Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

First diastereoselective [3+2] cycloaddition reaction of diethyl isocyanomethylphosphonate and maleimides

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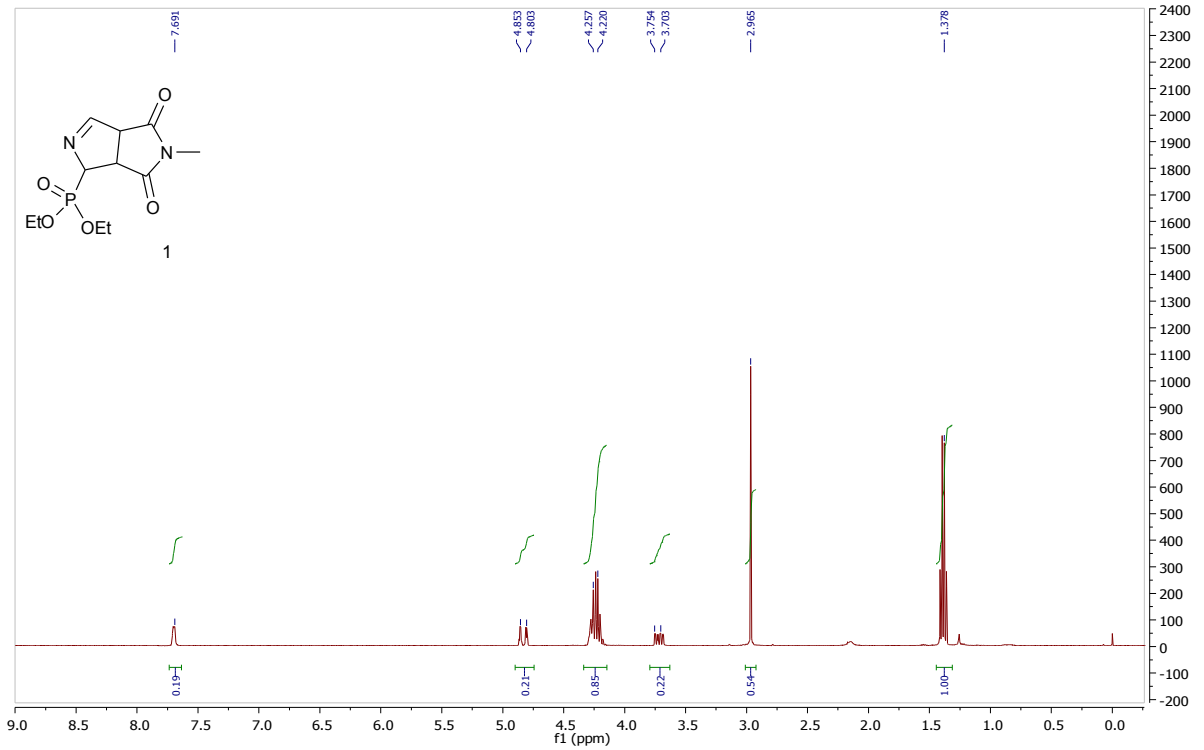

