	1.025330
1	−1.903185	1.538350	0.894821
1	−1.356373	−2.072439	−0.059554

Standard coordinate and geometry of H_2O:



8	0.000000	0.000000	0.119517
1	0.000000	0.762211	−0.478070
1	0.000000	−0.762211	−0.478070

Standard coordinate and geometry of 1,5-zwitterion:

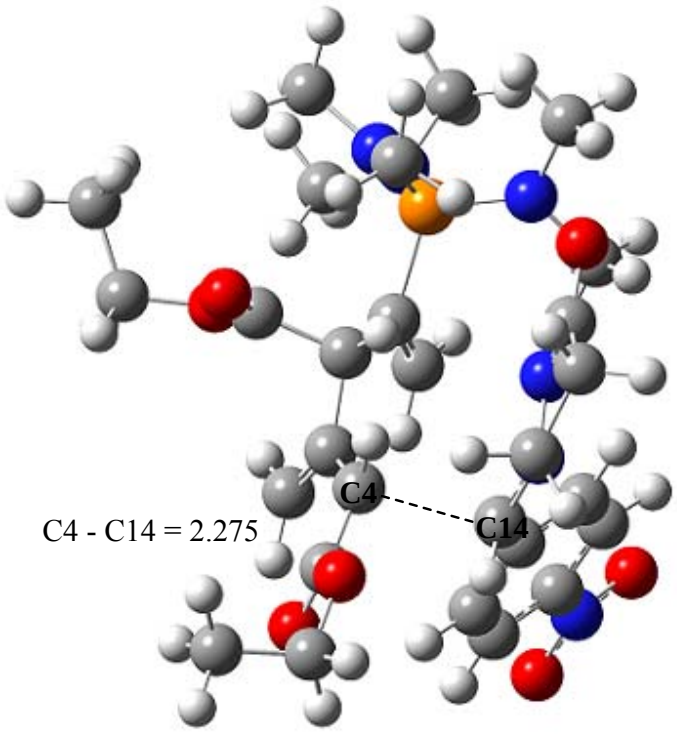


6	−1.058110	−1.385413	1.653301
1	−1.512105	−1.124263	2.606548
6	−1.911180	−2.225225	0.886790
8	−1.293304	−2.869560	−0.200523
8	−3.115471	−2.419792	1.097201
6	−2.081542	−3.866746	−0.858294
1	−1.355088	−4.577400	−1.269055

1	-2.703963	-4.378304	-0.119382
6	0.368654	-1.191560	1.562891
6	0.920572	-1.071488	0.134787
1	0.818770	-2.060586	-0.321530
6	1.185896	-1.008155	2.631863
1	2.235089	-0.744908	2.543293
1	0.806361	-1.140329	3.641479
6	2.390715	-0.688850	0.077943
8	2.817856	0.449199	-0.046534
8	3.182805	-1.768079	0.180635
6	4.612939	-1.542329	0.209167
1	5.007374	-2.396265	0.764722
1	4.814504	-0.623112	0.764485
6	0.107827	-0.122094	-0.743267
6	-0.139468	-0.428761	-2.028532
1	-0.653194	0.241624	-2.710353
1	0.161834	-1.393995	-2.427473
15	-0.520352	1.512899	-0.182421
7	-0.062718	2.540561	-1.467411
7	0.012513	2.218812	1.251028
7	-2.197455	1.536013	-0.062140
6	-0.519242	1.844982	2.568593
1	-1.390158	1.201550	2.457199
1	0.232689	1.287133	3.134567
1	-0.796301	2.758146	3.111965
6	1.297459	2.919127	1.325635
1	2.093598	2.256503	1.680152
1	1.584674	3.311354	0.350649
1	1.189999	3.763051	2.018321
6	-2.923351	2.578238	0.664986
1	-3.677587	3.034469	0.009056
1	-3.443221	2.148846	1.531411
1	-2.246453	3.357828	1.015007
6	-3.069219	0.454401	-0.539051

1	-2.502694	-0.288527	-1.093376
1	-3.544135	-0.060928	0.301511
1	-3.837632	0.879159	-1.198963
6	1.258696	2.509287	-2.103592
1	1.854428	1.678670	-1.729299
1	1.144895	2.415202	-3.192001
1	1.808346	3.439886	-1.900071
6	-0.801951	3.772027	-1.729182
1	-0.366873	4.643996	-1.216881
1	-0.783680	3.970863	-2.808027
1	-1.844637	3.667695	-1.428924
6	5.190279	-1.475779	-1.197081
1	4.799299	-0.606131	-1.732858
1	6.281798	-1.387458	-1.147282
1	4.944294	-2.380944	-1.761964
6	-2.958123	-3.293079	-1.966986
1	-2.356473	-2.734222	-2.694138
1	-3.475553	-4.100050	-2.501597
1	-3.709477	-2.625391	-1.537284

Standard coordinate and geometry of TS-1:

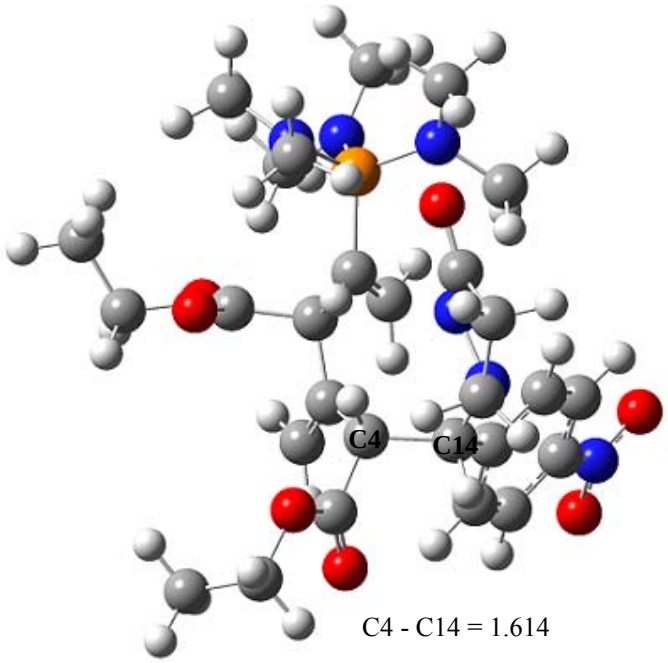


8	-1.066016	-0.381000	4.028413
8	-1.886763	-1.526260	-2.556609
8	-1.482609	-3.129757	-1.011308
8	3.503998	-3.088441	0.283318
8	3.662142	-1.966793	-1.691199
8	2.270797	5.780453	-1.088567
8	3.589348	4.863795	-2.563639
7	0.619509	0.055494	2.515805
7	1.956690	-0.350997	2.409616
7	2.902920	4.821532	-1.540522
6	0.107700	-0.508165	3.623234
6	1.162631	-1.368260	4.354150
1	0.734241	-2.323316	4.666734
1	1.500667	-0.840003	5.253975
6	2.259257	-1.495487	3.303520
1	3.280965	-1.403802	3.683280
1	2.183708	-2.431649	2.734446
6	2.655851	-0.154426	1.282758
1	3.602887	-0.684470	1.287048
6	1.778650	-1.612755	-0.227740
1	1.315626	-2.150689	0.592591
6	0.842996	-1.002171	-1.163194
6	-0.604905	-0.899255	-0.619432
6	-1.276106	0.472698	-0.651584
6	-0.793962	1.576426	-1.233612
1	-1.331484	2.520251	-1.215673
6	-1.385745	-1.977689	-1.377505
6	-2.255643	-2.534989	-3.534192
1	-1.547550	-3.362955	-3.453224
1	-2.113026	-2.033182	-4.494442
6	-3.686212	-3.024860	-3.374617
1	-3.803251	-3.579493	-2.440337
1	-3.935941	-3.696161	-4.204622
1	-4.395677	-2.190216	-3.390387

6	1.124241	-0.632791	-2.436663
1	2.119602	-0.772112	-2.837251
1	0.355321	-0.252580	-3.100226
6	3.021835	-2.209119	-0.668642
6	4.747387	-3.742635	-0.023371
1	5.176070	-3.996487	0.951151
1	5.408363	-3.038759	-0.536474
6	4.530285	-4.991189	-0.868877
1	3.833870	-5.677841	-0.375603
1	5.481834	-5.514602	-1.022335
1	4.124026	-4.719624	-1.847261
6	2.658783	1.124733	0.551801
6	3.405148	1.228536	-0.639927
1	3.901127	0.350923	-1.041712
6	3.488205	2.433132	-1.328000
1	4.052553	2.518943	-2.248365
6	2.826713	3.551517	-0.818116
6	2.089750	3.484029	0.366009
1	1.605906	4.377381	0.742101
6	2.004111	2.272880	1.041766
1	1.432779	2.195658	1.957971
1	0.164008	1.559376	-1.743482
1	-2.081896	3.425240	2.097282
6	-1.635975	2.429876	1.966118
7	-2.685988	1.441134	1.697501
1	-0.911638	2.463046	1.156247
1	-1.108239	2.129360	2.874455
15	-2.871016	0.630264	0.255650
6	-3.564716	1.213838	2.857833
7	-3.560483	-0.847942	0.659626
7	-3.889690	1.490245	-0.789524
1	-2.960332	0.796900	3.669298
1	-4.010815	2.168669	3.166529
1	-4.369123	0.521993	2.605656

6	-4.700260	-1.428475	-0.045305
6	-2.987561	-1.714915	1.707845
6	-4.985259	2.301451	-0.259969
6	-3.966259	1.238052	-2.231804
1	-4.416438	-2.371380	-0.525693
1	-5.509906	-1.635269	0.667679
1	-5.079557	-0.747702	-0.807547
1	-2.525764	-2.598736	1.253504
1	-2.252136	-1.179867	2.315957
1	-3.796747	-2.038791	2.374786
1	-5.050464	3.233570	-0.834382
1	-5.953404	1.784878	-0.332346
1	-4.798744	2.557986	0.783735
1	-3.181099	0.551807	-2.548155
1	-4.939687	0.803747	-2.501912
1	-3.852889	2.183077	-2.778202
1	-0.576041	-1.219242	0.424764

Standard coordinate and geometry of IN-1:



C4 - C14 = 1.614

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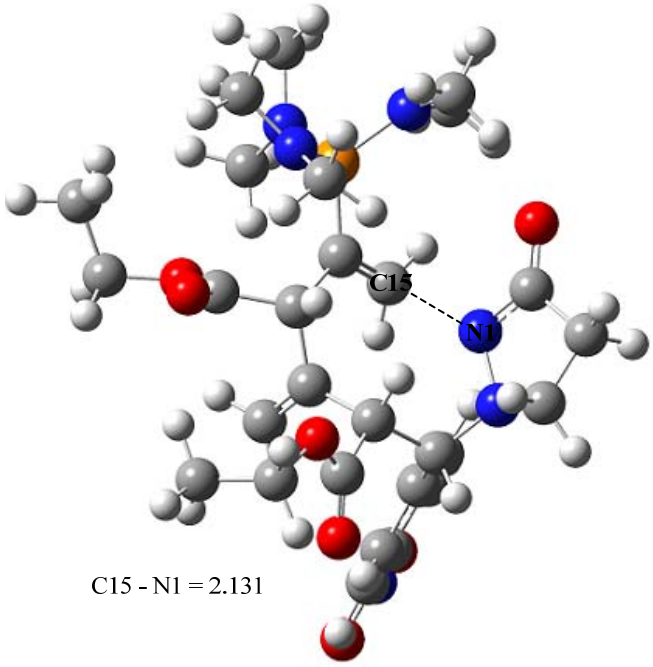
8	1.938464	1.416085	-2.400889
8	1.801868	2.964291	-0.756724

