

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121021\
 Data File : VN069974.D
 Acq On : 10 Dec 2021 21:56
 Operator : JC/MD
 Sample : M4970-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-22

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: VN069974.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.242	85	94	105	rBV6	54098	131153	1.61%	0.239%
2	5.189	1176	1193	1223	rVB2	81622	282341	3.46%	0.515%
3	5.377	1240	1263	1291	rBV3	124480	460559	5.64%	0.840%
4	5.621	1324	1354	1403	rBV2	1273613	4499725	55.13%	8.211%
5	6.501	1652	1682	1709	rVB4	75192	266304	3.26%	0.486%
6	7.847	2166	2184	2201	rVB5	60605	149967	1.84%	0.274%
7	8.024	2227	2250	2261	rBV	884960	2113704	25.90%	3.857%
8	8.086	2262	2273	2306	rVB	1460122	3327227	40.76%	6.071%
9	8.440	2384	2405	2424	rBV	1017667	2459351	30.13%	4.488%
10	8.536	2424	2441	2488	rVB	1672261	4050836	49.63%	7.392%
11	8.968	2581	2602	2632	rBV	2540072	5293638	64.85%	9.659%
12	9.974	2958	2977	2990	rBV4	67450	136110	1.67%	0.248%
13	10.207	3045	3064	3066	rBV3	281430	459640	5.63%	0.839%
14	10.237	3069	3075	3103	rVB3	485968	964690	11.82%	1.760%
15	10.443	3132	3152	3178	rBV	4022934	7600824	93.12%	13.869%
16	10.553	3179	3193	3218	rVB	543527	1096676	13.44%	2.001%
17	11.092	3369	3394	3400	rBV6	51940	115934	1.42%	0.212%
18	11.130	3401	3408	3422	rVV2	81289	148833	1.82%	0.272%
19	11.213	3424	3439	3469	rVB2	144650	342114	4.19%	0.624%
20	11.623	3569	3592	3619	rBV4	93020	269836	3.31%	0.492%
21	11.746	3619	3638	3668	rVV	4437288	8162287	100.00%	14.894%
22	11.864	3669	3682	3706	rVB5	80463	204934	2.51%	0.374%
23	12.733	3988	4006	4035	rBV	3362583	5945730	72.84%	10.849%
24	13.675	4340	4357	4384	rBV	3632206	6320632	77.44%	11.533%

