Preparation of aromatic γ-hydroxyketones by means of Heck coupling of aryl halides and 2,3-dihydrofuran, catalyzed by palladium(II) glycine complex under microwave irradiation

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Electronic Supplementary Material (ESI) for New Journal of Chemistry

SUPPORTING INFORMATION

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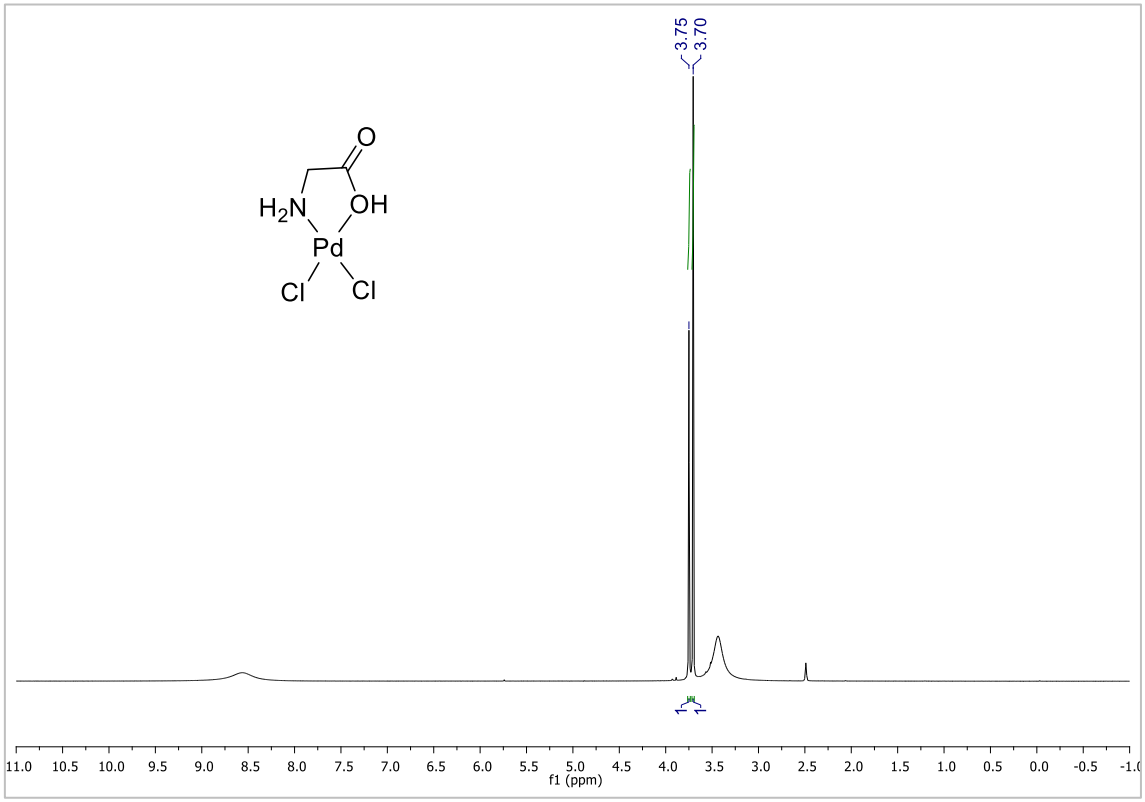
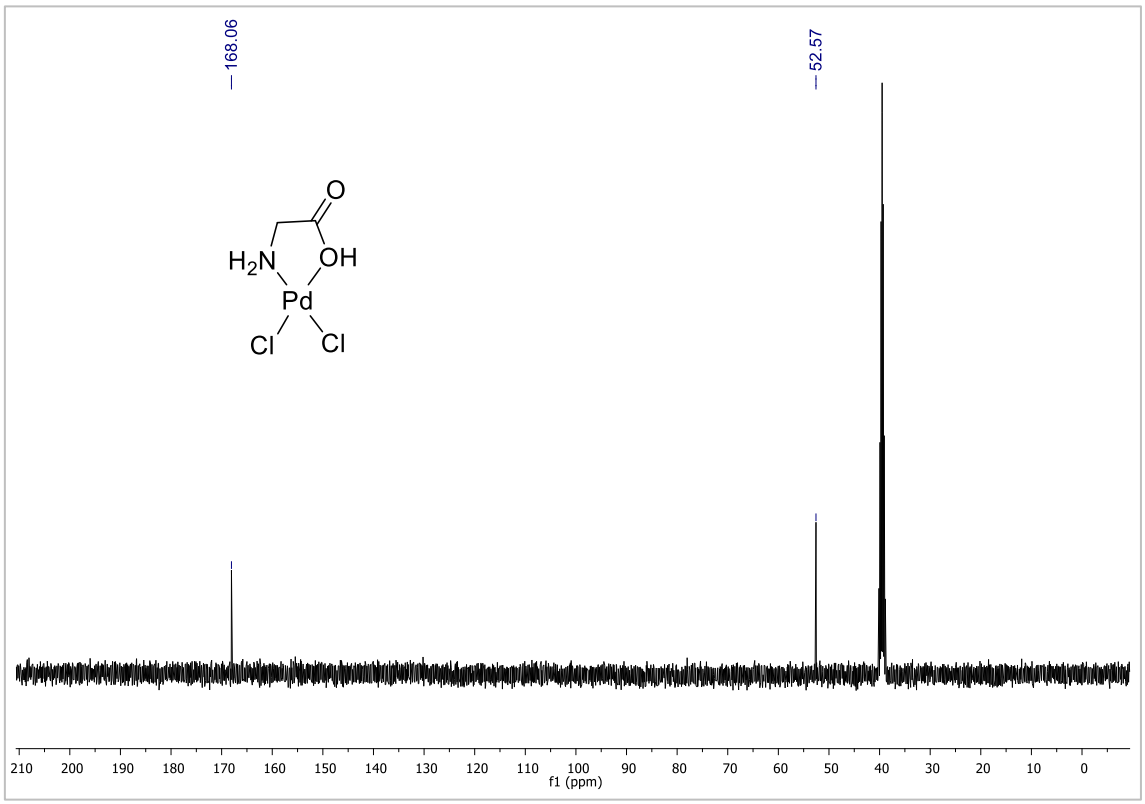
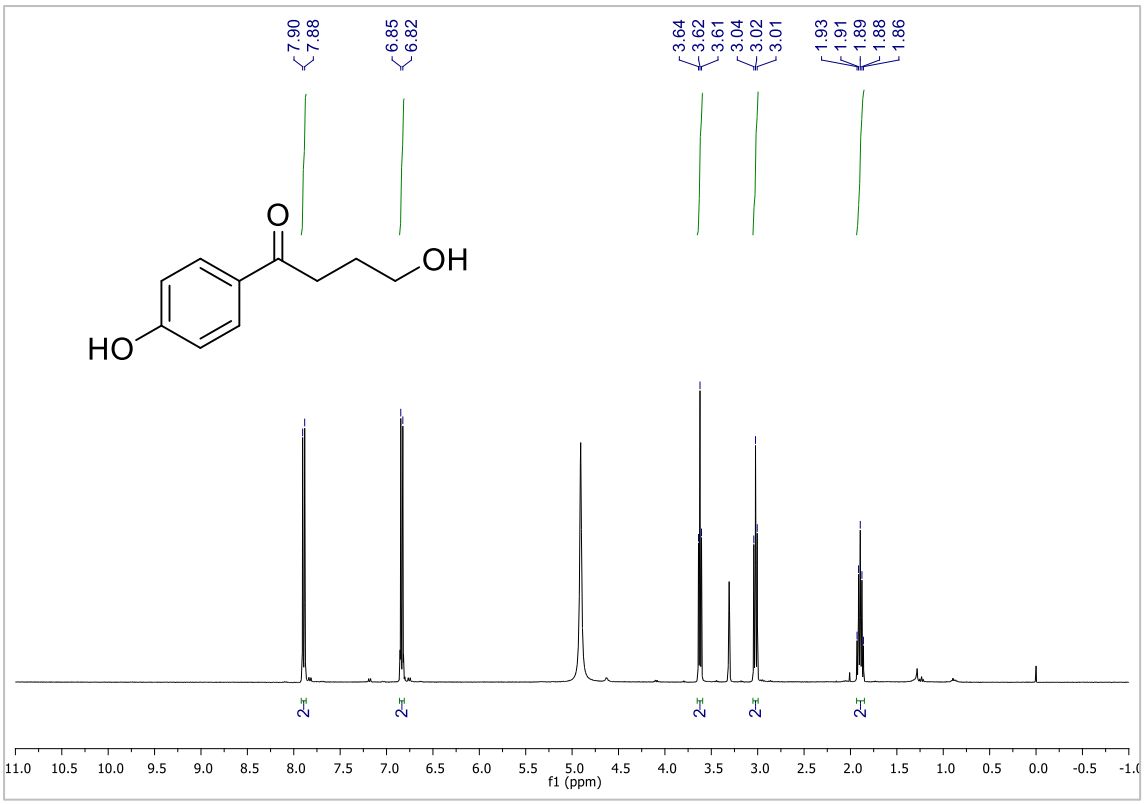
1. NMR spectra



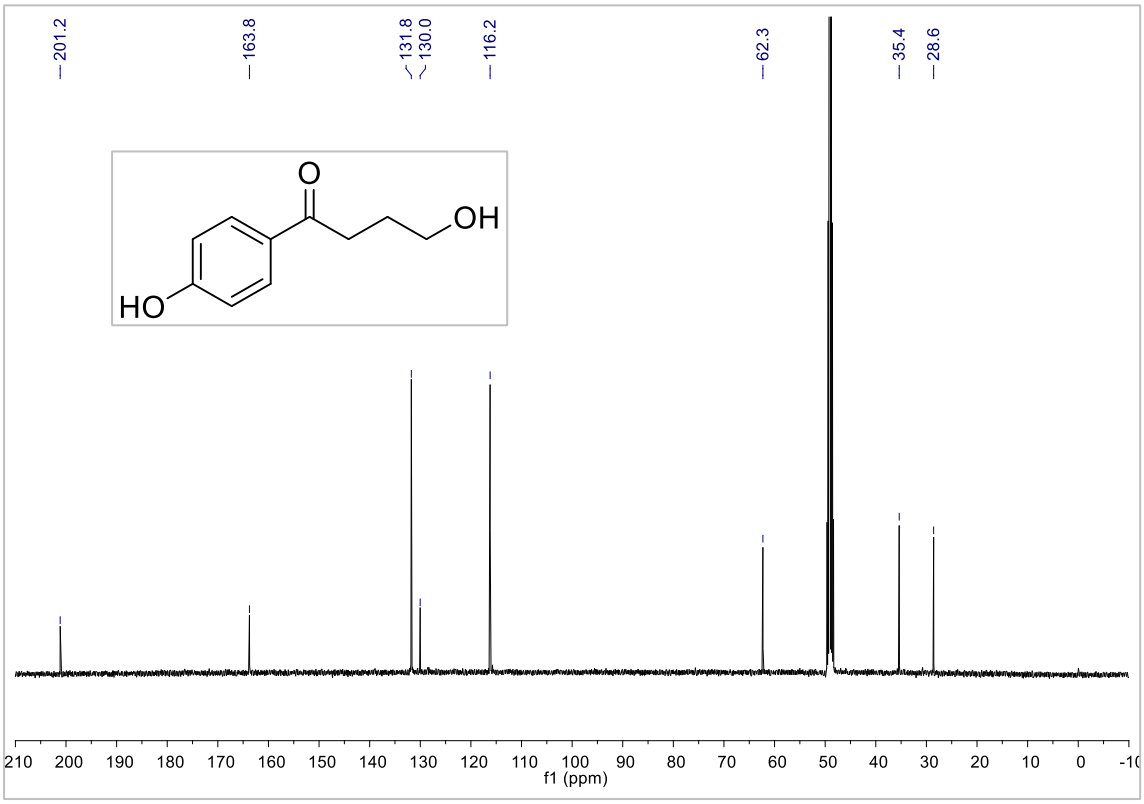
^{1}H NMR spectrum of catalyst **1** (400 MHz, DMSO-d_6).



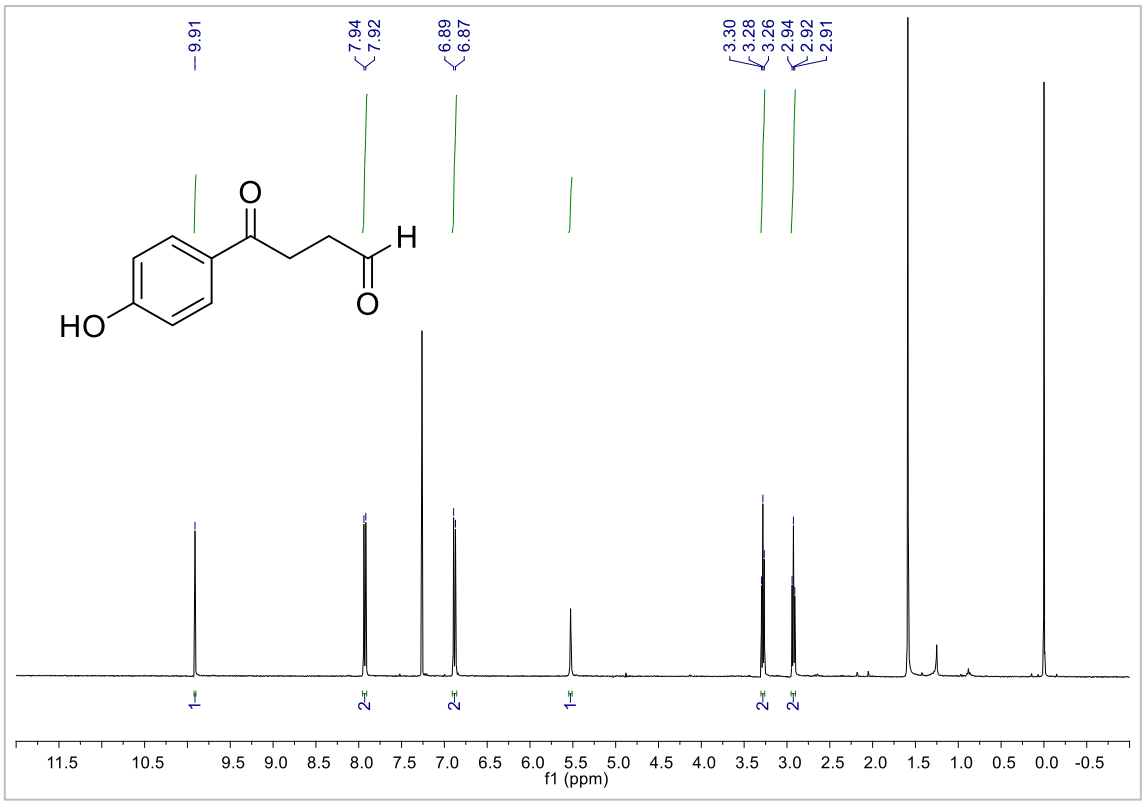
^{13}C NMR spectrum of catalyst **1** (100 MHz, DMSO-d_6).



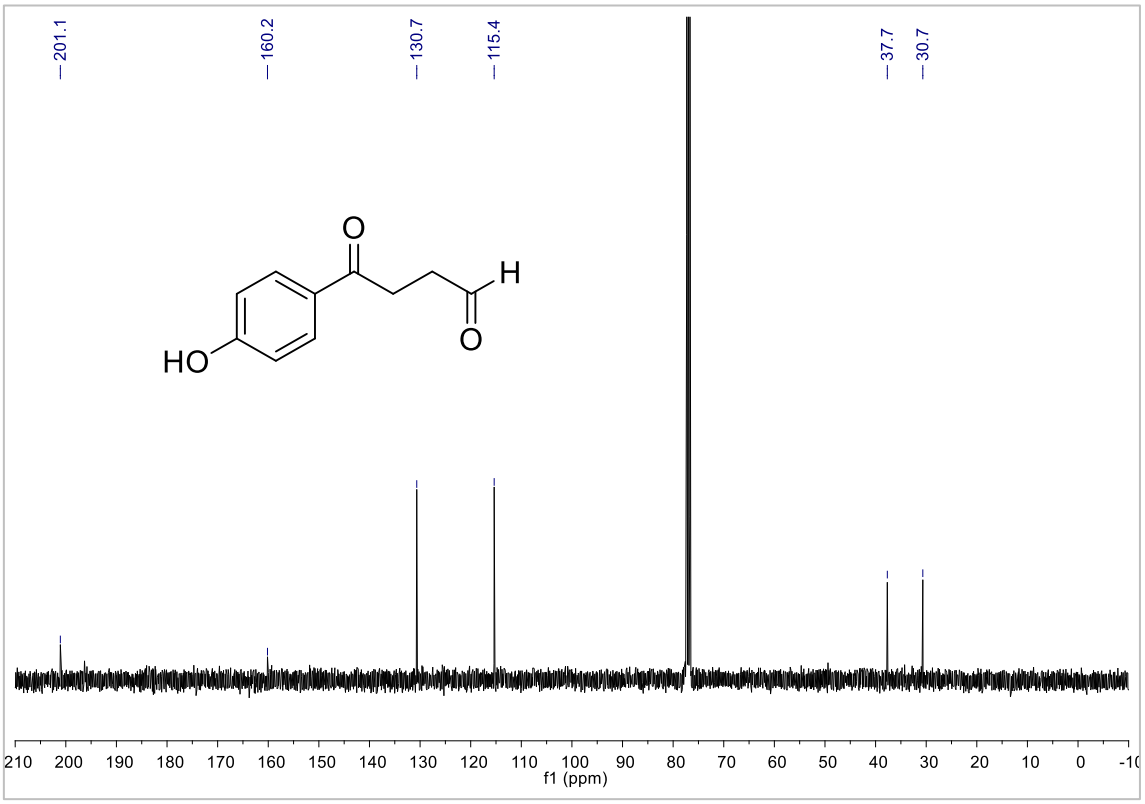
^{1}H NMR spectrum of **2** (400 MHz, CD_3OD).



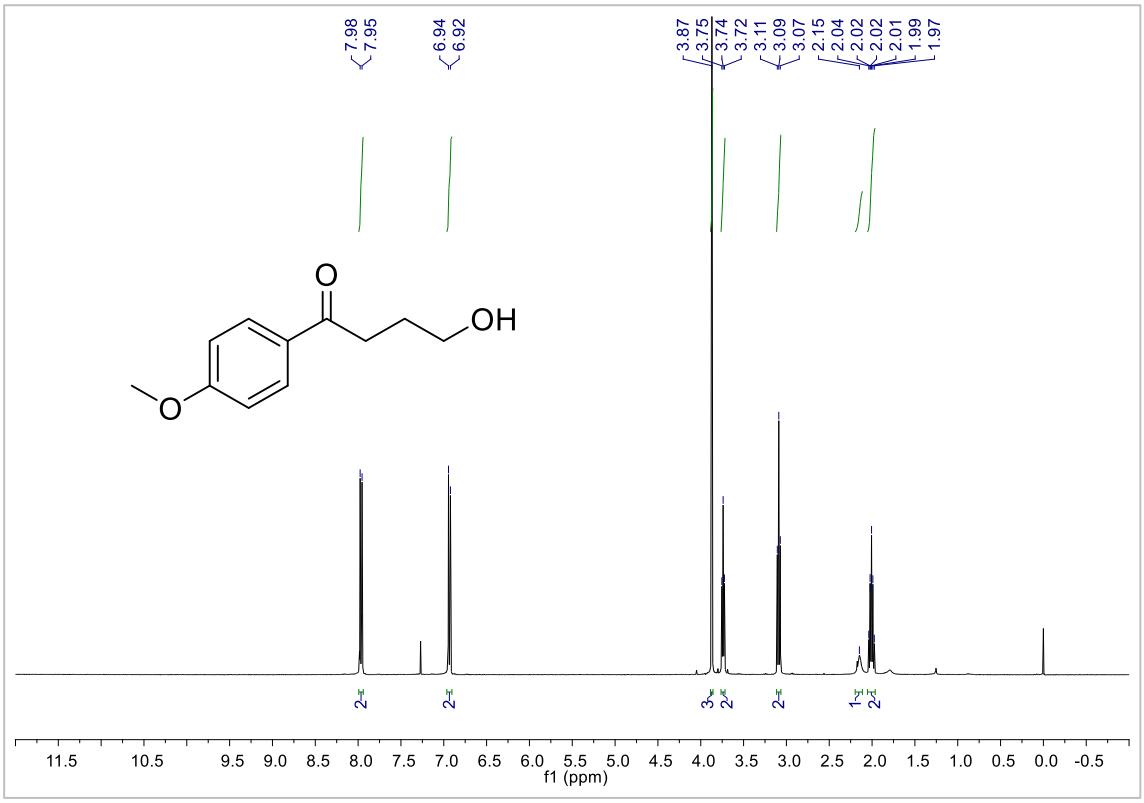
^{13}C NMR spectrum of **2** (100 MHz, CD_3OD).



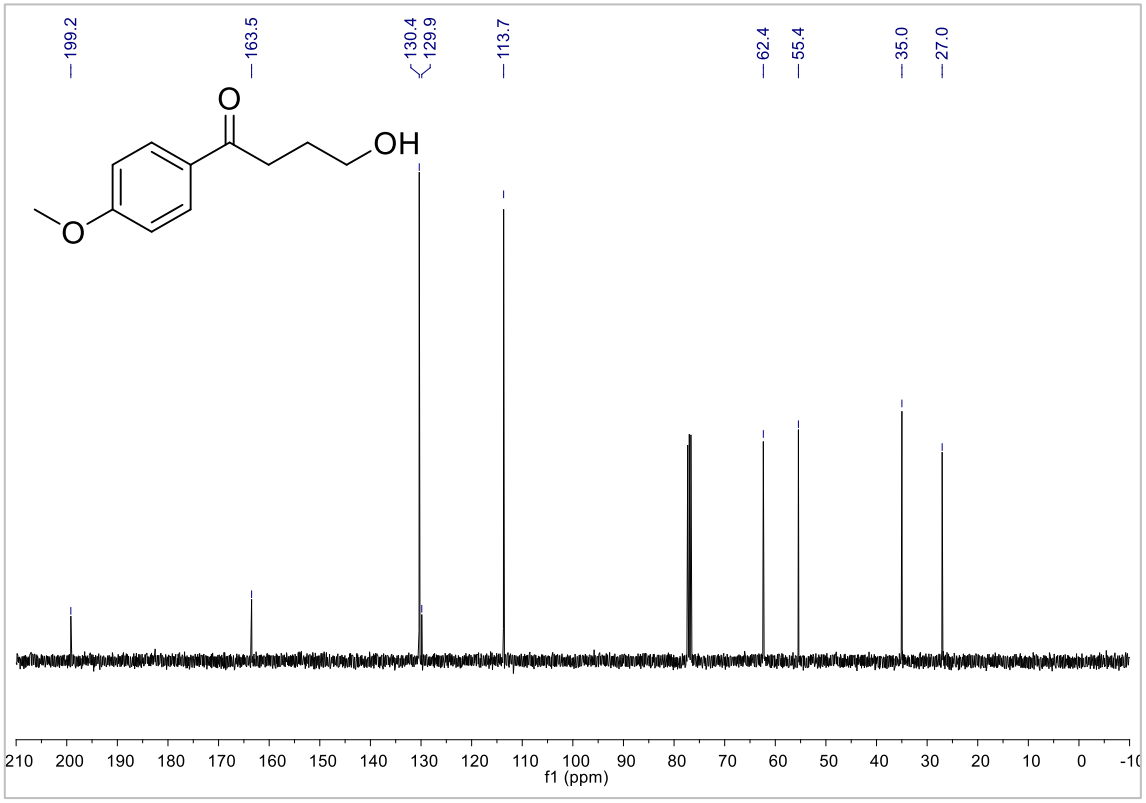
^{1}H NMR spectrum of **3** (400 MHz, $CDCl_3$).



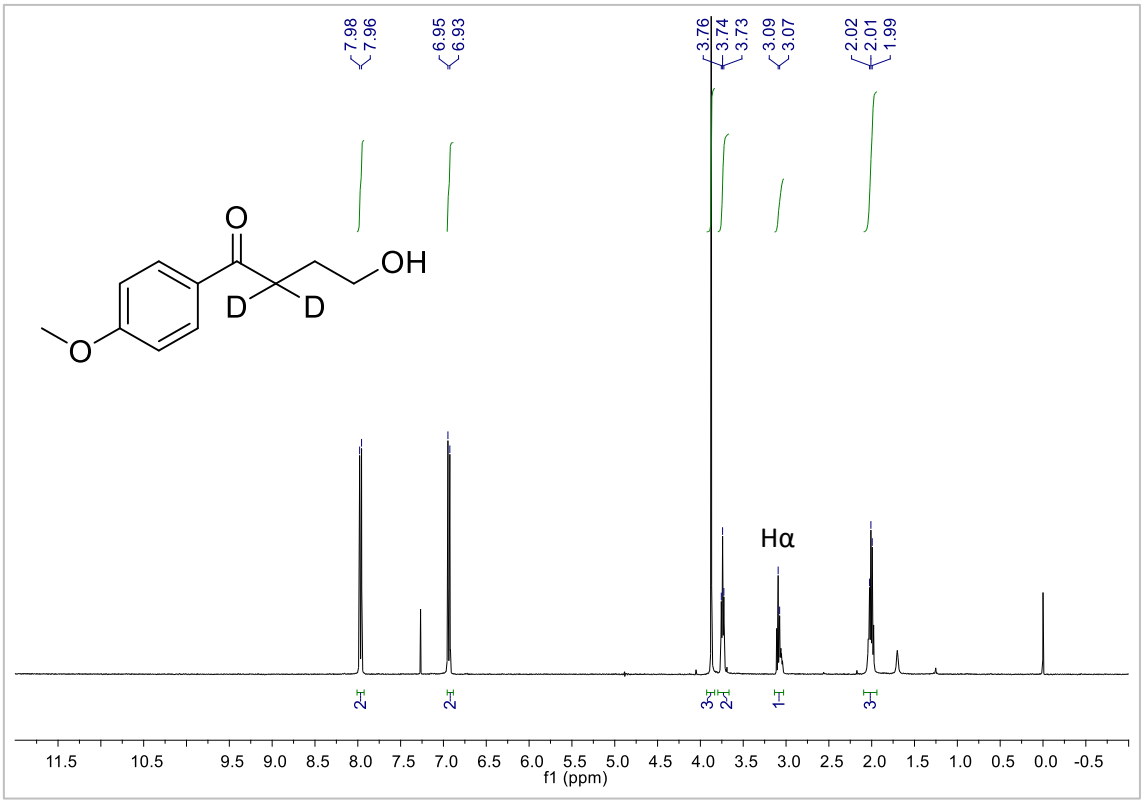
^{13}C NMR spectrum of **3** (100 MHz, $CDCl_3$).



