

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042523\
 Data File : VN077472.D
 Acq On : 25 Apr 2023 16:20
 Operator : JC\MD
 Sample : 02460-06 40X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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\82N042423W.M
 Title : SW846 8260

Signal : TIC: VN077472.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.519	94	99	106	rVB2	23620	41545	1.36%	0.209%
2	2.831	144	152	160	rVB4	38415	107728	3.52%	0.542%
3	3.254	214	224	238	rVB	344003	861795	28.15%	4.334%
4	3.648	283	291	302	rVB2	45966	119253	3.90%	0.600%
5	4.437	410	425	440	rBV5	37699	135025	4.41%	0.679%
6	5.295	558	571	574	rBV5	61483	211335	6.90%	1.063%
7	5.354	574	581	596	rVB5	103430	386873	12.64%	1.945%
8	5.819	647	660	673	rBV3	97305	339745	11.10%	1.708%
9	6.313	735	744	746	rBV3	21092	39832	1.30%	0.200%
10	7.083	868	875	885	rBV6	12802	34663	1.13%	0.174%
11	7.236	891	901	908	rBV5	21588	64825	2.12%	0.326%
12	7.336	908	918	926	rBV3	87063	239565	7.83%	1.205%
13	8.013	1026	1033	1042	rVB7	15623	39236	1.28%	0.197%
14	8.172	1049	1060	1065	rBV2	420971	1030206	33.66%	5.180%
15	8.230	1065	1070	1081	rVV	756645	1780064	58.15%	8.951%
16	8.336	1081	1088	1098	rVB2	75879	197568	6.45%	0.993%
17	8.454	1101	1108	1115	rBV3	38710	81115	2.65%	0.408%
18	8.583	1121	1130	1141	rVB	412984	940741	30.73%	4.730%
19	8.725	1145	1154	1158	rBV4	36619	84055	2.75%	0.423%
20	8.860	1172	1177	1185	rVB6	33571	76767	2.51%	0.386%
21	9.107	1208	1219	1241	rBV	1104121	2332092	76.19%	11.727%
22	9.607	1289	1304	1314	rBV2	90456	269029	8.79%	1.353%
23	9.783	1327	1334	1340	rVB4	16486	32931	1.08%	0.166%
