

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
 Data File : VN069969.D
 Acq On : 10 Dec 2021 19:48
 Operator : JC/MD
 Sample : M4969-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-28D2

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: VN069969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.588	942	969	998	rBV	52842	180026	1.88%	0.269%
2	5.377	1228	1263	1317	rBV	1467153	5435793	56.70%	8.132%
3	5.618	1325	1353	1405	rVB2	2730991	9586611	100.00%	14.341%
4	6.501	1655	1682	1708	rVB2	80832	267520	2.79%	0.400%
5	8.024	2227	2250	2261	rBV	895557	2170249	22.64%	3.247%
6	8.086	2261	2273	2302	rVB2	1491213	3439245	35.88%	5.145%
7	8.440	2381	2405	2423	rBV	1040179	2425470	25.30%	3.628%
8	8.536	2423	2441	2480	rVV	2234839	5312961	55.42%	7.948%
9	8.968	2583	2602	2633	rBV	2537540	5293412	55.22%	7.919%
10	10.202	3046	3062	3067	rBV	338158	614754	6.41%	0.920%
11	10.443	3132	3152	3178	rBV	4118552	7810106	81.47%	11.683%
12	10.553	3179	3193	3220	rVB	532335	1090180	11.37%	1.631%
13	11.213	3422	3439	3464	rBV3	170272	383179	4.00%	0.573%
14	11.744	3618	3637	3668	rBV	4509561	8261890	86.18%	12.359%
15	11.865	3671	3682	3695	rVV7	49555	114066	1.19%	0.171%
16	12.731	3989	4005	4028	rBV	3583487	6311525	65.84%	9.442%
17	13.675	4341	4357	4396	rBV	4096272	7387128	77.06%	11.051%
18	13.876	4425	4432	4444	rVB2	73296	121663	1.27%	0.182%
19	14.214	4547	4558	4572	rVB3	69357	123916	1.29%	0.185%
20	14.930	4812	4825	4838	rVB4	46666	96499	1.01%	0.144%
21	15.507	5026	5040	5055	rVB	158769	305331	3.18%	0.457%
22	16.617	5441	5454	5473	rVB2	52321	117032	1.22%	0.175%

