

Supporting Information

Enantioselective Hydrogenation of β -Ketophosphonates with Chiral Ru(II) Catalysts

Xiaoming Tao[†], Wanfang Li[†], Xin Ma[†], Xiaoming Li[†], Weizheng Fan[†], Lvfang Zhu[†],
Xiaomin Xie[†], and Zhaoguo Zhang^{†§*}

[†]*School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, 800
Dongchuan Road, Shanghai 200240, China,* [§]*State Key Laboratory of Organometallic
Chemistry, Shanghai Institute of Organic Chemistry, 345 Lingling Road, Shanghai 200032,
China*

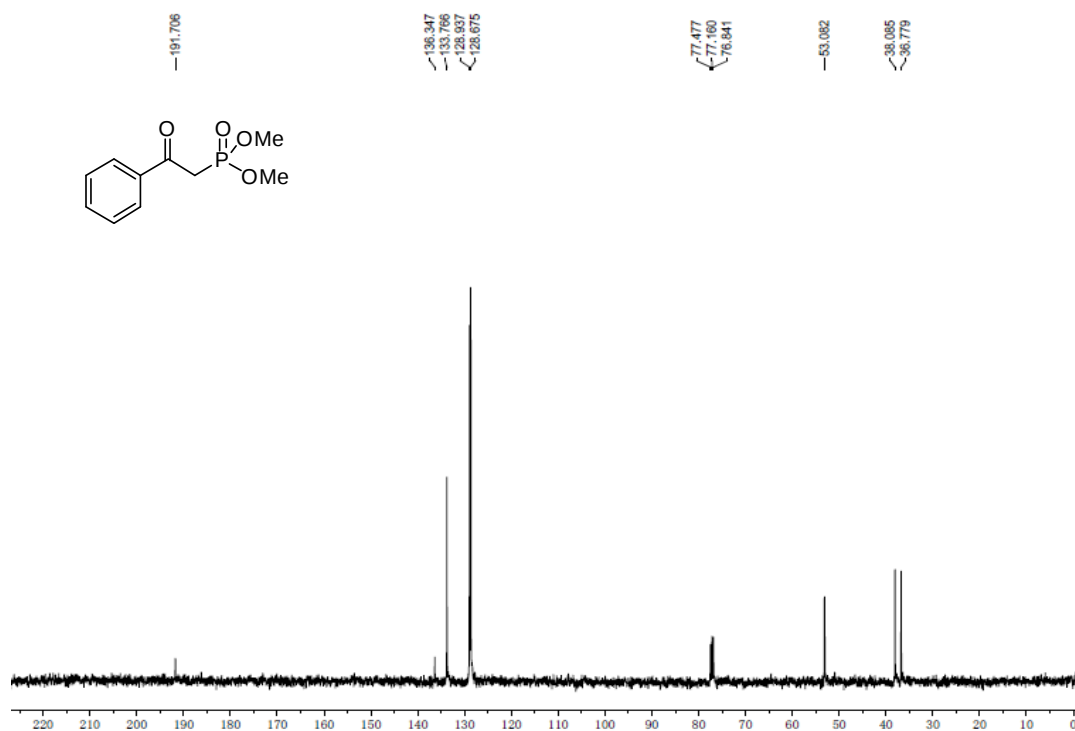
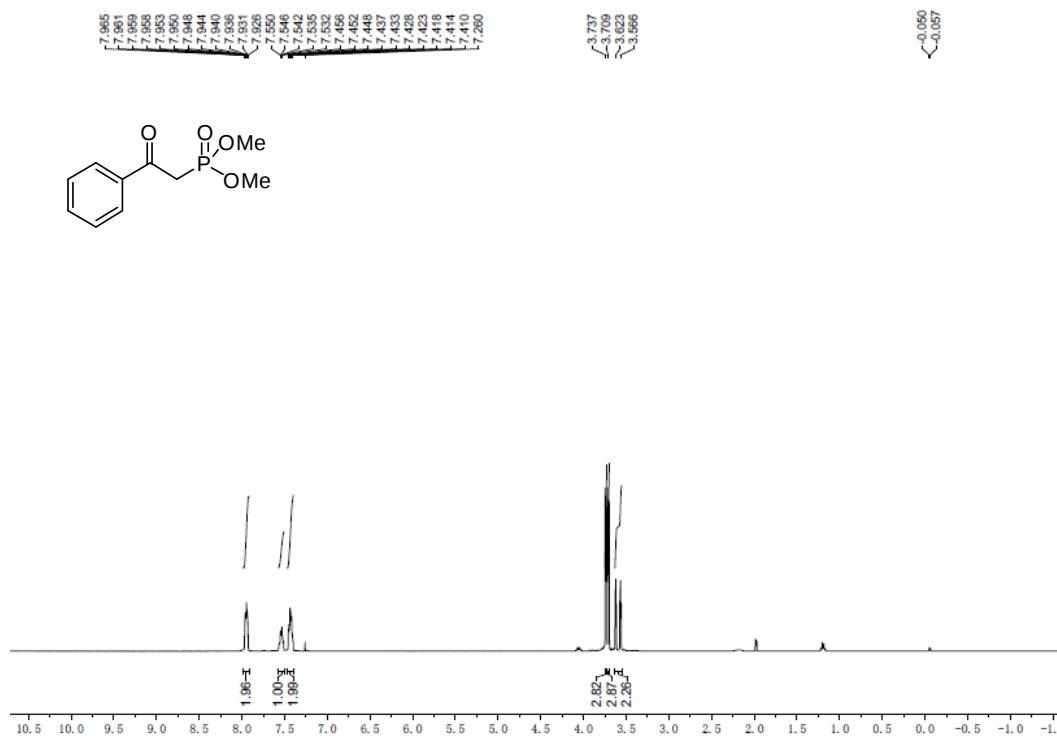
zhaoguo@sjtu.edu.cn

Table of contents

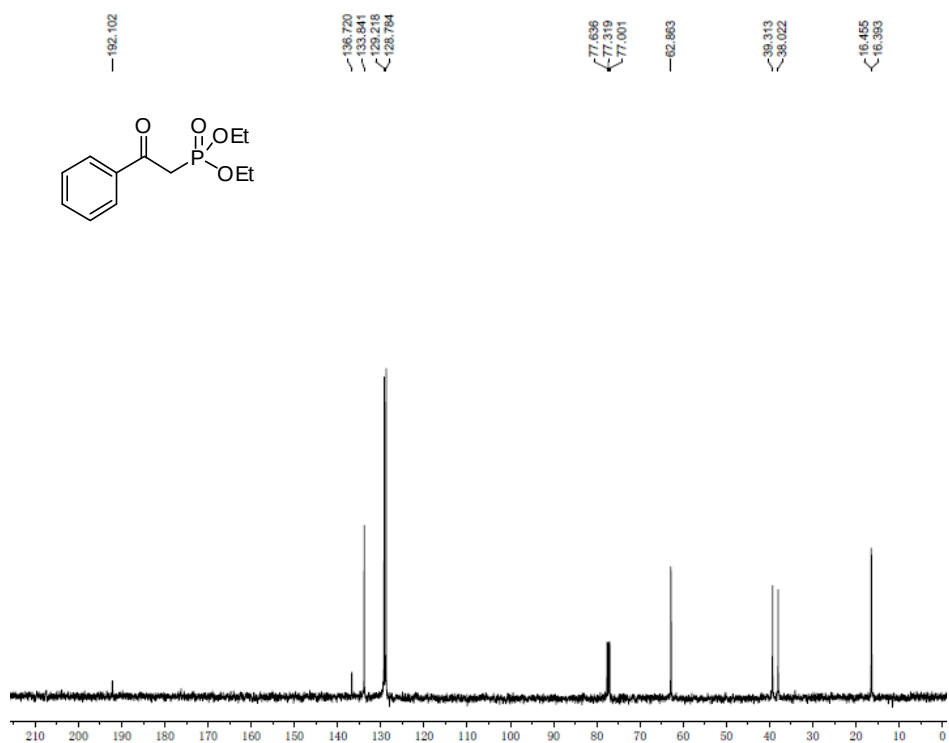
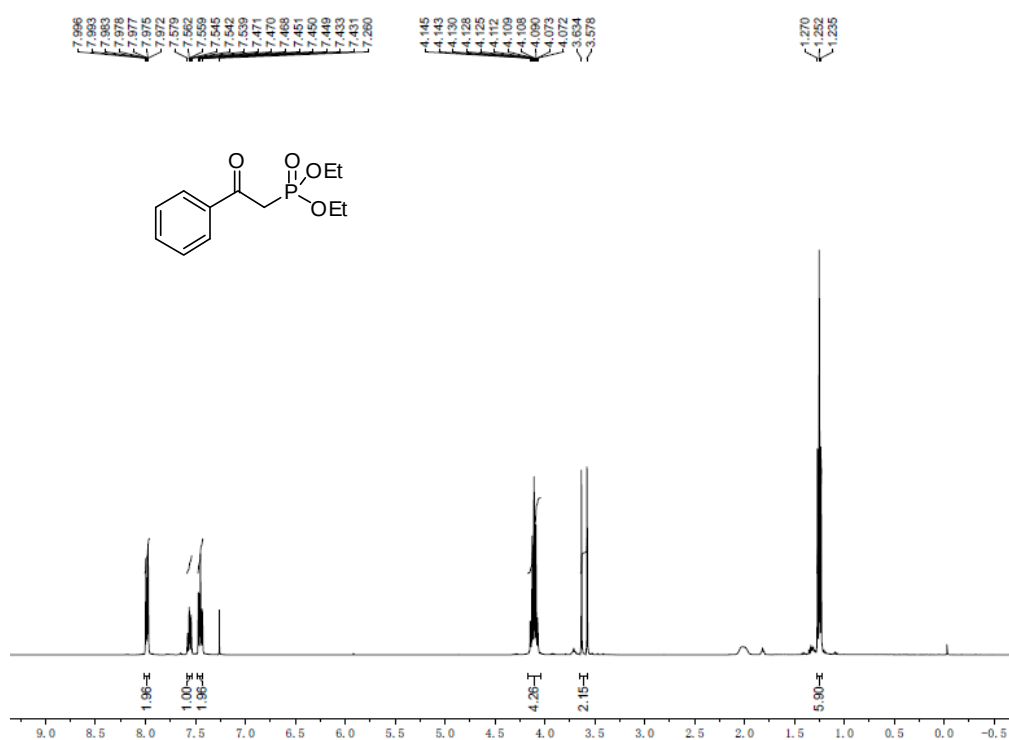
NMR data for compounds 1-3	2
HPLC for racemic and chiral compounds 2, 3m-s	59

NMR data for compounds 1-3

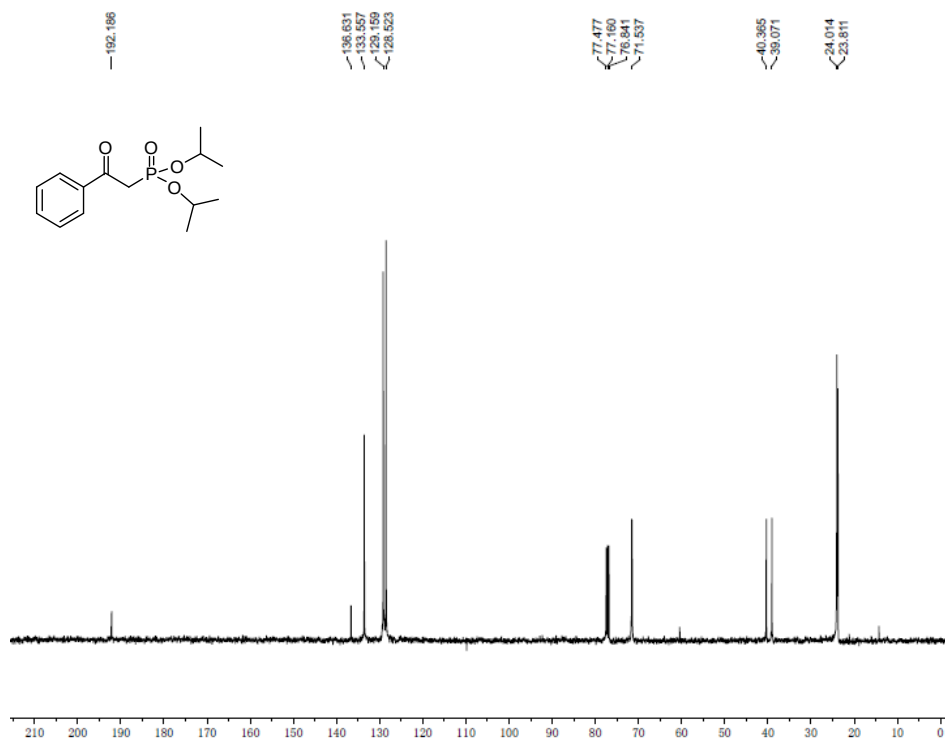
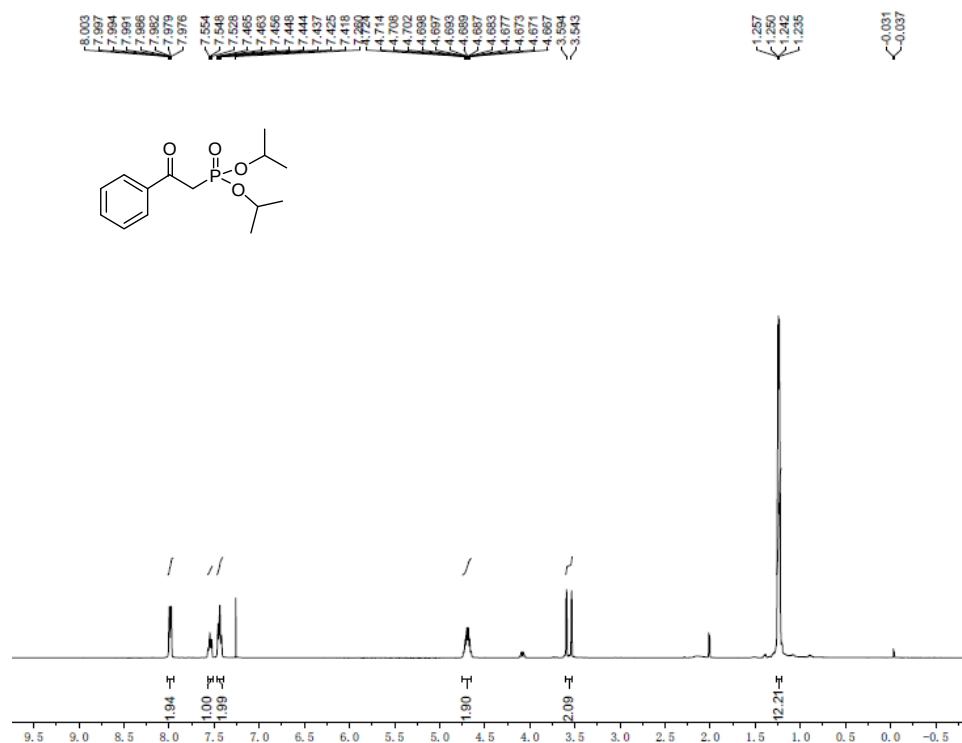
(1a) Dimethyl (2-oxo-2-phenyl)phosphonate



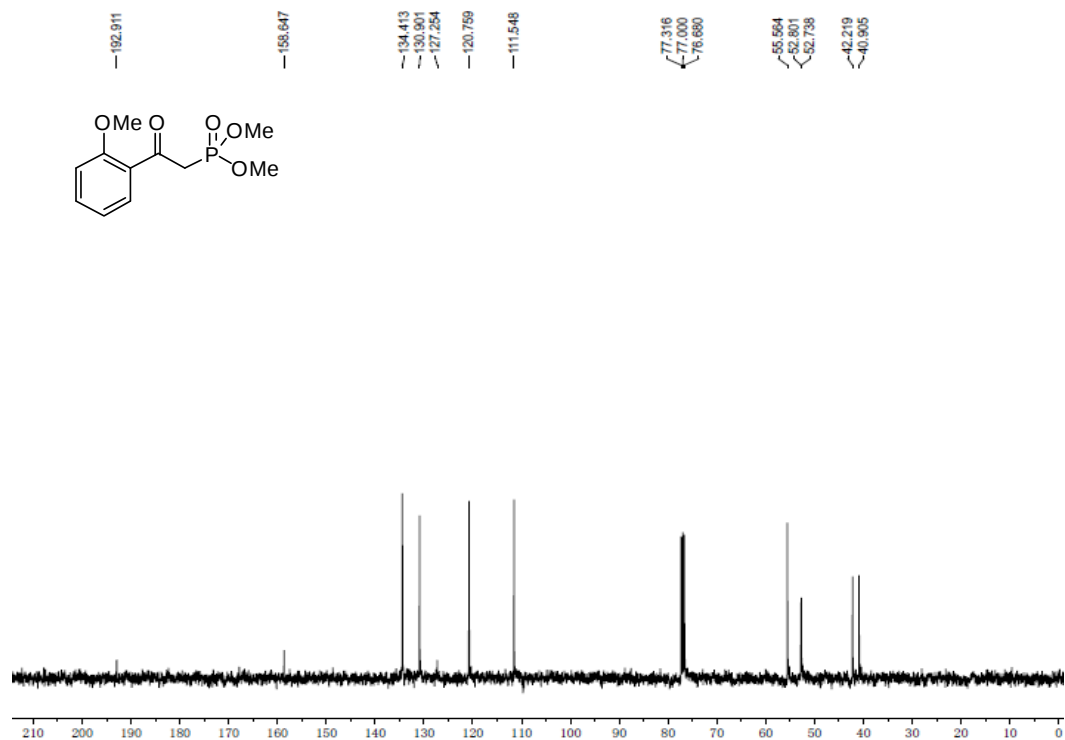
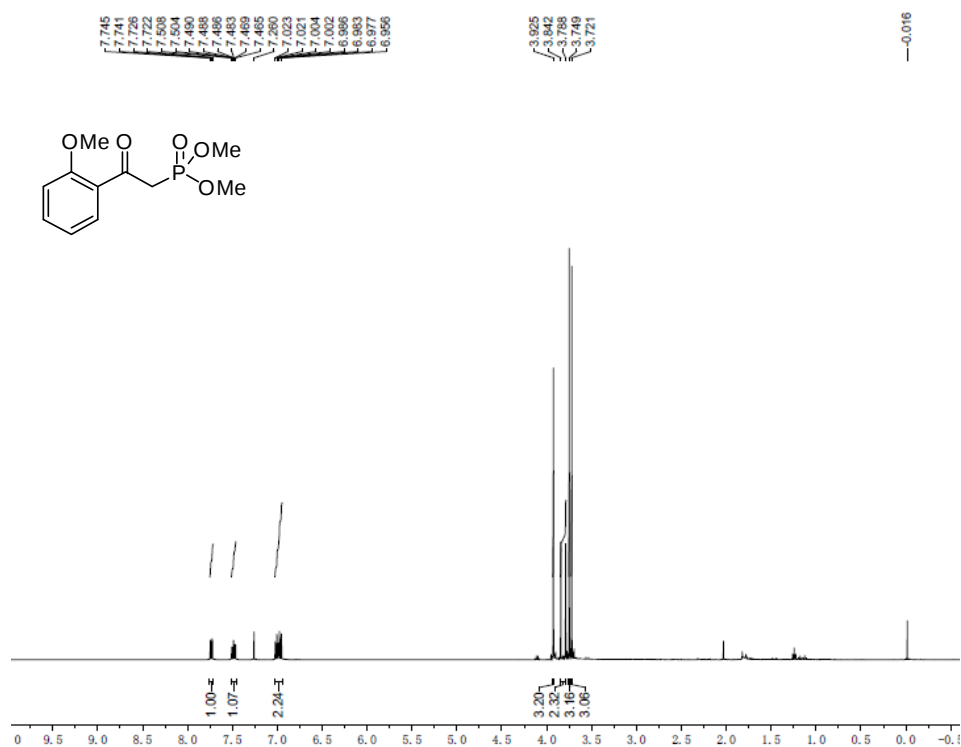
(2b) Diethyl (2-oxo-2-phenylethyl)phosphonate



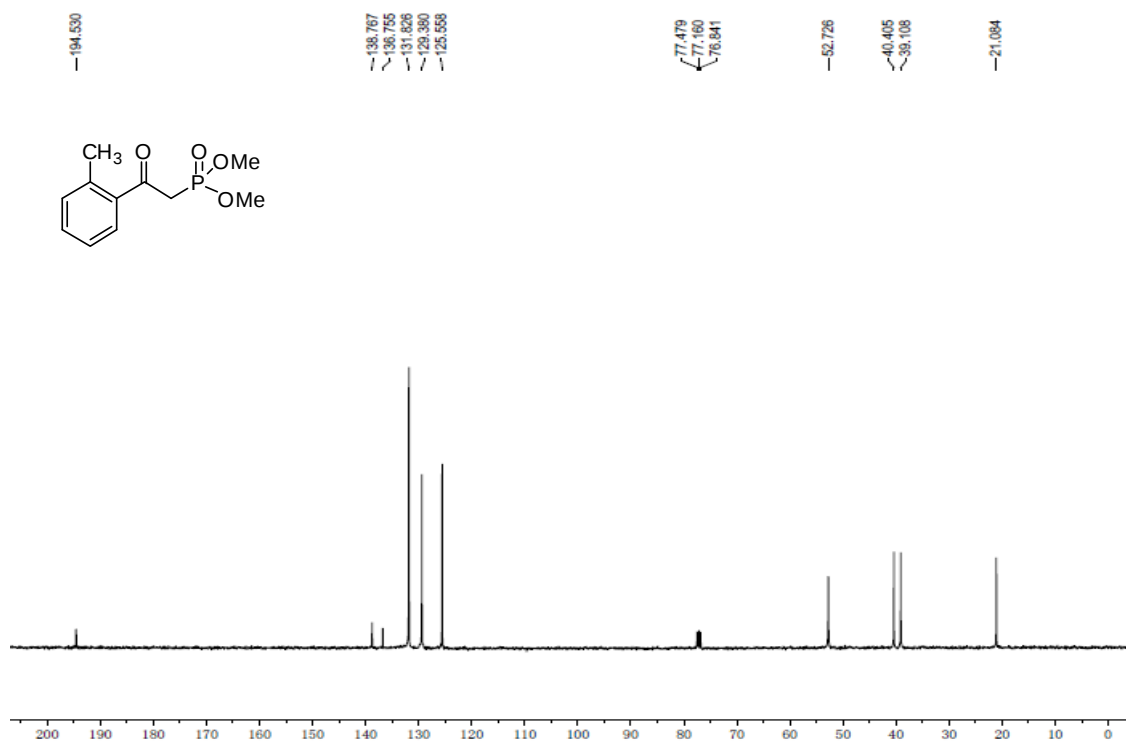
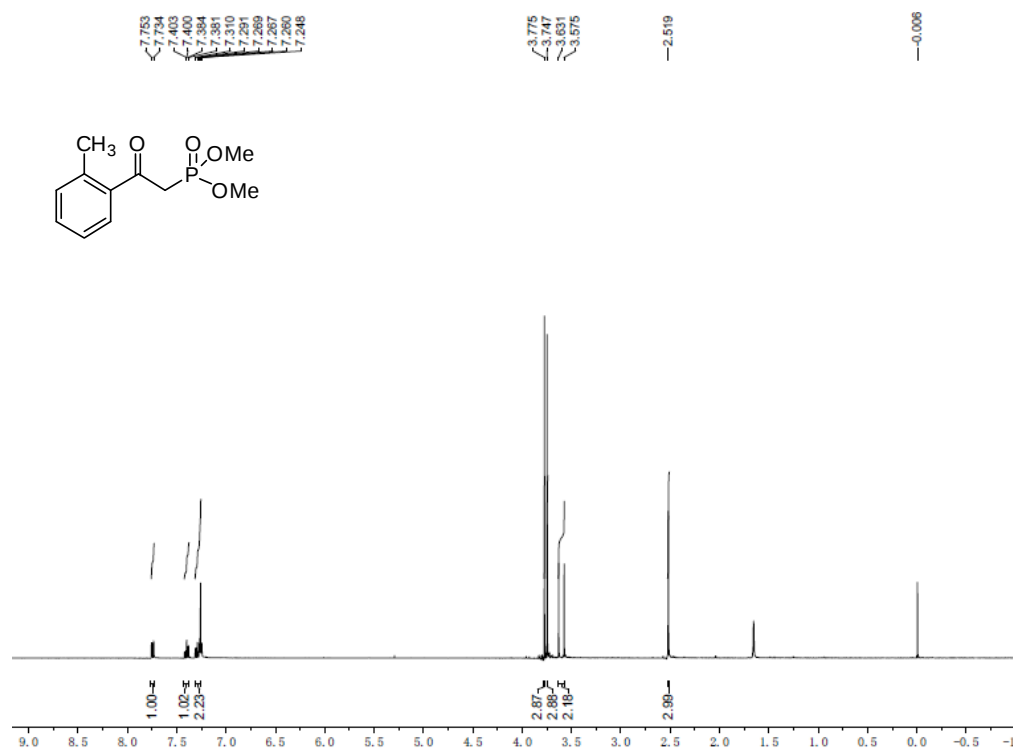
(1c) Diisopropyl (2-oxo-2-phenylethyl)phosphonate



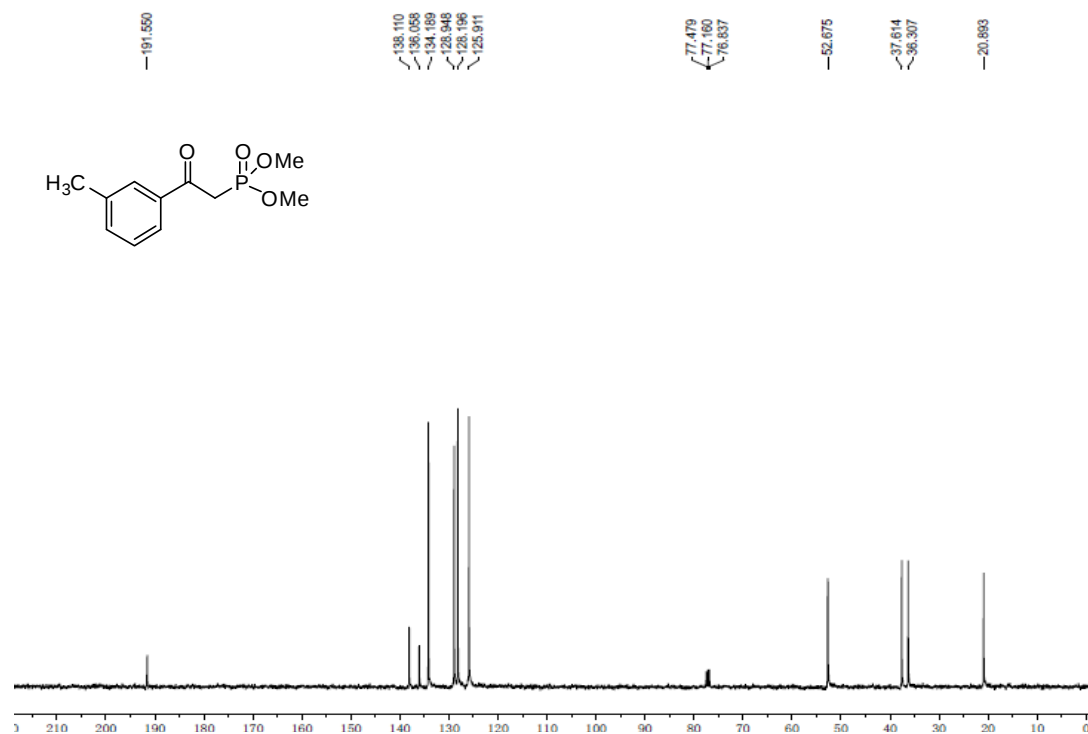
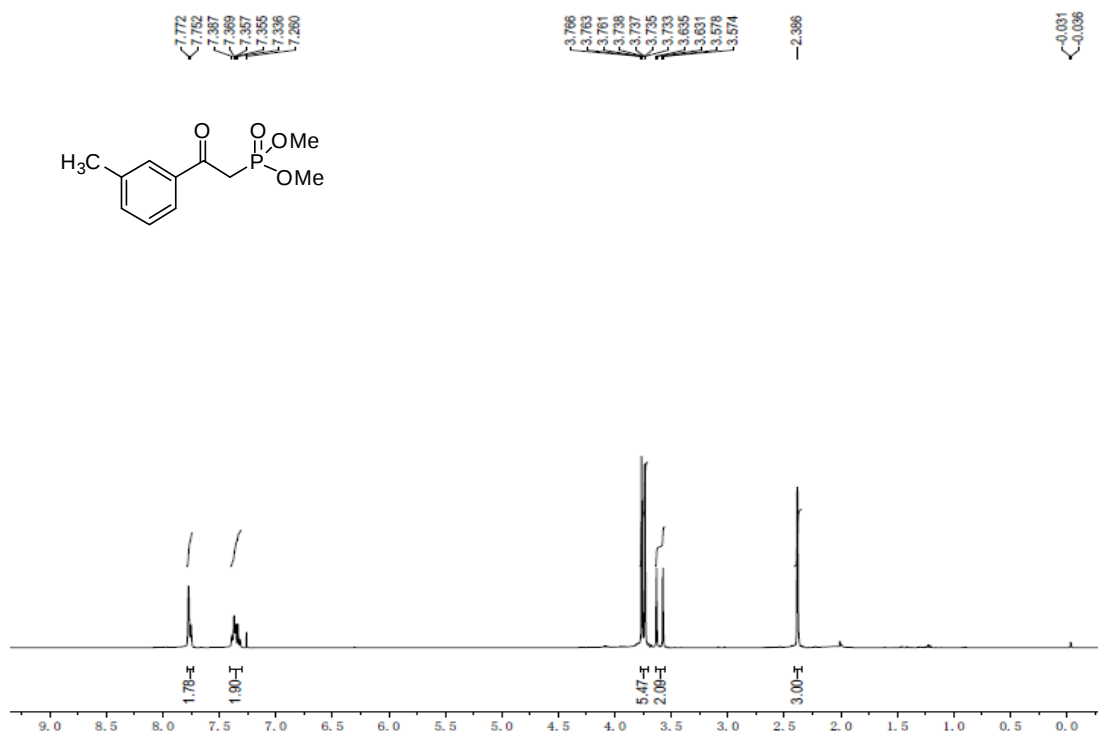
(1d) Dimethyl 2-*o*-methoxyphenyl-2-oxoethylphosphonate



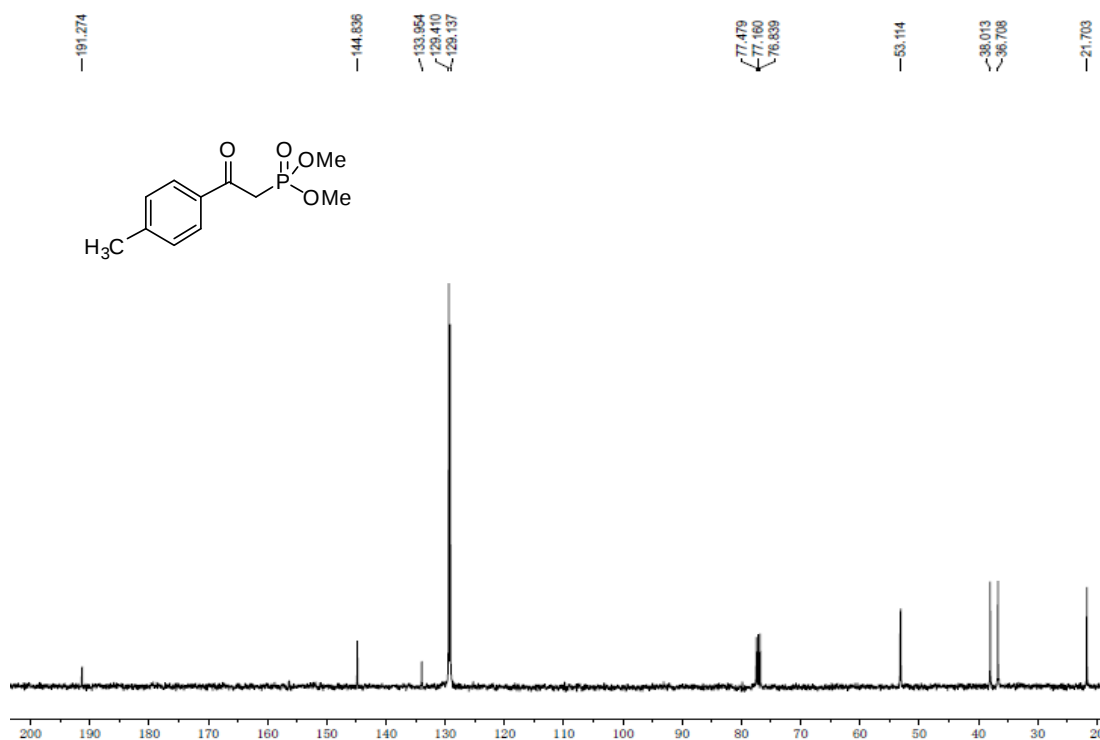
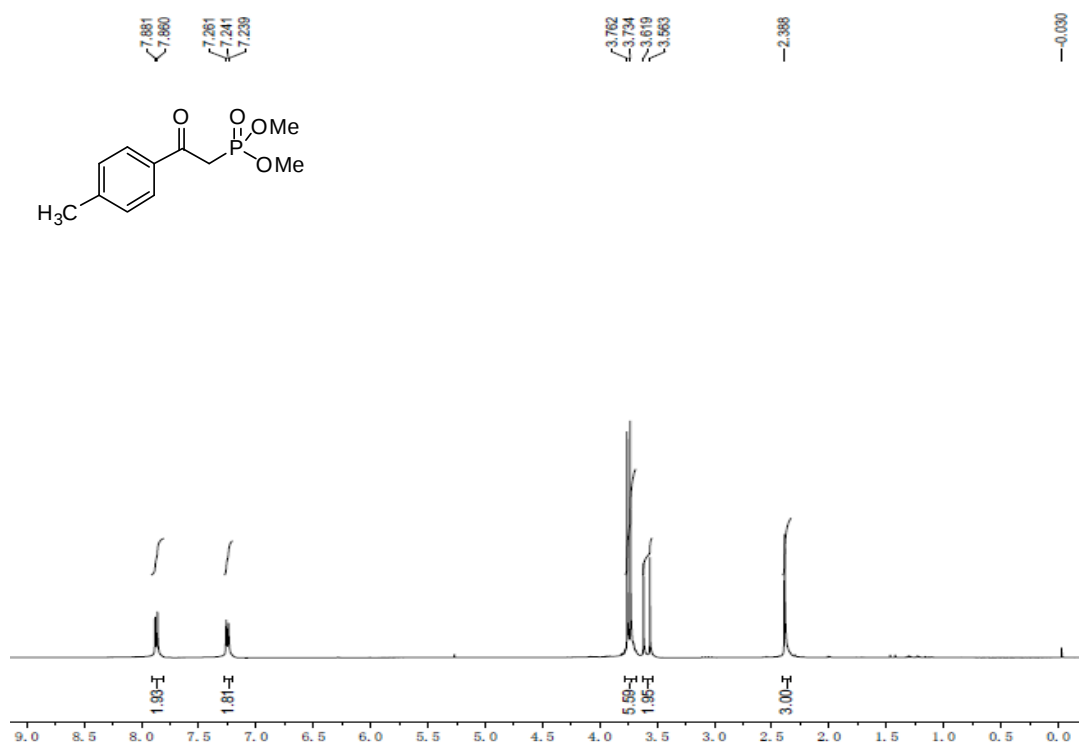
(1e) Dimethyl 2-*o*-methylphenyl-2-oxoethylphosphonate



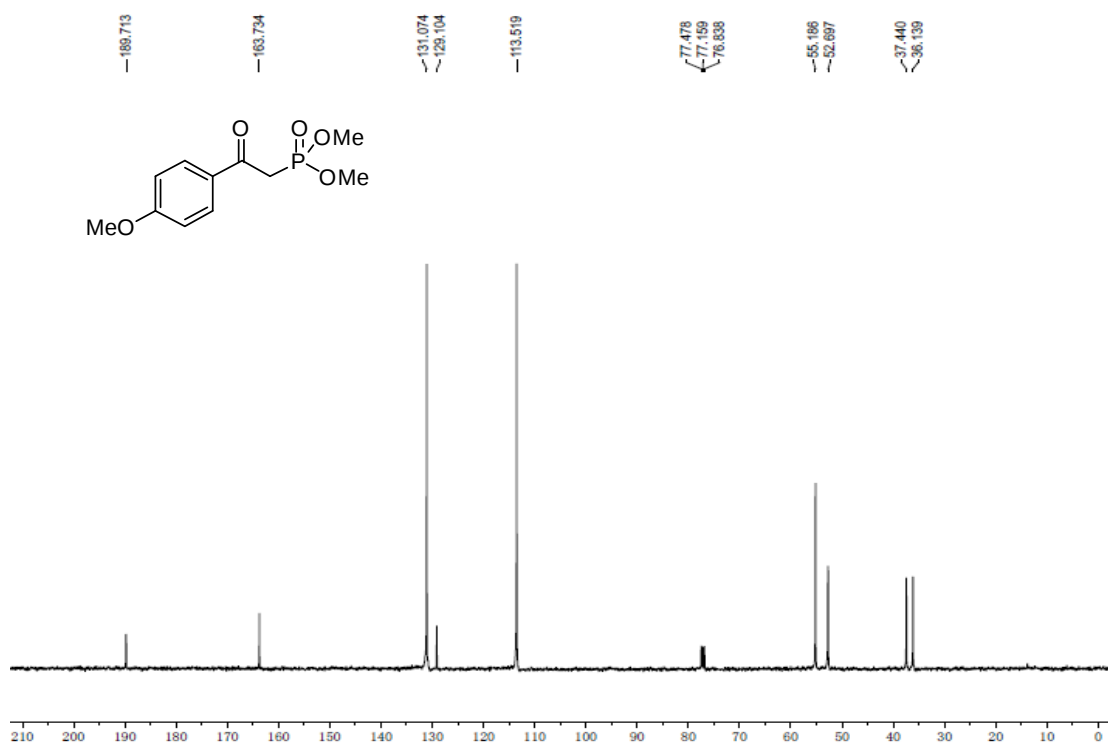
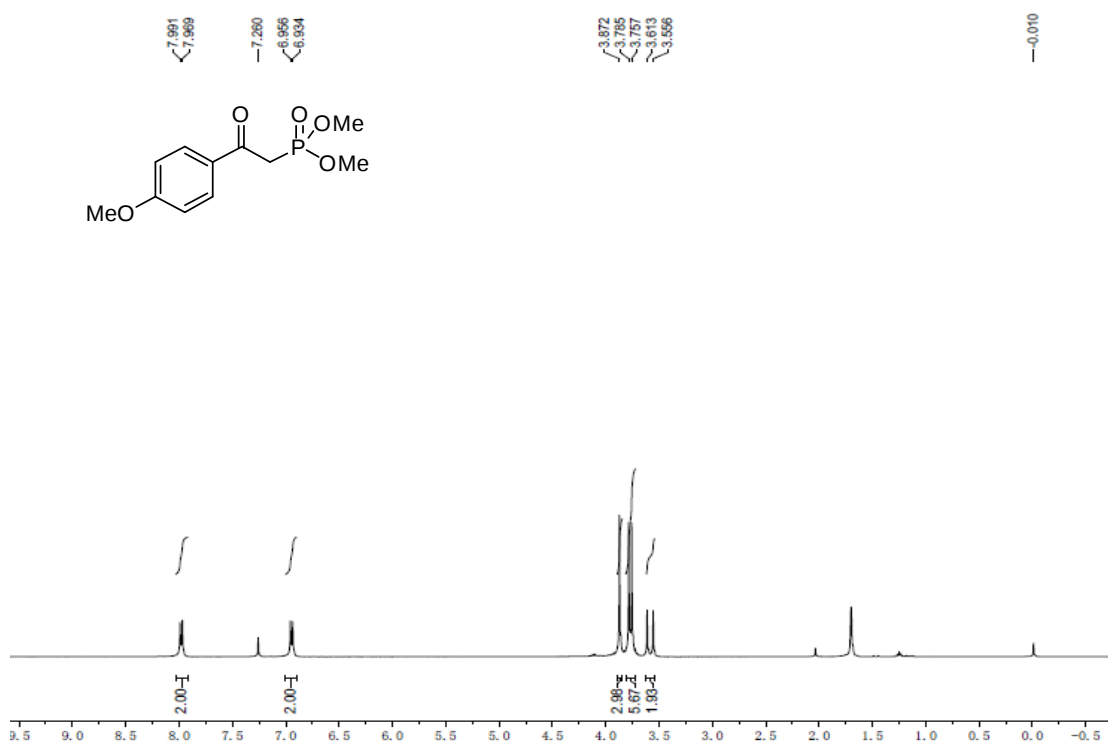
(1f) Dimethyl 2-*m*-methylphenyl-2-oxoethylphosphonate



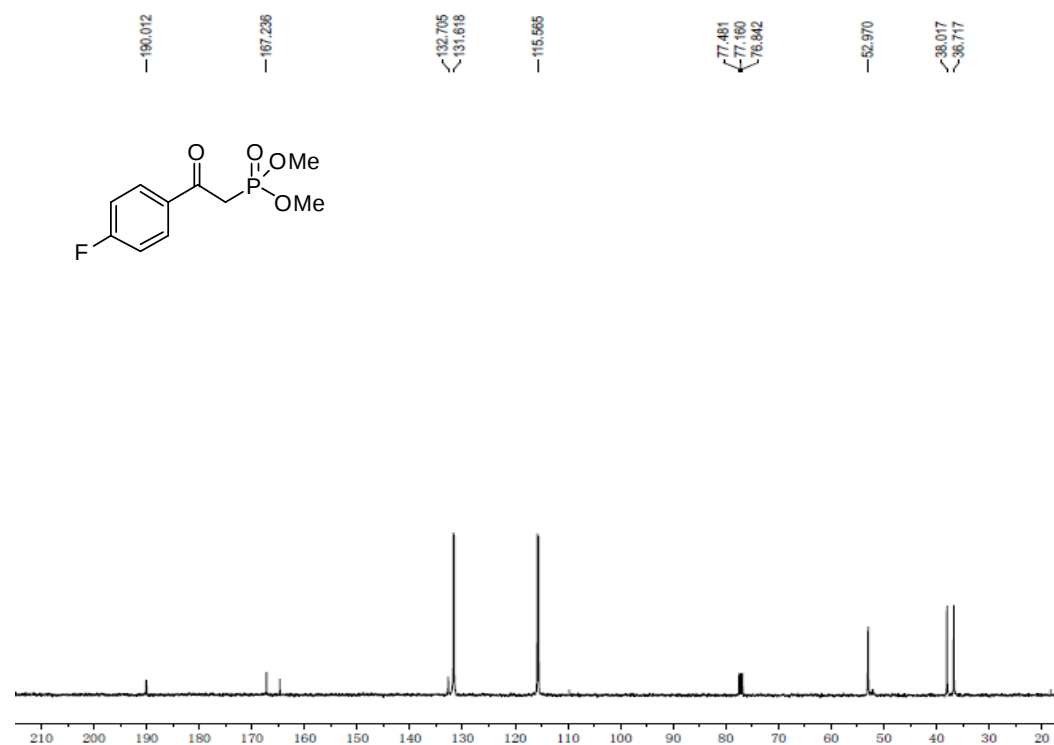
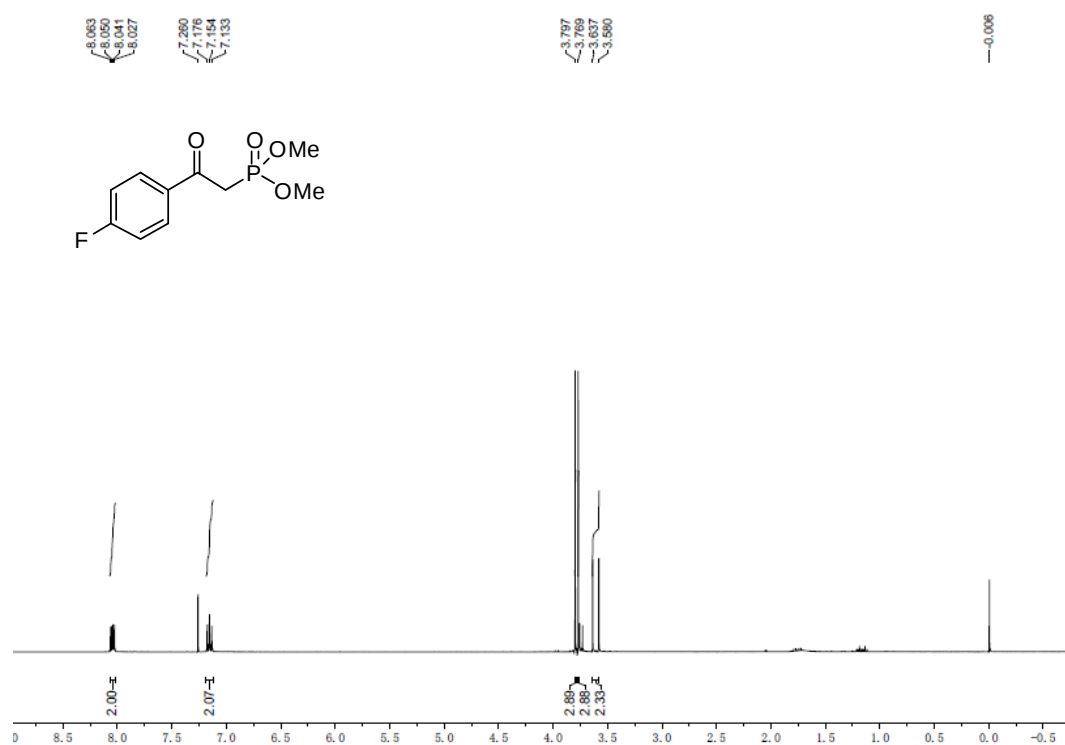
(1g) Dimethyl 2-*p*-methylphenyl-2-oxoethylphosphonate



