

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
 Data File : VN069927.D
 Acq On : 9 Dec 2021 21:51
 Operator : JC/MD
 Sample : M4970-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-19

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M

Title : SW846 8260

Signal : TIC: VN069927.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	80	92	100	rBV2	177763	355705	1.83%	0.499%
2	5.374	1231	1262	1299	rBV3	350261	1295099	6.65%	1.816%
3	5.618	1317	1353	1404	rBV	5483976	19474963	100.00%	27.311%
4	6.498	1657	1681	1709	rVB3	81004	261456	1.34%	0.367%
5	8.021	2227	2249	2261	rBV2	930409	2263385	11.62%	3.174%
6	8.086	2261	2273	2300	rVB	1585067	3657072	18.78%	5.128%
7	8.440	2384	2405	2423	rBV	1048672	2463096	12.65%	3.454%
8	8.534	2423	2440	2472	rVV	1603060	3878979	19.92%	5.440%
9	8.968	2582	2602	2650	rVB	2672744	5617893	28.85%	7.878%
10	10.202	3045	3062	3066	rBV2	362795	622104	3.19%	0.872%
11	10.440	3133	3151	3177	rBV	4304586	8028780	41.23%	11.259%
12	10.550	3178	3192	3220	rVB	577020	1184522	6.08%	1.661%
13	11.213	3422	3439	3468	rVB3	126251	293293	1.51%	0.411%
14	11.623	3569	3592	3616	rBV5	83710	237086	1.22%	0.332%
15	11.744	3619	3637	3668	rBV	4622957	8496387	43.63%	11.915%
16	12.731	3987	4005	4036	rBV	3561717	6325673	32.48%	8.871%
17	13.675	4339	4357	4385	rBV	3958303	6853712	35.19%	9.611%

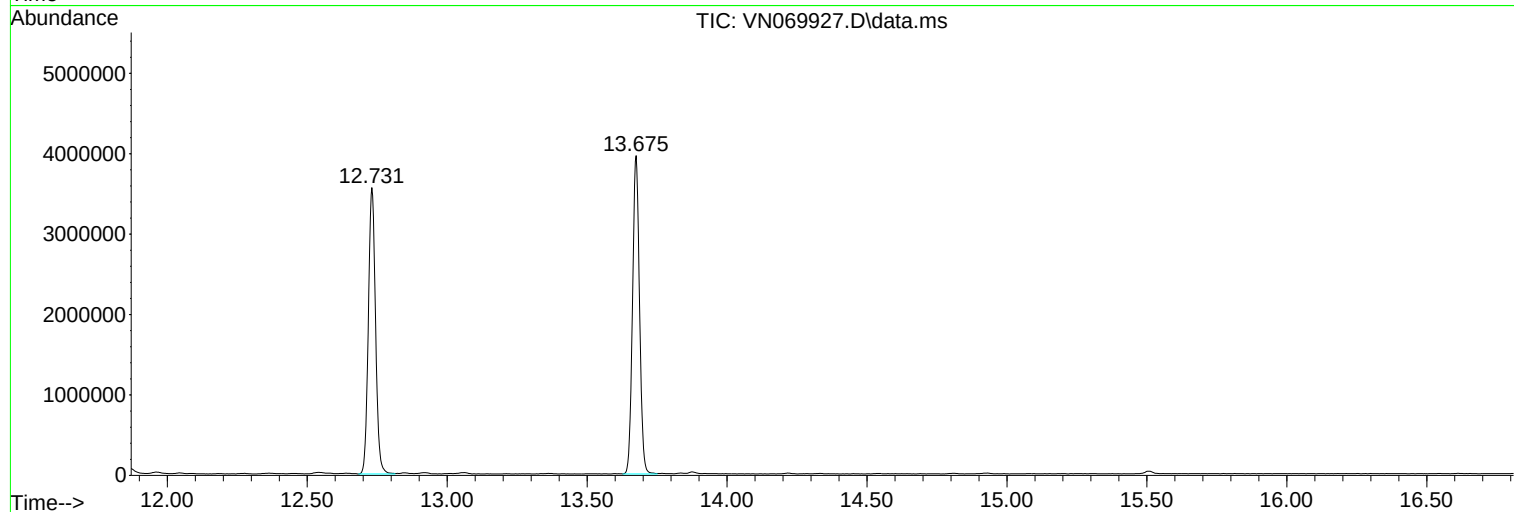
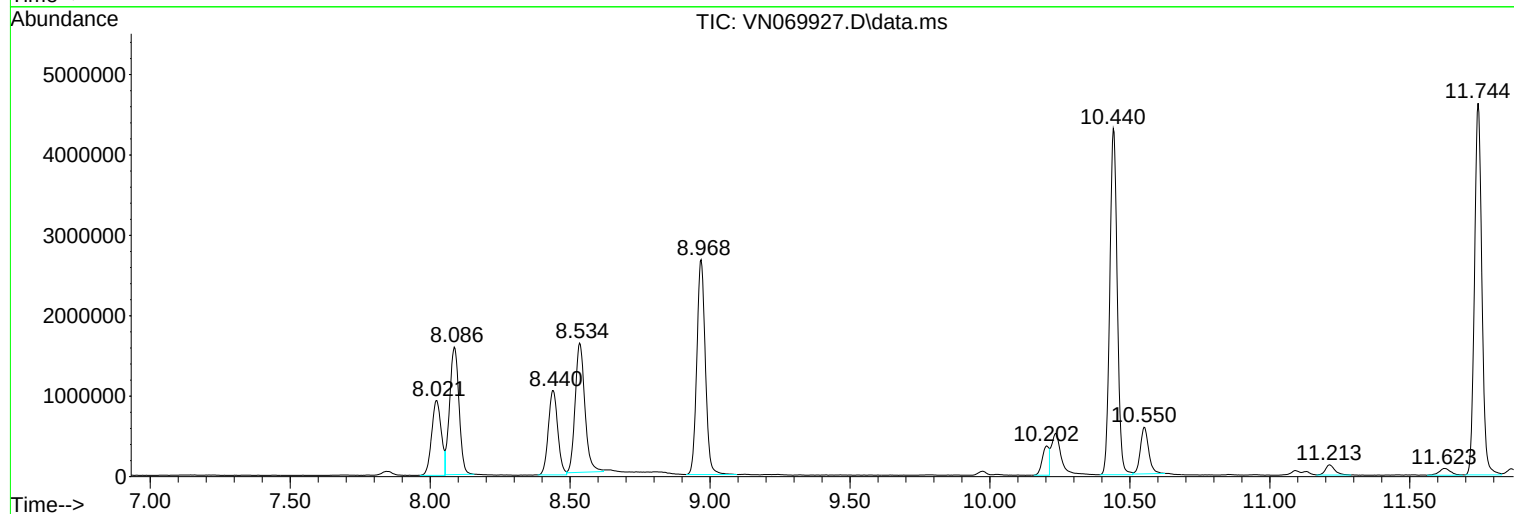
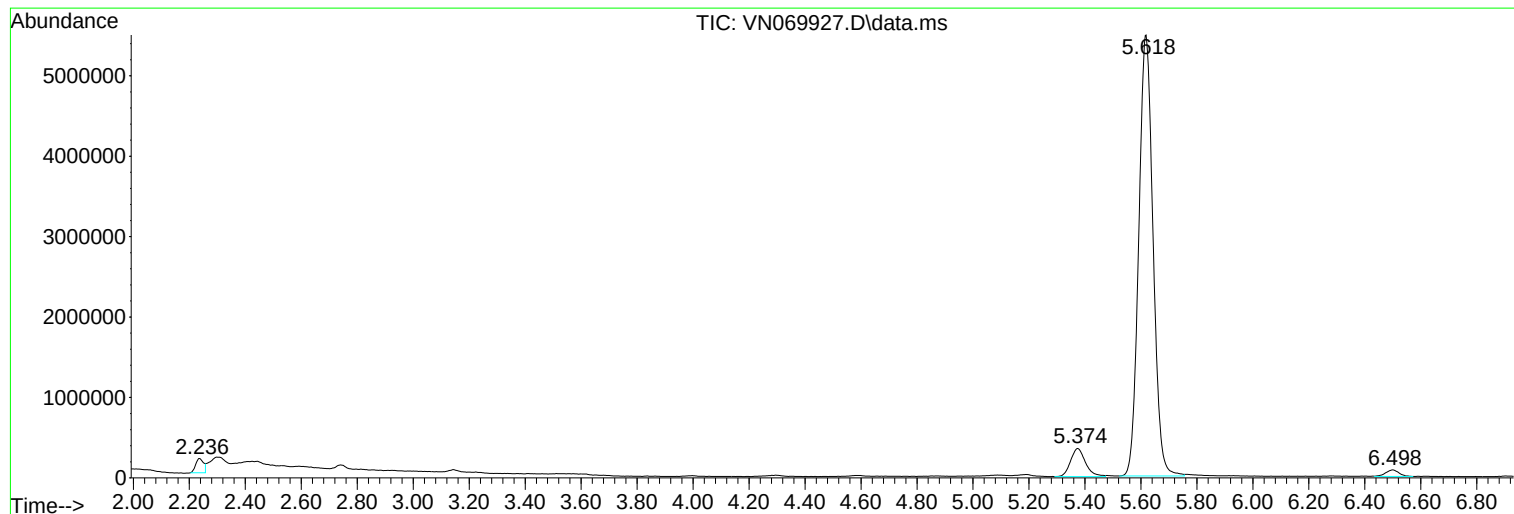
Sum of corrected areas: 71309205

