

Supporting information

Ru(II)-*p*-cymene complexes containing ester of chiral D/L-phenylalanine derived aroylthiourea ligands for enantioselective reduction of pro-chiral ketones

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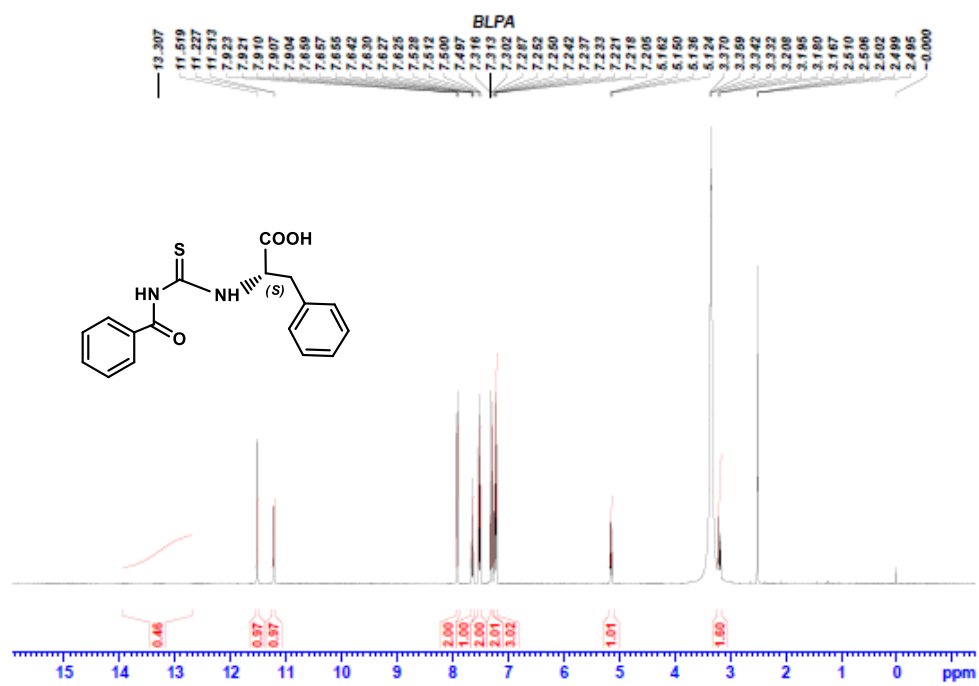
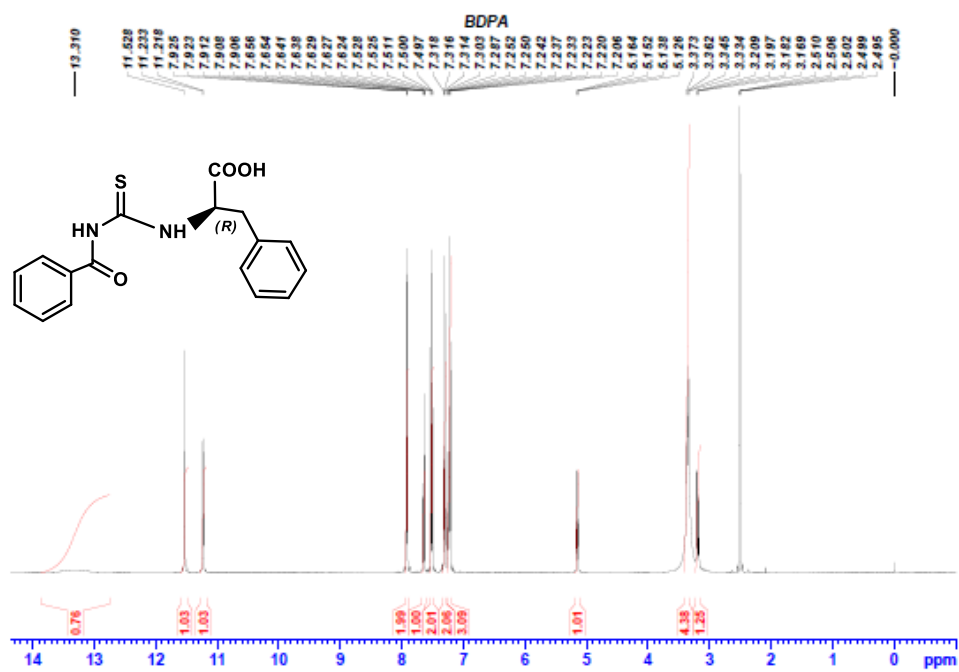
^c Department of Chemistry, Texas A & M University, College Station, TX 77842, USA

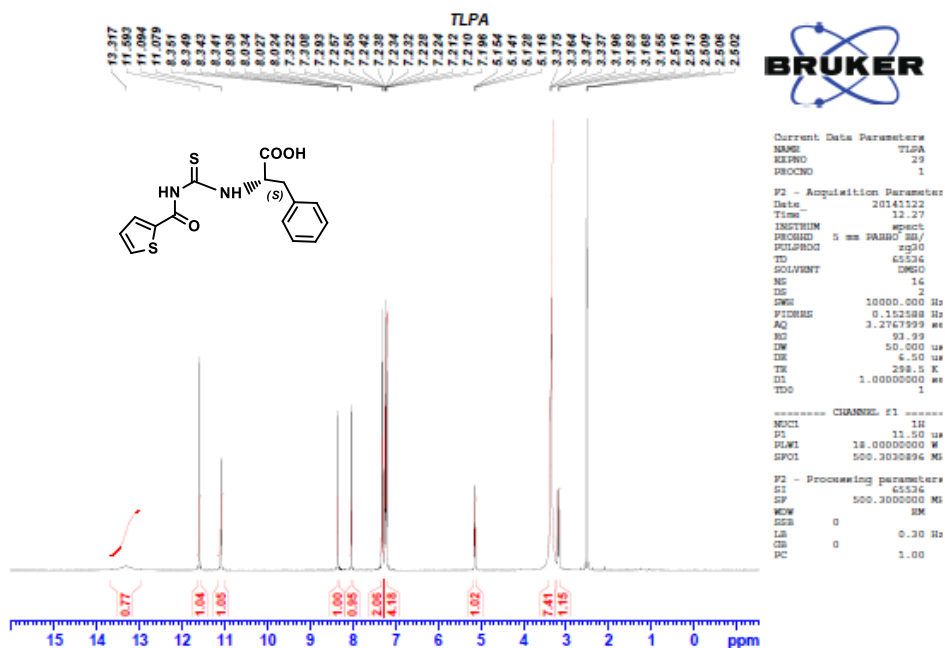
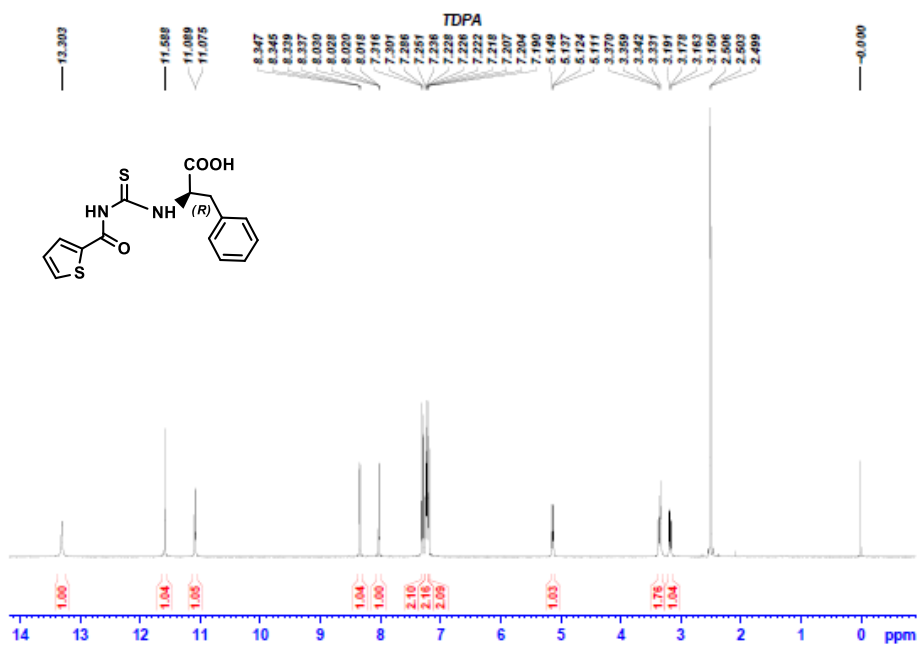
Supporting Information Table S1. Experimental details for the x-ray diffraction studies.

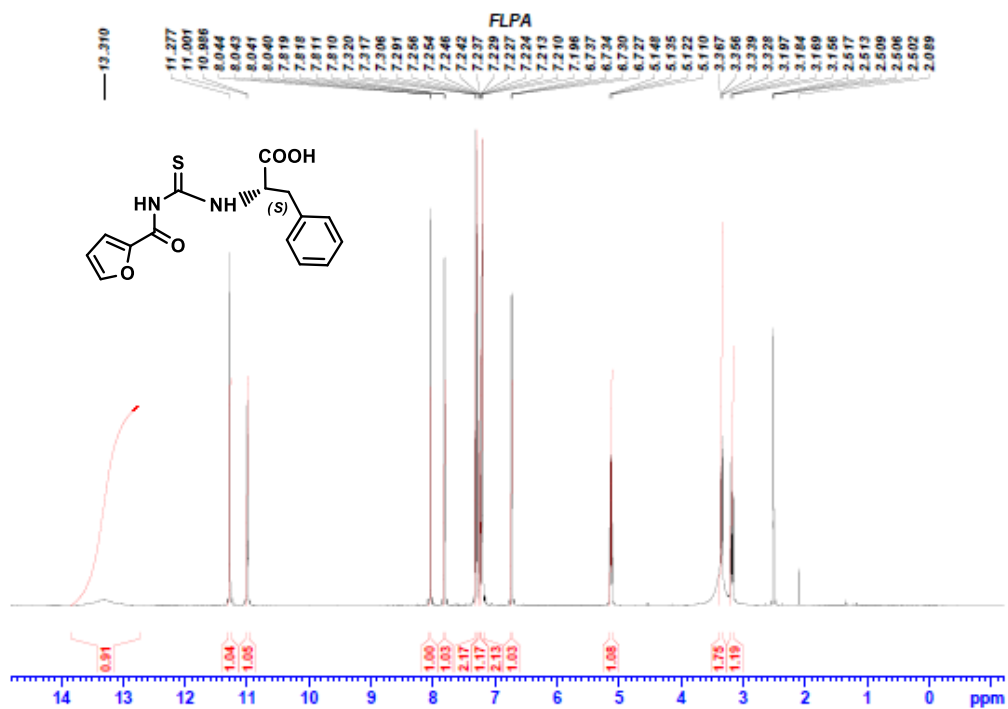
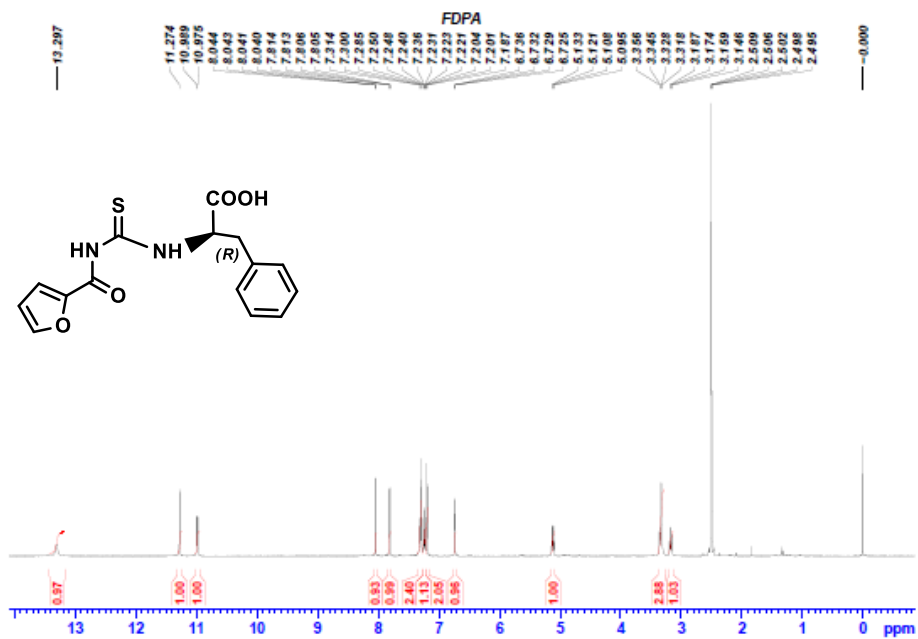
	L1	3	6
Identification code	L1	3	6
Empirical formula	C ₁₇ H ₁₆ N ₂ O ₃ S	C ₂₆ H ₃₀ Cl ₂ N ₂ O ₃ Ru S ₂	C ₂₆ H ₃₀ Cl ₂ N ₂ O ₄ Ru S
Formula weight	328.38	654.61	638.55
Temperature	110.0 K	150.15 K	150.15 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 11.9242(6) Å b = 26.5717(13) Å c = 5.0373(3) Å	a = 11.408(3) Å b = 13.270(5) Å c = 18.477(4) Å	a = 11.398(2) Å b = 13.064(3) Å c = 18.578(4) Å
Volume	1596.05(15) Å ³	2797.3(14) Å ³	2766.2(10) Å ³
Z	4	4	4
Density (calculated)	1.367 Mg/m ³	1.554 Mg/m ³	1.533 Mg/m ³
Absorption coefficient	0.219 mm ⁻¹	0.932 mm ⁻¹	0.870 mm ⁻¹
F(000)	688	1336	1304
Crystal size	0.442 x 0.13 x 0.078 mm ³	0.59 x 0.26 x 0.24 mm ³	0.38 x 0.22 x 0.2 mm ³
Theta range for data collection	2.295 to 27.472°.	1.889 to 27.554°.	1.906 to 27.492°.
Index ranges	-15<=h<=15, -34<=k<=34, -6<=l<=6	-14<=h<=14, -17<=k<=16, -23<=l<=23	-14<=h<=14, -16<=k<=16, -24<=l<=23
Reflections collected	33565	32747	32418
Independent reflections	3659 [R(int) = 0.0760]	6363 [R(int) = 0.0389]	6329 [R(int) = 0.0369]
Completeness to theta = 25.242°	99.9 %	99.7 %	100.0 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7436 and 0.6681	0.7456 and 0.6172	0.7456 and 0.6628
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	3659 / 0 / 209	6363 / 0 / 329	6329 / 0 / 329
Goodness-of-fit on F ²	1.104	1.051	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.1084	R1 = 0.0240, wR2 = 0.0579	R1 = 0.0273, wR2 = 0.0711
R indices (all data)	R1 = 0.0751, wR2 = 0.1138	R1 = 0.0263, wR2 = 0.0593	R1 = 0.0296, wR2 = 0.0727
Absolute structure parameter	0.03(3)	-0.002(12)	-0.003(13)
Extinction coefficient	n/a	n/a	n/a
Largest diff. peak and hole	0.480 and -0.365 e.Å ⁻³	0.743 and -0.420 e.Å ⁻³	1.124 and -0.484 e.Å ⁻³

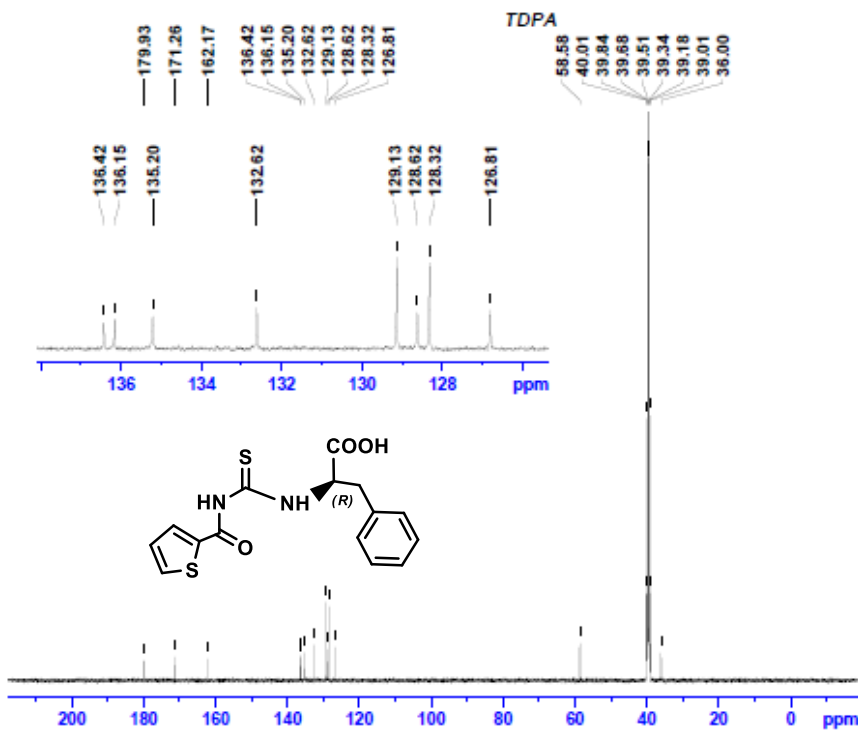
CCDC for L1 is 1474599 and complexes **3** and **6** is 1458027-1458028.

¹H NMR of ligands









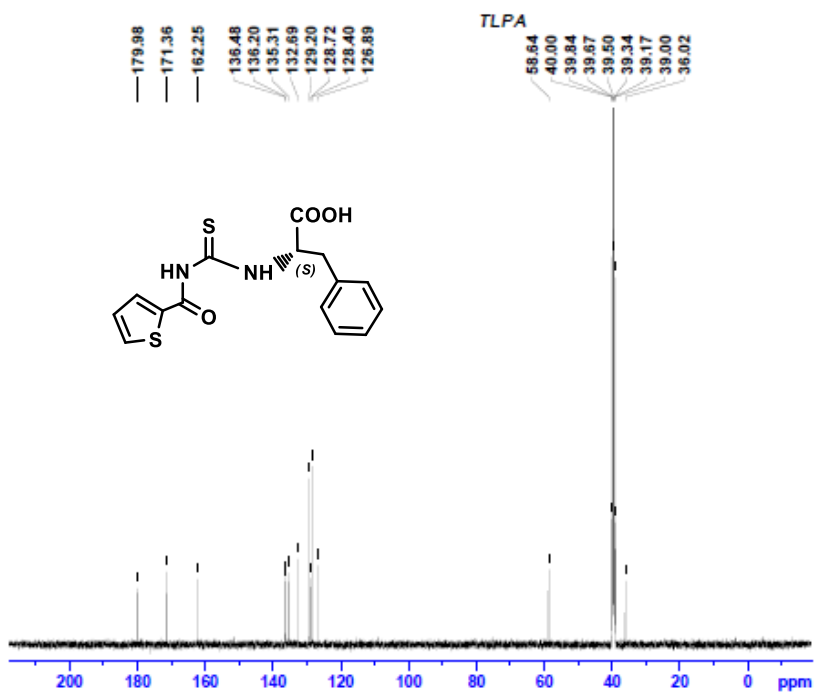
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 KEPRNO 9
 PROCNO 1

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 INSTRUM spect
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 PULPROG zgpg30
 TD 2336
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 186.93
 DW 16.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUCL 13C
 P1 9.73 usec
 PLW1 76.00000000 W
 SFO1 125.8131145 MS

----- CHANNEL f2 -----
 CPOPRG2 waltz16
 NUCL2 1H
 PCPRG2 80.00 usec
 PLW2 18.00000000 W
 PLW12 0.37195000 W
 PLW13 0.23805000 W
 SFO2 500.3020012 MS

F2 - Processing parameters
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 SF 125.8006023 MS
 KW 8M
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



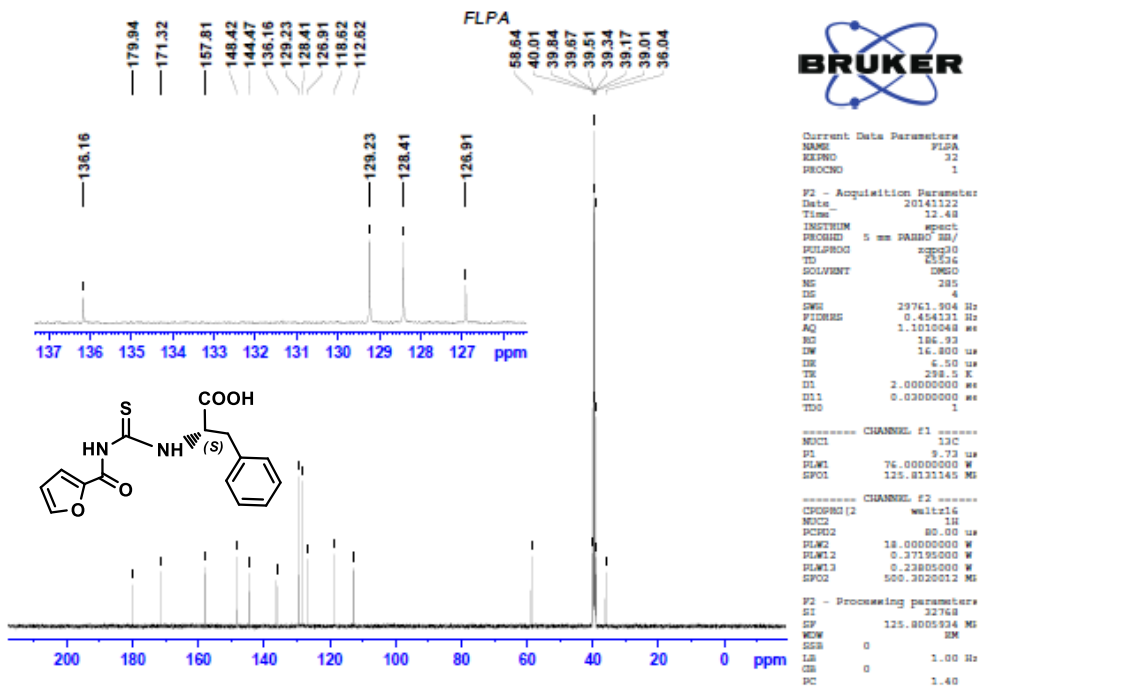
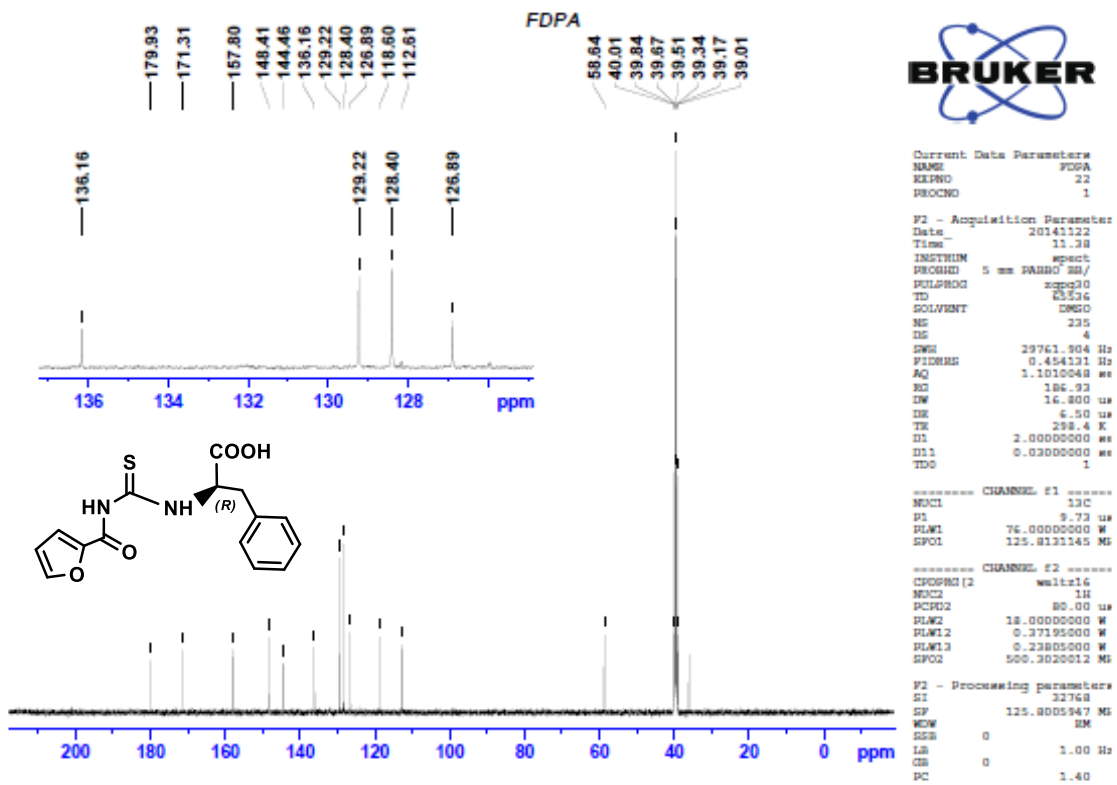
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 SOLVENT DMSO
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 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
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 DW 16.800 usec
 DE 6.50 usec
 TE 298.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