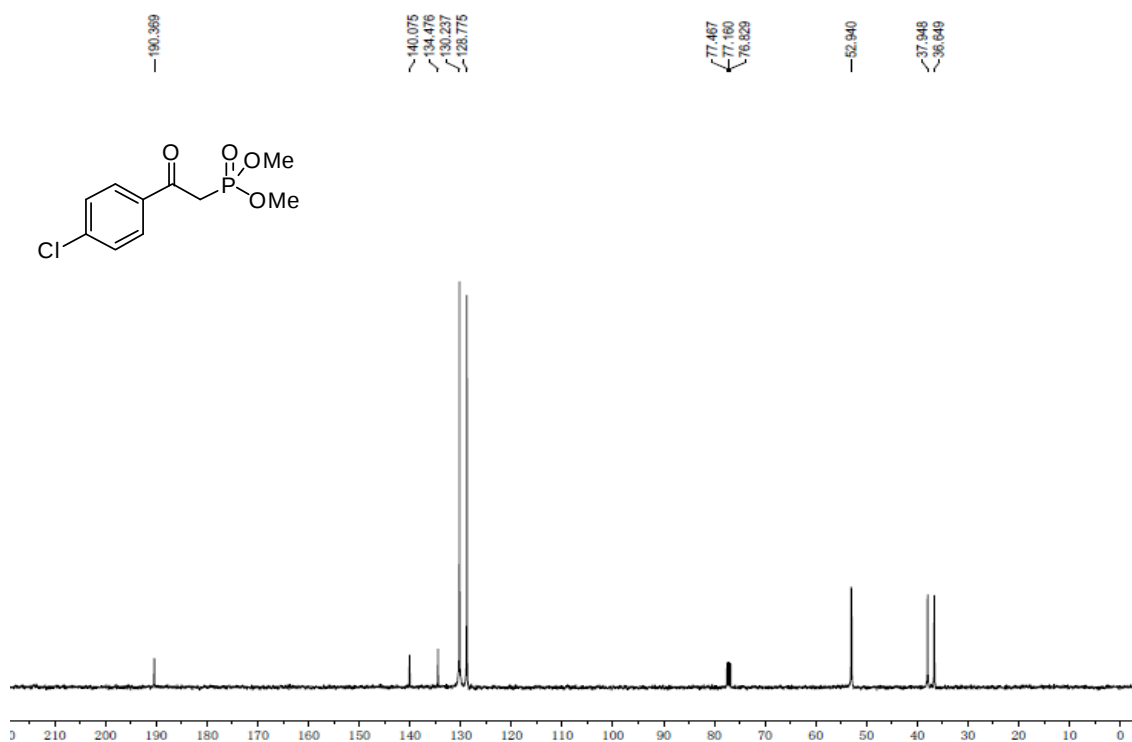
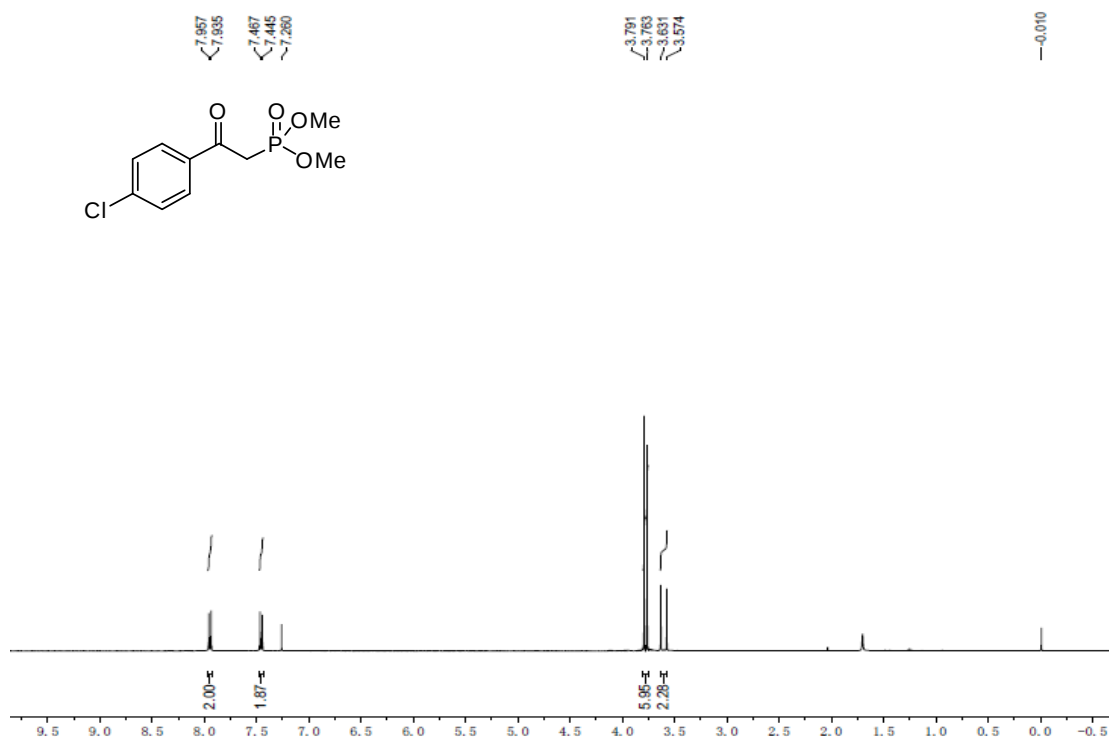
(1h) Dimethyl 2-*p*-methoxyphenyl-2-oxoethylphosphonate



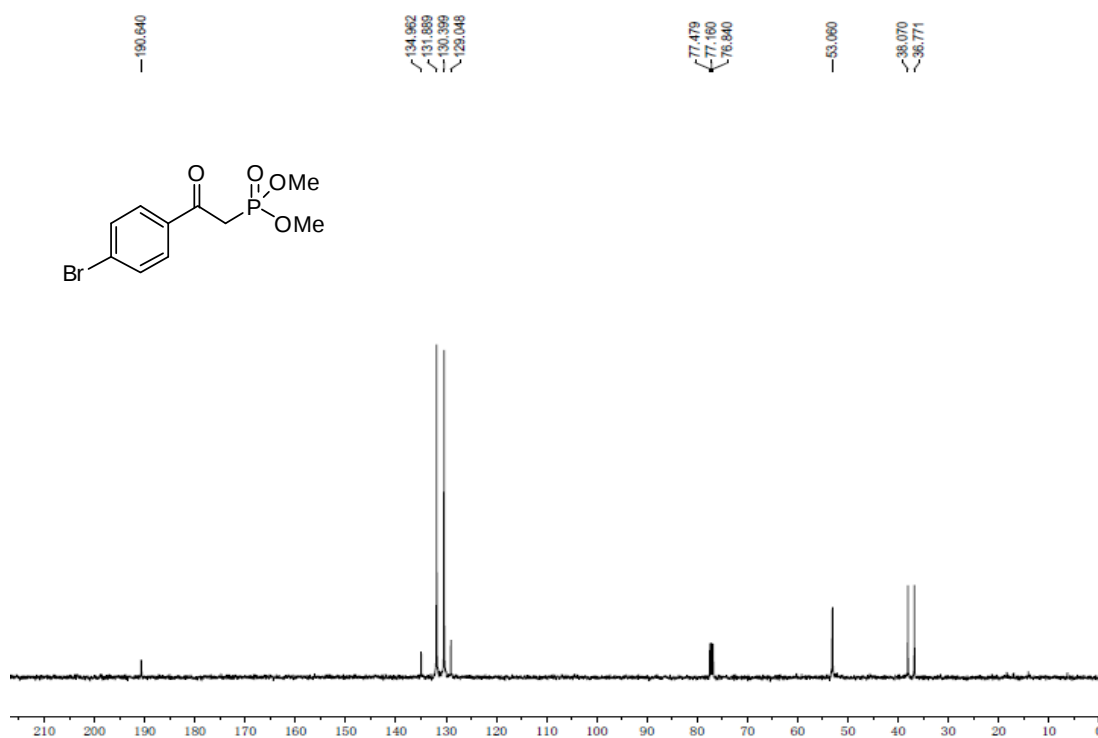
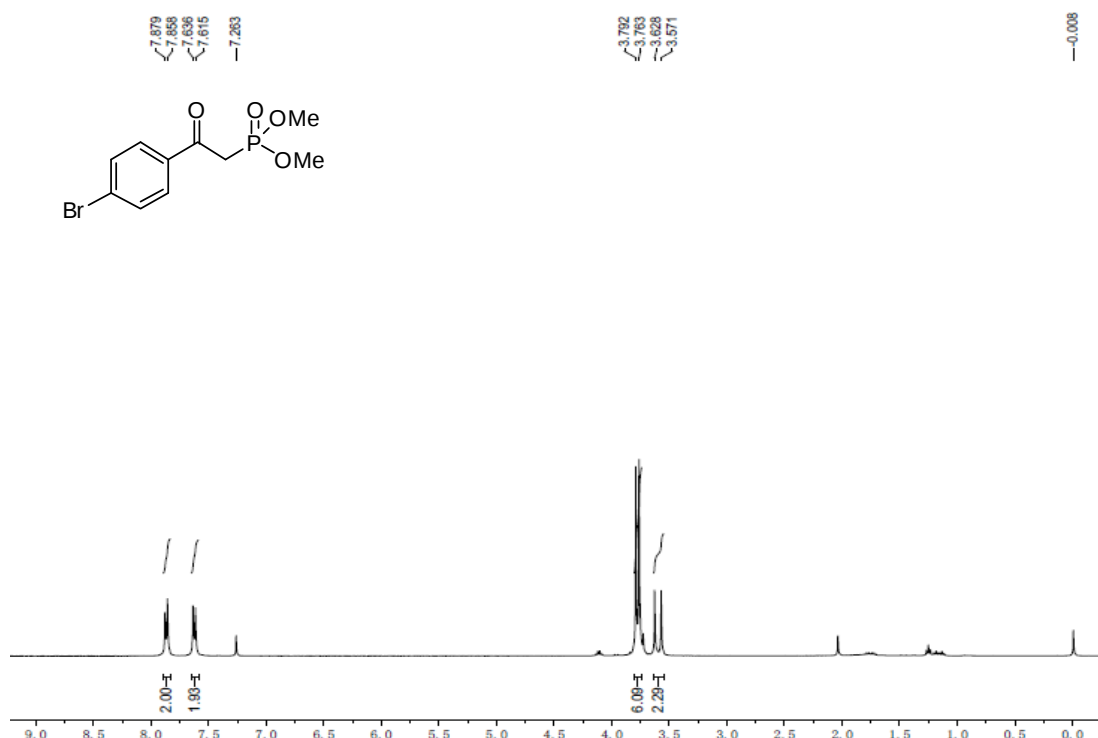
(1i) Dimethyl 2-*p*-fluorophenyl-2-oxoethylphosphonate



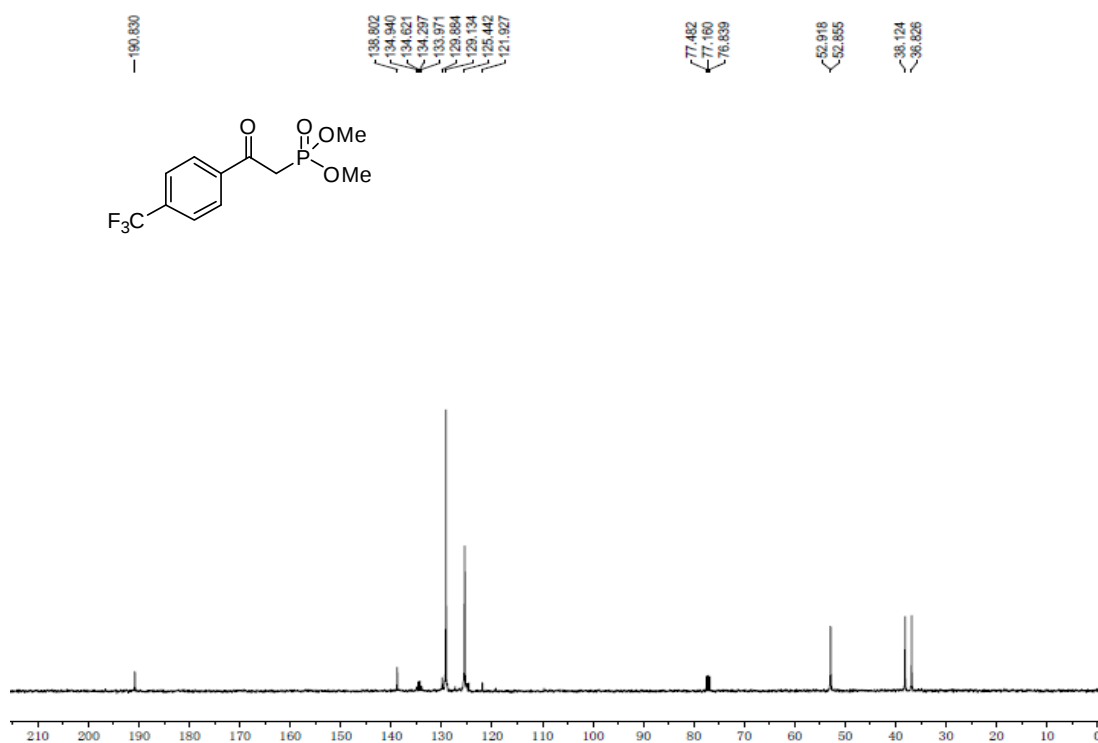
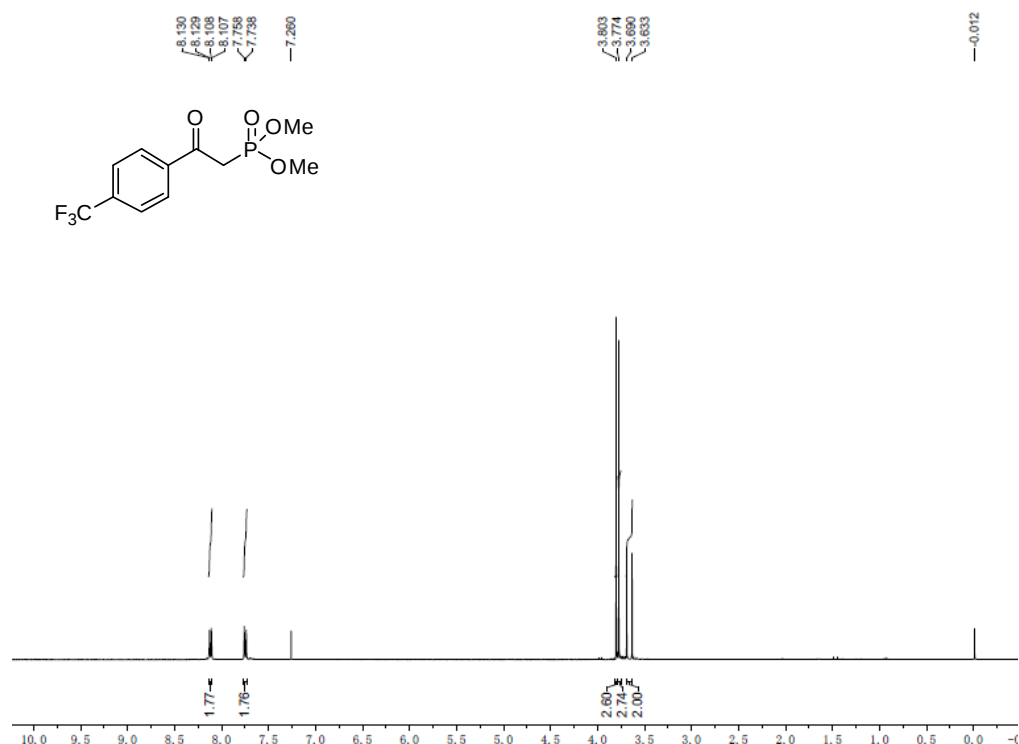
(1j) Dimethyl 2-*p*-chlorophenyl-2-oxoethylphosphonate



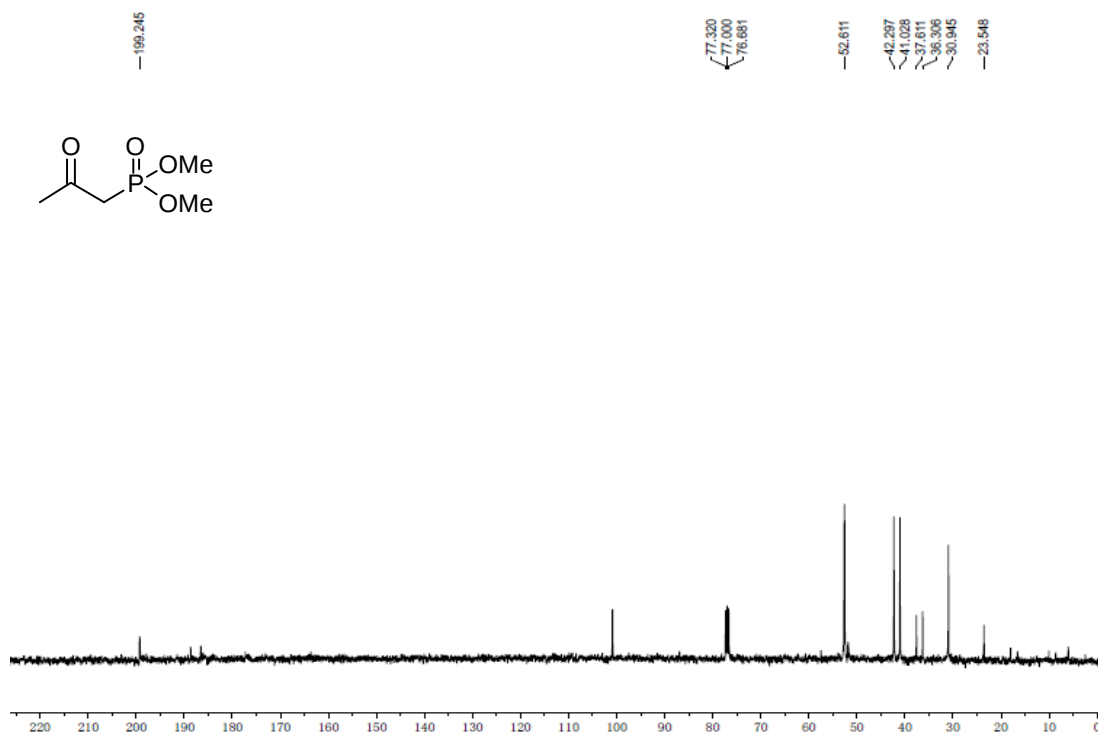
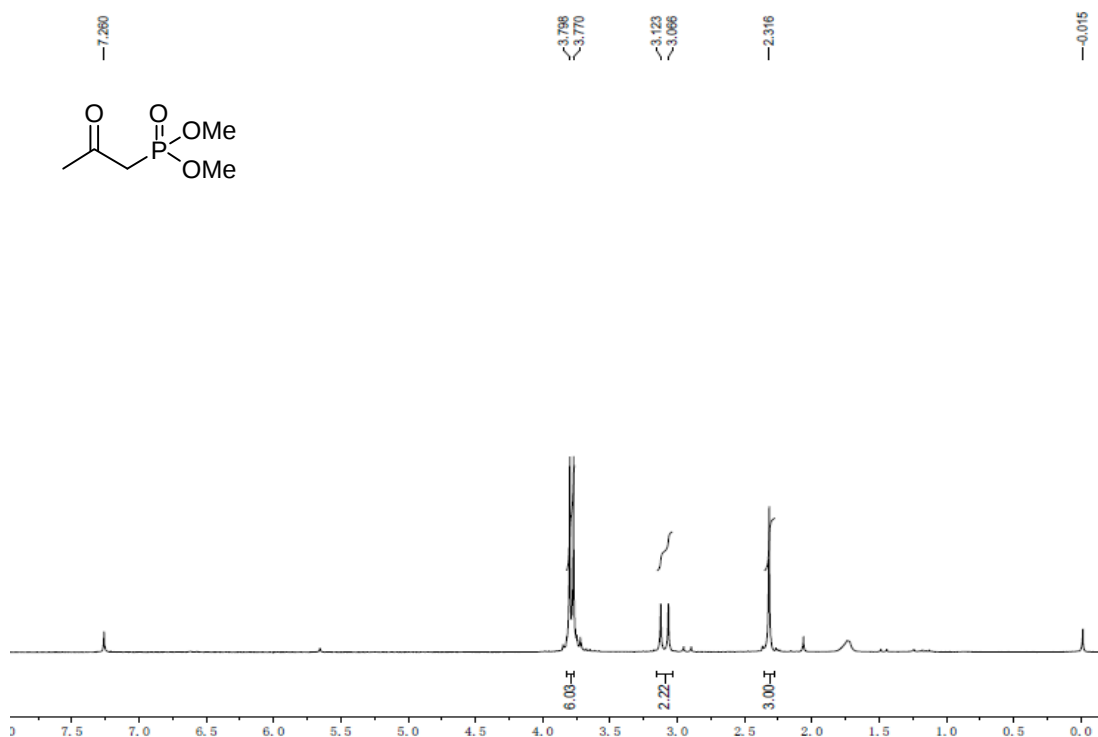
(1k) Dimethyl 2-*p*-bromophenyl-2-oxoethylphosphonate



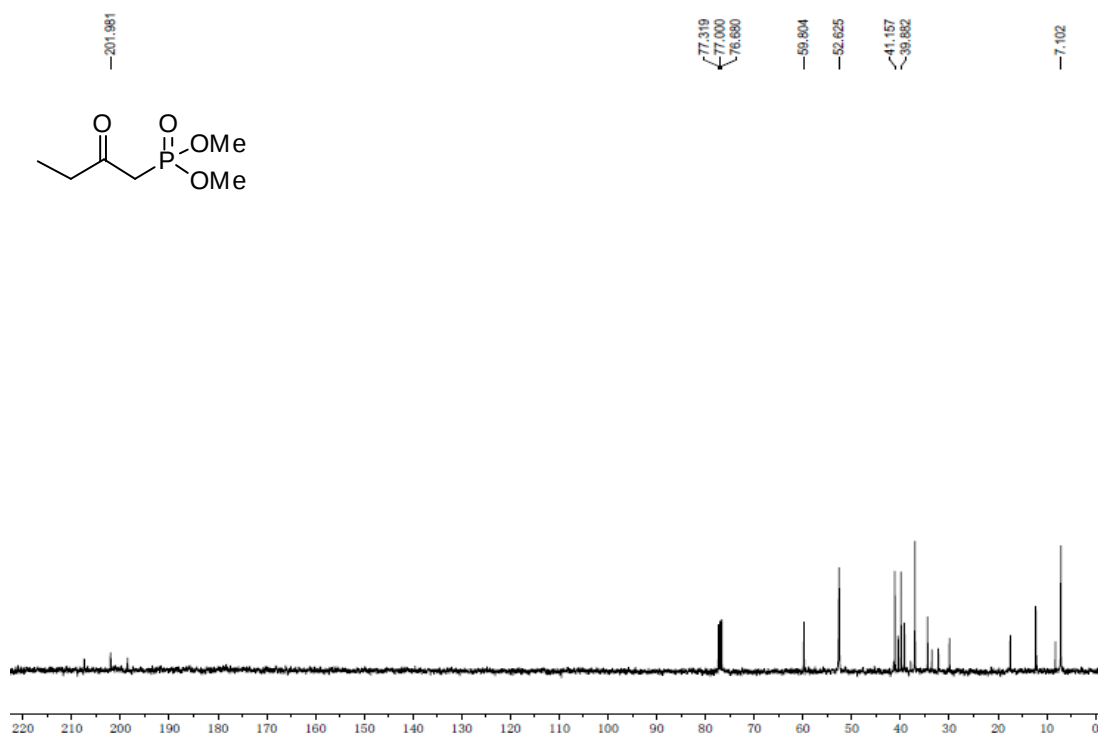
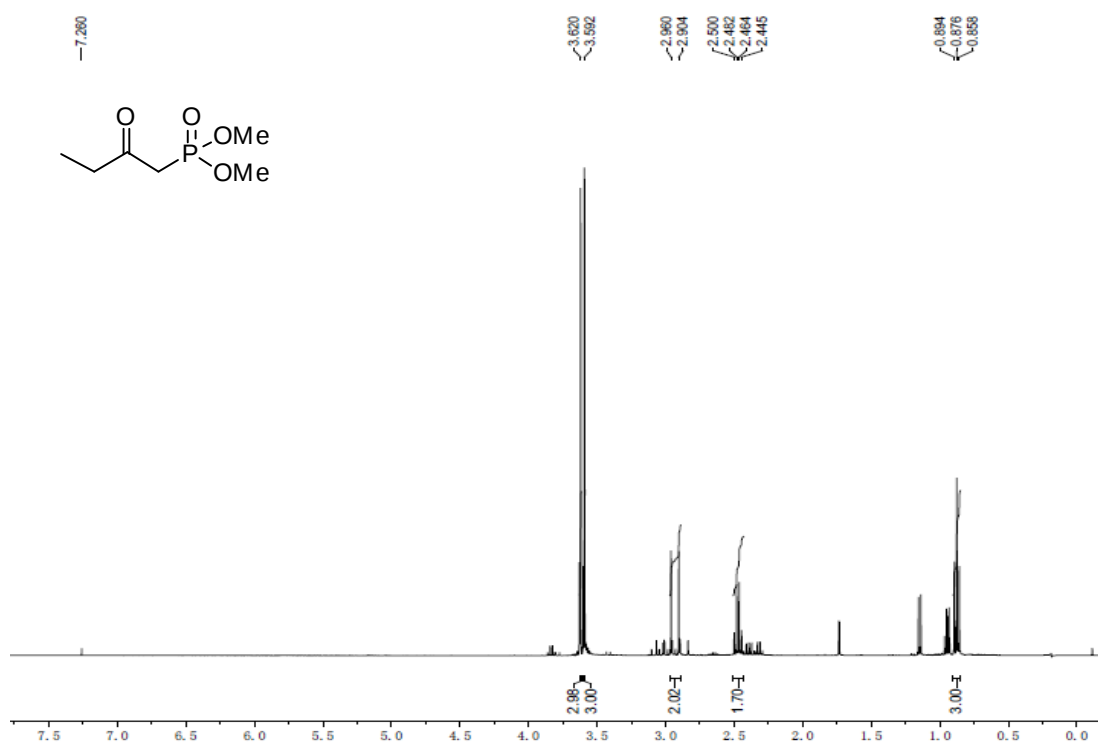
(1l) Dimethyl 2-*p*-trifluoromethylphenyl-2-oxoethylphosphonate



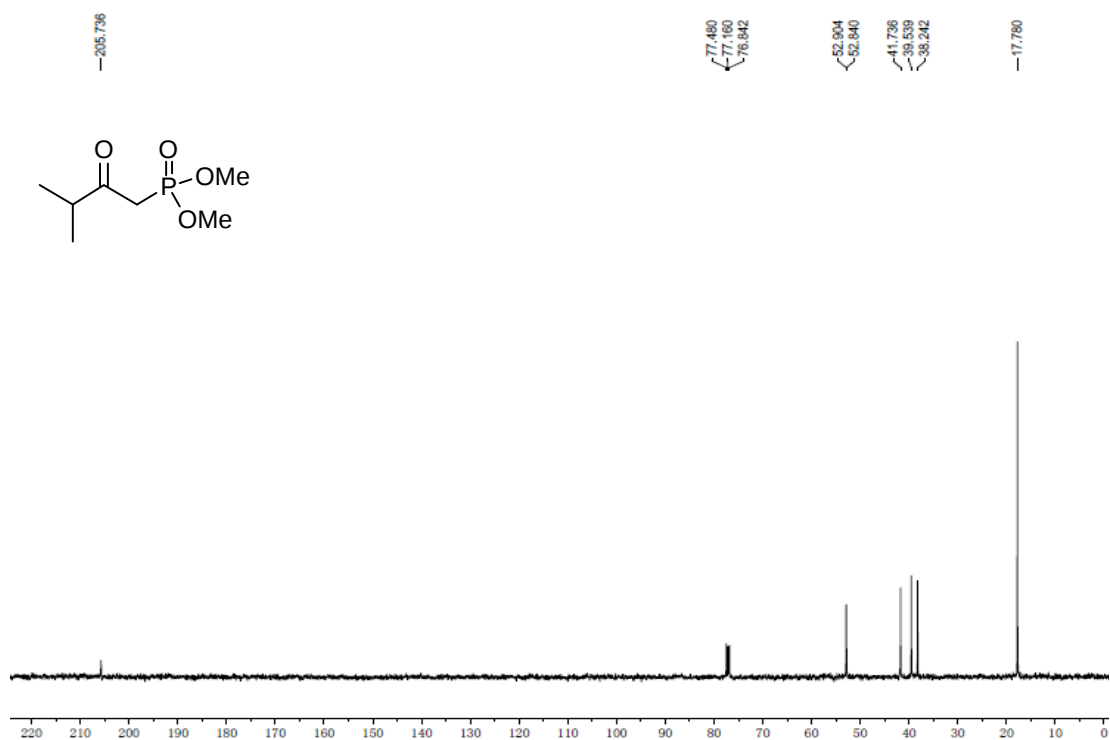
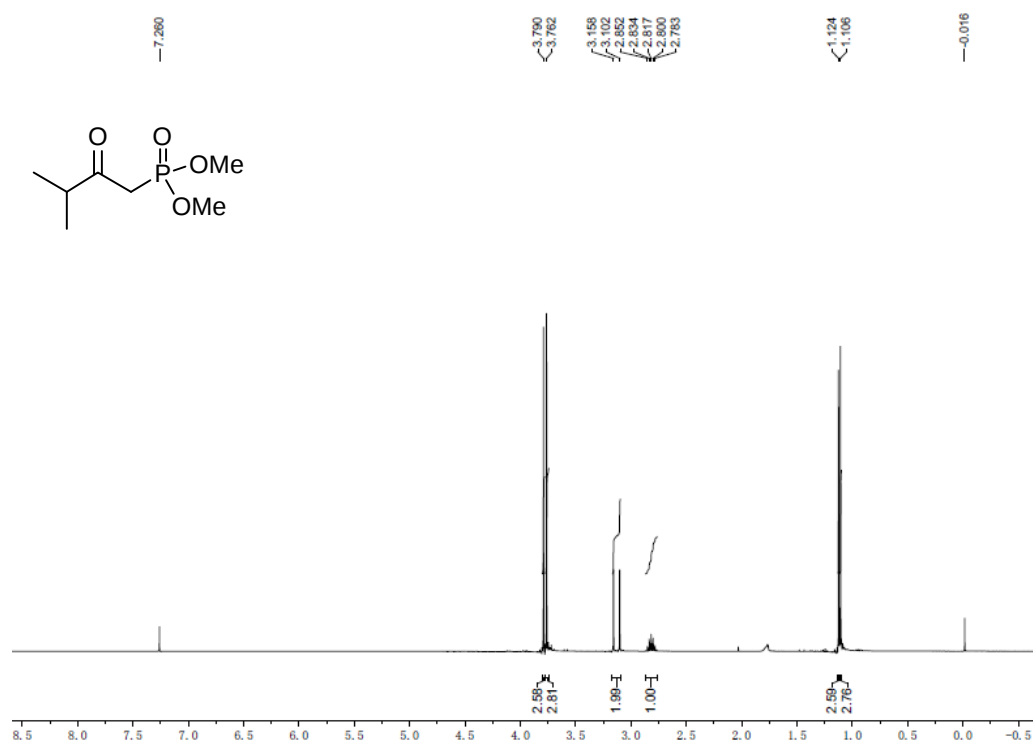
(1m) Dimethyl 2-oxopropylphosphonate



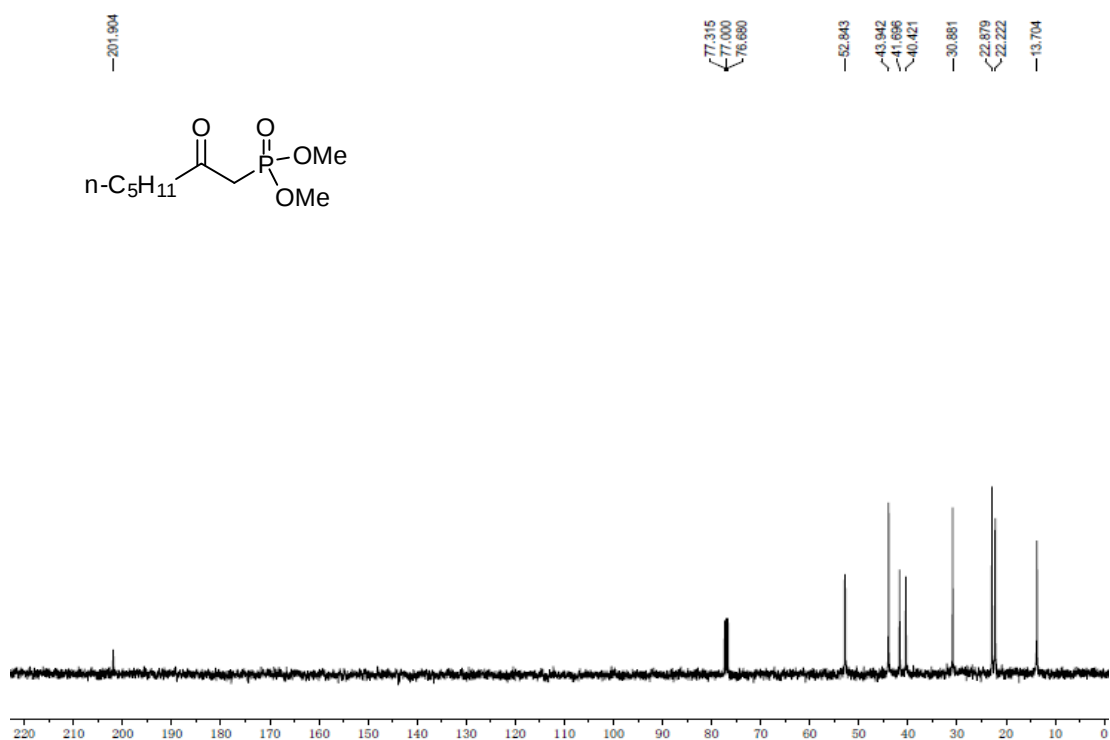
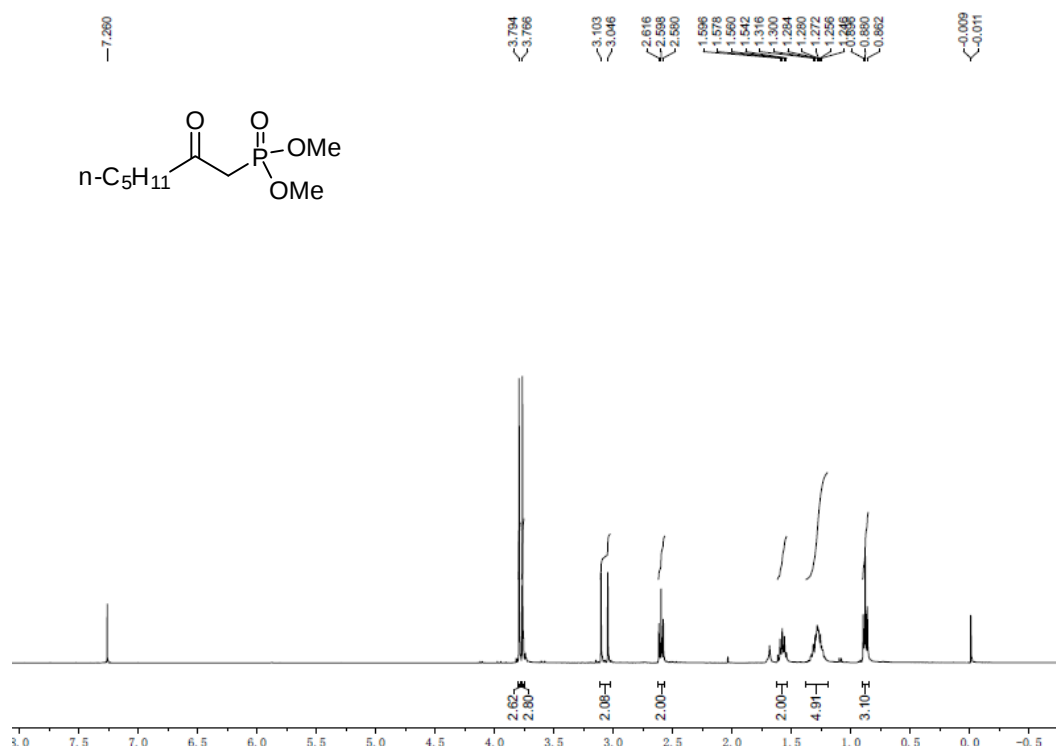
(1n) Dimethyl 2-oxobutylphosphonate



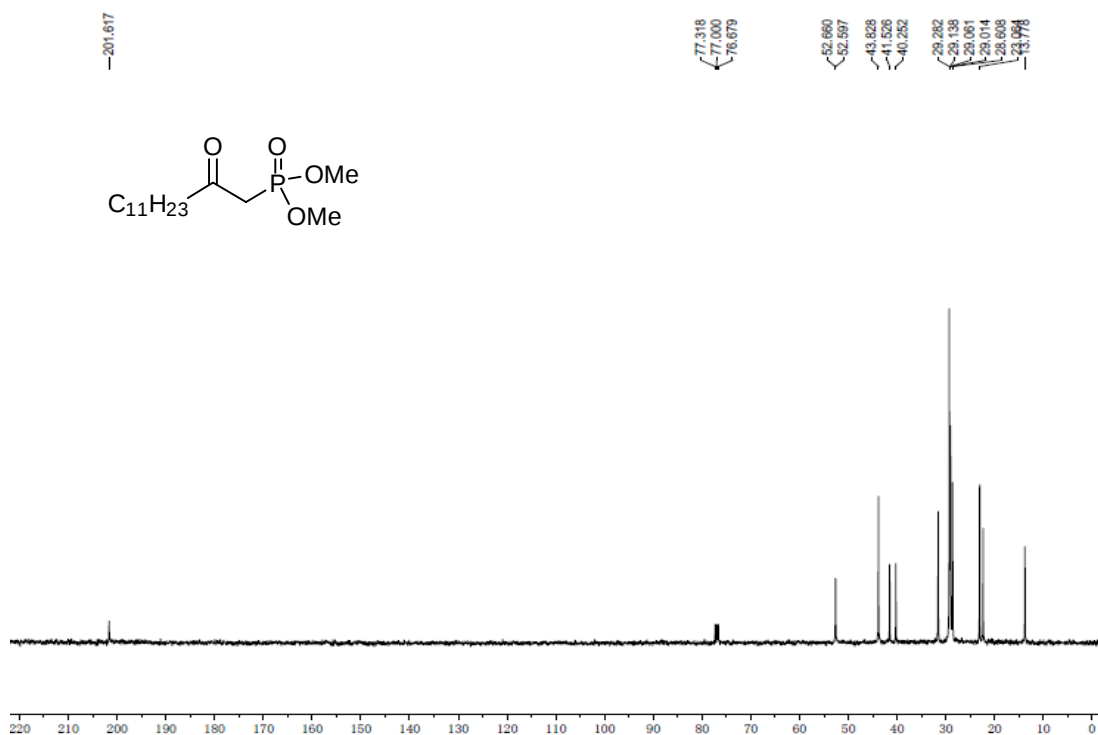
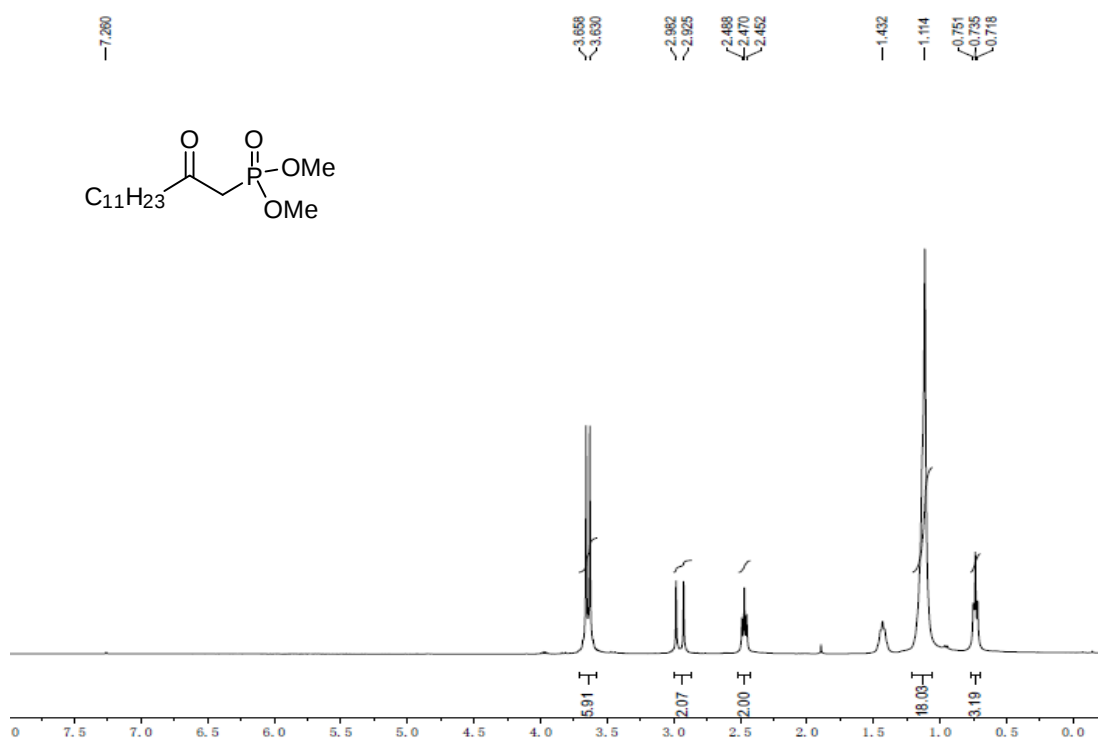
(1o) Dimethyl 3-methyl-2-oxobutylphosphonate



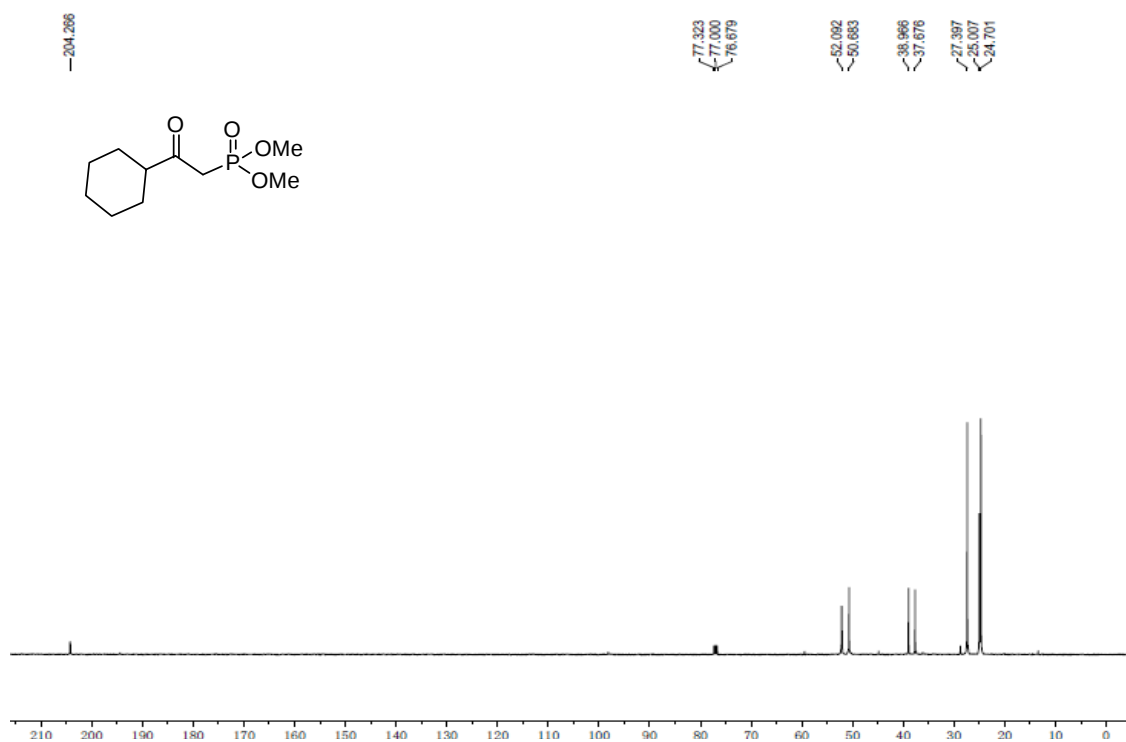
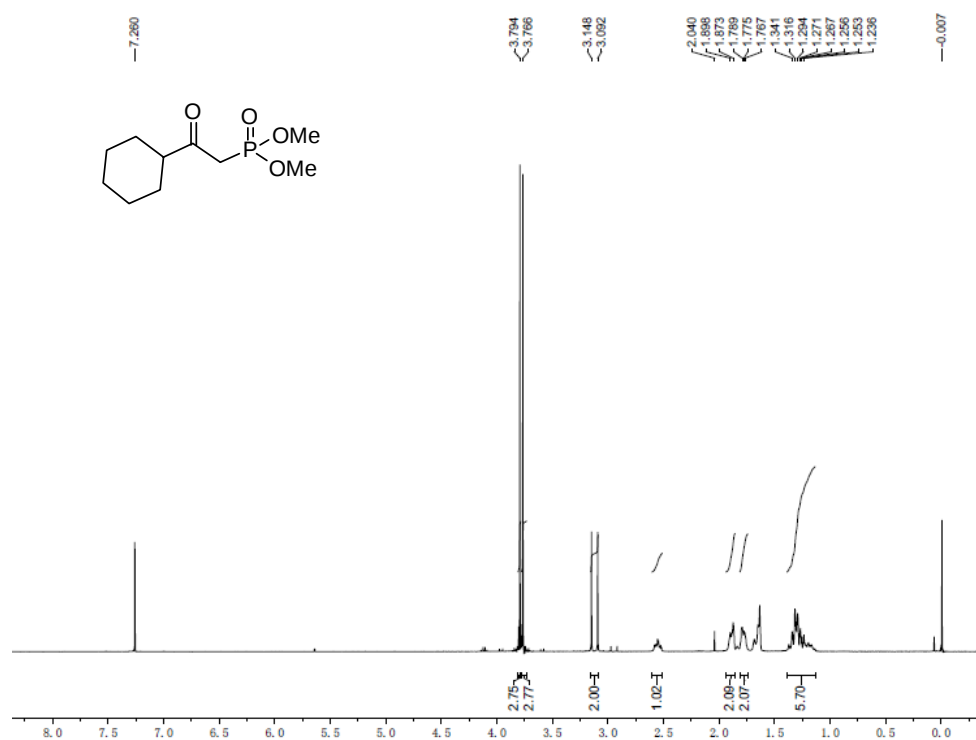
(1p) Dimethyl 2-oxoheptylphosphonate