24	10.013	1368	1373	1381	rVB4	26363	51426	1.68%	0.259%
25	10.101	1383	1388	1392	rBV3	23380	48109	1.57%	0.242%
26	10.154	1392	1397	1402	rVB5	37274	66821	2.18%	0.336%
27	10.571	1460	1468	1482	rBV	1603353	3061033	100.00%	15.392%
28	10.989	1533	1539	1548	rVB5	31490	85985	2.81%	0.432%
29	11.866	1681	1688	1701	rBV	1410659	2585910	84.48%	13.003%
30	11.971	1701	1706	1710	rVB3	25355	47334	1.55%	0.238%
31	12.695	1822	1829	1838	rBV	40842	68960	2.25%	0.347%
32	12.854	1848	1856	1866	rBV	1001486	1766439	57.71%	8.882%
33	13.042	1882	1888	1895	rVB2	102432	176235	5.76%	0.886%
34	13.618	1976	1986	1992	rBV2	27496	53472	1.75%	0.269%
35	13.795	2009	2016	2026	rVB	1161317	1977680	64.61%	9.945%
36	13.954	2036	2043	2047	rBV3	32071	54980	1.80%	0.276%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Title : SW846 8260

37	13.995	2047	2050	2055	rVV	32622	54770	1.79%	0.275%
38	14.059	2055	2061	2066	rVV5	24948	58459	1.91%	0.294%
39	14.330	2102	2107	2114	rVB3	37160	62884	2.05%	0.316%
40	14.448	2122	2127	2133	rVB2	49396	86982	2.84%	0.437%
41	14.930	2204	2209	2215	rVB3	22624	38530	1.26%	0.194%
42	15.048	2221	2229	2238	rBV5	27335	58578	1.91%	0.295%
43	15.589	2316	2321	2325	rBV2	21031	36218	1.18%	0.182%

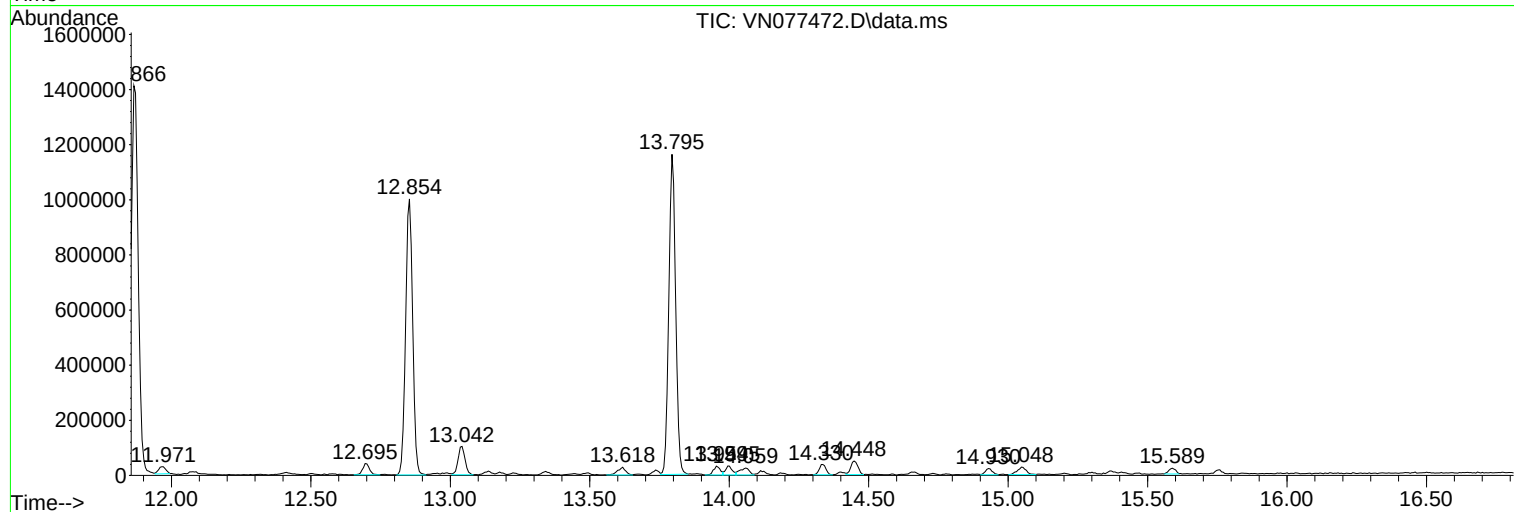
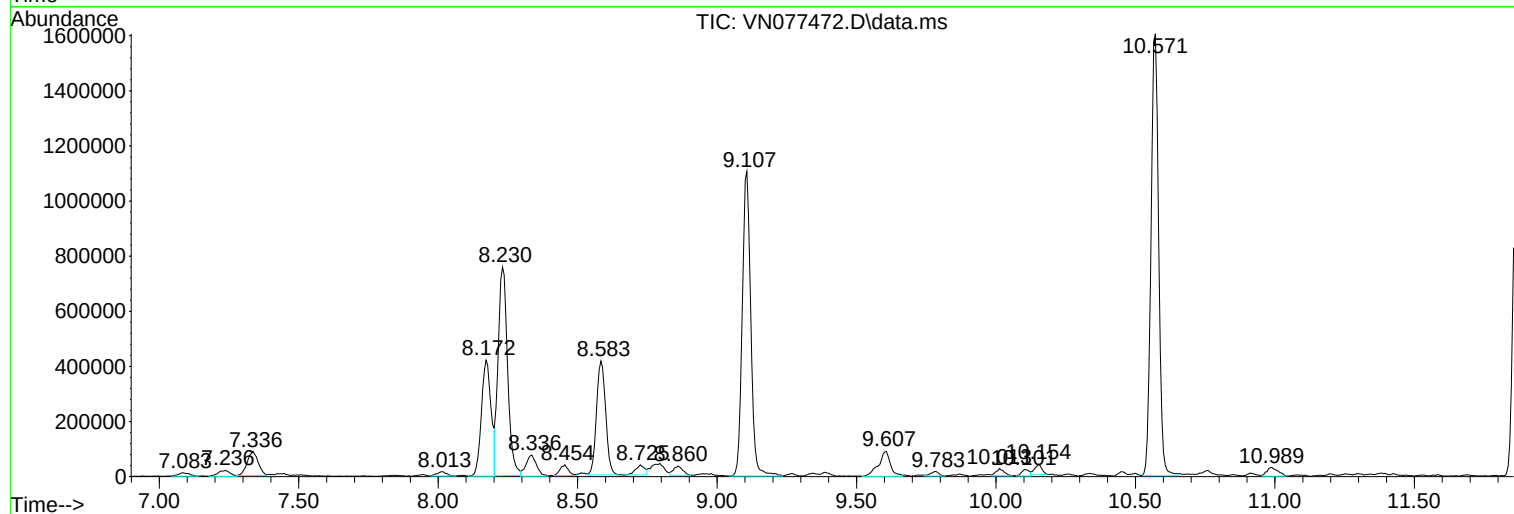
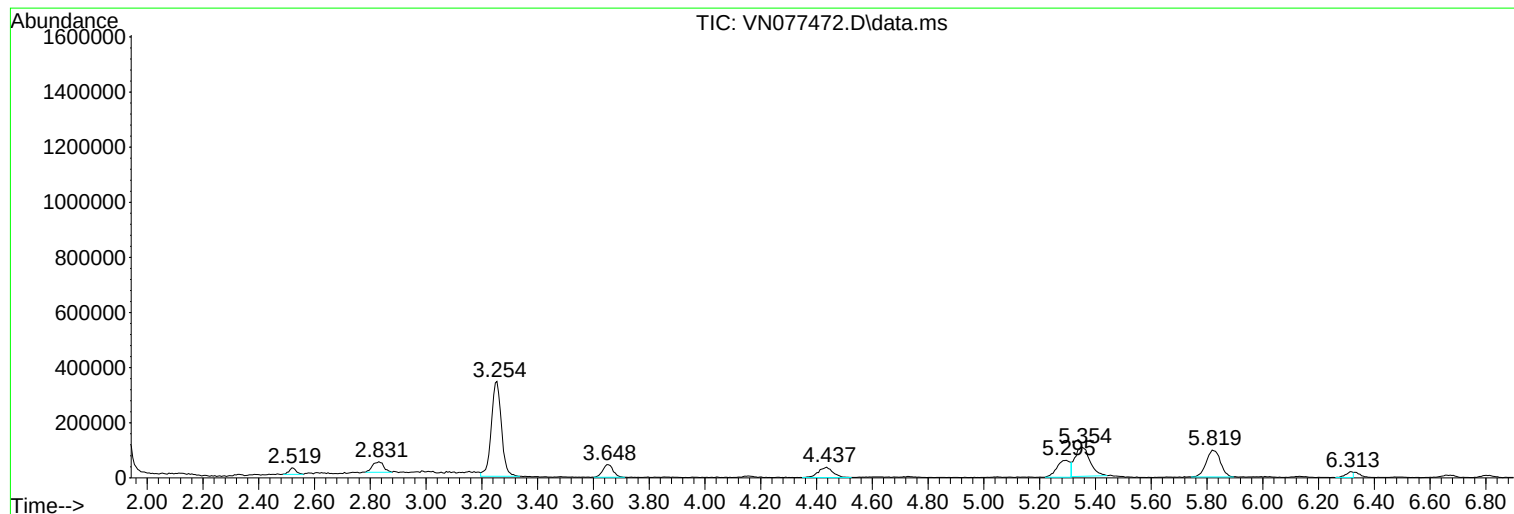
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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



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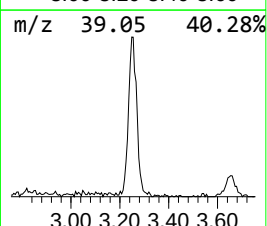
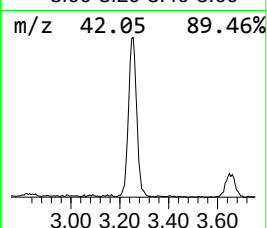
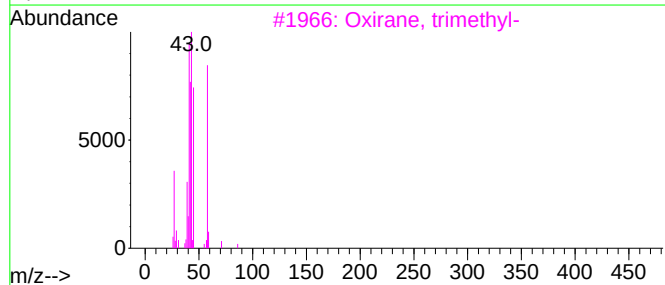