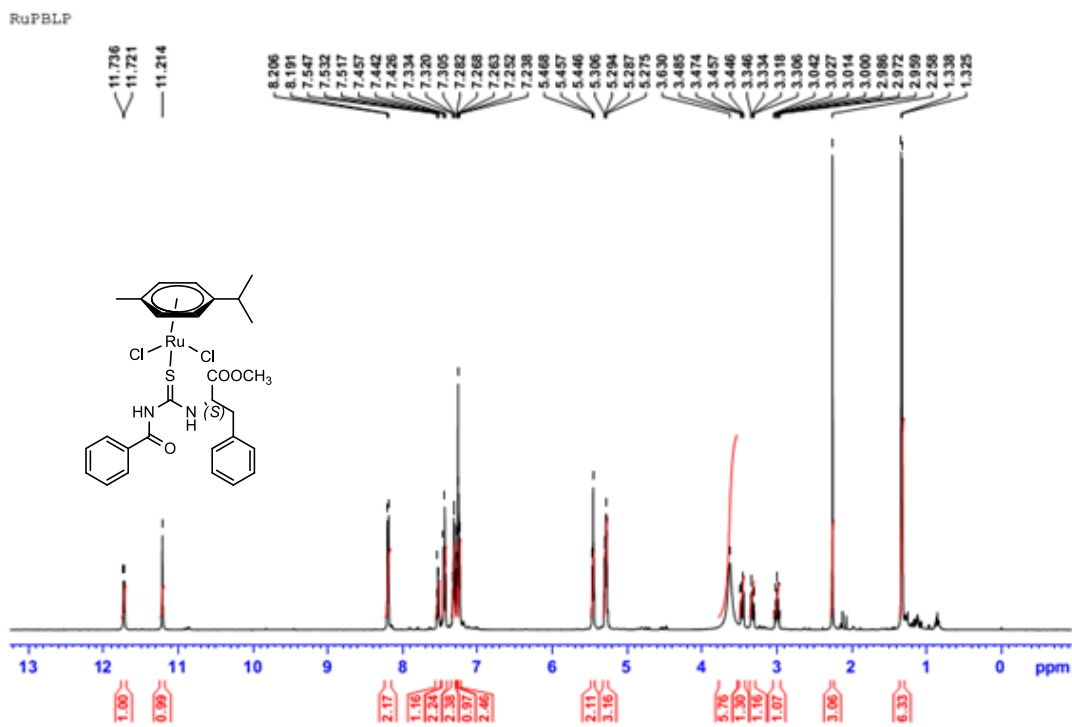
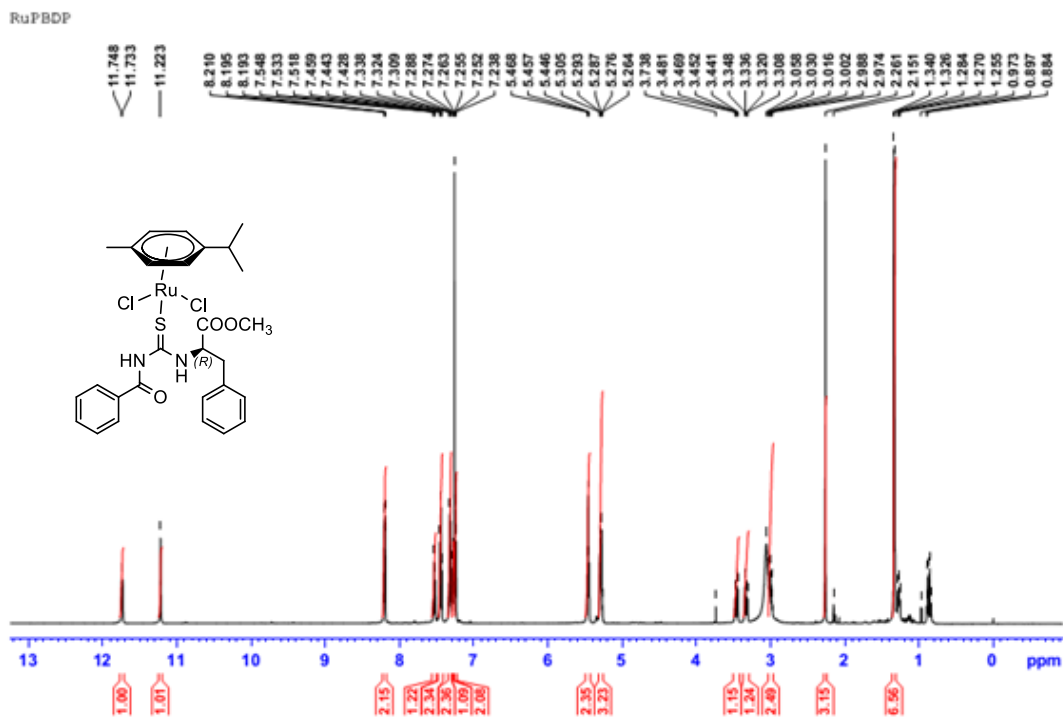
----- CHANNEL f1 -----
 NUCL 13C
 P1 9.73 usec
 PLW1 76.00000000 W
 SFO1 125.8131145 MS

----- CHANNEL f2 -----
 CPOPRG2 waltz16
 NUCL2 1H
 PCPRG2 80.00 usec
 PLW2 18.00000000 W
 PLW12 0.37195000 W
 PLW13 0.23805000 W
 SFO2 500.3020012 MS

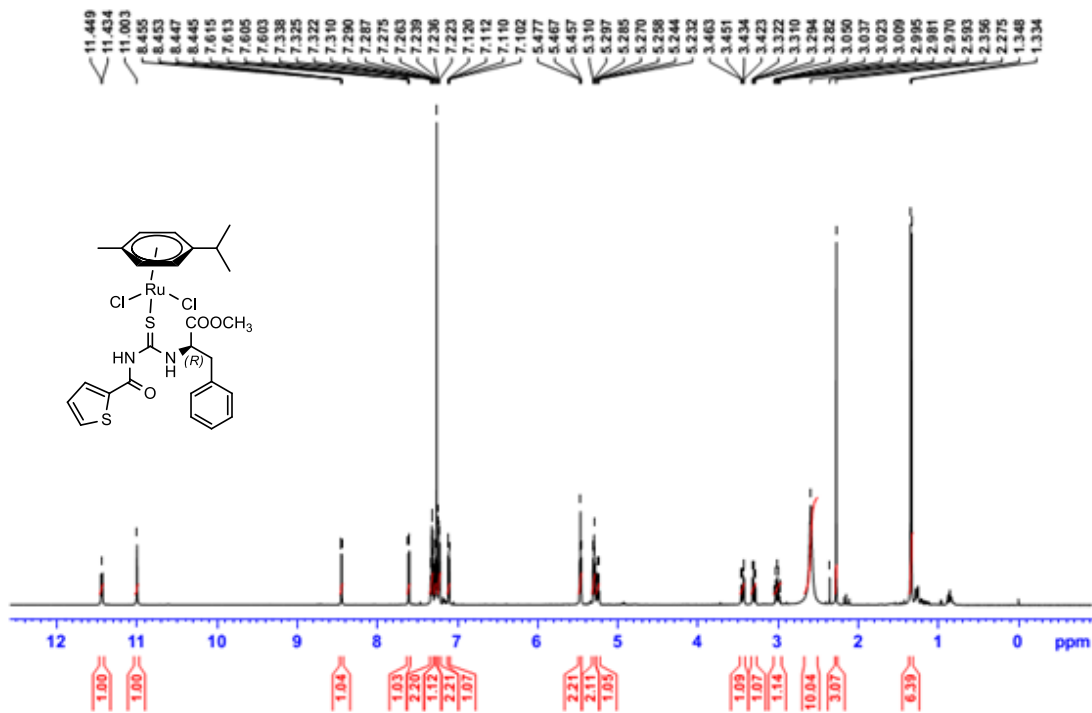
F2 - Processing parameters
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 LB 1.00 Hz
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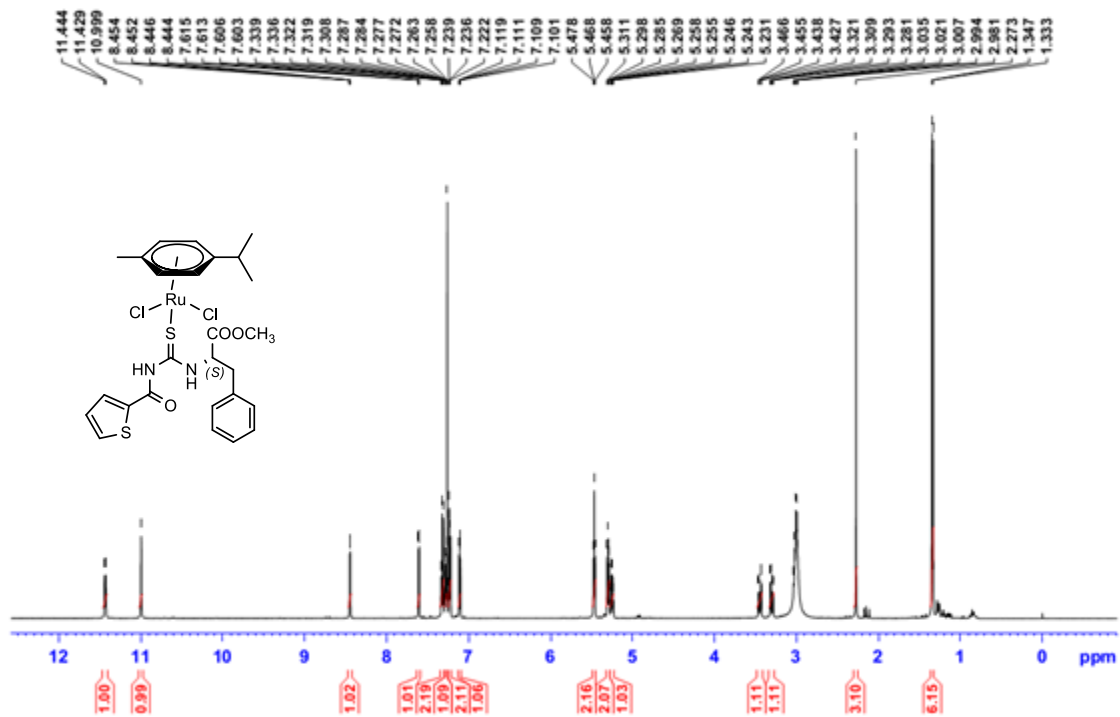
¹H NMR of complexes



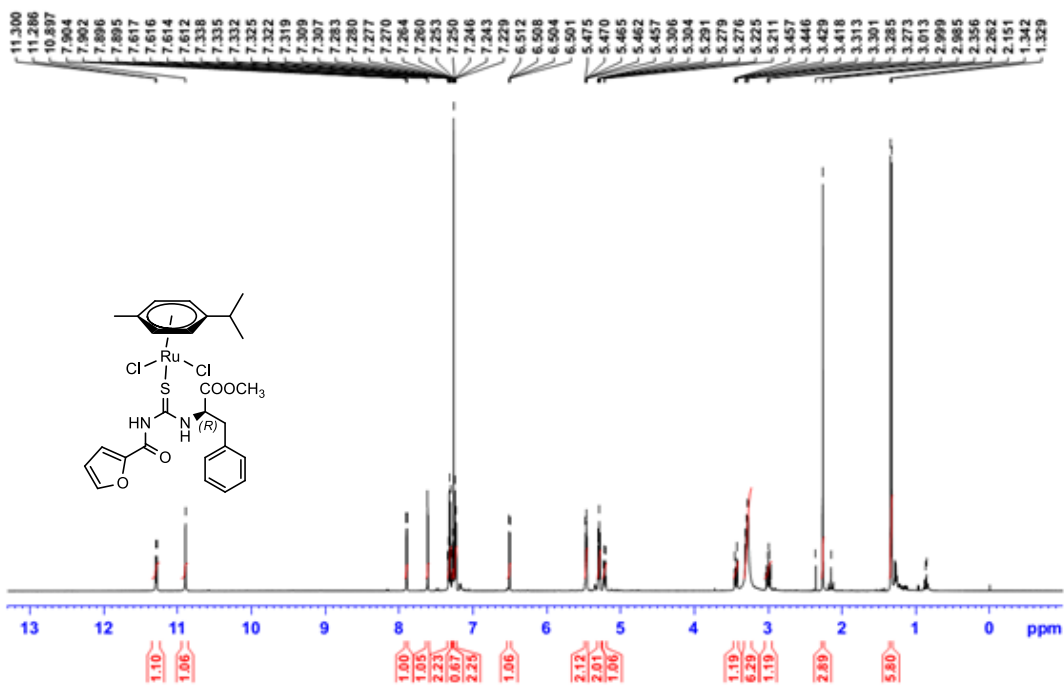
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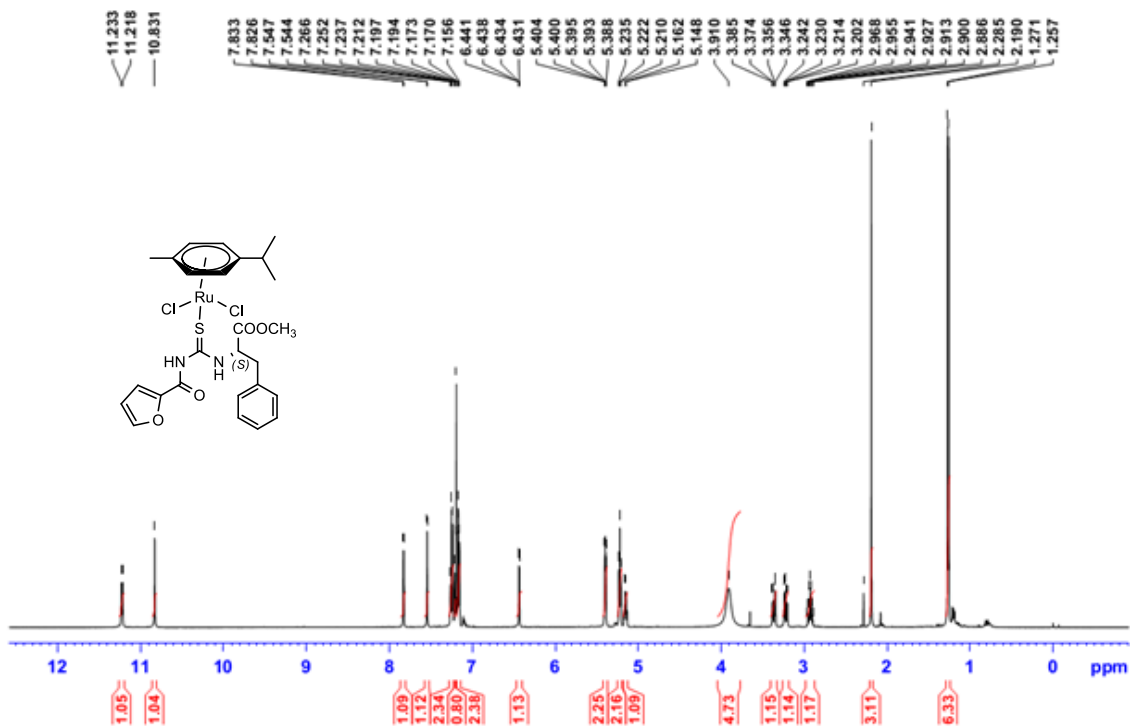
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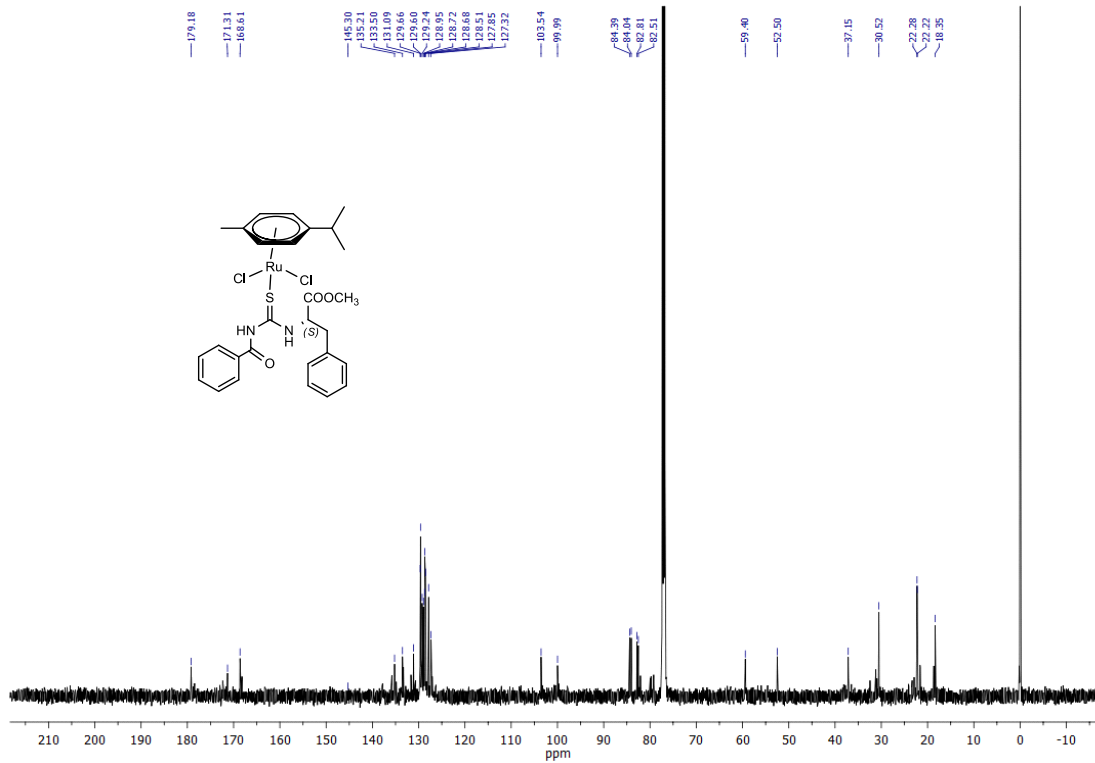
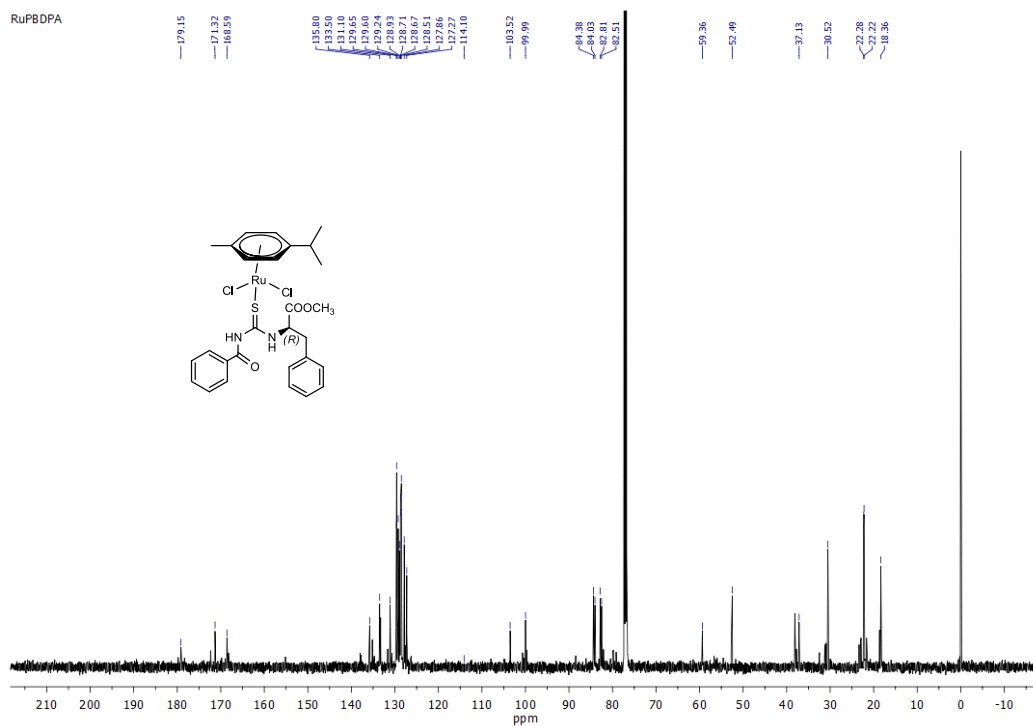
RuPFDP

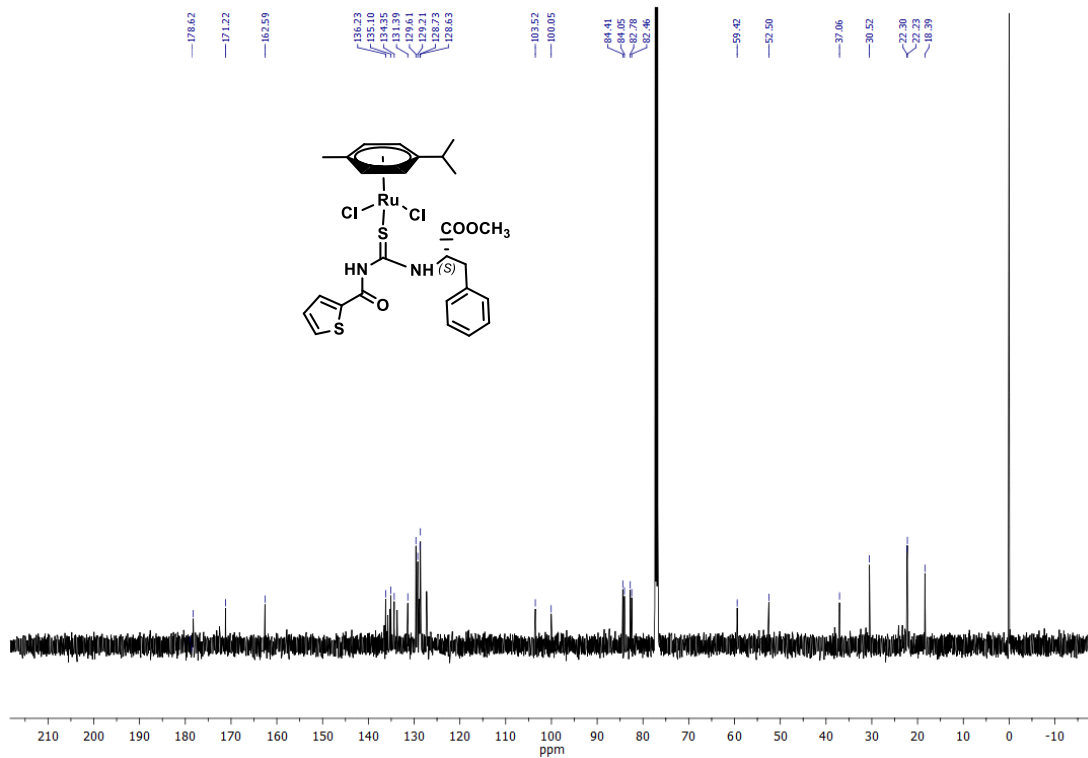
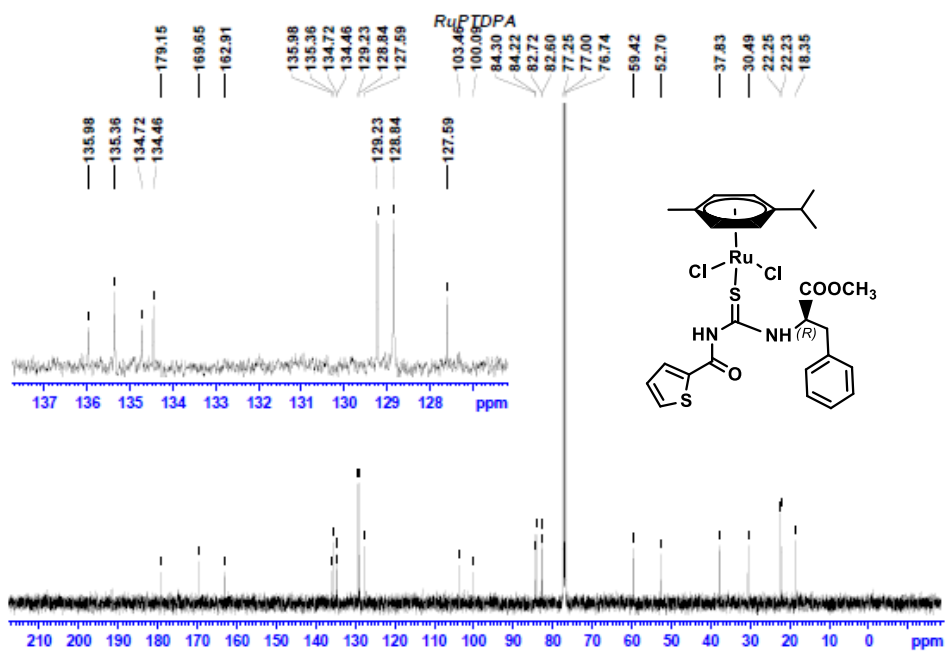


