

# Supporting Information

Kinetic Resolution of Racemic 5-Alkylcyclohexenones via Pd(II)-catalyzed  
1, 4-Additions of Arylboronic acids - Access to 3-alkyl-5-  
arylcyclohexanones

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1.1

#### Calculation of Selectivity Factor (s)

The selectivity factor was calculated based on conversion and selectivities of the product alkanone according to the following equation:

$$s = \{ \ln [ 1 - C ( 1 + ee ) ] \} / \{ \ln [ 1 - C ( 1 - ee ) ] \}$$

#### Determination of *dr*

Based on the assignment by Kolb *et. al.* for compound **3a**, the retention times are as follows, *trans*-(3*R*, 5*R*), *trans*-(3*S*, 5*S*), *cis*-(3*S*, 5*R*) and *cis*-(3*R*, 5*S*).

Therefore,  $dr = [trans-(3R, 5R) + trans-(3S, 5S)] : [cis-(3S, 5R) + cis-(3R, 5S)]$

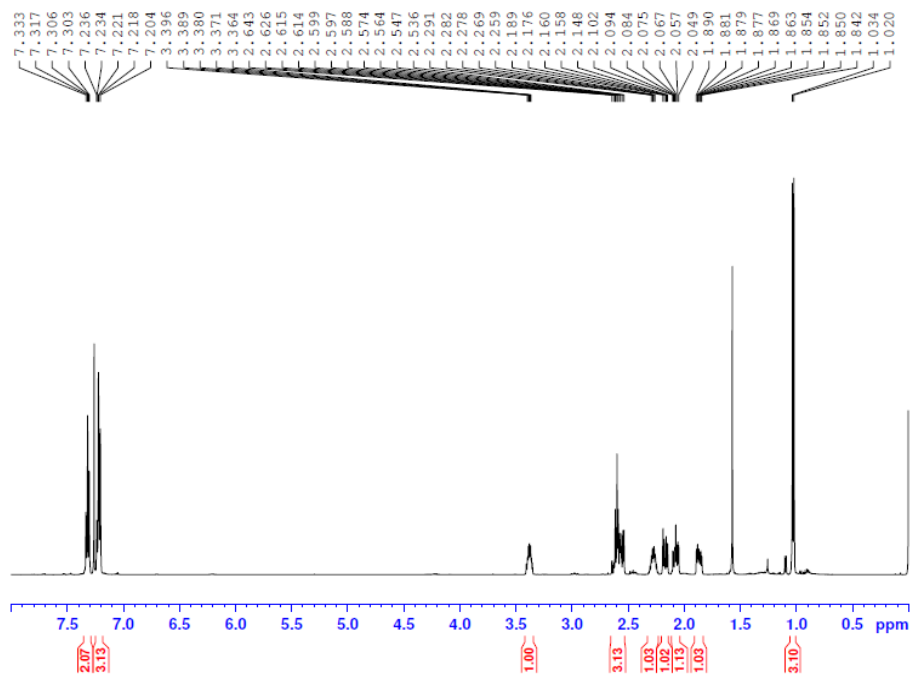
and,  $trans\ ee = [trans-(3R, 5R) - trans-(3S, 5S)] / [trans-(3R, 5R) + trans-(3S, 5S)]$

Consequent values of adducts are calculated based on the above.

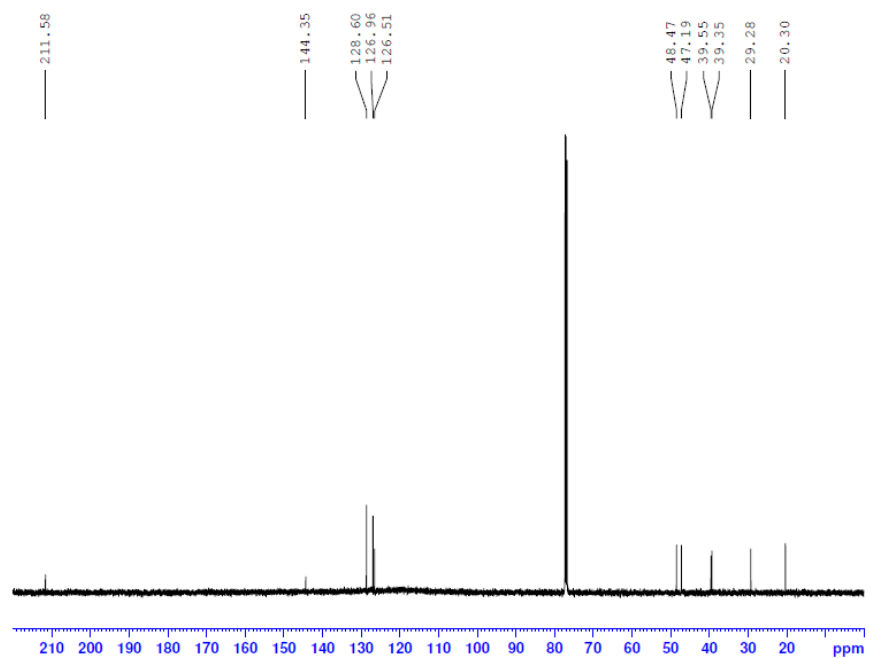
1.2.1

3-methyl-5-phenyl cyclohexanone (**3a**):

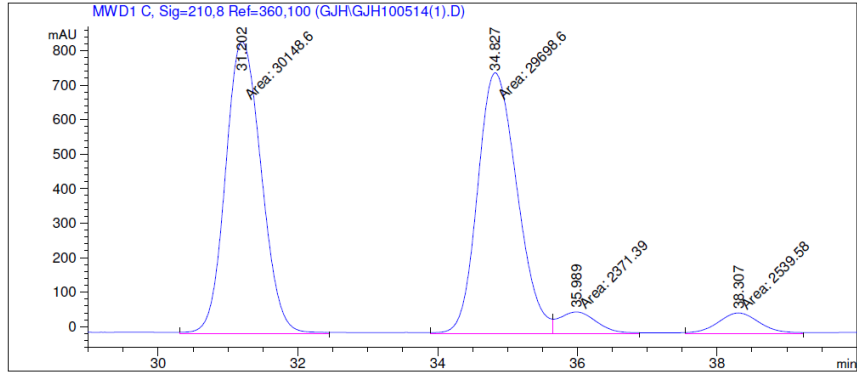
$^1\text{H}$  NMR: **3a**



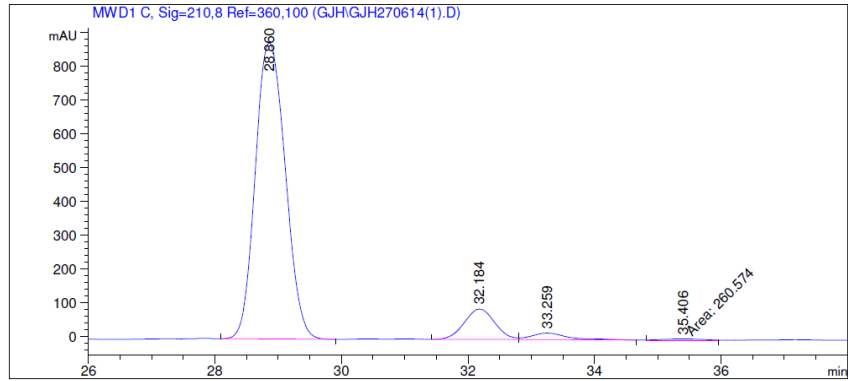
$^{13}\text{C}$  NMR: **3a**



HPLC Data: 3a



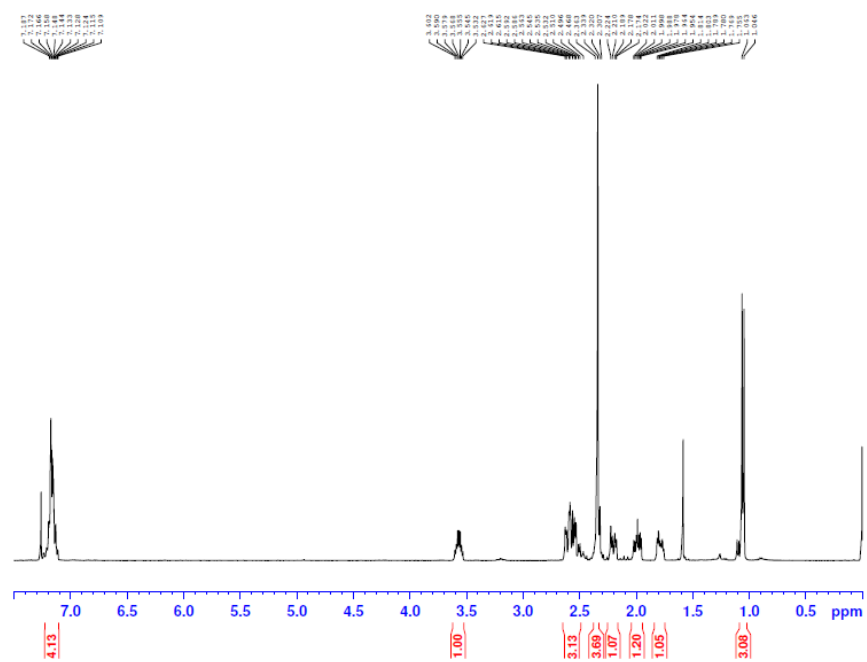
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.202	MM	0.5937	3.01486e4	846.37921	46.5557
2	34.827	MF	0.6548	2.96986e4	755.95355	45.8608
3	35.989	FM	0.6275	2371.38623	62.98321	3.6619
4	38.307	MM	0.7059	2539.58252	59.95761	3.9216



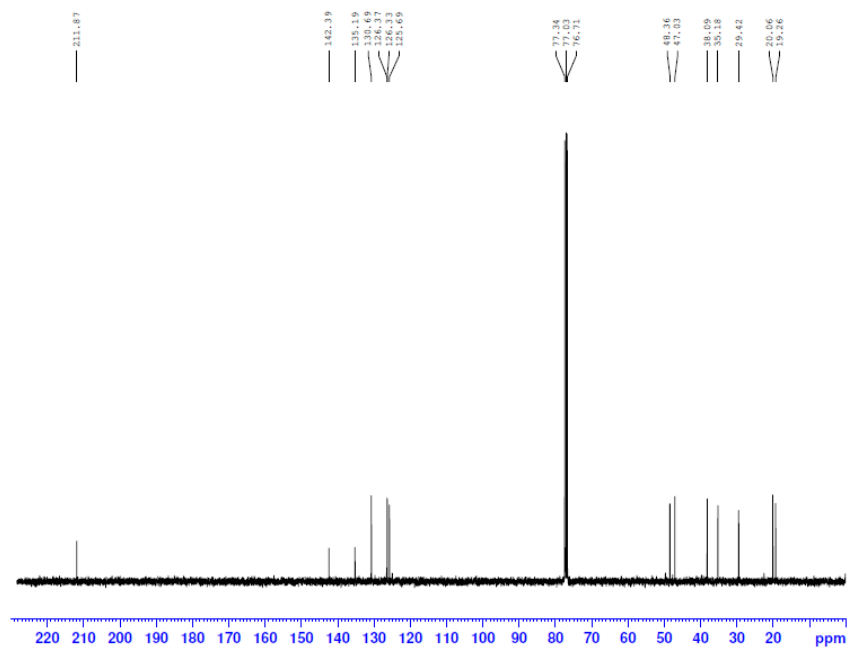
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.860	BB	0.5299	2.88330e4	876.25159	87.6686
2	32.184	BV	0.5219	3010.72681	90.07731	9.1543
3	33.259	VB	0.5818	784.31287	19.47725	2.3848
4	35.406	MM	0.7888	260.57355	5.50589	0.7923

3-methyl-5-(*o*-tolyl)cyclohexanone (**3b**):

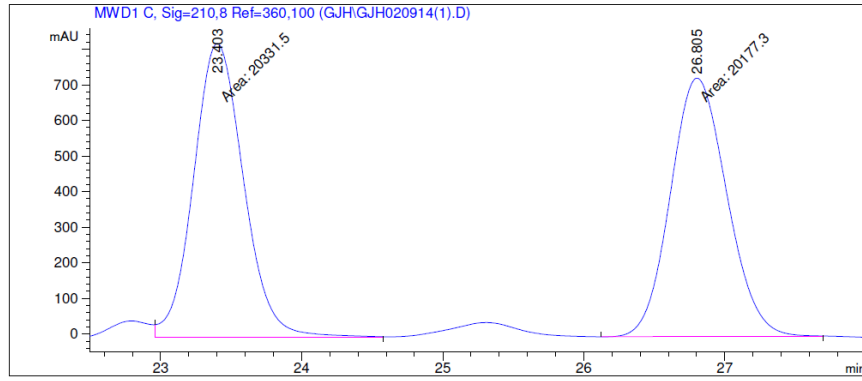
$^1\text{H}$  NMR: **3b**



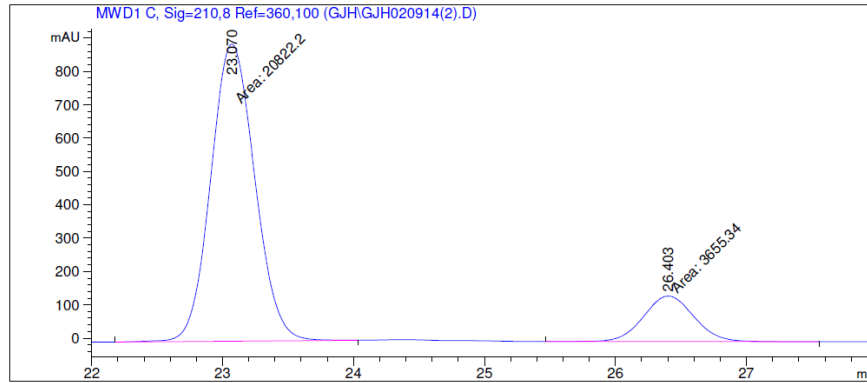
$^{13}\text{C}$  NMR: **3b**



HPLC Data: 3b



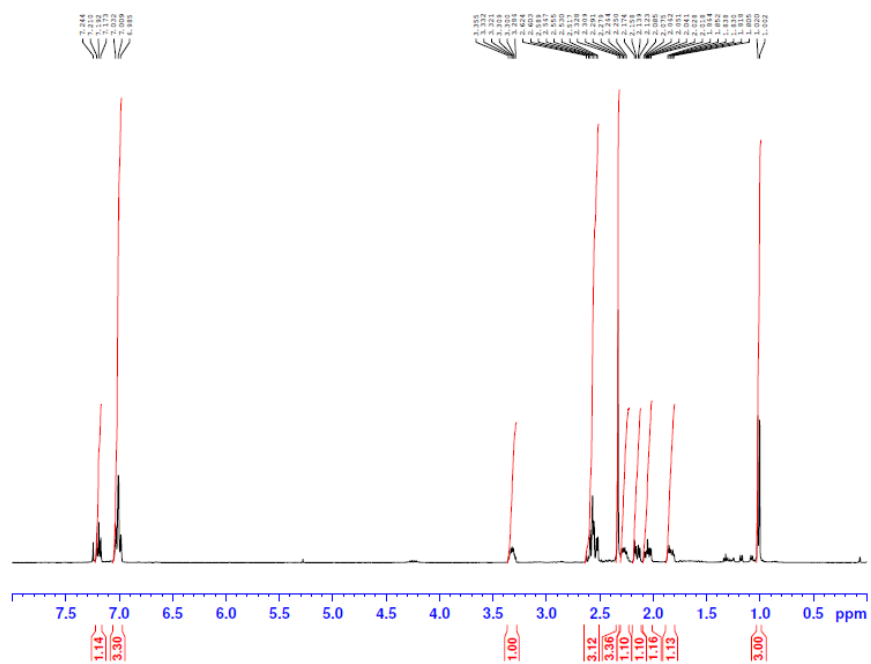
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.403	MM	0.4109	2.03315e4	824.76764	50.1903
2	26.805	MM	0.4632	2.01773e4	726.01483	49.8097



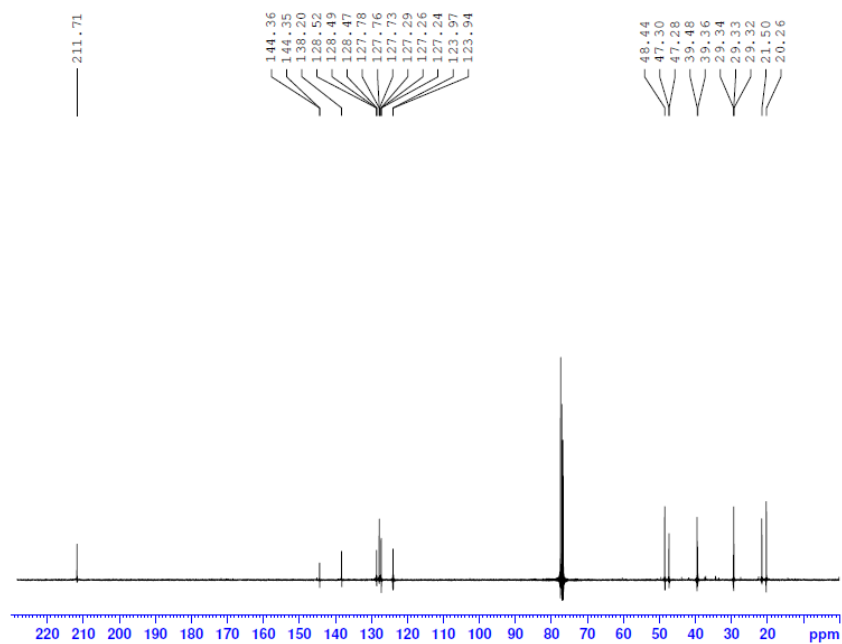
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.070	MM	0.3894	2.08222e4	891.17834	85.0665
2	26.403	MM	0.4466	3655.34204	136.41870	14.9335

3-methyl-5-(*m*-tolyl)cyclohexanone (**3c**):