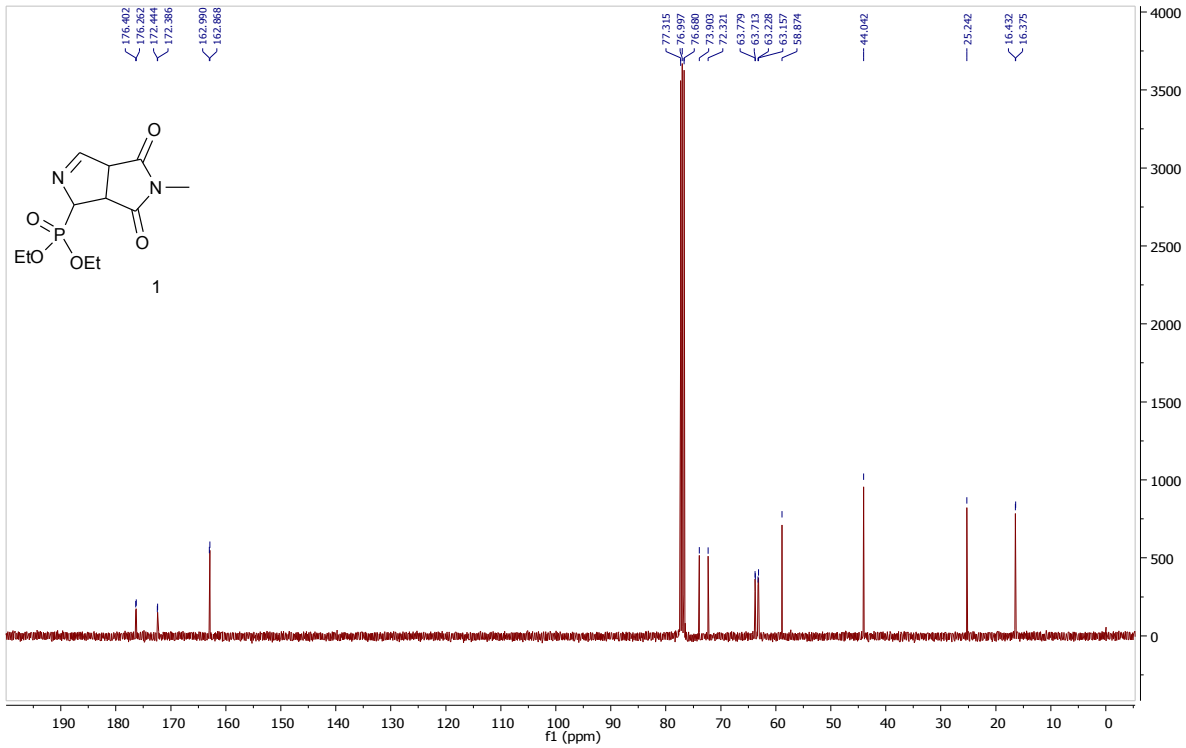

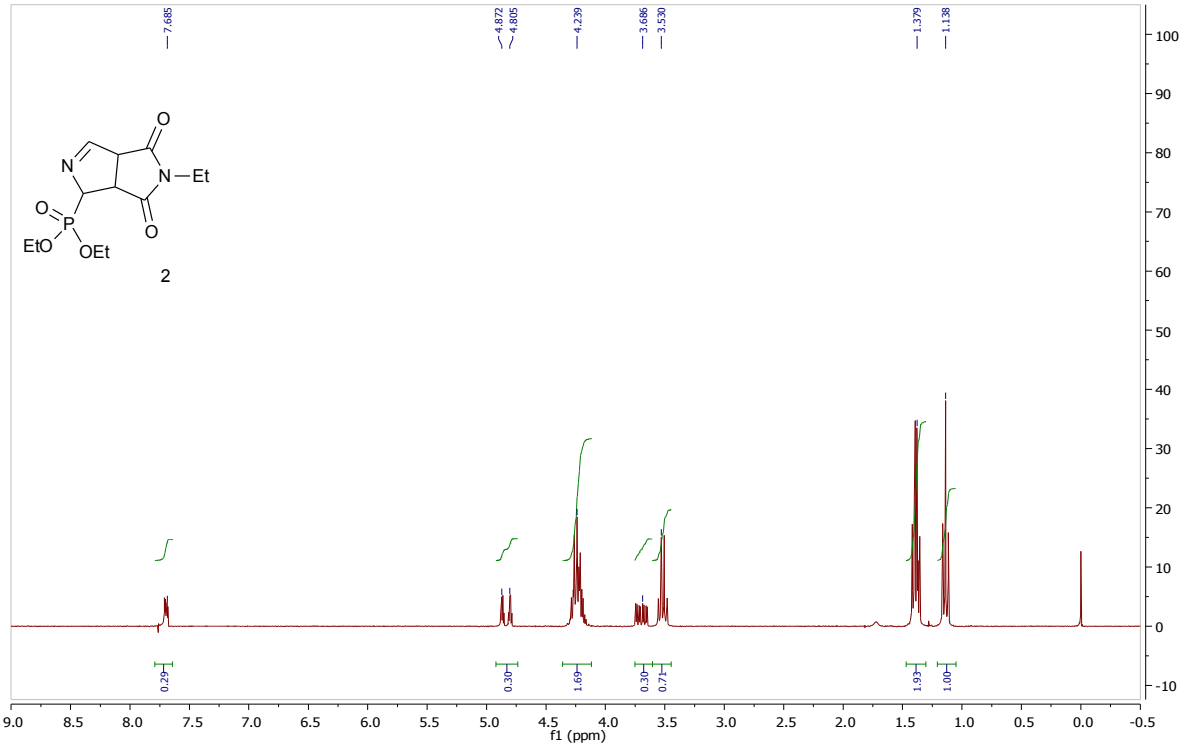

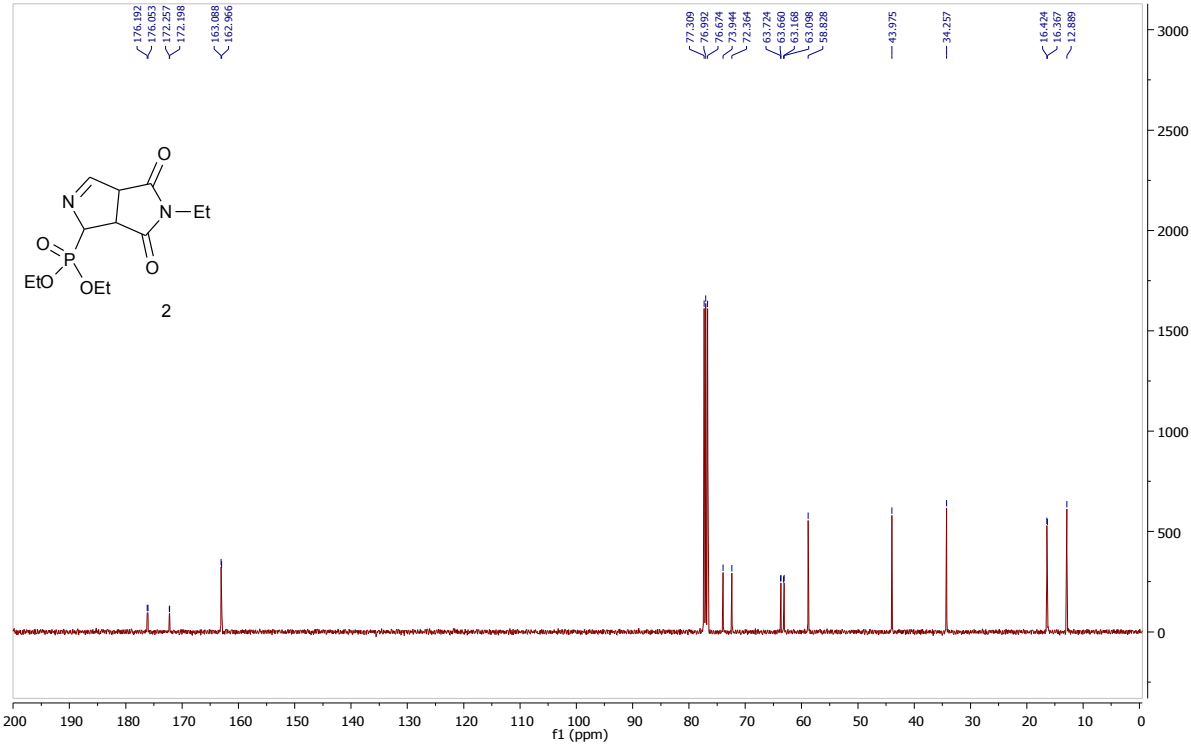

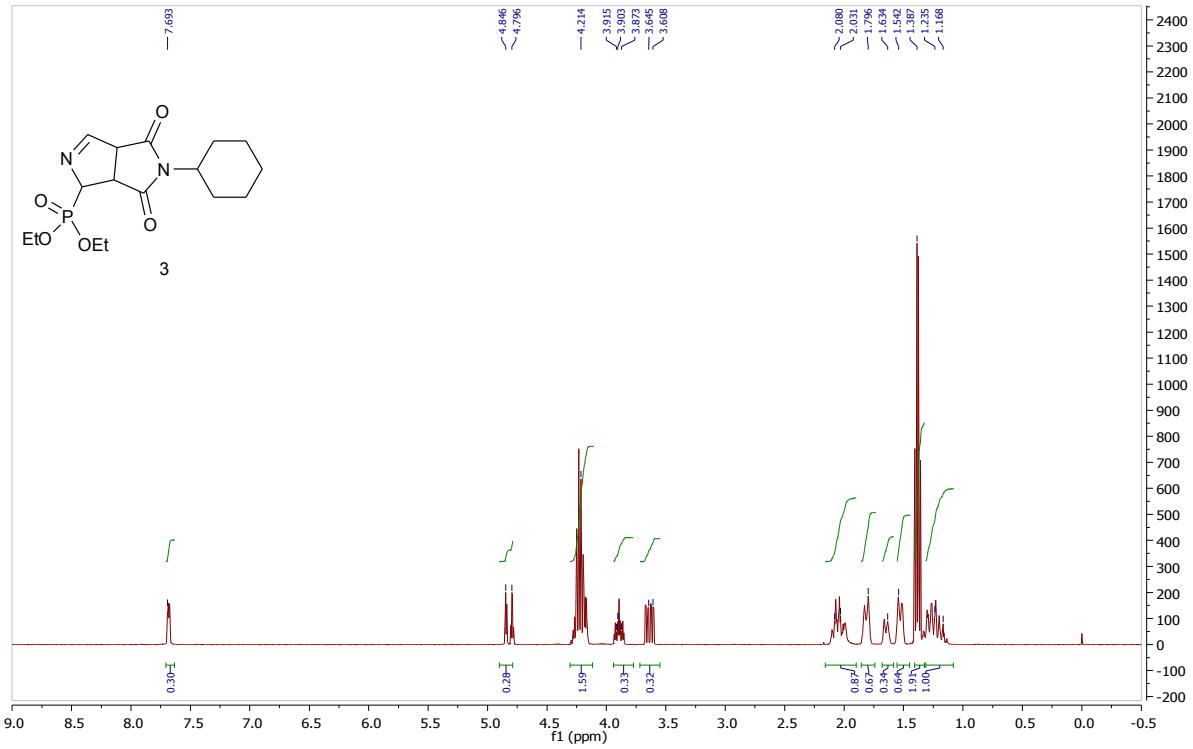

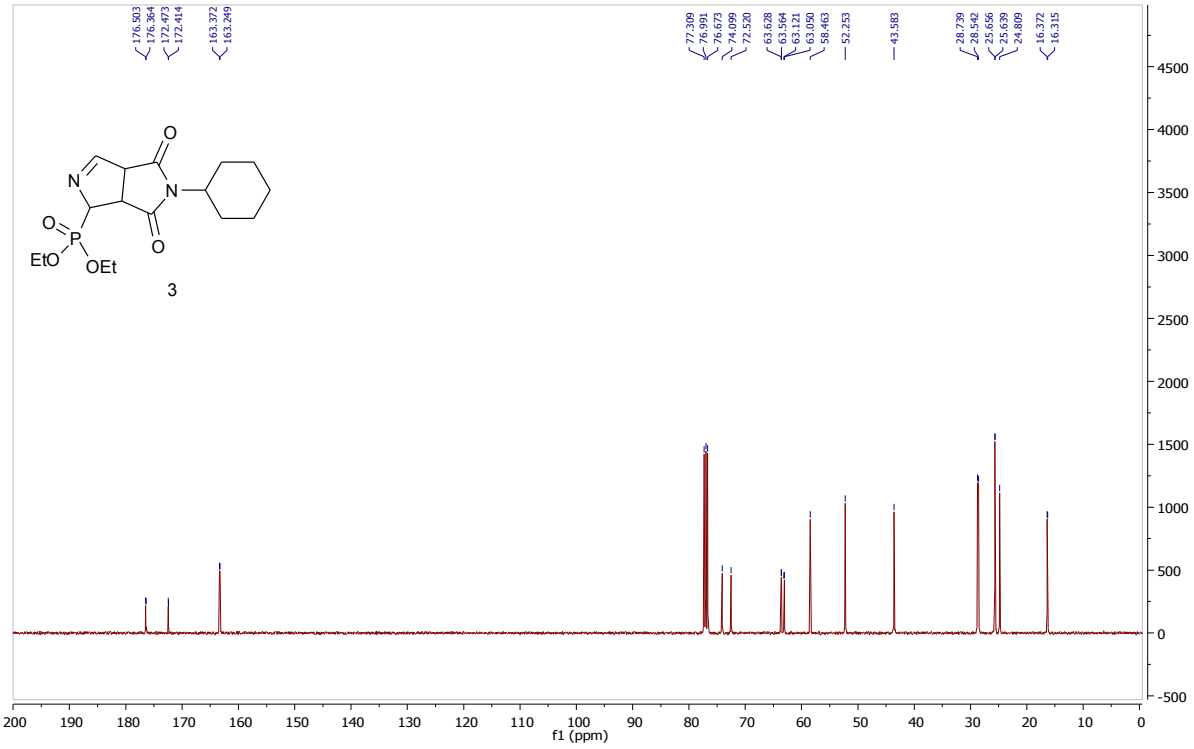

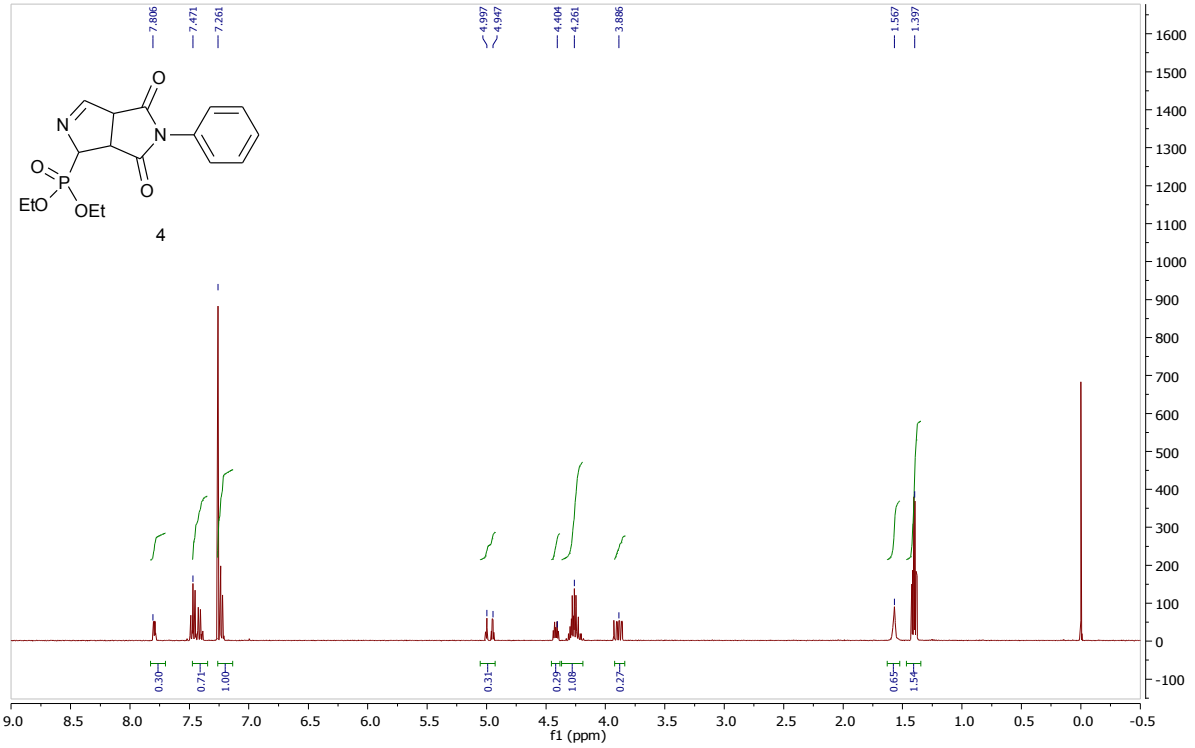
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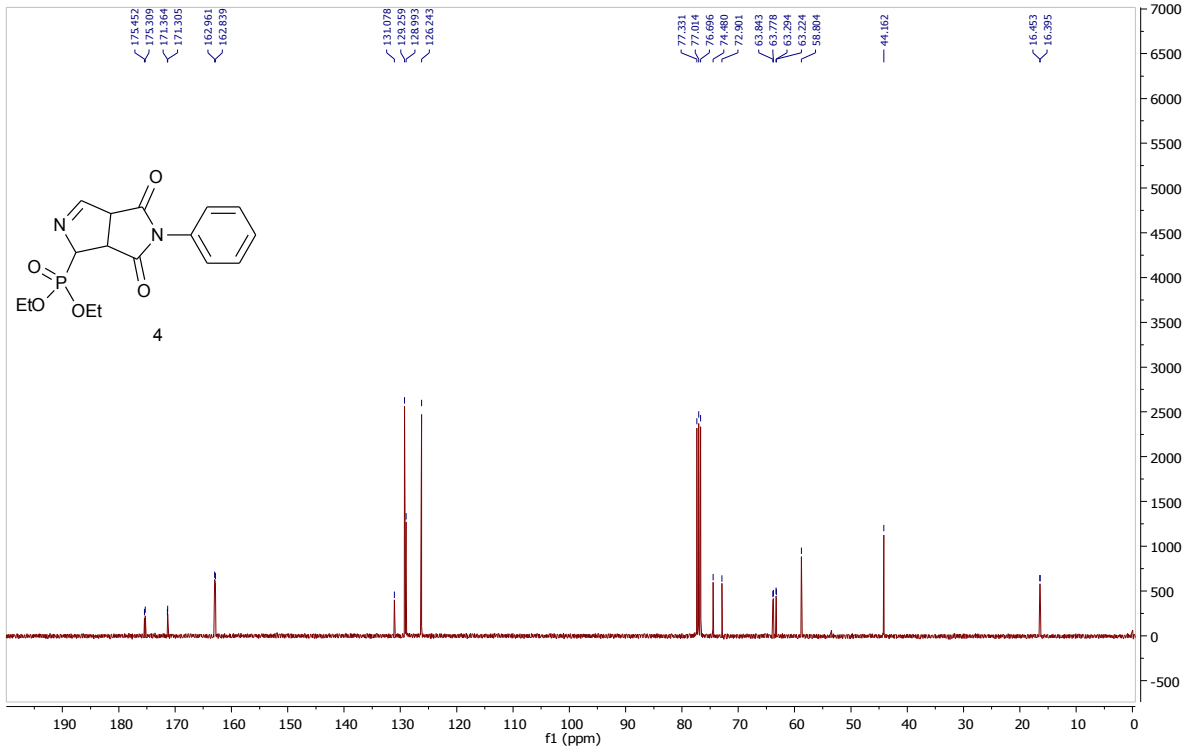