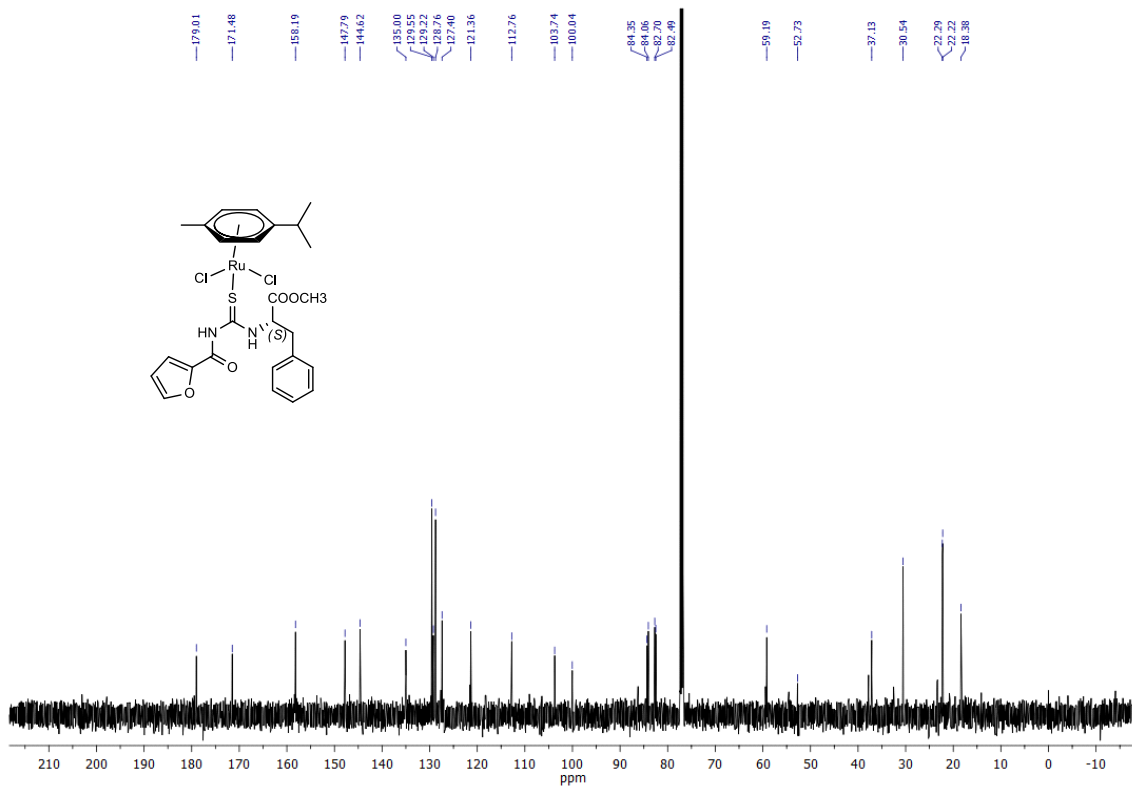
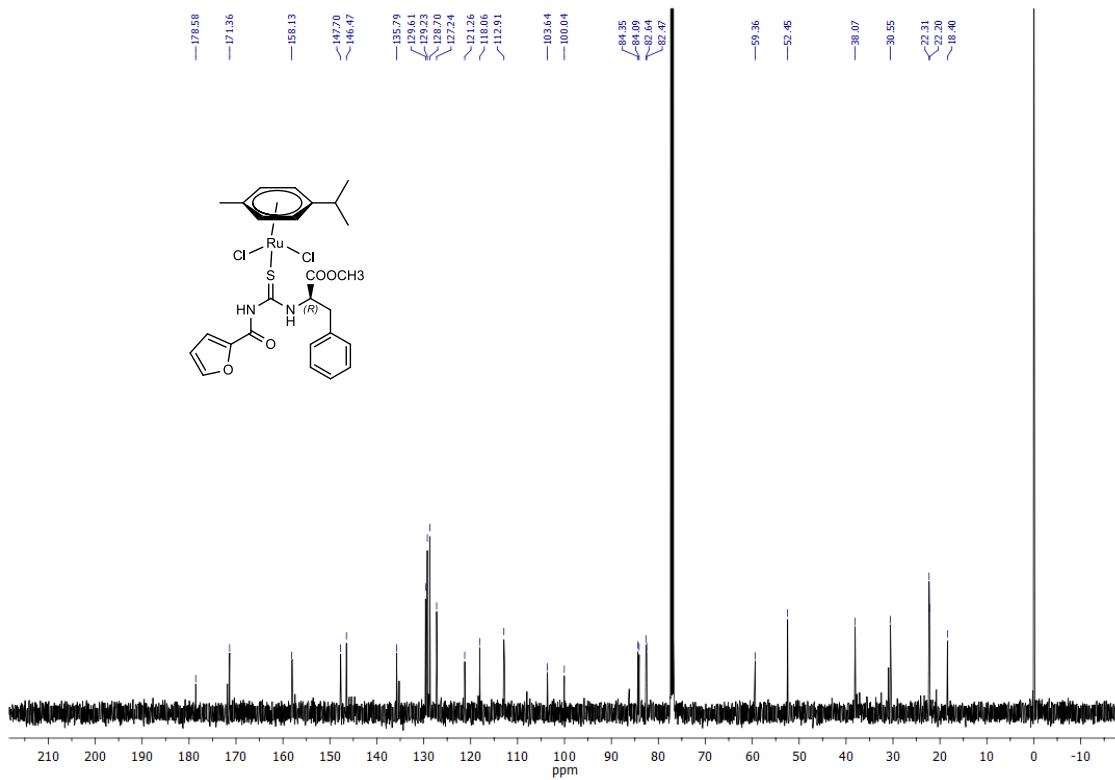
RuPFLP

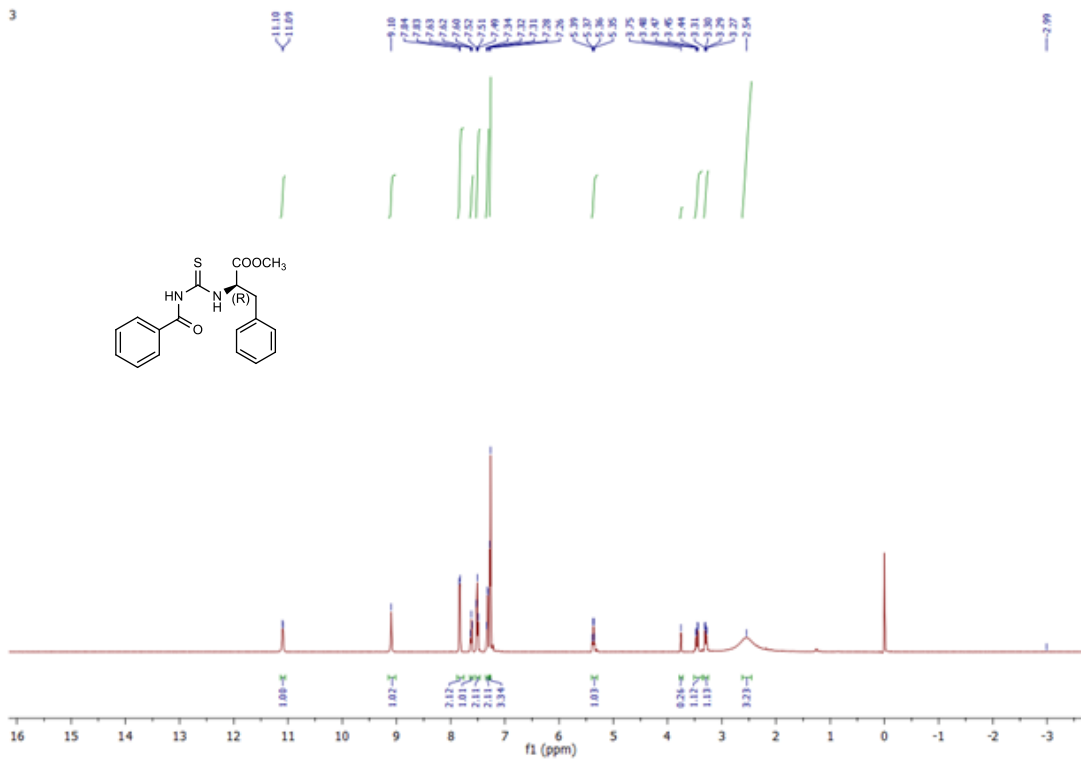


¹³C NMR of complexes



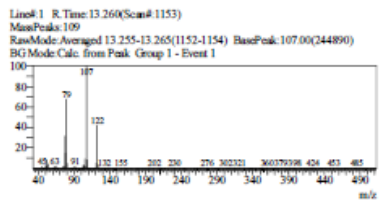
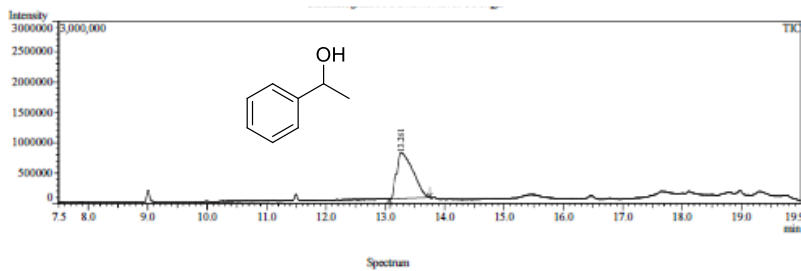






GC-MS data

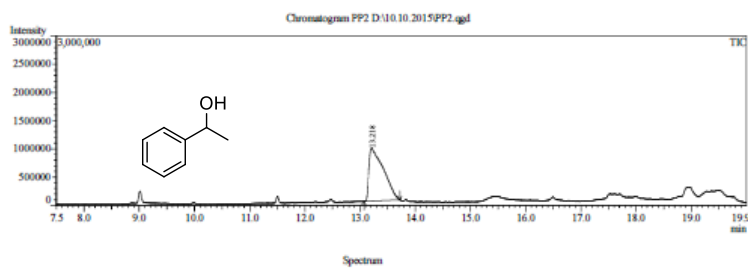
Entry 1



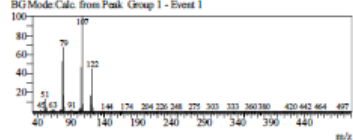
Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	13.261	14384928	100.00	Benzenemethanol, alpha-methyl-
		14384928	100.00	

Entry 2



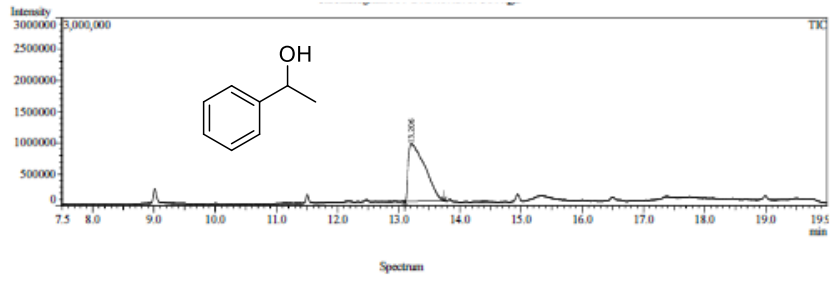
Line# 1 R-Time: 13.220(Scan# 1145)
 MassPeak: 111
 RawMode: Averaged 13.215-13.225(1144-1146) BasePeak: 107.00(250231)
 BG Mode Calc. from Peak Group 1 - Event 1



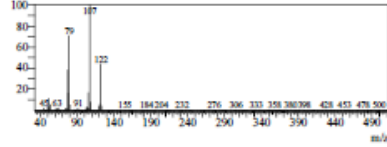
Peak Report TIC

Peak#	R-Time	Area	Area%	Name
1	13.218	1701902.4	100.00	Benzenemethanol, alpha-methyl-
		1701902.4	100.00	

Entry 3

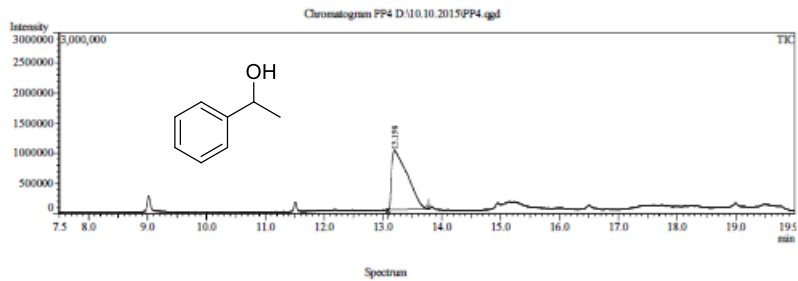


Line# 1 R.Time:13.205(Scan# 1142)
 MassPeak: 109
 RawMode:Averaged 13.200-13.210(1141-1143) BasePeak:107.00(266384)
 BG Mode Calc. from Peak Group 1 - Event 1

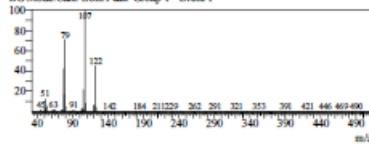


Peak Report TIC				
Peak#	R.Time	Area	Area%	Name
1	13.206	17345758	100.00	Benzenemethanol, alpha-methyl-
		17345758	100.00	

Entry 4

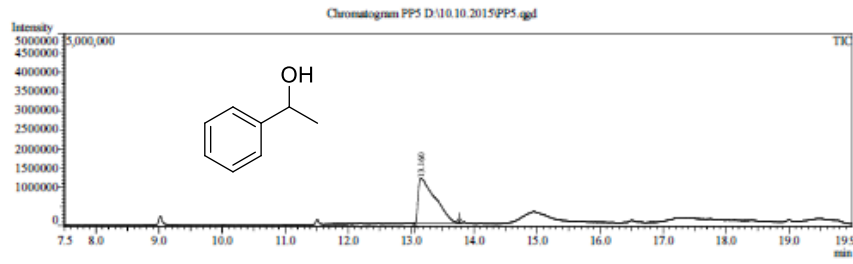


Line# 1 R.Time:13.200(Scan# 1141)
 MassPeak: 110
 RawMode:Averaged 13.195-13.205(1140-1142) BasePeak:107.05(273730)
 BG Mode Calc. from Peak Group 1 - Event 1



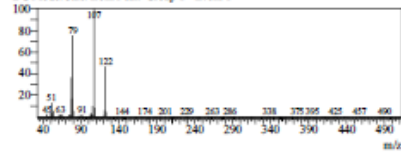
Peak Report TIC				
Peak#	R.Time	Area	Area%	Name
1	13.198	18091355	100.00	Benzenemethanol, alpha-methyl-
		18091355	100.00	

Entry 5



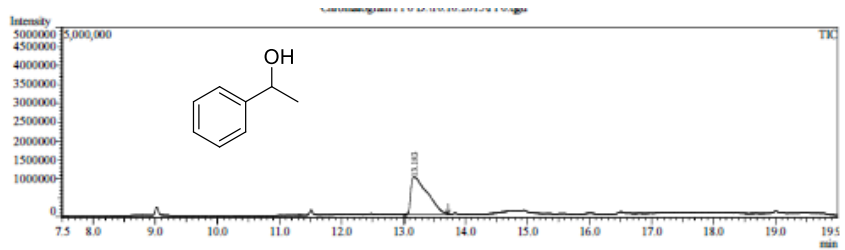
Spectrum

Line# 1 R.Time:13.160(Scan# 1133)
 MassPeaks:99
 RawMode:Averaged 13.155-13.165(1132-1134) BasePeak:107.00(336582)
 BG Mode Calc. from Peak Group 1 - Event 1



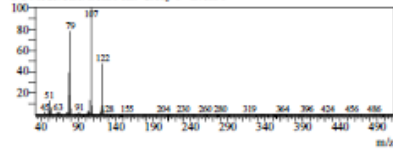
Peak Report TIC				
Peak#	R.Time	Area	Area%	Name
1	13.160	21666493	100.00	Benzenemethanol, alpha-methyl-
		21666493	100.00	

Entry 6



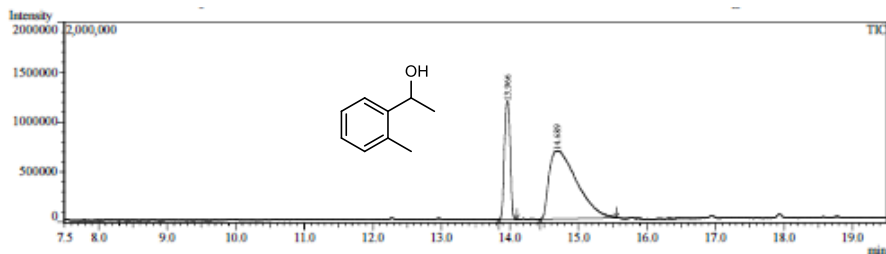
Spectrum

Line# 1 R.Time:13.185(Scan# 1138)
 MassPeaks:101
 RawMode:Averaged 13.180-13.190(1137-1139) BasePeak:107.00(272712)
 BG Mode Calc. from Peak Group 1 - Event 1



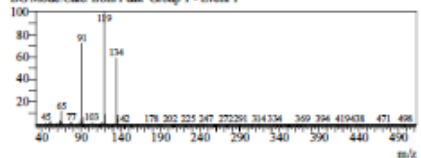
Peak Report TIC				
Peak#	R.Time	Area	Area%	Name
1	13.183	17787646	100.00	Benzenemethanol, alpha-methyl-
		17787646	100.00	

Entry 7

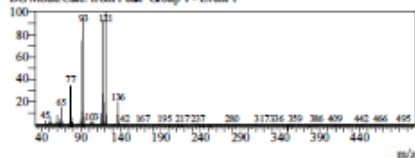


Spectrum

Line# 1 R. Time: 13.965(Scan# 1294)
 MassPeaks: 215
 RawMode: Averaged 13.960-13.970(1293-1295) BasePeak: 119.05(399140)
 BG Mode Calc: from Peak Group 1 - Event 1



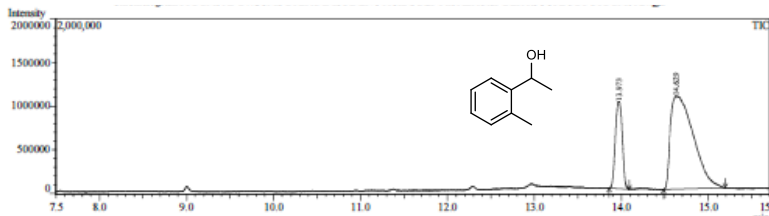
Line# 2 R. Time: 14.690(Scan# 1439)
 MassPeaks: 246
 RawMode: Averaged 14.685-14.695(1438-1440) BasePeak: 121.05(115941)
 BG Mode Calc: from Peak Group 1 - Event 1



Peak Report TIC

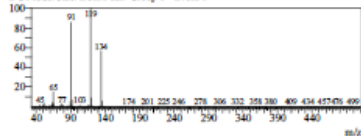
Peak#	R. Time	Area	Area%	Name
1	13.966	6780250	26.16	Ethanone, 1-(2-methylphenyl)- (CAS)
2	14.689	19135563	73.84	1-(2-Methylphenyl)ethanol
		25915813	100.00	

Entry 8

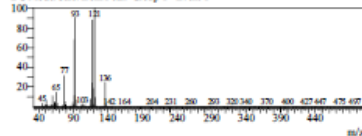


Spectrum

Line# 1 R. Time: 13.970(Scan# 1295)
 MassPeaks: 179
 RawMode: Averaged 13.965-13.975(1294-1296) BasePeak: 119.10(319343)
 BG Mode Calc: from Peak Group 1 - Event 1



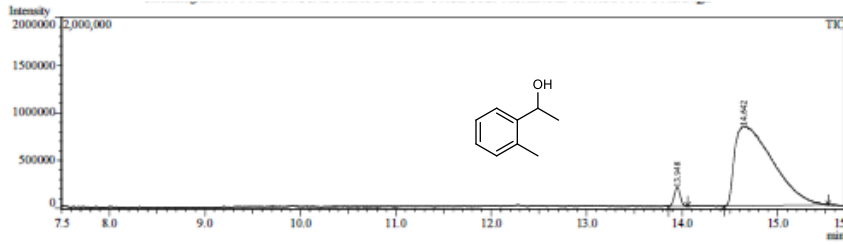
Line# 2 R. Time: 14.630(Scan# 1427)
 MassPeaks: 168
 RawMode: Averaged 14.625-14.635(1426-1428) BasePeak: 121.10(189930)
 BG Mode Calc: from Peak Group 1 - Event 1



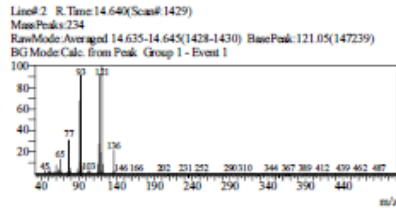
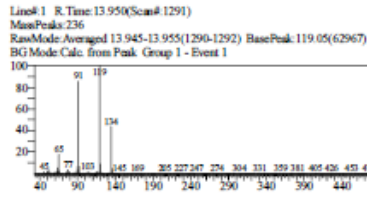
Peak Report TIC

Peak#	R. Time	Area	Area%	Name
1	13.973	5659722	22.47	Ethanone, 1-(2-methylphenyl)-
2	14.629	19526748	77.53	1-(2-Methylphenyl)ethanol
		25186470	100.00	

Entry 9



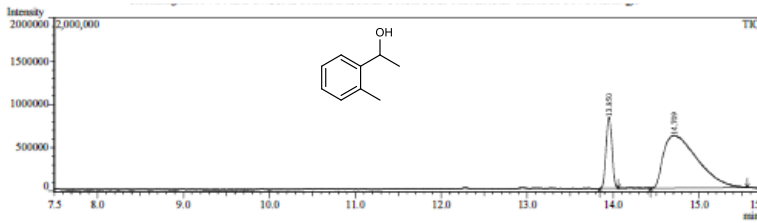
Spectrum



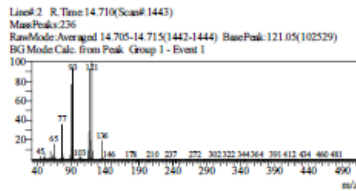
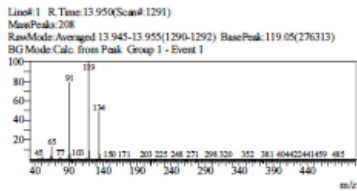
Peak Report TIC

Peak#	R. Time	Area	Area%	Name
1	13.948	887934	3.69	Ethanone, 1-(2-methylphenyl)-
2	14.642	23154703	96.31	1-(2-Methylphenyl)ethanol
		24042637	100.00	

Entry 10



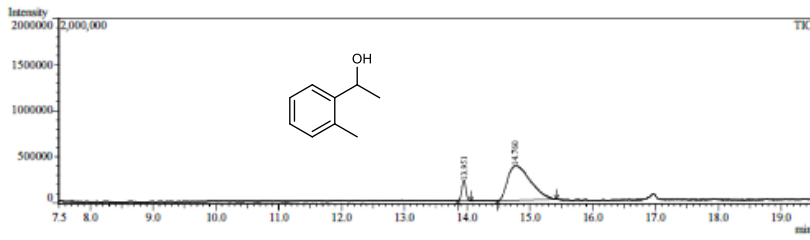
Spectrum



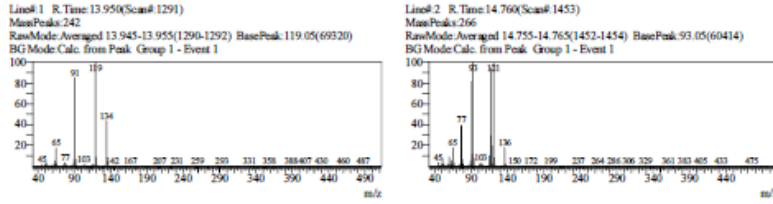
Peak Report TIC

Peak#	R. Time	Area	Area%	Name
1	13.950	4042567	19.61	Ethanone, 1-(2-methylphenyl)- (CAS)
2	14.709	16571375	80.39	1-(2-Methylphenyl)ethanol
		20613942	100.00	

Entry 11

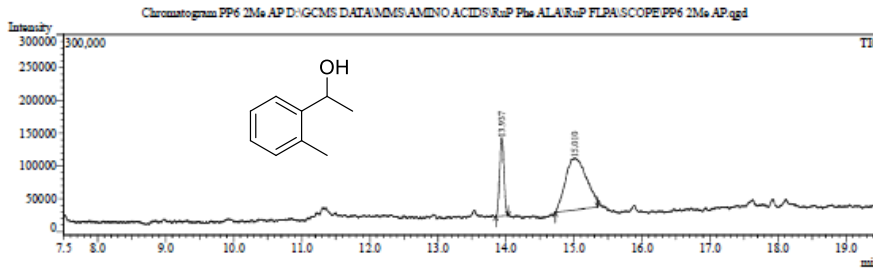


Spectrum

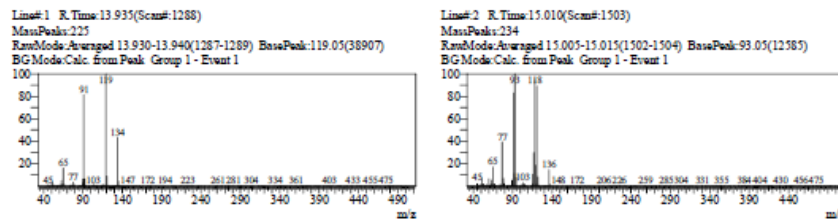


Peak Report TIC				
Peak#	R. Time	Area	Area%	Name
1	13.951	98589.5	9.56	Ethanone, 1-(2-methylphenyl)-
2	14.760	932903.1	90.44	Benzenemethanol, alpha, 4-dimethyl-
		1031492.6	100.00	

Entry 12

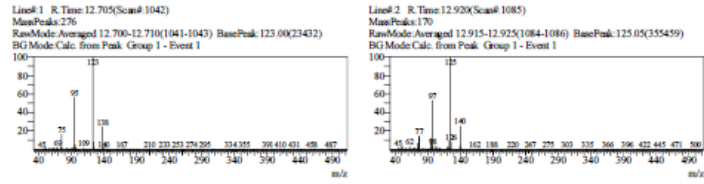
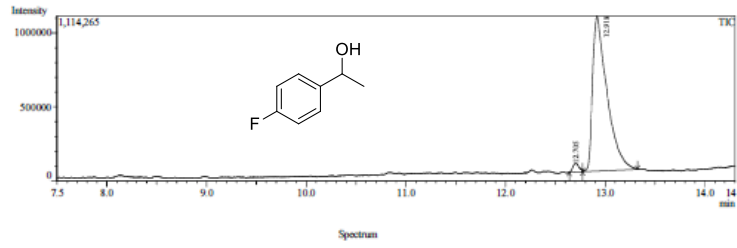


Spectrum



Peak Report TIC				
Peak#	R. Time	Area	Area%	Name
1	13.937	53049.2	23.88	Ethanone, 1-(2-methylphenyl)- (CAS)
2	15.010	169101.2	76.12	1-(2-Methylphenyl)ethanol

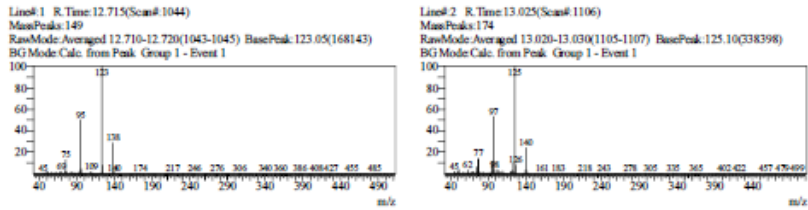
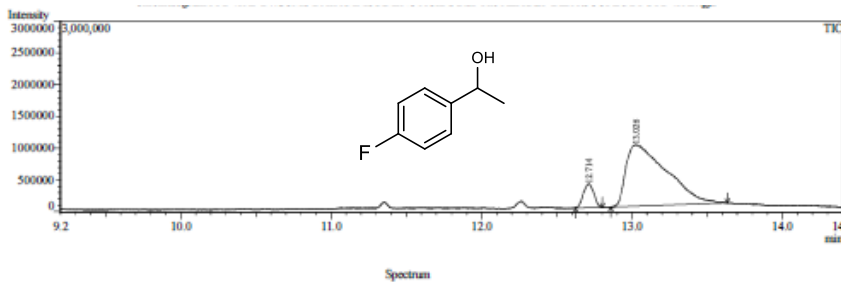
Entry 13



Peak Report TIC

Peak#	R. Time	Area	Area%	Name
1	12.705	255204	2.37	Ethanone, 1-(4-fluorophenyl)-
2	12.918	10531993	97.63	2-Fluorophenylmethylethanol
		10787287	100.00	