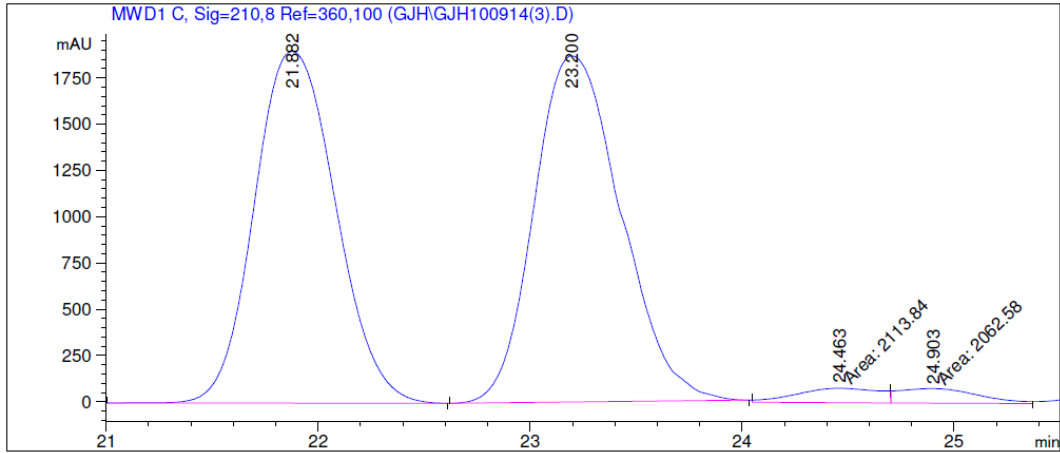
$^1\text{H}$  NMR: **3c**



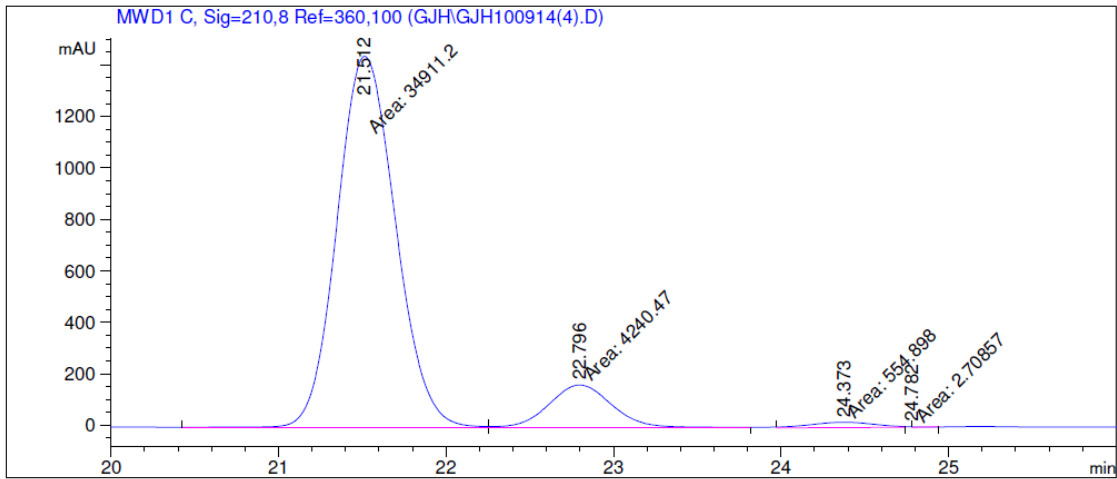
$^{13}\text{C}$  NMR: **3c**



HPLC Data: 3c



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.882	VB	0.4211	5.06967e4	1901.19153	46.8774
2	23.200	BB	0.4402	5.32743e4	1870.77722	49.2608
3	24.463	MF	0.4528	2113.83618	77.81053	1.9546
4	24.903	FM	0.4358	2062.57813	78.87357	1.9072

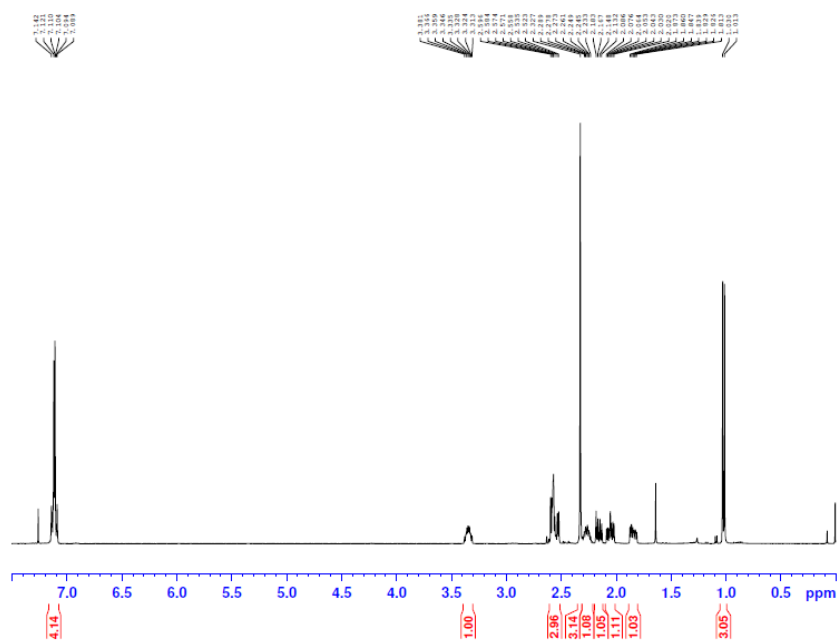


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.512	MF	0.4038	3.49112e4	1441.03577	87.9170
2	22.796	FM	0.4298	4240.47363	164.44882	10.6788
3	24.373	MM	0.4392	554.89795	21.05546	1.3974
4	24.782	MM	0.0286	2.70857	1.57646	6.821e-3

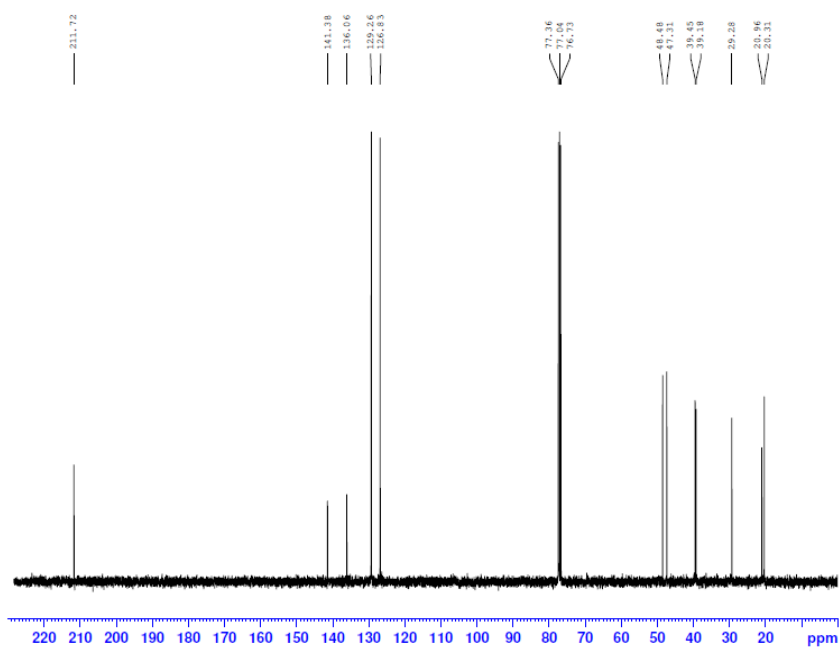


3-methyl-5-(*p*-tolyl)cyclohexanone (**3d**):

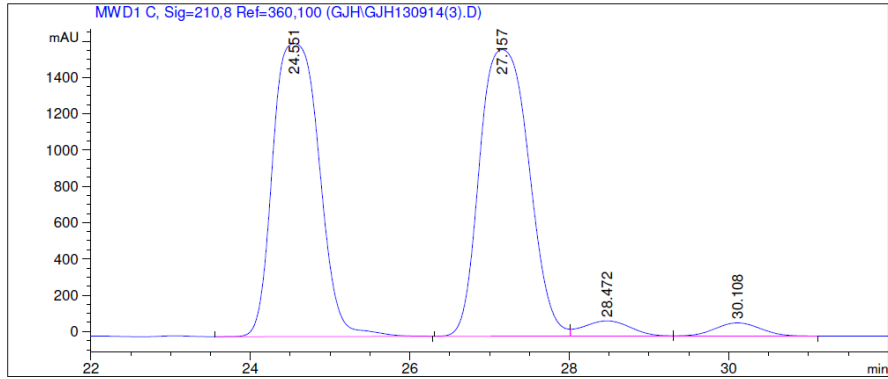
$^1\text{H}$  NMR: **3d**



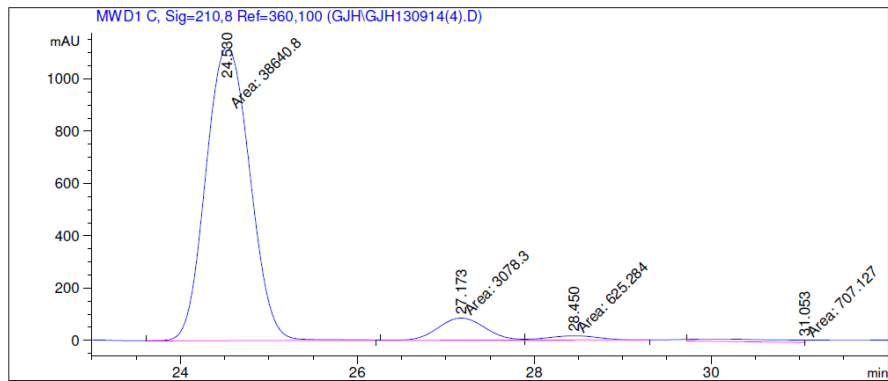
$^{13}\text{C}$  NMR: **3d**



HPLC Data: 3d



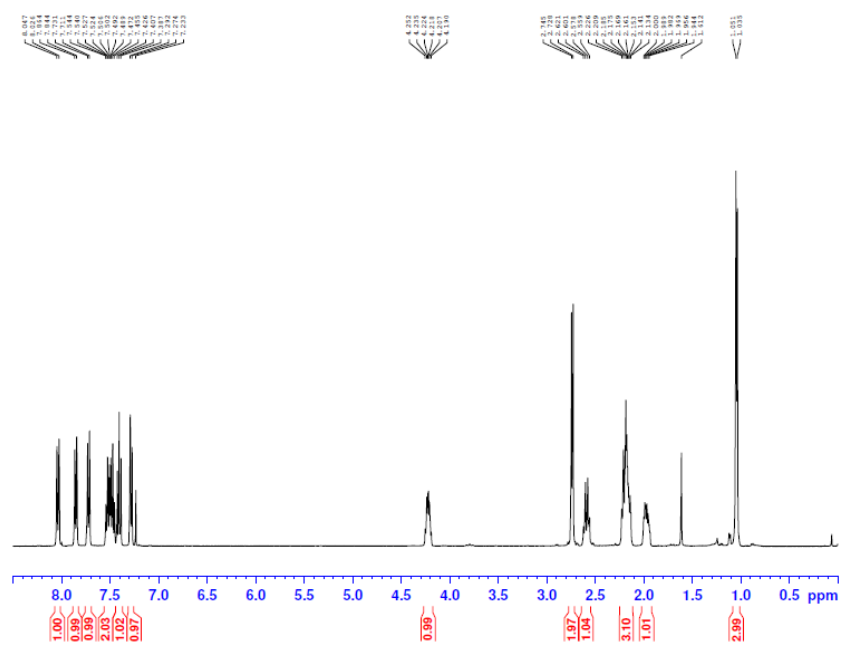
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.551	BB	0.6453	6.49943e4	1615.75574	46.7782
2	27.157	BV	0.6934	6.76299e4	1579.80139	48.6752
3	28.472	VV	0.6135	3426.80249	84.43647	2.4664
4	30.108	VB	0.6055	2890.34546	72.74877	2.0803



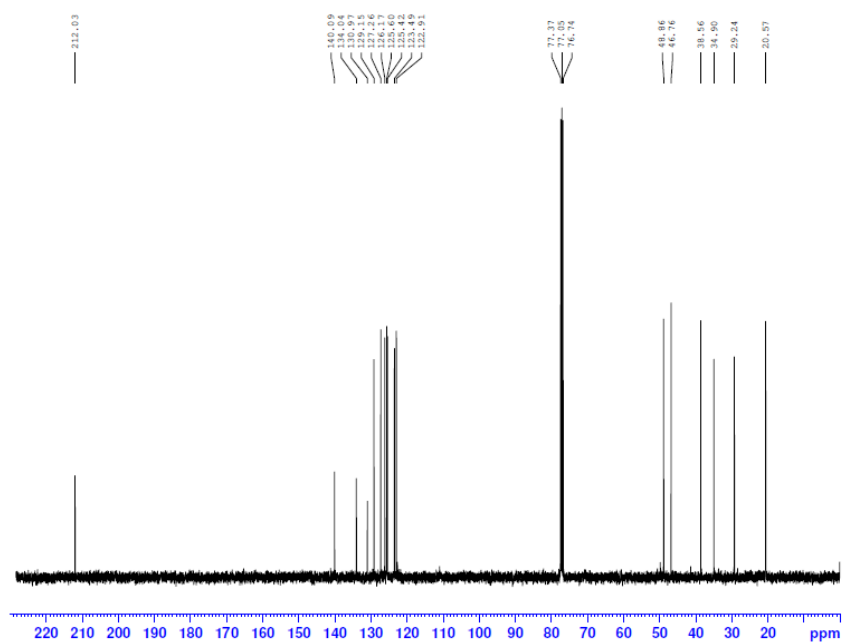
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.530	MM	0.5742	3.86408e4	1121.49304	89.7548
2	27.173	MF	0.6095	3078.29517	84.17308	7.1503
3	28.450	FM	0.6432	625.28406	16.20205	1.4524
4	31.053	MM	1.2235	707.12683	9.63274	1.6425

3-methyl-5-(1-naphthalene)cyclohexanone (**3e**):

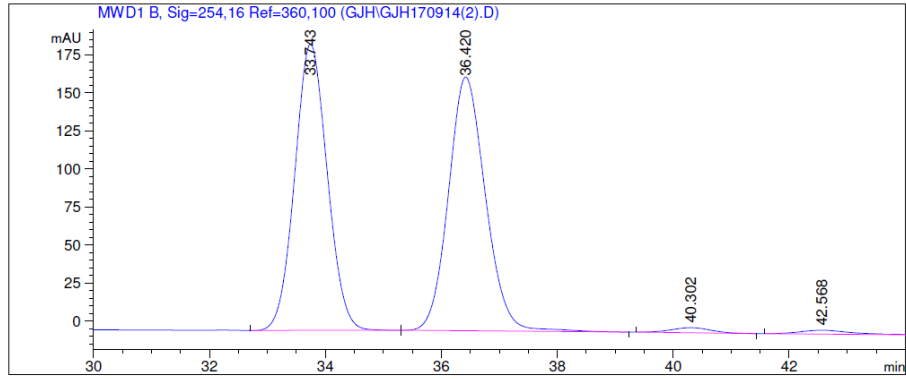
$^1\text{H}$  NMR: **3e**



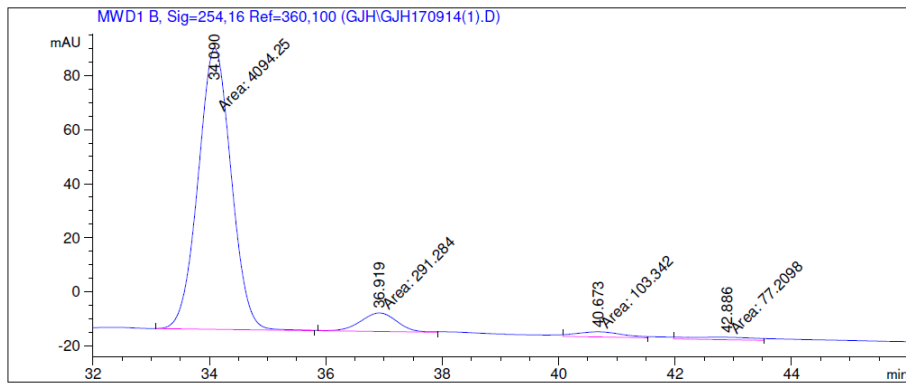
$^{13}\text{C}$ : **3e**



HPLC Data: 3e



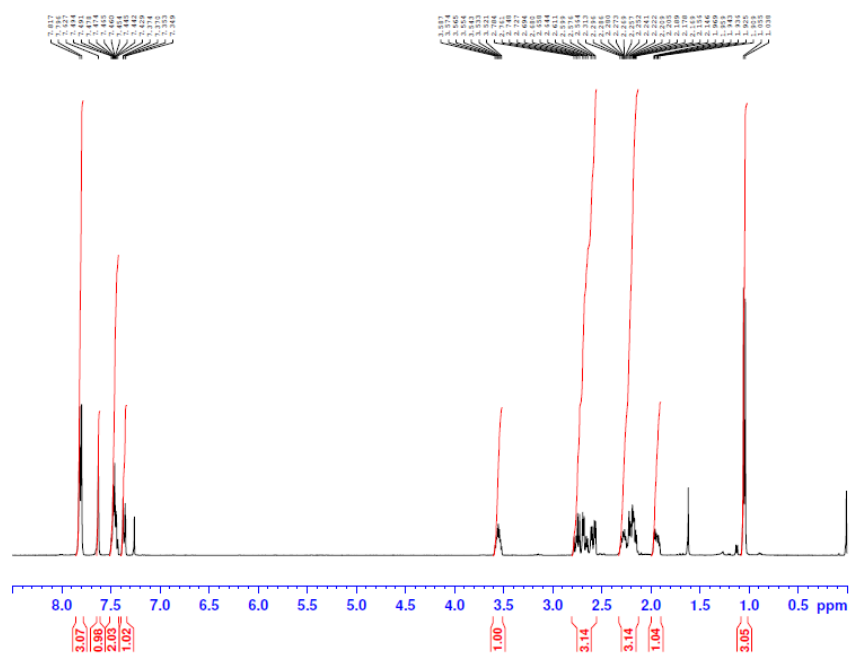
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.743	BB	0.6068	7342.55566	188.34312	48.6787
2	36.420	BB	0.6780	7407.92139	166.84525	49.1120
3	40.302	BB	0.6134	158.55989	3.39169	1.0512
4	42.568	BBA	0.8152	174.68863	2.58892	1.1581



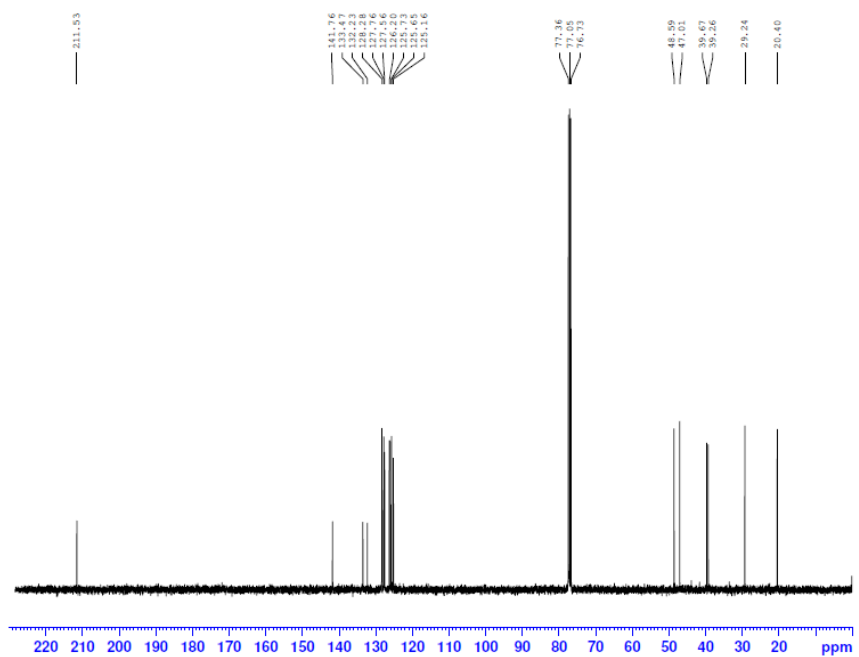
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	34.090	MM	0.6554	4094.25439	104.11782	89.6665
2	36.919	MM	0.7085	291.28369	6.85227	6.3793
3	40.673	MM	0.9171	103.34182	1.87808	2.2632
4	42.886	MM	1.3274	77.20979	9.69408e-1	1.6909

