

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
 Data File : VN066194.D
 Acq On : 12 Mar 2021 20:06
 Operator : JC/MD
 Sample : M1647-22
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP3-30788:89

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\82N031221W.M
 Title : SW846 8260

Signal : TIC: VN066194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.783	25	35	53	rVB3	81677	115933	4.71%	0.588%
2	1.966	93	103	115	rBV2	16183	25999	1.06%	0.132%
3	2.121	152	161	176	rBV3	37144	66214	2.69%	0.336%
4	2.274	206	218	236	rVB	198198	307907	12.52%	1.561%
5	3.205	550	565	583	rBV3	31880	80426	3.27%	0.408%
6	3.629	709	723	739	rVB2	16835	38423	1.56%	0.195%
7	3.741	749	765	783	rBV2	102782	254070	10.33%	1.288%
8	4.243	935	952	973	rVB2	44751	120185	4.89%	0.609%
9	4.696	1100	1121	1123	rBV7	26622	46583	1.89%	0.236%
10	5.849	1530	1551	1552	rBV3	31861	52903	2.15%	0.268%
11	6.453	1748	1776	1800	rBV2	289107	863856	35.11%	4.381%
12	6.745	1866	1885	1893	rBV2	17236	39937	1.62%	0.203%
13	7.509	2149	2170	2184	rBV2	303368	756314	30.74%	3.835%
14	7.587	2185	2199	2227	rVB	580654	1360271	55.29%	6.898%