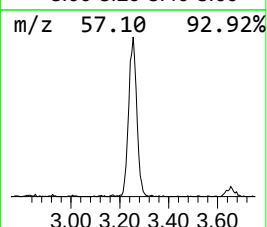
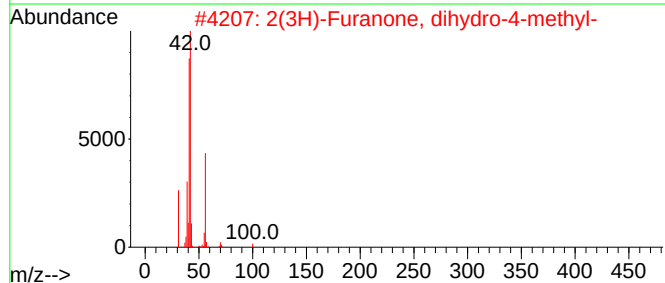
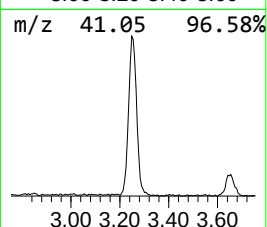
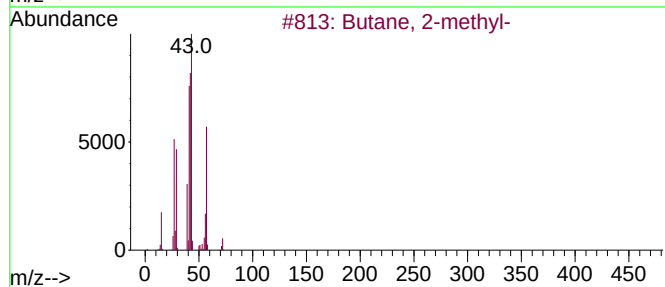
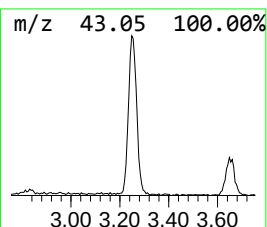
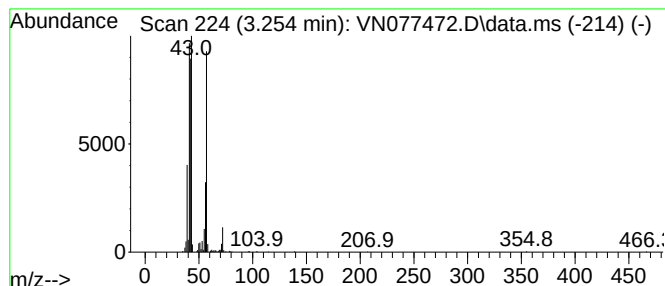
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.254	24.21 ug/l	861795	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	53
2			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	38
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	37
4			3-Buten-1-ol	72	C4H8O	000627-27-0	35
5			1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	35



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

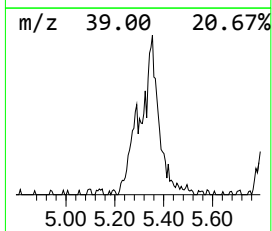
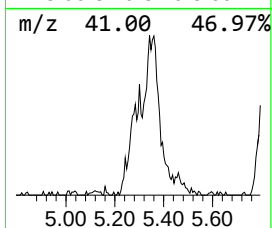
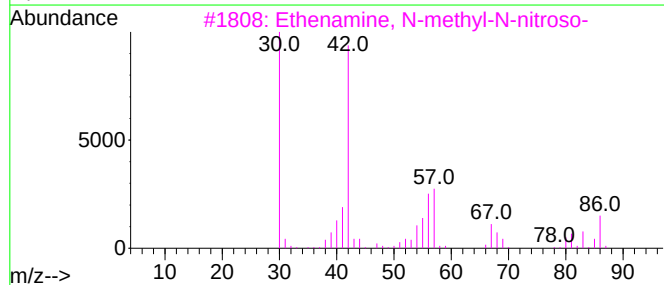
