Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Chemo- and Regioselective Hydroformylation of Alkenes with CO_2/H_2 over a Bifunctional Catalyst

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1 Material and Methods

General. All reactions and operations involving air- or moisture-sensitive compounds were performed in Ar-filled glove box. Unless otherwise noted, all commercially available reagents were used without further purification. Among these, extra-dry solvents with water⩽50 ppm (by K.F.) were bought from Energy Chemical. And all reactions were carried out in a Teflon-lined stainless steel reactor of 50 mL capacity equipped with a magnetic stirrer.

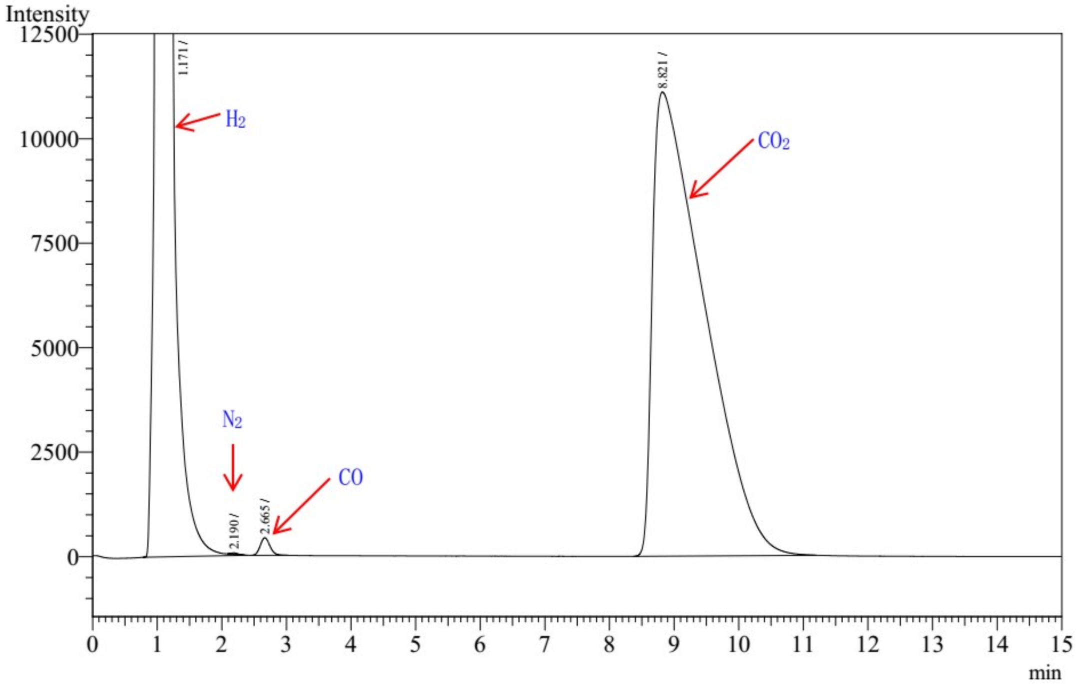
Instrumentation. GC analysis was performed on Shimadzu-2014 with a FID detector and a Stabilwax®-DA column (60 m, 0.53 mm, 0.5 μm). The gaseous mixture was collected and analyzed by gas chromatography equipped with thermal conductivity detector (Shimadzu GC-2014C) with Argon as the carrier gas. ESI-MS analysis was performed on WATERS 2695+ZQ2000. Detected masses are given in m/z and correlated to calculated masses of the respective species. High resolution MS (omni star gas analysis system) analyses were performed to detect ^{13}CO after $^{13}CO_2$ Isotope experiment. Detected masses are given in m/z and correlated to calculated masses of the respective species. ^1H- and ^{13}C- NMR spectra were recorded on Bruker Avance III 400 MHz spectrometers. Chemical shifts (δ values) were reported in ppm relative to internal TMS.

Calculation of the CO amount in the gaseous product. We quantified the gas from the reactor by the internal standard method (nitrogen as the internal standard). The relative correction factor (f) and correlation coefficients of each component are shown in the following table:

component	H_2	CO	CH_4	CO_2
Correction factor(f)	0.111738704	1.099931423	0.37969925	1.223846589
Correl	0.999999858	0.99933951	0.999991074	0.999999152

GC analysis of the gas sample clearly indicates the presence of CO, residual H_2 and CO_2 in the gas phase of the reaction system (Figure S1).

Figure S1 GC spectra of the gas phase after the reaction

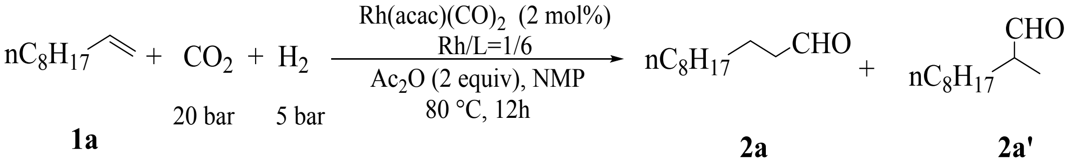


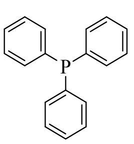
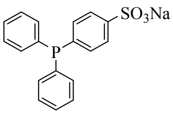
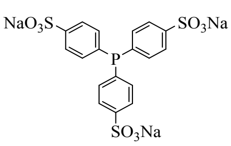
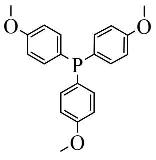
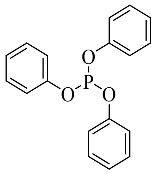
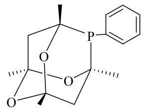
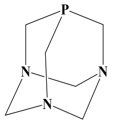
2 Typical procedure for hydroformylation of alkenes with CO_2/H_2

General procedure: All reactions were carried out in a Teflon-lined stainless steel reactor of 50 mL capacity equipped with a magnetic stirrer. Typically, in a glovebox, 1-decene (1.0 mmol), $Rh(acac)(CO)_2$ (0.02 mmol), ligand (0.12 mmol), Ac_2O (2.0 mmol) and NMP (4 mL) were loaded into the reactor. The autoclave was sealed and purged three times with CO_2 gas, subsequently charged with CO_2 (20 bar), then H_2 (5 bar) to total pressure of 5 bar. The autoclave was then heated at 80 °C for 12 h. After the reaction, the autoclave was cooled in ice water and then the gas was carefully vented into the airbag. The resulting clear solution was diluted with N-methyl-2-pyrrolidinone (10 mL) and added benzyl alcohol (0.5 mmol) or isooctane (0.3 mmol) as internal standard. The sample was filtered through a short cotton plug, and the filtrate was firstly analyzed by GC-MS to determine the structures of the aldehyde products, then immediately analyzed by GC to determine the conversion of alkenes, yields of the aldehydes, and the regioselectivity (n/iso ratio) as well as percentage of isomerization and hydrogenation products. Yields were found to be reproducible within Y = ±5% in three independent runs for selected experiments.

Gas chromatography method: Stabilwax®-DA column (60 m, 0.53 mm, 0.5 μm). Temperature: 35 °C for 4 min, then heated to 100 °C at 10 °C min^{-1} for 2 min, rated 10 °C/min to 240 °C and held 10 min, $t_{r\ major}$=21.2 min.

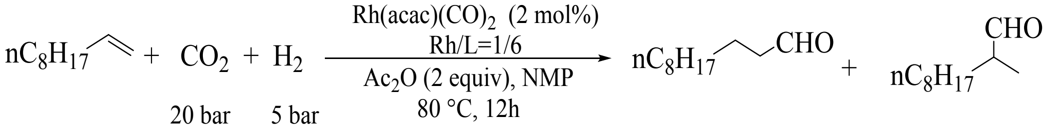
Table S1. The effect of monodentate phosphine ligands[a]



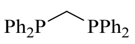
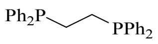
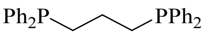
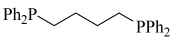
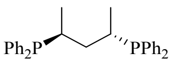
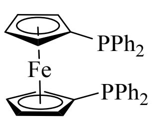
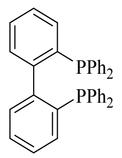
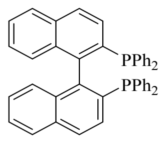
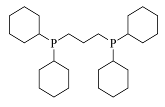
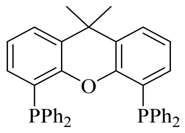
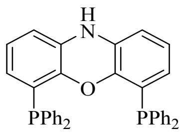
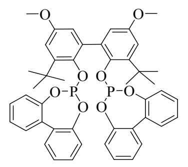
Ligand					
	L1	L2	L3	L4	L5
Y/l/b[b]	15%/3.3	16%/2.8	14%/9.0	26%/3.1	0/-
Ligand			Without Ligand		
	L6 (CgPPh)	L7	-		
Y/l/b[b]	18%/3.2	90%/8.1	3%/5.7		

[a] Reaction conditions: 1-decene (1 mmol), $Rh(acac)(CO)_2$ (0.02 mmol), ligand (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard. GC at page 18-25.

Table S2 The effect of bidentate phosphine ligands[a]



1a **2a** **2a'**

Ligand					
	L1	L2	L3	L4	L5
Y/l/b[b]	6%/2.0	0/-	57%/1.1	87%/4.0	11%/3.0
Ligand					
	L6	L7	L8	L9	L10
Y/l/b[b]	6%/13.0	20%/12.0	15%/6.0	15%/4.7	5%/1.2
Ligand					
	L11	L12			
Y/l/b[b]	6%/1.4	0/-			

[a] Reaction conditions: 1-decene (1 mmol), $Rh(acac)(CO)_2$ (0.02 mmol), ligand (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard. GC at page 26-37.

Table S3 The effect of Rh precursor[a]

Entry	Rh source	PTA/Rh	2a+2a'[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	GC at page
1	$(PPh_3)_3(CO)Rh\text{-}H$	-	17	65/35	47	36	38
2	$Rh(OAc)_3$	6	80	90/10	11	9	39
3	$RhCl(CO)_2$	6	17	93/7	77	6	40
4	$Rh(NO_3)_3$	6	0	-	98	2	41
5	$Rh(acac)(CO)_2$	6	90	89/11	7	3	42

[a] Reaction conditions: 1-decene (1 mmol), Rh precursor (0.02 mmol), PTA (0 or 0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard.

Table S4 The effect of PTA/Rh[a]

Entry	PTA/Rh	2a+2a’[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	GC at page
1	0	3	85/15	83	14	43
2	3	25	68/32	22	42	44
3	6	90	89/11	7	3	45
4	9	68	90/10	28	5	46

[a] Reaction conditions: 1-decene (1 mmol), Rh(acac)$(CO)_2$ (0.02 mmol), PTA (0 - 0.18 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard.

Table S5 The effect of the solvent[a]

Entry	Solvent	2a+2a'[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	GC at page
1	NMP	90	89/11	7	3	47
2	DMI	83	91/9	8	9	48
3	DMSO	73	89/11	26	1	49
4	DMF	68	86/14	26	6	50
5	THF	34	97/3	14	52	51
6	toluene	27	95/5	59	14	52
7	CH_3CN	26	90/10	49	25	53
8	1,4-Dioxane	16	92/8	17	68	54

[a] Reaction conditions: 1-decene (1 mmol), $Rh(acac)(CO)_2$ (0.02 mmol), PTA (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, solvent (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard.

Table S6 The effect of the temperature[a]

Entry	T/ºC	2a+2a’[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	GC at page
1	60	65	93/7	19	16	55
2	70	84	87/13	9	7	56
3	80	90	89/11	7	3	57
4	90	85	89/11	10	5	58
5	100	75	90/10	11	14	59
6	120	78	84/16	12	10	60

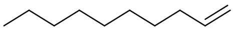
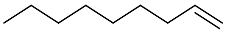
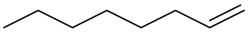
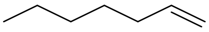
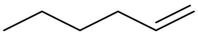
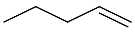
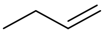
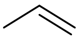
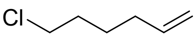
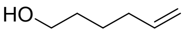
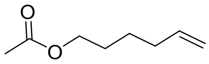
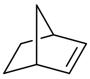
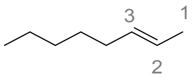
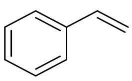
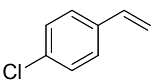
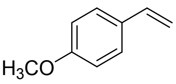
[a] Reaction conditions: 1-decene (1 mmol), Rh(acac)$(CO)_2$ (0.02 mmol), PTA (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard.

Table S7 The effect of the P_{CO2}/P_{H2}[a].

Entry	P_{CO2}/P_{H2} bar/bar	2a+2a'[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	GC at page
1	40/10	88	87/13	7	5	61
2	20/5	90	89/11	7	3	62
3	22/3	83	92/8	11	6	63
4	10/3	87	91/9	9	4	64
5	7/3	74	94/6	13	13	65
6	12/12	42	87/13	19	39	66

[a] Reaction conditions: 1-decene (1 mmol), Rh(acac)$(CO)_2$ (0.02 mmol), PTA (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard.

Table S8: Substrate scope.[a]

Entry	Alkene	Conv./%[b]	Yield [b]/%	l/b	Iso[b]/%	H[b]/%	GC at page
1		99	92	90/10	3	3	67
2		99	96	90/10	1	1	68
3		99	96	88/12	2	1	69
4		99	95	86/14	2	1	70
5		100	97	85/15	2	<1	71
6		99	95	86/14	2	2	72
7[c]		-	77	93/7	-	-	73
8[c]		-	73	85/15	-	-	74
9[c]		-	72	-	-	-	75
10		98	87	87/13	2	8	76
11		99	92	73/27	1	6	77
12		98	90	85/15	3	4	78
13[d]		76	75	-	0	1	79
14[e]		90	64	16/84	25	1	80
15		99	90	10/90	0	1	81
16		98	47	17/83	0	4	82
17		94	91	16/84	0	<1	83

[a] Alkene (1 mmol), Rh(acac)$(CO)_2$ (0.022 mmol), PTA (0.132 mmol), Ac_2O (2.0 mmol), NMP (4 mL), H_2/CO_2=5/20 bar, 80 ° C, 12 h,. [b] Determined by GC analysis with benzyl alcohol or isooctane as the internal standard. [c] alkene (3 mmol), Ac_2O (4.5 mmol). [d] T = 90 ºC. [e] T=100 ºC, 24 h. 1-CHO: 2-CHO: 3-CHO=16:60:24.

Table S9 Control experiments with different ligands.[a]

a) PPh_3

Entry	t/h	2a+2a'[b]/%	l/b[b]	CO/mmol	GC at page
1	0.5	8	82/18	0.10	84
2	1	10	90/10	0.12	86
3	2	13	76/24	0.08	88
4	6	13	80/20	0.08	90
5	12	15	74/26	trace	92

b) Xantphos

Entry	t/h	2a+2a'[b]/%	l/b[b]	CO/mmol	GC at page
1	0.5	0	0	0	94
2	1	3	60/40	trace	96
3	2	3	62/38	0.01	98
4	6	4	59/41	0.03	100
5	12	5	50/50	0.05	102

c) dppb

Entry	t/h	2a+2a'[b]/%	l/b[b]	CO/mmol	GC at page
1	0.5	58	79/21	0.25	104
2	1	61	82/18	0.39	106
3	2	73	80/20	0.66	108
4	6	87	80/20	0.61	110
5	12	92	78/22	0.51	112

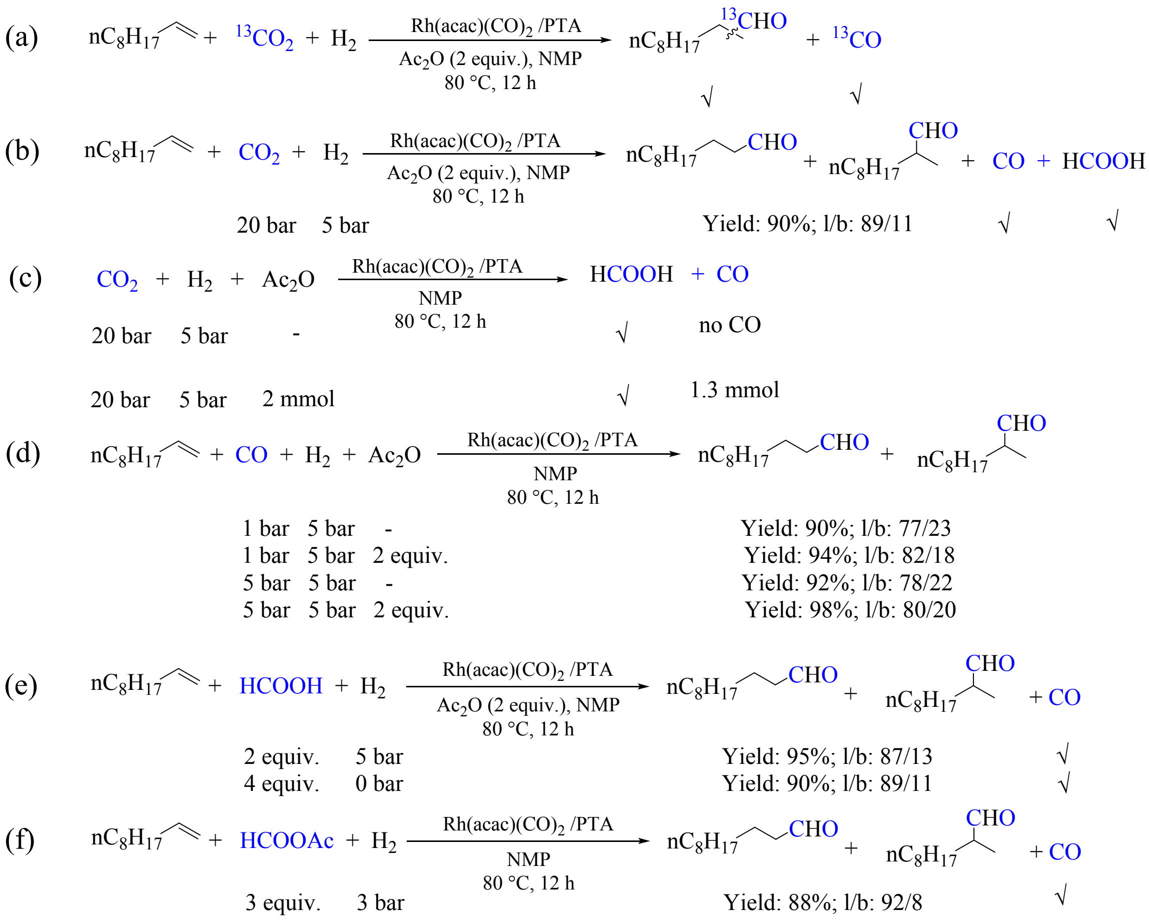
[a] Reaction conditions: 1-decene (1 mmol), $Rh(acac)(CO)_2$ (0.02 mmol), ligand (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard. The data of PTA please see Table S12.

Table S10 Control experiments with different acids additives.[a]

Entry	additive	2a+2a'[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	GC at page
1	-	90	89/11	7	3	114
2	PTSA	0	-	97	1	115
3	CH_3SO_3H	trace	-	84	15	116
4[c]	-	92	78/22	7	trace	117
5[c,d]	HCOOH	94	77/23	5	1	118
6[c,e]	HCOOH	94	74/26	5	trace	119
7[c,e]	Ac_2O	98	80/20	1	trace	120
8[c,f]	HCOOH+Ac_2O	91	84/16	9	trace	121

[a] Reaction conditions: 1-decene (1 mmol), Rh(acac)$(CO)_2$ (0.02 mmol), ligand (0.12 mmol), additive (0.1 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, 12 h, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard. [c] Reaction conditions: 1-decene (1 mmol), Rh(acac)$(CO)_2$ (0.02 mmol), ligand (0.12 mmol), H_2/CO = 5/5 bar, 80 °C, 12 h, NMP (4 mL). [d] additive (0.3 mmol). [e] additive (2.0 mmol). [f] HCOOH (0.3 mmol) and Ac_2O (2.0 mmol).

Table S11: Isotope-Labeling Experiments and Control Experiment



(a) nC_8H_{17} + $^{13}CO_2$ + H_2 $\xrightarrow[\text{Ac}_2\text{O (2 equiv.), NMP, 80 °C, 12 h}]{\text{Rh(acac)(CO)}_2\text{/PTA}}$ nC_8H_{17}–^{13}CHO + ^{13}CO

√ √

(b) nC_8H_{17} + CO_2 + H_2 $\xrightarrow[\text{Ac}_2\text{O (2 equiv.), NMP, 80 °C, 12 h}]{\text{Rh(acac)(CO)}_2\text{/PTA}}$ nC_8H_{17}–CHO + nC_8H_{17}–CHO + CO + HCOOH

20 bar 5 bar Yield: 90%; l/b: 89/11 √ √

(c) CO_2 + H_2 + Ac_2O $\xrightarrow[\text{NMP, 80 °C, 12 h}]{\text{Rh(acac)(CO)}_2\text{/PTA}}$ HCOOH + CO

CO_2	H_2	Ac_2O	HCOOH	CO
20 bar	5 bar	-	√	no CO
20 bar	5 bar	2 mmol	√	1.3 mmol

(d) nC_8H_{17} + CO + H_2 + Ac_2O $\xrightarrow[\text{NMP, 80 °C, 12 h}]{\text{Rh(acac)(CO)}_2\text{/PTA}}$ nC_8H_{17}–CHO + nC_8H_{17}–CHO

CO	H_2	Ac_2O	
1 bar	5 bar	-	Yield: 90%; l/b: 77/23
1 bar	5 bar	2 equiv.	Yield: 94%; l/b: 82/18
5 bar	5 bar	-	Yield: 92%; l/b: 78/22
5 bar	5 bar	2 equiv.	Yield: 98%; l/b: 80/20

(e) nC_8H_{17} + HCOOH + H_2 $\xrightarrow[\text{Ac}_2\text{O (2 equiv.), NMP, 80 °C, 12 h}]{\text{Rh(acac)(CO)}_2\text{/PTA}}$ nC_8H_{17}–CHO + nC_8H_{17}–CHO + CO

HCOOH	H_2		CO
2 equiv.	5 bar	Yield: 95%; l/b: 87/13	√
4 equiv.	0 bar	Yield: 90%; l/b: 89/11	√

(f) nC_8H_{17} + HCOOAc + H_2 $\xrightarrow[\text{NMP, 80 °C, 12 h}]{\text{Rh(acac)(CO)}_2\text{/PTA}}$ nC_8H_{17}–CHO + nC_8H_{17}–CHO + CO

3 equiv. 3 bar Yield: 88%; l/b: 92/8 √

√ **indicated the typical substance was detected.**

GC at page 122-130. NMR and Mass Spectra at page 147-153.

Table S12 Reaction profiles for the hydroformylation of **1a** with CO_2/H_2 catalyzed by Rh/PTA[a].

Entry	t/h	2a+2a'[b]/%	l/b[b]	1a+Iso[b]/%	H[b]/%	CO/mmol	GC at page
1	1/6	14	96/4	83	3	0.46	131
2	0.5	20	>96/4	75	5	0.91	133
3	1	57	<96/4	35	7	0.71	135
4	2	73	93/7	20	7	0.40	137
5	4	82	91/9	12	6	0.39	139
6	6	85	89/11	8	7	0.37	141
7	8	85	89/11	9	6	0.44	143
8	12	89	89/11	8	4	0.41	145

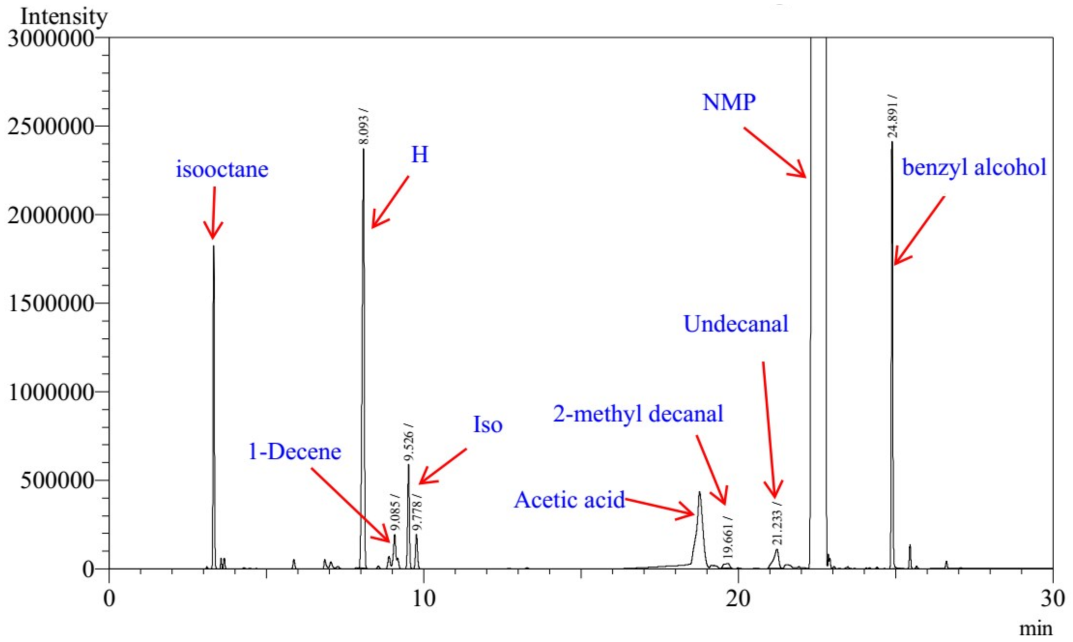
[a] Reaction conditions: 1-decene (1 mmol), $Rh(acac)(CO)_2$ (0.02 mmol), PTA (0.12 mmol), Ac_2O (2.0 mmol), H_2/CO_2 = 5/20 bar, 80 °C, NMP (4 mL). [b] Determined by GC with benzyl alcohol or isooctane as the internal standard.

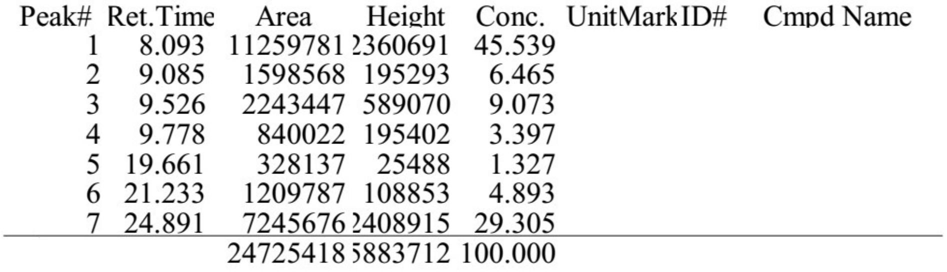
3 Gas chromatographic Data

In the following GC chromatograms, **H** represented the hydrogenation product of the corresponding alkene, and **Iso** represented the isomerization product of the alkene.

3.1 Gas chromatograms to Table S1

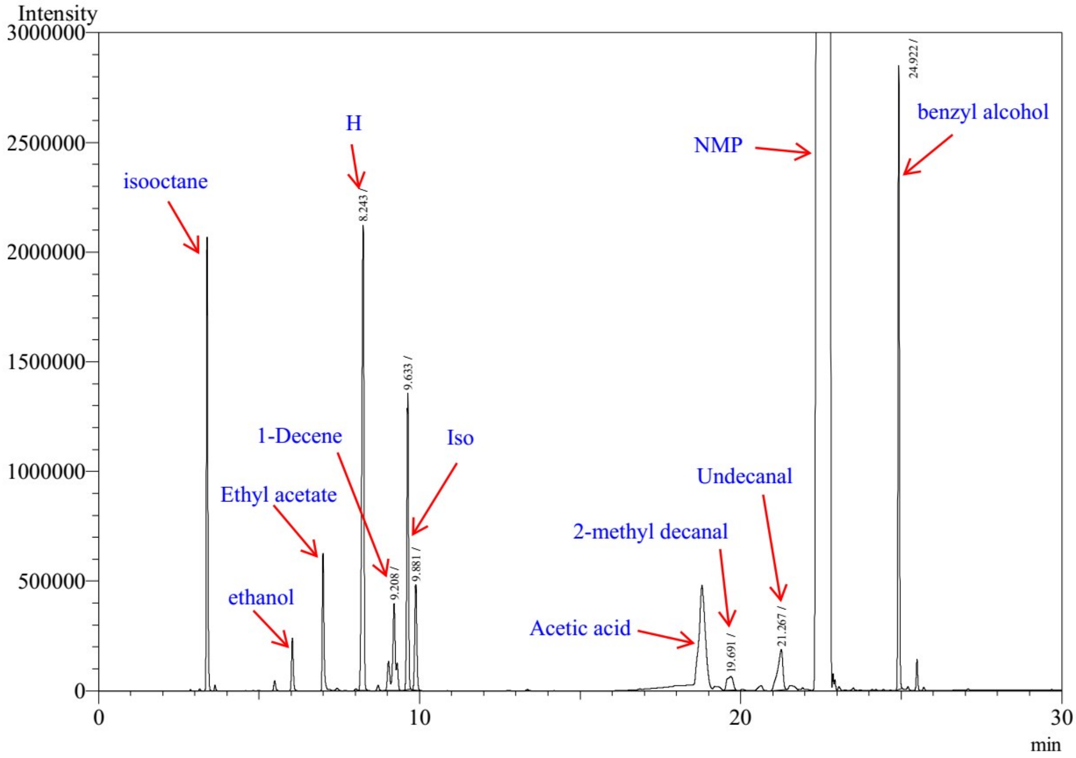
L1





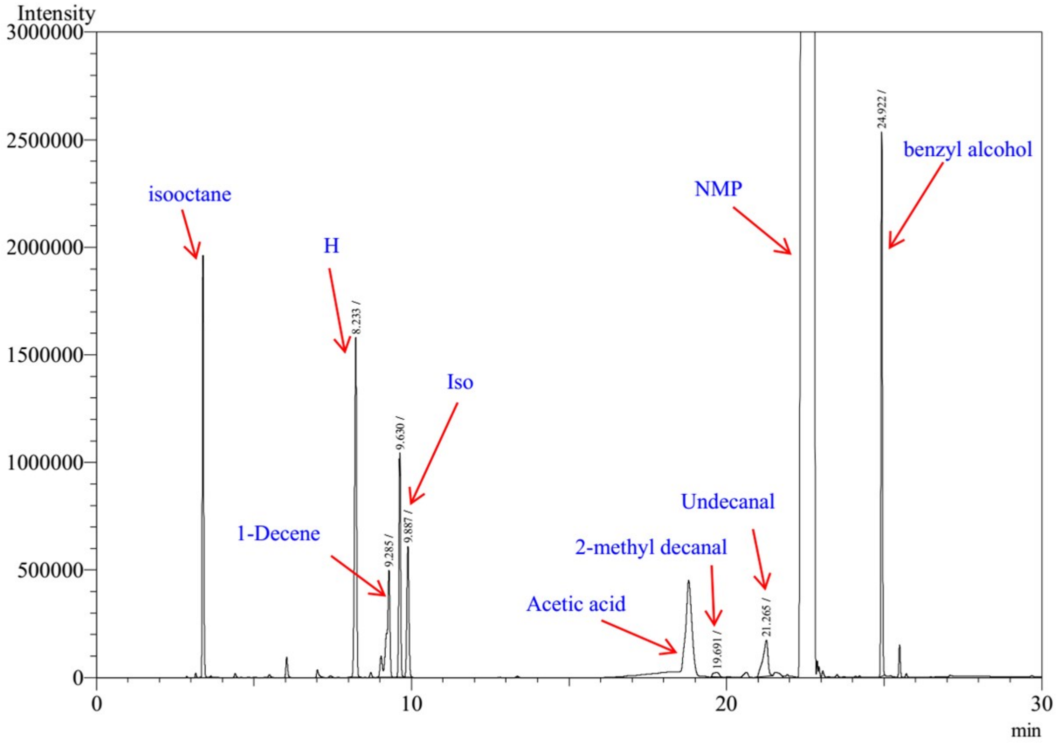
Peak#	Ret.Time	Area	Height	Conc.	UnitMark	ID#	Cmpd Name
1	8.093	11259781	2360691	45.539			
2	9.085	1598568	195293	6.465			
3	9.526	2243447	589070	9.073			
4	9.778	840022	195402	3.397			
5	19.661	328137	25488	1.327			
6	21.233	1209787	108853	4.893			
7	24.891	7245676	2408915	29.305			
		24725418	5883712	100.000			

L2



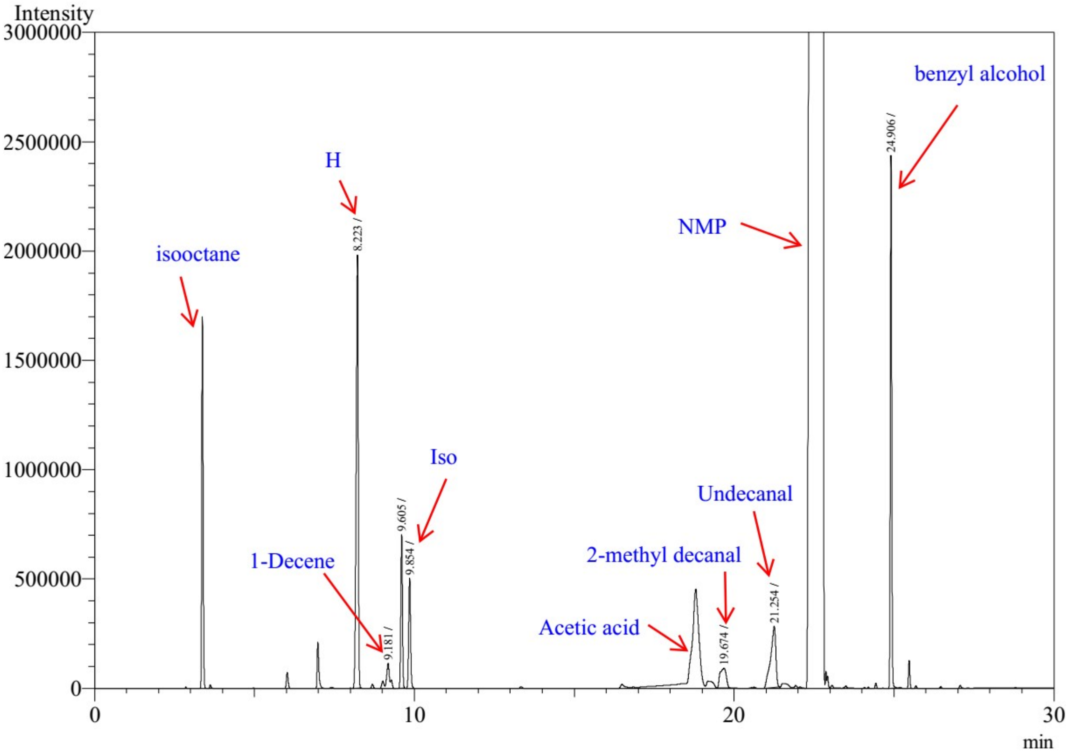
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.243	9612284	2115431	30.838				
2	9.208	3032469	394296	9.729				
3	9.633	4990646	1345481	16.011				
4	9.881	2169525	479975	6.960				
5	19.691	826326	62056	2.651				
6	21.267	2086756	184236	6.695				
7	24.922	8451935	2838164	27.116				
		31169941	7419639	100.000				

L3



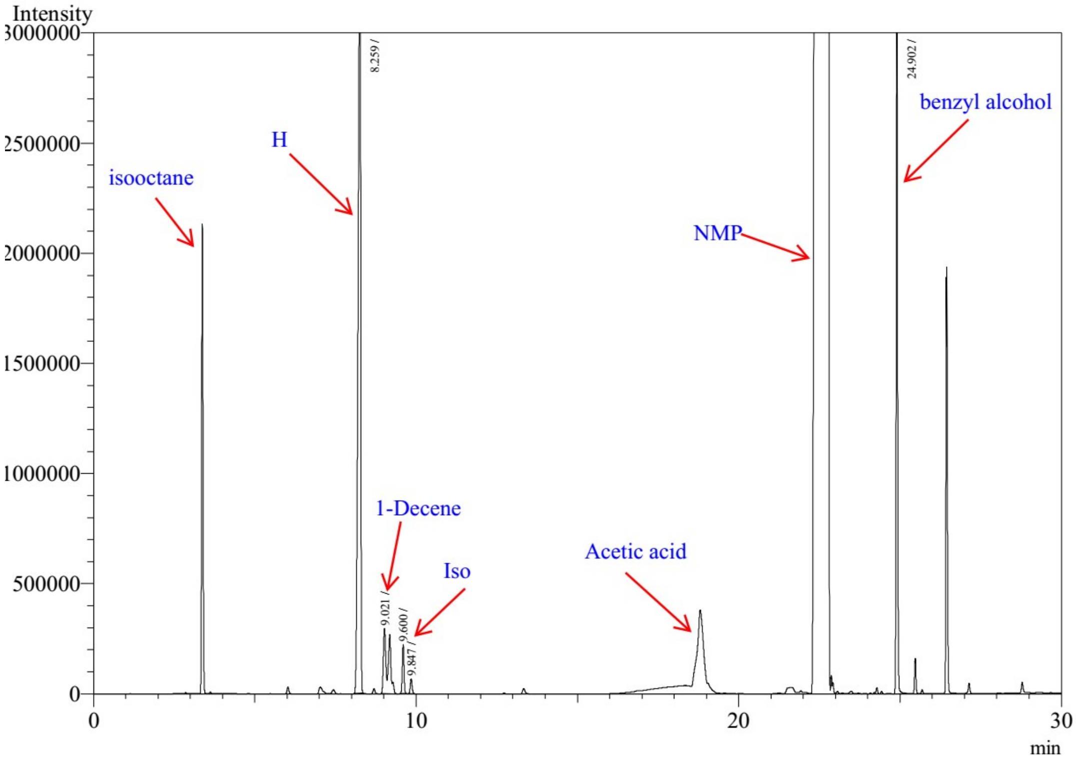
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.233	6988144	1573020	25.873				
2	9.285	3619236	495799	13.400				
3	9.630	3849909	1043045	14.254				
4	9.887	2784935	606745	10.311				
5	19.691	278711	21123	1.032				
6	21.265	1897187	167766	7.024				
7	24.922	7591621	2519832	28.107				
		27009743	6427330	100.000				

L4



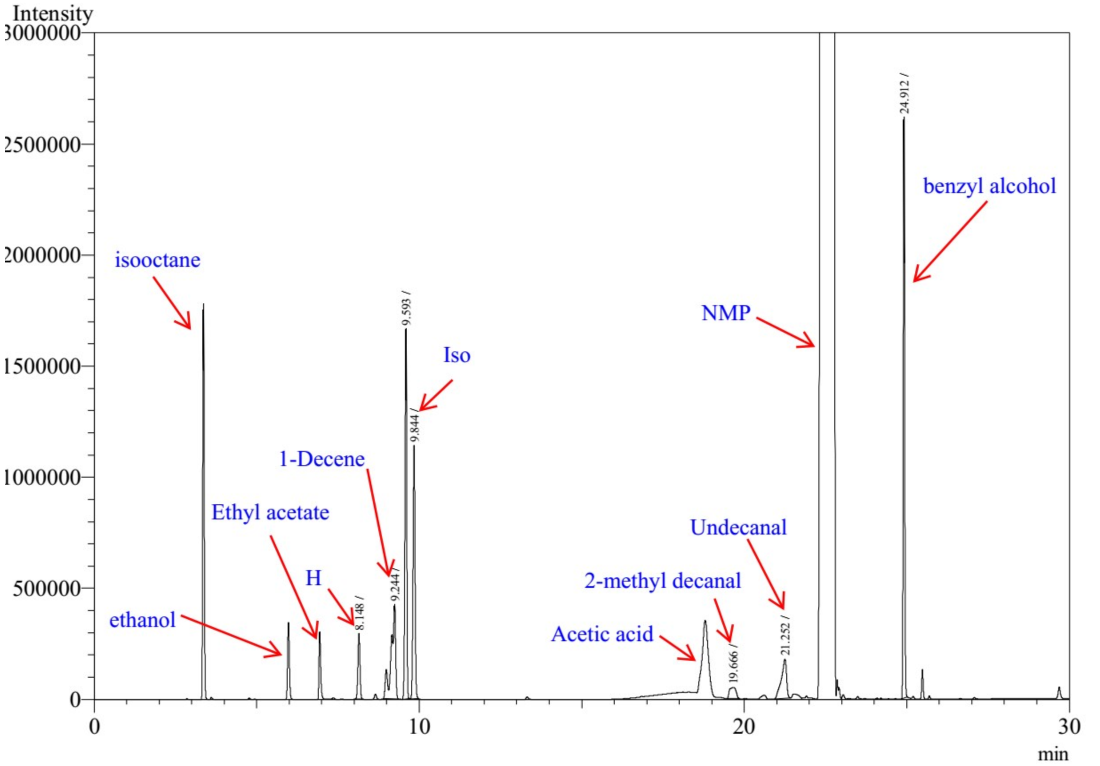
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.223	8865115	1969681	34.011				
2	9.181	936369	116326	3.592				
3	9.605	2529401	700607	9.704				
4	9.854	2065350	504528	7.924				
5	19.674	1200282	89379	4.605				
6	21.254	3160765	281316	12.126				
7	24.906	7307945	2406108	28.037				
		26065227	6067945	100.000				

L5



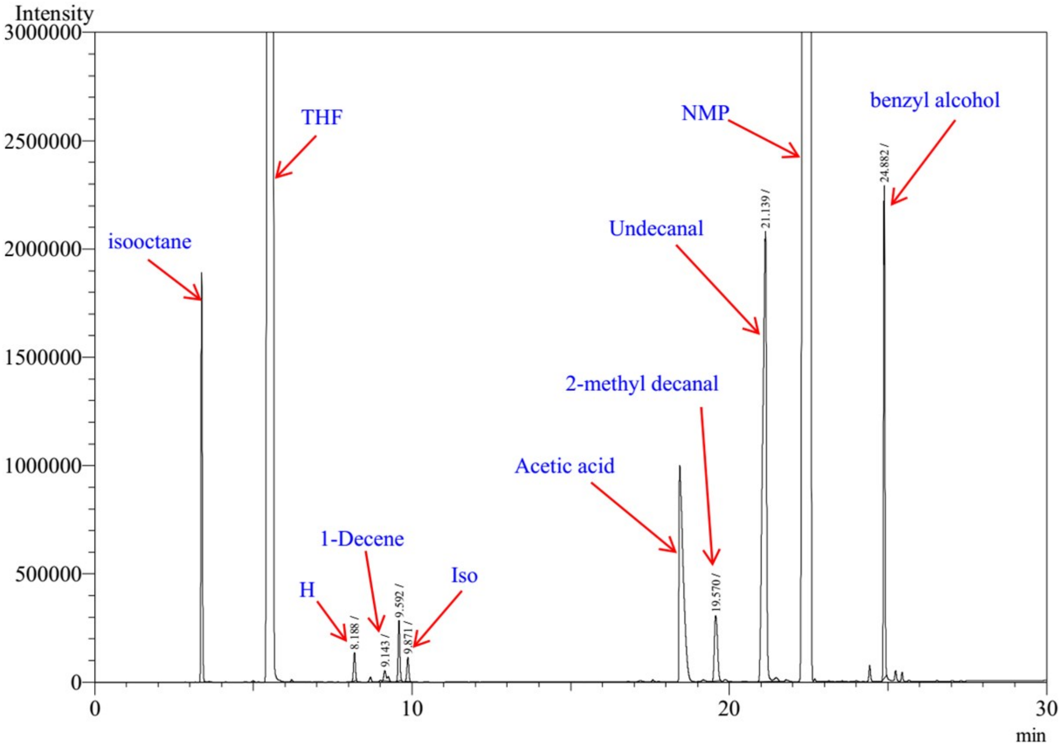
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.259	19696242	3802041	59.974				
2	9.021	3102503	295926	9.447				
3	9.600	785036	221182	2.390				
4	9.847	264755	66210	0.806				
5	24.902	8992854	2975202	27.383				
		32841390	7360561	100.000				

L6



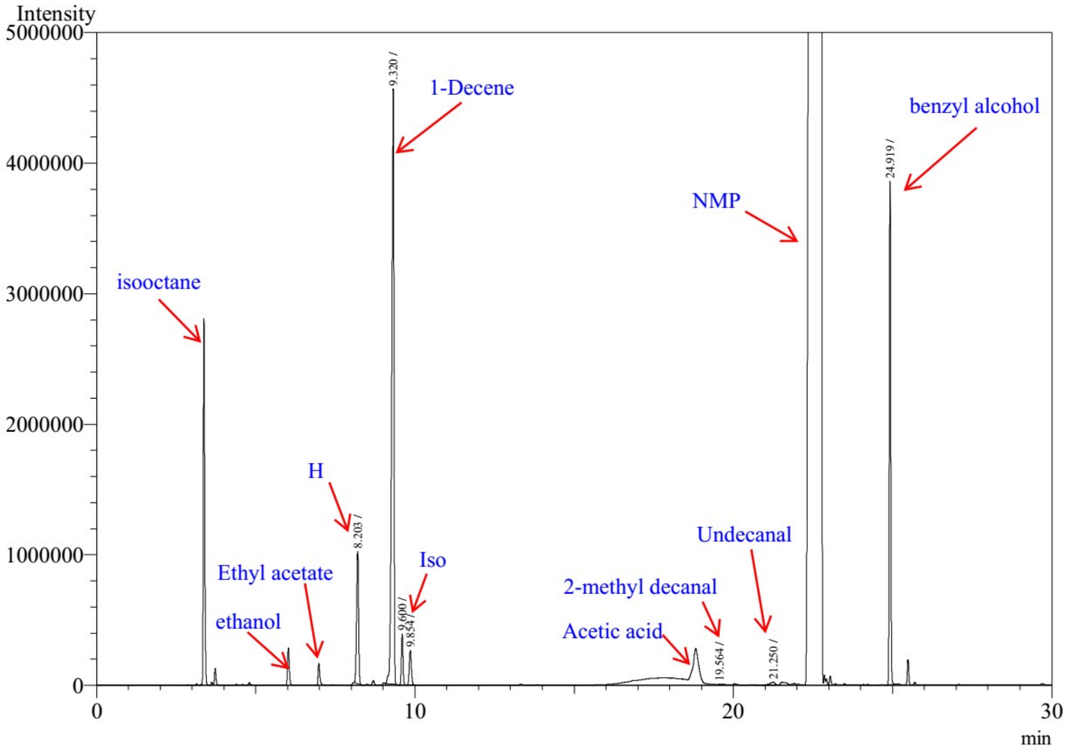
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.148	1267963	292841	4.721				
2	9.244	4026763	420554	14.991				
3	9.593	6182621	1665087	23.017				
4	9.844	4830129	1136897	17.982				
5	19.666	708449	51175	2.638				
6	21.252	1977679	177237	7.363				
7	24.912	7867002	2597458	29.288				
		26860606	6341249	100.000				

L7 (PTA)



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.188	525964	131807	1.863				
2	9.143	321902	48238	1.140				
3	9.592	1027430	278473	3.640				
4	9.871	450422	109733	1.596				
5	19.570	2058181	300500	7.292				
6	21.139	17112415	2068063	60.628				
7	24.882	6729007	2267694	23.840				
		28225321	5204508	100.000				

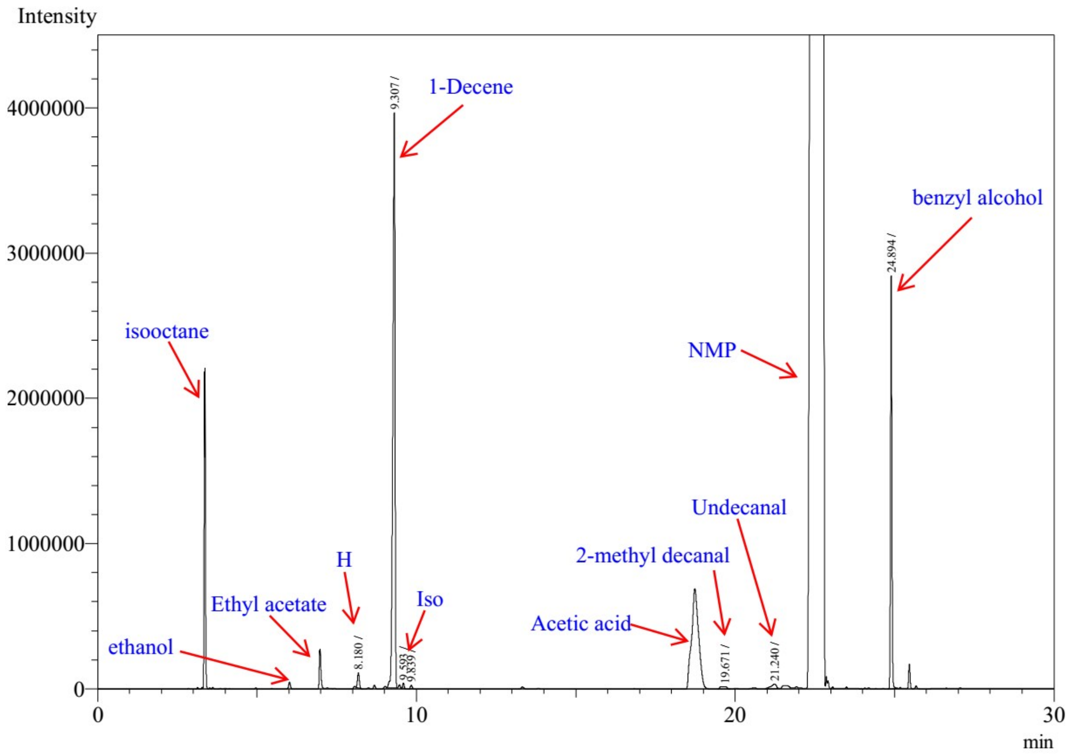
without Ligand



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.203	4370925	1013142	10.660				
2	9.320	22177586	4540904	54.088				
3	9.600	1375707	389838	3.355				
4	9.854	1210636	265845	2.953				
5	19.564	40745	3095	0.099				
6	21.250	233201	22021	0.569				
7	24.919	11594272	3846070	28.277				
[redacted]		41003072	10080915	100.000				