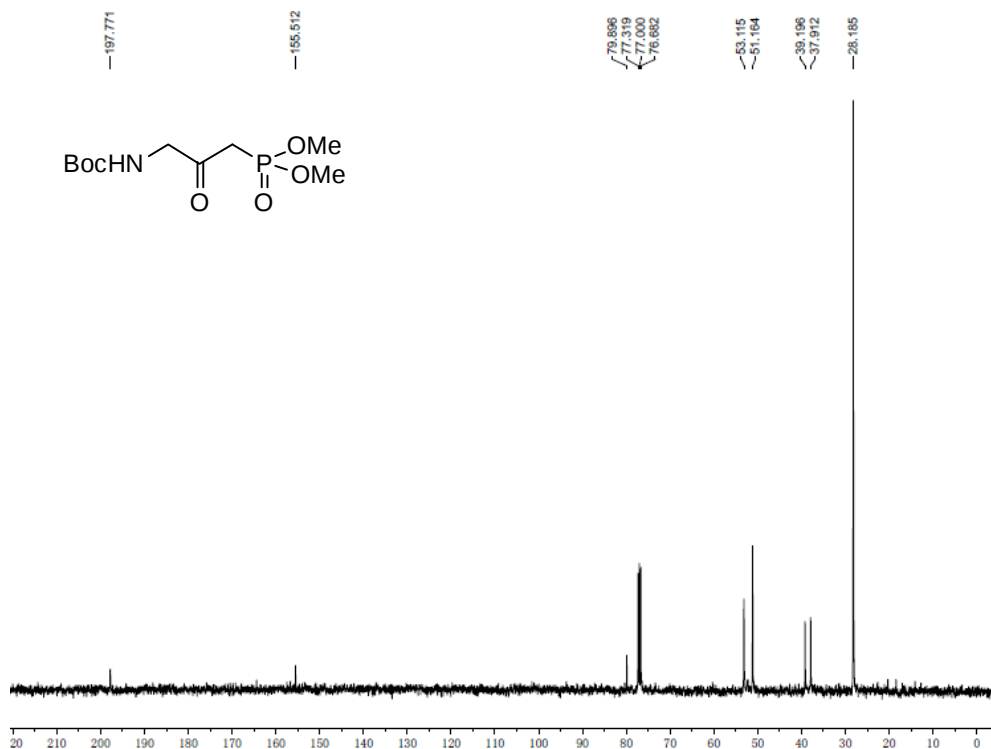
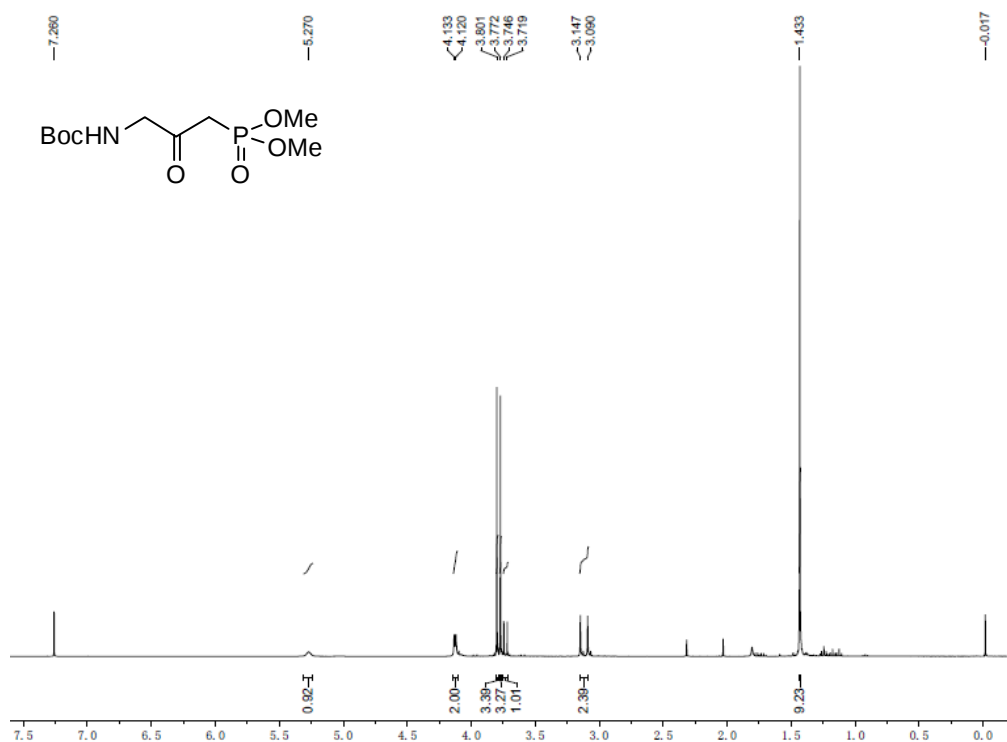
(1q) Dimethyl 2-oxotridecylphosphonate



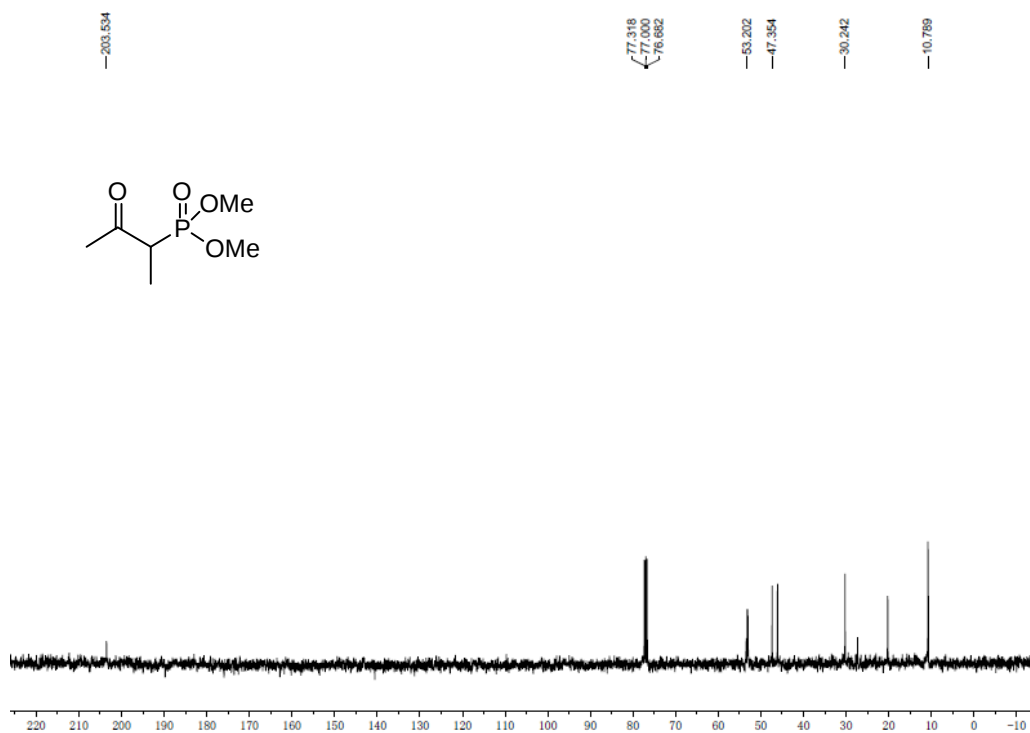
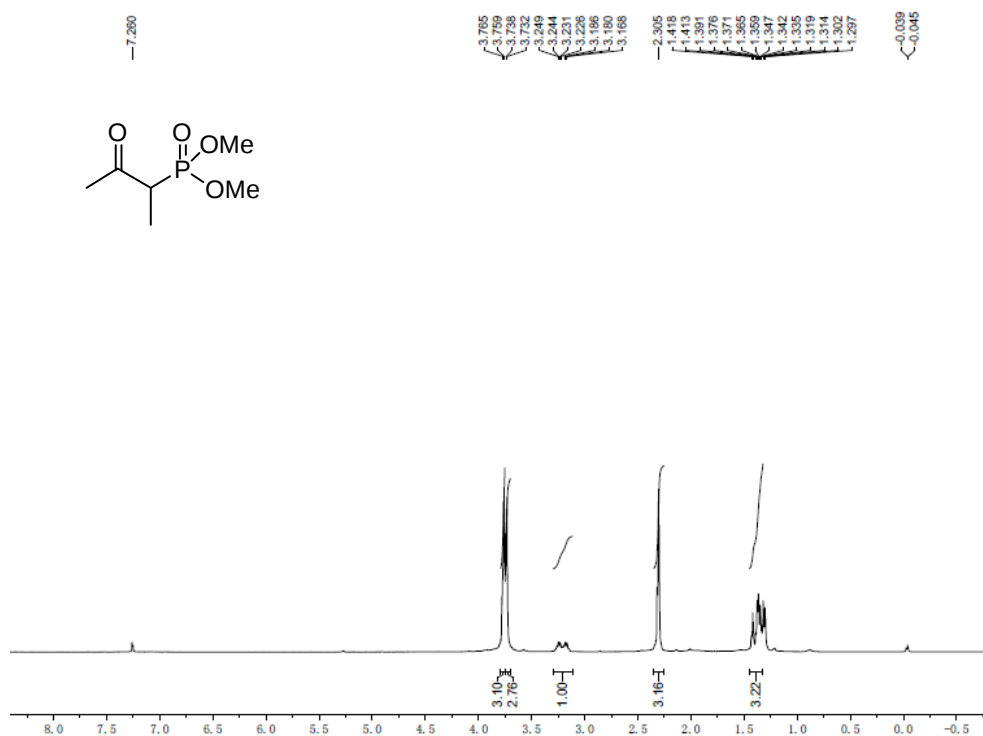
(1r) Dimethyl 2-cyclohexyl-2-oxoethylphosphonate



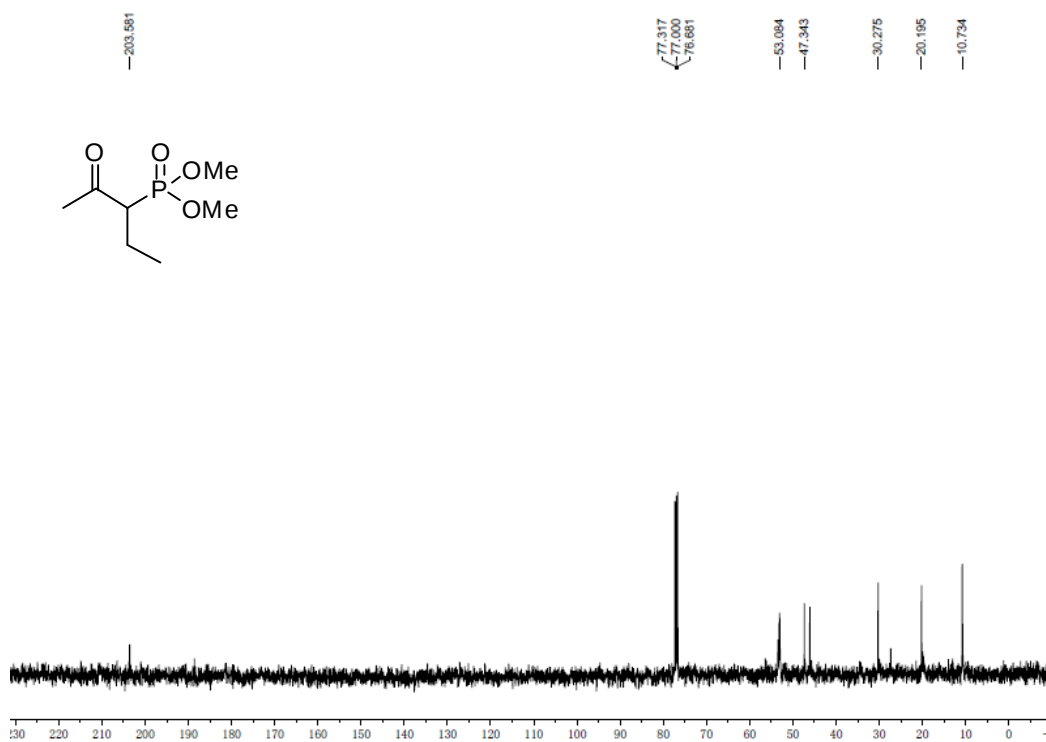
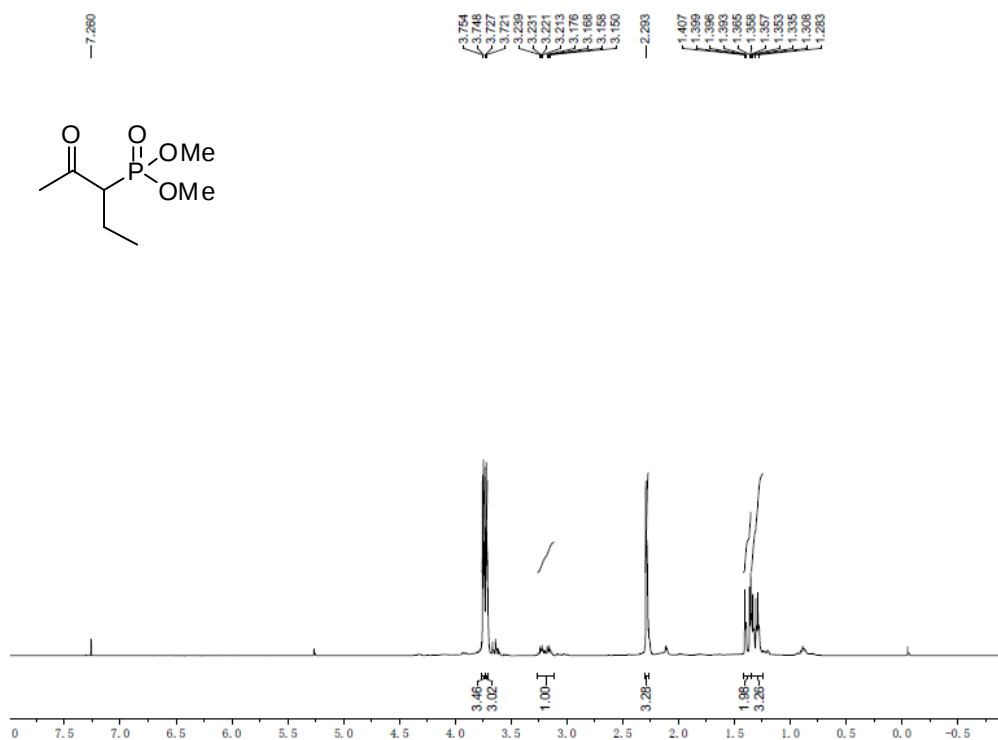
(1s) Dimethyl 2-oxo-3-(N-tert-butoxycarbonylamino)propane phosphonate



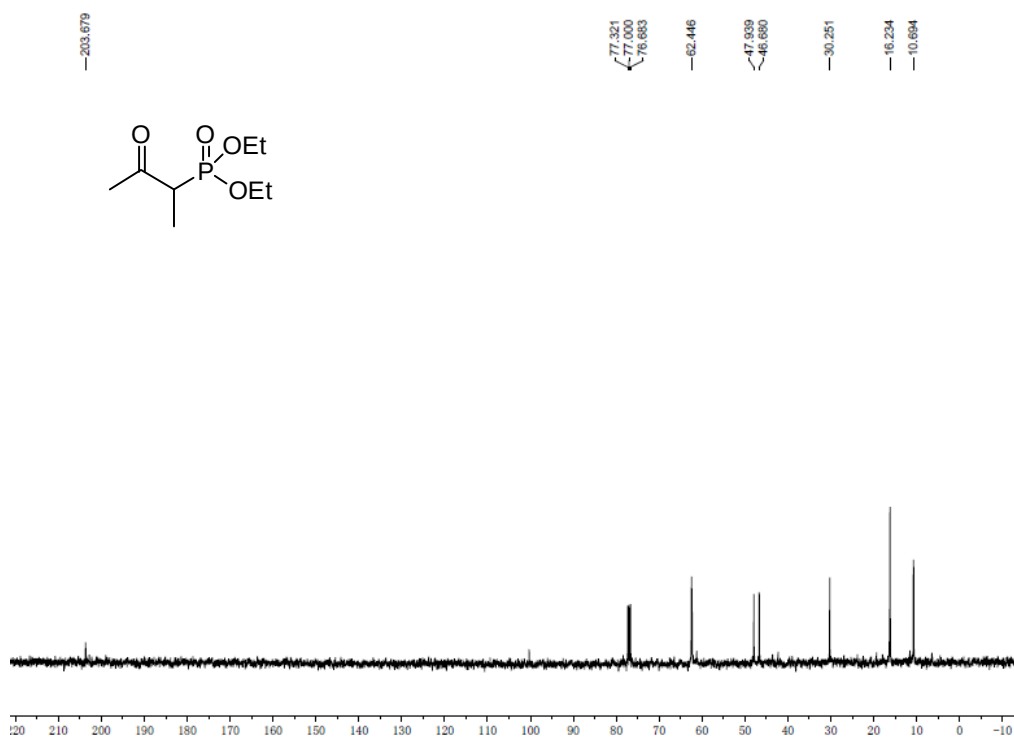
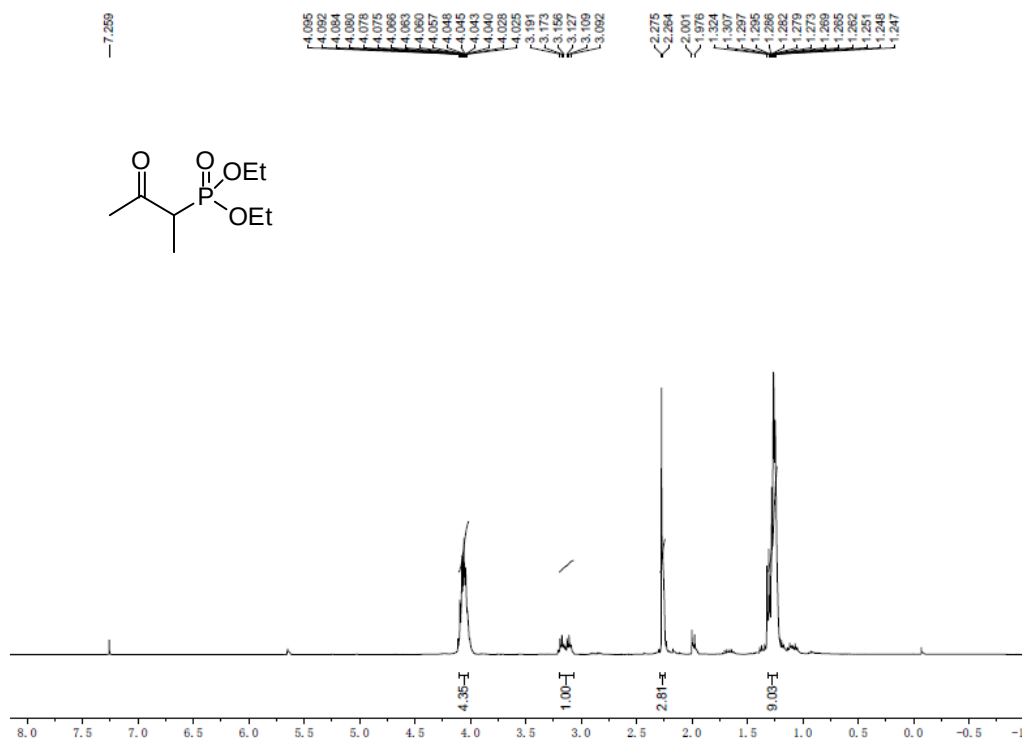
(1t) Dimethyl (1-methylacetyl)phosphonate



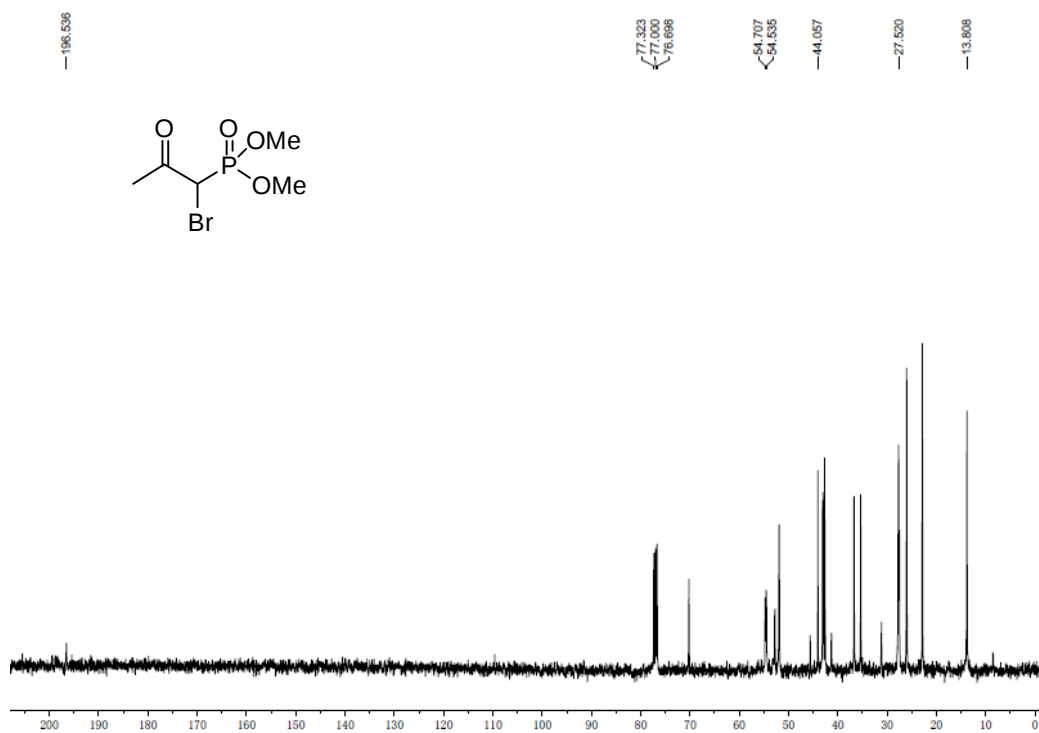
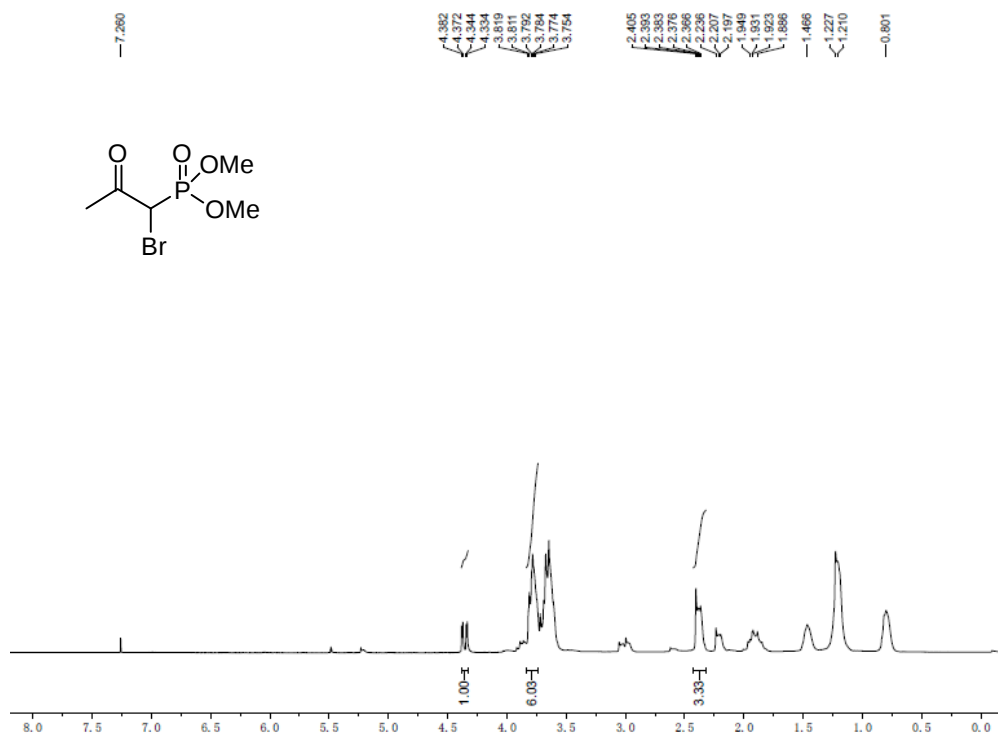
(1u) Dimethyl (1-ethylacetyl)phosphonate



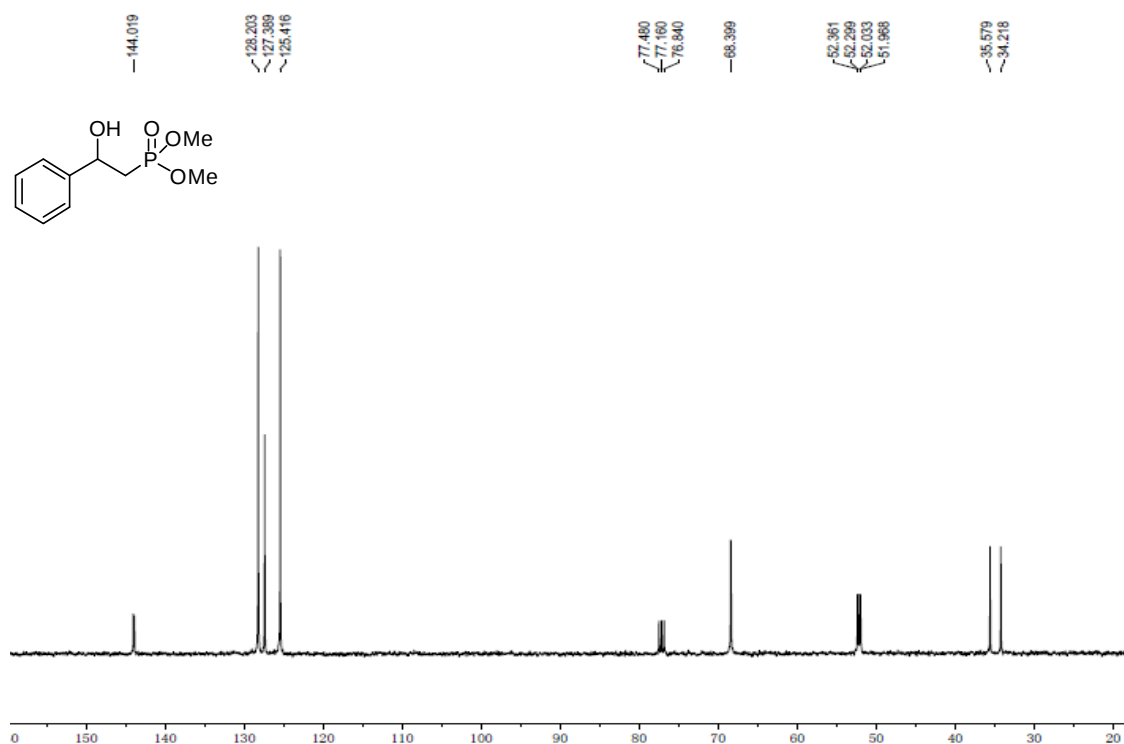
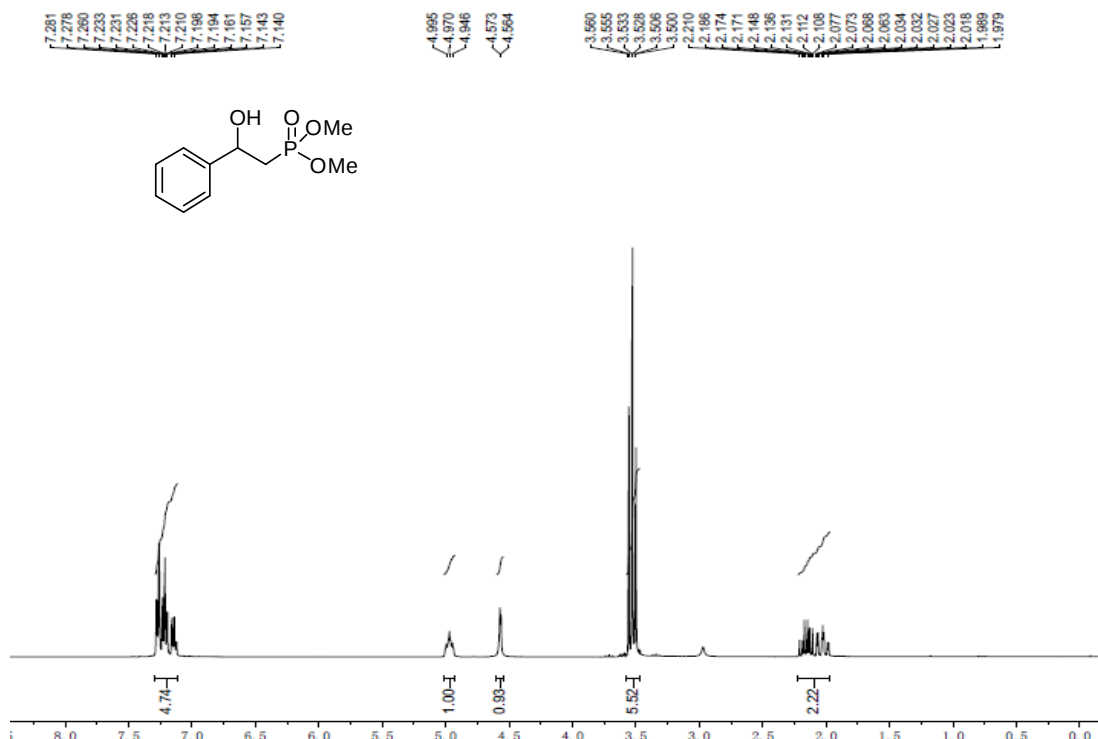
(1v) Diethyl (1-methylacetyl)phosphonate



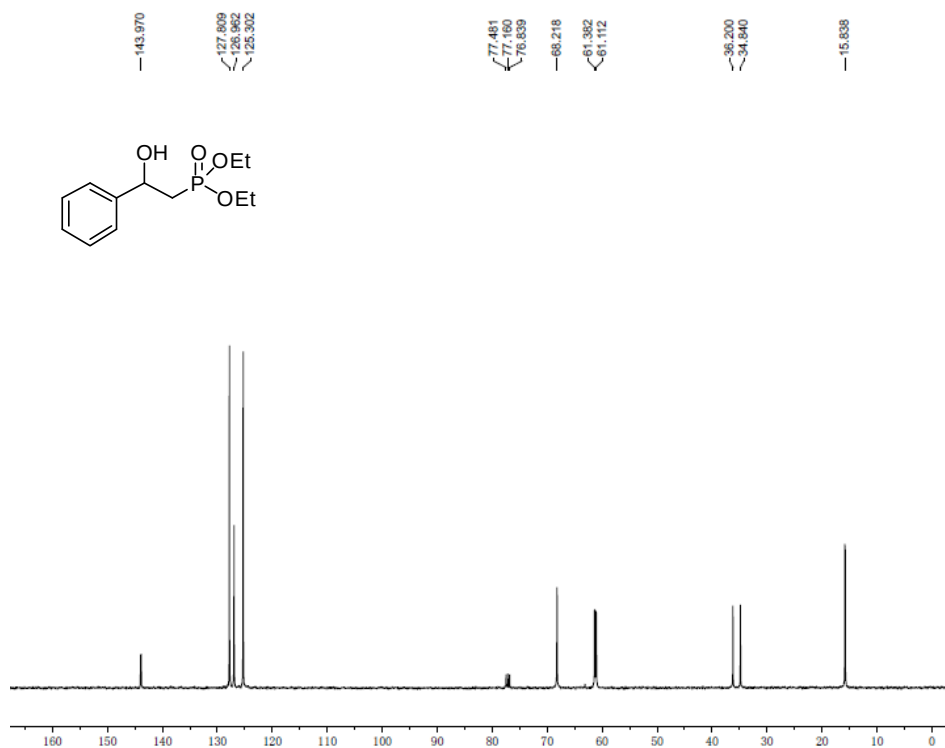
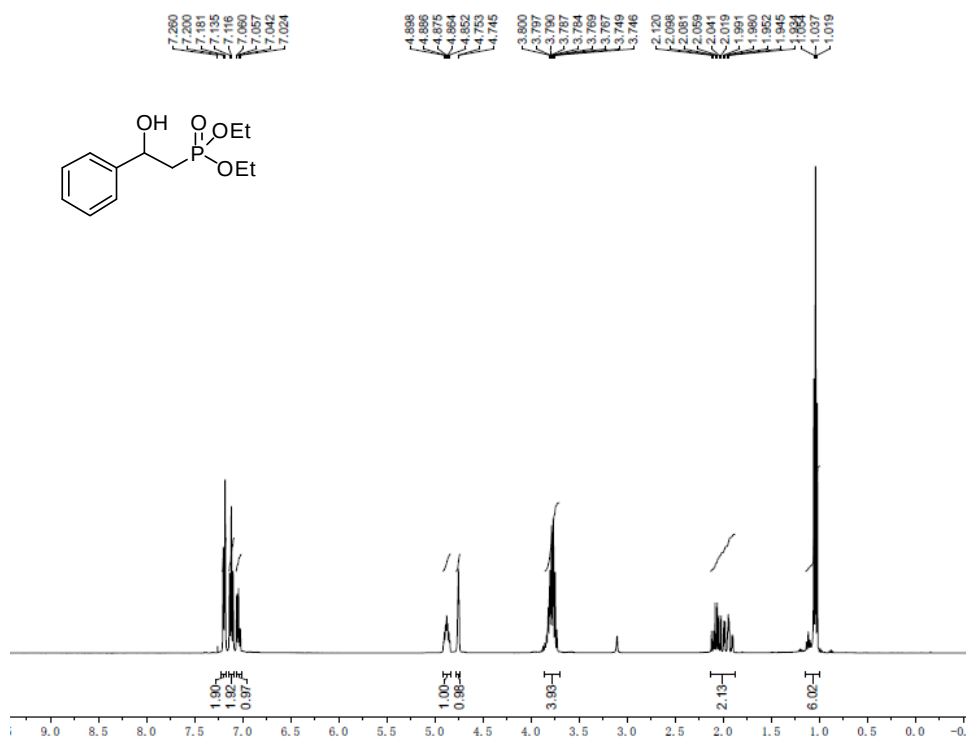
(1w) Dimethyl 1-bromo-2-oxopropylphosphonate



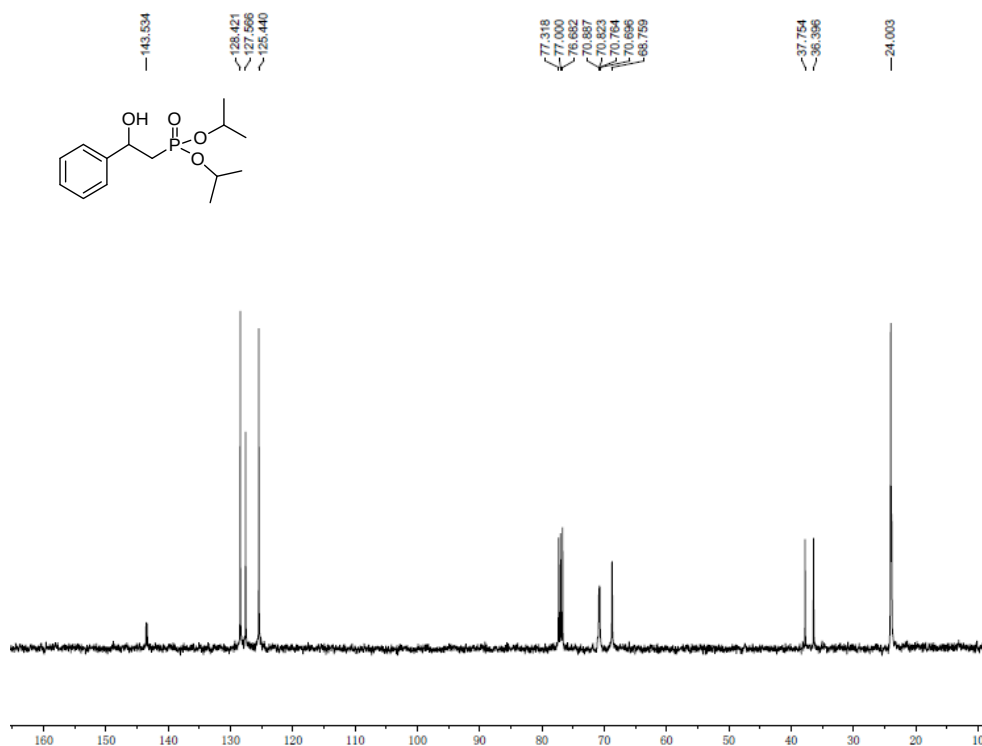
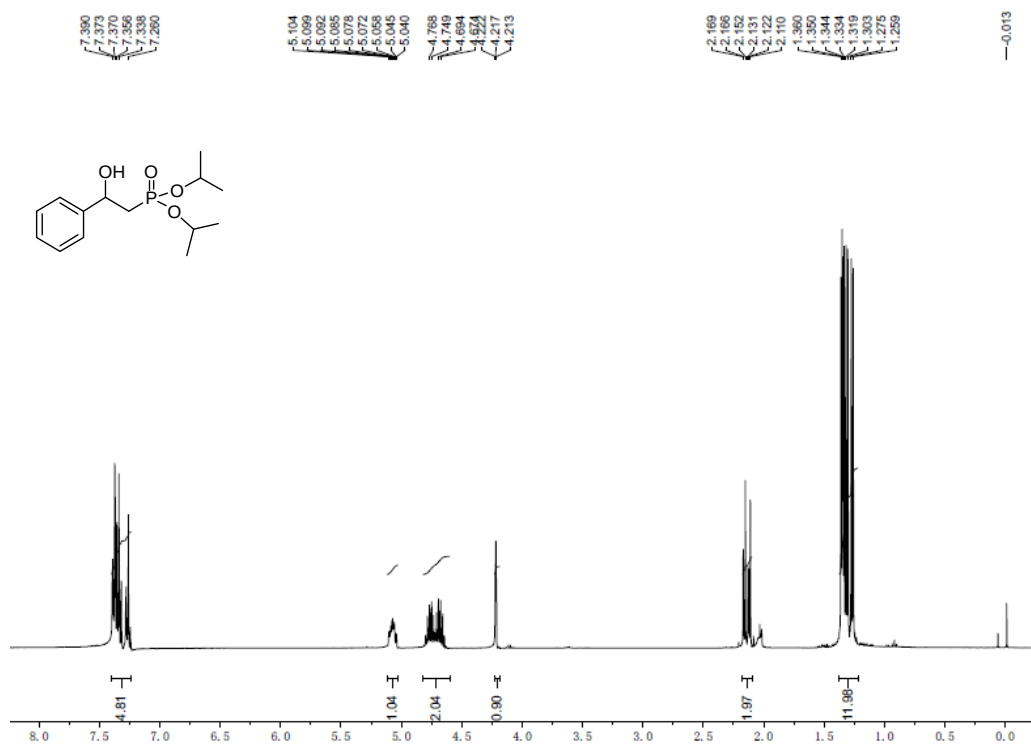
(2a) Dimethyl 2-hydroxy-2-phenylethylphosphonate



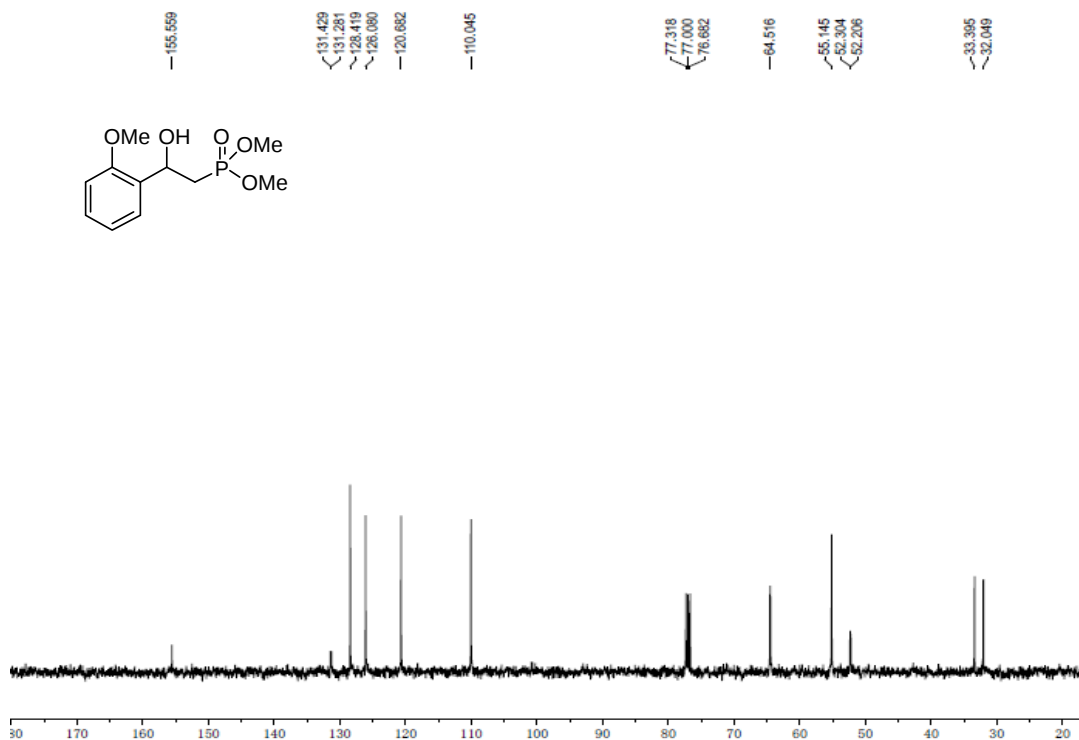
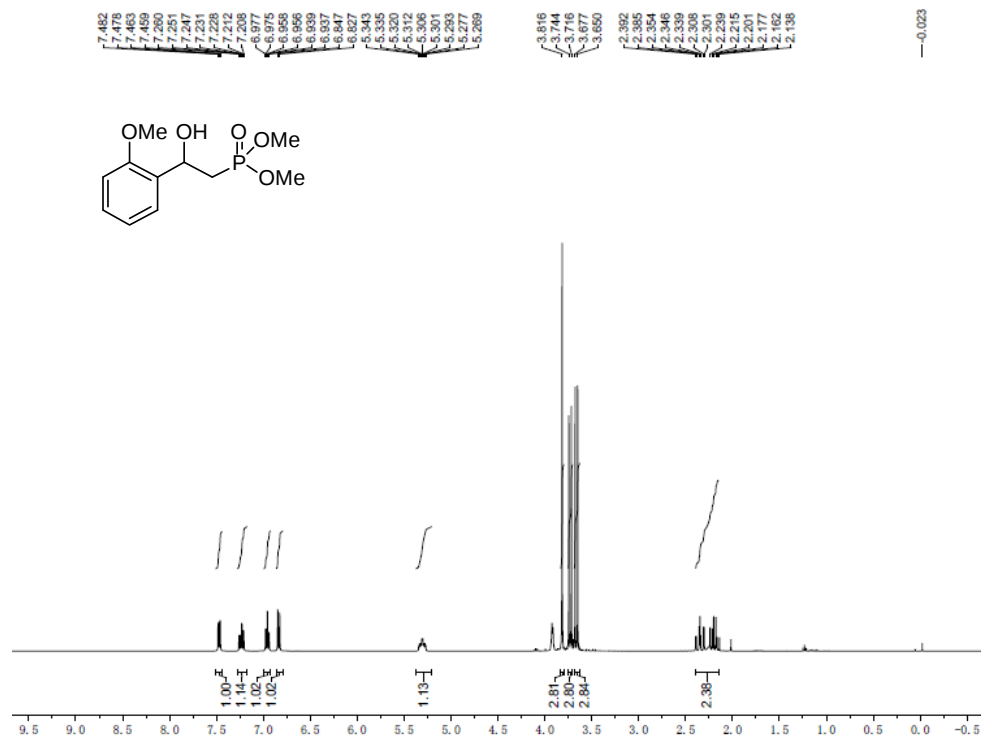
(2b) Diethyl 2-hydroxy-2-phenylethylphosphonate



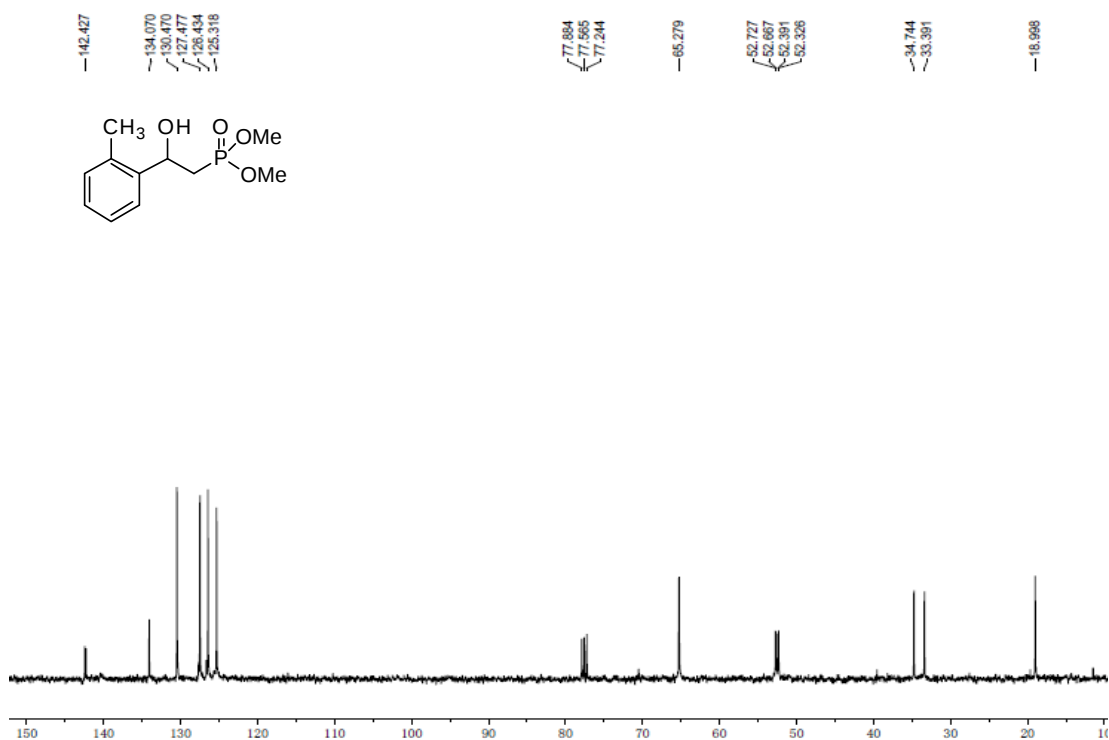
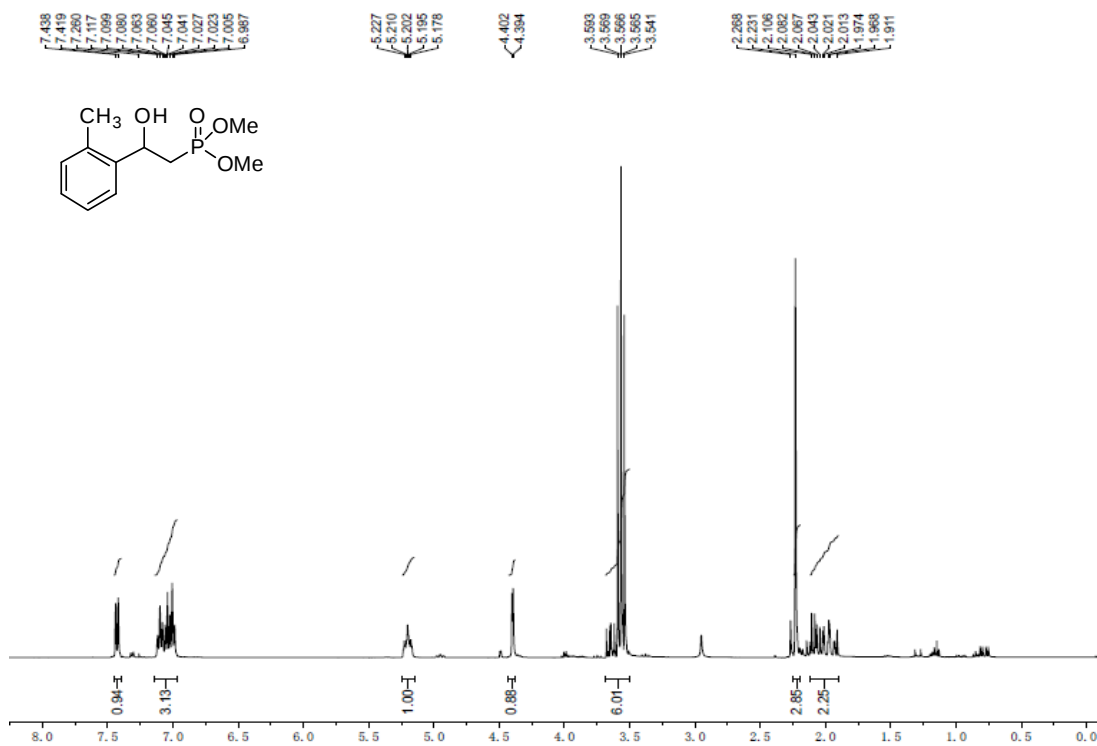
(2c) Diisopropyl 2-hydroxy-2-phenylethylphosphonate