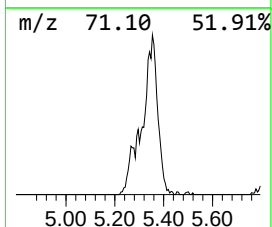
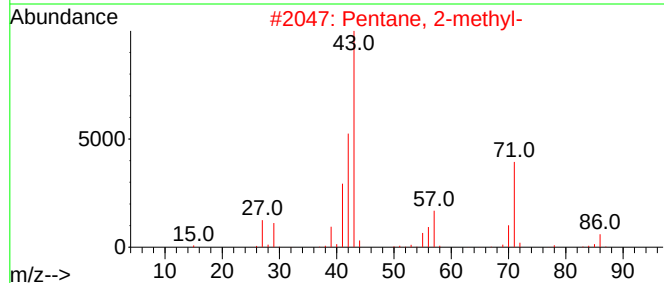
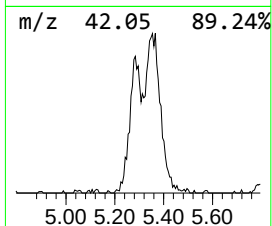
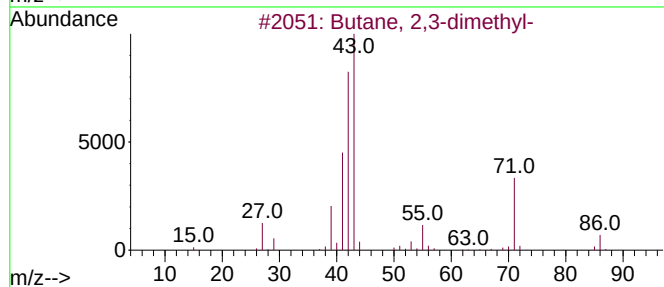
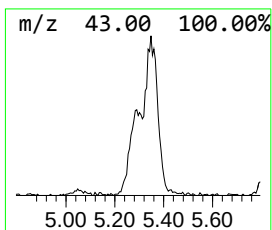
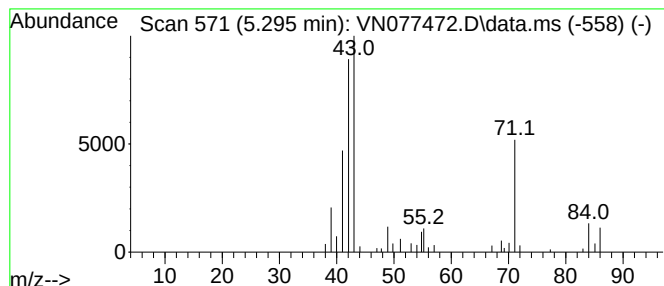
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.295	5.94 ug/l	211335	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-			86	C6H14	000079-29-8	80
2	Pentane, 2-methyl-			86	C6H14	000107-83-5	59
3	Ethenamine, N-methyl-N-nitroso-			86	C3H6N2O	004549-40-0	37
4	1,2,3-Trimethyldiaziridine			86	C4H10N2	113604-56-1	36
5	Cyclobutane, methyl-			70	C5H10	000598-61-8	35



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

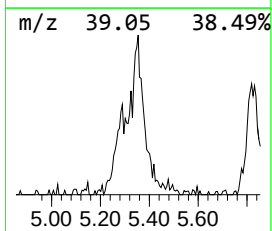
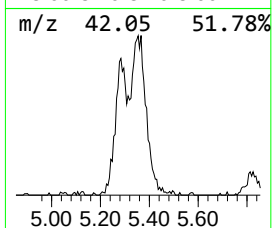
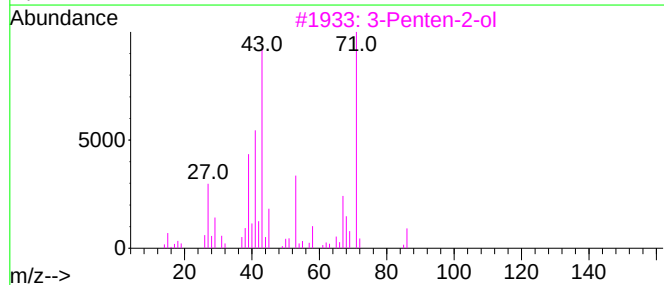