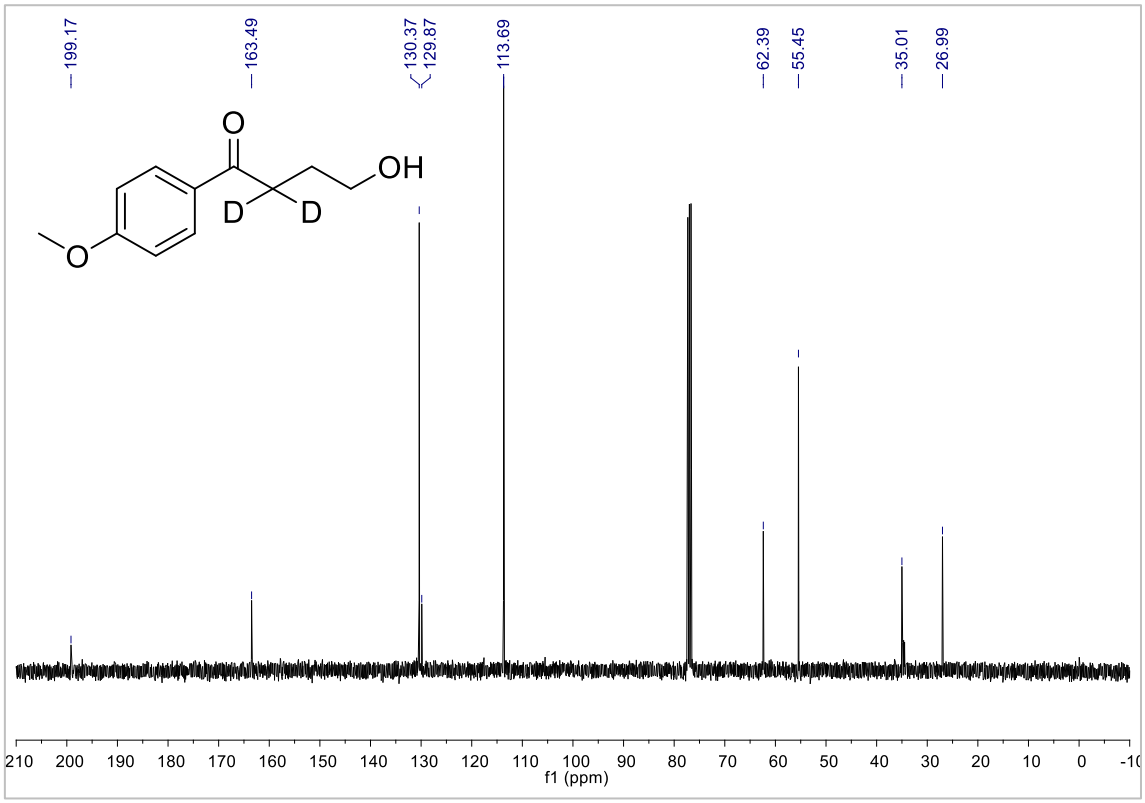
^{1}H NMR spectrum of **4** (400 MHz, $CDCl_3$).



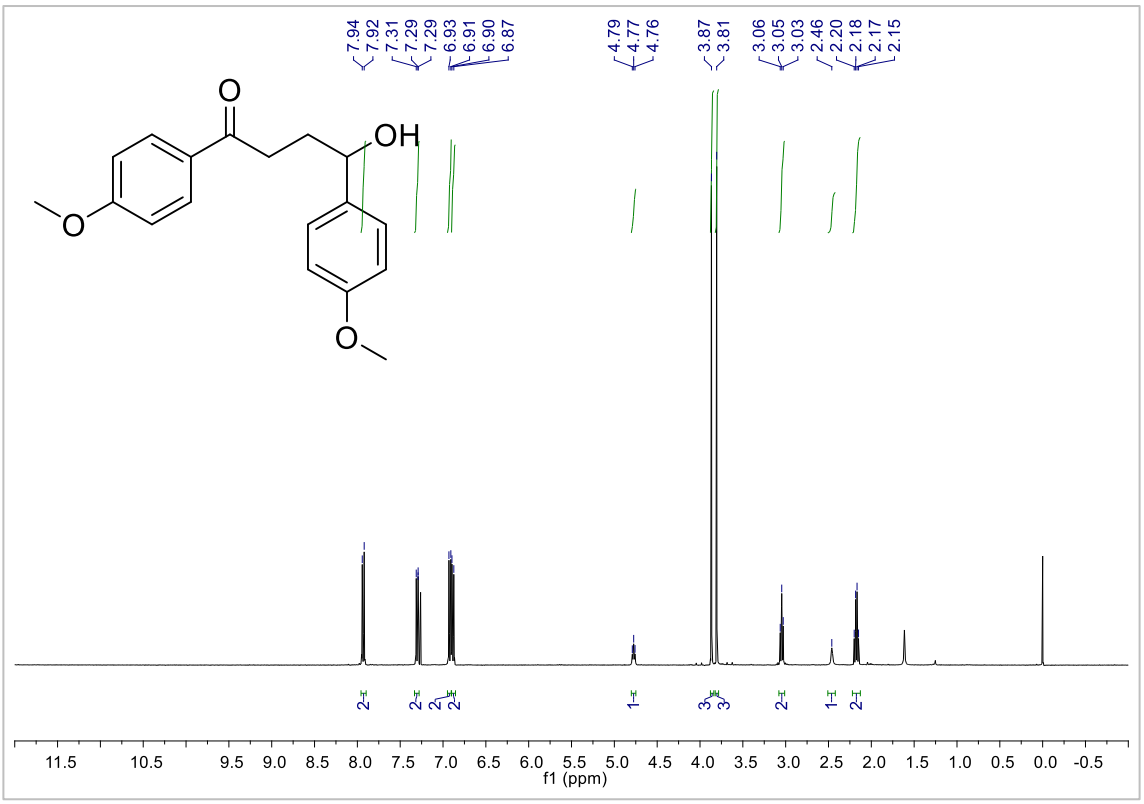
^{13}C NMR spectrum of **4** (100 MHz, $CDCl_3$).



^{1}H NMR spectrum of **4-d_2** (400 MHz, $CDCl_3$).



^{13}C NMR spectrum of **4-d_2** (100 MHz, $CDCl_3$).



^{1}H NMR spectrum of **5** (400 MHz, $CDCl_3$).

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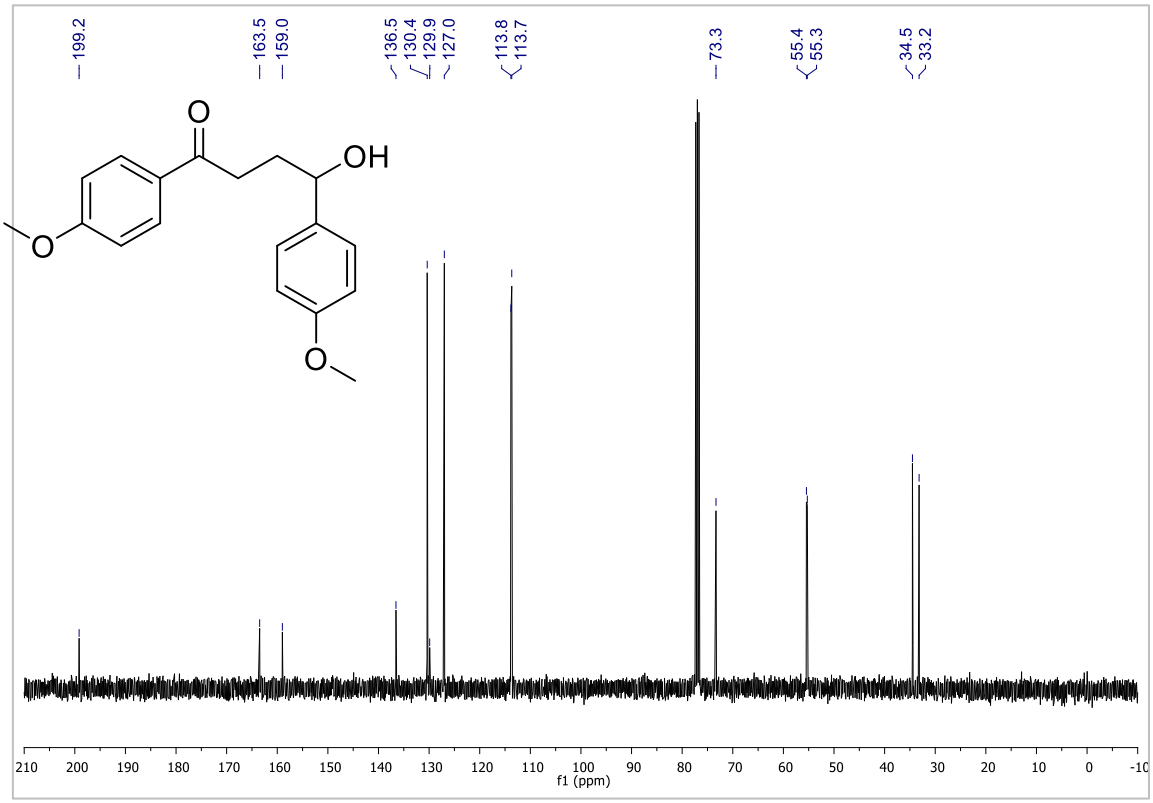
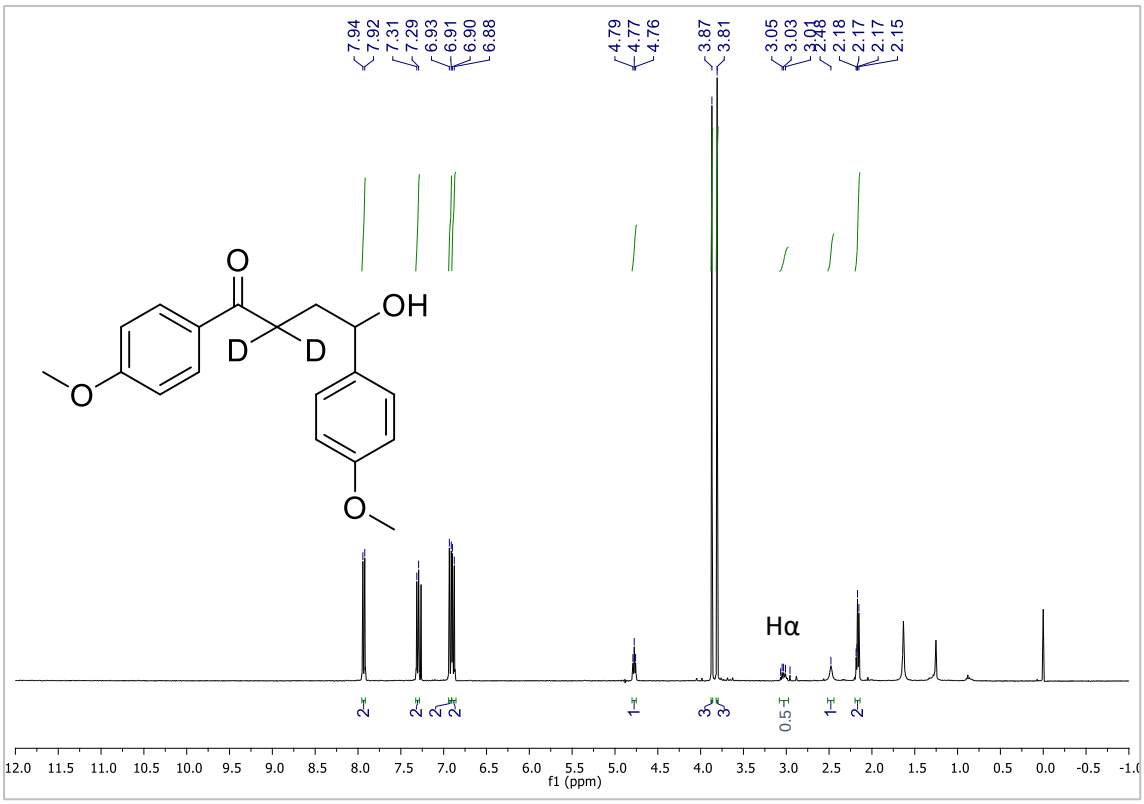
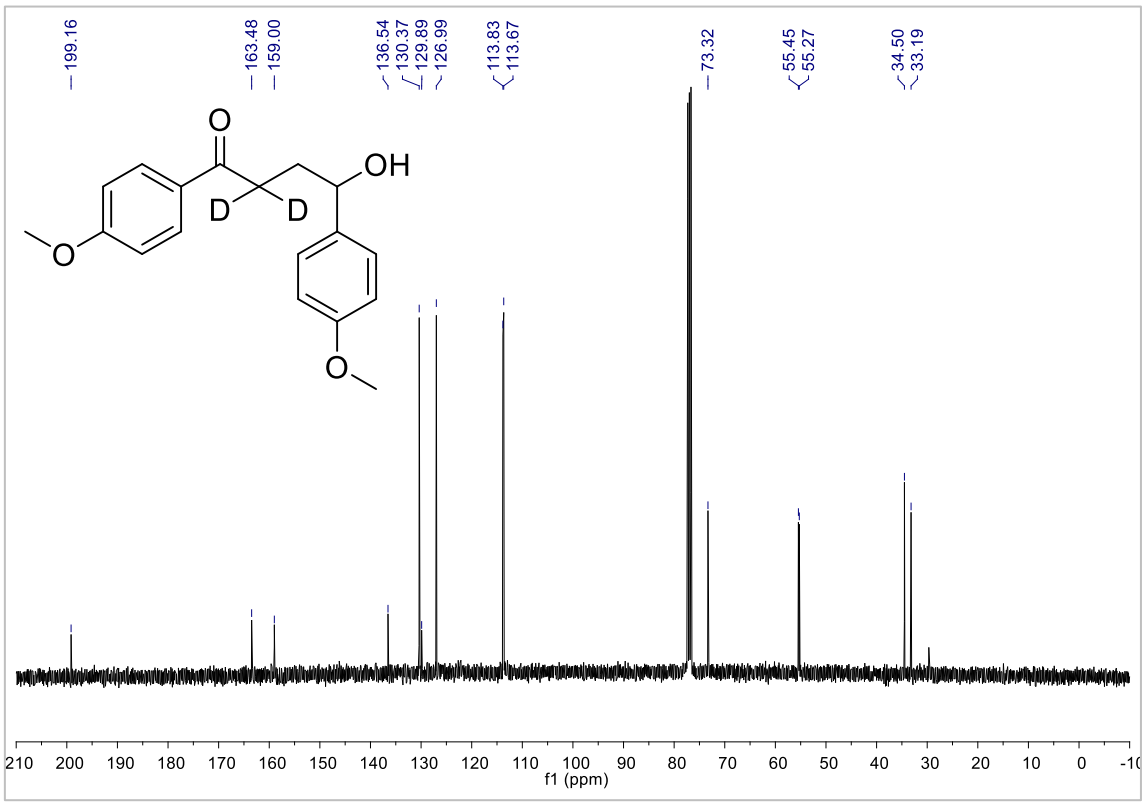


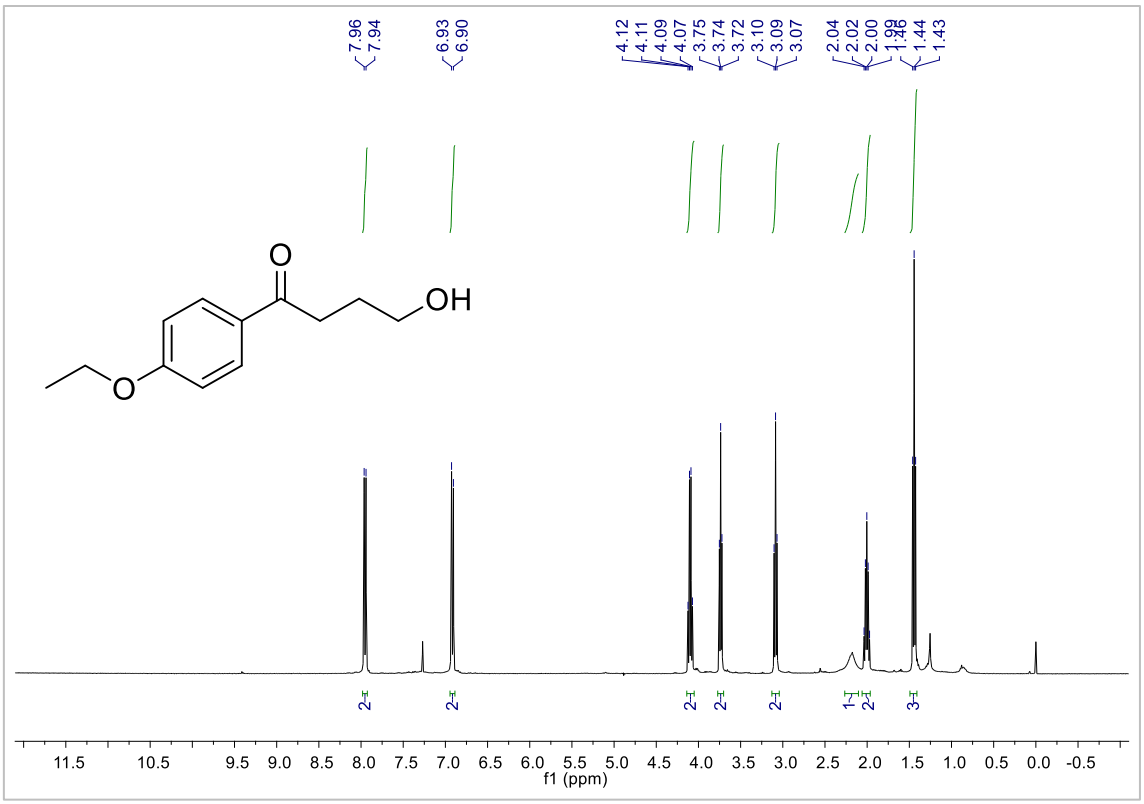
^{13}C NMR spectrum of **5** (100 MHz, $CDCl_3$).



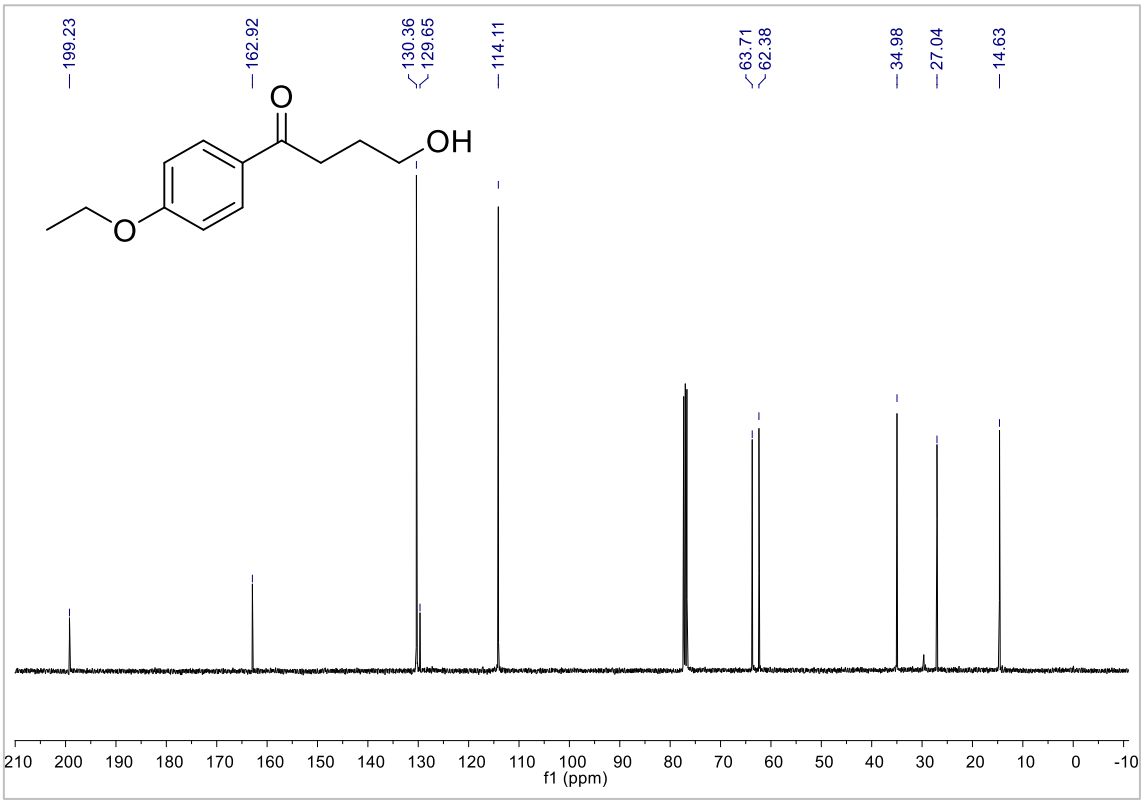
^{1}H NMR spectrum of **5-*d*$_2$** (400 MHz, $CDCl_3$



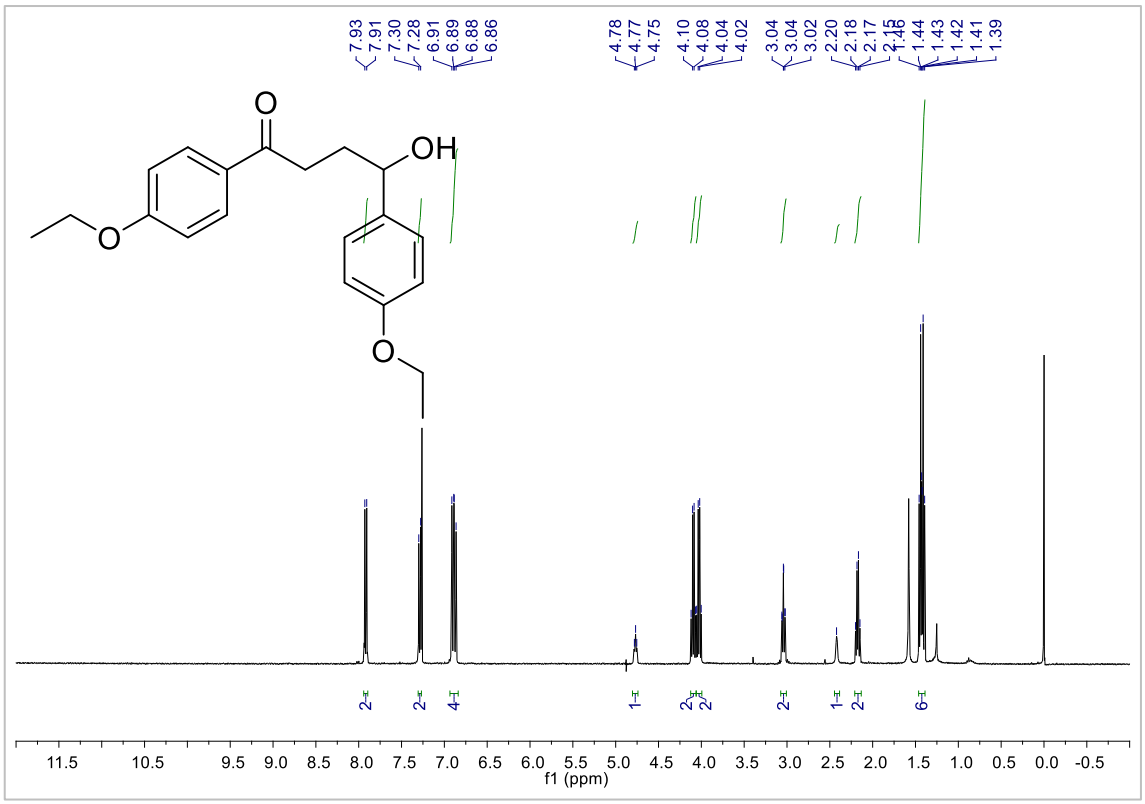
^{13}C NMR spectrum of **5-*d*$_2$** (100 MHz, $CDCl_3$).



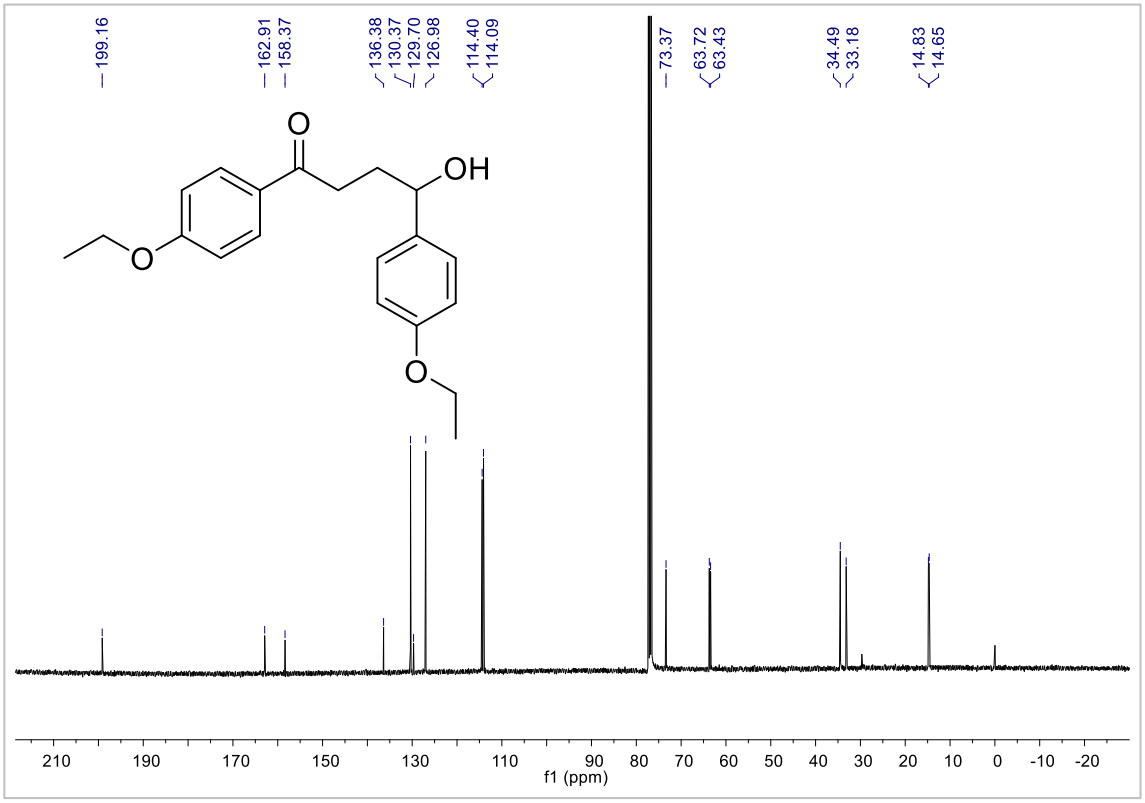
^{1}H NMR spectrum of **6** (400 MHz, $CDCl_3$).