15	7.957	2312	2337	2363	rBV5	633524	1674368	68.06%	8.491%
16	8.515	2526	2545	2574	rBV	883846	1813681	73.72%	9.197%
17	8.727	2605	2624	2641	rBV3	79364	183980	7.48%	0.933%
18	9.102	2749	2764	2784	rVB2	29555	65746	2.67%	0.333%
19	9.926	3057	3071	3083	rBV5	13459	25187	1.02%	0.128%
20	10.030	3090	3110	3123	rBV	1356155	2460206	100.00%	12.476%
21	10.092	3124	3133	3153	rVB	239128	446246	18.14%	2.263%
22	10.816	3390	3403	3421	rVB	165094	302477	12.29%	1.534%
23	11.350	3583	3602	3630	rBV	1209802	2264042	92.03%	11.481%
24	11.452	3632	3640	3655	rVB2	33228	61161	2.49%	0.310%
25	11.562	3668	3681	3699	rVB2	123315	229900	9.34%	1.166%
26	11.693	3717	3730	3749	rVB8	45389	92230	3.75%	0.468%
27	11.892	3793	3804	3817	rVV4	67871	136476	5.55%	0.692%
28	12.128	3883	3892	3902	rBV4	20089	33217	1.35%	0.168%
29	12.345	3958	3973	3994	rBV	814752	1399646	56.89%	7.098%
30	12.616	4064	4074	4091	rVB9	27113	61390	2.50%	0.311%
31	12.771	4120	4132	4135	rBV8	27183	42537	1.73%	0.216%
32	12.860	4152	4165	4191	rBV	194297	356451	14.49%	1.808%
33	12.978	4193	4209	4220	rVV	23928	60234	2.45%	0.305%
34	13.053	4226	4237	4252	rBV	107190	188913	7.68%	0.958%