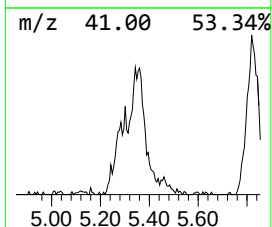
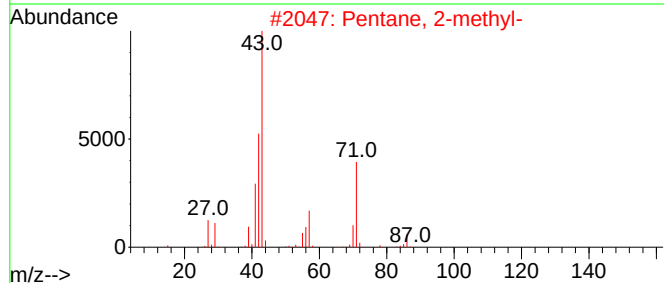
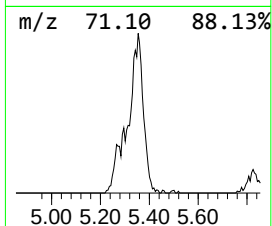
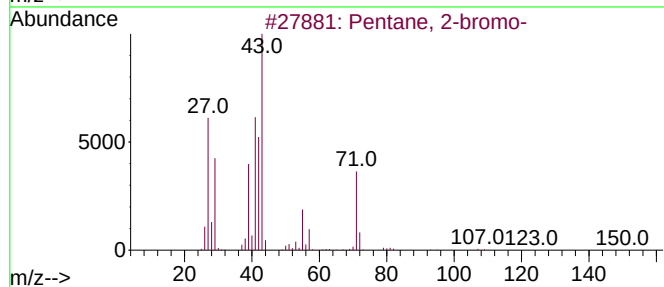
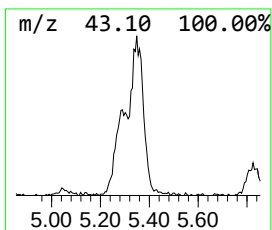
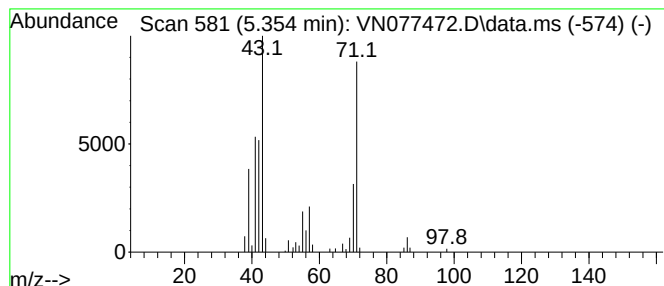
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2-bromo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.354	10.87 ug/l	386873	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	50
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	46
3			3-Penten-2-ol	86	C5H10O	001569-50-2	42
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	40
5			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	38



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1

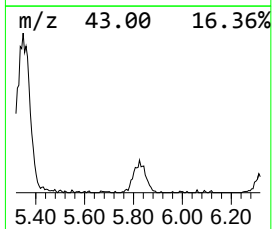
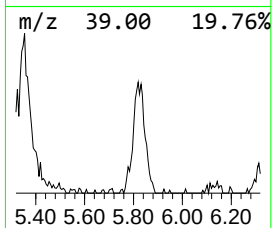