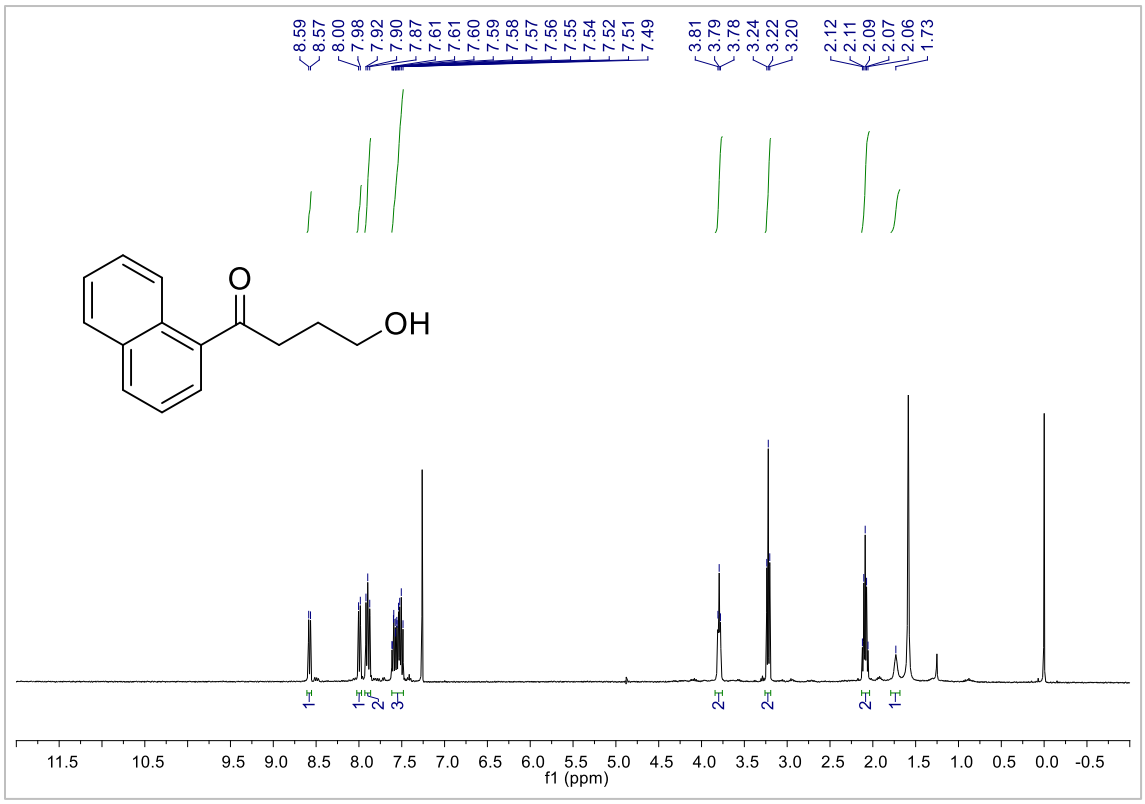
^{13}C NMR spectrum of **6** (100 MHz, $CDCl_3$).



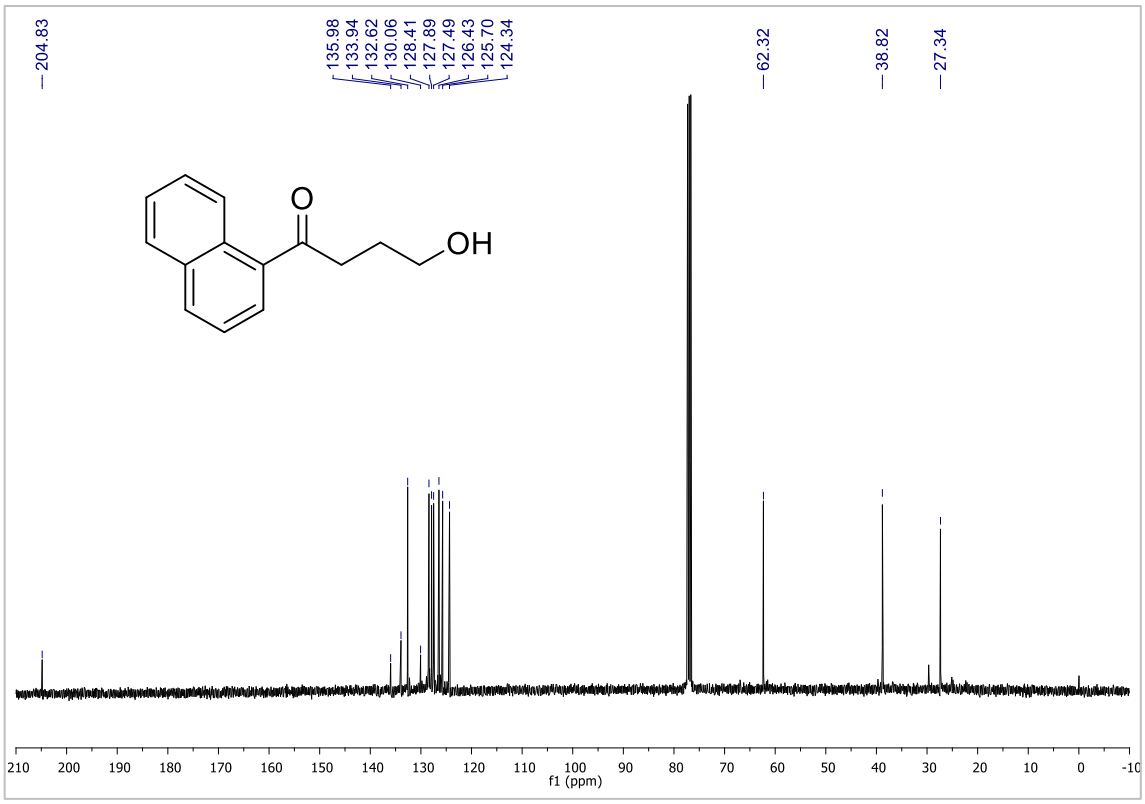
^{1}H NMR spectrum of **7** (400 MHz, $CDCl_3$).



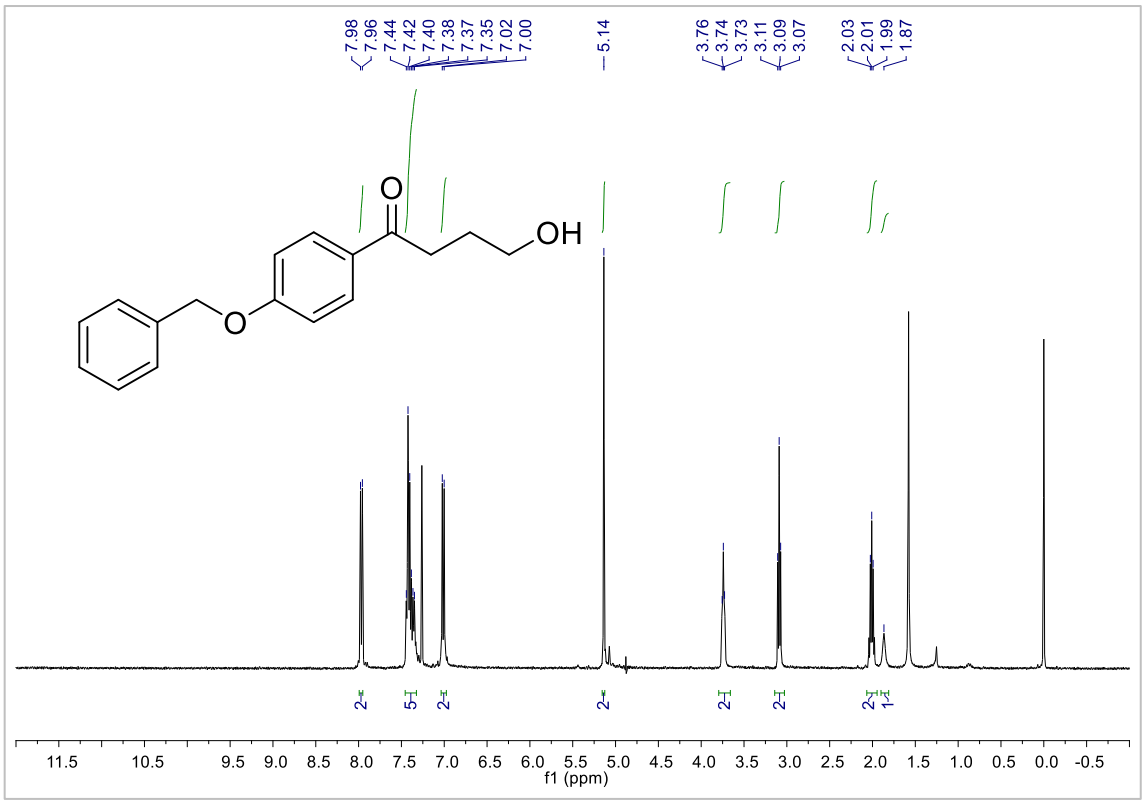
^{13}C NMR spectrum of **7** (100 MHz, $CDCl_3$).



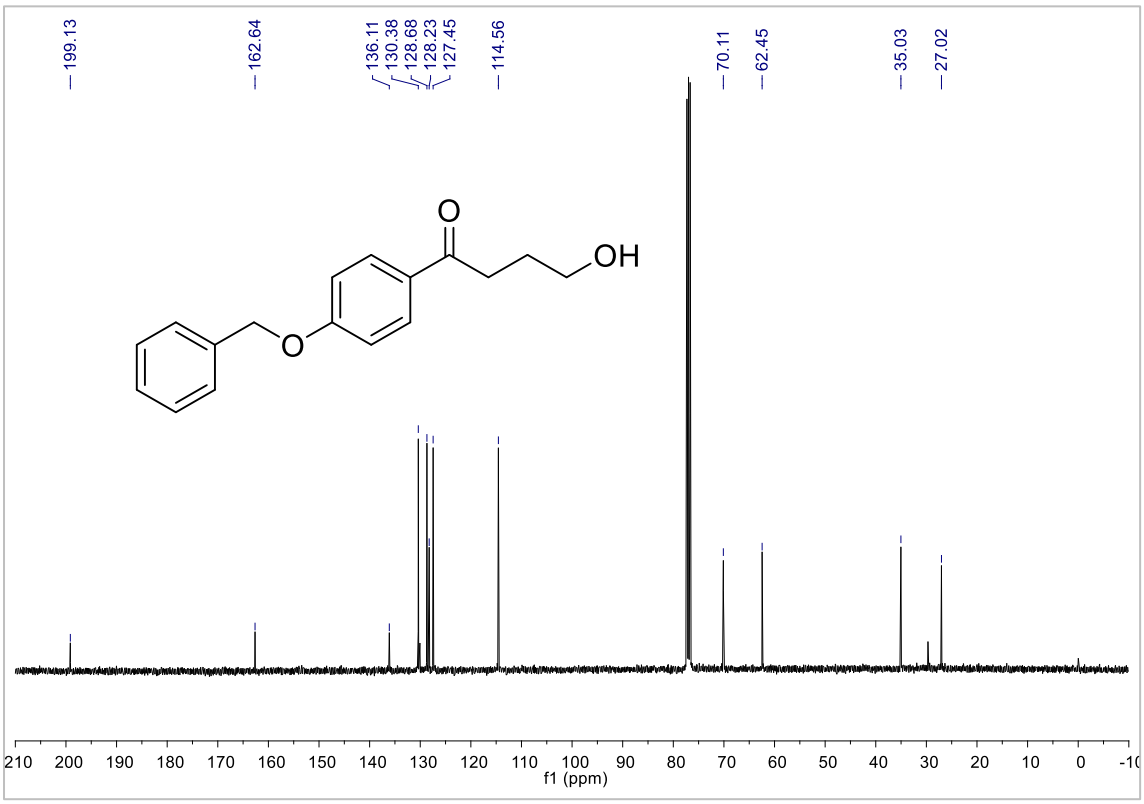
^{1}H NMR spectrum of **8** (400 MHz, $CDCl_3$).



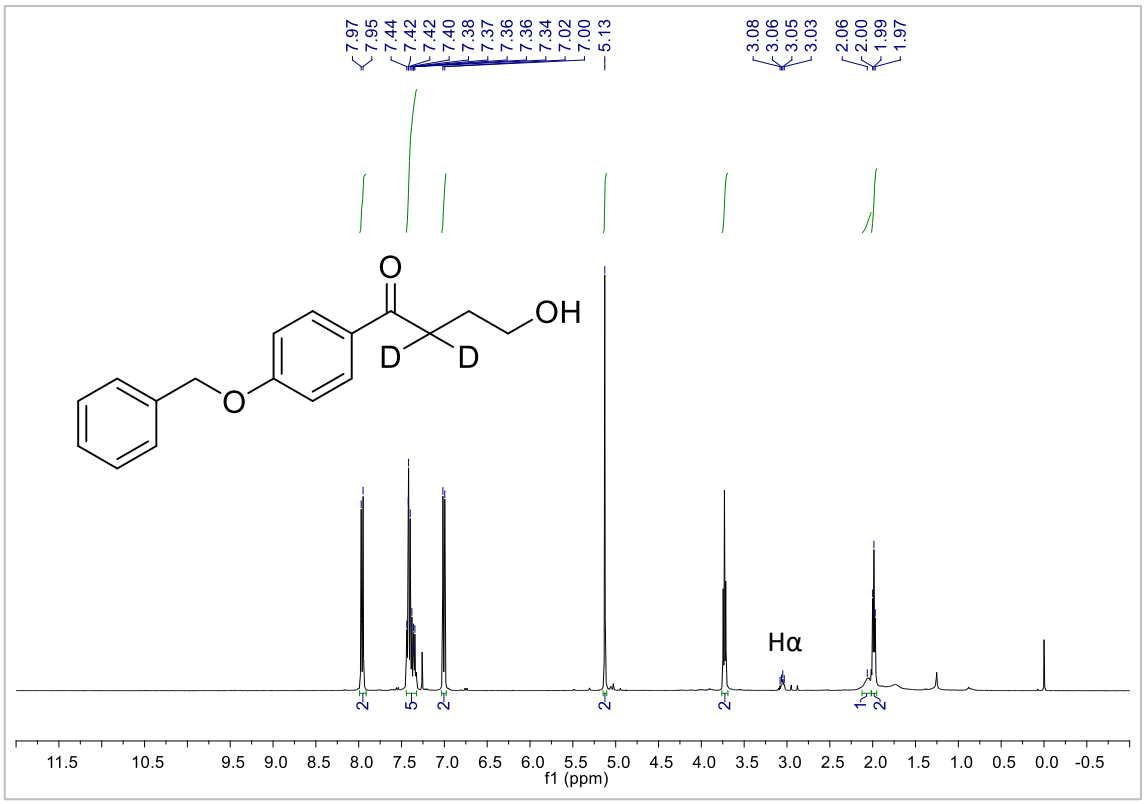
^{13}C NMR spectrum of **8** (100 MHz, $CDCl_3$).



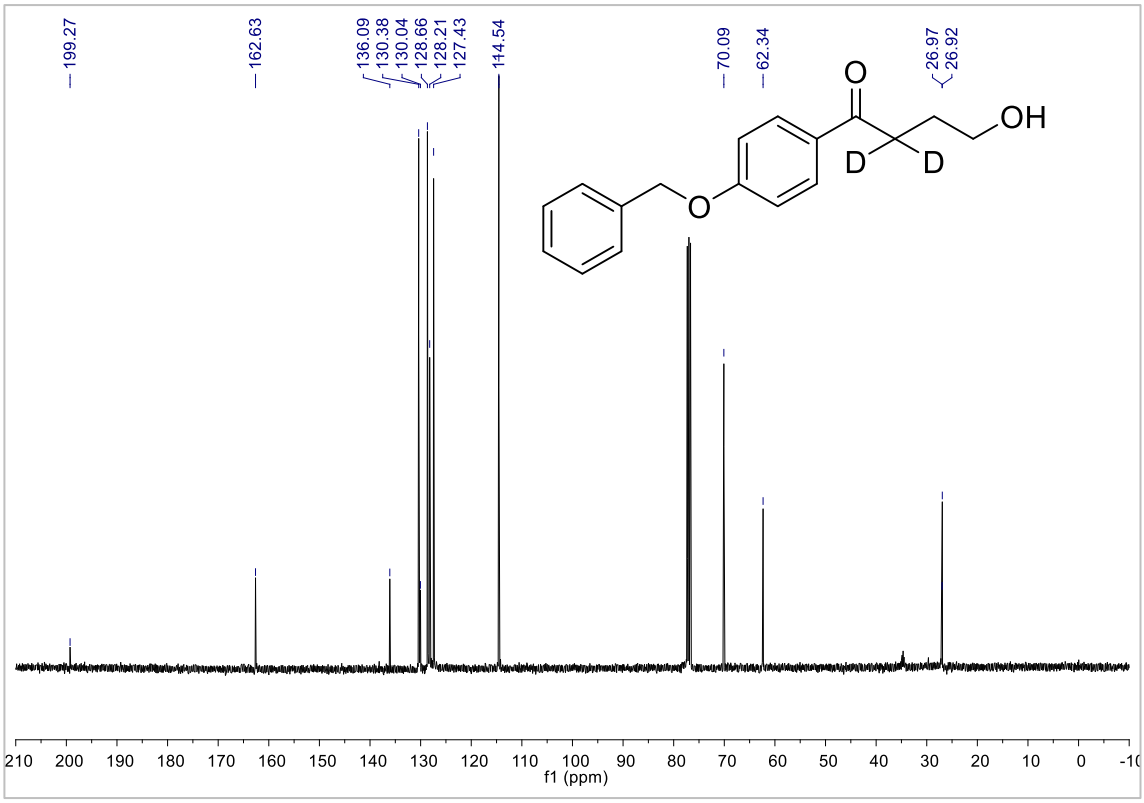
^{1}H NMR spectrum of **9** (400 MHz, $CDCl_3$).



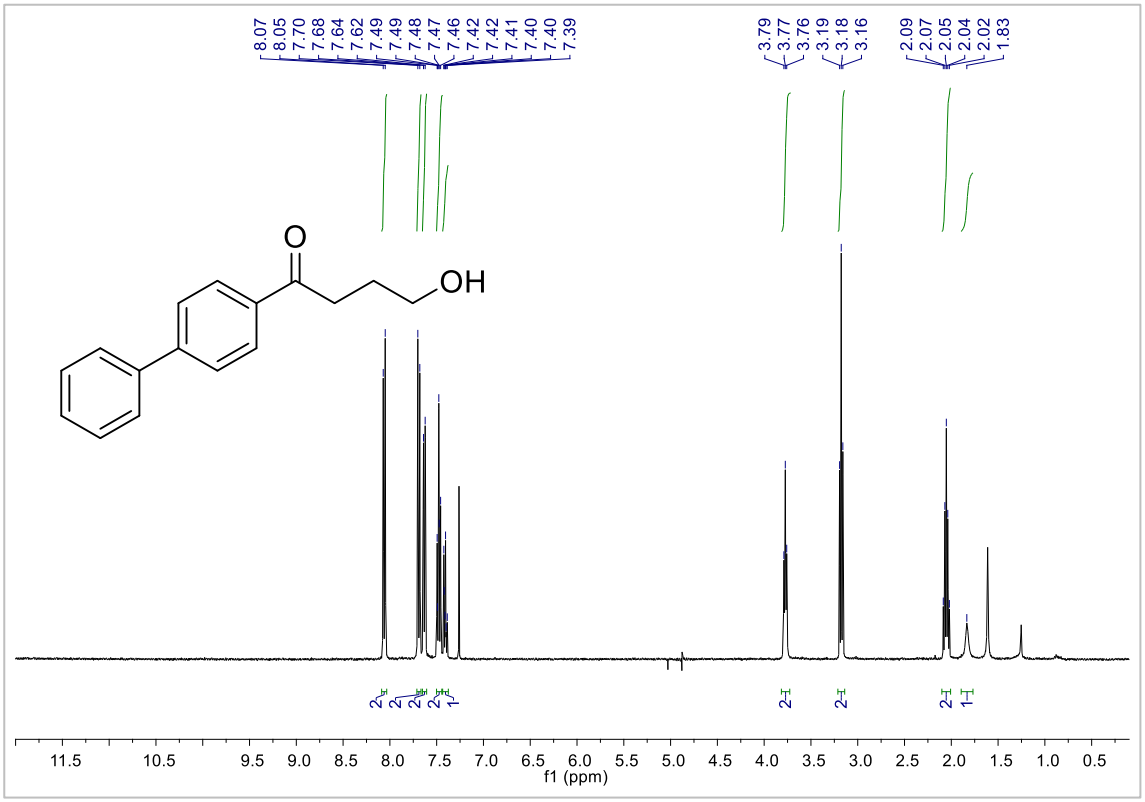
^{13}C NMR spectrum of **9** (100 MHz, $CDCl_3$).



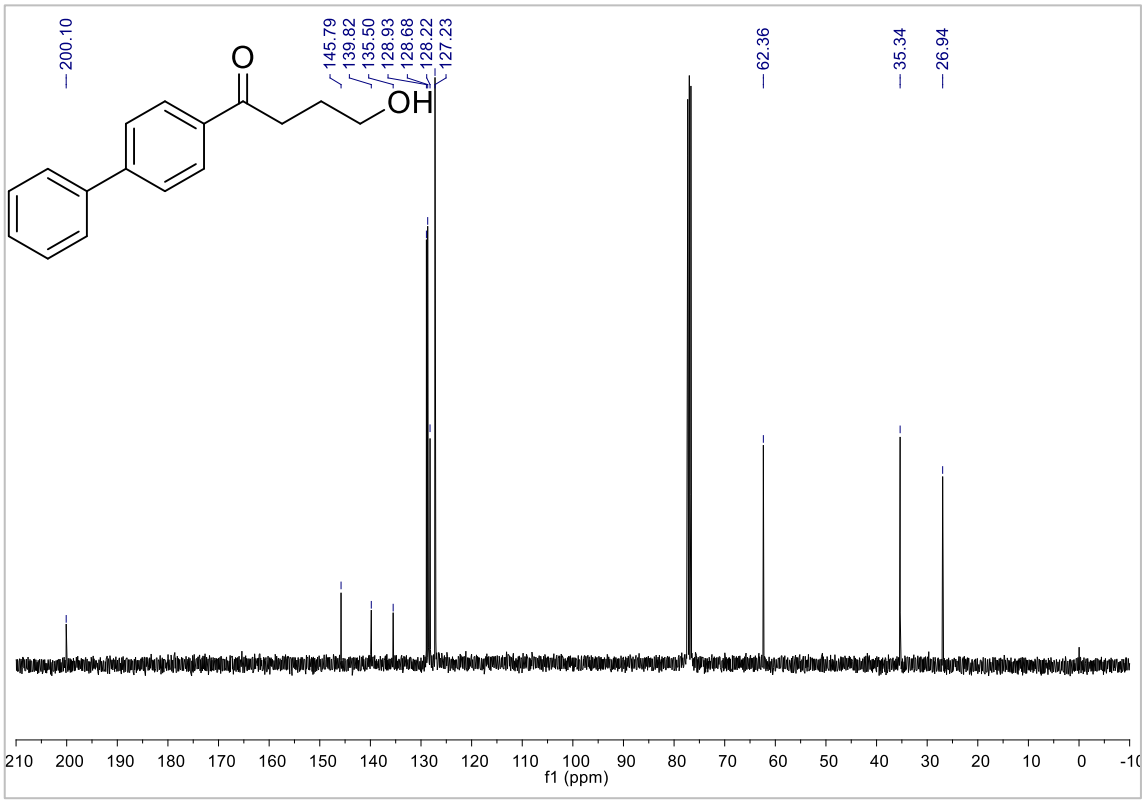
^{1}H NMR spectrum of **9-d_2** (400 MHz, $CDCl_3$).



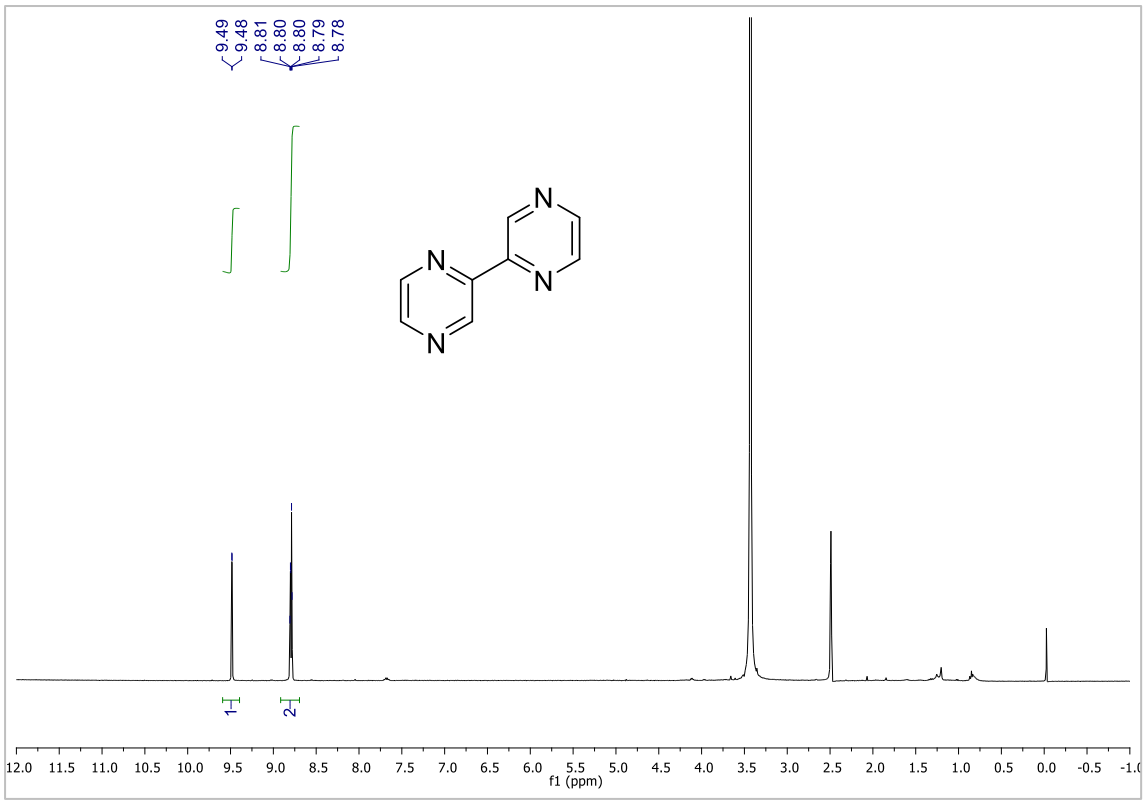
^{13}C NMR spectrum of **9-d_2** (100 MHz, $CDCl_3$).