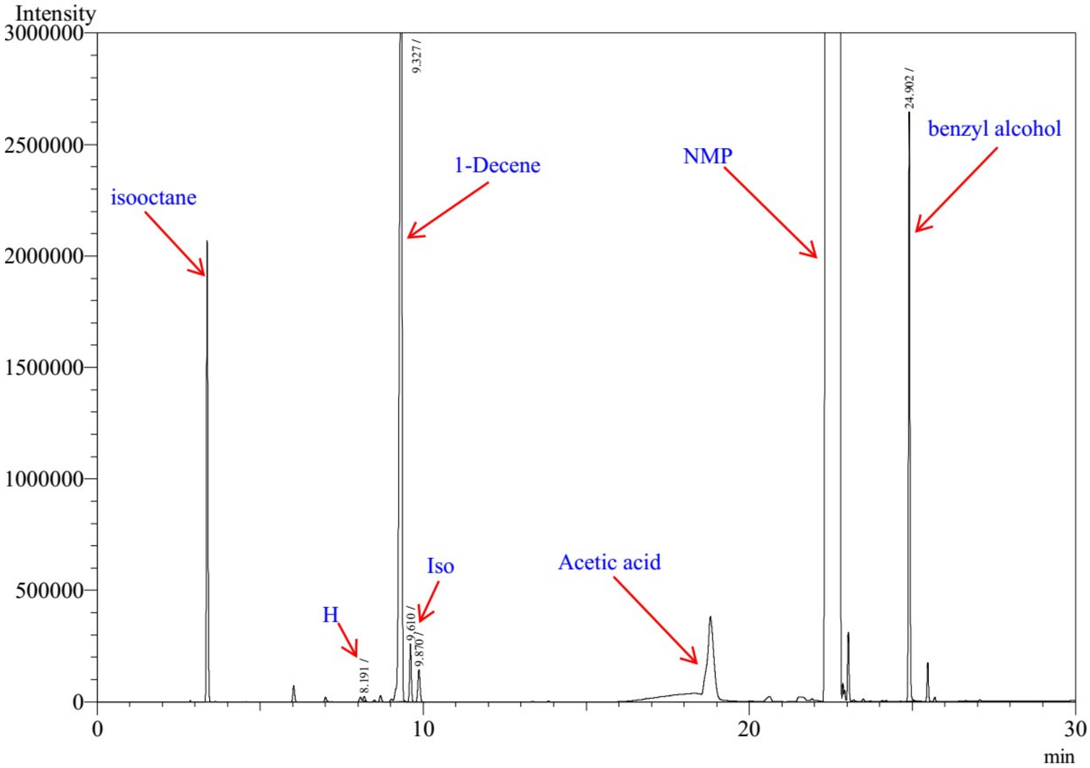
3.2 Gas chromatograms to Table S2

L1



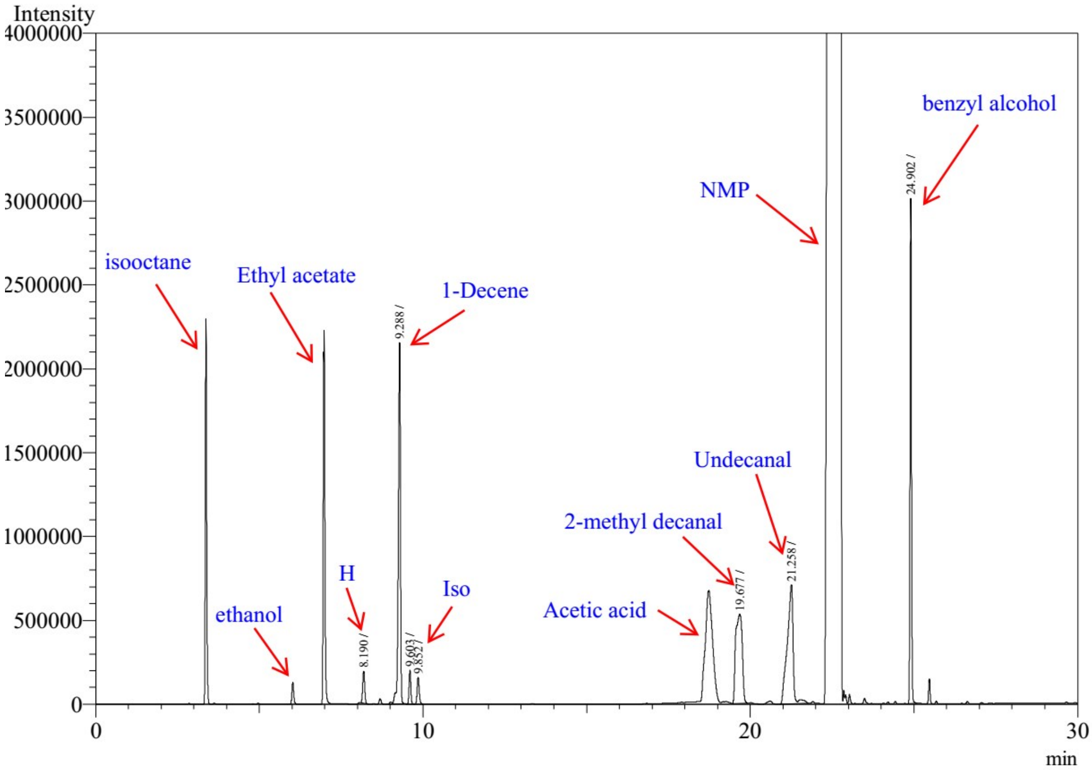
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.180	414773	102933	1.472				
2	9.307	18481521	3950500	65.569				
3	9.593	107745	35080	0.382				
4	9.839	92505	25016	0.328				
5	19.671	212233	15281	0.753				
6	21.240	377935	31802	1.341				
7	24.894	8499709	2831371	30.155				
		28186421	6991983	100.000				

L2



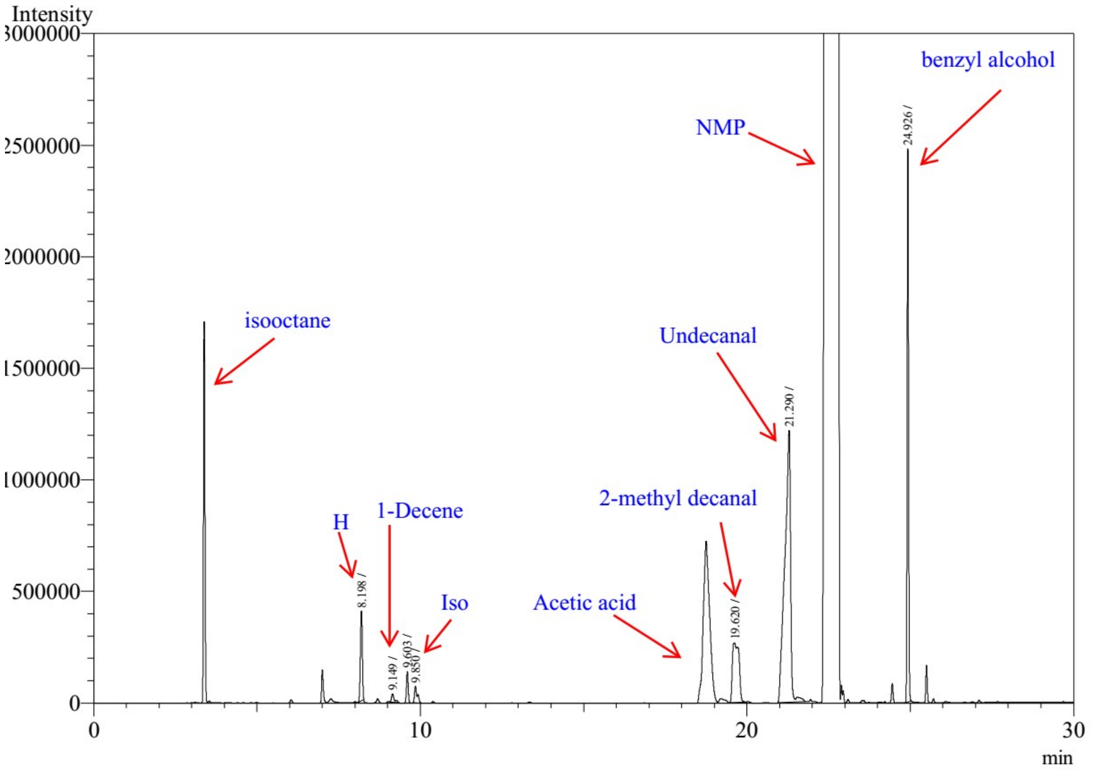
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.191	75391	20175	0.231				
2	9.327	23040688	4665315	70.697				
3	9.610	918027	259251	2.817				
4	9.870	671300	143140	2.060				
5	24.902	7885385	2618732	24.195				
		32590791	7706613	100.000				

L3



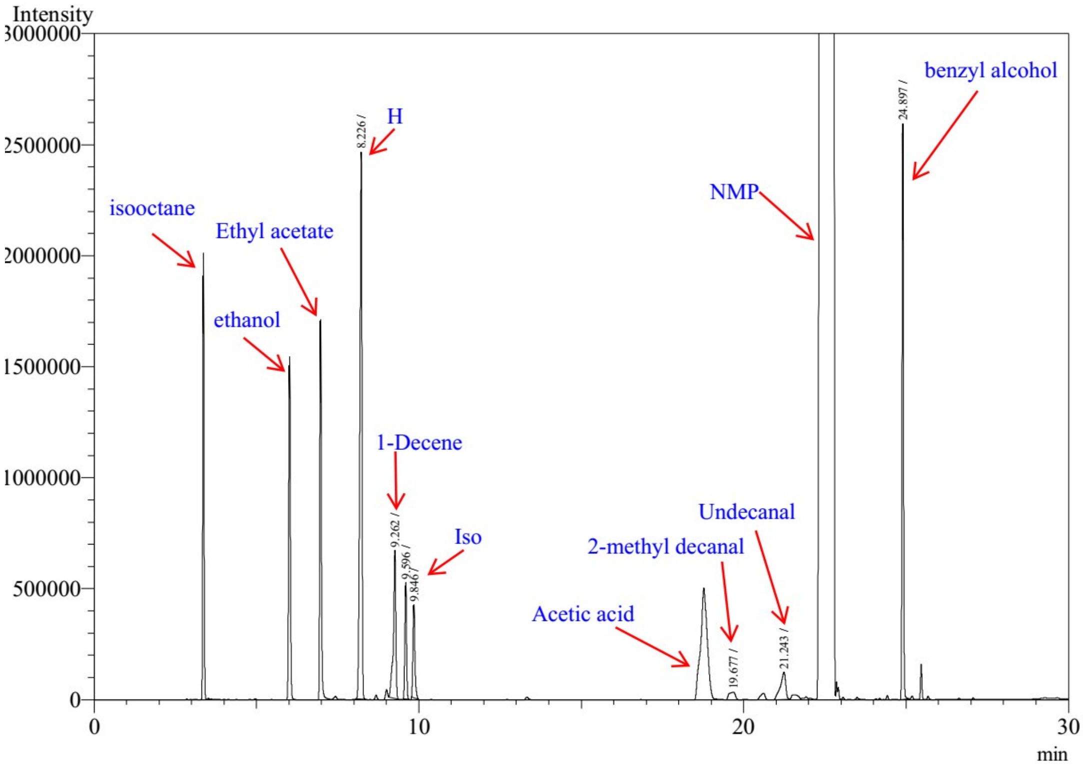
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.190	798169	190279	2.158				
2	9.288	9563199	2147429	25.860				
3	9.603	725535	198414	1.962				
4	9.852	690997	160384	1.869				
5	19.677	7405436	533830	20.025				
6	21.258	8740725	709685	23.636				
7	24.902	9056352	2977117	24.490				
		36980413	6917138	100.000				

L4



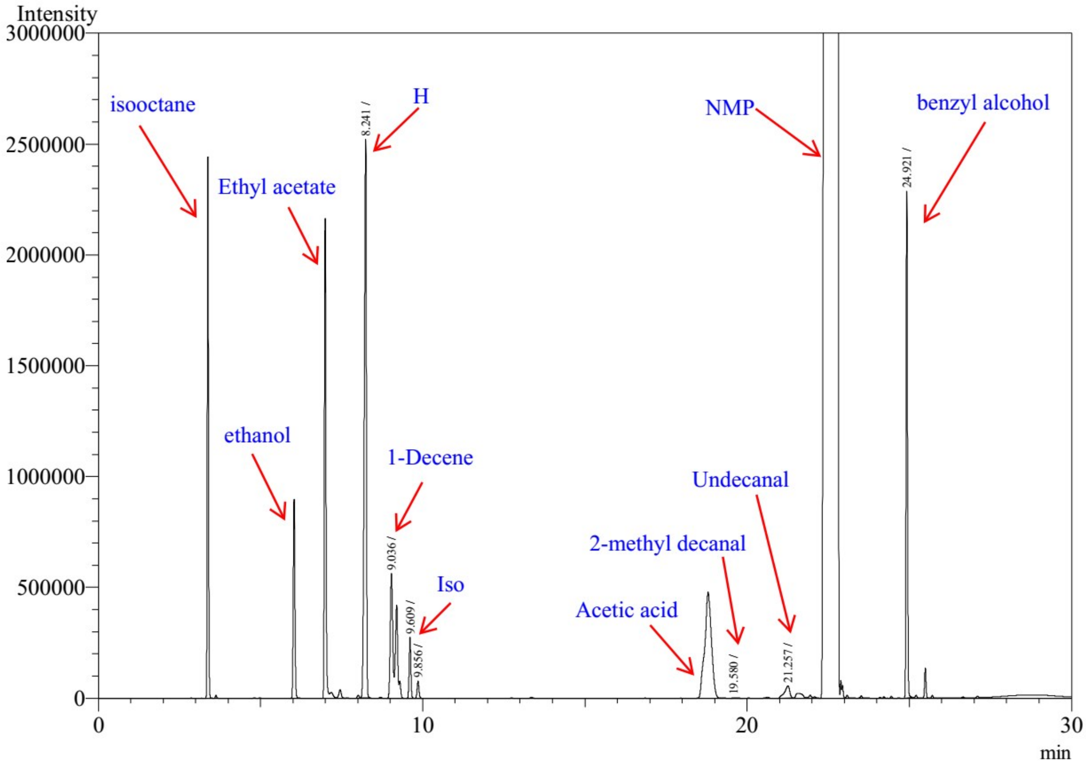
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.198	1635271	400056	5.676				
2	9.149	227786	39174	0.791				
3	9.603	507281	140045	1.761				
4	9.850	429319	73549	1.490				
5	19.620	3774655	267376	13.101				
6	21.290	14864151	1215617	51.592				
7	24.926	7372707	2459665	25.590				
全部		28811170	4595482	100.000				

L5



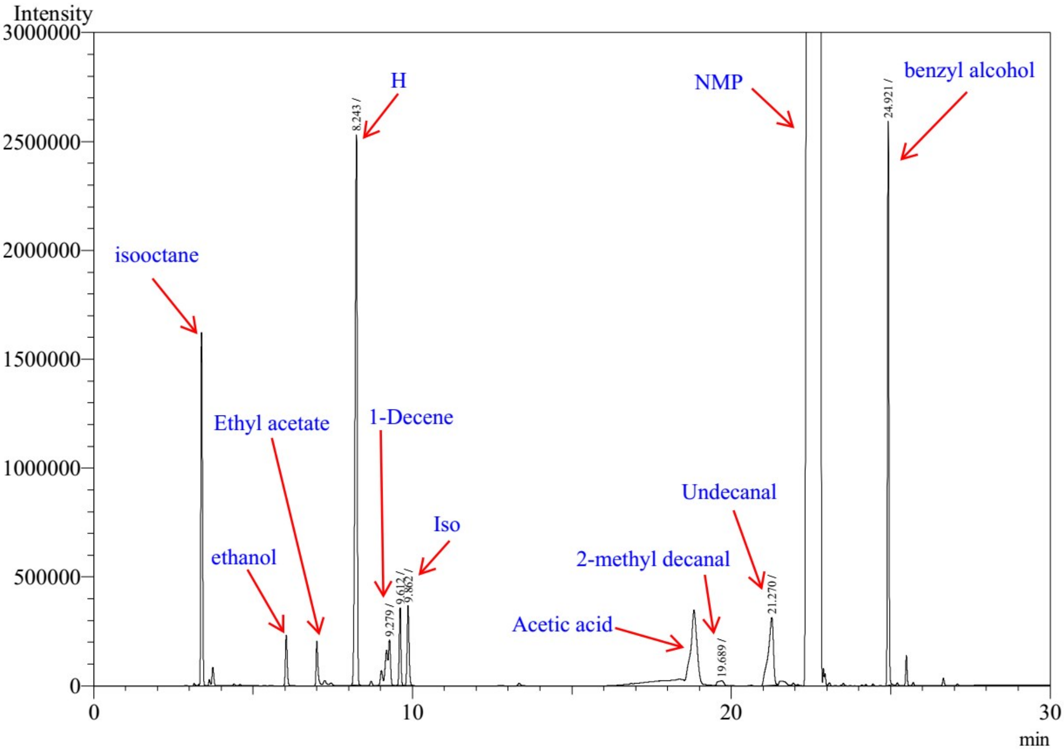
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.226	11327890	2462687	40.433				
2	9.262	3450232	658139	12.315				
3	9.596	1882149	524368	6.718				
4	9.846	1744076	416217	6.225				
5	19.677	459323	34341	1.639				
6	21.243	1388780	122563	4.957				
7	24.897	7763888	2565358	27.712				
[redacted]		28016338	6783673	100.000				

L6



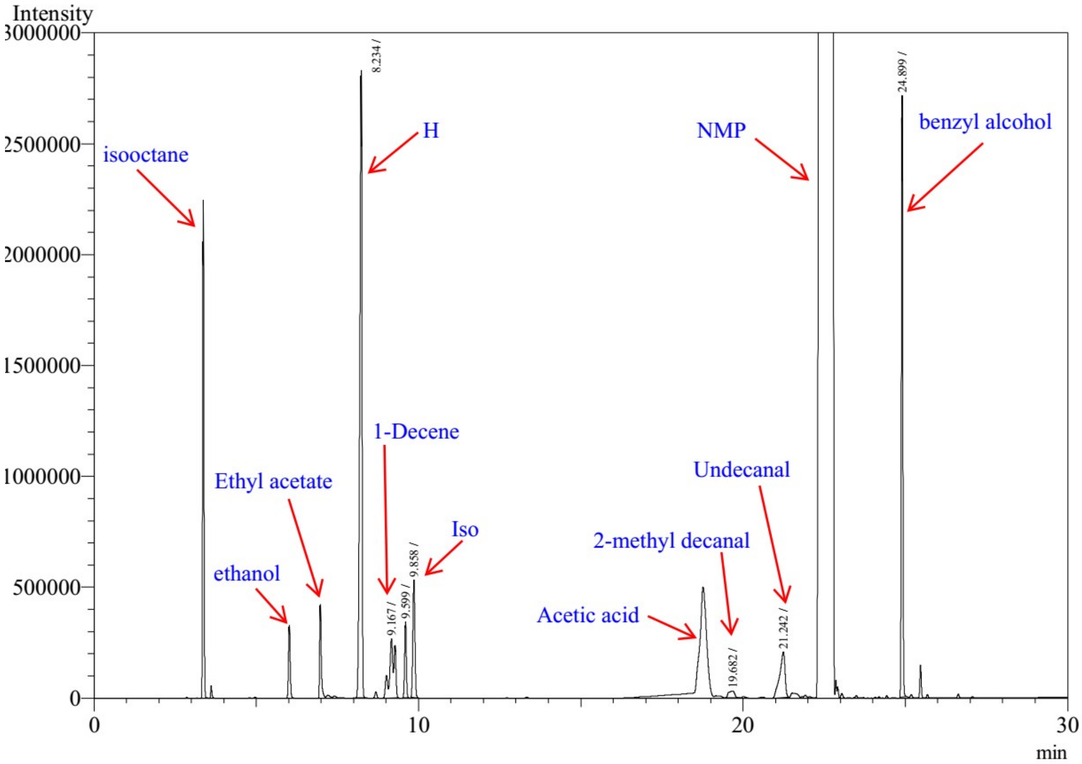
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.241	11366255	2493025	44.752				
2	9.036	5233534	562044	20.606				
3	9.609	986982	272157	3.886				
4	9.856	306519	76484	1.207				
5	19.580	49587	3582	0.195				
6	21.257	634833	55784	2.499				
7	24.921	6820691	2253778	26.855				
		25398401	5716854	100.000				

L7



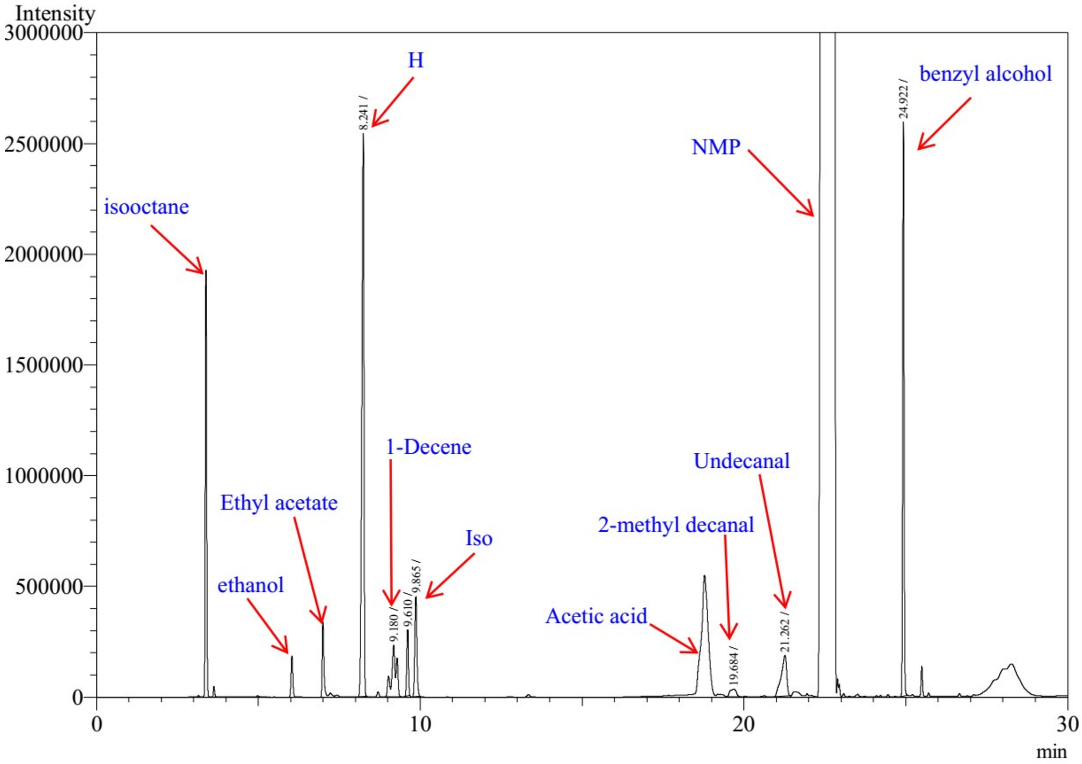
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.243	11656106	2524549	41.337				
2	9.279	2151801	209905	7.631				
3	9.612	1289172	355723	4.572				
4	9.862	1550035	365536	5.497				
5	19.689	302841	22156	1.074				
6	21.270	3524886	310212	12.501				
7	24.921	7722878	2559310	27.388				
[redacted]		28197719	6347391	100.000				

L8



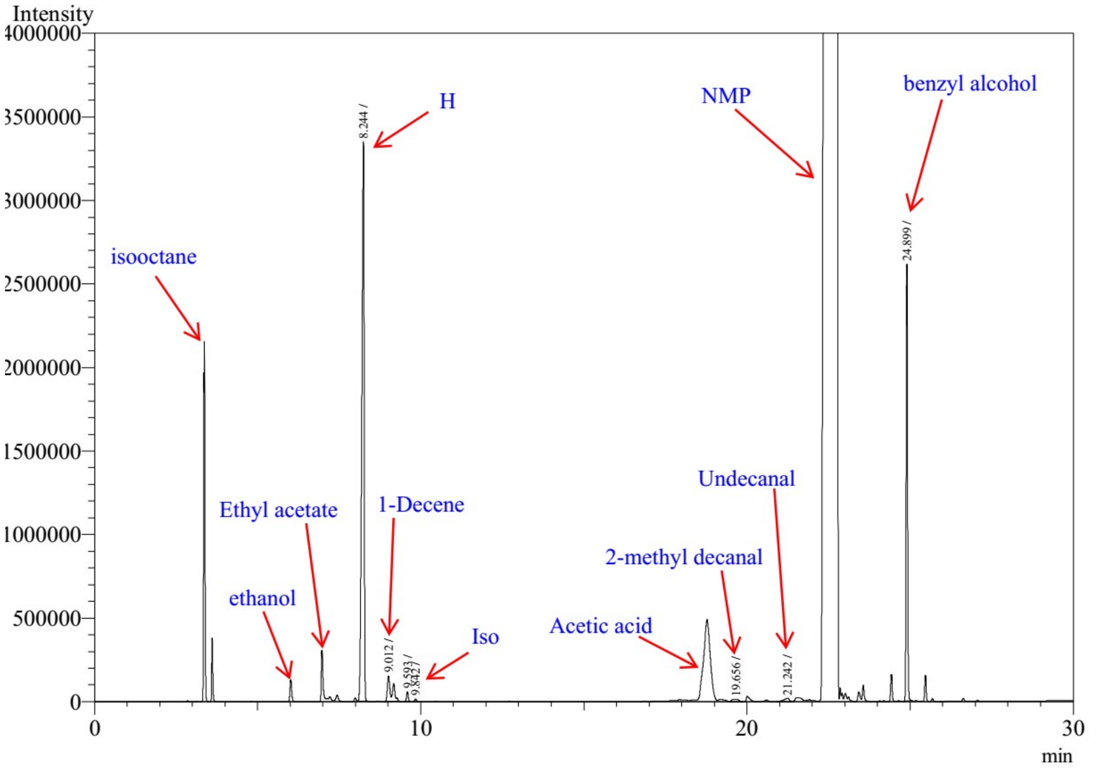
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.234	13339968	2825445	43.245				
2	9.167	3009412	267315	9.756				
3	9.599	1230546	337386	3.989				
4	9.858	2338053	529999	7.579				
5	19.682	411374	31211	1.334				
6	21.242	2355768	205808	7.637				
7	24.899	8162481	2703152	26.461				
		30847602	6900316	100.000				

L9



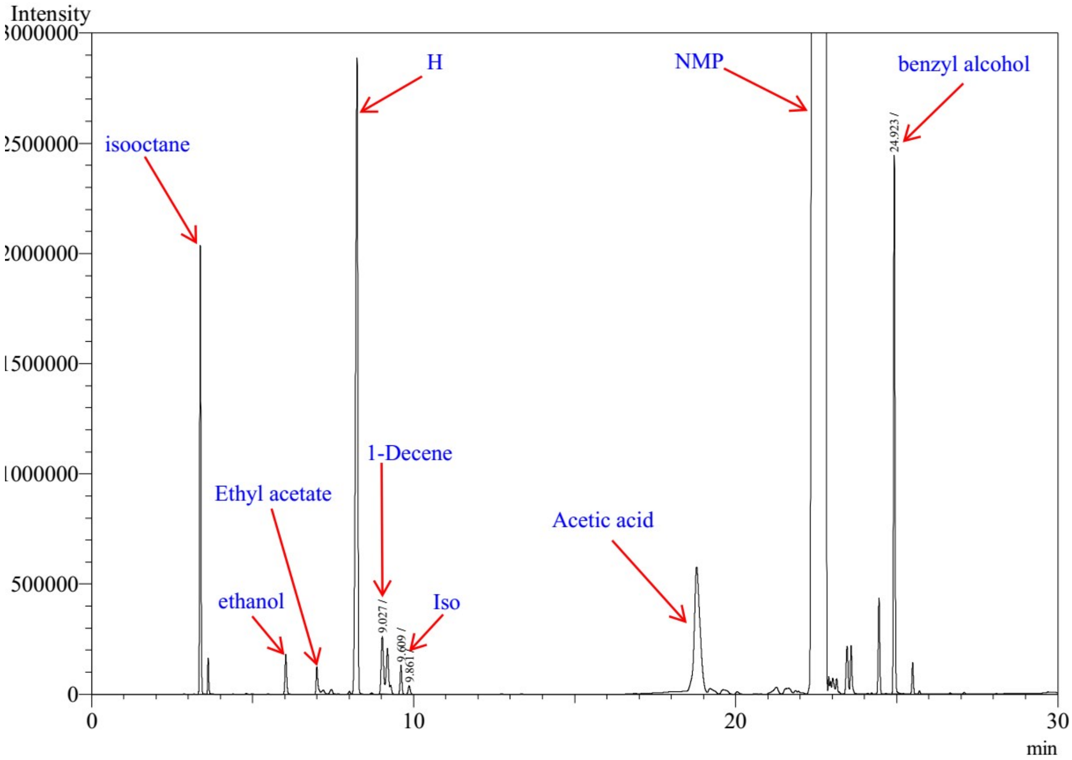
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.241	11625190	2512044	42.093				
2	9.180	2480055	233097	8.980				
3	9.610	1051915	297250	3.809				
4	9.865	1991777	447852	7.212				
5	19.684	461185	33482	1.670				
6	21.262	2169047	183799	7.854				
7	24.922	7838911	2583561	28.383				
		27618080	6291085	100.000				

L10



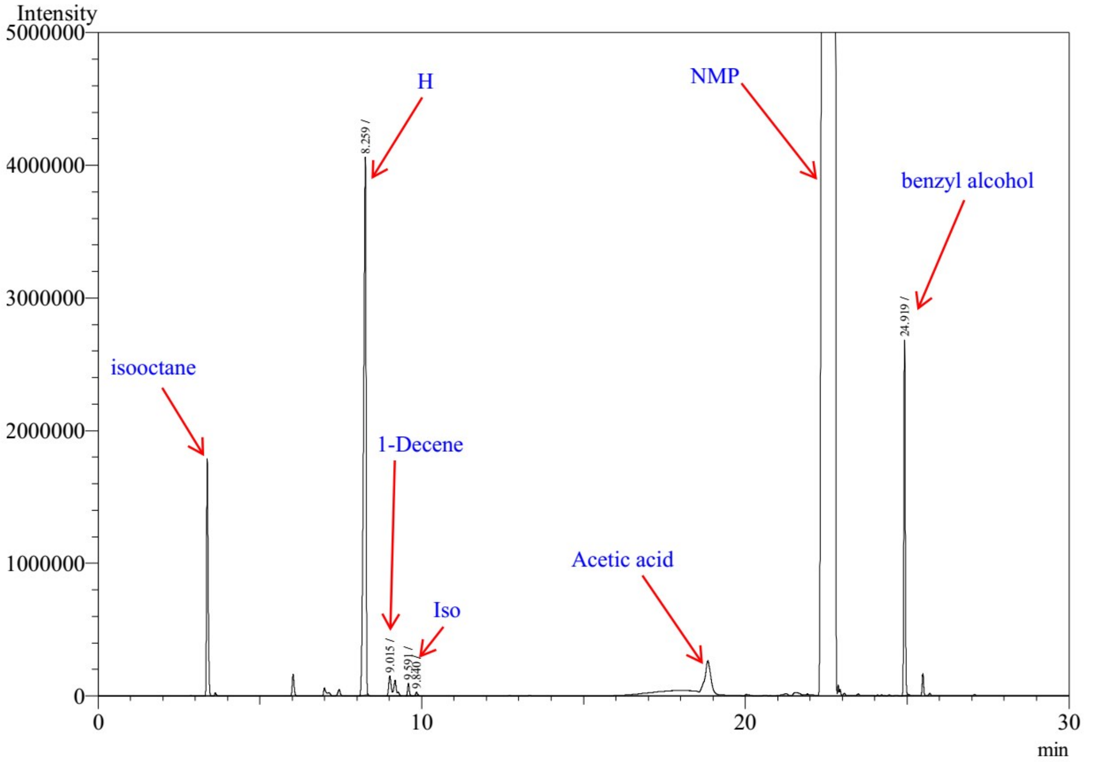
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.244	16439460	3344970	62.304				
2	9.012	1361408	152215	5.160				
3	9.593	216505	59691	0.821				
4	9.842	61205	15873	0.232				
5	19.656	190030	13337	0.720				
6	21.242	223008	19608	0.845				
7	24.899	7894382	2609399	29.919				
		26385998	6215093	100.000				

L11



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	9.027	2483875	260814	23.794				
2	9.609	485594	131713	4.652				
3	9.861	166178	37798	1.592				
4	24.923	7303370	2438849	69.962				
		10439017	2869174	100.000				

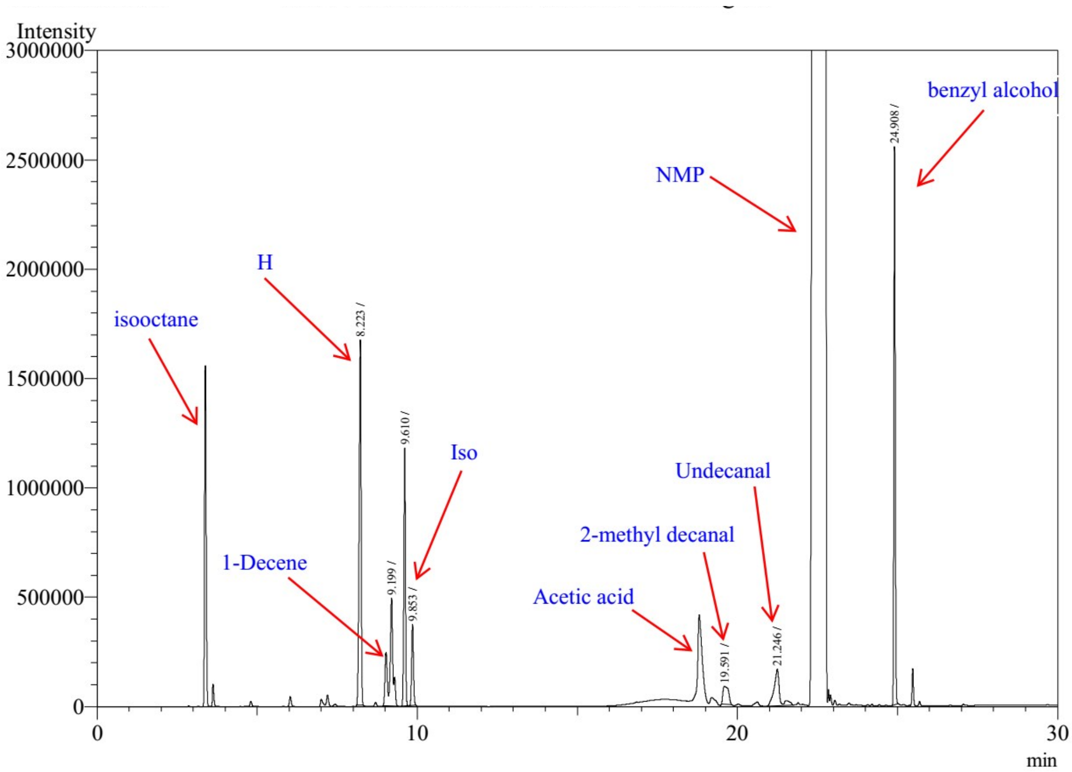
L12



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.259	21178373	4020921	67.978				
2	9.015	1438336	148268	4.617				
3	9.591	341884	93314	1.097				
4	9.840	98730	25723	0.317				
5	24.919	8097581	2620490	25.991				
[redacted]		31154904	6908716	100.000				

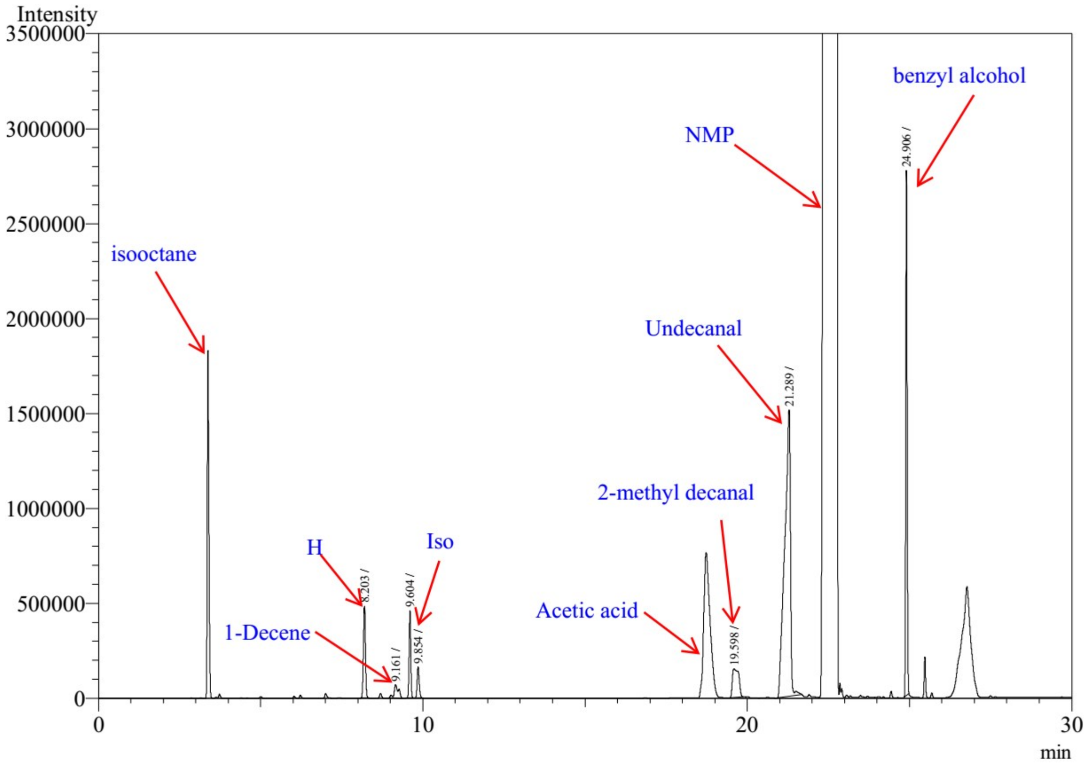
3.3 Gas chromatograms to Table S3

Entry 1



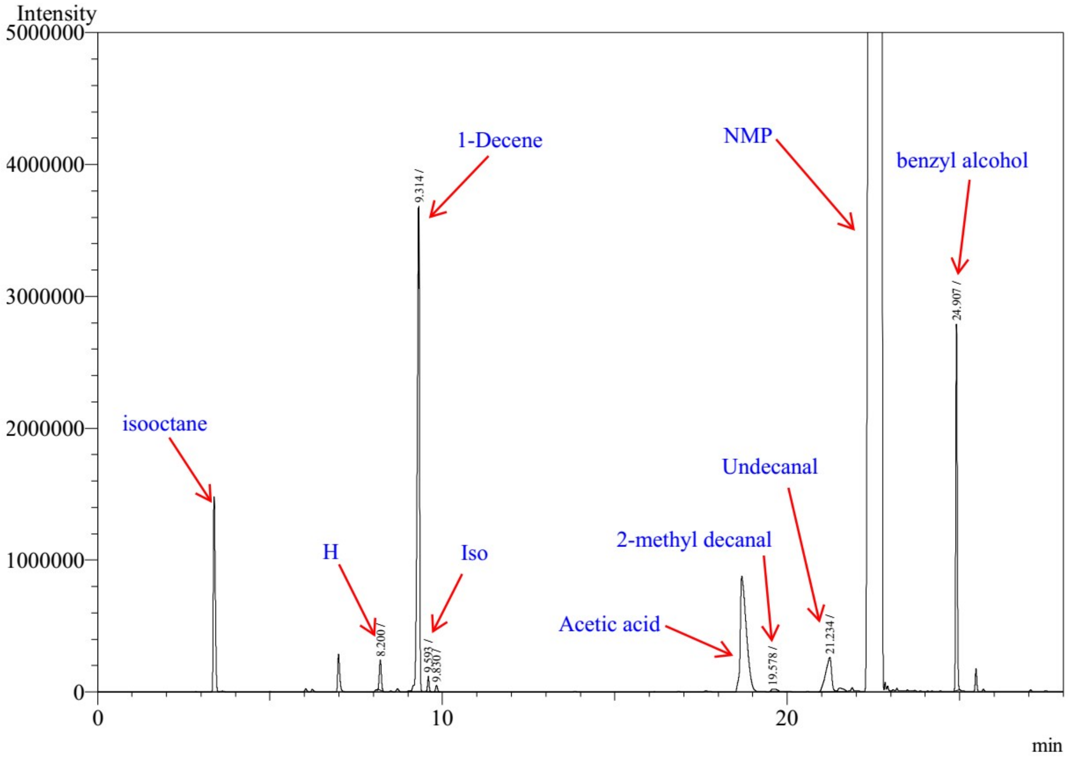
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.223	7192653	1662313	26.135				
2	9.199	4021241	492520	14.611				
3	9.610	4207932	1175266	15.290				
4	9.853	1481388	371547	5.383				
5	19.591	1007158	82721	3.660				
6	21.246	2005715	167718	7.288				
7	24.908	7605376	2543774	27.634				
		27521463	6495859	100.000				

Entry 2



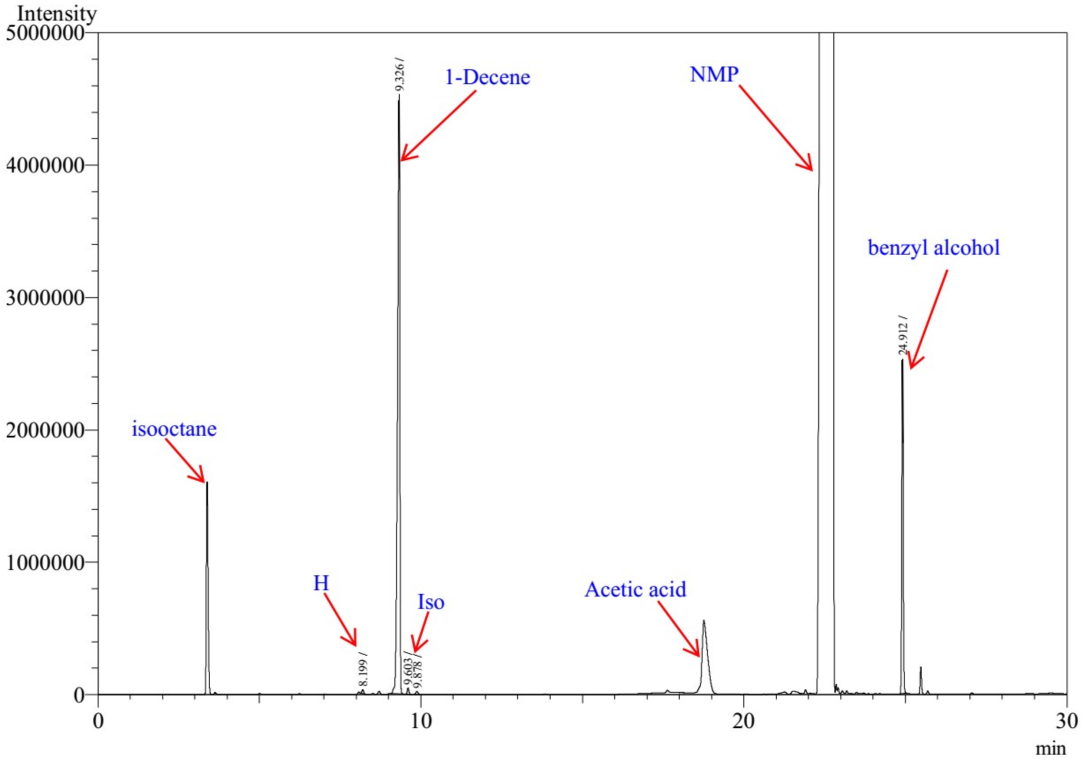
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.203	2093044	482509	6.174				
2	9.161	666811	70085	1.967				
3	9.604	1640681	457004	4.840				
4	9.854	714075	163715	2.106				
5	19.598	2075341	151984	6.122				
6	21.289	18441418	1506729	54.400				
7	24.906	8268182	2732477	24.390				
		33899552	5564503	100.000				

Entry 3



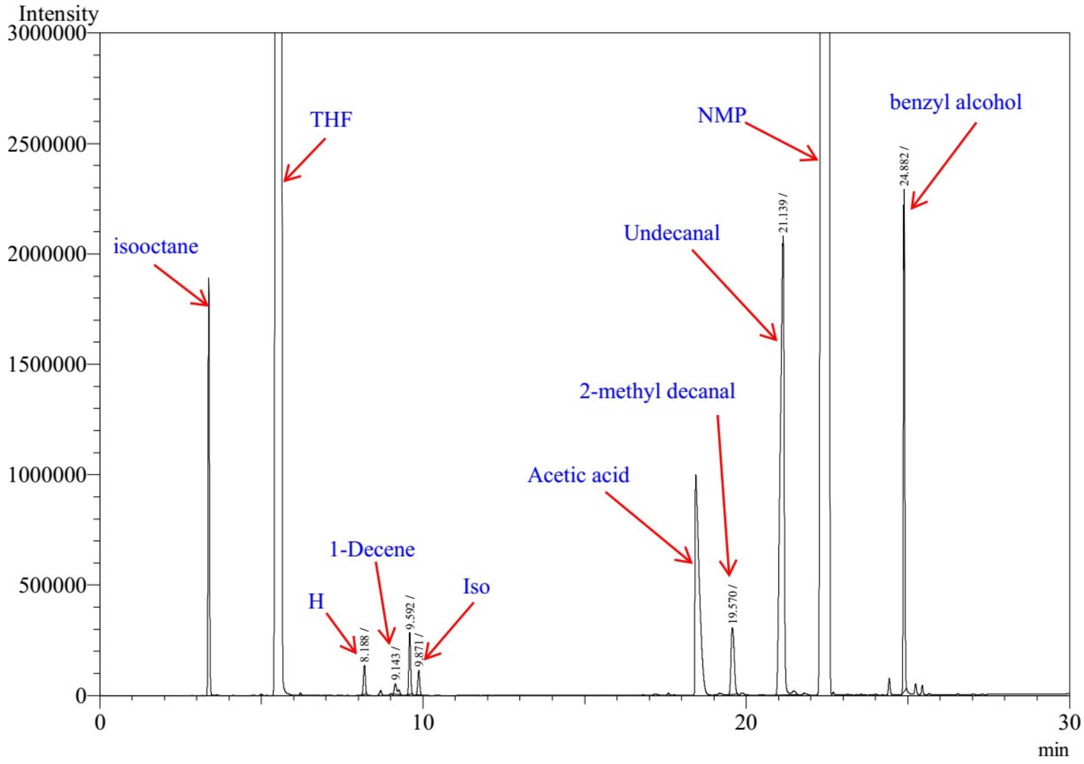
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.200	919430	228264	3.067				
2	9.314	16708245	3629041	55.730				
3	9.593	355721	116616	1.187				
4	9.830	187333	49766	0.625				
5	19.578	198057	18489	0.661				
6	21.234	3304365	257693	11.022				
7	24.907	8307517	2759008	27.710				
		29980668	7058877	100.000				

Entry 4



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.199	94510	26505	0.318				
2	9.326	21792369	4521552	73.375				
3	9.603	169399	46931	0.570				
4	9.878	109647	23320	0.369				
5	24.912	7533904	2510451	25.367				
		29699829	7128759	100.000				

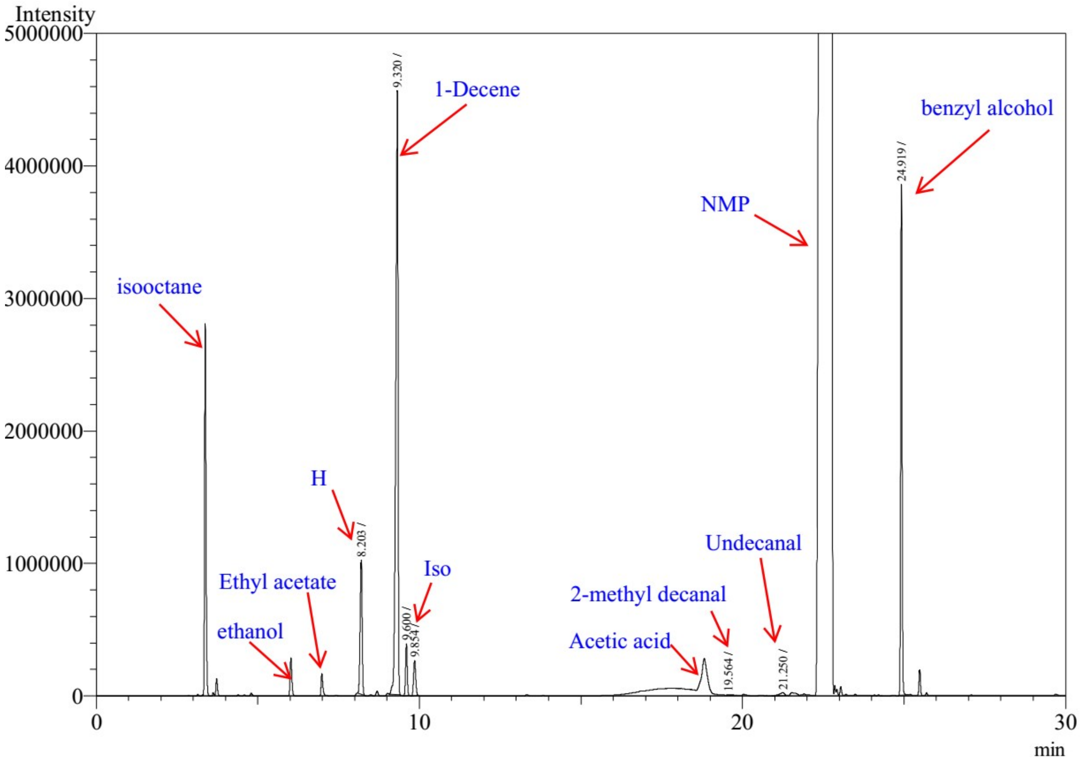
Entry 5



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.188	525964	131807	1.863				
2	9.143	321902	48238	1.140				
3	9.592	1027430	278473	3.640				
4	9.871	450422	109733	1.596				
5	19.570	2058181	300500	7.292				
6	21.139	17112415	2068063	60.628				
7	24.882	6729007	2267694	23.840				
		28225321	5204508	100.000				