Sum of corrected areas: 54803045

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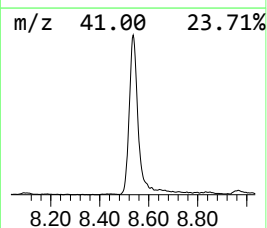
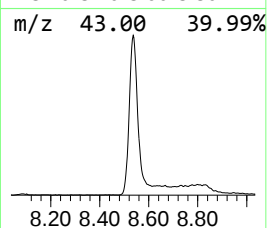
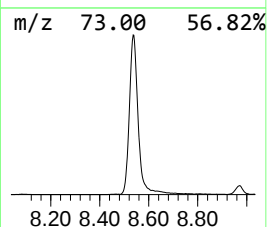
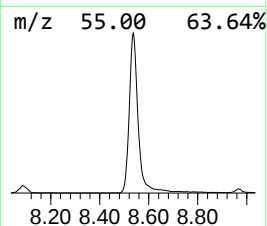
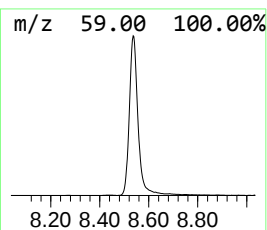
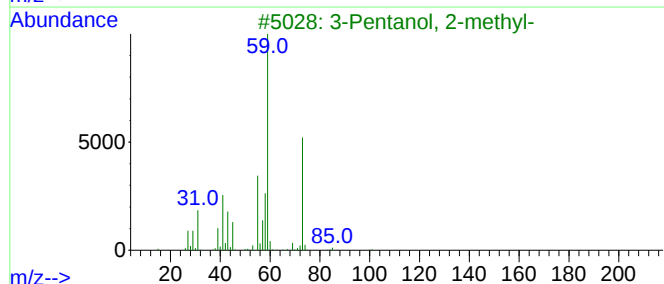
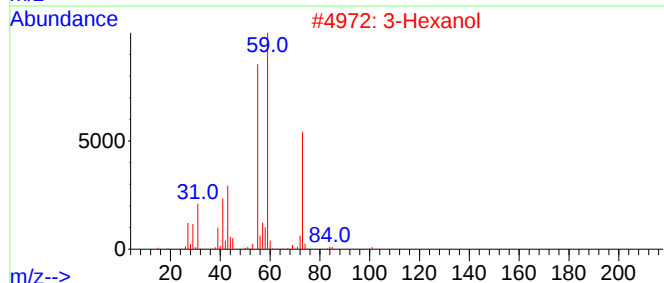
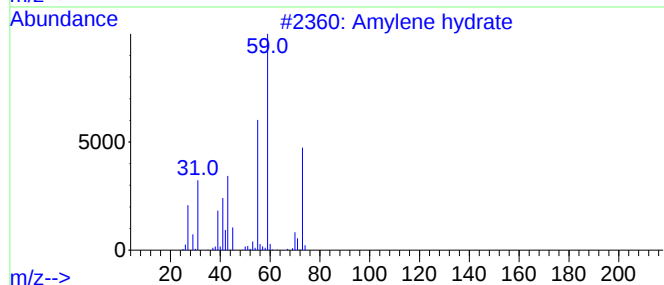
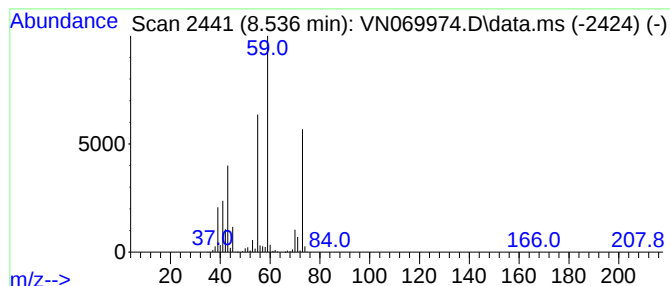
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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	38.26 ug/l	4050840	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-Hexanol	102	C6H14O	000623-37-0	38
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	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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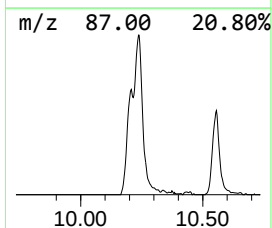
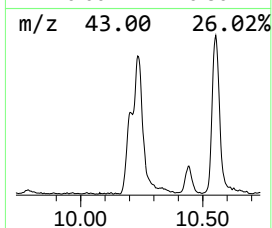
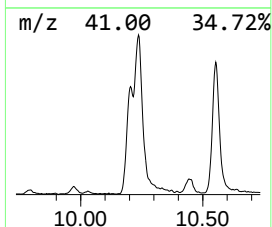
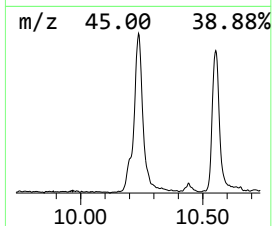
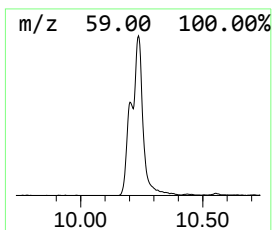
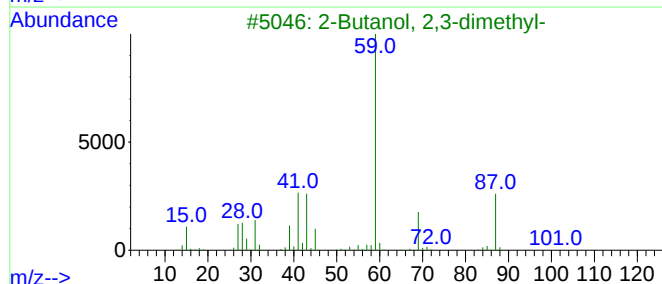
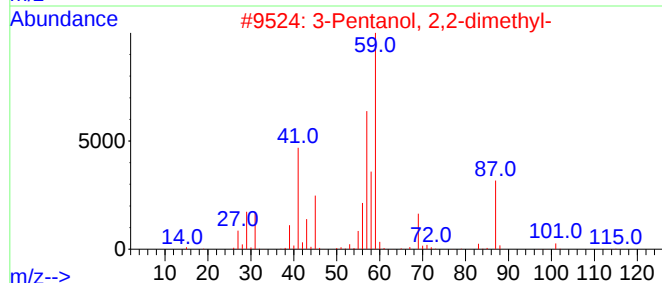
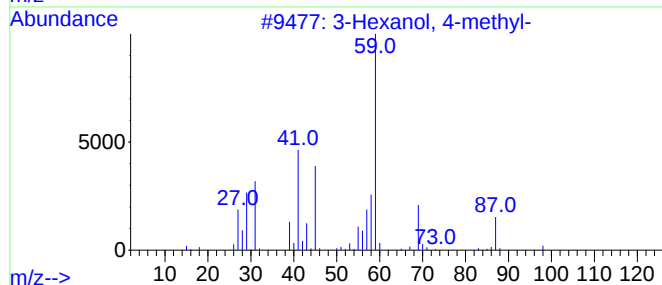
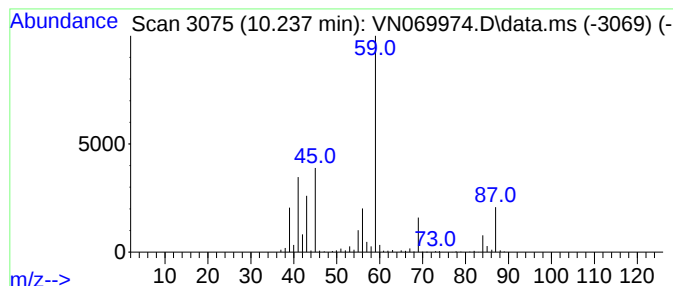
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Peak Number 2 3-Hexanol, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.236	9.11 ug/l	964690	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	50
2			3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40
3			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	40
4			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	40
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	37