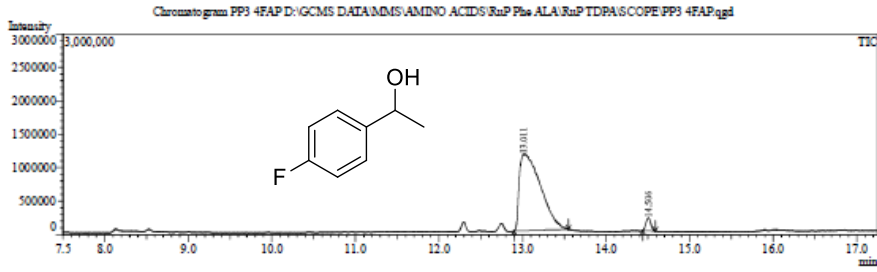
Entry 14



Peak Report TIC

Peak#	R. Time	Area	Area%	Name
1	12.714	1772121	8.94	ETHANONE, 1-(4-FLUOROPHENYL)-
2	13.026	18053847	91.06	4-Fluorophenylmethylethanol
		19825968	100.00	

Entry 15



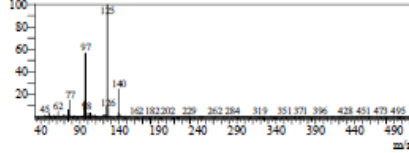
Spectrum

Line#1 R.Time:13.010(Scan#:1103)

MassPeak:220

RawMode: Averaged 13.005-13.015(1102-1104) BasePeak:125.05(381419)

BGMode: Calc. from Peak Group 1 - Event 1

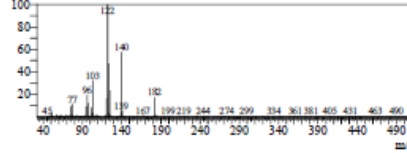


Line#2 R.Time:14.505(Scan#:1402)

MassPeak:253

RawMode: Averaged 14.500-14.510(1401-1403) BasePeak:122.05(45830)

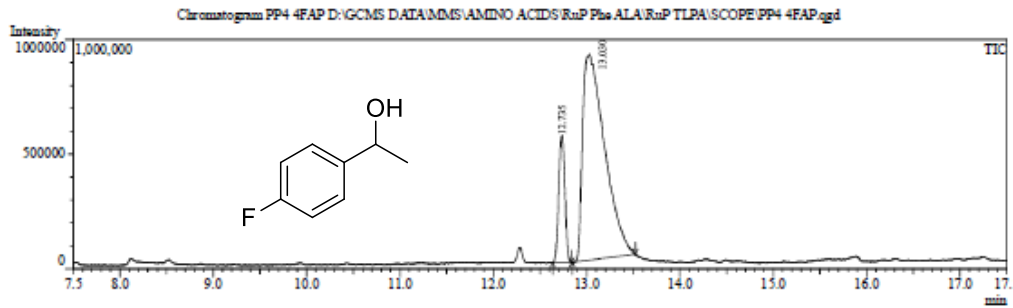
BGMode: Calc. from Peak Group 1 - Event 1



Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	13.011	20285203	96.37	4-Fluorophenylmethylethanol
2	14.506	765133	3.63	4-Fluoro- α -methylbenzyl alcohol, trifluoro-

Entry 16



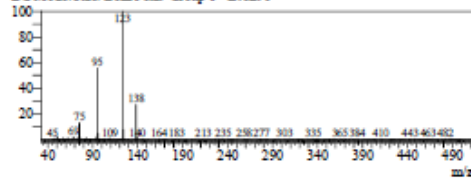
Spectrum

Line#1 R.Time:12.735(Scan#:1048)

MassPeak:232

RawMode: Averaged 12.730-12.740(1047-1049) BasePeak:123.05(230803)

BGMode: Calc. from Peak Group 1 - Event 1

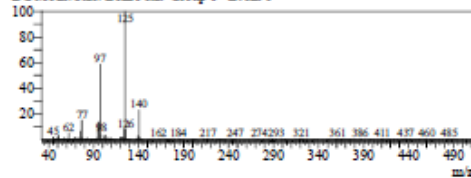


Line#2 R.Time:13.030(Scan#:1107)

MassPeak:209

RawMode: Averaged 13.025-13.035(1106-1108) BasePeak:125.05(296136)

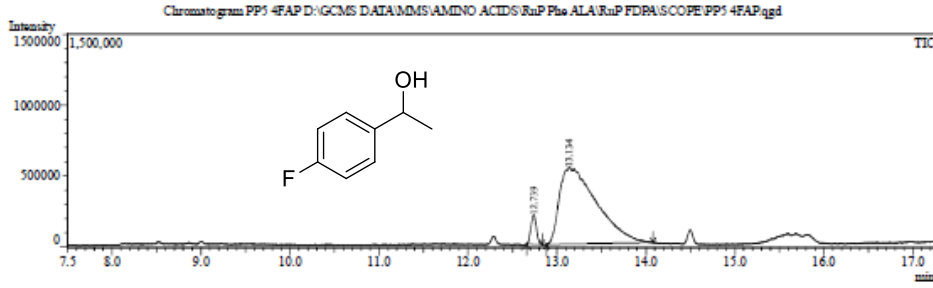
BGMode: Calc. from Peak Group 1 - Event 1



Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	12.735	2558854	14.77	Ethanone, 1-(4-fluorophenyl)-
2	13.030	14761276	85.23	2-Fluorophenylmethylethanol

Entry 17



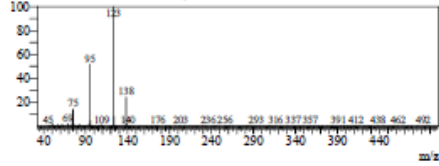
Spectrum

Line# 1 R.Time:12.740(Scan#:1049)

MassPeak:229

RawMode:Averaged 12.735-12.745(1048-1050) BasePeak:123.05(88696)

BGMode:Calc. from Peak Group 1 - Event 1

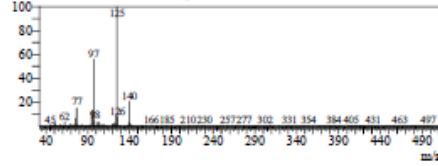


Line# 2 R.Time:13.135(Scan#:1128)

MassPeak:259

RawMode:Averaged 13.130-13.140(1127-1129) BasePeak:125.05(181610)

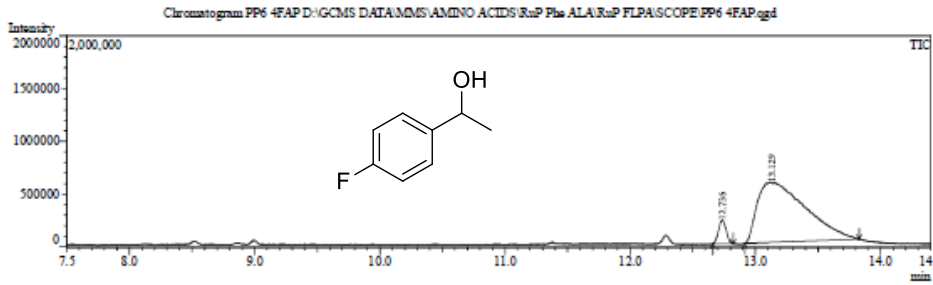
BGMode:Calc. from Peak Group 1 - Event 1



Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	12.739	885161	5.35	Ethanone, 1-(4-fluorophenyl)-
2	13.134	15675316	94.65	2-Fluorophenylmethylethanol

Entry 18



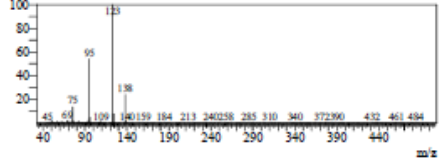
Spectrum

Line# 1 R.Time:12.735(Scan#:1048)

MassPeak:224

RawMode:Averaged 12.730-12.740(1047-1049) BasePeak:123.05(94954)

BGMode:Calc. from Peak Group 1 - Event 1

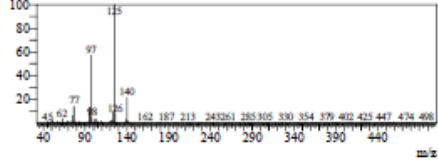


Line# 2 R.Time:13.130(Scan#:1127)

MassPeak:262

RawMode:Averaged 13.125-13.135(1126-1128) BasePeak:125.05(192976)

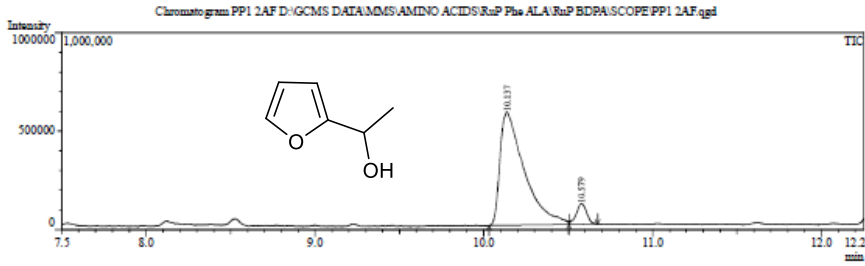
BGMode:Calc. from Peak Group 1 - Event 1



Peak Report TIC

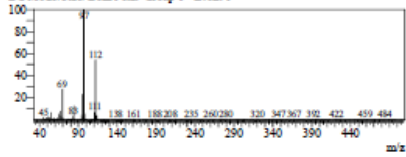
Peak#	R.Time	Area	Area%	Name
1	12.736	941499	5.81	Ethanone, 1-(4-fluorophenyl)-
2	13.129	15261577	94.19	2-Fluorophenylmethylethanol

Entry 19

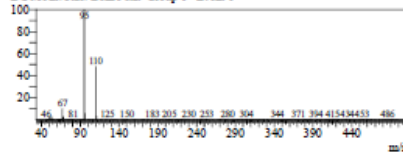


Spectrum

Line# 1 R.Time:10.135(Scan#:528)
 MassPeak:215
 RawMode:Averaged 10.130-10.140(527-529) BasePeak:97.00(197709)
 BG Mode Calc. from Peak Group 1 - Event 1



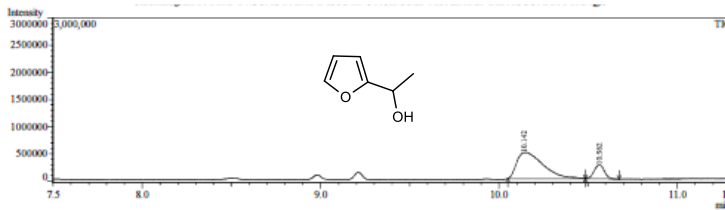
Line# 2 R.Time:10.580(Scan#:617)
 MassPeak:240
 RawMode:Averaged 10.575-10.585(616-618) BasePeak:95.00(34081)
 BG Mode Calc. from Peak Group 1 - Event 1



Peak Report TIC

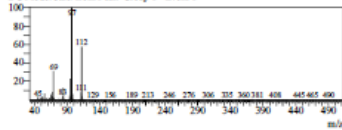
Peak#	R Time	Area	Area%	Name
1	10.137	5766098	92.74	4(3)-Methyl-2-furfuryl alcohol
2	10.579	451507	7.26	Ethanone, 1-(2-furanyl)- (CAS)

Entry 20

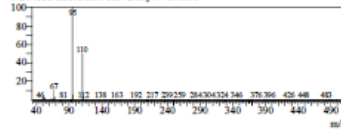


Spectrum

Line# 1 R.Time:10.140(Scan#:529)
 MassPeak:183
 RawMode:Averaged 10.135-10.145(528-530) BasePeak:97.05(196998)
 BG Mode Calc. from Peak Group 1 - Event 1



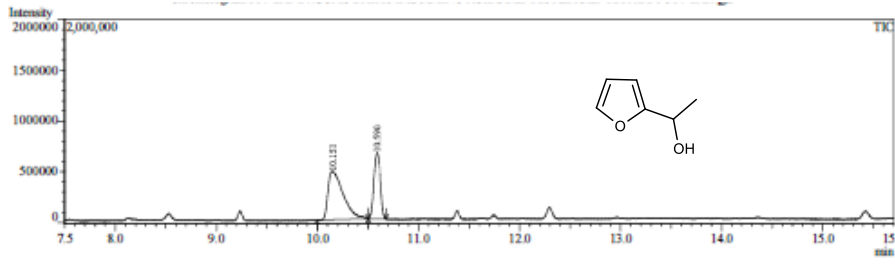
Line# 2 R.Time:10.560(Scan#:613)
 MassPeak:205
 RawMode:Averaged 10.555-10.565(612-614) BasePeak:95.00(193387)
 BG Mode Calc. from Peak Group 1 - Event 1



Peak Report TIC

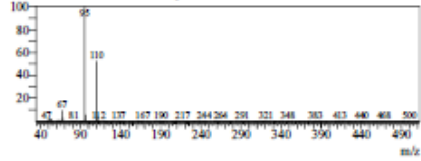
Peak#	R Time	Area	Area%	Name
1	10.142	4871556	83.13	4(3)-Methyl-2-furfuryl alcohol
2	10.562	988637	16.87	Ethanone, 1-(2-furanyl)-
		5860193	100.00	

Entry 21

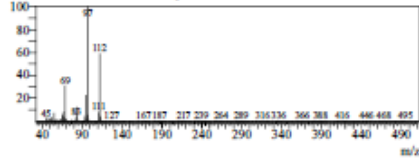


Spectrum

Line# 1 R.Time:10.590(Scan# 619)
 MassPeaks:183
 RawMode:Averaged 10.585-10.595(618-620) BasePeak:95.00(256564)
 BG Mode Calc: from Peak Group 1 - Event 1



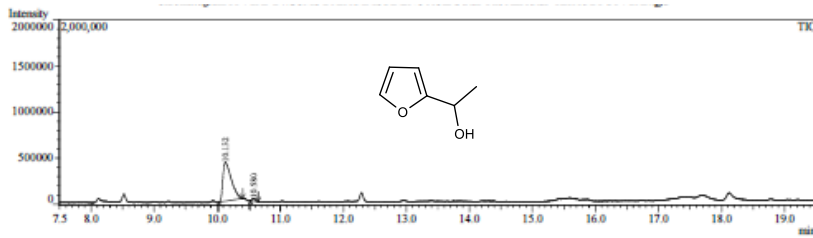
Line# 2 R.Time:10.150(Scan# 531)
 MassPeaks:209
 RawMode:Averaged 10.145-10.155(530-532) BasePeak:97.05(157707)
 BG Mode Calc: from Peak Group 1 - Event 1



Peak Report TIC

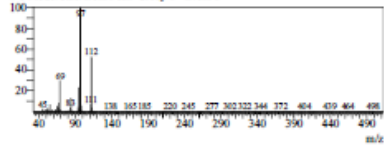
Peak#	R.Time	Area	Area%	Name
1	10.151	4904024	63.01	4(3)-Methyl-2-furfuryl alcohol
2	10.590	2879283	36.99	Ethanone, 1-(2-furanyl)- (CAS)
		7783307	100.00	

Entry 22

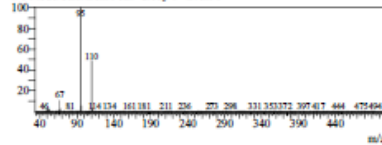


Spectrum

Line# 1 R.Time:10.130(Scan# 527)
 MassPeaks:225
 RawMode:Averaged 10.125-10.135(526-528) BasePeak:97.00(145130)
 BG Mode Calc: from Peak Group 1 - Event 1



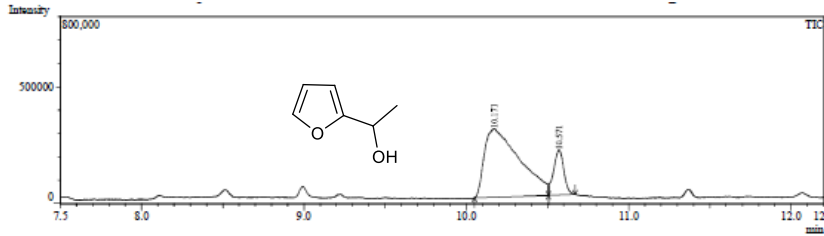
Line# 2 R.Time:10.580(Scan# 617)
 MassPeaks:229
 RawMode:Averaged 10.575-10.585(616-618) BasePeak:95.00(16228)
 BG Mode Calc: from Peak Group 1 - Event 1



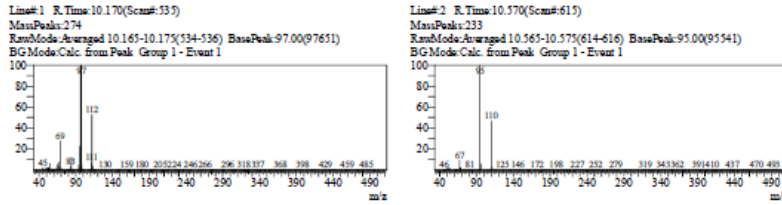
Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	10.132	3823516	97.42	4(3)-Methyl-2-furfuryl alcohol
2	10.580	101284	2.58	Ethanone, 1-(2-furanyl)- (CAS)
		3924800	100.00	

Entry 23



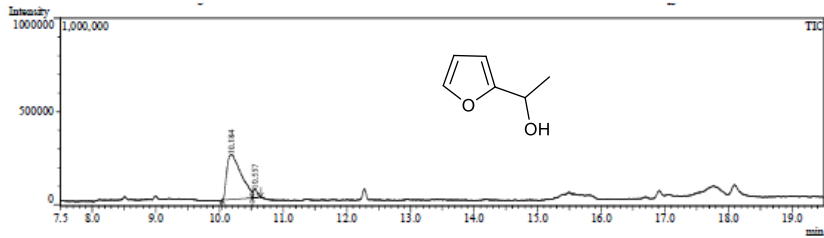
Spectrum



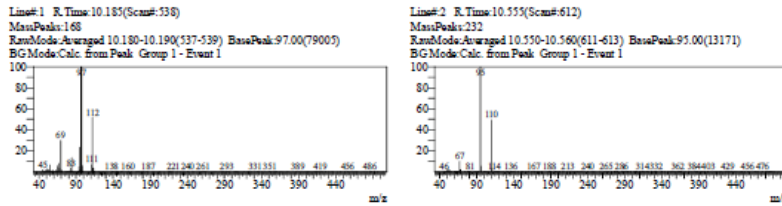
Peak Report TIC

Peak#	R Time	Area	Area%	Name
1	10.171	4396444	83.90	4(3)-Methyl-2-furfuryl alcohol
2	10.571	843645	16.10	Ethanone, 1-(2-furanyl)- (CAS)

Entry 24



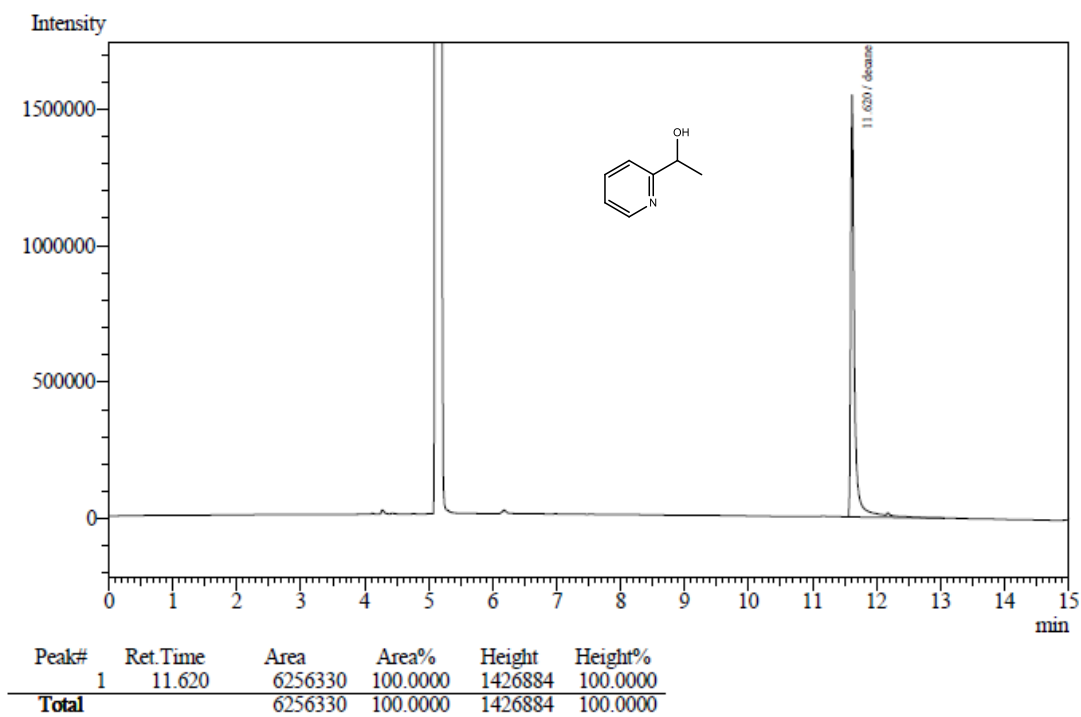
Spectrum



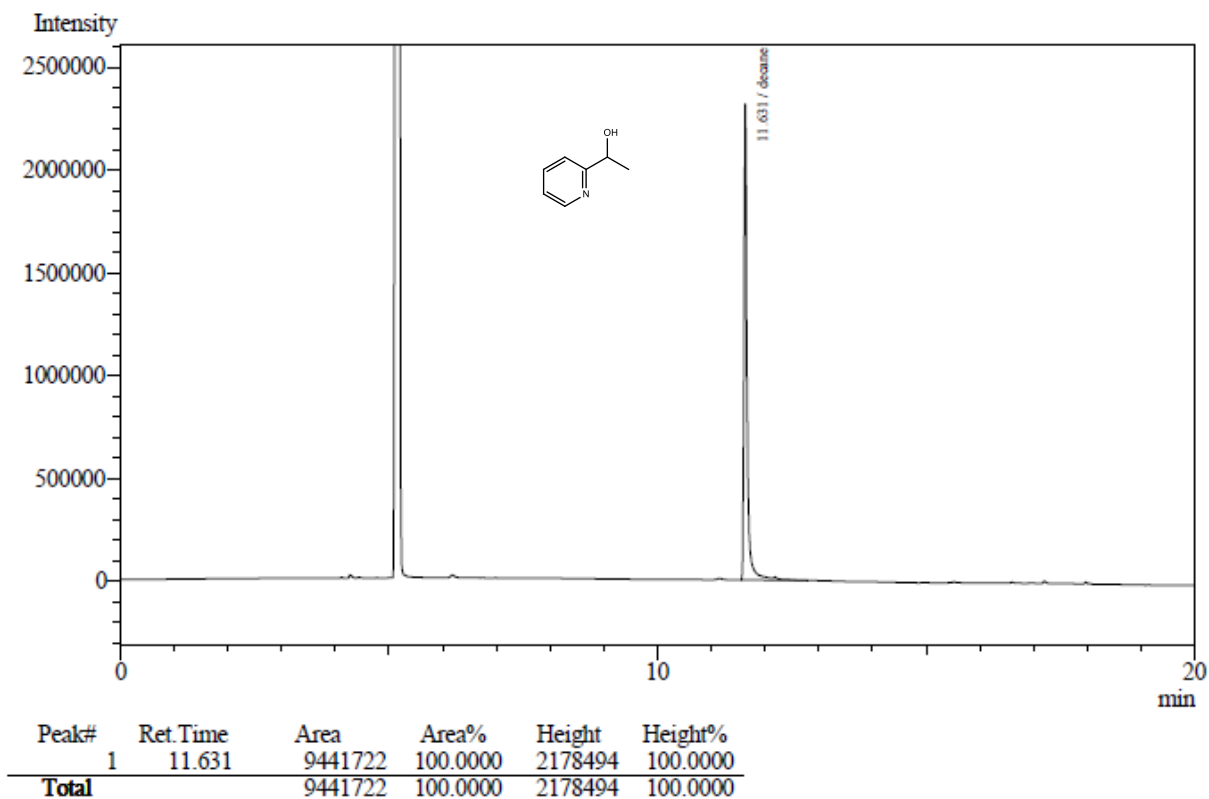
Peak Report TIC

Peak#	R Time	Area	Area%	Name
1	10.184	3742176	94.55	4(3)-Methyl-2-furfuryl alcohol
2	10.557	215522	5.45	Ethanone, 1-(2-furanyl)- (CAS)