3-methyl-5-(2-naphthalene)cyclohexanone (**3f**):

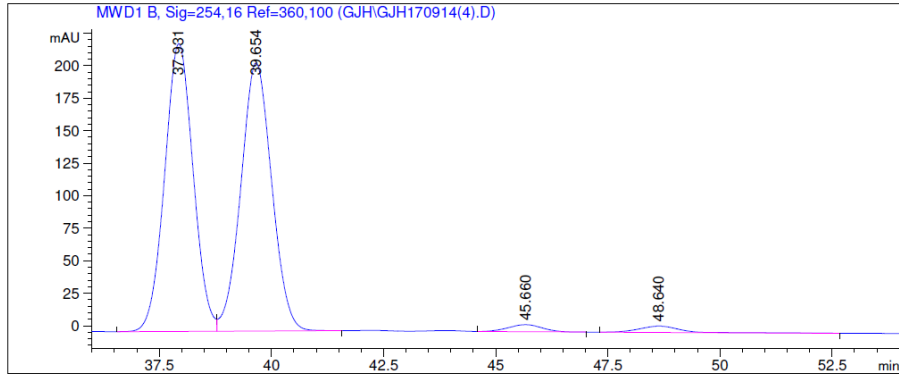
$^1\text{H}$  NMR: **3f**



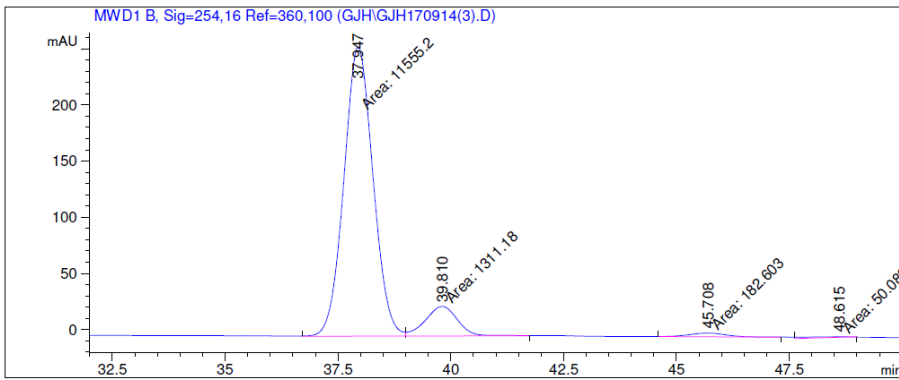
$^{13}\text{C}$  NMR: **3f**



HPLC Data: 3f



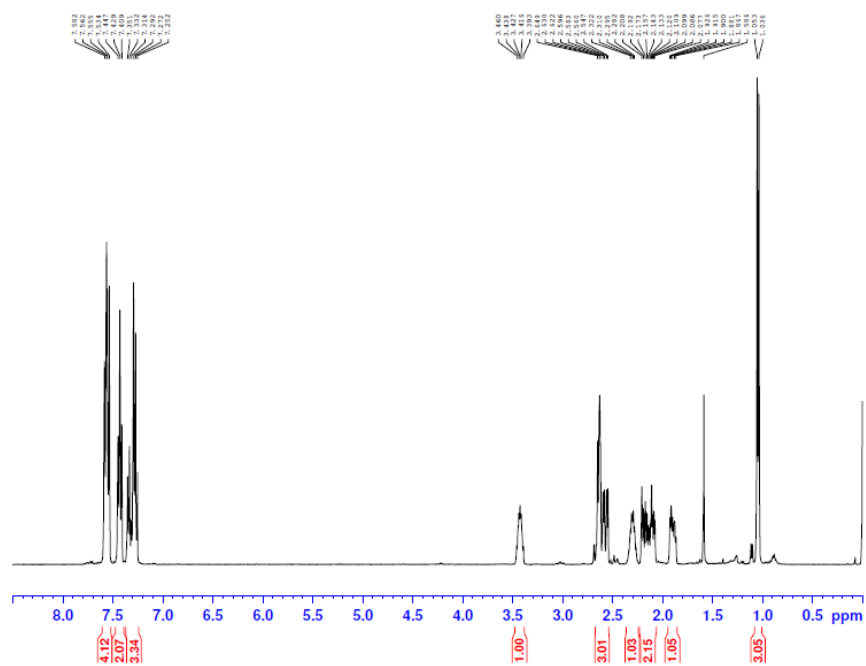
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.931	BV	0.6889	9805.44238	221.30238	48.3836
2	39.654	VB	0.7425	9874.68164	206.28798	48.7253
3	45.660	BB	0.7754	285.72226	5.36426	1.4099
4	48.640	BB	0.8049	300.18845	4.85795	1.4812



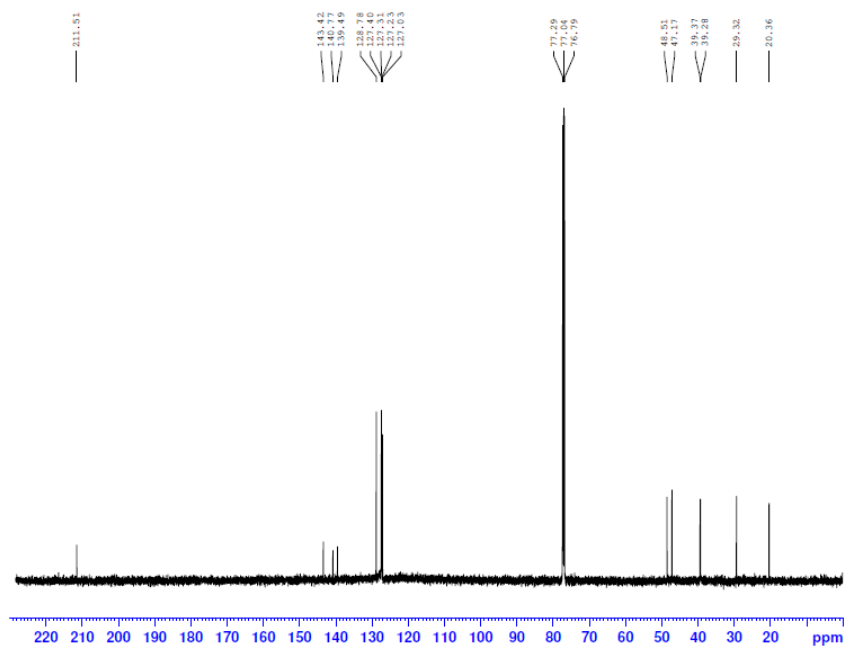
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.947	MF	0.7488	1.15552e4	257.20090	88.2140
2	39.810	FM	0.8283	1311.18030	26.38168	10.0097
3	45.708	MM	0.9201	182.60315	3.30750	1.3940
4	48.615	MM	1.3842	50.08234	4.25500e-1	0.3823

3-methyl-5-(Biphenyl-4)cyclohexanone (**3g**):

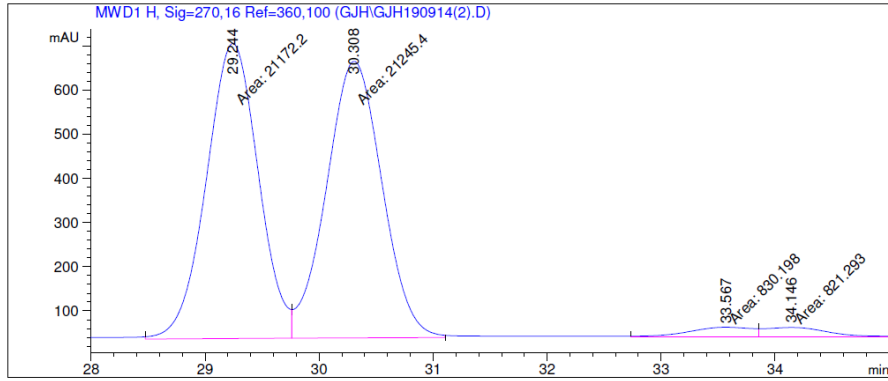
$^1\text{H}$  NMR: **3g**



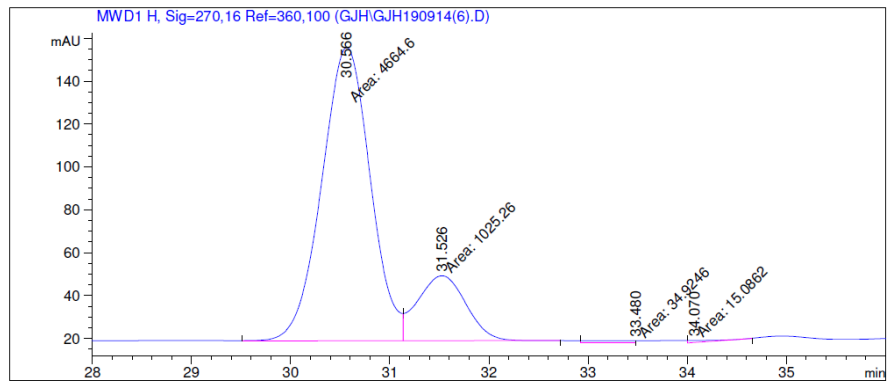
$^{13}\text{C}$  NMR: **3g**



HPLC Data: 3g



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.244	MF	0.5283	2.11722e4	667.87811	48.0433
2	30.308	FM	0.5658	2.12454e4	625.83911	48.2092
3	33.567	MF	0.6413	830.19849	21.57507	1.8839
4	34.146	FM	0.6520	821.29260	20.99288	1.8636

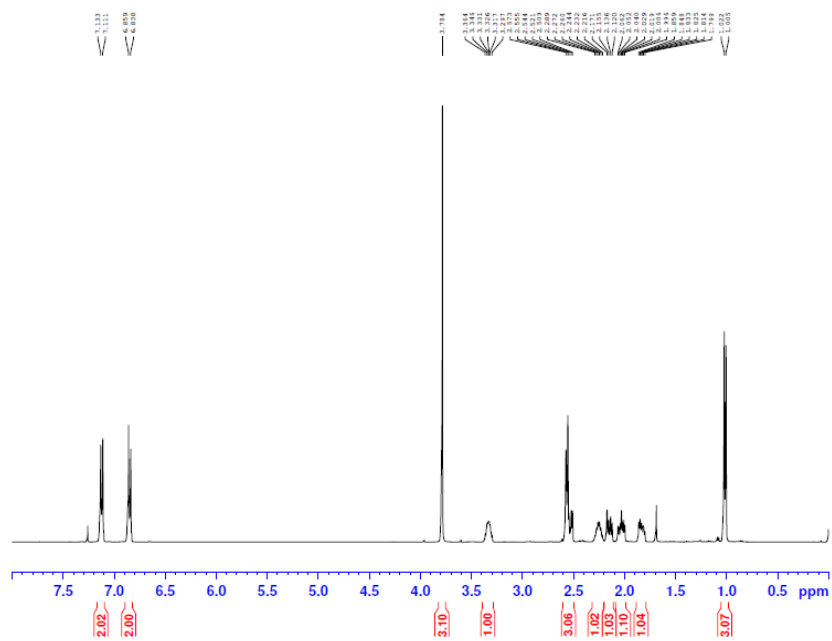


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.566	MF	0.5681	4664.60107	136.85965	81.2666
2	31.526	FM	0.5639	1025.26111	30.30319	17.8621
3	33.480	MM	0.5431	34.92465	1.07172	0.6085
4	34.070	MM	0.2604	15.08622	9.65540e-1	0.2628

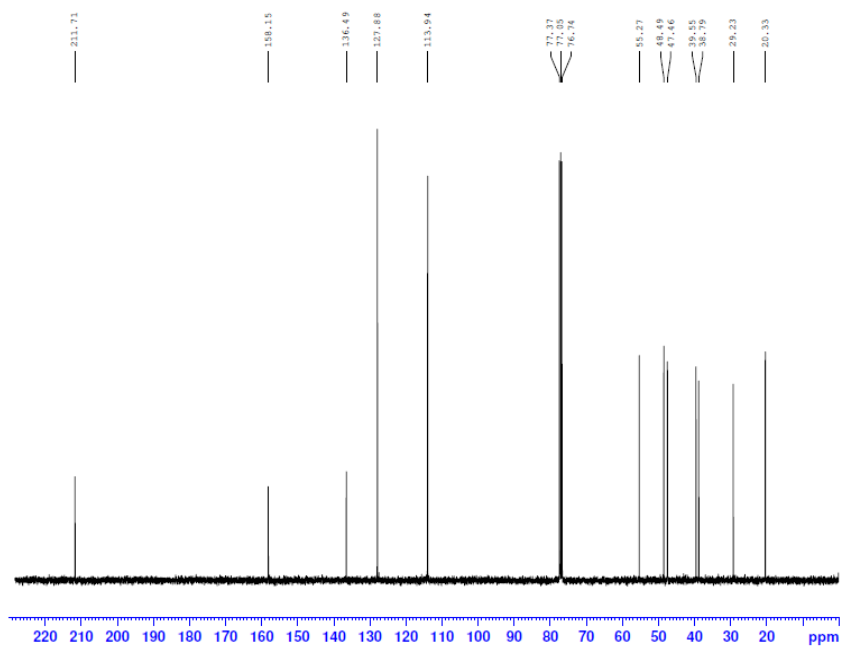


3-methyl-5- *p*-methoxyphenylcyclohexanone (**3h**):

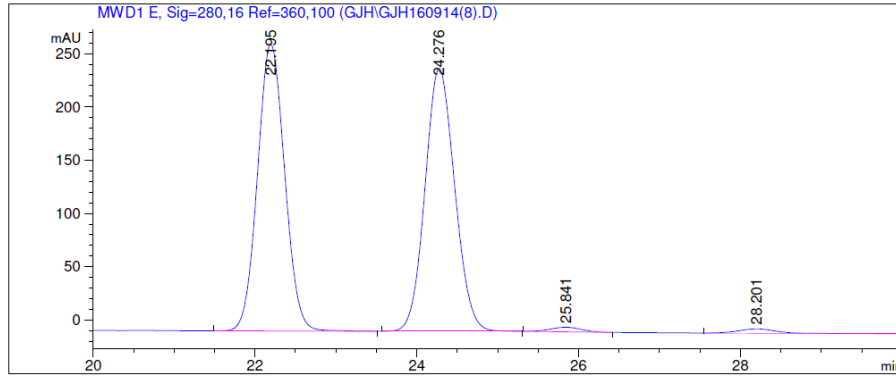
<sup>1</sup>H NMR: **3h**



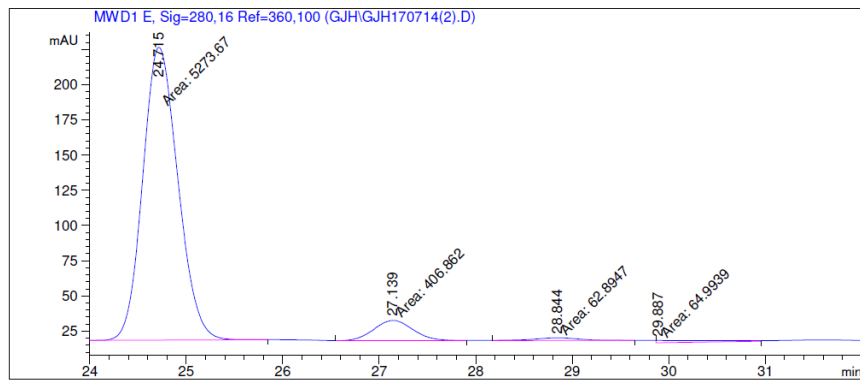
<sup>13</sup>C NMR: **3h**



HPLC Data: 3h



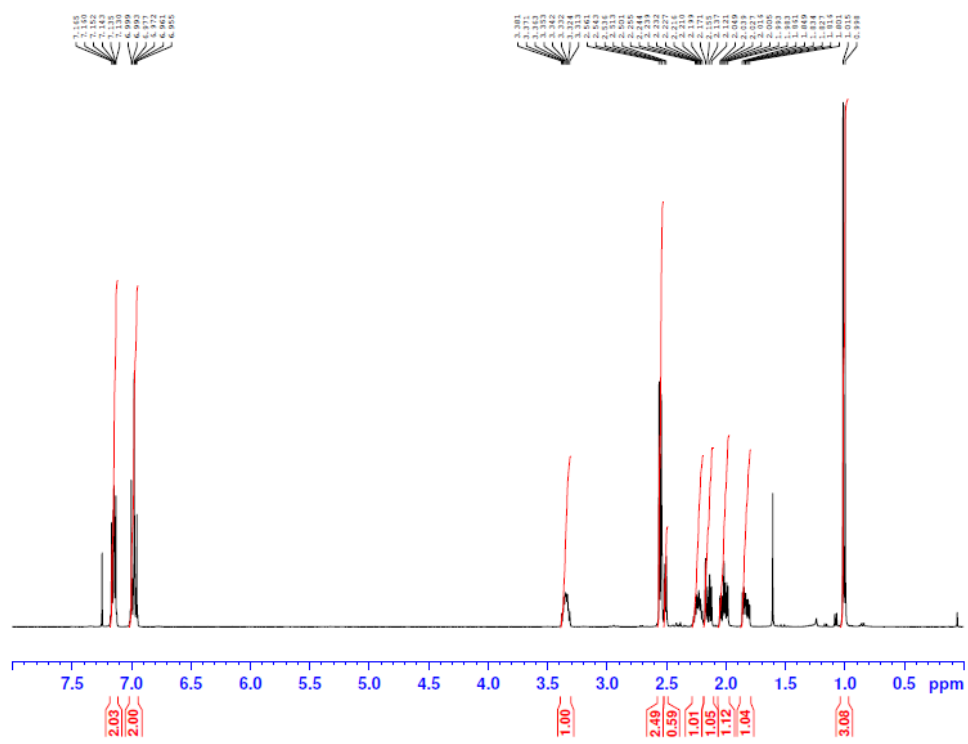
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.195	BB	0.3660	6282.16357	269.49600	49.0336
2	24.276	BB	0.3950	6282.26611	246.80898	49.0344
3	25.841	BB	0.4097	115.26737	4.37028	0.8997
4	28.201	BB	0.4714	132.26280	4.15446	1.0323