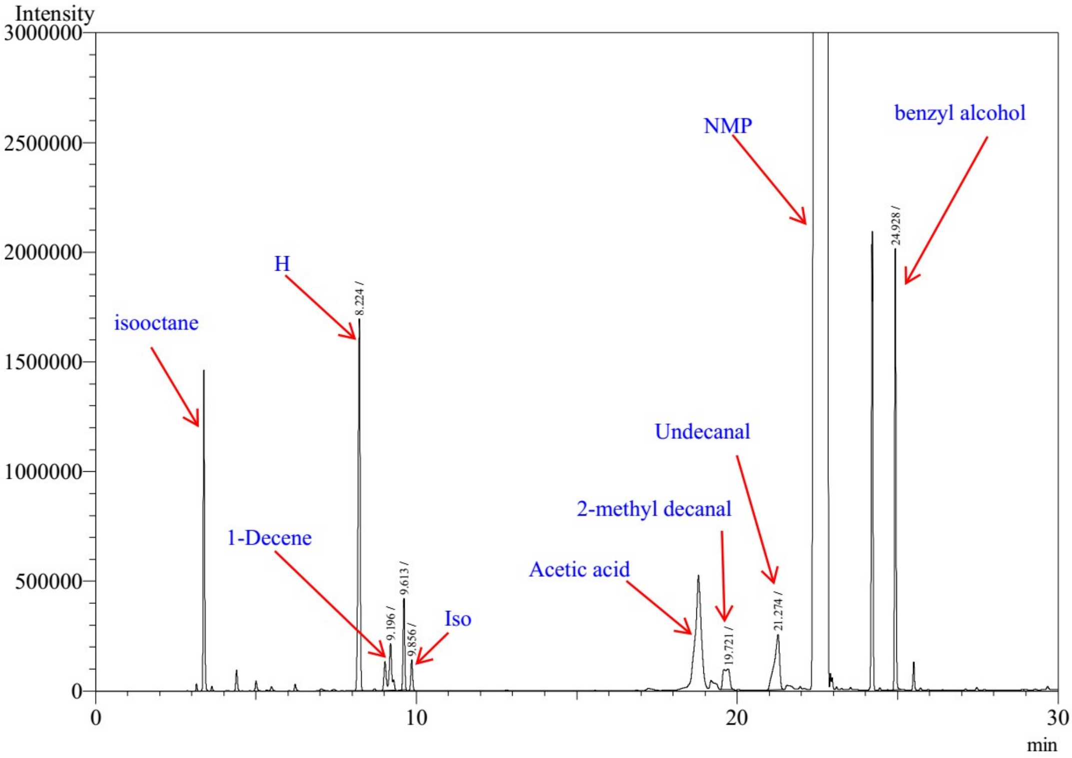
3.4 Gas chromatograms to Table S4

Entry 1



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.203	4370925	1013142	10.660				
2	9.320	22177586	4540904	54.088				
3	9.600	1375707	389838	3.355				
4	9.854	1210636	265845	2.953				
5	19.564	40745	3095	0.099				
6	21.250	233201	22021	0.569				
7	24.919	11594272	3846070	28.277				
		41003072	10080915	100.000				

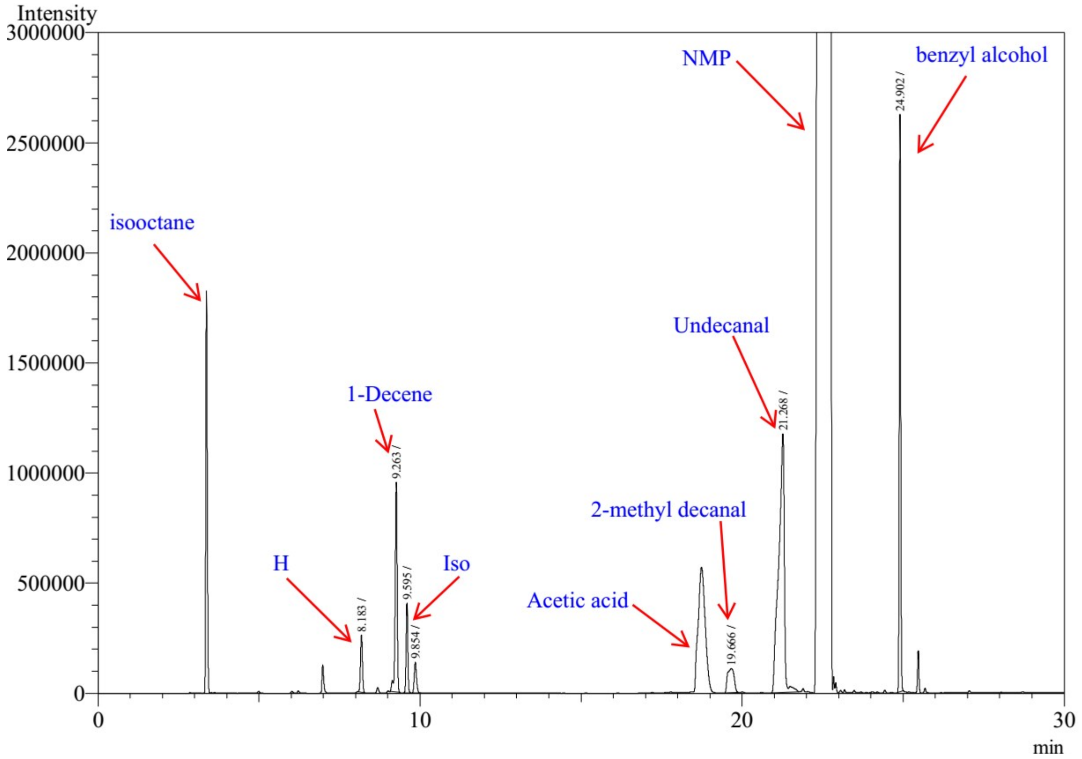
Entry 2



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.224	7406619	1690825	34.604				
2	9.196	1786382	213370	8.346				
3	9.613	1482195	413829	6.925				
4	9.856	532013	140236	2.486				
5	19.721	1352519	94302	6.319				
6	21.274	2891644	252085	13.510				
7	24.928	5952402	1963241	27.810				
		21403774	4767888	100.000				

Entry 3

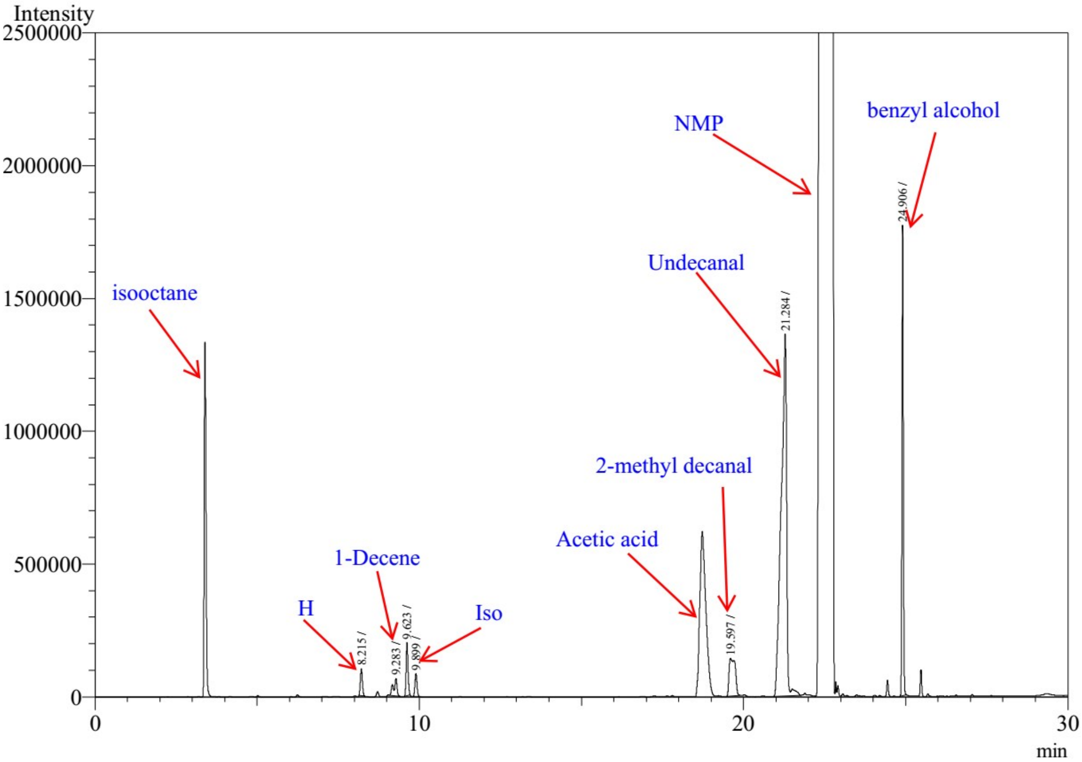
Entry 4



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.183	1077319	259919	3.464				
2	9.263	4123909	948349	13.262				
3	9.595	1454097	405226	4.676				
4	9.854	682662	139492	2.195				
5	19.666	1564273	109278	5.030				
6	21.268	14225786	1175060	45.747				
7	24.902	7968578	2602916	25.625				
		31096624	5640240	100.000				

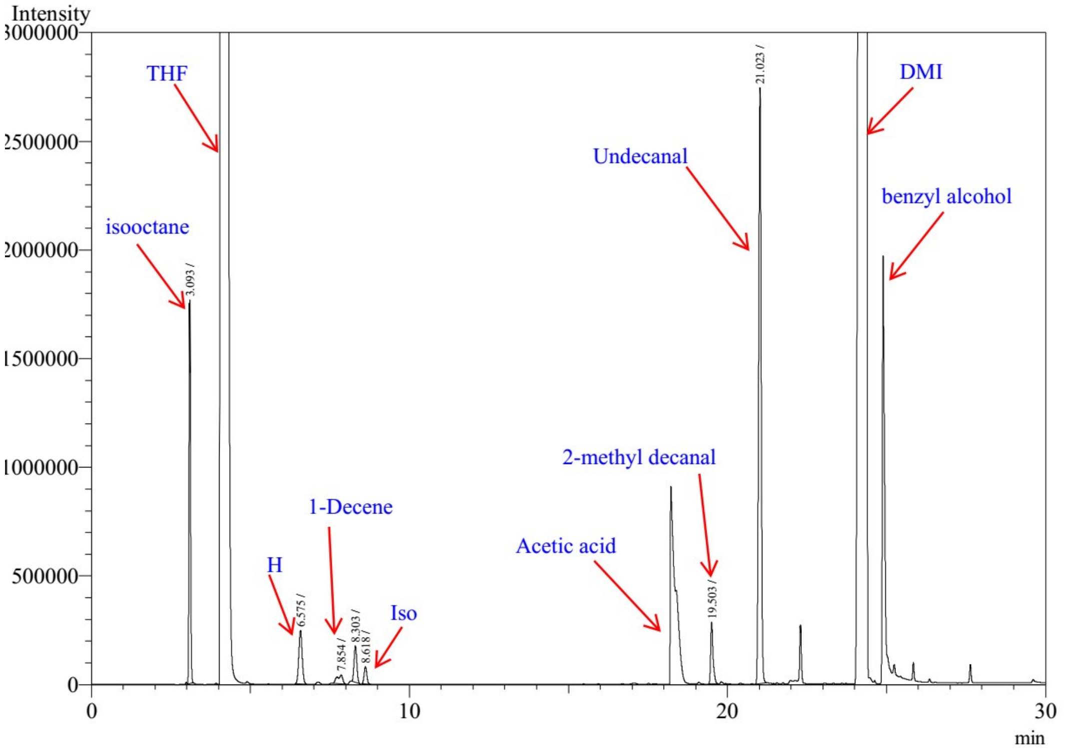
3.5 Gas chromatograms to Table S5

Entry 1



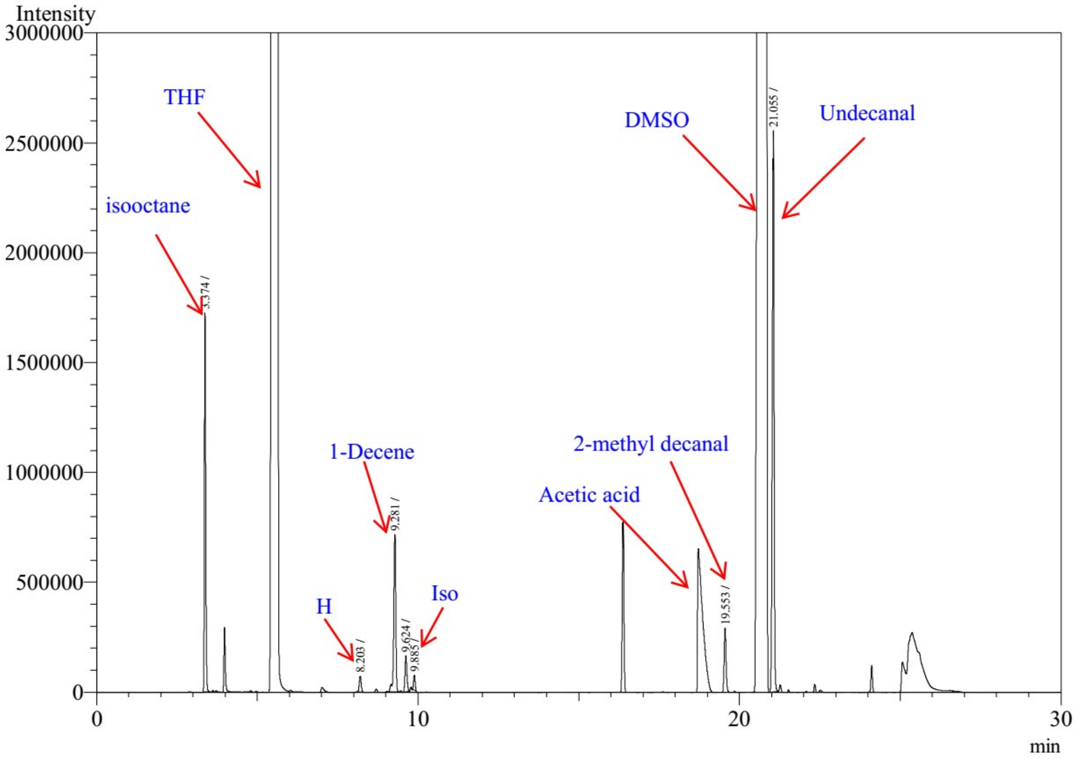
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.215	440025	101190	1.754				
2	9.283	472428	64613	1.883				
3	9.623	804617	198409	3.207				
4	9.899	385910	86955	1.538				
5	19.597	1882639	142718	7.504				
6	21.284	15859109	1359841	63.210				
7	24.906	5244856	1744648	20.905				
		25089584	3698374	100.000				

Entry 2



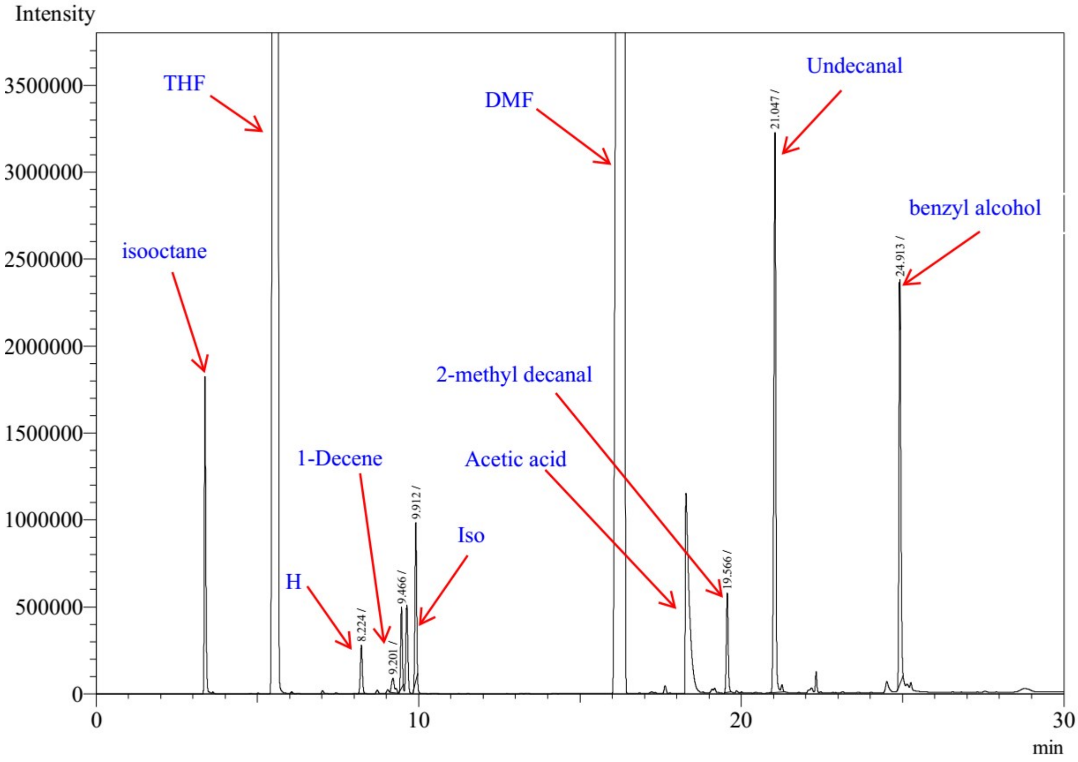
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.093	5676426	1729634	21.736				
2	6.575	1794691	245437	6.872				
3	7.854	489333	40990	1.874				
4	8.303	1007394	168273	3.857				
5	8.618	474227	80271	1.816				
6	19.503	1459599	281140	5.589				
7	21.023	15213815	2730727	58.256				
[redacted]		26115485	5276472	100.000				

Entry 3



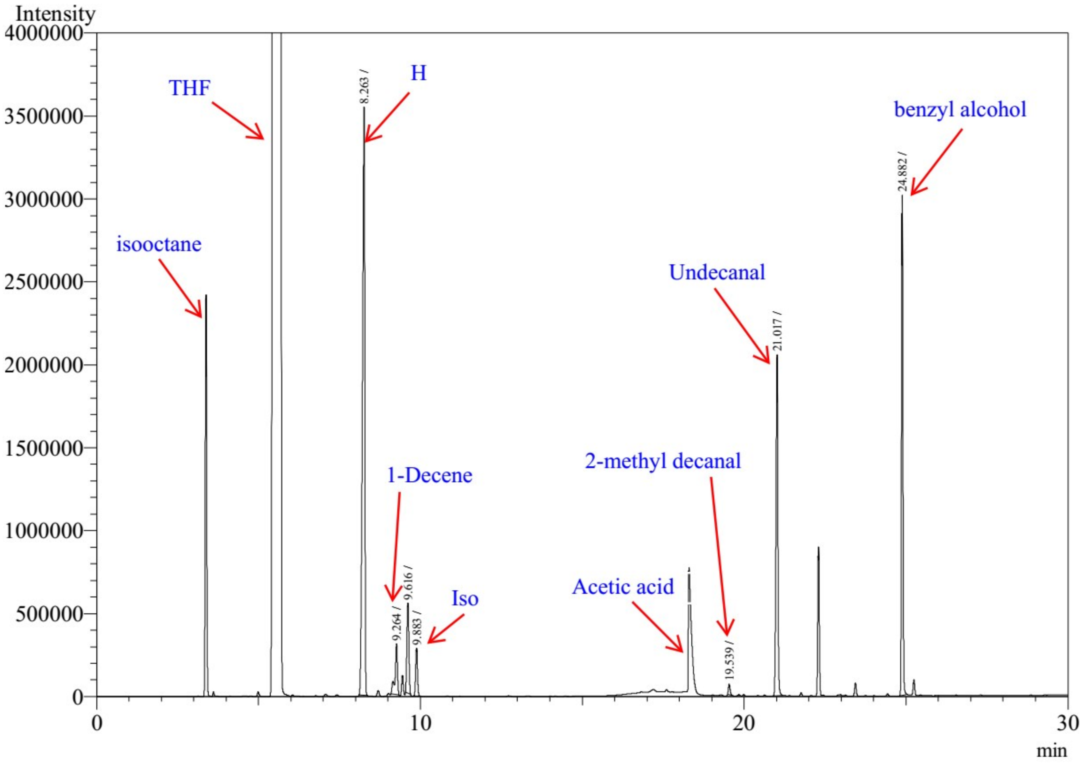
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.374	4856661	1685963	23.948				
2	8.203	302029	71712	1.489				
3	9.281	3105255	715163	15.312				
4	9.624	673471	163373	3.321				
5	9.885	229225	67430	1.130				
6	19.553	1237705	293094	6.103				
7	21.055	9875316	2550977	48.696				
		20279662	5547712	100.000				

Entry 4



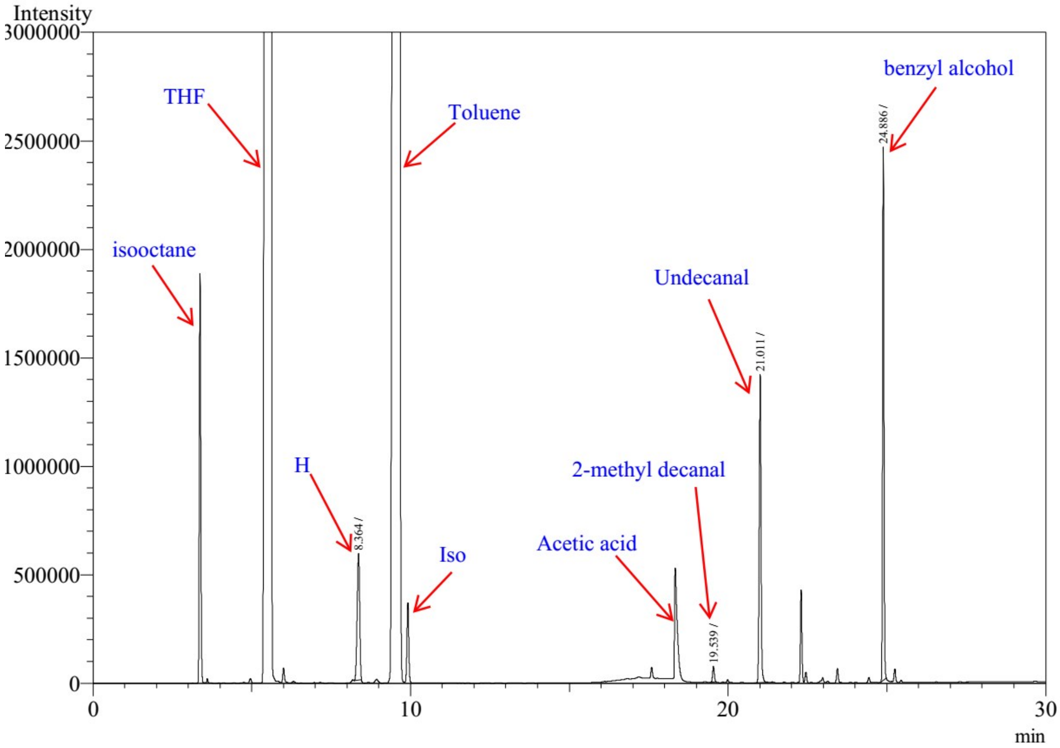
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.224	1185418	277025	3.749				
2	9.201	545415	81055	1.725				
3	9.466	1587125	462767	5.020				
4	9.912	3134379	904902	9.913				
5	19.566	2235124	562020	7.069				
6	21.047	13657905	3199026	43.197				
7	24.913	9272126	2321729	29.326				
		31617492	7808524	100.000				

Entry 5



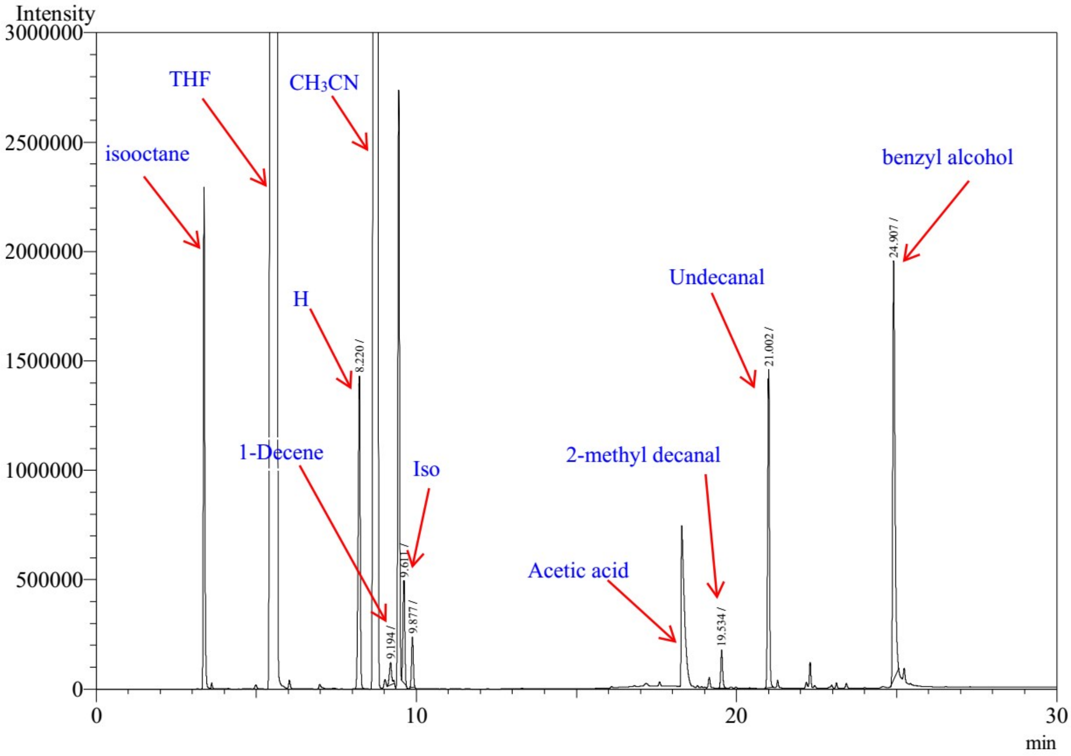
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.263	17573179	3544031	43.706				
2	9.264	1574127	305914	3.915				
3	9.616	2375110	546085	5.907				
4	9.883	1124845	285321	2.798				
5	19.539	237260	64723	0.590				
6	21.017	8192799	2051996	20.376				
7	24.882	9130304	2953533	22.708				
		40207624	9751603	100.000				

Entry 6



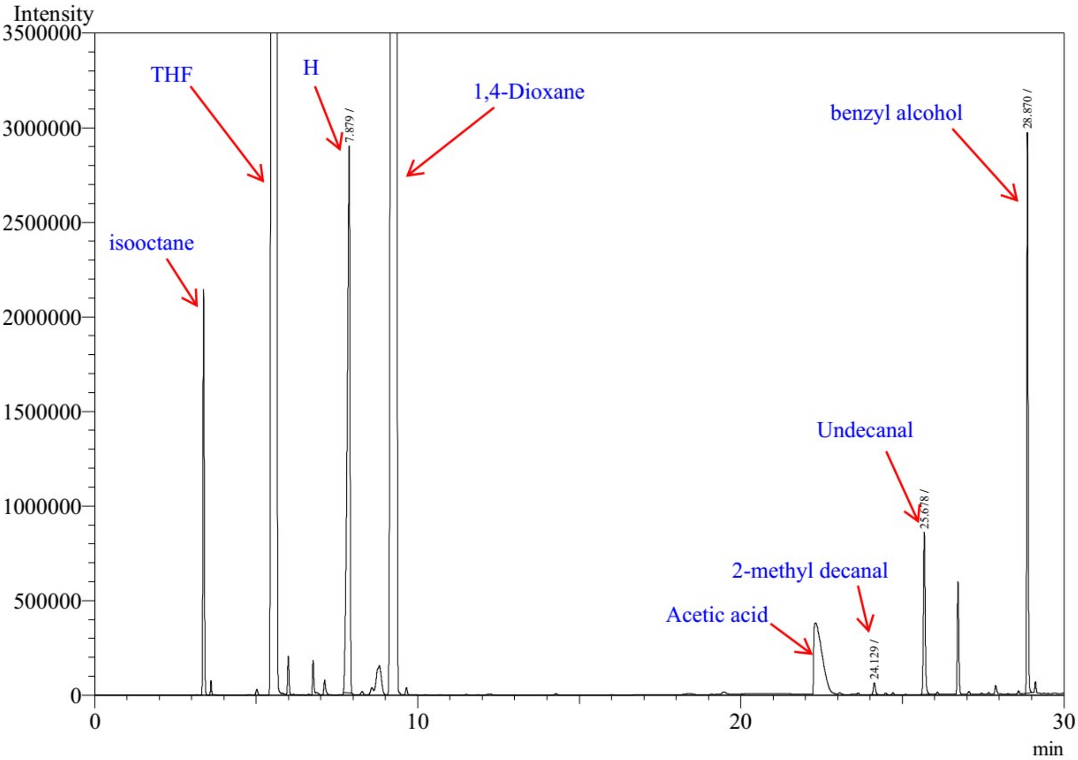
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.364	3253053	584443	19.806				
2	19.539	277186	73581	1.688				
3	21.011	5522251	1413536	33.622				
4	24.886	7372264	2397776	44.885				
		16424754	4469336	100.000				

Entry 7



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.220	6235370	1427413	24.779				
2	9.194	513660	101855	2.041				
3	9.611	1875911	468189	7.455				
4	9.877	900343	230546	3.578				
5	19.534	697612	172535	2.772				
6	21.002	5644153	1454121	22.430				
7	24.907	9296698	1912751	36.945				
		25163747	5767410	100.000				

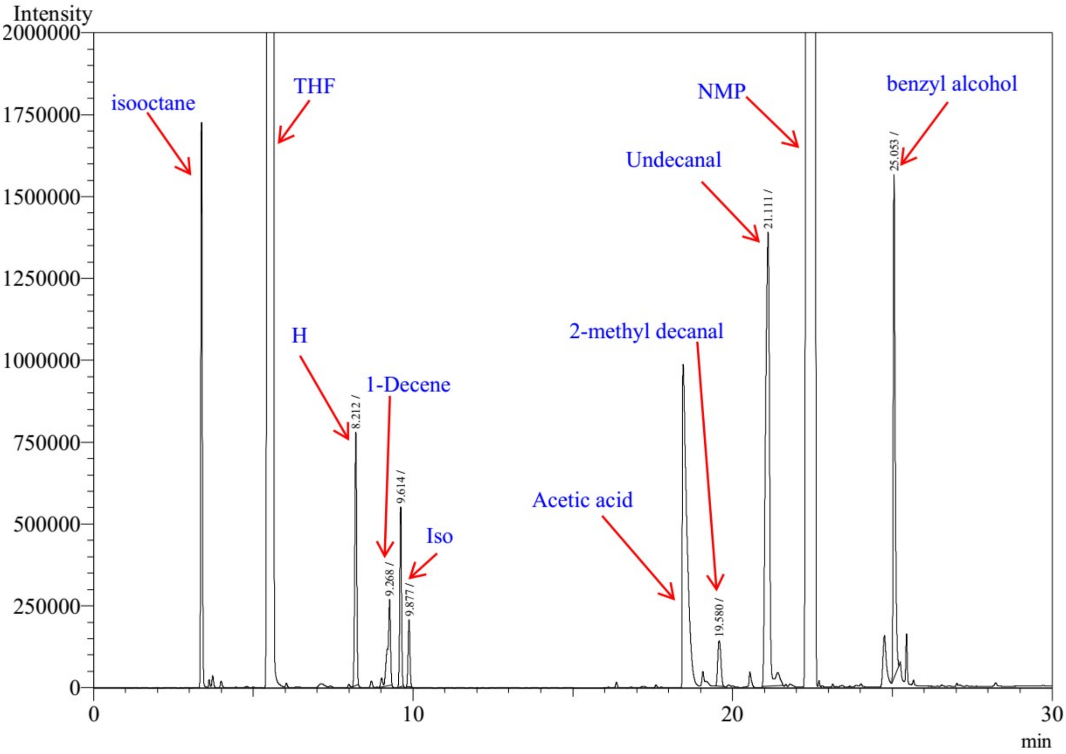
Entry 8



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	7.879	16974415	2889191	59.474				
2	24.129	284991	62551	0.999				
3	25.678	3234309	854350	11.332				
4	28.870	8046951	2951447	28.195				
		28540666	6757539	100.000				

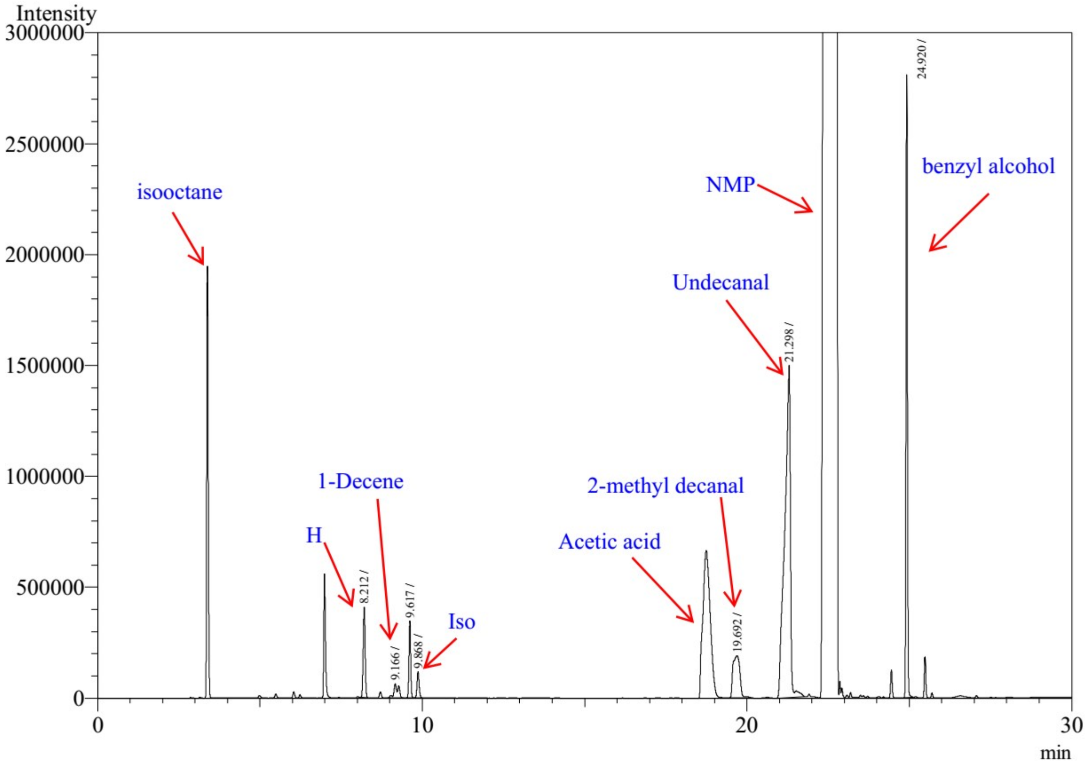
3.6 Gas chromatograms to Table S6

Entry 1



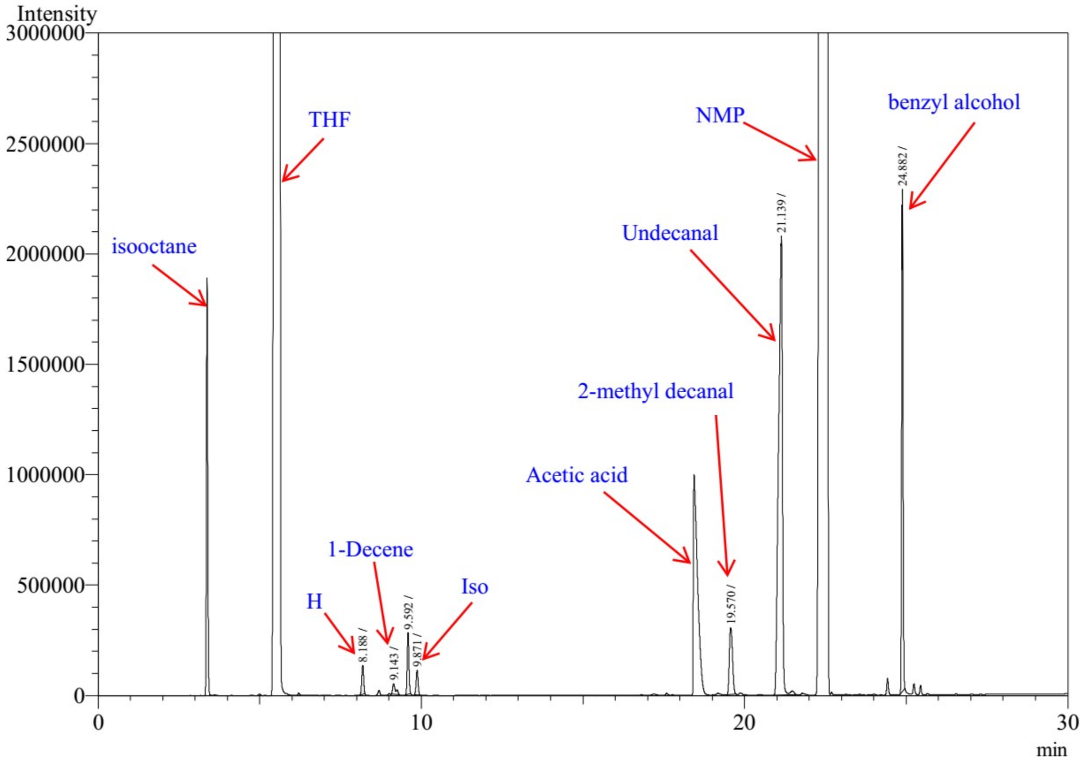
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.212	3233552	773785	11.834				
2	9.268	1722484	260852	6.304				
3	9.614	2030908	545506	7.433				
4	9.877	823277	204313	3.013				
5	19.580	950519	138190	3.479				
6	21.111	12047677	1382353	44.092				
7	25.053	6515643	1534877	23.846				
		27324060	4839876	100.000				

Entry 2



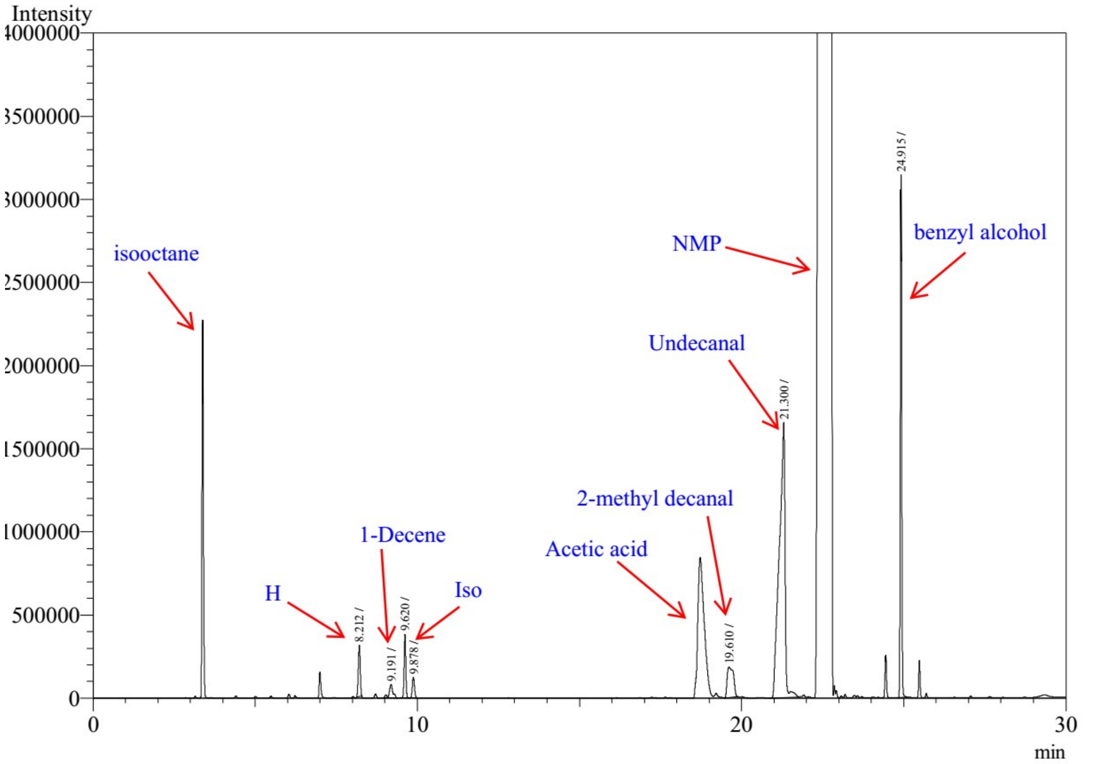
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.212	1729521	402193	5.175				
2	9.166	612686	63531	1.833				
3	9.617	1237231	341511	3.702				
4	9.868	515393	116909	1.542				
5	19.692	2846504	190022	8.517				
6	21.298	17974793	1489422	53.782				
7	24.920	8505263	2756027	25.449				
		33421391	5359615	100.000				

Entry 3



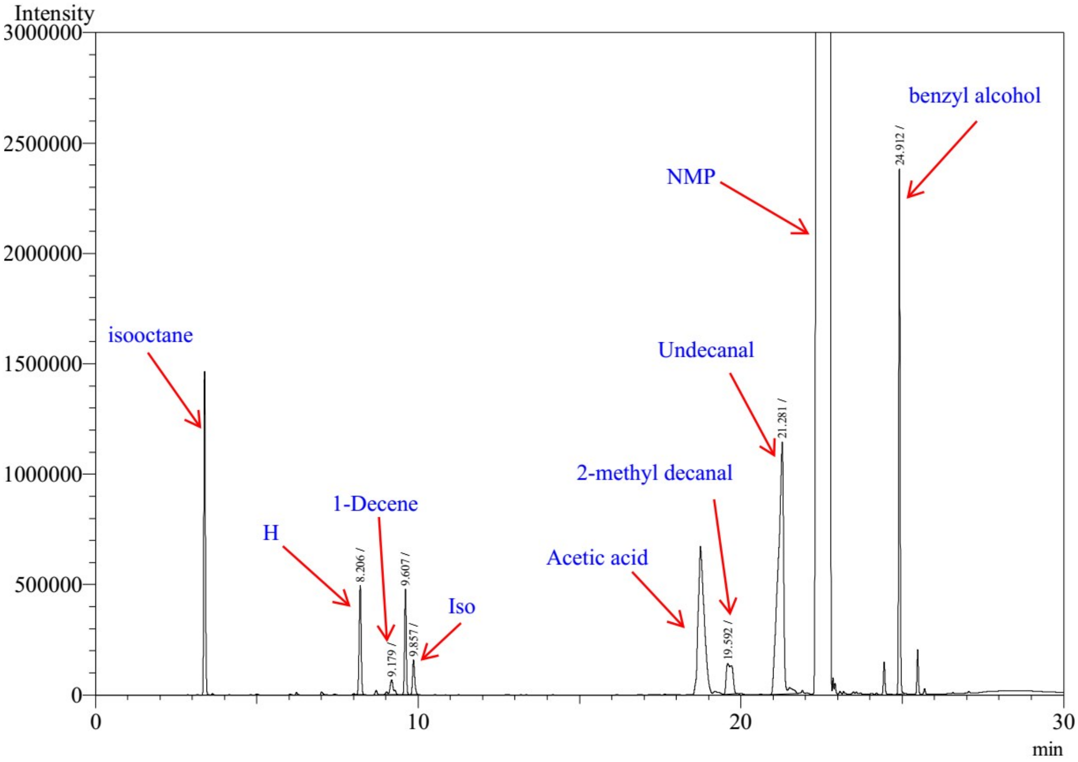
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.188	525964	131807	1.863				
2	9.143	321902	48238	1.140				
3	9.592	1027430	278473	3.640				
4	9.871	450422	109733	1.596				
5	19.570	2058181	300500	7.292				
6	21.139	17112415	2068063	60.628				
7	24.882	6729007	2267694	23.840				
		28225321	5204508	100.000				

Entry 4



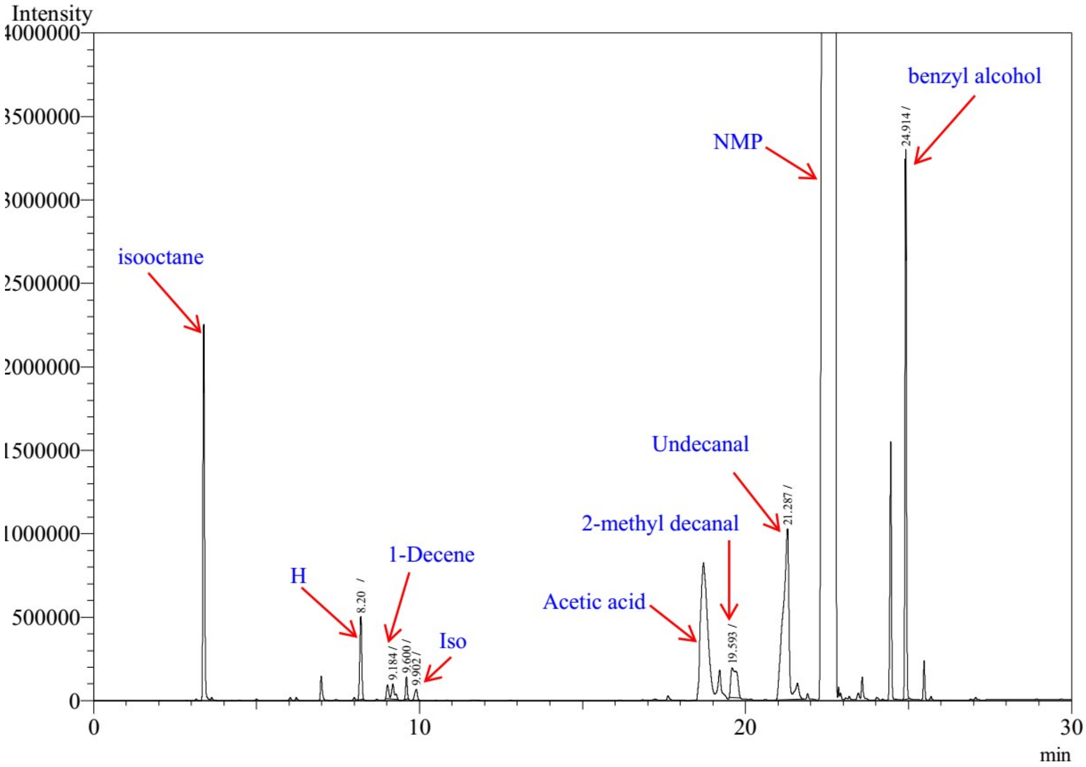
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.212	1278520	305847	3.529				
2	9.191	661323	80428	1.826				
3	9.620	1370562	381510	3.783				
4	9.878	573102	122698	1.582				
5	19.610	2464096	182553	6.802				
6	21.300	20476834	1652518	56.527				
7	24.915	9400729	3094717	25.951				
[redacted]		36225166	5820271	100.000				

Entry 5



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.206	2101495	493799	7.679				
2	9.179	540045	67543	1.973				
3	9.607	1704500	476487	6.229				
4	9.857	720633	156721	2.633				
5	19.592	1867702	139597	6.825				
6	21.281	13395228	1140812	48.949				
7	24.912	7035804	2360965	25.711				
		27365407	4835924	100.000				

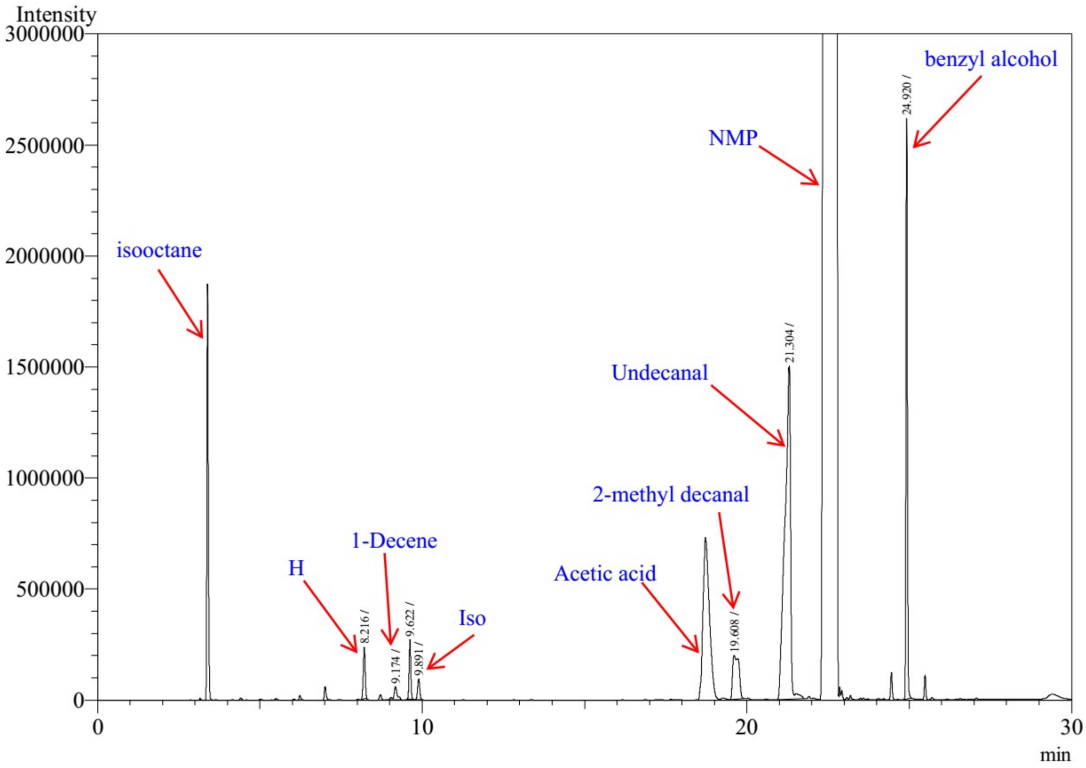
Entry 6



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.201	2106106	496581	7.141				
2	9.184	940861	90931	3.190				
3	9.600	467076	134991	1.584				
4	9.902	367585	65197	1.246				
5	19.593	2413894	178892	8.185				
6	21.287	13156041	1023421	44.609				
7	24.914	10040501	3287422	34.045				
		29492064	5277435	100.000				