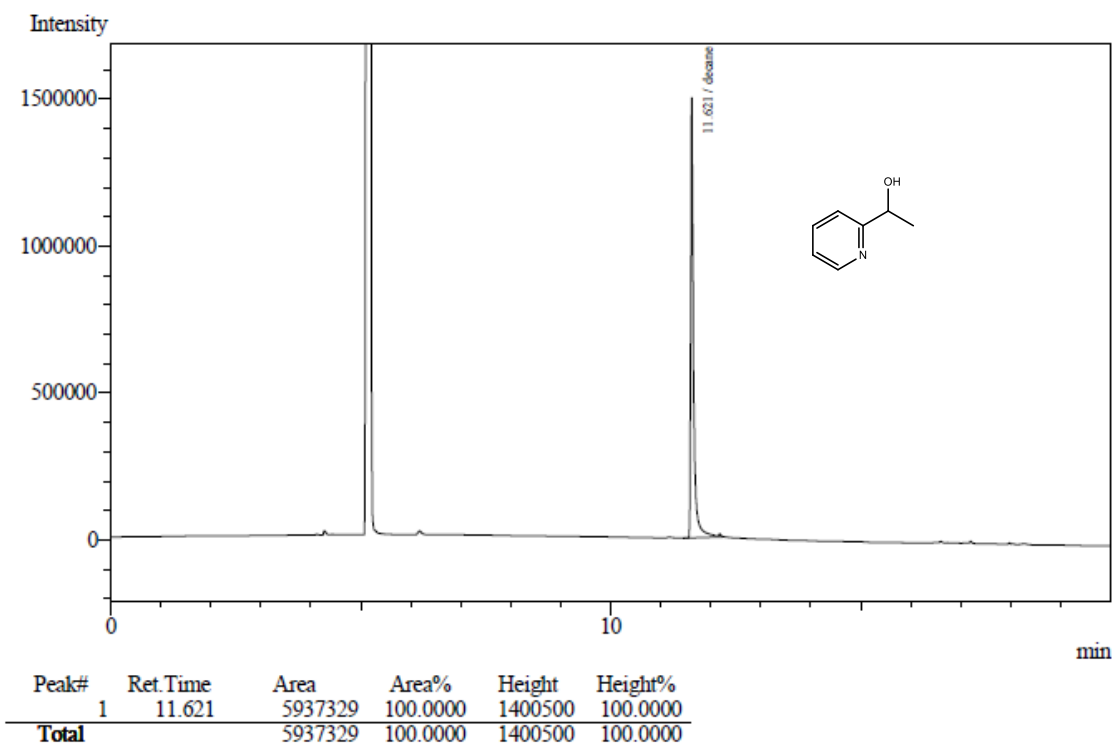
Entry 25



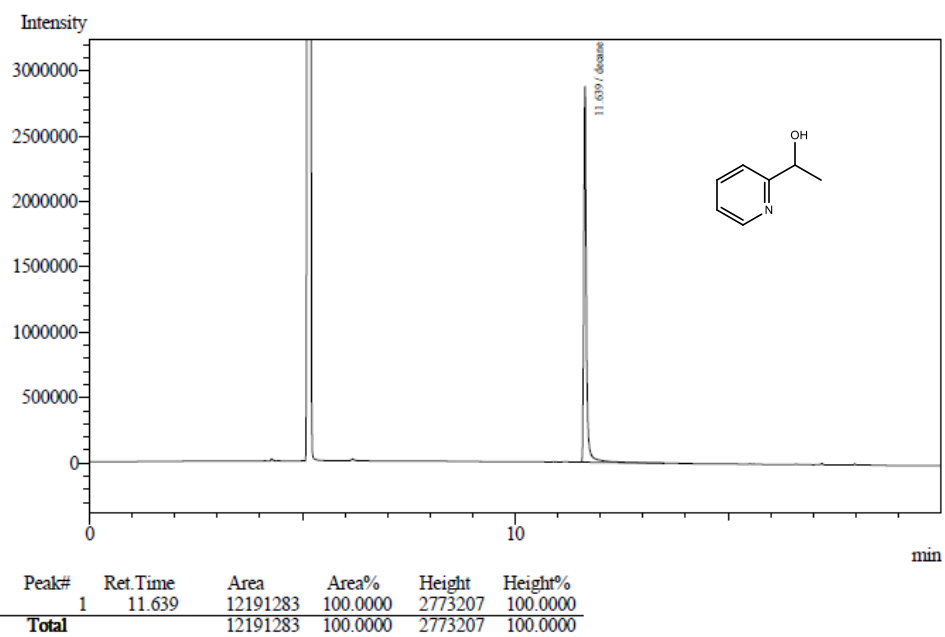
Entry 26



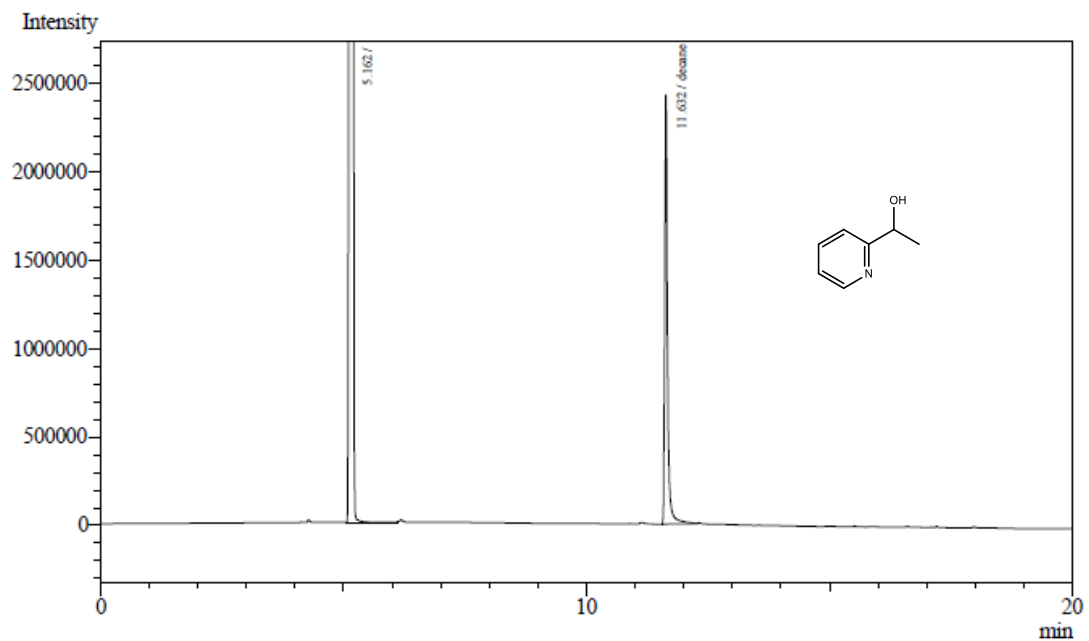
Entry 27



Entry 28

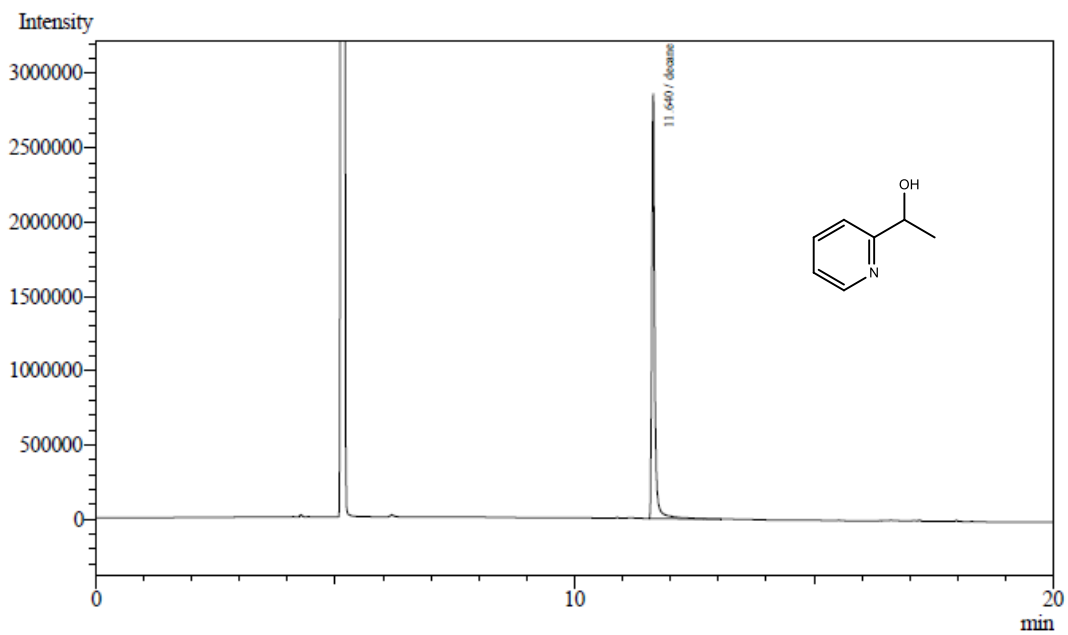


Entry 29



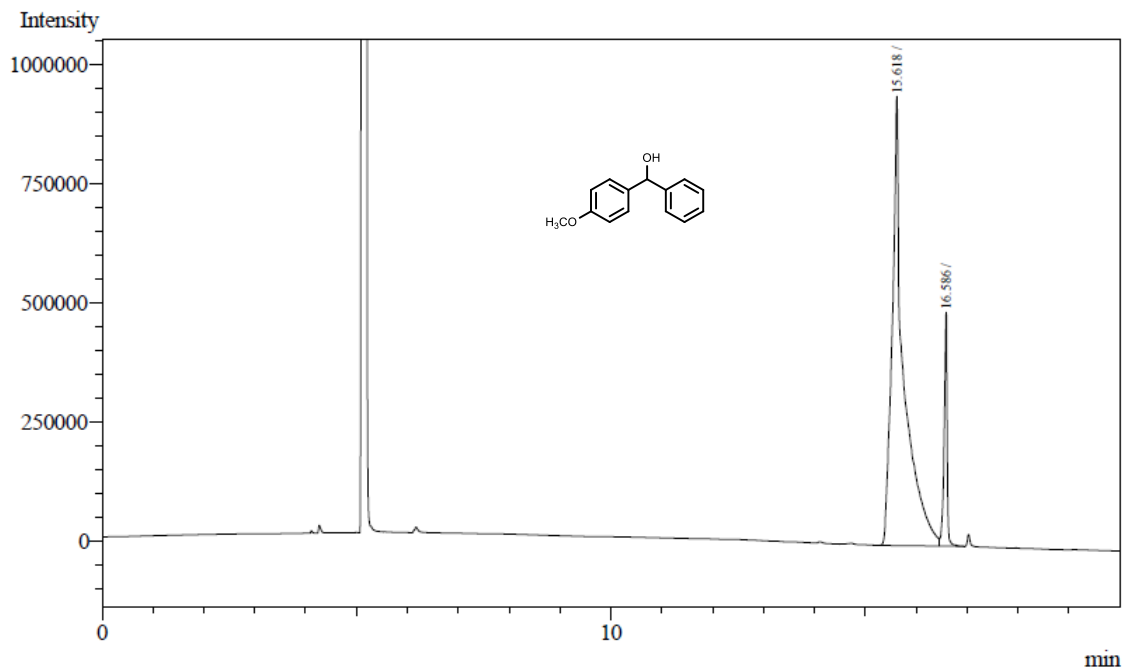
Peak#	Ret. Time	Area	Area%	Height	Height%
1	5.162	178386581	94.8600	47044945	95.4206
2	11.632	9665899	5.1400	2257792	4.5794
Total		188052480	100.0000	49302737	100.0000

Entry 30



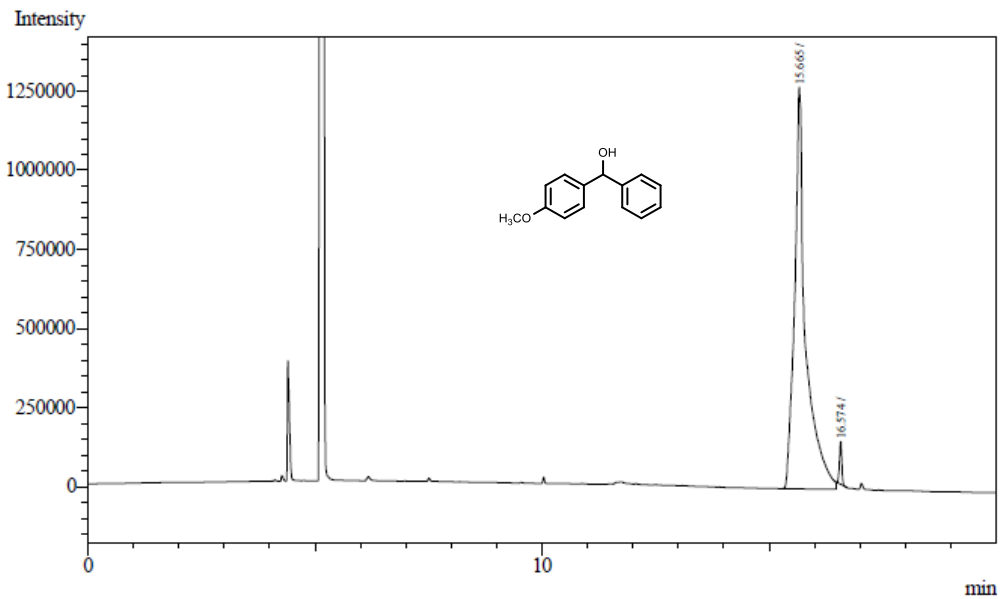
Peak#	Ret. Time	Area	Area%	Height	Height%
1	11.640	11959656	100.0000	2763029	100.0000
Total		11959656	100.0000	2763029	100.0000

Entry 31



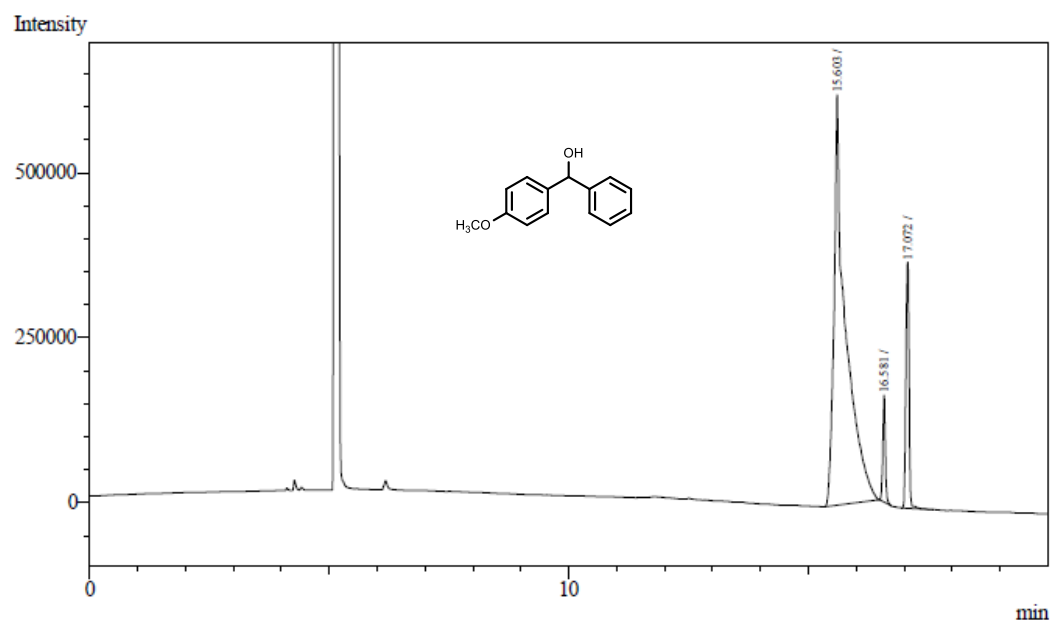
Peak#	Ret. Time	Area	Area%	Height	Height%
1	15.618	15001751	88.3126	915262	66.7003
2	16.586	1985354	11.6874	456938	33.2997
Total		16987105	100.0000	1372200	100.0000

Entry 32



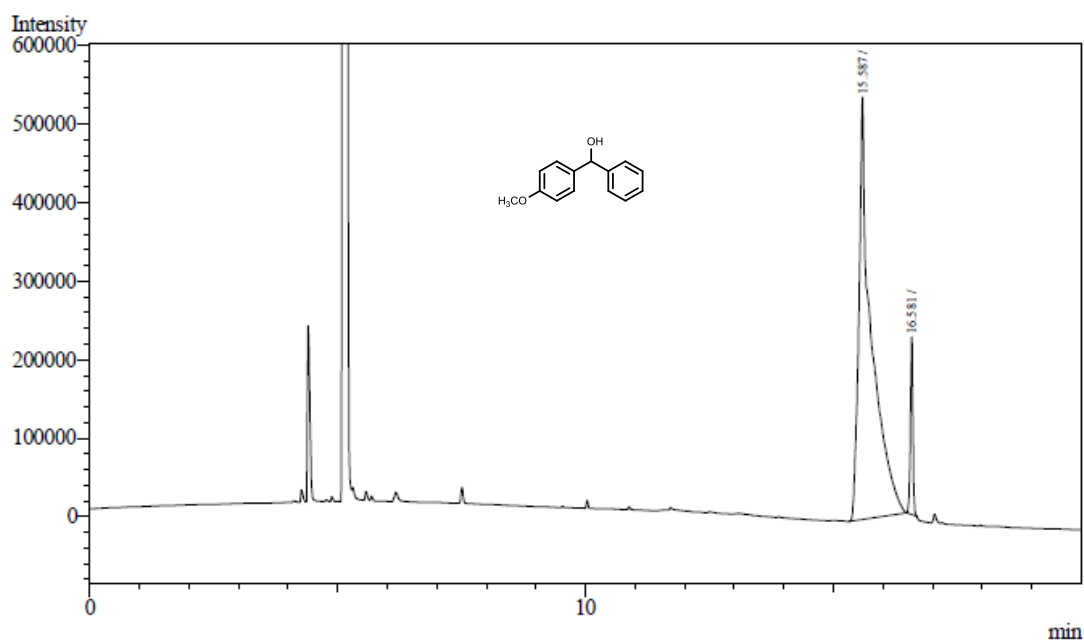
Peak#	Ret. Time	Area	Area%	Height	Height%
1	15.665	21720049	97.8160	1260633	90.5312
2	16.574	484961	2.1840	131852	9.4688
Total		22205010	100.0000	1392485	100.0000

Entry 33



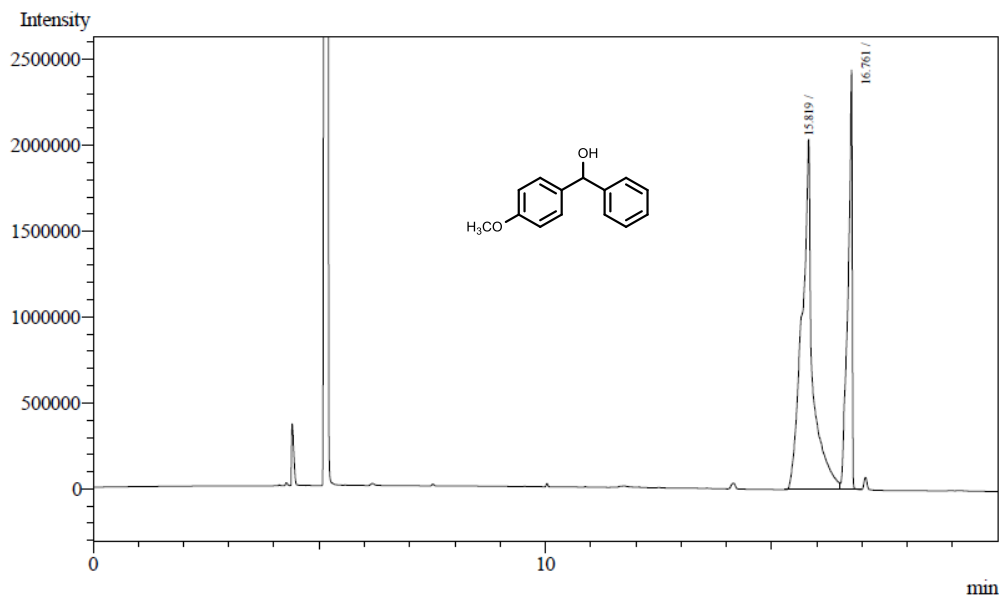
Peak#	Ret. Time	Area	Area%	Height	Height%
1	15.603	10515401	81.9472	608956	53.8971
2	16.581	593744	4.6271	152605	13.5067
3	17.072	1722779	13.4257	368288	32.5962
Total		12831924	100.0000	1129849	100.0000

Entry 34



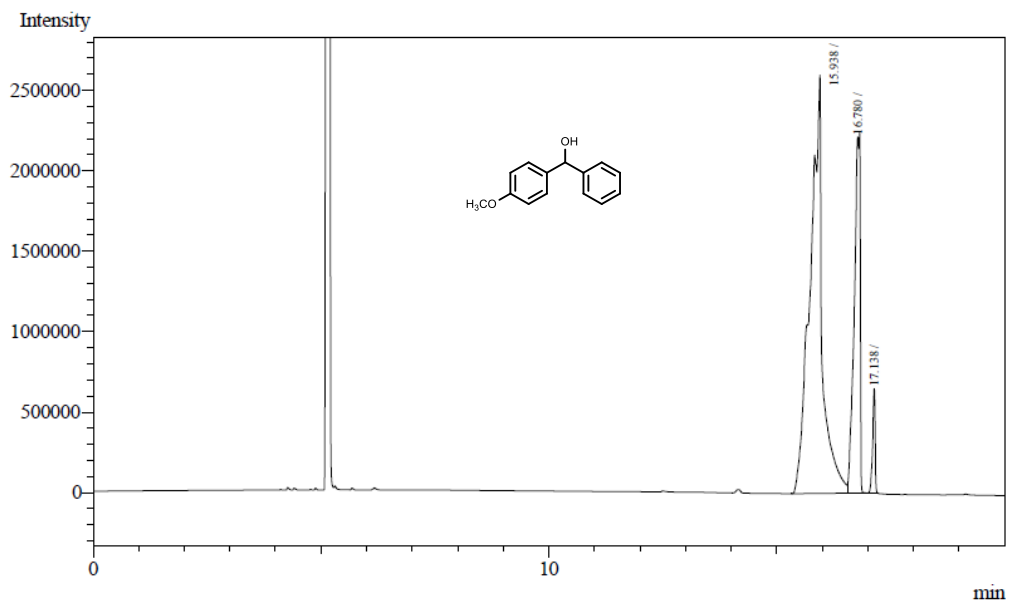
Peak#	Ret. Time	Area	Area%	Height	Height%
1	15.587	9509491	92.2553	529743	71.3348
2	16.581	798303	7.7447	212872	28.6652
Total		10307794	100.0000	742615	100.0000

Entry 35



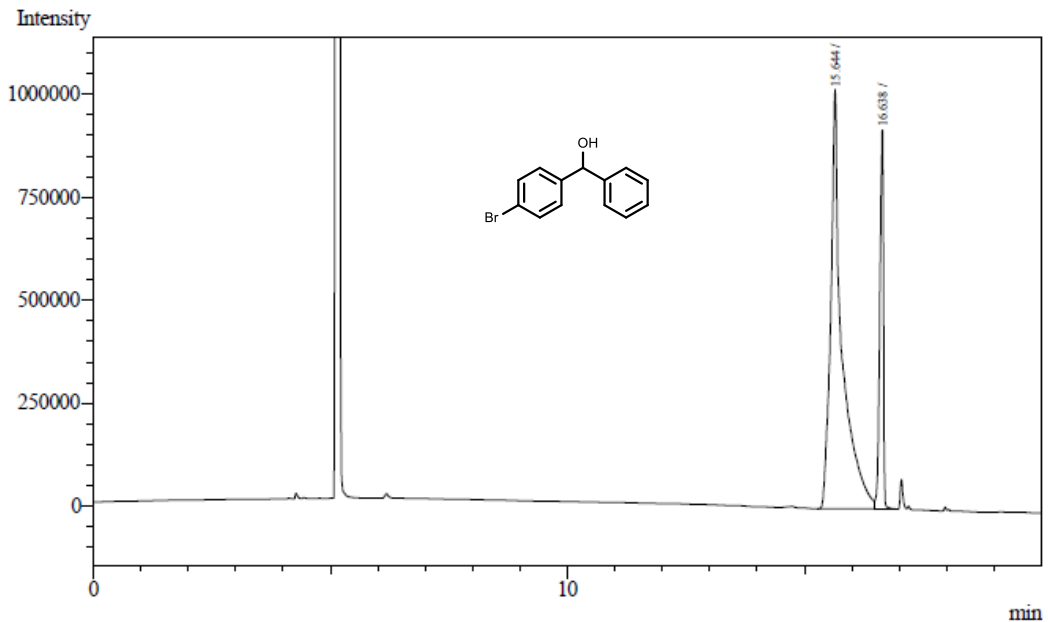
Peak#	Ret. Time	Area	Area%	Height	Height%
1	15.819	33447203	68.0872	2002239	46.6148
2	16.761	15676874	31.9128	2293045	53.3852
Total		49124077	100.0000	4295284	100.0000

Entry 36



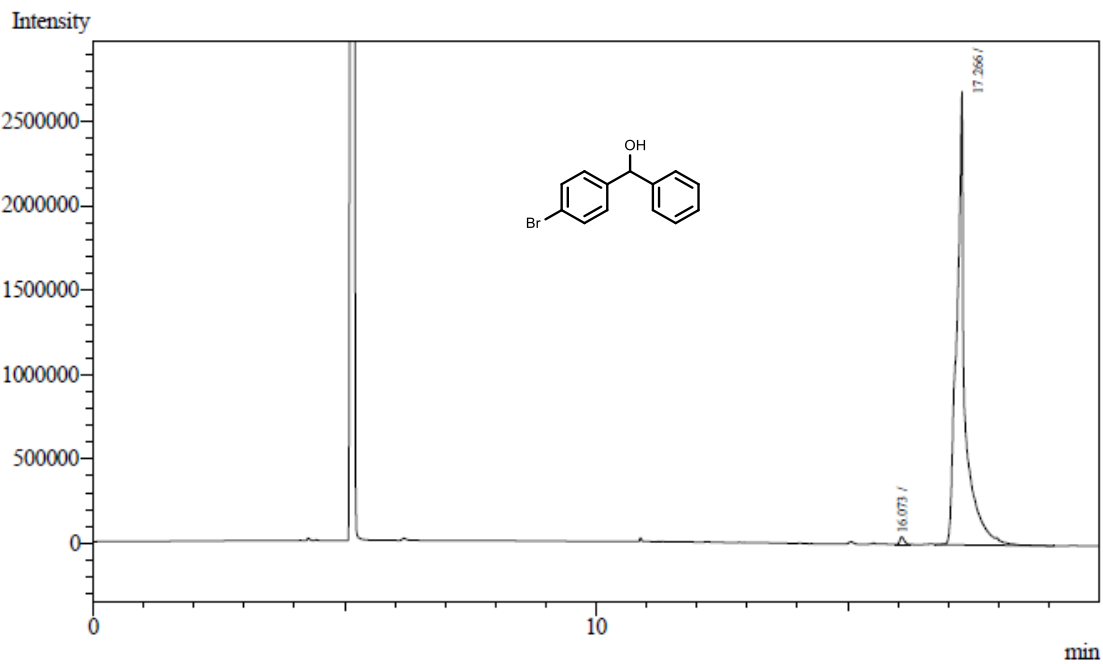
Peak#	Ret. Time	Area	Area%	Height	Height%
1	15.938	49282388	68.5744	2551149	47.4376
2	16.780	20150487	28.0386	2200179	40.9115
3	17.138	2434158	3.3870	626571	11.6509
Total		71867033	100.0000	5377899	100.0000