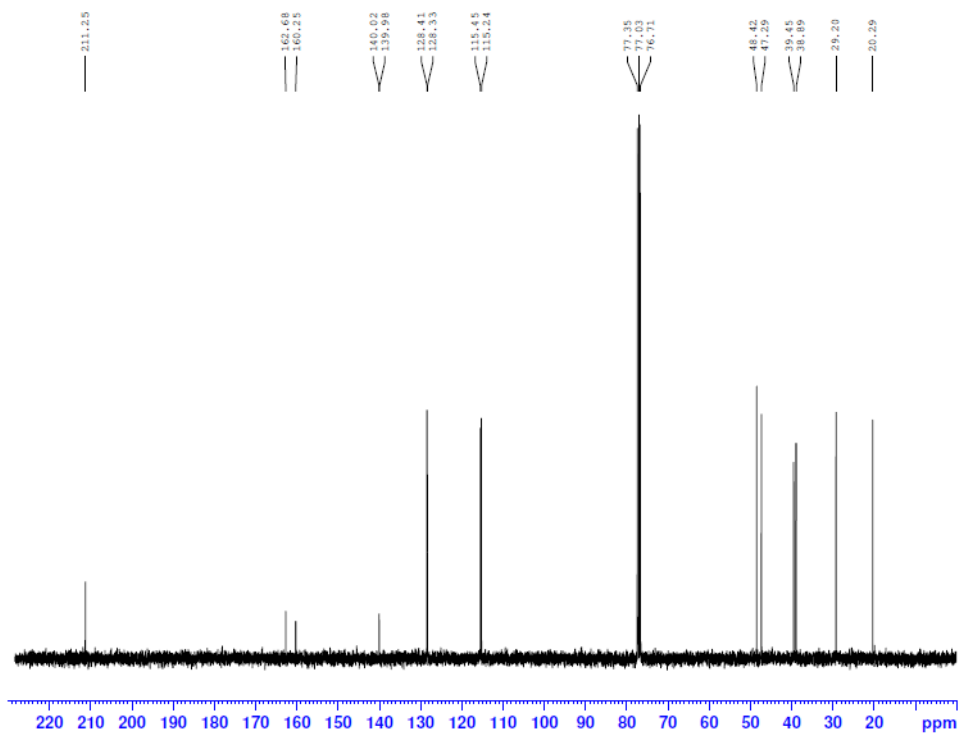
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.715	MM	0.4227	5273.67432	207.92404	90.7935
2	27.139	MM	0.4723	406.86227	14.35801	7.0047
3	28.844	MM	0.5412	62.89470	1.93700	1.0828
4	29.887	MM	0.6518	64.99390	1.66183	1.1190

3-methyl-5- *p*-fluorophenylcyclohexanone (**3i**):

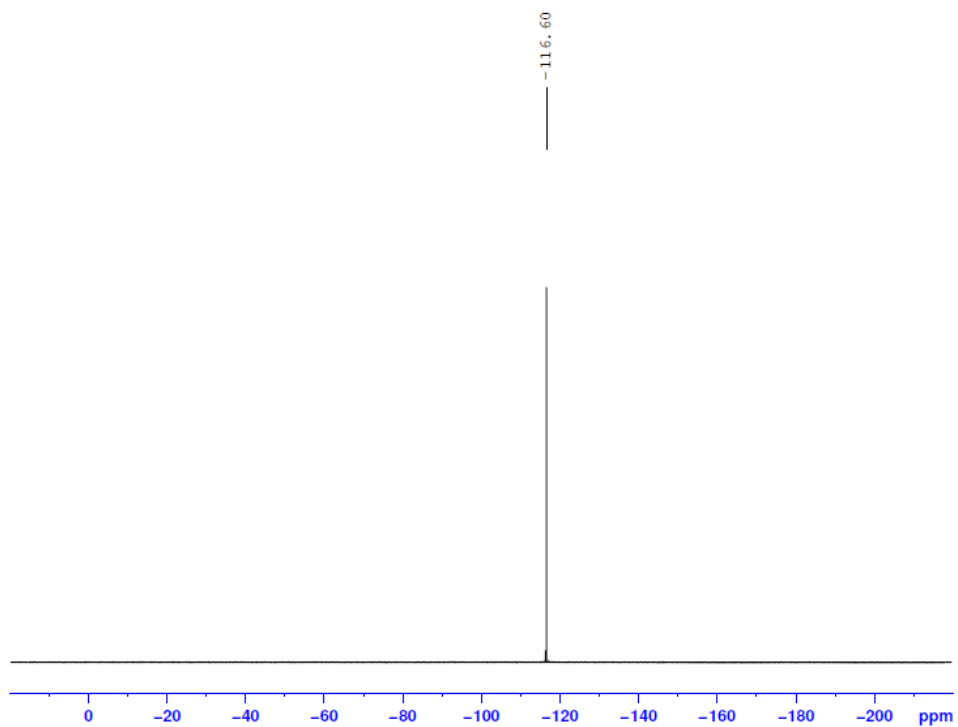
<sup>1</sup>H NMR: **3i**



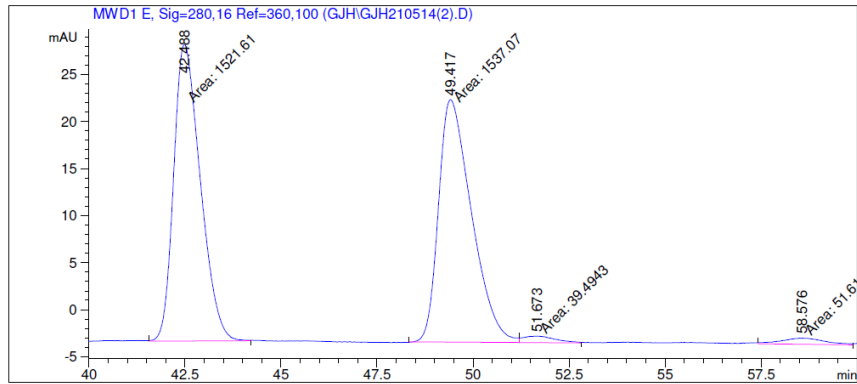
<sup>13</sup>C NMR: **3i**



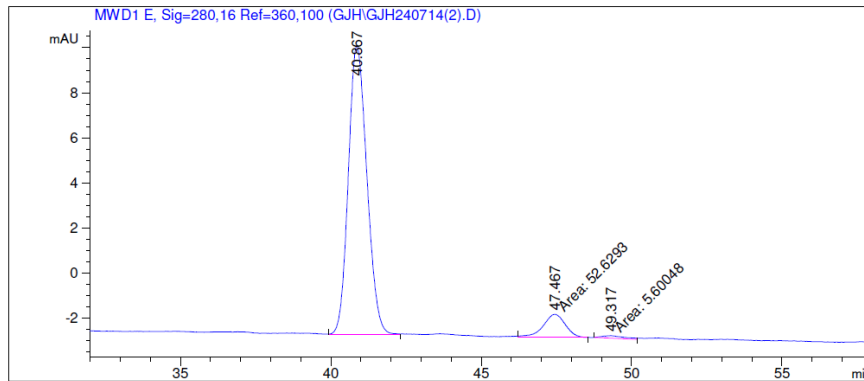
<sup>19</sup>F NMR: **3i**



HPLC Data: 3i



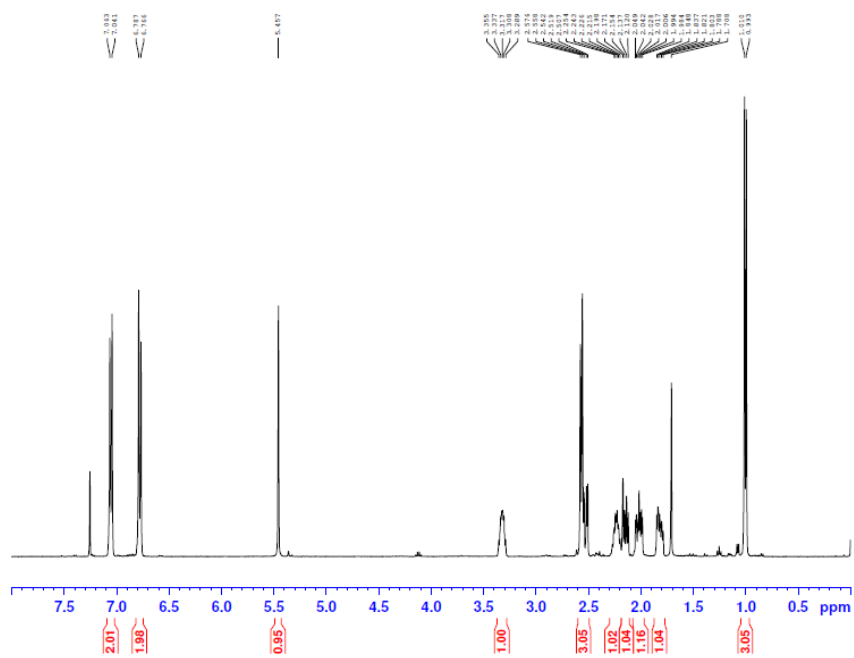
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	42.488	MM	0.8045	1521.61487	31.52444	48.3084
2	49.417	MF	0.9945	1537.06848	25.75908	48.7991
3	51.673	FM	0.9530	39.49427	6.90713e-1	1.2539
4	58.576	MM	1.3324	51.61390	6.45607e-1	1.6386



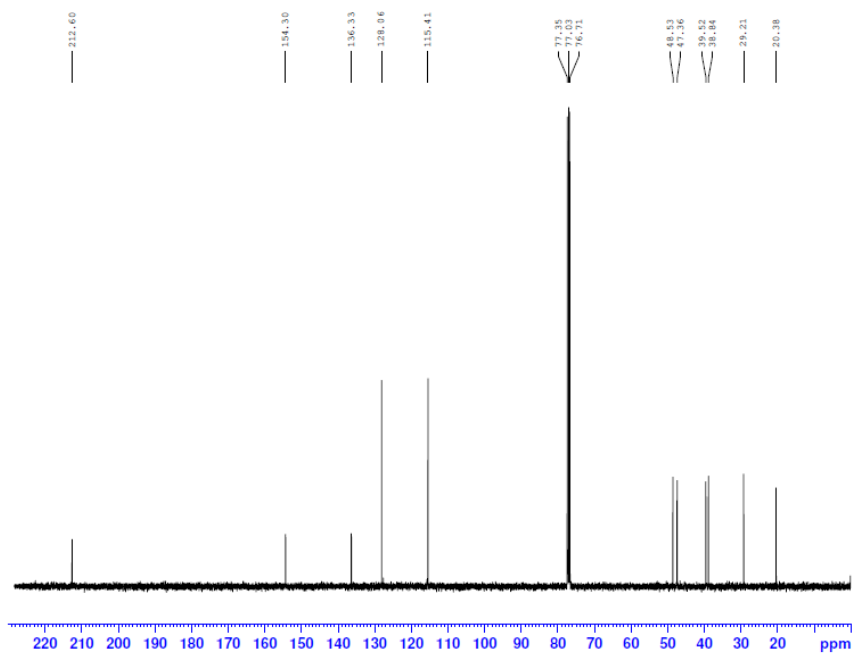
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	40.867	BB	0.6570	547.29919	12.79538	90.3837
2	47.467	MM	0.8604	52.62928	1.01942	8.6915
3	49.317	MM	0.8438	5.60048	1.10616e-1	0.9249

3-methyl-5- *p*-hydroxyphenylcyclohexanone (**3j**):

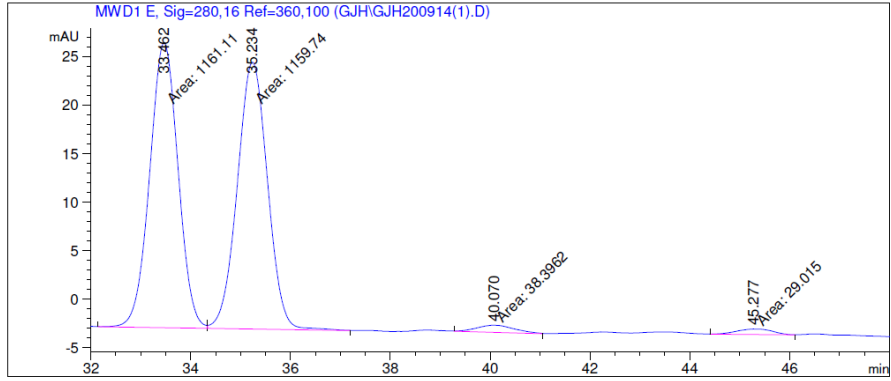
<sup>1</sup>H NMR: **3j**



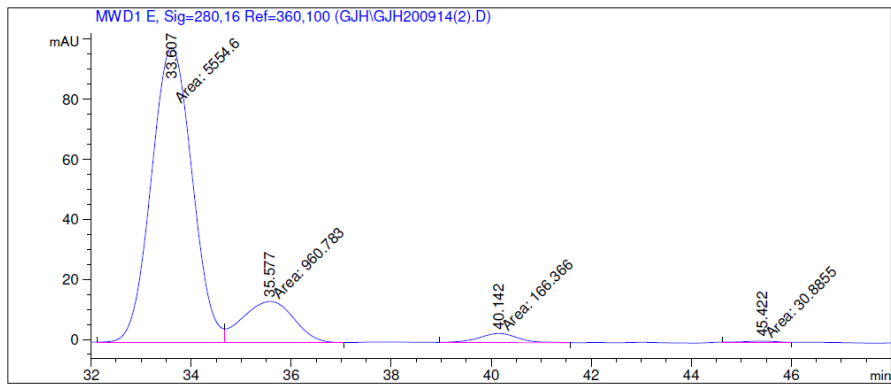
<sup>13</sup>C NMR: **3j**



HPLC Data: 3j



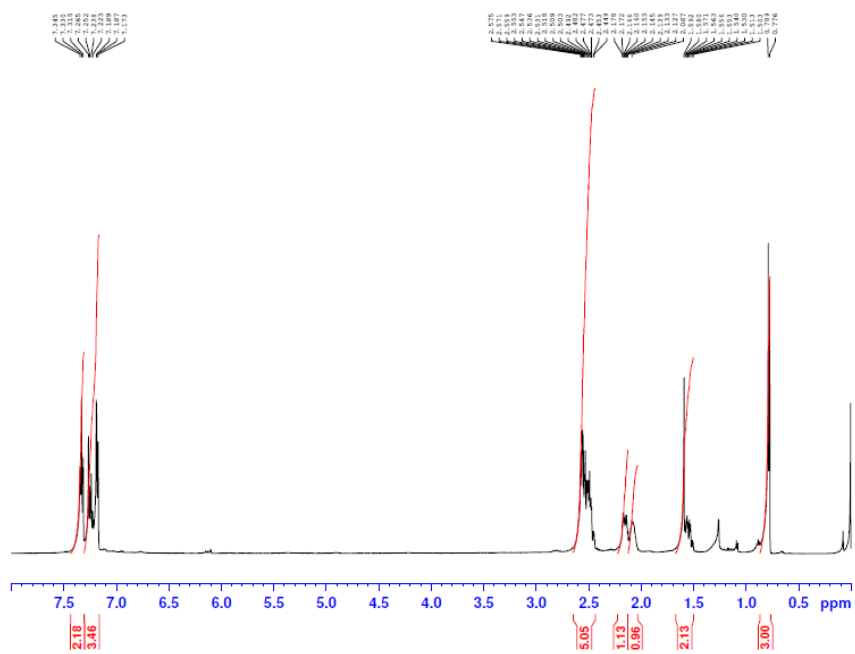
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.462	MF	0.6583	1161.10889	29.39500	48.6174
2	35.234	FM	0.7022	1159.73584	27.52764	48.5599
3	40.070	MM	0.8662	38.39620	7.38780e-1	1.6077
4	45.277	MM	0.8504	29.01501	5.68639e-1	1.2149



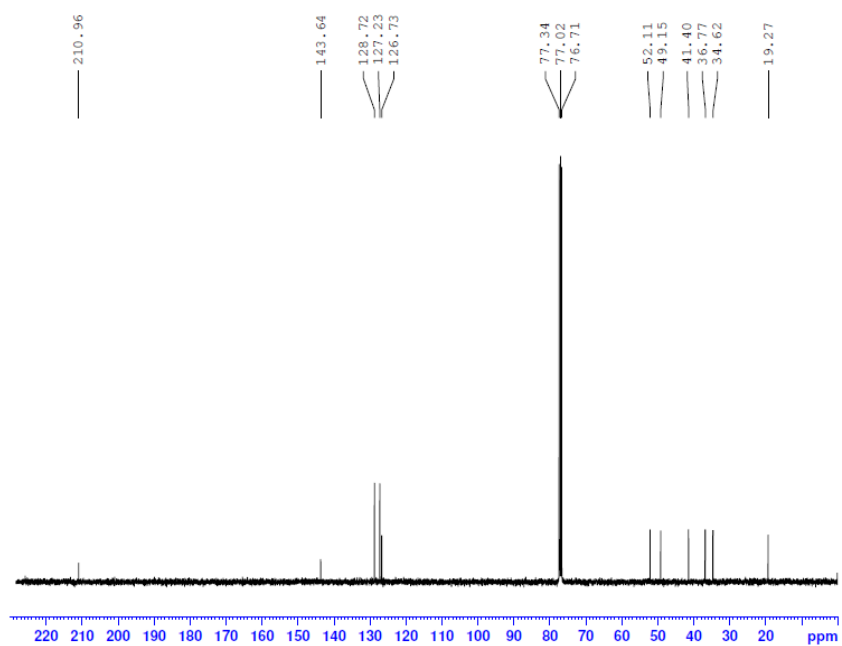
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.607	MF	0.9438	5554.59912	98.08818	82.7484
2	35.577	FM	1.1790	960.78345	13.58222	14.3131
3	40.142	MM	0.9129	166.36627	3.03731	2.4784
4	45.422	MM	0.9344	30.88548	5.50909e-1	0.4601

3-methyl-4-phenylcyclohexanone (**3k**):