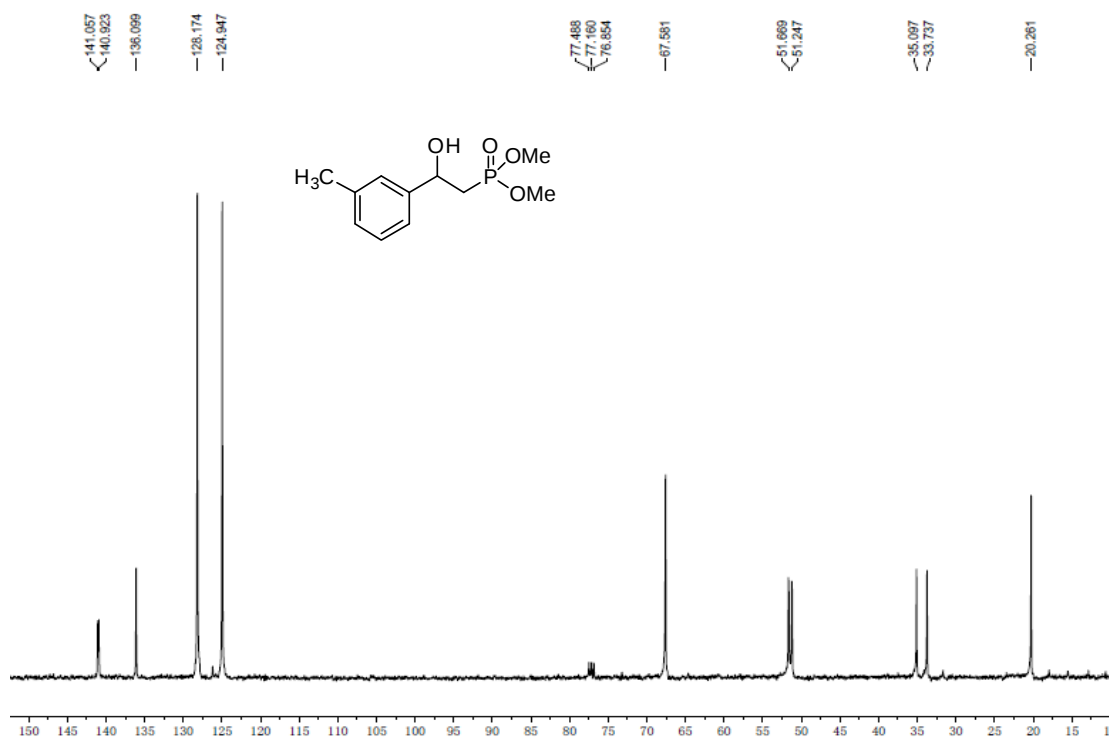
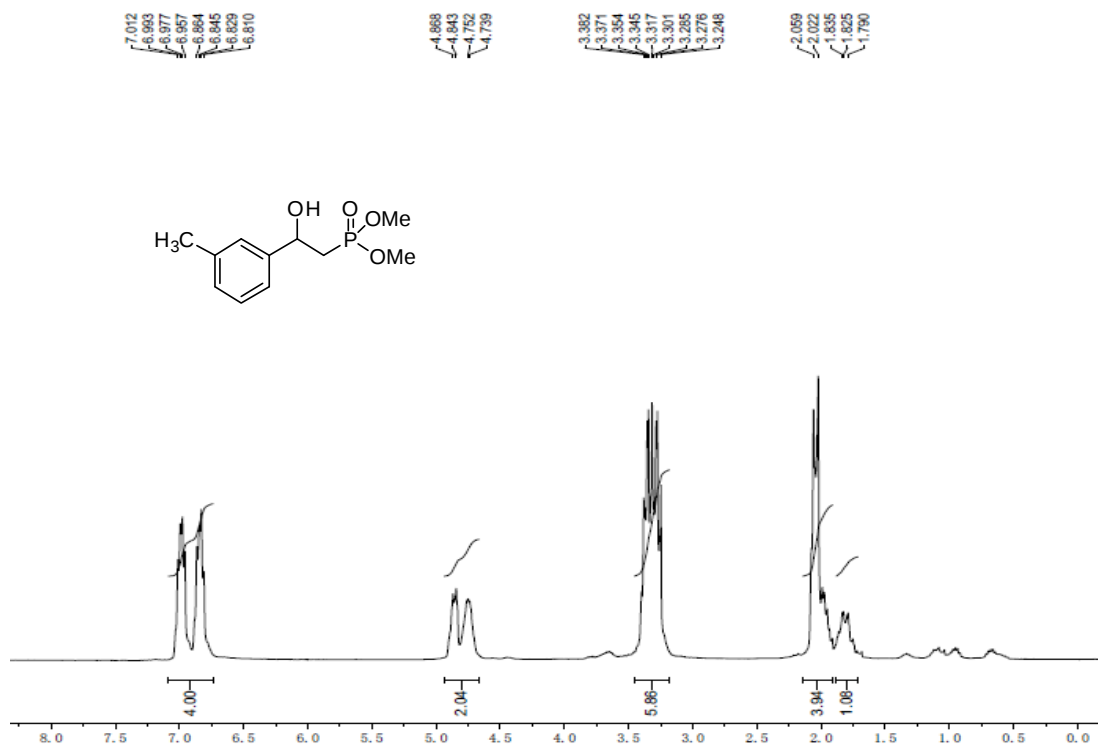
(2d) Dimethyl [2-hydroxy-2-(2-methoxyphenyl)ethyl]phosphonate



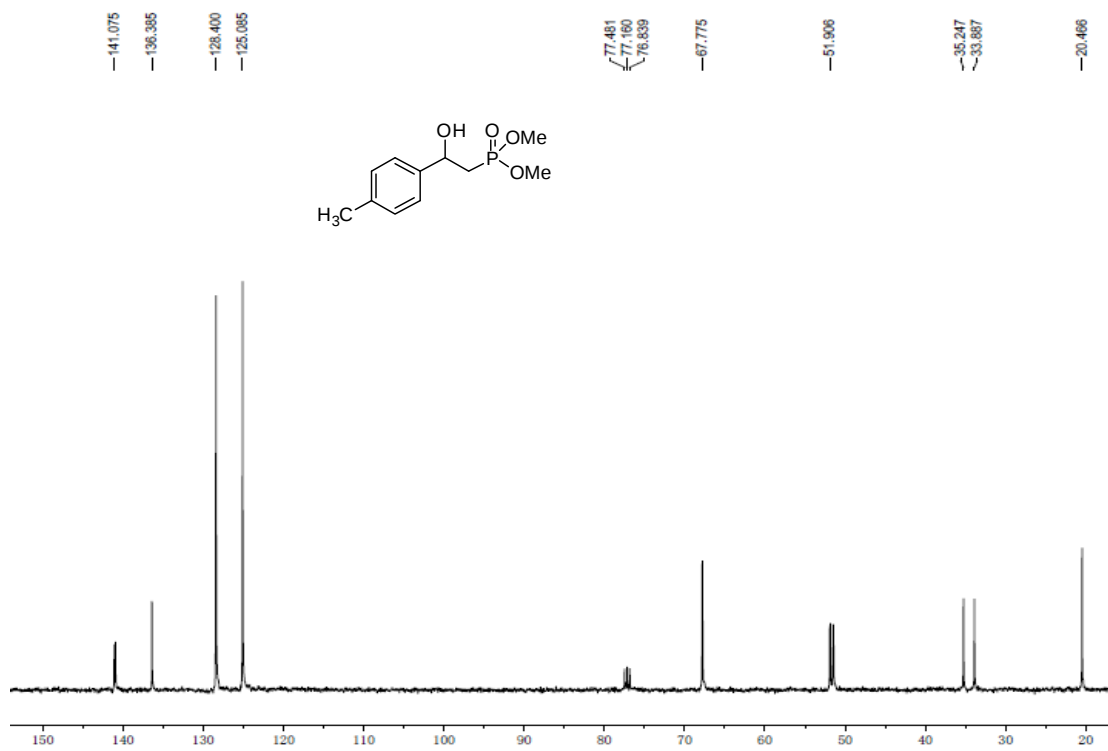
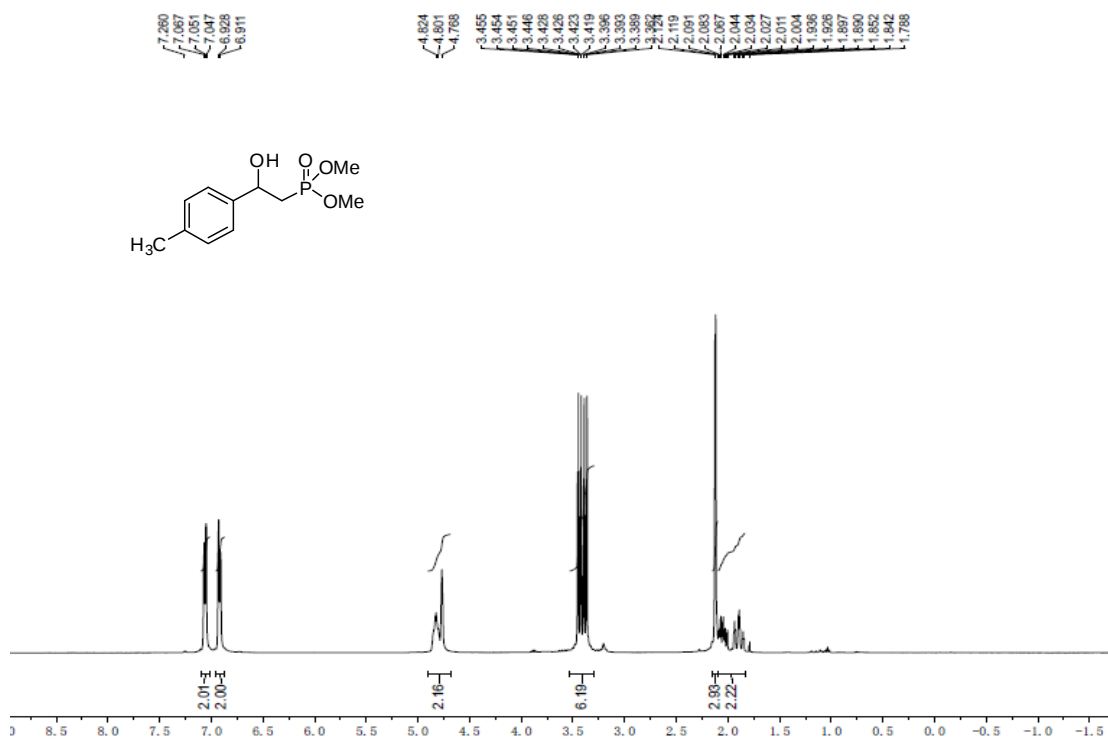
(2e) Dimethyl [2-hydroxy-2-(2-methylphenyl)ethyl]phosphonate



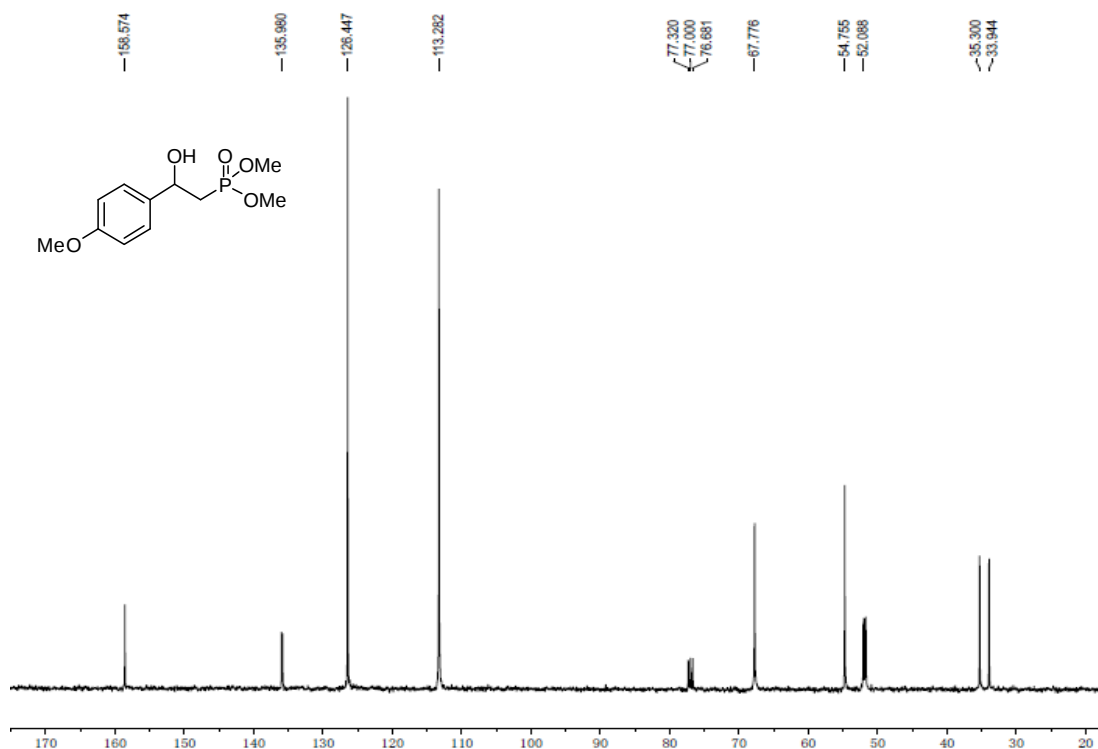
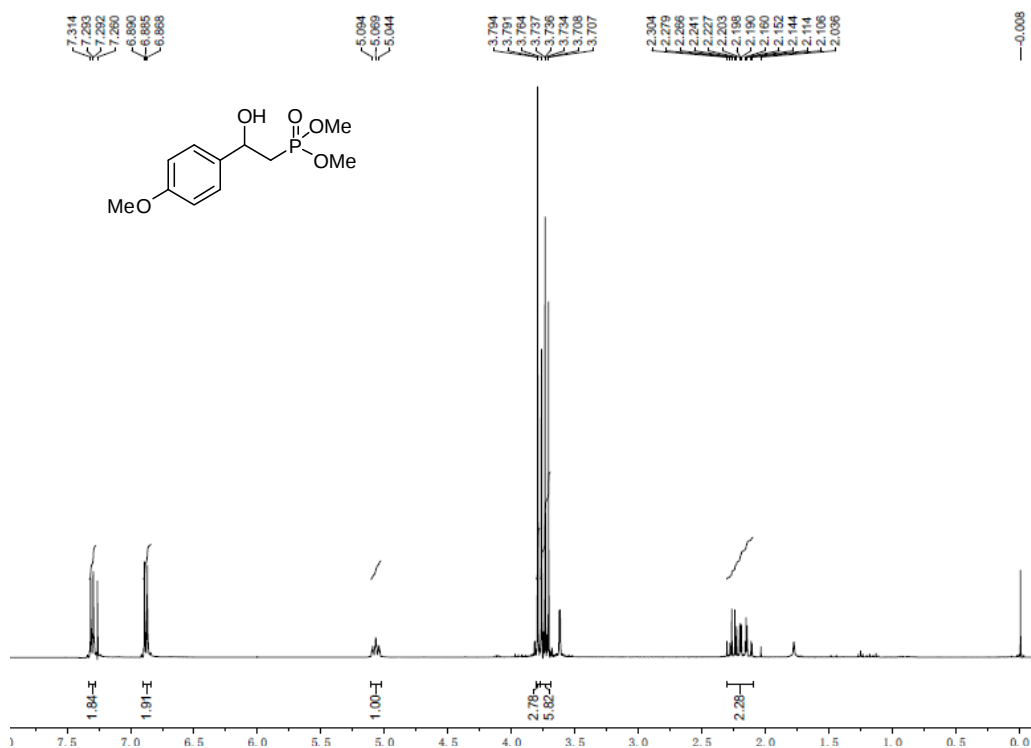
(2f) Dimethyl [2-hydroxy-2-(3-methylphenyl)ethyl]phosphonate



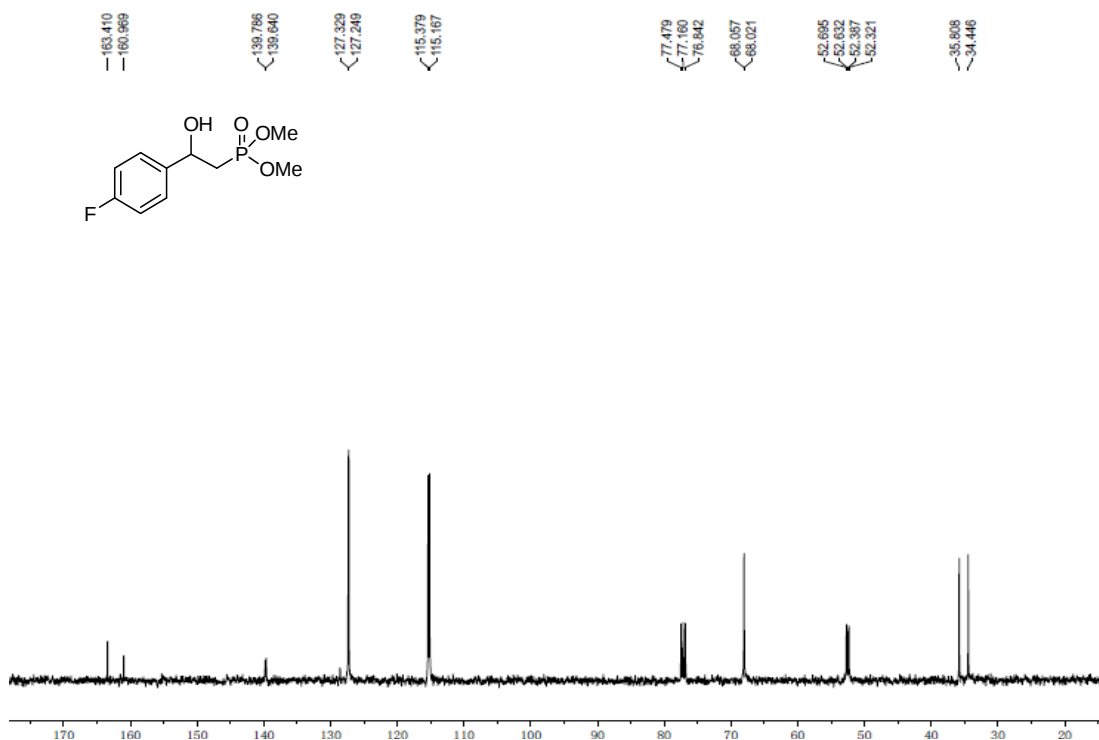
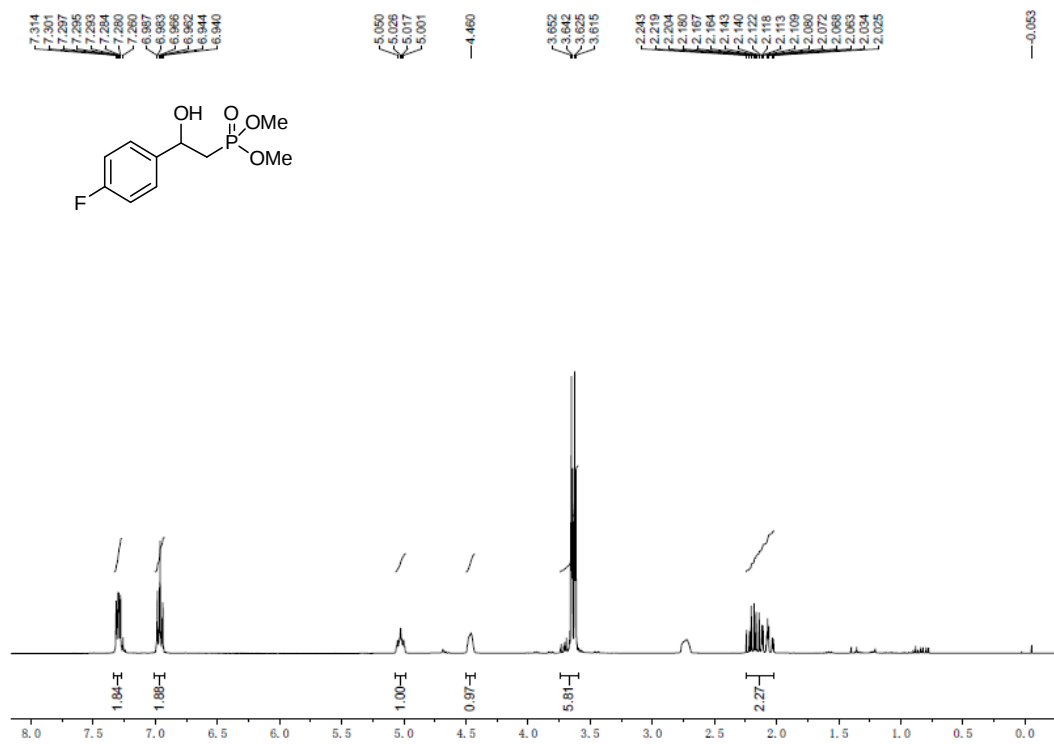
(2g) Dimethyl [2-hydroxy-2-(4-methylphenyl)ethyl]phosphonate



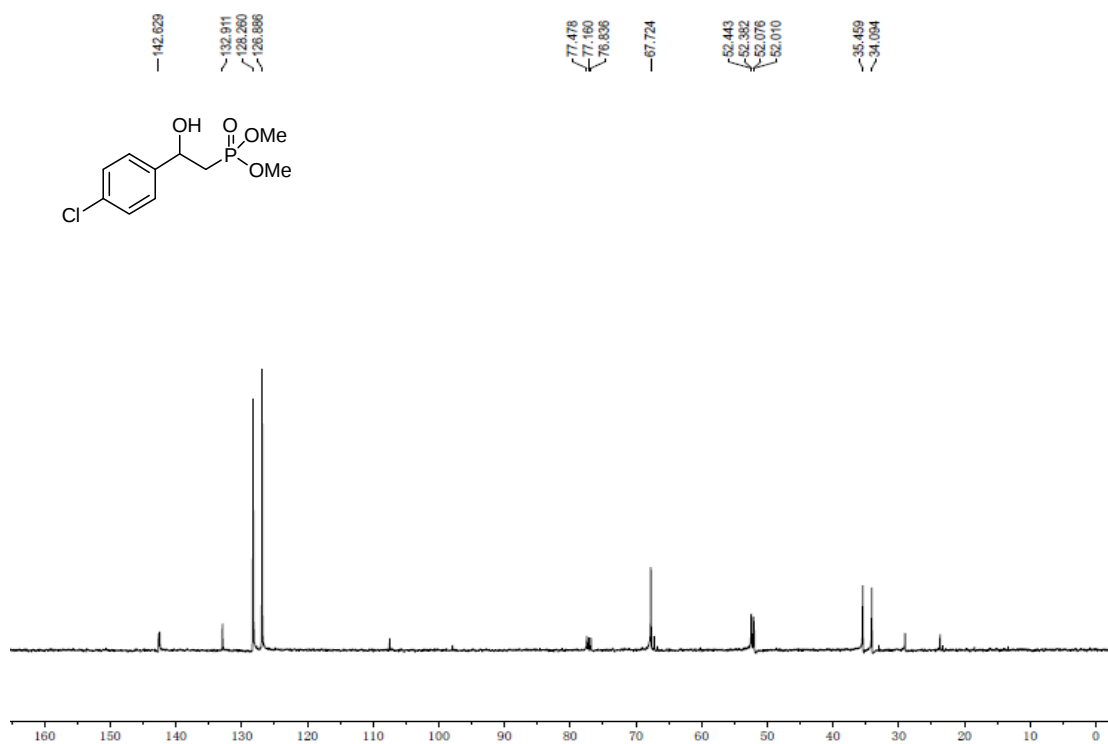
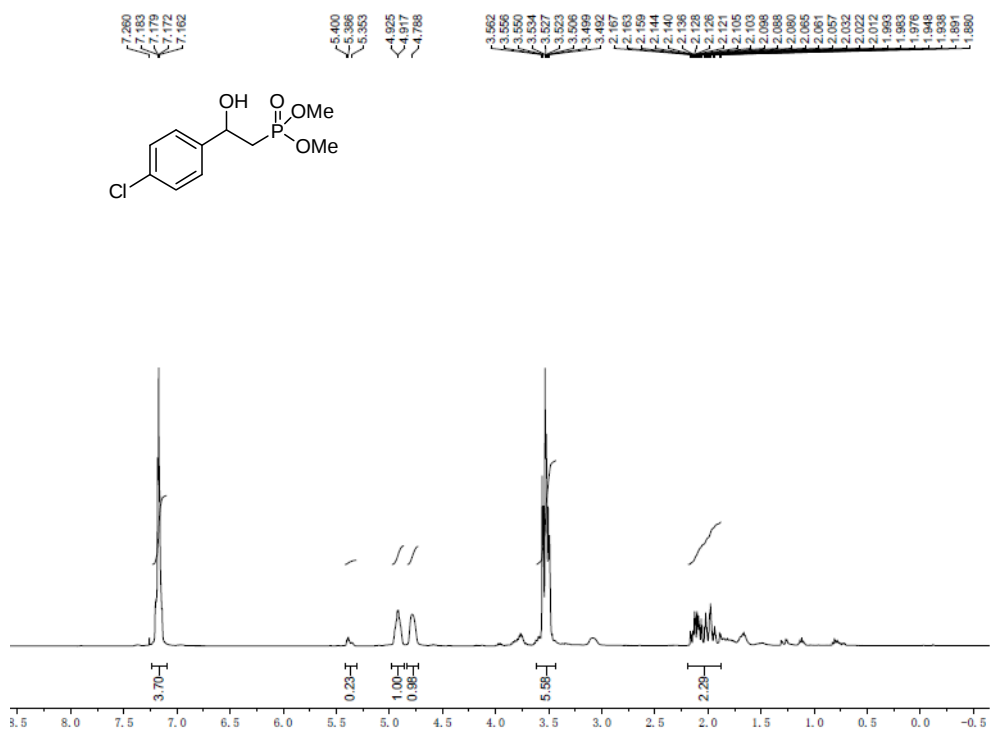
(2h) Dimethyl [2-hydroxy-2-(4-methoxyphenyl)ethyl]phosphonate



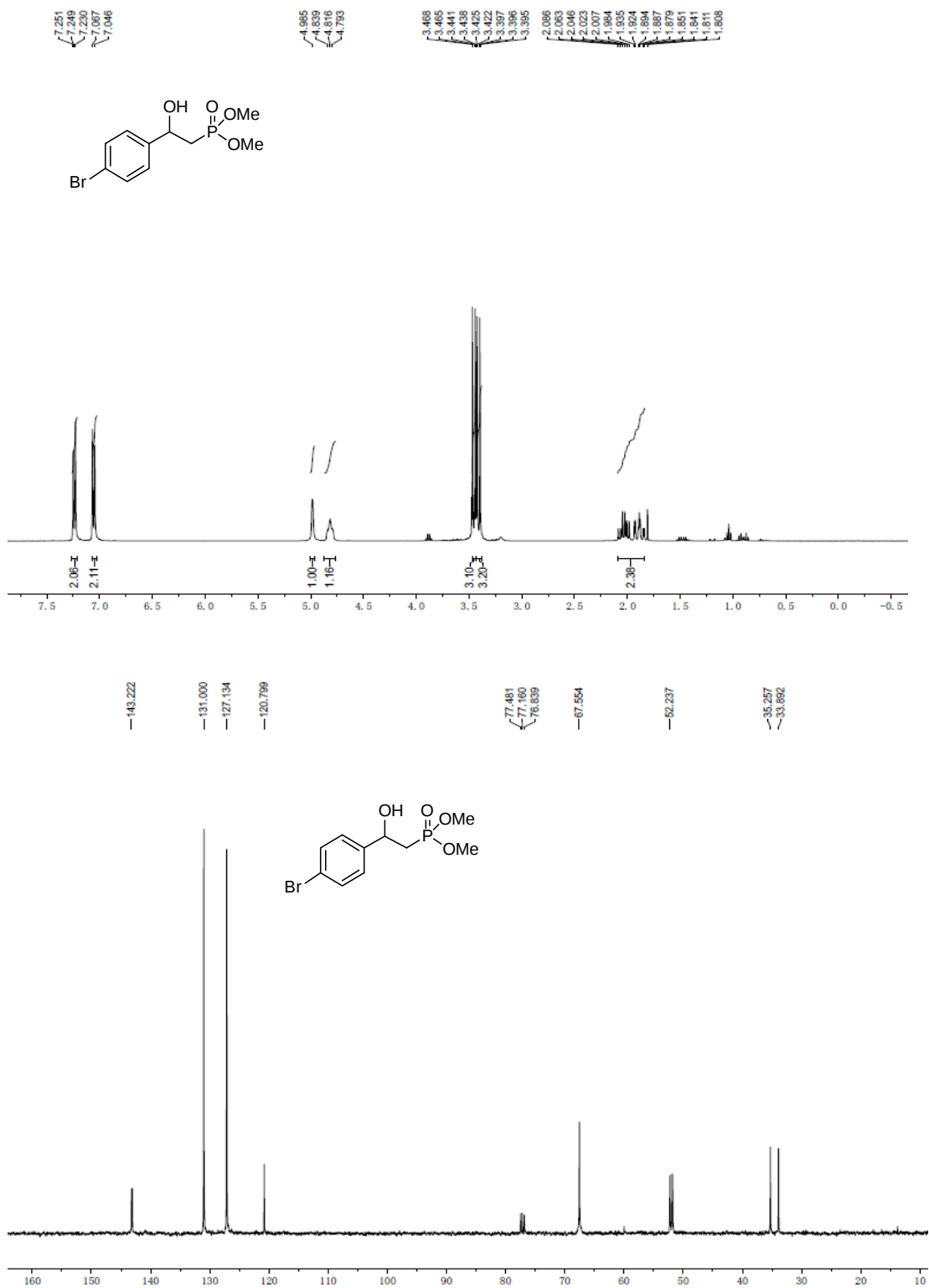
(2i) Dimethyl [2-hydroxy-2-(4-fluorophenyl)ethyl]phosphonate



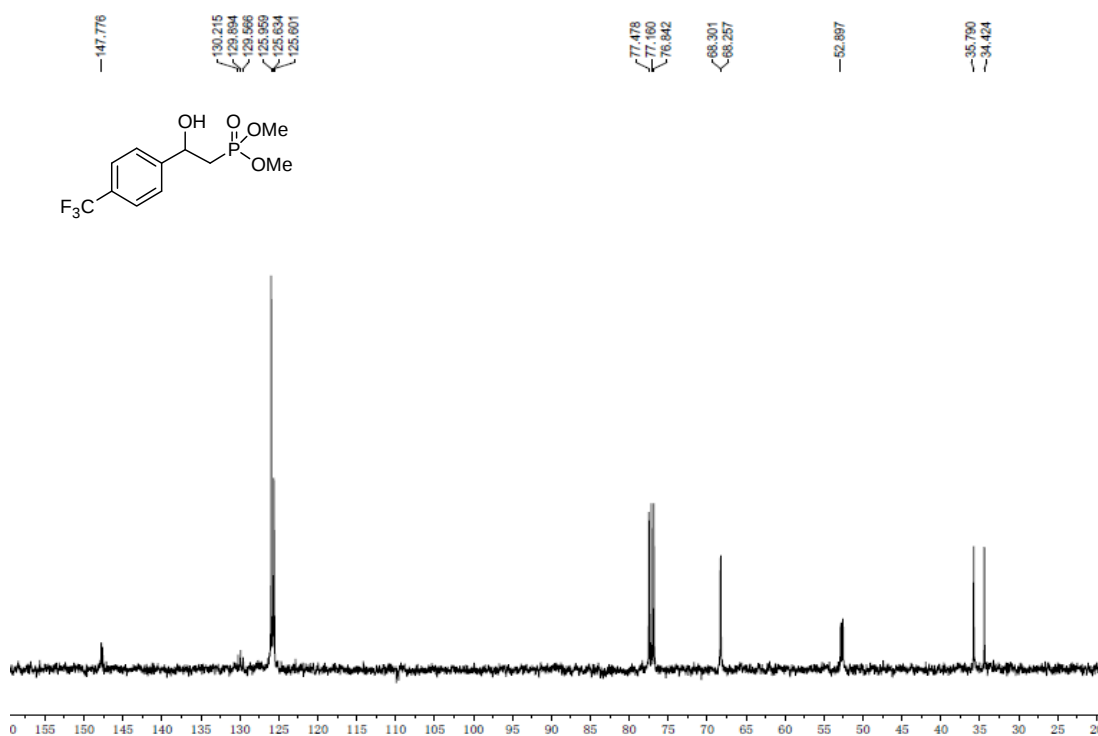
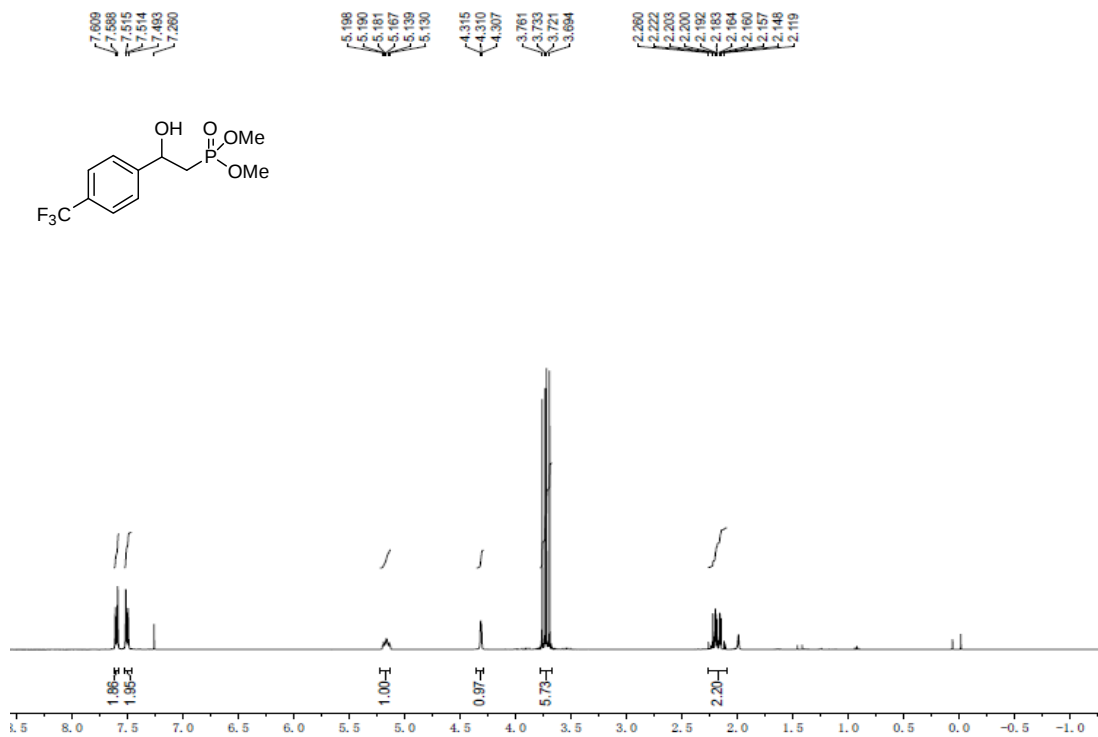
(2j) Dimethyl [2-hydroxy-2-(4-chlorophenyl)ethyl]phosphonate



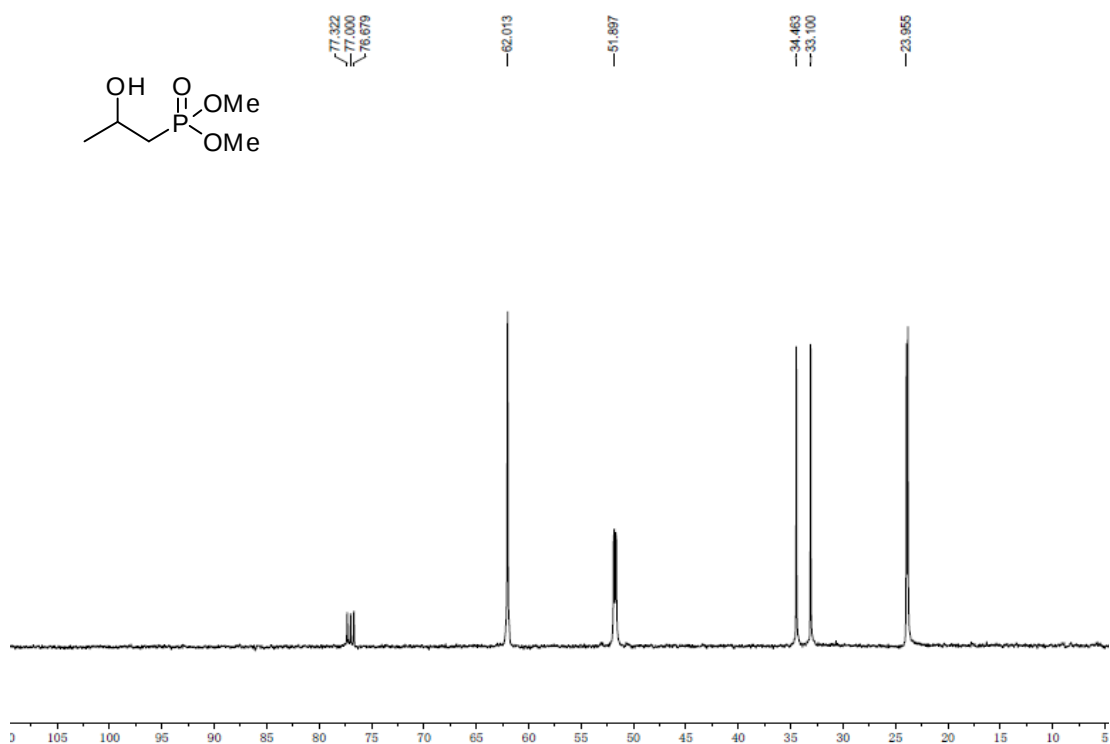
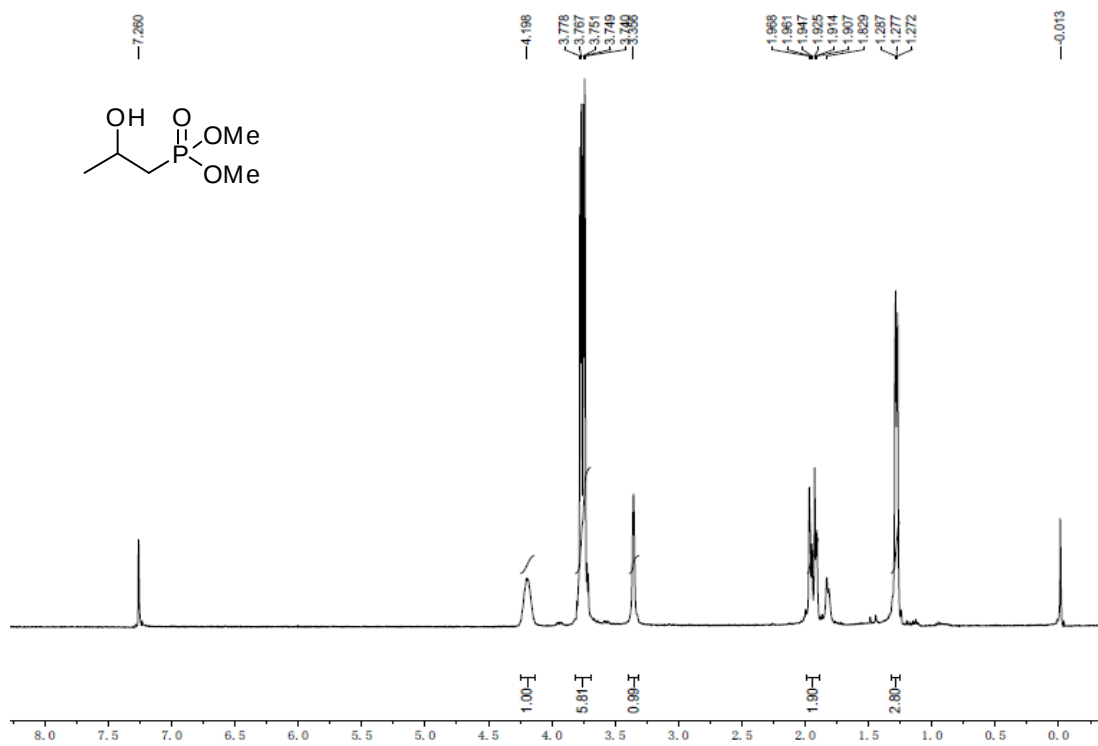
(2k) Dimethyl [2-hydroxy-2-(4-bromophenyl)ethyl]phosphonate



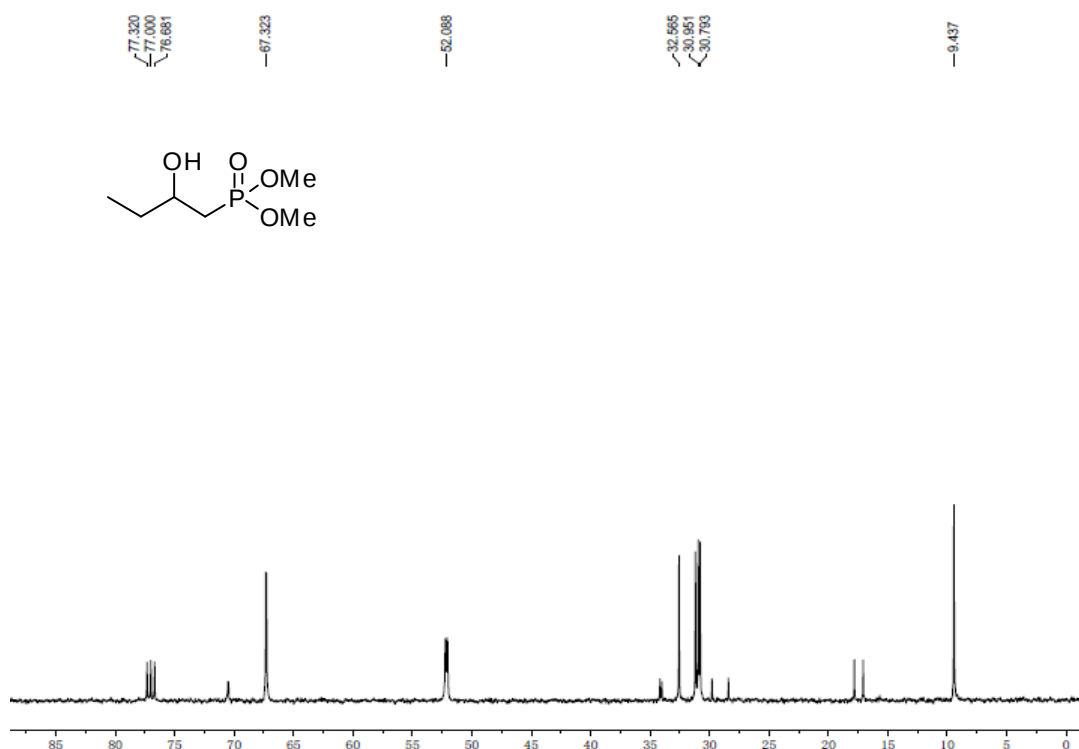
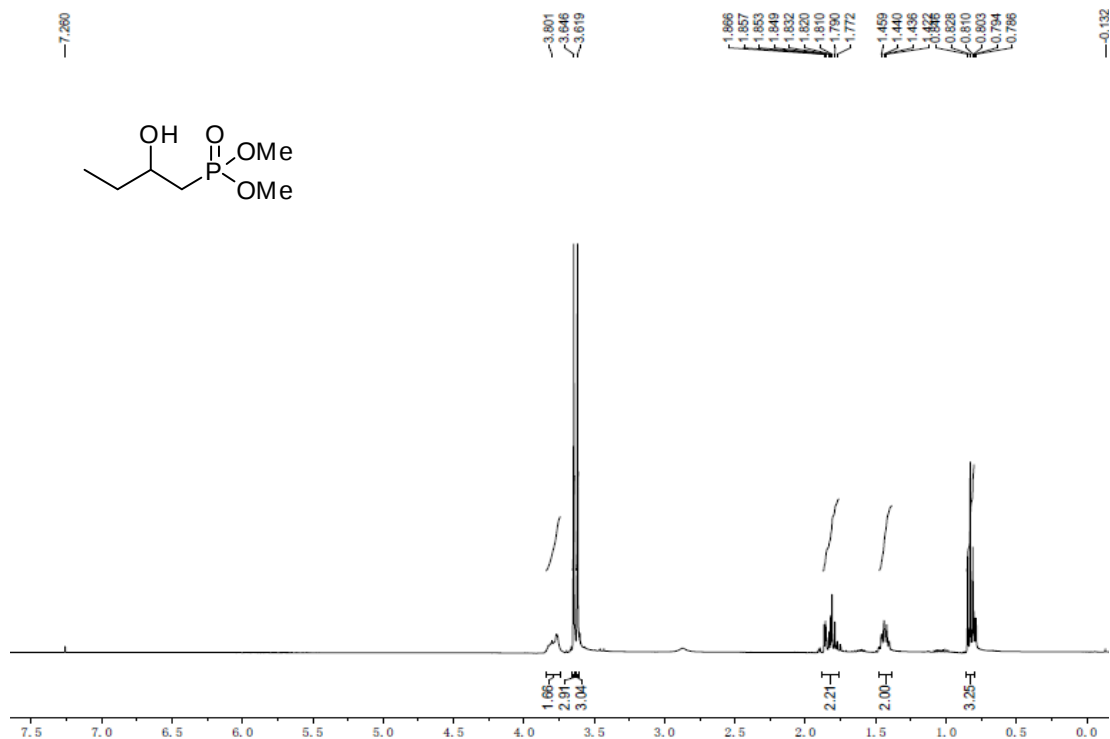
(2l) Dimethyl [2-hydroxy-2-(4- trifluoromethylphenyl)ethyl]phosphonate