Entry 37



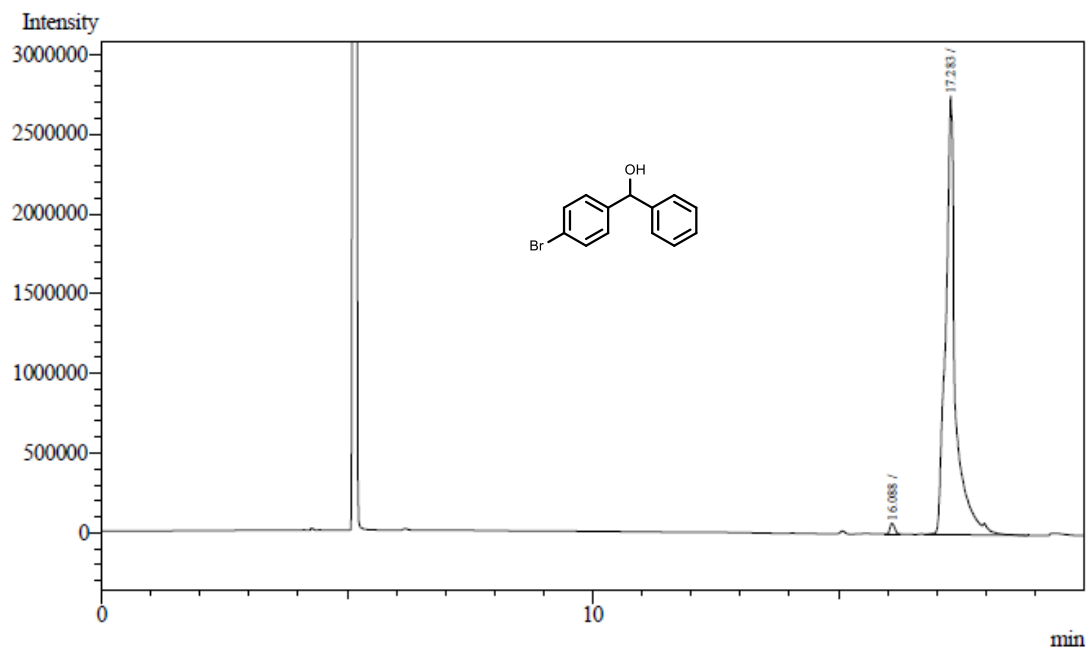
Peak#	Ret.Time	Area	Area%	Height	Height%
1	15.644	16977766	77.3083	1011285	52.4878
2	16.638	4983348	22.6917	915420	47.5122
Total		21961114	100.0000	1926705	100.0000

Entry 38



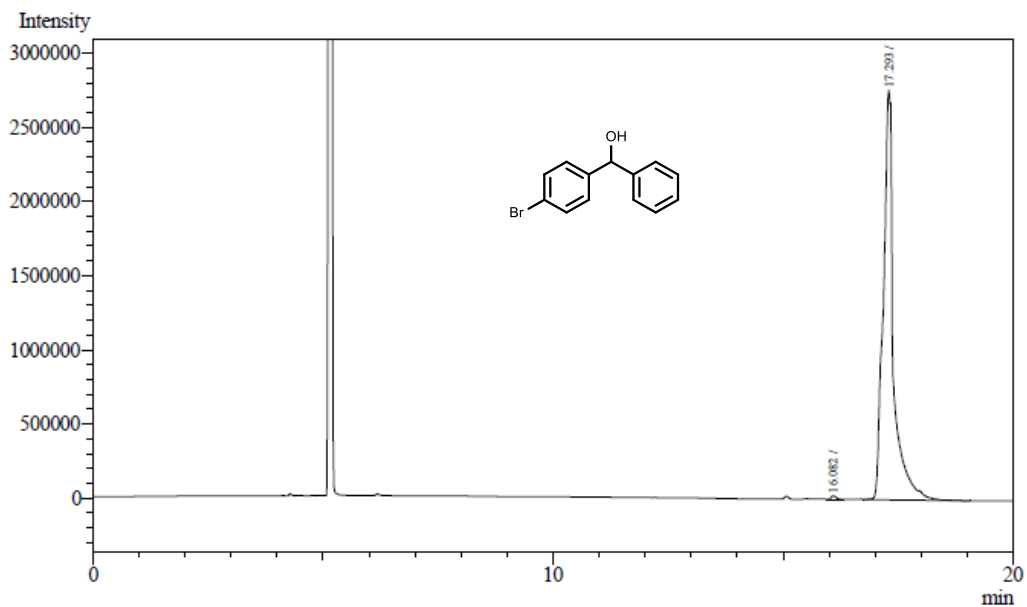
Peak#	Ret.Time	Area	Area%	Height	Height%
1	16.073	265371	0.8327	44364	1.7197
2	17.266	31603794	99.1673	2535415	98.2803
Total		31869165	100.0000	2579779	100.0000

Entry 39



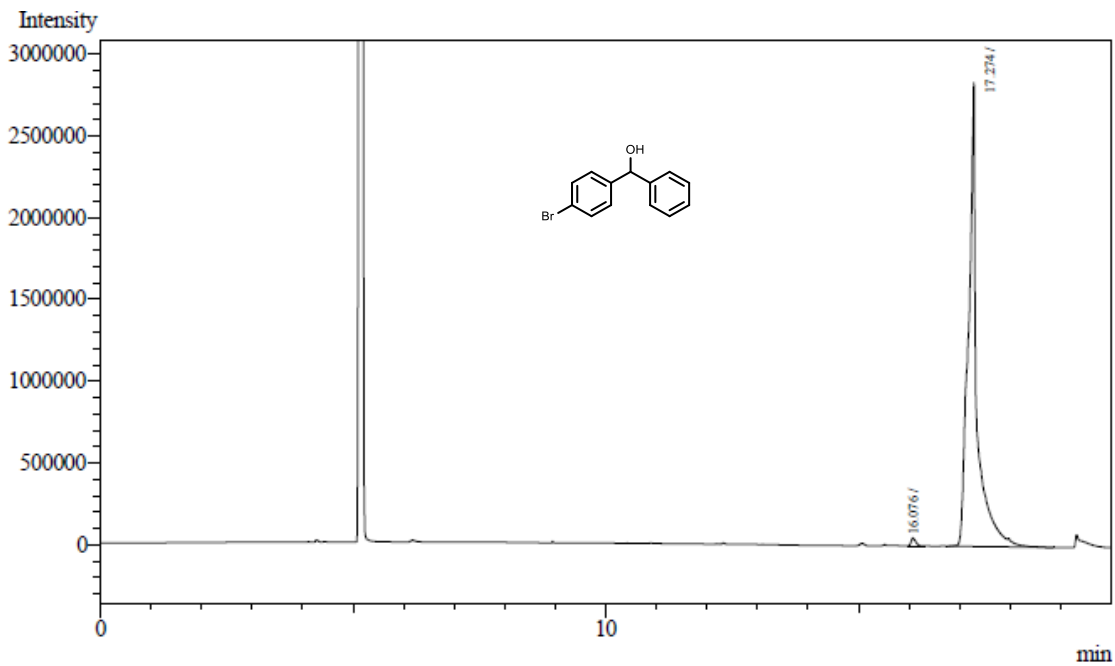
Peak#	Ret.Time	Area	Area%	Height	Height%
1	16.088	433076	1.1068	65536	2.3604
2	17.283	38695360	98.8932	2710907	97.6396
Total		39128436	100.0000	2776443	100.0000

Entry 40



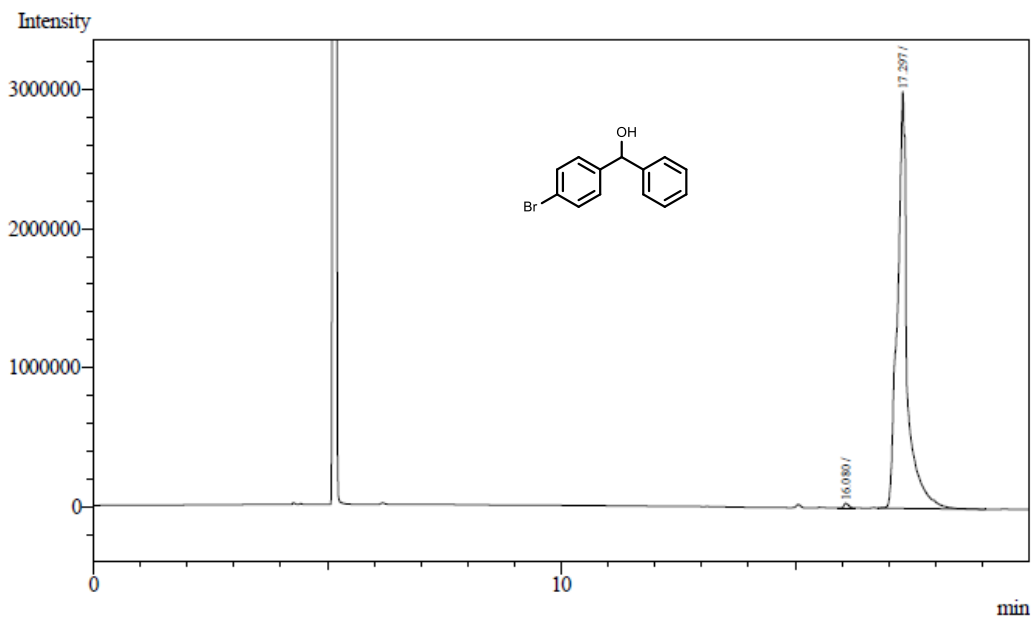
Peak#	Ret.Time	Area	Area%	Height	Height%
1	16.082	157476	0.3648	23161	0.8344
2	17.293	43007507	99.6352	2752732	99.1656
Total		43164983	100.0000	2775893	100.0000

Entry 41



Peak#	Ret. Time	Area	Area%	Height	Height%
1	16.076	294455	0.8734	48053	1.7022
2	17.274	33421058	99.1266	2774950	98.2978
Total		33715513	100.0000	2823003	100.0000

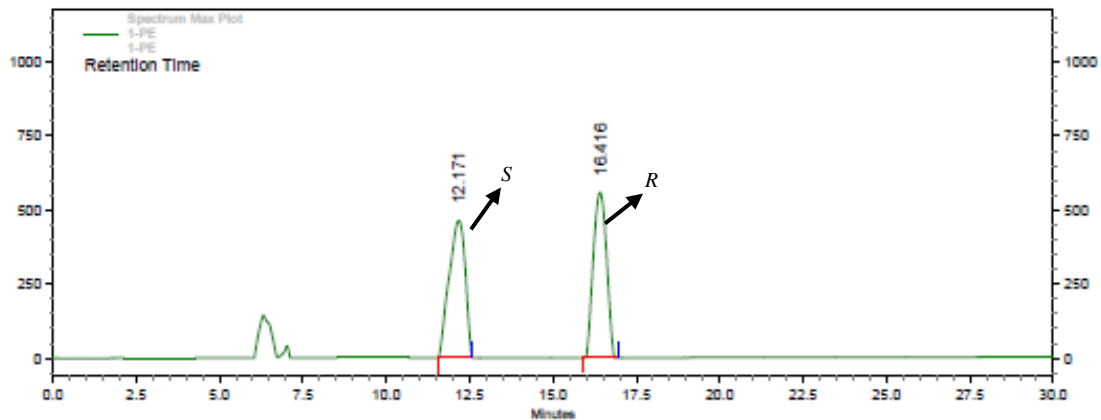
Entry 42



Peak#	Ret. Time	Area	Area%	Height	Height%
1	16.080	218270	0.4870	32642	1.0932
2	17.297	44603563	99.5130	2953156	98.9068
Total		44821833	100.0000	2985798	100.0000

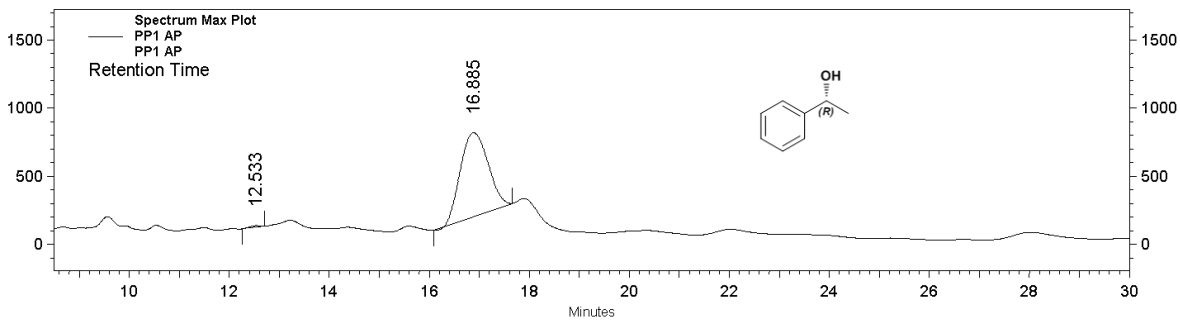
HPLC data

Racemic 1-Phenylethanol



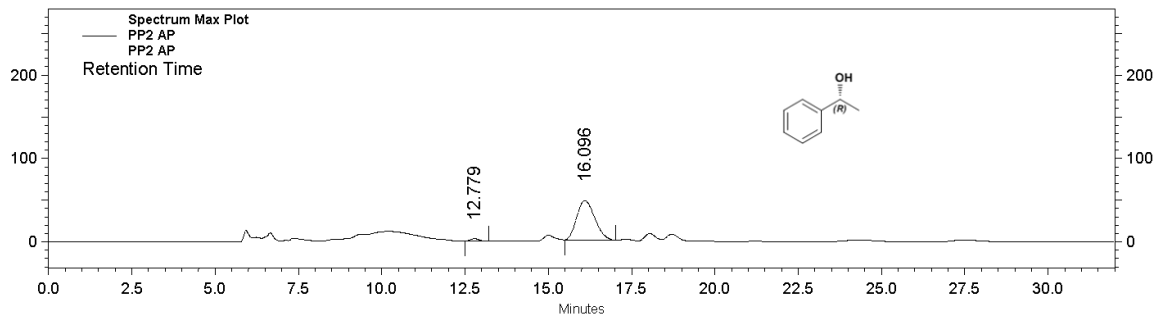
Pk #	Retention Time	Area	Area %	Height	Height %
1	12.171	15598325	50.267	462764	45.361
2	16.416	15432391	49.733	557424	54.639
Totals		31030716	100.000	1020188	100.000

Entry 1



Pk #	Retention Time	Area	Area %	Height	Height %
1	12.533	87177	0.725	5840	1.857
2	16.885	11931927	99.275	308652	98.143
Totals		12019104	100.000	314492	100.000

Entry 2

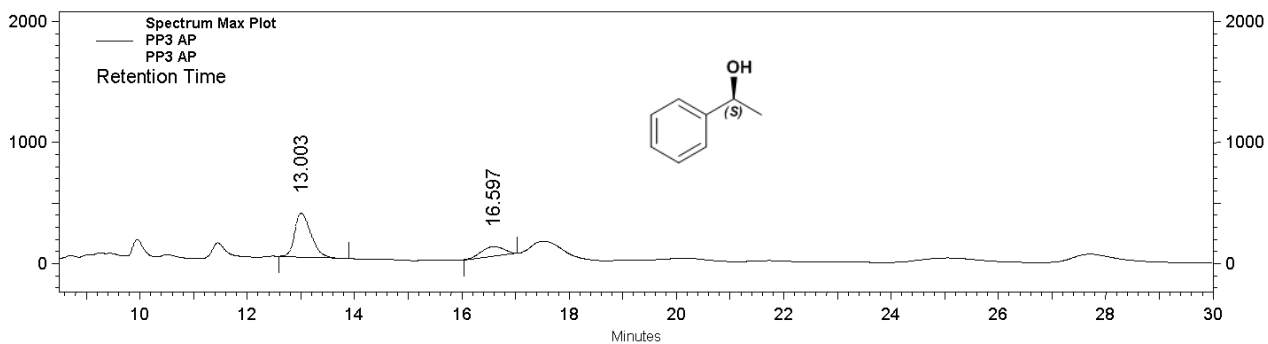


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	12.779	246570	2.671	13833	5.497
2	16.096	8983878	97.329	237821	94.503

Totals		9230448	100.000	251654	100.000
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Entry 3

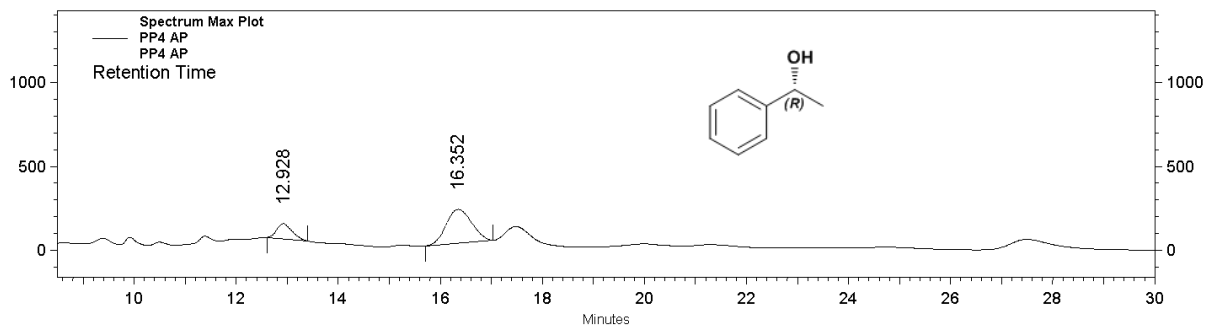


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	13.003	15269918	76.813	723222	82.375
2	16.597	4609320	23.187	154740	17.625

Totals		19879238	100.000	877962	100.000
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Entry 4

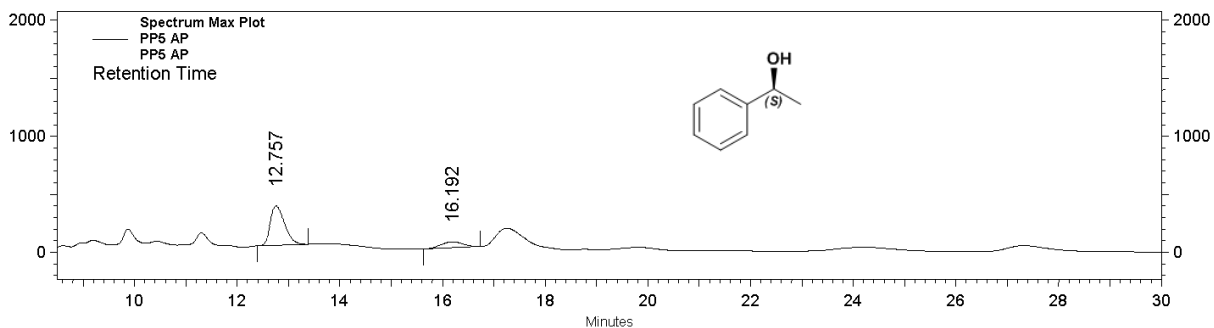


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	12.928	3763893	21.195	182698	31.201
2	16.352	13994626	78.805	402854	68.799

Totals		17758519	100.000	585552	100.000
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Entry 5

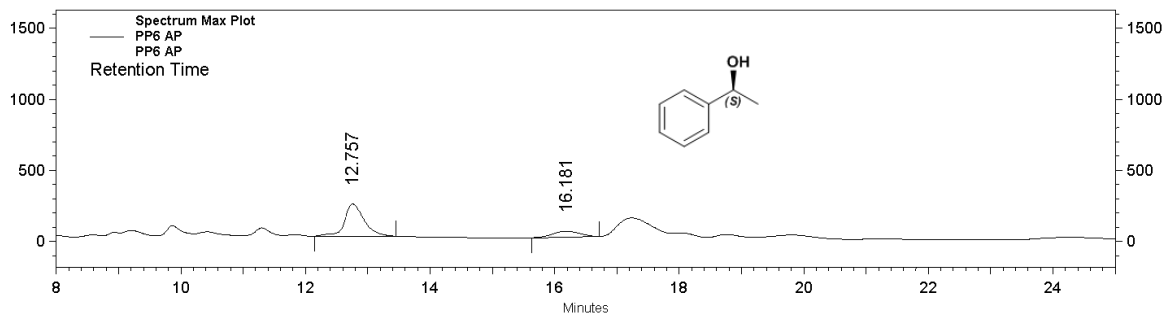


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	12.757	13186605	80.915	678279	86.657
2	16.192	3110328	19.085	104439	13.343

Totals		16296933	100.000	782718	100.000
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Entry 6

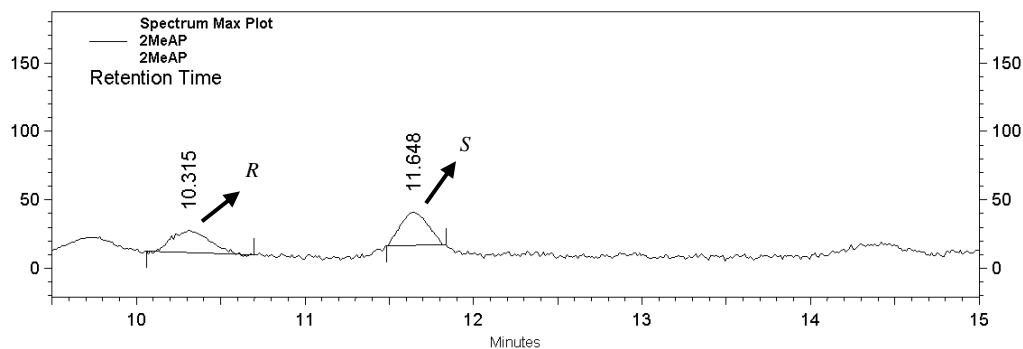


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	12.757	16418675	80.026	751280	84.493
2	16.181	4097946	19.974	137887	15.507

Totals		20516621	100.000	889167	100.000
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Racemic 1-(o-tolyl)ethanol

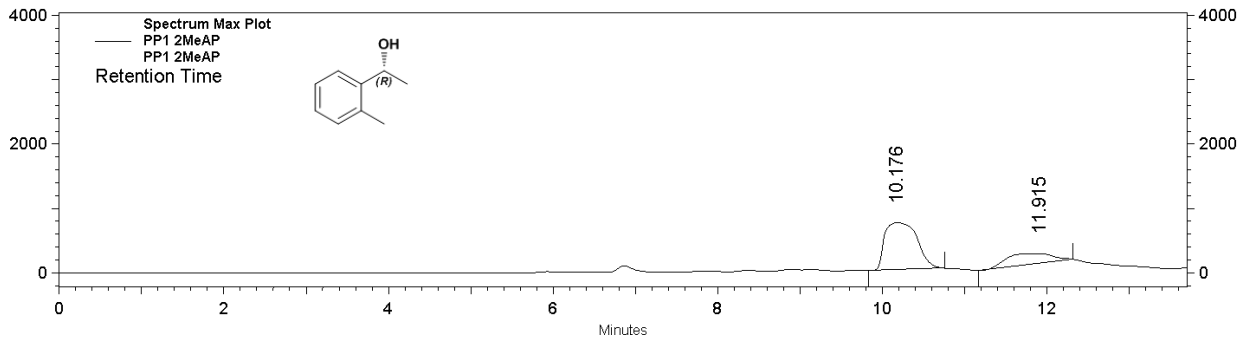


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.315	243757	46.808	15966	40.107
2	11.648	276999	53.192	23843	59.893

Totals		520756	100.000	39809	100.000
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Entry 7

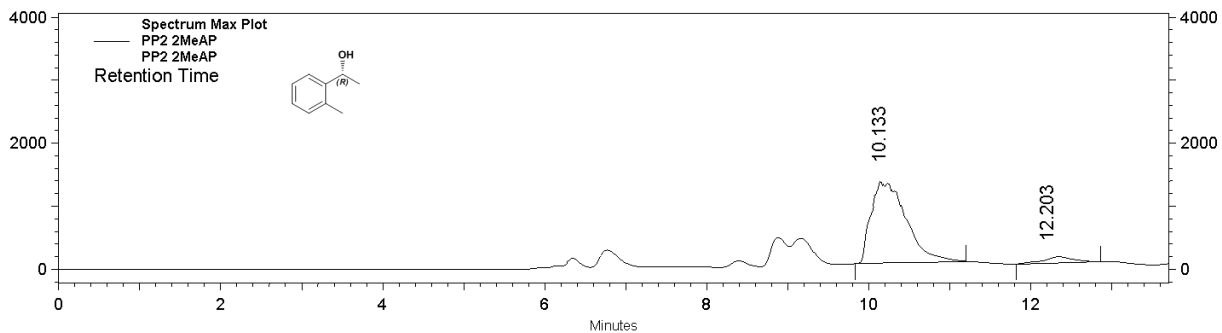


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.176	39285728	75.553	1455559	82.995
2	11.915	12711517	24.447	298230	17.005

Totals		51997245	100.000	1753789	100.000
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Entry 8

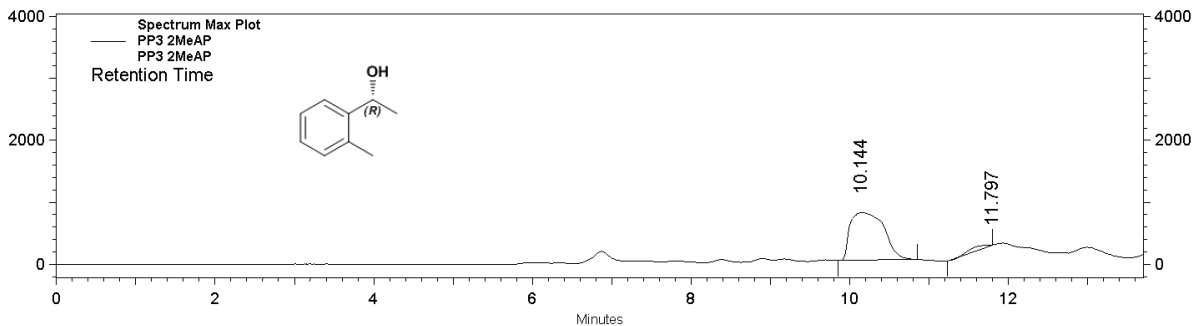


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.133	77473383	94.031	2586113	95.960
2	12.203	4918152	5.969	108891	4.040

Totals		82391535	100.000	2695004	100.000
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Entry 9