8	-2.280707	3.947060	0.313901
8	-3.604517	2.559490	-0.879897
8	-3.451555	-5.375258	-1.141135
8	-4.548597	-4.218456	-2.627066
7	-0.452050	0.064724	2.354746
7	-1.878153	0.299903	2.466236
7	-3.868738	-4.310480	-1.602878
6	0.118681	0.456959	3.492904
6	-0.932460	1.052618	4.453385
1	-0.544514	1.926087	4.983190
1	-1.215438	0.296369	5.197945
6	-2.070849	1.351872	3.485505
1	-3.078502	1.284861	3.911548
1	-1.941385	2.365389	3.060629
6	-2.491243	0.566004	1.181708
1	-3.457135	1.035220	1.410685
6	-1.675114	1.660920	0.320399
1	-1.018167	2.137529	1.050782
6	-0.779131	1.168785	-0.815921
6	0.678906	0.839057	-0.426077
6	1.111251	-0.610491	-0.631556
6	0.413822	-1.549377	-1.279361
1	0.782054	-2.564165	-1.393220
6	1.550608	1.854503	-1.173444
6	2.462809	2.421221	-3.308635
1	1.896949	3.344093	-3.160497
1	2.244324	2.018779	-4.300975
6	3.952670	2.663018	-3.126104
1	4.153624	3.103717	-2.146375
1	4.306841	3.359618	-3.894936
1	4.519156	1.731083	-3.226569
6	-1.166927	1.123538	-2.098806
1	-2.169951	1.401229	-2.400249
1	-0.482250	0.820461	-2.884259

6	-2.629985	2.737249	-0.168906
6	-3.112543	5.071118	-0.064041
1	-2.978824	5.788192	0.749446
1	-4.154513	4.743572	-0.094730
6	-2.675510	5.653789	-1.399790
1	-1.617660	5.934649	-1.373039
1	-3.265784	6.549370	-1.626146
1	-2.829609	4.929049	-2.204401
6	-2.831912	-0.721548	0.433909
6	-3.615648	-0.682435	-0.732114
1	-3.958473	0.275996	-1.108336
6	-3.963810	-1.851693	-1.401997
1	-4.567718	-1.832207	-2.301009
6	-3.525463	-3.074780	-0.893436
6	-2.771300	-3.147901	0.277496
1	-2.467813	-4.116715	0.655617
6	-2.434692	-1.968865	0.937616
1	-1.866818	-1.995721	1.858090
1	-0.557718	-1.331144	-1.709851
1	1.409772	-3.542062	2.487075
6	1.203703	-2.741413	1.769916
7	2.472158	-2.026729	1.524966
1	0.833485	-3.204212	0.853928
1	0.452260	-2.049045	2.165987
15	2.706454	-1.134423	0.135963
6	3.293723	-1.842904	2.737712
7	3.720693	0.153246	0.500918
7	3.426376	-2.134152	-1.027585
1	2.735282	-1.246783	3.468654
1	3.534435	-2.833925	3.141542
1	4.229085	-1.339766	2.489390
6	4.984806	0.397947	-0.188820
6	3.427883	1.111841	1.587983
6	4.334047	-3.210249	-0.631287

6	3.473766	-1.796211	-2.452576
1	4.985979	1.396223	-0.641281
1	5.817632	0.346428	0.525987
1	5.158593	-0.338733	-0.972996
1	3.213681	2.100080	1.166808
1	2.587633	0.787510	2.217003
1	4.311315	1.184791	2.235342
1	4.126519	-4.099075	-1.239898
1	5.388081	-2.932272	-0.777898
1	4.174585	-3.465842	0.416999
1	2.839931	-0.936379	-2.668872
1	4.501197	-1.562618	-2.767527
1	3.123539	-2.649772	-3.047163
1	0.772036	1.056775	0.641065

Standard coordinate and geometry of TS-2a:



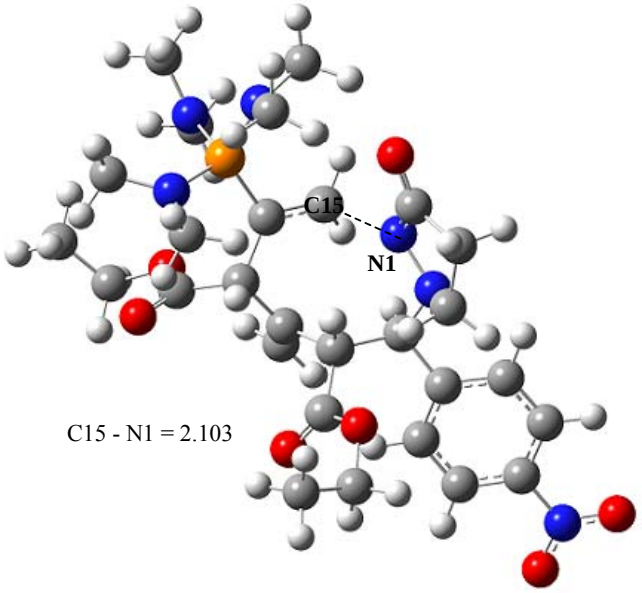
8	-1.137070	-3.233502	-2.279491
8	-1.509676	1.801044	2.211247
8	-2.026719	3.082436	0.427023
8	0.607889	3.025453	-2.336364
8	2.817923	2.761050	-1.911934
8	5.990612	-2.351328	3.216763

8	6.929474	-0.410074	2.899098
7	0.595992	-1.869800	-1.590510
7	1.829469	-1.395557	-2.199506
7	6.087712	-1.270077	2.633495
6	-0.081662	-2.596122	-2.482911
6	0.656870	-2.565851	-3.835386
1	-0.042589	-2.486329	-4.671196
1	1.229930	-3.494993	-3.950952
6	1.565781	-1.357281	-3.650468
1	2.512622	-1.396159	-4.199725
1	1.026282	-0.437683	-3.951212
6	2.358367	-0.152308	-1.643662
1	2.998417	0.252541	-2.436336
6	1.242084	0.950782	-1.426932
1	0.428767	0.642267	-2.088267
6	0.617026	1.170173	-0.038522
6	-0.909830	0.975931	0.014730
6	-1.289571	-0.494137	0.271796
6	-0.303514	-1.462069	0.298370
1	-0.553549	-2.509427	0.412561
6	-1.557283	2.058466	0.884446
6	-1.938159	2.869764	3.095215
1	-1.574167	3.818167	2.692655
1	-1.425860	2.654852	4.036071
6	-3.447479	2.902217	3.280413
1	-3.945582	3.143756	2.338386
1	-3.709392	3.671456	4.016215
1	-3.820269	1.940054	3.647131
6	1.325759	1.593265	1.014508
1	2.390754	1.778837	0.949240
1	0.860861	1.758771	1.979975
6	1.683058	2.326476	-1.915983
6	0.798179	4.429365	-2.641469
1	0.031674	4.649979	-3.388398

1	1.787663	4.564284	-3.084245
6	0.616724	5.270966	-1.387160
1	-0.343336	5.045995	-0.911731
1	0.645257	6.336423	-1.643199
1	1.418567	5.069657	-0.669924
6	3.308892	-0.438574	-0.479971
6	4.301922	0.495387	-0.137154
1	4.350400	1.436678	-0.676297
6	5.215257	0.231588	0.878958
1	5.985920	0.943213	1.148973
6	5.135130	-0.985951	1.554705
6	4.178597	-1.943236	1.221382
1	4.158941	-2.885605	1.755044
6	3.277400	-1.667572	0.195638
1	2.553892	-2.415973	-0.106556
1	0.689303	-1.195144	0.629927
1	-3.827899	-4.467136	0.110247
6	-3.020562	-3.723226	0.128633
7	-3.565095	-2.429442	-0.321351
1	-2.658979	-3.642957	1.157330
1	-2.206708	-4.038395	-0.531675
15	-2.992938	-0.994128	0.382667
6	-4.044826	-2.473417	-1.710602
7	-3.909402	0.305367	-0.218202
7	-3.405427	-1.267846	2.008022
1	-3.220017	-2.642553	-2.410331
1	-4.756799	-3.304898	-1.787492
1	-4.585579	-1.558001	-1.953922
6	-5.144992	0.762188	0.407936
6	-3.705120	0.826959	-1.573589
6	-4.647982	-1.942436	2.387130
6	-2.512524	-1.028598	3.139395
1	-5.200383	1.854188	0.320794
1	-6.040204	0.334259	-0.068601

1	-5.150241	0.509804	1.468359
1	-3.493122	1.901973	-1.528219
1	-2.869672	0.321192	-2.062559
1	-4.599085	0.666910	-2.192235
1	-4.432485	-2.912657	2.856474
1	-5.205421	-1.333174	3.111935
1	-5.275259	-2.119356	1.513746
1	-1.589549	-0.561098	2.806226
1	-2.993207	-0.369293	3.874443
1	-2.277785	-1.979944	3.638547
1	-1.255512	1.261802	-0.982280

Standard coordinate and geometry of TS-2b:



8	-1.187334	3.858633	0.241655
8	-2.486639	-2.725051	-1.244622
8	-2.406897	-3.026565	0.991034
8	2.506489	-0.458957	2.326955
8	1.992647	-2.471946	1.434512
8	8.356041	0.711293	-1.572126
8	8.098478	-1.431957	-1.266568
7	0.270620	2.221282	-0.488997
7	1.688308	1.954035	-0.305128
7	7.666064	-0.280347	-1.332266

6	-0.073074	3.296239	0.228092
6	1.145788	3.774725	1.037832
1	0.854427	4.104741	2.038145
1	1.614453	4.621035	0.518413
6	2.025227	2.529355	1.018050
1	3.099677	2.719020	1.090415
1	1.742425	1.855601	1.841967
6	1.987430	0.547701	-0.536458
6	1.126929	-0.422191	0.409536
1	0.553947	0.286513	1.016861
6	0.120317	-1.265754	-0.365153
6	-1.333705	-1.059113	0.083669
6	-1.950096	0.207618	-0.555243
6	-1.204858	1.026006	-1.393101
1	-1.645052	1.914476	-1.827161
6	-2.140564	-2.359064	0.011786
6	-3.059493	-4.051264	-1.394718
1	-2.520696	-4.734740	-0.734035
1	-2.849251	-4.311785	-2.434887
6	-4.552955	-4.085463	-1.107212
1	-4.749898	-3.837975	-0.061545
1	-4.937091	-5.093918	-1.300538
1	-5.097011	-3.386649	-1.750906
6	0.486767	-2.085194	-1.354536
1	1.529823	-2.200834	-1.634196
1	-0.231464	-2.670603	-1.916173
6	1.908151	-1.261227	1.416838
6	3.317811	-1.107303	3.337117
1	4.041810	-0.343208	3.629928
1	3.842310	-1.948273	2.877800
6	2.473612	-1.561508	4.518526
1	1.916288	-0.720746	4.945093
1	3.121154	-1.975932	5.299935
1	1.767116	-2.337429	4.210714