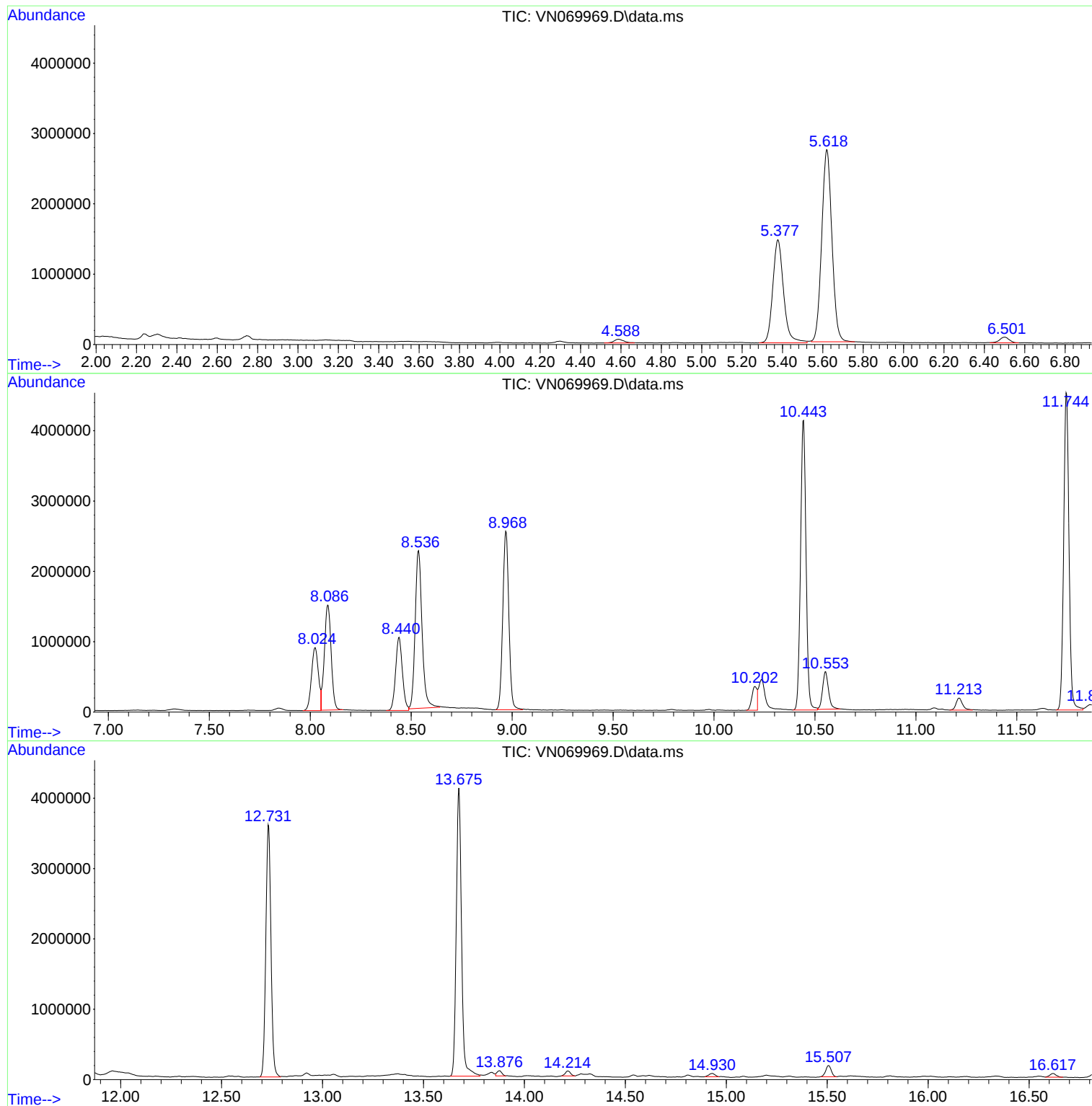
Sum of corrected areas: 66848556

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



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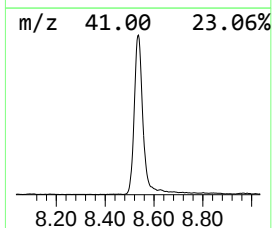
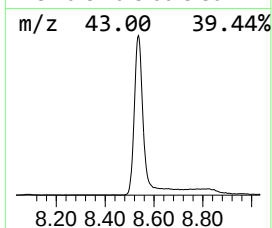
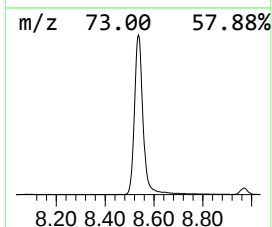
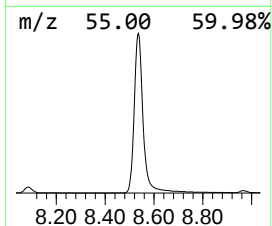
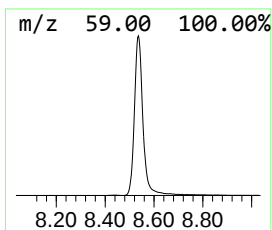
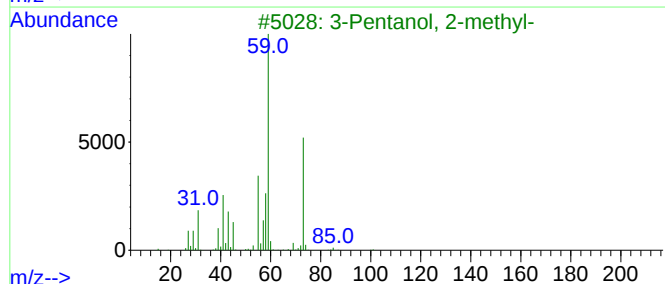
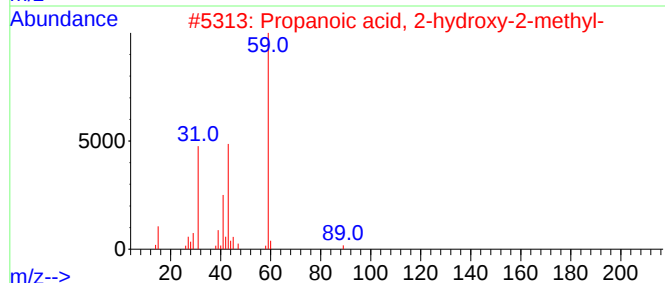
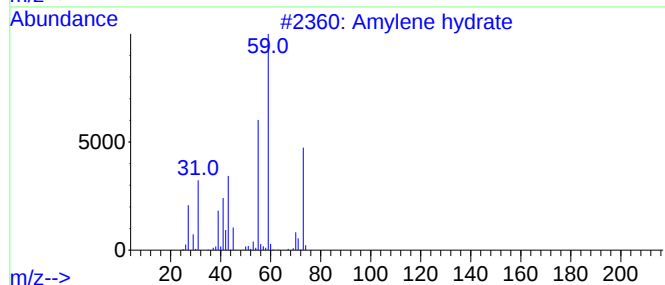
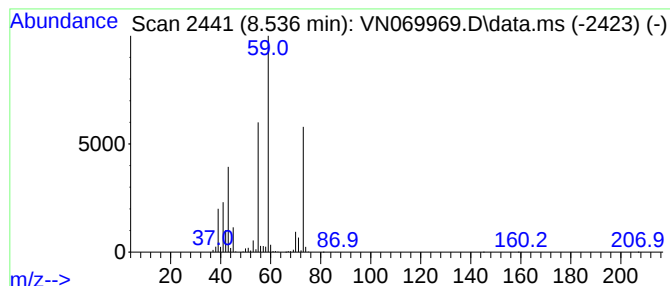
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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.
8.536	50.18 ug/l	5312960	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	40
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	11
5			2-Methyl-1-butene	70	C5H10	000563-46-2	9