35	13.144	4263	4271	4279	rBV3	30883	53400	2.17%	0.271%
36	13.195	4283	4290	4310	rVV4	83691	151714	6.17%	0.769%

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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

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37	13.286	4311	4324	4346	rVB	853523	1445315	58.75%	7.329%
38	13.396	4352	4365	4390	rBV	818654	1530996	62.23%	7.764%
39	15.067	4970	4988	4998	rBV4	189152	511027	20.77%	2.591%

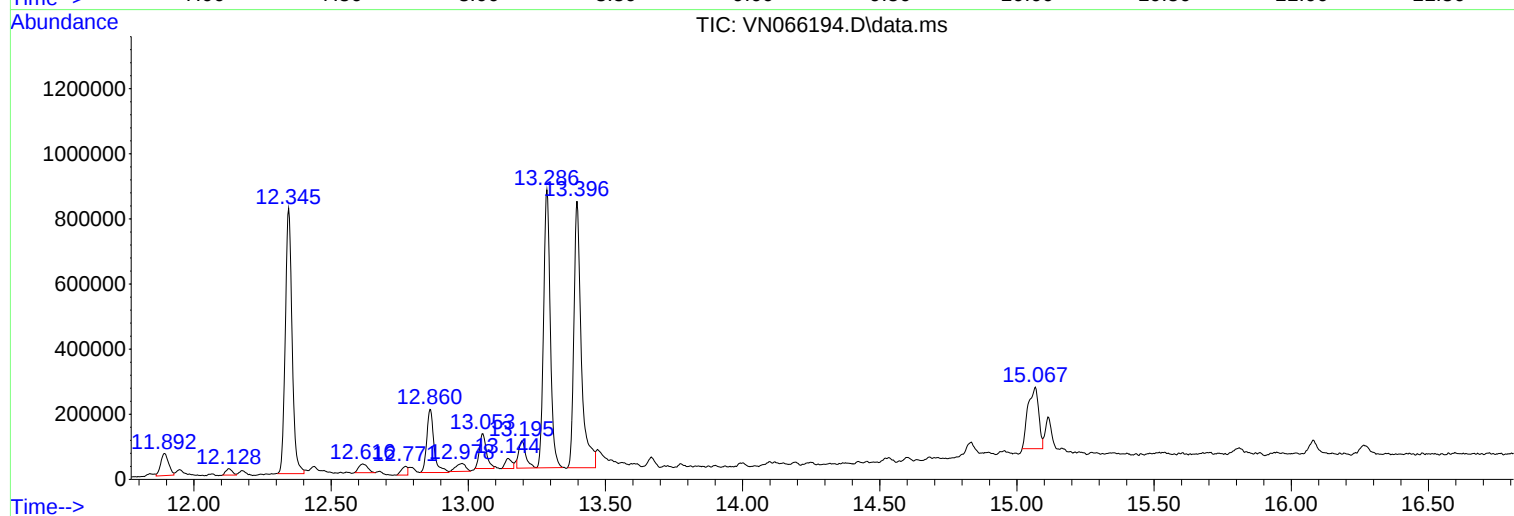
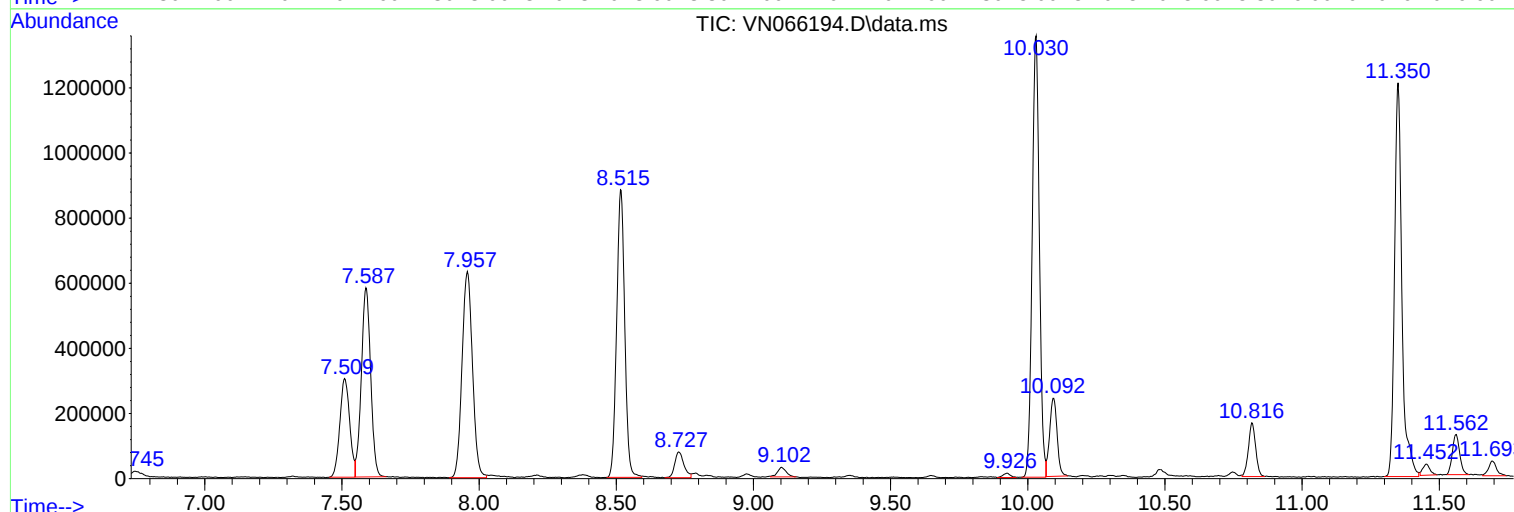
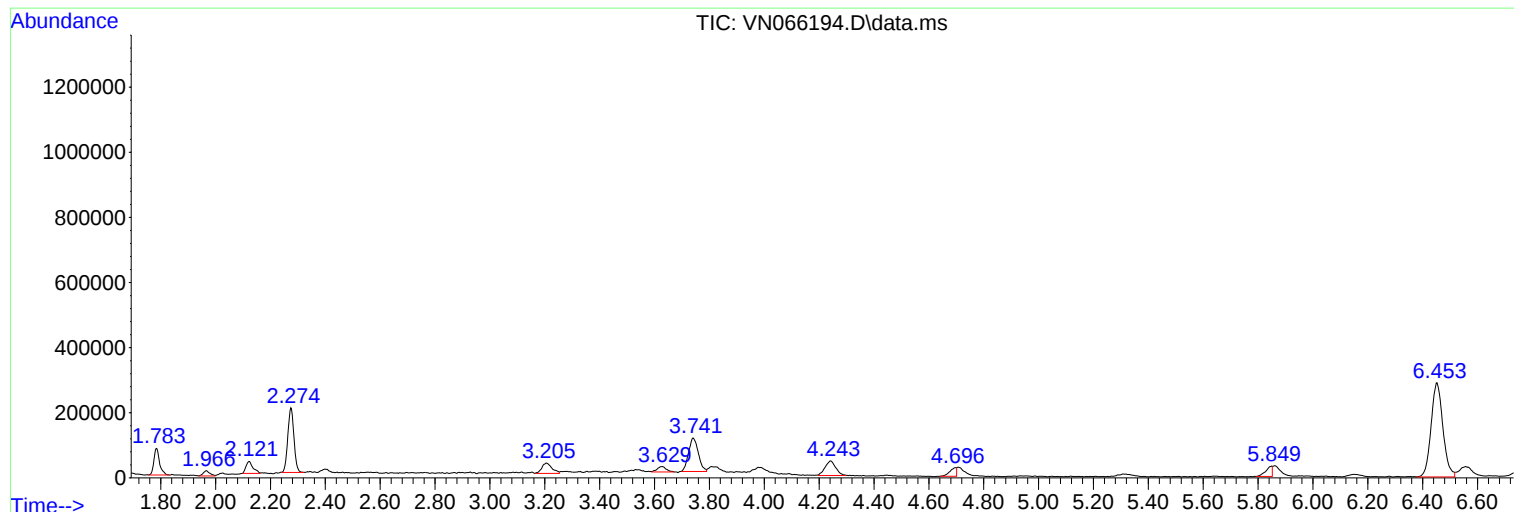
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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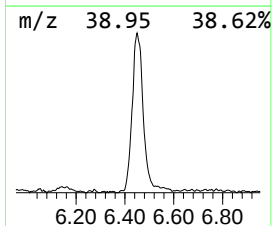
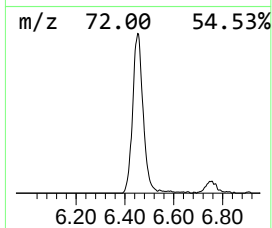
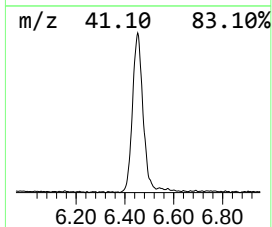
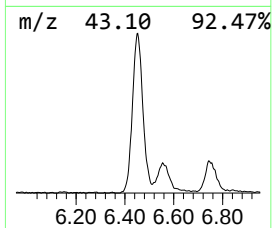
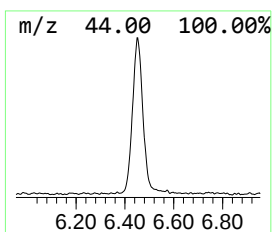
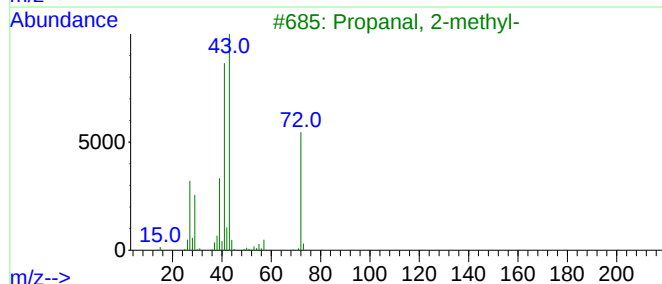
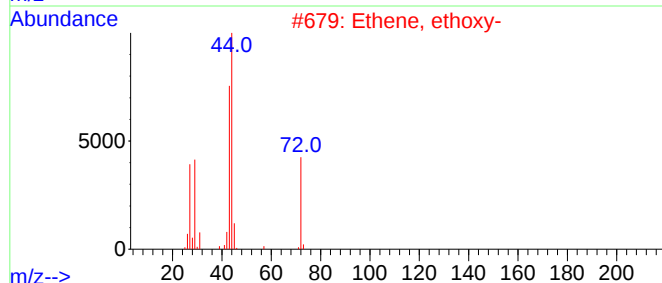
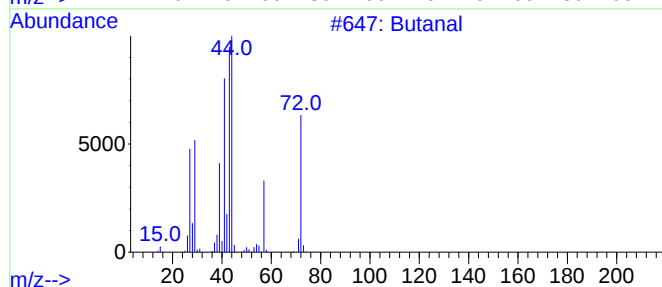
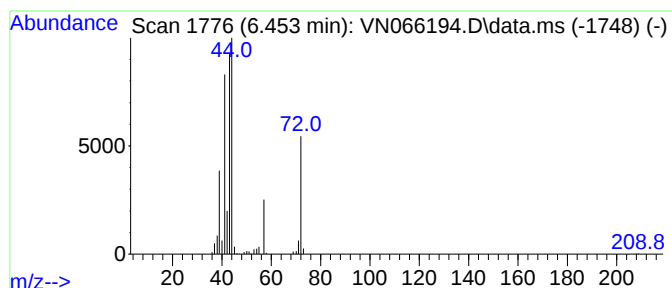