<sup>1</sup>H NMR: **3k**

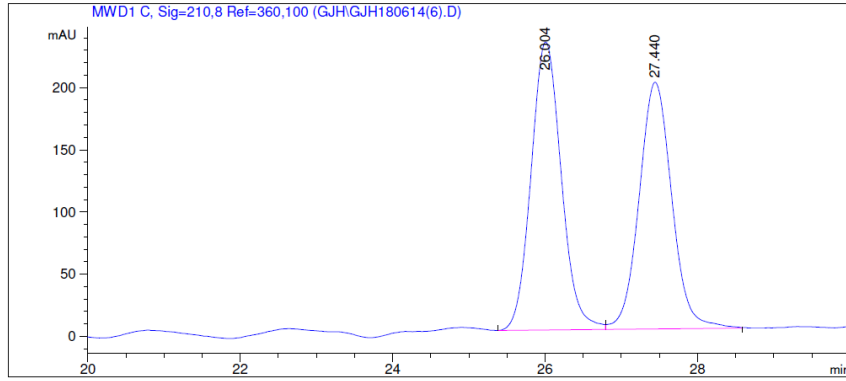


<sup>13</sup>C NMR: **3k**

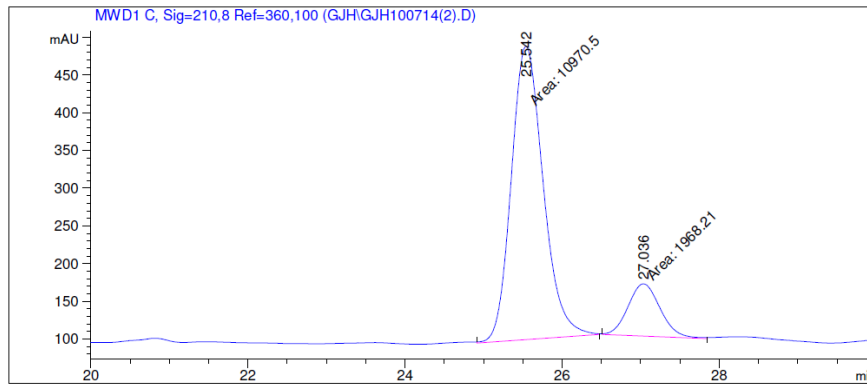




HPLC Data: 3k



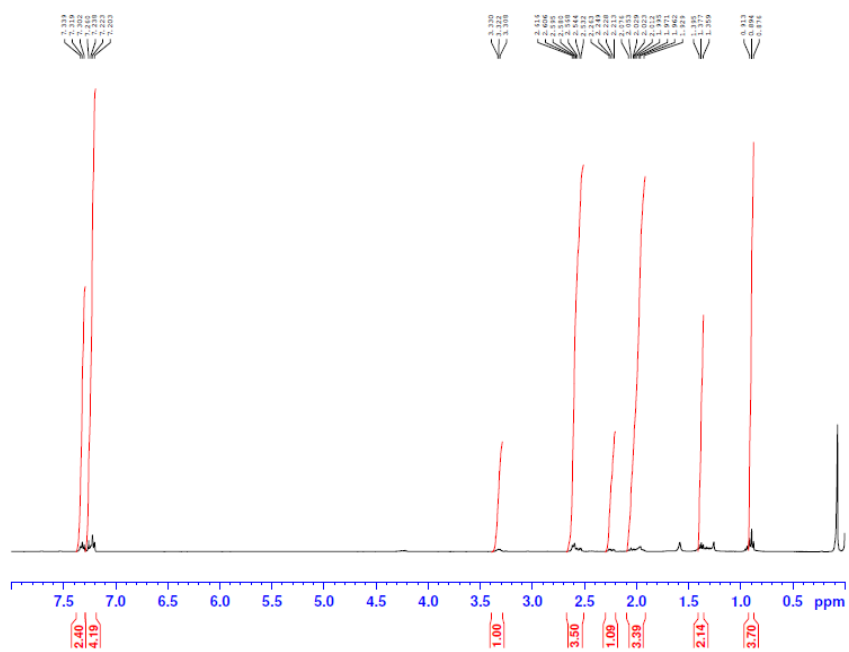
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.004	BV	0.4297	6387.42090	231.60951	47.3919
2	27.440	VV	0.4624	5925.37012	198.40744	43.9637



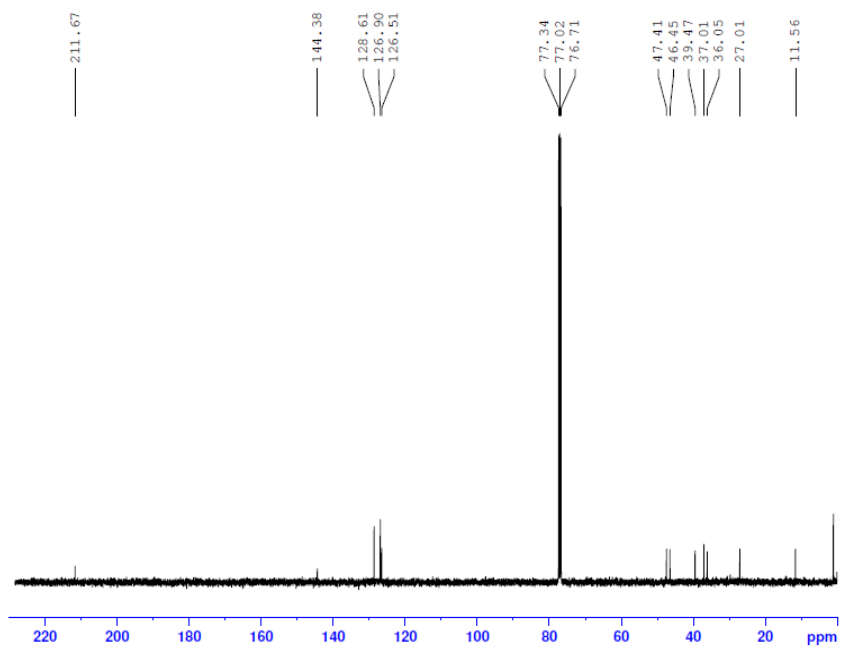
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.542	MM	0.4704	1.09705e4	388.68365	84.7882
2	27.036	MM	0.4736	1968.21350	69.26700	15.2118

3-ethyl-5-phenylcyclohexanone (**3I**):

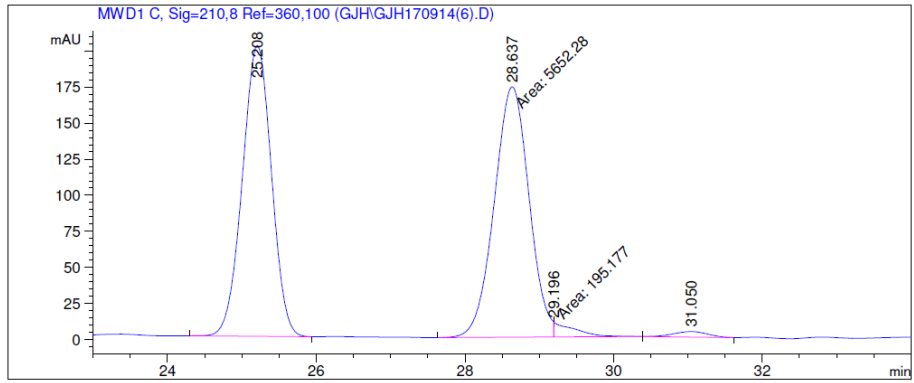
$^1\text{H}$  NMR: **3I**



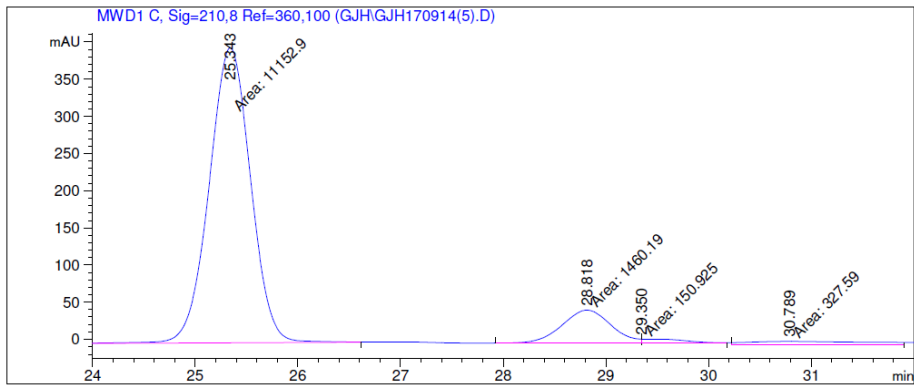
$^{13}\text{C}$  NMR: **3I**



HPLC Data: 3I



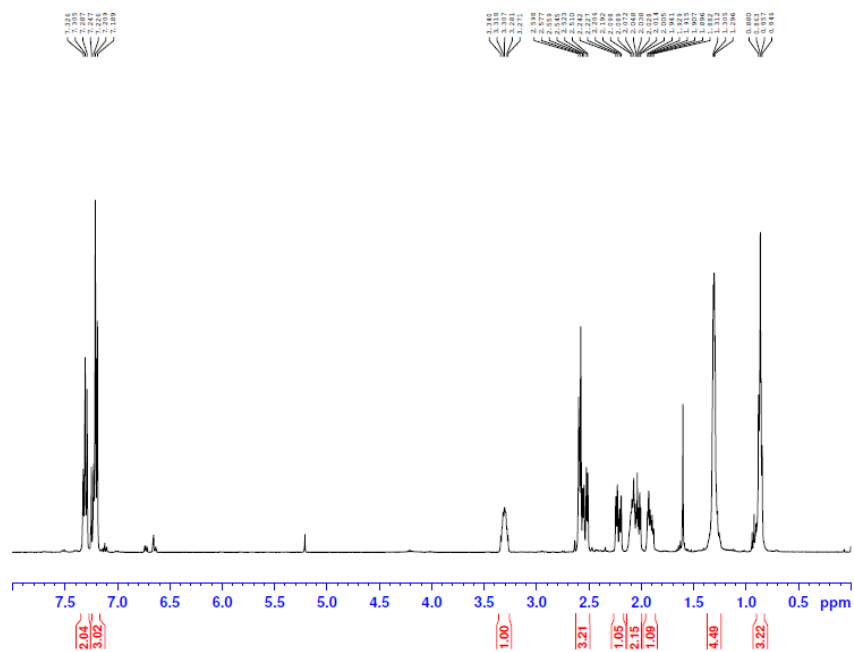
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.208	BB	0.4259	5485.90674	201.32001	47.8861
2	28.637	MF	0.5431	5652.28076	173.45670	49.3384
3	29.196	FM	0.3107	195.17708	10.47091	1.7037
4	31.050	BB	0.4395	122.78938	3.87711	1.0718



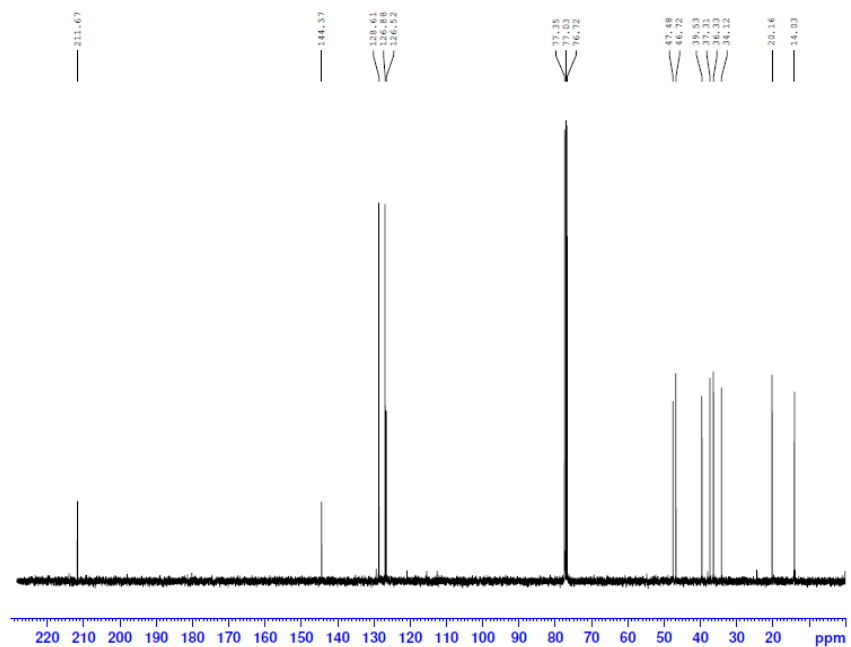
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.343	MM	0.4682	1.11529e4	397.03714	85.1913
2	28.818	MF	0.5501	1460.18933	44.23964	11.1536
3	29.350	FM	0.4068	150.92473	5.23982	1.1528
4	30.789	MM	1.3662	327.58966	3.99642	2.5023

3-propyl-5-phenylcyclohexanone (**3m**):

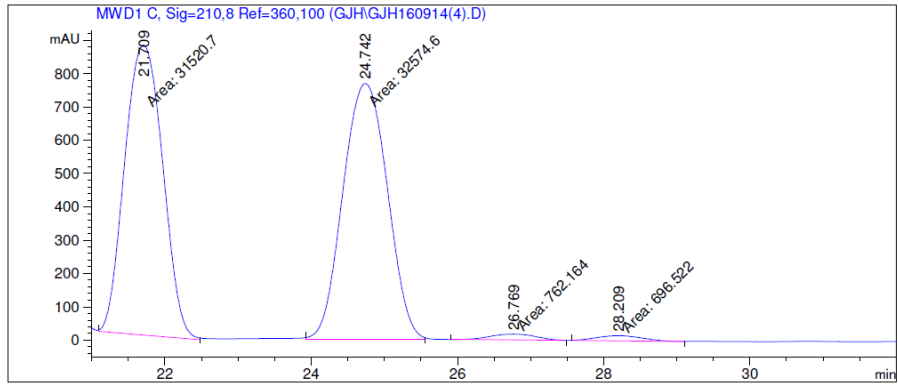
<sup>1</sup>H NMR: **3m**



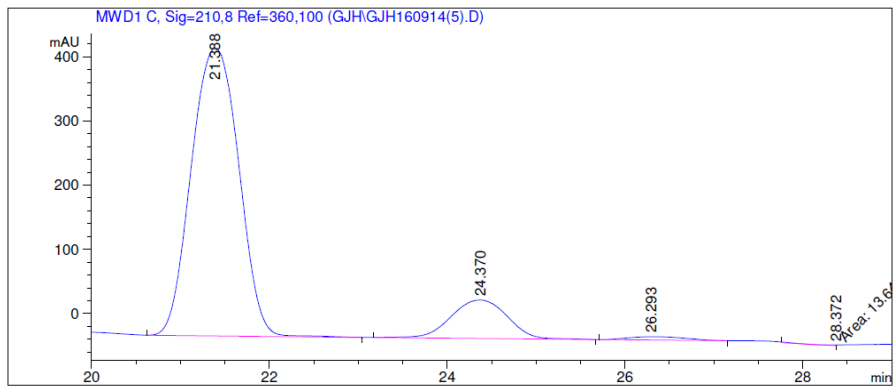
<sup>13</sup>C NMR: **3m**



HPLC Data: 3m



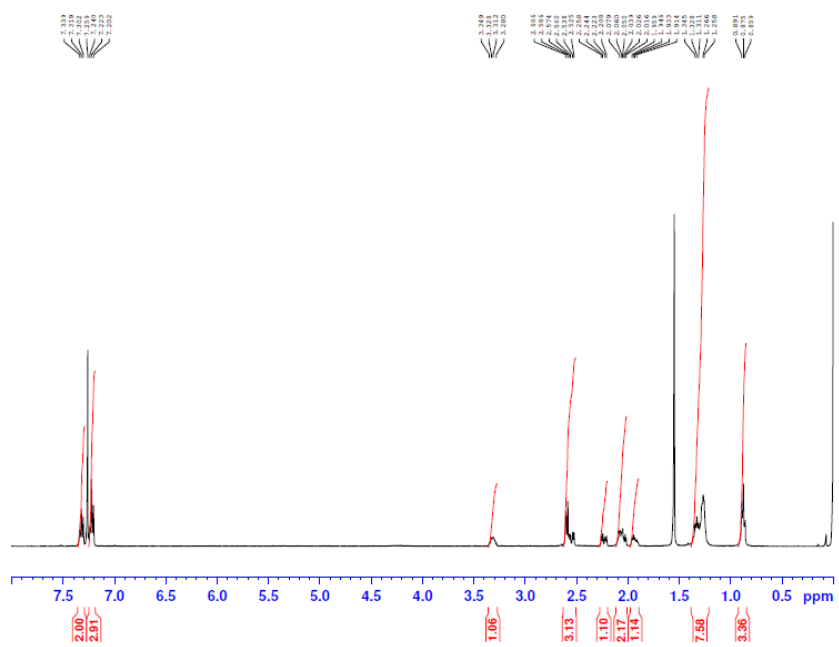
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.709	MM	0.6035	3.15207e4	870.50464	48.0835
2	24.742	MM	0.7056	3.25746e4	769.40942	49.6913
3	26.769	MM	0.7278	762.16425	17.45461	1.1627
4	28.209	MM	0.7518	696.52191	15.44068	1.0625



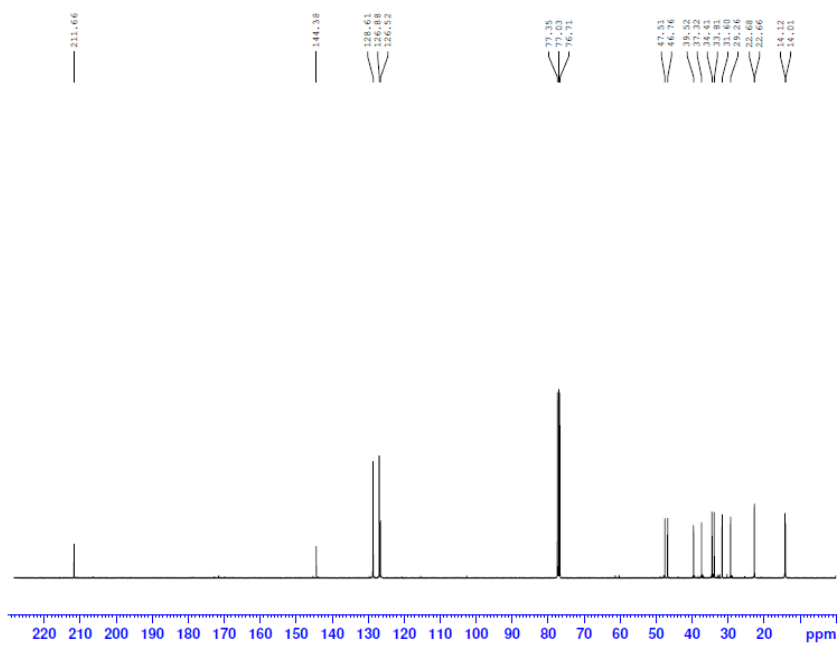
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.388	BB	0.5327	1.66249e4	448.25552	85.2768
2	24.370	VB	0.5895	2633.90259	59.83903	13.5105
3	26.293	BB	0.5336	222.76559	5.02065	1.1427
4	28.372	MM	0.1810	13.64805	1.25680	0.0700

3-butyl-5-phenylcyclohexanone (**3n**):