6	3.495669	0.314431	-0.658257
6	4.058185	-0.973347	-0.621865
1	3.442342	-1.840827	-0.417710
6	5.419083	-1.174909	-0.839046
1	5.853844	-2.166288	-0.805078
6	6.229958	-0.075556	-1.108183
6	5.703347	1.212457	-1.180298
1	6.356614	2.045503	-1.409654
6	4.341406	1.395772	-0.964145
1	3.908008	2.384460	-1.052635
1	-0.413088	0.589273	-1.985172
1	-4.762747	3.962641	-1.030328
6	-3.928725	3.249867	-1.077118
7	-4.046044	2.316874	0.057518
1	-4.002432	2.706603	-2.023180
1	-2.976342	3.786522	-1.025800
15	-3.612534	0.687669	-0.151302
6	-3.926557	2.994349	1.356647
7	-4.043879	-0.167185	1.249480
7	-4.672769	0.238539	-1.402964
1	-2.928738	3.424510	1.491398
1	-4.668844	3.802472	1.377868
1	-4.170448	2.306660	2.167096
6	-5.290157	-0.909212	1.398678
6	-3.265422	-0.065886	2.485624
6	-6.045801	0.742773	-1.457763
6	-4.257352	-0.438078	-2.629078
1	-5.070878	-1.876627	1.867358
1	-6.016492	-0.374421	2.028981
1	-5.738324	-1.101248	0.424002
1	-2.930665	-1.063780	2.794128
1	-2.392583	0.575491	2.342698
1	-3.870735	0.369137	3.293473
1	-6.173332	1.435327	-2.301909

1	−6.748816	−0.090288	−1.594175
1	−6.298940	1.275666	−0.541472
1	−3.238722	−0.806790	−2.537840
1	−4.919244	−1.290265	−2.831184
1	−4.320583	0.249493	−3.485833
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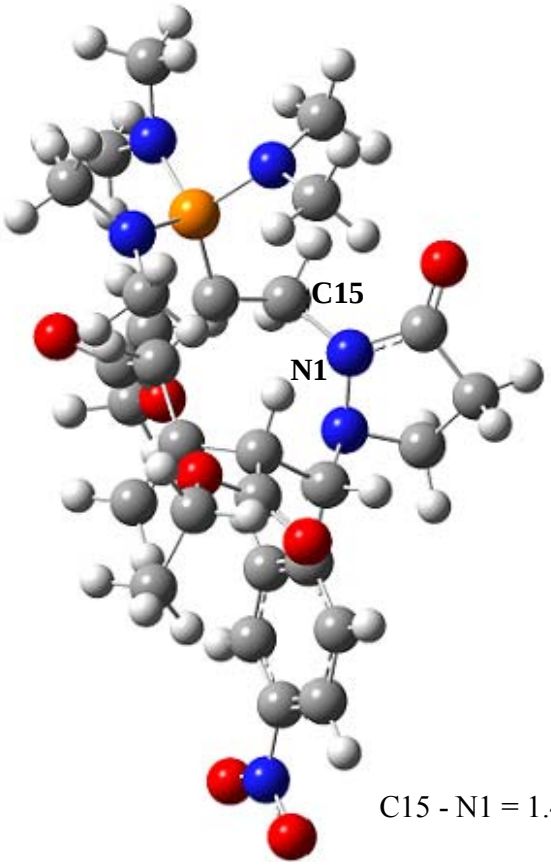
1	1.601983	0.344256	−1.541933

Standard coordinate and geometry of IN-2:



C15 - N1 = 1.490

8	1.764688	−0.346760	3.952596
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8	1.295544	−2.089888	−2.896105
8	−0.460779	3.260890	−0.931206
8	−1.978684	3.180687	0.733252
8	−7.032031	−1.975289	−1.200863
8	−7.809276	−0.130766	−0.337891
7	0.434946	−0.588227	2.071403
7	−0.947438	−0.788970	1.756689
7	−6.893770	−0.915231	−0.589152

6	0.665970	-0.441062	3.419945
6	-0.694542	-0.491452	4.120459
1	-1.045404	0.522061	4.348848
1	-0.603381	-1.034688	5.063635
6	-1.542446	-1.201905	3.060250
1	-1.437688	-2.289054	3.152339
1	-2.605256	-0.956822	3.082964
6	-1.594982	0.460153	1.256861
1	-1.710740	1.190021	2.071094
6	-0.684699	1.177876	0.208907
1	0.297821	1.265662	0.699415
6	-0.439451	0.431724	-1.093537
6	0.906740	-0.315922	-1.279263
6	1.839318	-0.384639	-0.069341
6	1.445363	-1.181986	1.151714
1	2.306991	-1.367627	1.794715
6	0.694549	-1.696035	-1.912872
6	-0.434468	-3.795054	-1.775427
1	-0.396336	-3.749565	-2.866146
1	-1.451993	-4.036254	-1.457145
6	0.567560	-4.803664	-1.233465
1	1.579202	-4.561594	-1.570904
1	0.316653	-5.807486	-1.595967
1	0.552452	-4.821093	-0.138580
6	-1.323979	0.461477	-2.095377
1	-2.257627	1.012529	-2.032631
1	-1.143715	-0.064237	-3.030884
6	-1.150106	2.624568	0.037912
6	-0.774448	4.660155	-1.143851
1	0.135868	5.071976	-1.586376
1	-0.955242	5.133394	-0.175785
6	-1.968438	4.824831	-2.072075
1	-1.798949	4.303402	-3.019637
1	-2.127635	5.887950	-2.286451

1	-2.876047	4.429921	-1.607003
6	-2.987090	0.101418	0.752710
6	-4.075799	0.947856	1.016389
1	-3.910333	1.873503	1.555927
6	-5.357232	0.625657	0.576282
1	-6.204992	1.269897	0.773977
6	-5.543886	-0.562284	-0.127895
6	-4.484959	-1.426617	-0.402280
1	-4.672383	-2.340573	-0.952470
6	-3.208708	-1.089004	0.039442
1	-2.370089	-1.744929	-0.159067
1	1.020787	-2.154574	0.874650
1	5.652327	-0.026990	2.697450
6	4.703060	-0.387289	2.275356
7	4.209094	0.581323	1.287602
1	4.884550	-1.353282	1.802382
1	3.982775	-0.519317	3.091054
15	3.483224	0.094960	-0.196338
6	3.761097	1.823030	1.917712
7	3.589484	1.355989	-1.354130
7	4.676236	-1.049738	-0.681285
1	2.917759	1.659741	2.601617
1	4.593284	2.243868	2.497981
1	3.479582	2.562438	1.166699
6	4.706965	1.496340	-2.279919
6	2.741078	2.541508	-1.309195
6	6.113580	-0.853976	-0.517872
6	4.333258	-2.217244	-1.481263
1	4.329947	1.888318	-3.233673
1	5.476780	2.192840	-1.911121
1	5.170145	0.531567	-2.478866
1	2.308947	2.734547	-2.300679
1	1.917412	2.400028	-0.613154
1	3.310566	3.436150	-1.009696

1	6.553274	-1.682795	0.056288
1	6.624576	-0.820154	-1.492313
1	6.313905	0.077239	0.013276
1	3.254496	-2.301455	-1.595928
1	4.771141	-2.156103	-2.489319
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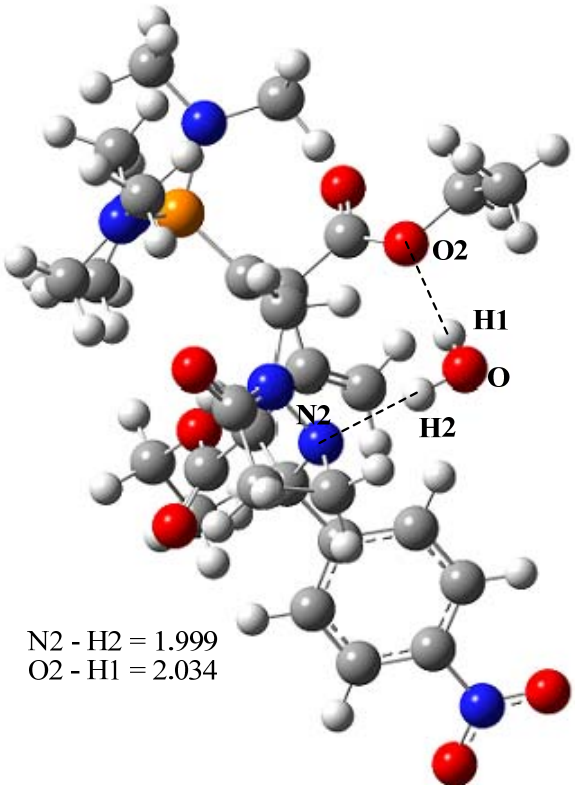
Standard coordinate and geometry of IN-3:



8	1.571969	-0.654517	3.924790
8	1.107603	-2.299554	-2.011471
8	2.126184	-0.785159	-3.347188
8	-0.879005	2.892786	-1.305019
8	-1.953382	3.037831	0.675183
8	-7.477021	-1.648265	-1.007429
8	-8.014693	0.247008	-0.073664
7	0.331175	-0.807316	1.978082
7	-1.037212	-1.035454	1.591297
7	-7.199739	-0.620507	-0.389496
6	0.499928	-0.754640	3.342376

6	-0.878708	-0.911783	3.984107
1	-1.274840	0.066043	4.282733
1	-0.798840	-1.529067	4.881429
6	-1.664799	-1.563157	2.845992
1	-1.525587	-2.649628	2.854240
1	-2.734161	-1.352776	2.844817
6	-1.692416	0.245934	1.164470
1	-1.739947	0.936124	2.018038
6	-0.785920	0.981018	0.125798
1	0.150526	1.155656	0.679923
6	-0.374972	0.197361	-1.112837
6	1.142905	0.001566	-1.269303
6	1.915756	-0.201988	0.039833
6	1.440746	-1.211646	1.054972
1	2.243897	-1.490642	1.739909
6	1.499526	-1.034634	-2.338144
6	1.461145	-3.371338	-2.926665
1	2.388106	-3.100788	-3.435872
1	0.667881	-3.438065	-3.679974
6	1.584604	-4.655904	-2.124632
1	2.430041	-4.602032	-1.430258
1	1.753188	-5.498463	-2.804681
1	0.679030	-4.848778	-1.542228
6	-1.243253	-0.172932	-2.059196
1	-2.299386	0.063564	-1.998011
1	-0.929014	-0.706562	-2.952025
6	-1.305786	2.395087	-0.129778
6	-1.268660	4.254894	-1.617659
1	-0.491296	4.603304	-2.301860
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6	-2.643254	4.296907	-2.267476
1	-2.670217	3.667114	-3.162469
1	-2.882714	5.325177	-2.561926
1	-3.411089	3.952915	-1.568793

6	-3.132339	-0.018406	0.728139
6	-4.119974	0.925149	1.064567
1	-3.836035	1.821467	1.603992
6	-5.449842	0.740676	0.698156
1	-6.213904	1.465084	0.951807
6	-5.796388	-0.412518	-0.002504
6	-4.848090	-1.376225	-0.336337
1	-5.154283	-2.266426	-0.872016
6	-3.517937	-1.176626	0.029495
1	-2.790303	-1.939212	-0.225675
1	1.086374	-2.131400	0.577057
1	5.512043	-0.054937	3.109613
6	4.621815	-0.398425	2.563390
7	4.085192	0.709544	1.764492
1	4.918630	-1.223956	1.914110
1	3.882781	-0.758767	3.287668
15	3.493697	0.457926	0.171266
6	3.549833	1.786566	2.596854
7	3.537721	1.938814	-0.692258
7	4.815832	-0.442858	-0.459009
1	2.672688	1.469127	3.174122
1	4.329151	2.099928	3.304235
1	3.295667	2.655685	1.989785
6	4.494737	2.252624	-1.746052
6	2.588482	3.015188	-0.439168
6	6.207620	-0.053424	-0.259968
6	4.636453	-1.680661	-1.201946
1	3.957798	2.658670	-2.614382
1	5.235485	3.001179	-1.424585
1	5.015840	1.354700	-2.072877
1	2.050885	3.280769	-1.360607
1	1.849809	2.705972	0.300791
1	3.096444	3.919648	-0.070596
1	6.751318	-0.823691	0.307129