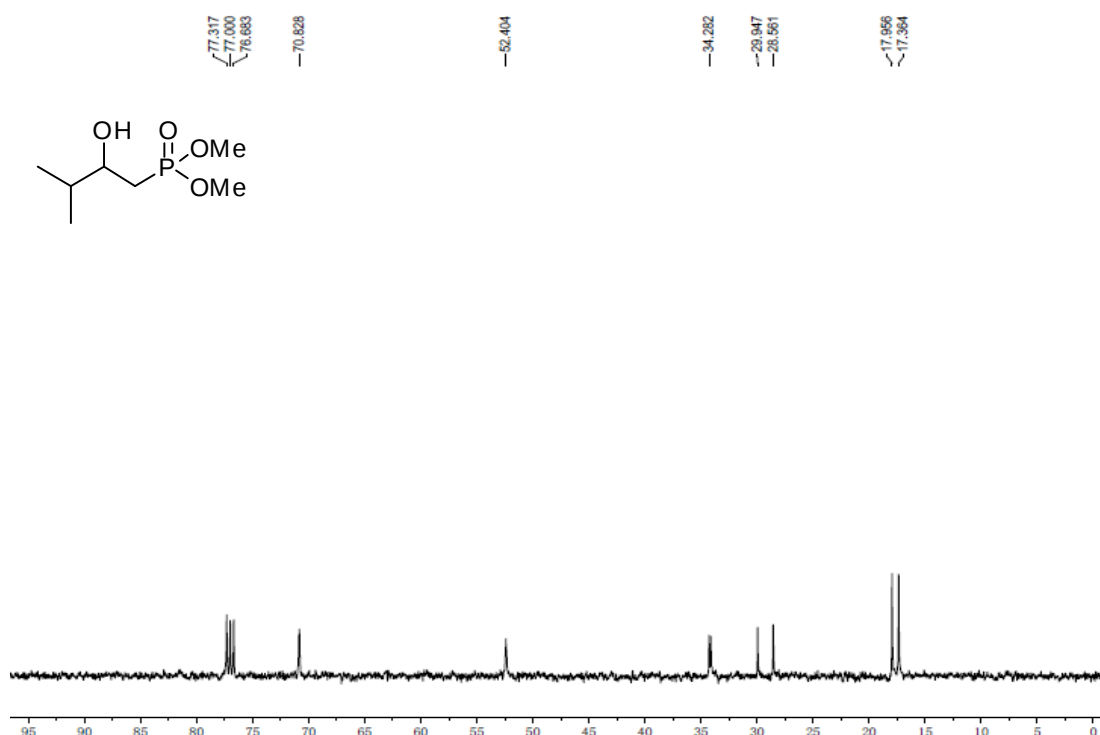
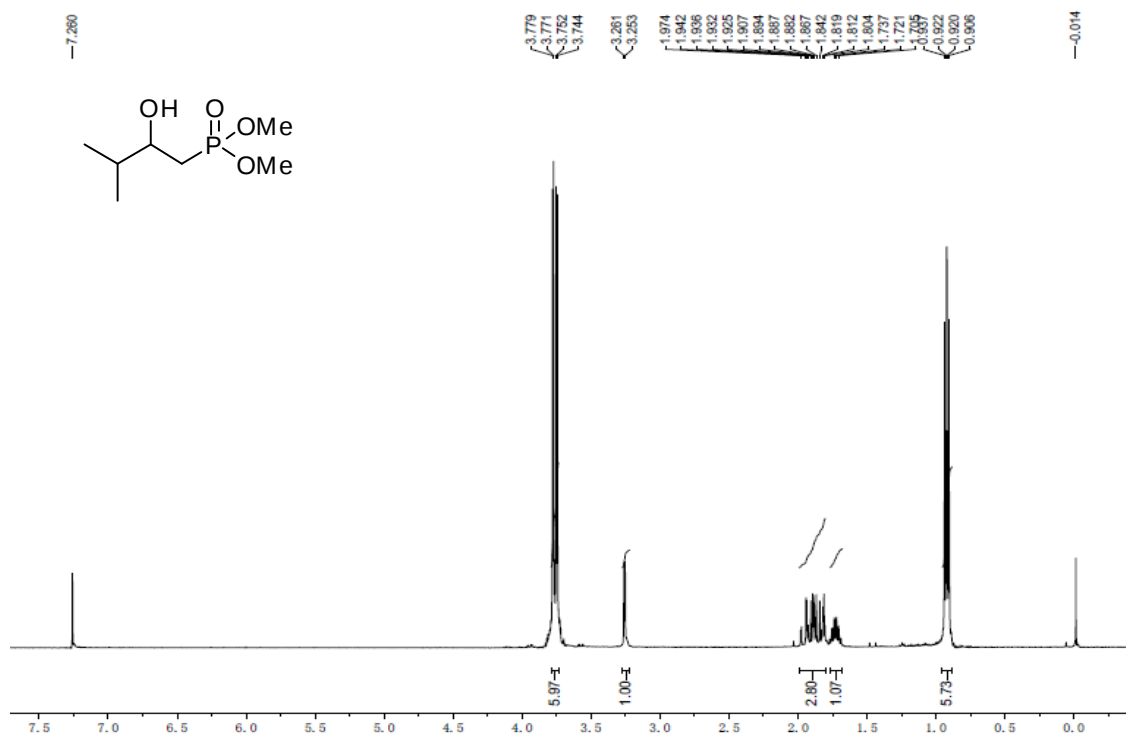
(2m) Dimethyl 2-hydroxypropylphosphonate



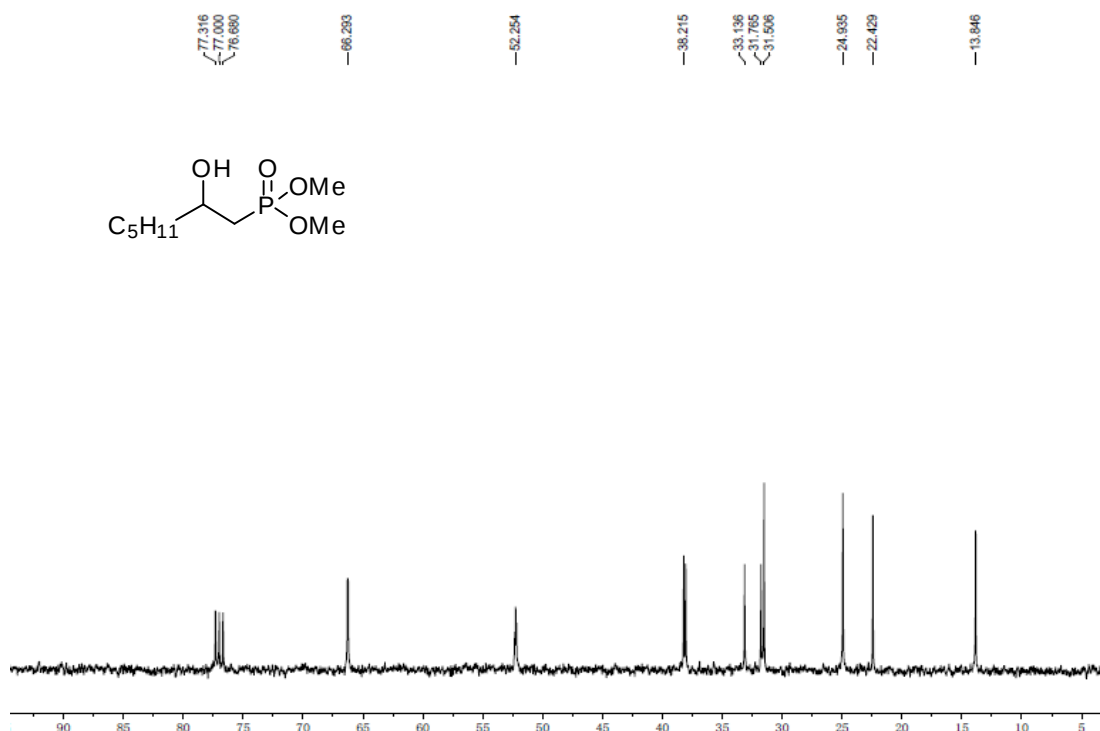
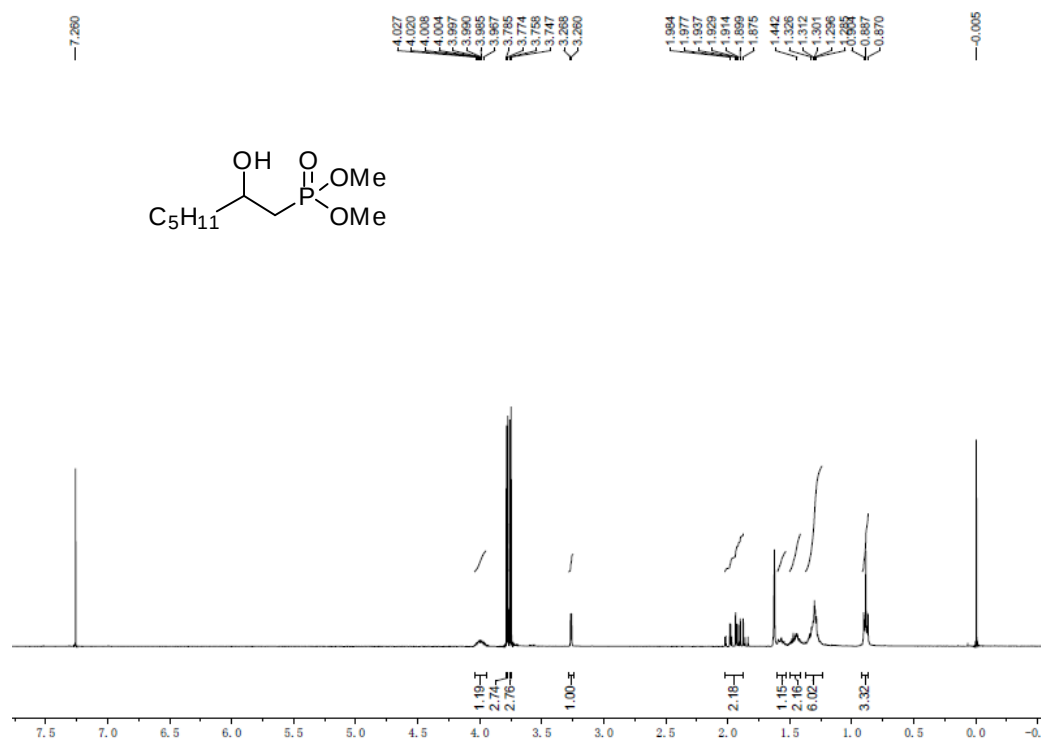
(2n) Dimethyl 2-hydroxybutylphosphonate



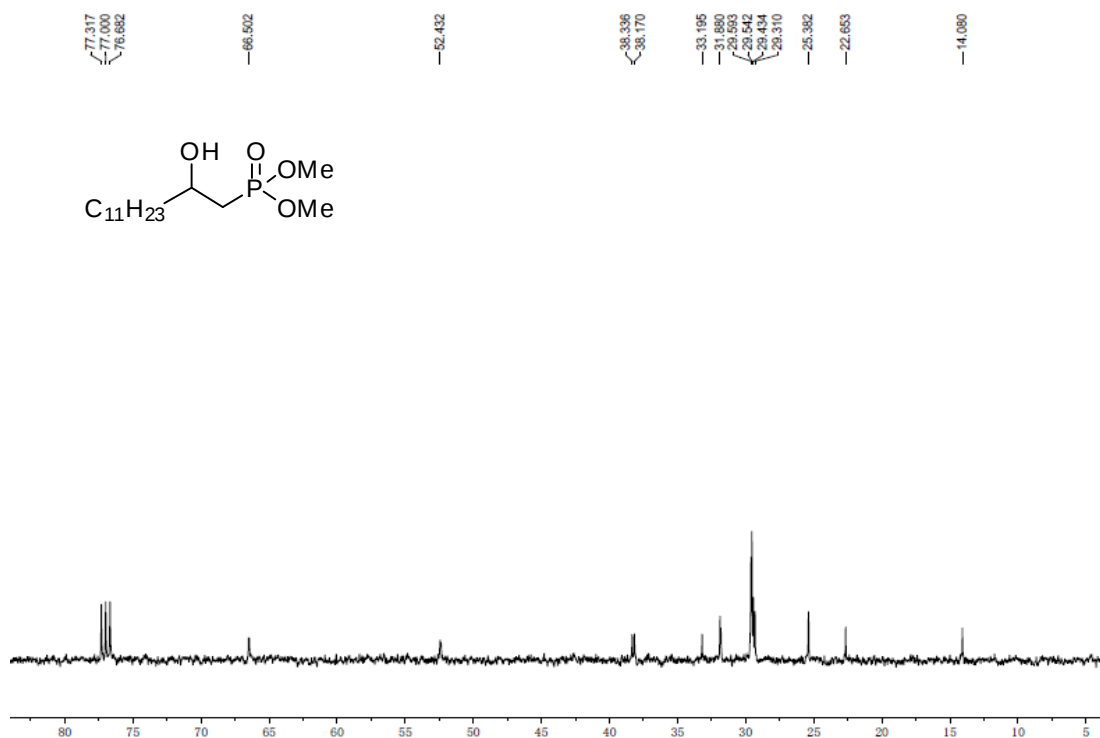
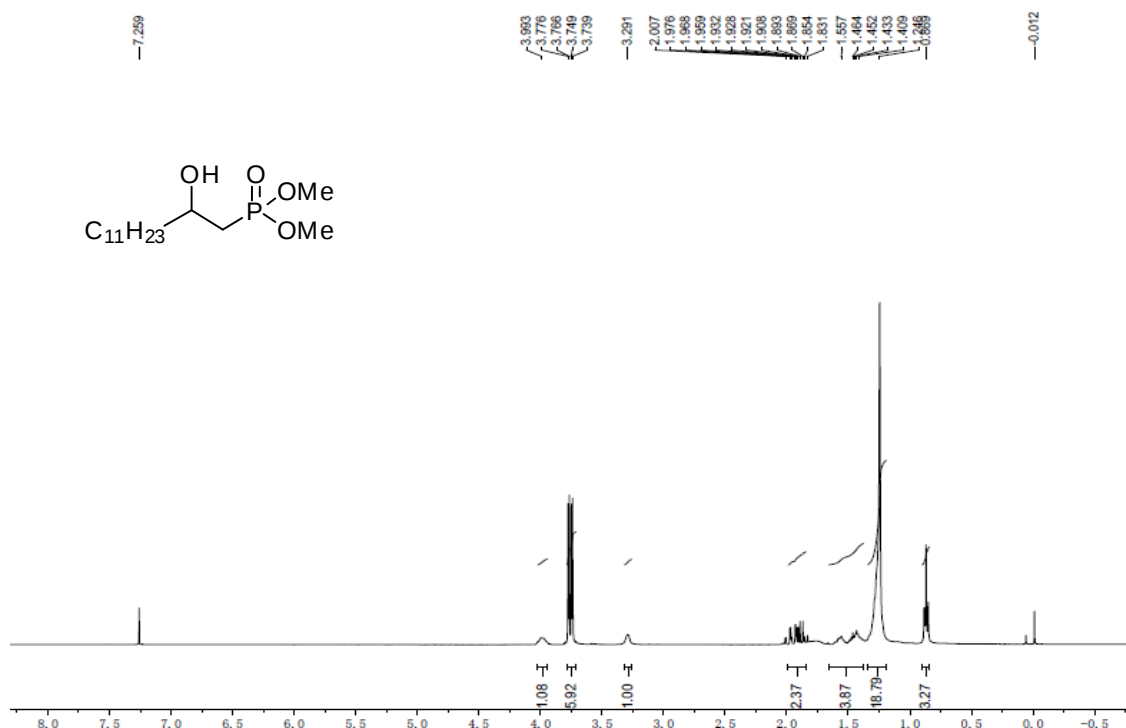
(2o) Dimethyl (2-hydroxy-3-methylbutyl)phosphonate



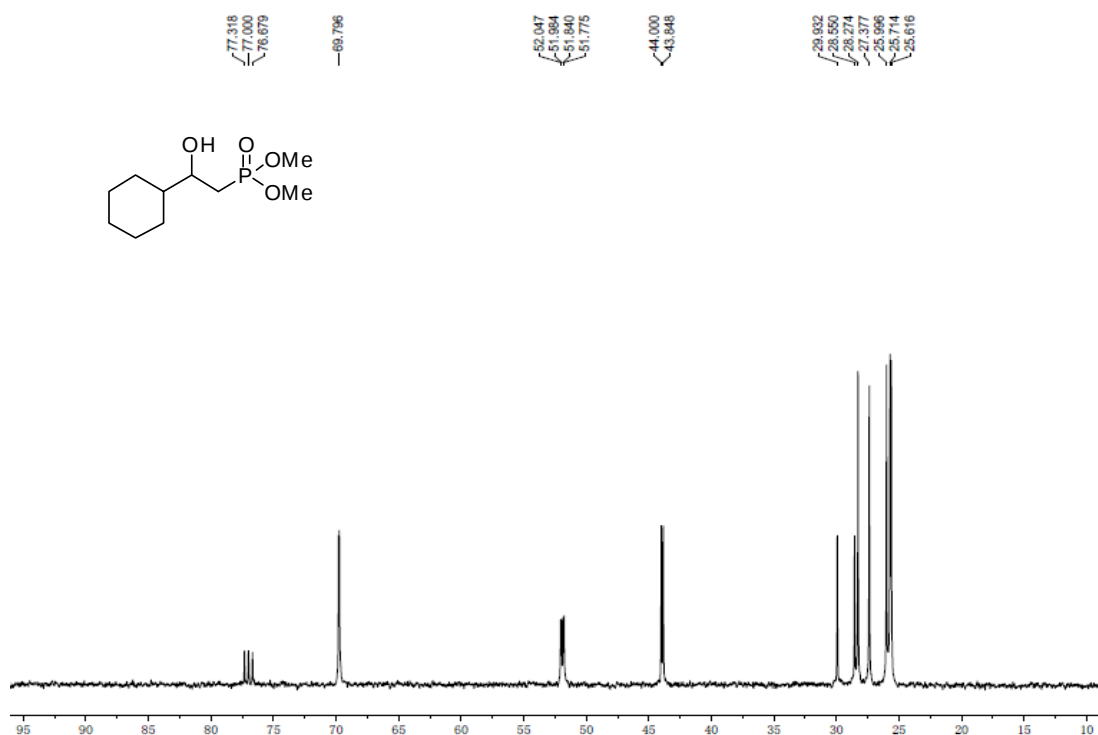
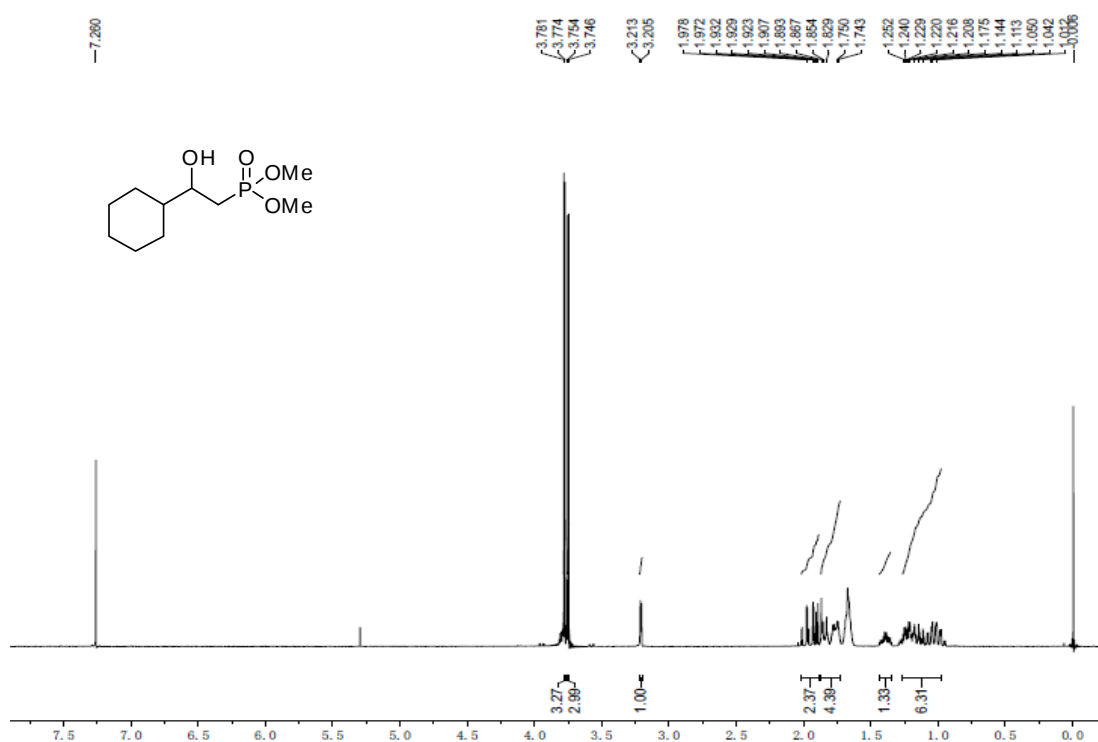
(2p) Dimethyl 2-hydroxyheptylphosphonate



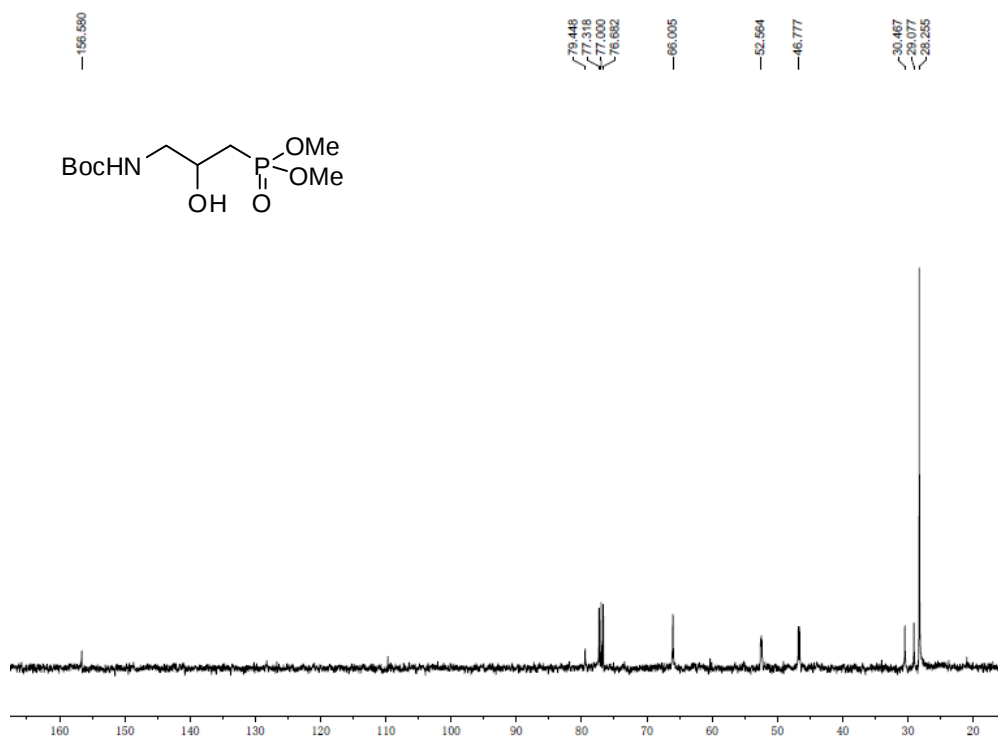
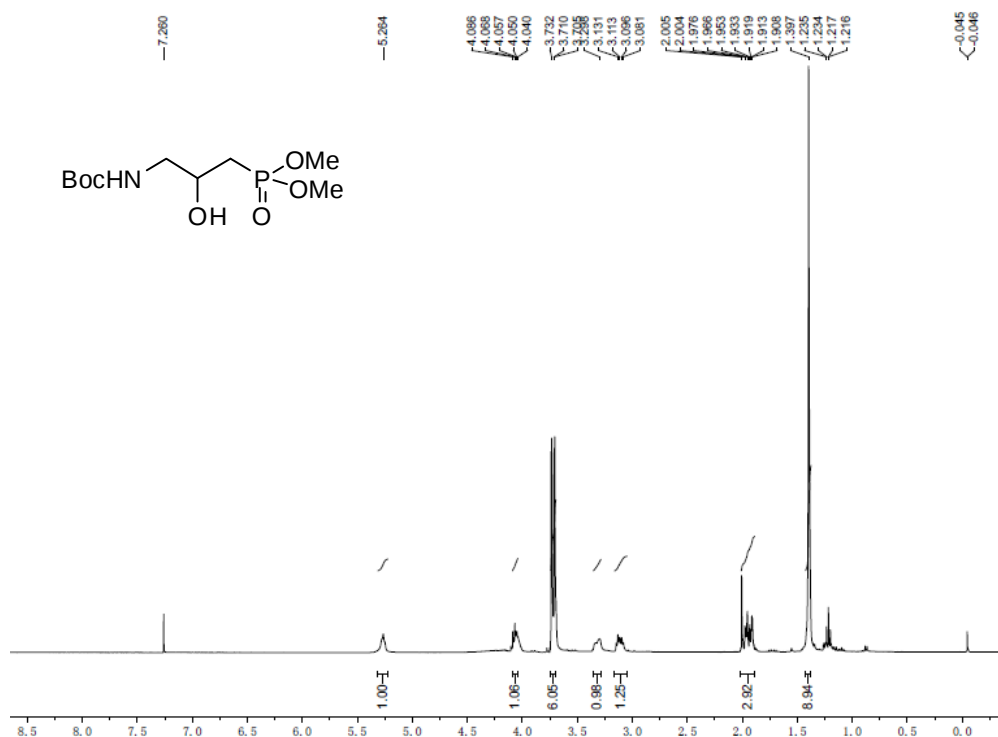
(2q) Dimethyl 2-hydroxytridecylphosphonate



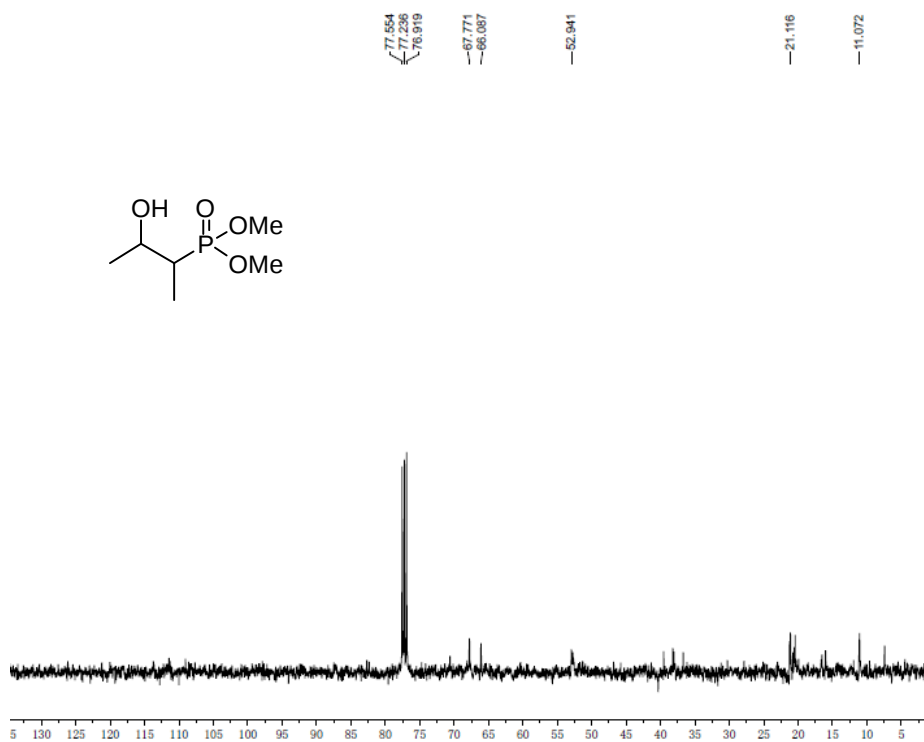
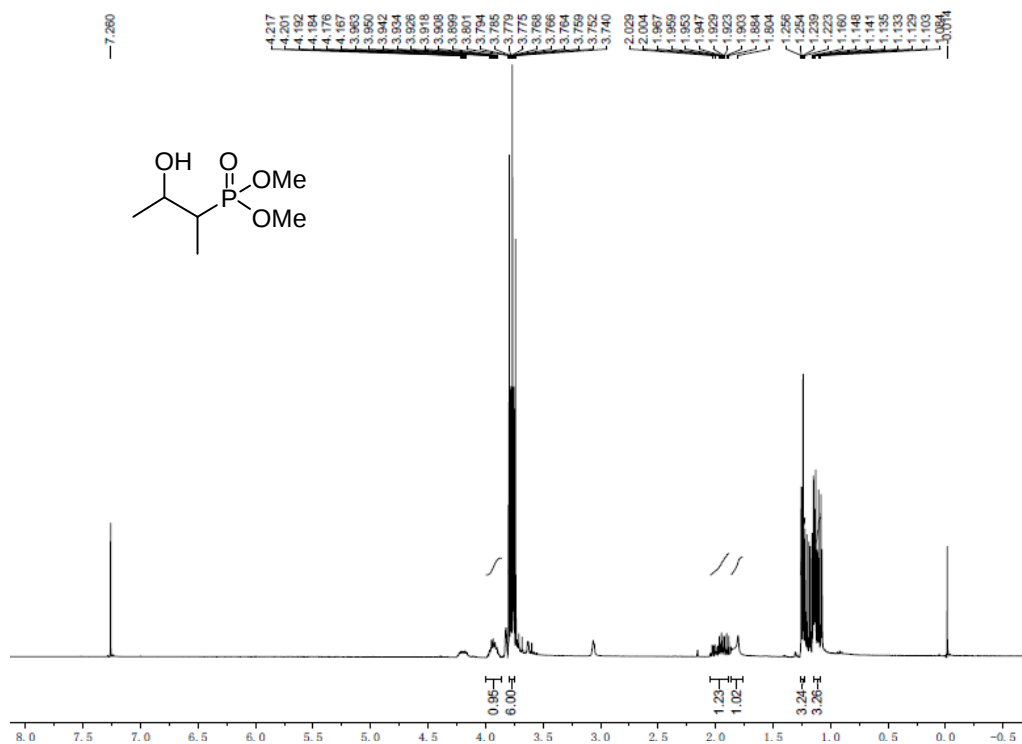
(2r) Dimethyl 2-hydroxycyclohexylphosphonate



(2s) Dimethyl 2-hydroxy-3-(N-tert-butoxycarbonylamino)phosphonate



(2t) Dimethyl 3-hydroxybut-2-ylphosphonate



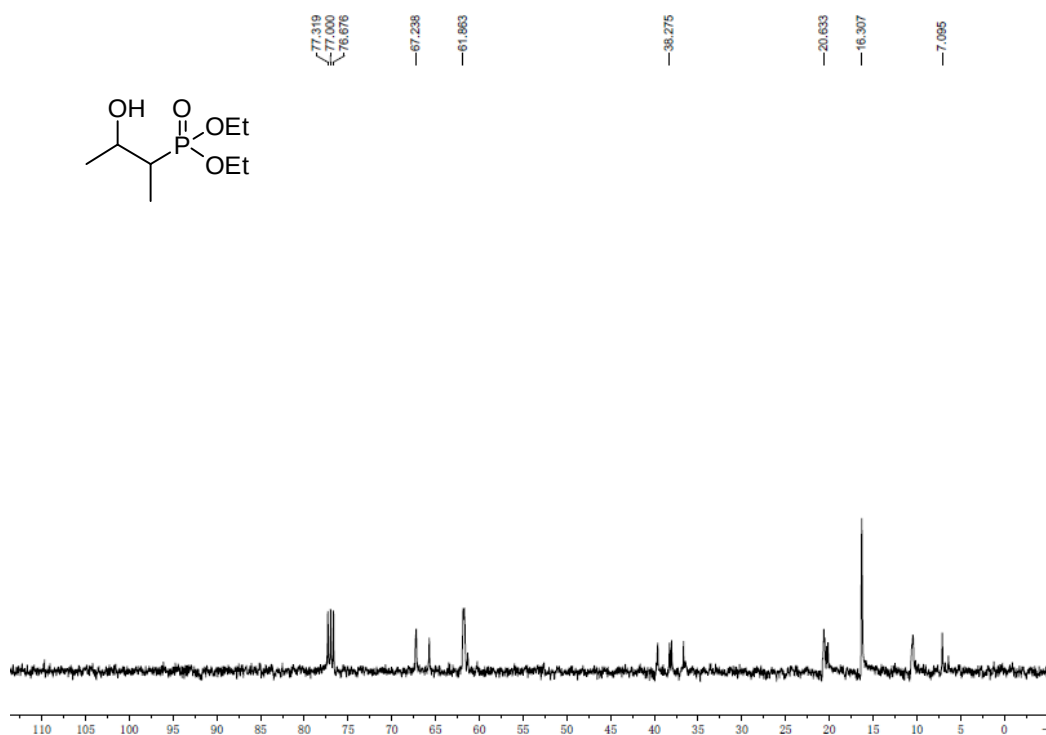
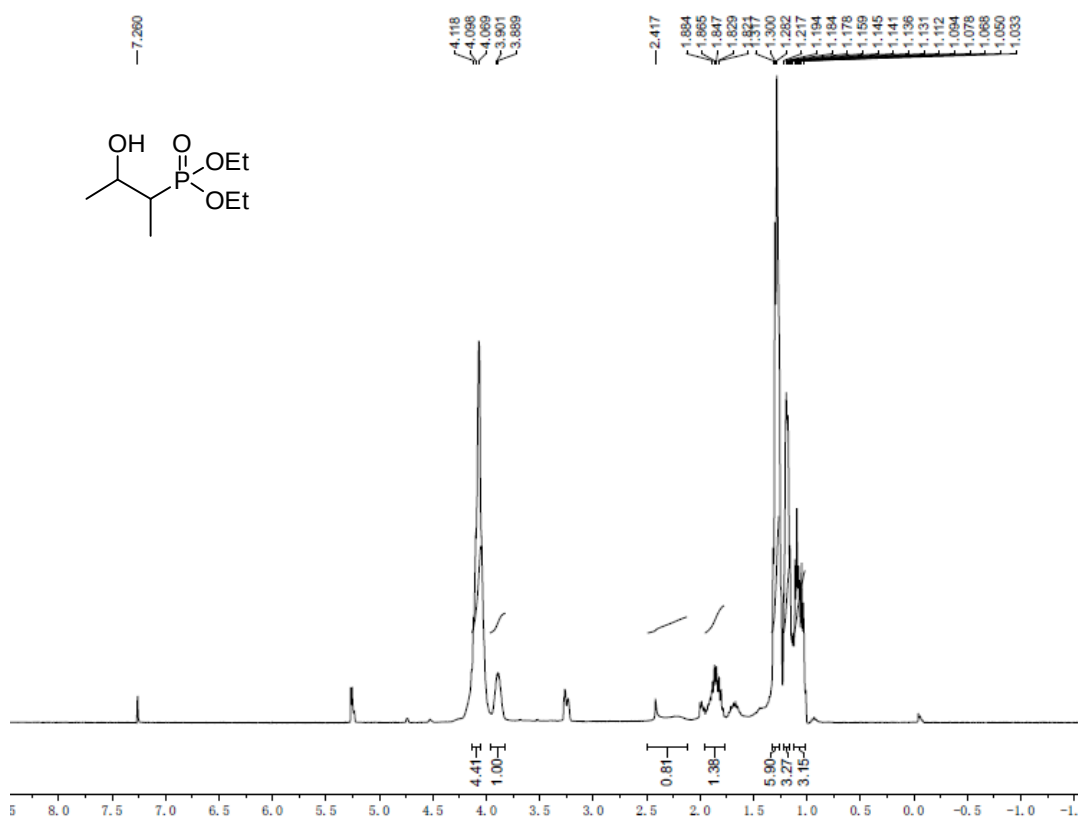
Chemical structure: CC(C)C(O)c1ccccc1

¹H NMR spectrum (CDCl₃) data:

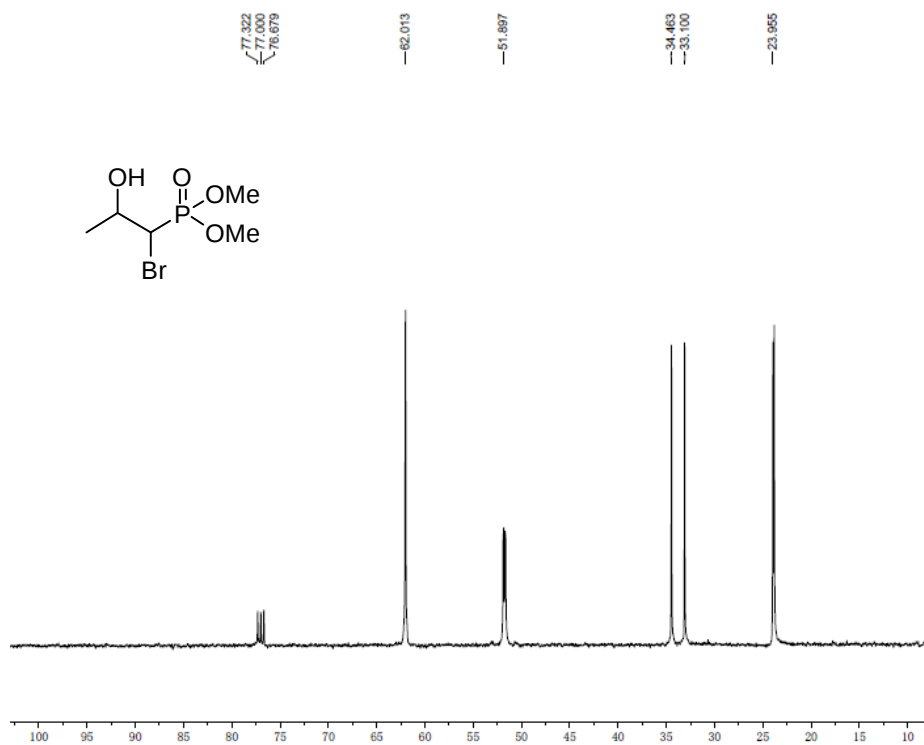
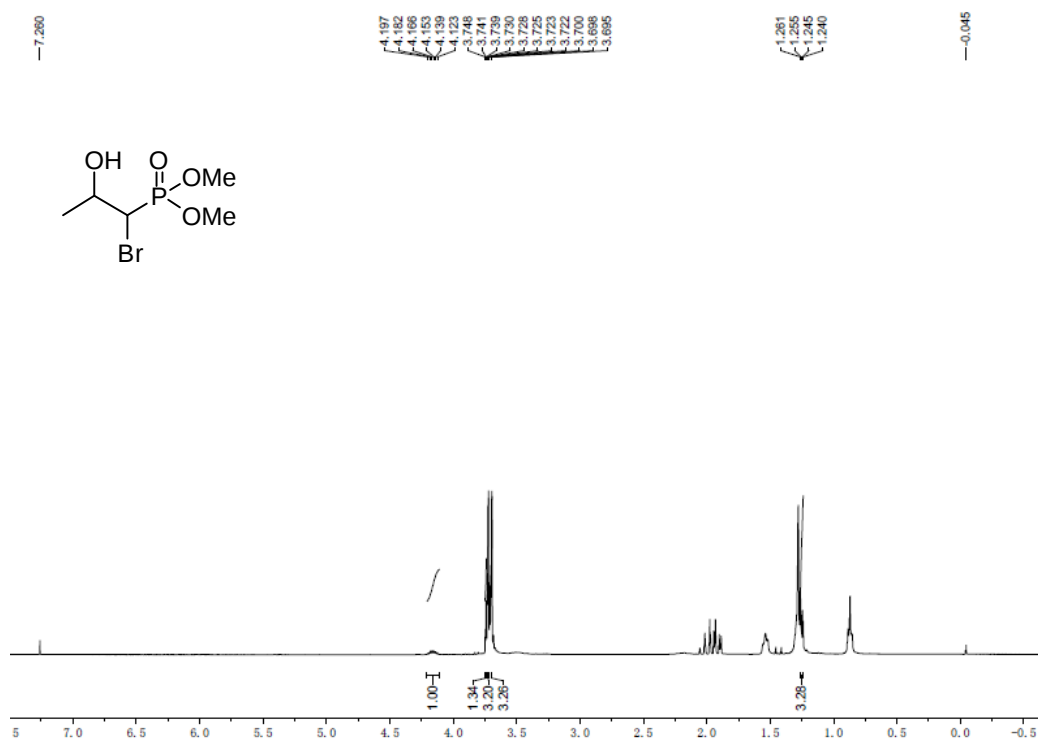
Chemical Shift (ppm)	Integration
7.260 (broad singlet)	1.00
7.201 - 7.160 (multiplet)	1.23
3.948 - 3.643 (multiplet)	2.86
1.272 - 1.069 (multiplet)	3.22



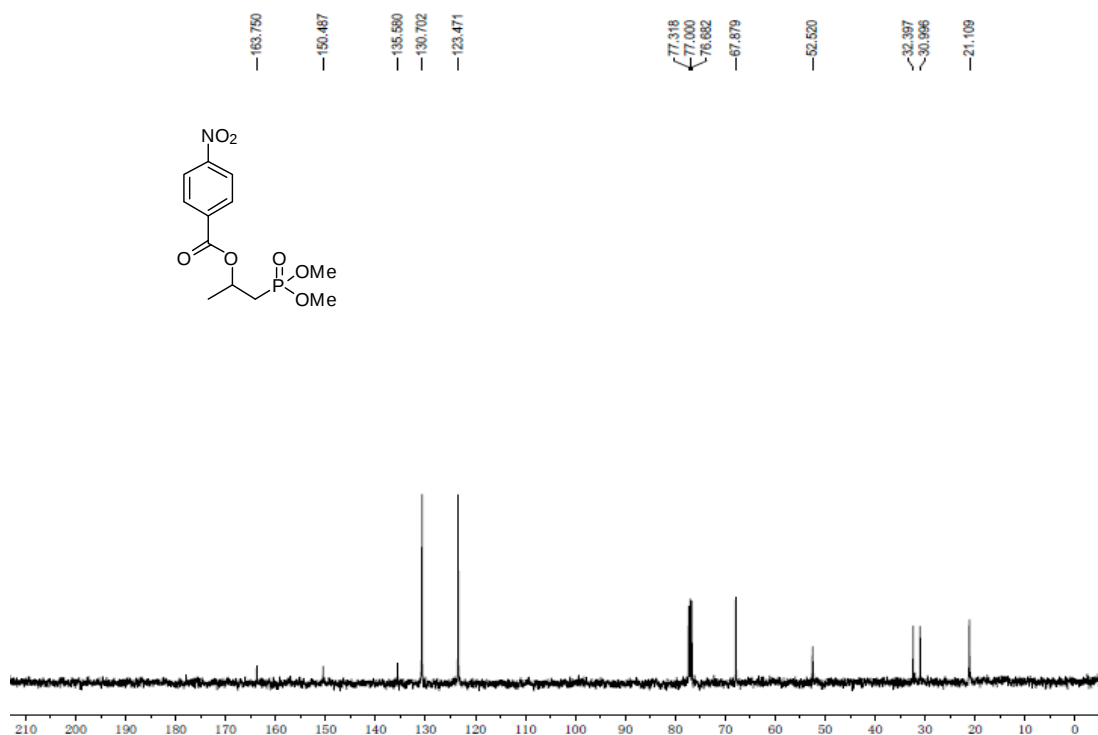
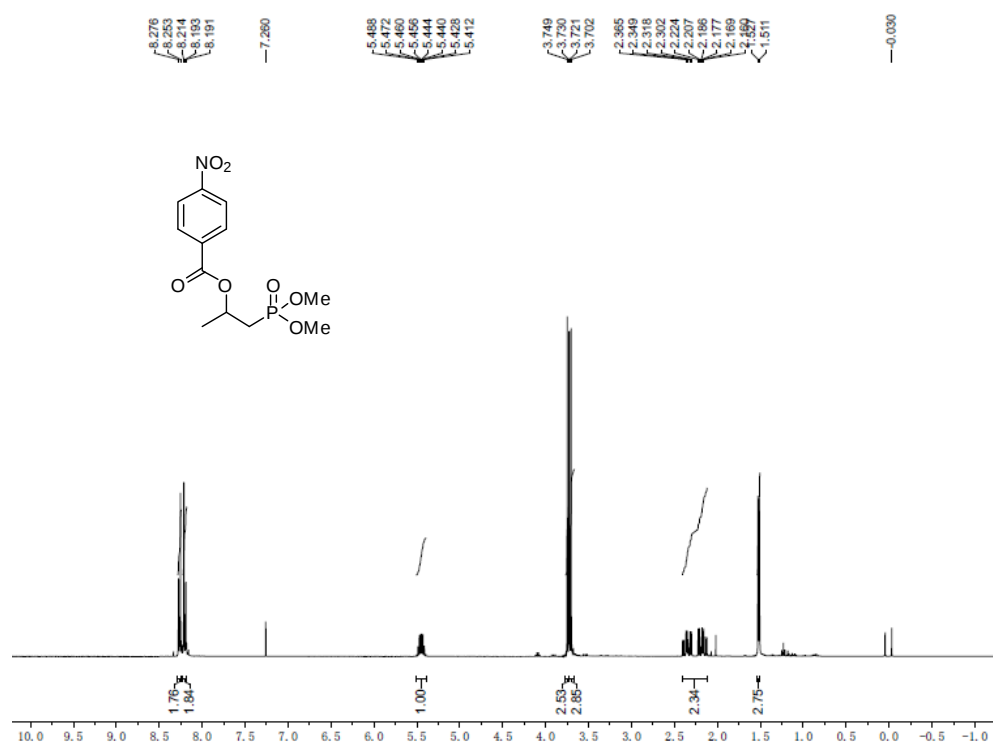
(2v) Diethyl 3-hydroxybut-2-ylphosphonate