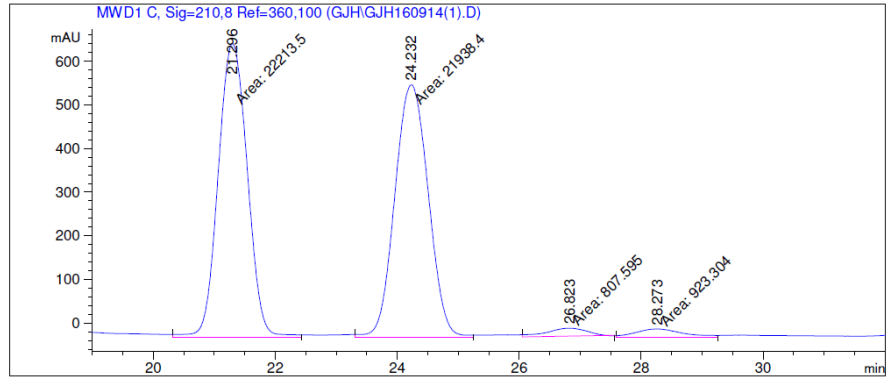
<sup>1</sup>H NMR: **3n**



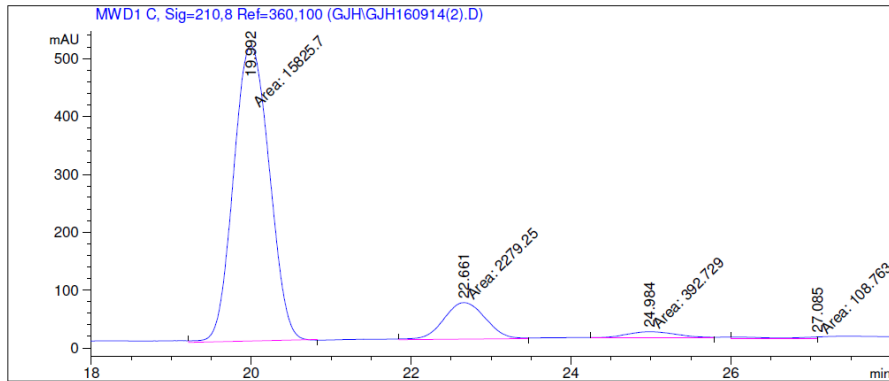
<sup>13</sup>C NMR: **3n**



HPLC Data: 3n



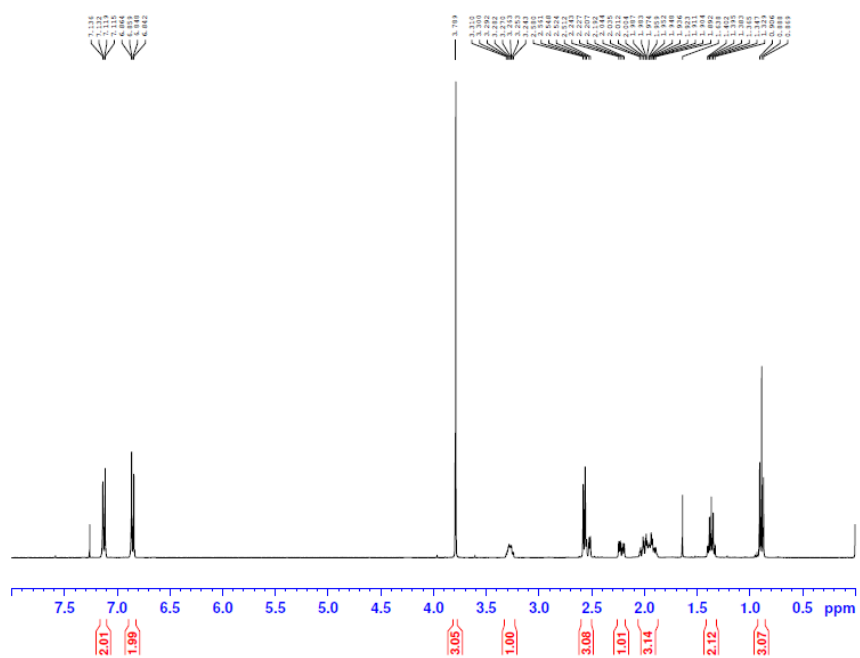
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.296	MM	0.5513	2.22135e4	671.57471	48.4135
2	24.232	MM	0.6336	2.19384e4	577.10693	47.8140
3	26.823	MM	0.7617	807.59485	17.67075	1.7601
4	28.273	MM	0.8609	923.30389	17.87581	2.0123



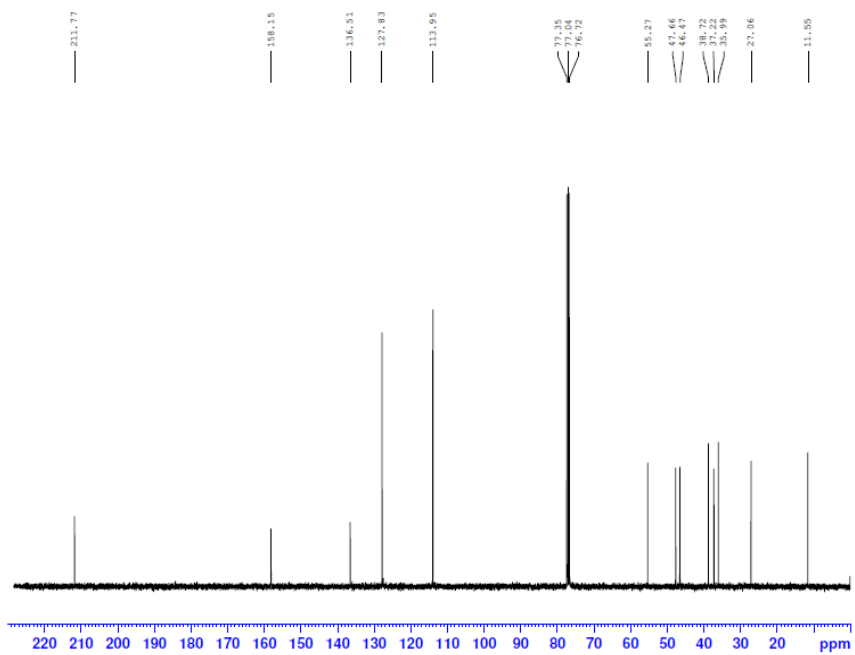
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.992	MM	0.5171	1.58257e4	510.09460	85.0549
2	22.661	MM	0.6025	2279.24585	63.05064	12.2498
3	24.984	MM	0.6745	392.72897	9.70410	2.1107
4	27.085	MM	0.6596	108.76315	2.74835	0.5845

3-ethyl-5-*p*-methoxyphenylcyclohexanone (**3o**):

<sup>1</sup>H NMR: **3o**

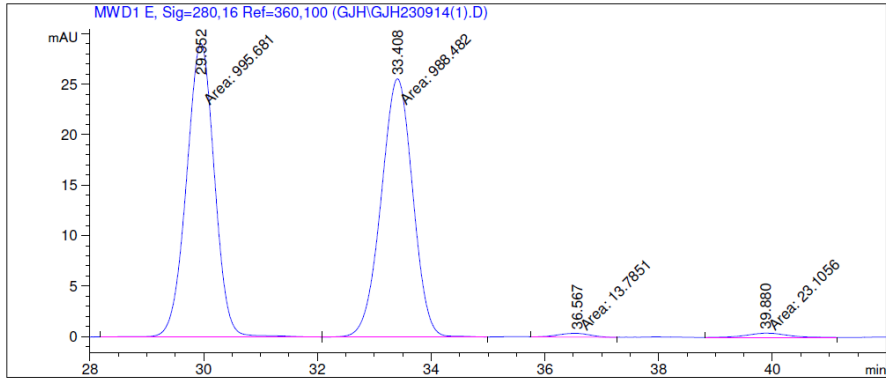


<sup>13</sup>C NMR: **3o**

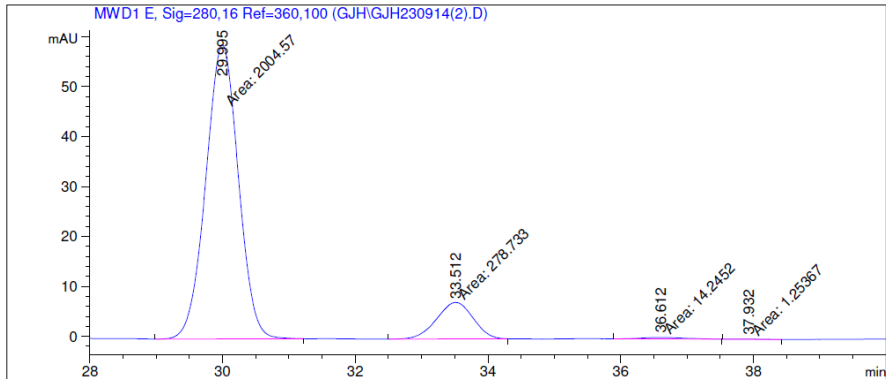




HPLC Data: 3o



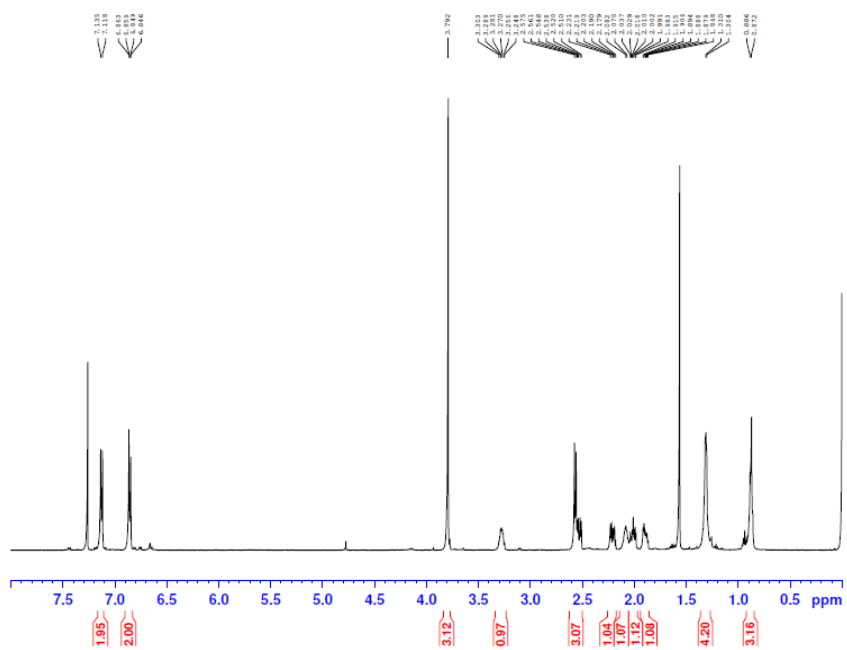
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.952	MF	0.5708	995.68146	29.07209	49.2655
2	33.408	FM	0.6442	988.48193	25.57559	48.9092
3	36.567	MM	0.6226	13.78510	3.69015e-1	0.6821
4	39.880	MM	0.8613	23.10562	4.47105e-1	1.1432



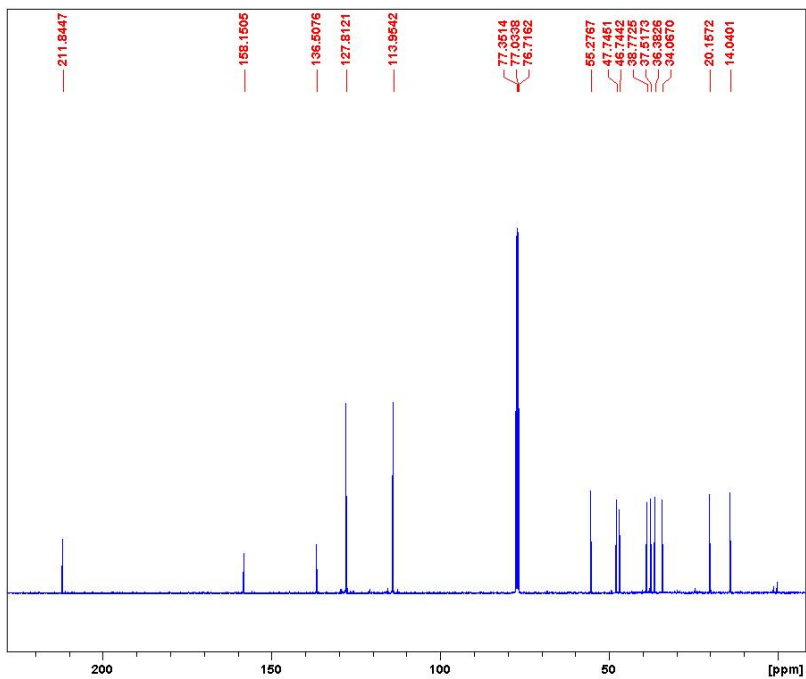
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.995	MM	0.5675	2004.57336	58.87435	87.2007
2	33.512	MM	0.6374	278.73306	7.28848	12.1251
3	36.612	MM	0.7564	14.24523	3.13894e-1	0.6197
4	37.932	MM	0.4511	1.25367	4.63169e-2	0.0545

3-propyl-5-*p*-methoxyphenylcyclohexanone (**3p**):

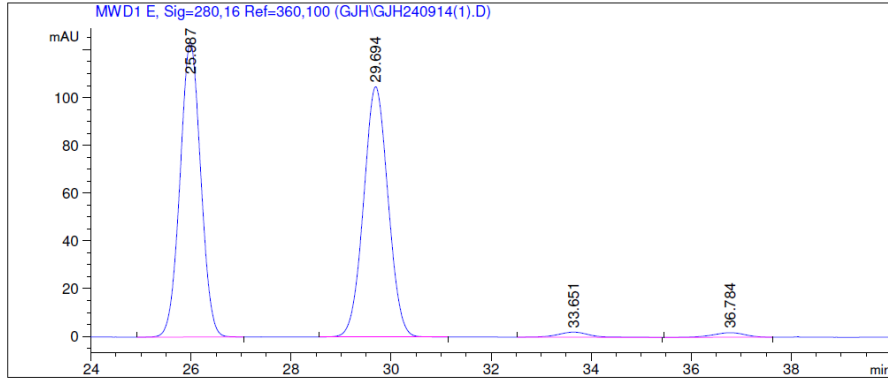
<sup>1</sup>H NMR: **3p**



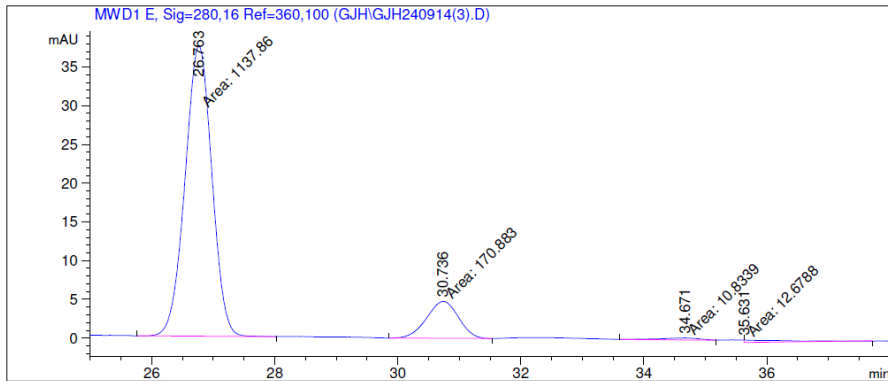
<sup>13</sup>C NMR: **3p**



HPLC Data: 3p



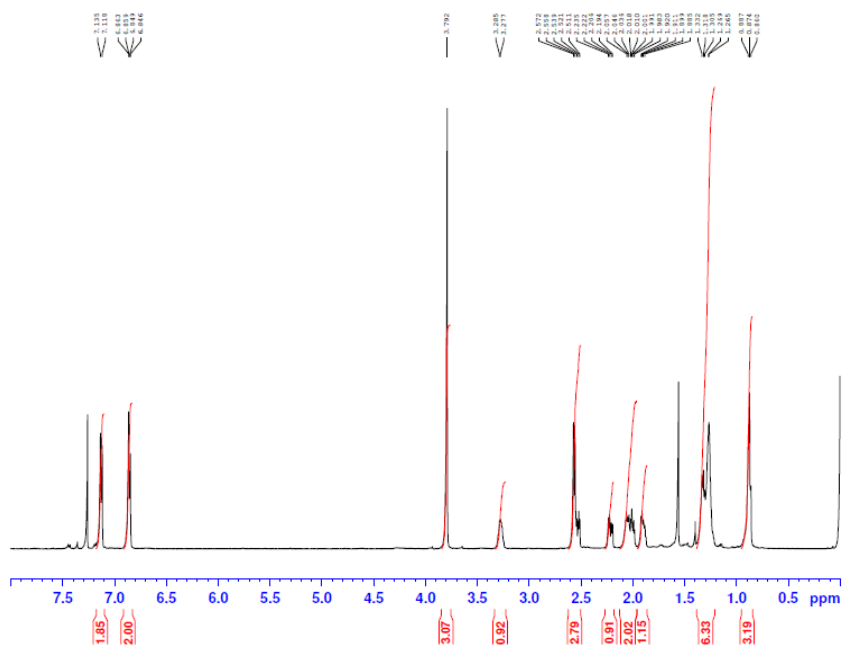
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.987	BB	0.4460	3548.25952	123.21095	48.5950
2	29.694	BB	0.5278	3571.70972	104.76304	48.9162
3	33.651	BB	0.5677	94.63482	2.18304	1.2961
4	36.784	BB	0.5616	87.08992	1.96304	1.1927



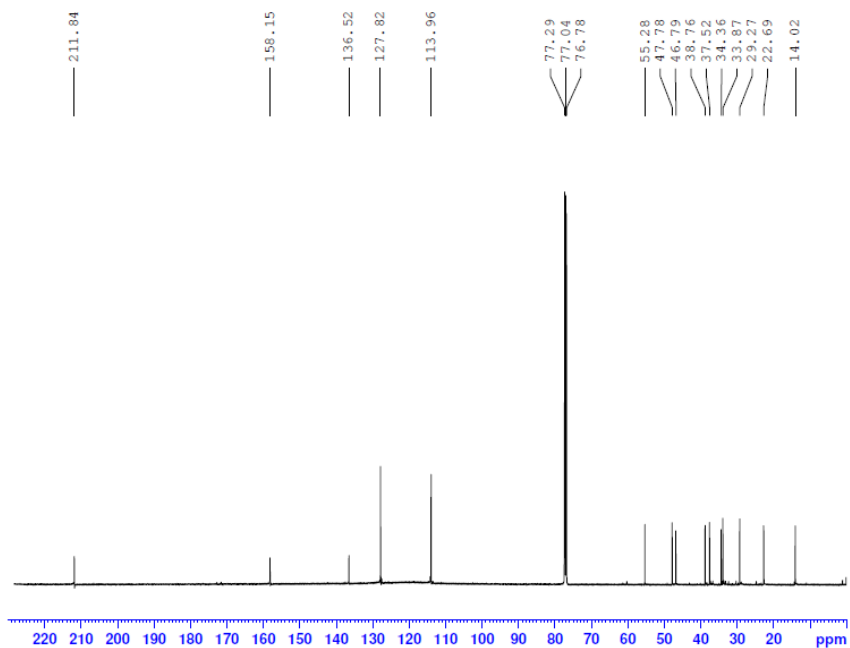
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.763	MM	0.5056	1137.85803	37.51098	85.4085
2	30.736	MM	0.5986	170.88254	4.75775	12.8266
3	34.671	MM	0.6941	10.83387	2.60153e-1	0.8132
4	35.631	MM	0.6863	12.67878	3.07884e-1	0.9517