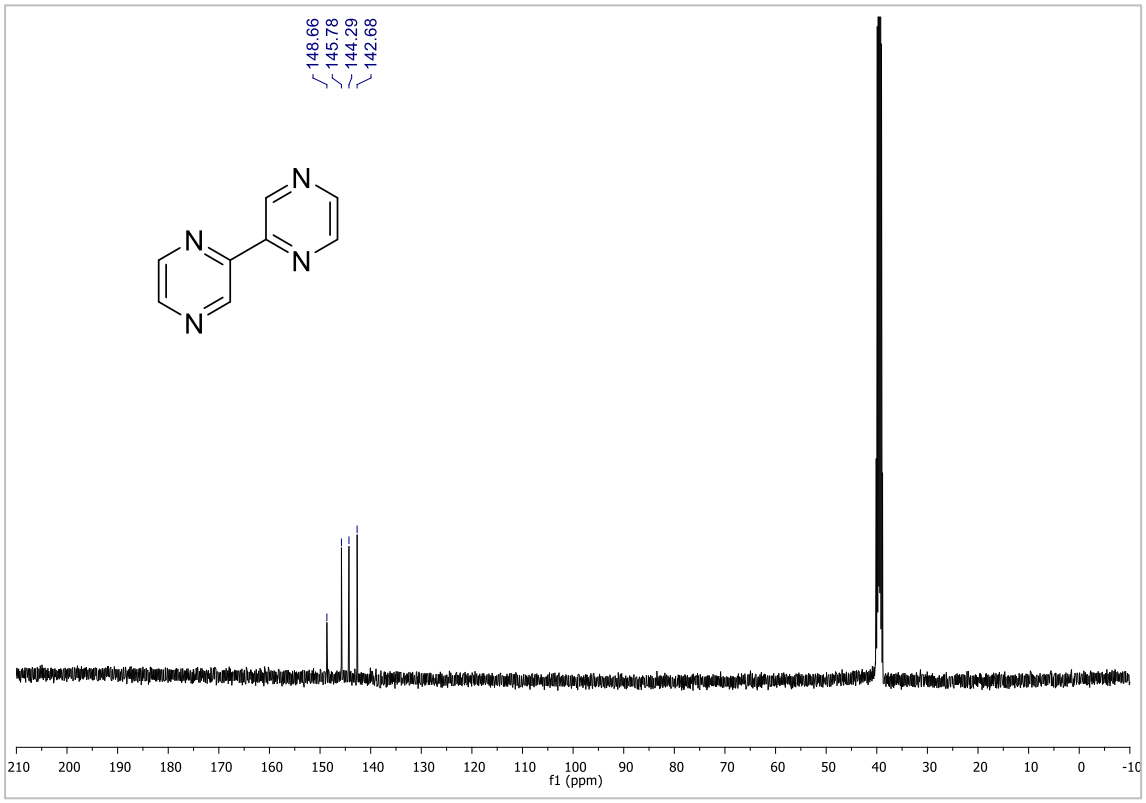
^{1}H NMR spectrum of **10** (400 MHz, $CDCl_3$).



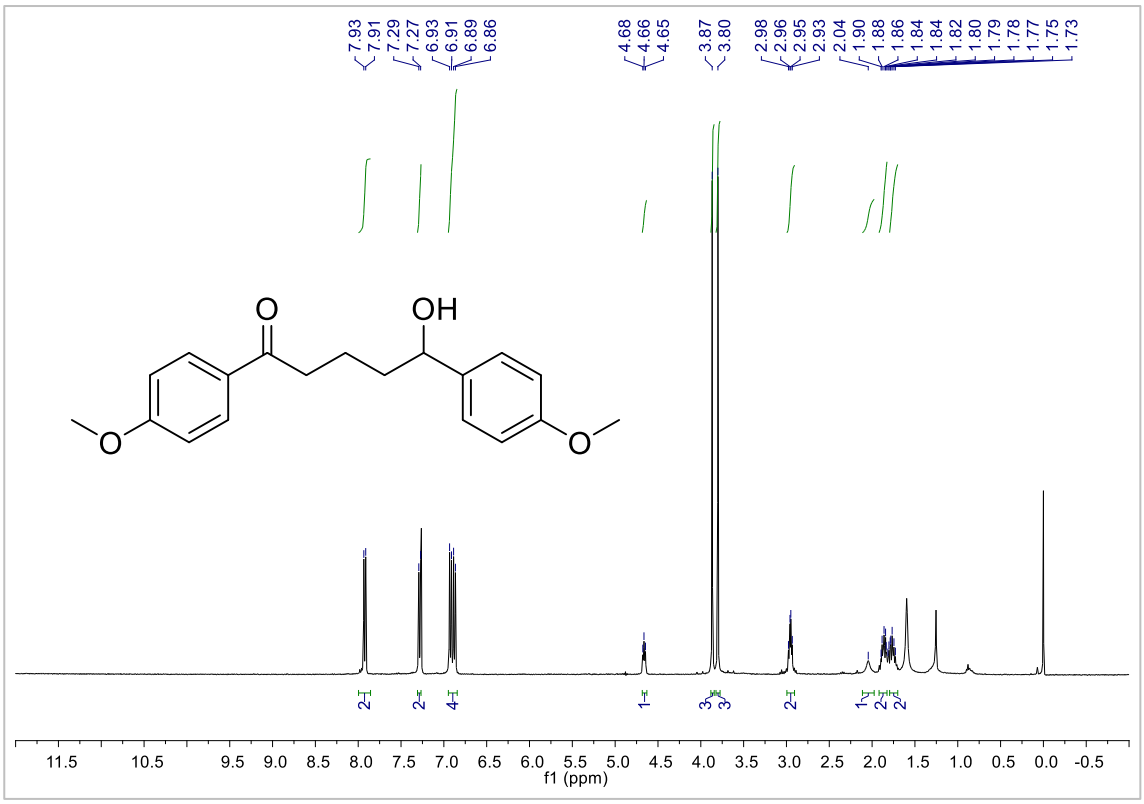
^{13}C NMR spectrum of **10** (100 MHz, $CDCl_3$).



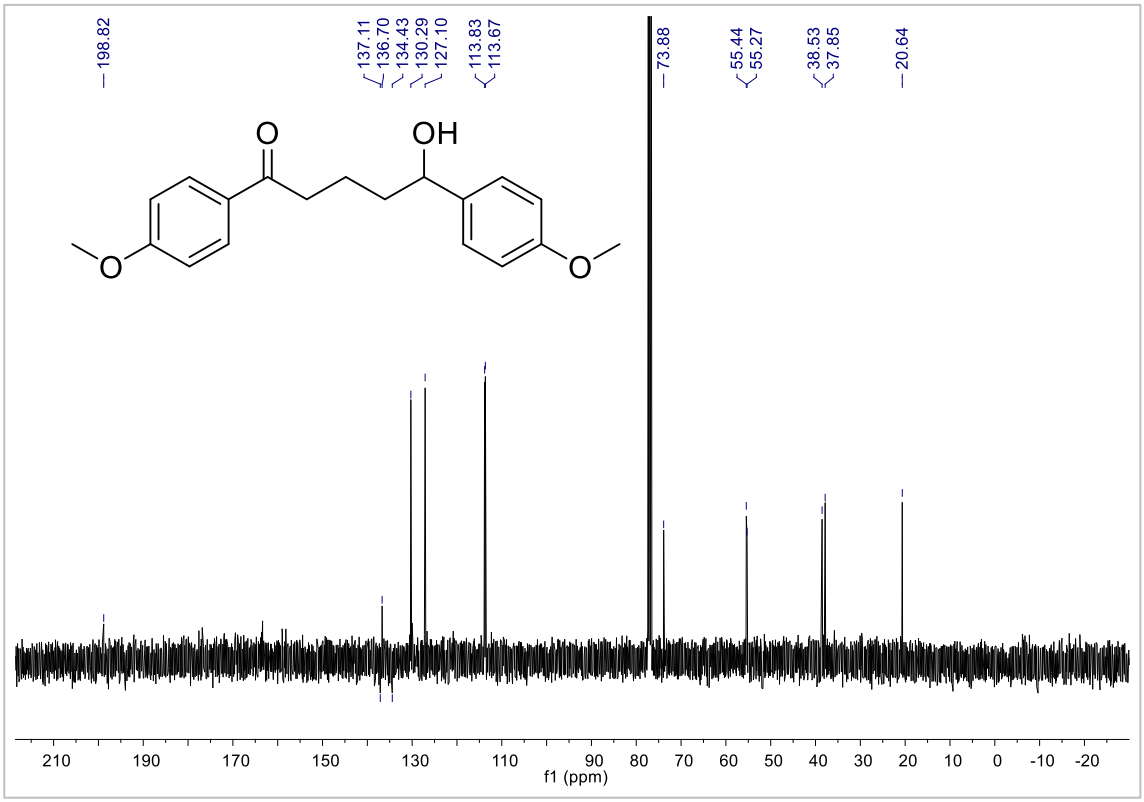
^{1}H NMR spectrum of **11** (400 MHz, DMSO-d_6).



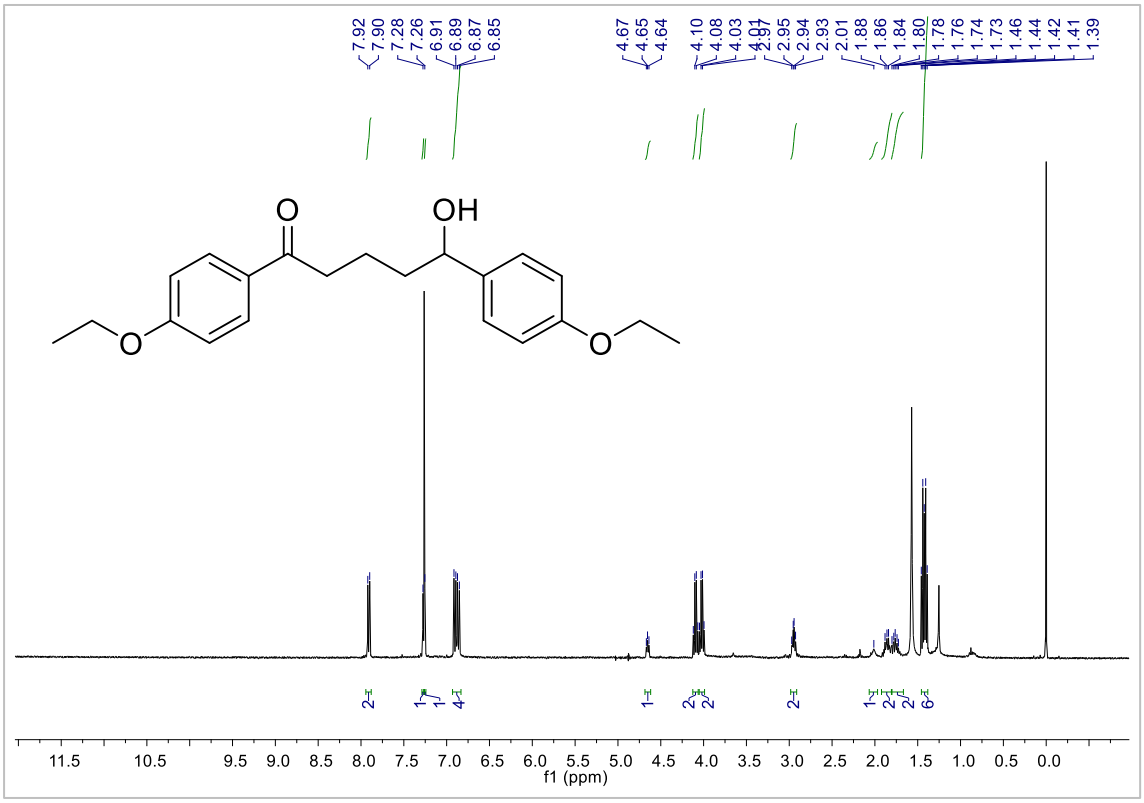
^{13}C NMR spectrum of **11** (100 MHz, DMSO-d_6).



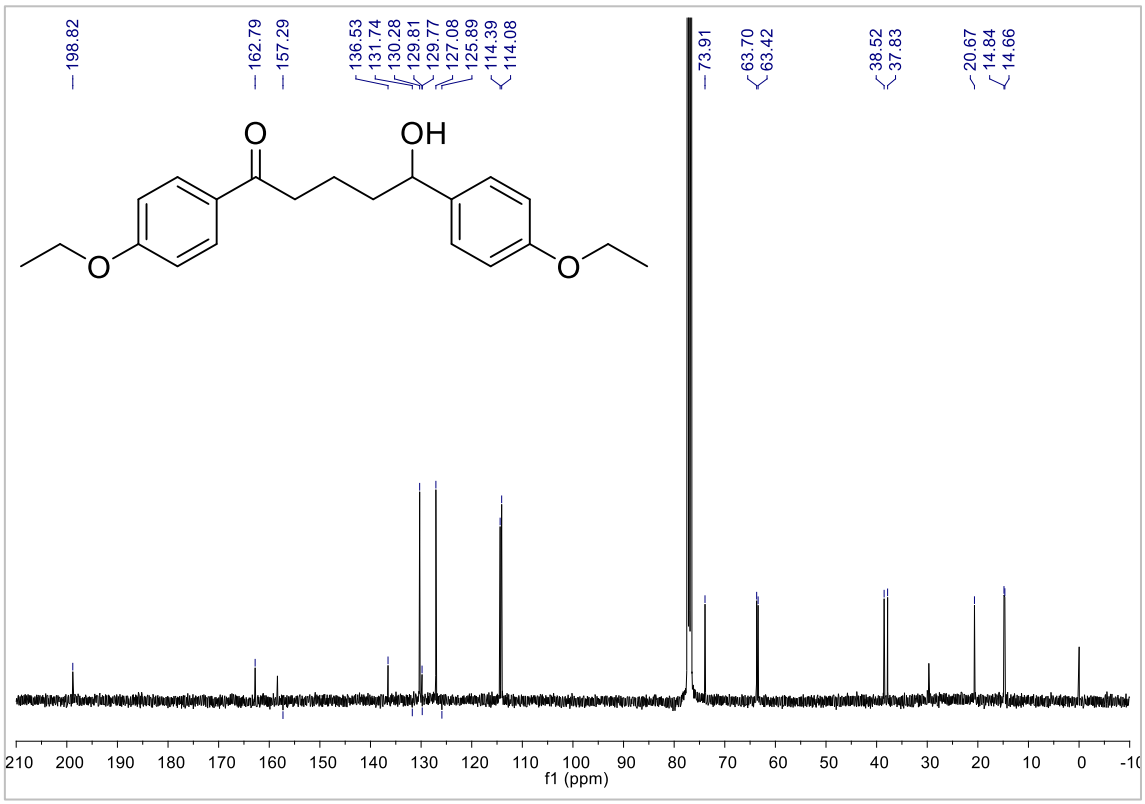
^{1}H NMR spectrum of **12** (400 MHz, $CDCl_3$).



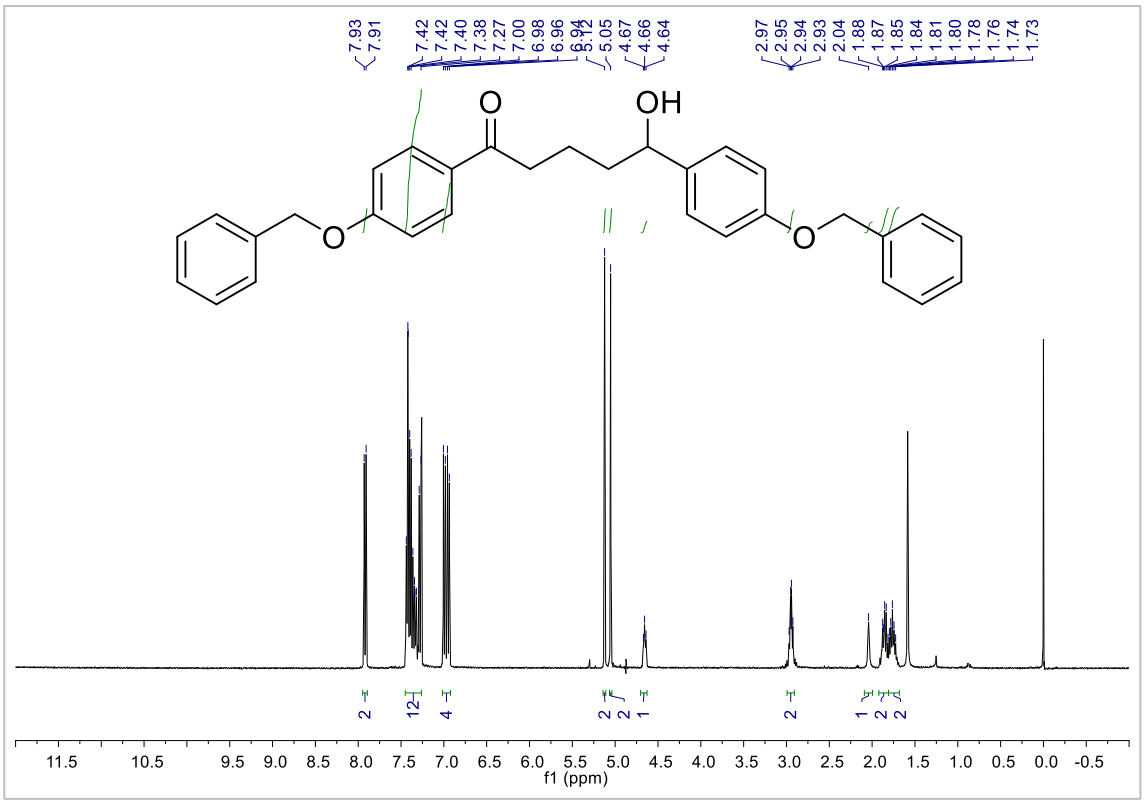
^{13}C NMR spectrum of **12** (100 MHz, $CDCl_3$).



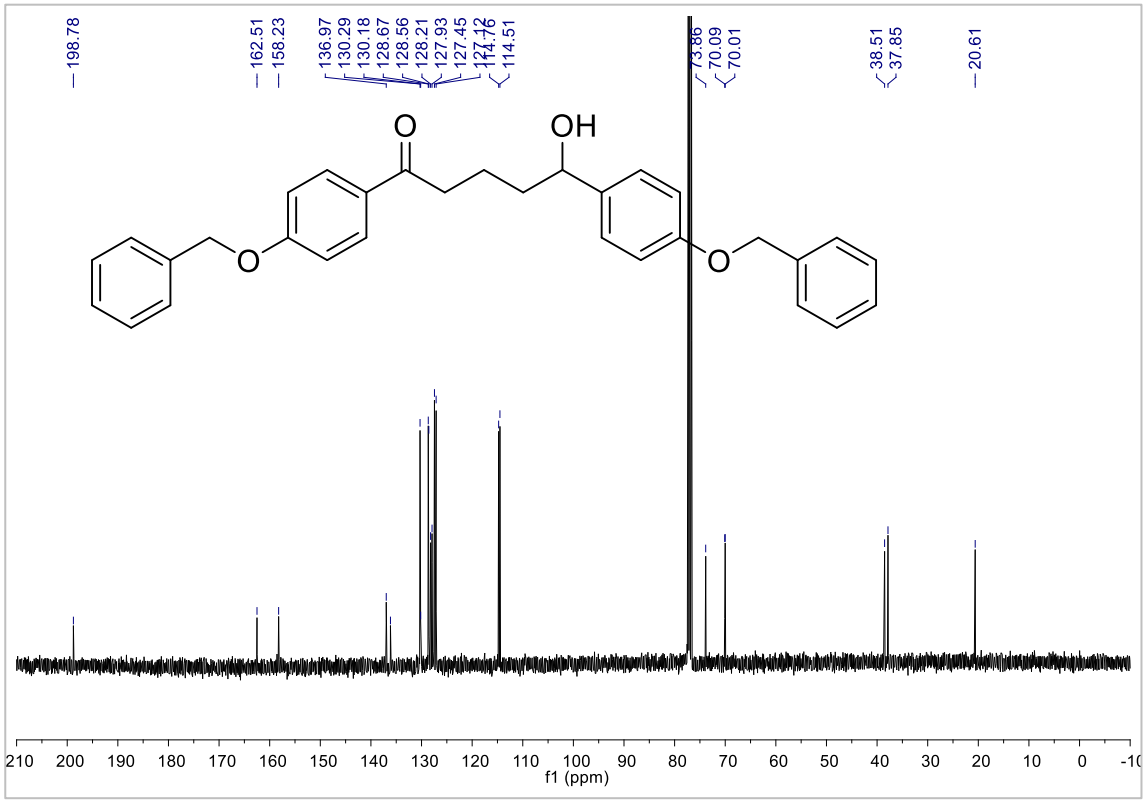
^{1}H NMR spectrum of **13** (400 MHz, $CDCl_3$).



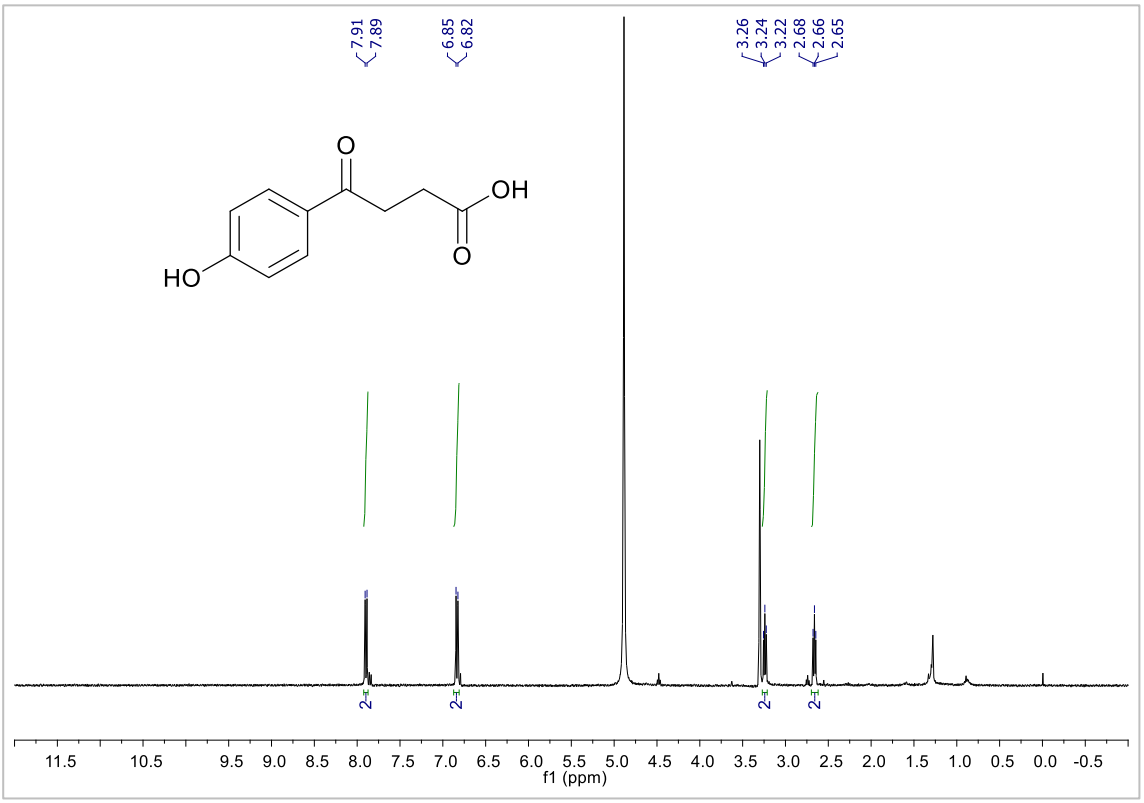
^{13}C NMR spectrum of **13** (100 MHz, $CDCl_3$).



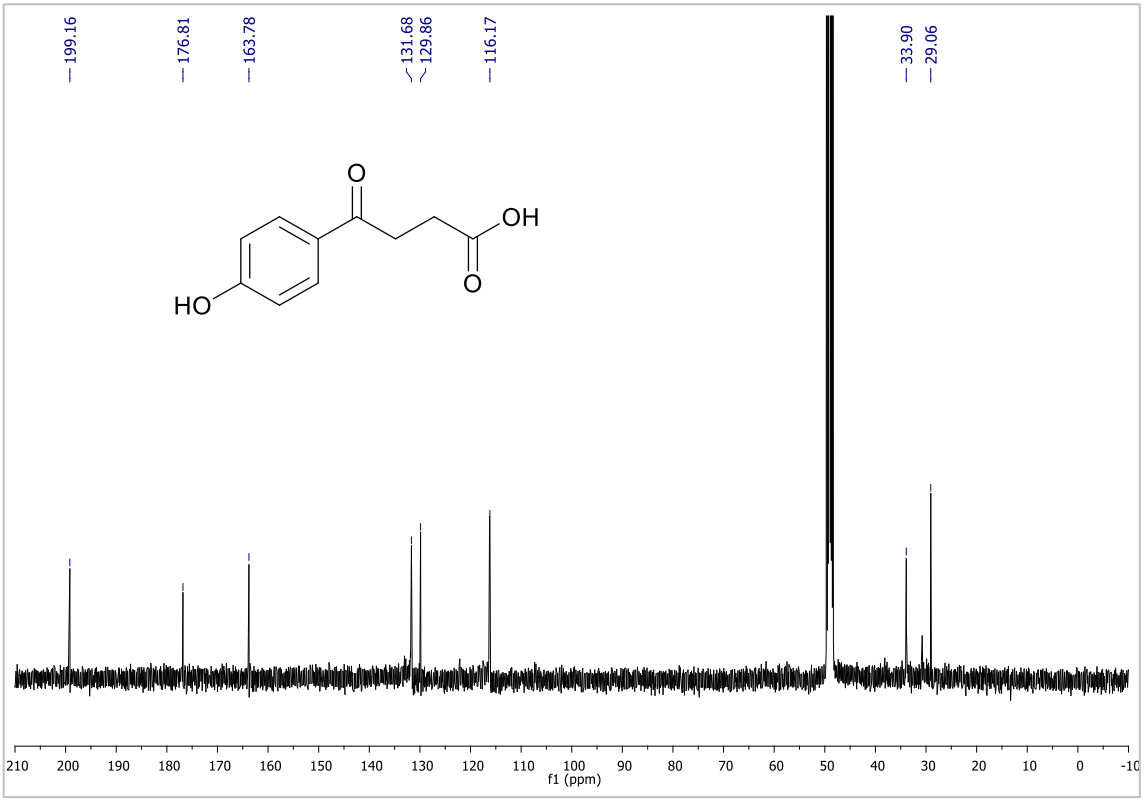
^{13}H NMR spectrum of **14** (400 MHz, $CDCl_3$).



^{13}C NMR spectrum of **14** (100 MHz, $CDCl_3$).