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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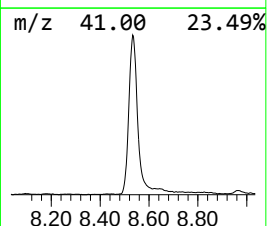
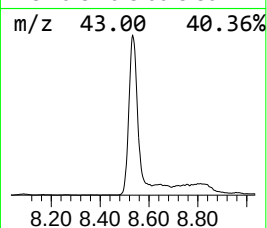
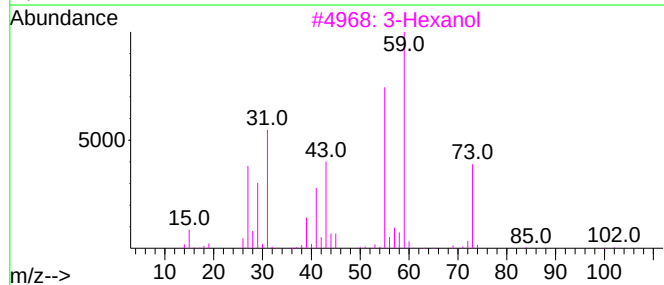
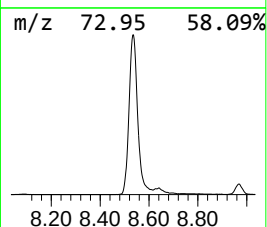
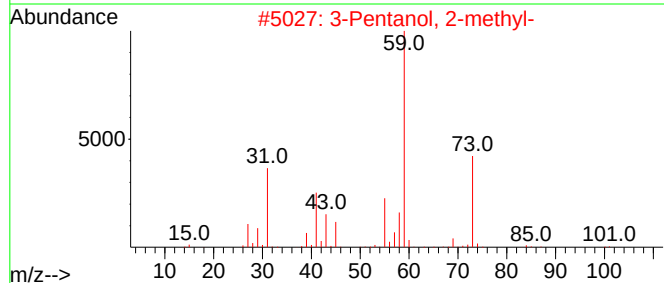
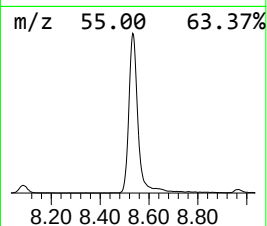
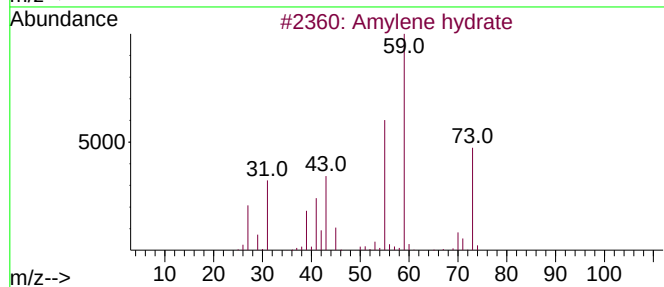
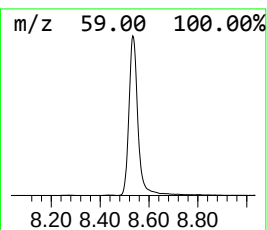
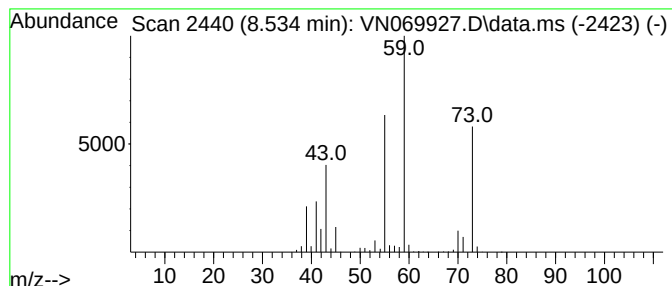
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.534	34.52 ug/l	3878980	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
3			3-Hexanol	102	C6H14O	000623-37-0	38
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
5			2-Pentene, (E)-	70	C5H10	000646-04-8	11



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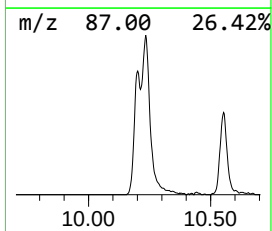