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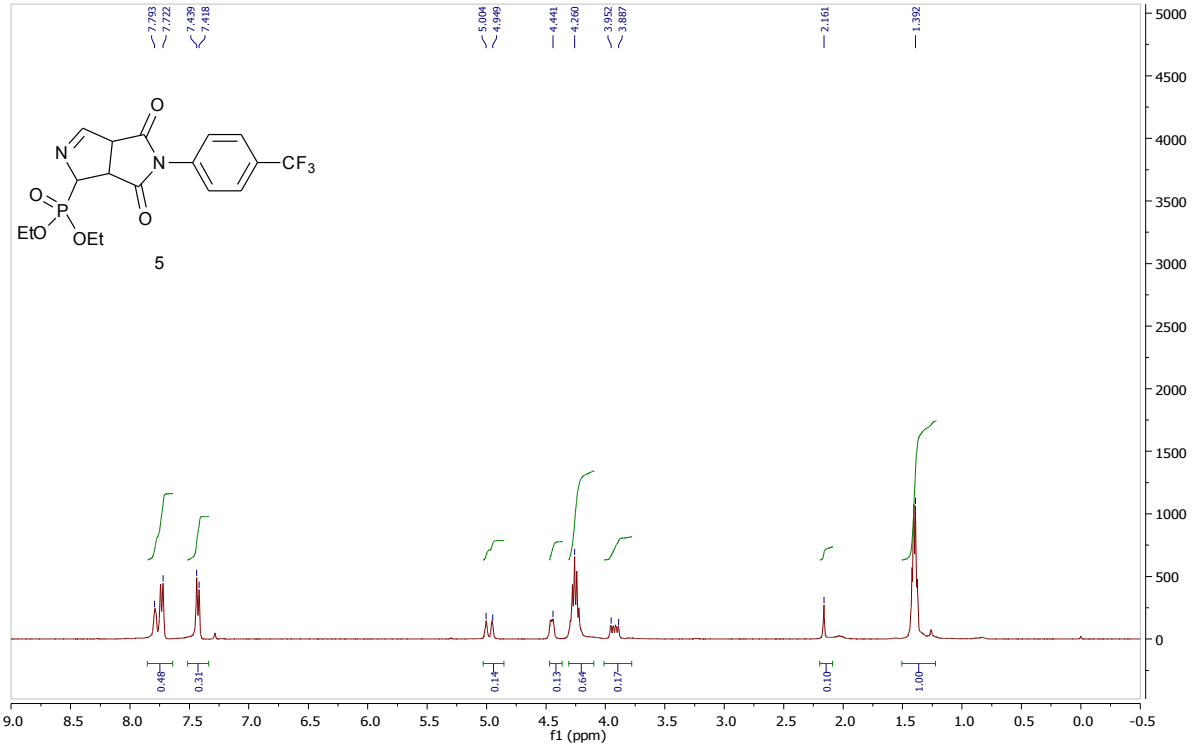
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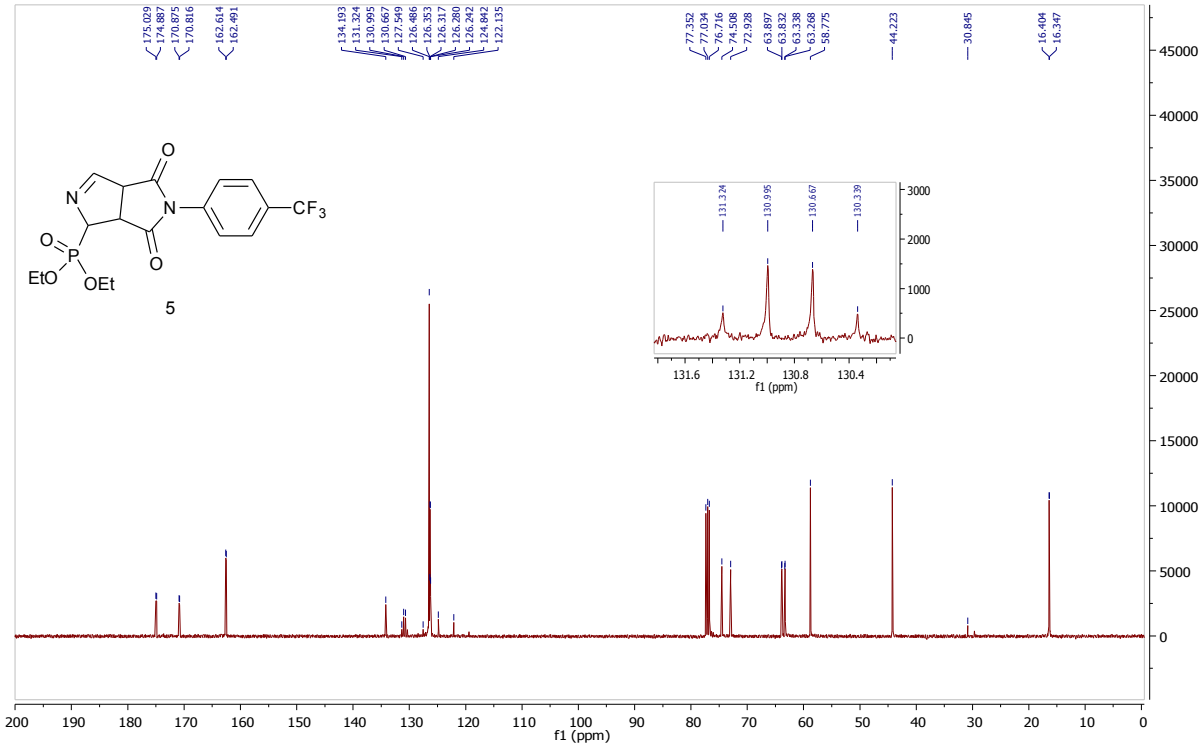
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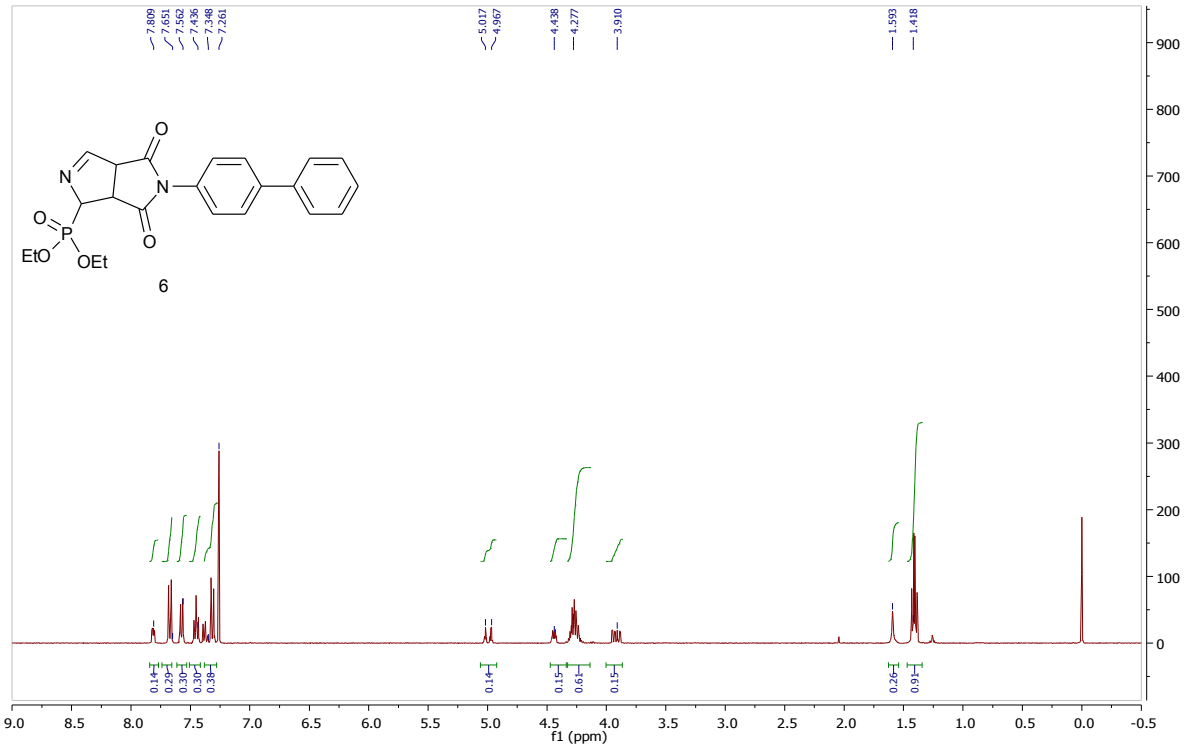