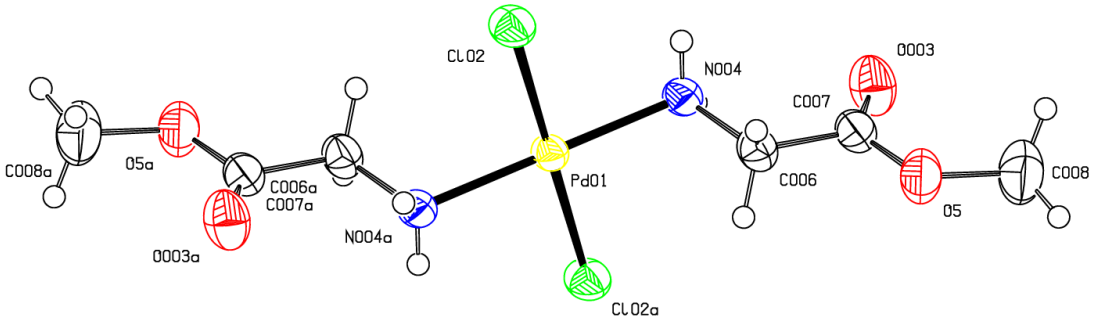


^{13}H NMR spectrum of **15** (400 MHz, $CDCl_3$).



^{13}C NMR spectrum of **15** (100 MHz, $CDCl_3$).

2. Crystal data and X-ray crystallographic structure of compund 1 (methyl ester).



Empirical formula C6H14Cl2N2O4Pd
Formula weight 355.51
Temperature/K 298.15
Crystal system monoclinic
Space group P21/c
a/Å 9.0537(3)
b/Å 12.1660(4)
c/Å 5.4933(2)
α/° 90
β/° 96.5990(10)
γ/° 90
Volume/Å3 601.06(4)
Z 2
ρcalcg/cm3 1.9642
μ/mm-1 1.985
F(000) 350.8
Crystal size/mm3 0.3 × 0.14 × 0.04
Radiation Mo Kα (λ = 0.71073)
2Θ range for data collection/° 5.64 to 56.06
Index ranges -11 ≤ h ≤ 11, -16 ≤ k ≤ 16, -7 ≤ l ≤ 7
Reflections collected 23919
Independent reflections 1443 [Rint = 0.0483, Rsigma = 0.0169]
Data/restraints/parameters 1443/0/79
Goodness-of-fit on F2 1.130
Final R indexes [I>=2σ (I)] R1 = 0.0247, wR2 = 0.0505
Final R indexes [all data] R1 = 0.0309, wR2 = 0.0536
Largest diff. peak/hole / e Å-3 0.40/-0.50

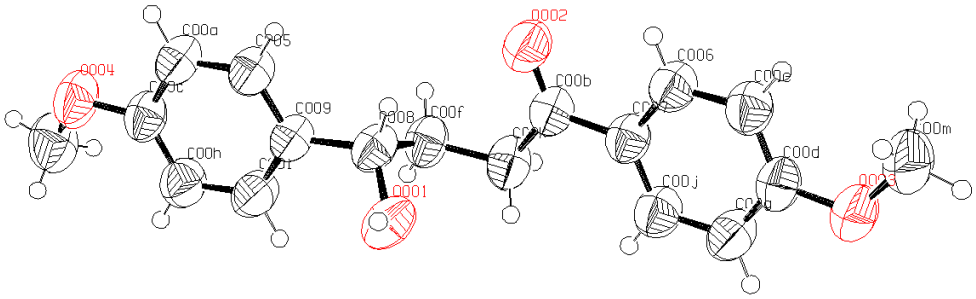
Bond Lengths for 1
Atom Atom Length/Å Atom Atom Length/Å
Pd01 Cl02 2.2947(7)
Pd01 Cl02-1 2.2947(7)
Pd01 N004 2.040(2)
O003 C007 1.195(4)

N004 C006 1.459(4)
O5 C007 1.328(4)
O5 C008 1.472(4)
Pd01 N004-1 2.040(2)
C006 C007 1.507(4)

Bond Angles for 1

Atom Atom Atom Angle/° Atom Atom Atom Angle/°
Cl021 Pd01 Cl02 180.0 C006 N004 Pd01 112.41(17)
N004 Pd01 Cl02 90.48(8) C008 O5 C007 117.4(3)
N004 Pd01 Cl021 89.52(8) C007 C006 N004 112.9(2)
N0041Pd01 Cl02 89.52(8) O5 C007 O003 124.9(3)
N0041Pd01 Cl021 90.48(8) C006 C007 O003 125.1(3)
N0041Pd01 N004 180.0 C006 C007 O5 110.0(2)

Crystal data and X-ray crystallographic structure of compund 5.



Empirical formula $C_{18}H_{20}O_4$
Formula weight 300.34
Temperature/K 273.15
Crystal system monoclinic
Space group P21
a/Å 11.1124(5)
b/Å 5.2113(2)
c/Å 13.3792(6)
α/° 90
β/° 93.648(2)
γ/° 90
Volume/Å3 773.22(6)
Z 2
ρcalcg/cm3 1.290
μ/mm-1 0.736
F(000) 320.0
Crystal size/mm3 0.3 × 0.1 × 0.04
Radiation CuKα (λ = 1.54178)
2Θ range for data collection/° 6.62 to 125.08

Index ranges -12 ≤ h ≤ 12, -5 ≤ k ≤ 5, -15 ≤ l ≤ 15
Reflections collected 18846
Independent reflections 2454 [Rint = 0.0703, Rsigma = 0.0402]
JAV_JC_11_0m
23/10/
2454/1/203
Goodness-of-fit on F2 1.072
Final R indexes [I>=2σ (I)] R1 = 0.0511, wR2 = 0.1338
Final R indexes [all data] R1 = 0.0584, wR2 = 0.1435
Largest diff. peak/hole / e Å-3 0.17/-0.13
Flack parameter 0.04(14).

Bond Lengths for 5

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	C00B	1.226(5)	C00D	C00G	1.387(6)
O002	C008	1.435(5)	C00E	C007	1.384(5)
O003	C00D	1.366(4)	C00F	C00K	1.528(5)
O003	C00M	1.428(6)	C00F	C008	1.518(6)
O004	C00C	1.379(4)	C00G	C00J	1.371(6)
O004	C00L	1.422(7)	C00H	C00I	1.383(6)
C00A	C00C	1.382(6)	C00I	C009	1.392(6)
C00A	C006	1.382(5)	C00J	C005	1.383(6)
C00B	C00K	1.501(6)	C005	C007	1.391(6)
C00B	C005	1.497(5)	C006	C009	1.380(5)
C00C	C00H	1.368(6)	C008	C009	1.503(5)

Bond Angles for 5

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C00D	O003	C00M	118.1(4)	C00C	C00H	C00I	120.2(4)
C00C	O004	C00L	116.8(4)	C00H	C00I	C009	121.5(4)
C006	C00A	C00C	119.9(4)	C00G	C00J	C005	121.3(4)
O001	C00B	C00K	121.3(4)	C00B	C00K	C00F	114.7(4)
O001	C00B	C005	120.2(4)	C00J	C005	C00B	123.7(4)
C005	C00B	C00K	118.5(4)	C00J	C005	C007	118.0(4)
O004	C00C	C00A	115.3(4)	C007	C005	C00B	118.2(4)
C00H	C00C	O004	125.2(4)	C009	C006	C00A	121.7(4)
C00H	C00C	C00A	119.5(4)	C00E	C007	C005	121.4(4)
O003	C00D	C00E	124.1(4)	O002	C008	C00F	107.8(3)
O003	C00D	C00G	116.0(4)	O002	C008	C009	111.5(3)
C00E	C00D	C00G	120.0(4)	C009	C008	C00F	112.4(3)
C00D	C00E	C007	119.3(4)	C00I	C009	C008	121.4(4)
C008	C00F	C00K	114.0(4)	C006	C009	C00I	117.2(3)
C00J	C00G	C00D	120.0(4)	C006	C009	C008	121.3(4)

3. Figures and Coordinates of structures of minima along the Catalytic Cycle.

Geometries along the catalytic cycle where calculated. Single points at the PBE0/TZDP(COSMO-DMF) over full optimizations at the PBE0/DZ level of theory where performed using the Amsterdam Density Functional software.[1] The final minimum geometries along the catalytic cycle where confirmed by calculation of frequencies.

Color code in figures: carbon atoms as grey spheres, nitrogen atoms as blue spheres, oxygen atoms as red spheres, hydrogen atoms as white spheres, palladium atoms as orange spheres, chlorine atoms as green spheres, iodine atoms as purple spheres.