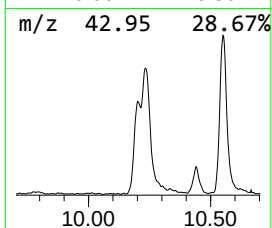
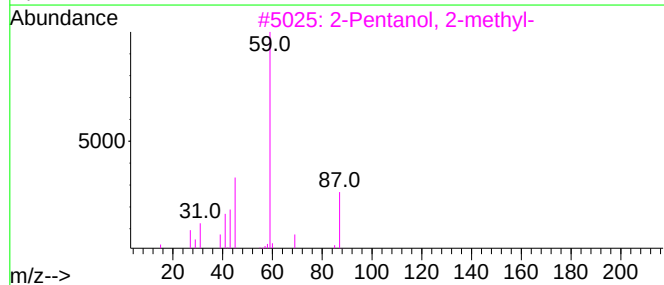
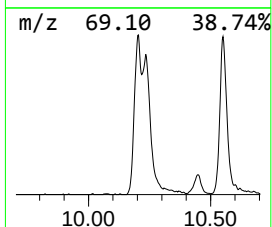
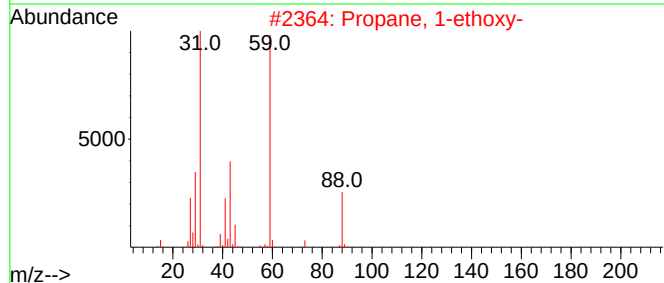
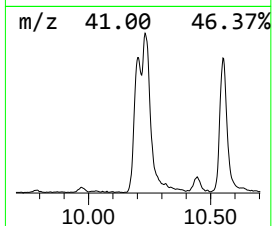
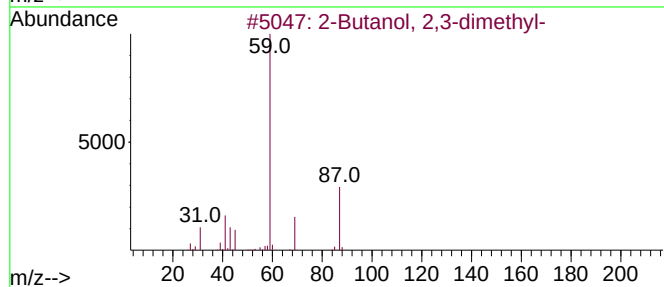
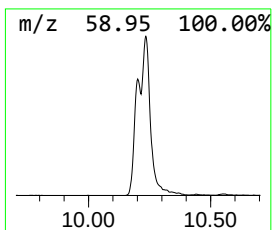
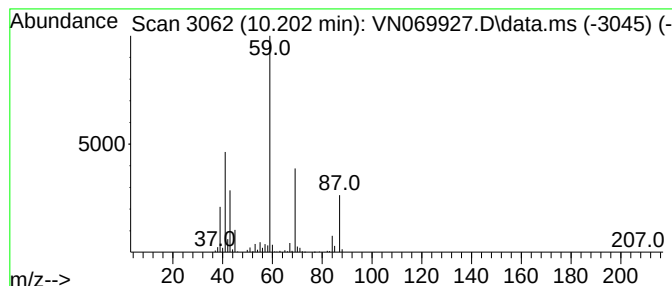
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.202	5.54 ug/l	622104	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	78
2	Propane, 1-ethoxy-			88	C5H12O	000628-32-0	50
3	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	50
4	DL-Lactamide, N,O-dimethyl-			117	C5H11NO2	1000452-56-3	45
5	3-Pentanol, 2,2-dimethyl-			116	C7H16O	003970-62-5	39



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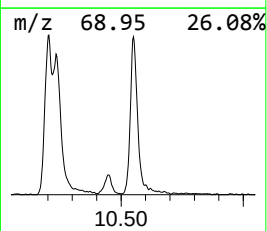