3.7 Gas chromatograms to Table S7

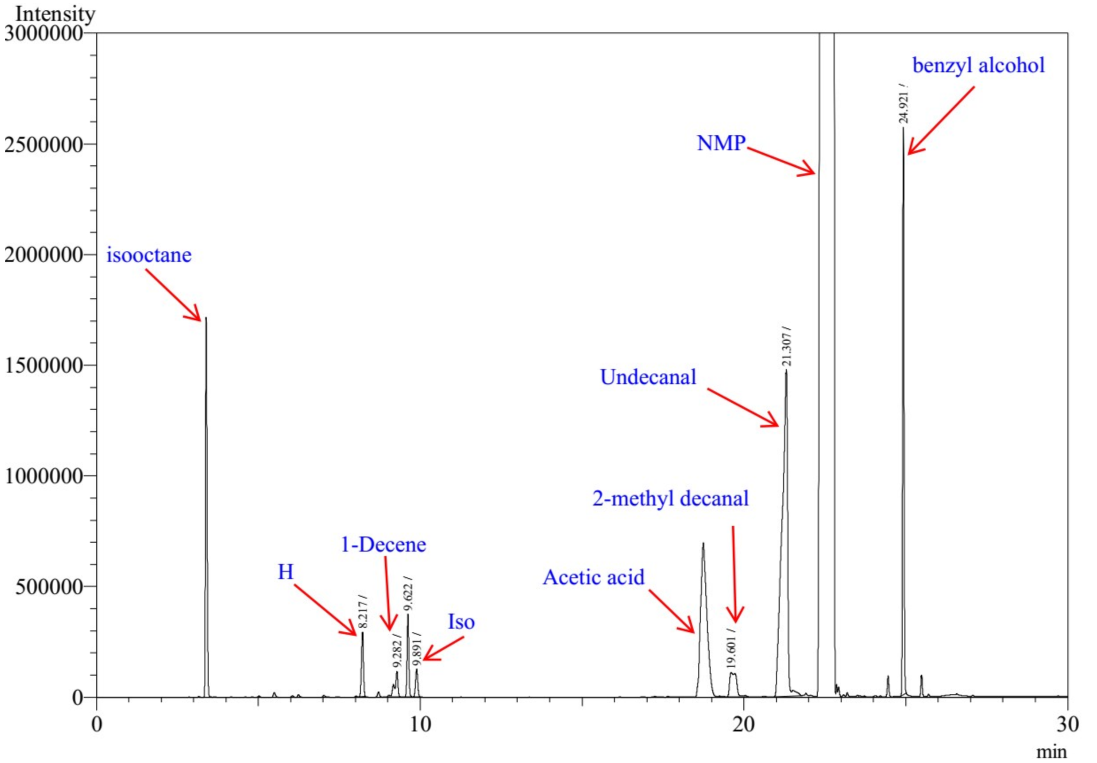
Entry 1



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.216	963490	231689	3.075				
2	9.174	415740	58885	1.327				
3	9.622	964583	264204	3.078				
4	9.891	436136	93955	1.392				
5	19.608	2679056	196332	8.550				
6	21.304	18093976	1499954	57.747				
7	24.920	7780408	2580584	24.831				
		31333389	4925603	100.000				

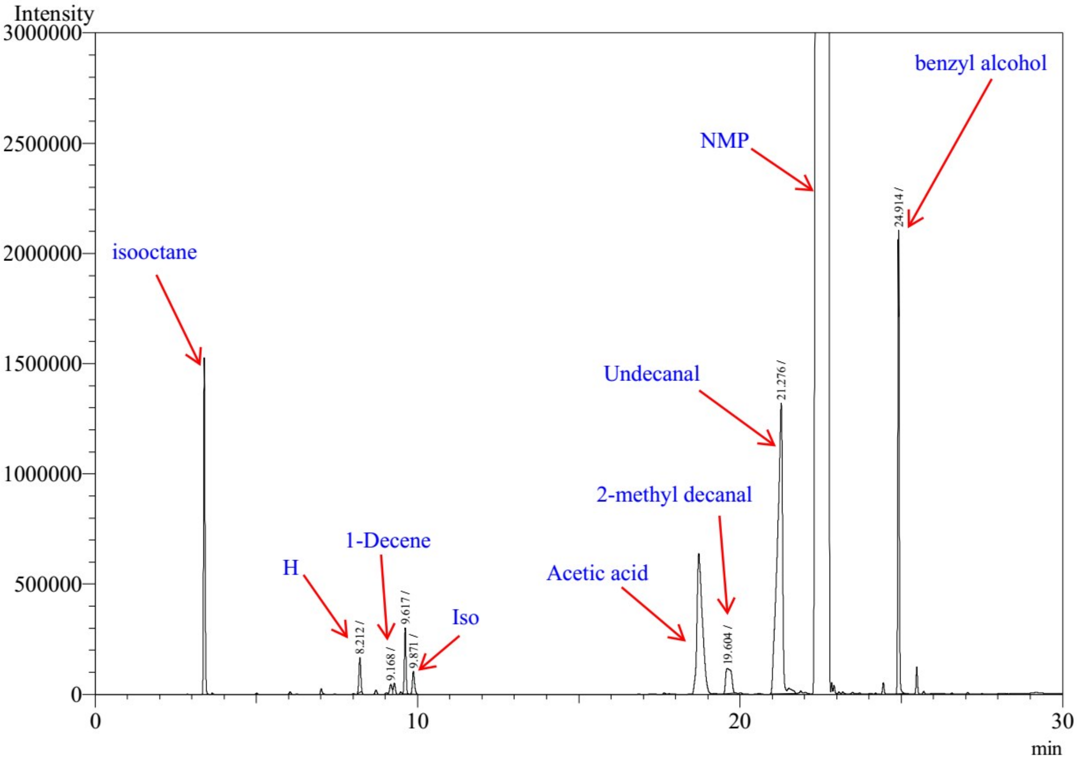
Entry 2

Entry 3



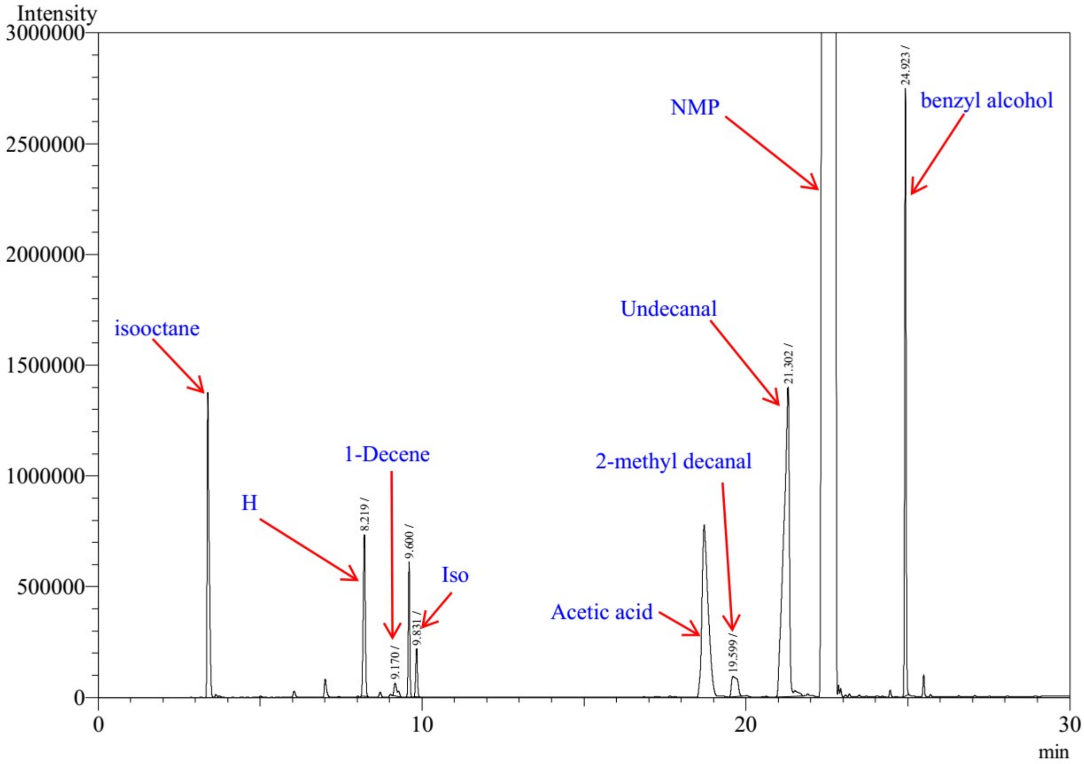
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.217	1226539	288741	3.944				
2	9.282	818010	114886	2.631				
3	9.622	1377392	371156	4.430				
4	9.891	590722	125344	1.900				
5	19.601	1604879	110981	5.161				
6	21.307	17861266	1472447	57.440				
7	24.921	7616843	2546407	24.495				
[redacted]		31095651	5029962	100.000				

Entry 4



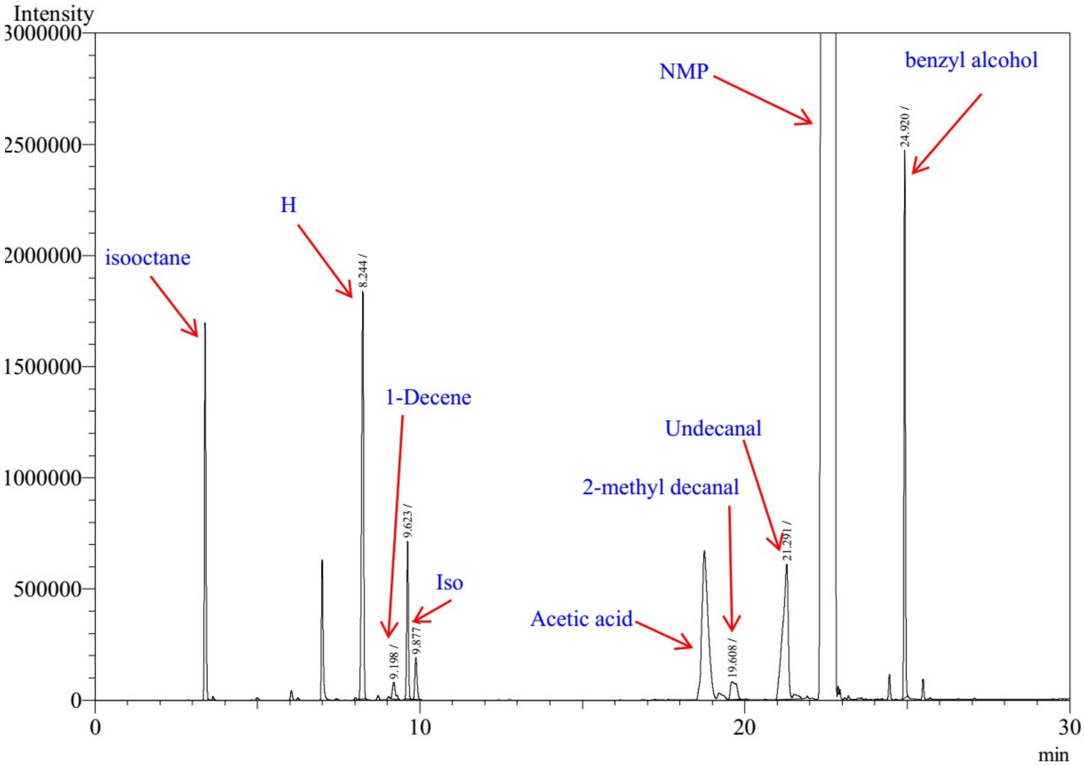
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.212	629513	156582	2.529				
2	9.168	251829	47668	1.012				
3	9.617	1045493	295836	4.199				
4	9.871	477865	104179	1.919				
5	19.604	1440189	114957	5.785				
6	21.276	14745835	1318564	59.230				
7	24.914	6305264	2054005	25.326				
		24895988	4091791	100.000				

Entry 5



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.219	3250913	727776	9.887				
2	9.170	407905	57761	1.241				
3	9.600	1919553	603977	5.838				
4	9.831	811773	217835	2.469				
5	19.599	1201023	91183	3.653				
6	21.302	16902683	1395758	51.406				
7	24.923	8386695	2738491	25.507				
		32880545	5832781	100.000				

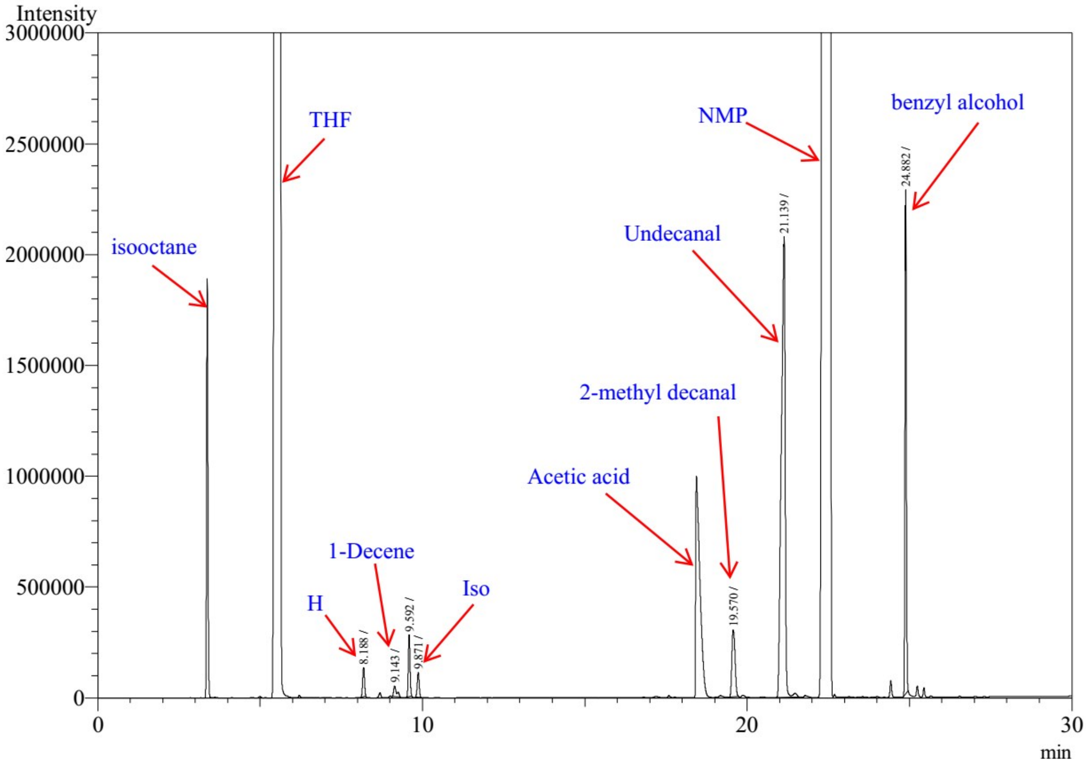
Entry 6



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.244	8095621	1832646	29.102				
2	9.198	483809	75124	1.739				
3	9.623	2528300	704299	9.089				
4	9.877	887514	187608	3.190				
5	19.608	1068469	80511	3.841				
6	21.291	7427628	607984	26.701				
7	24.920	7326390	2435324	26.337				
		27817731	5923496	100.000				

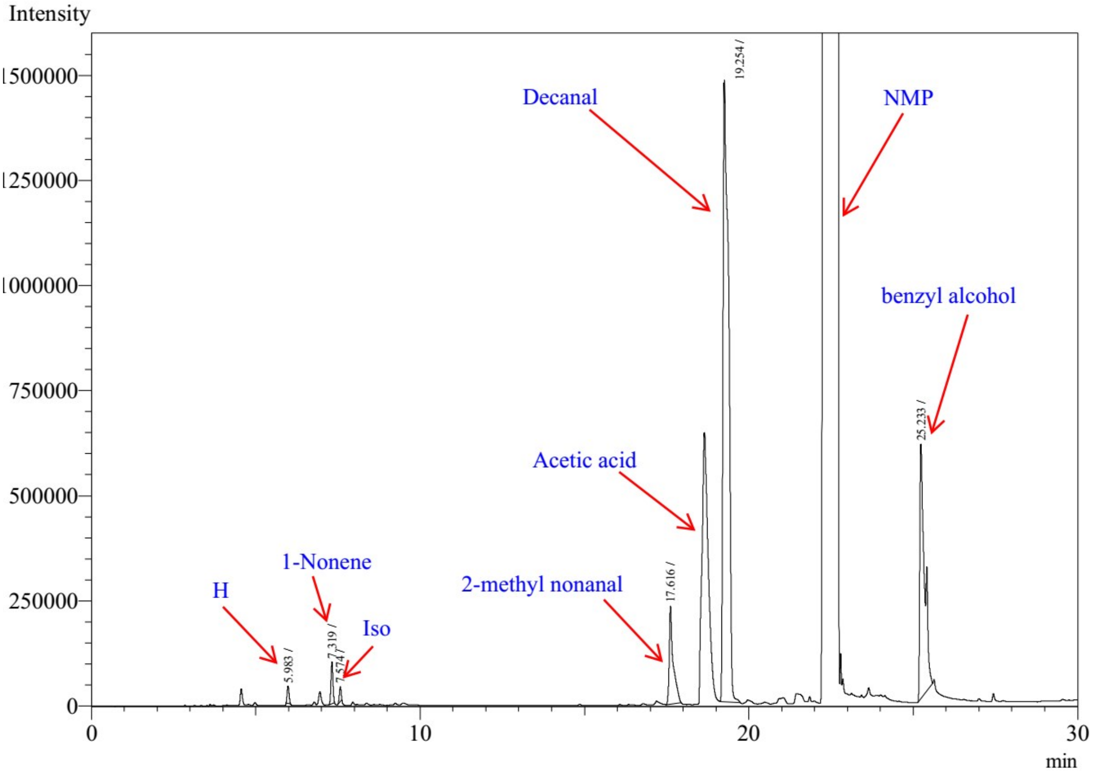
3.8 Gas chromatograms to Table S8

Entry 1



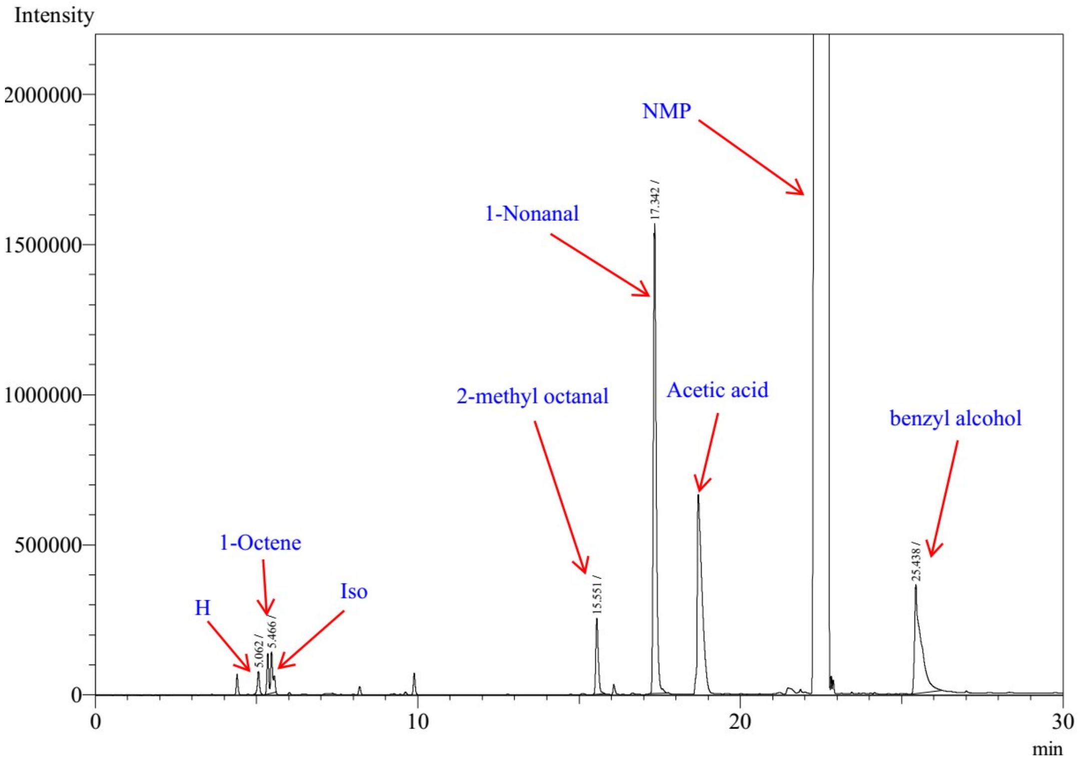
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.188	525964	131807	1.863				
2	9.143	321902	48238	1.140				
3	9.592	1027430	278473	3.640				
4	9.871	450422	109733	1.596				
5	19.570	2058181	300500	7.292				
6	21.139	17112415	2068063	60.628				
7	24.882	6729007	2267694	23.840				
[redacted]		28225321	5204508	100.000				

Entry 2



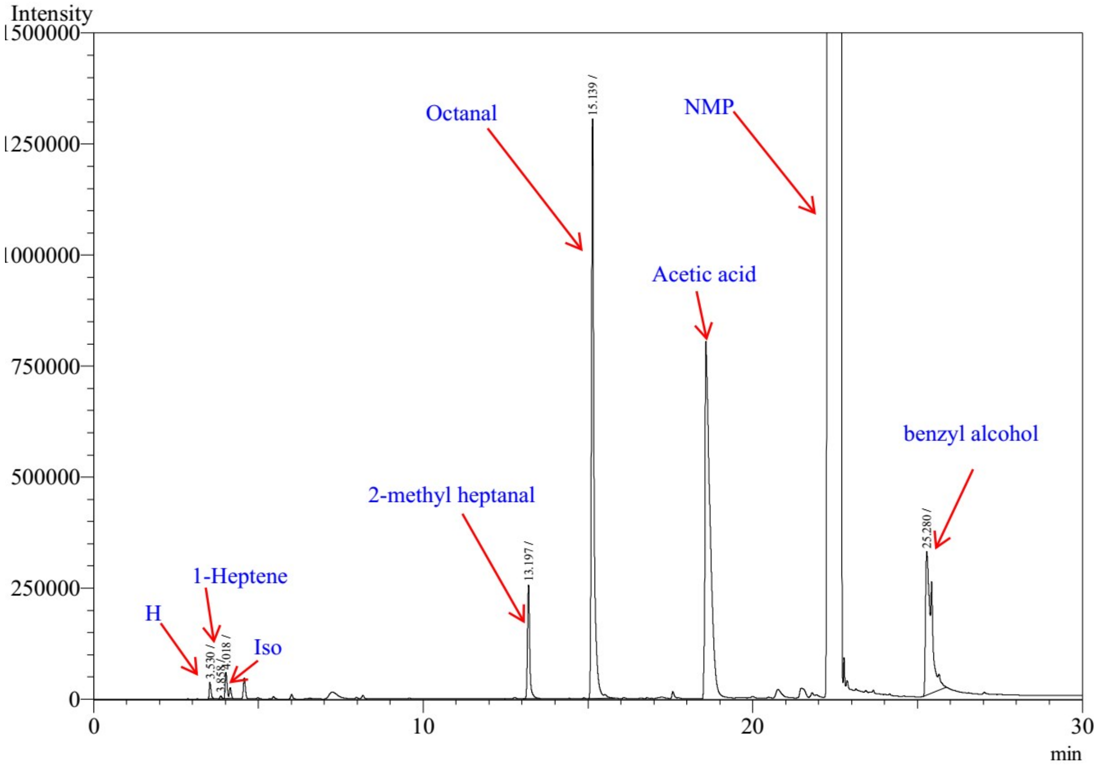
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	5.983	168923	41565	0.655				
2	7.319	417544	99349	1.619				
3	7.574	130279	35155	0.505				
4	17.616	1928270	231253	7.475				
5	19.254	17125060	1471719	66.384				
6	25.233	6026724	604225	23.362				
		25796800	2483266	100.000				

Entry 3



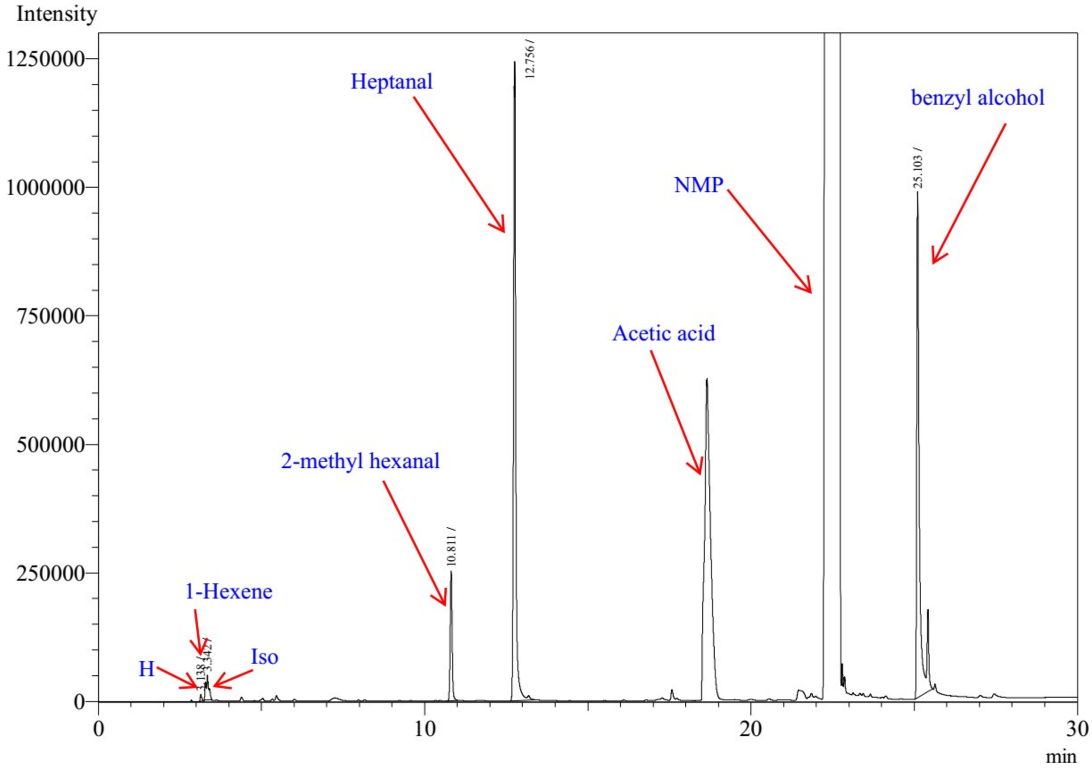
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	5.062	351600	76983	1.980				
2	5.466	1251506	137868	7.049				
3	15.551	1372773	253008	7.732				
4	17.342	9779828	1562154	55.086				
5	25.438	4998090	361045	28.152				
		17753797	2391058	100.000				

Entry 4



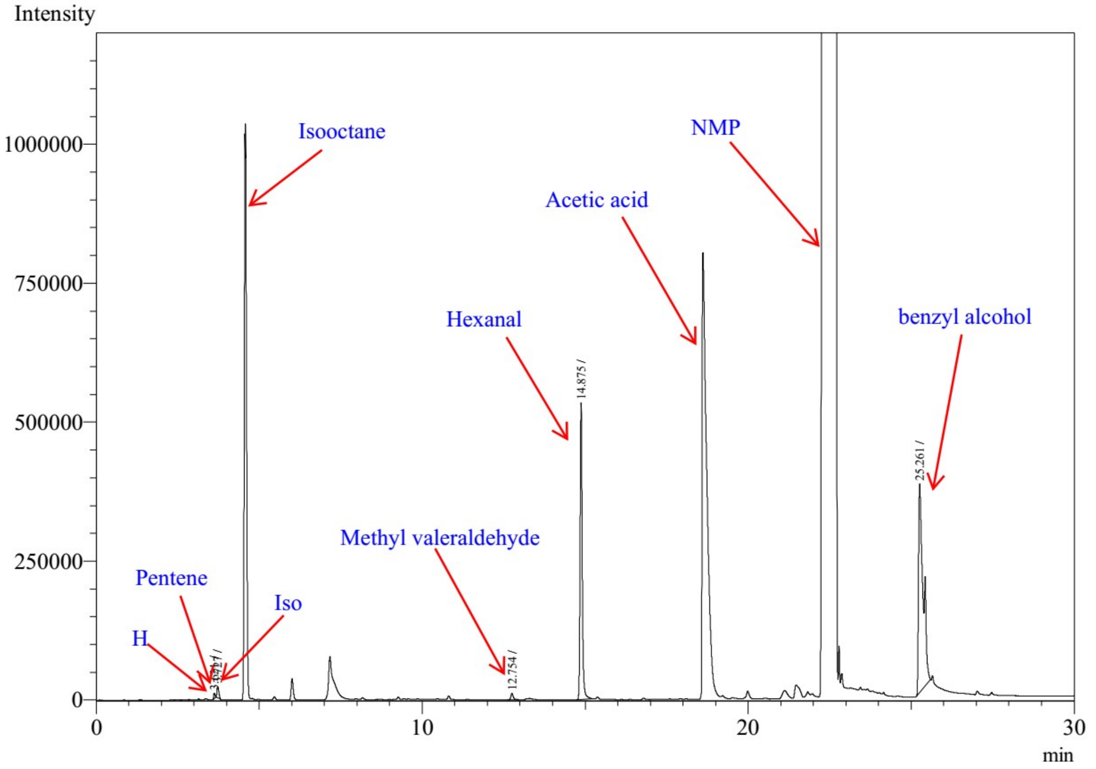
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.530	136372	36848	1.060				
2	3.858	22546	6080	0.175				
3	4.018	314979	58135	2.447				
4	13.197	1228075	254675	9.542				
5	15.139	7017881	1300207	54.530				
6	25.280	4149850	323389	32.245				
		12869703	1979334	100.000				

Entry 5



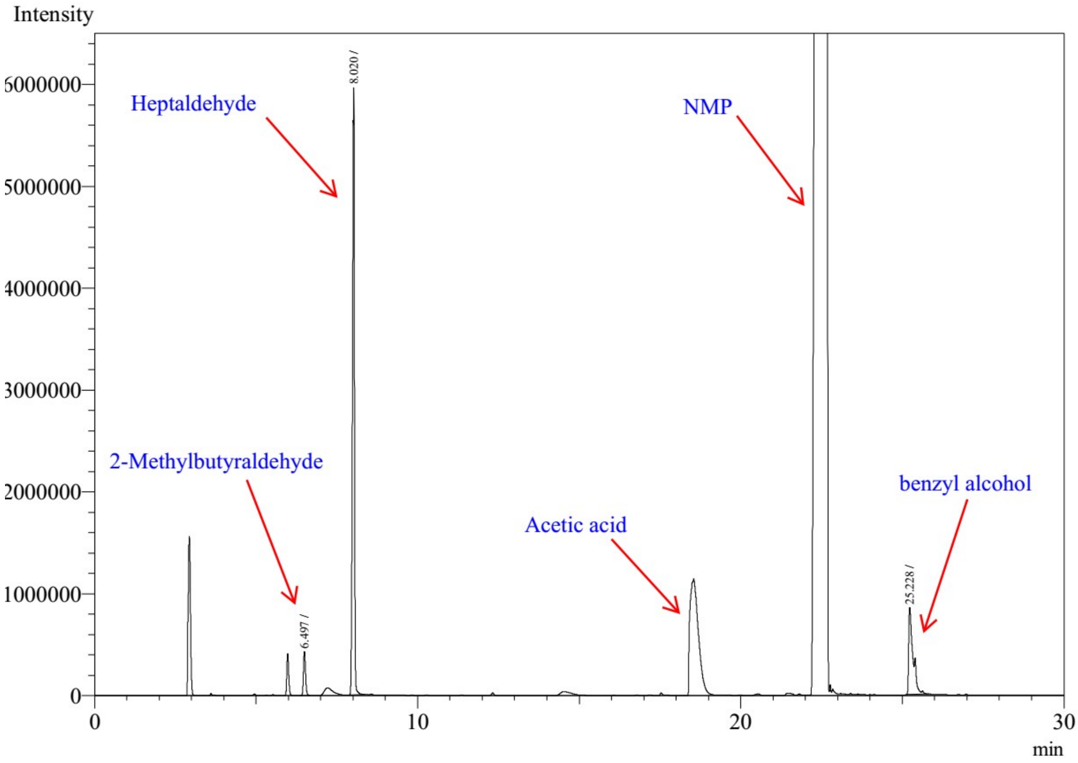
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.138	43208	13406	0.333				
2	3.342	306829	48374	2.366				
3	10.811	1055356	252135	8.138				
4	12.756	5915196	1241980	45.610				
5	25.103	5648382	980390	43.553				
		12968971	2536285	100.000				

Entry 6



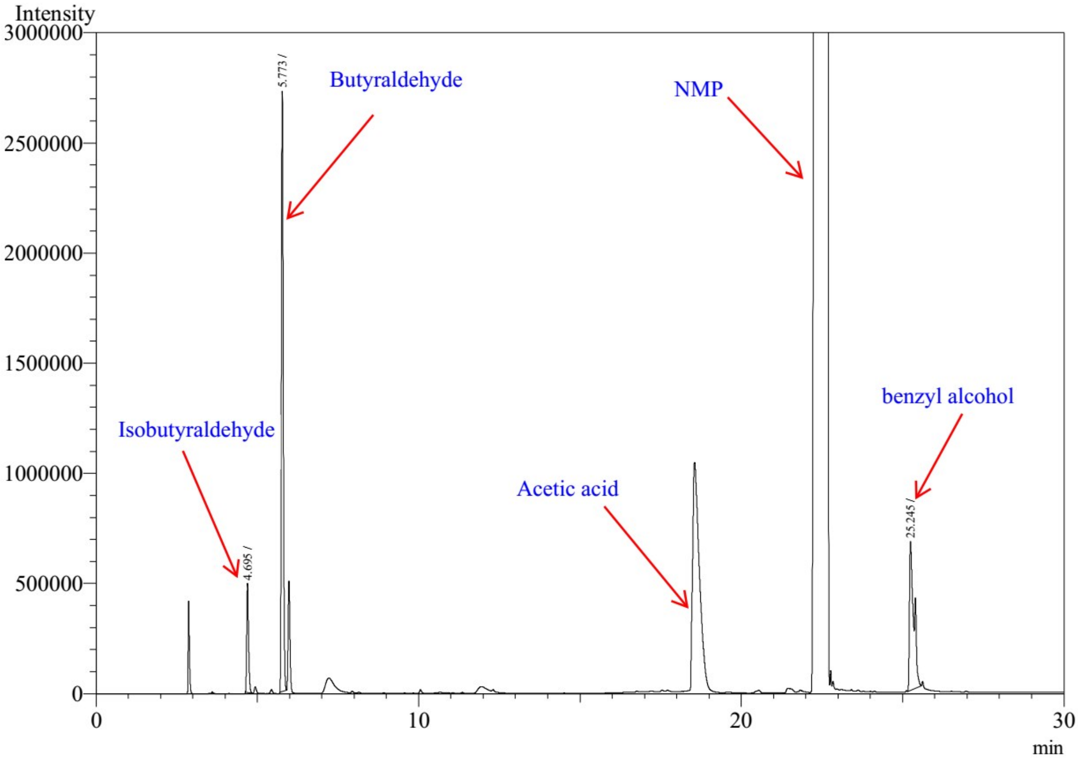
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.621	27974	9745	0.446				
2	3.727	83275	20548	1.327				
3	12.754	56739	11989	0.904				
4	14.875	2421314	532718	38.589				
5	25.261	3685262	374847	58.733				
		6274564	949847	100.000				

Entry 7



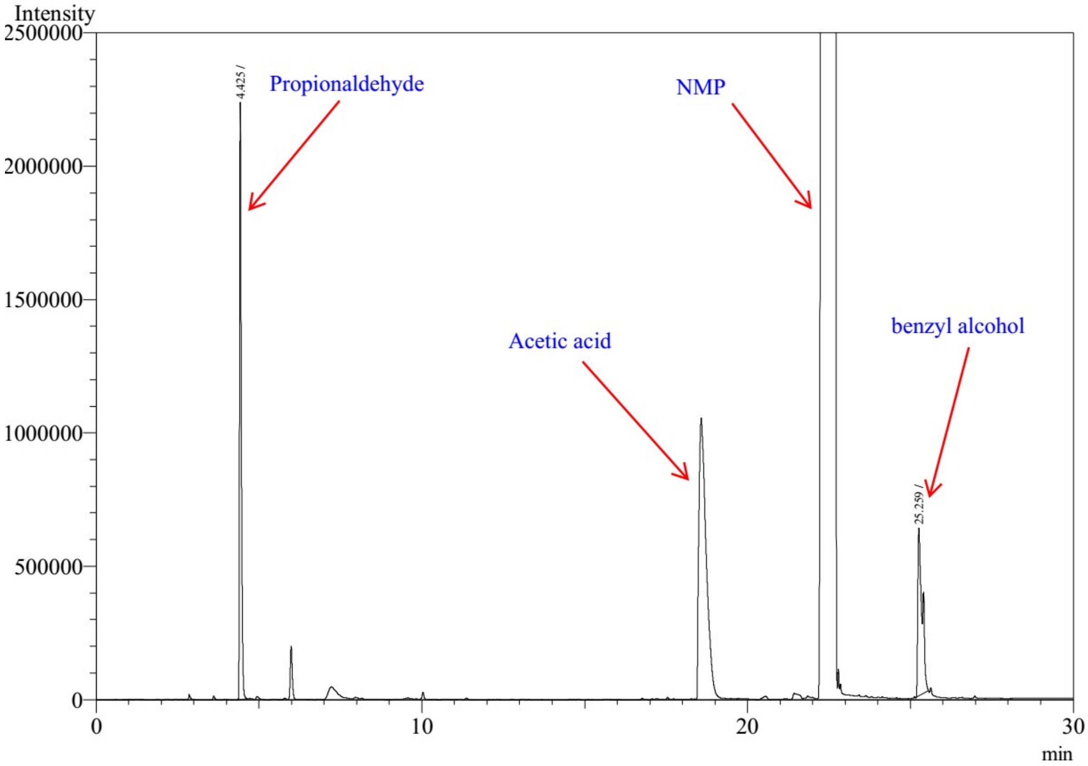
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	6.497	1903891	428590	5.476				
2	8.020	24826152	5953317	71.406				
3	25.228	8037695	852072	23.118				
		34767738	7233979	100.000				

Entry 8



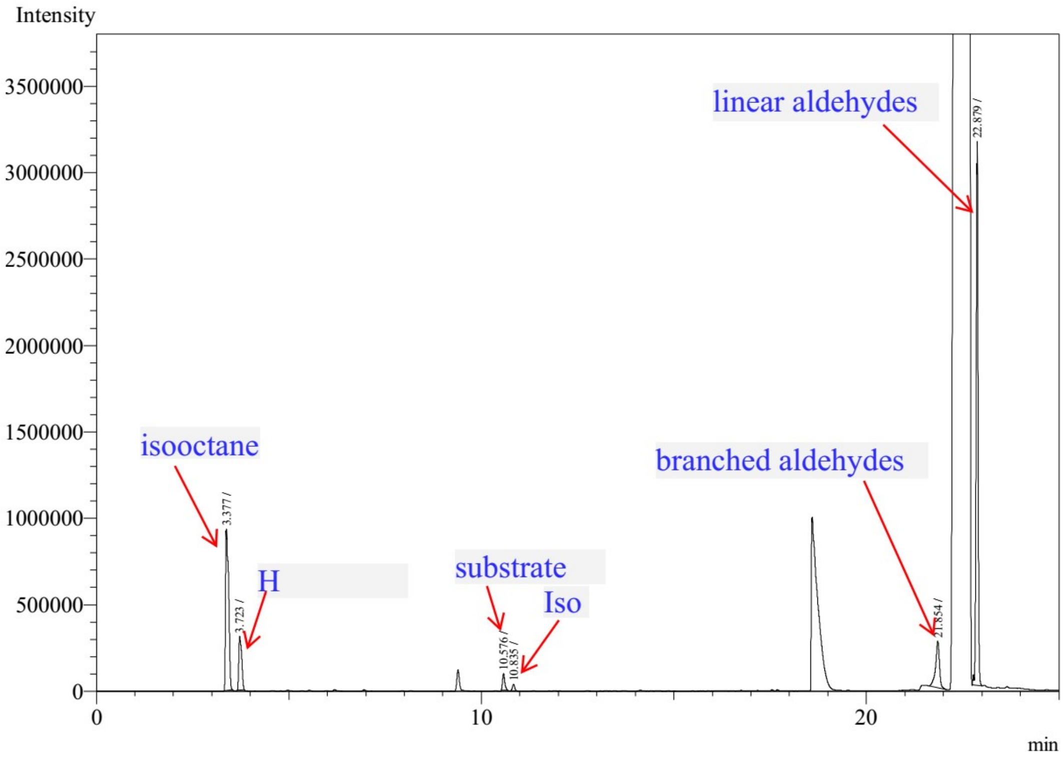
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	4.695	1957234	493841	10.180				
2	5.773	10881986	2714895	56.602				
3	25.245	6386146	671789	33.217				
[redacted]		19225366	3880525	100.000				

Entry 9



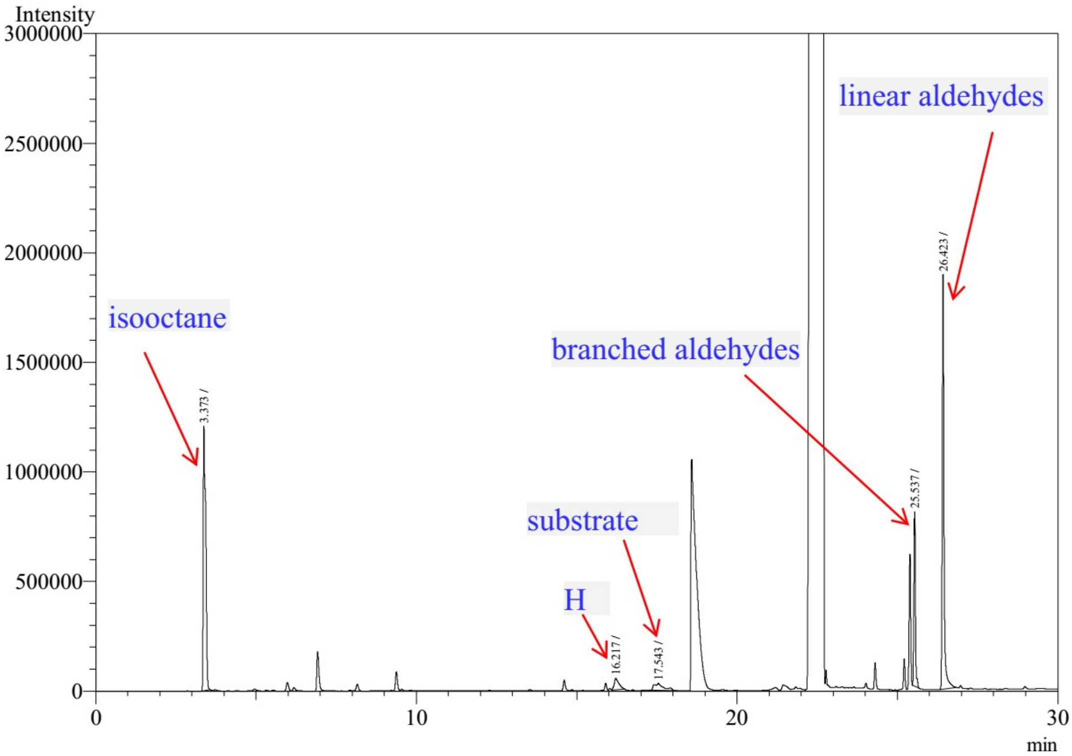
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	4.425	8416074	2228361	59.182				
2	25.259	5804504	629582	40.818				
		14220578	2857943	100.000				

Entry 10



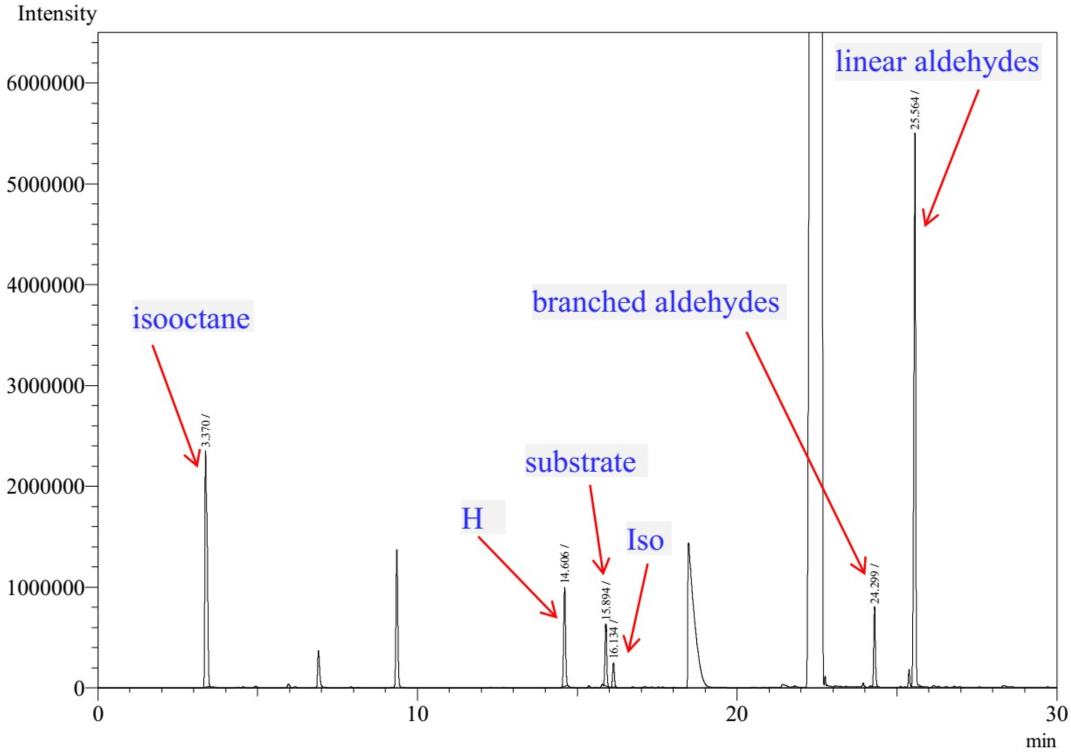
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.377	5101246	930725	25.448				
2	3.723	1639368	308538	8.178				
3	10.576	390781	96573	1.949				
4	10.835	152901	38726	0.763				
5	21.854	1881364	268373	9.385				
6	22.879	10880442	3141022	54.277				
[redacted]		20046102	4783957	100.000				

Entry 11



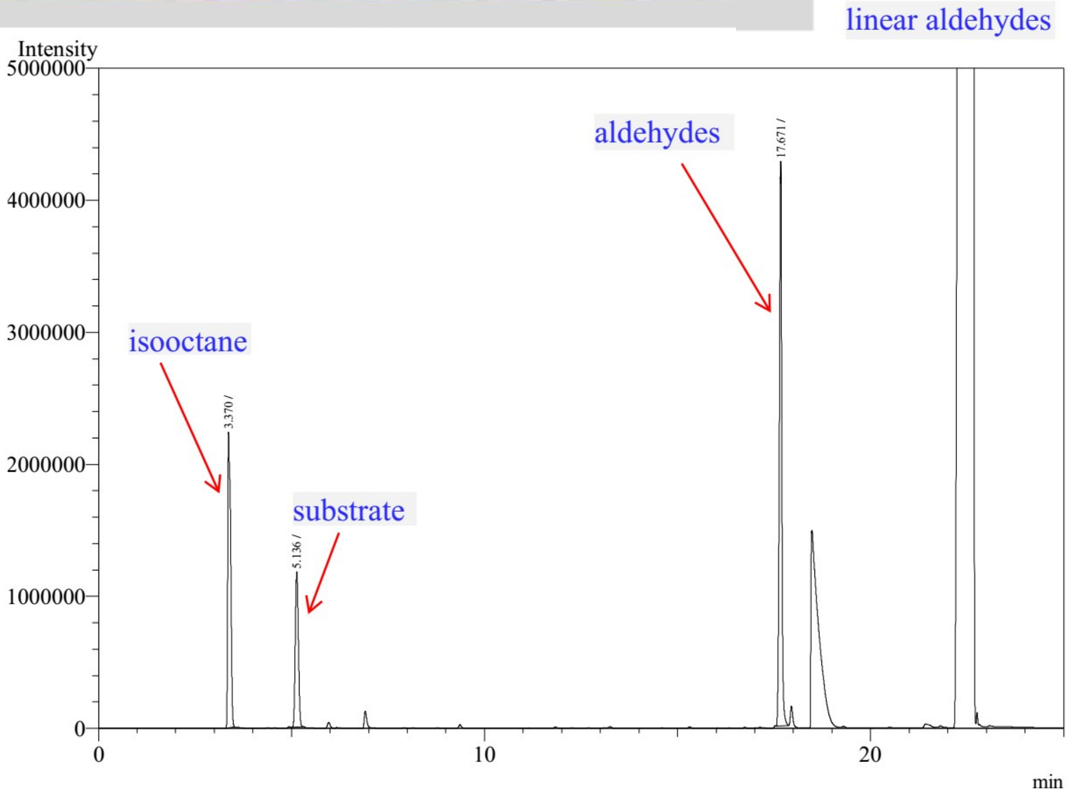
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.373	6518664	1189265	37.150				
2	16.217	527220	51829	3.005				
3	17.543	663894	32188	3.784				
4	25.537	2647913	793392	15.091				
5	26.423	7189172	1876193	40.971				
		17546863	3942867	100.000				