Orbital energies obtained for the structure B)
(Observe the value of HOMO, -0.1615798267550 a.u.)

```
                        * R E S U L T S *
                         ******************

*** Setting up for NEW gradients in focky
*** Using FIT density in focky

Hartree-Fock exchange energy:   -212.667061628707

Hartree-Fock exchange energy:   -212.667061628707

Scaled ZORA Orbital Energies, per Irrep and Spin:
================================================
               Occup          E (au)          E (eV)     Diff (eV) with prev. cycle
               -----     --------------------    ------    --------------------------
A
        54     2.000    -0.27758236254402E+00     -7.553          6.03E-07

        55     2.000    -0.26391480935024E+00     -7.181         -4.62E-06

        56     2.000    -0.26319378959403E+00     -7.162          2.65E-06

        57     2.000    -0.26282260328150E+00     -7.152          4.24E-06

        58     2.000    -0.25319125167616E+00     -6.890          7.97E-07

        59     2.000    -0.19704457485430E+00     -5.362          7.13E-07

        60     2.000    -0.19688296347595E+00     -5.357          7.99E-07

        61     2.000    -0.18996638342079E+00     -5.169          7.51E-07

        62     2.000    -0.18983829531572E+00     -5.166          7.93E-07

        63     2.000    -0.16157982675508E+00     -4.397          7.65E-07

        64     0.000     0.11481474614491E-01      0.312

        65     0.000     0.28407103515336E-01      0.773

        66     0.000     0.30158997703452E-01      0.821

        67     0.000     0.42131354385244E-01      1.146

        68     0.000     0.44694194954064E-01      1.216

        69     0.000     0.55014895772756E-01      1.497

        70     0.000     0.72146537486032E-01      1.963

        71     0.000     0.86032407694840E-01      2.341

        72     0.000     0.99456272376864E-01      2.706

        73     0.000     0.10311295621141E+00      2.806

HOMO :     63 A          -0.16157982675508E+00
LUMO :     64 A           0.11481474614491E-01

 COSMO charges converged: Iteration #   34 Conv  3.148105E-09
 The total uncorrected surface charge :      1.90365020
 cosmo_calcen: solen (Hartrees) =   -0.289858

 Solvation energy (screening term,uncorrected) =   -181.888922 kcal/mol

 Solvation energy (dispersion and cavitation terms) =      1.349174 kcal/mol
 Solvation Energy Contributions (Hartrees)
        esola        esolb        esolc
    0.28985845    0.00000000   -0.57971690
 esol   -0.28985845
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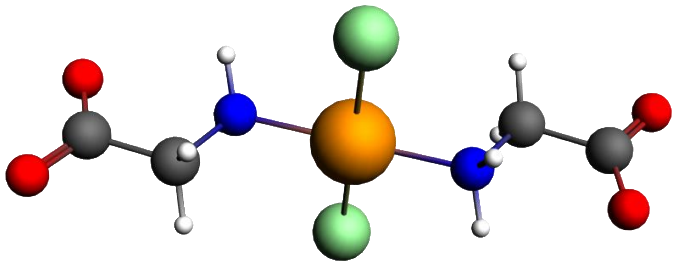
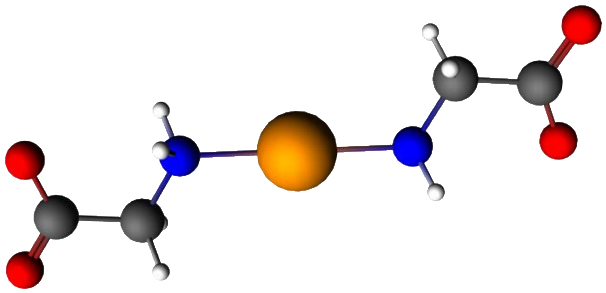


Compound **A** Coordinates (Cartesian)

==========

Atom	bohr			angstrom			Geometric Variables		
X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)			
1 Pd	-1.938416	8.935767	2.324136	-1.025765	4.728604	1.229880	1	2	3
2 C	3.621910	9.399524	1.293919	1.916632	4.974014	0.684712	4	5	6
3 C	5.946153	11.048082	0.555078	3.146569	5.846393	0.293735	7	8	9
4 N	1.237051	10.879944	1.240011	0.654619	5.757418	0.656185	10	11	12
5 O	8.036448	9.859519	0.419373	4.252705	5.217433	0.221923	13	14	15
6 O	5.499345	13.399499	0.184366	2.910128	7.090709	0.097562	16	17	18
7 H	3.882940	8.665515	3.201160	2.054763	4.585593	1.693981	19	20	21
8 H	0.958181	11.525397	-0.557848	0.507048	6.098977	-0.295200	22	23	24
9 H	1.477660	12.430619	2.365663	0.781944	6.578000	1.251855	25	26	27
10 H	-5.361120	5.473755	2.216569	-2.836983	2.896586	1.172958	28	29	30
11 H	3.444712	7.821276	-0.016479	1.822863	4.138841	-0.008720	31	32	33
12 C	-7.482989	8.471579	3.434041	-3.959827	4.482967	1.817216	34	35	36
13 C	-9.796964	6.830240	4.220224	-5.184330	3.614407	2.233246	37	38	39
14 N	-5.107608	6.977358	3.401262	-2.702830	3.692259	1.799870	40	41	42
15 O	-11.891388	8.013966	4.336796	-6.292652	4.240808	2.294934	43	44	45
16 O	-9.337430	4.491901	4.650870	-4.941155	2.377012	2.461134	46	47	48
17 H	-7.256342	10.028423	4.762971	-3.839891	5.306813	2.520456	49	50	51
18 H	-7.793817	9.237588	1.547196	-4.124311	4.888321	0.818741	52	53	54
19 H	-4.814973	6.260790	5.169798	-2.547974	3.313067	2.735739	55	56	57
20 Cl	-1.095880	9.936826	6.686076	-0.579915	5.258342	3.538119	58	59	60
21 Cl	-2.754809	7.893776	-2.036454	-1.457782	4.177206	-1.077645	61	62	63



Compound **B**: Coordinates (Cartesian)

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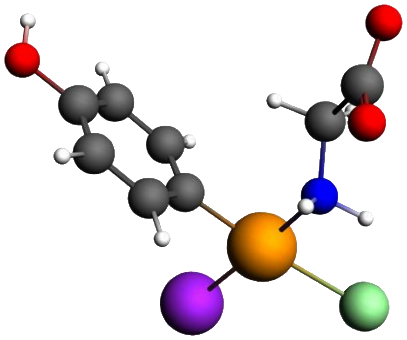
Atom	bohr			angstrom			Geometric Variables		
X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)			
1 Pd	-1.942665	9.014107	2.372684	-1.028014	4.770060	1.255571	1	2	3
2 C	3.505334	10.648020	0.830225	1.854943	5.634689	0.439336	4	5	6
3 C	6.346135	10.951985	1.509580	3.358230	5.795541	0.798836	7	8	9
4 N	1.969201	9.541420	2.901869	1.042056	5.049102	1.535603	10	11	12
5 O	7.729817	11.872497	-0.247430	4.090443	6.282655	-0.130934	13	14	15
6 O	7.010762	10.262349	3.737446	3.709936	5.430601	1.977771	16	17	18
7 H	3.328363	9.447725	-0.834707	1.761294	4.999521	-0.441708	19	20	21
8 H	2.206440	10.639512	4.469450	1.167598	5.630187	2.365131	22	23	24
9 H	2.725485	7.826913	3.356946	1.442265	4.141824	1.776419	25	26	27
10 H	-6.614142	10.214081	1.454423	-3.500053	5.405059	0.769647	28	29	30
11 H	2.723459	12.491317	0.344749	1.441193	6.610120	0.182433	31	32	33
12 C	-7.374899	7.304684	3.887275	-3.902629	3.865472	2.057057	34	35	36
13 C	-10.209609	6.972389	3.196042	-5.402692	3.689630	1.691272	37	38	39
14 N	-5.854486	8.485302	1.844997	-3.098061	4.490229	0.976330	40	41	42
15 O	-11.591126	6.035145	4.945820	-6.133760	3.193661	2.617215	43	44	45
16 O	-10.870783	7.653043	0.964338	-5.752570	4.049816	0.510305	46	47	48
17 H	-6.565171	5.461406	4.325660	-3.474139	2.890052	2.289040	49	50	51
18 H	-7.217271	8.464147	5.582558	-3.819216	4.479034	2.954163	52	53	54
19 H	-6.103757	7.440895	0.242733	-3.229969	3.937552	0.128449	55	56	57



Compound **C**: Coordinates (Cartesian)

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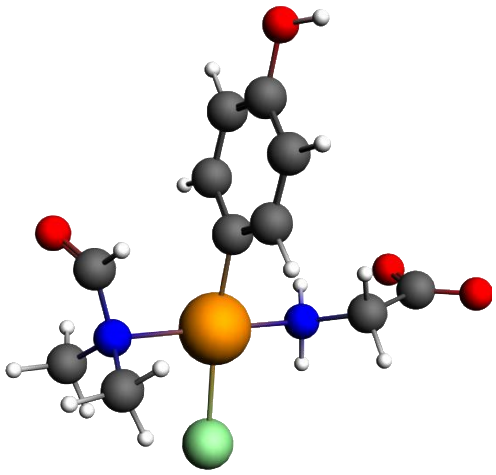
Atom	bohr			angstrom			Geometric Variables		
X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)			
1 Pd	-1.245896	0.470207	-0.551269	-0.659300	0.248823	-0.291719	1	2	3
2 C	4.432511	-1.041360	-0.951261	2.345584	-0.551064	-0.503386	4	5	6
3 C	7.223960	-0.124124	-0.923506	3.822755	-0.065684	-0.488698	7	8	9
4 N	2.666411	0.959911	-0.098016	1.411004	0.507963	-0.051868	10	11	12
5 O	7.543645	2.278123	-0.824572	3.991925	1.205531	-0.436345	13	14	15
6 O	8.894093	-1.860034	-1.065961	4.706551	-0.984288	-0.564082	16	17	18
7 H	4.219568	-2.694594	0.256019	2.232899	-1.425918	0.135480	19	20	21
8 H	3.296010	2.612513	-0.886871	1.744173	1.382482	-0.469312	22	23	24
9 H	2.766475	1.172402	1.823108	1.463955	0.620408	0.964747	25	26	27
10 I	-6.251136	-0.153157	-1.315806	-3.307959	-0.081047	-0.696295	28	29	30
11 H	3.940103	-1.566366	-2.884948	2.085013	-0.828885	-1.526649	31	32	33
12 C	-0.689016	-0.014491	-4.234732	-0.364611	-0.007668	-2.240924	34	35	36
13 C	-0.877218	-2.410984	-5.349647	-0.464204	-1.275838	-2.830911	37	38	39
14 C	-0.278641	-2.802378	-7.892339	-0.147451	-1.482955	-4.176446	40	41	42
15 C	0.519145	-0.778179	-9.359561	0.274720	-0.411794	-4.952866	43	44	45
16 C	0.697971	1.622666	-8.331668	0.369350	0.858678	-4.408929	46	47	48
17 C	0.089397	1.988263	-5.787676	0.047307	1.052143	-3.062706	49	50	51
18 H	-1.527070	-3.992433	-4.225707	-0.808091	-2.112705	-2.236148	52	53	54
19 H	-0.469934	-4.673013	-8.717149	-0.248678	-2.472852	-4.612917	55	56	57
20 O	1.155981	-1.063467	-11.967274	0.611719	-0.562762	-6.332809	58	59	60
21 H	1.335845	3.161964	-9.520503	0.706899	1.673239	-5.038033	61	62	63
22 H	0.243388	3.874344	-5.004894	0.128795	2.050215	-2.648476	64	65	66
23 H	1.577577	-2.832492	-12.324564	0.834818	-1.498890	-6.521878	67	68	69

24 Cl	-1.402871	1.118894	4.142911	-0.742367	0.592093	2.192334	70	71	72



Compound D: Coordinates (Cartesian)

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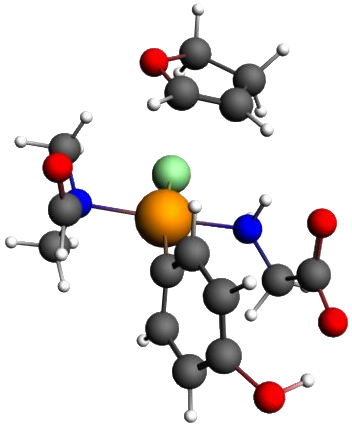
Atom	bohr			angstrom			Geometric Variables		
X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)			
1 Pd	-0.215629	0.971185	0.072629	-0.114106	0.513929	0.038434	1	2	3
2 C	5.198959	-0.713787	-1.334519	2.751171	-0.377720	-0.706197	4	5	6
3 C	6.941461	-3.095332	-1.411134	3.673263	-1.637979	-0.746740	7	8	9
4 N	2.936602	-1.265980	0.236993	1.553983	-0.669928	0.125411	10	11	12
5 O	5.868457	-5.146390	-0.688680	3.105454	-2.723352	-0.364434	13	14	15
6 O	9.160176	-2.724079	-2.235508	4.847356	-1.441521	-1.182980	16	17	18
7 H	4.599250	-0.322380	-3.263484	2.433818	-0.170596	-1.726961	19	20	21
8 H	3.425717	-1.145631	2.104891	1.812811	-0.606242	1.113861	22	23	24
9 H	2.553191	-3.145500	-0.114512	1.351091	-1.664527	-0.060597	25	26	27
10 Cl	0.712249	2.249110	4.493869	0.376906	1.190178	2.378053	28	29	30
11 H	6.214805	0.901706	-0.568210	3.288733	0.477162	-0.300684	31	32	33
12 C	-0.518610	0.020369	-3.578148	-0.274436	0.010779	-1.893474	34	35	36
13 C	0.731214	1.483334	-5.392017	0.386942	0.784946	-2.853333	37	38	39
14 C	0.645900	0.855555	-7.955088	0.341796	0.452740	-4.209651	40	41	42
15 C	-0.689215	-1.275242	-8.710425	-0.364717	-0.674829	-4.609358	43	44	45
16 C	-1.953208	-2.755176	-6.952584	-1.033593	-1.457977	-3.679149	46	47	48
17 C	-1.867841	-2.099564	-4.402921	-0.988419	-1.111041	-2.329926	49	50	51
18 H	1.824227	3.121758	-4.823528	0.965339	1.651963	-2.552501	52	53	54
19 H	1.636622	2.010707	-9.329649	0.866063	1.064020	-4.937038	55	56	57

20 O	-0.862401	-2.033538	-11.260720	-0.456363	-1.076102	-5.958916	58	59	60
21 H	-2.964682	-4.407468	-7.607566	-1.568842	-2.332332	-4.025751	61	62	63
22 H	-2.875767	-3.264920	-3.054943	-1.521791	-1.727721	-1.616606	64	65	66
23 H	0.431194	-1.216931	-12.308299	0.228178	-0.643972	-6.513271	67	68	69
24 C	-4.914720	2.674875	-2.256571	-2.600758	1.415483	-1.194126	70	71	72
25 C	-5.190121	2.590626	2.310645	-2.746493	1.370900	1.222741	73	74	75
26 O	-6.819575	1.345831	-2.364330	-3.608764	0.712183	-1.251150	76	77	78
27 H	-4.044500	3.516325	-3.923481	-2.140257	1.860759	-2.076217	79	80	81
28 H	-5.705867	0.606067	2.190392	-3.019415	0.320717	1.159106	82	83	84
29 H	-6.921925	3.724924	2.366162	-3.662925	1.971145	1.252119	85	86	87
30 H	-4.031467	2.905204	3.974791	-2.133360	1.537368	2.103369	88	89	90
31 H	-1.494468	6.085964	1.797223	-0.790839	3.220553	0.951050	91	92	93
32 H	-1.577827	6.287673	-1.545541	-0.834950	3.327294	-0.817865	94	95	96
33 H	-4.272516	7.258025	0.252796	-2.260918	3.840782	0.133774	97	98	99
34 N	-3.682476	3.279642	0.048194	-1.948682	1.735512	0.025503	100	101	102
35 C	-2.700427	5.912650	0.140499	-1.429004	3.128840	0.074349	103	104	105

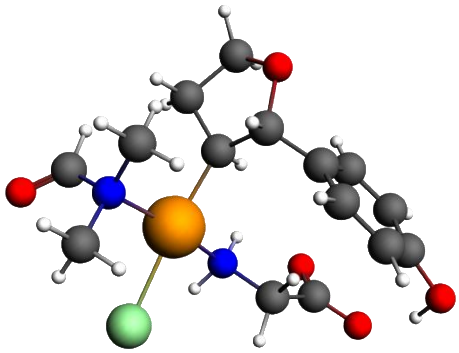


Compound **E**: Coordinates (Cartesian)

==========

Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.668986	1.132952	-0.111027	-0.354012	0.599533	-0.058753	1	2	3
2 C	4.755917	-0.868769	-1.859966	2.516723	-0.459733	-0.984252	4	5	6
3 C	4.651418	-3.349158	-3.438470	2.461425	-1.772298	-1.819560	7	8	9
4 N	2.723830	-0.909281	0.091892	1.441389	-0.481171	0.048627	10	11	12
5 O	3.418843	-5.158152	-2.419881	1.809174	-2.729577	-1.280546	13	14	15
6 O	5.826921	-3.320844	-5.545460	3.083474	-1.757315	-2.934531	16	17	18
7 H	4.583259	0.752126	-3.100739	2.425356	0.398008	-1.640840	19	20	21
8 H	3.354715	-0.356145	1.829104	1.775239	-0.188464	0.967920	22	23	24
9 H	2.166070	-2.781413	0.137624	1.146235	-1.471860	0.072827	25	26	27
10 Cl	0.015653	2.022192	4.478561	0.008283	1.070098	2.369953	28	29	30
11 H	6.604789	-0.812767	-0.931407	3.495104	-0.430098	-0.492879	31	32	33
12 C	-0.463107	0.660936	-3.863514	-0.245066	0.349752	-2.044483	34	35	36
13 C	0.878720	2.453908	-5.274394	0.464998	1.298552	-2.791089	37	38	39
14 C	2.095540	1.751062	-7.510617	1.108912	0.926622	-3.974447	40	41	42
15 C	1.949866	-0.742876	-8.315508	1.031825	-0.393113	-4.400377	43	44	45
16 C	0.288160	-2.411227	-7.160041	0.152488	-1.275966	-3.788930	46	47	48
17 C	-0.911342	-1.710421	-4.925026	-0.482261	-0.905116	-2.606212	49	50	51
18 H	1.194191	4.342724	-4.537962	0.631939	2.298071	-2.401386	52	53	54
19 H	3.333672	3.039273	-8.508717	1.764103	1.608314	-4.502619	55	56	57
20 O	3.733904	-1.673331	-10.059474	1.975897	-0.885488	-5.323245	58	59	60
21 H	0.164993	-4.328721	-7.858692	0.087310	-2.290661	-4.158641	61	62	63

22 H	-2.010640	-3.105506	-3.916232	-1.063985	-1.643363	-2.072381	64	65	66
23 H	4.973596	-2.626346	-8.978850	2.631914	-1.389803	-4.751403	67	68	69
24 C	-5.363748	1.997169	-2.511659	-2.838373	1.056856	-1.329113	70	71	72
25 C	-5.767565	2.601895	2.028385	-3.052064	1.376864	1.073375	73	74	75
26 O	-6.988626	0.334596	-2.433663	-3.698221	0.177061	-1.287839	76	77	78
27 H	-4.664983	2.800169	-4.274073	-2.468603	1.481785	-2.261742	79	80	81
28 H	-6.049750	0.579213	2.271185	-3.201390	0.306506	1.201859	82	83	84
29 H	-7.608947	3.536498	1.856438	-4.026481	1.871434	0.982384	85	86	87
30 H	-4.711925	3.334489	3.628006	-2.493443	1.764535	1.919858	88	89	90
31 H	-2.380562	6.317675	0.995796	-1.259739	3.343170	0.526953	91	92	93
32 H	-2.513043	6.038202	-2.344482	-1.329845	3.195279	-1.240646	94	95	96
33 H	-5.270516	6.967833	-0.626533	-2.789037	3.687218	-0.331547	97	98	99
34 N	-4.273213	3.083831	-0.300410	-2.261287	1.631893	-0.158970	100	101	102
35 C	-3.568952	5.784370	-0.595216	-1.888608	3.060957	-0.314975	103	104	105
36 O	-5.342903	-3.437599	3.107794	-2.827343	-1.819099	1.644574	106	107	108
37 H	-0.840420	-7.084321	4.678754	-0.444731	-3.748861	2.475890	109	110	111
38 C	-4.235482	-4.337099	0.862237	-2.241320	-2.295094	0.456276	112	113	114
39 C	-3.481721	-3.905009	5.182727	-1.842447	-2.066442	2.742581	115	116	117
40 C	-1.943196	-5.318084	1.159657	-1.028295	-2.814209	0.613664	118	119	120
41 C	-1.180817	-5.190058	3.921416	-0.624861	-2.746461	2.075124	121	122	123
42 H	-4.437139	-5.104783	6.554861	-2.348033	-2.701335	3.468683	124	125	126
43 H	-5.406821	-4.071373	-0.781961	-2.861166	-2.154478	-0.413796	127	128	129
44 H	-0.736697	-6.074510	-0.307599	-0.389843	-3.214492	-0.162775	130	131	132
45 H	0.532143	-4.070816	4.202763	0.281598	-2.154183	2.224006	133	134	135
46 H	-3.014023	-2.070461	5.982734	-1.594952	-1.095641	3.165926	136	137	138



Compound **F**: Coordinates (Cartesian)

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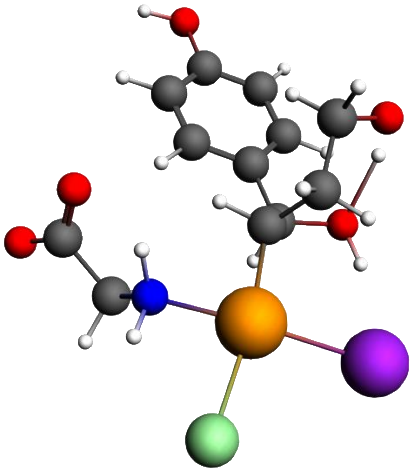
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.456903	0.444844	-0.203521	-0.241783	0.235401	-0.107699	1	2	3
2 C	3.794581	-3.305745	-1.044519	2.008006	-1.749325	-0.552736	4	5	6
3 C	4.301124	-6.054439	-1.920082	2.276057	-3.203871	-1.016064	7	8	9
4 N	1.177770	-3.081370	-0.017596	0.623249	-1.630591	-0.009312	10	11	12
5 O	2.444534	-7.576182	-1.785161	1.293592	-4.009143	-0.944666	13	14	15
6 O	6.531708	-6.486940	-2.763653	3.456431	-3.432741	-1.462462	16	17	18
7 H	4.011229	-2.051541	-2.657934	2.122651	-1.085629	-1.406518	19	20	21
8 H	1.234303	-3.387038	1.890720	0.653165	-1.792343	1.000526	22	23	24
9 H	0.182871	-4.546779	-0.821063	0.096771	-2.406052	-0.434488	25	26	27
10 Cl	1.996030	1.031320	3.762863	1.056253	0.545751	1.991221	28	29	30
11 H	5.143794	-2.739874	0.402897	2.721978	-1.449879	0.213204	31	32	33
12 C	1.005983	-0.994278	-6.811203	0.532343	-0.526149	-3.604333	34	35	36
13 C	3.211181	0.447355	-6.931099	1.699284	0.236730	-3.667780	37	38	39
14 C	5.567202	-0.710835	-7.161890	2.946036	-0.376158	-3.789909	40	41	42
15 C	5.717143	-3.333841	-7.276330	3.025382	-1.764193	-3.850468	43	44	45
16 C	3.507238	-4.765424	-7.438507	1.855951	-2.521754	-3.936289	46	47	48
17 C	1.173812	-3.600545	-7.196461	0.621154	-1.905326	-3.808203	49	50	51
18 H	3.104003	2.485406	-6.744270	1.642568	1.315220	-3.568914	52	53	54
19 H	7.304382	0.366627	-7.123920	3.865313	0.194010	-3.769816	55	56	57
20 O	8.047372	-4.524958	-7.028853	4.258486	-2.394505	-3.719509	58	59	60
21 H	3.653214	-6.797779	-7.602264	1.933197	-3.597230	-4.022945	61	62	63
22 H	-0.532923	-4.727036	-7.252197	-0.282011	-2.501440	-3.837697	64	65	66
23 H	7.926127	-5.586908	-5.416777	4.194326	-2.956464	-2.866435	67	68	69
24 C	-4.346646	3.552664	1.310311	-2.300146	1.879989	0.693386	70	71	72

25 C	-0.465172	5.996890	1.580333	-0.246158	3.173418	0.836276	73	74	75
26 O	-4.780803	4.003170	3.548657	-2.529892	2.118386	1.877868	76	77	78
27 H	-5.690510	2.582456	0.089326	-3.011288	1.366577	0.047269	79	80	81
28 H	-0.252559	5.232100	3.468716	-0.133649	2.768708	1.835565	82	83	84
29 H	-1.343428	7.870552	1.665638	-0.710912	4.164917	0.881418	85	86	87
30 H	1.385075	6.103463	0.696644	0.732950	3.229813	0.368648	88	89	90
31 H	-0.703809	5.527586	-3.455694	-0.372440	2.925073	-1.828675	91	92	93
32 H	-3.759589	4.172775	-3.599006	-1.989489	2.208137	-1.904512	94	95	96
33 H	-3.354170	7.259701	-2.323775	-1.774951	3.841668	-1.229689	97	98	99
34 N	-2.087286	4.292779	0.051896	-1.104544	2.271641	0.027462	100	101	102
35 C	-2.514459	5.373375	-2.500288	-1.330594	2.843467	-1.323095	103	104	105
36 O	-3.542268	-0.503927	-7.812288	-1.874488	-0.266667	-4.134085	106	107	108
37 C	-1.445640	0.173696	-6.016154	-0.765000	0.091916	-3.183612	109	110	111
38 C	-2.359934	-0.794635	-3.427678	-1.248823	-0.420503	-1.813849	112	113	114
39 C	-5.256173	-0.695871	-3.641535	-2.781447	-0.368239	-1.927017	115	116	117
40 C	-5.657978	-1.589353	-6.365857	-2.994073	-0.841049	-3.368667	118	119	120
41 H	-6.179290	-1.918350	-2.257942	-3.269939	-1.015147	-1.194851	121	122	123
42 H	-1.283356	2.223964	-6.116141	-0.679123	1.176871	-3.236522	124	125	126
43 H	-7.394691	-0.905076	-7.237683	-3.913102	-0.478946	-3.830017	127	128	129
44 H	-1.902494	-2.812548	-3.405861	-1.006756	-1.488336	-1.802304	130	131	132
45 H	-6.033731	1.209639	-3.461275	-3.192913	0.640113	-1.831628	133	134	135
46 H	-5.584428	-3.652024	-6.487235	-2.955152	-1.932568	-3.432897	136	137	13



Compound **G**: Coordinates (Cartesian)

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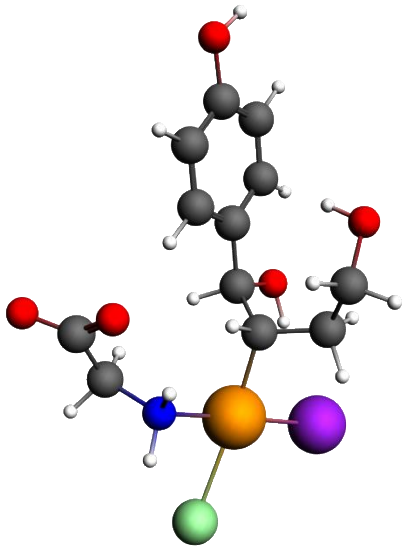
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.179924	0.985276	0.424943	-0.095212	0.521386	0.224870	1	2	3
2 C	4.130186	-2.808720	1.042423	2.185600	-1.486311	0.551627	4	5	6
3 C	4.660735	-5.589026	0.270168	2.466355	-2.957585	0.142967	7	8	9
4 N	1.408174	-2.425529	1.638955	0.745174	-1.283534	0.867298	10	11	12
5 O	2.701863	-6.856533	-0.425777	1.429764	-3.628321	-0.225312	13	14	15
6 O	6.957743	-6.291294	0.305748	3.681879	-3.329210	0.161795	16	17	18
7 H	4.686055	-1.597162	-0.532766	2.479754	-0.845182	-0.281928	19	20	21
8 H	1.142709	-2.229394	3.544101	0.604696	-1.179745	1.875457	22	23	24
9 H	0.495936	-4.005959	0.968772	0.262438	-2.119862	0.512652	25	26	27
10 Cl	0.344563	2.186262	5.042908	0.182335	1.156920	2.668592	28	29	30
11 H	5.281848	-2.292449	2.668549	2.795033	-1.213112	1.412135	31	32	33
12 C	2.151072	-1.510334	-7.006905	1.138298	-0.799234	-3.707894	34	35	36
13 C	2.931808	-3.922921	-6.262467	1.551446	-2.075920	-3.313955	37	38	39
14 C	3.881148	-5.634827	-8.023728	2.053815	-2.981822	-4.245974	40	41	42
15 C	4.046966	-4.943346	-10.547568	2.141562	-2.615906	-5.581533	43	44	45
16 C	3.283737	-2.562253	-11.332521	1.737679	-1.355886	-5.996912	46	47	48
17 C	2.352512	-0.855274	-9.558973	1.244896	-0.452592	-5.058391	49	50	51
18 H	2.814856	-4.552096	-4.316654	1.489558	-2.408866	-2.284275	52	53	54
19 H	4.488411	-7.481467	-7.373671	2.375165	-3.959022	-3.901979	55	56	57
20 O	4.992776	-6.603150	-12.424839	2.642063	-3.494236	-6.574942	58	59	60
21 H	3.425518	-2.079460	-13.314914	1.812706	-1.100403	-7.045949	61	62	63
22 H	1.769966	1.014334	-10.137979	0.936626	0.536763	-5.364788	64	65	66

23 H	5.510810	-8.212643	-11.664341	2.916195	-4.345944	-6.172503	67	68	69
24 H	-2.686931	-3.402411	-6.920601	-1.421863	-1.800478	-3.662224	70	71	72
25 O	-3.904355	0.023651	-8.540601	-2.066096	0.012516	-4.519491	73	74	75
26 C	1.232739	0.398553	-5.060547	0.652338	0.210905	-2.677926	76	77	78
27 C	-0.622700	-0.668070	-3.095191	-0.329519	-0.353527	-1.637905	79	80	81
28 C	-3.411770	-0.693313	-3.893445	-1.805431	-0.366885	-2.060323	82	83	84
29 C	-3.989615	-1.846776	-6.499688	-2.111213	-0.977272	-3.439487	85	86	87
30 H	-4.423016	-1.776088	-2.444693	-2.340560	-0.939865	-1.293676	88	89	90
31 H	2.910243	1.124944	-4.083181	1.540034	0.595295	-2.160726	91	92	93
32 H	-5.923308	-2.568906	-6.543123	-3.134480	-1.359406	-3.462471	94	95	96
33 H	-0.071018	-2.628207	-2.744617	-0.037581	-1.390787	-1.452389	97	98	99
34 H	-4.221440	1.208290	-3.861894	-2.233890	0.639399	-2.043626	100	101	102
35 I	-1.789159	5.640487	-1.079724	-0.946782	2.984817	-0.571365	103	104	105
36 H	-0.380411	3.841735	-5.250275	-0.201305	2.032959	-2.778326	106	107	108
37 O	0.128278	2.520410	-6.486541	0.067882	1.333743	-3.432529	109	110	111
38 H	-2.462008	1.179722	-8.187910	-1.302838	0.624282	-4.332855	112	113	114



Compound **I**: Coordinates (Cartesian)

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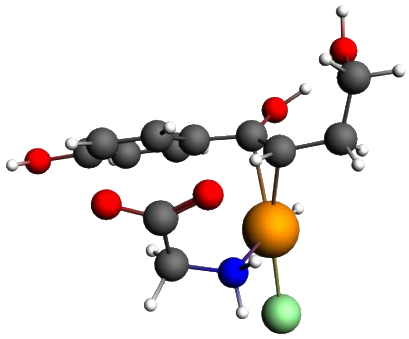
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.325607	0.975521	0.411512	-0.172304	0.516223	0.217763	1	2	3
2 C	3.534753	-3.282539	1.393766	1.870511	-1.737045	0.737549	4	5	6
3 C	3.893879	-5.945432	0.217745	2.060552	-3.146187	0.115225	7	8	9
4 N	0.807653	-2.631813	1.598984	0.427392	-1.392696	0.846146	10	11	12
5 O	1.952049	-6.831112	-0.955354	1.032980	-3.614869	-0.505551	13	14	15
6 O	6.068781	-6.932509	0.459078	3.211461	-3.668526	0.242933	16	17	18