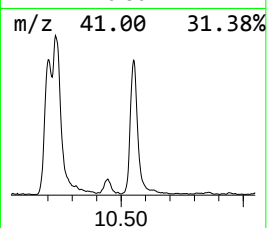
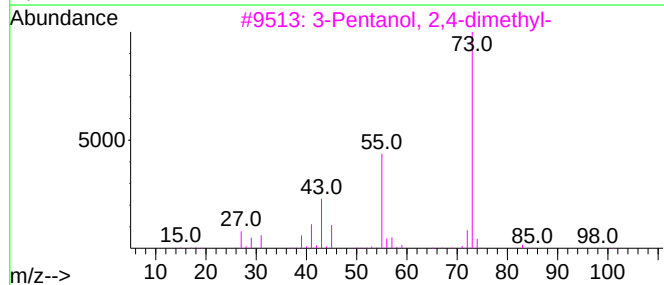
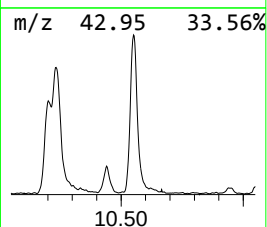
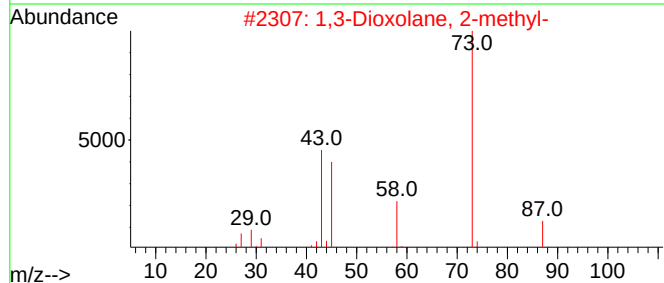
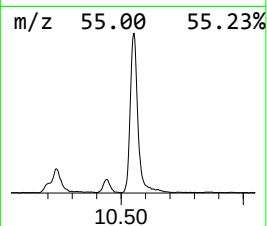
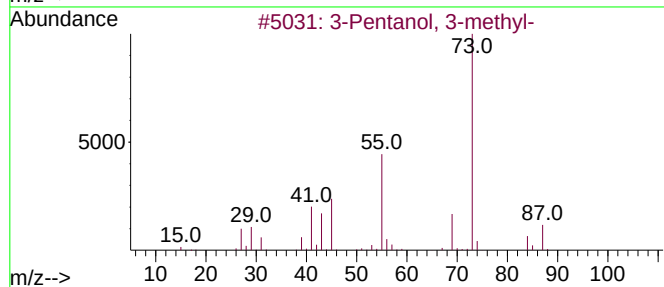
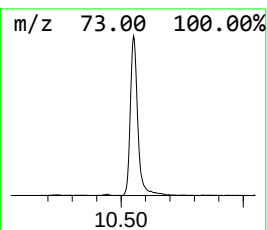
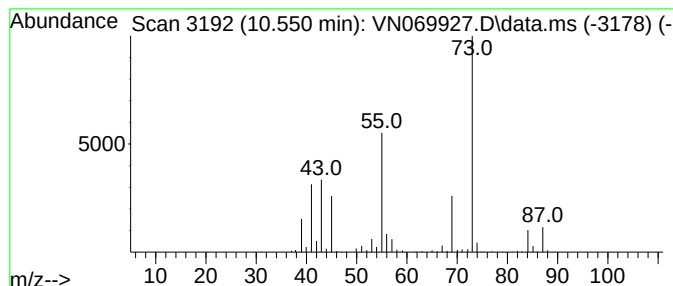
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Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.550	6.97 ug/l	1184520	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37
5			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	8.534	34.5	ug/l	3878980	2	8.968	5617890	50.0
2-Butanol, 2,3-...	10.202	5.5	ug/l	622104	2	8.968	5617890	50.0
3-Pentanol, 3-m...	10.550	7.0	ug/l	1184520	3	11.744	8496390	50.0