Entry 12



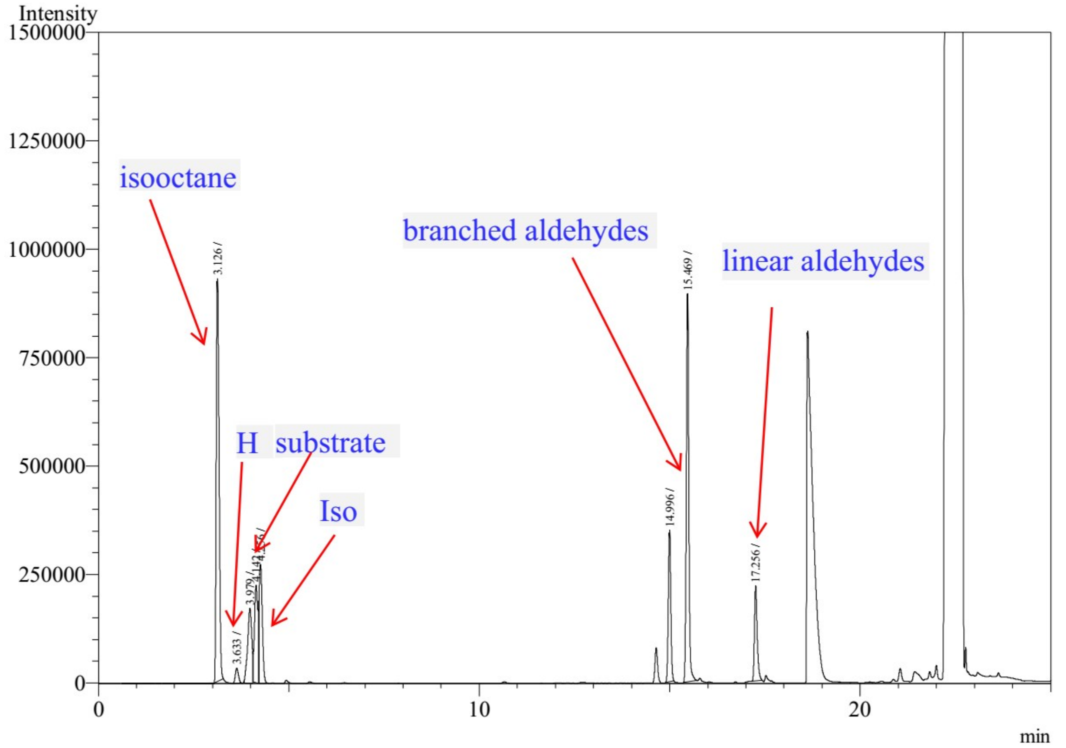
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.370	11787688	2331993	27.586				
2	14.606	3942965	968754	9.227				
3	15.894	2328067	613068	5.448				
4	16.134	905538	243429	2.119				
5	24.299	2743472	785282	6.420				
6	25.564	21023324	5432083	49.199				
		42731054	10374609	100.000				

Entry 13



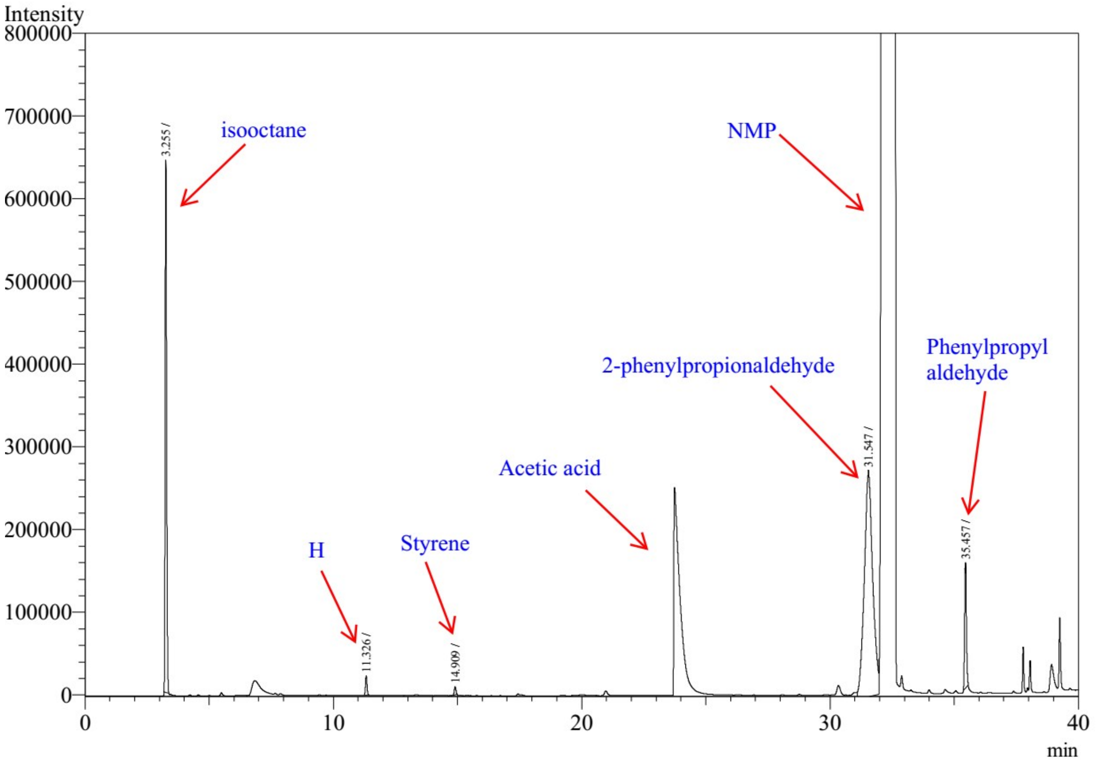
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.370	11612361	2223886	31.431				
2	5.136	6590600	1174450	17.838				
3	17.671	18743103	4272290	50.731				
		36946064	7670626	100.000				

Entry 14



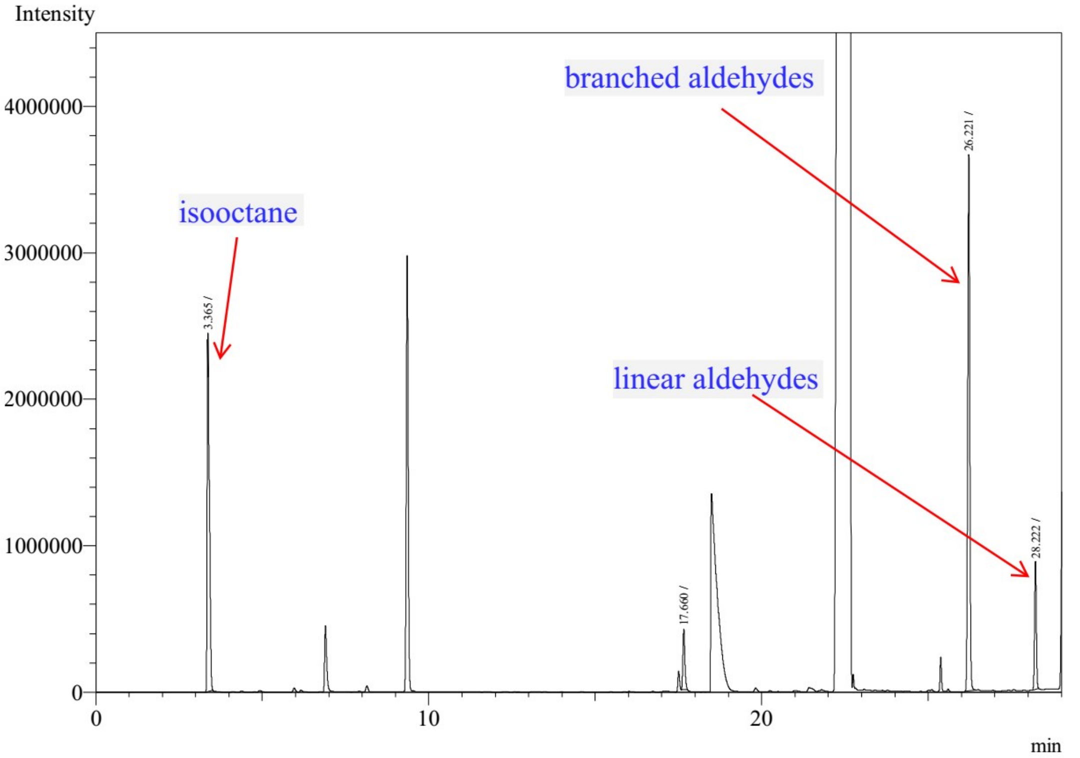
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.126	4801417	929330	30.463				
2	3.633	191767	34579	1.217				
3	3.979	1274898	173220	8.089				
4	4.142	1337187	225778	8.484				
5	4.256	1474861	273824	9.357				
6	14.996	1571954	348543	9.973				
7	15.469	4016916	884343	25.486				
8	17.256	1092557	219386	6.932				
		15761557	3089003	100.000				

Entry 15



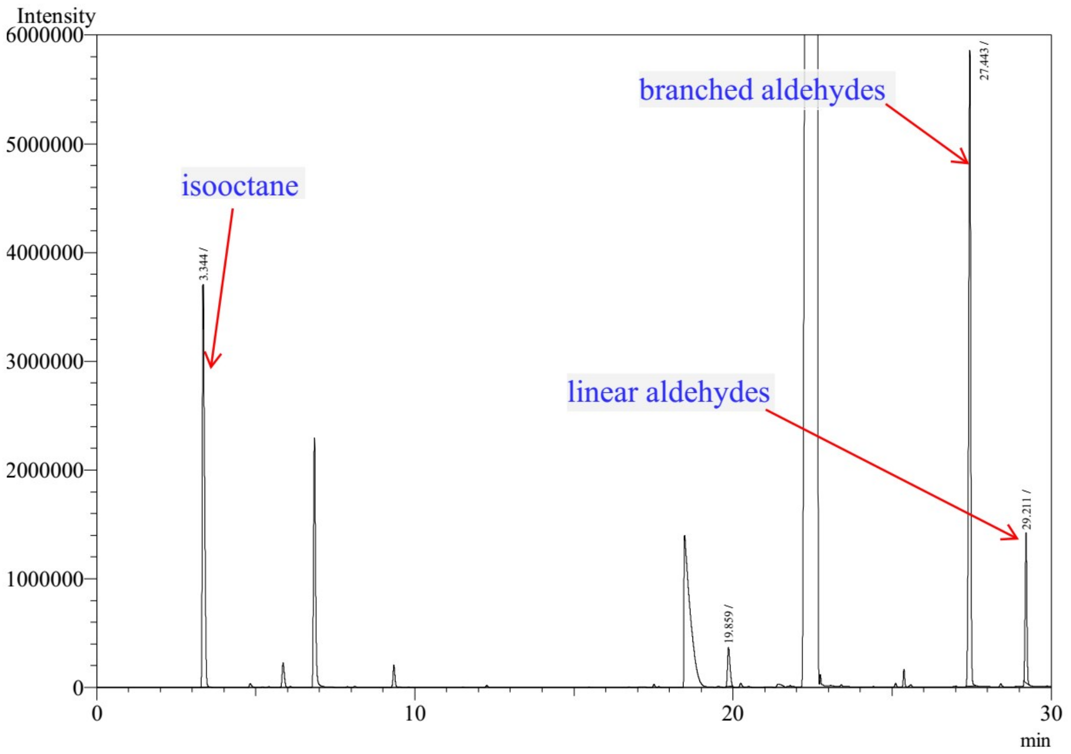
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.255	2688317	642937	26.767				
2	11.326	97316	23173	0.969				
3	14.909	47706	10002	0.475				
4	31.547	6478843	274287	64.509				
5	35.457	731199	150571	7.280				
		10043381	1100970	100.000				

Entry 16



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.365	11187330	2421872	35.489				
2	17.660	1698385	412620	5.388				
3	26.221	15463636	3624638	49.055				
4	28.222	3173979	870588	10.069				
		31523330	7329718	100.000				

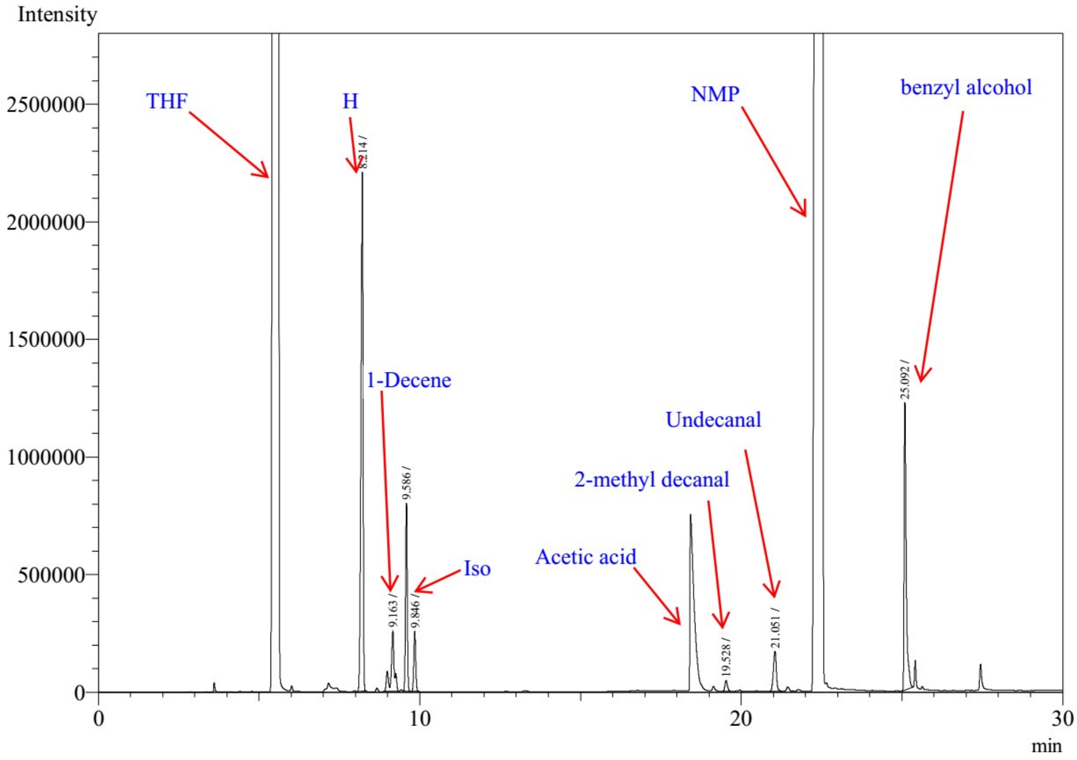
Entry 17



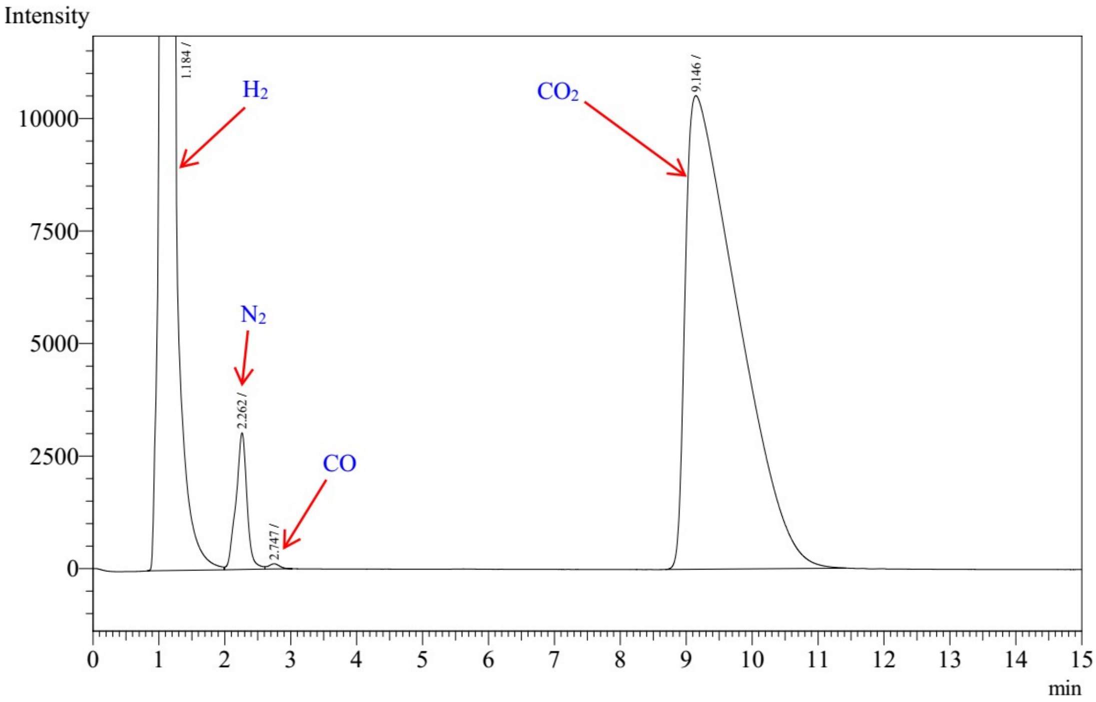
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.344	17602025	3699848	34.963				
2	19.859	1933647	360079	3.841				
3	27.443	25669817	5838910	50.988				
4	29.211	5139513	1379364	10.209				
		50345002	11278201	100.000				

3.9 Gas chromatograms to Table S9

PPh$_3$ Entry 1

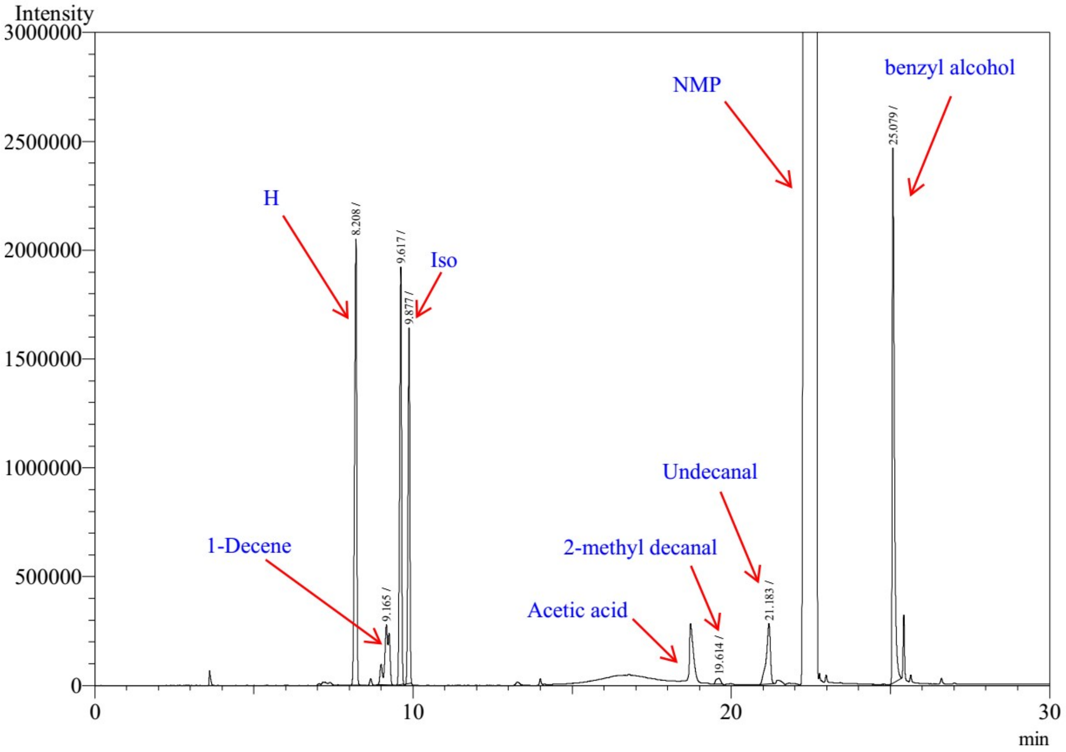


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.214	9925307	2194525	43.636				
2	9.163	1902660	256871	8.365				
3	9.586	2932134	796275	12.891				
4	9.846	1044651	252230	4.593				
5	19.528	236943	45331	1.042				
6	21.051	1093269	168580	4.807				
7	25.092	5610637	1207177	24.667				
		22745601	4920989	100.000				

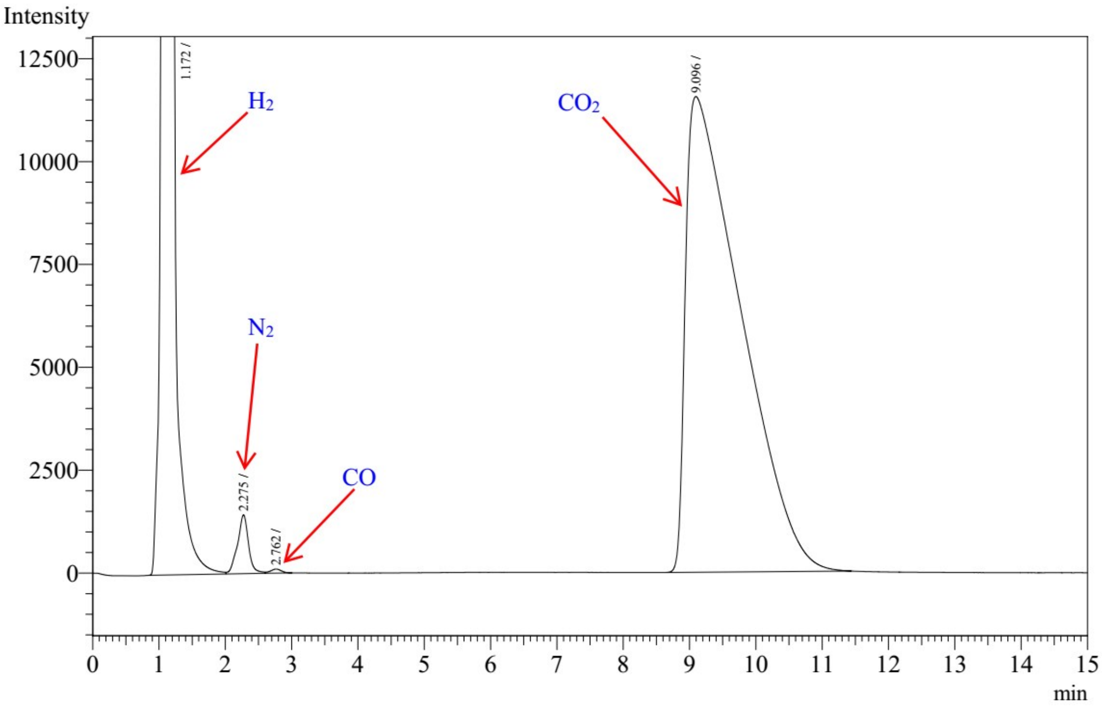


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.184	1485401	176877	70.672				
2	2.262	35396	3036	1.684		V		
3	2.747	1377	116	0.066		V		
4	9.146	579646	10519	27.578				
[redacted]		2101820	190548					

PPh$_3$ Entry 2

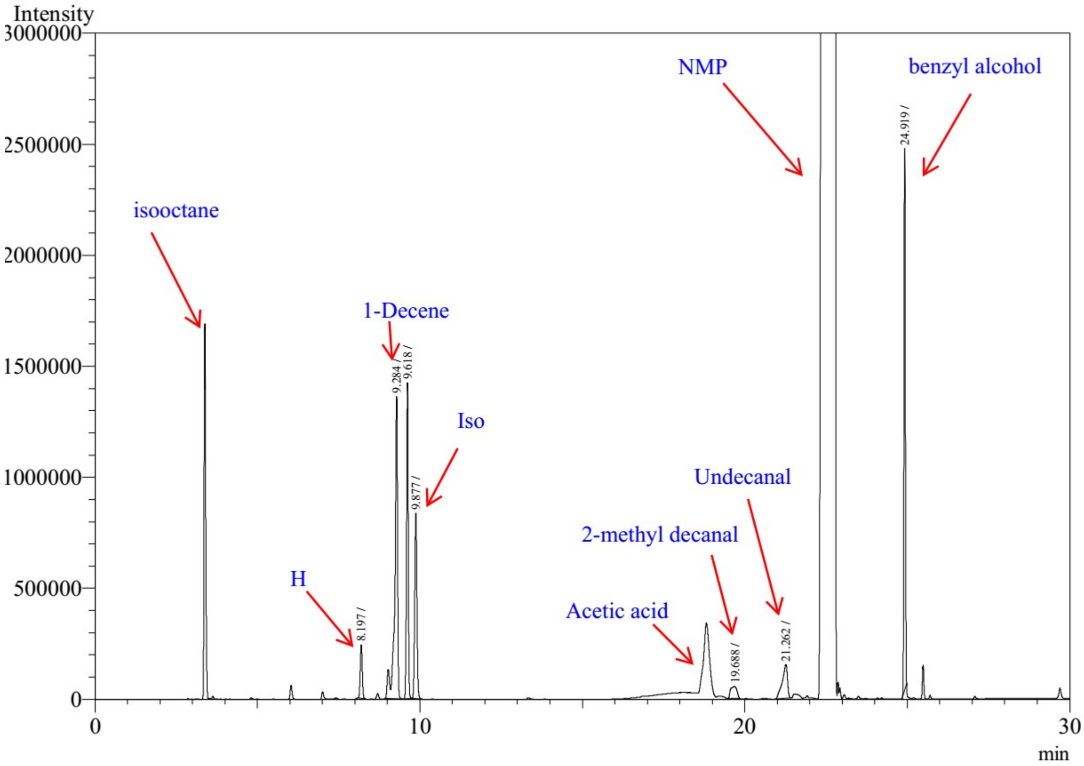


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.208	9521242	2029574	22.981				
2	9.165	3012808	276248	7.272				
3	9.617	8261923	1917047	19.941				
4	9.877	6552723	1631800	15.816				
5	19.614	263968	26642	0.637				
6	21.183	2481983	277030	5.991				
7	25.079	11337147	2443575	27.363				
		41431794	8601916	100.000				

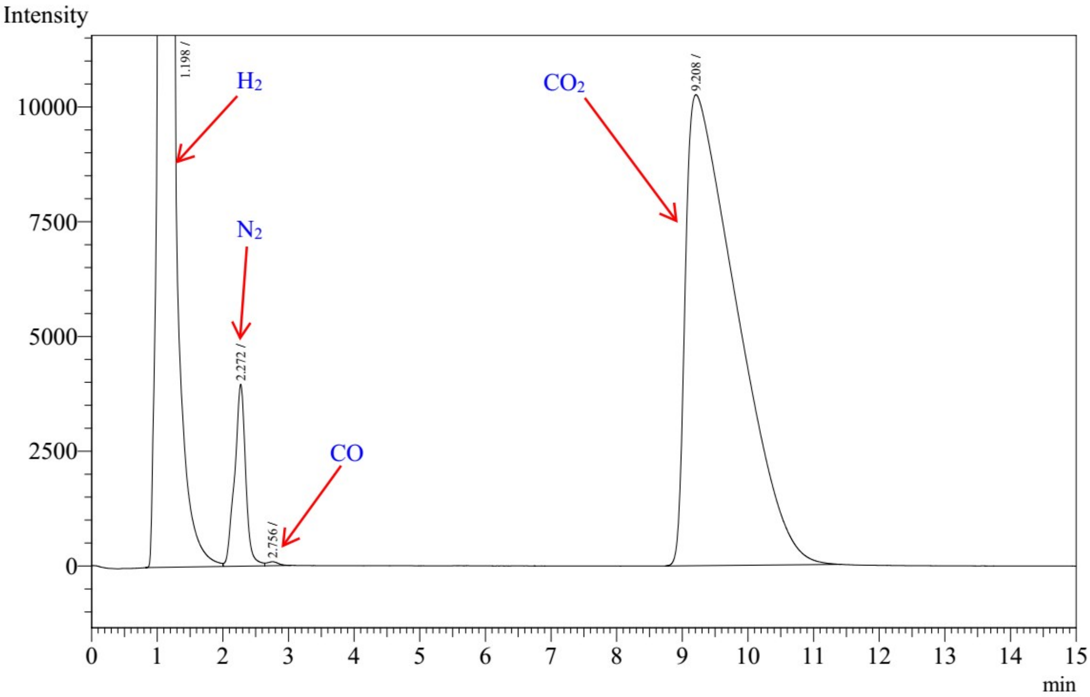


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.172	1065690	146488	60.824				
2	2.275	16565	1430	0.945		V		
3	2.762	1148	100	0.066		V		
4	9.096	668693	11557	38.165				
		1752096	159575					

PPh$_3$ Entry 3

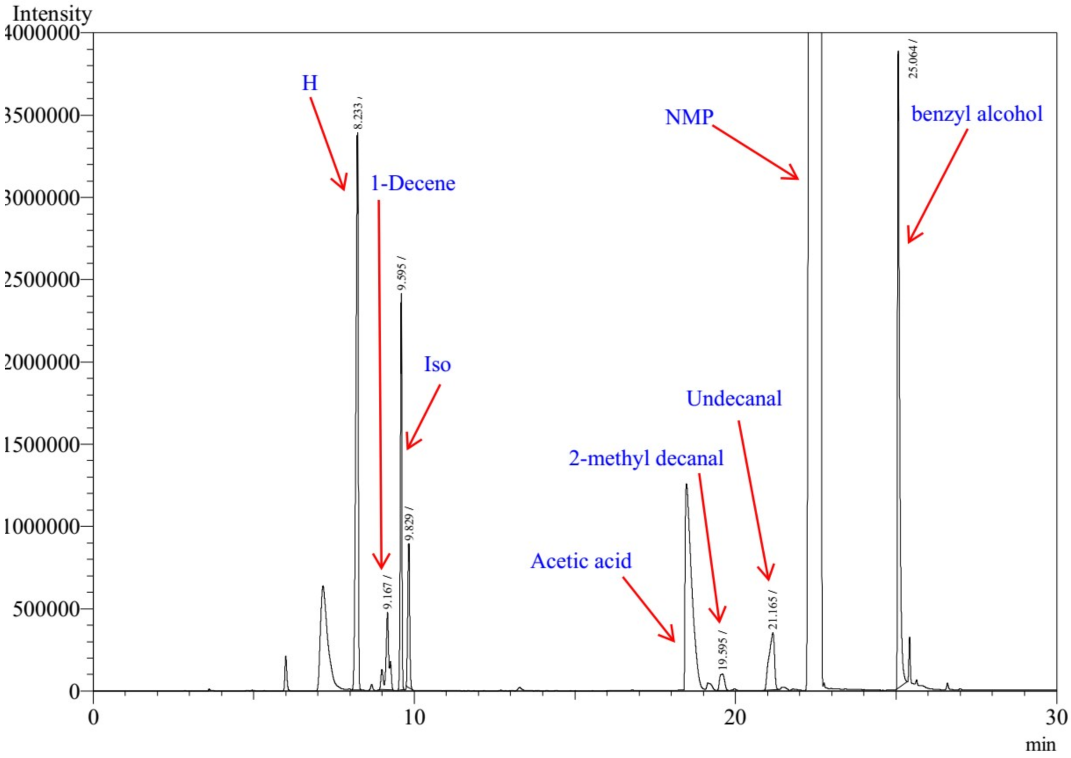


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.197	1038754	240702	3.745				
2	9.284	7881951	1361197	28.414				
3	9.618	5232428	1415414	18.863				
4	9.877	3972289	833469	14.320				
5	19.688	741665	54184	2.674				
6	21.262	1693254	153359	6.104				
7	24.919	7179055	2400701	25.880				
		27739396	6459026	100.000				

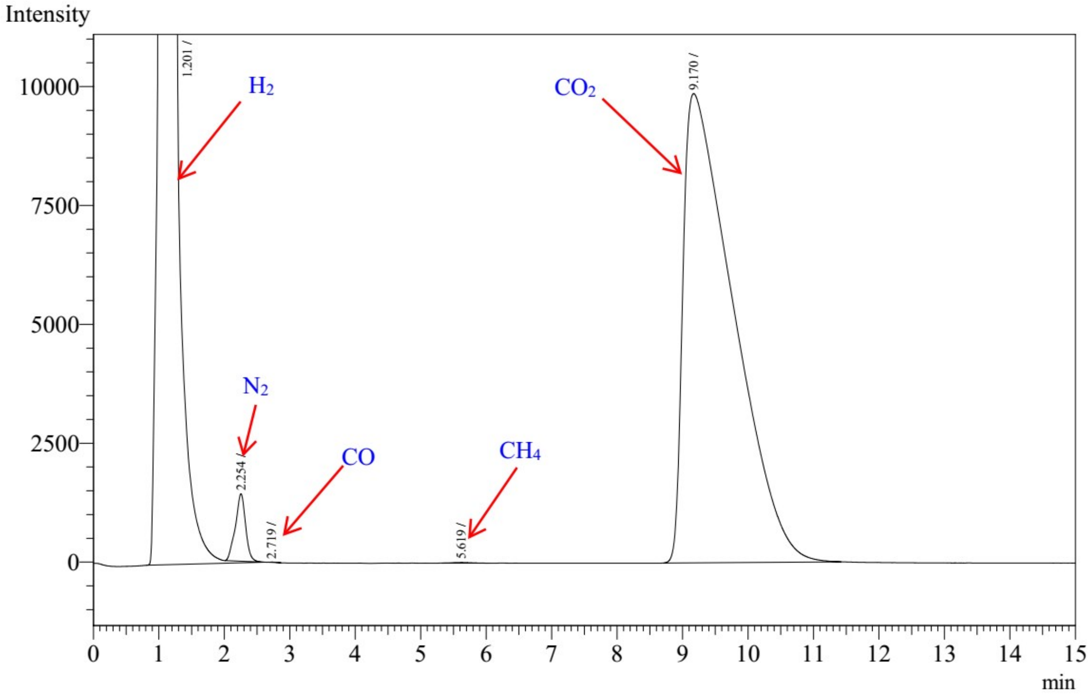


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.198	1702274	189346	73.739				
2	2.272	46451	3963	2.012		V		
3	2.756	1060	86	0.046		V		
4	9.208	558714	10258	24.202				
[redacted]		2308499	203653					

PPh$_3$ Entry 4

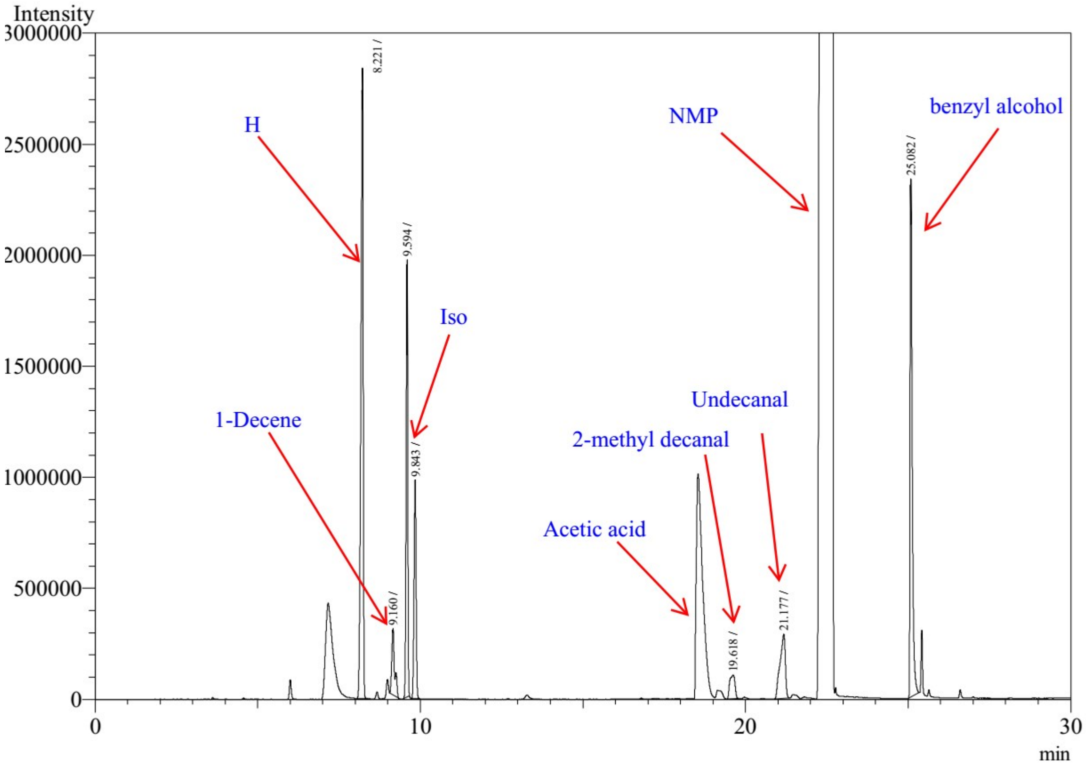


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.233	17051035	3383778	31.229				
2	9.167	3543660	471933	6.490				
3	9.595	7747759	2391615	14.190				
4	9.829	3668879	872143	6.719				
5	19.595	1045755	99346	1.915				
6	21.165	4119192	348160	7.544				
7	25.064	17424277	3833275	31.912				
		54600557	11400250	100.000				

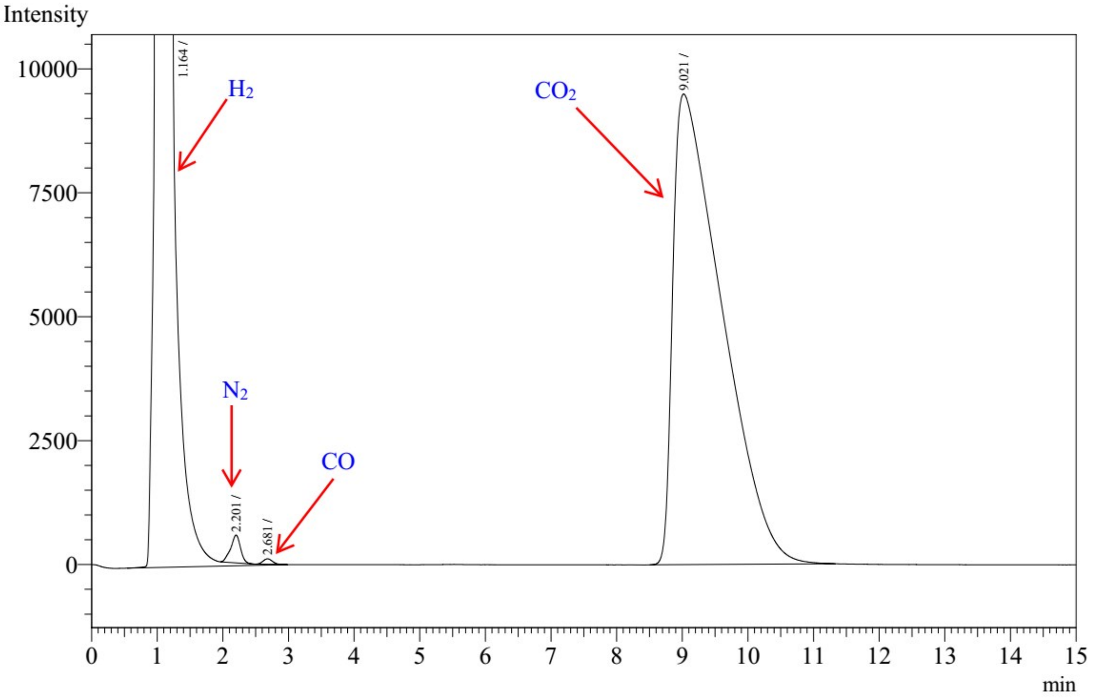


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.201	2012894	207082	78.798		S		
2	2.254	15442	1418	0.604		T		
3	2.719	58	7	0.002				
4	5.619	253	13	0.010				
5	9.170	525851	9866	20.585				
		2554498	218386					

PPh$_3$ Entry 5

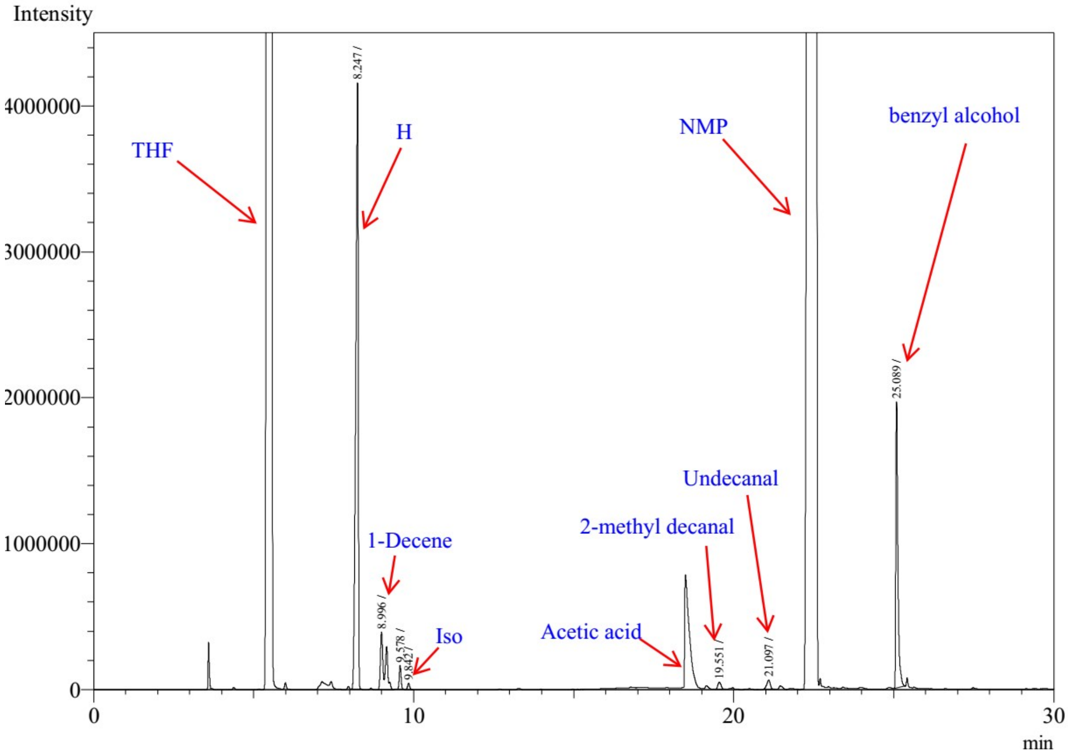


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.221	13643348	2806517	32.858				
2	9.160	1815257	295861	4.372				
3	9.594	6684691	1934536	16.099				
4	9.843	4280916	983024	10.310				
5	19.618	1188956	105596	2.863				
6	21.177	3291452	289160	7.927				
7	25.082	10617409	2307585	25.571				
[redacted]		41522029	8722279	100.000				

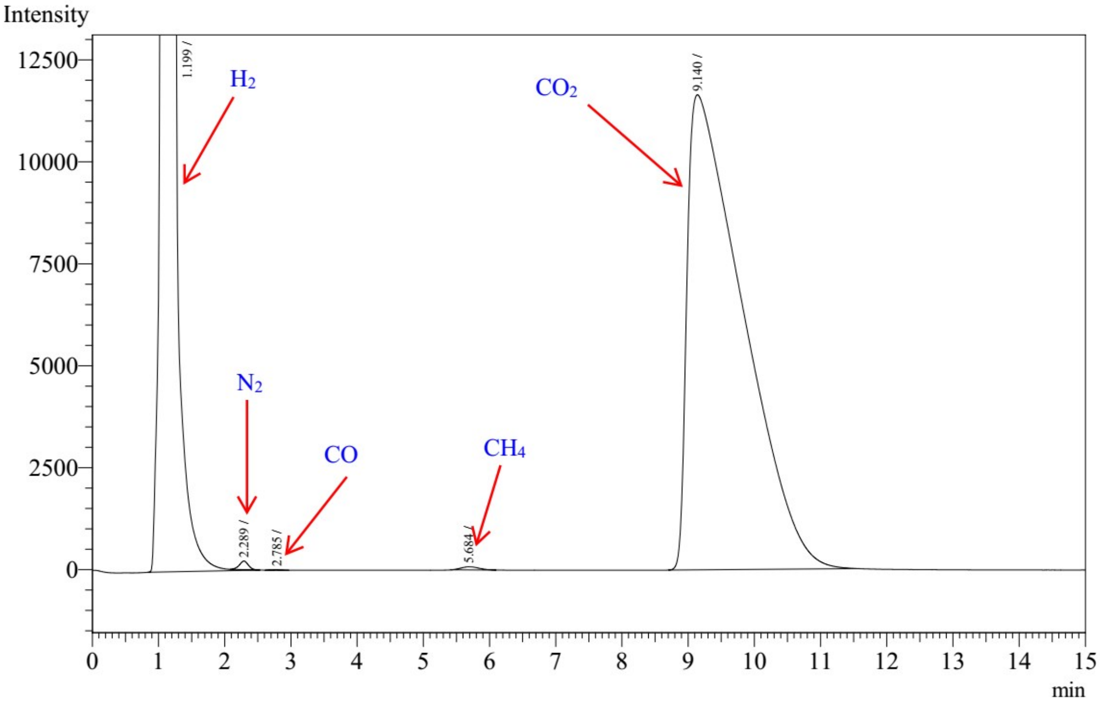


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.164	1865664	201572	78.876		S		
2	2.201	5851	561	0.247		T		
3	2.681	1097	110	0.046		T		
4	9.021	492706	9495	20.830		S		
		2365318	211738					

Xantphos Entry 1

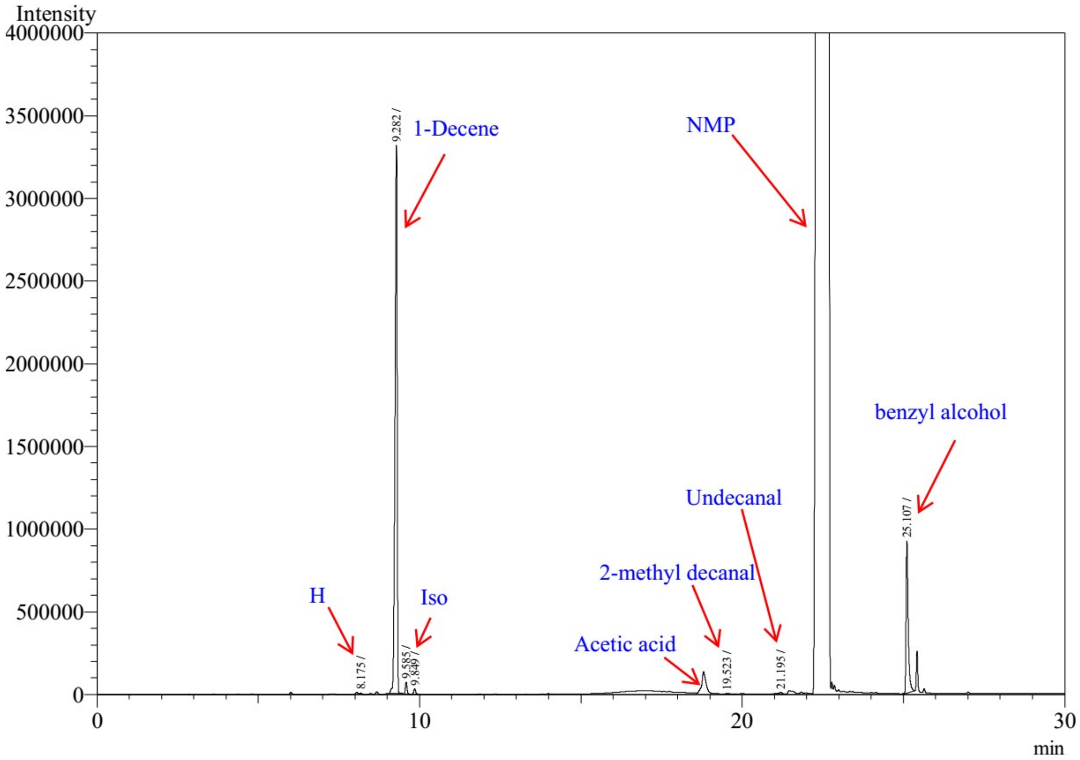


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.247	22018001	4140549	61.115				
2	8.996	3616558	392190	10.038				
3	9.578	634174	164253	1.760				
4	9.842	184421	44357	0.512				
5	19.551	335438	47975	0.931				
6	21.097	482967	62370	1.341				
7	25.089	8755315	1951165	24.302				
		36026874	6802859	100.000				

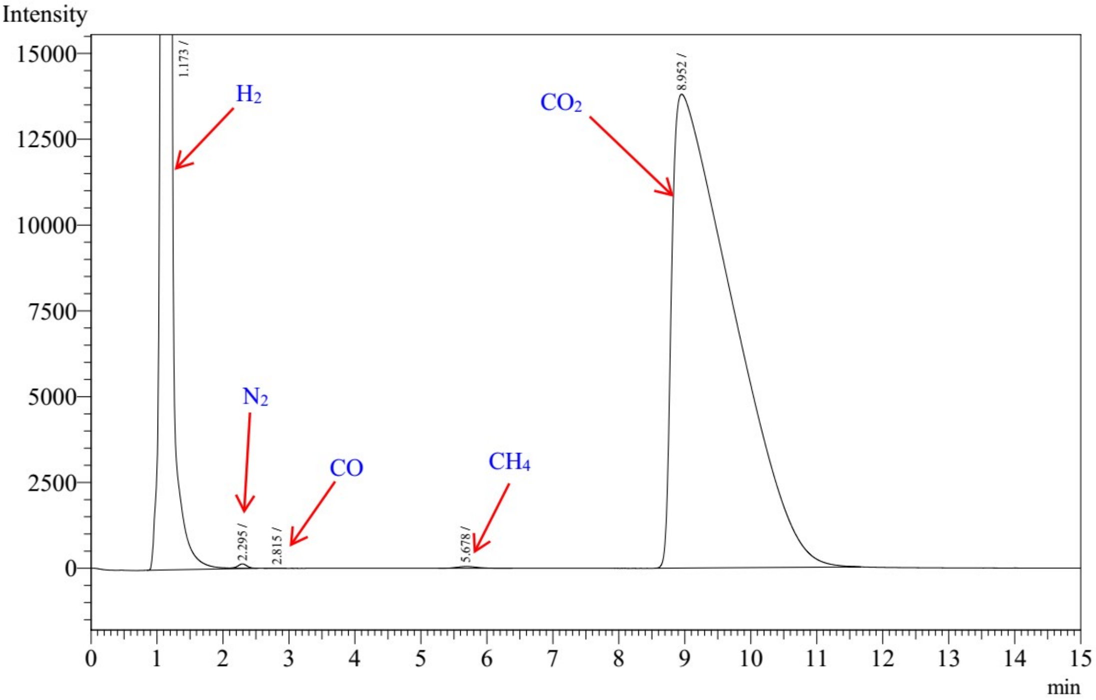


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.199	1493602	176840	68.573		S		
2	2.289	1993	210	0.092		T		
3	2.785	56	6	0.003				
4	5.684	1485	78	0.068				
5	9.140	680977	11652	31.265				
[redacted]		2178113	188786					