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.453	31.75 ug/l	863856	Pentafluorobenzene	7.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	90
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5			Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	17



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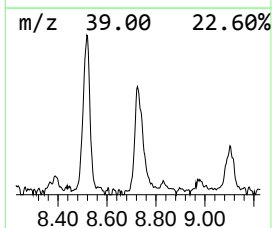
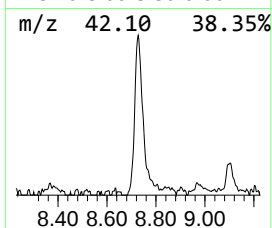
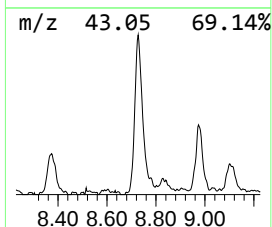
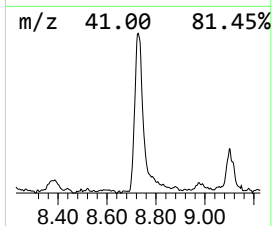
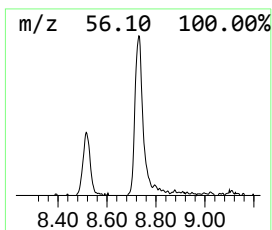
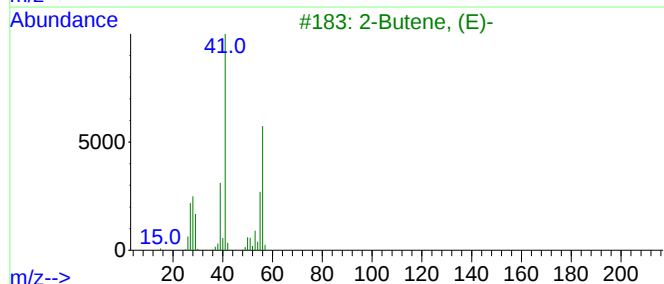
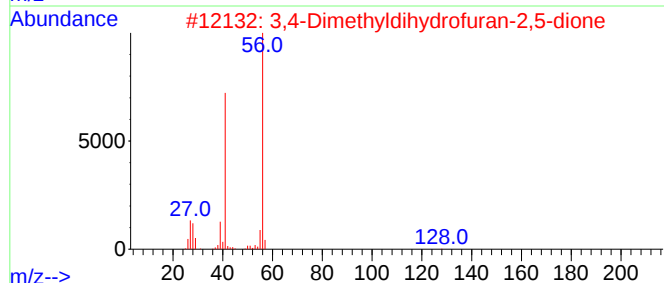
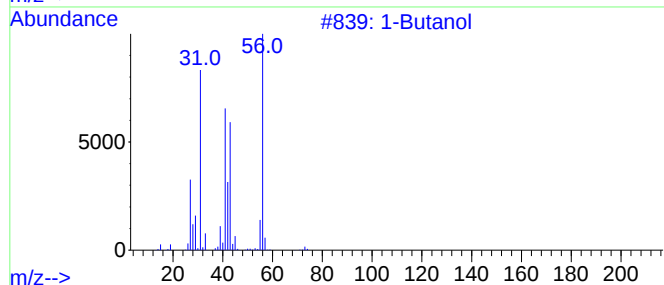
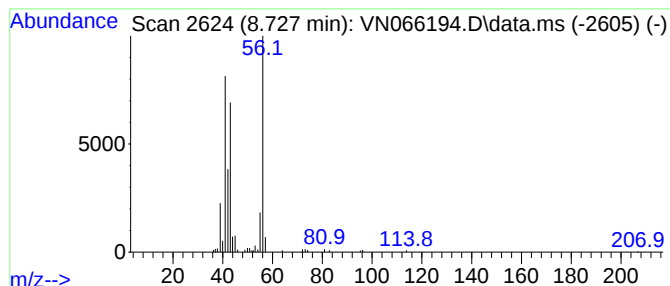
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Peak Number 3 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.727	5.07 ug/l	183980	1,4-Difluorobenzene	8.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	86
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
3			2-Butene, (E)-	56	C4H8	000624-64-6	40
4			1-Hexanol	102	C6H14O	000111-27-3	40
5			Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	40



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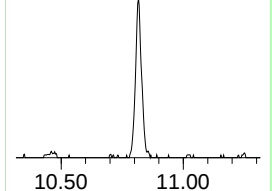