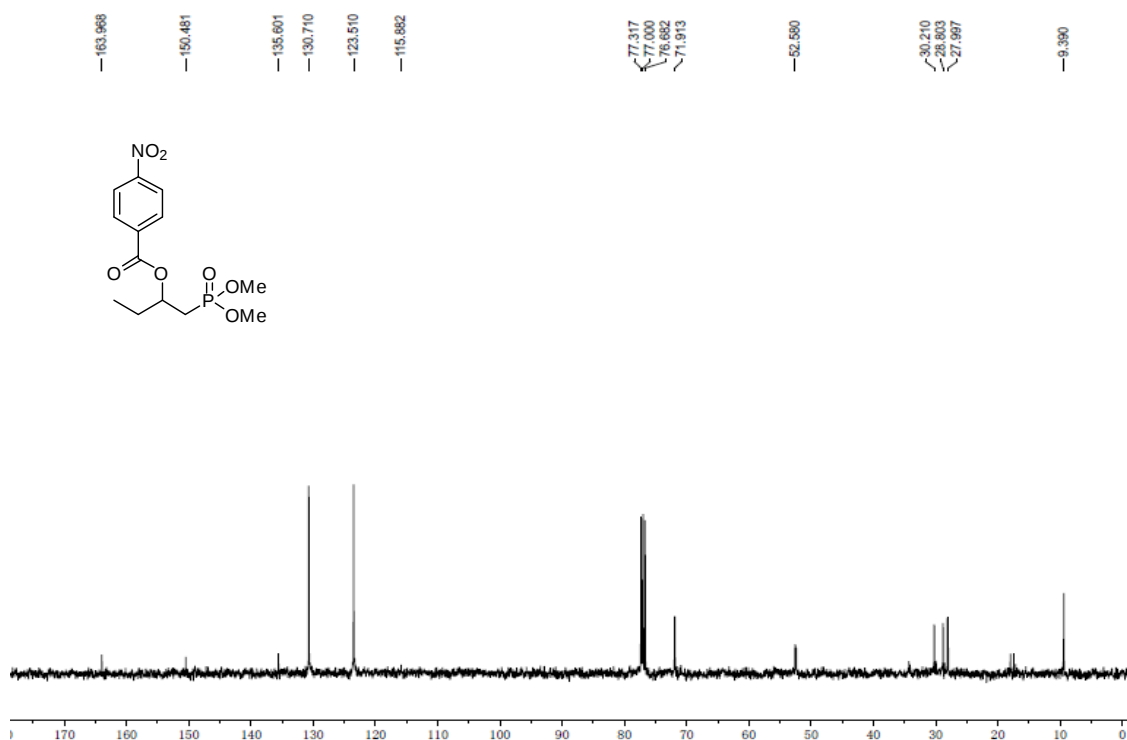
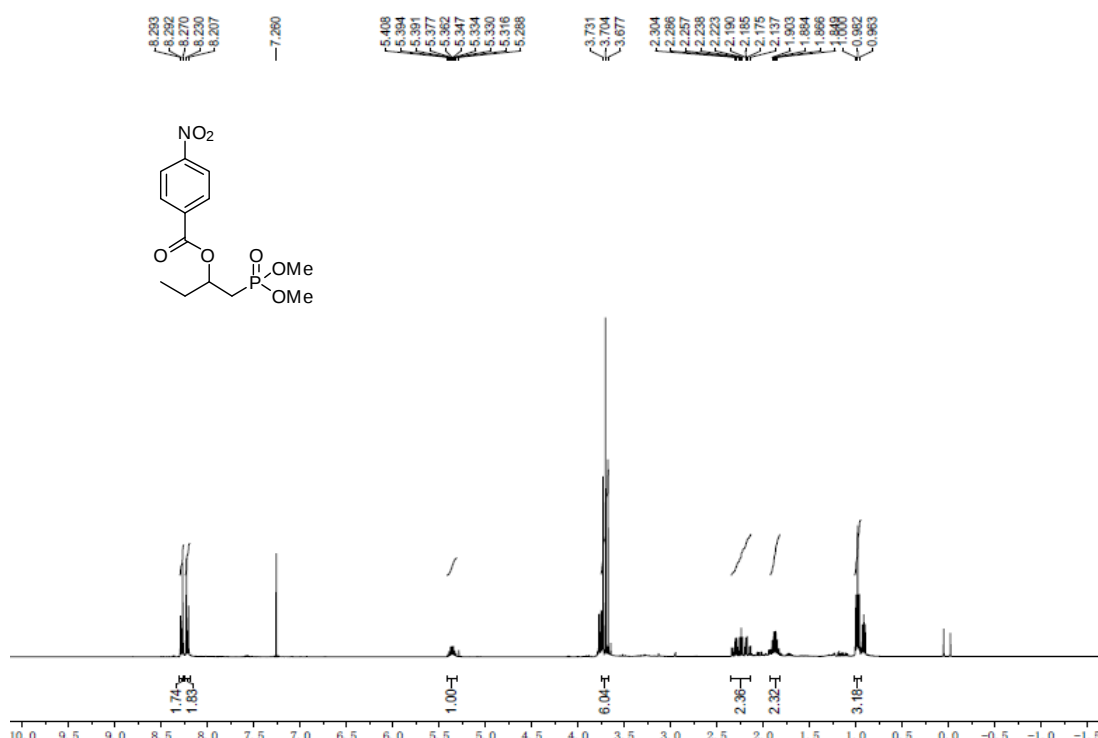
(2w) Dimethyl 1-bromo-2-hydroxypropylphosphonate



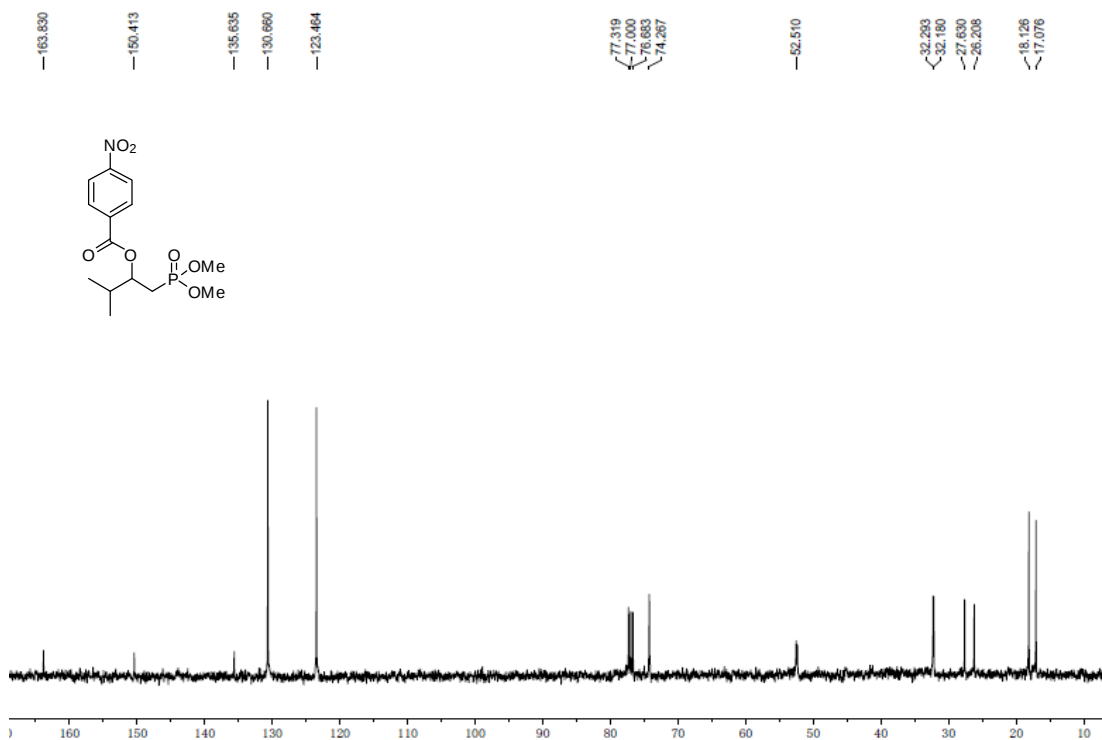
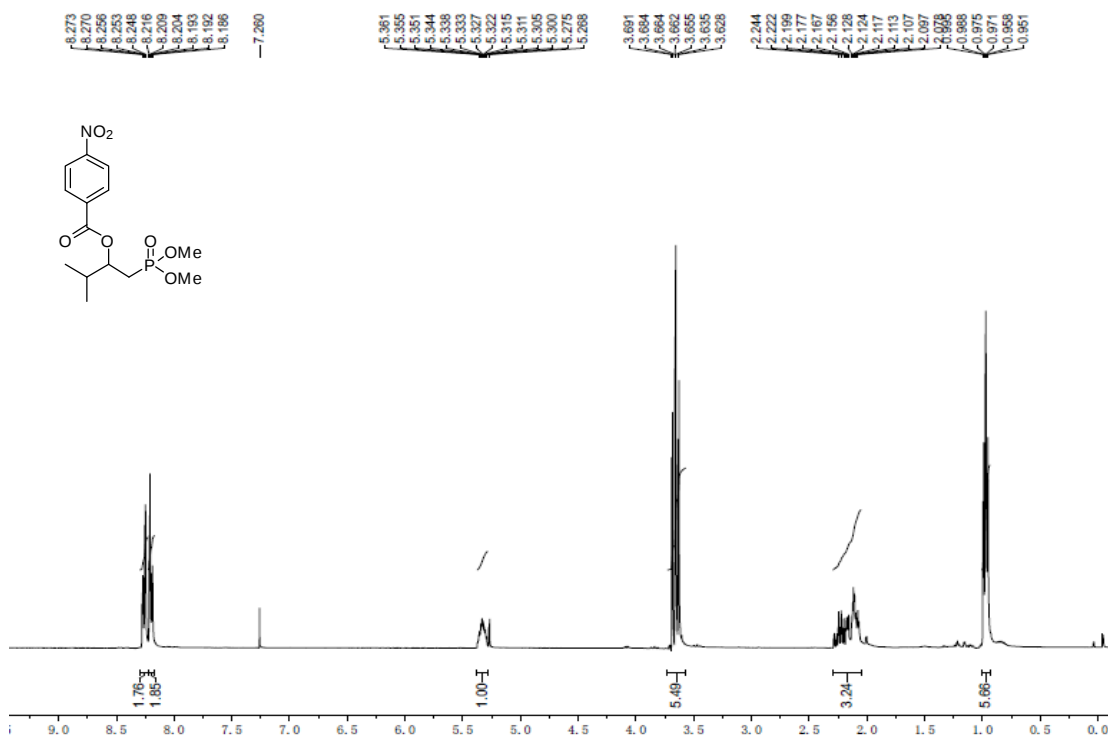
(3m) 1-(Dimethoxyphosphoryl)propan-2-yl 4-nitrobenzoate



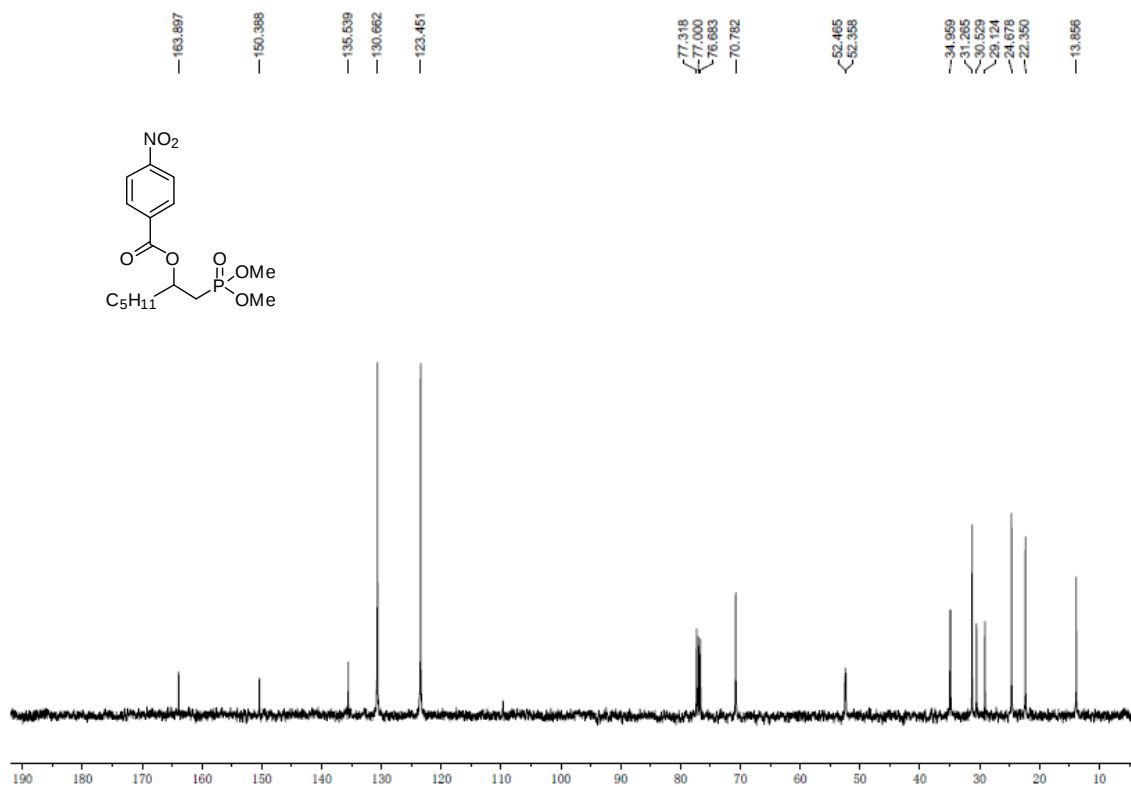
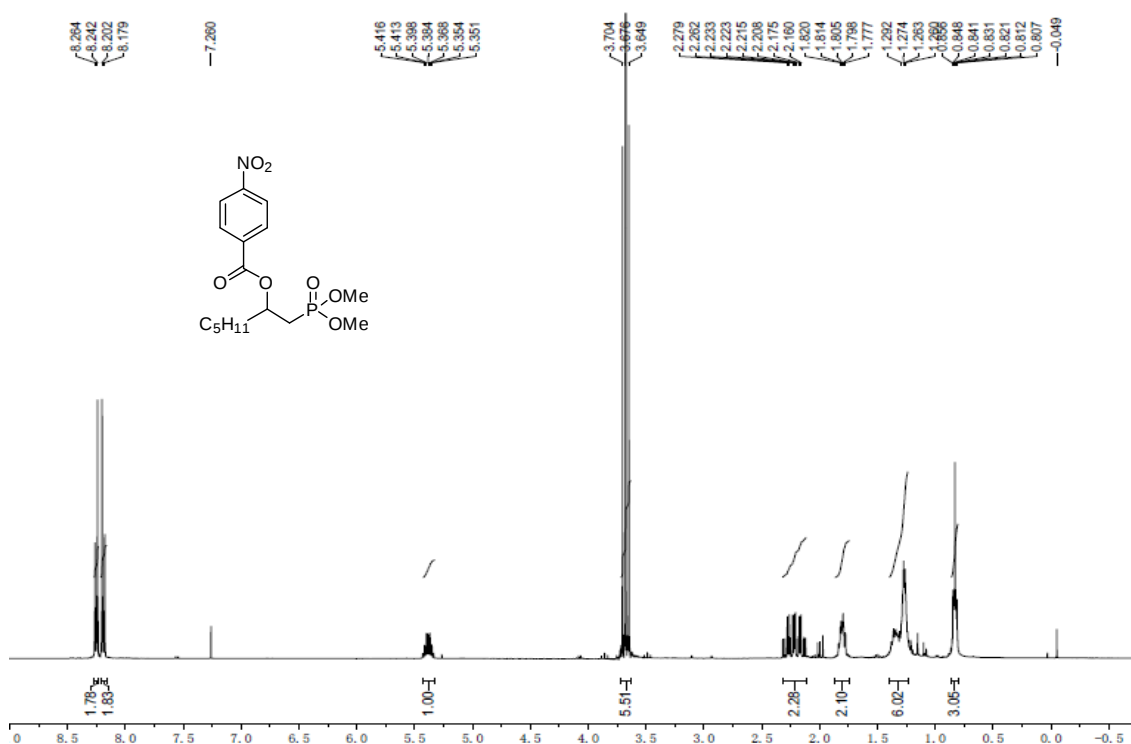
(3n) 1-(Dimethoxyphosphoryl)butan-2-yl 4-nitrobenzoate



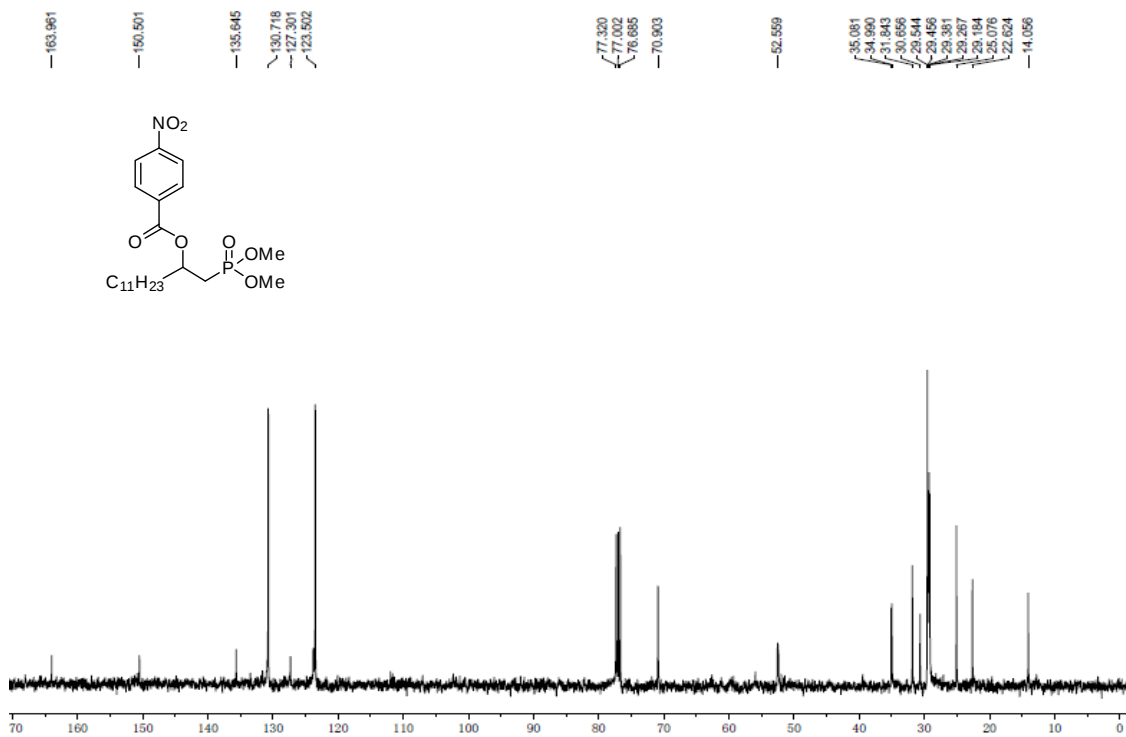
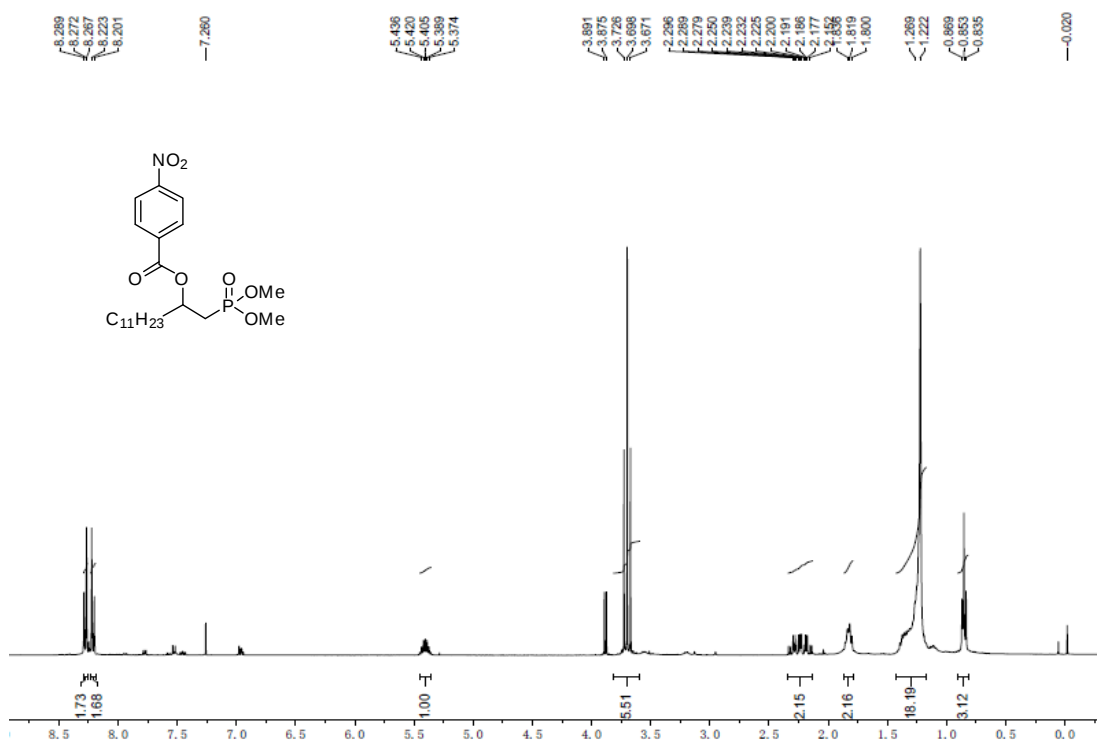
(3o) 1-(Dimethoxyphosphoryl)-3methylbutan-2-yl 4-nitrobenzoate



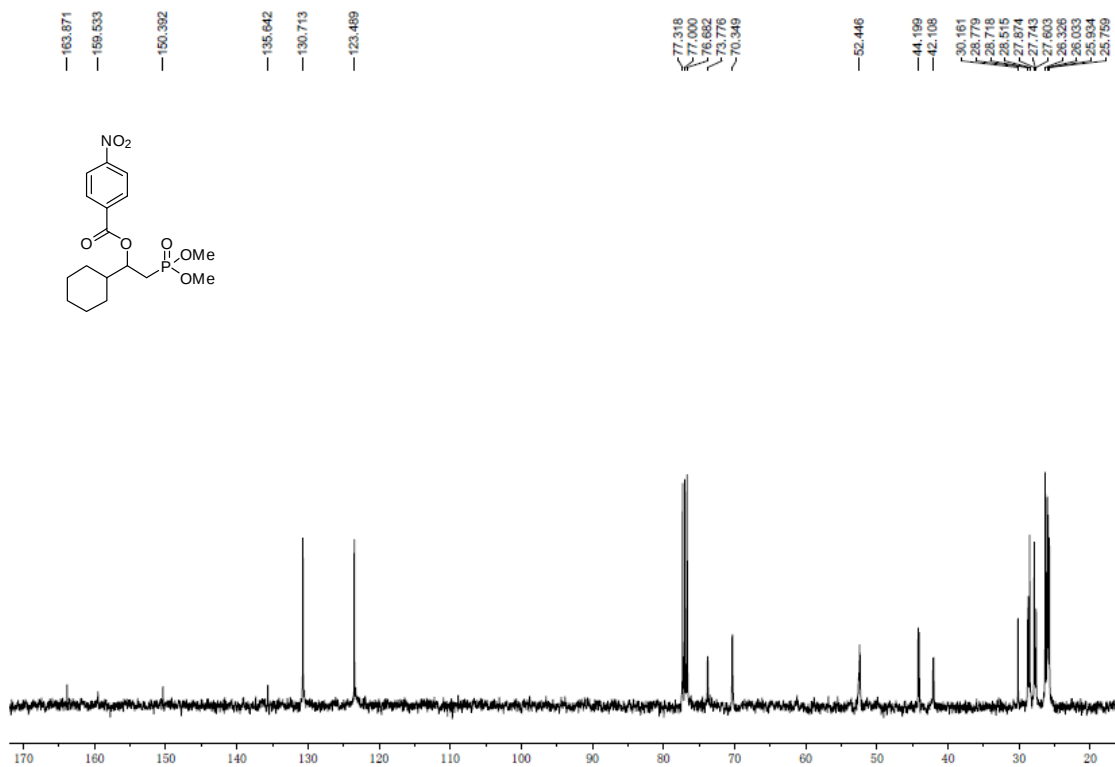
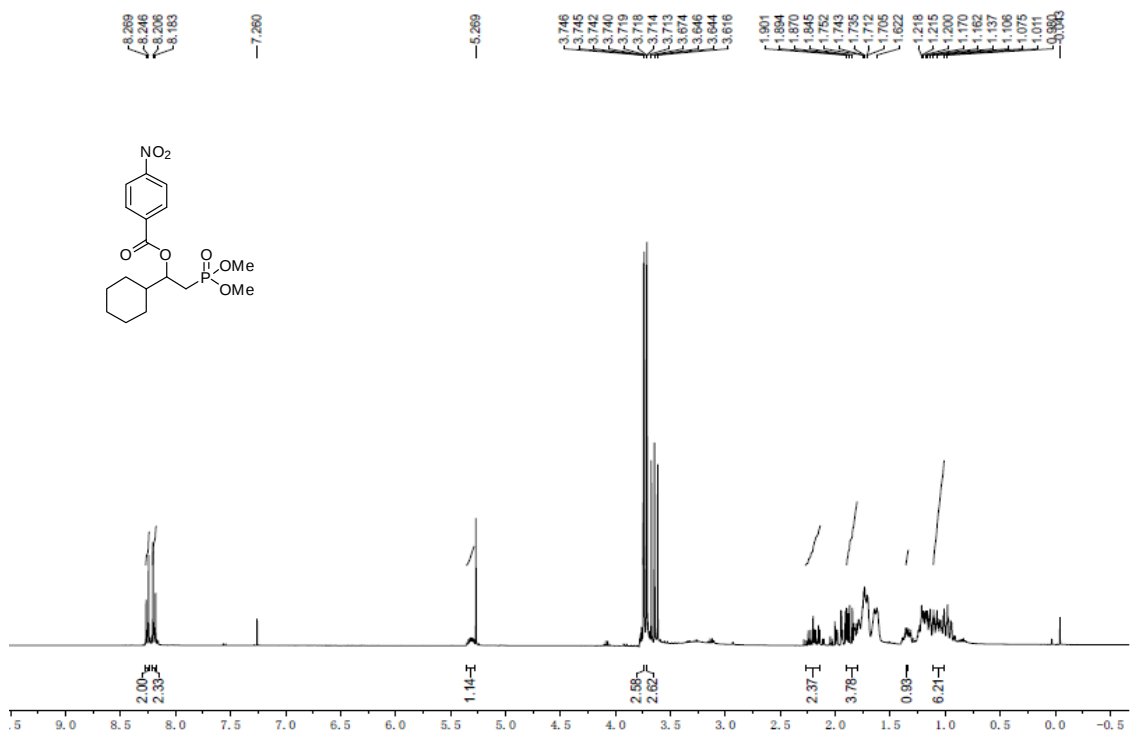
(3p) 1-(Dimethoxyphosphoryl)heptan-2-yl 4-nitrobenzoate



(3q) 1-(Dimethoxyphosphoryl)tridecan-2-yl 4-nitrobenzoate

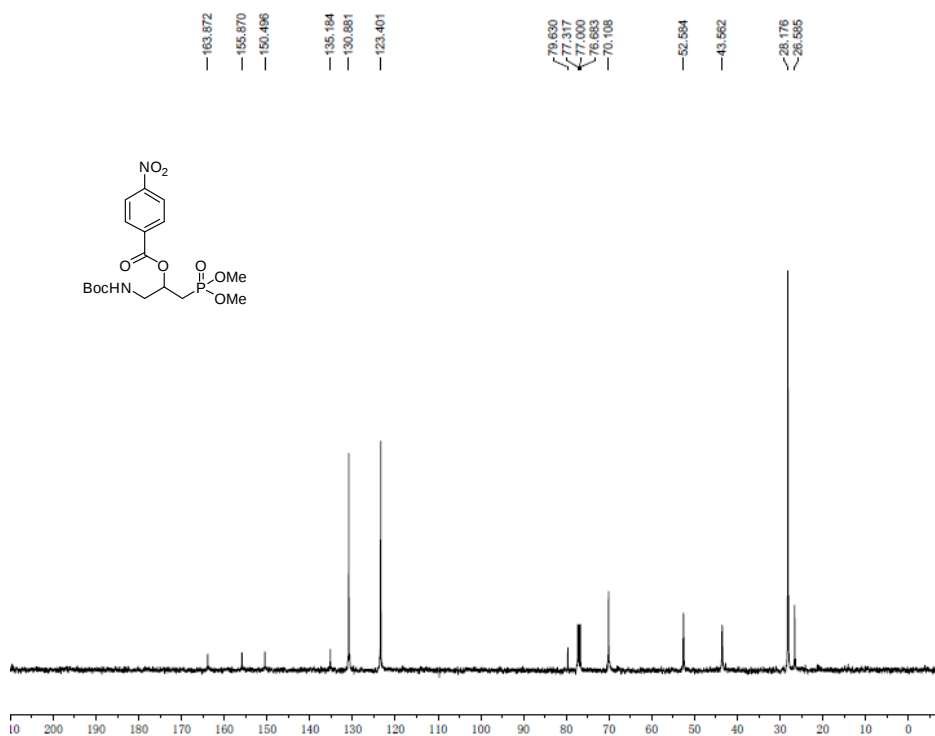
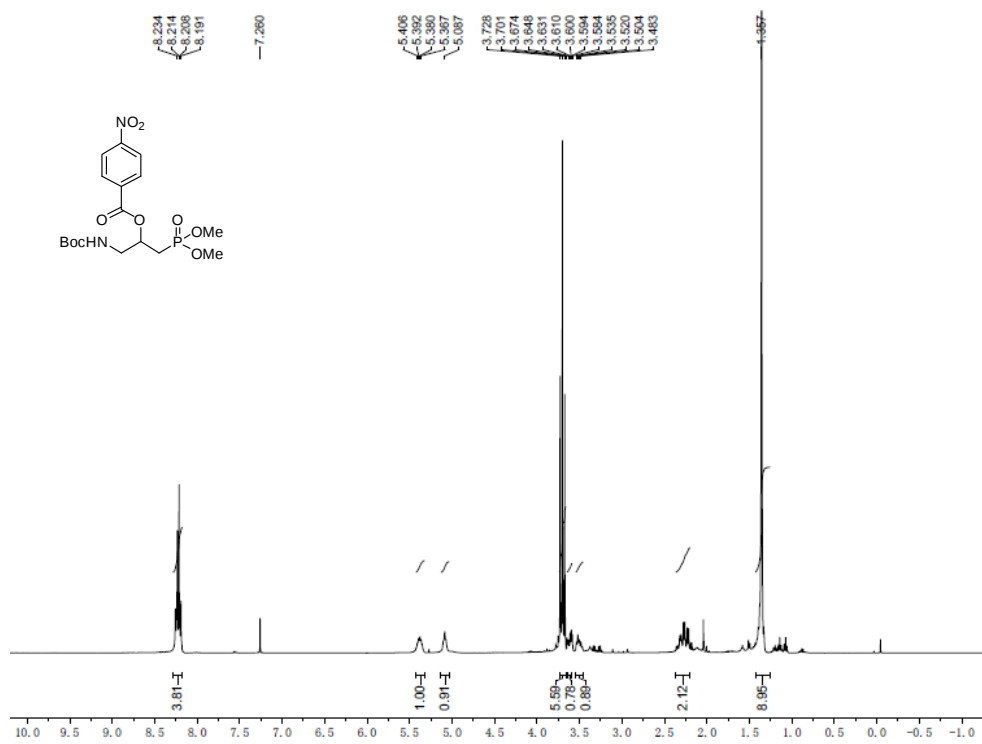


(3r) 1-Cyclohexyl-2-(dimethoxyphosphoryl)ethyl 4-nitrobenzoate

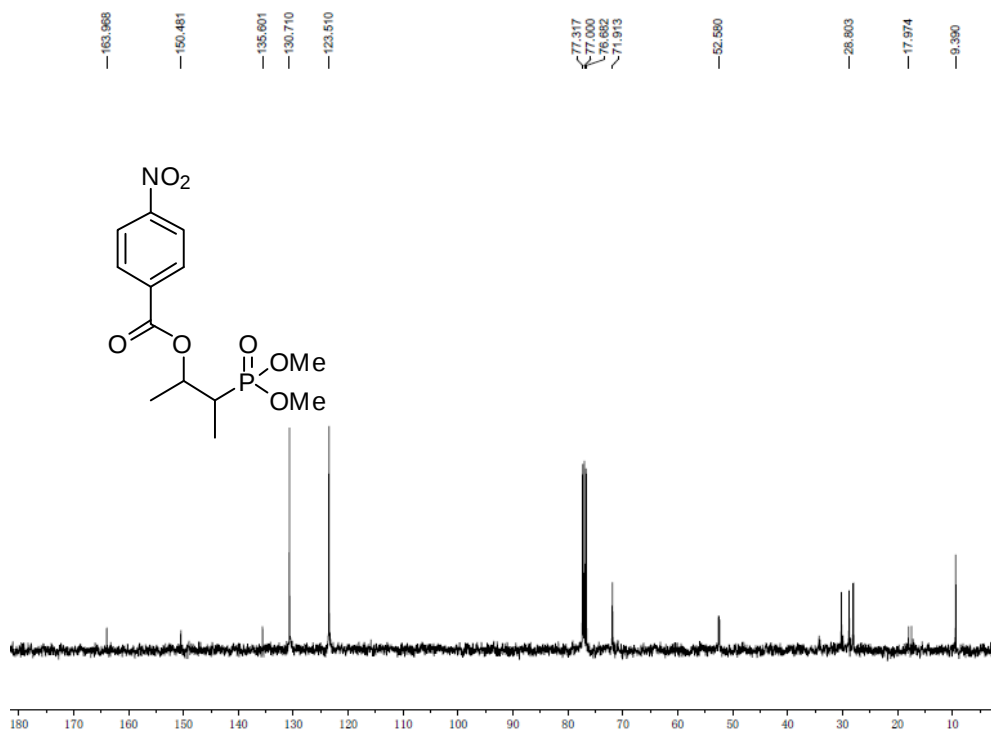
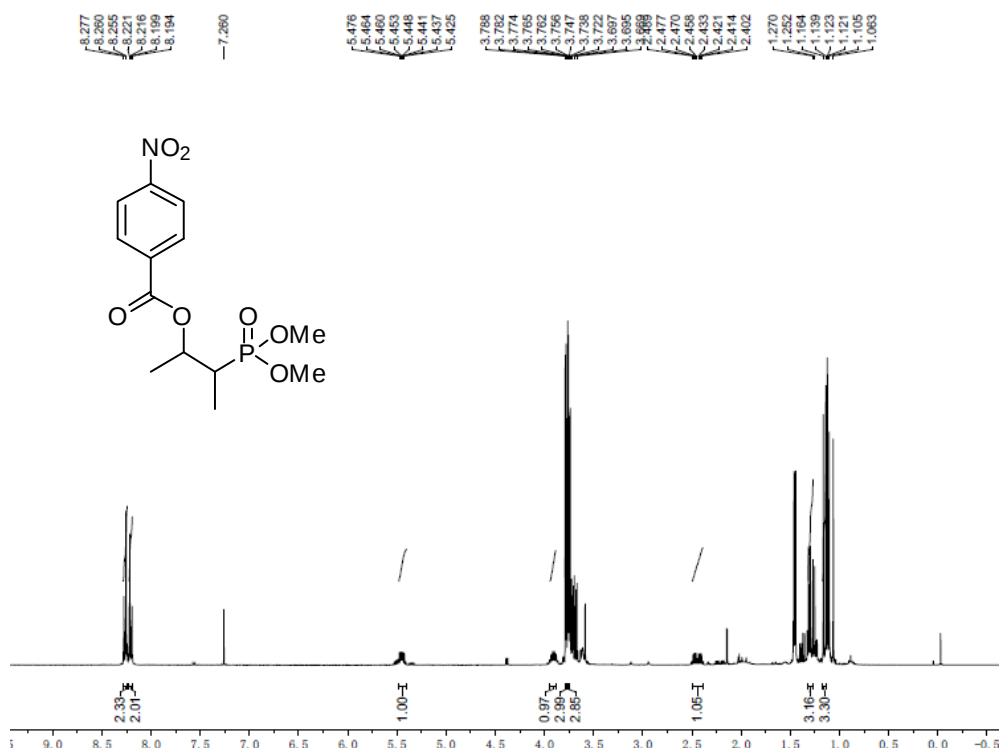


(3s) 1-[(Tert-butoxycarbonyl)amino-3-(dimethoxyphosphoryl)propan-2-yl
nitrobenzoate

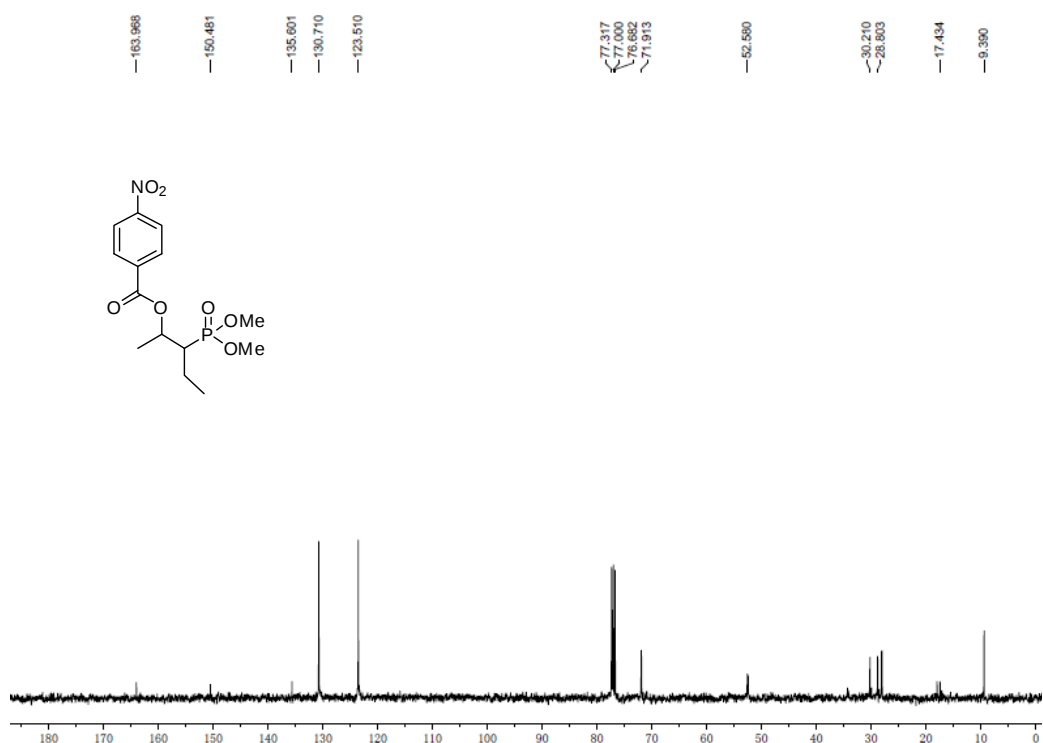
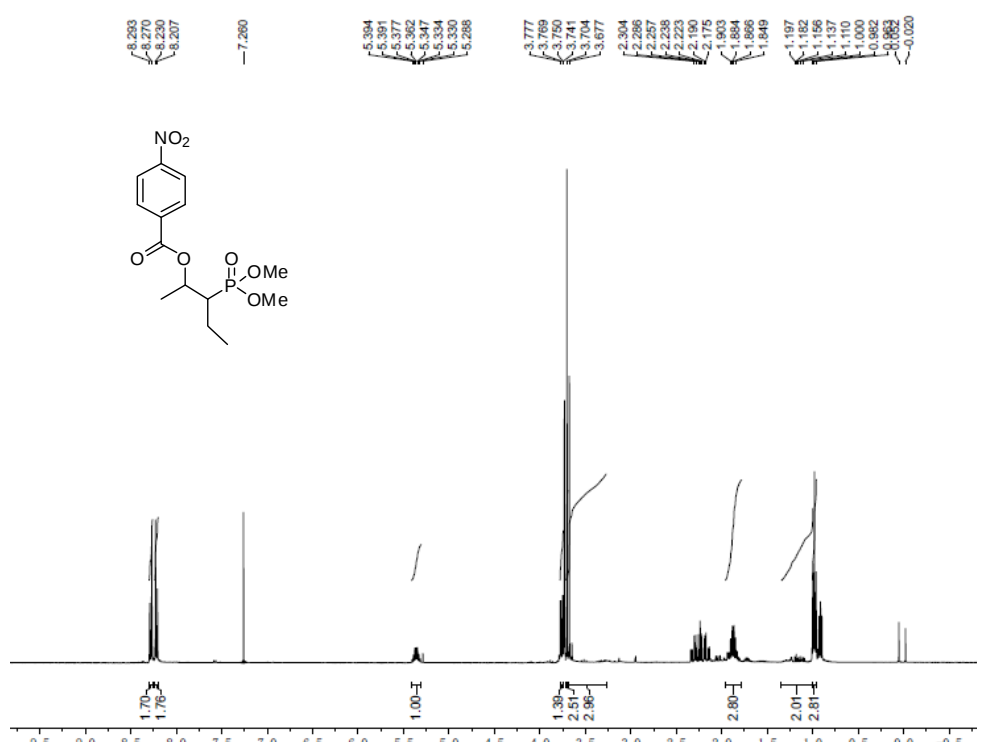
4-



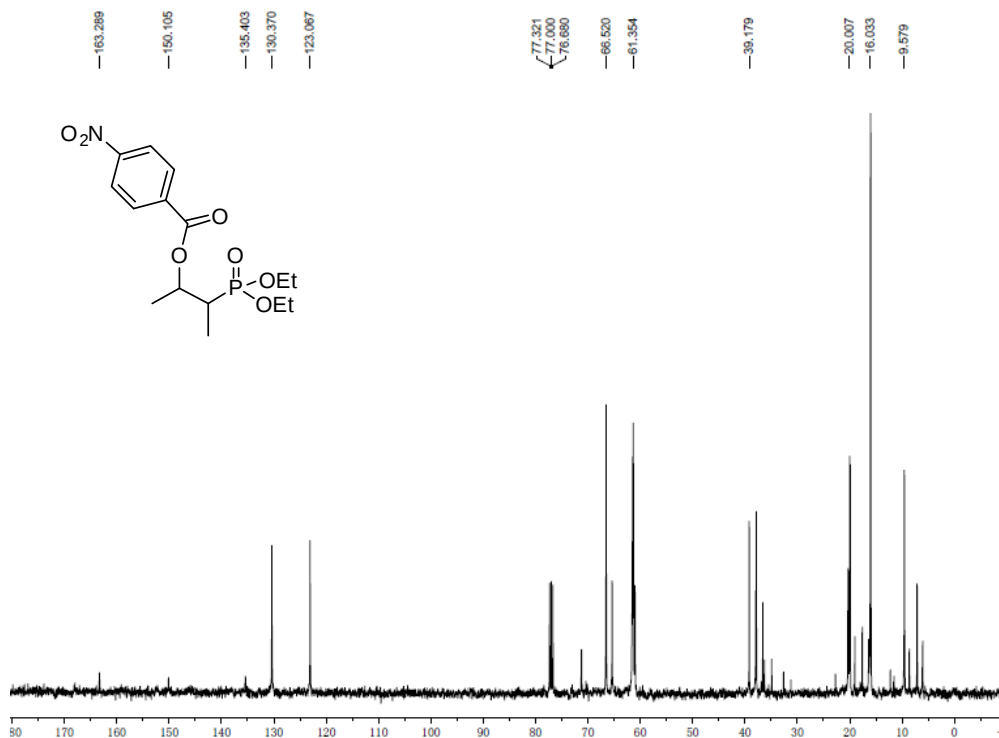
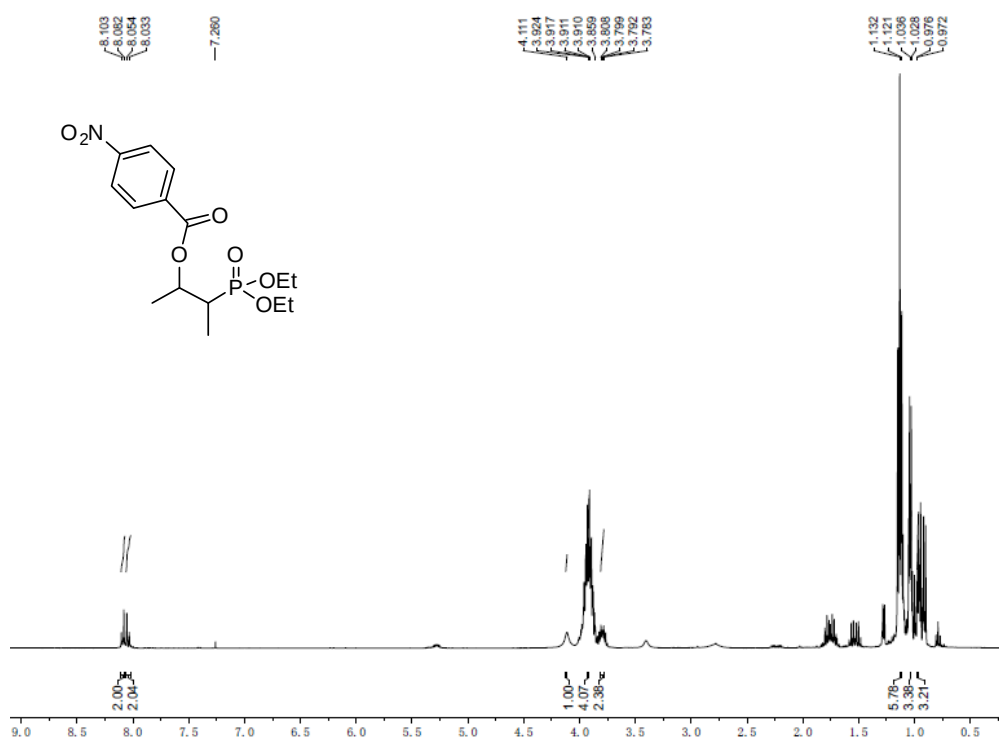
(3t) 3-(Dimethoxyphosphoryl)butan-2-yl 4-nitrobenzoate