1	6.724574	0.081306	-1.221551
1	6.262575	0.881953	0.299373
1	5.276419	-2.467741	-0.776408
1	3.599849	-2.010445	-1.128879
1	4.892943	-1.566425	-2.264871
1	1.508689	0.931768	-1.718392
1	-1.037038	-2.655122	0.420284
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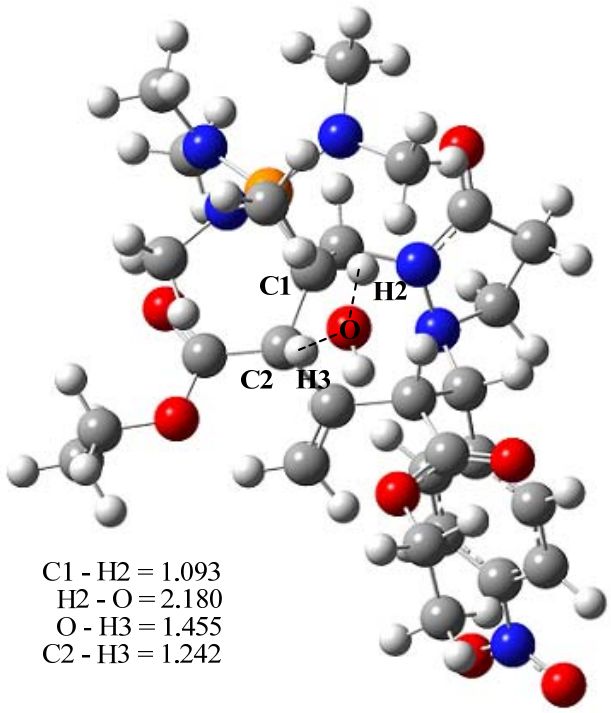
Standard coordinate and geometry of TS-3a:



8	1.580901	-4.038529	-0.048350
8	1.123917	3.323280	-0.890188
8	2.344960	1.815996	-2.039518
8	-1.467502	1.841520	2.338986
8	-2.253116	-0.162700	3.012079
8	-7.409537	0.294930	-2.445886
8	-8.114258	-0.054940	-0.412794
7	0.222818	-2.223998	-0.498608
7	-1.161484	-1.943960	-0.738326
7	-7.226622	-0.000437	-1.264435

6	0.470439	-3.541797	-0.176321
6	-0.882774	-4.243612	-0.101147
1	-1.219574	-4.309950	0.940320
1	-0.797998	-5.258880	-0.494255
6	-1.741531	-3.304031	-0.953292
1	-1.638758	-3.551744	-2.016133
1	-2.801948	-3.304230	-0.701848
6	-1.832633	-1.257855	0.409847
1	-1.931290	-1.939270	1.267110
6	-0.972686	-0.067659	0.962040
1	-0.103766	-0.528671	1.441931
6	-0.456154	0.940276	-0.065501
6	1.056650	1.075057	-0.136749
6	1.793965	-0.290167	-0.178930
6	1.252742	-1.391478	-1.126823
1	2.036129	-2.092325	-1.427893
6	1.555129	2.059515	-1.130299
6	1.586793	4.358679	-1.782280
1	2.637333	4.180689	-2.025382
1	1.503934	5.275455	-1.192637
6	0.746813	4.442876	-3.050170
1	0.838903	3.522683	-3.633919
1	1.091088	5.279157	-3.670268
1	-0.308911	4.608338	-2.810680
6	-1.320773	1.689878	-0.764627
1	-2.386874	1.639315	-0.579482
1	-1.001106	2.426744	-1.490389
6	-1.657588	0.522650	2.199578
6	-2.003411	2.454476	3.537137
1	-1.358089	3.320158	3.704542
1	-1.899693	1.754010	4.369093
6	-3.453192	2.871068	3.338648
1	-3.550802	3.539918	2.477402
1	-3.813745	3.399668	4.228778

1	-4.088166	1.994986	3.179013
6	-3.248451	-0.900985	-0.041984
6	-4.311015	-0.959228	0.875476
1	-4.109066	-1.230427	1.905609
6	-5.613762	-0.657959	0.485795
1	-6.438827	-0.698986	1.186198
6	-5.853440	-0.309335	-0.841695
6	-4.825365	-0.256771	-1.781604
1	-5.051657	0.012187	-2.806095
6	-3.527864	-0.554814	-1.375434
1	-2.715056	-0.525272	-2.090762
1	0.809110	-0.943538	-2.019408
1	5.520882	-3.144374	1.008913
6	4.690809	-2.873730	0.341053
7	3.961425	-1.726309	0.878497
1	5.102415	-2.645522	-0.642393
1	4.014456	-3.729827	0.243234
15	3.671731	-0.312160	-0.001351
6	3.253874	-2.004124	2.140596
7	4.458144	0.923509	0.845054
7	4.501010	-0.365958	-1.466619
1	2.559354	-2.840282	1.995635
1	3.985525	-2.289214	2.909230
1	2.706096	-1.121822	2.496310
6	4.344314	2.310147	0.379649
6	4.712625	0.834223	2.294448
6	5.962263	-0.263516	-1.485320
6	3.904718	-0.634698	-2.773846
1	3.504022	2.823377	0.863141
1	5.273167	2.834049	0.636719
1	4.215851	2.340703	-0.702369
1	3.790519	1.065551	2.843029
1	5.069971	-0.163847	2.550588
1	5.511943	1.548214	2.525245

1	6.419095	-1.191564	-1.856415
1	6.266056	0.557255	-2.148030
1	6.342020	-0.057435	-0.484578
1	2.869784	-0.306069	-2.798264
1	4.439460	-0.038204	-3.521571
1	3.985340	-1.694748	-3.054589
1	1.364814	1.333220	1.038804
8	1.733514	0.872038	2.369077
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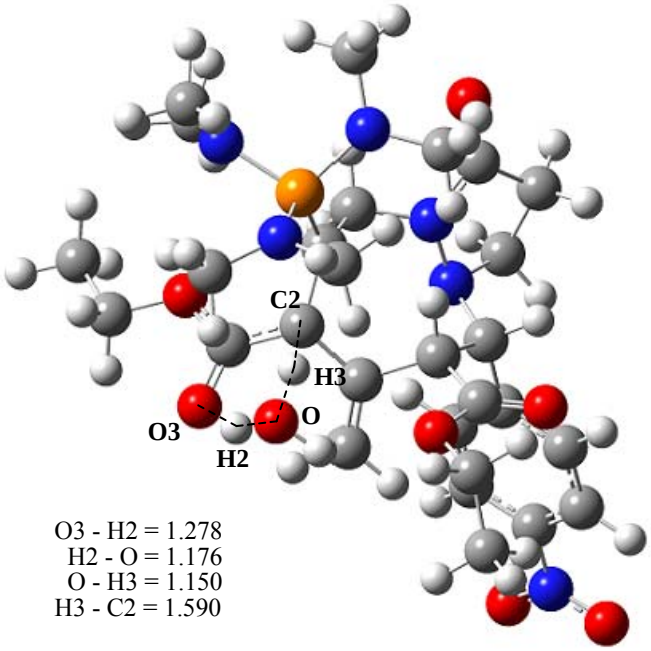
Standard coordinate and geometry of TS-3b:



8	1.322227	4.228003	-0.594116
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8	-0.870193	-2.062210	-2.228123
8	-2.146938	-0.349682	-2.949653
8	-7.352961	-0.309638	2.467665
8	-8.057087	-0.269805	0.405035
7	0.144357	2.362489	0.111575
7	-1.201162	2.018511	0.469308
7	-7.175202	-0.162414	1.258011

6	0.268650	3.655874	-0.346570
6	-1.139442	4.247556	-0.422191
1	-1.525156	4.185283	-1.447196
1	-1.115690	5.300974	-0.135079
6	-1.886735	3.343350	0.559165
1	-1.768061	3.713275	1.584216
1	-2.952177	3.234341	0.356919
6	-1.840832	1.140848	-0.553143
1	-1.950080	1.670497	-1.511599
6	-0.912250	-0.078213	-0.871838
1	0.031728	0.374483	-1.215985
6	-0.520100	-0.964984	0.307018
6	0.950157	-0.912697	0.660741
6	1.711974	0.329832	0.298613
6	1.264446	1.679131	0.820677
1	2.067865	2.419229	0.778186
6	1.325237	-1.664395	1.838274
6	2.562552	-1.905473	3.866087
1	3.358425	-2.560862	3.494327
1	1.743596	-2.538311	4.214246
6	3.057160	-0.976654	4.960020
1	3.883336	-0.349925	4.611487
1	3.409785	-1.568402	5.812057
1	2.250299	-0.322633	5.306023
6	-1.454210	-1.758900	0.871067
1	-2.472761	-1.775727	0.502067
1	-1.237824	-2.410899	1.710019
6	-1.416610	-0.822020	-2.101285
6	-1.203963	-2.797646	-3.436211
1	-0.356269	-3.472764	-3.578351
1	-1.252827	-2.093884	-4.269617
6	-2.509642	-3.561558	-3.278392
1	-2.468032	-4.241882	-2.421078
1	-2.699698	-4.157593	-4.178387

1	-3.346122	-2.871134	-3.140638
6	-3.241292	0.781494	-0.065839
6	-4.297014	0.663990	-0.984200
1	-4.100424	0.807896	-2.040683
6	-5.585871	0.348002	-0.560581
1	-6.406491	0.253195	-1.260955
6	-5.817095	0.162698	0.800824
6	-4.794995	0.286096	1.741129
1	-5.015034	0.139896	2.791478
6	-3.510957	0.593211	1.301141
1	-2.702792	0.697244	2.014527
1	0.927363	1.591309	1.863036
1	5.273097	2.199554	-2.434581
6	4.650268	2.418445	-1.552379
7	3.465711	1.572306	-1.485180
1	5.259281	2.303146	-0.658158
1	4.332700	3.467399	-1.609986
15	3.263615	0.245747	-0.421330
6	2.484133	1.903591	-2.514697
7	3.644209	-1.225565	-1.225132
7	4.648112	0.324095	0.618662
1	2.188226	2.953577	-2.419529
1	2.894327	1.739473	-3.524237
1	1.593712	1.285932	-2.394387
6	4.096778	-2.422562	-0.516796
6	3.147048	-1.487753	-2.568962
6	6.009686	0.029026	0.189120
6	4.562693	0.991723	1.907302
1	3.332584	-3.208072	-0.524623
1	5.004393	-2.822262	-0.994694
1	4.337261	-2.175205	0.518222
1	2.206357	-2.057958	-2.569830
1	2.989727	-0.553592	-3.109436
1	3.895345	-2.070177	-3.124518