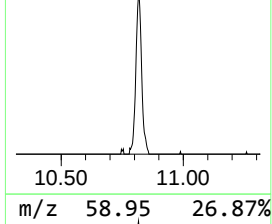
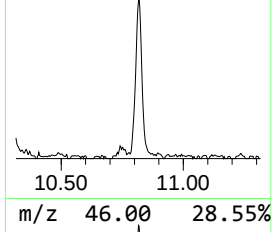
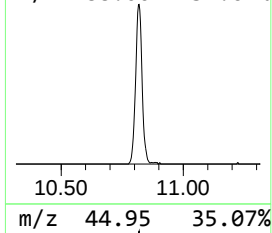
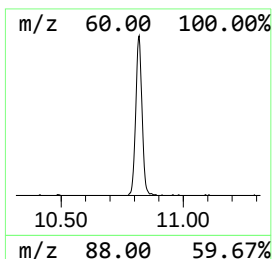
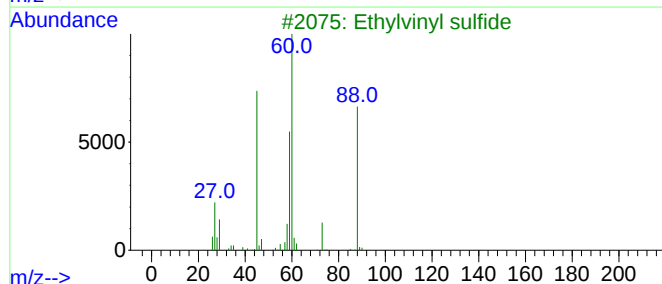
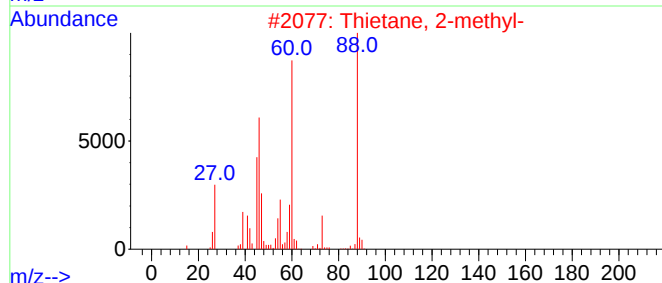
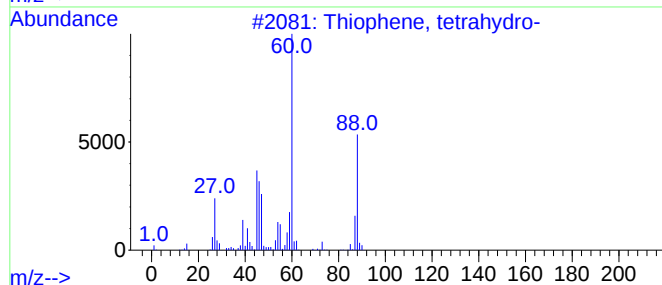
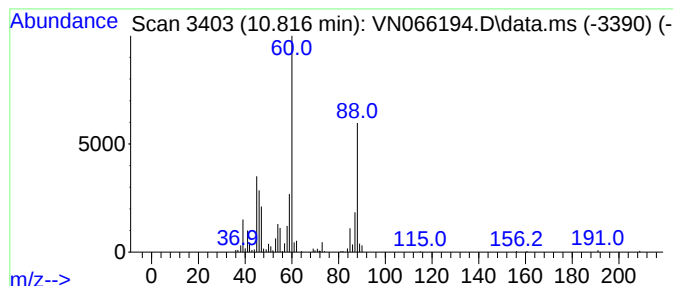
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophene, tetrahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	6.68 ug/l	302477	Chlorobenzene-d5	11.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4			Ethenol, 2-ethoxy-, acetate	130	C6H10O3	089489-60-1	28
5			Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	25



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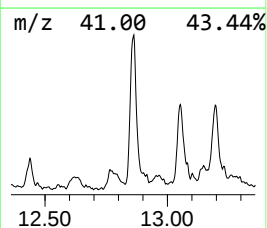
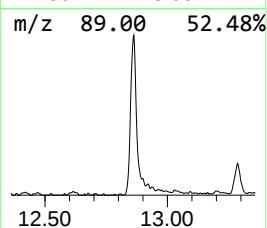
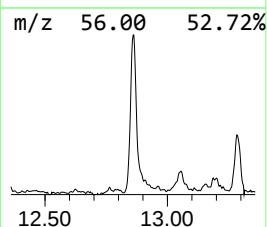
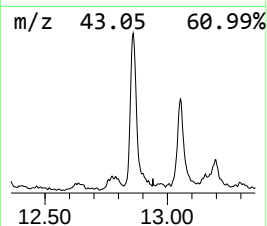
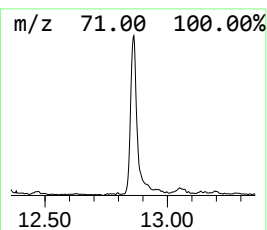
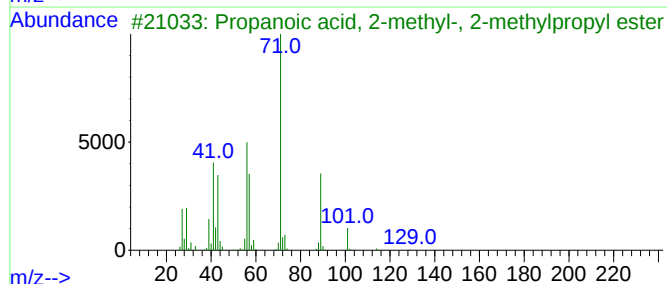
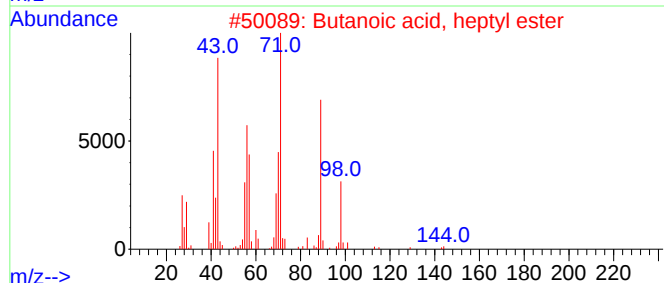
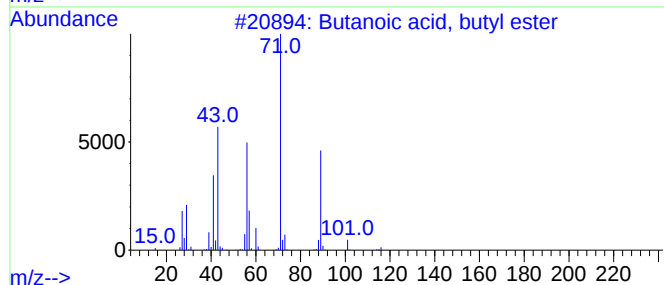
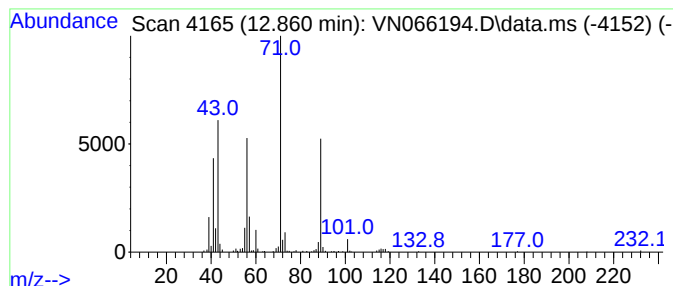