Xantphos Entry 2



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.175	19590	5162	0.099				
2	9.282	15112260	3290563	76.134				
3	9.585	265202	71436	1.336				
4	9.849	141879	33581	0.715				
5	19.523	23467	1920	0.118				
6	21.195	89592	9156	0.451				
7	25.107	4197544	910658	21.147				
		19849534	4322476	100.000				



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Peak#  Ret.Time      Area    Height   Conc.  UnitMark ID#    Cmpd Name
    1     1.173    890853    132390  50.023       S
    2     2.295      1131       123   0.064       T
    3     2.815        32         4   0.002
    4     5.678      1074        52   0.060
    5     8.952    887781     13807  49.851
                  1780871    146376
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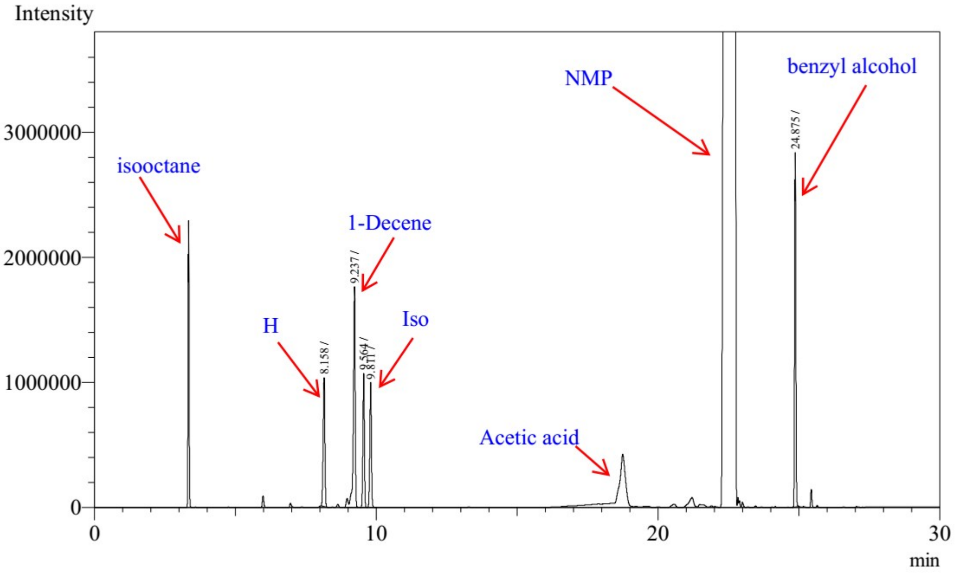
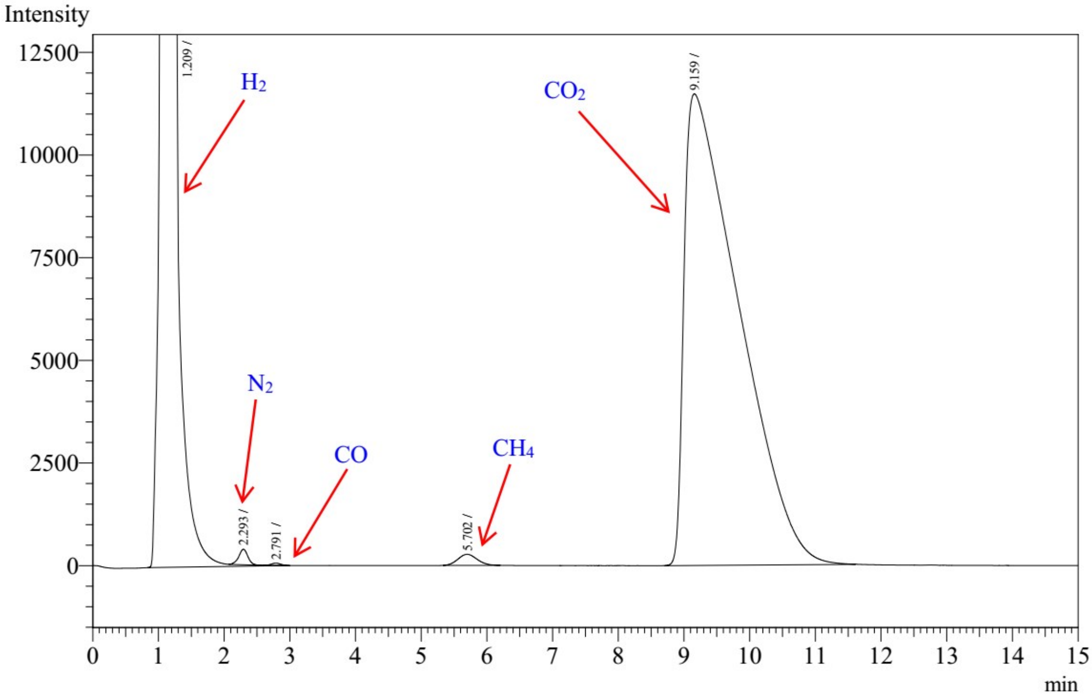
Xantphos Entry 3

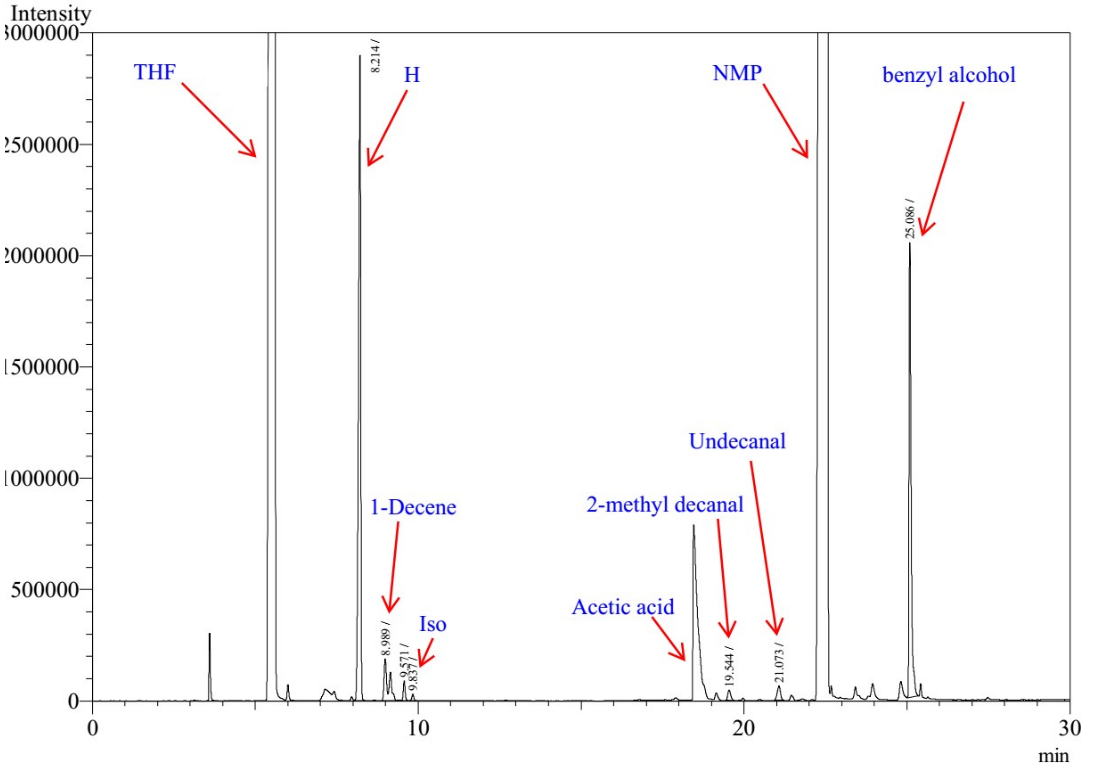


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.158	4324477	1024530	14.938				
2	9.237	8374504	1757606	28.927				
3	9.564	3857020	1069793	13.323				
4	9.811	3893031	994893	13.447				
5	24.875	8501034	2821801	29.364				
		28950066	7668623	100.000				

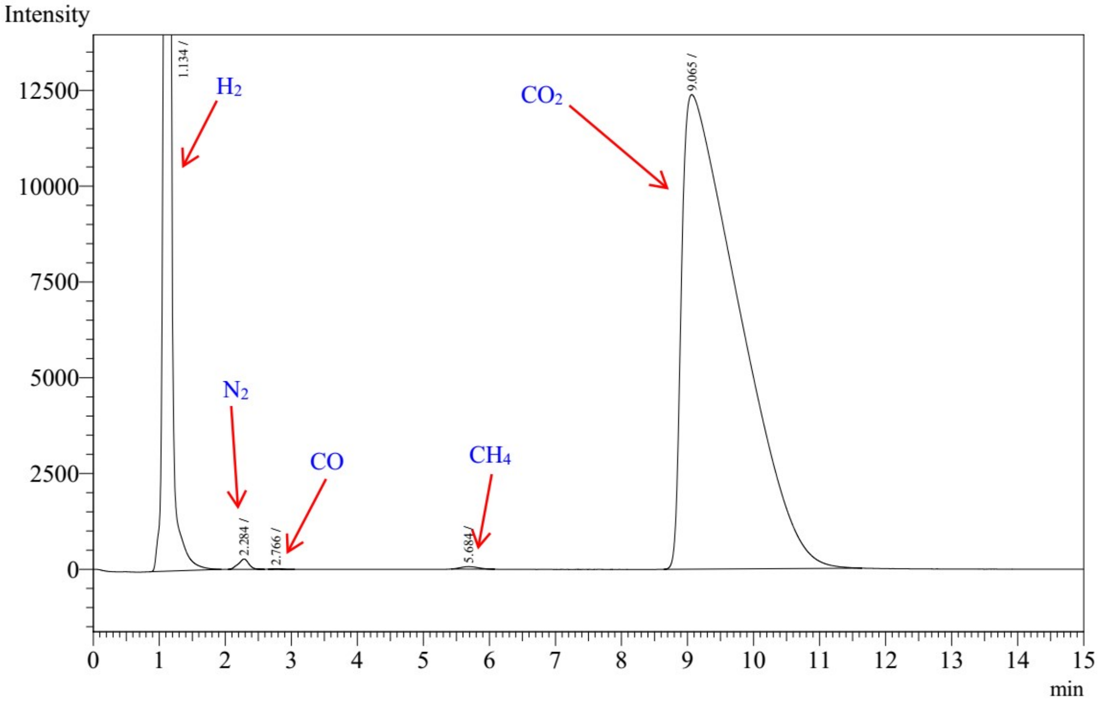


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.209	1676079	187120	71.284		S		
2	2.293	3653	378	0.155		T		
3	2.791	504	53	0.021		T		
4	5.702	5468	269	0.233				
5	9.159	665580	11484	28.307				
		2351284	199304					

Xantphos Entry 4

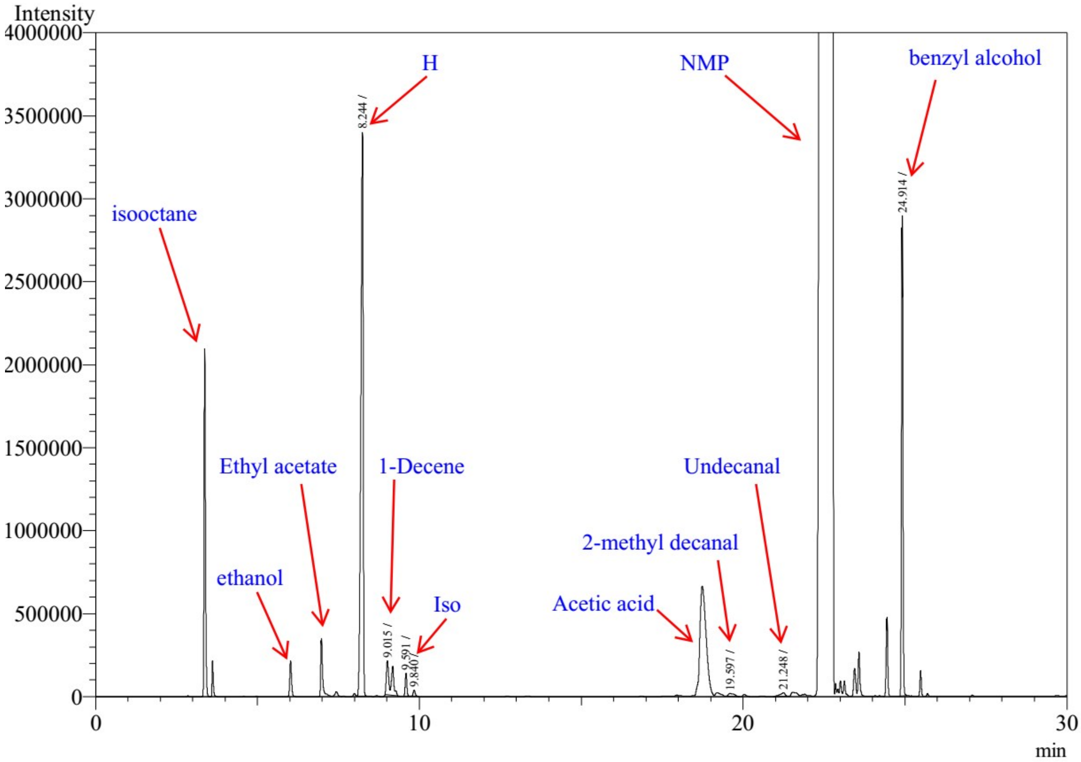


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.214	13359505	2887010	53.015				
2	8.989	1692875	186493	6.718				
3	9.571	340528	88250	1.351				
4	9.837	119925	28591	0.476				
5	19.544	280195	45514	1.112				
6	21.073	427443	63606	1.696				
7	25.086	8979136	2040224	35.632				
		25199607	5339688	100.000				

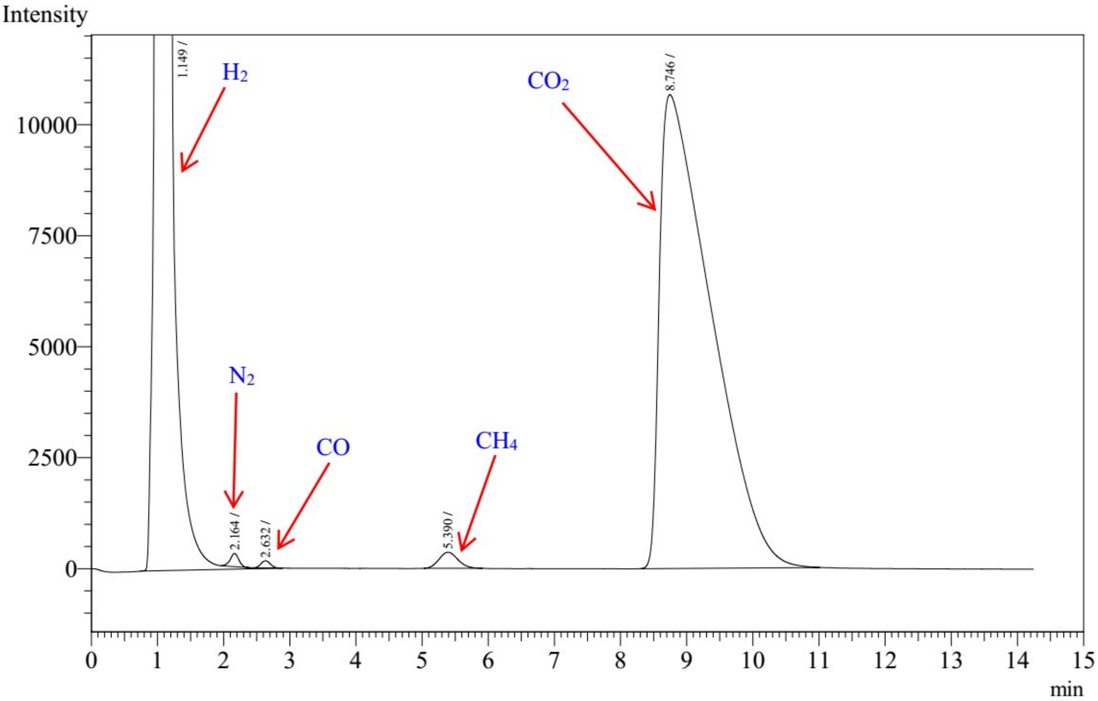


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.134	382090	72646	33.681				
2	2.284	2985	269	0.263				
3	2.766	106	12	0.009				
4	5.684	1209	65	0.107				
5	9.065	748057	12388	65.940				
		1134447	85380					

Xantphos Entry 5

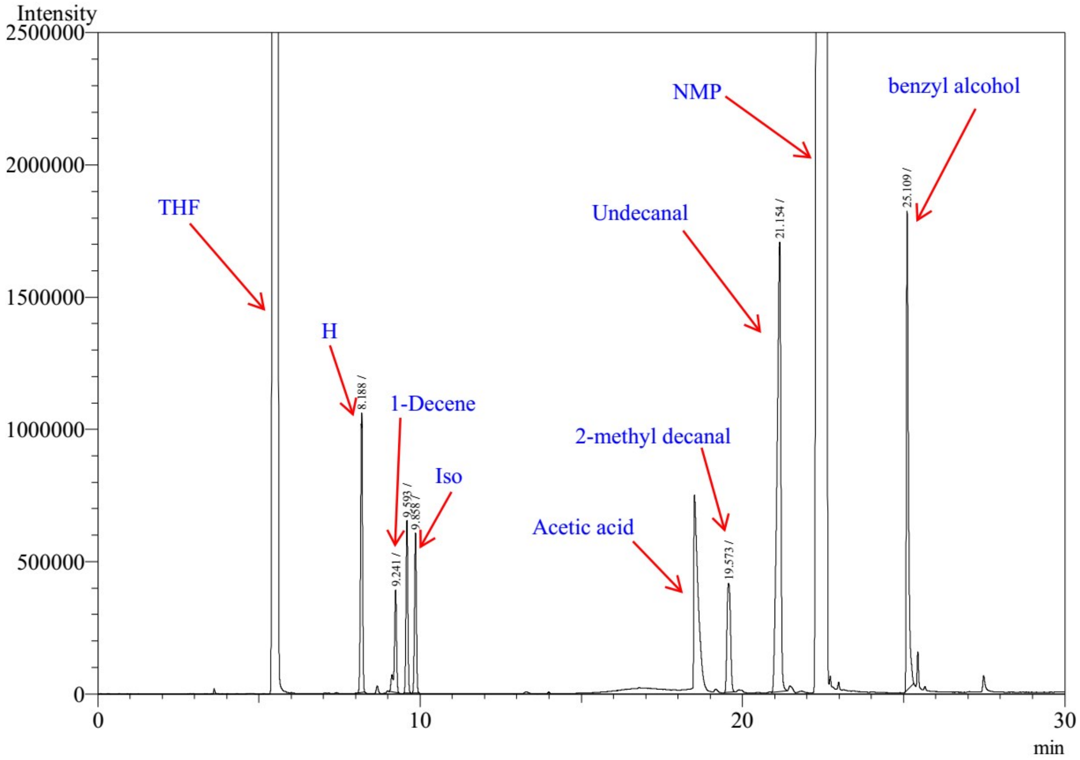


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.244	16672845	3392426	58.663				
2	9.015	1975914	205877	6.952				
3	9.591	490094	138494	1.724				
4	9.840	149231	37249	0.525				
5	19.597	223581	17432	0.787				
6	21.248	236894	20414	0.834				
7	24.914	8672627	2840523	30.515				
		28421186	6652415	100.000				

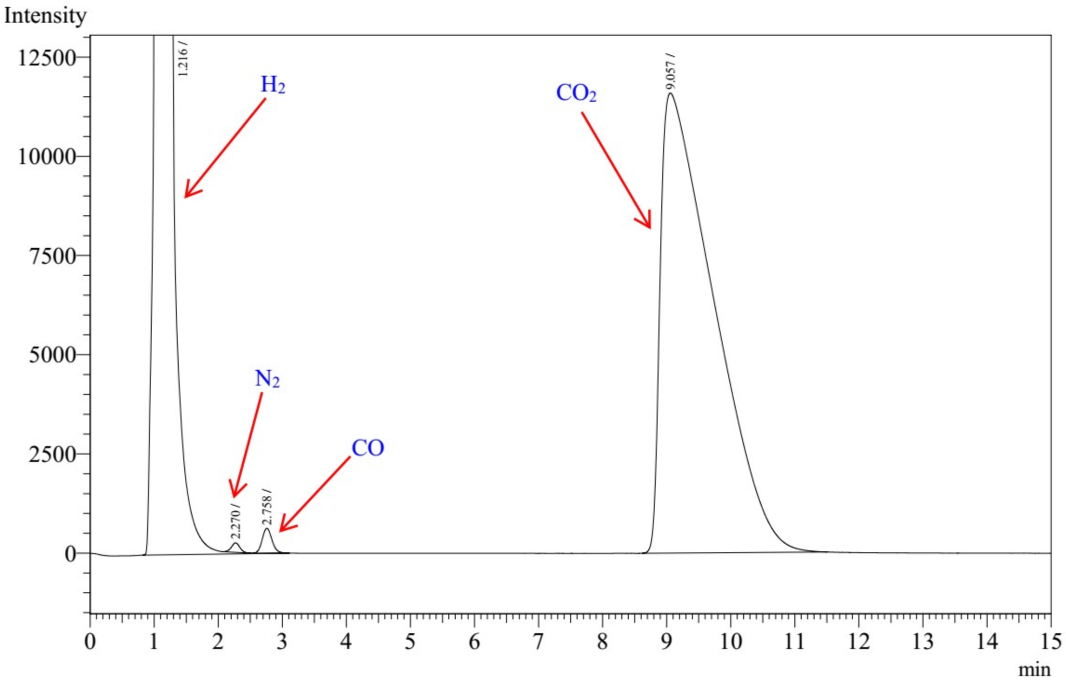


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.149	1876950	204650	76.126		S		
2	2.164	2681	297	0.109		T		
3	2.632	1602	163	0.065		T		
4	5.390	7215	362	0.293				
5	8.746	577120	10672	23.407				
		2465568	216144					

dppb Entry 1

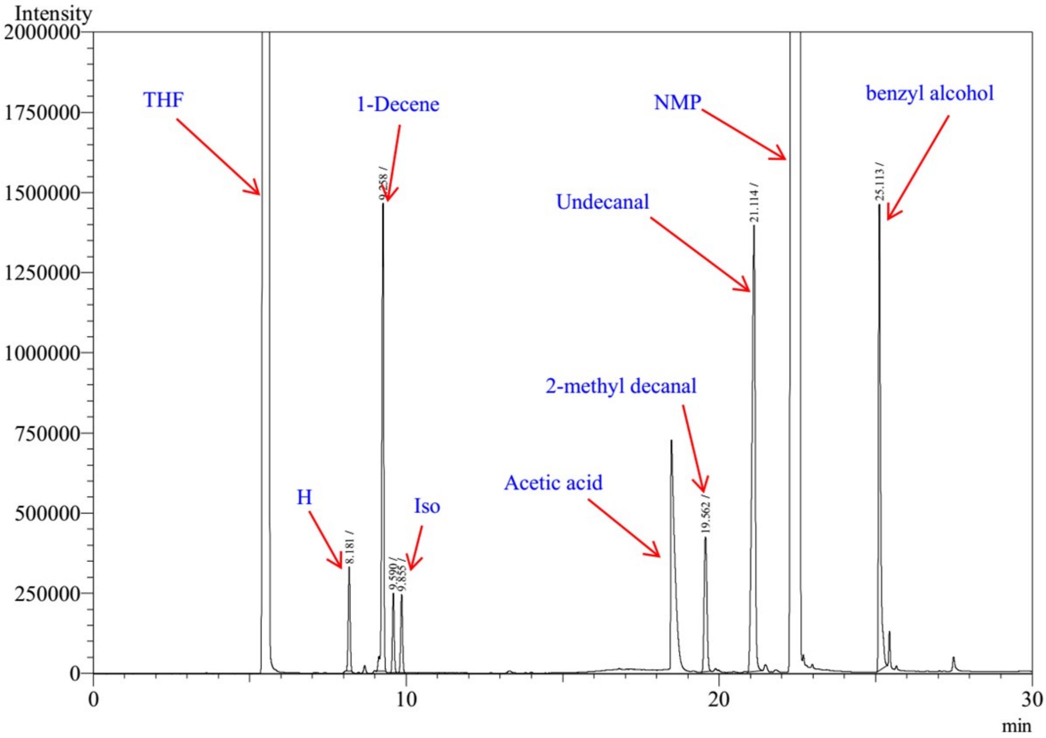


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.188	4455686	1054720	12.259				
2	9.241	1884823	385062	5.186				
3	9.593	2598538	652743	7.149				
4	9.858	2434974	603378	6.699				
5	19.573	3119154	412266	8.582				
6	21.154	13797692	1695178	37.961				
7	25.109	8055827	1809042	22.164				
[redacted]		36346694	6612389	100.000				

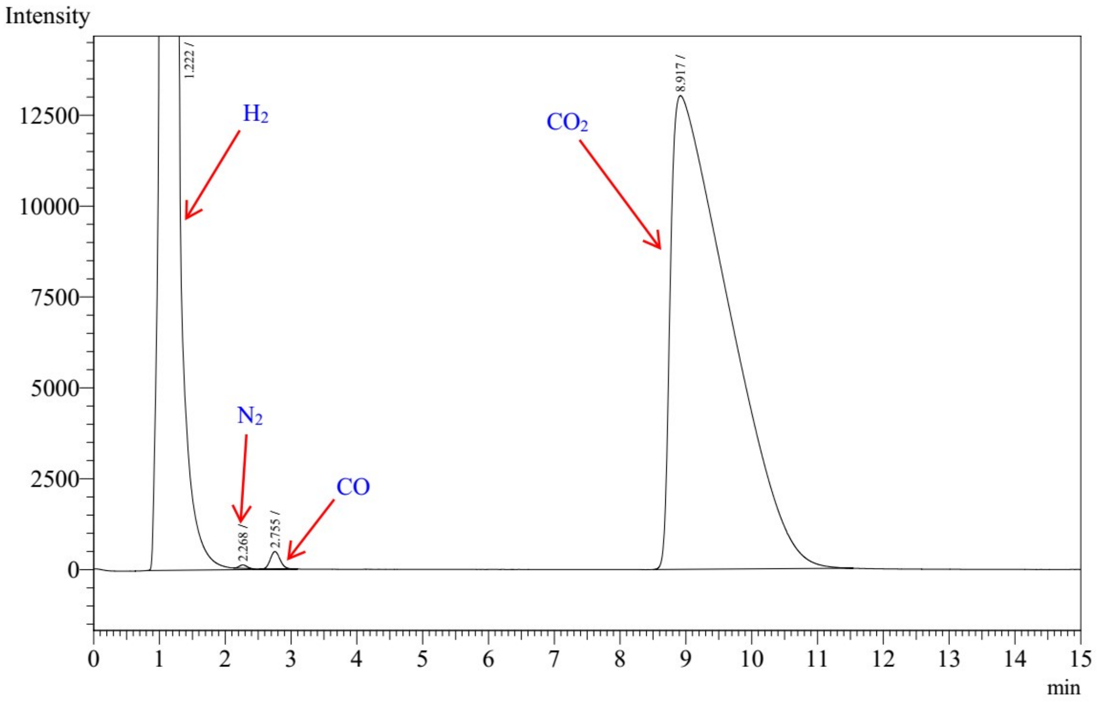


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.216	2119947	212434	75.725		S		
2	2.270	2170	238	0.078		T		
3	2.758	6577	625	0.235		T		
4	9.057	670838	11592	23.962				
		2799532	224889					

dppb Entry 2

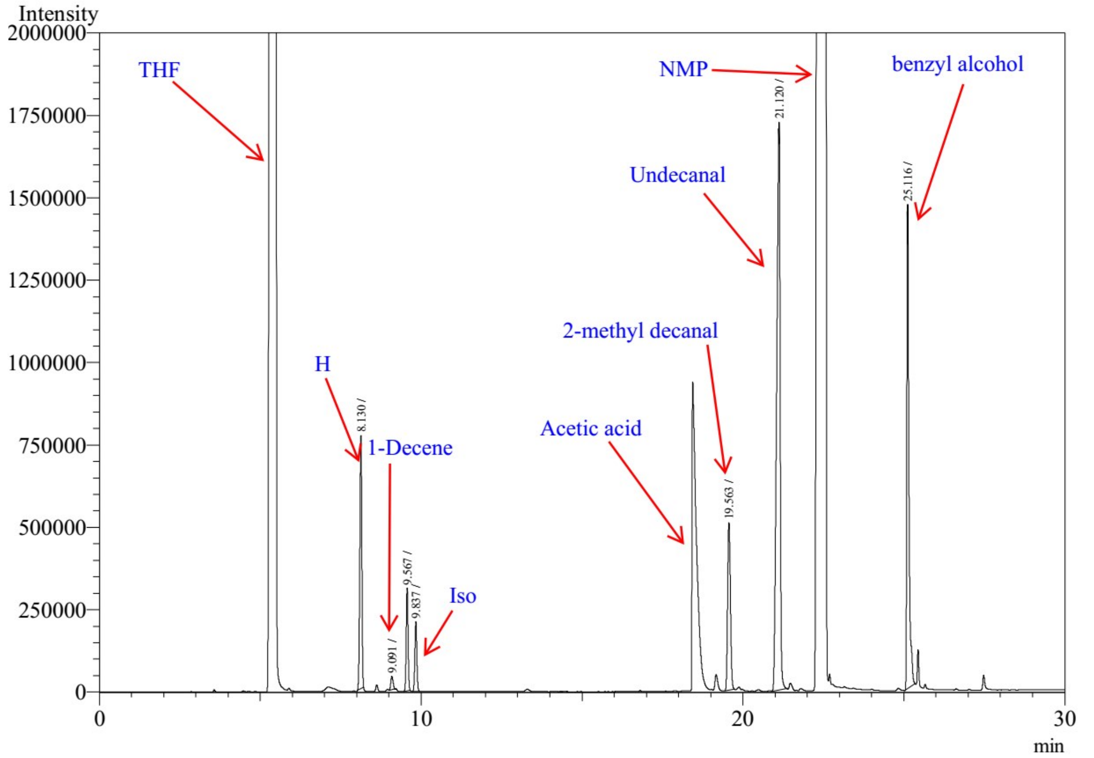


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.181	1345941	322567	4.688				
2	9.258	6218787	1458825	21.662				
3	9.590	961447	245510	3.349				
4	9.855	991302	244425	3.453				
5	19.562	2586658	421145	9.010				
6	21.114	9918009	1391074	34.548				
7	25.113	6685806	1450178	23.289				
		28707950	5533724	100.000				

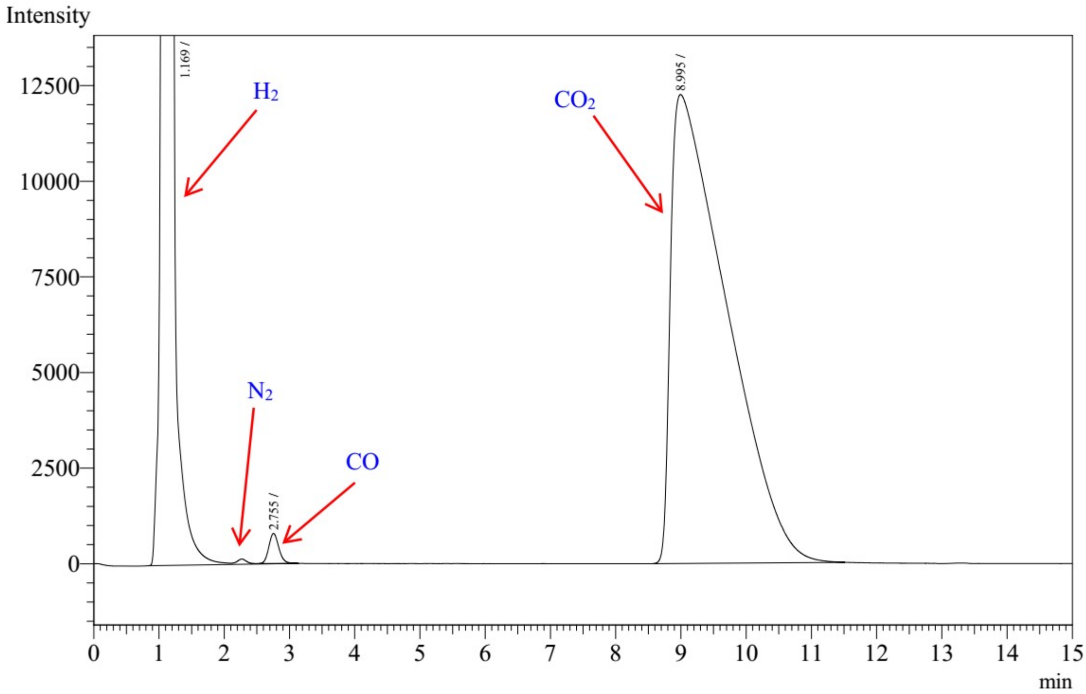


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.222	2319837	221119	74.126		S		
2	2.268	742	93	0.024		T		
3	2.755	5041	483	0.161		T		
4	8.917	803968	13030	25.689				
		3129588	234725					

dppb Entry 3

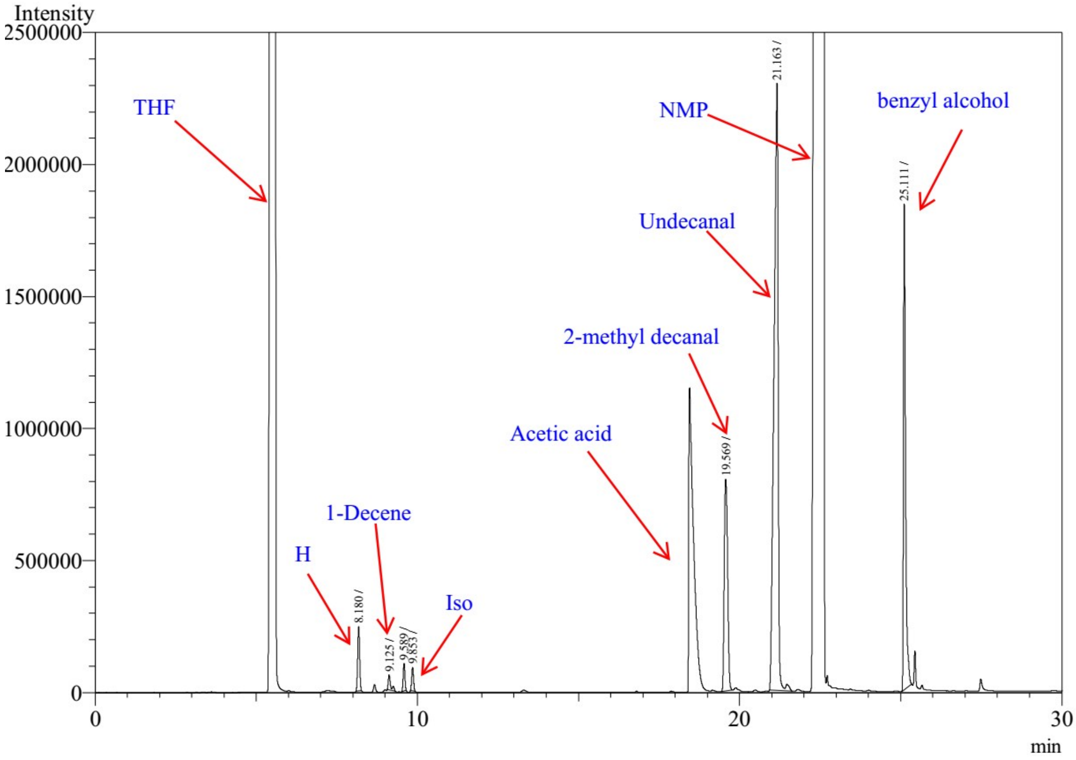


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.130	3336130	764349	11.928				
2	9.091	197227	40712	0.705				
3	9.567	1238799	309390	4.429				
4	9.837	890899	209977	3.185				
5	19.563	3062417	506848	10.949				
6	21.120	12644192	1722250	45.207				
7	25.116	6599945	1460223	23.597				
[redacted]		27969609	5013749	100.000				

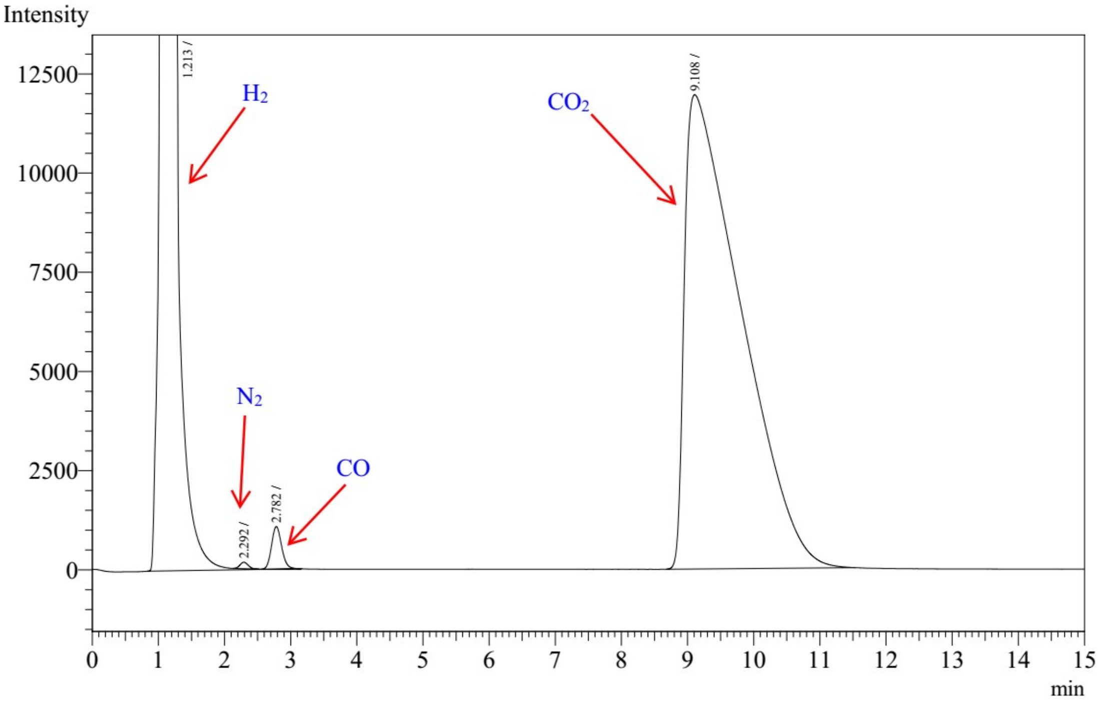


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.169	1088859	149523	59.552		S		
2	2.755	8323	787	0.455		T		
3	8.995	731220	12259	39.992				
[redacted]		1828402	162569					

dppb Entry 4



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.180	1023571	241284	2.798				
2	9.125	304501	57298	0.832				
3	9.589	385291	104903	1.053				
4	9.853	340621	87991	0.931				
5	19.569	5825135	801132	15.925				
6	21.163	20470176	2289077	55.962				
7	25.111	8229195	1811964	22.497				
		36578490	5393649	100.000				