1	6.652035	0.923165	0.208209
1	6.467370	-0.719206	0.853655
1	6.007743	-0.369532	-0.826770
1	4.971182	2.015459	1.879136
1	3.524174	1.029564	2.237381
1	5.136135	0.426167	2.655806
1	1.177115	-2.219459	-0.216320
1	0.096012	-3.296271	-0.751759
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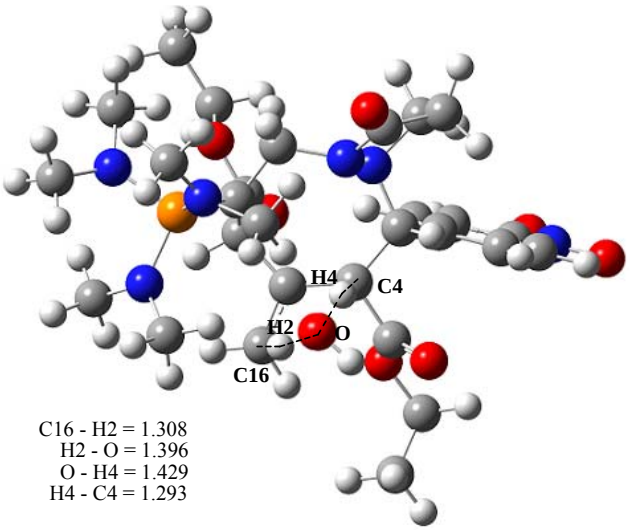
Standard coordinate and geometry of TS-3c:



8	1.464463	-1.133693	3.982599
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8	-2.572751	2.259536	-1.082301
8	-2.164528	3.013177	1.007645
8	-7.166259	-1.737687	-1.479785
8	-7.869373	-0.672671	0.287687
7	0.520757	-0.906451	1.878401
7	-0.735165	-1.196909	1.239422
7	-6.975759	-1.093364	-0.448114
6	0.500168	-1.189628	3.237601
6	-0.911193	-1.673641	3.582081
1	-1.518047	-0.859671	3.996163

1	-0.853632	-2.465314	4.332371
6	-1.387240	-2.138277	2.202813
1	-0.999865	-3.140455	1.986709
1	-2.467333	-2.153881	2.066815
6	-1.516166	0.058391	1.086190
1	-1.603292	0.558599	2.063433
6	-0.853425	1.150208	0.190660
1	0.018069	1.832031	0.858923
6	0.078143	1.043787	-0.915680
6	1.102961	-0.083712	-1.167090
6	2.071506	-0.302707	-0.023056
6	1.720463	-1.250540	1.083128
1	2.532763	-1.310039	1.809715
6	0.408664	-1.306167	-1.772854
6	0.610725	-3.572136	-2.418524
1	0.387124	-3.309858	-3.457347
1	-0.335314	-3.825101	-1.930052
6	1.621307	-4.699367	-2.319616
1	2.563757	-4.426223	-2.805253
1	1.226416	-5.593228	-2.814924
1	1.830498	-4.950642	-1.274704
6	0.435658	2.306158	-1.480706
1	1.202208	2.299965	-2.252549
6	-1.905835	2.259469	0.087050
6	-3.665086	3.204840	-1.215458
1	-4.191189	3.266045	-0.260127
1	-4.317981	2.746962	-1.961895
6	-3.175623	4.573106	-1.666054
1	-2.532790	5.025134	-0.905273
1	-4.033084	5.236720	-1.827044
1	-2.620083	4.500203	-2.607065
6	-2.949117	-0.264842	0.649713
6	-4.016028	0.177837	1.447946
1	-3.810548	0.743886	2.352177

6	-5.338605	-0.084357	1.097254
1	-6.167842	0.253183	1.706619
6	-5.585302	-0.805692	-0.068078
6	-4.548095	-1.257785	-0.883920
1	-4.781153	-1.809003	-1.786726
6	-3.232425	-0.981206	-0.523930
1	-2.423629	-1.307775	-1.165764
1	1.529911	-2.267869	0.704555
1	6.232501	1.003124	2.048951
6	5.523545	0.162050	1.992900
7	4.223228	0.565607	1.474640
1	5.961811	-0.627161	1.383533
1	5.393677	-0.232894	3.008977
15	3.678781	0.266491	-0.109209
6	3.428341	1.339122	2.437775
7	3.900396	1.628761	-1.129052
7	4.847987	-0.797321	-0.812857
1	3.192711	0.717337	3.310430
1	3.995039	2.220766	2.772224
1	2.491914	1.680908	1.994509
6	4.204953	1.547797	-2.550042
6	3.822685	2.989807	-0.605299
6	6.212824	-0.407135	-1.144018
6	4.600705	-2.229896	-0.880137
1	3.438967	2.069810	-3.143349
1	5.175136	2.015194	-2.781669
1	4.242830	0.506678	-2.874111
1	3.231736	3.616289	-1.285903
1	3.321552	3.019025	0.361849
1	4.823248	3.440670	-0.513158
1	6.951850	-0.945757	-0.531511
1	6.434112	-0.628229	-2.198935
1	6.355088	0.663357	-0.981981
1	5.150665	-2.787573	-0.104645

1	3.532705	-2.423857	-0.773443
1	4.920678	-2.616736	-1.858852
1	1.683876	0.281240	-2.024113
1	0.283683	3.600117	1.333114
8	0.921532	2.923189	1.048767
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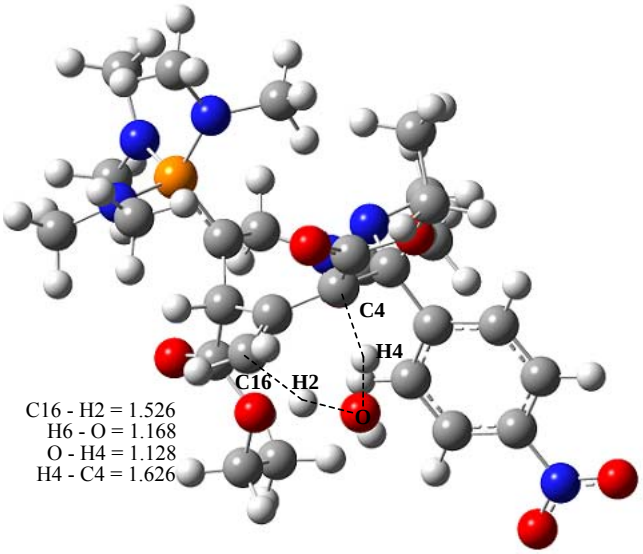
Standard coordinate and geometry of TS-3d:



8	-1.036061	-2.946254	2.517994
8	-0.836923	-2.229931	-1.889601
8	0.994348	-3.352980	-1.201703
8	-0.697841	3.628135	-0.248186
8	0.925929	3.148487	-1.735124
8	-6.937400	-1.341655	-0.456126
8	-7.474009	0.618135	0.336709
7	-0.192711	-1.011314	1.557968
7	-0.316694	0.399067	1.737067
7	-6.651900	-0.235632	0.004053
6	-1.012390	-1.731391	2.426412
6	-1.799708	-0.726168	3.271341
1	-1.829835	-1.075915	4.306451
1	-2.830353	-0.645969	2.911531
6	-0.982161	0.553319	3.064122

1	-1.571732	1.471998	3.089090
1	-0.198403	0.632963	3.827576
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1	-1.089781	2.114657	1.045443
6	-0.331435	1.320453	-0.727276
6	0.362219	0.349472	-1.583583
6	1.115174	-0.943933	-1.175788
6	1.851885	-0.919323	0.136644
6	1.188255	-1.520391	1.333662
1	1.782728	-1.350376	2.241390
6	0.423810	-2.300086	-1.396150
6	-1.451980	-3.509332	-2.216599
1	-0.688260	-4.146753	-2.666946
1	-2.203295	-3.257718	-2.969899
6	-2.073642	-4.182178	-1.000857
1	-1.332510	-4.333760	-0.212354
1	-2.474705	-5.159458	-1.294056
1	-2.898672	-3.592577	-0.589197
6	0.396853	0.595834	-2.960410
1	0.314293	1.613159	-3.337772
1	0.970196	-0.070487	-3.600467
6	0.064738	2.734810	-0.970818
6	-0.399597	5.025342	-0.435604
1	-1.335852	5.536532	-0.192760
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1	0.504758	5.287467	1.520351
1	0.882365	6.573163	0.354803
1	1.664436	4.986529	0.201843
6	-2.511835	0.700132	0.465976
6	-3.510351	1.637120	0.787946
1	-3.218724	2.622582	1.140241
6	-4.864590	1.343927	0.644906
1	-5.633498	2.066355	0.890554

6	-5.228545	0.087992	0.165846
6	-4.269902	-0.867090	-0.174345
1	-4.592178	-1.834155	-0.542207
6	-2.919860	-0.555882	-0.024577
1	-2.173423	-1.291177	-0.293930
1	1.042631	-2.603268	1.239242
1	4.842268	2.901483	0.140551
6	5.035896	1.930600	0.620007
7	3.787641	1.205990	0.817497
1	5.711718	1.360699	-0.019839
1	5.545512	2.128768	1.576185
15	3.458504	-0.363863	0.199526
6	2.847108	1.859478	1.716876
7	4.222007	-0.224180	-1.330775
7	4.335816	-1.439414	1.207202
1	3.231783	1.899269	2.749160
1	2.671903	2.892720	1.384425
1	1.888093	1.334540	1.709908
6	4.798665	-1.391873	-1.983770
6	3.954468	0.894942	-2.235753
6	5.471381	-1.053860	2.032784
6	4.154399	-2.886904	1.095256
1	4.104429	-1.871031	-2.692340
1	5.694059	-1.089150	-2.543813
1	5.102230	-2.135763	-1.245959
1	3.391823	0.565175	-3.120213
1	3.363076	1.667568	-1.742100
1	4.900602	1.336377	-2.582488
1	5.424446	-1.591135	2.989746
1	6.437222	-1.295641	1.561082
1	5.443200	0.013544	2.247183
1	3.335270	-3.110662	0.409386
1	5.069765	-3.376996	0.728247
1	3.917533	-3.317007	2.078572

1	-1.588098	1.306058	-1.759716
1	1.886739	-1.007185	-1.952293
8	-2.144586	0.997286	-2.691004
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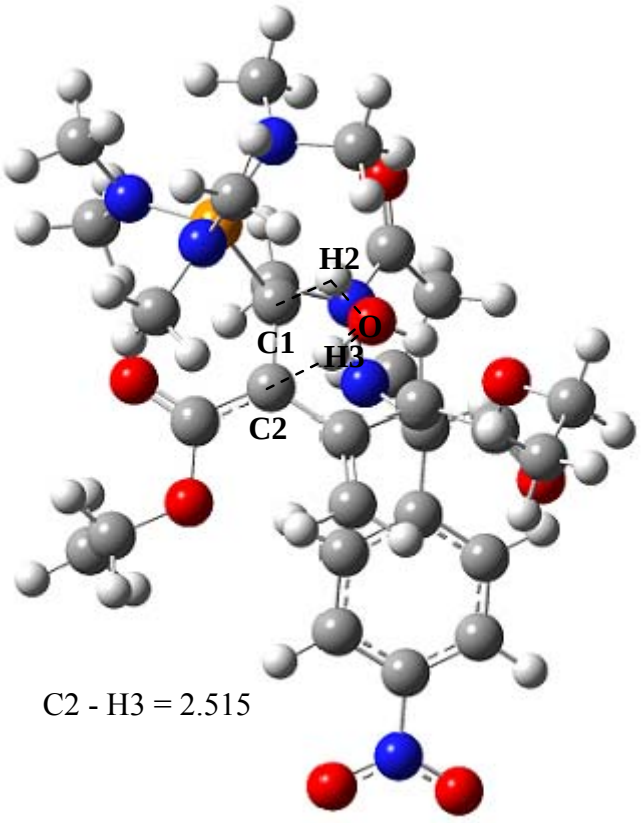
1	-1.125843	0.543024	-3.036590