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Peak Number 5 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.860	12.33 ug/l	356451	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56



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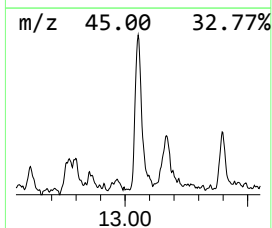
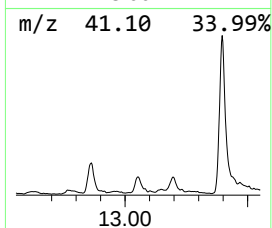
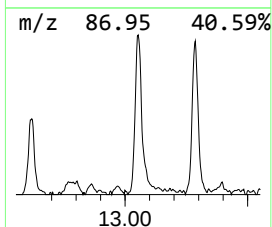
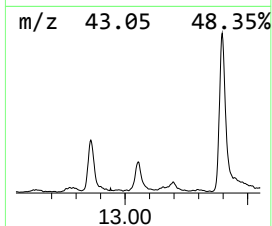
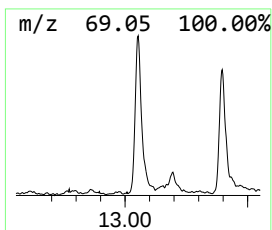
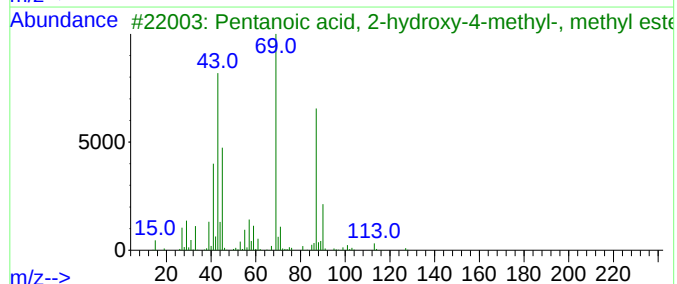
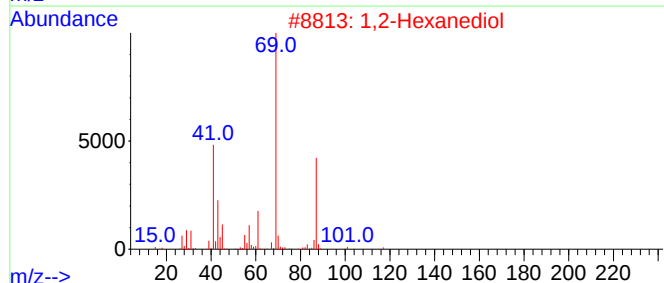
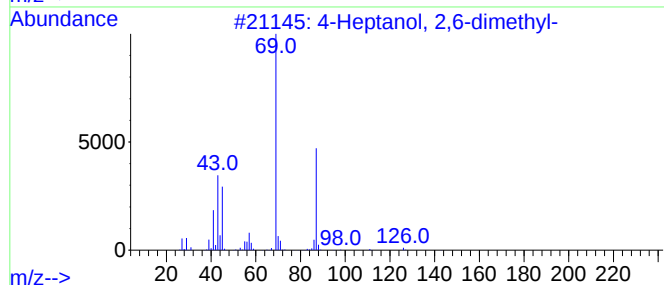
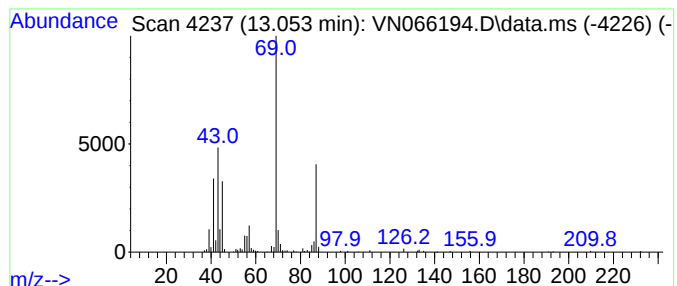
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4-Heptanol, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.053	6.54 ug/l	188913	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2			1,2-Hexanediol	118	C6H14O2	006920-22-5	78
3			Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	78
4			5-Nonanol	144	C9H20O	000623-93-8	78
5			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066194.D
Acq On : 12 Mar 2021 20:06
Operator : JC/MD
Sample : M1647-22
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP3-30788:89