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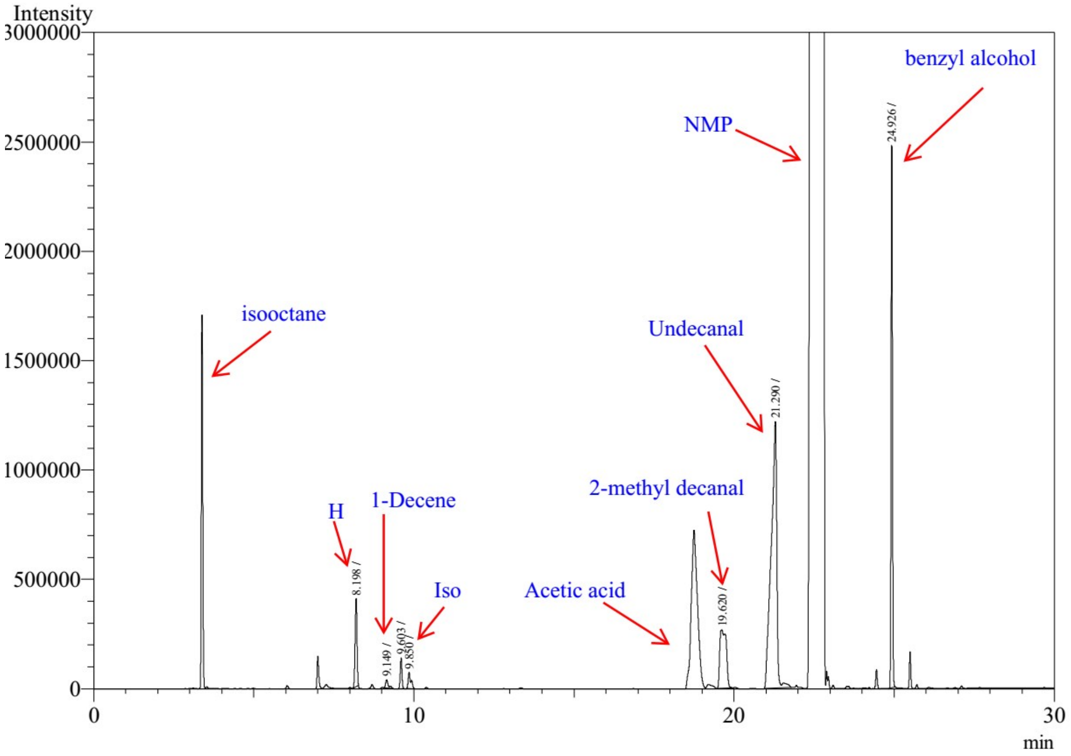
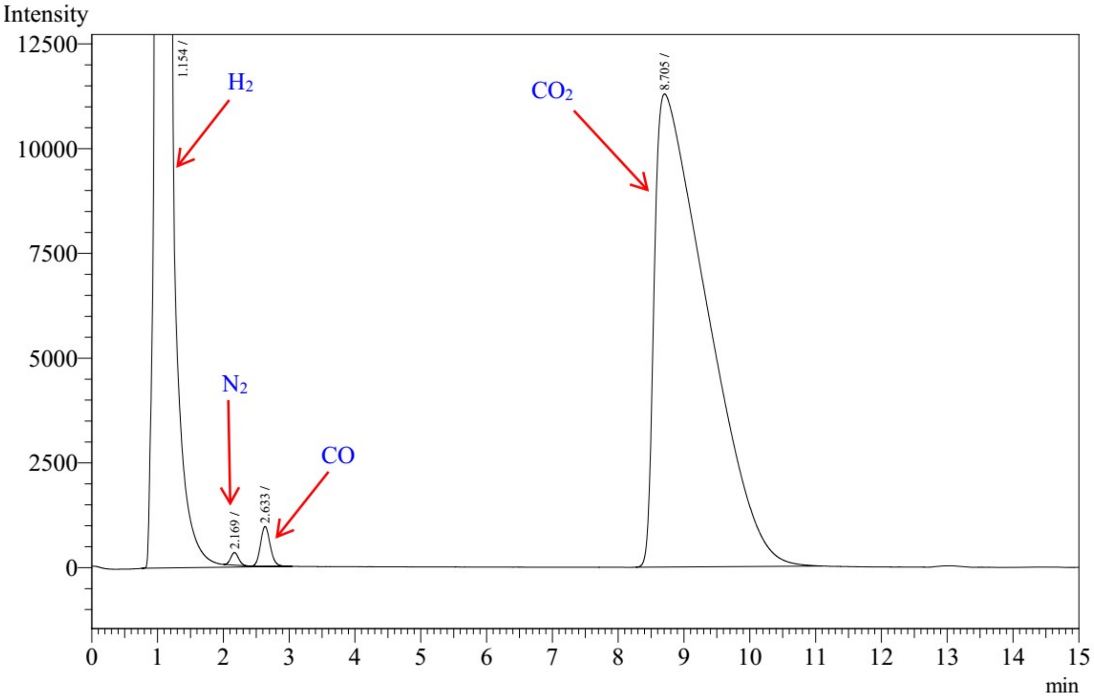
Peak#  Ret.Time      Area     Height    Conc.   UnitMark ID#    Cmpd Name
    1     1.213   1758483   192616   70.950        S
    2     2.292      1425      165    0.057        T
    3     2.782     11418     1073    0.461        T
    4     9.108    707146    11955   28.532
[redacted]          2478472   205809
```

dppb Entry 5



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.198	1635271	400056	5.676				
2	9.149	227786	39174	0.791				
3	9.603	507281	140045	1.761				
4	9.850	429319	73549	1.490				
5	19.620	3774655	267376	13.101				
6	21.290	14864151	1215617	51.592				
7	24.926	7372707	2459665	25.590				
		28811170	4595482	100.000				

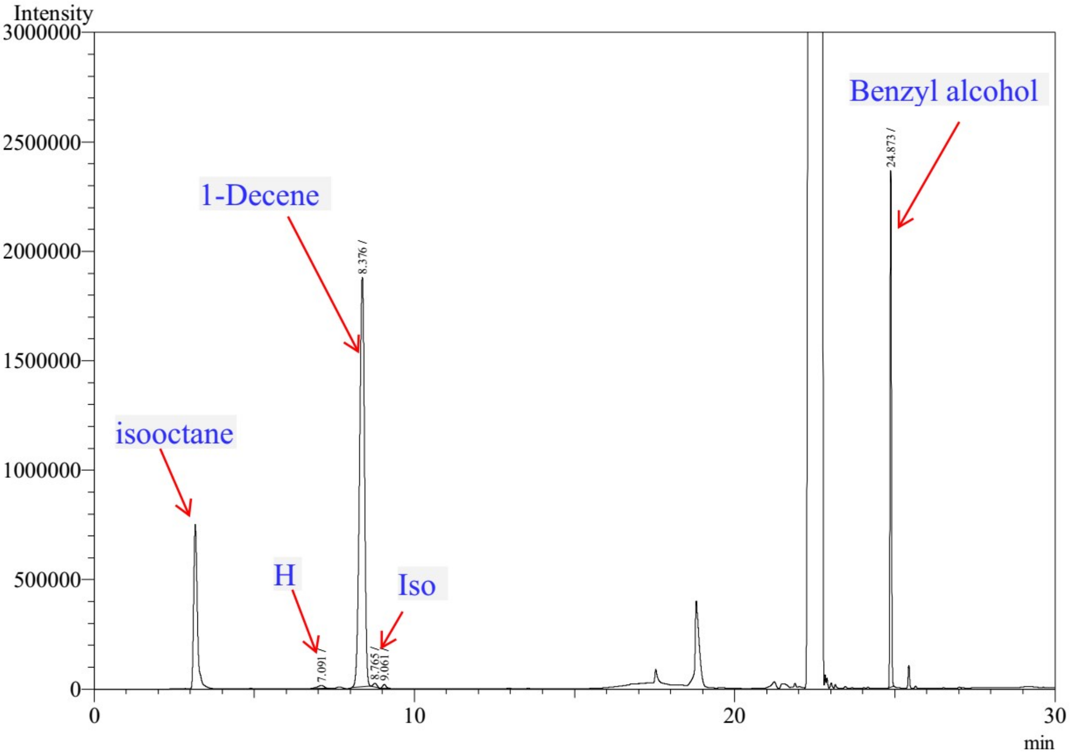


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.154	1965475	209490	75.415		S		
2	2.169	2497	298	0.096		T		
3	2.633	9682	947	0.372		T		
4	8.705	628555	11291	24.118				
[redacted]		2606209	222026					

3.10 Gas chromatograms to Table S10

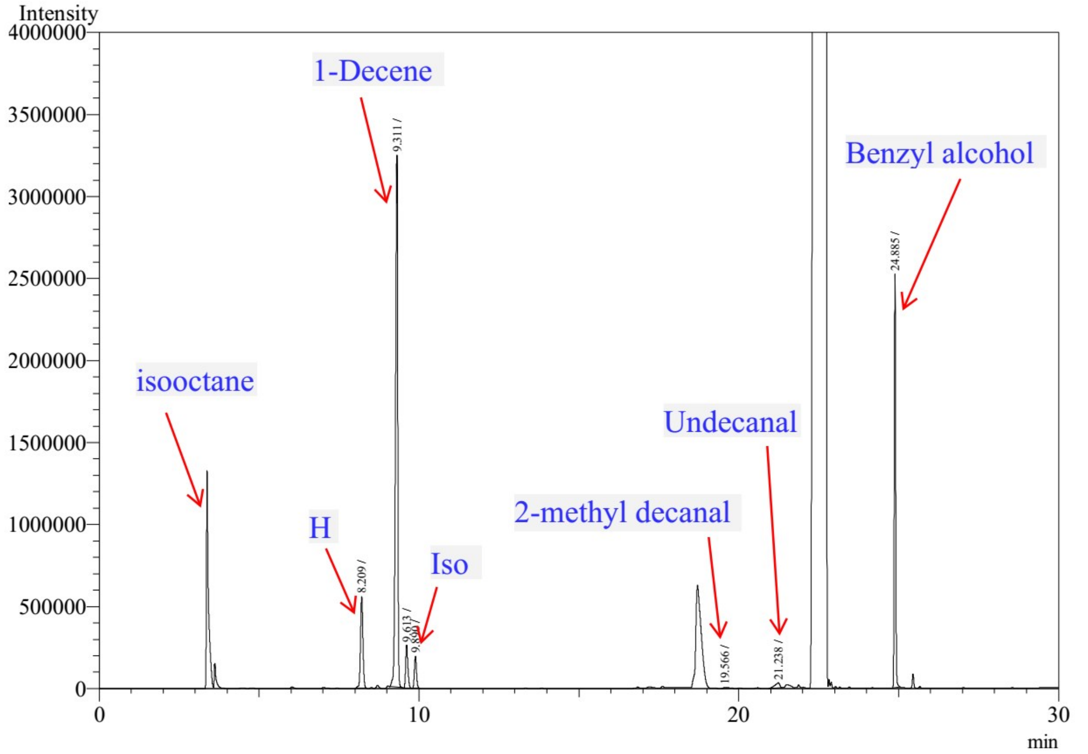
Entry 1

Entry 2



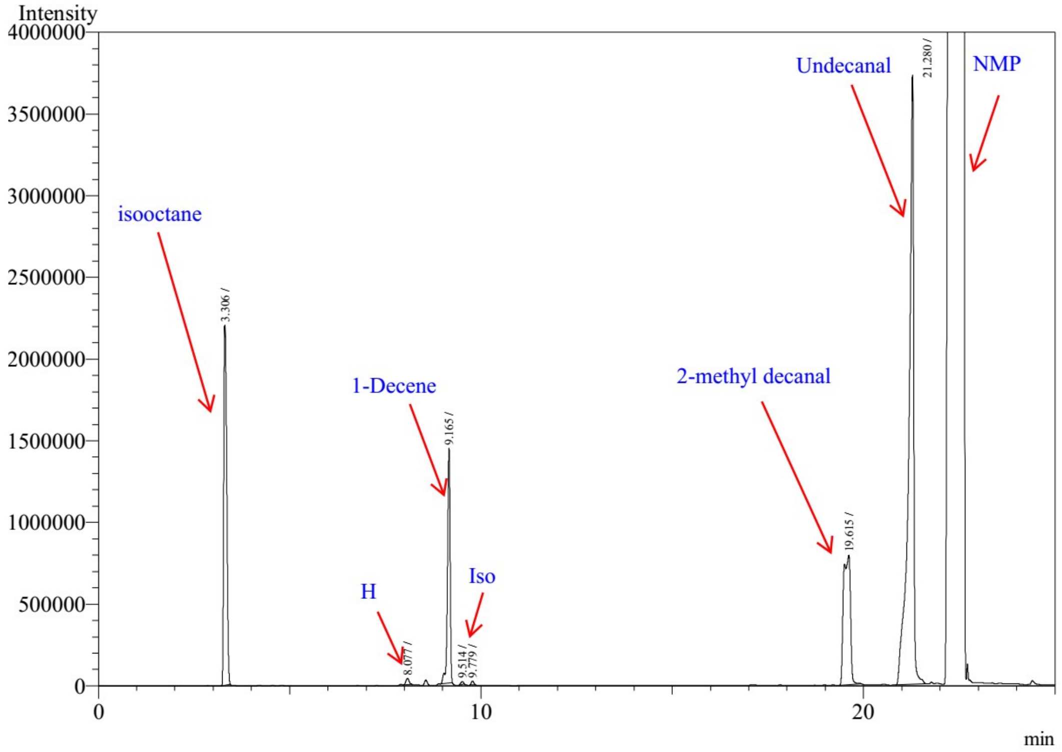
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	7.091	209340	14305	0.760				
2	8.376	20090353	1869829	72.936				
3	8.765	136175	16853	0.494				
4	9.061	135675	17869	0.493				
5	24.873	6973594	2313095	25.317				
		27545137	4231951	100.000				

Entry 3



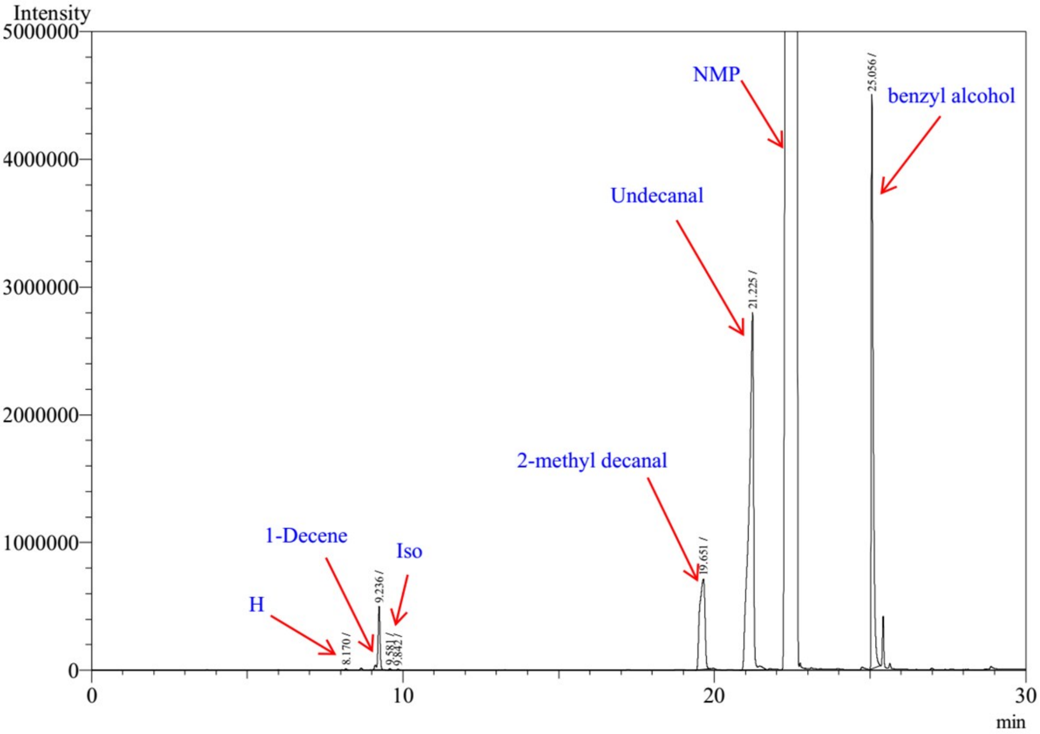
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.209	2954061	555983	10.297				
2	9.311	15688510	3231458	54.687				
3	9.613	1235379	260394	4.306				
4	9.890	883141	195033	3.078				
5	19.566	52722	4627	0.184				
6	21.238	340881	31484	1.188				
7	24.885	7533351	2515105	26.260				
[redacted]		28688045	6794084	100.000				

Entry 4



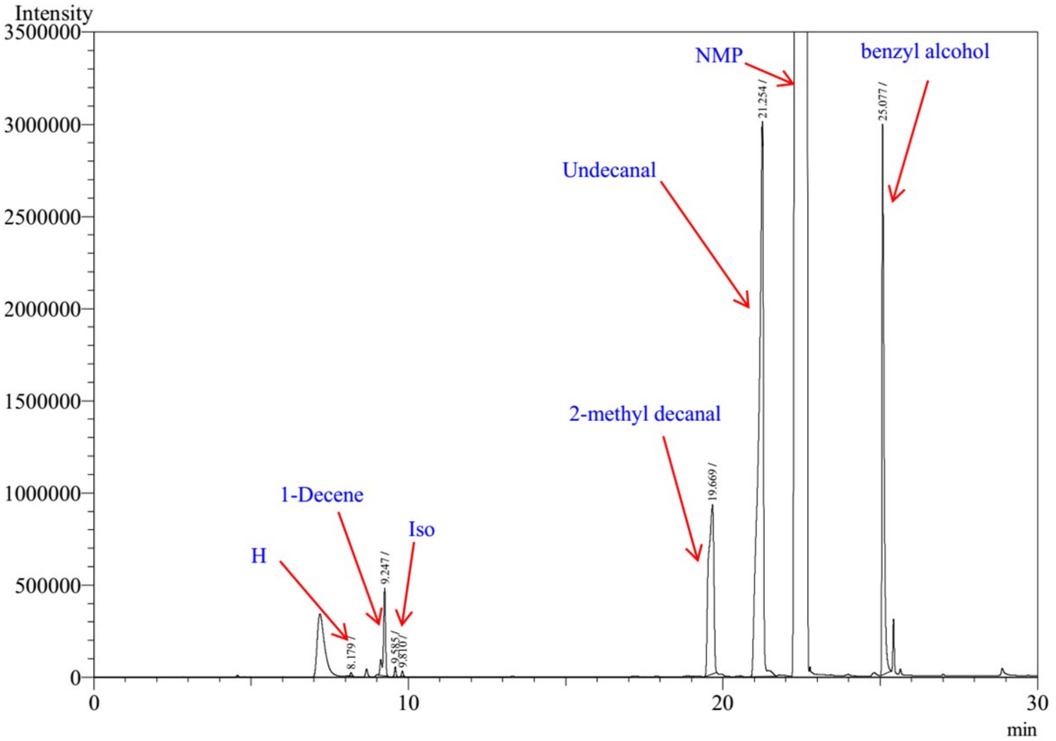
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.306	11905712	2203368	19.329				
2	8.077	225363	39671	0.366				
3	9.165	6760912	1426248	10.976				
4	9.514	88250	18616	0.143				
5	9.779	99588	23325	0.162				
6	19.615	9929273	792249	16.120				
7	21.280	32586094	3716473	52.904				
[redacted]		61595192	8219950	100.000				

Entry 5



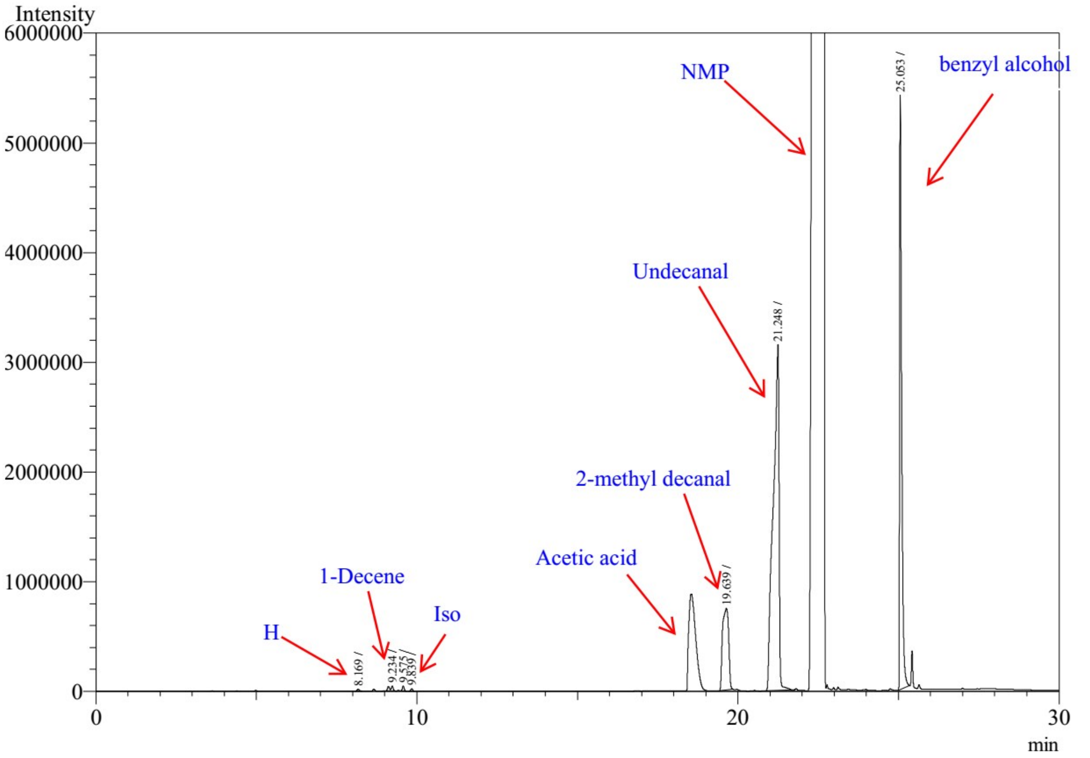
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.170	42926	9951	0.073				
2	9.236	2256186	493327	3.845				
3	9.581	46837	12450	0.080				
4	9.842	36866	9279	0.063				
5	19.651	8221311	708147	14.010				
6	21.225	28128456	2797519	47.933				
7	25.056	19950079	4474189	33.997				
		58682661	8504862	100.000				

Entry 6



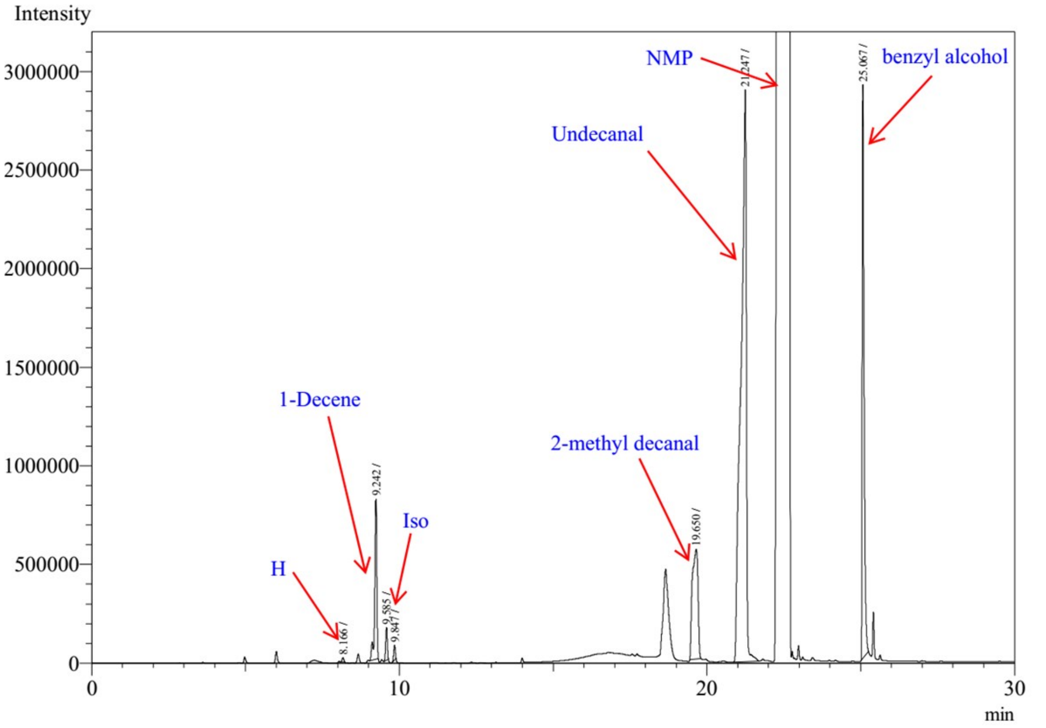
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.179	68014	17398	0.120				
2	9.247	2327490	478066	4.093				
3	9.585	172283	53022	0.303				
4	9.810	102425	28093	0.180				
5	19.669	10627868	916384	18.690				
6	21.254	30379513	3008378	53.425				
7	25.077	13185840	2940762	23.189				
[redacted]		56863433	7442103	100.000				

Entry 7



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.169	92211	18900	0.125				
2	9.234	369803	44462	0.501				
3	9.575	171366	46520	0.232				
4	9.839	92370	22406	0.125				
5	19.639	9844968	747525	13.325				
6	21.248	39237074	3146003	53.106				
7	25.053	24076111	5411642	32.586				
		73883903	9437458	100.000				

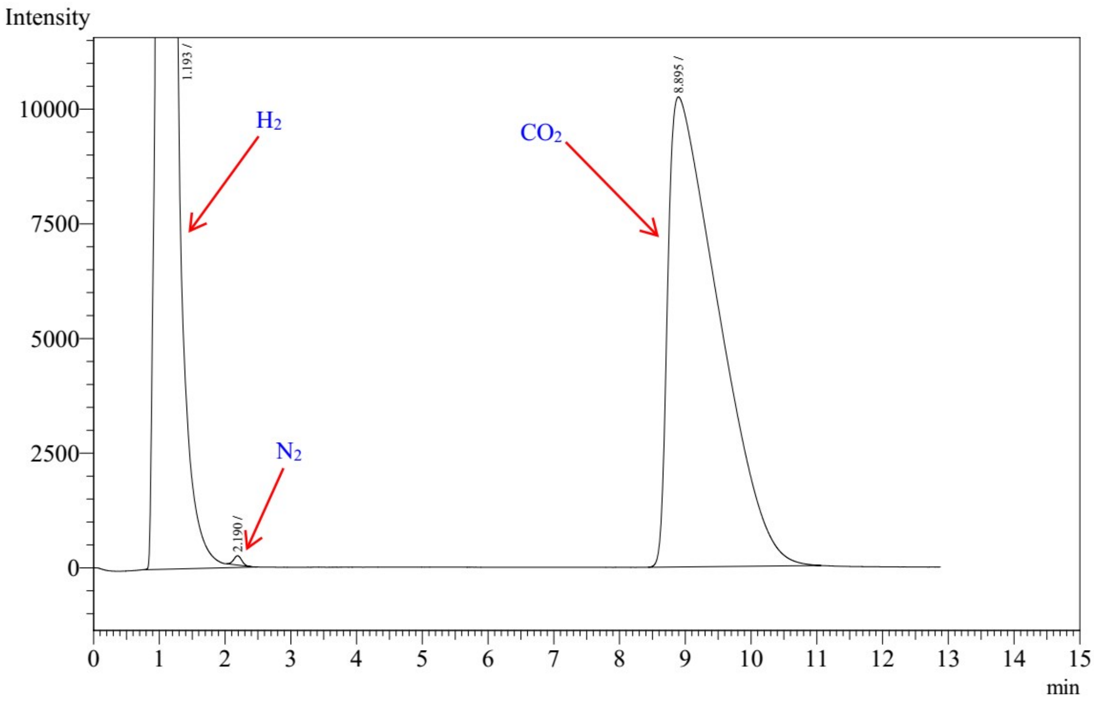
Entry 8



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.166	87829	22005	0.149				
2	9.242	3743884	809802	6.333				
3	9.585	621178	164105	1.051				
4	9.847	252168	73208	0.427				
5	19.650	7107625	556932	12.024				
6	21.247	34926275	2891955	59.084				
7	25.067	12374410	2903331	20.933				
		59113369	7421338	100.000				

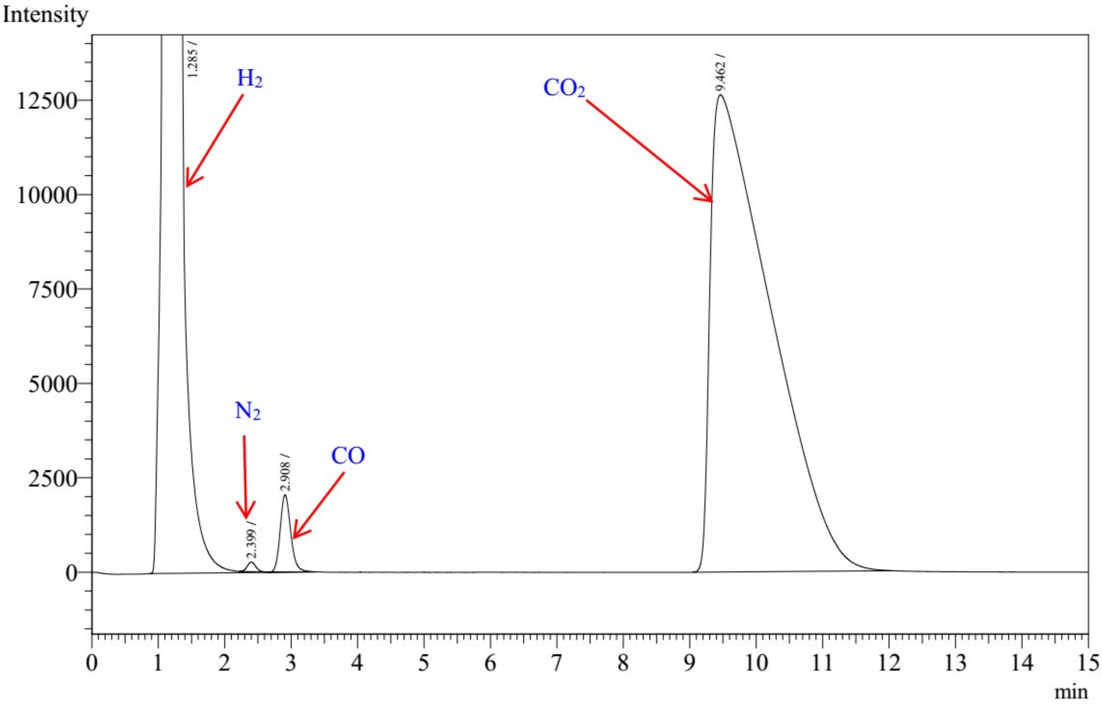
3.11 Gas chromatograms to Table S11

equation (c) without Ac_2O



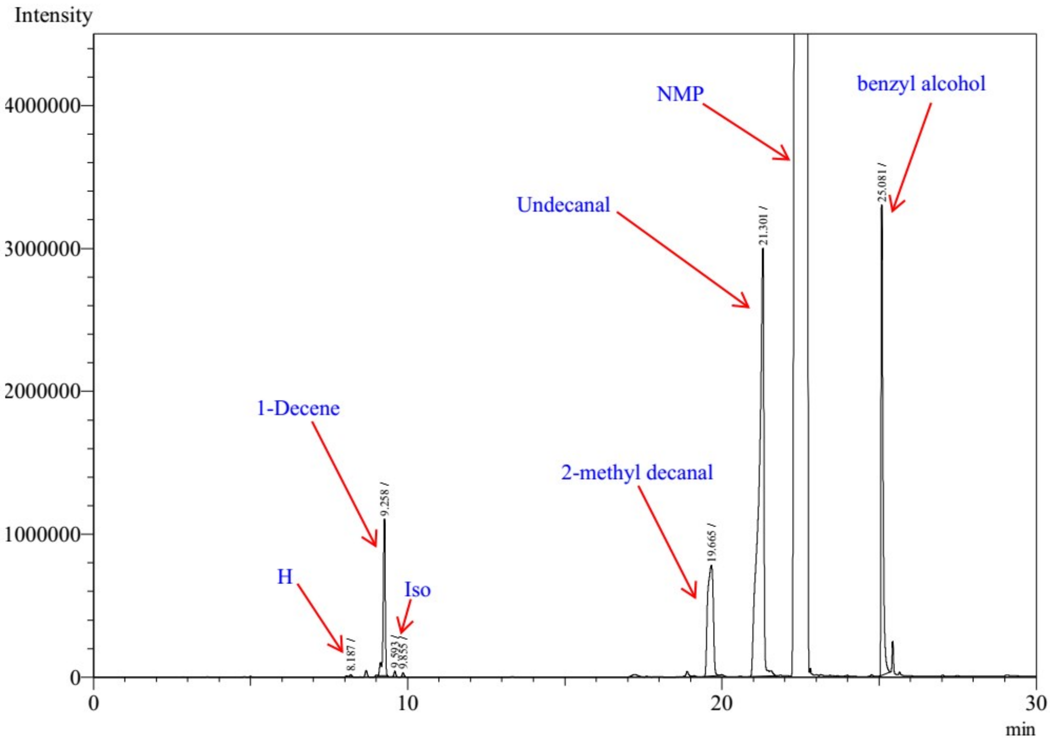
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.193	2732420	243831	83.259		S		
2	2.190	1714	203	0.052		T		
3	8.895	547708	10247	16.689				
[redacted]		3281842	254281					

equation (c) with Ac_2O



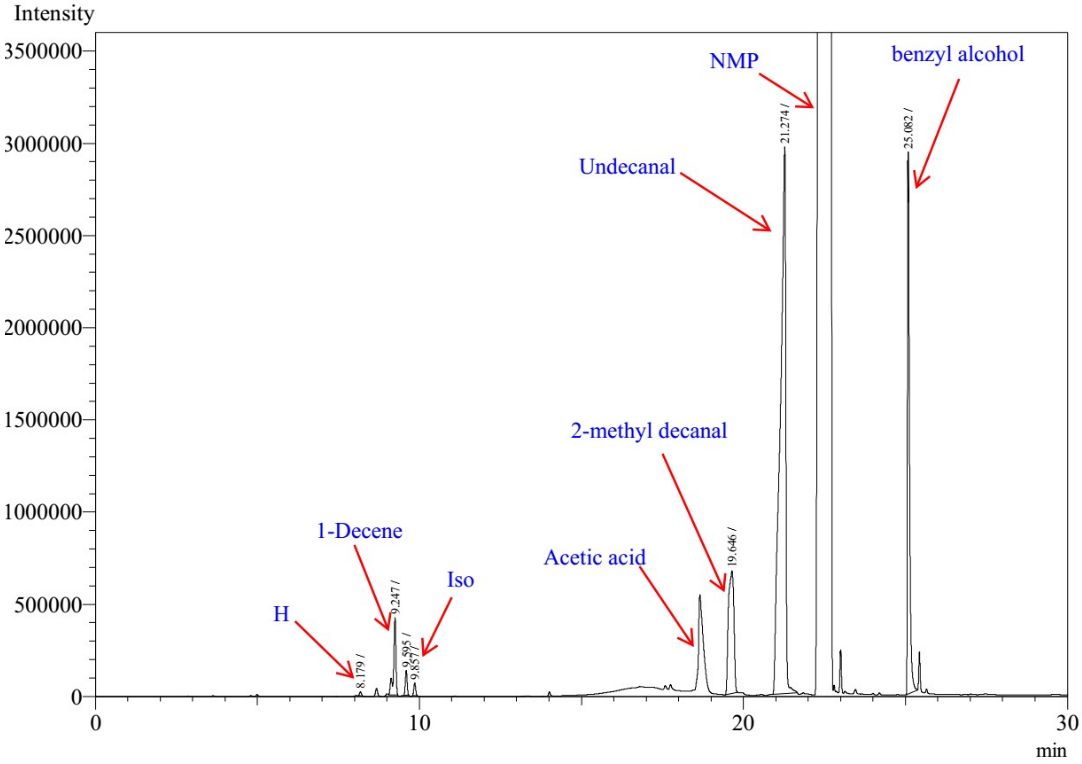
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.285	2251267	212847	73.249		S		
2	2.399	2246	255	0.073		T		
3	2.908	22423	2043	0.730		T		
4	9.462	797492	12635	25.948				
		3073428	227780					

equation (d) Entry 1



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.187	58556	14597	0.095				
2	9.258	4984710	1089111	8.119				
3	9.593	142096	39829	0.231				
4	9.855	109140	28056	0.178				
5	19.665	9591520	773650	15.622				
6	21.301	32448842	2993487	52.852				
7	25.081	14060773	3285176	22.902				
		61395637	8223906	100.000				

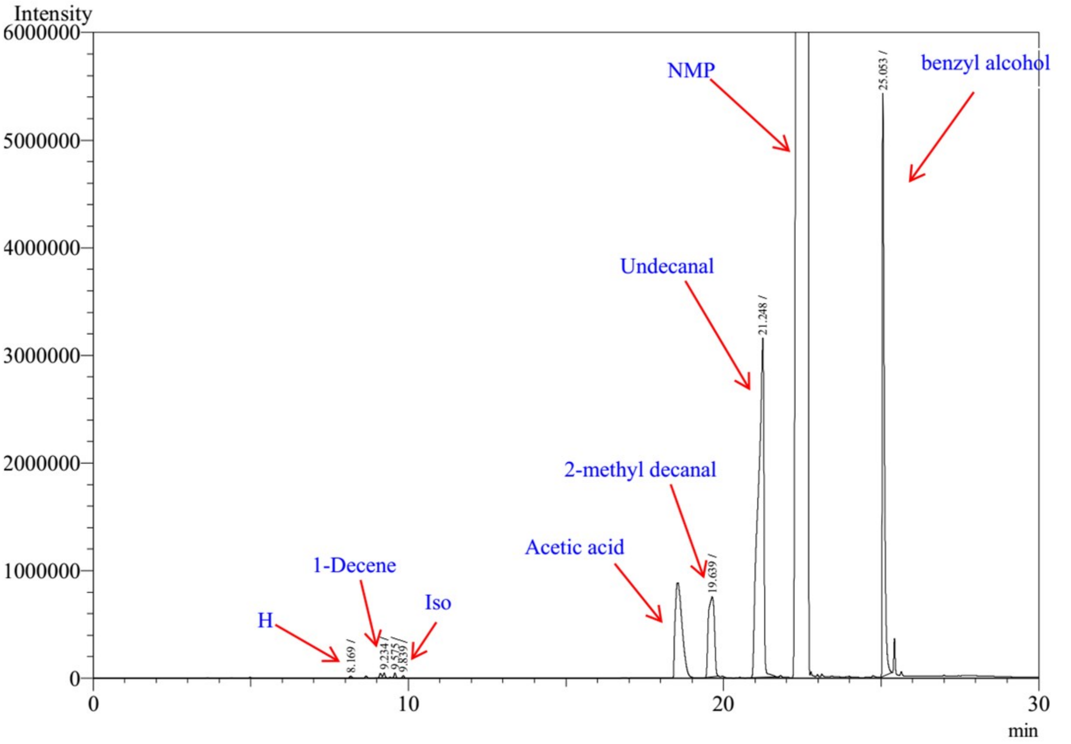
equation (d) Entry 2



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.179	78555	20574	0.135				
2	9.247	2117457	418047	3.636				
3	9.595	514151	132937	0.883				
4	9.857	270613	69054	0.465				
5	19.646	7784184	663323	13.368				
6	21.274	34904314	2963496	59.942				
7	25.082	12561161	2892480	21.571				
		58230435	7159911	100.000				

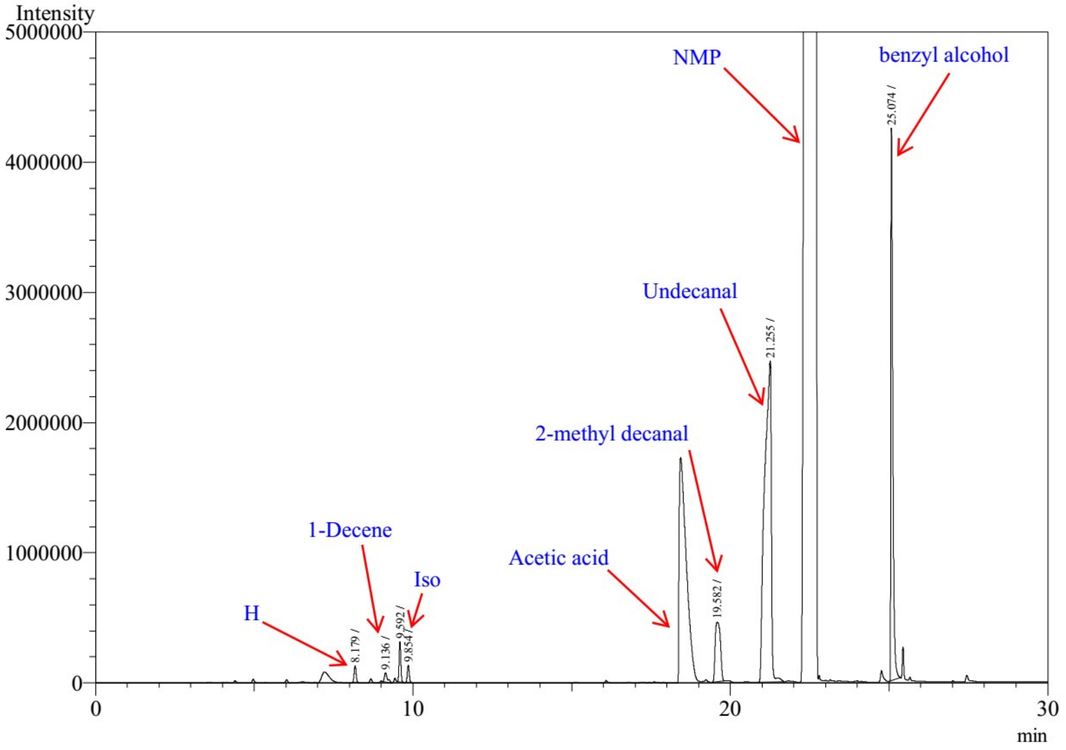
equation (d) Entry 3

equation (d) Entry 4



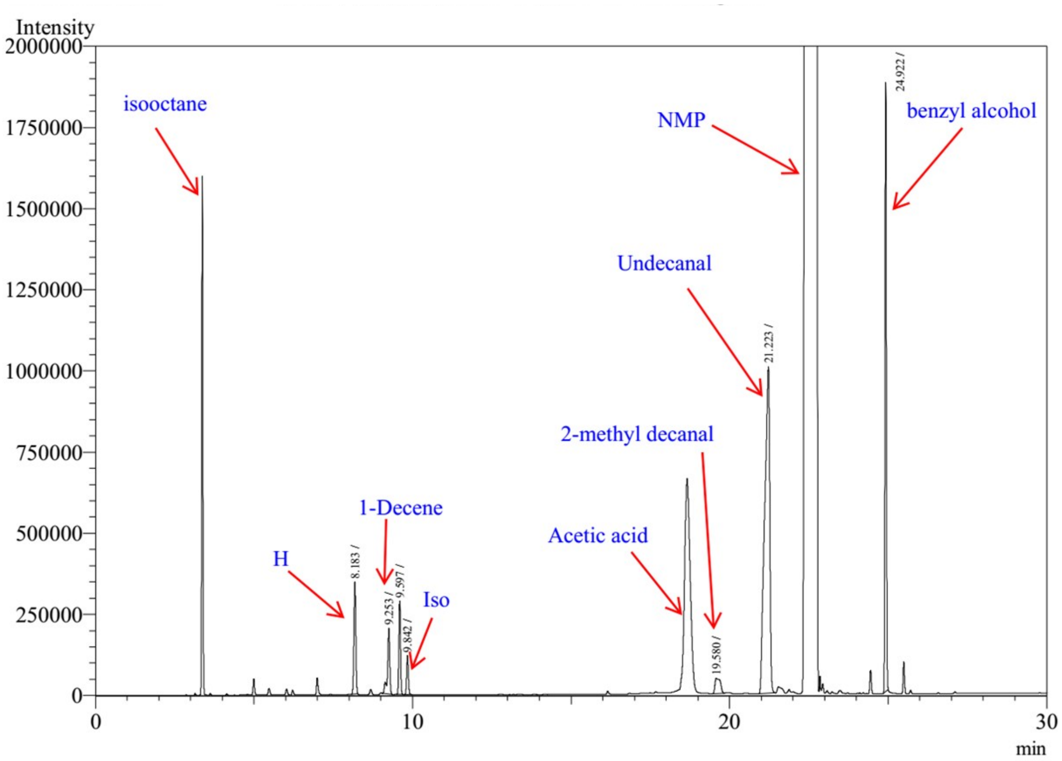
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.169	92211	18900	0.125				
2	9.234	369803	44462	0.501				
3	9.575	171366	46520	0.232				
4	9.839	92370	22406	0.125				
5	19.639	9844968	747525	13.325				
6	21.248	39237074	3146003	53.106				
7	25.053	24076111	5411642	32.586				
[redacted]		73883903	9437458	100.000				

equation (e) Entry 1



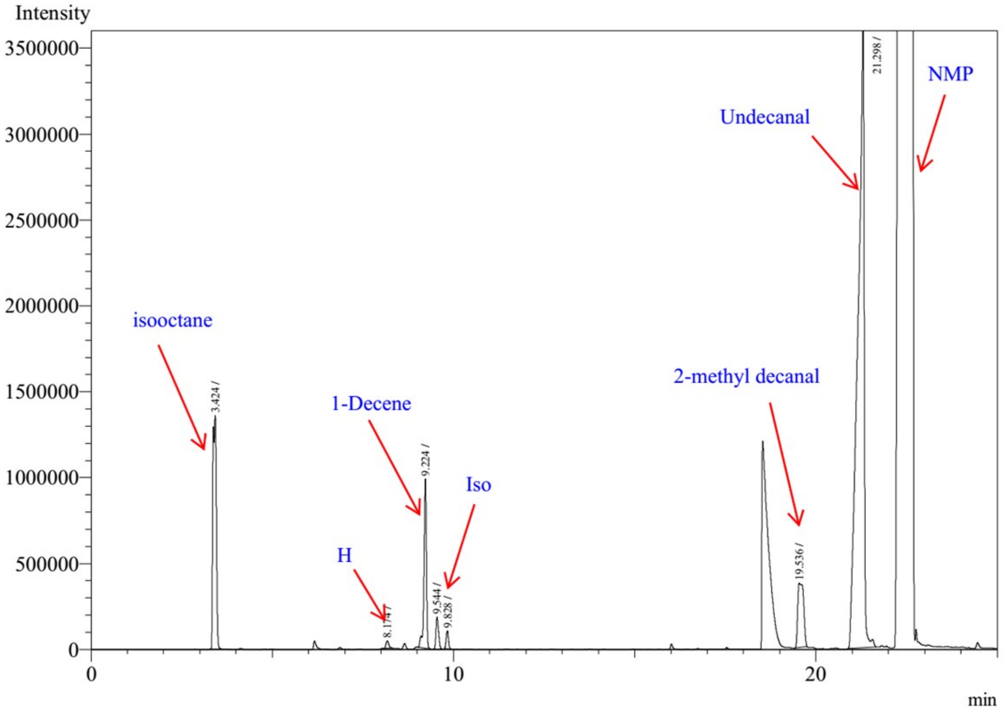
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.179	541697	128387	0.874				
2	9.136	447373	70684	0.722				
3	9.592	1155613	309927	1.865				
4	9.854	537417	132537	0.867				
5	19.582	5214317	457233	8.413				
6	21.255	35865783	2467725	57.869				
7	25.074	18215484	4217518	29.390				
		61977684	7784011	100.000				

equation (e) Entry 2



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.183	1420466	345834	6.701				
2	9.253	969032	200953	4.571				
3	9.597	1031693	287672	4.867				
4	9.842	446346	118631	2.105				
5	19.580	548675	47199	2.588				
6	21.223	11177407	1004477	52.726				
7	24.922	5605616	1872087	26.443				
		21199235	3876853	100.000				

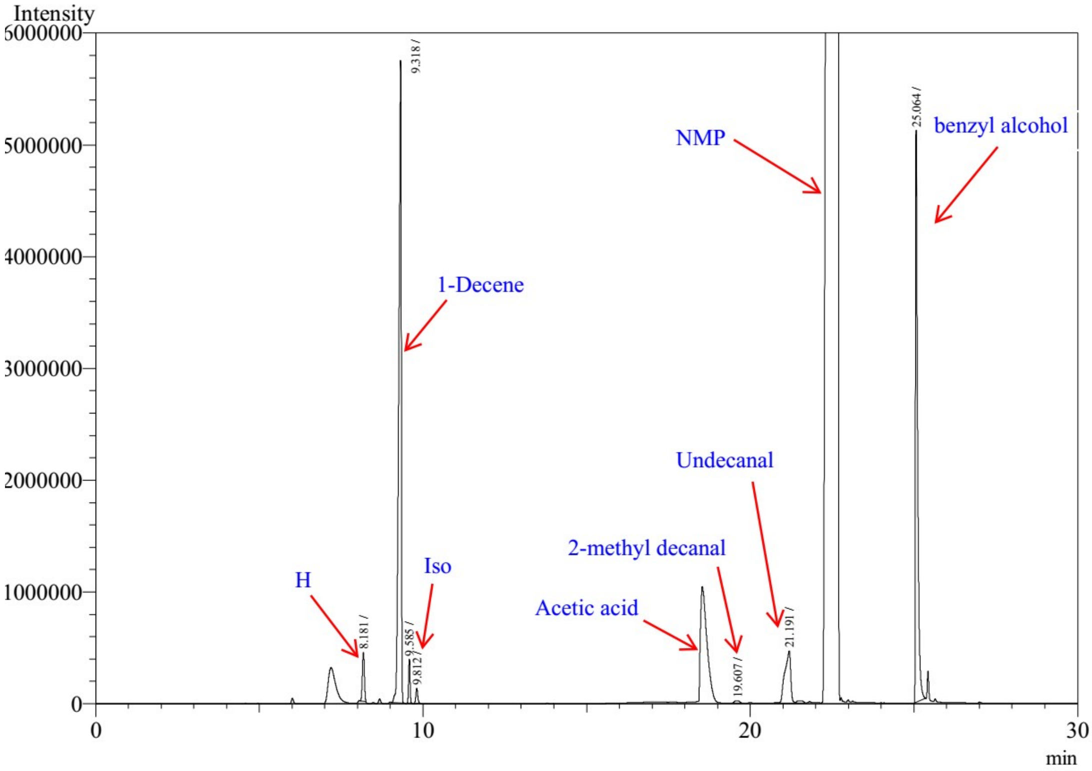
equation (f) Entry 1