7 H	4.508108	-1.921998	0.188506	2.385588	-1.017078	0.099753	19	20	21
8 H	0.257635	-2.502683	3.448073	0.136335	-1.324363	1.824642	22	23	24
9 H	-0.139298	-4.052277	0.669500	-0.073713	-2.144373	0.354284	25	26	27
10 Cl	-0.435556	1.794950	5.158358	-0.230486	0.949847	2.729685	28	29	30
11 H	4.418619	-3.219197	3.253029	2.338232	-1.703526	1.721429	31	32	33
12 C	2.593695	-1.498412	-6.908023	1.372524	-0.792926	-3.655569	34	35	36
13 C	3.013838	-0.467527	-9.299635	1.594854	-0.247405	-4.921155	37	38	39
14 C	3.558951	-2.022172	-11.362853	1.883316	-1.070087	-6.012963	40	41	42
15 C	3.712073	-4.616157	-11.014474	1.964344	-2.442765	-5.828608	43	44	45
16 C	3.338543	-5.676497	-8.642429	1.766681	-3.003873	-4.573376	46	47	48
17 C	2.783855	-4.125755	-6.593258	1.473153	-2.183255	-3.489002	49	50	51
18 H	2.907122	1.563553	-9.492485	1.538383	0.827397	-5.023207	52	53	54
19 H	3.872671	-1.191279	-13.211919	2.049329	-0.630398	-6.991446	55	56	57
20 O	4.262942	-6.296498	-13.025027	2.255852	-3.331963	-6.892548	58	59	60

21	H	3.497951	-7.701464	-8.414056	1.851036	-4.075439	-4.452526	61	62	63
22	H	2.511342	-5.003576	-4.752990	1.328945	-2.647778	-2.515174	64	65	66
23	H	4.373694	-5.380274	-14.632298	2.314459	-2.847119	-7.743078	67	68	69
24	H	-3.530112	-3.688813	-5.717249	-1.868055	-1.952036	-3.025438	70	71	72
25	O	-3.141087	-1.529632	-9.045443	-1.662191	-0.809446	-4.786643	73	74	75
26	C	2.039823	0.208635	-4.669533	1.079428	0.110405	-2.471010	76	77	78
27	C	-0.403372	-0.446603	-3.248166	-0.213455	-0.236332	-1.718855	79	80	81
28	C	-2.889930	0.214832	-4.590820	-1.529285	0.113684	-2.429357	82	83	84
29	C	-3.960466	-1.780342	-6.399074	-2.095788	-0.942116	-3.386244	85	86	87
30	H	-4.313195	0.519894	-3.118964	-2.282445	0.275116	-1.650484	88	89	90
31	H	3.627420	-0.012055	-3.354359	1.919548	-0.006379	-1.775051	91	92	93
32	H	-6.006612	-1.571837	-6.539442	-3.178562	-0.831780	-3.460524	94	95	96
33	H	-0.369794	-2.487517	-2.901580	-0.195686	-1.316337	-1.535450	97	98	99
34	H	-2.726296	2.006243	-5.607823	-1.442693	1.061658	-2.967532	100	101	102
35	I	-1.511834	5.811937	-0.894554	-0.800028	3.075545	-0.473378	103	104	105
36	H	1.330536	3.923236	-4.334940	0.704089	2.076087	-2.293952	106	107	108
37	O	2.057616	2.790923	-5.637597	1.088844	1.476893	-2.983288	109	110	111
38	H	-1.287202	-1.571634	-9.124523	-0.681158	-0.831673	-4.828490	112	113	114



Structure **K** (X=Cl) Coordinates (Cartesian)

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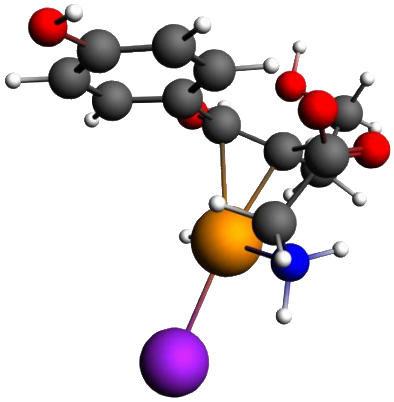
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-2.350742	3.293786	-7.221541	-1.243959	1.742997	-3.821475	1	2	3
2 C	1.496148	5.853679	-3.300682	0.791727	3.097633	-1.746646	4	5	6
3 C	1.500228	4.385233	-0.774619	0.793886	2.320566	-0.409911	7	8	9
4 N	-1.103486	6.006578	-4.335222	-0.583940	3.178544	-2.294101	10	11	12
5 O	-0.670008	3.606845	0.007665	-0.354553	1.908660	0.004056	13	14	15
6 O	3.648020	4.044016	0.242856	1.930449	2.140001	0.128514	16	17	18
7 H	2.742638	4.900623	-4.637195	1.451341	2.593298	-2.453898	19	20	21
8 H	-1.408704	7.626424	-5.335617	-0.745454	4.035730	-2.823487	22	23	24
9 H	-2.312862	5.835820	-2.831788	-1.223914	3.088183	-1.498518	25	26	27
10 Cl	-2.584096	6.839398	-10.060103	-1.367445	3.619253	-5.323577	28	29	30
11 H	2.265047	7.739008	-2.927478	1.198611	4.095307	-1.549155	31	32	33
12 C	1.291452	-0.869604	-6.008654	0.683407	-0.460175	-3.179643	34	35	36
13 C	2.655277	-1.245676	-8.247630	1.405112	-0.659183	-4.364458	37	38	39
14 C	5.259610	-0.971208	-8.271552	2.783266	-0.513941	-4.377117	40	41	42
15 C	6.511349	-0.331064	-6.045958	3.445657	-0.175192	-3.199383	43	44	45
16 C	5.202110	-0.037047	-3.794399	2.752838	-0.019605	-2.007910	46	47	48
17 C	2.590903	-0.339792	-3.779171	1.371047	-0.179810	-1.999851	49	50	51
18 H	1.633965	-1.708572	-9.956522	0.864657	-0.904137	-5.268765	52	53	54
19 H	6.350401	-1.195268	-9.985719	3.360487	-0.632509	-5.284215	55	56	57
20 O	9.142845	-0.007671	-6.213994	4.838185	-0.004060	-3.288304	58	59	60
21 H	6.126807	0.519477	-2.054564	3.242167	0.274896	-1.087228	61	62	63
22 H	1.593264	-0.131592	-2.007770	0.843119	-0.069635	-1.062466	64	65	66
23 H	9.840131	0.677591	-4.636944	5.207173	0.358566	-2.453765	67	68	69
24 H	-5.419659	-2.852765	-1.197987	-2.867960	-1.509618	-0.633947	70	71	72

25	O	-5.946532	-4.688727	-4.705419	-3.146769	-2.481167	-2.490001	73	74	75
26	C	-1.491888	-1.036307	-6.057100	-0.789473	-0.548390	-3.205279	76	77	78
27	C	-3.063451	0.292475	-4.422680	-1.621108	0.154771	-2.340381	79	80	81
28	C	-5.873750	-0.188146	-4.261653	-3.108255	-0.099562	-2.255170	82	83	84
29	C	-6.548762	-2.630920	-2.911376	-3.465456	-1.392223	-1.540634	85	86	87
30	H	-3.397835	1.687196	-9.421645	-1.798057	0.892826	-4.985720	88	89	90
31	H	-3.926190	-3.707117	-6.980603	-2.077650	-1.961722	-3.693976	91	92	93
32	H	-8.565333	-2.714487	-2.474822	-4.532579	-1.436445	-1.309620	94	95	96
33	O	-2.354488	-2.906702	-7.673227	-1.245941	-1.538161	-4.060497	97	98	99
34	H	-6.736199	-0.227606	-6.142372	-3.564643	-0.120444	-3.250403	100	101	102
35	H	-5.939377	-6.355852	-3.907585	-3.142983	-3.363372	-2.067805	103	104	105
36	H	-6.727741	1.389100	-3.237465	-3.560167	0.735080	-1.713193	106	107	108
37	H	-2.221584	1.226145	-2.786535	-1.175612	0.648848	-1.474571	109	110	111



Structure **K** (X=I) Coordinates (Cartesian)

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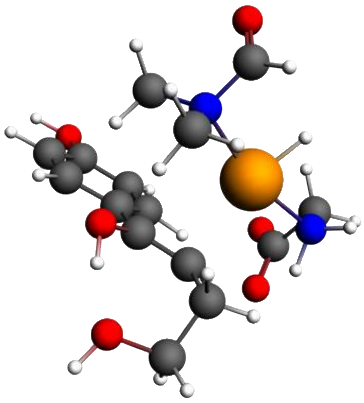
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-2.431180	3.390216	-7.173960	-1.286525	1.794025	-3.796296	1	2	3
2 C	1.050476	6.018410	-3.028715	0.555888	3.184805	-1.602727	4	5	6
3 C	1.056810	4.470429	-0.548080	0.559240	2.365649	-0.290031	7	8	9
4 N	-1.532238	6.074064	-4.125898	-0.810825	3.214256	-2.183331	10	11	12
5 O	-1.093494	3.552936	0.135128	-0.578652	1.880133	0.071506	13	14	15
6 O	3.185619	4.208611	0.527492	1.685757	2.227101	0.279137	16	17	18
7 H	2.378297	5.165879	-4.355366	1.258541	2.733666	-2.304760	19	20	21
8 H	-1.930735	7.756712	-4.973948	-1.021701	4.104675	-2.632100	22	23	24
9 H	-2.750892	5.697266	-2.663805	-1.455709	3.014863	-1.409625	25	26	27
10 I	-2.771621	7.128506	-10.520472	-1.466679	3.772243	-5.567194	28	29	30
11 H	1.714694	7.925569	-2.579579	0.907377	4.194031	-1.365055	31	32	33
12 C	1.256944	-0.770894	-5.864798	0.665146	-0.407939	-3.103518	34	35	36
13 C	2.732431	-1.101145	-8.039083	1.445940	-0.582701	-4.254100	37	38	39
14 C	5.322888	-0.723487	-7.949346	2.816751	-0.382853	-4.206613	40	41	42
15 C	6.448750	-0.022899	-5.675447	3.412532	-0.012118	-3.003317	43	44	45
16 C	5.029632	0.227653	-3.485055	2.661566	0.120469	-1.844211	46	47	48
17 C	2.435115	-0.180179	-3.582863	1.288608	-0.095347	-1.895970	49	50	51
18 H	1.807693	-1.610996	-9.788937	0.956590	-0.852503	-5.180082	52	53	54
19 H	6.496372	-0.912165	-9.612612	3.437732	-0.482697	-5.086775	55	56	57
20 O	9.069472	0.402449	-5.727909	4.799358	0.212967	-3.031079	58	59	60
21 H	5.853411	0.826697	-1.708438	3.097491	0.437469	-0.904066	61	62	63
22 H	1.352977	-0.008705	-1.857478	0.715964	-0.004606	-0.982935	64	65	66
23 H	9.670437	1.112377	-4.122519	5.117375	0.588645	-2.181543	67	68	69

24	H	-5.753772	-3.027473	-1.492158	-3.044765	-1.602070	-0.789616	70	71	72
25	O	-5.991040	-4.778312	-5.072360	-3.170322	-2.528574	-2.684178	73	74	75
26	C	-1.513278	-1.037787	-6.036761	-0.800792	-0.549173	-3.194516	76	77	78
27	C	-3.199176	0.224533	-4.477482	-1.692931	0.118818	-2.369382	79	80	81
28	C	-6.007806	-0.288607	-4.513391	-3.179194	-0.152724	-2.388384	82	83	84
29	C	-6.752336	-2.773426	-3.280332	-3.573182	-1.467634	-1.735877	85	86	87
30	H	-3.214537	1.780951	-9.481436	-1.701060	0.942438	-5.017360	88	89	90
31	H	-3.841055	-3.721232	-7.170602	-2.032599	-1.969191	-3.794519	91	92	93
32	H	-8.795328	-2.887761	-3.002076	-4.654287	-1.528137	-1.588630	94	95	96
33	O	-2.242290	-2.879373	-7.743558	-1.186569	-1.523699	-4.097714	97	98	99
34	H	-6.741180	-0.282158	-6.449117	-3.567279	-0.149312	-3.412726	100	101	102
35	H	-6.023363	-6.464859	-4.317822	-3.187426	-3.421056	-2.284893	103	104	105
36	H	-6.948098	1.251065	-3.507748	-3.676775	0.662035	-1.856220	106	107	108
37	H	-2.470200	1.161016	-2.790673	-1.307174	0.614383	-1.476760	109	110	111



Structure **K** (X=DFM) Coordinates (Cartesian)

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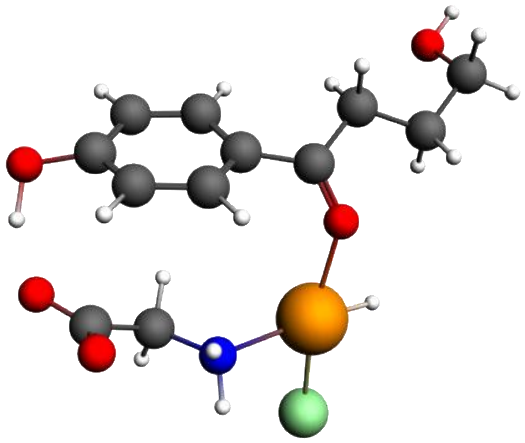
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-1.066763	-0.217799	-0.386557	-0.564507	-0.115254	-0.204557	1	2	3
2 C	0.557224	-5.145840	1.906841	0.294870	-2.723061	1.009057	4	5	6
3 C	0.810987	-6.920479	-0.408985	0.429156	-3.662160	-0.216425	7	8	9
4 N	-1.771033	-3.591668	1.490128	-0.937190	-1.900629	0.788542	10	11	12
5 O	-1.249221	-7.124191	-1.719437	-0.661059	-3.769959	-0.909887	13	14	15
6 O	2.931913	-7.906014	-0.809661	1.551502	-4.183683	-0.428454	16	17	18
7 H	2.227338	-3.968592	2.091920	1.178657	-2.100089	1.106996	19	20	21
8 H	-2.680561	-3.187128	3.135406	-1.418492	-1.686556	1.659185	22	23	24
9 H	-2.847545	-4.757411	0.333358	-1.506856	-2.517513	0.176405	25	26	27
10 H	-8.012333	-0.656993	-9.250796	-4.239944	-0.347666	-4.895311	28	29	30
11 H	0.341930	-6.316243	3.598459	0.180941	-3.342412	1.904222	31	32	33
12 C	0.921146	-1.478106	-6.601410	0.487450	-0.782180	-3.493316	34	35	36
13 C	2.124737	0.000173	-8.435355	1.124362	0.000092	-4.463797	37	38	39
14 C	4.580755	-0.537692	-9.191654	2.424031	-0.284535	-4.864014	40	41	42
15 C	5.843979	-2.587292	-8.127264	3.092501	-1.369136	-4.300763	43	44	45
16 C	4.644622	-4.139731	-6.370989	2.457828	-2.190651	-3.371382	46	47	48
17 C	2.198067	-3.596454	-5.633321	1.163167	-1.903162	-2.981025	49	50	51
18 H	1.109507	1.556997	-9.284084	0.587126	0.823927	-4.912925	52	53	54
19 H	5.484447	0.621797	-10.617869	2.902245	0.329041	-5.618734	55	56	57
20 O	8.312476	-3.230841	-8.758532	4.398773	-1.709687	-4.634815	58	59	60
21 H	5.627350	-5.761332	-5.606347	2.977866	-3.048766	-2.966751	61	62	63
22 H	1.274999	-4.905646	-4.368452	0.674700	-2.595956	-2.311685	64	65	66

23	H	9.072978	-2.096117	-10.014591	4.801213	-1.109217	-5.299493	67	68	69
24	H	-7.092440	-4.122071	-6.447593	-3.753157	-2.181306	-3.411919	70	71	72
25	O	-7.083759	-0.334103	-7.685641	-3.748564	-0.176800	-4.067066	73	74	75
26	C	-1.638839	-0.810381	-5.768997	-0.867236	-0.428835	-3.052822	76	77	78
27	C	-3.049695	-2.136689	-4.051142	-1.613829	-1.130687	-2.143772	79	80	81
28	C	-5.803431	-1.564066	-3.526583	-3.071043	-0.827668	-1.866187	82	83	84
29	C	-7.549444	-2.252380	-5.708714	-3.994993	-1.191908	-3.020921	85	86	87
30	H	-6.401121	-2.652245	-1.875371	-3.387327	-1.403508	-0.992403	88	89	90
31	H	2.628794	5.717955	-3.427039	1.391098	3.025812	-1.813511	91	92	93
32	H	-9.529107	-2.142065	-5.140884	-5.042586	-1.133532	-2.720439	94	95	96
33	H	0.790306	3.520758	-5.208966	0.418212	1.863105	-2.756466	97	98	99
34	H	-6.125587	0.432828	-3.084657	-3.241521	0.229043	-1.632330	100	101	102
35	H	-0.281498	0.529115	2.335535	-0.148962	0.279996	1.235912	103	104	105
36	H	-4.431478	1.065020	-7.380626	-2.345037	0.563584	-3.905659	106	107	108
37	O	-2.591112	1.337673	-6.922024	-1.371158	0.707866	-3.662978	109	110	111
38	C	0.900526	4.498077	1.008156	0.476538	2.380280	0.533493	112	113	114
39	O	3.165164	4.829732	1.354859	1.674932	2.555784	0.716960	115	116	117
40	H	-0.538651	4.913395	2.426906	-0.285042	2.600057	1.284263	118	119	120
41	N	-0.123643	3.660174	-1.363182	-0.065429	1.936881	-0.721365	121	122	123
42	C	-2.537708	4.972314	-1.990043	-1.342897	2.631235	-1.053085	124	125	126
43	H	3.244144	2.438165	-3.170467	1.716727	1.290221	-1.677739	127	128	129
44	H	-2.184506	6.985093	-2.321054	-1.155991	3.696352	-1.228249	130	131	132
45	H	-3.874432	4.747906	-0.439563	-2.050261	2.512484	-0.232607	133	134	135
46	H	-3.295095	4.134467	-3.704125	-1.743689	2.187866	-1.960139	136	137	138
47	C	1.765117	3.838956	-3.438277	0.934060	2.031488	-1.819458	139	140	141
48	H	-2.428398	-4.044129	-3.578624	-1.285053	-2.140061	-1.893726	142	143	144



Structure **M** (X=Cl) Coordinates (Cartesian)

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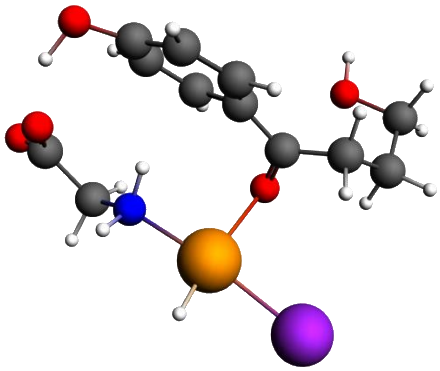
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	0.372885	-1.729978	2.465157	0.197322	-0.915465	1.304505	1	2	3
2 C	6.265143	-1.496083	1.697448	3.315371	-0.791693	0.898251	4	5	6
3 C	8.640158	-3.109200	1.192946	4.572175	-1.645318	0.631280	7	8	9
4 N	4.308077	-2.937670	3.100944	2.279736	-1.554548	1.640949	10	11	12
5 O	8.735372	-5.294168	2.161501	4.622560	-2.801553	1.143817	13	14	15
6 O	10.289572	-2.098149	-0.307880	5.445007	-1.110293	-0.162923	16	17	18
7 H	5.514937	-0.873604	-0.119935	2.918379	-0.462291	-0.063467	19	20	21
8 H	4.438620	-2.548475	4.987190	2.348817	-1.348595	2.639107	22	23	24
9 H	4.698167	-4.818972	2.873664	2.486163	-2.550090	1.520677	25	26	27
10 Cl	0.864121	0.944378	6.058510	0.457273	0.499743	3.206025	28	29	30
11 H	6.780021	0.193823	2.761527	3.587833	0.102567	1.461337	31	32	33
12 C	2.164610	-3.512194	-4.026520	1.145462	-1.858573	-2.130743	34	35	36
13 C	3.850751	-5.173353	-2.827016	2.037730	-2.737620	-1.495993	37	38	39
14 C	6.402982	-5.070059	-3.338428	3.388312	-2.682960	-1.766620	40	41	42
15 C	7.354659	-3.160887	-4.917154	3.891918	-1.672669	-2.602046	43	44	45
16 C	5.671430	-1.655797	-6.298767	3.001192	-0.876210	-3.333164	46	47	48
17 C	3.093410	-1.854390	-5.879666	1.636962	-0.981301	-3.111385	49	50	51
18 H	3.117253	-6.529682	-1.481334	1.649579	-3.455359	-0.783888	52	53	54
19 H	7.704807	-6.347880	-2.414238	4.077208	-3.359153	-1.277560	55	56	57
20 O	9.880457	-2.659397	-4.983876	5.228513	-1.407292	-2.637354	58	59	60
21 H	6.446363	-0.251248	-7.565539	3.411269	-0.132954	-4.003511	61	62	63
22 H	1.823184	-0.587770	-6.864355	0.964787	-0.311035	-3.632460	64	65	66

23	H	10.508669	-2.523454	-3.080232	5.560948	-1.335355	-1.629989	67	68	69
24	H	-7.376921	-4.286970	-6.764635	-3.903699	-2.268567	-3.579691	70	71	72
25	O	-6.606782	-0.417222	-7.315126	-3.496158	-0.220784	-3.870998	73	74	75
26	C	-0.446574	-3.476543	-3.158538	-0.236317	-1.839707	-1.671427	76	77	78
27	C	-2.566249	-3.125957	-5.012833	-1.358001	-1.654185	-2.652677	79	80	81
28	C	-5.116446	-2.756867	-3.733963	-2.707507	-1.458871	-1.975928	82	83	84
29	C	-7.230208	-2.550456	-5.645519	-3.826061	-1.349643	-2.987480	85	86	87
30	H	-5.488513	-4.321646	-2.439301	-2.904396	-2.286917	-1.290822	88	89	90
31	H	-2.317914	-0.622440	2.310129	-1.226588	-0.329381	1.222467	91	92	93
32	H	-9.029076	-2.198355	-4.688566	-4.777981	-1.163319	-2.481082	94	95	96
33	H	-2.178889	-1.508927	-6.238152	-1.153018	-0.798490	-3.301088	97	98	99
34	H	-5.057090	-1.034306	-2.596603	-2.676097	-0.547331	-1.374063	100	101	102
35	H	-7.974308	-0.099943	-8.525690	-4.219822	-0.052887	-4.511601	103	104	105
36	H	-2.585897	-4.789618	-6.255676	-1.368398	-2.534557	-3.310361	106	107	108
37	O	-0.955248	-3.821503	-0.856218	-0.505495	-2.022252	-0.453091	109	110	111



Structure **M** (X=I) Coordinates (Cartesian)

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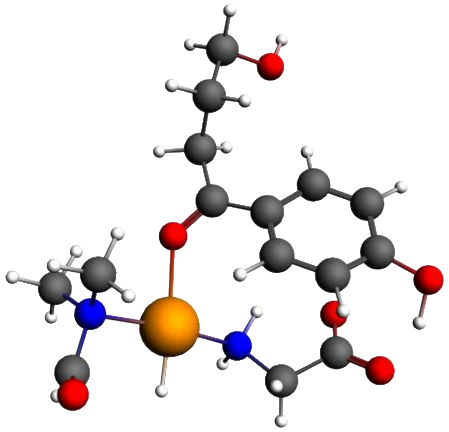
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.099259	-2.622389	2.761081	-0.052525	-1.387709	1.461101	1	2	3
2 C	5.605784	-2.049120	1.527827	2.966453	-1.084347	0.808491	4	5	6
3 C	7.943000	-2.978591	0.033758	4.203255	-1.576203	0.017864	7	8	9
4 N	3.491800	-3.893222	1.525438	1.847781	-2.060204	0.807227	10	11	12
5 O	7.817638	-5.281245	-0.801834	4.136916	-2.794714	-0.424312	13	14	15
6 O	9.703483	-1.410744	-0.281039	5.134862	-0.746534	-0.148719	16	17	18
7 H	4.958513	-0.282509	0.693282	2.623932	-0.149497	0.366869	19	20	21
8 H	4.002666	-5.420377	2.581823	2.118120	-2.868340	1.366242	22	23	24
9 H	3.267452	-4.563085	-0.269615	1.729061	-2.414681	-0.142674	25	26	27
10 H	-3.212440	2.127268	-7.635010	-1.699950	1.125702	-4.040273	28	29	30
11 H	6.147575	-1.662119	3.478715	3.253156	-0.879555	1.840857	31	32	33
12 C	0.255368	-2.991228	-3.928185	0.135135	-1.582890	-2.078706	34	35	36
13 C	2.502965	-1.607166	-4.190522	1.324512	-0.850476	-2.217529	37	38	39
14 C	4.722539	-2.802667	-4.866401	2.499060	-1.483107	-2.575189	40	41	42
15 C	4.755716	-5.436206	-5.180302	2.516617	-2.876716	-2.741298	43	44	45
16 C	2.478102	-6.774219	-5.215827	1.311355	-3.584762	-2.760097	46	47	48
17 C	0.232858	-5.550495	-4.606640	0.123223	-2.937195	-2.437729	49	50	51
18 H	2.463782	0.393184	-3.764079	1.303777	0.208064	-1.991865	52	53	54
19 H	6.482072	-1.769412	-5.017371	3.430165	-0.936333	-2.655078	55	56	57
20 O	7.012962	-6.710765	-5.227242	3.711100	-3.551184	-2.766138	58	59	60
21 H	2.544461	-8.789746	-5.550372	1.346471	-4.651333	-2.937130	61	62	63
22 H	-1.495312	-6.638897	-4.465576	-0.791285	-3.513153	-2.363081	64	65	66
23 H	7.922263	-6.250613	-3.518066	4.192281	-3.307682	-1.861681	67	68	69

24 H	-6.998162	-0.059634	-6.885191	-3.703268	-0.031557	-3.643486	70	71	72
25 O	-3.498404	1.558517	-5.896366	-1.851276	0.824732	-3.120223	73	74	75
26 C	-1.825219	-1.803122	-2.544726	-0.965864	-0.954171	-1.346611	76	77	78
27 C	-4.530748	-2.592037	-2.924608	-2.397569	-1.371647	-1.547636	79	80	81
28 C	-6.283441	-0.291354	-2.878751	-3.325054	-0.154178	-1.523369	82	83	84
29 C	-6.179192	1.103034	-5.378422	-3.269888	0.583700	-2.846138	85	86	87
30 H	-8.226531	-0.876239	-2.489878	-4.353293	-0.463686	-1.317587	88	89	90
31 H	0.294731	-4.203845	5.128829	0.155965	-2.224579	2.714060	91	92	93
32 H	-7.199090	2.898209	-5.262204	-3.809594	1.533666	-2.784638	94	95	96
33 H	-4.745487	-3.646985	-4.686400	-2.511204	-1.929901	-2.479936	97	98	99
34 H	-5.664233	0.946289	-1.346560	-2.997383	0.500755	-0.712569	100	101	102
35 I	-4.598248	-1.860593	4.806432	-2.433288	-0.984584	2.543454	103	104	105
36 H	-5.015966	-3.824654	-1.327757	-2.654335	-2.023920	-0.702619	106	107	108
37 O	-1.294789	-0.224201	-0.846656	-0.685173	-0.118642	-0.448031	109	110	111



Structure **M** (X=DMF) Coordinates (Cartesian)

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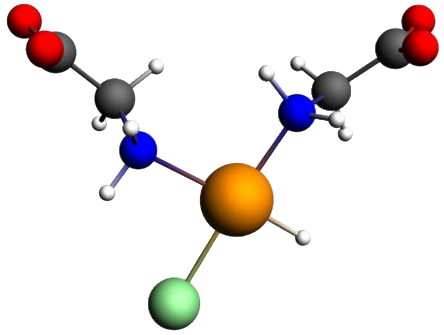
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	1.812887	0.859103	2.189987	0.959339	0.454618	1.158891	1	2	3
2 C	5.416375	-3.629690	2.282568	2.866222	-1.920749	1.207883	4	5	6
3 C	5.327977	-6.051803	0.674097	2.819444	-3.202476	0.356717	7	8	9
4 N	2.751724	-2.859301	2.887312	1.456150	-1.513077	1.527900	10	11	12
5 O	7.390780	-6.625197	-0.484605	3.911032	-3.505903	-0.256442	13	14	15
6 O	3.212544	-7.162494	0.530733	1.700005	-3.790229	0.280852	16	17	18
7 H	6.378183	-2.152394	1.233194	3.375189	-1.138998	0.652578	19	20	21
8 H	2.376991	-3.183813	4.748945	1.257849	-1.684801	2.513034	22	23	24
9 H	1.637693	-4.100812	1.857870	0.866630	-2.170056	0.983142	25	26	27
10 H	-8.060474	-6.316873	-6.946527	-4.265419	-3.342745	-3.675944	28	29	30
11 H	6.466439	-3.990574	4.021027	3.421892	-2.111721	2.127836	31	32	33
12 C	0.089963	-2.675443	-3.411057	0.047606	-1.415783	-1.805053	34	35	36
13 C	2.614934	-1.822170	-3.290771	1.383763	-0.964251	-1.741401	37	38	39
14 C	4.565342	-3.357760	-4.047769	2.415875	-1.776850	-2.141987	40	41	42
15 C	4.048289	-5.859640	-4.810851	2.142262	-3.100788	-2.545793	43	44	45
16 C	1.548906	-6.582206	-5.305434	0.819646	-3.483153	-2.807515	46	47	48
17 C	-0.409798	-5.012052	-4.613210	-0.216856	-2.652264	-2.441206	49	50	51
18 H	3.012792	0.069628	-2.609516	1.594301	0.036846	-1.380896	52	53	54
19 H	6.510822	-2.737031	-3.971733	3.445379	-1.448374	-2.101750	55	56	57
20 O	5.921425	-7.594400	-4.911942	3.133483	-4.018783	-2.599288	58	59	60
21 H	1.212652	-8.465527	-6.020748	0.641708	-4.479764	-3.186043	61	62	63
22 H	-2.336811	-5.656793	-4.873609	-1.236587	-2.993446	-2.579003	64	65	66

23	H	6.941067	-7.525430	-3.184494	3.673055	-3.982286	-1.685162	67	68	69
24	H	-9.097311	-2.088356	-5.511646	-4.814090	-1.105111	-2.916638	70	71	72
25	O	-6.730399	-5.191328	-6.318161	-3.561574	-2.747133	-3.343427	73	74	75
26	C	-1.876302	-1.273289	-2.170102	-0.992896	-0.673796	-1.148368	76	77	78
27	C	-4.592685	-1.655735	-2.886727	-2.430344	-0.876177	-1.527590	79	80	81
28	C	-5.142912	-1.047555	-5.678435	-2.721512	-0.554342	-3.004898	82	83	84
29	C	-7.407758	-2.522095	-6.623515	-3.920017	-1.334635	-3.505013	85	86	87
30	H	-5.477176	0.979095	-5.912816	-2.898396	0.518115	-3.128928	88	89	90
31	H	-5.739799	-0.486915	-1.632627	-3.037371	-0.257664	-0.863949	91	92	93
32	H	-7.759435	-2.095375	-8.613516	-4.106116	-1.108825	-4.558076	94	95	96
33	H	-5.092416	-3.635211	-2.546078	-2.694791	-1.923671	-1.347326	97	98	99
34	H	-3.519157	-1.553941	-6.849718	-1.862258	-0.822310	-3.624715	100	101	102
35	H	3.872650	1.361523	4.183234	2.049318	0.720487	2.213672	103	104	105
36	H	-0.336689	4.409671	-1.854248	-0.178168	2.333497	-0.981226	106	107	108
37	O	-1.391585	0.294409	-0.393641	-0.736395	0.155794	-0.208306	109	110	111
38	C	2.938522	5.959608	3.320136	1.554999	3.153689	1.756940	112	113	114
39	O	4.739460	7.062289	2.371251	2.508014	3.737203	1.254812	115	116	117
40	H	2.654926	5.790690	5.356581	1.404926	3.064301	2.834581	118	119	120
41	N	0.977385	4.810342	1.857798	0.517210	2.545523	0.983105	121	122	123
42	C	-1.581914	5.075057	3.004646	-0.837113	2.685605	1.589990	124	125	126
43	H	2.924616	5.254474	-1.593199	1.547640	2.780548	-0.843084	127	128	129
44	H	-2.235152	7.030360	2.835834	-1.182791	3.720306	1.500659	130	131	132
45	H	-1.510682	4.533909	4.990286	-0.799419	2.399241	2.640745	133	134	135
46	H	-2.862085	3.810707	2.012844	-1.514550	2.016539	1.065151	136	137	138
47	C	1.034839	5.554778	-0.846012	0.547613	2.939462	-0.447690	139	140	141