Standard coordinate and geometry of IN-4:



8	1.656506	1.143718	4.016847
8	-0.450398	-2.319918	-1.897871
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8	-0.353377	3.484437	-1.122258
8	-2.509598	3.122854	-0.546292
8	-6.767488	-2.531467	-0.752242
8	-7.801827	-0.720045	-0.120603
7	0.324260	0.272662	2.339141
7	-1.055732	-0.018354	2.095921
7	-6.781498	-1.387865	-0.295382
6	0.554122	0.879748	3.560574
6	-0.812629	1.066581	4.221801

1	-1.168492	2.094372	4.081730
1	-0.731137	0.884367	5.295622
6	-1.650945	0.027669	3.462114
1	-1.537166	-0.962187	3.918371
1	-2.716137	0.254277	3.397961
6	-1.734529	0.981241	1.201044
1	-1.965388	1.894098	1.773574
6	-0.804311	1.464093	0.041160
1	0.116537	1.778953	0.538431
6	-0.463382	0.420072	-1.043625
6	0.616300	-0.535188	-0.744465
6	1.666179	-0.175000	0.279643
6	1.327831	-0.599275	1.731868
1	2.189730	-0.554461	2.405448
6	0.601924	-1.898466	-1.114633
6	-0.471574	-3.710192	-2.251888
1	0.546413	-4.048882	-2.461222
1	-1.061186	-3.750516	-3.173280
6	-1.104165	-4.571048	-1.164774
1	-0.501759	-4.528850	-0.253061
1	-1.162995	-5.615857	-1.493880
1	-2.119841	-4.229133	-0.935918
6	-1.228672	0.414640	-2.161471
1	-2.091777	1.065139	-2.263242
1	-1.059334	-0.297368	-2.958518
6	-1.357818	2.749746	-0.563787
6	-0.725614	4.672190	-1.873379
1	0.092897	5.374588	-1.696342
1	-1.648336	5.072753	-1.450326
6	-0.870635	4.336509	-3.349864
1	0.040645	3.863063	-3.729561
1	-1.055070	5.251869	-3.923661
1	-1.709883	3.653399	-3.511322
6	-3.058275	0.364232	0.771784

6	-4.255534	1.074743	0.938558
1	-4.227015	2.086878	1.328685
6	-5.480219	0.512684	0.589111
1	-6.411145	1.051389	0.714036
6	-5.494328	-0.779609	0.068165
6	-4.321871	-1.511733	-0.112621
1	-4.374089	-2.511778	-0.525085
6	-3.105792	-0.935248	0.242741
1	-2.188516	-1.494308	0.109677
1	0.925341	-1.614396	1.721030
1	5.743448	1.211103	2.251986
6	4.852756	0.584746	2.115699
7	4.320999	0.807016	0.765389
1	5.145884	-0.456654	2.249518
1	4.119247	0.850623	2.889848
15	3.515499	-0.457571	-0.069225
6	3.879032	2.196391	0.569489
7	3.967065	-0.241950	-1.674223
7	4.203501	-1.895867	0.471016
1	3.191483	2.506004	1.370820
1	4.753124	2.859811	0.599937
1	3.379601	2.324424	-0.394855
6	3.456149	-1.151751	-2.705782
6	4.848279	0.813272	-2.179698
6	5.612278	-2.149866	0.163436
6	3.564355	-2.915241	1.304081
1	2.811638	-0.616050	-3.413737
1	4.304318	-1.574963	-3.261632
1	2.891049	-1.966763	-2.250579
1	4.273681	1.570648	-2.723377
1	5.388923	1.285766	-1.360338
1	5.583402	0.357768	-2.856335
1	6.223468	-2.169320	1.076677
1	5.710626	-3.120893	-0.338335

1	6.009065	-1.379050	-0.499139
1	2.494371	-2.933106	1.115892
1	3.954374	-3.893219	1.000082
1	3.784622	-2.772771	2.371828
1	1.579979	1.235318	-2.248564
8	1.948843	2.136112	-2.261828
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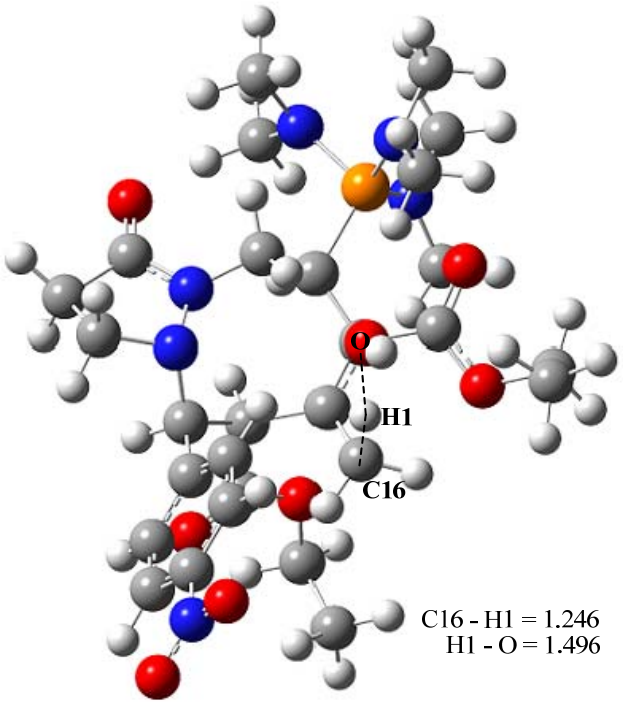
Standard coordinate and geometry of TS-4a:



8	-1.695453	3.937323	0.565451
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8	0.972961	-1.240337	3.196806
8	2.597015	0.327768	3.203461
8	6.876270	-0.546178	-2.932512
8	7.924938	-0.031713	-1.092834
7	-0.230569	2.277278	-0.093660
7	1.157012	2.109084	-0.372099
7	6.899877	-0.149926	-1.766613
6	-0.558428	3.534477	0.350370
6	0.749157	4.323157	0.447115

1	1.099130	4.345502	1.486516
1	0.586948	5.354287	0.125685
6	1.657800	3.505022	-0.481090
1	1.537850	3.831926	-1.520166
1	2.719462	3.539103	-0.231756
6	1.891404	1.351204	0.684439
1	2.157654	2.016307	1.519479
6	0.972160	0.286264	1.372569
1	0.126515	0.874549	1.748184
6	0.420955	-0.901676	0.581400
6	-0.932480	-0.966256	0.284537
6	-1.789086	0.305668	0.222204
6	-1.170190	1.373607	-0.747686
1	-1.944896	1.998934	-1.194708
6	-1.563613	-2.134707	-0.305459
6	-1.328826	-4.345530	-1.176437
1	-2.379888	-4.187464	-1.422648
1	-1.231850	-5.275264	-0.608501
6	-0.440909	-4.329069	-2.415338
1	-0.364031	-3.303784	-2.794778
1	-0.854234	-4.988009	-3.188299
1	0.571636	-4.671075	-2.176237
6	1.406406	-1.818942	0.031078
1	2.422972	-1.635787	0.378426
1	1.161184	-2.874248	0.076299
6	1.643036	-0.201142	2.668743
6	1.481079	-1.785634	4.440266
1	0.607445	-2.253041	4.901056
1	1.829358	-0.963391	5.070038
6	2.587039	-2.798269	4.184651
1	2.241874	-3.586115	3.507850
1	2.891594	-3.261149	5.130480
1	3.461539	-2.312249	3.743048
6	3.201959	0.890739	0.048316

6	4.404674	1.014143	0.760717
1	4.383779	1.369654	1.785181
6	5.621273	0.669101	0.176691
1	6.557148	0.760406	0.713780
6	5.620799	0.206154	-1.137127
6	4.440608	0.073018	-1.869038
1	4.483042	-0.300925	-2.884765
6	3.229445	0.419907	-1.276635
1	2.294887	0.282605	-1.820481
1	-0.608859	0.846482	-1.529179
1	-5.431071	3.177862	-0.933720
6	-4.411657	2.766113	-0.930797
7	-4.332153	1.672282	0.045211
1	-4.180136	2.407690	-1.932231
1	-3.710617	3.564968	-0.666435
15	-3.603705	0.145289	-0.250214
6	-4.474897	2.180266	1.415558
7	-4.454069	-0.732764	0.942512
7	-3.873879	0.055707	-1.926893
1	-3.699845	2.925867	1.628515
1	-5.458408	2.656841	1.529354
1	-4.407467	1.366246	2.137375
6	-5.915454	-0.786061	0.899967
6	-3.872686	-1.791617	1.767884
6	-5.256648	0.034390	-2.412410
6	-2.945016	-0.535663	-2.905478
1	-6.279456	-1.685884	0.382628
1	-6.301920	-0.804070	1.926884
1	-6.318771	0.098798	0.406748
1	-4.034227	-2.788714	1.342915
1	-2.802121	-1.640935	1.906168
1	-4.350680	-1.743345	2.755108
1	-5.298921	0.538259	-3.385894
1	-5.621983	-0.994444	-2.545171

1	-5.925424	0.563490	-1.732467
1	-1.901895	-0.551682	-2.581751
1	-3.234282	-1.564575	-3.147625
1	-3.011550	0.074871	-3.816118
1	-1.902415	0.783112	1.206036
8	0.440024	-0.963288	-2.329014
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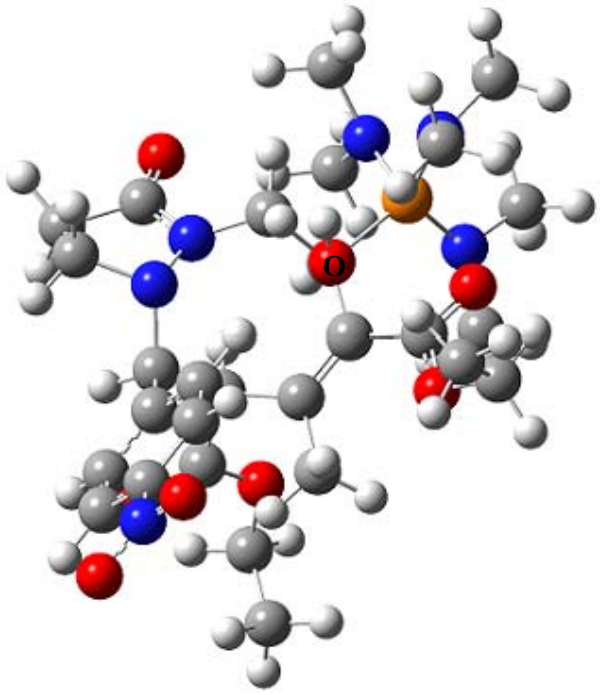
Standard coordinate and geometry of IN-5:



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8	-0.622513	-2.430006	2.712846
8	-2.343705	-3.235808	1.486593
8	-6.335571	2.912391	-1.054003
8	-7.533726	1.189638	-0.467947
7	0.433584	-1.428018	-1.903069
7	-0.976667	-1.242579	-1.993091
7	-6.460892	1.723894	-0.756938
6	0.882300	-2.565151	-2.528693