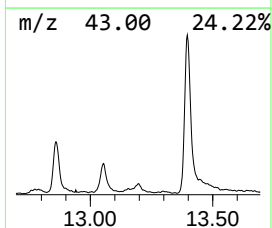
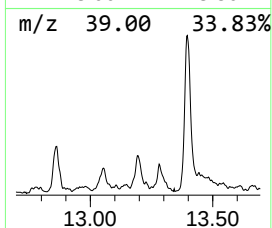
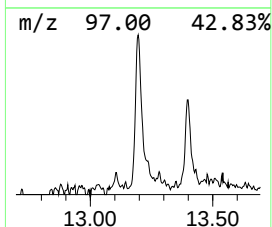
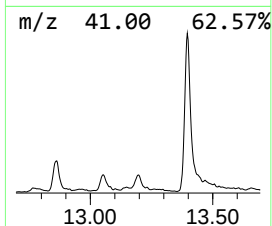
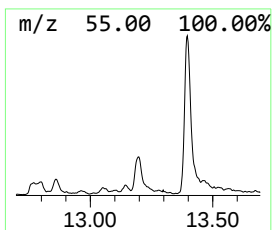
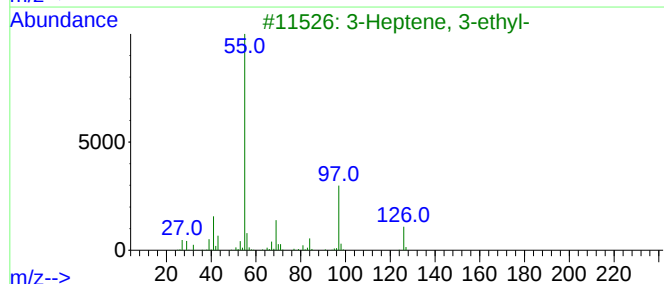
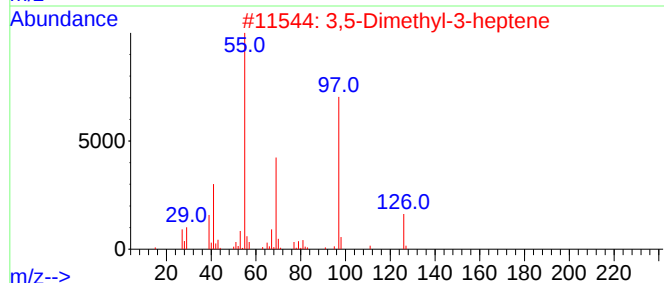
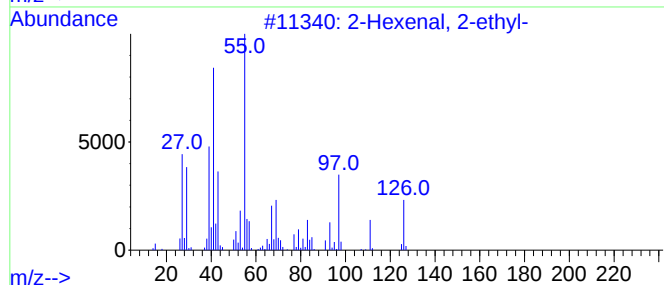
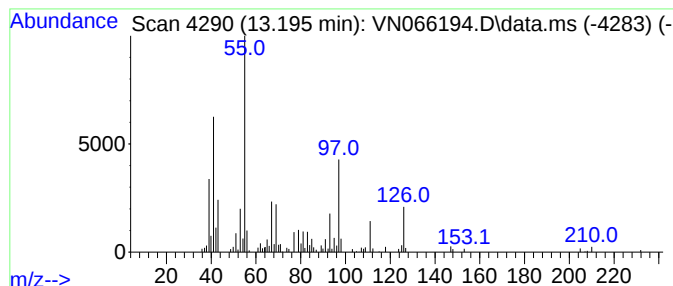
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Hexenal, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.195	5.25 ug/l	151714	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	83
2			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	47
3			3-Heptene, 3-ethyl-	126	C9H18	074764-46-8	47
4			2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	47
5			Cycloheptane, bromo-	176	C7H13Br	002404-35-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066194.D
Acq On : 12 Mar 2021 20:06
Operator : JC/MD
Sample : M1647-22
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP3-30788:89

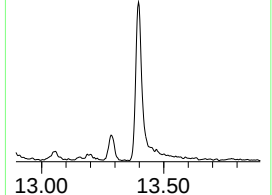
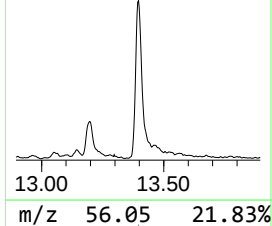
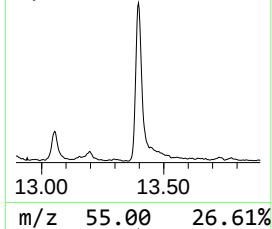