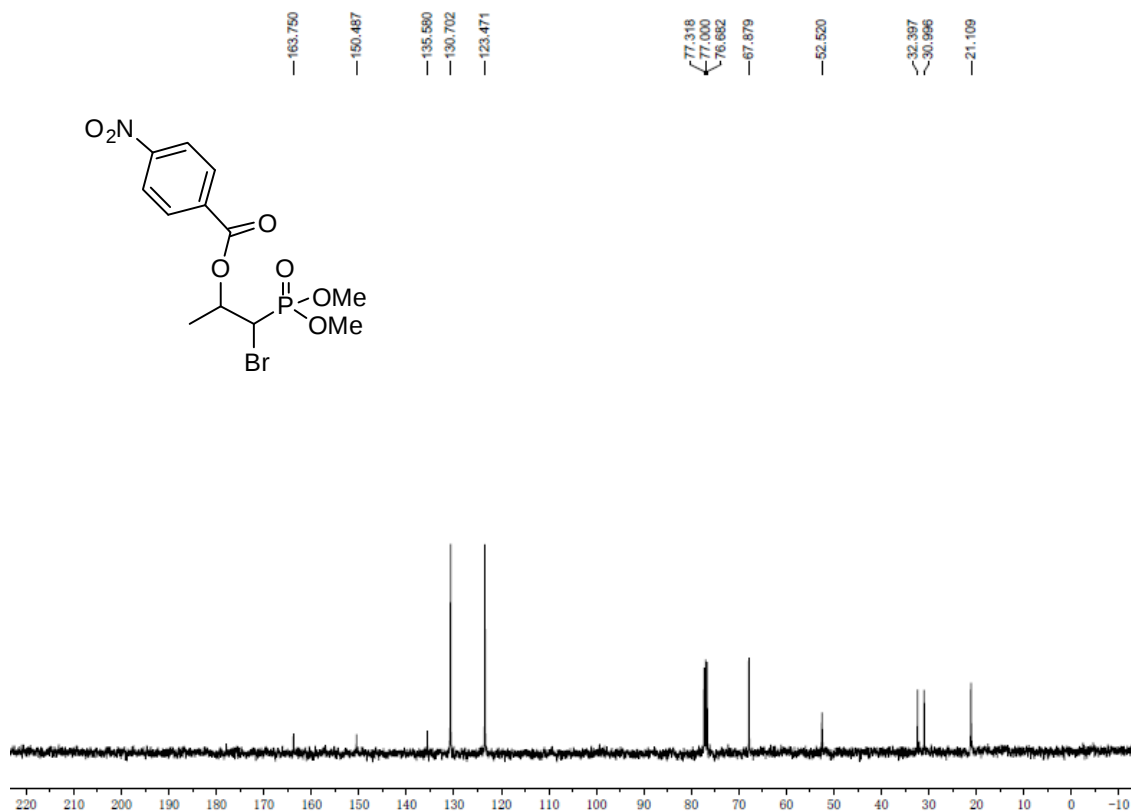
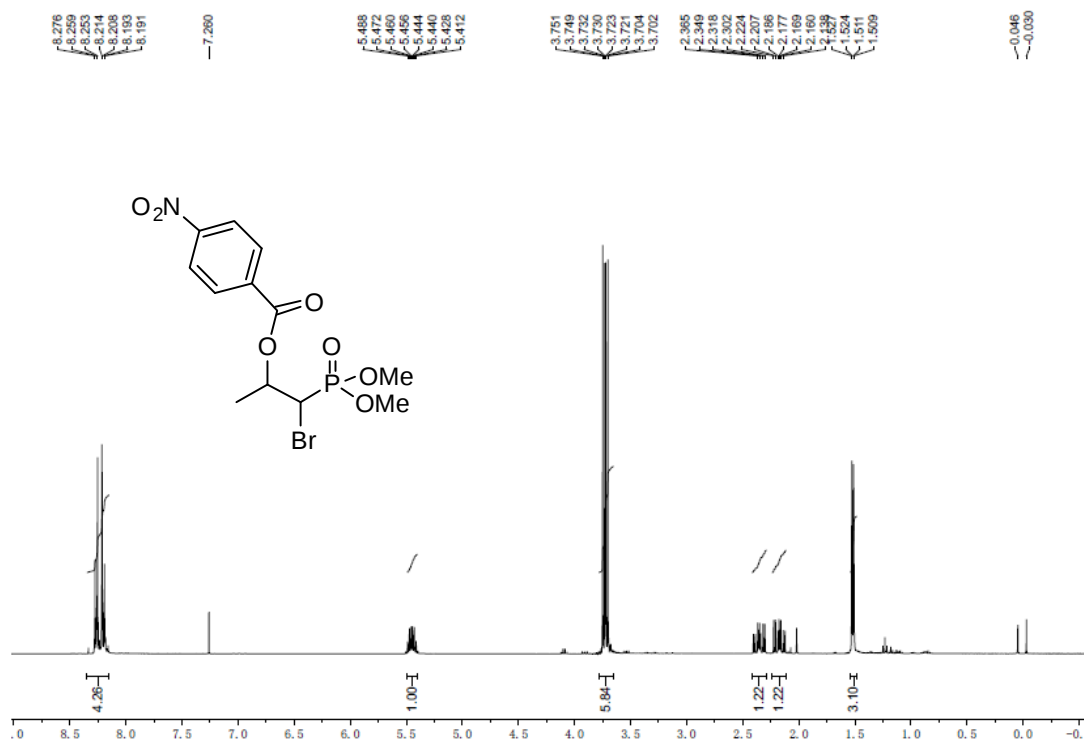
(3u) 3-(Dimethoxyphosphoryl)pentan-2-yl 4-nitrobenzoate



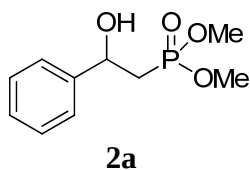
(3v) 3-(Diethoxyphosphoryl)butan-2-nitrobenzoate



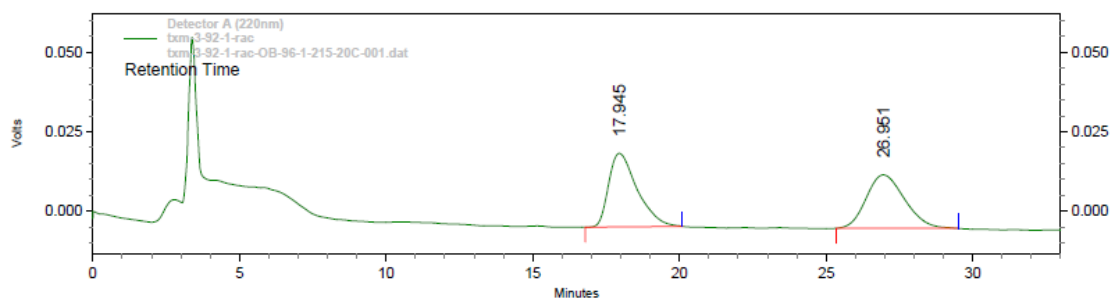
(3w) 1-Bromo-1-(dimethoxyphosphoryl)propan-2-yl 4-nitrobenzoate



HPLC for racemic and chiral compounds 2, 3m-s

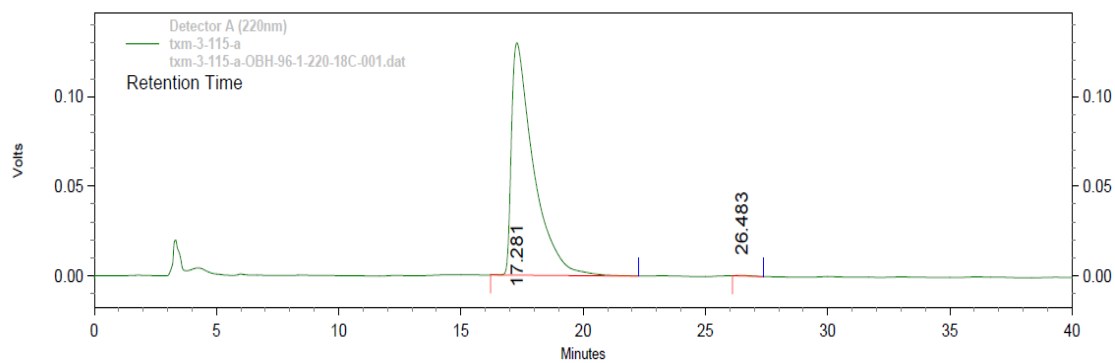


Racemate:



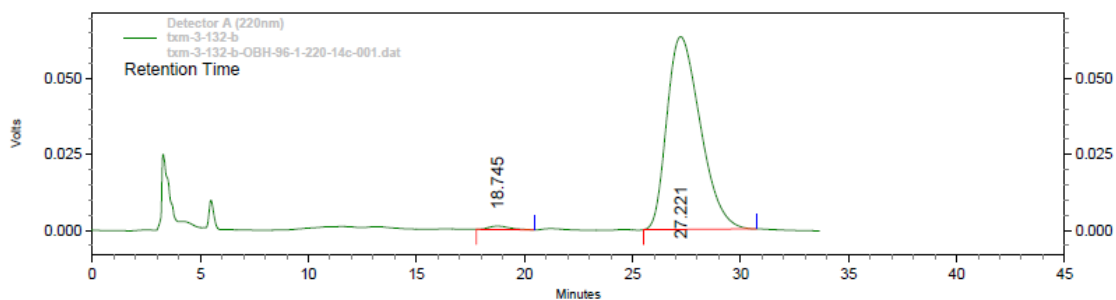
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.945	1562666	50.602	23074	57.917
2	26.951	1525461	49.398	16766	42.083

Table 1, entry 1: L1 as ligand



Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.281	8112186	99.871	129737	99.817
2	26.483	10508	0.129	238	0.183

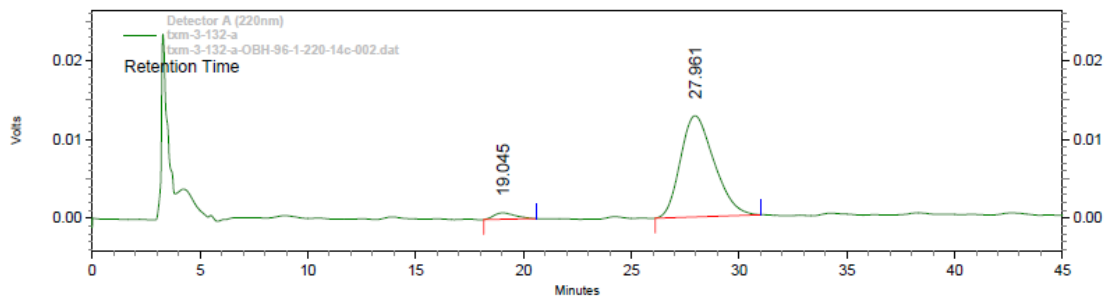
Table 1, entry 2: L2 as ligand



Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	18.745	77899	1.124	1149	1.776
2	27.221	6850006	98.876	63558	98.224

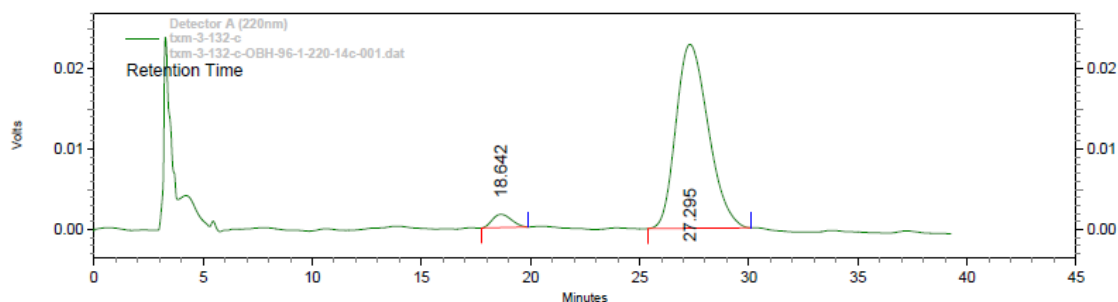
Table 1, entry 3: L3 as ligand



Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.045	55832	3.840	805	5.894
2	27.961	1398293	96.160	12858	94.106

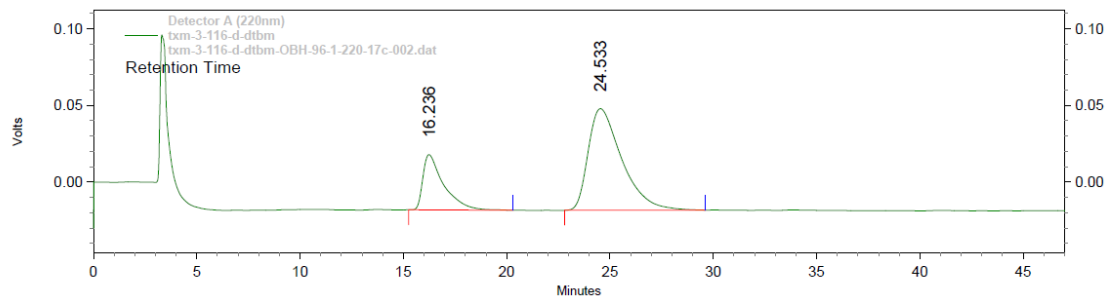
Table 1, entry 4: L4 as ligand



Detector A (220nm)

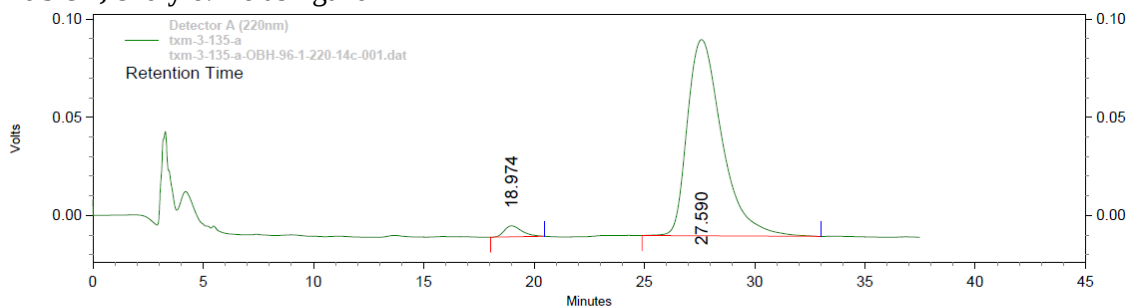
Pk #	Retention Time	Area	Area %	Height	Height %
1	18.642	100034	4.055	1652	6.716
2	27.295	2366692	95.945	22941	93.284

Table 1, entry 5: L5 as ligand



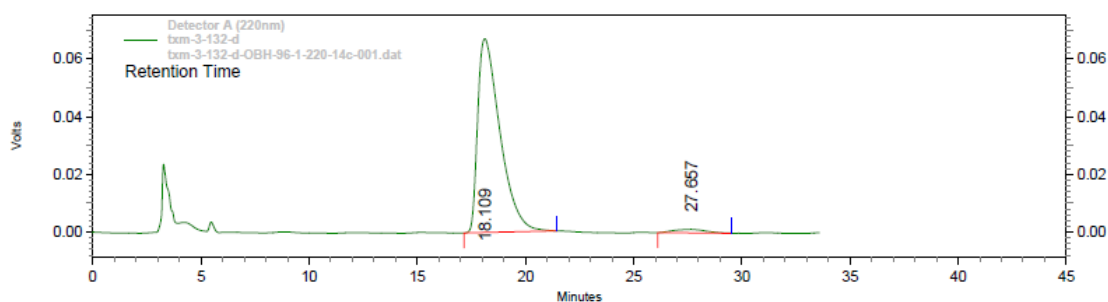
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	16.236	2519352	25.110	36065	35.237
2	24.533	7513891	74.890	66283	64.763

Table 1, entry 6: L6 as ligand



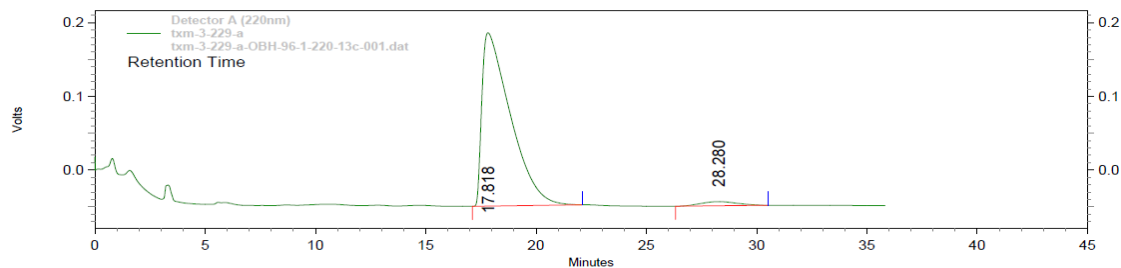
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	18.974	311767	2.770	5616	5.318
2	27.590	10942748	97.230	99995	94.682

Table 1, entry 7: L7 as ligand



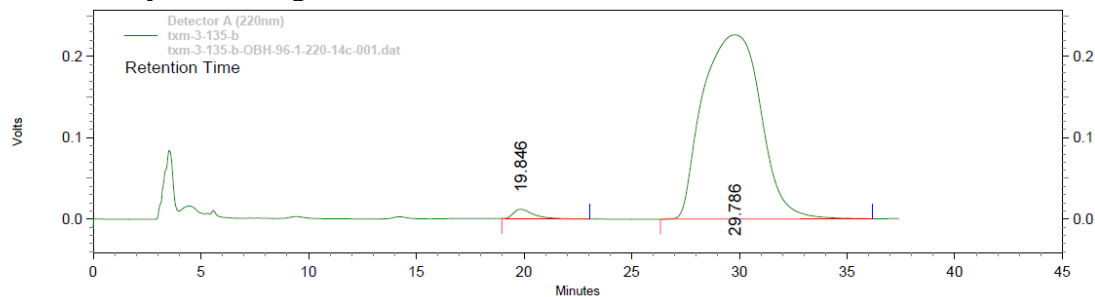
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	18.109	4807346	97.483	67072	98.229
2	27.657	124142	2.517	1209	1.771

Table 1, entry 8: L8 as ligand



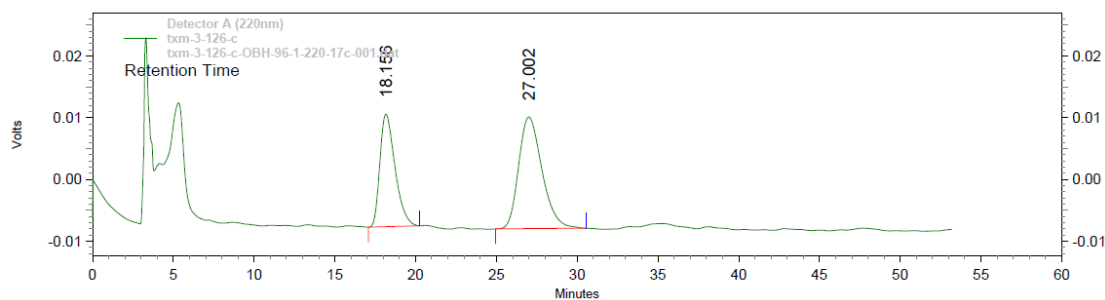
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.818	21086419	97.009	235461	97.630
2	28.280	650229	2.991	5715	2.370

Table 1, entry 9: L9 as ligand



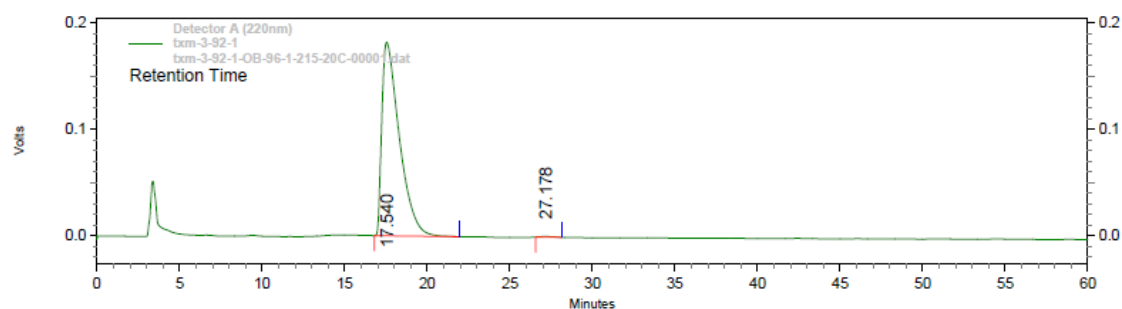
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	19.846	763305	1.763	11717	4.915
2	29.786	42540183	98.237	226684	95.085

Table 1, entry 10: L10 as ligand



Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	18.156	1186671	39.550	18218	50.195
2	27.002	1813728	60.450	18076	49.805

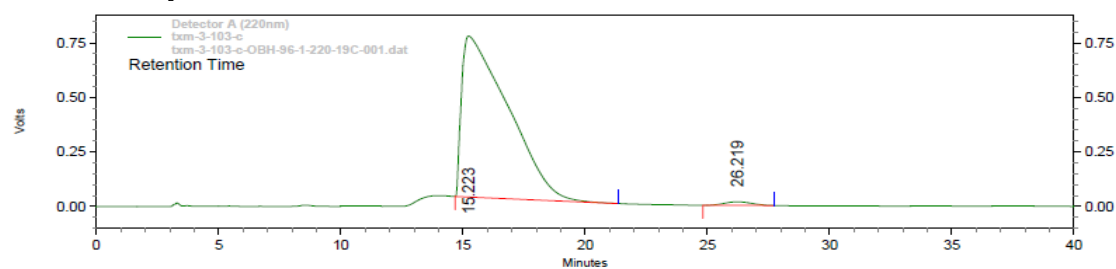
Table 2, entry 1



Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	17.540	13403798	99.792	181662	99.692
2	27.178	27910	0.208	561	0.308

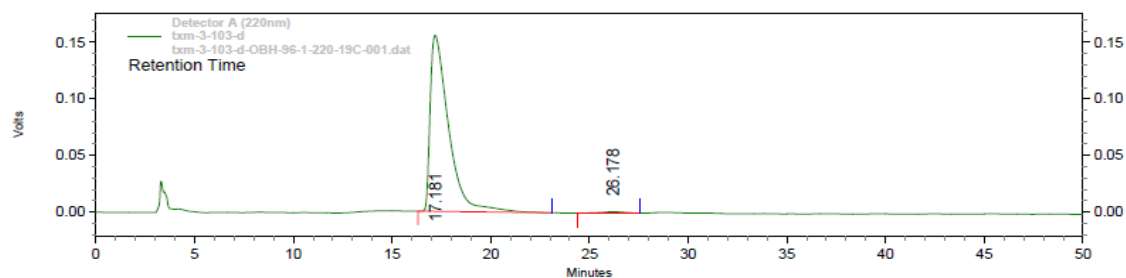
Table 2, entry 2



Detector A (220nm)

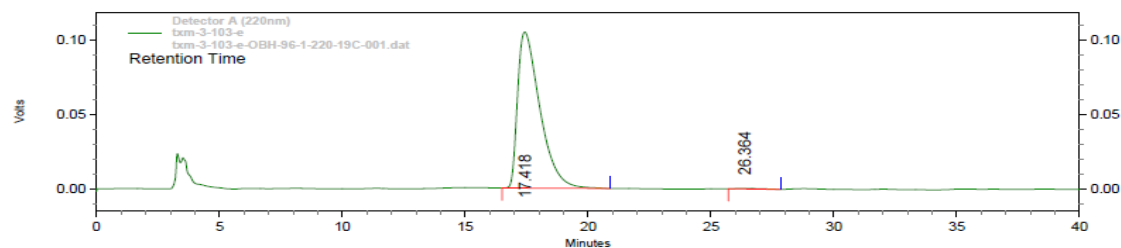
Pk #	Retention Time	Area	Area %	Height	Height %
1	15.223	97726117	98.739	738367	97.853
2	26.219	1248437	1.261	16199	2.147

Table 2, entry 3



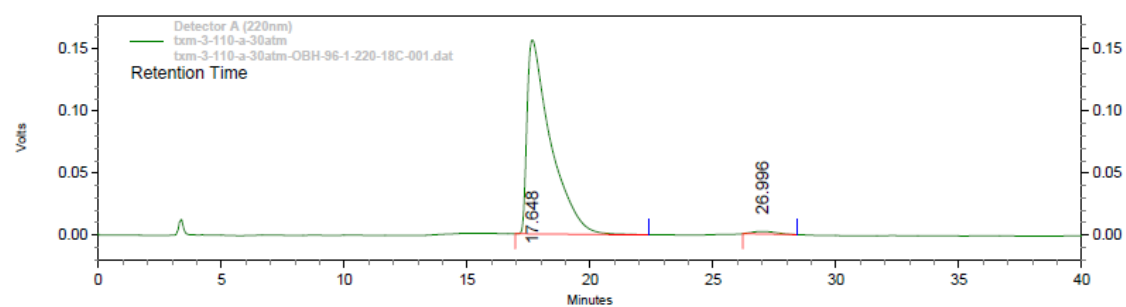
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.181	10097305	98.961	155654	99.235
2	26.178	106042	1.039	1201	0.765

Table 2, entry 4



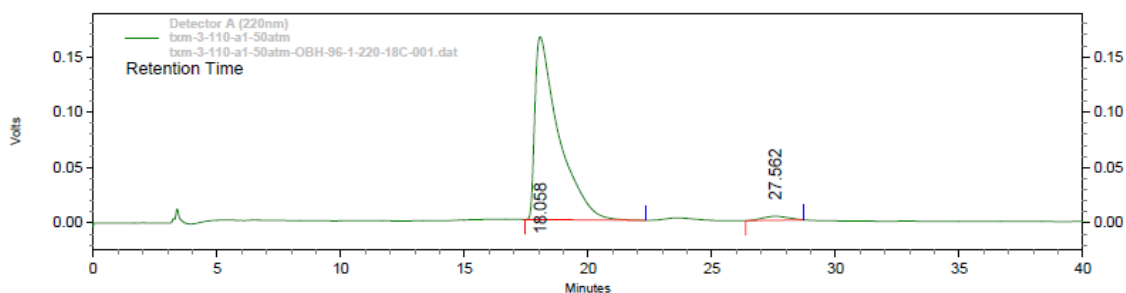
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.418	6617220	99.622	104896	99.682
2	26.364	25126	0.378	335	0.318

Table 2, entry 5



Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.648	10469559	98.661	156537	98.700
2	26.996	147050	1.339	2061	1.299

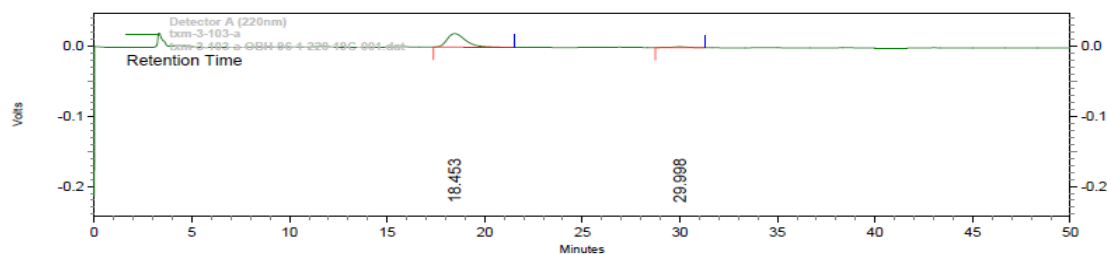
Table 2, entry 6



Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	18.058	11069319	97.744	165140	97.916
2	27.562	255461	2.256	3514	2.084

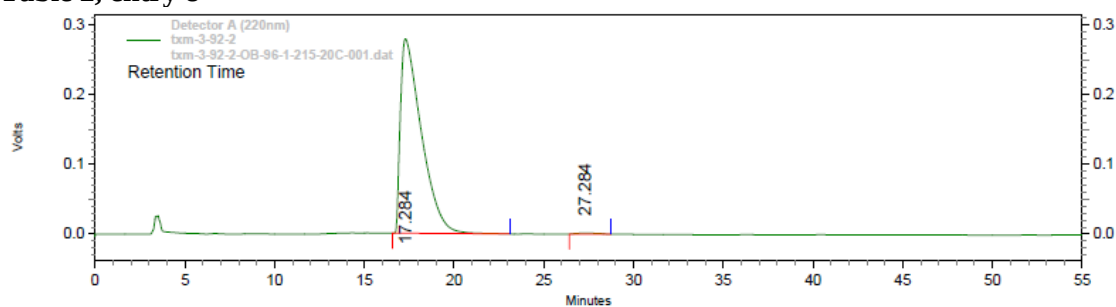
Table 2, entry 7



Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	18.453	1275717	94.757	19349	94.653
2	29.998	70591	5.243	1093	5.347

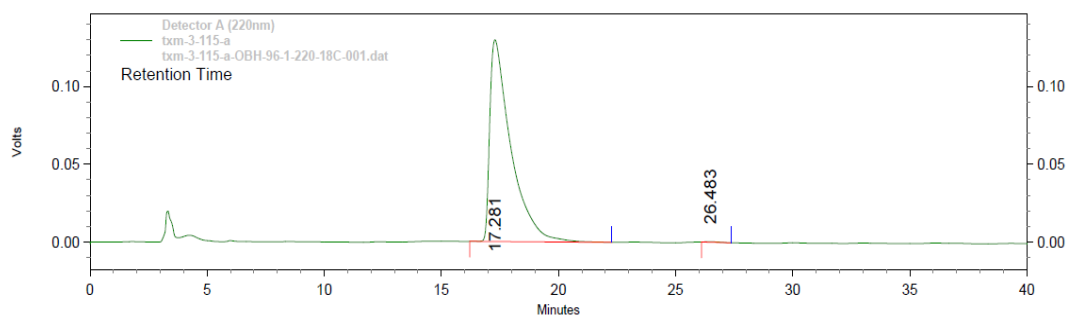
Table 2, entry 8



Detector A (220nm)

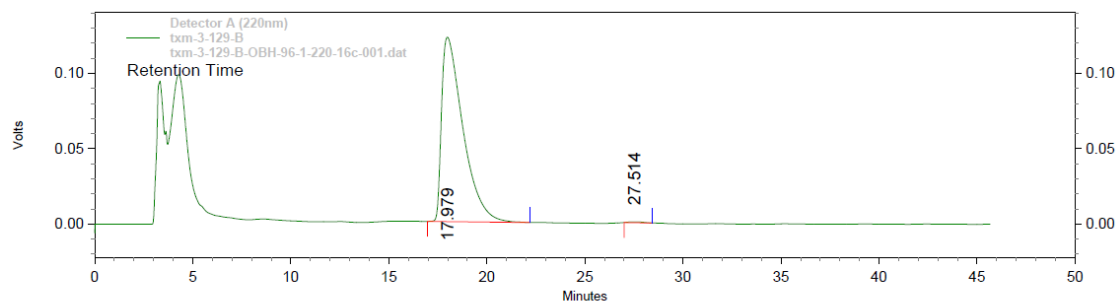
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.284	22710340	99.537	278743	99.548
2	27.284	105744	0.463	1267	0.452

Table 3, entry 1

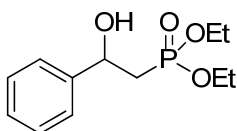


Detector A (220nm)						
Pk #	Retention Time	Area	Area %	Height	Height %	
1	17.281	8112186	99.871	129737	99.817	
2	26.483	10508	0.129	238	0.183	

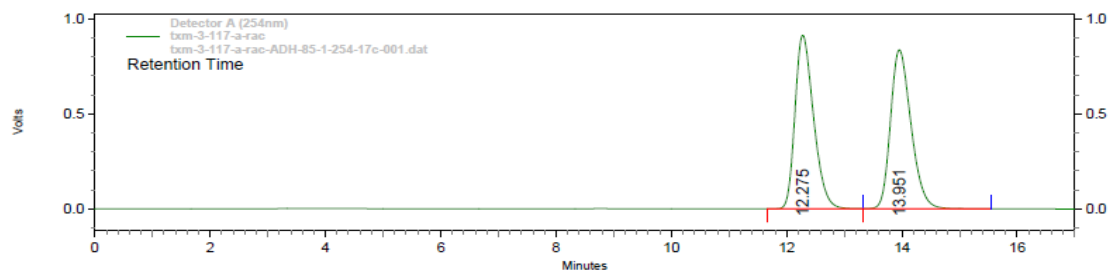
Table 3, entry 2



Detector A (220nm)						
Pk #	Retention Time	Area	Area %	Height	Height %	
1	17.979	9255821	99.687	122381	99.527	
2	27.514	29086	0.313	581	0.473	

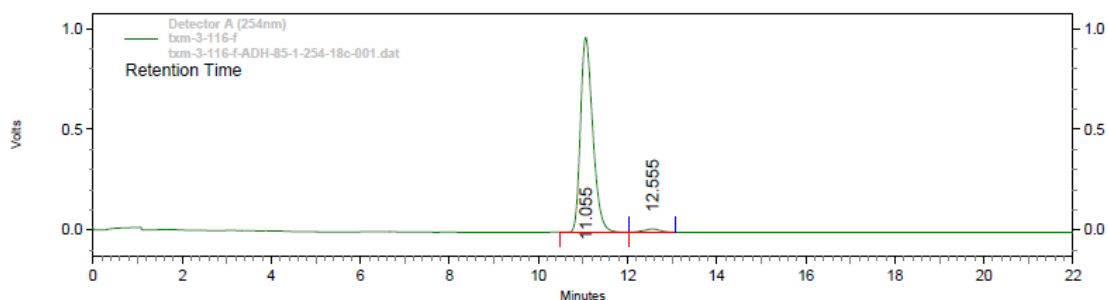


Racemate:



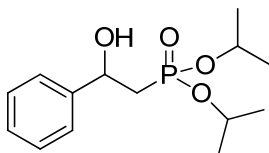
Detector A (254nm)						
Pk #	Retention Time	Area	Area %	Height	Height %	
1	12.275	20435180	49.705	912644	52.192	
2	13.951	20677799	50.295	835984	47.808	

Table 3, entry 3

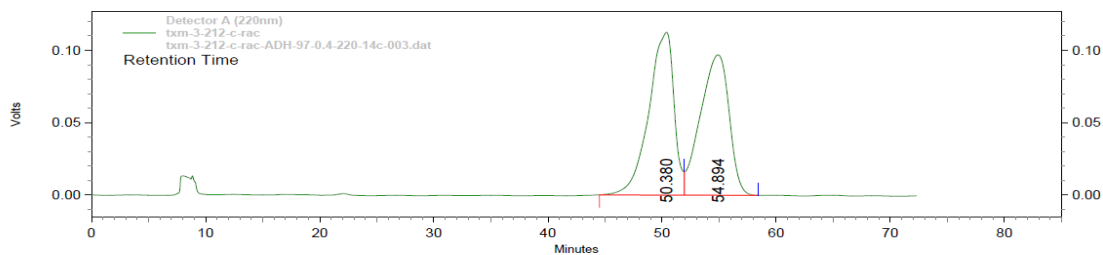


Detector A (254nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	11.055	18546256	97.862	968114	98.352
2	12.555	405178	2.138	16217	1.648



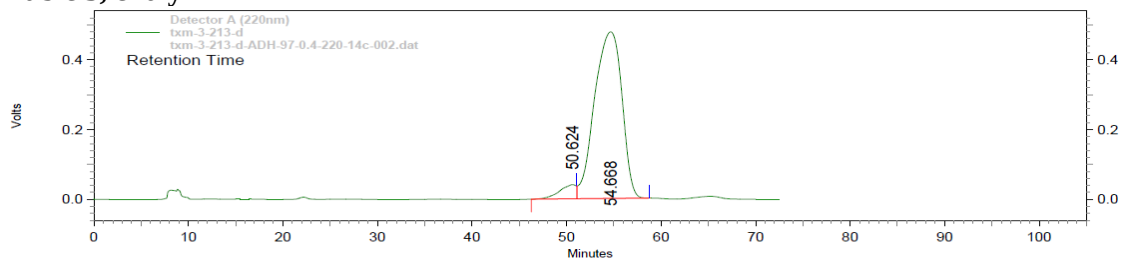
Racemate:



Detector A (220nm)

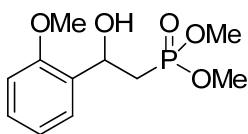
Pk #	Retention Time	Area	Area %	Height	Height %
1	50.380	17306647	50.545	112491	53.698
2	54.894	16933600	49.455	96999	46.302

Table 3, entry 4

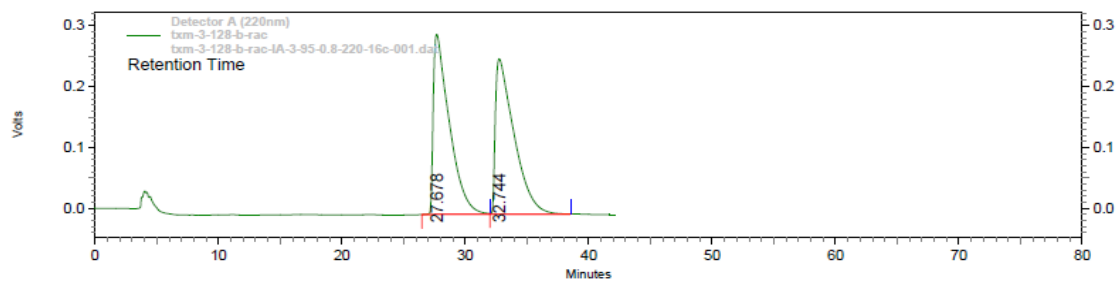


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	50.624	4963428	4.913	40790	7.883
2	54.668	96057276	95.087	476668	92.117



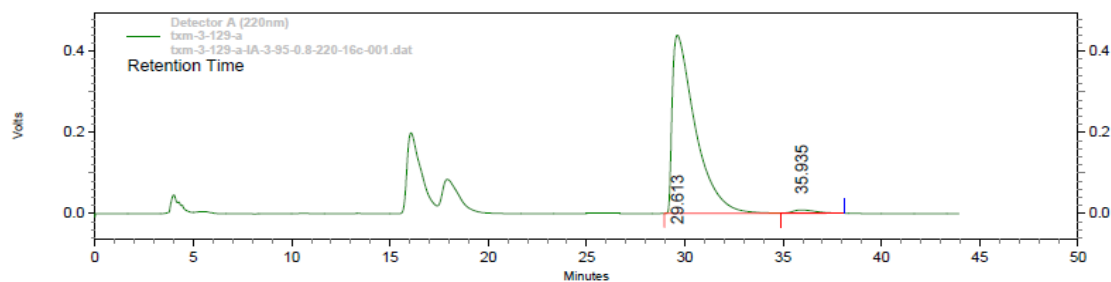
Racemate:



Detector A (220nm)

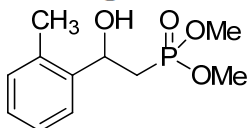
Pk #	Retention Time	Area	Area %	Height	Height %
1	27.678	26821423	49.919	296097	53.678
2	32.744	26907959	50.081	255520	46.322

Table 3, entry 5

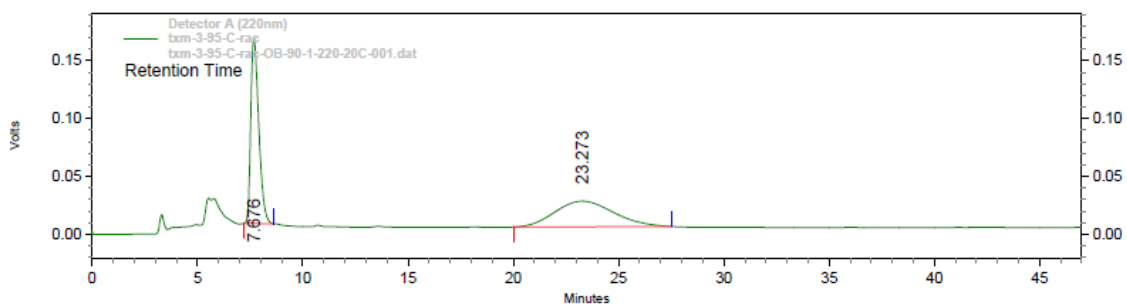


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	29.613	35797363	98.313	439431	98.245
2	35.935	614392	1.687	7850	1.755



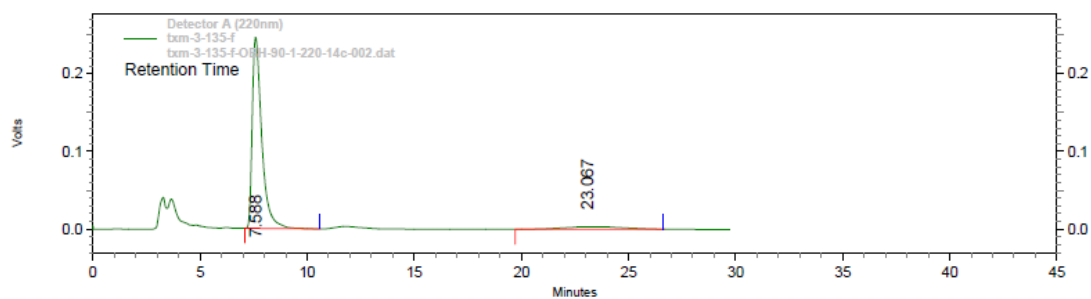
Racemate:



Detector A (220nm)

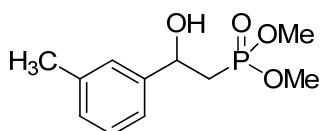
Pk #	Retention Time	Area	Area %	Height	Height %
1	7.676	4231695	49.578	160780	87.901
2	23.273	4303687	50.422	22131	12.099

Table 3, entry 6

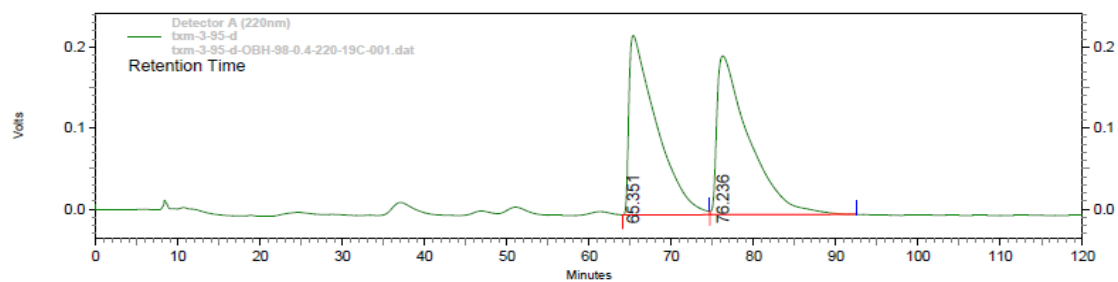


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	7.588	7627016	92.267	245788	98.694
2	23.067	639197	7.733	3253	1.306

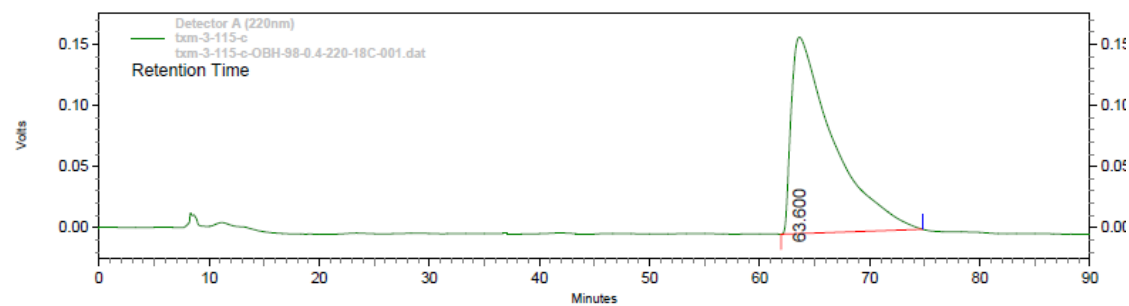


Racemate:

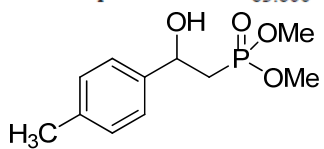


Detector A (220nm)					
PK #	Retention Time	Area	Area %	Height	Height %
1	65.351	51245165	49.124	221083	53.065
2	76.236	53072277	50.876	195548	46.935

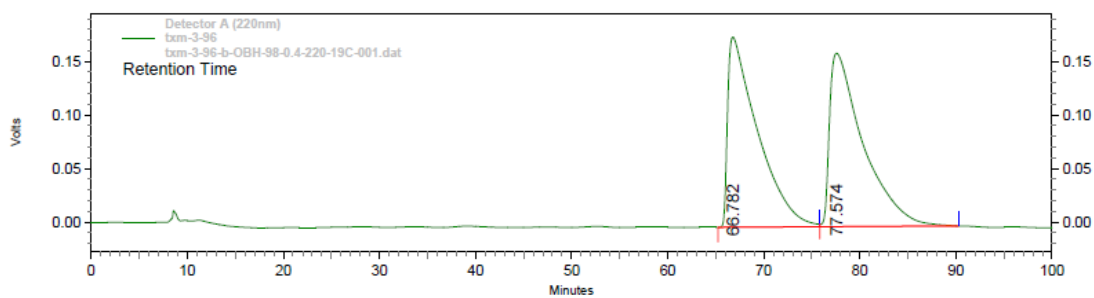
Table 3, entry 7



Detector A (220nm)					
PK #	Retention Time	Area	Area %	Height	Height %
1	63.600	42724601	100.000	160825	100.000

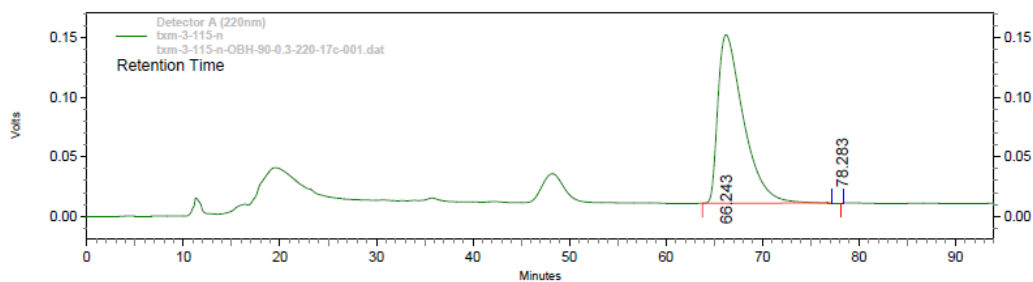


Racemate:

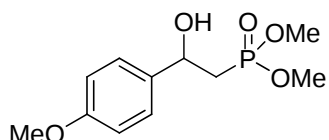


Detector A (220nm)					
PK #	Retention Time	Area	Area %	Height	Height %
1	66.782	38481972	49.468	177708	52.308
2	77.574	39309066	50.532	162024	47.692

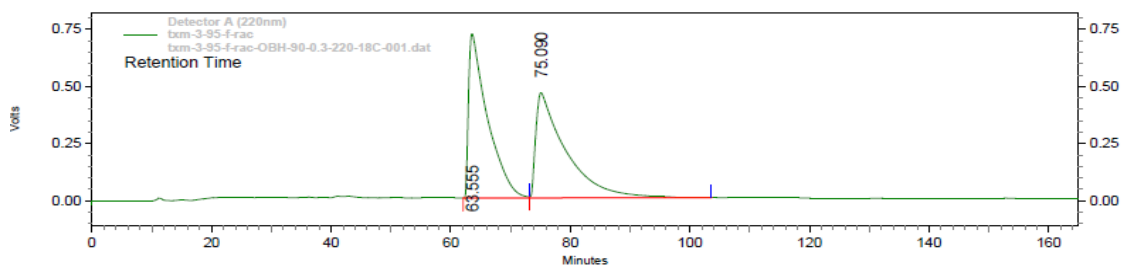
Table 3, entry 8



Detector A (220nm)					
PK #	Retention Time	Area	Area %	Height	Height %
1	66.243	25994107	100.000	141534	99.997
2	78.283	43	0.000	4	0.003