48	H	0.574725	7.563069	-1.030856	0.304132	4.002204	-0.545505	142	143	144



Structure **N** (X=Cl) Coordinates (Cartesian)

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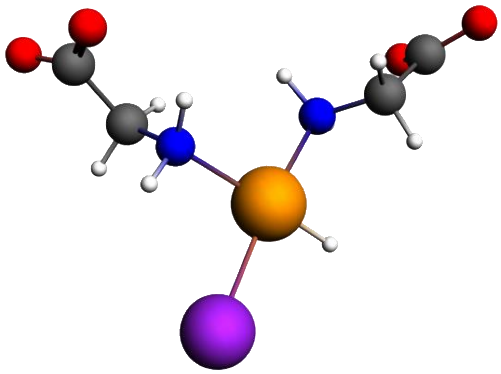
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	1.424429	0.726572	4.803920	0.753775	0.384485	2.542125	1	2	3
2 C	6.154400	-3.012809	4.569169	3.256768	-1.594310	2.417900	4	5	6
3 C	7.051196	-5.815046	4.626425	3.731332	-3.077190	2.448199	7	8	9
4 N	3.569538	-2.714139	5.612428	1.888918	-1.436260	2.969969	10	11	12
5 O	9.418120	-6.169048	4.344495	4.983854	-3.264519	2.299008	13	14	15
6 O	5.290333	-7.464109	4.889930	2.799523	-3.949837	2.587639	16	17	18
7 H	6.179675	-2.377610	2.602536	3.270143	-1.258177	1.377203	19	20	21
8 H	3.653698	-2.554556	7.536287	1.933454	-1.351813	3.988031	22	23	24
9 H	2.646377	-4.376000	5.217391	1.400402	-2.315680	2.760924	25	26	27
10 Cl	1.607753	1.658004	9.296929	0.850786	0.877378	4.919723	28	29	30
11 H	7.470259	-1.835069	5.627535	3.953091	-0.971077	2.977963	31	32	33
12 H	-0.136123	3.188230	4.371213	-0.072033	1.687139	2.313146	34	35	36
13 C	2.238863	1.972315	-0.810835	1.184755	1.043704	-0.429076	37	38	39
14 C	0.893253	1.944072	-3.426199	0.472689	1.028758	-1.813066	40	41	42
15 N	1.086756	0.092715	0.946338	0.575087	0.049063	0.500780	43	44	45
16 O	-1.211436	0.738338	-3.500126	-0.641064	0.390712	-1.852187	46	47	48
17 O	1.991050	3.178320	-5.177460	1.053618	1.681894	-2.739794	49	50	51
18 H	4.245553	1.577477	-1.040481	2.246650	0.834765	-0.550599	52	53	54
19 H	1.811813	-1.653077	0.562967	0.958770	-0.874770	0.297909	55	56	57
20 H	2.027942	3.846336	0.013209	1.073141	2.035393	0.006990	58	59	60
21 H	-0.786535	0.024437	0.431796	-0.416217	0.012931	0.228497	61	62	63



Structure **N** (X=I) Coordinates (Cartesian)

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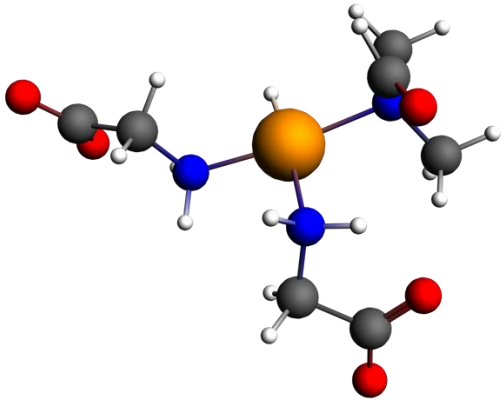
Atom	bohr			angstrom			Geometric Variables		
X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)			
1 Pd	0.381428	-1.024569	3.734204	0.201843	-0.542178	1.976056	1	2	3
2 C	5.957435	-1.952268	2.427965	3.152539	-1.033096	1.284824	4	5	6
3 C	7.878277	-3.985393	1.520603	4.169005	-2.108979	0.804668	7	8	9
4 N	3.335318	-2.576545	1.603001	1.764974	-1.363449	0.848271	10	11	12
5 O	6.899277	-6.051734	0.710085	3.650940	-3.202440	0.375761	13	14	15
6 O	10.201892	-3.398371	1.752515	5.398609	-1.798340	0.927391	16	17	18
7 H	6.492436	-0.099994	1.708393	3.435649	-0.052915	0.904043	19	20	21
8 H	3.255452	-4.517035	1.616539	1.722711	-2.390312	0.855436	22	23	24
9 H	3.111253	-2.041543	-0.236244	1.646404	-1.080338	-0.125015	25	26	27
10 I	-3.156333	0.677196	6.951305	-1.670259	0.358357	3.678472	28	29	30
11 H	5.995015	-1.892614	4.485603	3.172425	-1.001528	2.373679	31	32	33
12 H	1.258915	-2.785154	5.921379	0.666189	-1.473840	3.133459	34	35	36
13 C	-2.456740	0.145770	-1.339360	-1.300051	0.077138	-0.708759	37	38	39
14 C	-2.650956	1.805552	-3.759610	-1.402825	0.955457	-1.989500	40	41	42
15 N	-1.001522	1.416294	0.698751	-0.529982	0.749471	0.369763	43	44	45
16 O	-1.077246	3.648896	-3.884791	-0.570054	1.930912	-2.055743	46	47	48
17 O	-4.302356	1.118544	-5.374090	-2.276709	0.591908	-2.843846	49	50	51
18 H	-1.512976	-1.620702	-1.848154	-0.800633	-0.857639	-0.978001	52	53	54
19 H	-2.163502	2.640478	1.635755	-1.144876	1.397281	0.865604	55	56	57
20 H	0.332952	2.500058	-0.203963	0.176191	1.322974	-0.107933	58	59	60
21 H	-4.339400	-0.322386	-0.650903	-2.296312	-0.170599	-0.344443	61	62	63



Structure **N** (X=DMF) Coordinates (Cartesian)

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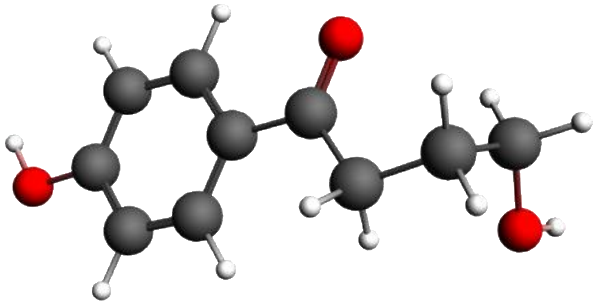
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-1.050612	-2.541164	1.804521	-0.555960	-1.344726	0.954911	1	2	3
2 C	-0.214582	-8.312582	1.398584	-0.113552	-4.398829	0.740099	4	5	6
3 C	2.268280	-9.185872	2.731884	1.200322	-4.860954	1.445651	7	8	9
4 N	-1.546170	-6.448593	3.036310	-0.818198	-3.412448	1.606746	10	11	12
5 O	2.479801	-8.467501	5.042321	1.312254	-4.480809	2.668282	13	14	15
6 O	3.754949	-10.494066	1.399885	1.987034	-5.553220	0.740787	16	17	18
7 H	-1.370562	-9.994795	1.072768	-0.725270	-5.289018	0.567684	19	20	21
8 H	-0.768231	-6.712878	4.813947	-0.406531	-3.552302	2.547431	22	23	24
9 H	-3.444284	-6.764727	3.123837	-1.822636	-3.579739	1.653063	25	26	27
10 H	4.531768	-2.500979	4.160506	2.398108	-1.323461	2.201645	28	29	30
11 H	0.304554	-7.493973	-0.418613	0.161163	-3.965640	-0.221521	31	32	33
12 C	-1.182144	-1.660215	6.772217	-0.625563	-0.878548	3.583703	34	35	36
13 O	-1.417724	-3.520382	8.150826	-0.750227	-1.862906	4.313231	37	38	39
14 H	-2.593814	-0.151960	6.678593	-1.372587	-0.080414	3.534159	40	41	42
15 N	0.925045	-1.230706	5.178881	0.489513	-0.651261	2.740546	43	44	45
16 C	1.573788	1.487873	4.883542	0.832813	0.787349	2.584259	46	47	48
17 H	4.047847	-2.186275	7.486207	2.142029	-1.156927	3.961530	49	50	51
18 H	2.830711	1.693490	3.274779	1.497948	0.896156	1.732938	52	53	54
19 H	2.517876	2.161734	6.599274	1.332403	1.143940	3.492185	55	56	57
20 H	-0.125128	2.589855	4.525895	-0.066215	1.370492	2.395000	58	59	60
21 C	3.198823	-2.793847	5.698151	1.692744	-1.478440	3.015332	61	62	63
22 H	-0.832027	0.184436	0.707385	-0.440290	0.097600	0.374332	64	65	66
23 H	2.756109	-4.807821	5.809547	1.458470	-2.544189	3.074280	67	68	69

24 C	-5.700669	-2.542393	-1.494246	-3.016664	-1.345376	-0.790721	70	71	72
25 C	-6.386054	-1.488287	-4.170172	-3.379354	-0.787567	-2.206760	73	74	75
26 N	-2.965276	-3.263801	-1.476467	-1.569157	-1.727129	-0.781313	76	77	78
27 O	-4.459800	-1.077025	-5.589307	-2.360024	-0.569937	-2.957734	79	80	81
28 O	-8.712337	-1.124225	-4.573168	-4.610370	-0.594914	-2.420016	82	83	84
29 H	-6.890942	-4.160605	-1.047943	-3.646530	-2.201697	-0.554547	85	86	87
30 H	-2.258019	-2.247378	-3.007329	-1.194892	-1.189261	-1.591410	88	89	90
31 H	-2.777762	-5.131169	-1.922010	-1.469928	-2.715297	-1.017084	91	92	93
32 H	-6.029715	-1.048953	-0.118864	-3.190788	-0.555082	-0.062900	94	95	96



Structure **P2** Coordinates (Cartesian)

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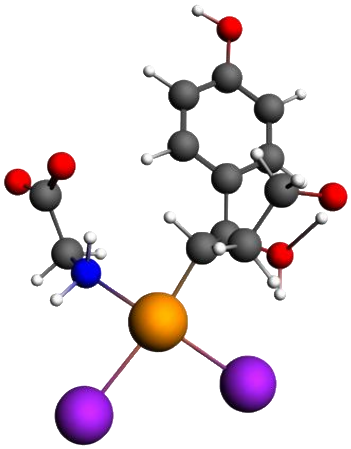
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 C	-4.841558	0.603371	-1.233680	-2.562042	0.319290	-0.652836	1	2	3
2 H	-4.501240	2.605951	-4.732477	-2.381954	1.379010	-2.504319	4	5	6
3 C	-0.919666	-0.958956	-5.423064	-0.486666	-0.507458	-2.869762	7	8	9
4 H	-5.908969	2.111059	-0.307344	-3.126891	1.117124	-0.162640	10	11	12
5 C	-5.164237	0.764058	-4.075290	-2.732796	0.404322	-2.156550	13	14	15
6 H	-4.214892	-3.136902	-4.517368	-2.230425	-1.659977	-2.390488	16	17	18
7 H	-7.179637	0.587671	-4.496850	-3.799300	0.310982	-2.379630	19	20	21
8 H	-5.638699	-2.162239	1.333250	-2.983871	-1.144207	0.705526	22	23	24
9 C	-3.744607	-1.342605	-5.433223	-1.981561	-0.710476	-2.875138	25	26	27
10 H	-4.367911	-1.462570	-7.406106	-2.311399	-0.773959	-3.919142	28	29	30
11 O	0.034542	0.995300	-4.519833	0.018279	0.526690	-2.391793	31	32	33
12 C	0.717659	-2.937715	-6.542449	0.379769	-1.554572	-3.462115	34	35	36
13 C	3.326357	-2.513103	-6.616080	1.760232	-1.329877	-3.501079	37	38	39
14 C	4.949978	-4.293120	-7.648017	2.619416	-2.271821	-4.047157	40	41	42
15 C	3.957256	-6.531708	-8.618887	2.094090	-3.456431	-4.560919	43	44	45
16 C	1.368431	-6.995472	-8.562330	0.724142	-3.701845	-4.530990	46	47	48
17 C	-0.237914	-5.203149	-7.527511	-0.125899	-2.753388	-3.983387	49	50	51
18 H	4.043722	-0.757079	-5.847752	2.139846	-0.400629	-3.094497	52	53	54
19 H	6.966287	-3.936950	-7.693547	3.686400	-2.083344	-4.071250	55	56	57
20 O	5.443998	-8.415355	-9.686388	2.880840	-4.453214	-5.125816	58	59	60
21 H	0.675806	-8.757661	-9.331156	0.357621	-4.634354	-4.937835	61	62	63
22 H	-2.244021	-5.591687	-7.488543	-1.187485	-2.958994	-3.962766	64	65	66
23 H	7.256693	-8.016739	-9.687878	3.840077	-4.242276	-5.126604	67	68	69
24 H	-2.848884	0.742810	-0.719095	-1.507564	0.393078	-0.380529	70	71	72
25 O	-5.860162	-1.875485	-0.484222	-3.101064	-0.992464	-0.256239	73	74	75



Structure **H**: Coordinates (Cartesian)

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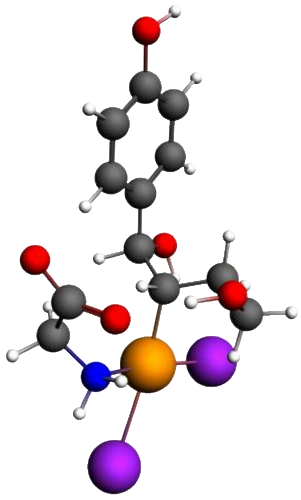
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.154356	0.885734	0.236855	-0.081682	0.468710	0.125338	1	2	3
2 C	4.169946	-2.862222	0.893391	2.206641	-1.514623	0.472762	4	5	6
3 C	4.805619	-5.598362	0.047858	2.543024	-2.962525	0.025325	7	8	9
4 N	1.409771	-2.574739	1.374974	0.746019	-1.362493	0.727605	10	11	12
5 O	2.920870	-6.855952	-0.848139	1.545658	-3.628014	-0.448816	13	14	15
6 O	7.102501	-6.274465	0.221644	3.758481	-3.320304	0.117289	16	17	18
7 H	4.749438	-1.581714	-0.617214	2.513294	-0.837007	-0.326615	19	20	21
8 H	1.055772	-2.606231	3.273140	0.558690	-1.379158	1.732071	22	23	24
9 H	0.576976	-4.112659	0.522670	0.305322	-2.176325	0.276585	25	26	27
10 I	0.367443	2.330852	5.386043	0.194443	1.233434	2.850171	28	29	30
11 H	5.229645	-2.363376	2.585231	2.767409	-1.250645	1.368045	31	32	33
12 C	2.135973	-1.540578	-7.248163	1.130308	-0.815239	-3.835562	34	35	36
13 C	2.976484	-3.935672	-6.511960	1.575087	-2.082668	-3.445981	37	38	39
14 C	3.929637	-5.631474	-8.286676	2.079474	-2.980048	-4.385120	40	41	42
15 C	4.042389	-4.941233	-10.813913	2.139140	-2.614788	-5.722476	43	44	45
16 C	3.224591	-2.575122	-11.589231	1.706380	-1.362696	-6.132757	46	47	48
17 C	2.289761	-0.883416	-9.803060	1.211689	-0.467483	-5.187556	49	50	51
18 H	2.903878	-4.570736	-4.564854	1.536666	-2.418729	-2.415617	52	53	54
19 H	4.576362	-7.466997	-7.643096	2.421706	-3.951365	-4.044552	55	56	57
20 O	4.987963	-6.585404	-12.703719	2.639516	-3.484846	-6.722519	58	59	60
21 H	3.326003	-2.092340	-13.574063	1.760045	-1.107219	-7.183085	61	62	63
22 H	1.661819	0.973446	-10.375618	0.879397	0.515125	-5.490541	64	65	66

23	H	5.554405	-8.181663	-11.949769	2.939265	-4.329550	-6.323545	67	68	69
24	H	-2.691596	-3.514732	-7.095636	-1.424331	-1.859916	-3.754849	70	71	72
25	O	-3.991225	-0.109525	-8.694466	-2.112065	-0.057958	-4.600913	73	74	75
26	C	1.200555	0.354685	-5.294867	0.635306	0.187691	-2.801923	76	77	78
27	C	-0.610390	-0.754949	-3.311083	-0.323004	-0.399502	-1.752150	79	80	81
28	C	-3.410926	-0.816923	-4.056350	-1.804984	-0.432297	-2.146528	82	83	84
29	C	-4.012313	-1.980253	-6.654187	-2.123224	-1.047905	-3.521244	85	86	87
30	H	-4.383022	-1.914877	-2.592423	-2.319396	-1.013309	-1.371851	88	89	90
31	H	2.872105	1.118232	-4.336549	1.519852	0.591743	-2.294803	91	92	93
32	H	-5.934366	-2.733216	-6.664616	-3.140331	-1.446356	-3.526763	94	95	96
33	H	-0.021090	-2.706500	-2.983414	-0.011160	-1.432218	-1.578755	97	98	99
34	H	-4.246223	1.073111	-4.011886	-2.247004	0.567866	-2.122999	100	101	102
35	I	-1.761792	5.524916	-1.282016	-0.932300	2.923659	-0.678414	103	104	105
36	H	-0.460851	3.773193	-5.478919	-0.243872	1.996688	-2.899319	106	107	108
37	O	0.036269	2.446852	-6.714340	0.019193	1.294818	-3.553076	109	110	111
38	H	-2.554254	1.064114	-8.373071	-1.351653	0.563105	-4.430838	112	113	114



Structure J: Coordinates (Cartesian)

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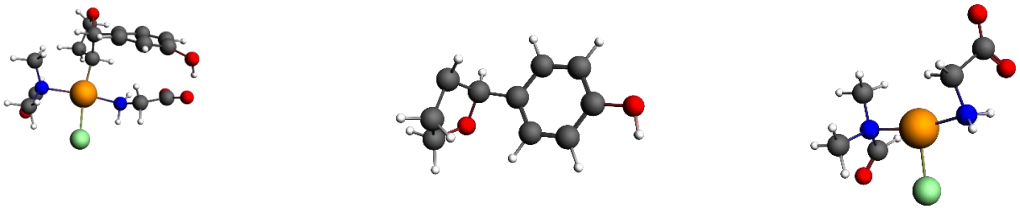
Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	0.065190	0.964957	0.126352	0.034497	0.510633	0.066862	1	2	3
2 C	3.151847	-4.132963	0.675284	1.667885	-2.187070	0.357345	4	5	6
3 C	2.265372	-6.371511	-0.991979	1.198783	-3.371658	-0.524933	7	8	9
4 N	0.960479	-2.655454	1.586968	0.508263	-1.405206	0.839787	10	11	12
5 O	-0.142822	-6.662256	-1.166397	-0.075578	-3.525514	-0.617230	13	14	15
6 O	4.000938	-7.665659	-2.022403	2.117205	-4.056492	-1.070209	16	17	18
7 H	4.442485	-2.949356	-0.407084	2.350862	-1.560732	-0.215419	19	20	21
8 H	1.081025	-2.215805	3.463228	0.572054	-1.172553	1.832661	22	23	24
9 H	-0.608303	-3.750063	1.235419	-0.321900	-1.984448	0.653756	25	26	27
10 I	-0.155463	2.339347	5.394850	-0.082267	1.237929	2.854832	28	29	30
11 H	4.204388	-4.923881	2.271388	2.224866	-2.605606	1.201967	31	32	33
12 C	3.430924	-1.092323	-7.224256	1.815567	-0.578032	-3.822912	34	35	36
13 C	3.261202	0.024927	-9.604181	1.725754	0.013191	-5.082313	37	38	39
14 C	3.737608	-1.370969	-11.790488	1.977857	-0.725486	-6.239257	40	41	42
15 C	4.387657	-3.904092	-11.587225	2.321848	-2.065957	-6.131696	43	44	45
16 C	4.577572	-5.052329	-9.238252	2.422347	-2.673577	-4.888673	46	47	48
17 C	4.105862	-3.645877	-7.065404	2.172729	-1.929315	-3.738851	49	50	51
18 H	2.763505	2.004119	-9.692511	1.462384	1.060534	-5.129056	52	53	54
19 H	3.604640	-0.468525	-13.628886	1.907494	-0.247933	-7.212096	55	56	57
20 O	4.902890	-5.422443	-13.738683	2.594498	-2.869433	-7.270198	58	59	60
21 H	5.052184	-7.036977	-9.120671	2.673501	-3.723808	-4.826451	61	62	63

22 H	4.243124	-4.615050	-5.264519	2.245364	-2.442180	-2.785864	64	65	66
23 H	4.411197	-4.536724	-15.290563	2.334305	-2.400731	-8.091418	67	68	69
24 H	-4.271468	-1.437631	-1.907036	-2.260363	-0.760762	-1.009160	70	71	72
25 O	-3.877029	-4.641526	-4.273845	-2.051635	-2.456190	-2.261622	73	74	75
26 C	2.846283	0.441104	-4.863144	1.506188	0.233422	-2.573465	76	77	78
27 C	0.475364	-0.543771	-3.508940	0.251552	-0.287751	-1.856851	79	80	81
28 C	-1.930125	-0.412882	-5.085478	-1.021378	-0.218488	-2.691119	82	83	84
29 C	-4.099508	-1.914587	-3.918224	-2.169366	-1.013156	-2.073435	85	86	87
30 H	-2.514221	1.552868	-5.343476	-1.330468	0.821742	-2.827646	88	89	90
31 H	4.465342	0.279680	-3.575797	2.362957	0.148000	-1.892230	91	92	93
32 H	-5.871495	-1.427382	-4.856958	-3.107062	-0.755338	-2.570191	94	95	96
33 H	0.836108	-2.533578	-3.098719	0.442449	-1.340712	-1.639772	97	98	99
34 H	-1.572115	-1.229790	-6.966565	-0.831927	-0.650777	-3.686547	100	101	102
35 I	-1.527938	5.608732	-1.351986	-0.808550	2.968013	-0.715440	103	104	105
36 H	1.692758	4.041251	-4.412500	0.895769	2.138538	-2.334994	106	107	108
37 O	2.638292	3.062133	-5.694918	1.396124	1.620411	-3.013621	109	110	111
38 H	-2.511455	-5.410356	-3.222222	-1.329005	-2.863037	-1.705126	112	113	114

Elimination of the catalyzer from structure **F**

F ⟺ Free ligand + Free catalyzer



ΔE=114.37 (E(products)-E(reactants)).

Coordinates of F: full optimization at PBE0//TZDP level of theory:

Coordinates (Cartesian)
==========

Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Pd	-0.417837	0.418599	-0.196029	-0.221110	0.221513	-0.103734	1	2	3
2 C	3.823038	-3.407330	-1.077804	2.023065	-1.803082	-0.570349	4	5	6
3 C	4.203491	-6.193243	-1.902162	2.224392	-3.277323	-1.006581	7	8	9
4 N	1.273394	-3.059516	0.003696	0.673851	-1.619026	0.001956	10	11	12
5 O	2.335356	-7.591557	-1.644652	1.235817	-4.017279	-0.870312	13	14	15
6 O	6.342585	-6.724995	-2.771358	3.356351	-3.558714	-1.466540	16	17	18
7 H	4.055801	-2.203450	-2.726410	2.146238	-1.166015	-1.442754	19	20	21
8 H	1.404414	-3.273252	1.907389	0.743184	-1.732130	1.009347	22	23	24
9 H	0.308992	-4.612236	-0.652976	0.163511	-2.440690	-0.345540	25	26	27
10 Cl	1.877586	1.080775	3.680861	0.993576	0.571922	1.947828	28	29	30
11 H	5.242565	-2.856069	0.305776	2.774246	-1.511367	0.161810	31	32	33
12 C	0.982732	-0.940157	-6.898661	0.520039	-0.497510	-3.650614	34	35	36
13 C	3.166497	0.512004	-6.973414	1.675638	0.270941	-3.690172	37	38	39
14 C	5.536117	-0.603544	-7.152603	2.929587	-0.319382	-3.784995	40	41	42
15 C	5.739694	-3.221258	-7.236670	3.037315	-1.704616	-3.829481	43	44	45
16 C	3.543993	-4.658843	-7.496357	1.875400	-2.465354	-3.966901	46	47	48
17 C	1.204573	-3.529412	-7.302488	0.637433	-1.867685	-3.864310	49	50	51
18 H	3.031569	2.546014	-6.731814	1.604237	1.347293	-3.562323	52	53	54
19 H	7.244279	0.517487	-7.015102	3.833508	0.273842	-3.712232	55	56	57
20 O	7.995218	-4.369283	-6.876269	4.230887	-2.312125	-3.638765	58	59	60
21 H	3.714492	-6.694480	-7.615473	1.965624	-3.542566	-4.029935	61	62	63
22 H	-0.479878	-4.695202	-7.336175	-0.253940	-2.484594	-3.882137	64	65	66
23 H	7.683529	-5.476638	-5.379015	4.065949	-2.898112	-2.846452	67	68	69
24 C	-4.254067	3.549054	1.392460	-2.251155	1.878078	0.736858	70	71	72
25 C	-0.469386	6.072080	1.424884	-0.248389	3.213206	0.754016	73	74	75
26 O	-4.631105	4.034449	3.570170	-2.450675	2.134939	1.889253	76	77	78
27 H	-5.591279	2.503908	0.194627	-2.958777	1.325011	0.102992	79	80	81

28 H	-0.057917	5.310916	3.281163	-0.030648	2.810416	1.736317	82	83	84
29 H	-1.449114	7.887033	1.582546	-0.766838	4.173638	0.837447	85	86	87
30 H	1.293453	6.307085	0.394305	0.684466	3.337566	0.208657	88	89	90
31 H	-0.963033	5.522478	-3.559863	-0.509615	2.922370	-1.883798	91	92	93
32 H	-3.972245	4.084703	-3.470210	-2.102022	2.161532	-1.836356	94	95	96
33 H	-3.564767	7.196533	-2.251024	-1.886393	3.808241	-1.191191	97	98	99
34 N	-2.065732	4.285717	0.024349	-1.093138	2.267904	0.012885	100	101	102
35 C	-2.690875	5.330571	-2.464997	-1.423950	2.820817	-1.304420	103	104	105
36 O	-3.536010	-0.448734	-7.731501	-1.871176	-0.237460	-4.091334	106	107	108
37 C	-1.480538	0.170739	-6.045739	-0.783467	0.090351	-3.199267	109	110	111
38 C	-2.281268	-0.827058	-3.433875	-1.207195	-0.437660	-1.817128	112	113	114
39 C	-5.159249	-0.833143	-3.625146	-2.730157	-0.440880	-1.918345	115	116	117
40 C	-5.520987	-1.616272	-6.365958	-2.921581	-0.855294	-3.368720	118	119	120
41 H	-6.037626	-2.147867	-2.300344	-3.194974	-1.136602	-1.217289	121	122	123
42 H	-1.299239	2.231677	-6.079314	-0.687528	1.180953	-3.217034	124	125	126
43 H	-7.314341	-0.993757	-7.185010	-3.870582	-0.525874	-3.802143	127	128	129
44 H	-1.750219	-2.823454	-3.449500	-0.926176	-1.494107	-1.825397	130	131	132
45 H	-6.028270	1.021911	-3.340323	-3.190023	0.540772	-1.767623	133	134	135
46 H	-5.405489	-3.680862	-6.549091	-2.860461	-1.947828	-3.465630	136	137	138

Coordinates of free ligand: full optimization at PBE0//TZDP level of theory:

Coordinates (Cartesian)
==========

Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 H	-6.013998	-3.499287	-7.111980	-3.182471	-1.851743	-3.763498	1	2	3
2 O	-3.546909	-0.663536	-7.994989	-1.876944	-0.351128	-4.230766	4	5	6
3 C	-1.5								
99528	0.532193	-6.529669	-0.846434	0.281624	-3.455352	7	8	9	
4 C	-2.540705	0.490129	-3.821277	-1.344483	0.259365	-2.022133	10	11	12
5 C	-4.083890	-1.901406	-3.775021	-2.161102	-1.006181	-1.997655	13	14	15
6 C	-5.387390	-1.684929	-6.318697	-2.850884	-0.891626	-3.343710	16	17	18
7 H	-3.041670	-3.744072	-3.724765	-1.609582	-1.981277	-1.971061	19	20	21
8 H	-1.319443	2.454737	-7.286810	-0.698219	1.298991	-3.856014	22	23	24
9 H	-7.015685	-0.402489	-6.192759	-3.712541	-0.212988	-3.277067	25	26	27
10 H	-1.009752	0.568889	-2.434353	-0.534338	0.301043	-1.288204	28	29	30
11 H	-5.458178	-1.963450	-2.226136	-2.888344	-1.039013	-1.178020	31	32	33
12 C	0.856245	-0.890456	-6.843931	0.453105	-0.471209	-3.621652	34	35	36
13 C	3.156531	0.345922	-6.433105	1.670364	0.183054	-3.404252	37	38	39
14 C	5.447136	-0.917218	-6.446817	2.882500	-0.485371	-3.411509	40	41	42
15 C	5.499080	-3.501518	-6.894331	2.909988	-1.852923	-3.648323	43	44	45
16 C	3.256001	-4.767103	-7.370170	1.723001	-2.522642	-3.900126	46	47	48
17 C	0.971819	-3.475111	-7.372617	0.514265	-1.838949	-3.901421	49	50	51
18 H	3.134187	2.366969	-6.073000	1.658540	1.252546	-3.213693	52	53	54

19 H	7.210024	0.078996	-6.127621	3.815380	0.041803	-3.242597	55	56	57
20 O	7.810096	-4.715281	-6.898504	4.132925	-2.495219	-3.650531	58	59	60
21 H	3.294200	-6.783080	-7.779567	1.743216	-3.589451	-4.116769	61	62	63
22 H	-0.759408	-4.464212	-7.826155	-0.401861	-2.362359	-4.141423	64	65	66
23 H	7.502692	-6.471084	-7.222712	3.970254	-3.424350	-3.822094	67	68	69

Coordinates of free catalyzer: full optimization at PBE0//TZDP level of theory:

Coordinates (Cartesian)

Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 C	-4.178815	2.899382	0.794803	-2.211334	1.534287	0.420592	1	2	3
2 C	-0.739579	5.743844	-0.151848	-0.391368	3.039512	-0.080355	4	5	6
3 O	-4.991984	4.414490	2.232390	-2.641644	2.336047	1.181330	7	8	9
4 H	-5.085596	1.079946	0.349408	-2.691181	0.571483	0.184899	10	11	12
5 H	-0.377046	5.938162	1.859701	-0.199524	3.142340	0.984111	13	14	15
6 H	-2.025861	7.237918	-0.759083	-1.072039	3.830141	-0.401689	16	17	18
7 H	1.023339	5.870242	-1.201578	0.541528	3.106398	-0.635848	19	20	21
8 H	-0.591580	2.858974	-4.367621	-0.313051	1.512904	-2.311245	22	23	24
9 H	-3.270238	0.993786	-3.606725	-1.730535	0.525889	-1.908596	25	26	27
10 H	-3.603371	4.307142	-4.081056	-1.906822	2.279241	-2.159602	28	29	30
11 N	-1.868933	3.246525	-0.621867	-0.988997	1.717987	-0.329078	31	32	33
12 C	-2.370073	2.826135	-3.337057	-1.254188	1.495526	-1.765895	34	35	36
13 Pd	0.657966	0.323045	0.581774	0.348180	0.170948	0.307862	37	38	39
14 Cl	-0.047933	1.085734	4.718985	-0.025365	0.574546	2.497179	40	41	42
15 C	3.415661	-2.320213	-1.775617	1.807490	-1.227804	-0.939616	43	44	45
16 N	3.145996	-2.458570	0.904605	1.664789	-1.301019	0.478696	46	47	48
17 H	4.708687	-2.115510	1.954389	2.491730	-1.119480	1.034218	49	50	51
18 H	2.364931	-4.238682	1.221468	1.251467	-2.243014	0.646373	52	53	54
19 H	5.122108	-1.382692	-2.425921	2.710503	-0.731689	-1.283742	55	56	57
20 C	2.902412	-5.131261	-2.968566	1.535890	-2.715347	-1.570897	58	59	60
21 O	1.907378	-6.505535	-1.364208	1.009341	-3.442581	-0.721908	61	62	63
22 O	3.561636	-5.326666	-5.158980	1.884737	-2.818750	-2.730015	64	65	66
23 H	1.704637	-1.271375	-2.592907	0.902055	-0.672782	-1.372107	67	68	69

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