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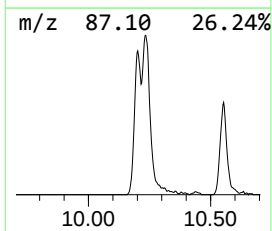
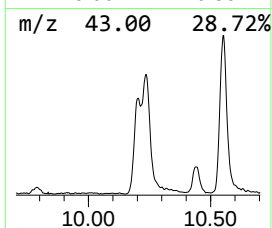
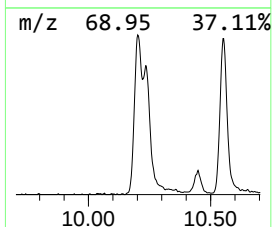
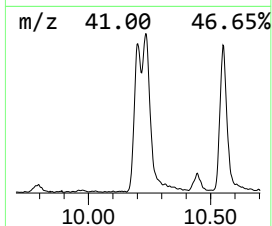
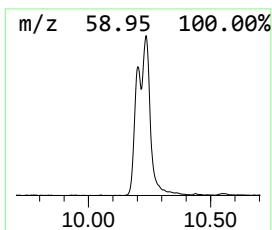
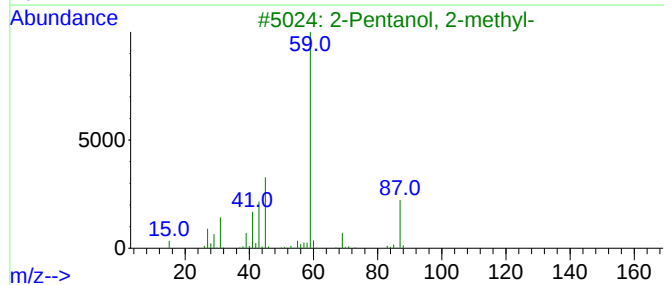
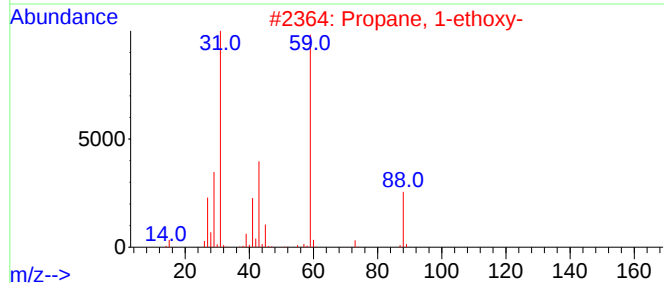
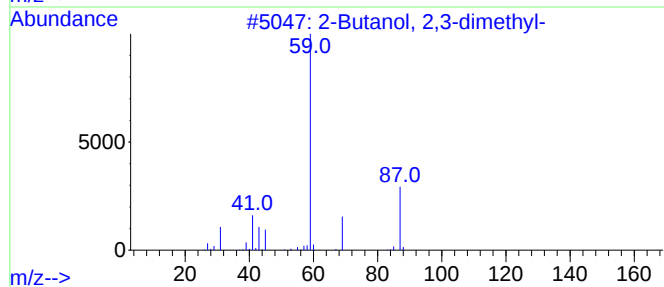
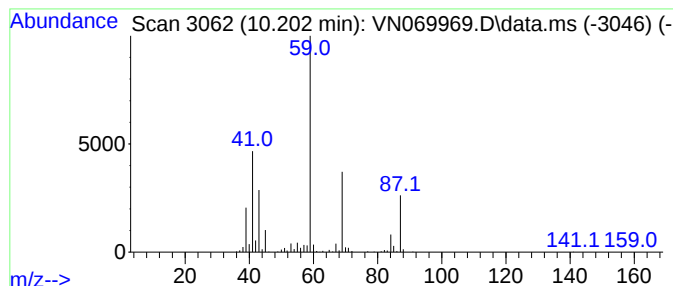
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Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.202	5.81 ug/l	614754	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	83
2		Propane, 1-ethoxy-	88	C5H12O	000628-32-0	58
3		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
4		3-Heptanol	116	C7H16O	000589-82-2	39
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39