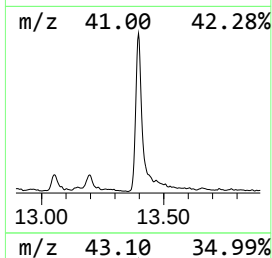
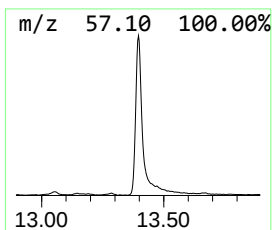
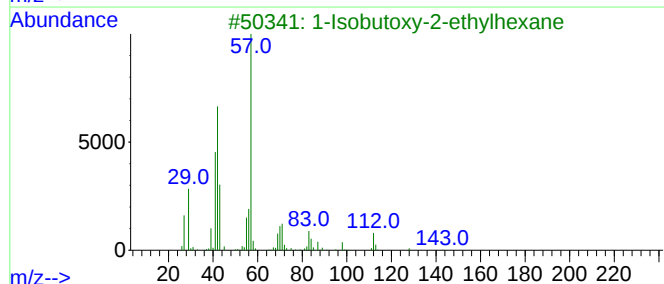
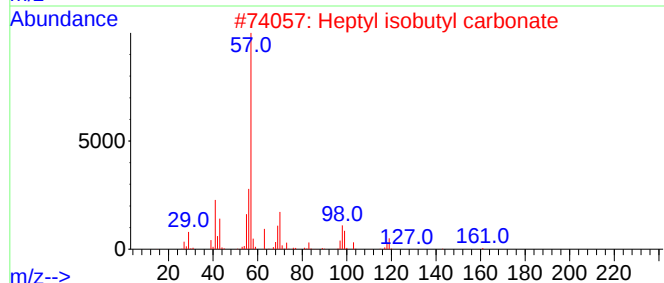
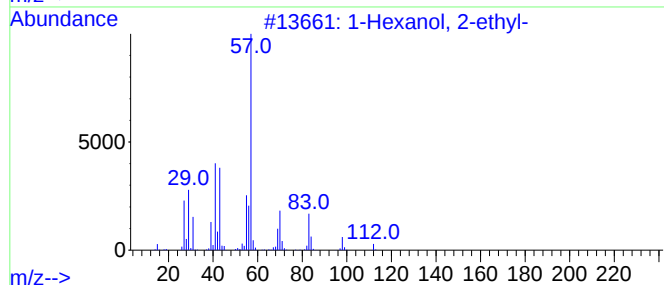
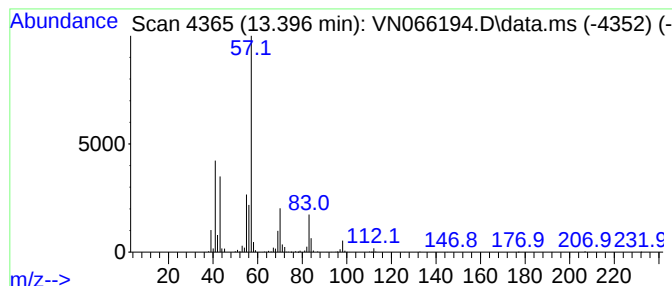
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	52.96 ug/l	1531000	1,4-Dichlorobenzene-d4	13.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			2-Propyl-1-pentanol, methyl ether	144	C9H20O	1000365-12-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066194.D
Acq On : 12 Mar 2021 20:06
Operator : JC/MD
Sample : M1647-22
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP3-30788:89

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	6.453	31.8	ug/l	863856	1	7.587	1360270	50.0
1-Butanol	8.727	5.1	ug/l	183980	2	8.518	1813680	50.0
Thiophene, tetr...	10.816	6.7	ug/l	302477	3	11.350	2264040	50.0
Butanoic acid, ...	12.860	12.3	ug/l	356451	4	13.286	1445320	50.0
4-Heptanol, 2,6...	13.053	6.5	ug/l	188913	4	13.286	1445320	50.0
2-Hexenal, 2-et...	13.195	5.3	ug/l	151714	4	13.286	1445320	50.0
1-Hexanol, 2-et...	13.396	53.0	ug/l	1531000	4	13.286	1445320	50.0