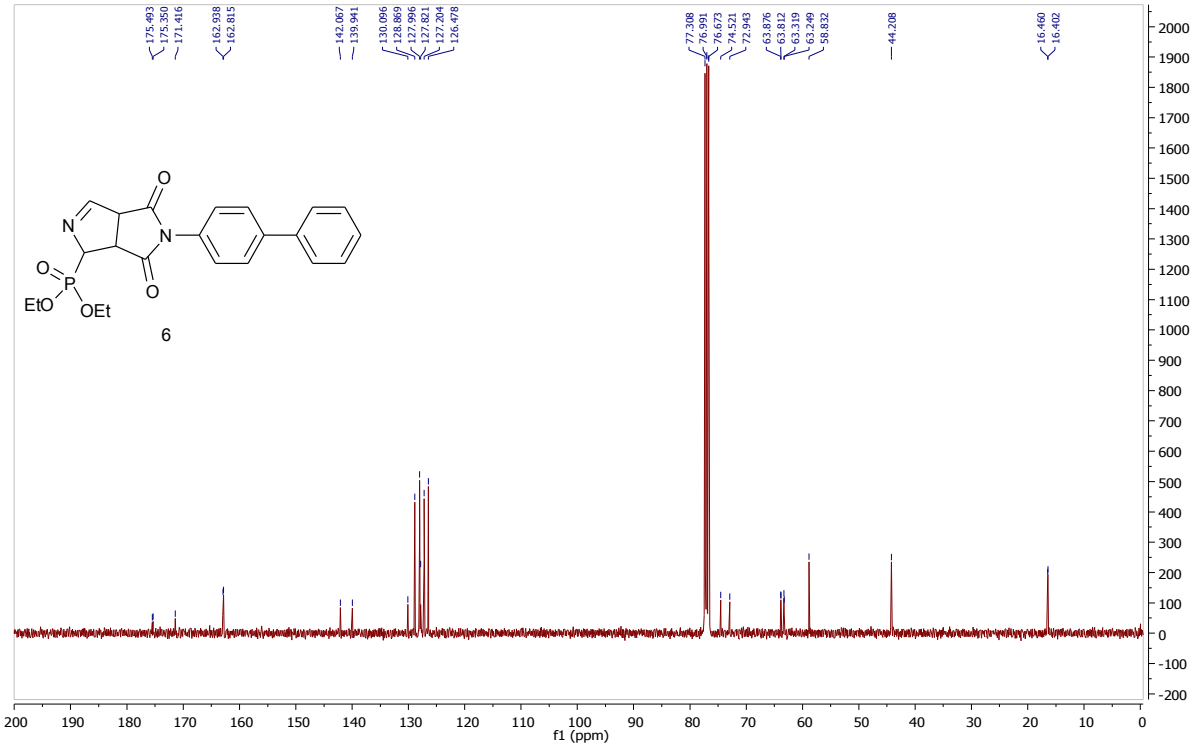

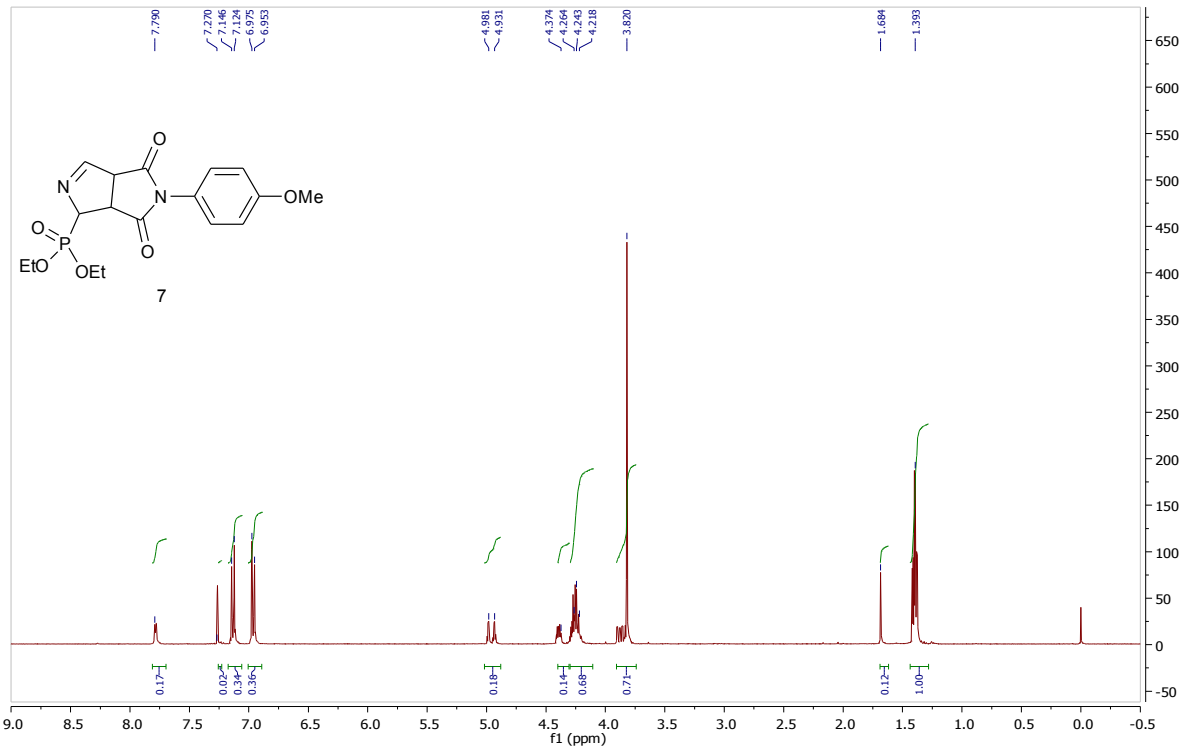

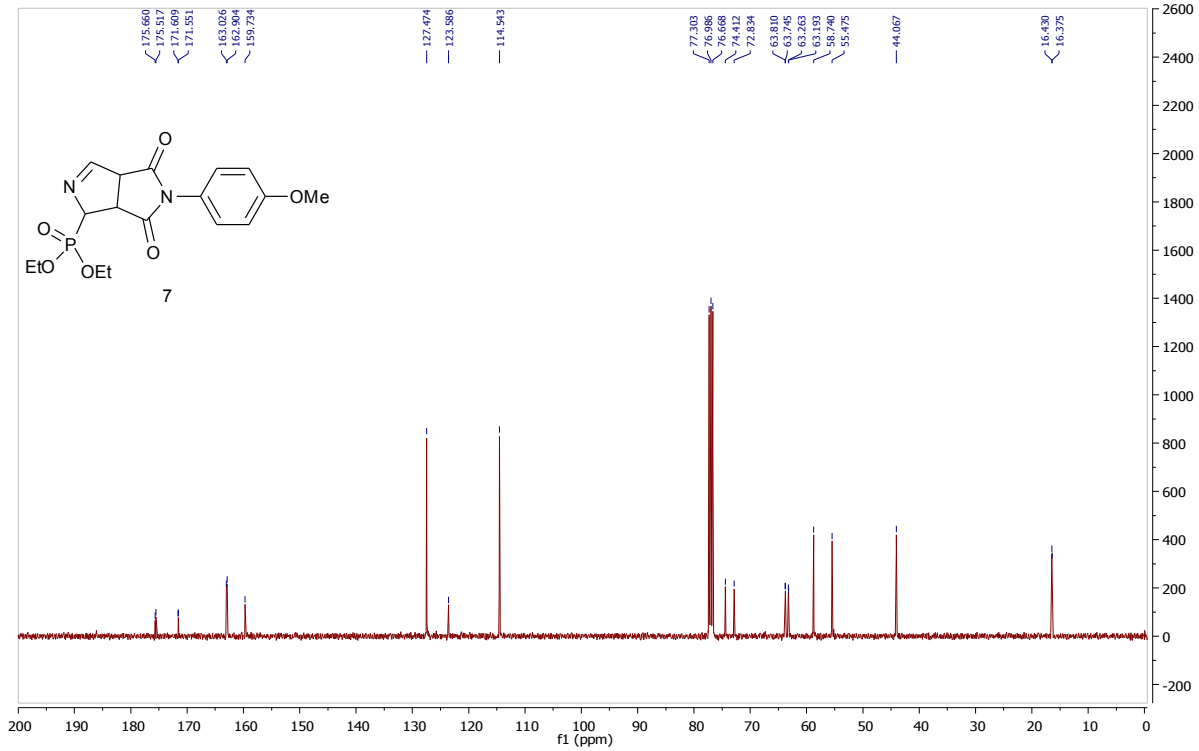

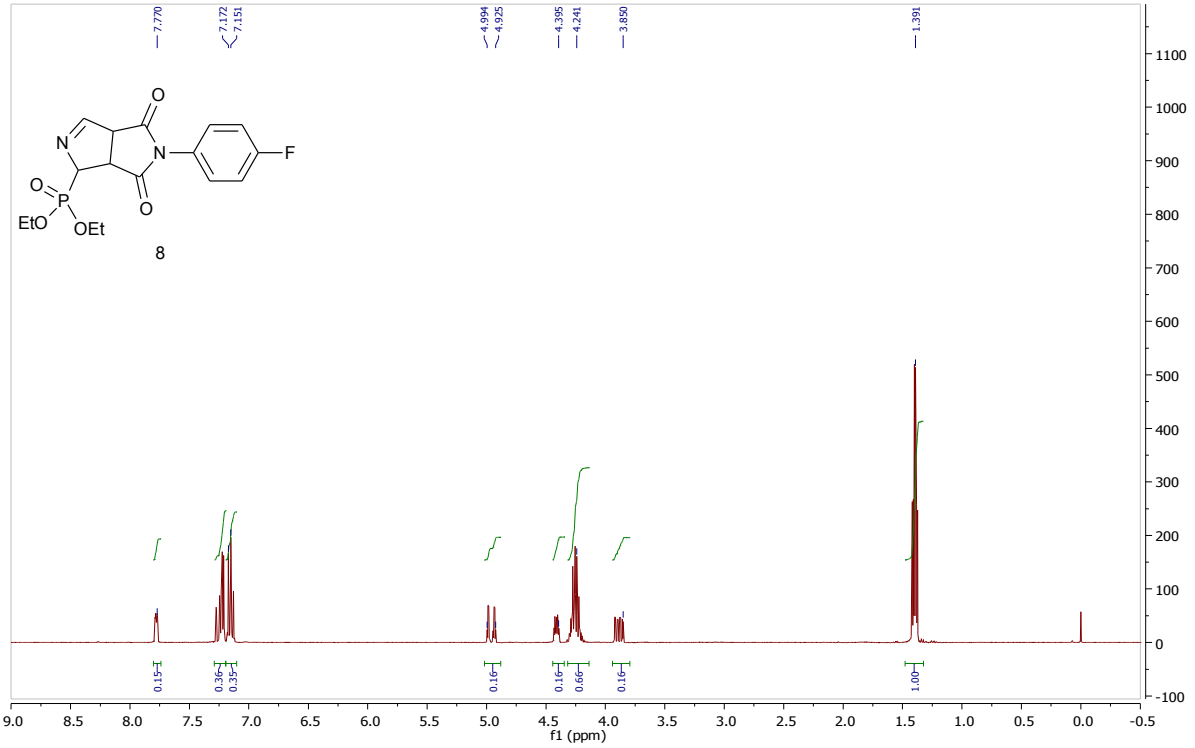
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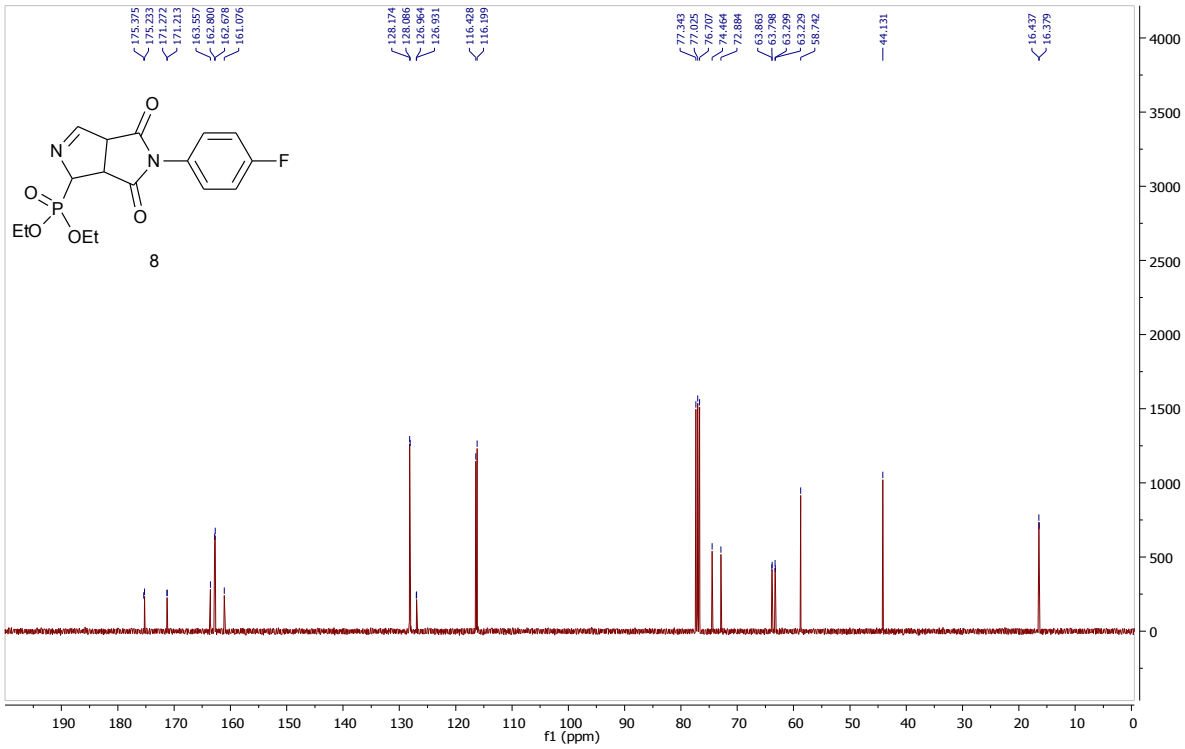
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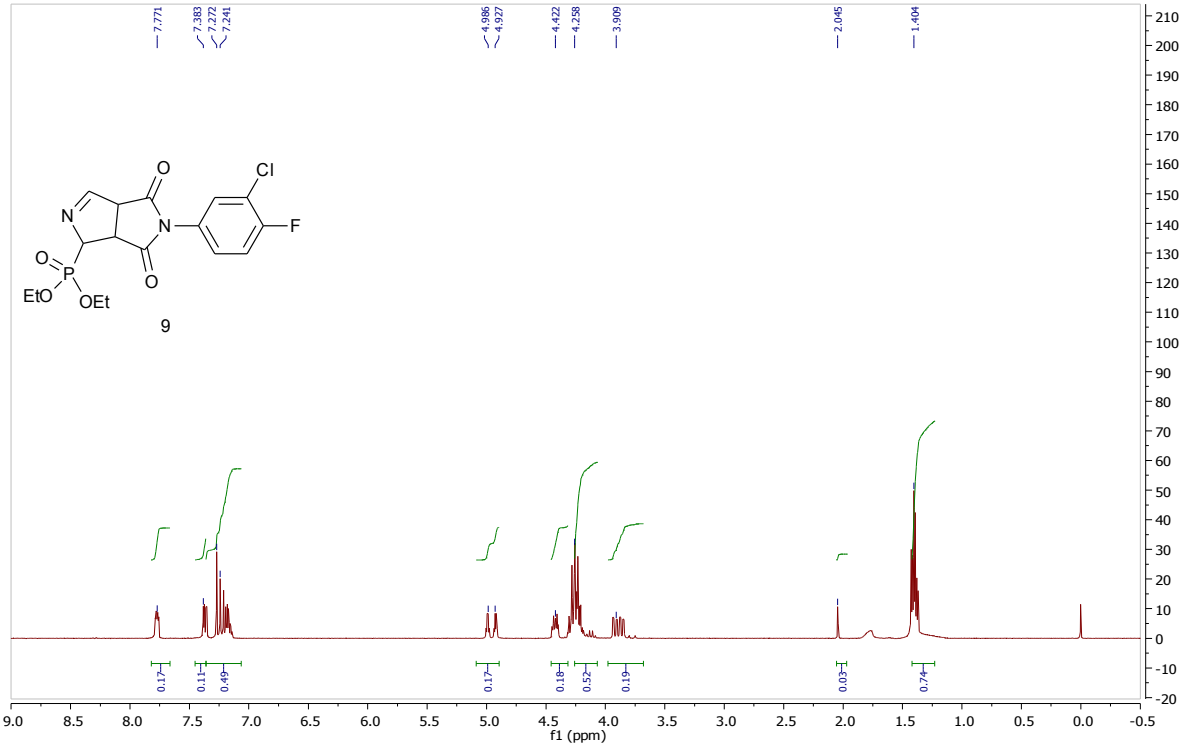
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F