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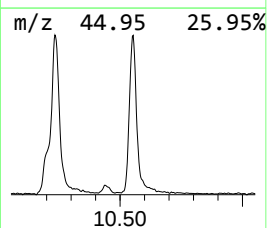
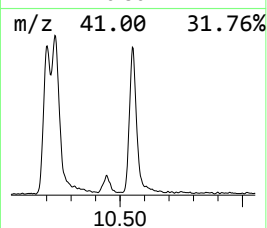
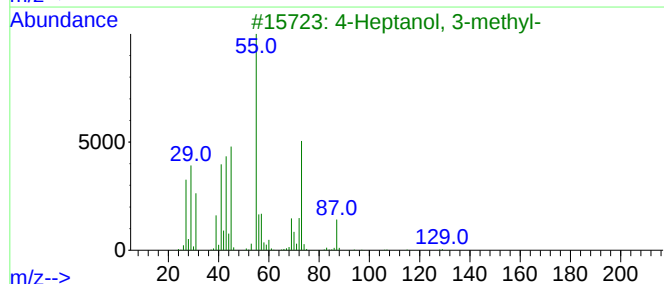
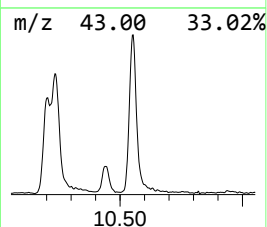
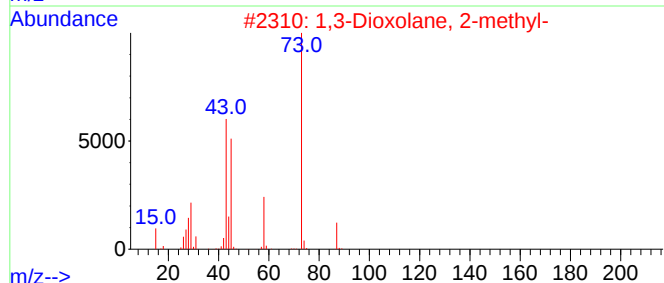
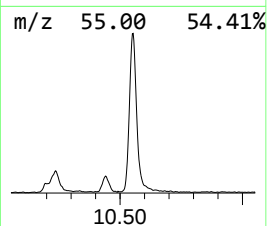
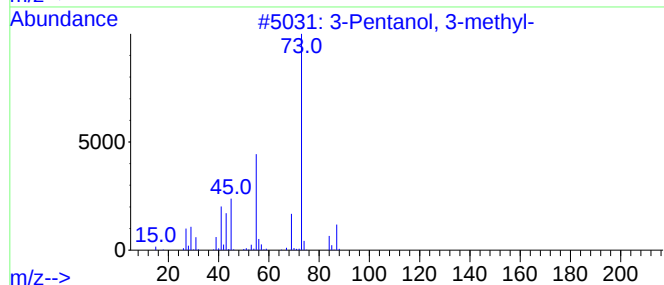
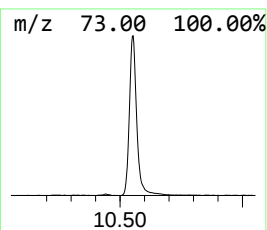
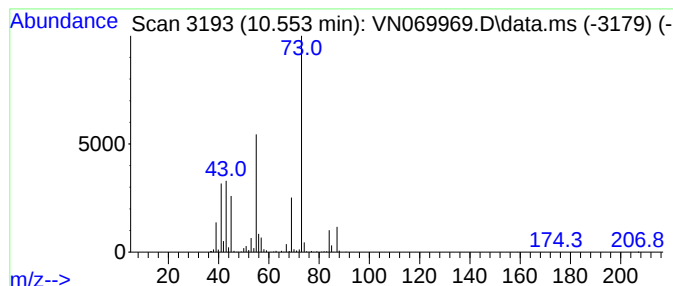
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Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.553	6.60 ug/l	1090180	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	42
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	8.536	50.2	ug/l	5312960	2	8.968	5293410	50.0
2-Butanol, 2,3-...	10.202	5.8	ug/l	614754	2	8.968	5293410	50.0
3-Pentanol, 3-m...	10.553	6.6	ug/l	1090180	3	11.744	8261890	50.0