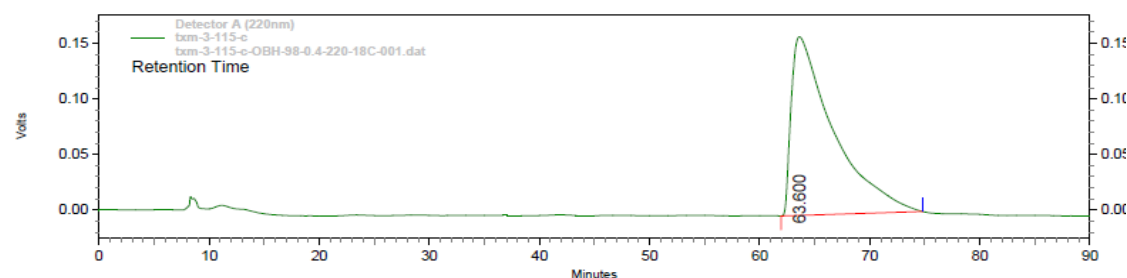
Racemate:



Detector A (220nm)

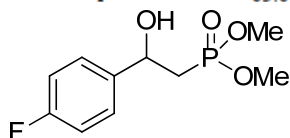
Pk #	Retention Time	Area	Area %	Height	Height %
1	63.555	157610118	49.619	718595	60.960
2	75.090	160031841	50.381	460198	39.040

Table 3, entry 9

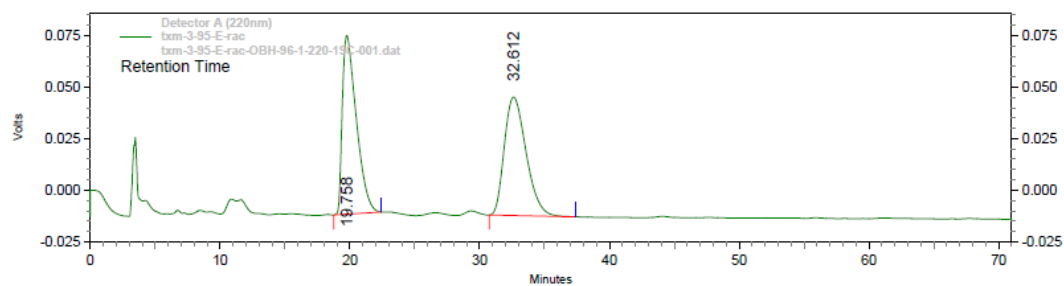


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	63.600	42724601	100.000	160825	100.000



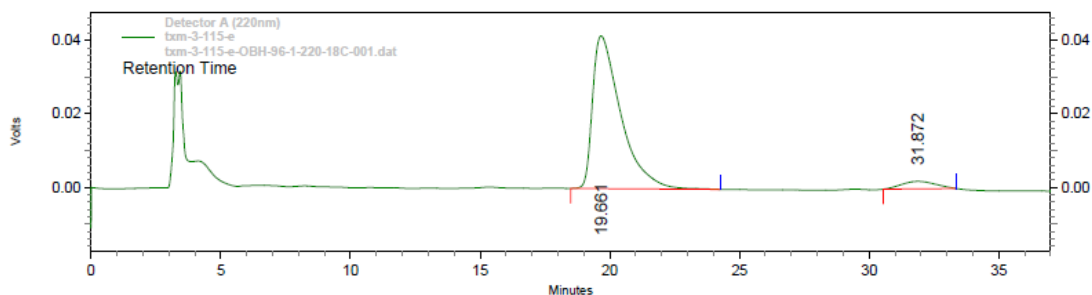
Racemate:



Detector A (220nm)

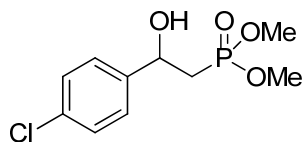
Pk #	Retention Time	Area	Area %	Height	Height %
1	19.758	6480193	49.138	86716	60.128
2	32.612	6707642	50.862	57504	39.872

Table 3, entry 10

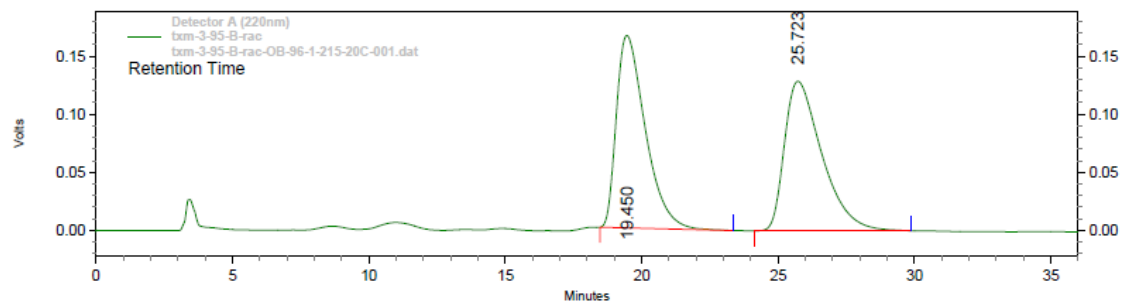


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.661	3138615	94.372	41538	95.293
2	31.872	187191	5.628	2052	4.707



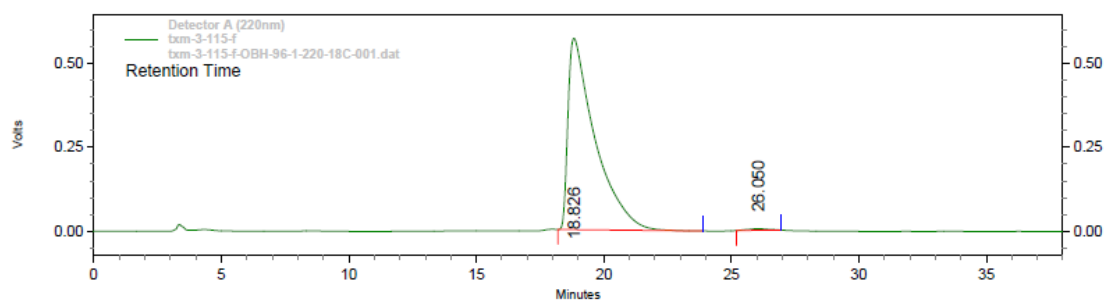
Racemate:



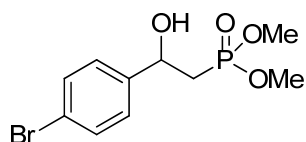
Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.450	12213419	49.812	165575	56.254
2	25.723	12305610	50.188	128760	43.746

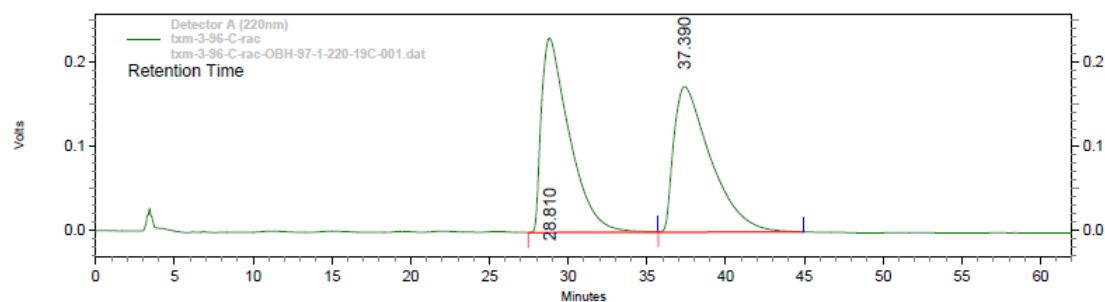
Table 3, entry 11



Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	18.826	42020081	99.361	570416	99.249
2	26.050	270351	0.639	4316	0.751

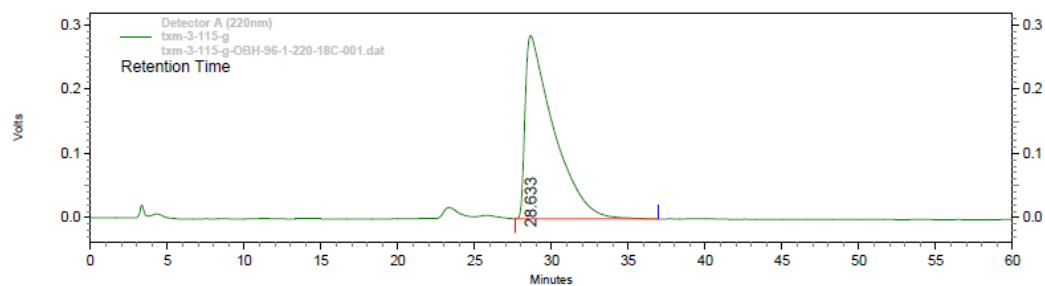


Racemate:



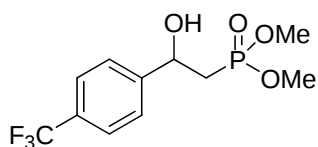
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	28.810	28569716	50.284	231151	57.194
2	37.390	28247487	49.716	173005	42.806

Table 3, entry 12

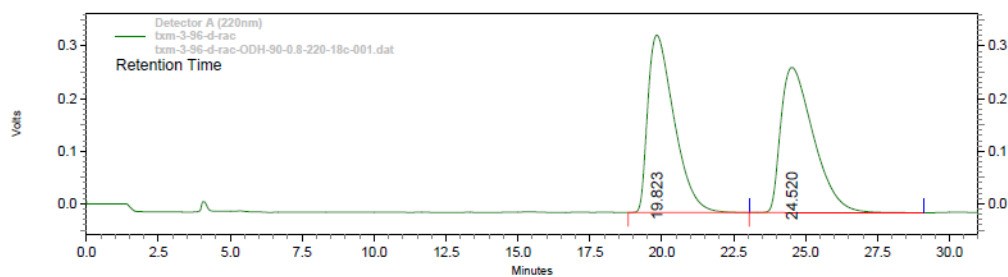


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	28.633	36672934	100.000	285071	100.000



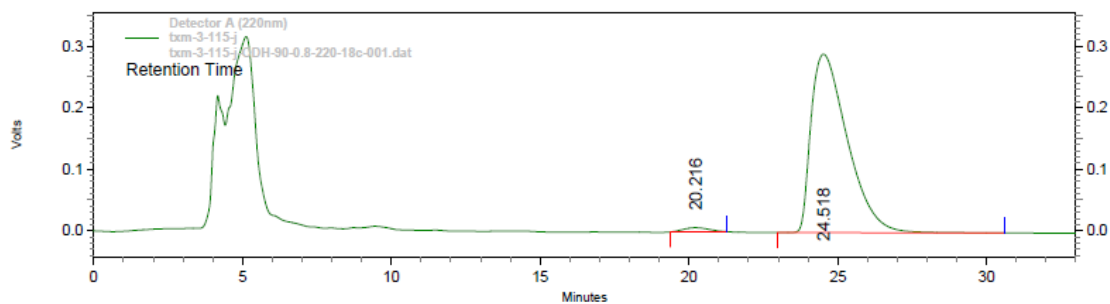
Racemate:



Detector A (220nm)

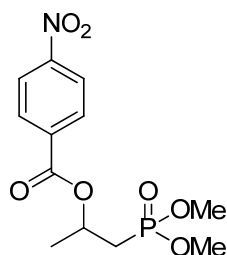
Pk #	Retention Time	Area	Area %	Height	Height %
1	19.823	21432834	49.629	336783	54.977
2	24.520	21753073	50.371	275805	45.023

Table 3, entry 13

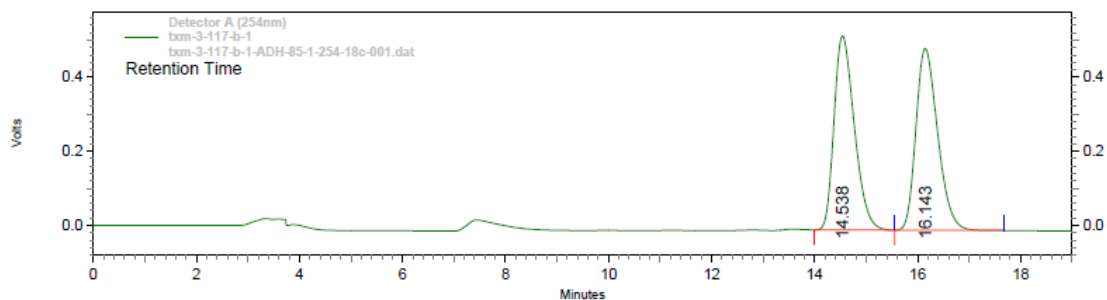


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	20.216	408432	1.634	6711	2.264
2	24.518	24593958	98.366	289688	97.736

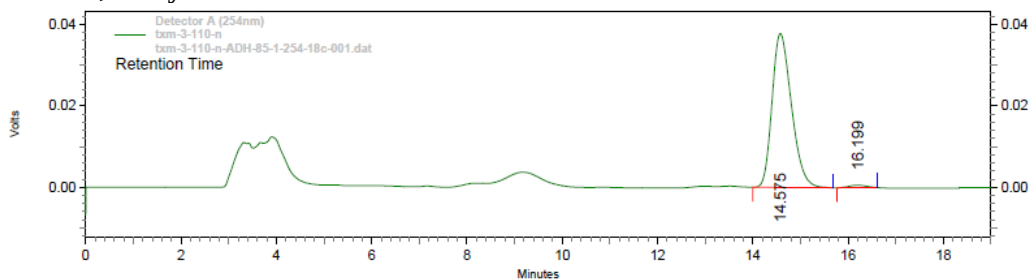


Racemate:

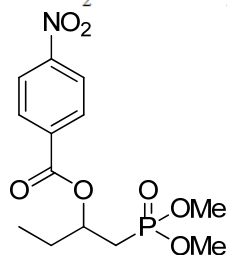


Detector A (254nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	14.538	14346465	49.918	524236	51.666
2	16.143	14393447	50.082	490431	48.334

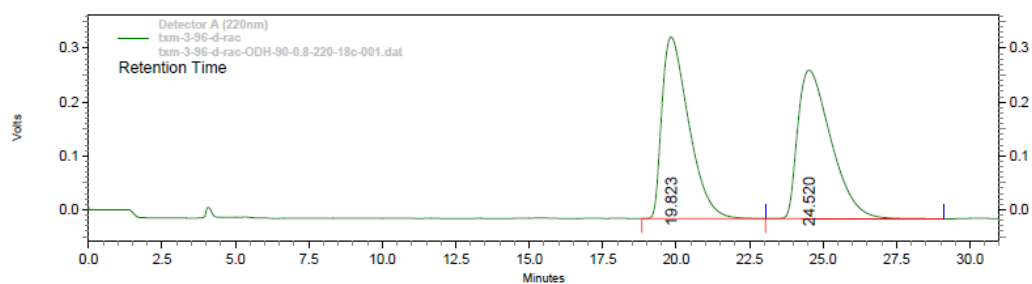
Table 3, entry 14



Detector A (254nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	14.575	1068718	98.623	37795	98.456
2	16.199	14925	1.377	593	1.544

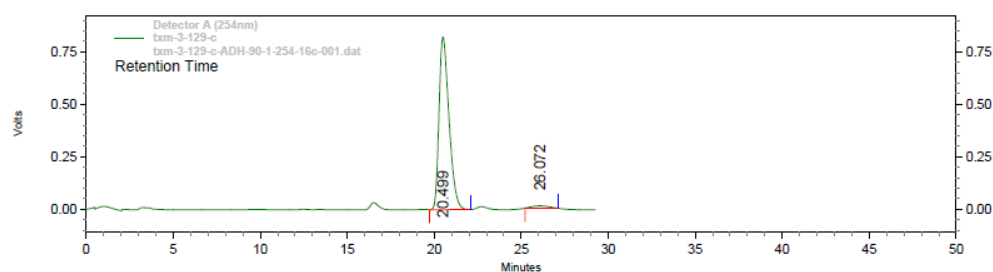


Racemate:

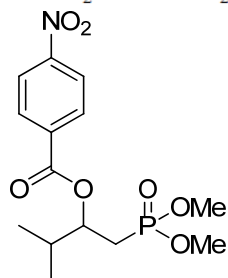


Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	19.823	21432834	49.629	336783	54.977
2	24.520	21753073	50.371	275805	45.023

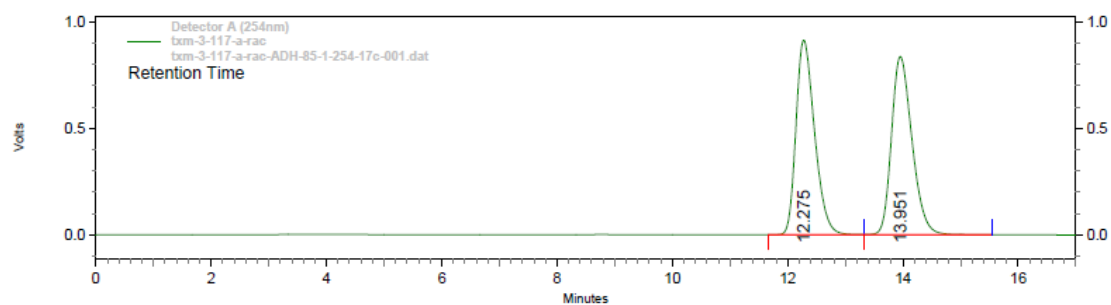
Table 3, entry 15



Detector A (254nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	20.499	32756835	97.651	823145	98.640
2	26.072	787950	2.349	11350	1.360

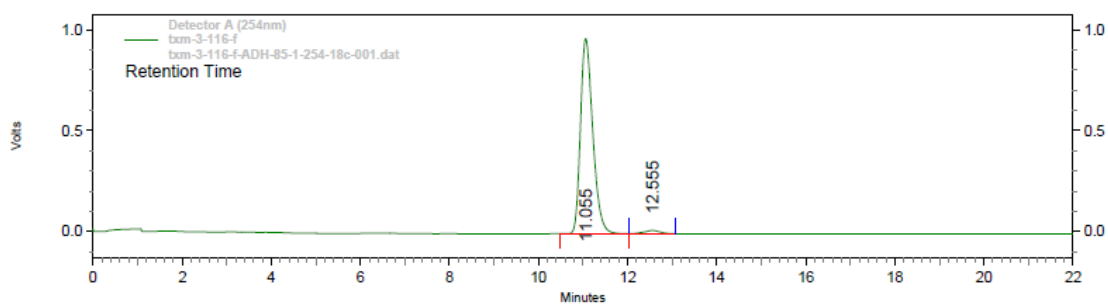


Racemate:

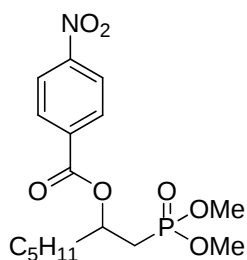


Detector A (254nm)						
Pk #	Retention Time	Area	Area %	Height	Height %	
1	12.275	20435180	49.705	912644	52.192	
2	13.951	20677799	50.295	835984	47.808	

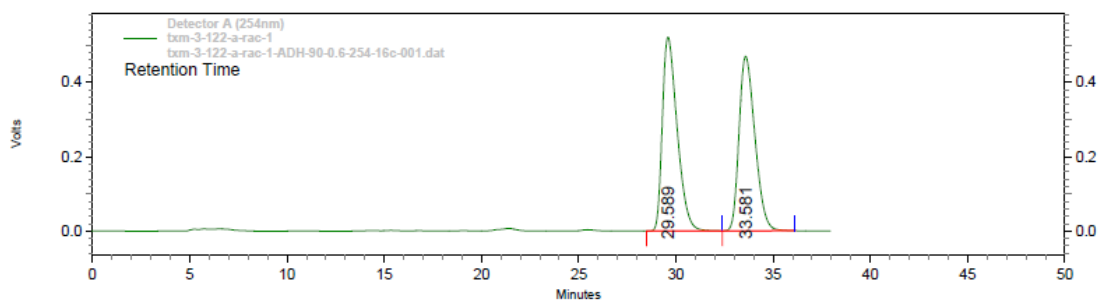
Table 3, entry 16



Detector A (254nm)						
Pk #	Retention Time	Area	Area %	Height	Height %	
1	11.055	18546256	97.862	968114	98.352	
2	12.555	405178	2.138	16217	1.648	



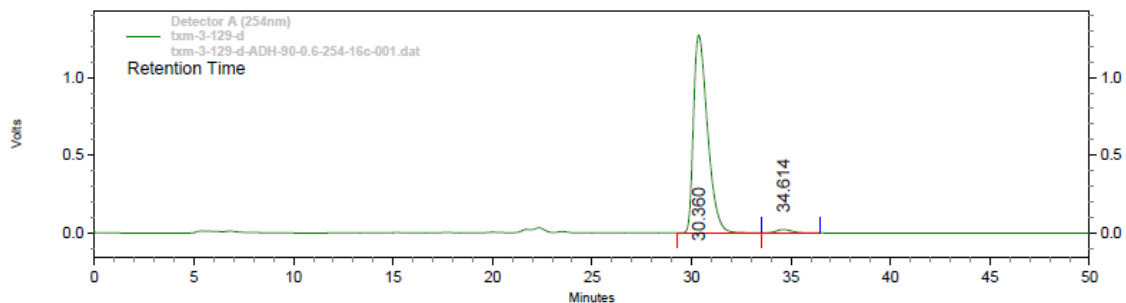
Racemate:



Detector A (254nm)

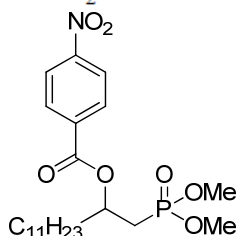
Pk #	Retention Time	Area	Area %	Height	Height %
1	29.589	27639090	50.860	521785	52.627
2	33.581	26704875	49.140	469694	47.373

Table 3, entry 17

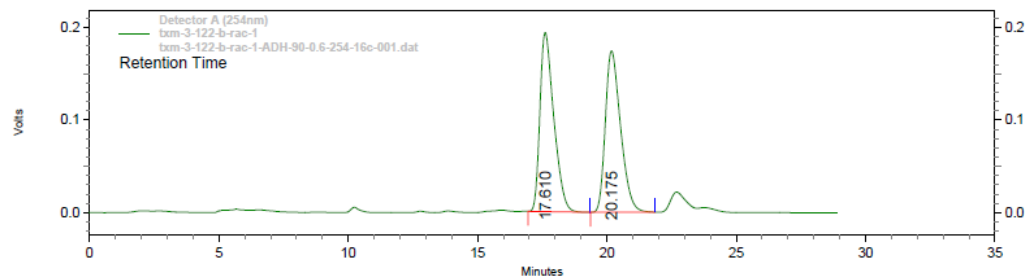


Detector A (254nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	30.360	62535197	98.160	1273961	98.321
2	34.614	1172523	1.840	21760	1.679



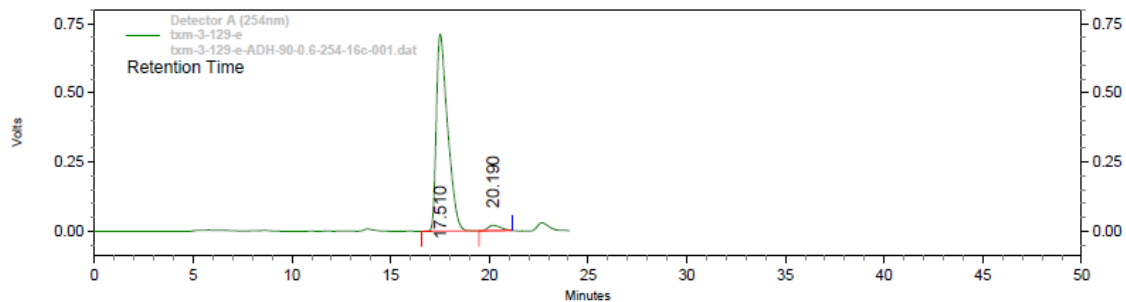
Racemate:



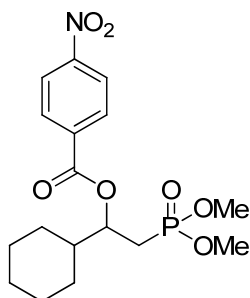
Detector A (254nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	17.610	7203316	50.194	193259	52.591
2	20.175	7147573	49.806	174217	47.409

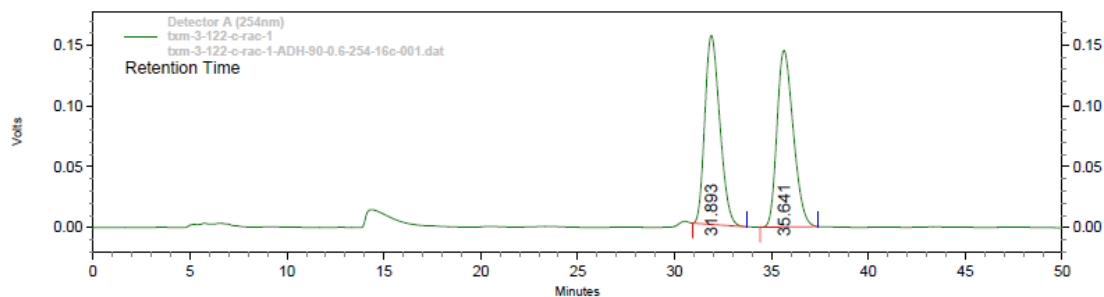
Table 3, entry 18



Detector A (254nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.510	28317381	97.003	712075	97.315
2	20.190	874796	2.997	19645	2.685

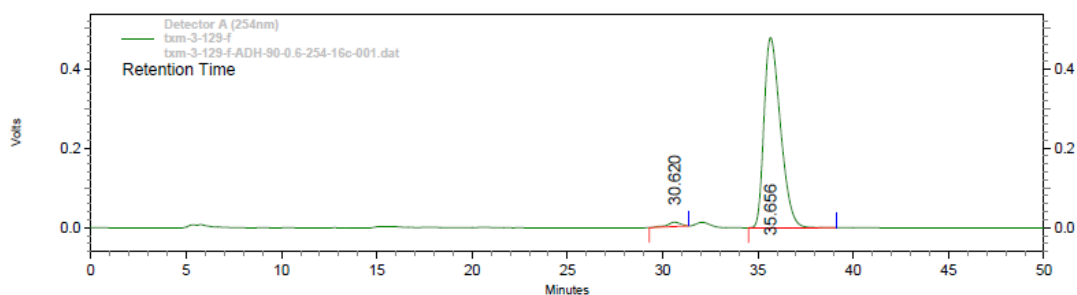


Racemate:



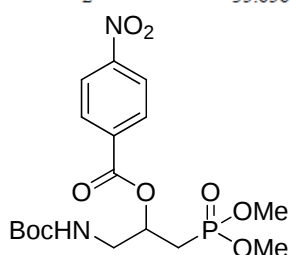
Detector A (254nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	31.893	8330788	49.477	155535	51.696
2	35.641	8506841	50.523	145329	48.304

Table 3, entry 19

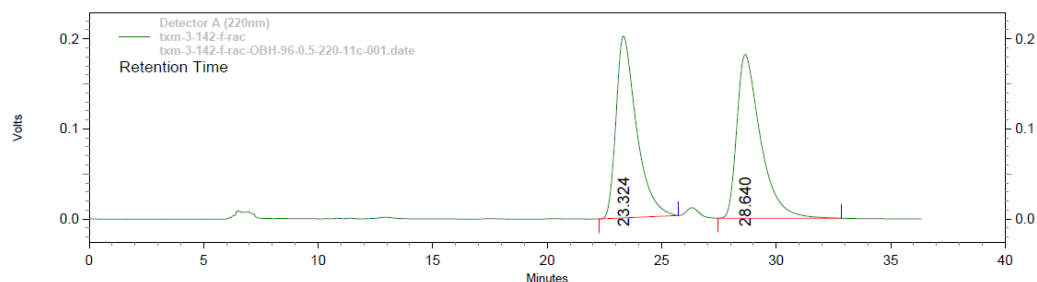


Detector A (254nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	30.620	529732	1.812	10975	2.243
2	35.656	28703496	98.188	478269	97.757



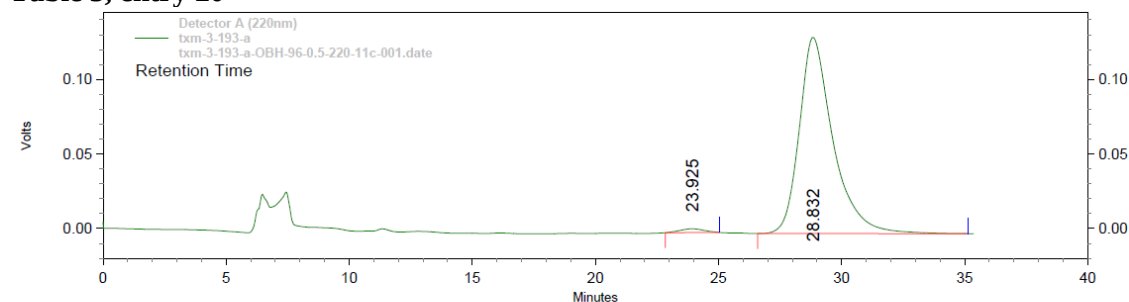
Racemate:



Detector A (220nm)

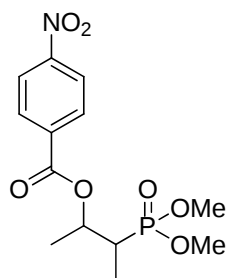
Pk #	Retention Time	Area	Area %	Height	Height %
1	23.324	12555573	49.070	201839	52.625
2	28.640	13031736	50.930	181706	47.375

Table 3, entry 20

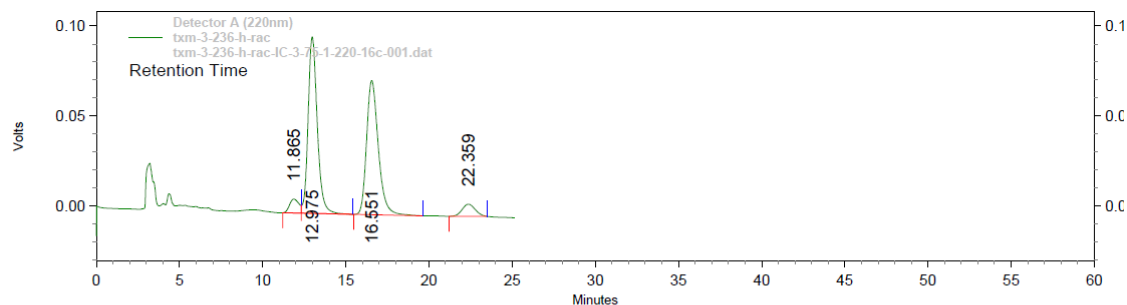


Detector A (220nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	23.925	169050	1.329	2511	1.871
2	28.832	12550897	98.671	131675	98.129



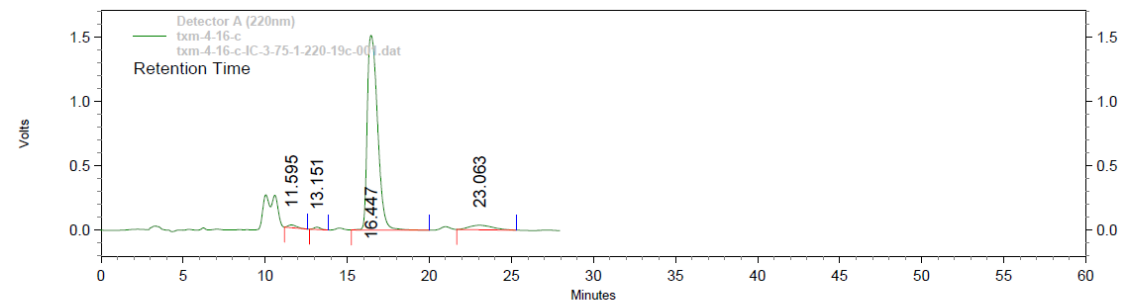
Racemate:



Detector A (220nm)

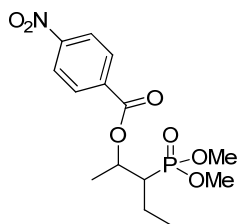
PK #	Retention Time	Area	Area %	Height	Height %
1	11.865	302501	3.735	7725	4.131
2	12.975	3757726	46.400	98047	52.433
3	16.551	3667322	45.284	74467	39.823
4	22.359	371031	4.581	6755	3.612

Table 3, entry 21

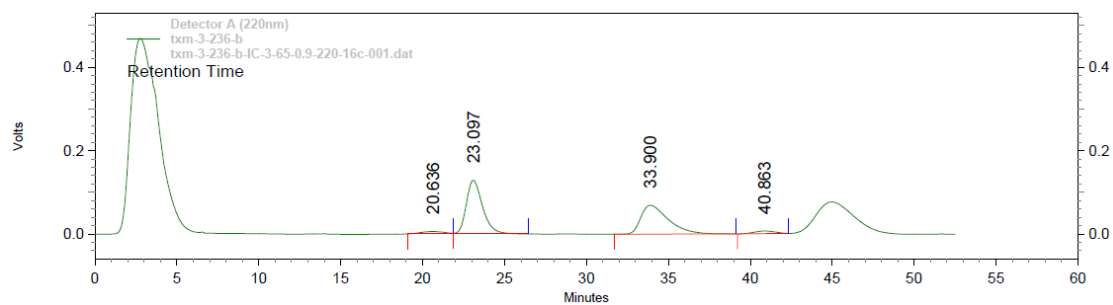


Detector A (220nm)

PK #	Retention Time	Area	Area %	Height	Height %
1	11.595	776707	1.093	21780	1.370
2	13.151	495075	0.697	17841	1.123
3	16.447	66292640	93.302	1514570	95.303
4	23.063	3487050	4.908	35025	2.204



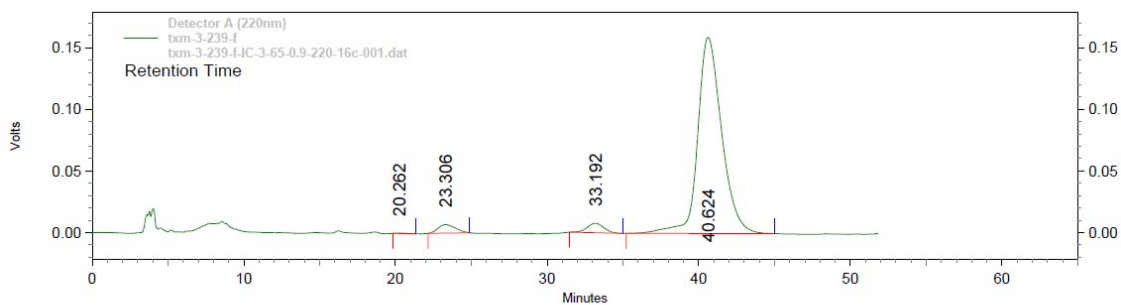
Racemate:



Detector A (220nm)

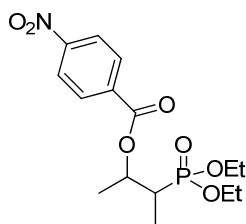
PK #	Retention Time	Area	Area %	Height	Height %
1	20.636	554953	3.070	5690	2.716
2	23.097	8884594	49.144	128446	61.312
3	33.900	8095422	44.779	69138	33.002
4	40.863	543655	3.007	6223	2.970

Table 3, entry 22

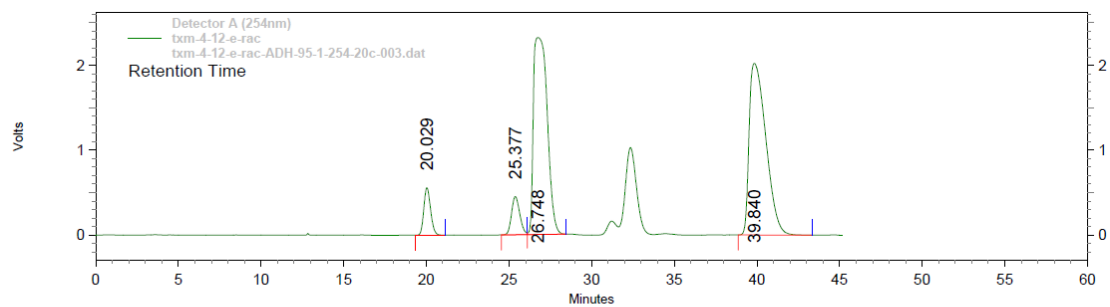


Detector A (220nm)

PK #	Retention Time	Area	Area %	Height	Height %
1	20.262	16077	0.086	316	0.182
2	23.306	546734	2.925	6901	3.964
3	33.192	593075	3.173	7659	4.399
4	40.624	17538092	93.817	159217	91.455



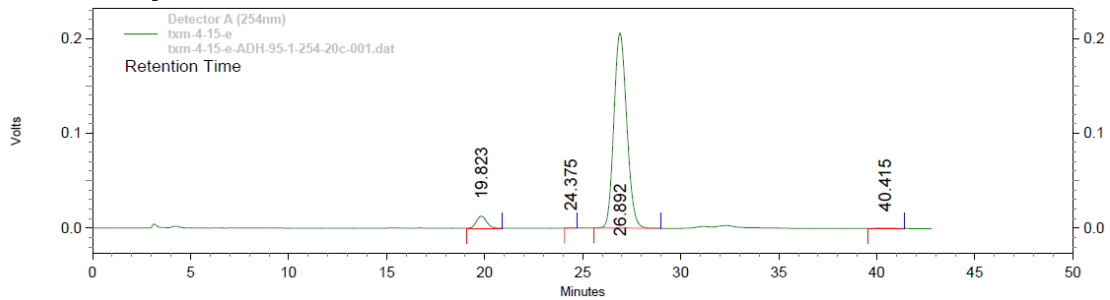
Racemate:



Detector A (254nm)

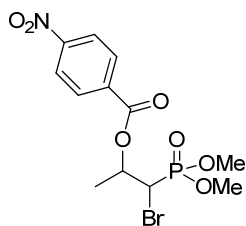
Pk #	Retention Time	Area	Area %	Height	Height %
1	20.029	15885242	5.158	557992	10.445
2	25.377	15491499	5.030	448445	8.394
3	26.748	134688167	43.733	2317387	43.378
4	39.840	141915336	46.079	2018437	37.782

Table 3, entry 23

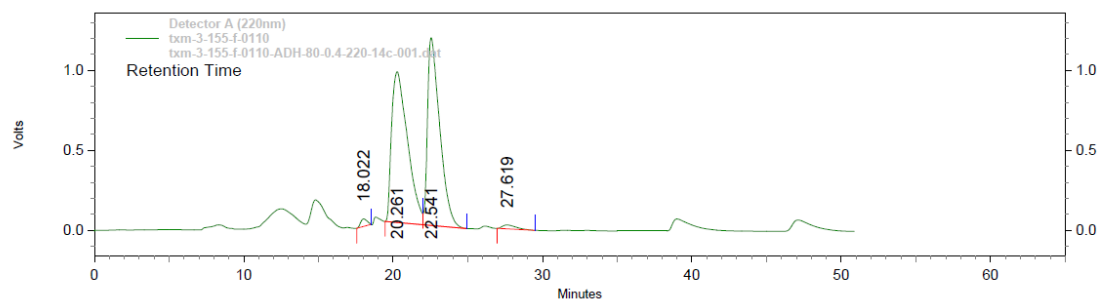


Detector A (254nm)

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.823	453909	4.609	12597	5.761
2	24.375	1528	0.016	61	0.028
3	26.892	9368897	95.130	205572	94.009
4	40.415	24139	0.245	444	0.203

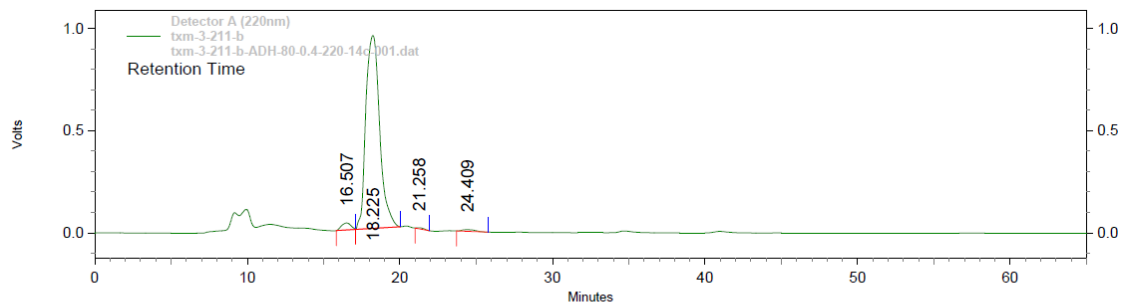


Racemate:



Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	18.022	1423973	1.016	47134	2.152
2	20.261	70109064	50.046	943189	43.066
3	22.541	67000562	47.827	1175195	53.660
4	27.619	1555464	1.110	24559	1.121

Table 3, entry 24

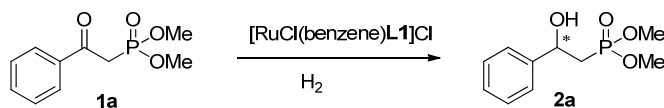


Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	16.507	1457461	2.370	34014	3.436
2	18.225	59358921	96.539	942701	95.228
3	21.258	171056	0.278	4673	0.472
4	24.409	499654	0.813	8556	0.864

Table 4. Optimization of Temperature and Time

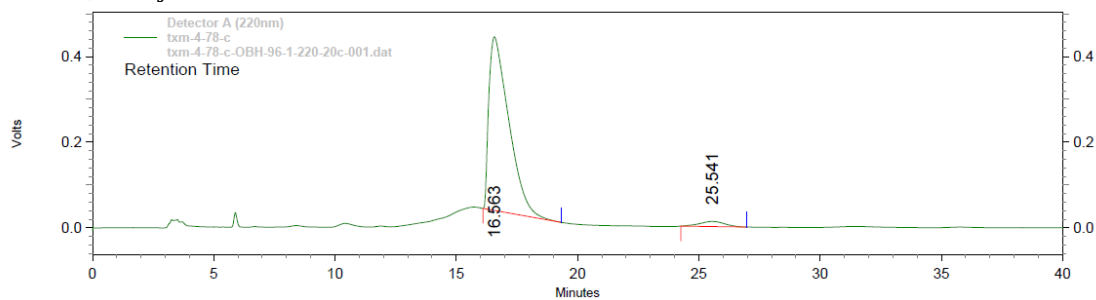
entry	T (°C)	t (h)	con (%)	yield (2m:2u)	ee (%)	dr
1	50	4	80	92:8	99.6	96:4
2	50	10	95	89:11	99.5	95:5
3	50	19	99	87:13	99.7	96:4
4	70	4	90	85:15	99.3	95:5
5	30	38	96	90:10	97.0	95:5

All reactions were carried out with **1u** (1 mmol) concentration of 0.5 M in MeOH under 10 atm of H₂, S/C = 200/1. Ee and dr values were determined by HPLC.

Table 5. Optimization of Time ^a

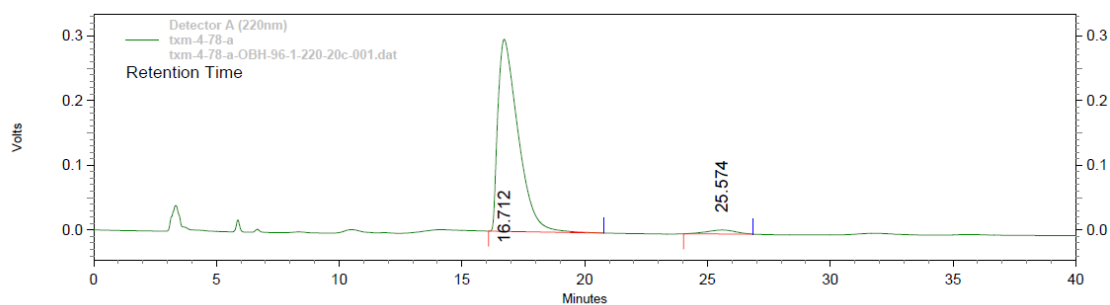
entry	time (h)	con (%) ^b	ee (%) ^c
1	3	20	92.9
2	8	85	94.3
3	13	>99	99.7
4	19	>99	99.5

^a All reactions were carried out with a substrate (1 mmol) concentration of 0.5 M in MeOH under 10 bar of H₂ at 50 °C, S/C = 200:1. ^b Conversion were determined by NMR. ^c Ee values were determined by HPLC on a Chiralpak OB-H column.

Table 5, entry 1

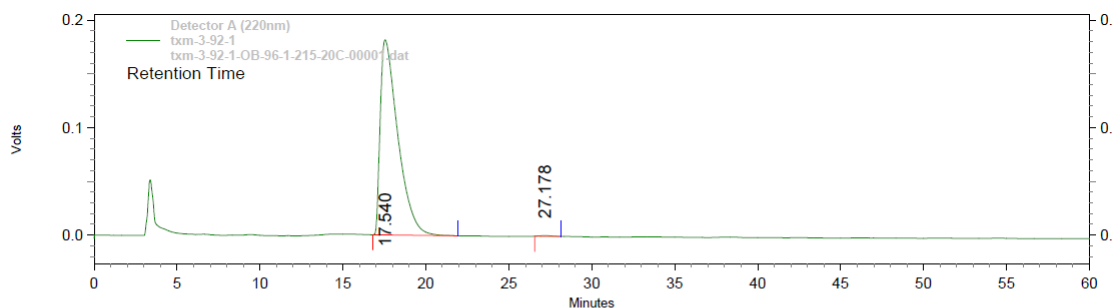
Detector A (220nm)					
PK #	Retention Time	Area	Area %	Height	Height %
1	16.563	23224121	96.429	405369	97.134
2	25.541	860006	3.571	11960	2.866

Table 5, entry 2



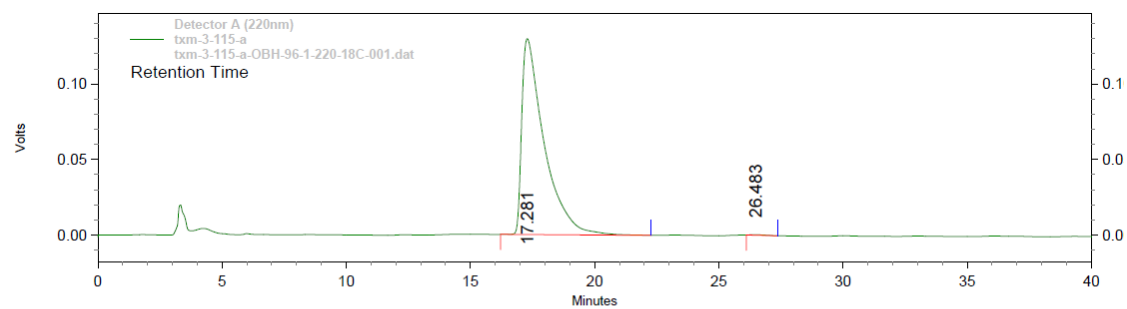
Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	16.712	16978086	97.146	296917	97.988
2	25.574	498747	2.854	6098	2.012

Table 5, entry 3



Detector A (220nm)					
Pk #	Retention Time	Area	Area %	Height	Height %
1	17.540	13403798	99.792	181662	99.692
2	27.178	27910	0.208	561	0.308

Table 5, entry 4



Detector A (220nm)						
Pk #	Retention Time	Area	Area %	Height	Height %	
1	17.281	8112186	99.871	129737	99.817	
2	26.483	10508	0.129	238	0.183	