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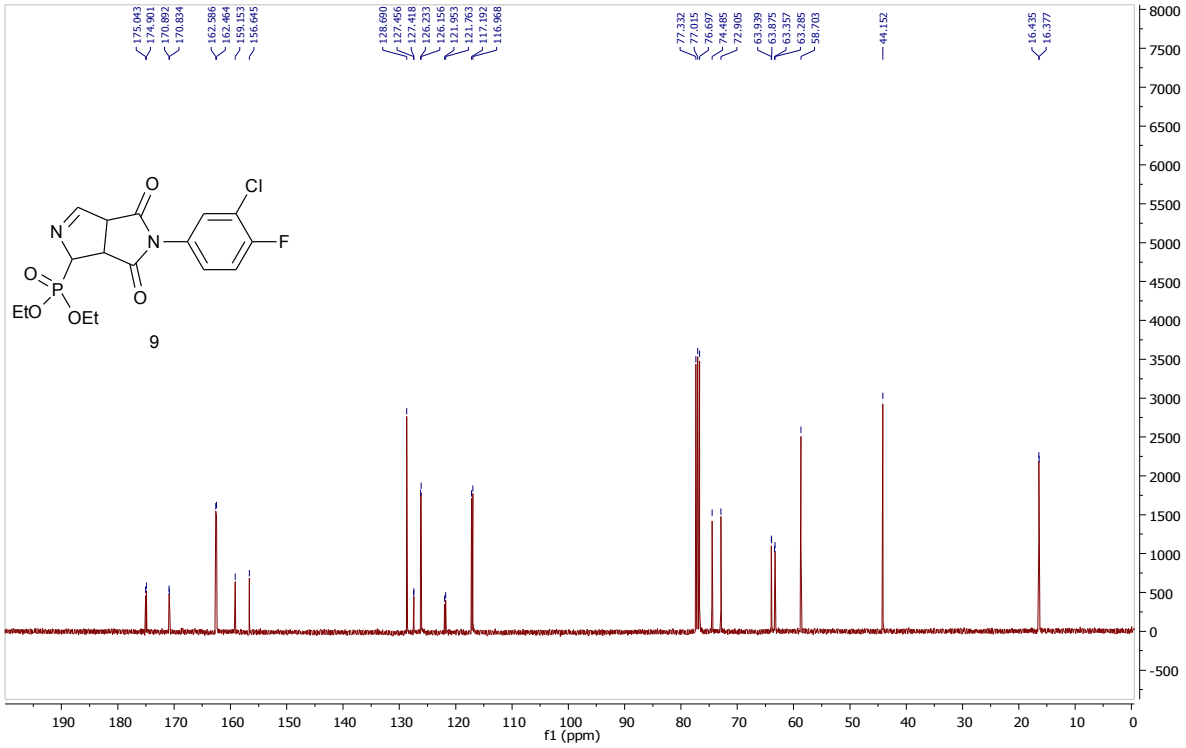
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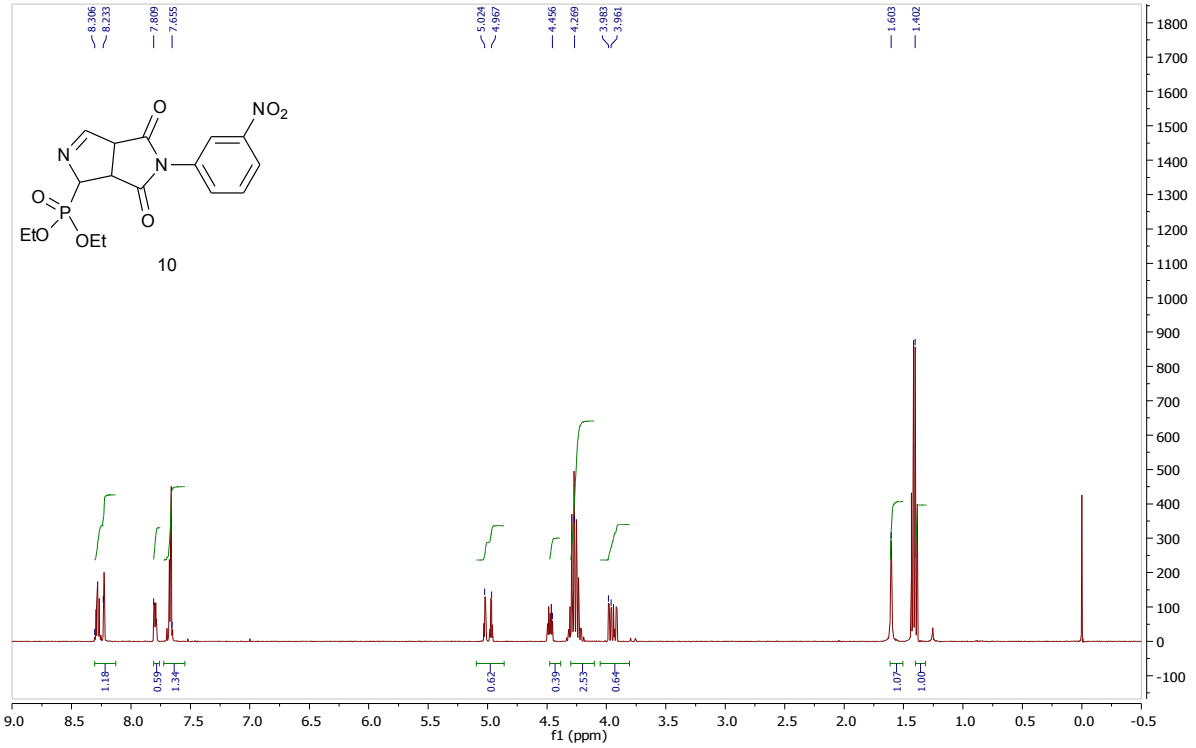
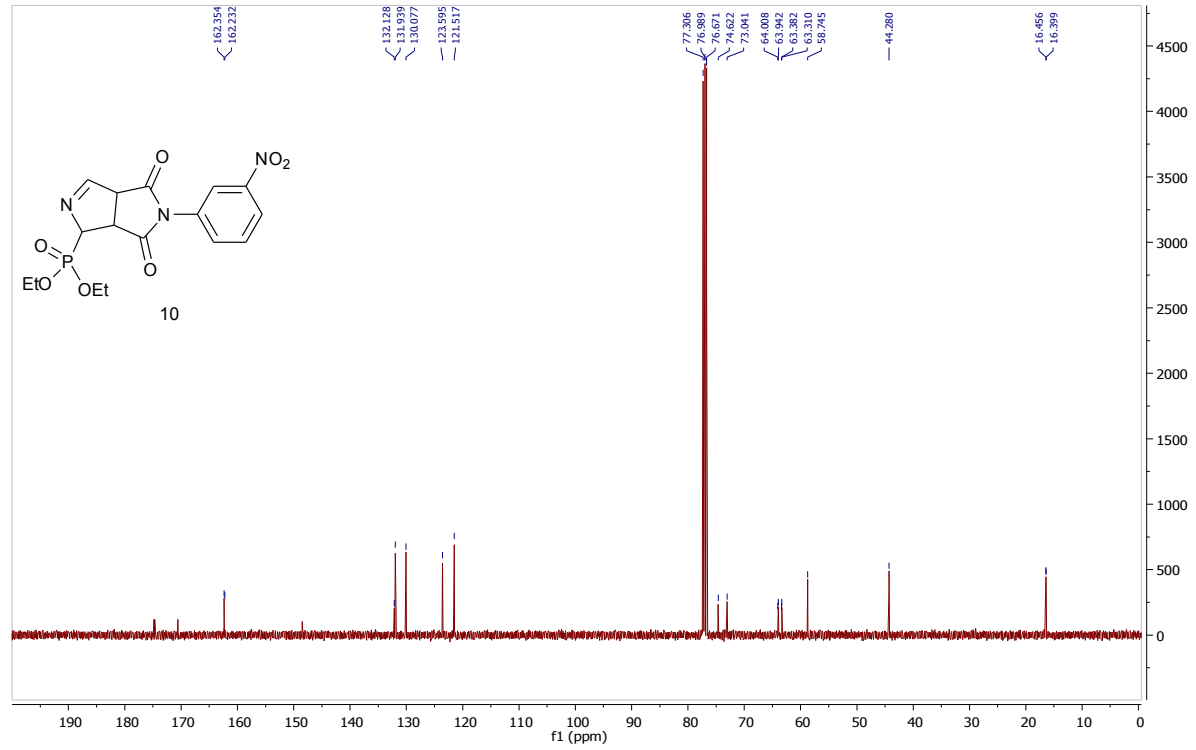
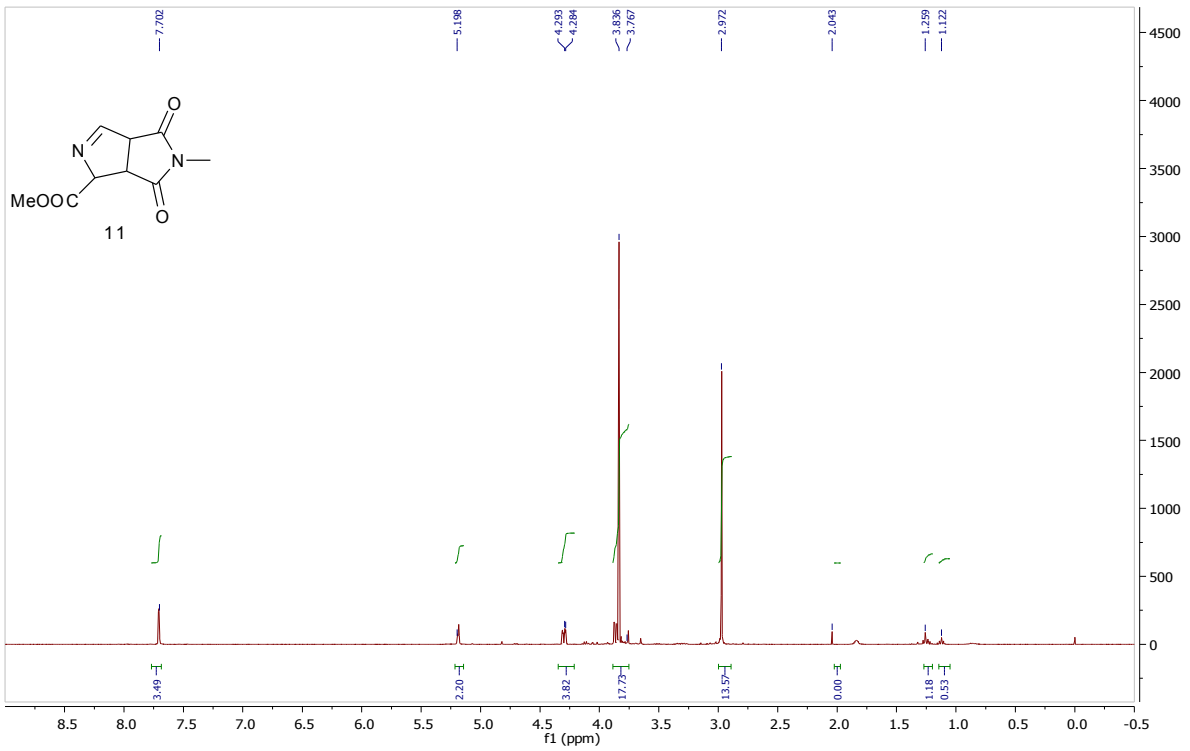
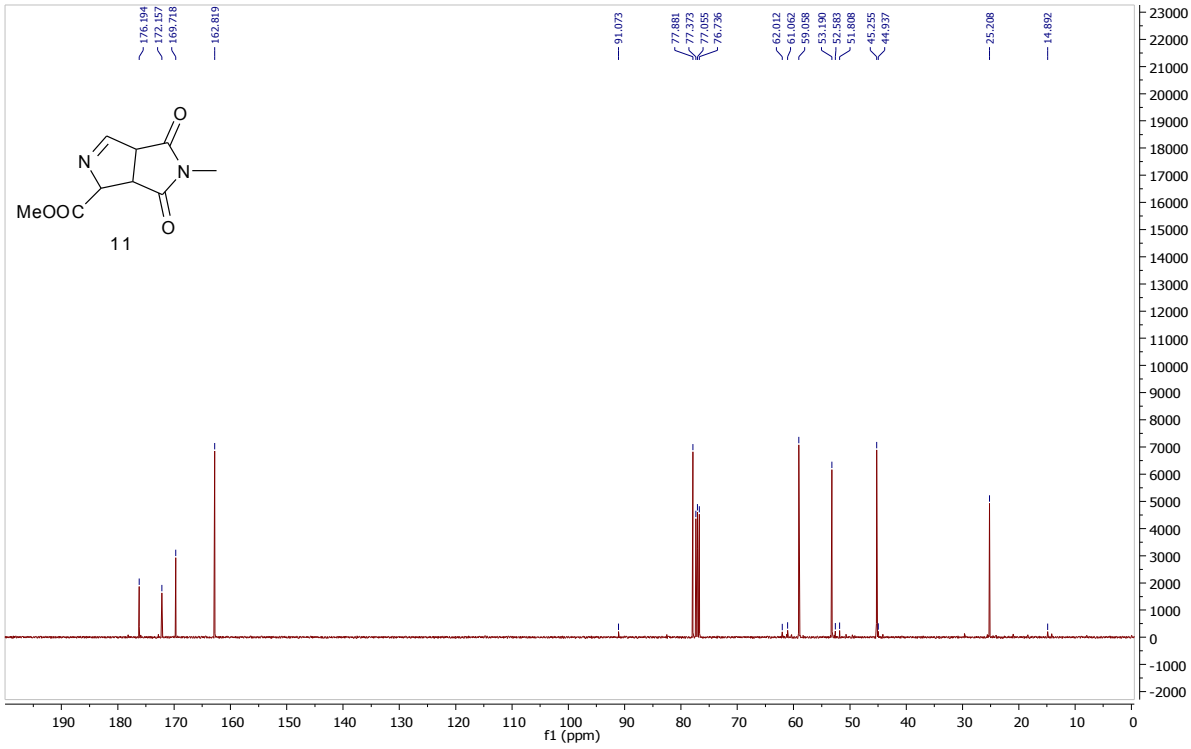
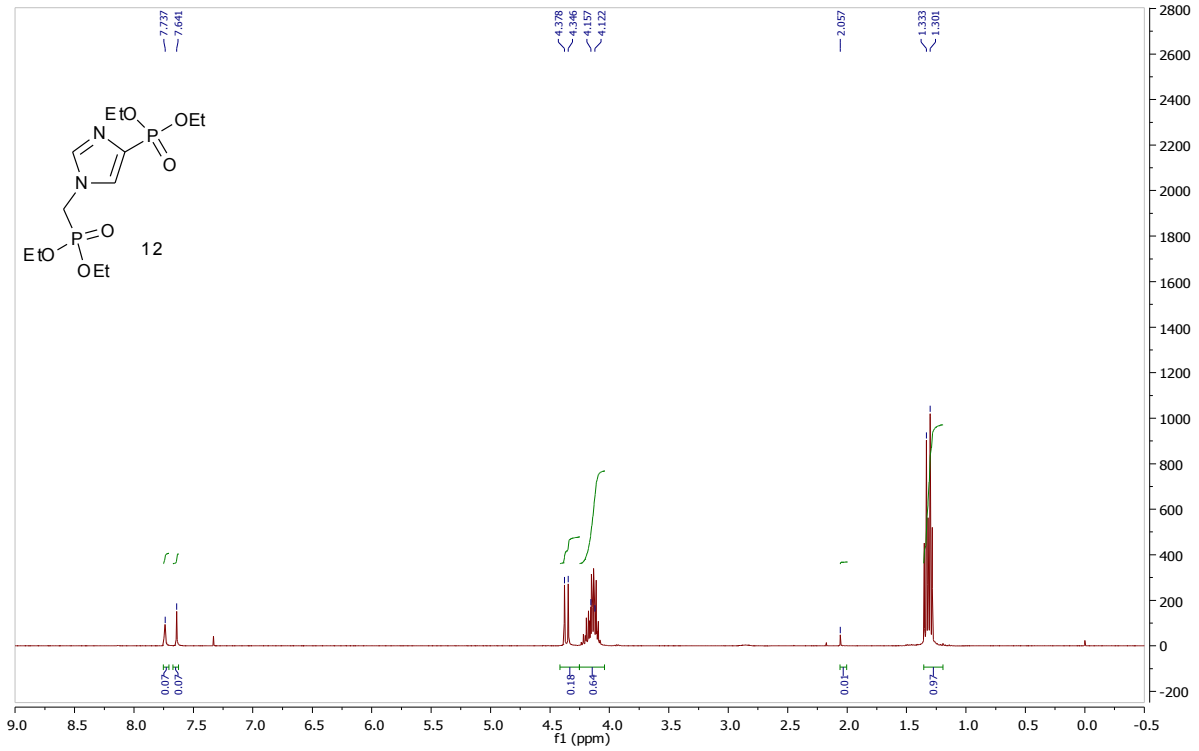
f1 (ppm)