6	-0.351343	-3.268502	-3.102076
1	-0.652421	-4.093374	-2.443816
1	-0.119508	-3.689979	-4.082804
6	-1.365532	-2.115582	-3.128821
1	-1.264130	-1.539542	-4.055666
1	-2.409840	-2.417065	-3.027060
6	-1.737237	-1.588957	-0.747864
1	-2.078895	-2.631875	-0.793063
6	-0.841577	-1.547129	0.532707
1	0.093994	-2.032720	0.236711
6	-0.542527	-0.157750	1.082859
6	0.605151	0.486385	0.754411
6	1.679595	-0.173915	-0.116887
6	1.260277	-0.264203	-1.623603
1	2.134009	-0.336551	-2.273254
6	0.916936	1.884275	1.162805
6	0.042719	4.032526	1.733628
1	1.091860	4.290209	1.582292
1	-0.251011	4.315588	2.749108
6	-0.859630	4.621762	0.659483
1	-0.671407	4.069543	-0.272564
1	-0.651358	5.691552	0.535445
1	-1.915574	4.505113	0.927503
6	-1.632576	0.426974	1.962737
1	-2.423243	-0.305487	2.143424
1	-1.237739	0.752078	2.929336
6	-1.396108	-2.487572	1.608361
6	-0.980024	-3.309954	3.809822
1	-0.041607	-3.453718	4.350922
1	-1.311837	-4.265927	3.397697
6	-2.047782	-2.690273	4.698363
1	-1.727247	-1.711825	5.070383
1	-2.234443	-3.341907	5.559728
1	-2.986582	-2.570782	4.150481

6	-2.972235	-0.693059	-0.727412
6	-4.221440	-1.245116	-0.406575
1	-4.289621	-2.295939	-0.140908
6	-5.372127	-0.460324	-0.411175
1	-6.344932	-0.870905	-0.170919
6	-5.252508	0.887435	-0.744285
6	-4.020678	1.461397	-1.062035
1	-3.968604	2.515793	-1.305488
6	-2.871900	0.671756	-1.060437
1	-1.900823	1.140369	-1.282919
1	0.667926	0.665148	-1.816915
1	5.756181	-1.076396	-2.381557
6	4.696916	-0.825591	-2.231805
7	4.407344	-0.799520	-0.790879
1	4.503426	0.147452	-2.680853
1	4.079974	-1.579472	-2.733023
15	3.459202	0.409307	-0.034100
6	4.495897	-2.143416	-0.206351
7	4.038567	0.212111	1.561342
7	3.849220	1.737118	-0.999719
1	3.805460	-2.830339	-0.712205
1	5.517391	-2.527536	-0.328864
1	4.270184	-2.112244	0.860007
6	5.463892	0.409019	1.833990
6	3.216847	0.321026	2.767501
6	5.251192	2.157495	-1.089335
6	2.920479	2.803780	-1.416478
1	5.684648	1.436703	2.157162
1	5.768306	-0.273468	2.637214
1	6.061443	0.174120	0.952842
1	3.186801	1.342347	3.163146
1	2.196498	-0.012839	2.581032
1	3.651817	-0.343111	3.525381
1	5.439045	2.539783	-2.099939

1	5.474787	2.962176	−0.374380
1	5.933300	1.324455	−0.914781
1	1.854950	2.523046	−1.343770
1	3.082716	3.705064	−0.813536
1	3.155679	3.035455	−2.464845
1	1.851782	−1.197479	0.241623
8	−0.118072	2.208504	−1.316004
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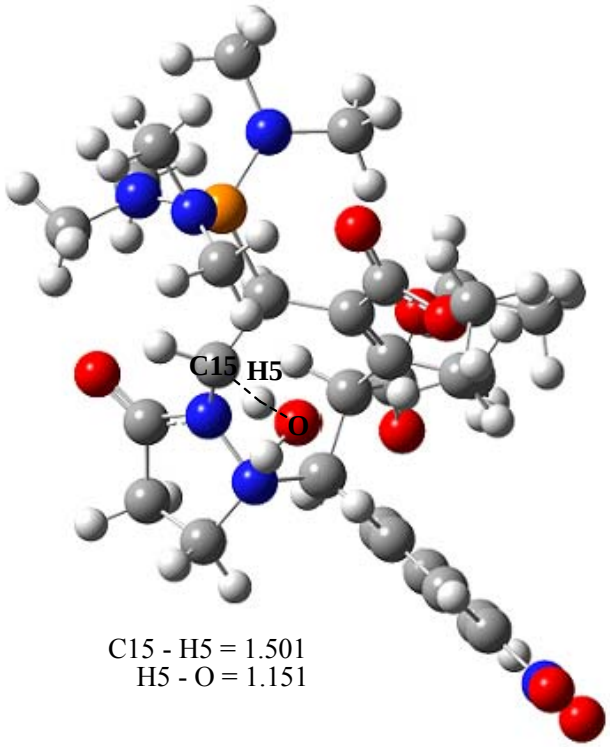
Standard coordinate and geometry of TS-5:



8	2.024645	−2.676726	−2.808609
8	−0.140967	2.643810	1.577606
8	2.072617	2.351003	1.269479
8	−0.590097	−2.425921	2.609701
8	−2.251911	−3.273400	1.332137
8	−6.571687	2.738797	−0.833353
8	−7.638061	0.949733	−0.192449
7	0.447338	−1.189881	−1.983614
7	−0.975399	−1.006930	−2.037308
7	−6.615704	1.543087	−0.540945

6	0.861929	-2.295545	-2.681853
6	-0.375979	-2.921800	-3.333906
1	-0.687738	-3.812297	-2.773417
1	-0.142556	-3.237166	-4.354047
6	-1.380973	-1.765507	-3.244508
1	-1.281410	-1.104498	-4.113310
1	-2.427676	-2.069511	-3.166335
6	-1.712230	-1.492705	-0.830061
1	-1.990803	-2.550610	-0.942544
6	-0.820813	-1.485365	0.454801
1	0.117552	-1.942596	0.126039
6	-0.528792	-0.116056	1.059612
6	0.632169	0.529951	0.777877
6	1.694029	-0.111928	-0.129969
6	1.276320	-0.046689	-1.634108
1	2.153539	-0.090132	-2.283494
6	0.924787	1.920254	1.226320
6	0.016256	4.078930	1.727708
1	1.080299	4.317438	1.702681
1	-0.381839	4.321595	2.717851
6	-0.757192	4.760496	0.608791
1	-0.437411	4.353566	-0.355622
1	-0.582011	5.842610	0.638233
1	-1.832616	4.582492	0.712697
6	-1.625420	0.441062	1.949631
1	-2.364307	-0.328209	2.186909
1	-1.224970	0.832289	2.888342
6	-1.345309	-2.482218	1.491572
6	-0.914618	-3.365050	3.666898
1	0.021715	-3.476312	4.219132
1	-1.184983	-4.322039	3.214235
6	-2.029798	-2.841066	4.558886
1	-1.771546	-1.861021	4.972954
1	-2.192174	-3.534588	5.391998

1	-2.965307	-2.754562	3.999257
6	-3.002025	-0.680761	-0.740257
6	-4.198490	-1.301433	-0.350246
1	-4.192752	-2.355191	-0.089833
6	-5.387973	-0.580160	-0.280092
1	-6.320285	-1.045383	0.015248
6	-5.365981	0.773652	-0.609612
6	-4.191047	1.415896	-1.002470
1	-4.216404	2.470625	-1.248288
6	-3.006333	0.686434	-1.073134
1	-2.079672	1.179429	-1.370942
1	0.492727	1.227982	-1.750728
1	5.752609	-1.209791	-2.353460
6	4.723903	-0.853547	-2.205812
7	4.411201	-0.899509	-0.768674
1	4.652329	0.167041	-2.579268
1	4.034438	-1.491699	-2.767547
15	3.501533	0.309616	0.017848
6	4.356621	-2.283324	-0.277560
7	4.027249	0.034853	1.620631
7	4.006805	1.687571	-0.817156
1	3.620279	-2.863192	-0.847667
1	5.342334	-2.750192	-0.404140
1	4.104685	-2.302054	0.783793
6	5.455909	0.073108	1.939085
6	3.181831	0.170456	2.806753
6	5.423440	2.058411	-0.789515
6	3.149430	2.793004	-1.265970
1	5.775894	1.062907	2.296117
1	5.661627	-0.656544	2.732251
1	6.049827	-0.205085	1.068356
1	3.216217	1.179382	3.233826
1	2.146406	-0.080607	2.580172
1	3.541317	-0.545597	3.556894

1	5.698802	2.476702	-1.765567
1	5.627056	2.819973	-0.022831
1	6.060016	1.191686	-0.608653
1	2.096400	2.517256	-1.347686
1	3.234985	3.651103	-0.589090
1	3.501091	3.092755	-2.262812
1	1.804843	-1.162553	0.188873
8	-0.051990	2.237736	-1.654880
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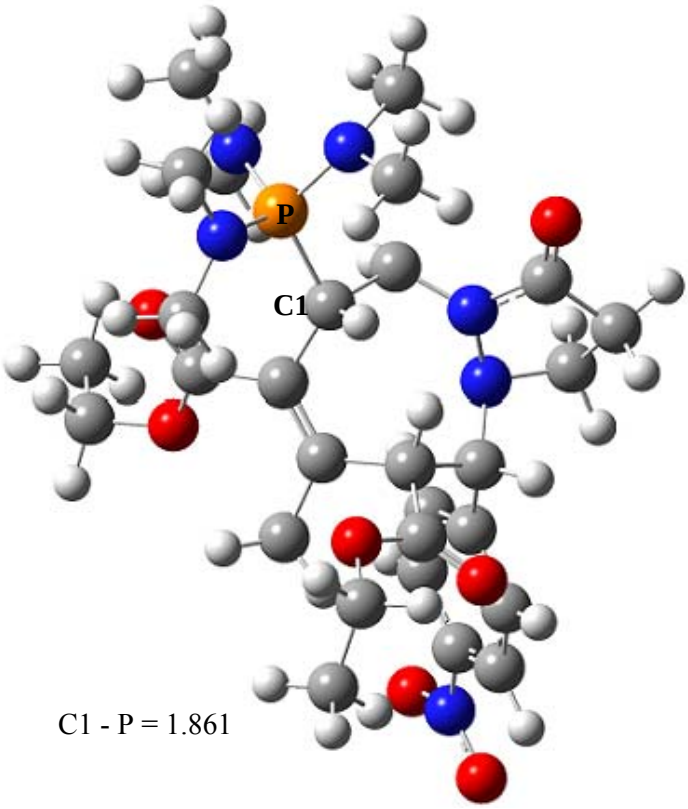
Standard coordinate and geometry of IN-6:



8	1.772573	-3.746741	-1.668567
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8	2.237445	2.716656	0.385095
8	-0.784872	-0.843736	3.266536
8	-2.314124	-2.273755	2.416531
8	-6.783543	2.106189	-1.960574
8	-7.757769	0.741431	-0.567264
7	0.465711	-1.835483	-1.422201

7	-0.964152	-1.502413	-1.567723
7	-6.770639	1.156051	-1.176387
6	0.695506	-3.162607	-1.711316
6	-0.635081	-3.797334	-2.129846
1	-1.059802	-4.382684	-1.304804
1	-0.467276	-4.480346	-2.966139
6	-1.467684	-2.561036	-2.480079
1	-1.268056	-2.244847	-3.510305
1	-2.547177	-2.686306	-2.364569
6	-1.729271	-1.534618	-0.284523
1	-1.964223	-2.566808	0.016754
6	-0.876858	-0.990290	0.904548
1	0.044098	-1.576685	0.835335
6	-0.538106	0.498559	0.869379
6	0.683346	0.903374	0.422123
6	1.695119	-0.143035	-0.095576
6	1.451788	-0.791126	-1.448356
1	1.146402	-0.058074	-2.200107
6	1.074488	2.338151	0.348536
6	0.352791	4.613665	0.188122
1	1.241665	4.795540	0.795663
1	-0.513279	5.089677	0.655400
6	0.545384	5.101100	-1.240005
1	1.425805	4.637338	-1.694276
1	0.689103	6.187791	-1.244585
1	-0.331297	4.867850	-1.852810
6	-1.639572	1.421294	1.361240
1	-2.442414	0.850318	1.833585
1	-1.268777	2.148017	2.089298
6	-1.449110	-1.437307	2.252223
6	-1.152551	-1.244144	4.611643
1	-0.258449	-1.034973	5.203846
1	-1.347838	-2.319092	4.615455
6	-2.354437	-0.462004	5.119212