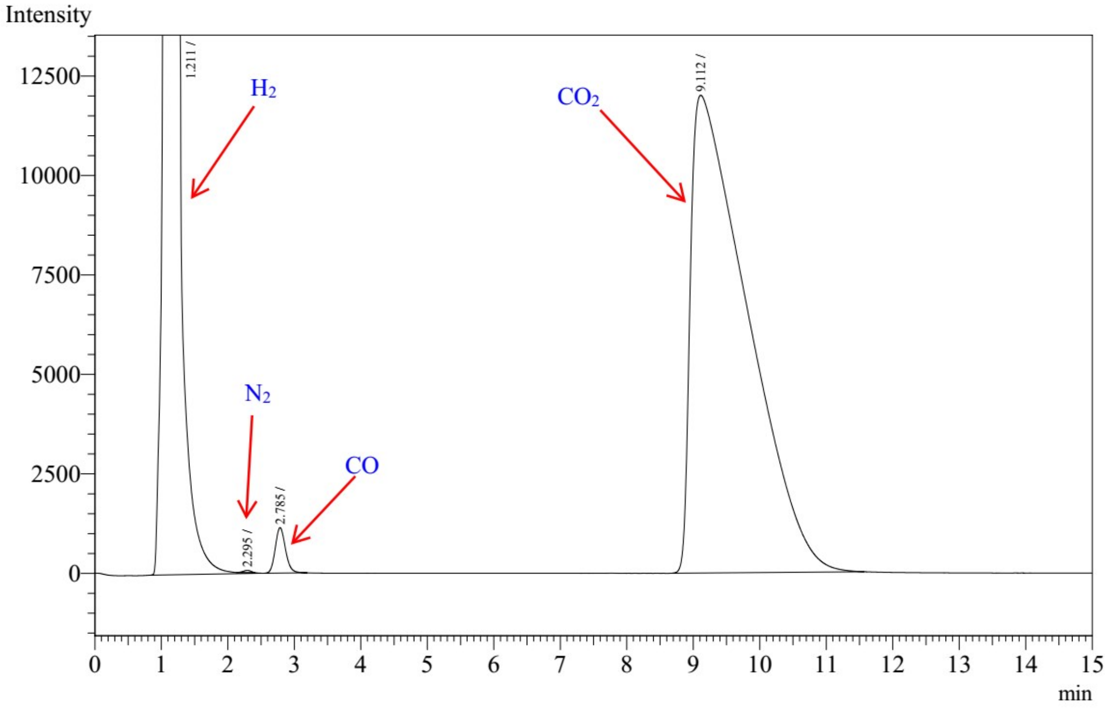
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.424	9153167	1360159	14.450				
2	8.174	234852	43839	0.371				
3	9.224	4615346	984215	7.286				
4	9.544	923219	185788	1.457				
5	9.828	447021	102516	0.706				
6	19.536	4223925	375610	6.668				
7	21.298	43746943	3688640	69.062				
[redacted]		63344473	6740767	100.000				

3.12 Gas chromatograms to Table S12

Entry 1

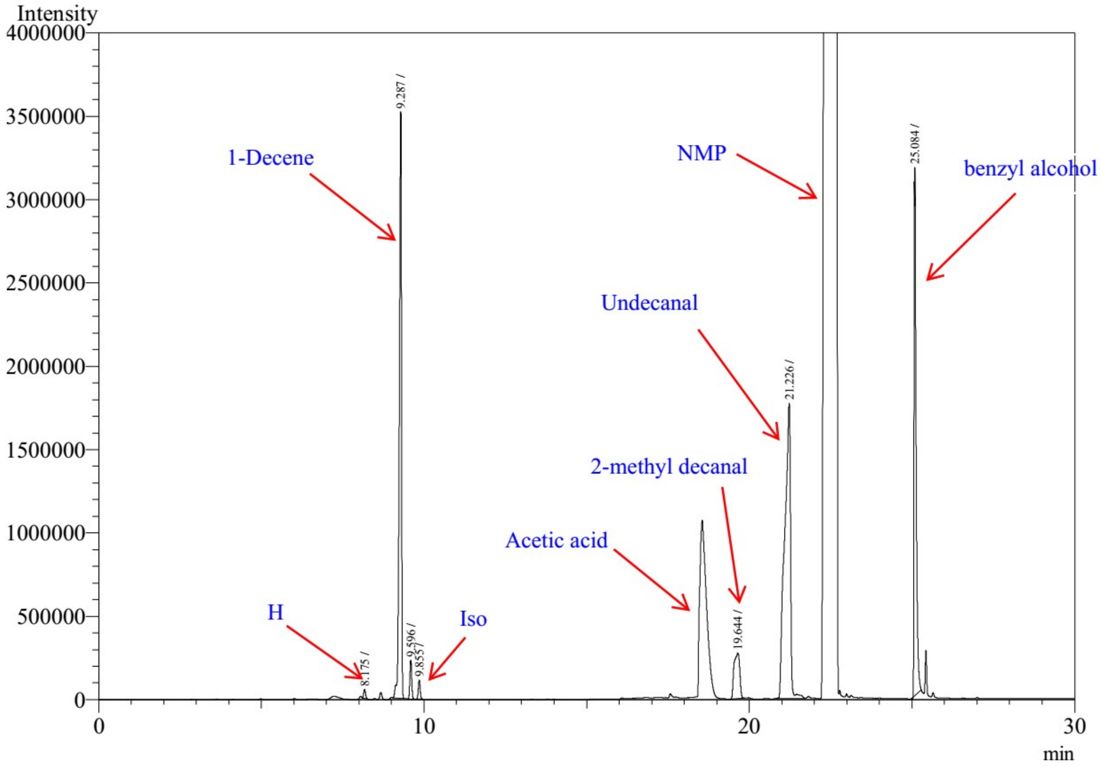


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.181	1881248	437686	2.967				
2	9.318	30351027	5671334	47.860				
3	9.585	1173165	386482	1.850				
4	9.812	519746	132925	0.820				
5	19.607	230063	19325	0.363				
6	21.191	6002794	464958	9.466				
7	25.064	23257912	5060427	36.675				
[redacted]		63415955	12173137	100.000				

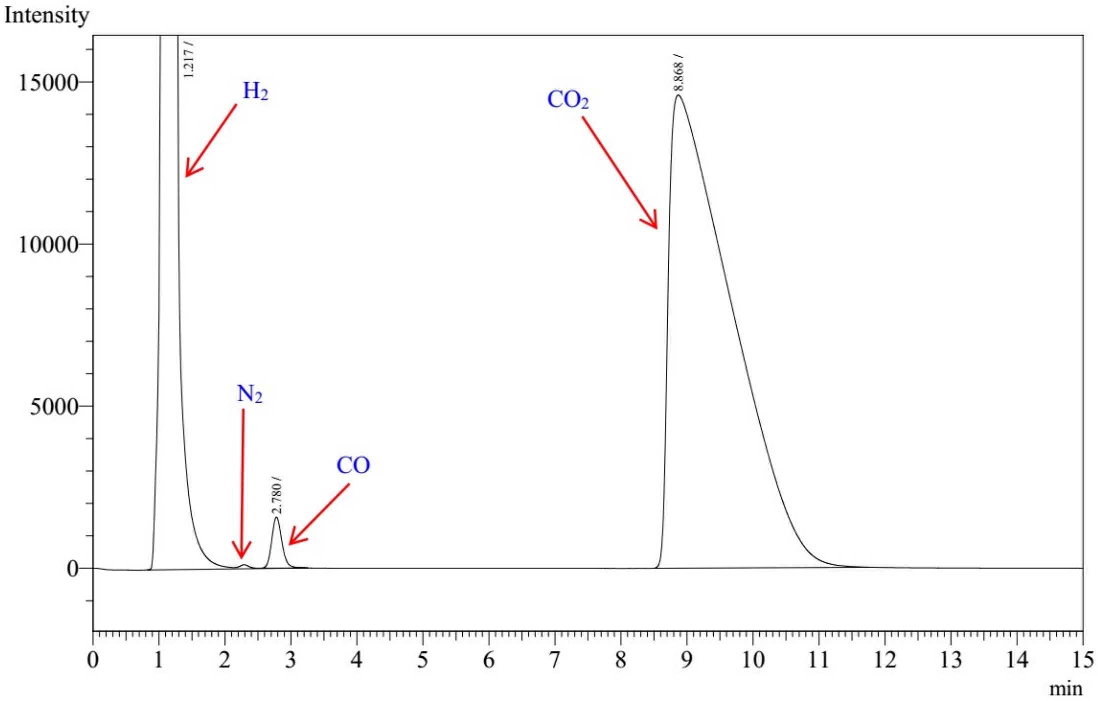


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.211	1671589	187668	69.746		S		
2	2.295	408	53	0.017		T		
3	2.785	12221	1143	0.510				
4	9.112	712463	12008	29.727				
		2396681	200872					

Entry 2



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.175	222542	53963	0.389				
2	9.287	16342569	3499372	28.553				
3	9.596	902202	232533	1.576				
4	9.855	463503	114867	0.810				
5	19.644	3333838	272550	5.825				
6	21.226	22058184	1770853	38.539				
7	25.084	13913654	3154942	24.309				
		57236492	9099080	100.000				



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Peak#  Ret.Time     Area    Height    Conc.  UnitMark ID#    Cmpd Name
    1     1.217  1806542   195558   64.666        S
    2     2.780    16825     1578    0.602        T
    3     8.868   970276    14595   34.732
                 2793643   211731
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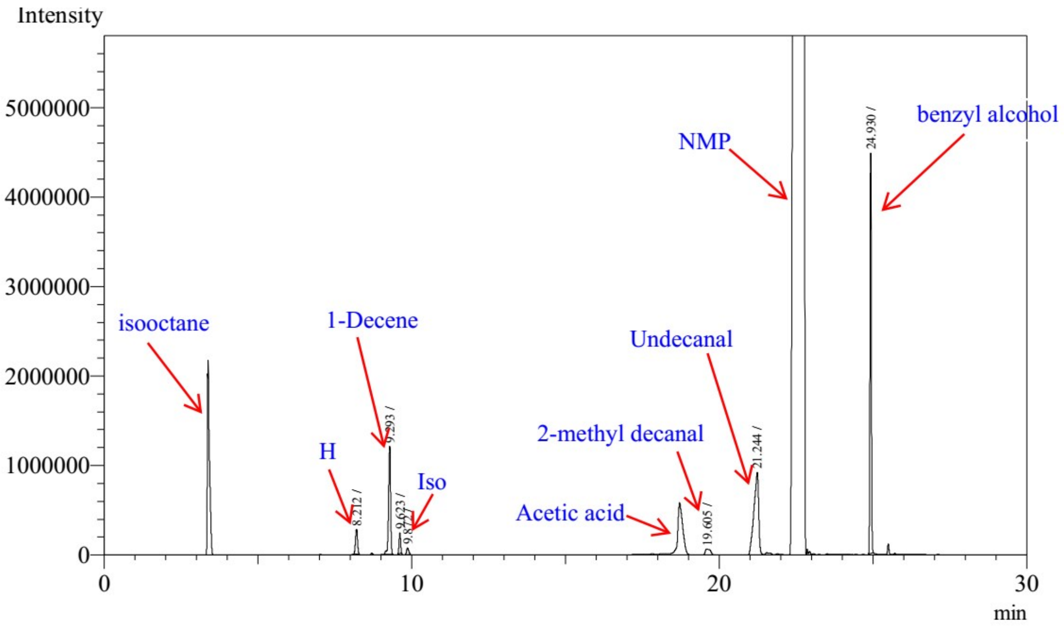
Entry 3



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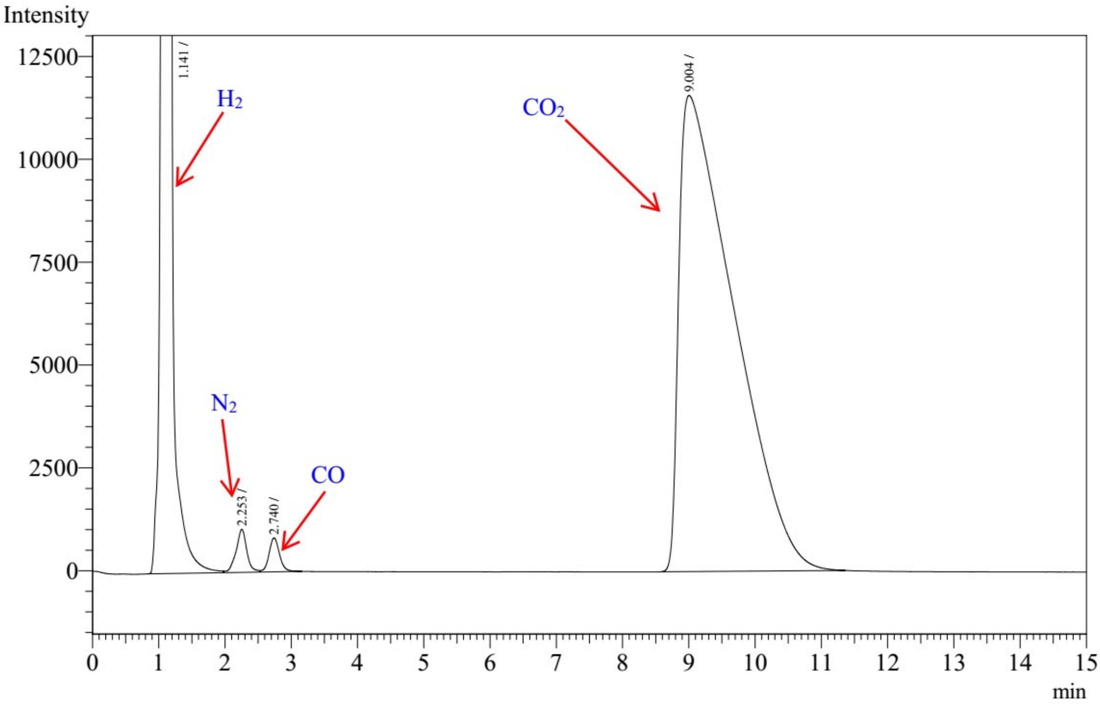
1	8.212	1264287	272688	3.947				
2	9.293	5398692	1203203	16.856				
3	9.623	798297	227607	2.492				
4	9.872	375006	78473	1.171				
5	19.605	765882	66281	2.391				
6	21.244	10111178	919519	31.570				
7	24.930	13314911	4436689	41.572				
		32028253	7204460	100.000				



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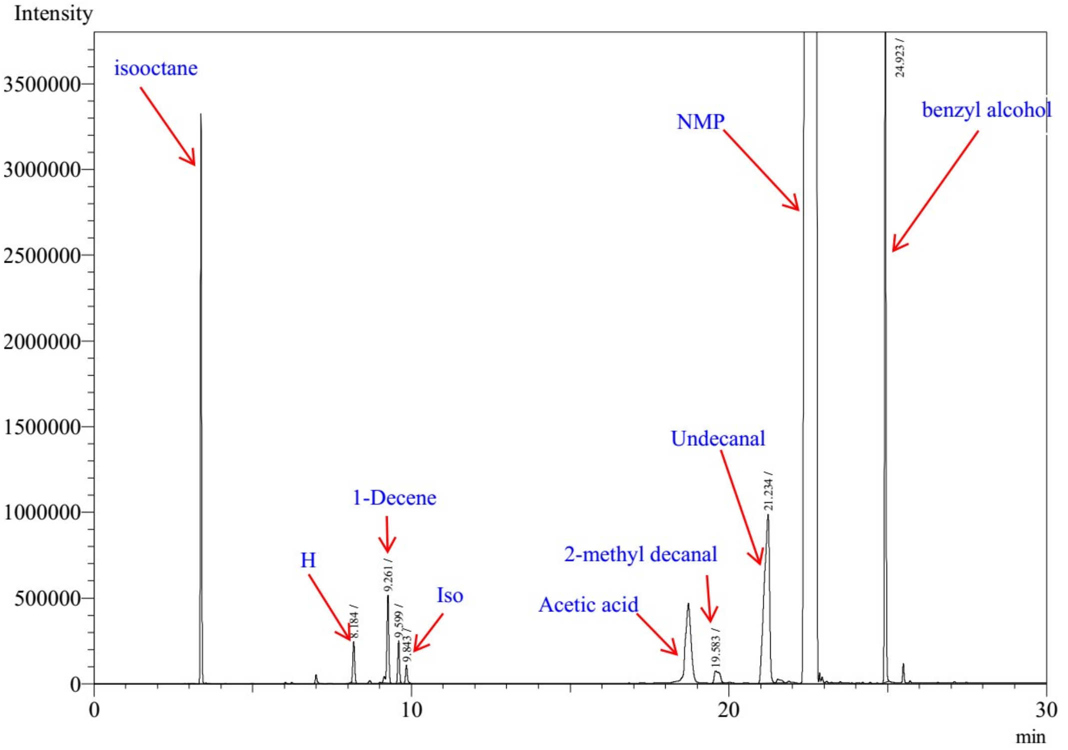
1	1.141	738098	117921	51.784				
2	2.253	11804	1048	0.828		V		
3	2.740	9068	826	0.636		V		
4	9.004	666357	11574	46.751				
		1425327	131369					

Entry 4



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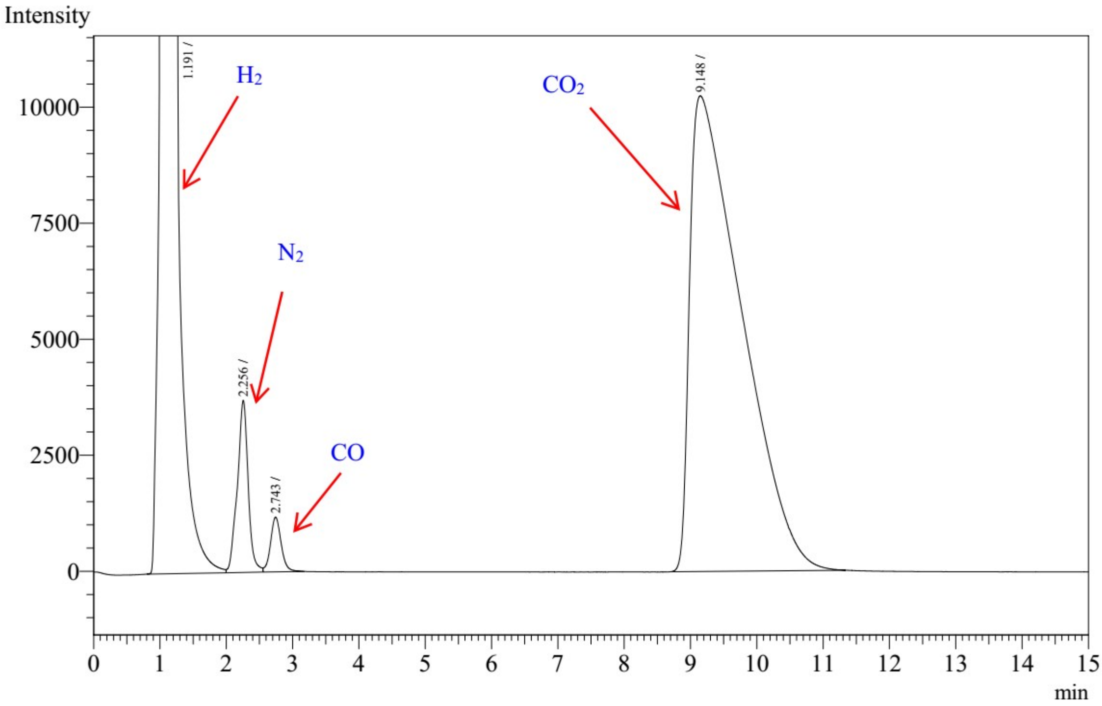
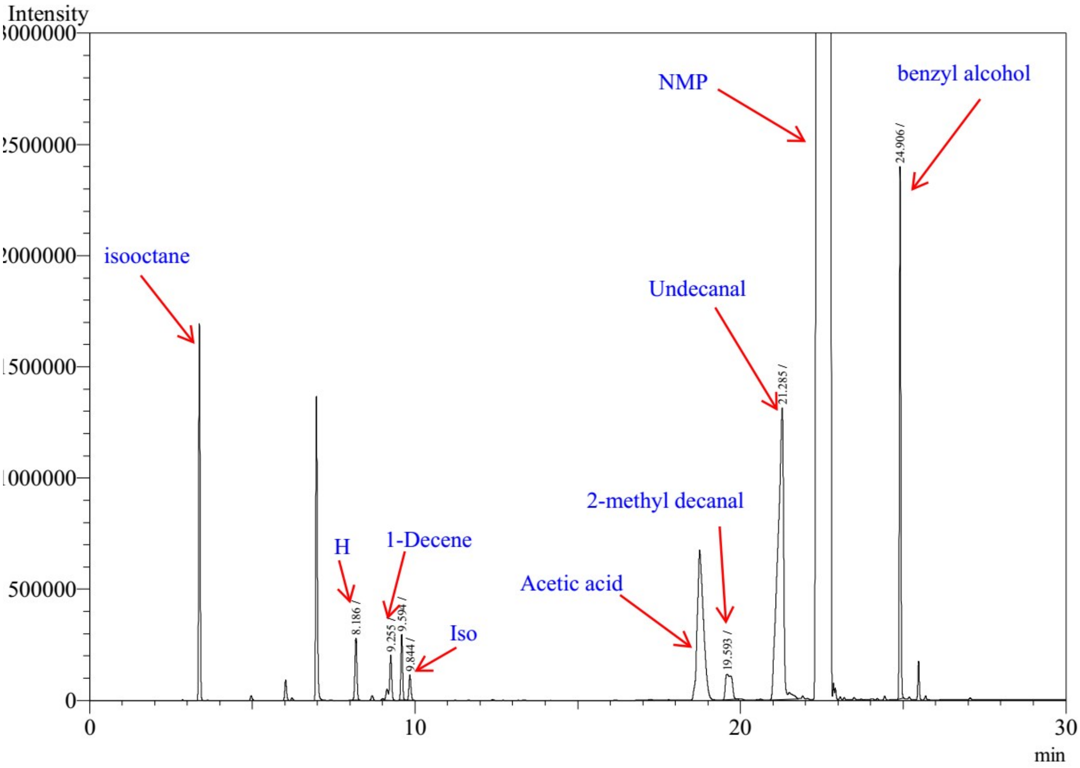
1	8.184	978356	242146	3.402				
2	9.261	2202964	511536	7.660				
3	9.599	878219	245434	3.054				
4	9.843	409943	105834	1.425				
5	19.583	834173	70701	2.901				
6	21.234	11613210	982907	40.381				
7	24.923	11842376	3928316	41.178				
[redacted]		28759241	6086874	100.000				

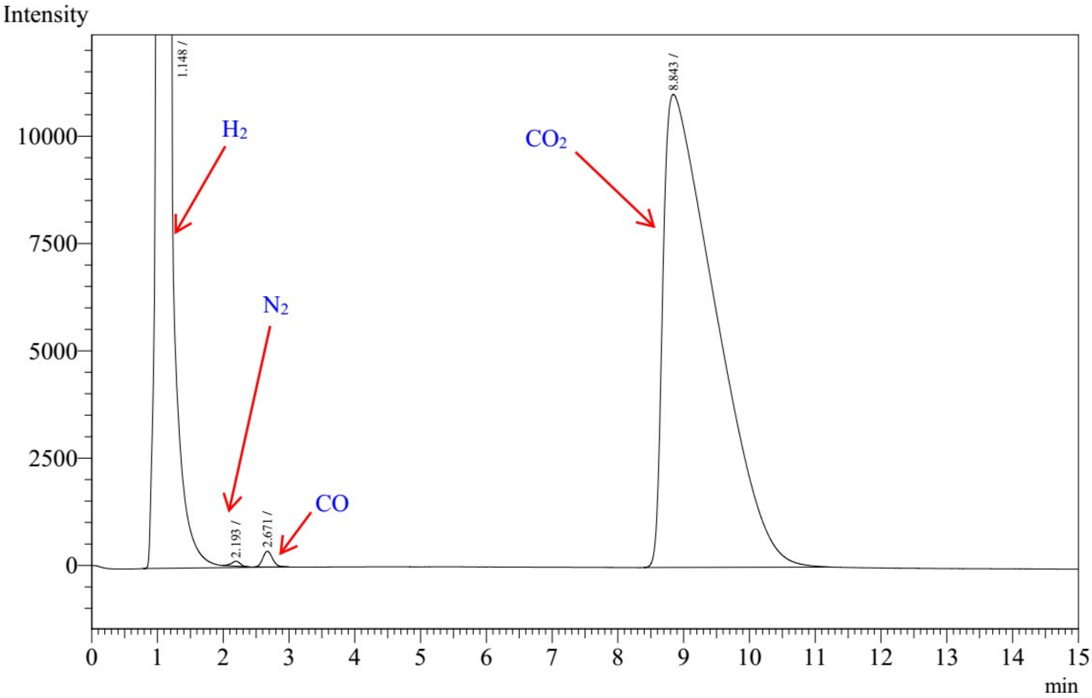


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.191	1720418	190778	73.763				
2	2.256	42243	3707	1.811		V		
3	2.743	13137	1180	0.563		V		
4	9.148	556546	10250	23.862				
		2332344	205915					

Entry 5



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.186	1161517	276953	4.046				
2	9.255	1092072	201589	3.804				
3	9.594	1059747	293433	3.692				
4	9.844	486702	114191	1.695				
5	19.593	1604330	115802	5.589				
6	21.285	16192450	1310982	56.407				
7	24.906	7109417	2366572	24.766				
		28706235	4679522	100.000				



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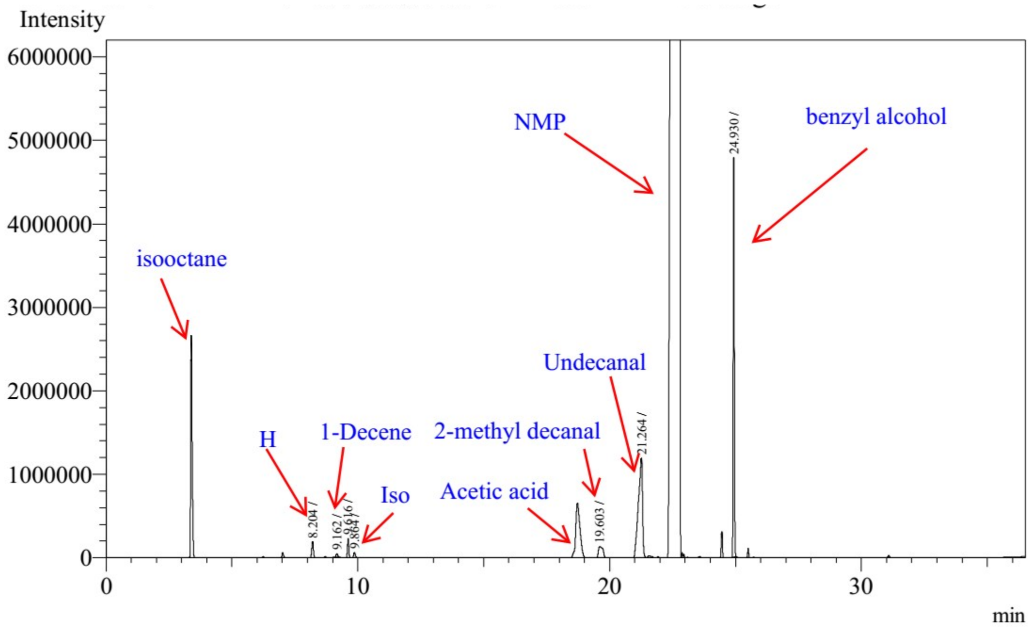
1	1.148	1483604	179921	70.683		S		
2	2.193	1073	115	0.051		T		
3	2.671	3790	368	0.181		T		
4	8.843	610498	11022	29.086				
		2098965	191426					

Entry 6



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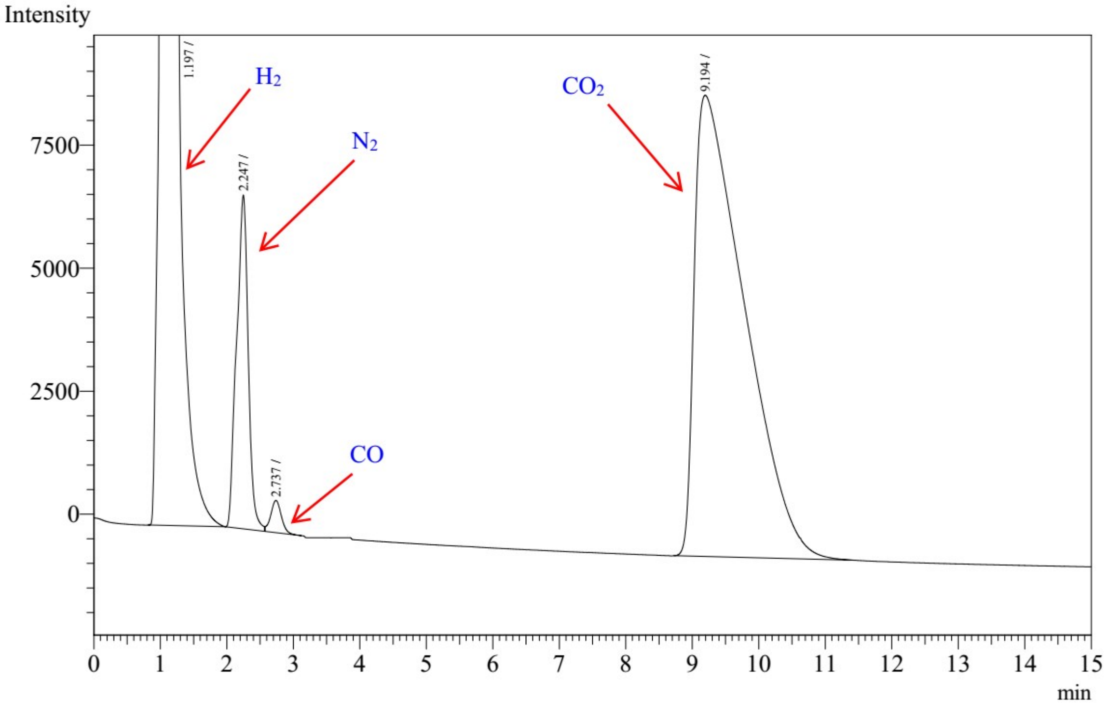
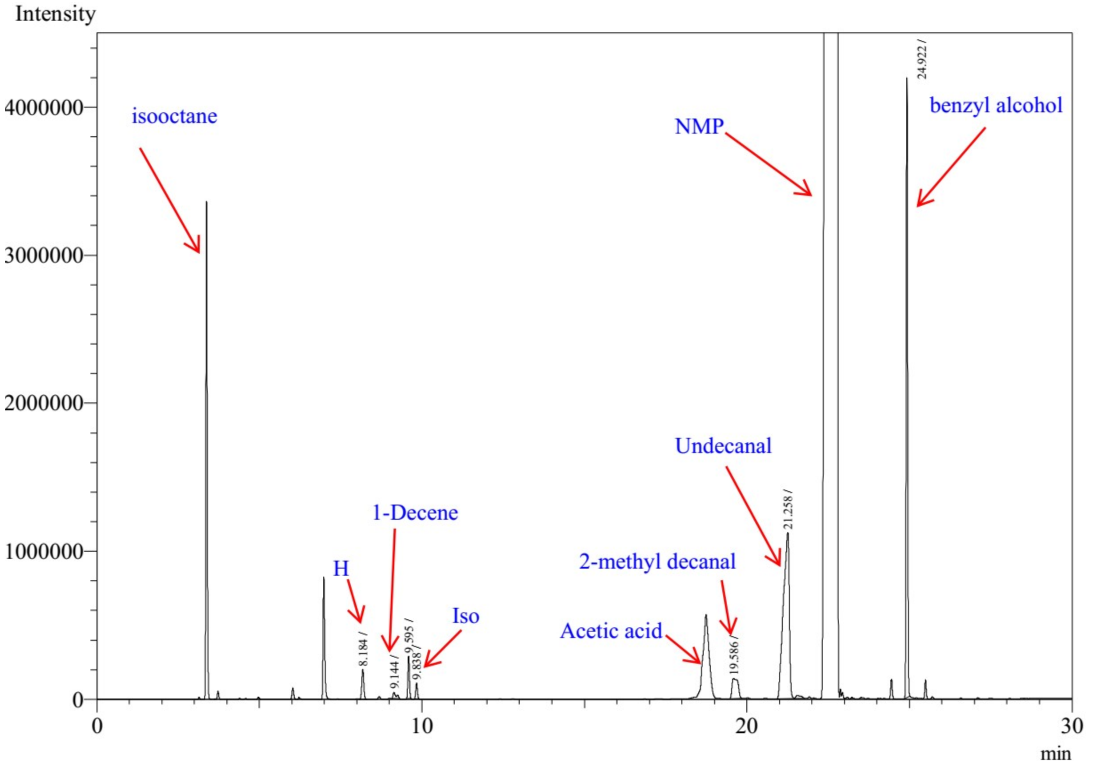
1	8.204	845192	192921	2.634				
2	9.162	169884	38987	0.530				
3	9.616	844912	227846	2.634				
4	9.864	298721	67602	0.931				
5	19.603	1715399	138251	5.347				
6	21.264	13924988	1200938	43.403				
7	24.930	14283962	4754744	44.522				
		32083058	5621289	100.000				

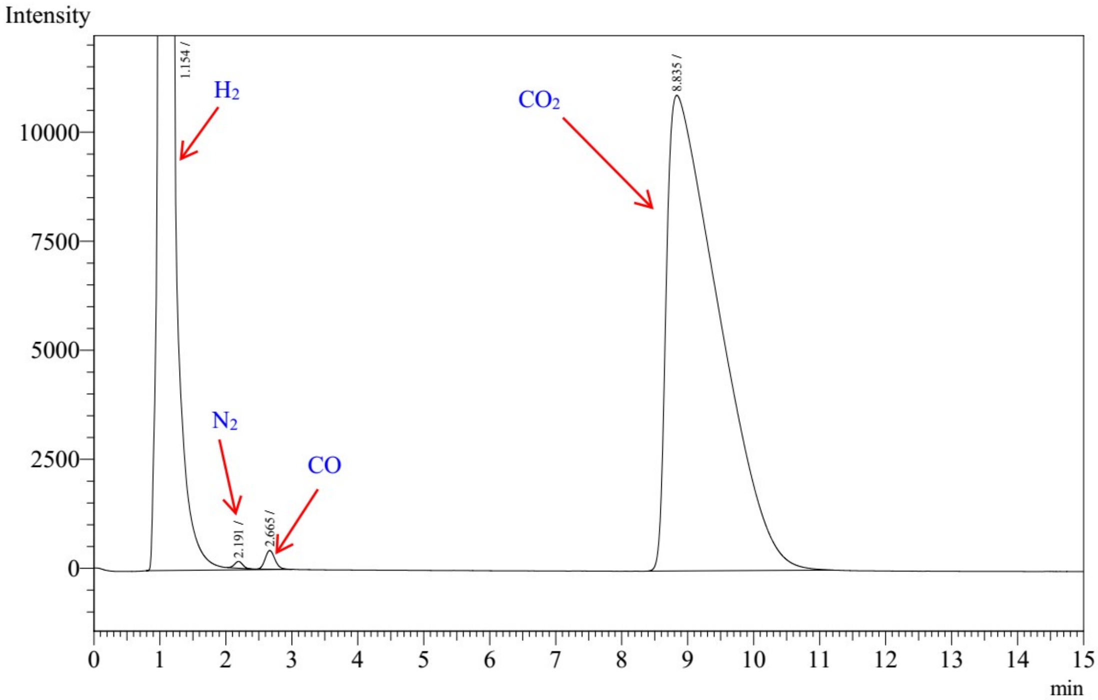


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.197	1959943	204044	77.131				
2	2.247	82621	6783	3.251				
3	2.737	7228	656	0.284		V		
4	9.194	491267	9373	19.333				
		2541059	220856					

Entry 7

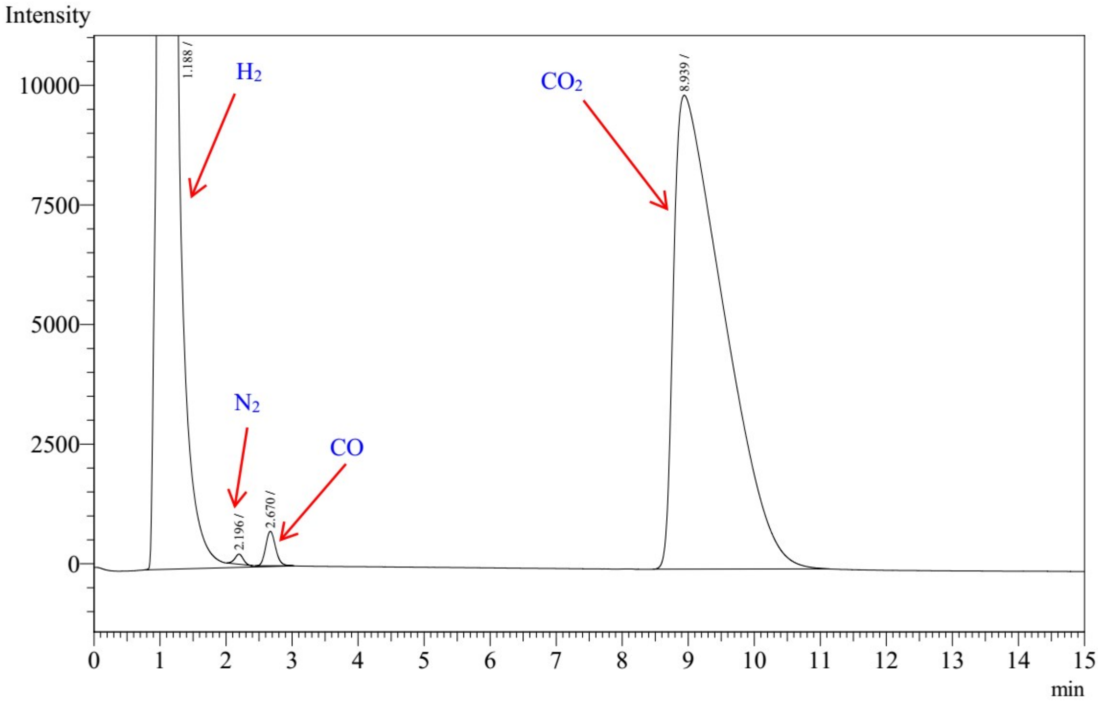


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.184	841229	201214	2.718				
2	9.144	279042	39931	0.902				
3	9.595	946161	284833	3.058				
4	9.838	395332	107556	1.278				
5	19.586	1706511	135481	5.515				
6	21.258	14352169	1121530	46.380				
7	24.922	12424553	4167139	40.150				
[redacted]		30944997	6057684	100.000				



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.154	1655753	190685	73.235		S		
2	2.191	1341	156	0.059		T		
3	2.665	4436	431	0.196		T		
4	8.835	599353	10906	26.510				
		2260883	202178					

Entry 8



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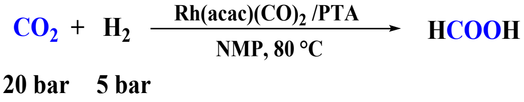
1	1.188	2482628	232918	82.378		S		
2	2.196	1885	213	0.063		T		
3	2.670	7522	721	0.250		T		
4	8.939	521660	9906	17.310				
[redacted]		3013695	243758					

4 NMR, ESI-MS and Mass Spectra

Figure S2 ^1H NMR ($CDCl_3$, 400 MHz) spectra of the reaction mixture for CO_2 hydrogenation in NMP



$$\underset{\text{20 bar}}{CO_2} + \underset{\text{5 bar}}{H_2} \xrightarrow[\text{NMP, 80 °C}]{\text{Rh(acac)(CO)}_2\text{ /PTA}} HCOOH$$

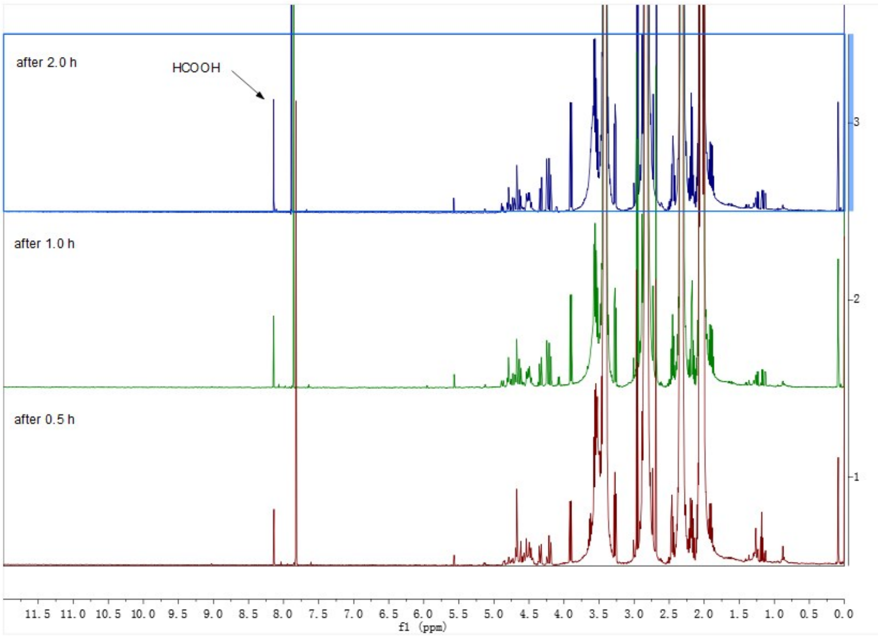


Figure S3 ESI-MS spectra of the Rh/PTA

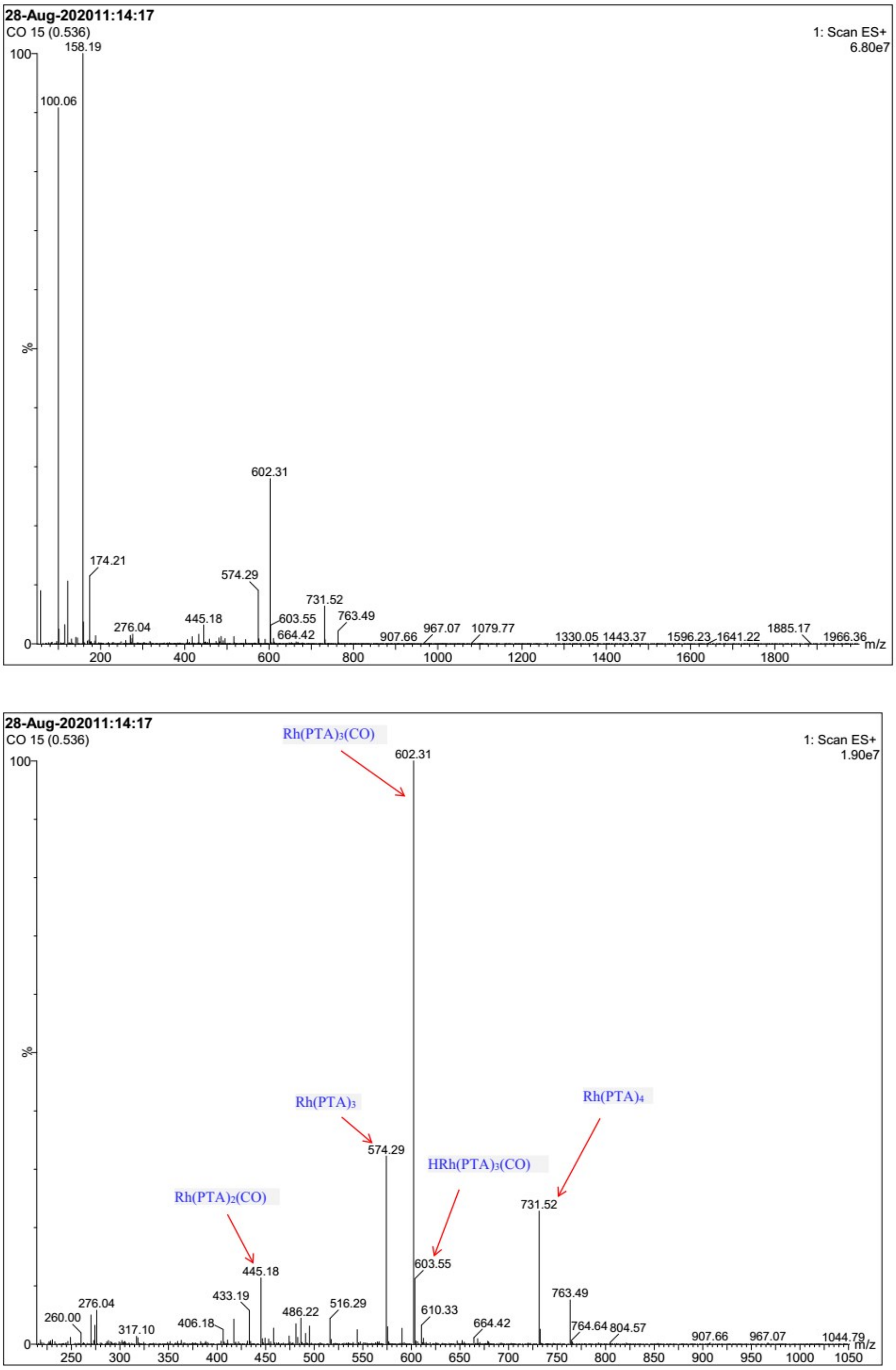


Figure S4 ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of the reaction system with $^{13}CO_2$ (Table S10 (a))

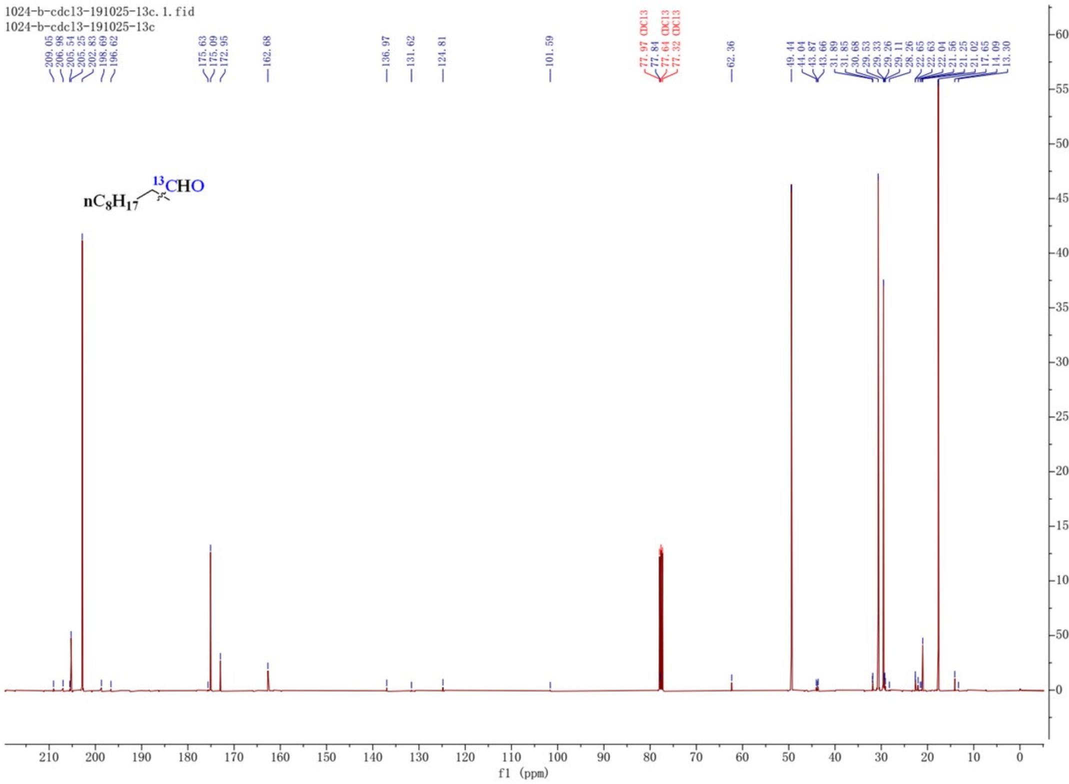
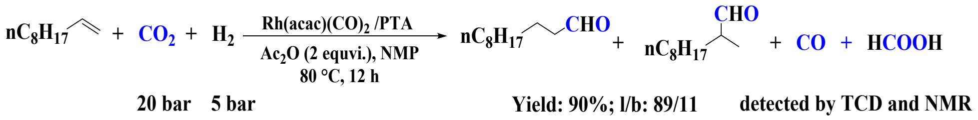
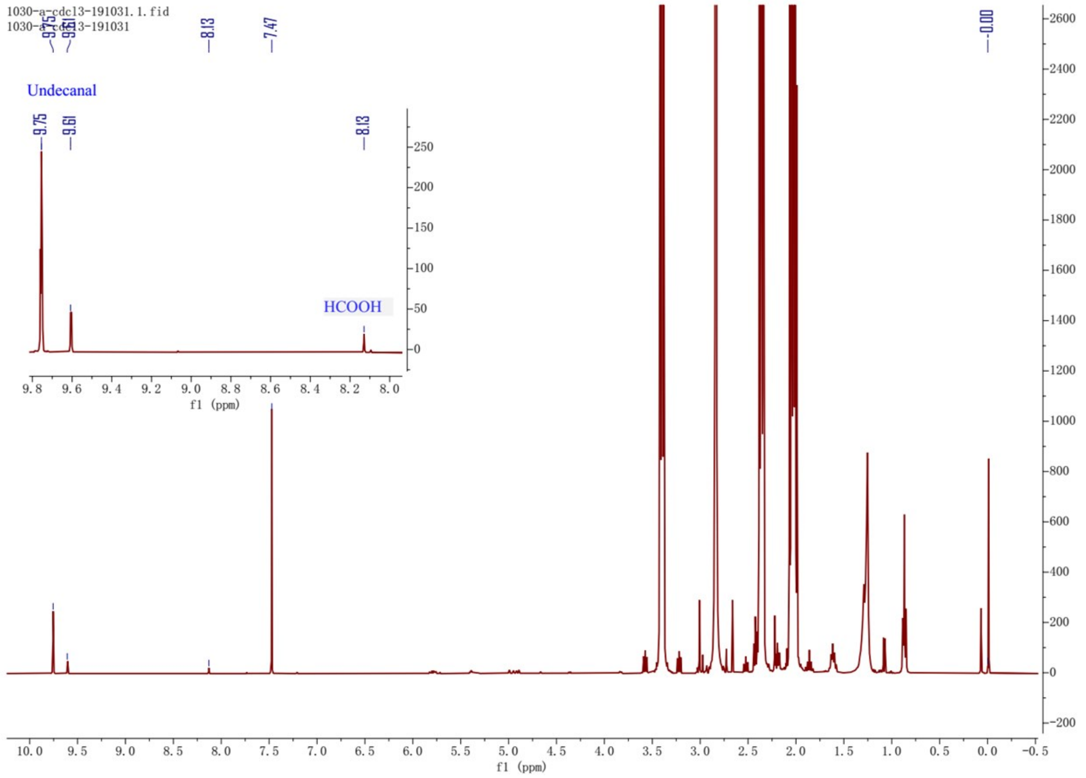


Figure S5 ^{1}H and ^{13}C NMR ($CDCl_3$, 400 MHz) spectra of the reaction system (Table S10 (b))





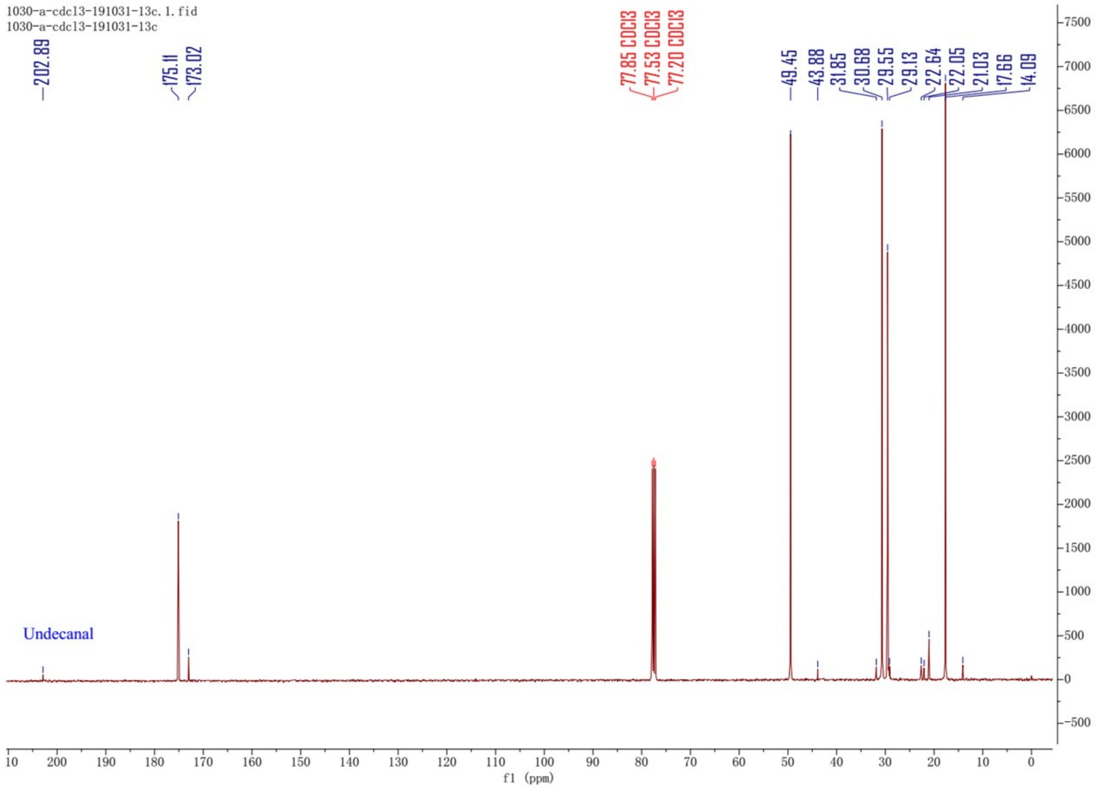


Figure S6 MS spectra of the reaction gas for the isotope-labeling experiments

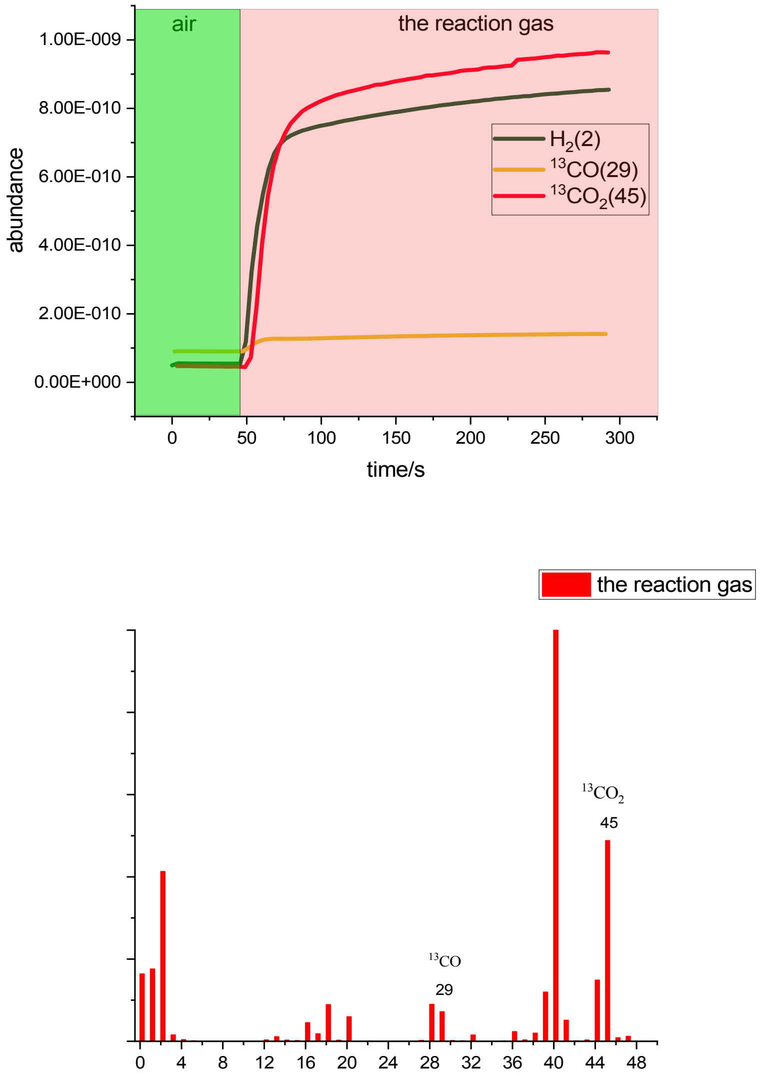


Figure S7 ^1H NMR ($CDCl_3$, 400 MHz) spectra of the reaction system (c, Table S10)

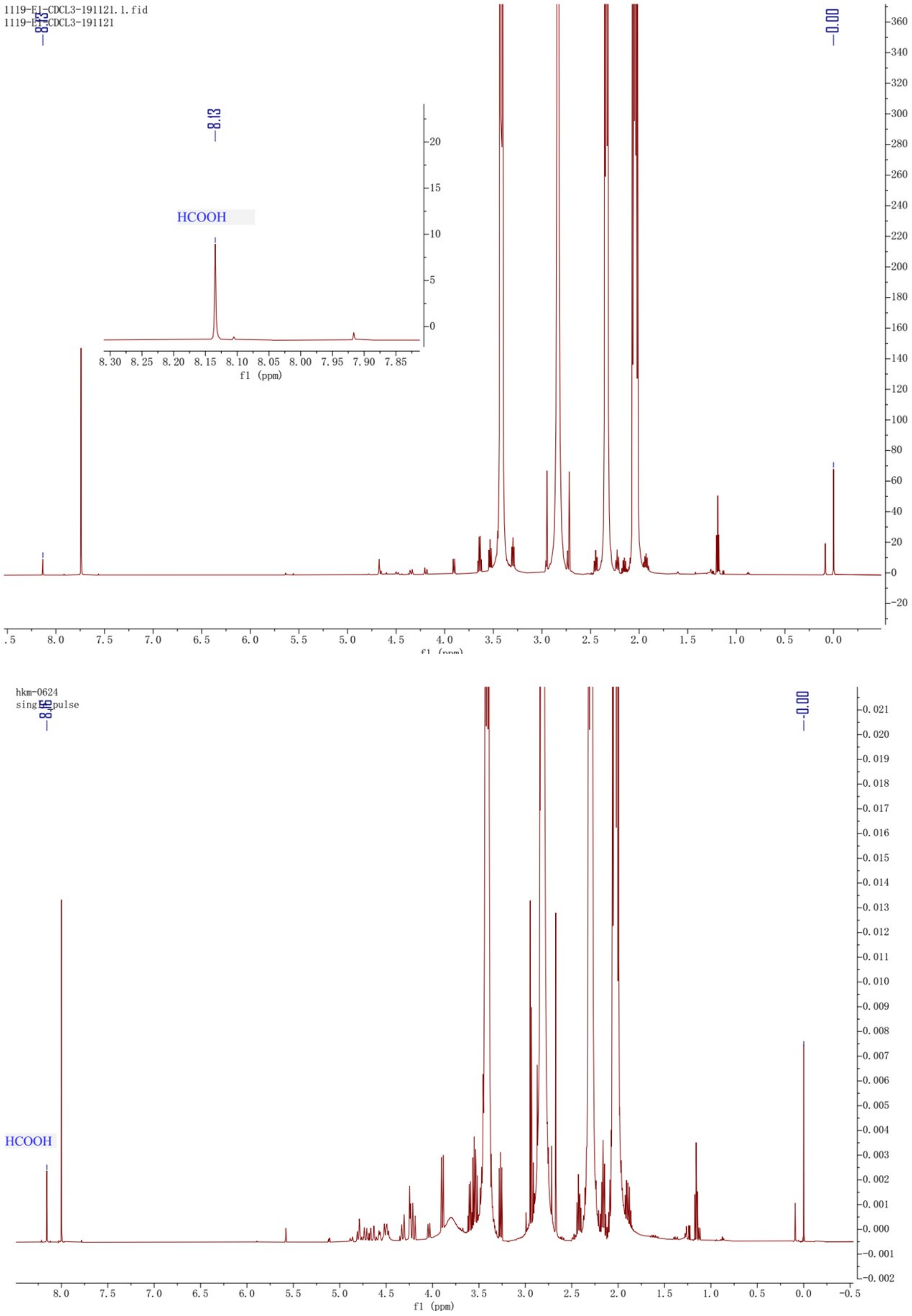


Figure S8 ^{1}H NMR (CDCl$_3$, 400 MHz) spectra of HCOOAc