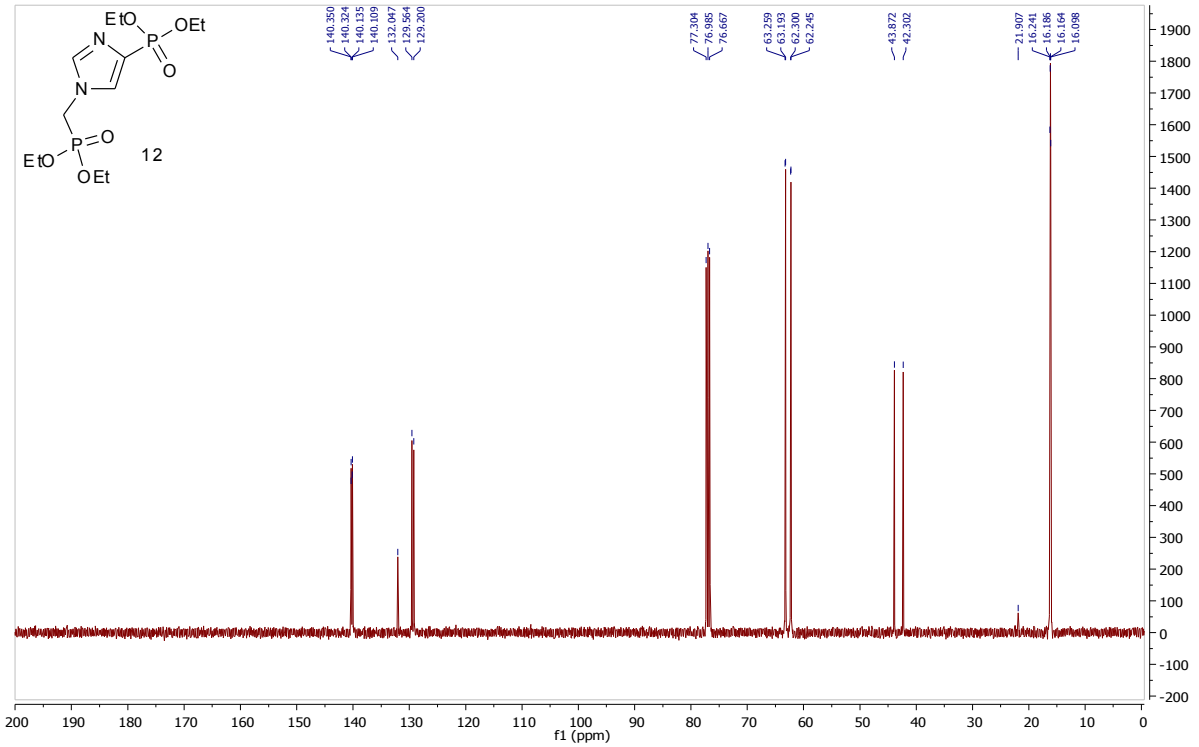


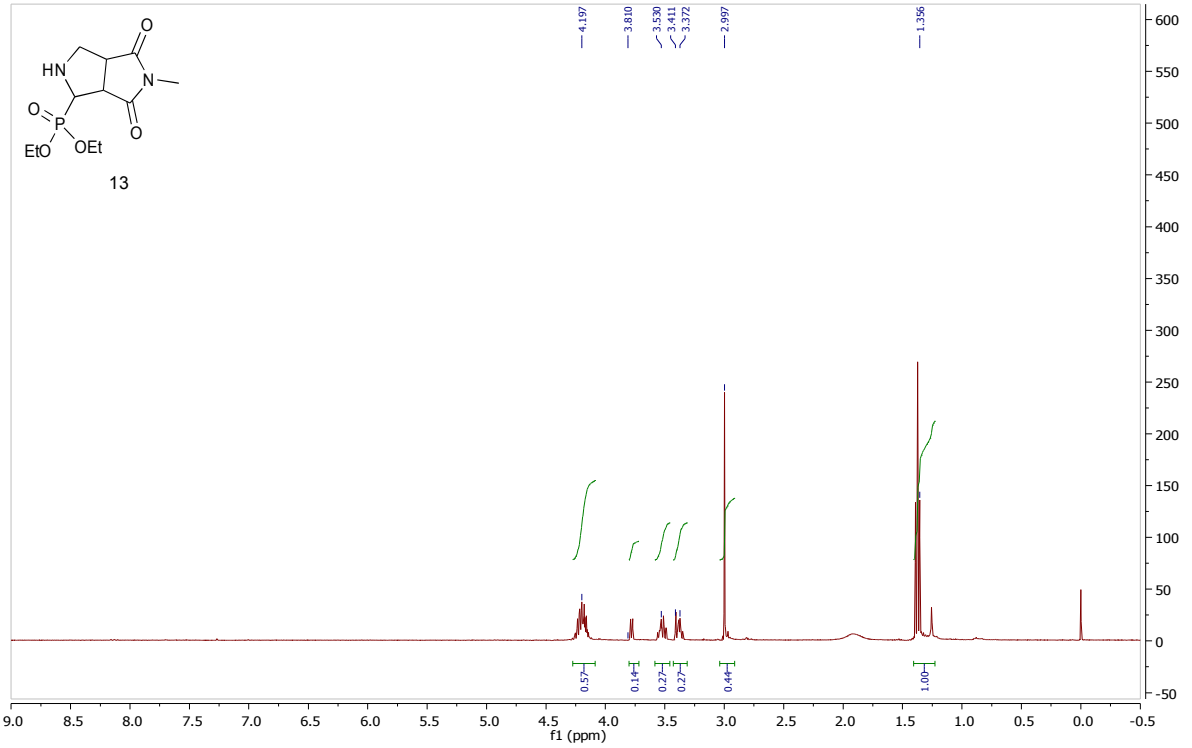








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O
O
P
EtO
OEt
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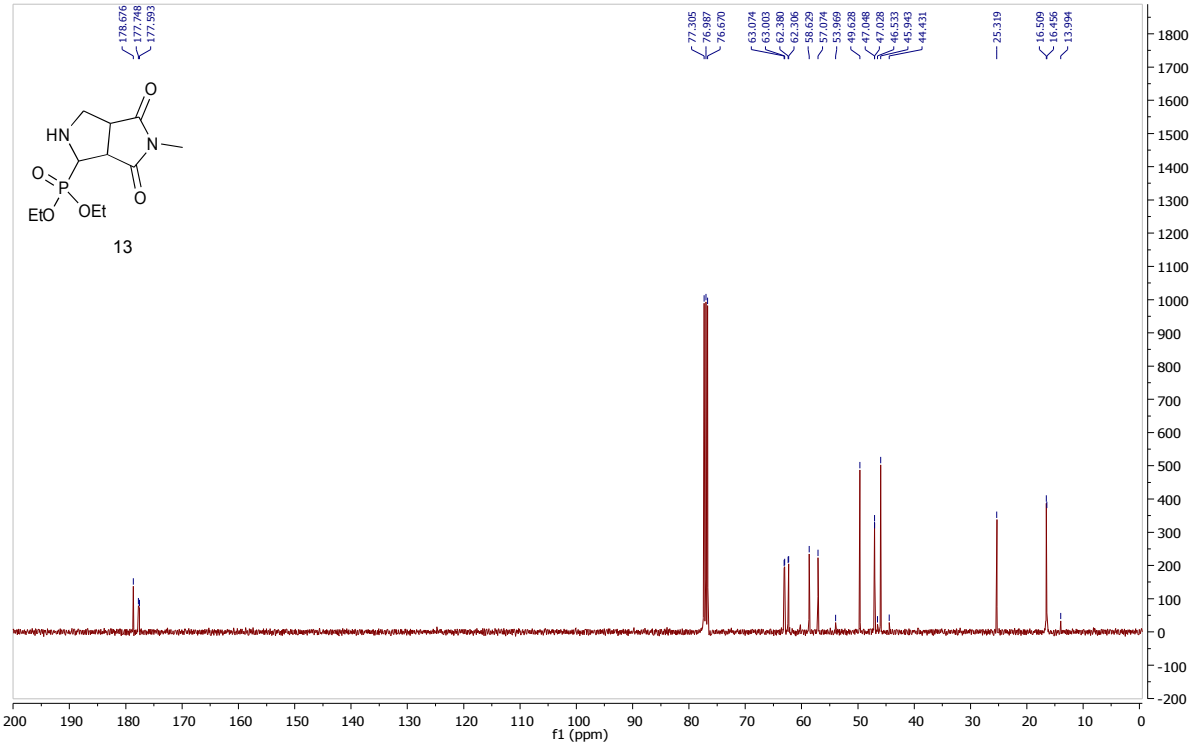
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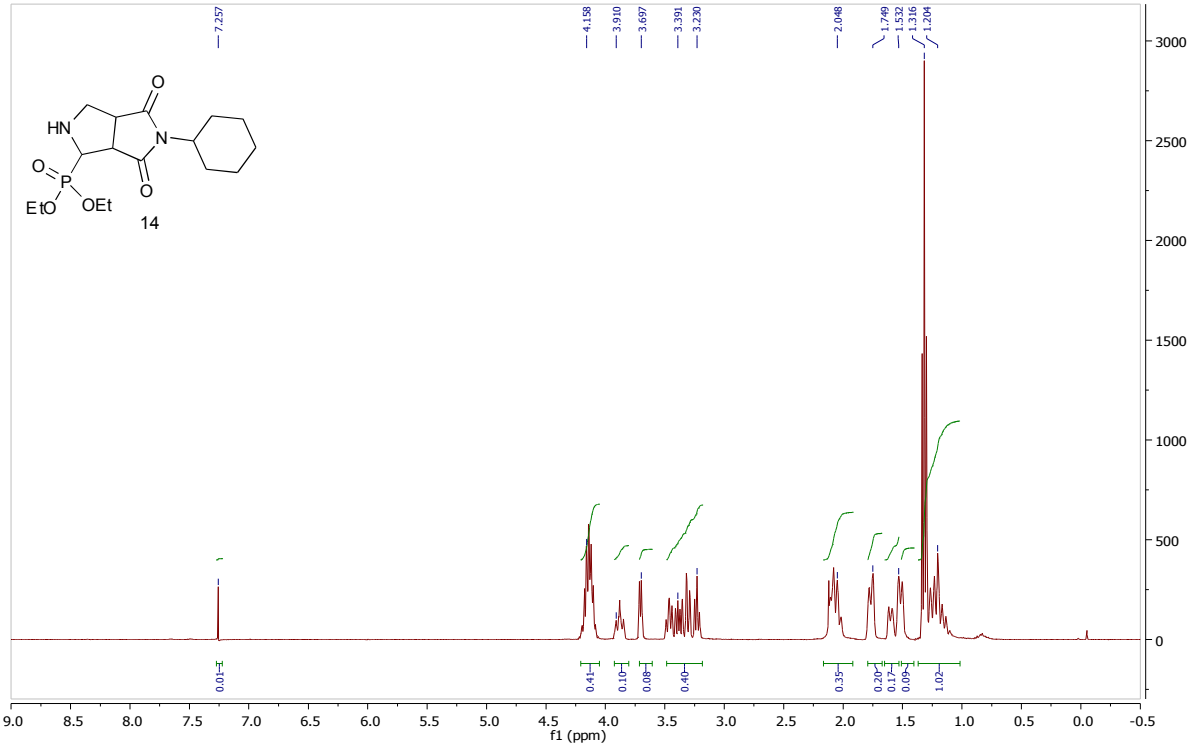
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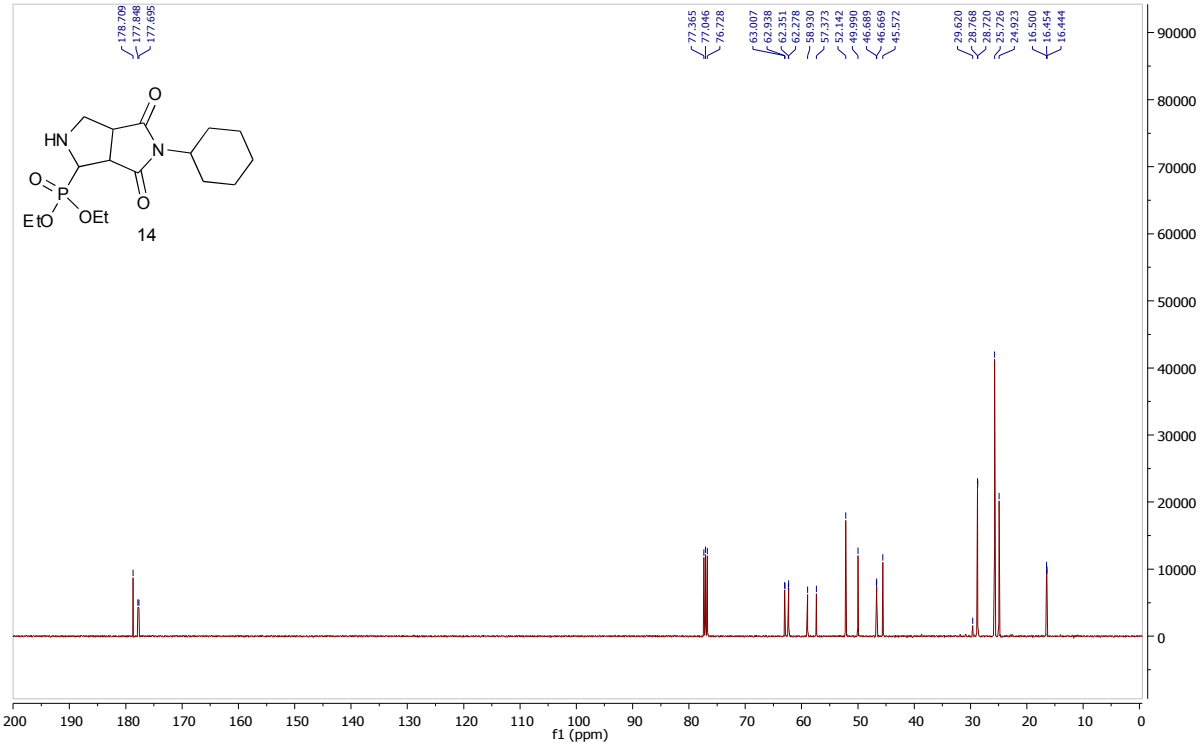
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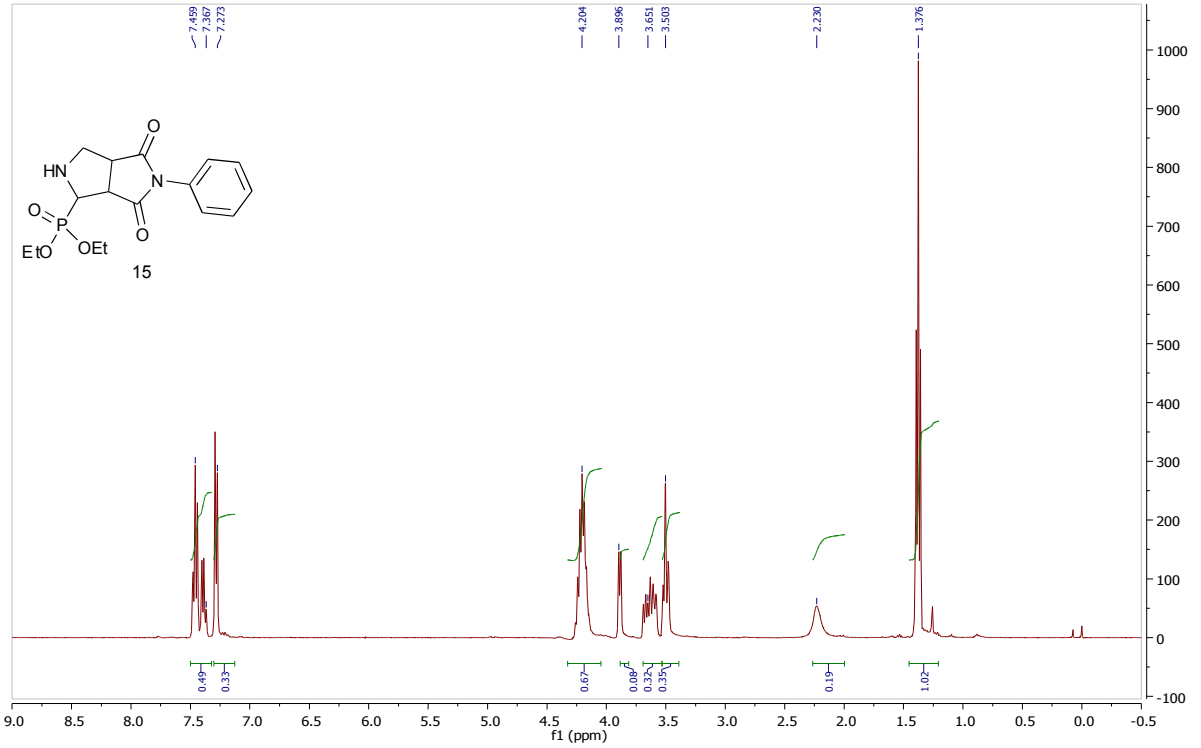
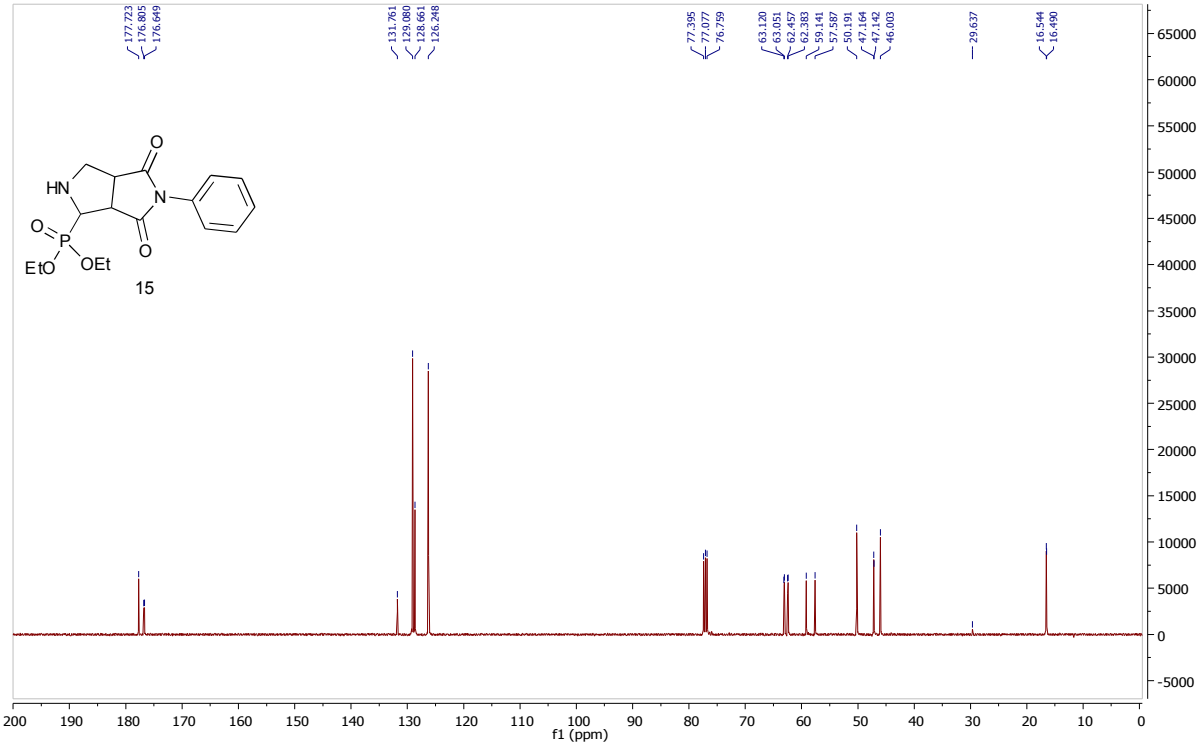




2. X-Ray crystallography

Diethyl 4,6-dioxo-5-phenyl-1,3a,4,5,6,6a-hexahydropyrrolo[3,4-*c*]pyrrole-1-phosphonate, (4).

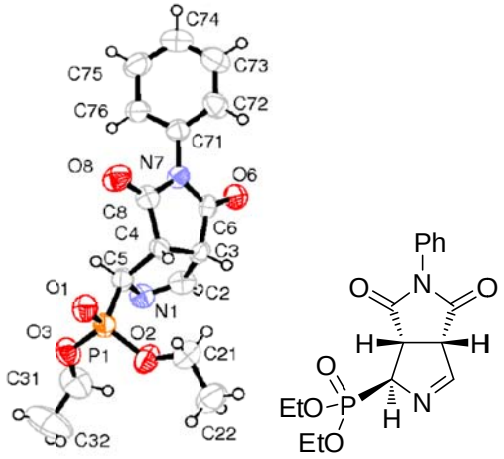


Table 1. Crystal data and structure refinement for **4**.

Identification code	Jb93	
Empirical formula	C16 H19 N2 O5 P	
Formula weight	350.30	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.116(6) Å	α= 111.01(7)°.
	b = 11.264(7) Å	β= 92.49(7)°.
	c = 13.284(9) Å	γ = 101.66(8)°.
Volume	829.9(10) Å^3	
Z	2	
Density (calculated)	1.402 Mg/m^3	
Absorption coefficient	0.195 mm^{-1}	
F(000)	368	
Crystal size	0.42 x 0.21 x 0.03 mm^3	
Theta range for data collection	1.66 to 24.98°.	
Index ranges	-7<=h<=7, -13<=k<=12, 0<=l<=15	
Reflections collected	3115	
Independent reflections	2918 [R(int) = 0.0595]	
Completeness to theta = 24.98°	99.9 %	
Max. and min. transmission	0.9942 and 0.9227	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2918 / 0 / 219	
Goodness-of-fit on F^2	0.898	
Final R indices [I>2sigma(I)]	R1 = 0.0659, wR2 = 0.1378	
R indices (all data)	R1 = 0.1876, wR2 = 0.1696	
Largest diff. peak and hole	0.205 and -0.230 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jb93. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	-1021(3)	3883(2)	6326(1)	57(1)
O(1)	-2033(6)	4536(4)	5726(3)	62(1)
O(2)	1266(6)	4657(4)	7066(3)	75(1)
O(3)	-2592(6)	3546(4)	7124(3)	71(1)
O(6)	4413(6)	193(4)	3577(3)	68(1)
O(8)	-1588(7)	1739(4)	2874(3)	73(1)
N(1)	526(8)	1700(4)	6003(4)	60(1)
N(7)	1329(7)	770(4)	2975(4)	53(1)
C(2)	2396(10)	1541(5)	5661(5)	63(2)
C(3)	3039(8)	2014(5)	4774(4)	53(1)
C(4)	1008(8)	2524(5)	4550(4)	50(1)
C(5)	-547(9)	2353(5)	5413(4)	55(2)
C(6)	3076(8)	875(5)	3736(4)	51(1)
C(8)	6(9)	1652(5)	3378(5)	57(2)
C(21)	3107(11)	5402(7)	6771(5)	88(2)
C(22)	4609(11)	6342(6)	7701(5)	91(2)
C(31)	-1996(12)	3256(7)	8054(5)	93(2)
C(32)	-2996(16)	3982(9)	8979(6)	149(4)
C(71)	917(9)	-174(6)	1877(4)	55(1)
C(72)	2620(10)	-227(6)	1237(5)	68(2)
C(73)	2222(12)	-1097(7)	178(5)	82(2)
C(74)	122(13)	-1899(7)	-242(5)	82(2)
C(75)	-1612(11)	-1855(6)	397(5)	78(2)
C(76)	-1212(10)	-973(6)	1482(5)	65(2)

Table 3. Bond lengths [Å] and angles [°] for **4**.