3-butyl-5-*p*-methoxyphenylcyclohexanone (**3q**):

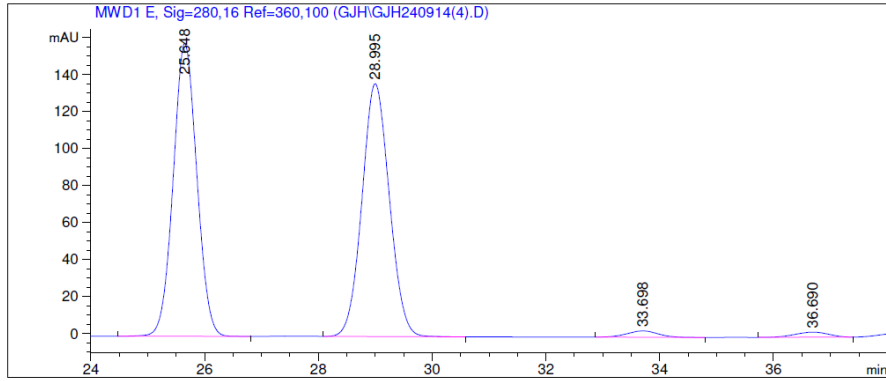
<sup>1</sup>H NMR: **3q**



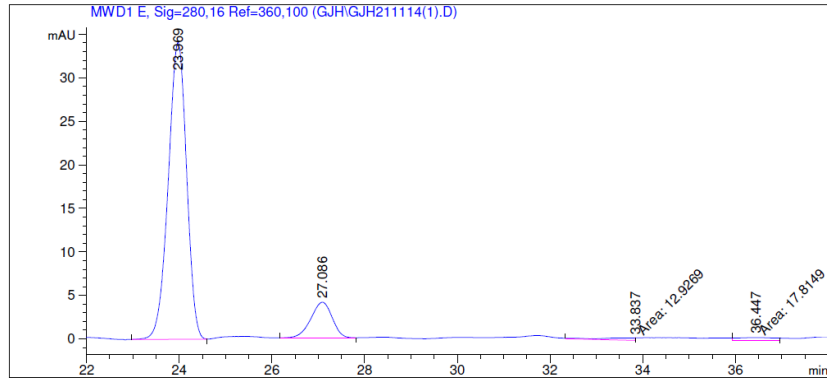
<sup>13</sup>C NMR: **3q**



HPLC Data: 3q



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.648	BB	0.4485	4561.59375	158.16008	48.6387
2	28.995	BB	0.5164	4572.13379	136.64035	48.7511
3	33.698	BB	0.5671	130.67569	3.36480	1.3933
4	36.690	BB	0.5733	114.12888	2.80149	1.2169



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.969	BB	0.4270	938.76880	34.11982	85.2806
2	27.086	BB	0.4845	131.28900	4.09043	11.9267
3	33.837	MM	0.7626	12.92695	2.82538e-1	1.1743
4	36.447	MM	0.9104	17.81489	3.26152e-1	1.6184

## 1.4

### Computational Details

DFT calculations were performed with the Gaussian 09 package.<sup>[1]</sup> Both intermediates and transition state structures involved in the rate-determining step are fully optimized by BP86<sup>[2]</sup> method using general basis set: 6-31G(d)<sup>[3]</sup> for H, C, O and P, SDD<sup>[4]</sup> for Fe and Pd. The SDD ECP is used for Fe and Pd as well. Also, harmonic vibrational frequencies are calculated on the optimized geometries to validate whether they are local minimum or transition state.

### Computational Results and Discussions

Table 1 Energetic information of the Intermediates and Transition States

The Intermediate	ZPE-corrected Energy (a.u.)	Relative Energy (kcal/mol)	Transition States (TS)	ZPE-corrected Energy (a.u.)	Activation Energy (kcal/mol)	Product
1	-2442.4315	1.63	1	-2442.4170	9.10	<b>3R, 5R</b>
2	-2442.4341	0.00	2	-2442.4192	9.35	3R, 5S
3	-2442.4323	1.75	3	-2442.4143	11.29	3S, 5S
4	-2442.4347	2.00	4	-2442.4171	11.04	3S, 5R

The calculation results show that the formation of Intermediate 1 is slight energy favored than that of Intermediate 2, and the activation barrier in the pathway from Intermediate 1 to TS1 is slighter lower than that in the pathway from Intermediate 2 to TS2. So the first reaction pathway is more preferred and it leads to the formation of the main product with 3R, 5R chirality. This conclusion is in agreement with the experimental result.

#### Intermediate 1

Fe -1.791424 -2.869574 -0.108136  
Pd -1.339982 0.713223 -0.205715  
C -1.234435 -1.129494 -1.101130  
C -0.096766 -2.014472 -0.878008  
C -0.361633 -3.287992 -1.503796  
H 0.293030 -4.162865 -1.487912  
C -1.657767 -3.209630 -2.119430  
H -2.167123 -4.020495 -2.644770  
C -2.193264 -1.899101 -1.864755  
H -3.179826 -1.559189 -2.174541  
C -1.531847 -3.229309 1.906221  
H -0.636282 -3.004481 2.486190  
C -1.802159 -4.454147 1.202883  
H -1.142863 -5.322182 1.149779  
C -3.079123 -4.322993 0.552292  
H -3.552928 -5.069360 -0.087342  
C -3.598518 -3.014546 0.851842  
H -4.531851 -2.593596 0.476647  
C -2.645138 -2.342080 1.693029  
H -2.729831 -1.321934 2.067766  
C 1.201842 -1.586203 -0.249531

H	1.553053	-2.315014	0.500681
C	2.293951	-1.463028	-1.334212
H	2.144184	-0.583756	-1.983395
H	2.184721	-2.328471	-2.019880
C	3.730558	-1.493176	-0.823873
O	4.458074	-0.926274	-3.105498
C	4.797601	-1.230587	-1.797138
C	6.175726	-1.241966	-1.669060
H	6.715850	-1.453911	-0.748402
C	6.710468	-0.929486	-2.952937
H	7.759624	-0.847764	-3.233136
C	5.625962	-0.748531	-3.783997
H	5.522410	-0.500893	-4.838455
C	2.179064	1.173584	0.399886
C	3.127171	1.521795	1.382308
H	3.057173	1.089573	2.383544
C	4.159111	2.424995	1.084343
H	4.884357	2.687821	1.861460
C	4.264010	2.988938	-0.195910
H	5.074498	3.688720	-0.424963
C	3.315547	2.662671	-1.178306
H	3.376947	3.110182	-2.176091
C	2.271304	1.775090	-0.877671
H	1.505561	1.561672	-1.633157
C	0.945906	-0.519173	2.471835
C	2.048939	-1.296981	2.895639
H	2.833930	-1.567807	2.180766
C	2.138585	-1.723758	4.229357
H	2.997785	-2.324775	4.545871
C	1.134419	-1.387292	5.151303
H	1.205546	-1.726865	6.190073
C	0.038353	-0.616748	4.736499
H	-0.748899	-0.349617	5.448880
C	-0.054263	-0.183338	3.405505
H	-0.907761	0.419046	3.090624
O	4.033967	-1.775094	0.344405
P	0.774362	0.009676	0.708908
C	-3.028173	0.889332	-1.411459
C	-2.925758	1.297212	-2.757194
C	-4.312241	0.577270	-0.912282
C	-4.065138	1.391312	-3.578034
H	-1.943167	1.530715	-3.184196
C	-5.453009	0.663325	-1.731697
H	-4.431235	0.251214	0.128470
C	-5.333759	1.071616	-3.069973
H	-3.956120	1.709555	-4.621854
H	-6.437204	0.408866	-1.320181
H	-6.220445	1.139228	-3.709574
C	-1.462284	2.491853	1.314177
H	-1.972637	1.956295	2.124437
C	-2.188707	2.888720	0.191650

H	-3.261390	2.686124	0.168769
C	-0.225623	3.215237	1.729218
C	-1.662866	3.944534	-0.766536
H	-1.048388	3.472013	-1.555214
H	-2.512611	4.421565	-1.285653
C	-0.803542	5.003746	-0.029528
C	0.305259	4.282781	0.771684
H	0.913708	4.985956	1.365712
H	0.994320	3.774958	0.068378
H	-0.315401	5.633050	-0.798733
O	0.295885	3.011447	2.829959
C	-1.650885	5.926500	0.864803
H	-1.017556	6.685654	1.356472
H	-2.419308	6.456050	0.274380
H	-2.167801	5.360714	1.660343

#### TS1

Fe	-1.438963	-3.030753	-0.169848
Pd	-1.319020	0.612149	-0.084140
C	-1.102592	-1.173047	-1.063219
C	0.116126	-1.959272	-0.951058
C	-0.057043	-3.207094	-1.657596
H	0.674059	-4.015115	-1.741731
C	-1.389393	-3.212477	-2.202023
H	-1.847073	-4.031821	-2.761053
C	-2.031067	-1.979735	-1.822533
H	-3.064291	-1.719585	-2.049898
C	-1.018415	-3.455644	1.799607
H	-0.122515	-3.154110	2.344461
C	-1.185832	-4.668411	1.044062
H	-0.432968	-5.445637	0.902304
C	-2.507789	-4.659075	0.474669
H	-2.930066	-5.424539	-0.178593
C	-3.156820	-3.439615	0.877499
H	-4.155511	-3.117747	0.580004
C	-2.239159	-2.699164	1.701338
H	-2.417417	-1.717921	2.141803
C	1.368631	-1.460099	-0.277410
H	1.724257	-2.173756	0.484287
C	2.512954	-1.270305	-1.296398
H	2.395652	-0.359935	-1.908474
H	2.456386	-2.105045	-2.024918
C	3.914479	-1.319402	-0.695011
O	4.786656	-0.511046	-2.849704
C	5.039644	-0.943213	-1.558060
C	6.405696	-0.954152	-1.334373
H	6.884027	-1.253958	-0.403969
C	7.022899	-0.507901	-2.539089
H	8.087439	-0.387821	-2.734654
C	5.995493	-0.254007	-3.422190
H	5.961381	0.099083	-4.450795



C	2.074856	1.411999	0.261680
C	3.094147	1.786265	1.159699
H	3.155767	1.312020	2.143056
C	4.028953	2.769112	0.799050
H	4.810523	3.055555	1.510403
C	3.965162	3.381379	-0.461374
H	4.698239	4.145861	-0.739310
C	2.951198	3.017187	-1.362157
H	2.888462	3.496225	-2.345183
C	2.004471	2.048396	-0.998491
H	1.193672	1.785936	-1.688921
C	1.069229	-0.259498	2.451927
C	2.050454	-1.175812	2.894851
H	2.729255	-1.650441	2.179038
C	2.190993	-1.448800	4.264959
H	2.953567	-2.162590	4.594525
C	1.368991	-0.808761	5.204949
H	1.479672	-1.028137	6.272307
C	0.416588	0.125852	4.771483
H	-0.211299	0.651401	5.498546
C	0.262951	0.399650	3.404372
H	-0.444431	1.168771	3.083545
O	4.143069	-1.712545	0.458675
P	0.818669	0.115862	0.659149
C	-3.273729	0.850639	-1.033480
C	-3.367702	0.995673	-2.435904
C	-4.335972	0.189916	-0.364769
C	-4.468070	0.488285	-3.146472
H	-2.566080	1.496710	-2.987923
C	-5.427890	-0.329916	-1.072180
H	-4.308836	0.087634	0.726992
C	-5.501598	-0.177673	-2.469549
H	-4.512709	0.609729	-4.234686
H	-6.231096	-0.844841	-0.532956
H	-6.362259	-0.568790	-3.022185
C	-1.840760	2.424069	1.061089
H	-2.266583	2.008919	1.987426
C	-2.750256	2.568093	-0.063170
H	-3.807313	2.597427	0.220142
C	-0.777261	3.412623	1.327425
C	-2.372676	3.568288	-1.155612
H	-1.628173	3.118457	-1.836276
H	-3.261009	3.807611	-1.766337
C	-1.744667	4.852098	-0.560092
C	-0.486892	4.455997	0.243203
H	-0.021705	5.324805	0.739783
H	0.273599	4.030176	-0.440540
H	-1.428415	5.483260	-1.413805
O	-0.185900	3.450834	2.418170
C	-2.737366	5.669651	0.286289
H	-2.269897	6.604485	0.641929

H -3.633763 5.940560 -0.299725  
H -3.071052 5.109398 1.177889

Intermediate 2

Fe -2.193228 -2.589057 -0.481735  
Pd -1.280546 0.899517 -0.031493  
C -1.442375 -0.783922 -1.191675  
C -0.421803 -1.825851 -1.164929  
C -0.857322 -2.931248 -1.985114  
H -0.320045 -3.869928 -2.141415  
C -2.145591 -2.592488 -2.524911  
H -2.763643 -3.233961 -3.156939  
C -2.506188 -1.290254 -2.032071  
H -3.448273 -0.785517 -2.237989  
C -1.925777 -3.320169 1.426598  
H -0.994259 -3.304195 1.993139  
C -2.362439 -4.364851 0.539650  
H -1.814088 -5.278982 0.305978  
C -3.631231 -3.976056 -0.017574  
H -4.209471 -4.540073 -0.751242  
C -3.979740 -2.689478 0.525038  
H -4.866312 -2.106491 0.273108  
C -2.928897 -2.287897 1.421431  
H -2.878604 -1.346950 1.969429  
C 0.925083 -1.683181 -0.508685  
H 1.172164 -2.563443 0.108997  
C 2.028900 -1.542560 -1.579668  
H 1.986970 -0.575082 -2.106728  
H 1.822351 -2.295652 -2.368299  
C 3.445847 -1.818108 -1.086922  
O 4.292532 -0.823016 -3.174475  
C 4.559729 -1.446848 -1.966717  
C 5.925802 -1.626092 -1.832519  
H 6.413369 -2.094240 -0.979672  
C 6.528309 -1.087948 -3.006664  
H 7.588794 -1.051311 -3.251552  
C 5.492871 -0.615721 -3.784231  
H 5.447053 -0.128259 -4.755931  
C 2.280216 0.773578 0.532994  
C 3.280507 0.825091 1.524651  
H 3.163215 0.252581 2.448410  
C 4.428945 1.609043 1.334006  
H 5.193603 1.641314 2.117130  
C 4.600835 2.344532 0.151776  
H 5.501815 2.949379 0.005410  
C 3.604601 2.312377 -0.837163  
H 3.720528 2.895056 -1.757221  
C 2.445694 1.546835 -0.640494  
H 1.649884 1.562822 -1.394871  
C 0.828282 -1.031951 2.354933  
C 1.795216 -2.028272 2.626556

H	2.524894	-2.308984	1.858838
C	1.822089	-2.660113	3.879322
H	2.575508	-3.429816	4.078154
C	0.889851	-2.312357	4.870121
H	0.911297	-2.811597	5.844676
C	-0.069909	-1.324187	4.606718
H	-0.798948	-1.044820	5.374209
C	-0.099692	-0.686532	3.357545
H	-0.840875	0.090049	3.163288
O	3.689863	-2.387618	-0.012975
P	0.726807	-0.217400	0.699311
C	-2.952055	1.475167	-1.128645
C	-2.827837	2.074335	-2.398982
C	-4.253095	1.255604	-0.625074
C	-3.963786	2.443022	-3.143338
H	-1.832856	2.245198	-2.826919
C	-5.391502	1.617280	-1.369377
H	-4.387668	0.783432	0.355789
C	-5.251125	2.213511	-2.632993
H	-3.838624	2.904899	-4.130133
H	-6.390793	1.429057	-0.958602
H	-6.136100	2.495008	-3.213895
C	-1.163880	2.446810	1.729073
H	-1.790684	1.895860	2.441739
C	-1.761910	3.113697	0.661054
H	-2.851120	3.109730	0.587357
C	0.157140	2.879457	2.268869
C	-1.021986	4.180113	-0.126516
H	-0.444330	3.723936	-0.953796
H	-1.752546	4.858515	-0.600849
C	-0.051944	4.968622	0.783718
C	0.890740	3.981764	1.504109
H	1.555913	4.493327	2.221052
H	1.544208	3.492097	0.754202
O	0.590999	2.429700	3.334143
H	-0.661862	5.483787	1.554401
C	0.728305	6.031153	-0.003124
H	0.045835	6.748186	-0.493255
H	1.401650	6.603168	0.659276
H	1.348555	5.562615	-0.789339

#### TS2

Fe	-1.746452	-2.847176	-0.450603
Pd	-1.278879	0.712700	0.035817
C	-1.232021	-0.948861	-1.157141
C	-0.096254	-1.858940	-1.142361
C	-0.394864	-3.005539	-1.968333
H	0.251575	-3.869647	-2.141611
C	-1.722766	-2.824275	-2.491862
H	-2.261182	-3.533331	-3.124844
C	-2.237318	-1.578731	-1.982777

H -3.239797 -1.196654 -2.172354  
C -1.371194 -3.489651 1.470261  
H -0.455761 -3.306133 2.033971  
C -1.625902 -4.607524 0.601919  
H -0.934282 -5.423797 0.386670  
C -2.939887 -4.442496 0.037564  
H -3.415076 -5.107928 -0.685251  
C -3.496612 -3.221086 0.556692  
H -4.465947 -2.795905 0.293819  
C -2.530078 -2.636706 1.447364  
H -2.637361 -1.694291 1.985078  
C 1.203047 -1.553452 -0.443320  
H 1.513580 -2.387783 0.207752  
C 2.334688 -1.307904 -1.463175  
H 2.252021 -0.325059 -1.958036  
H 2.215627 -2.044434 -2.284132  
C 3.743234 -1.498811 -0.909281  
O 4.614998 -0.518248 -2.991280  
C 4.869825 -1.091653 -1.756190  
C 6.237498 -1.192597 -1.567737  
H 6.717129 -1.608574 -0.683884  
C 6.853871 -0.656780 -2.735813  
H 7.919278 -0.569818 -2.943796  
C 5.824379 -0.264248 -3.564003  
H 5.788959 0.192602 -4.550875  
C 2.172877 1.138986 0.485227  
C 3.220831 1.279351 1.416088  
H 3.232411 0.664215 2.319750  
C 4.246608 2.210228 1.191236  
H 5.050254 2.314405 1.927624  
C 4.245427 3.002940 0.033960  
H 5.049798 3.725703 -0.138422  
C 3.203209 2.873140 -0.898063  
H 3.188642 3.494674 -1.799819  
C 2.166373 1.957178 -0.667120  
H 1.333758 1.879097 -1.376782  
C 0.993989 -0.721682 2.422489  
C 1.943879 -1.720288 2.738438  
H 2.618603 -2.104814 1.966431  
C 2.050737 -2.195937 4.055047  
H 2.788771 -2.970818 4.288462  
C 1.224286 -1.680498 5.065810  
H 1.308915 -2.057909 6.090498  
C 0.299531 -0.670688 4.760591  
H -0.333528 -0.246497 5.546859  
C 0.181757 -0.192877 3.447113  
H -0.507110 0.625463 3.225913  
O 3.972534 -2.025550 0.189569  
P 0.795012 -0.076905 0.702809  
C -3.185372 1.269496 -0.877114  
C -3.239577 1.610677 -2.247116