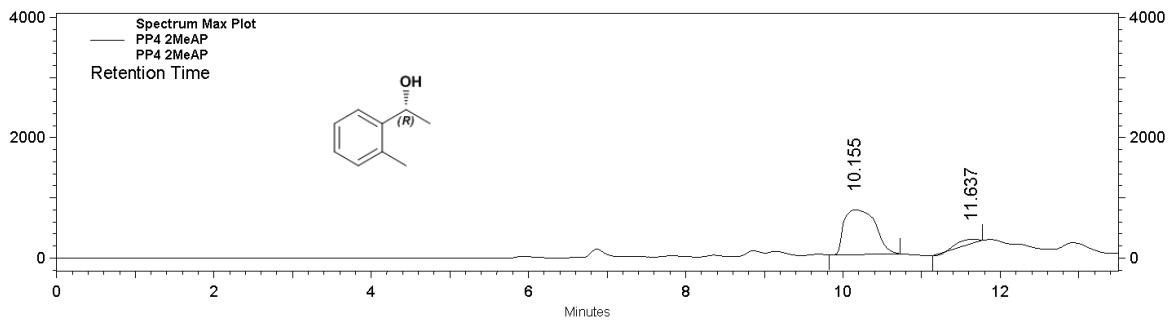


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.144	45028319	96.456	1531838	99.588
2	11.797	1654289	3.544	6339	0.412

Totals		46682608	100.000	1538177	100.000
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Entry 10

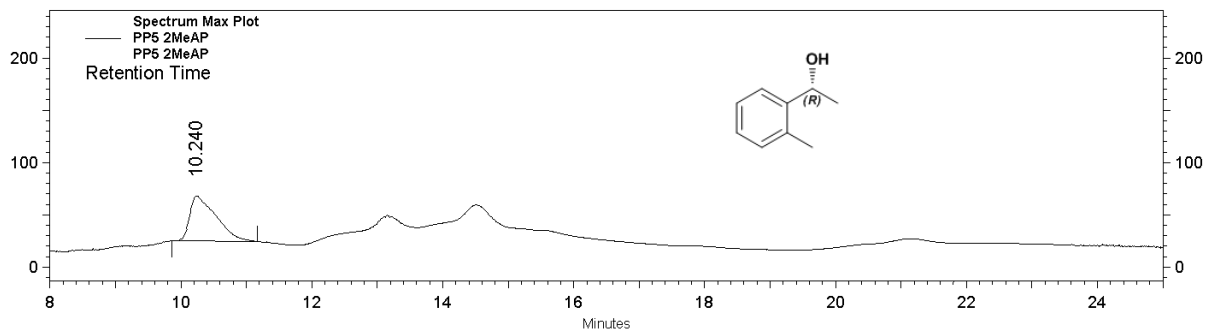


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.155	40429599	93.590	1479584	91.750
2	11.637	2769137	6.410	133050	8.250

Totals		43198736	100.000	1612634	100.000
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Entry 11

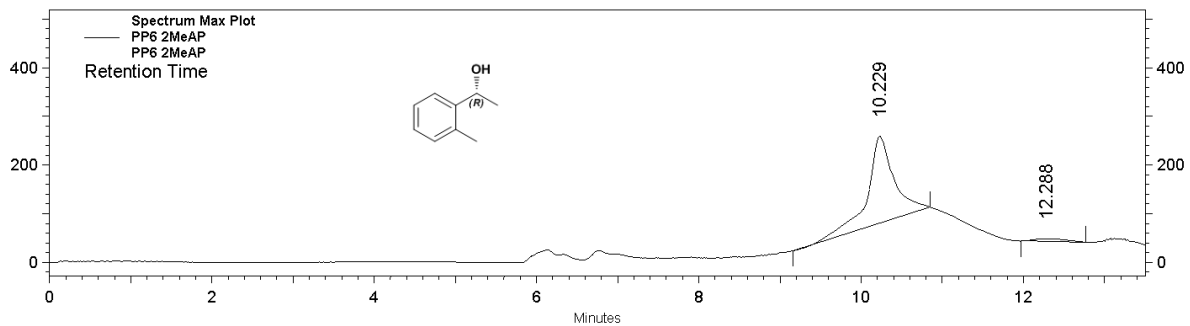


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.240	3003353	100.000	107675	100.000

Totals		3003353	100.000	107675	100.000
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Entry 12

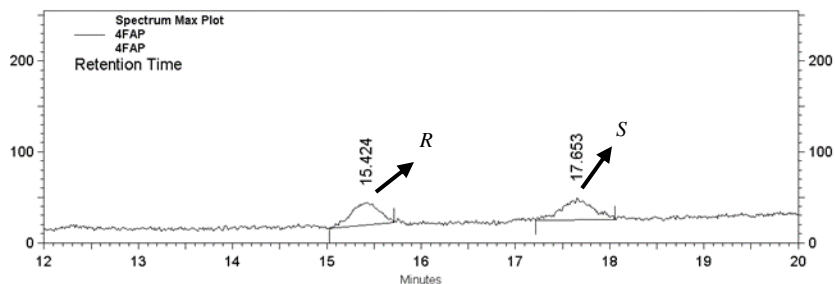


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	10.229	8203886	96.368	356728	96.911
2	12.288	309182	3.632	11369	3.089

Totals		8513068	100.000	368097	100.000
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Racemic 1-(4-fluorophenyl)ethanol

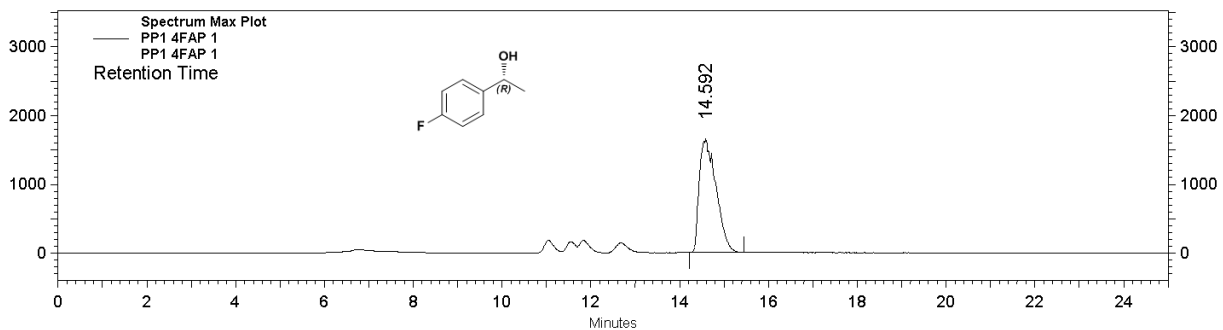


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.424	508489	48.176	24551	50.479
2	17.653	546993	51.824	24085	49.521

Totals		1055482	100.000	48636	100.000
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Entry 13

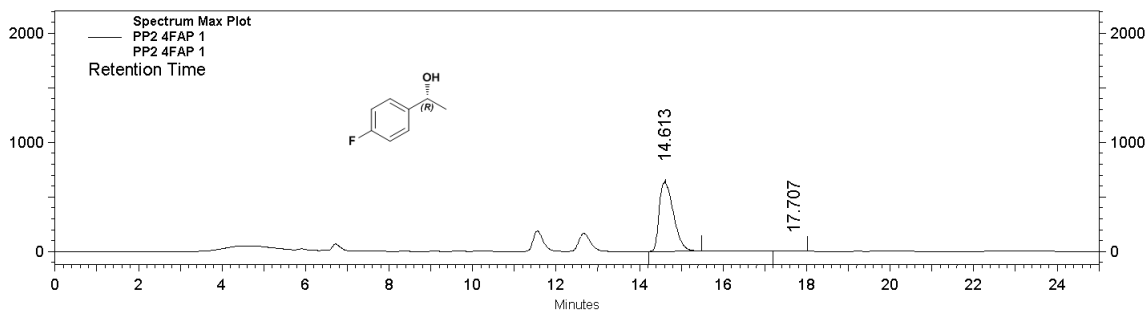


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	14.592	86694201	100.000	3307094	100.000

Totals		86694201	100.000	3307094	100.000
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Entry 14

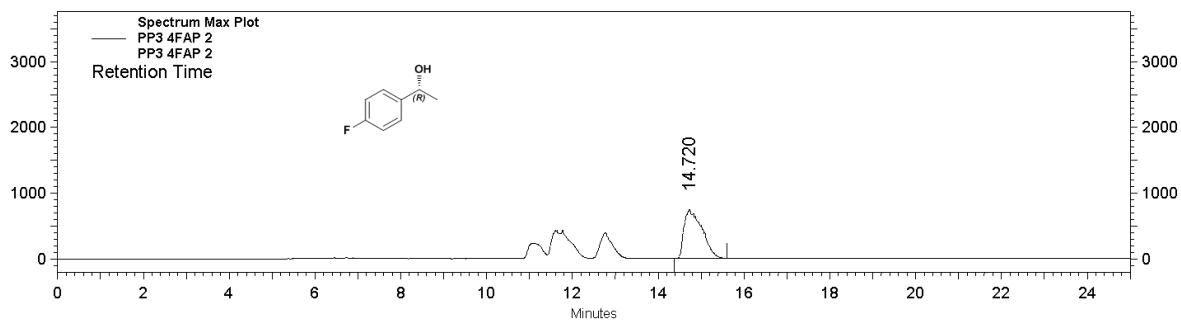


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	14.613	49665792	99.898	2189511	99.889
2	17.707	50710	0.102	2426	0.111

Totals		49716502	100.000	2191937	100.000
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Entry 15

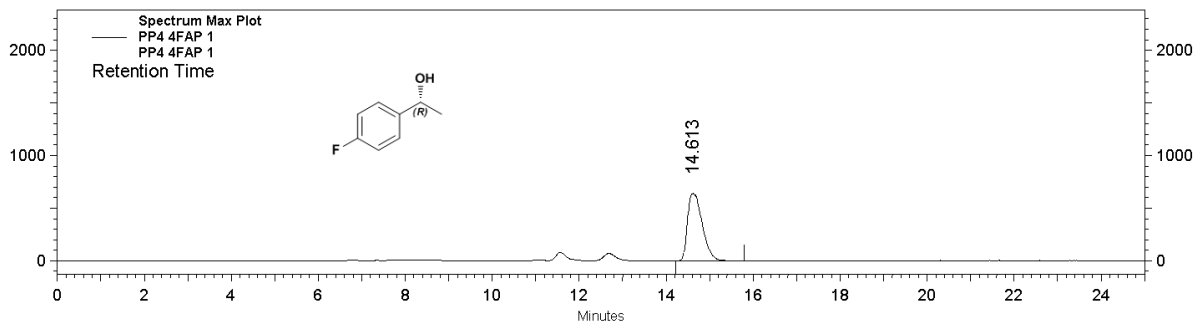


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	14.720	107694134	100.000	3719068	100.000

Totals		107694134	100.000	3719068	100.000
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Entry 16

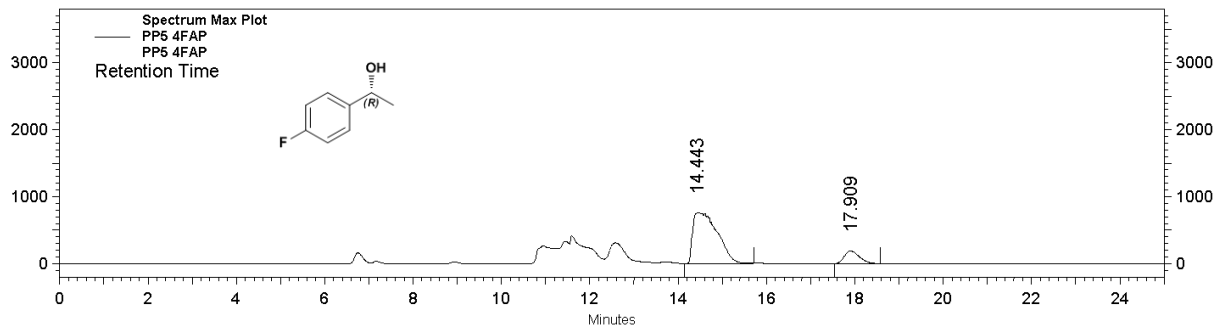


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	14.613	49787551	100.000	2127101	100.000

Totals		49787551	100.000	2127101	100.000
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Entry 17

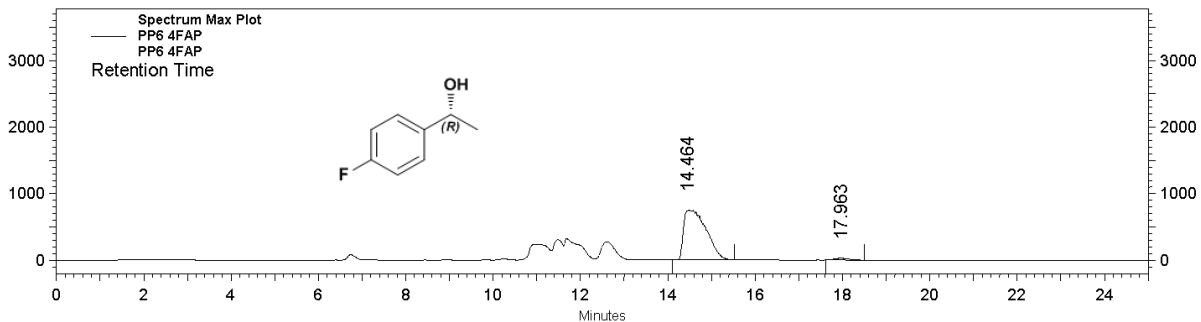


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	14.443	146222986	86.941	3787786	80.179
2	17.909	21962529	13.059	936384	19.821

Totals		168185515	100.000	4724170	100.000
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Entry 18

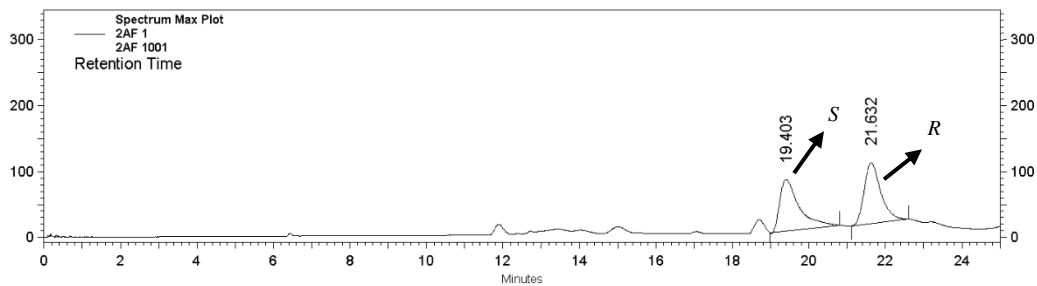


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	14.464	133959754	97.649	3736982	96.342
2	17.963	3225486	2.351	141899	3.658

Totals		137185240	100.000	3878881	100.000
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Racemic 1-(furan-2-yl)ethanol

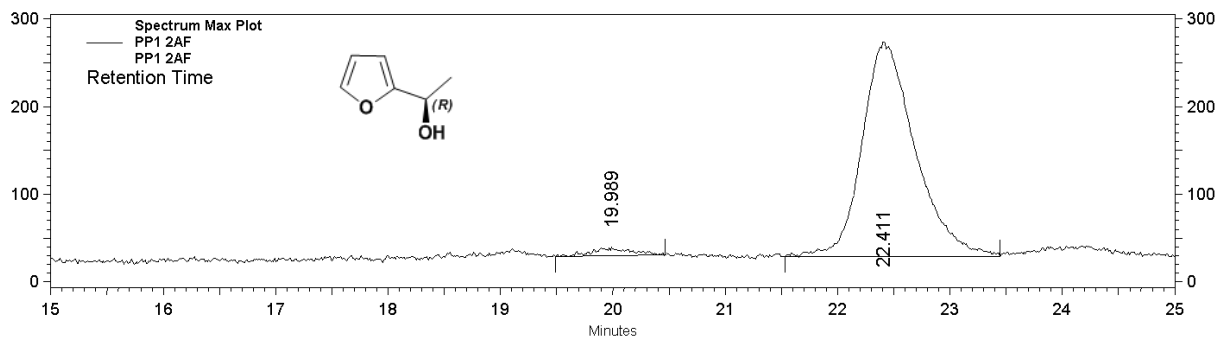


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.403	1399334	50.055	39238	45.952
2	21.632	1396254	49.945	46152	54.048

Totals		2795588	100.000	85390	100.000
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Entry 19

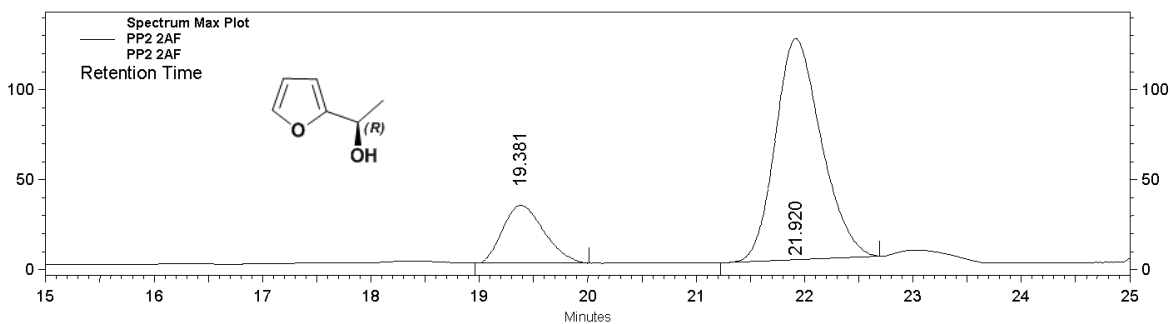


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.989	218889	2.659	10072	3.954
2	22.411	8013375	97.341	244637	96.046

Totals		8232264	100.000	254709	100.000
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Entry 20

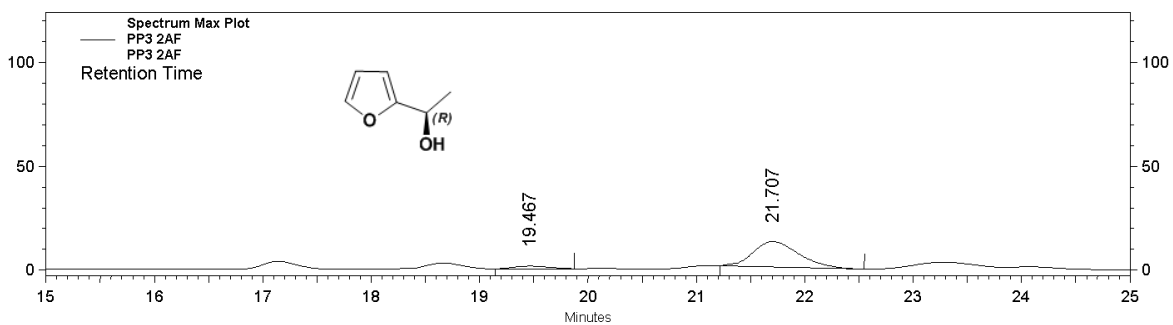


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.381	844268	18.912	31966	20.645
2	21.920	3620001	81.088	122873	79.355

Totals		4464269	100.000	154839	100.000
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Entry 21

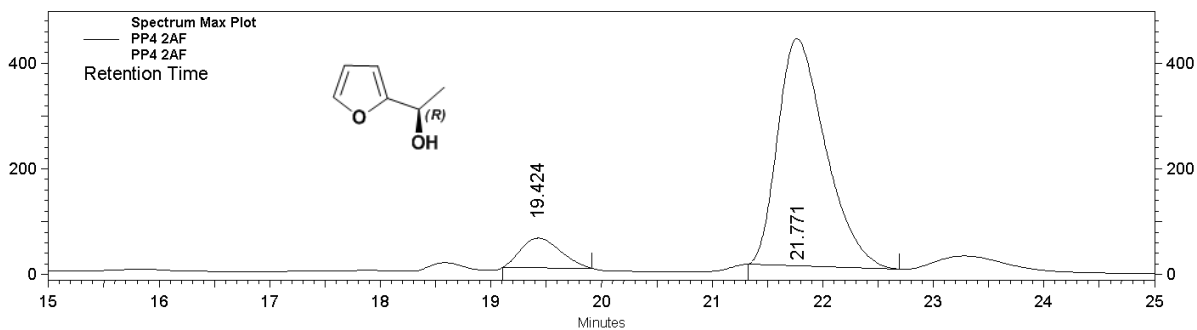


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.467	141014	7.326	6395	9.497
2	21.707	1783945	92.674	60941	90.503

Totals		1924959	100.000	67336	100.000
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Entry 22

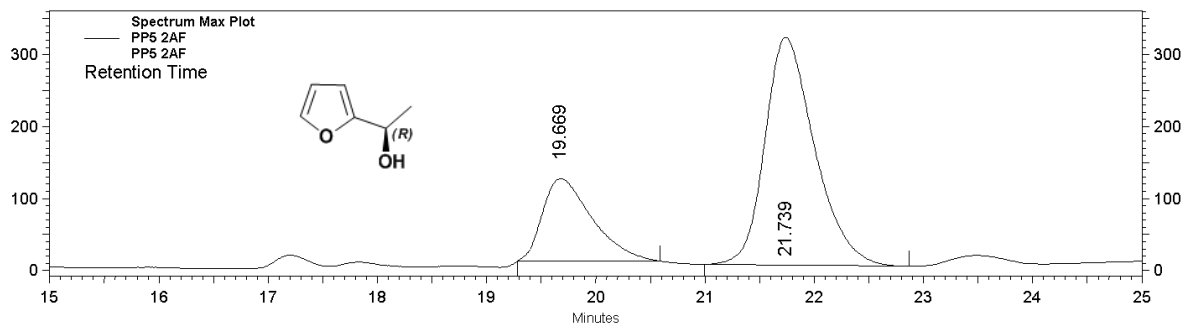


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.424	1407363	9.843	56549	11.630
2	21.771	12890807	90.157	429665	88.370

Totals		14298170	100.000	486214	100.000
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Entry 23

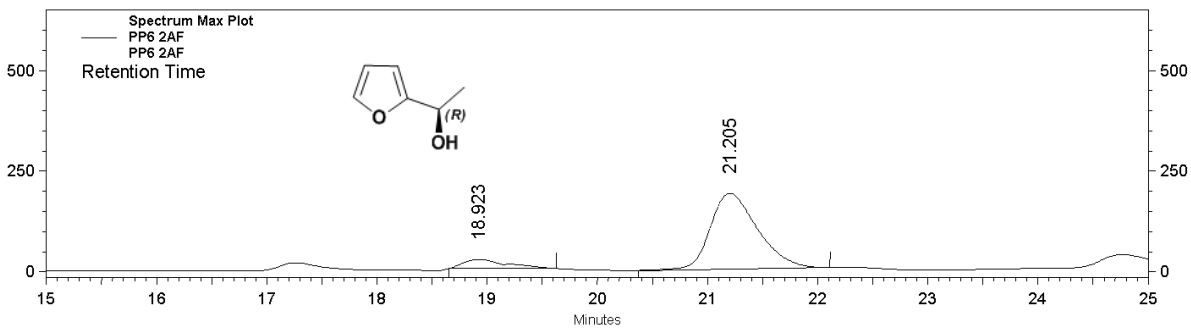


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	19.669	3611698	26.467	114217	26.534
2	21.739	10034490	73.533	316232	73.466

Totals		13646188	100.000	430449	100.000
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Entry 24

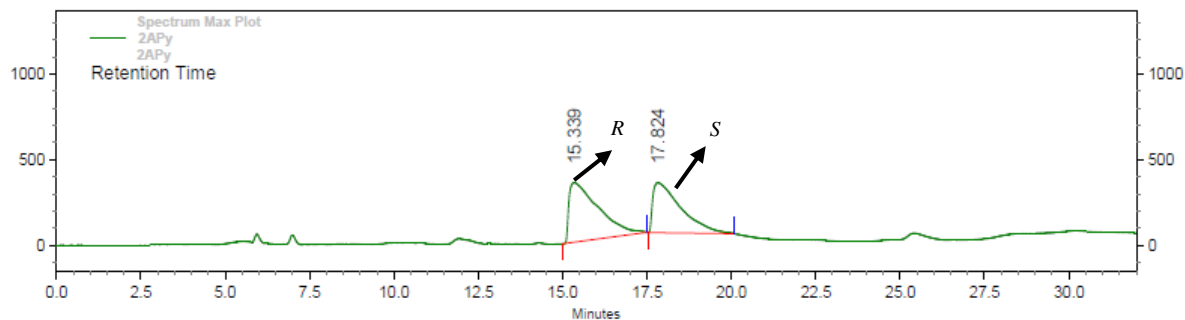


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	18.923	2083369	10.122	75724	10.799
2	21.205	18499209	89.878	625462	89.201

Totals		20582578	100.000	701186	100.000
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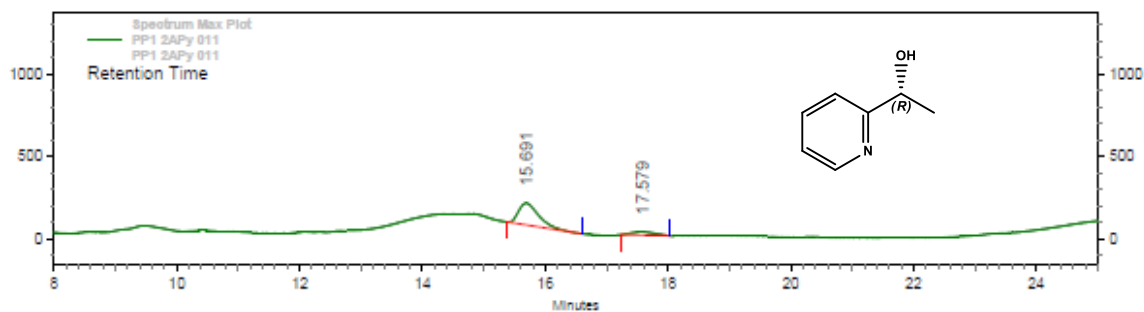
Racemic 1-(pyridin-2-yl)ethanol



Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.339	69784216	55.323	1159527	54.368
2	17.824	56355467	44.677	973229	45.632
Totals		126139683	100.000	2132756	100.000