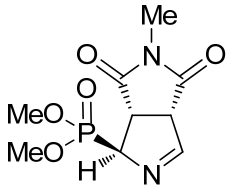
P(1)-O(1)	1.455(4)
P(1)-O(3)	1.556(4)
P(1)-O(2)	1.567(4)
P(1)-C(5)	1.805(6)
O(2)-C(21)	1.421(7)
O(3)-C(31)	1.437(7)
O(6)-C(6)	1.206(6)
O(8)-C(8)	1.198(6)
N(1)-C(2)	1.271(7)
N(1)-C(5)	1.465(7)
N(7)-C(8)	1.382(6)
N(7)-C(6)	1.395(6)
N(7)-C(71)	1.438(7)
C(2)-C(3)	1.494(7)
C(3)-C(6)	1.514(7)
C(3)-C(4)	1.529(7)
C(4)-C(8)	1.531(8)
C(4)-C(5)	1.561(7)
C(21)-C(22)	1.436(8)
C(31)-C(32)	1.448(8)
C(71)-C(72)	1.370(7)
C(71)-C(76)	1.381(7)
C(72)-C(73)	1.373(8)
C(73)-C(74)	1.372(8)
C(74)-C(75)	1.385(8)
C(75)-C(76)	1.403(8)
O(1)-P(1)-O(3)	111.4(2)
O(1)-P(1)-O(2)	117.2(2)
O(3)-P(1)-O(2)	103.7(2)
O(1)-P(1)-C(5)	110.9(3)
O(3)-P(1)-C(5)	106.5(3)
O(2)-P(1)-C(5)	106.5(3)
C(21)-O(2)-P(1)	125.4(4)
C(31)-O(3)-P(1)	128.0(4)
C(2)-N(1)-C(5)	109.6(5)
C(8)-N(7)-C(6)	113.6(5)
C(8)-N(7)-C(71)	122.8(4)
C(6)-N(7)-C(71)	123.5(4)
N(1)-C(2)-C(3)	116.9(5)
C(2)-C(3)-C(6)	110.6(5)
C(2)-C(3)-C(4)	102.5(4)
C(6)-C(3)-C(4)	105.2(4)
C(3)-C(4)-C(8)	105.1(4)
C(3)-C(4)-C(5)	104.2(4)
C(8)-C(4)-C(5)	113.8(4)
N(1)-C(5)-C(4)	106.7(4)
N(1)-C(5)-P(1)	111.5(4)
C(4)-C(5)-P(1)	112.8(4)
O(6)-C(6)-N(7)	125.4(5)
O(6)-C(6)-C(3)	126.4(5)
N(7)-C(6)-C(3)	108.2(4)
O(8)-C(8)-N(7)	125.4(5)
O(8)-C(8)-C(4)	126.7(5)
N(7)-C(8)-C(4)	107.8(5)
O(2)-C(21)-C(22)	112.3(6)

O(3)-C(31)-C(32)	110.3(6)
C(72)-C(71)-C(76)	121.6(6)
C(72)-C(71)-N(7)	119.3(5)
C(76)-C(71)-N(7)	119.1(5)
C(71)-C(72)-C(73)	119.7(6)
C(74)-C(73)-C(72)	120.2(6)
C(73)-C(74)-C(75)	120.7(6)
C(74)-C(75)-C(76)	119.4(6)
C(71)-C(76)-C(75)	118.5(6)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	48(1)	65(1)	59(1)	25(1)	7(1)	14(1)
O(1)	56(2)	71(3)	71(3)	37(2)	5(2)	22(2)
O(2)	55(2)	88(3)	77(3)	35(3)	-6(2)	0(2)
O(3)	63(2)	91(3)	73(3)	44(3)	20(2)	20(2)
O(6)	57(2)	77(3)	70(3)	25(2)	7(2)	25(2)
O(8)	73(3)	81(3)	70(3)	28(2)	-7(2)	32(2)
N(1)	63(3)	66(3)	62(3)	33(3)	9(2)	17(3)
N(7)	49(3)	53(3)	56(3)	20(2)	1(2)	14(2)
C(2)	78(4)	59(4)	59(4)	30(3)	4(3)	19(3)
C(3)	44(3)	49(3)	58(4)	14(3)	-3(3)	9(3)
C(4)	47(3)	49(3)	51(3)	16(3)	9(3)	13(3)
C(5)	48(3)	59(4)	59(4)	24(3)	6(3)	11(3)
C(6)	39(3)	52(3)	62(4)	25(3)	4(3)	4(3)
C(8)	58(4)	60(4)	60(4)	31(3)	8(3)	17(3)
C(21)	72(5)	104(6)	76(5)	25(4)	-4(4)	13(4)
C(22)	83(5)	77(5)	92(5)	15(4)	-14(4)	12(4)
C(31)	109(6)	114(6)	90(5)	68(5)	28(4)	43(5)
C(32)	235(11)	184(10)	89(6)	78(7)	73(7)	121(9)
C(71)	58(4)	56(4)	52(4)	23(3)	3(3)	12(3)
C(72)	67(4)	70(4)	69(4)	28(4)	18(3)	11(3)
C(73)	94(5)	81(5)	70(5)	26(4)	25(4)	18(4)
C(74)	106(6)	80(5)	55(4)	19(4)	5(4)	24(5)
C(75)	73(4)	75(5)	68(5)	12(4)	-8(4)	10(4)
C(76)	63(4)	70(4)	55(4)	21(4)	6(3)	6(3)

3. Computational details



1a

COMPOUND 1a

B3LYP/6-31+G(d): -1177.85946511 hartrees

Imaginary Frequencies: none found

Zero-point correction= 0.231518 (Hartree/Particle)

Thermal correction to Energy= 0.249234

Thermal correction to Enthalpy= 0.250179

Thermal correction to Gibbs Free Energy= 0.183860

Sum of electronic and zero-point Energies= -1177.627947

Sum of electronic and thermal Energies= -1177.610231

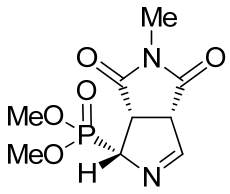
Sum of electronic and thermal Enthalpies= -1177.609286

Sum of electronic and thermal Free Energies= -1177.675605

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.938917	0.526998	-0.210941
2	6	0	1.688650	1.145295	-0.195778
3	6	0	0.707224	0.227875	0.523133
4	6	0	-0.451575	-0.275555	-0.399142
5	7	0	-0.179368	-1.689232	-0.693364
6	6	0	0.836486	-2.082821	-0.031274
7	6	0	1.515670	-1.041578	0.842540
8	6	0	2.944121	-0.732820	0.386840

9	6	0	4.132686	1.122545	-0.798726
10	8	0	3.923725	-1.442094	0.493578
11	8	0	1.443481	2.233287	-0.682580
12	15	0	-2.114917	-0.078845	0.427655
13	8	0	-2.018343	-0.134488	1.909323
14	8	0	-2.703924	1.296523	-0.197881
15	6	0	-2.400128	2.581510	0.388353
16	8	0	-3.095948	-1.173309	-0.202013
17	6	0	-3.377436	-1.282546	-1.612988
18	1	0	0.331870	0.733379	1.416125
19	1	0	-0.494170	0.280263	-1.342818
20	1	0	1.197360	-3.106975	-0.108201
21	1	0	1.527101	-1.344864	1.894800
22	1	0	3.854673	2.098960	-1.197660
23	1	0	4.907963	1.232736	-0.035546
24	1	0	4.514604	0.482163	-1.598606
25	1	0	-3.113792	3.284528	-0.044532
26	1	0	-2.524189	2.542689	1.473899
27	1	0	-1.380543	2.885107	0.128729
28	1	0	-3.734702	-0.326443	-2.005779
29	1	0	-2.483683	-1.617885	-2.146882
30	1	0	-4.161699	-2.036119	-1.699385



1b

COMPOUND 1b

B3LYP/6-31+G(d): -1177.85224786 hartrees

Imaginary Frequencies: none found

Zero-point correction= 0.230956 (Hartree/Particle)

Thermal correction to Energy= 0.248877

Thermal correction to Enthalpy= 0.249821

Thermal correction to Gibbs Free Energy= 0.182828

Sum of electronic and zero-point Energies= -1177.621292

Sum of electronic and thermal Energies= -1177.603371

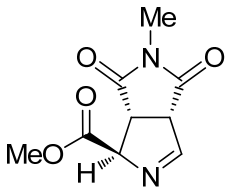
Sum of electronic and thermal Enthalpies= -1177.602427

Sum of electronic and thermal Free Energies= -1177.669420

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.191036	-0.943152	-0.167145
2	6	0	1.039223	-0.867085	-0.956185
3	6	0	0.746855	0.611688	-1.243372
4	6	0	-0.488360	1.317368	-0.553654
5	7	0	0.045071	2.305594	0.393645
6	6	0	1.316207	2.316402	0.341303
7	6	0	1.957204	1.354219	-0.638076
8	6	0	2.804598	0.281970	0.051556
9	6	0	2.728620	-2.211624	0.304849

10	8	0	3.833624	0.459798	0.673926
11	8	0	0.450398	-1.837208	-1.382044
12	15	0	-1.799215	0.330754	0.303176
13	8	0	-2.881647	1.130532	0.933385
14	8	0	-2.331743	-0.721718	-0.805282
15	6	0	-3.616510	-0.552848	-1.437775
16	8	0	-0.886494	-0.579103	1.271553
17	6	0	-1.506478	-1.472804	2.220342
18	1	0	0.664056	0.714959	-2.328040
19	1	0	-1.056727	1.870154	-1.313393
20	1	0	1.901202	2.982727	0.972703
21	1	0	2.591184	1.882325	-1.360365
22	1	0	2.011441	-2.692807	0.975764
23	1	0	2.915847	-2.874857	-0.544107
24	1	0	3.658536	-2.002951	0.835608
25	1	0	-3.533753	0.151594	-2.272742
26	1	0	-3.896513	-1.536929	-1.818088
27	1	0	-4.357529	-0.191371	-0.720949
28	1	0	-2.264948	-0.942015	2.802687
29	1	0	-0.707015	-1.818526	2.877399
30	1	0	-1.951553	-2.322831	1.694146



15a

COMPOUND 15a

B3LYP/6-31+G(d): -759.427467391 hartrees

Imaginary Frequencies: none found

Zero-point correction= 0.192456 (Hartree/Particle)

Thermal correction to Energy= 0.206345

Thermal correction to Enthalpy= 0.207289

Thermal correction to Gibbs Free Energy= 0.149964

Sum of electronic and zero-point Energies= -759.235011

Sum of electronic and thermal Energies= -759.221123

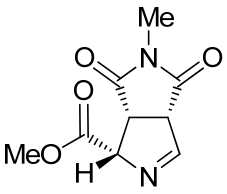
Sum of electronic and thermal Enthalpies= -759.220179

Sum of electronic and thermal Free Energies= -759.277504

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.427503	0.360093	-0.206070
2	6	0	-1.290978	1.164531	-0.290609
3	6	0	-0.069300	0.261397	-0.454523
4	6	0	0.948873	0.388793	0.724613
5	7	0	0.786986	-0.823630	1.551423
6	6	0	-0.026300	-1.625295	0.987501
7	6	0	-0.629725	-1.165606	-0.330326
8	6	0	-2.149308	-1.005085	-0.248530

9	6	0	-3.770817	0.909077	-0.066656
10	8	0	-2.976427	-1.893332	-0.205615
11	8	0	-1.306610	2.378073	-0.242696
12	6	0	2.407911	0.496512	0.273294
13	8	0	3.183111	1.343801	0.654999
14	8	0	2.722637	-0.478740	-0.603863
15	6	0	4.090347	-0.498871	-1.063507
16	1	0	0.391972	0.474626	-1.421830
17	1	0	0.762058	1.272307	1.339857
18	1	0	-0.276840	-2.584239	1.438616
19	1	0	-0.382234	-1.854065	-1.145343
20	1	0	-3.975823	1.597860	-0.890339
21	1	0	-4.474782	0.076060	-0.084943
22	1	0	-3.856809	1.454128	0.877779
23	1	0	4.152304	-1.345444	-1.747338
24	1	0	4.330091	0.435431	-1.577468
25	1	0	4.767773	-0.633042	-0.216601



15b

COMPOUND 15b

B3LYP/6-31+G(d): -759.426881110 hartrees

Imaginary Frequencies: none found

Zero-point correction=	0.192610 (Hartree/Particle)
Thermal correction to Energy=	0.206398
Thermal correction to Enthalpy=	0.207343
Thermal correction to Gibbs Free Energy=	0.150339
Sum of electronic and zero-point Energies=	-759.234271
Sum of electronic and thermal Energies=	-759.220483
Sum of electronic and thermal Enthalpies=	-759.219538
Sum of electronic and thermal Free Energies=	-759.276542

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.709479	-0.790007	-0.597602
2	6	0	-0.927684	-0.853647	0.553640
3	6	0	-0.633719	0.571394	1.020460
4	6	0	0.858971	1.058547	0.877737
5	7	0	0.860325	2.149332	-0.109907
6	6	0	-0.318613	2.341807	-0.549151
7	6	0	-1.409098	1.465503	0.036960
8	6	0	-2.037243	0.506411	-0.980800
9	6	0	-2.105370	-1.978188	-1.342703

10	8	0	-2.709682	0.810126	-1.945610
11	8	0	-0.577321	-1.885253	1.091483
12	6	0	1.817637	-0.031183	0.390865
13	8	0	1.722758	-0.573690	-0.689222
14	8	0	2.762112	-0.303178	1.303074
15	6	0	3.696734	-1.346440	0.951412
16	1	0	-0.958384	0.662253	2.059816
17	1	0	1.233224	1.447901	1.827446
18	1	0	-0.522654	3.102178	-1.300977
19	1	0	-2.209426	2.069026	0.481052
20	1	0	-1.222571	-2.450524	-1.783460
21	1	0	-2.591009	-2.688780	-0.669296
22	1	0	-2.794301	-1.665566	-2.128504
23	1	0	4.366278	-1.430659	1.807157
24	1	0	3.161501	-2.283418	0.780301
25	1	0	4.248798	-1.066945	0.050707

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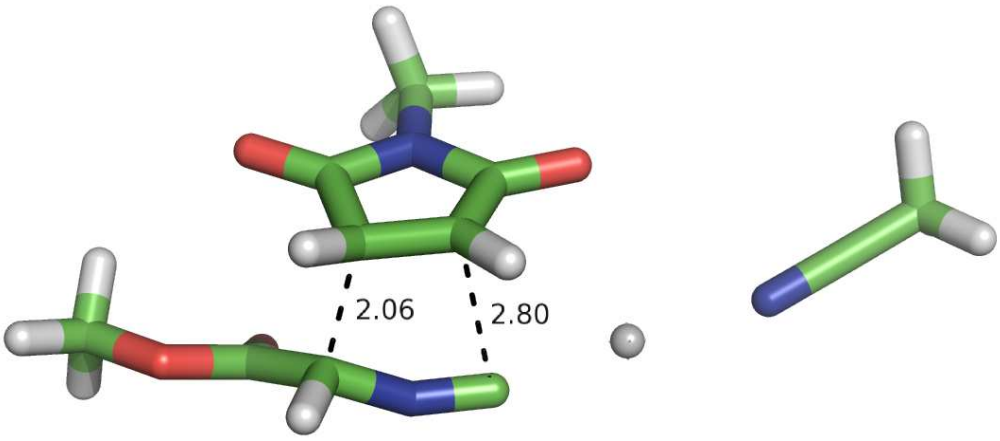