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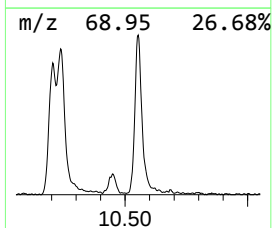
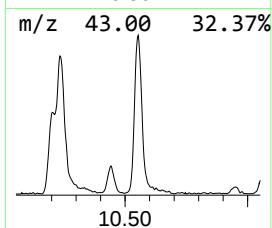
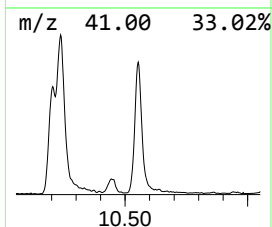
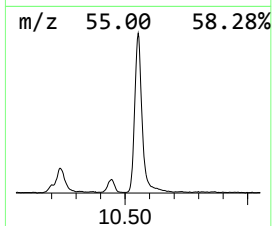
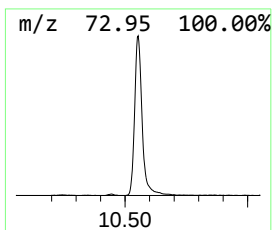
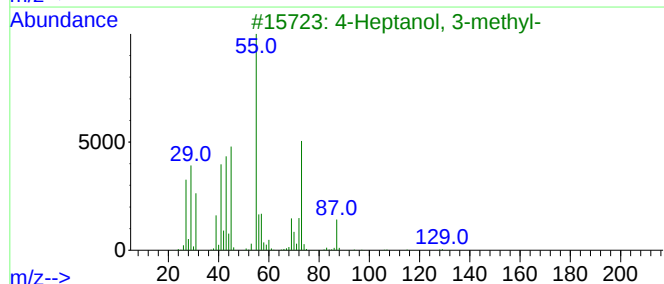
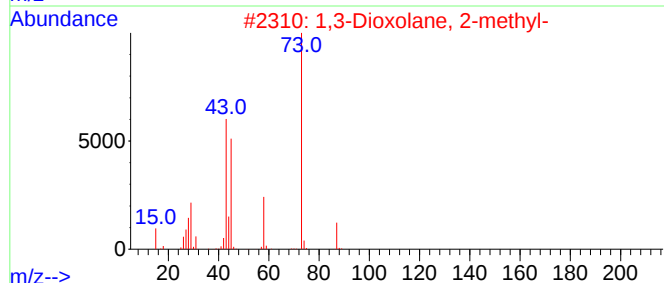
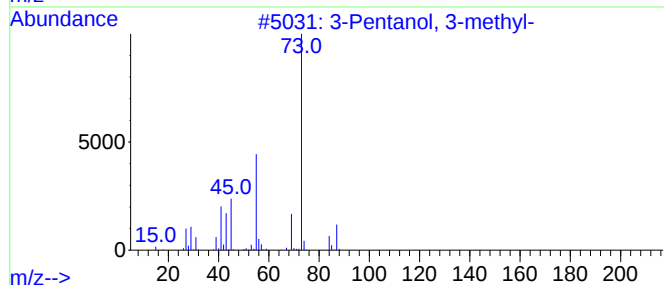
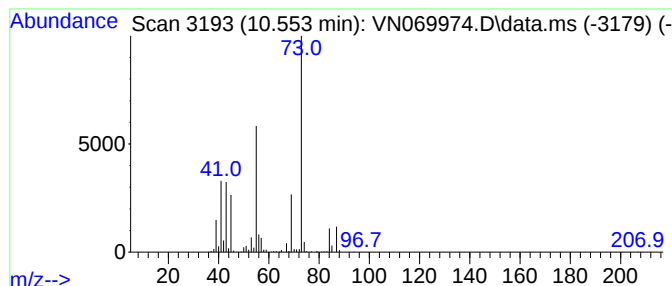
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Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.553	6.72 ug/l	1096680	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	64
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	42
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	8.536	38.3	ug/l	4050840	2	8.968	5293640	50.0
3-Hexanol, 4-me...	10.236	9.1	ug/l	964690	2	8.968	5293640	50.0
3-Pentanol, 3-m...	10.553	6.7	ug/l	1096680	3	11.746	8162290	50.0