1	-2.167482	0.615774	5.072673
1	-2.556554	-0.731045	6.162364
1	-3.244519	-0.693862	4.527705
6	-3.057680	-0.815163	-0.515456
6	-4.222864	-1.245960	0.140025
1	-4.166933	-2.082932	0.827391
6	-5.441389	-0.604748	-0.068601
1	-6.346069	-0.927979	0.431571
6	-5.490307	0.473559	-0.950318
6	-4.354765	0.917104	-1.627803
1	-4.434901	1.752256	-2.312909
6	-3.144458	0.266566	-1.407825
1	-2.250842	0.576043	-1.937807
1	5.494379	-2.352022	-1.925036
6	4.526441	-1.835724	-1.853691
7	4.373723	-1.353259	-0.469839
1	4.520890	-0.996911	-2.547976
1	3.709574	-2.513013	-2.114078
15	3.540916	0.091234	-0.151477
6	4.219328	-2.475837	0.467071
7	4.150251	0.398019	1.425935
7	4.088001	1.115951	-1.381985
1	3.378230	-3.112737	0.166132
1	5.135854	-3.079338	0.451954
1	4.070023	-2.107519	1.483794
6	5.584997	0.418450	1.704996
6	3.361049	1.027706	2.481419
6	5.508278	1.415334	-1.524880
6	3.233333	1.927416	-2.236804
1	6.000956	1.437370	1.678369
1	5.762019	0.009597	2.708831
1	6.120074	-0.207405	0.990427
1	3.511399	2.113415	2.529731
1	2.297148	0.834768	2.346112

1	3.660825	0.587733	3.442391
1	5.776717	1.407309	-2.589946
1	5.759191	2.405592	-1.115977
1	6.119156	0.661992	-1.027178
1	2.187567	1.656758	-2.119989
1	3.347607	2.995036	-2.008463
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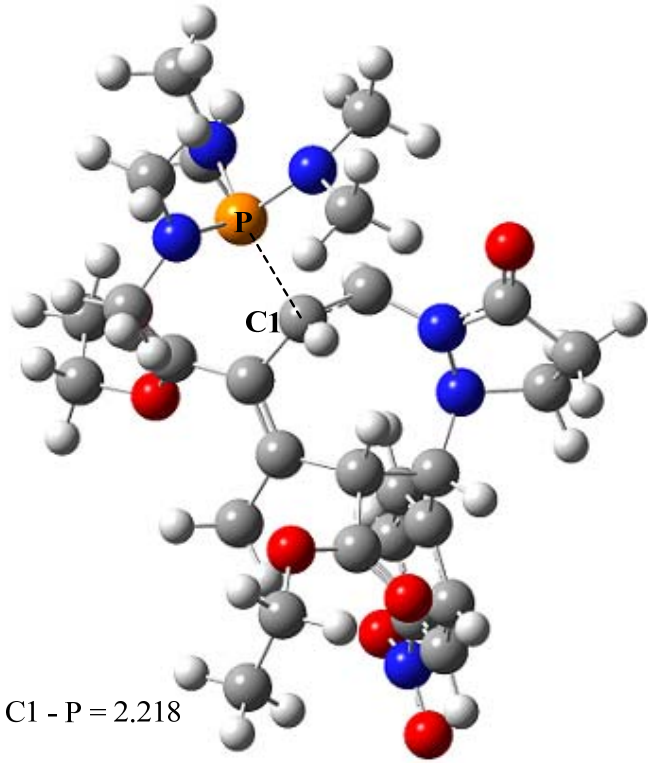
Standard coordinate and geometry of TS-6:



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8	2.160205	2.681277	0.551077
8	-0.797965	-0.936583	3.266948
8	-2.431790	-2.260087	2.441867
8	-6.719589	2.248396	-1.994013
8	-7.754897	0.959041	-0.573466
7	0.321739	-1.912035	-1.484401
7	-1.119256	-1.691188	-1.565441
7	-6.751231	1.313296	-1.192987

6	0.673760	-3.199750	-1.793389
6	-0.621409	-3.981044	-2.040218
1	-0.897250	-4.552587	-1.144724
1	-0.476093	-4.691687	-2.857013
6	-1.604315	-2.850231	-2.358366
1	-1.548770	-2.586032	-3.420915
1	-2.647999	-3.064686	-2.116446
6	-1.841681	-1.595385	-0.257121
1	-2.114668	-2.596454	0.105732
6	-0.968929	-1.020867	0.908256
1	-0.047673	-1.605200	0.843940
6	-0.618050	0.475609	0.900762
6	0.587771	0.880781	0.414073
6	1.470535	-0.208449	-0.186924
6	1.106808	-0.716736	-1.456936
1	0.755360	-0.004657	-2.202506
6	1.006541	2.307555	0.398560
6	0.290635	4.583369	0.174537
1	1.147602	4.757815	0.828239
1	-0.599770	5.047974	0.606852
6	0.550240	5.097044	-1.233536
1	1.454149	4.645066	-1.652546
1	0.688683	6.184242	-1.212345
1	-0.293856	4.870777	-1.892951
6	-1.672683	1.403795	1.475771
1	-2.423890	0.846102	2.040061
1	-1.242189	2.156712	2.140680
6	-1.527071	-1.469141	2.265239
6	-1.140549	-1.344818	4.616615
1	-0.215092	-1.200316	5.179019
1	-1.397621	-2.406647	4.605898
6	-2.275785	-0.506317	5.183917
1	-2.027735	0.559601	5.152879
1	-2.455612	-0.786829	6.228108

1	-3.198840	-0.673159	4.621606
6	-3.139489	-0.828447	-0.507344
6	-4.320458	-1.187446	0.161670
1	-4.303320	-2.011269	0.866743
6	-5.506753	-0.490670	-0.056373
1	-6.424630	-0.758696	0.452260
6	-5.504827	0.571723	-0.958040
6	-4.351478	0.946310	-1.646838
1	-4.392122	1.772614	-2.345985
6	-3.174780	0.238864	-1.419734
1	-2.269787	0.493763	-1.959077
1	5.499502	-2.198132	-2.120027
6	4.521731	-1.711611	-1.982845
7	4.382317	-1.312515	-0.575423
1	4.477235	-0.834212	-2.627210
1	3.726794	-2.405917	-2.268726
15	3.653472	0.173761	-0.109147
6	4.245762	-2.472847	0.310310
7	4.426957	0.374096	1.425442
7	4.236030	1.195374	-1.358843
1	3.424517	-3.122259	-0.017732
1	5.175341	-3.059409	0.292032
1	4.074320	-2.146947	1.338727
6	5.864874	0.234067	1.635319
6	3.740468	1.058594	2.515368
6	5.657692	1.455902	-1.544530
6	3.364449	2.096603	-2.096534
1	6.381936	1.206550	1.643269
1	6.049566	-0.252391	2.603636
1	6.297471	-0.393531	0.854618
1	4.013905	2.120853	2.588901
1	2.659994	1.000308	2.384793
1	4.001183	0.567549	3.463677
1	5.888026	1.507078	-2.618248

1	5.967937	2.407693	-1.085634
1	6.254853	0.649116	-1.117359
1	2.329054	1.762622	-2.037697
1	3.422897	3.130135	-1.727931
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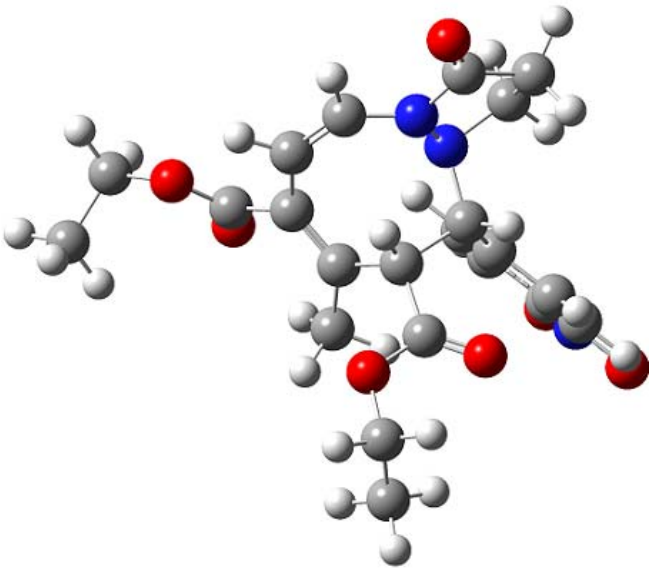
Standard coordinate and geometry of 7a:



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8	-0.871806	-0.290635	3.290940
8	1.046103	0.863521	2.975622
8	4.969698	-2.421051	-2.390462
8	6.124708	-1.583158	-0.741829
7	-1.347629	2.644475	-0.676556
7	-0.172423	1.894054	-0.982319
7	5.091386	-1.699917	-1.400635
6	-1.172606	4.029684	-0.752189
6	0.280274	4.254051	-1.152906
1	0.870795	4.529445	-0.270113
1	0.349159	5.074350	-1.870476

6	0.659001	2.883743	-1.726371
1	0.383668	2.821665	-2.784689
1	1.713806	2.629086	-1.627665
6	0.502389	1.396965	0.252887
1	0.862730	2.229575	0.873264
6	-0.538182	0.626716	1.134362
1	-1.371276	1.320732	1.299058
6	-1.096126	-0.608376	0.446627
6	-2.176261	-0.464159	-0.369853
6	-2.967924	0.770524	-0.526872
6	-2.613043	2.067843	-0.610153
1	-3.377846	2.837578	-0.637449
6	-2.722948	-1.650075	-1.122752
6	-4.713833	-2.674476	-1.948033
1	-4.094490	-2.916826	-2.814748
1	-5.655693	-2.234097	-2.284554
6	-4.951011	-3.900751	-1.078942
1	-4.000351	-4.342339	-0.767465
1	-5.510179	-4.653758	-1.646266
1	-5.531580	-3.640727	-0.187671
6	-0.414990	-1.925023	0.745870
1	0.654928	-1.781268	0.924700
1	-0.835096	-2.352919	1.665218
6	0.007008	0.404075	2.545229
6	-0.535834	-0.486943	4.689873
1	-1.504722	-0.615255	5.177808
1	-0.057340	0.421398	5.063362
6	0.355946	-1.703183	4.886741
1	-0.114587	-2.604741	4.481104
1	0.531649	-1.860827	5.957092
1	1.324046	-1.557927	4.399297
6	1.703860	0.562693	-0.175347
6	2.915520	0.656821	0.526125
1	2.979121	1.300440	1.396279

6	4.027213	-0.085257	0.134728
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6	3.918288	-0.920842	-0.974798
6	2.730389	-1.034924	-1.694948
1	2.684155	-1.696750	-2.550980
6	1.626736	-0.288784	-1.291020
1	0.695571	-0.363861	-1.841235
1	-0.538323	-2.642790	-0.061798
1	-4.037421	0.601090	-0.591963