B3LYP/6•31+G(d): -1037.29810817

Imaginary Frequencies: 1 (-311.6939)

Zero-point correction=	0.221847
Thermal correction to Energy=	0.244158
Thermal correction to Enthalpy=	0.245103
Thermal correction to Gibbs Free Energy=	0.164754
Sum of electronic and zero-point Energies=	-1037.076261
Sum of electronic and thermal Energies=	-1037.053950
Sum of electronic and thermal Enthalpies=	-1037.053006
Sum of electronic and thermal Free Energies=	-1037.133354

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.941970	1.940283	-0.084414
2	6	0	-2.164653	1.556128	0.435454
3	6	0	-1.864744	0.563011	1.545620
4	6	0	-2.347695	-1.228657	0.660942
5	7	0	-1.114334	-1.633733	0.205742
6	6	0	0.053808	-1.556385	0.096642
7	6	0	-0.472848	0.636421	1.752628
8	6	0	0.121682	1.398841	0.694133
9	6	0	-0.780697	2.813913	-1.228698
10	8	0	1.318457	1.600103	0.402812
11	8	0	-3.254330	1.953673	0.048377
12	6	0	-3.376700	-1.031767	-0.387253
13	8	0	-3.165465	-0.880337	-1.577178
14	8	0	-4.604005	-0.984879	0.181328
15	6	0	-5.674285	-0.564119	-0.683089
16	1	0	-2.602468	0.474397	2.336450
17	1	0	-2.685020	-1.799756	1.523429
18	1	0	0.100855	0.207068	2.562973
19	1	0	-1.160242	3.818748	-1.009874
20	1	0	0.286600	2.869390	-1.453152
21	1	0	-1.325792	2.414615	-2.090112
22	1	0	-6.570396	-0.584009	-0.061416
23	1	0	-5.478012	0.447435	-1.046612
24	1	0	-5.775716	-1.250722	-1.528191
25	47	0	2.055473	-0.925884	-0.067293
26	7	0	4.168699	-0.402662	-0.241513
27	6	0	5.194977	0.127539	-0.292700

28	6	0	6.482683	0.807628	-0.354262
29	1	0	6.906380	0.716105	-1.359355
30	1	0	6.348160	1.868012	-0.117443
31	1	0	7.175227	0.364250	0.368144

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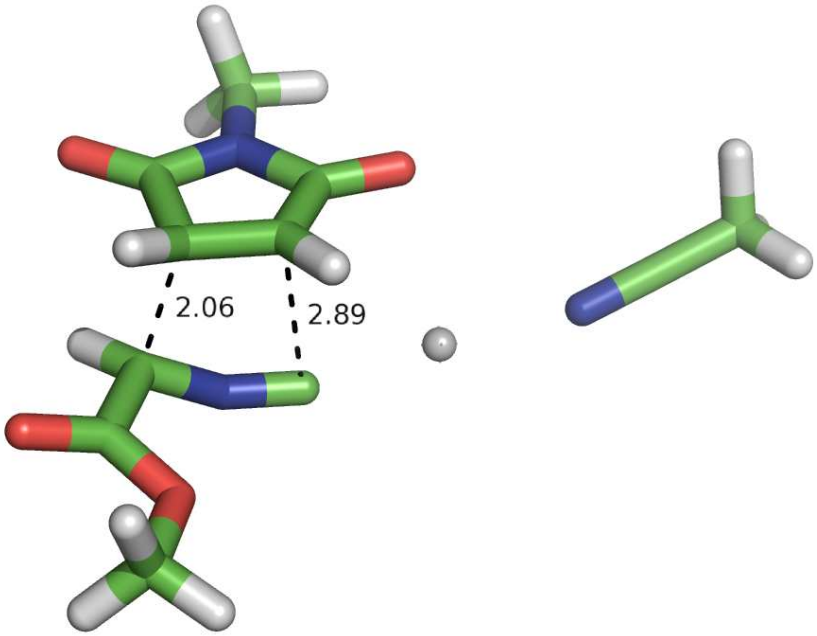

B3LYP/6•31+G(d): -1037.29817948

Imaginary Frequencies: 1 (-317.4587)

Zero-point correction=	0.221736
Thermal correction to Energy=	0.244151
Thermal correction to Enthalpy=	0.245095
Thermal correction to Gibbs Free Energy=	0.163847
Sum of electronic and zero-point Energies=	-1037.076443
Sum of electronic and thermal Energies=	-1037.054028
Sum of electronic and thermal Enthalpies=	-1037.053084
Sum of electronic and thermal Free Energies=	-1037.134333

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.517561	2.545031	0.101175
2	6	0	-1.885530	2.355041	0.187245
3	6	0	-2.087711	1.044737	0.932977
4	6	0	-2.673621	-0.113950	-0.667154
5	7	0	-1.456909	-0.595891	-1.086603
6	6	0	-0.305091	-0.818570	-1.017200
7	6	0	-0.816619	0.668839	1.402397
8	6	0	0.174623	1.528179	0.825293
9	6	0	0.111690	3.661525	-0.573629
10	8	0	1.421177	1.485338	0.860343
11	8	0	-2.732009	3.101489	-0.282805
12	6	0	-3.634641	-1.091057	-0.115448
13	8	0	-4.808674	-0.831665	0.090235
14	8	0	-3.059417	-2.272129	0.225298
15	6	0	-3.934975	-3.232780	0.838186
16	1	0	-3.018246	0.924241	1.478986
17	1	0	-3.130321	0.616005	-1.328731
18	1	0	-0.573516	-0.134763	2.084432
19	1	0	-0.136073	4.607603	-0.078518
20	1	0	1.191607	3.503152	-0.536231
21	1	0	-0.222864	3.719470	-1.614872
22	1	0	-3.313243	-4.108344	1.029876

23	1	0	-4.344342	-2.837925	1.772314
24	1	0	-4.758548	-3.484934	0.164270
25	47	0	1.739161	-0.793879	-0.521820
26	7	0	3.863154	-0.902864	-0.032782
27	6	0	4.931965	-0.729432	0.372871
28	6	0	6.274539	-0.499609	0.891527
29	1	0	6.606822	-1.368565	1.468233
30	1	0	6.971516	-0.330611	0.064632
31	1	0	6.269438	0.381261	1.541658

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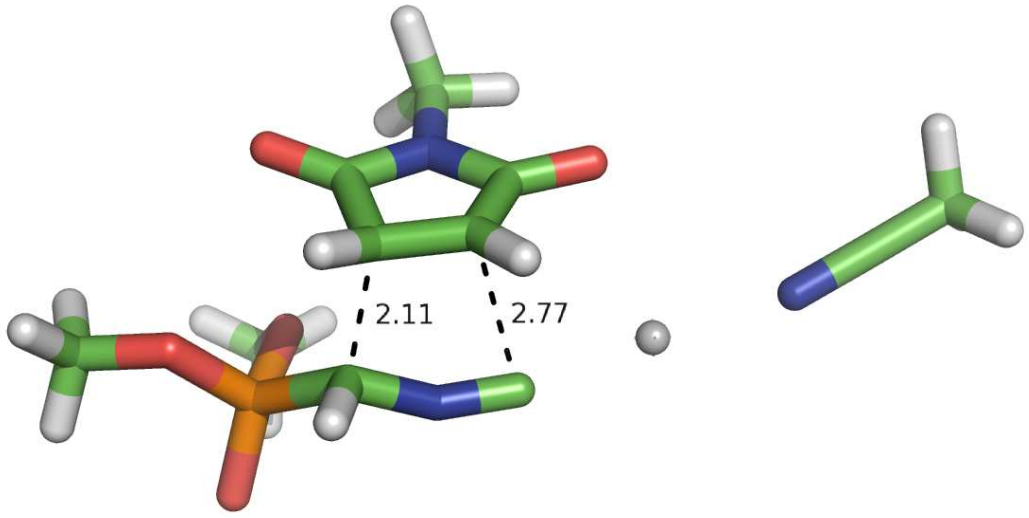


B3LYP/6•31+G(d): -1455.71652601

Imaginary Frequencies: 1 (-268.8965)

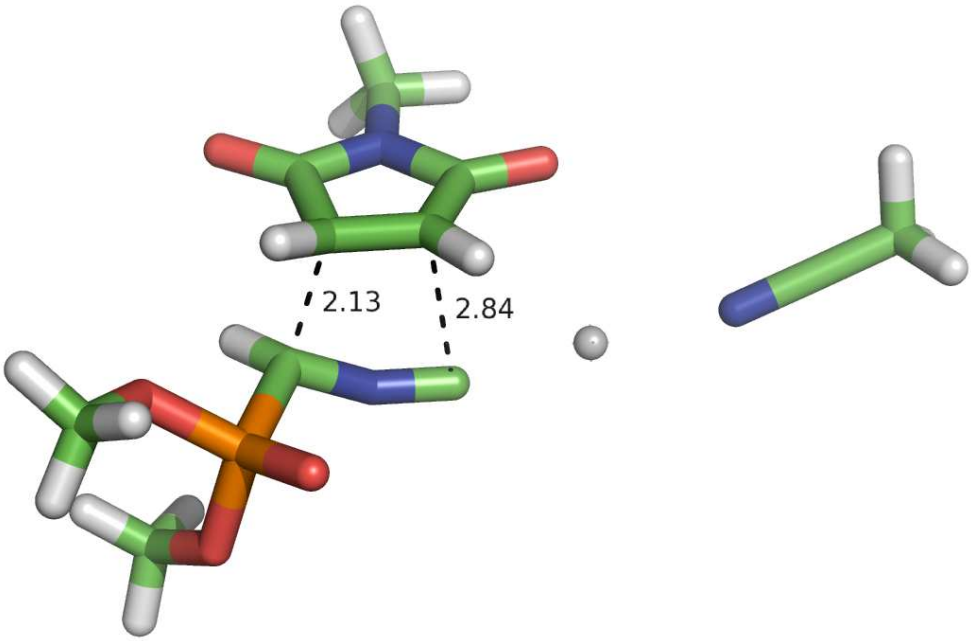
Zero-point correction=	0.260233
Thermal correction to Energy=	0.286809
Thermal correction to Enthalpy=	0.287753
Thermal correction to Gibbs Free Energy=	0.195809
Sum of electronic and zero-point Energies=	-1455.456293
Sum of electronic and thermal Energies=	-1455.429717
Sum of electronic and thermal Enthalpies=	-1455.428773
Sum of electronic and thermal Free Energies=	-1455.520717

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.296192	2.140927	0.250240
2	6	0	1.503017	1.992358	-0.424721
3	6	0	1.203261	1.129368	-1.638192
4	6	0	-0.197315	1.101792	-1.740942
5	6	0	-0.772388	1.640284	-0.538209
6	6	0	0.140940	2.896689	1.475022
7	8	0	-1.959461	1.694020	-0.157519
8	8	0	2.555984	2.511325	-0.095004
9	1	0	1.889560	1.199926	-2.474158
10	1	0	-0.795669	0.746682	-2.569325
11	1	0	0.354481	3.960545	1.313711
12	1	0	-0.892897	2.781350	1.807714
13	1	0	0.826283	2.518390	2.239860
14	6	0	1.850141	-0.806147	-1.106910
15	7	0	0.666065	-1.340848	-0.658317
16	6	0	-0.497161	-1.340882	-0.474098
17	47	0	-2.525370	-0.916240	-0.114985
18	7	0	-4.660807	-0.611123	0.221252
19	6	0	-5.730402	-0.204323	0.386822
20	6	0	-7.074663	0.319880	0.593832
21	1	0	-7.441985	0.027694	1.582675
22	1	0	-7.056328	1.412474	0.527022
23	1	0	-7.751785	-0.074365	-0.170480
24	15	0	3.251943	-1.028791	0.011817
25	8	0	3.784321	-2.397570	0.292162
26	8	0	4.291282	-0.059728	-0.755571

27	6	0	5.666159	0.020711	-0.349541
28	8	0	2.745487	-0.272355	1.354777
29	6	0	3.152341	-0.710229	2.662295
30	1	0	2.107377	-1.190008	-2.096881
31	1	0	6.193510	0.530632	-1.157935
32	1	0	5.751645	0.614241	0.567339
33	1	0	6.085167	-0.979043	-0.197723
34	1	0	3.342859	-1.786765	2.670328
35	1	0	2.332665	-0.463753	3.341488
36	1	0	4.053741	-0.168092	2.968278

Trans PTS



B3LYP/6•31+G(d): -1455.72100294

Imaginary Frequencies: 1 (-280.6074)

Zero-point correction=	0.260289
Thermal correction to Energy=	0.286816
Thermal correction to Enthalpy=	0.287761
Thermal correction to Gibbs Free Energy=	0.196013
Sum of electronic and zero-point Energies=	-1455.460714
Sum of electronic and thermal Energies=	-1455.434187
Sum of electronic and thermal Enthalpies=	-1455.433242
Sum of electronic and thermal Free Energies=	-1455.524990

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.274814	2.700370	-0.236211
2	6	0	-1.083593	2.592094	0.018872
3	6	0	-1.243514	1.417911	0.963183
4	6	0	0.047760	1.039458	1.344498
5	6	0	1.005926	1.768422	0.556947
6	6	0	0.865940	3.680358	-1.123788
7	8	0	2.245334	1.675503	0.485565
8	8	0	-1.948103	3.310071	-0.465258
9	1	0	-2.121371	1.383286	1.596113
10	1	0	0.326993	0.333550	2.114414
11	1	0	0.705909	4.697199	-0.746754
12	1	0	1.937498	3.475551	-1.174319
13	1	0	0.424088	3.609755	-2.123398
14	6	0	-2.009148	0.058791	-0.487586
15	7	0	-0.840398	-0.548969	-0.854377
16	6	0	0.299739	-0.833641	-0.768846
17	47	0	2.358283	-0.905751	-0.369708
18	7	0	4.479851	-1.114170	0.079975
19	6	0	5.578262	-1.007795	0.424768
20	6	0	6.960189	-0.863117	0.864940
21	1	0	7.201932	-1.639397	1.597800

22	1	0	7.637178	-0.954531	0.009711
23	1	0	7.096639	0.120136	1.326630
24	15	0	-3.183874	-1.035664	0.341078
25	8	0	-2.687177	-1.755583	1.541347
26	8	0	-4.379060	0.037288	0.583616
27	6	0	-5.409267	-0.250928	1.548606
28	8	0	-3.795774	-2.103161	-0.730403
29	6	0	-4.372384	-1.683779	-1.975742
30	1	0	-2.435999	0.713499	-1.246032
31	1	0	-6.053548	-1.062499	1.192595
32	1	0	-4.966367	-0.527963	2.509370
33	1	0	-5.991475	0.666667	1.650245
34	1	0	-5.157317	-0.936590	-1.815581
35	1	0	-3.604027	-1.274071	-2.641722
36	1	0	-4.802428	-2.579562	-2.428726