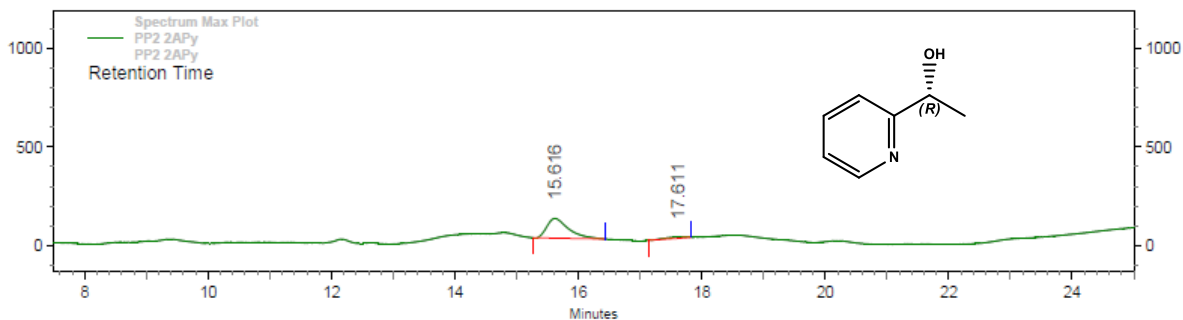
Entry 25



Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.691	2996478	85.227	131181	87.265
2	17.579	519418	14.773	19144	12.735
Totals		3515896	100.000	150325	100.000

Entry 26

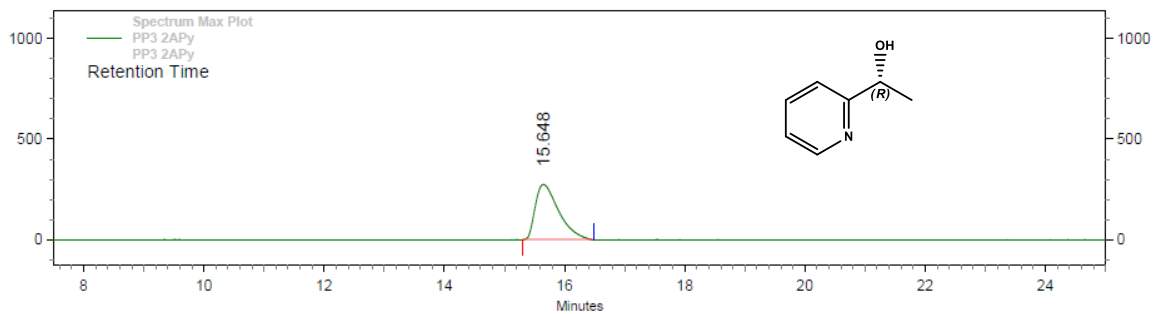


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.616	2444973	94.480	100344	94.685
2	17.611	142843	5.520	5633	5.315

Totals		2587816	100.000	105977	100.000
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Entry 27

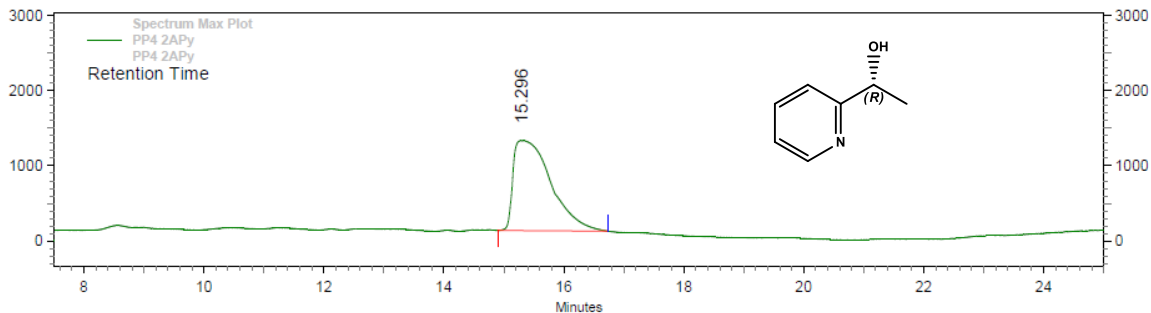


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.648	14767104	100.000	547707	100.000

Totals		14767104	100.000	547707	100.000
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Entry 28

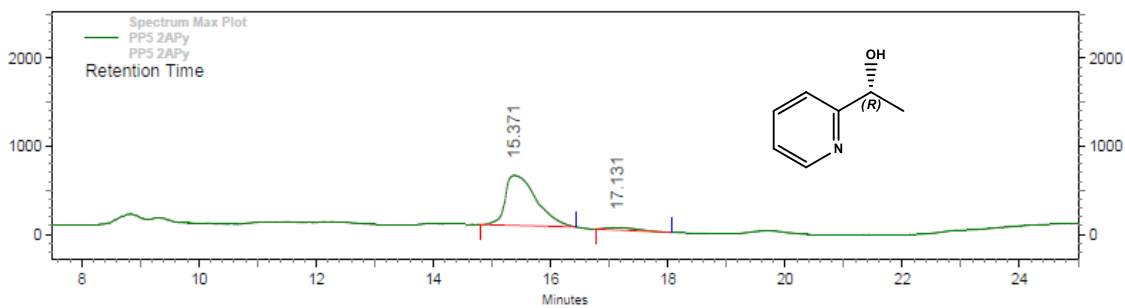


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.296	104787843	100.000	2392178	100.000

Totals		104787843	100.000	2392178	100.000
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Entry 29

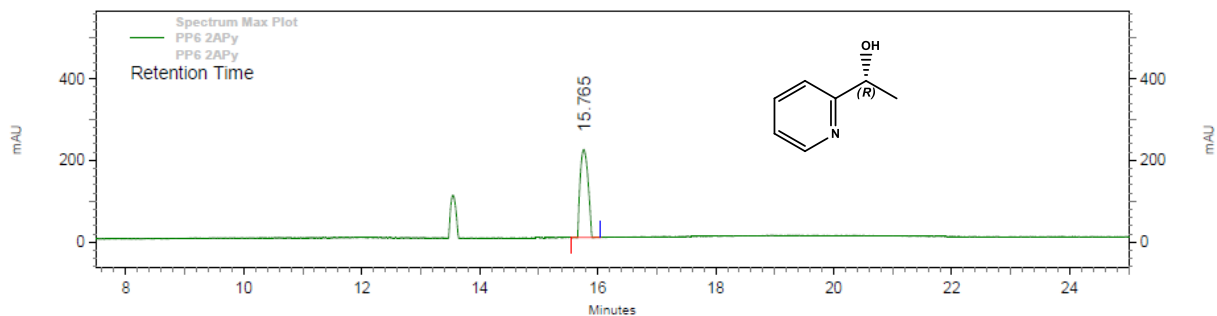


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.371	69515998	95.319	1883452	95.322
2	17.131	3413997	4.681	92439	4.678

Totals		72929995	100.000	1975891	100.000
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Entry 30

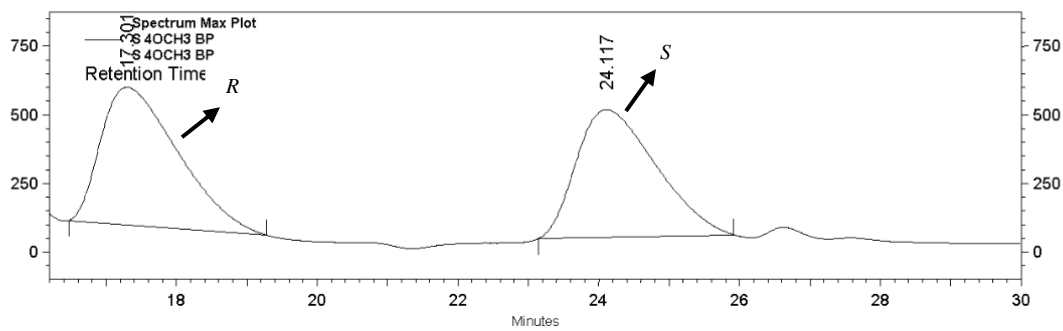


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	15.765	199979	100.000	21537	100.000

Totals		199979	100.000	21537	100.000
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Racemic (4-methoxyphenyl)(phenyl)methanol

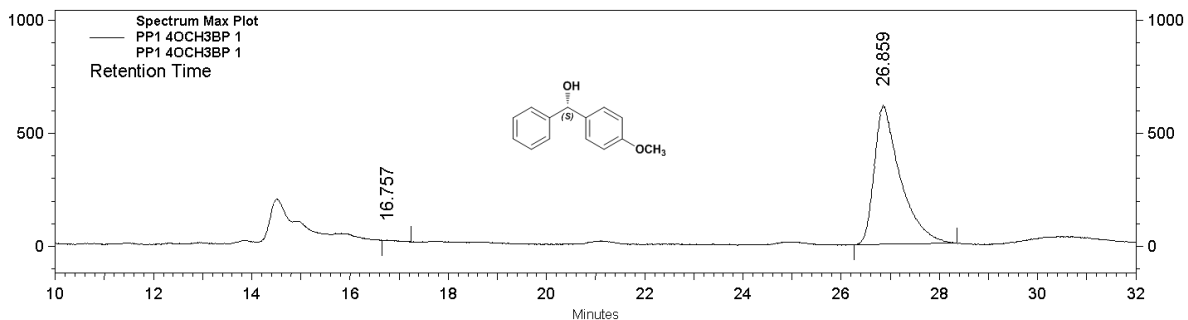


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	17.301	38217289	51.131	500784	51.853
2	24.117	36527002	48.869	465001	48.147

Totals		74744291	100.000	965785	100.000
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Entry 31

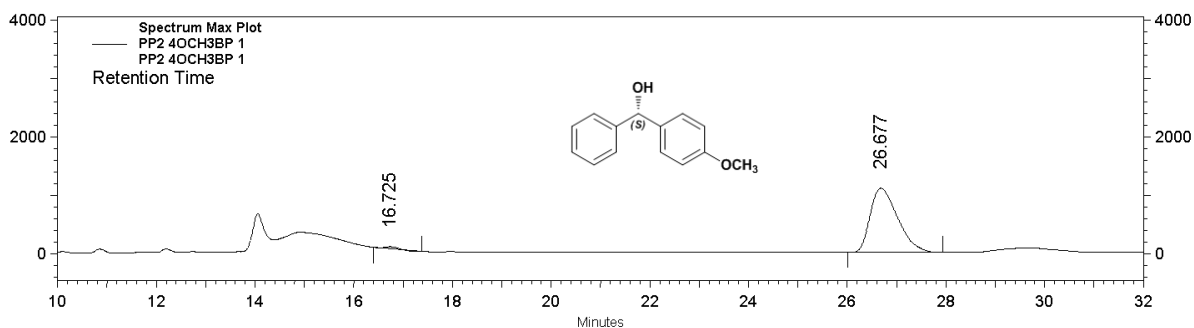


Spectrum Max Plot

PK #	Retention Time	Area	Area %	Height	Height %
1	16.757	43456	0.115	5431	0.527
2	26.859	37627474	99.885	1025271	99.473

Totals		37670930	100.000	1030702	100.000
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Entry 32

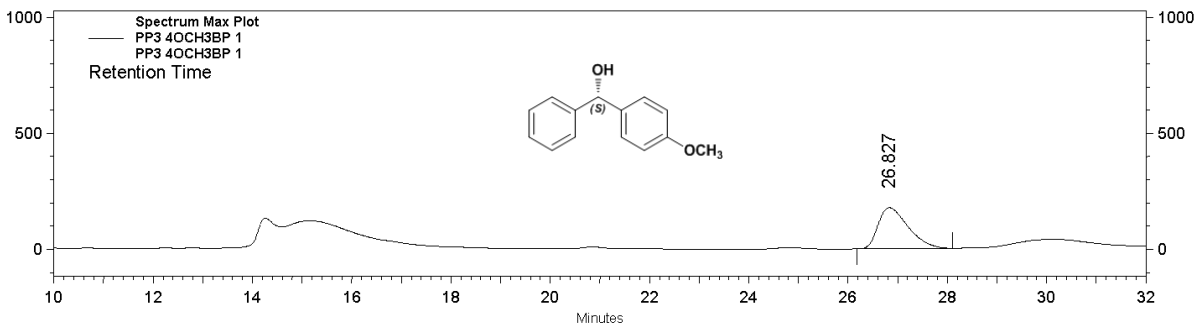


Spectrum Max Plot

PK #	Retention Time	Area	Area %	Height	Height %
1	16.725	106596	1.261	7144	3.176
2	26.677	8346065	98.739	217805	96.824

Totals		8452661	100.000	224949	100.000
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Entry 33

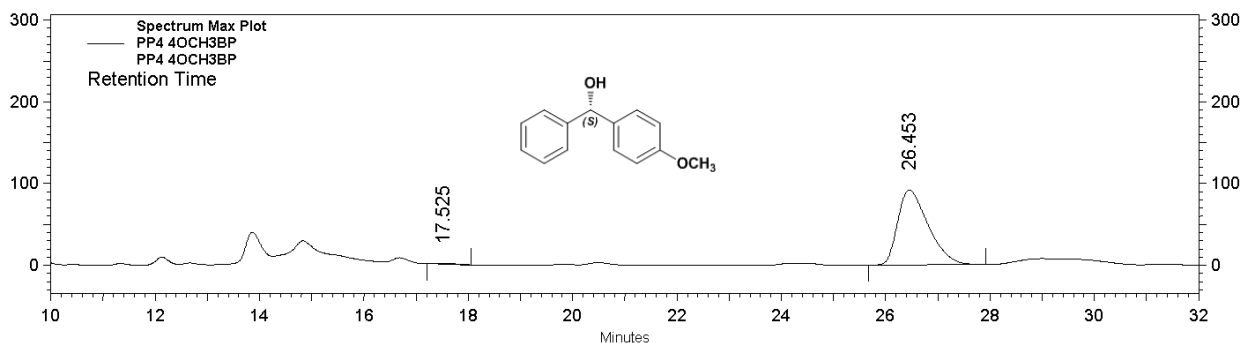


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	26.827	14777964	100.000	353287	100.000

Totals		14777964	100.000	353287	100.000
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Entry 34

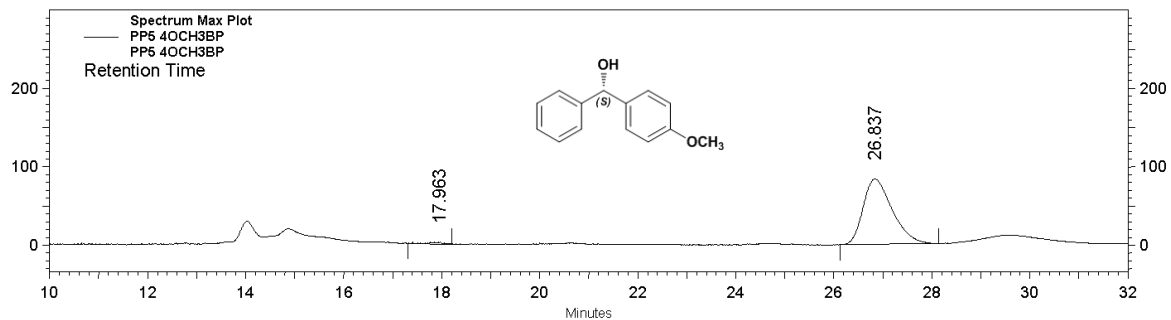


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	17.525	107901	0.862	3965	1.284
2	26.453	12408754	99.138	304898	98.716

Totals		12516655	100.000	308863	100.000
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Entry 35

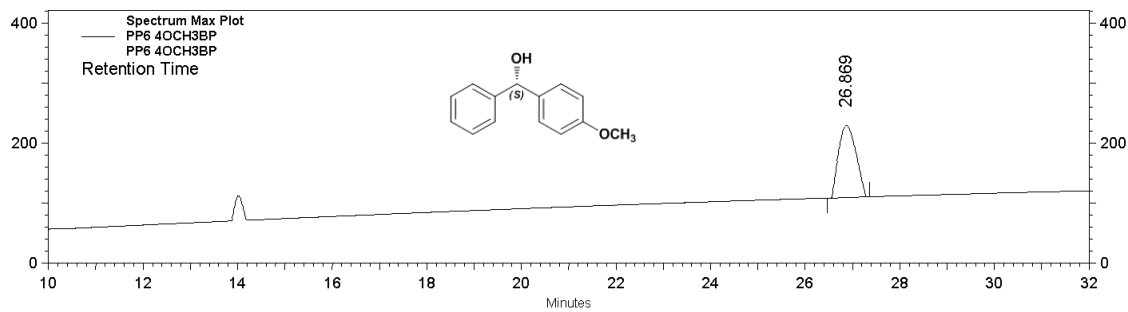


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	17.963	61097	1.052	4329	3.020
2	26.837	5745621	98.948	139038	96.980

Totals		5806718	100.000	143367	100.000
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Entry 36

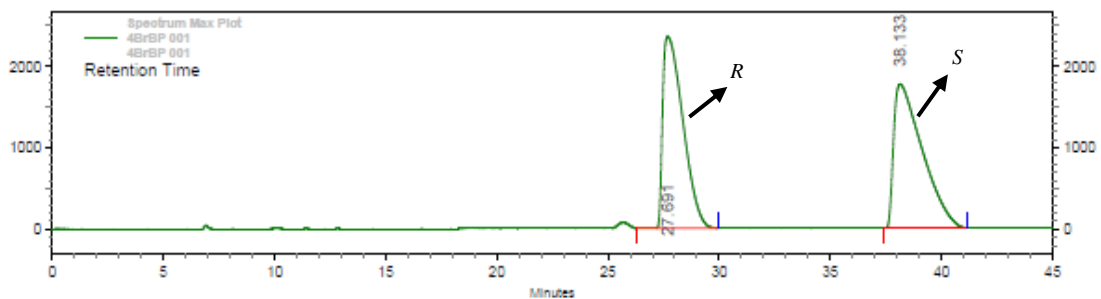


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	26.869	614391	100.000	23948	100.000

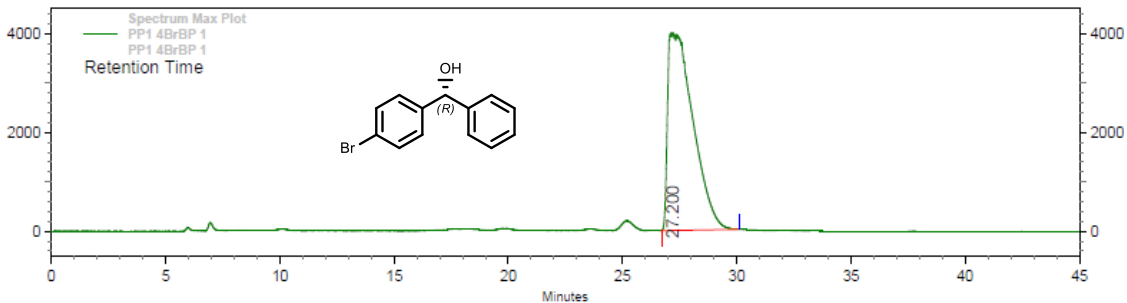
Totals		614391	100.000	23948	100.000
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Racemic (4-bromophenyl)(phenyl)methanol



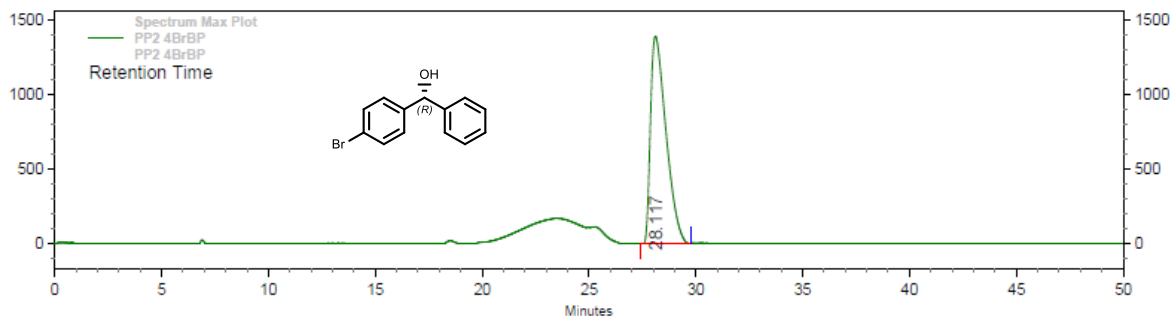
Spectrum Max Plot					
Pk #	Retention Time	Area	Area %	Height	Height %
1	27.691	148509642	48.541	2362179	57.231
2	38.133	157436009	51.459	1765248	42.769
Totals		305945651	100.000	4127427	100.000

Entry 37



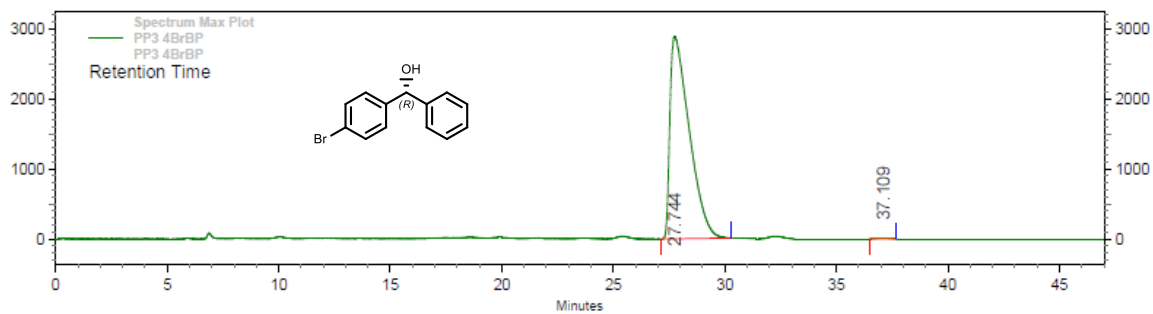
Spectrum Max Plot					
Pk #	Retention Time	Area	Area %	Height	Height %
1	27.200	309107929	100.000	4010725	100.000
Totals		309107929	100.000	4010725	100.000

Entry 38



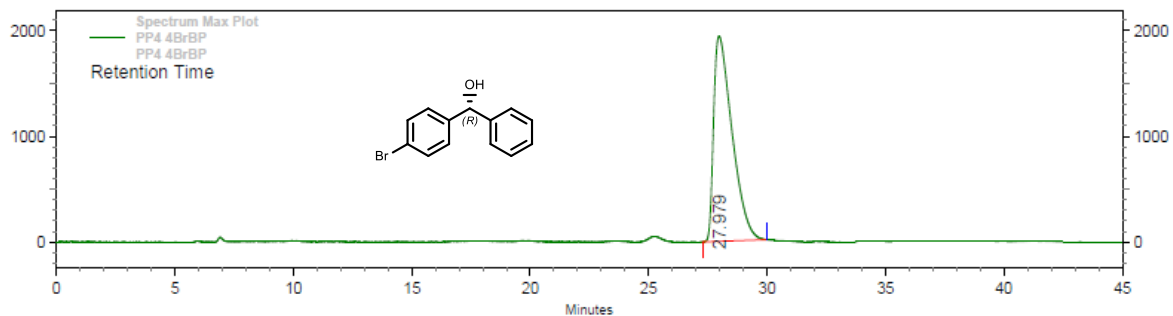
Spectrum Max Plot					
Pk #	Retention Time	Area	Area %	Height	Height %
1	28.117	69888064	100.000	1392453	100.000
Totals		69888064	100.000	1392453	100.000

Entry 39



Spectrum Max Plot					
Pk #	Retention Time	Area	Area %	Height	Height %
1	27.744	173419757	99.805	2883061	99.698
2	37.109	338305	0.195	8725	0.302
Totals		173758062	100.000	2891786	100.000

Entry 40

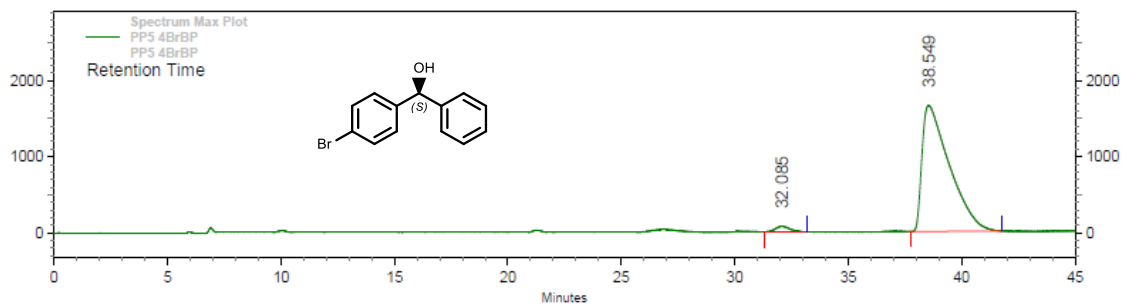


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	27.979	104999494	100.000	1943610	100.000

Totals	Area	Area %	Height	Height %
	104999494	100.000	1943610	100.000

Entry 41

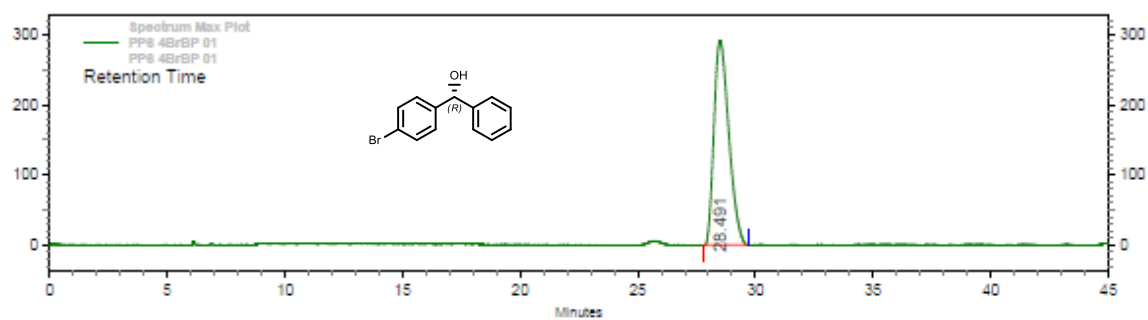


Spectrum Max Plot

Pk #	Retention Time	Area	Area %	Height	Height %
1	32.085	3361370	2.364	73858	4.266
2	38.549	138811124	97.636	1657328	95.734

Totals	Area	Area %	Height	Height %
	142172494	100.000	1731186	100.000

Entry 42



Spectrum Max Plot					
Pk #	Retention Time	Area	Area %	Height	Height %
1	28.491	12777641	100.000	291162	100.000
Totals		12777641	100.000	291162	100.000