C	-4.318598	0.634977	-0.307393
C	-4.371663	1.313945	-3.024210
H	-2.383224	2.100478	-2.721715
C	-5.444260	0.326879	-1.082668
H	-4.319099	0.383500	0.760206
C	-5.477356	0.670005	-2.447283
H	-4.385101	1.582790	-4.086526
H	-6.303581	-0.172706	-0.621105
H	-6.362087	0.443315	-3.051439
C	-1.642951	2.387878	1.421526
H	-2.128183	1.892125	2.276125
C	-2.507075	2.779121	0.322225
H	-3.562375	2.881597	0.596473
C	-0.487976	3.210048	1.833075
C	-2.009015	3.878361	-0.613699
H	-1.286297	3.467448	-1.343379
H	-2.854813	4.283995	-1.196221
C	-1.290049	4.994241	0.176866
C	-0.090617	4.378524	0.924238
H	0.429833	5.120549	1.554103
H	0.650449	4.009914	0.186104
O	0.091589	3.022029	2.913742
H	-1.997868	5.396676	0.931182
C	-0.863265	6.145404	-0.746091
H	-1.732923	6.601393	-1.252088
H	-0.346813	6.938815	-0.177620
H	-0.167387	5.786526	-1.527268

### Intermediate 3

Fe	-1.147615	-3.069000	0.336154
Pd	-1.199949	0.525358	-0.617964
C	-0.845391	-1.465331	-0.958084
C	0.414721	-2.081458	-0.554933
C	0.398814	-3.474584	-0.932851
H	1.191416	-4.203475	-0.746086
C	-0.860944	-3.738632	-1.571626
H	-1.200174	-4.707928	-1.943298
C	-1.622277	-2.518404	-1.575648
H	-2.635493	-2.418705	-1.960613
C	-0.930191	-3.012883	2.385338
H	-0.115920	-2.535418	2.931040
C	-0.954516	-4.371862	1.915786
H	-0.157155	-5.107161	2.035947
C	-2.201662	-4.585418	1.230090
H	-2.509323	-5.505821	0.731009
C	-2.949167	-3.356478	1.273592
H	-3.921212	-3.180921	0.811244
C	-2.165209	-2.387250	1.991242
H	-2.439920	-1.348148	2.171009
C	1.591764	-1.331584	0.012044
H	2.001621	-1.831834	0.906025

C	2.728992	-1.233925	-1.025996
H	2.499894	-0.526807	-1.841372
H	2.812004	-2.218250	-1.531139
C	4.103456	-0.930665	-0.435405
O	4.924821	-0.596198	-2.730416
C	5.193828	-0.635639	-1.371842
C	6.539024	-0.386571	-1.160709
H	7.024114	-0.358371	-0.186970
C	7.125549	-0.182570	-2.443682
H	8.167579	0.038746	-2.669761
C	6.102620	-0.321061	-3.356998
H	6.052409	-0.256876	-4.442021
C	2.120164	1.633566	0.195642
C	2.909411	2.281515	1.166760
H	2.826734	1.993244	2.217661
C	3.796930	3.302309	0.794535
H	4.399641	3.797628	1.562939
C	3.909832	3.692638	-0.548139
H	4.602490	4.491462	-0.833027
C	3.118289	3.065099	-1.522753
H	3.186782	3.371792	-2.571878
C	2.222371	2.051792	-1.152187
H	1.578271	1.592950	-1.912558
C	0.906459	0.156759	2.435204
C	2.058270	-0.328751	3.097498
H	2.952583	-0.587644	2.519069
C	2.054560	-0.483859	4.492076
H	2.951711	-0.860268	4.995093
C	0.909151	-0.163084	5.238770
H	0.909608	-0.288815	6.326648
C	-0.237244	0.314192	4.586432
H	-1.135279	0.562354	5.161240
C	-0.237966	0.473649	3.192560
H	-1.134752	0.840333	2.688079
O	4.343745	-0.975094	0.780059
P	0.869495	0.329564	0.597777
C	-2.820668	0.156262	-1.849280
C	-2.732522	0.265314	-3.253154
C	-4.054989	-0.256073	-1.298815
C	-3.838157	-0.012960	-4.077568
H	-1.784805	0.560213	-3.720164
C	-5.162808	-0.540839	-2.120363
H	-4.154941	-0.381608	-0.213713
C	-5.059001	-0.417824	-3.514788
H	-3.740668	0.082382	-5.165744
H	-6.106359	-0.866395	-1.665855
H	-5.918616	-0.640272	-4.156233
C	-2.099230	2.747165	-1.072887
H	-1.793130	2.758979	-2.125009
C	-1.110619	2.829229	-0.096392
H	-0.064954	2.999322	-0.371092

C	-3.562042	3.040485	-0.792281
C	-1.464190	3.149008	1.314185
C	-2.950285	3.069905	1.659093
C	-3.806490	3.749176	0.562527
H	-3.944817	3.666679	-1.620675
H	-4.147540	2.104820	-0.842686
O	-0.608441	3.495814	2.133919
H	-3.237091	2.000516	1.731206
H	-3.101996	3.530255	2.649976
H	-4.872094	3.613457	0.828026
C	-3.529797	5.262886	0.490837
H	-4.188123	5.746410	-0.252215
H	-3.708644	5.745865	1.467674
H	-2.484705	5.475765	0.202434

### TS3

Fe	-1.091367	-3.072270	0.499876
Pd	-1.158708	0.483900	-0.555352
C	-0.787204	-1.512420	-0.851840
C	0.468402	-2.112236	-0.420341
C	0.461166	-3.518828	-0.746033
H	1.251485	-4.242234	-0.530074
C	-0.796686	-3.806018	-1.383232
H	-1.129186	-4.788772	-1.725693
C	-1.558941	-2.584952	-1.435771
H	-2.570606	-2.499267	-1.830878
C	-0.864656	-2.898449	2.536995
H	-0.049185	-2.383919	3.046698
C	-0.883302	-4.283159	2.147498
H	-0.080060	-5.005236	2.303621
C	-2.132938	-4.542340	1.482087
H	-2.439815	-5.492476	1.041682
C	-2.886973	-3.316571	1.459523
H	-3.864703	-3.175445	0.997124
C	-2.106071	-2.302988	2.117271
H	-2.383206	-1.255790	2.238168
C	1.618327	-1.310056	0.136424
H	1.999897	-1.731268	1.082157
C	2.793100	-1.258562	-0.861986
H	2.585552	-0.600569	-1.724413
H	2.910633	-2.268024	-1.306351
C	4.136946	-0.890042	-0.239607
O	5.063118	-0.772020	-2.515160
C	5.267639	-0.672125	-1.148669
C	6.598019	-0.380496	-0.901426
H	7.035802	-0.248143	0.086049
C	7.242464	-0.294706	-2.169884
H	8.291242	-0.079007	-2.368525
C	6.265858	-0.540400	-3.111004
H	6.266399	-0.584077	-4.198184
C	2.052408	1.685375	0.027204

C	2.915756	2.354784	0.915332
H	2.900163	2.113393	1.981084
C	3.788589	3.344821	0.440277
H	4.447606	3.864131	1.143833
C	3.813247	3.675786	-0.922515
H	4.493629	4.452243	-1.287750
C	2.951800	3.017797	-1.814619
H	2.954601	3.278466	-2.878403
C	2.070230	2.036231	-1.341161
H	1.370157	1.548841	-2.030954
C	0.835025	0.417865	2.398727
C	1.951667	-0.013704	3.150856
H	2.855900	-0.360469	2.637957
C	1.900385	0.003111	4.553450
H	2.769663	-0.333250	5.128538
C	0.744092	0.444063	5.216765
H	0.708008	0.451290	6.311254
C	-0.367002	0.870673	4.473671
H	-1.273215	1.211525	4.984969
C	-0.321406	0.856853	3.072101
H	-1.188309	1.177252	2.487845
O	4.320988	-0.813604	0.984367
P	0.851695	0.386082	0.556866
C	-2.924555	0.364120	-1.860219
C	-2.593190	0.326496	-3.238798
C	-4.067024	-0.354519	-1.442187
C	-3.347164	-0.422256	-4.150448
H	-1.726927	0.894876	-3.599573
C	-4.838546	-1.091874	-2.357111
H	-4.359197	-0.358034	-0.386951
C	-4.481392	-1.131162	-3.713496
H	-3.057837	-0.445749	-5.207063
H	-5.719442	-1.640207	-2.004307
H	-5.084710	-1.701648	-4.427413
C	-2.765573	2.242099	-1.106406
H	-2.878074	2.588304	-2.139607
C	-1.506873	2.645131	-0.494403
H	-0.701702	2.974354	-1.167636
C	-4.033848	2.387440	-0.260587
C	-1.458525	3.354725	0.803911
C	-2.780633	3.530533	1.569606
C	-3.996615	3.653222	0.627291
H	-4.920813	2.380563	-0.918089
H	-4.137680	1.523737	0.418674
O	-0.417065	3.872692	1.230568
H	-2.927723	2.655050	2.234830
H	-2.663319	4.412410	2.222606
H	-4.917691	3.642637	1.242579
C	-3.984912	4.965473	-0.176510
H	-4.857719	5.025188	-0.850943
H	-4.018816	5.838094	0.498964



H -3.072994 5.060649 -0.792030

Intermediate 4

Fe -1.081616 -3.007373 0.559319  
Pd -1.170837 0.485249 -0.726978  
C -0.779089 -1.523747 -0.871473  
C 0.482102 -2.077369 -0.388012  
C 0.497944 -3.499281 -0.636375  
H 1.298021 -4.192550 -0.364958  
C -0.743023 -3.844177 -1.272776  
H -1.056206 -4.849105 -1.564274  
C -1.524197 -2.643802 -1.405242  
H -2.528703 -2.600116 -1.821638  
C -0.887677 -2.764873 2.594512  
H -0.083116 -2.231428 3.101266  
C -0.894369 -4.160971 2.249304  
H -0.089016 -4.872761 2.438233  
C -2.132640 -4.447723 1.573771  
H -2.428391 -5.412859 1.159312  
C -2.891914 -3.227657 1.499780  
H -3.861623 -3.105438 1.015742  
C -2.124603 -2.190000 2.135081  
H -2.409735 -1.141495 2.218087  
C 1.633458 -1.259605 0.137466  
H 2.017853 -1.664619 1.088997  
C 2.804428 -1.248021 -0.866783  
H 2.602330 -0.614043 -1.747593  
H 2.907826 -2.271021 -1.282903  
C 4.155641 -0.881320 -0.258163  
O 5.077772 -0.849135 -2.538327  
C 5.287335 -0.710036 -1.175998  
C 6.622984 -0.433502 -0.940425  
H 7.065211 -0.277950 0.041684  
C 7.265804 -0.398517 -2.212166  
H 8.317705 -0.207368 -2.419236  
C 6.283084 -0.657008 -3.143423  
H 6.280463 -0.735371 -4.228651  
C 2.131219 1.712464 0.049345  
C 2.898743 2.446699 0.974597  
H 2.793037 2.256334 2.045360  
C 3.793955 3.431107 0.530476  
H 4.379637 3.995393 1.263675  
C 3.935365 3.698944 -0.839303  
H 4.633834 4.470264 -1.180295  
C 3.165098 2.984418 -1.770011  
H 3.255829 3.195428 -2.840830  
C 2.261703 2.006783 -1.328086  
H 1.633501 1.478311 -2.056150  
C 0.845268 0.447929 2.379638  
C 1.972287 0.048819 3.135037

H	2.894252	-0.250071	2.623642
C	1.907543	0.028586	4.536811
H	2.785890	-0.282040	5.112647
C	0.725642	0.399217	5.198566
H	0.678568	0.377618	6.292438
C	-0.396864	0.790691	4.453913
H	-1.323897	1.074347	4.962588
C	-0.335956	0.815529	3.052728
H	-1.215341	1.108390	2.473577
O	4.343959	-0.771948	0.962339
P	0.878538	0.441553	0.534833
C	-2.783463	-0.030187	-1.924336
C	-2.695136	-0.033498	-3.332461
C	-4.003613	-0.437652	-1.341741
C	-3.788091	-0.417279	-4.131143
H	-1.757278	0.255843	-3.822667
C	-5.098846	-0.826557	-2.136541
H	-4.100285	-0.479537	-0.249851
C	-4.995660	-0.816144	-3.536437
H	-3.690812	-0.408454	-5.223471
H	-6.032097	-1.145169	-1.656583
H	-5.845544	-1.120040	-4.157125
C	-2.160614	2.604674	-1.348371
H	-1.944413	2.514440	-2.418000
C	-1.100352	2.832833	-0.475215
H	-0.084359	2.982860	-0.854366
C	-3.603876	2.888360	-0.968282
C	-1.341806	3.321982	0.911710
C	-2.797836	3.321606	1.376617
C	-3.732382	3.822136	0.253821
H	-4.111304	3.333593	-1.844270
H	-4.143780	1.943323	-0.770378
O	-0.423836	3.752939	1.615254
H	-3.090160	2.284423	1.646093
H	-2.868491	3.938833	2.288291
H	-3.379521	4.830807	-0.045549
C	-5.188176	3.942425	0.725599
H	-5.276295	4.646705	1.571508
H	-5.842372	4.305910	-0.086871
H	-5.578427	2.963072	1.058535

#### TS4

Fe	-1.086198	-2.967710	0.792980
Pd	-1.107801	0.434236	-0.701448
C	-0.729132	-1.584696	-0.731470
C	0.506901	-2.122531	-0.179949
C	0.509753	-3.559013	-0.329867
H	1.288102	-4.247619	0.008218
C	-0.724579	-3.926904	-0.971567
H	-1.046599	-4.945853	-1.198693
C	-1.481666	-2.723429	-1.204302

H -2.476793 -2.687252 -1.646865  
C -0.969258 -2.491427 2.792049  
H -0.209576 -1.859873 3.253246  
C -0.891803 -3.915583 2.606891  
H -0.057021 -4.555887 2.897082  
C -2.090947 -4.343948 1.936164  
H -2.321985 -5.364111 1.624898  
C -2.910452 -3.183165 1.706055  
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C -2.219415 -2.039654 2.239586  
H -2.559262 -1.004917 2.194653  
C 1.635120 -1.254989 0.320632  
H 1.977190 -1.556442 1.325631  
C 2.848107 -1.321953 -0.629358  
H 2.671286 -0.780548 -1.575320  
H 2.986065 -2.378843 -0.936466  
C 4.164014 -0.865471 -0.006324  
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C 5.331288 -0.756203 -0.888028  
C 6.648831 -0.423250 -0.624956  
H 7.043204 -0.161030 0.354807  
C 7.346403 -0.495126 -1.865819  
H 8.401897 -0.297137 -2.046510  
C 6.411659 -0.868361 -2.807527  
H 6.458751 -1.051167 -3.879080  
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C 2.884952 2.500624 0.708463  
H 2.814429 2.399018 1.794345  
C 3.775183 3.432832 0.155277  
H 4.391505 4.047883 0.819239  
C 3.871409 3.584463 -1.235762  
H 4.565529 4.315903 -1.662823  
C 3.063175 2.804983 -2.078489  
H 3.121583 2.925521 -3.165536  
C 2.163510 1.881683 -1.528550  
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C 1.837842 0.419643 3.170078  
H 2.772793 0.036433 2.745824  
C 1.717031 0.599916 4.556921  
H 2.564455 0.358730 5.207446  
C 0.519041 1.080615 5.109419  
H 0.429008 1.215053 6.192502  
C -0.565062 1.380921 4.270805  
H -1.504506 1.748998 4.696054  
C -0.449558 1.204806 2.884362  
H -1.295997 1.423391 2.227113  
O 4.295080 -0.630964 1.204161  
P 0.852871 0.476824 0.499563  
C -2.796143 0.158453 -2.079490  
C -2.374484 0.000588 -3.424914

C	-3.963980	-0.525578	-1.674070
C	-3.066264	-0.832637	-4.312077
H	-1.488793	0.542434	-3.779234
C	-4.673267	-1.346737	-2.567933
H	-4.324939	-0.433264	-0.644745
C	-4.226515	-1.506637	-3.888295
H	-2.707971	-0.949742	-5.341000
H	-5.576267	-1.865465	-2.226353
H	-4.780520	-2.143532	-4.585841
C	-2.711188	2.094048	-1.482370
H	-2.842447	2.343778	-2.541395
C	-1.463666	2.585373	-0.914744
H	-0.656579	2.849023	-1.613485
C	-3.978260	2.280084	-0.646985
C	-1.433572	3.422643	0.305386
C	-2.767020	3.672025	1.030267
C	-3.976312	3.641808	0.077895
H	-4.869147	2.164294	-1.288773
H	-4.044746	1.497496	0.131693
O	-0.401053	3.989154	0.689815
H	-2.910784	2.895175	1.810744
H	-2.672269	4.636186	1.559090
H	-3.842882	4.443956	-0.677296
C	-5.300773	3.886158	0.816120
H	-5.289190	4.856496	1.343071
H	-6.156559	3.889385	0.117548
H	-5.483827	3.097661	1.569892

## References

- [1] Gaussian 09, Revision **B.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.
- [2] (a) A. D. Becke, *Chem. Phys.* **1993**, *98*, 1372–1377 (b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652 (c) C. H. Holder, L. Zou, A. N. Marziale, P. Liu, Y. Lan, M. Gatti, K. Kikushima, K. N. Houk, B. M. Stoltz, *J. Am. Chem. Soc.* **2013**, *135*, 14996–15007 (d) S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais, *Phys. Rev. B* **1992**, *46*, 6671–6687 (e) Perdew, J. P., *Phys. Rev. B* **1986**, *33*, 8822–8824.
- [3] (a) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, **1972**, *56*, 2257 (b) P. C. Hariharan, J. A. Pople, *Theor. Chem. Acc.*, **1973**, *28*, 213 (c) M. J. Frisch, J. A. Pople, J. S. Binkley, *J. Chem. Phys.*, **1984**, *80*, 3265.
- [4] (a) A. Bergner, M. Dolg, W. Kuechle, H. Stoll, H. Preuss, *Mol. Phys.* **1993**, *80*, 1431 (b) M. Kaupp, P. v. R. Schleyer, H. Stoll, H. Preuss, *J. Chem. Phys.* **1991**, *94*, 1360 (c) M. Dolg, M. Stoll, H. Preuss, R. M. Pitzer, *J. Phys. Chem.* **1993**, *97*, 5852.