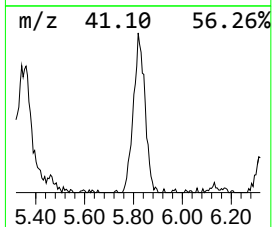
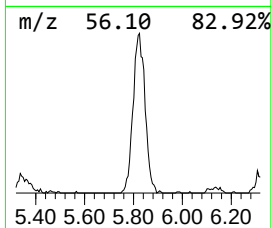
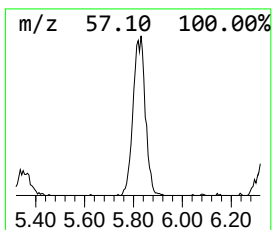
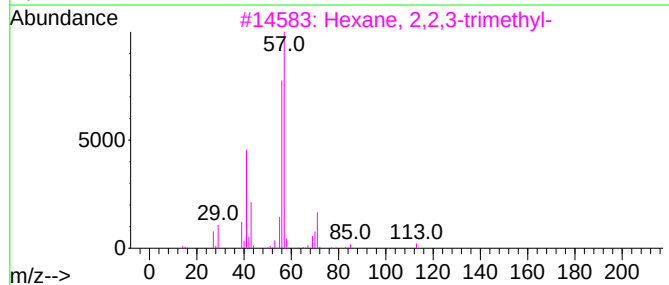
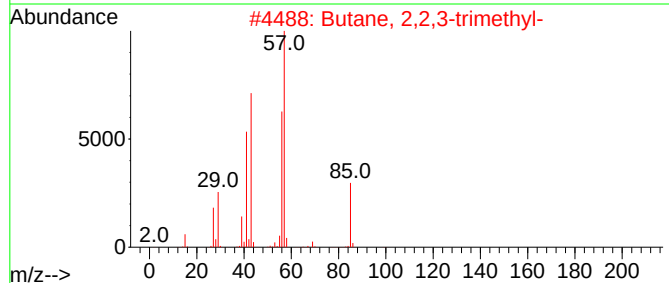
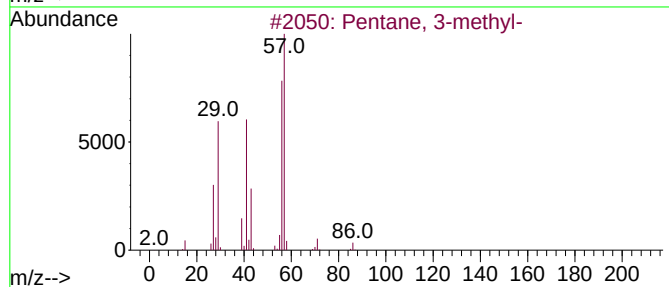
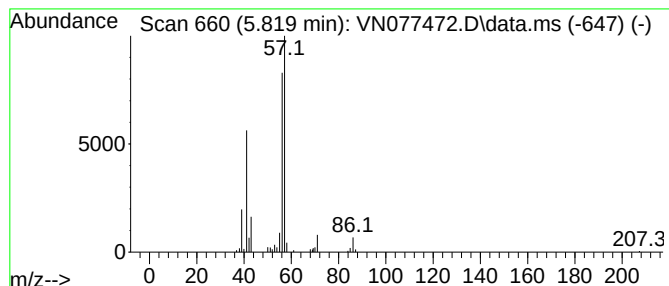
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.819	9.54 ug/l	339745	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	64



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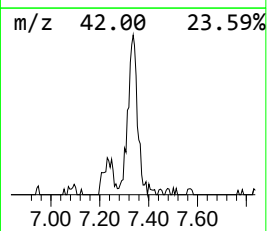
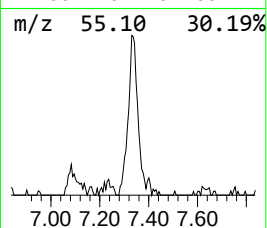
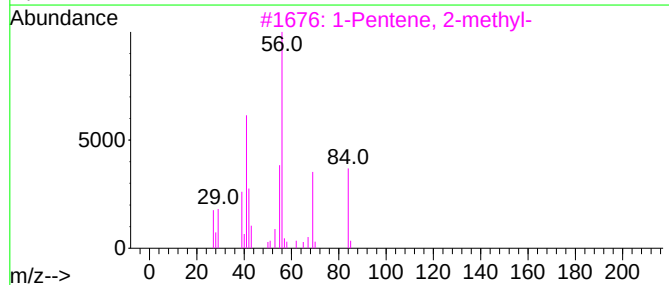
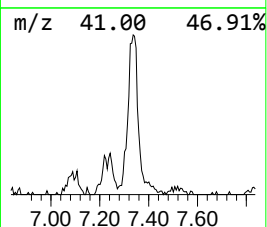
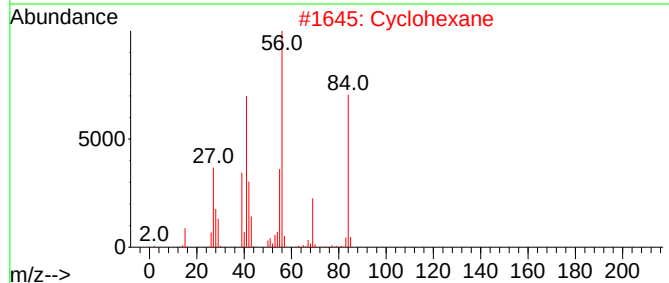
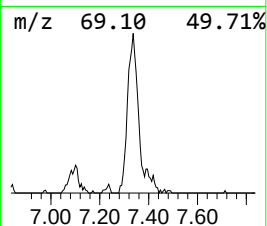
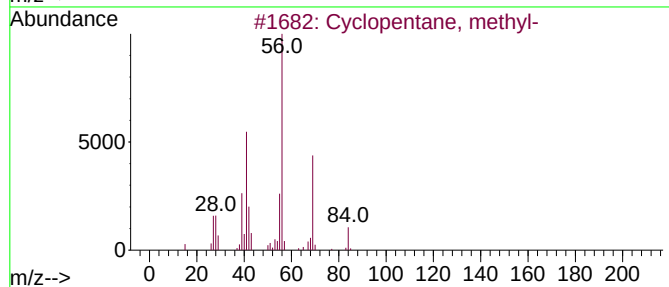
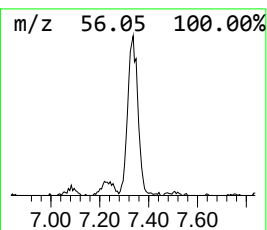
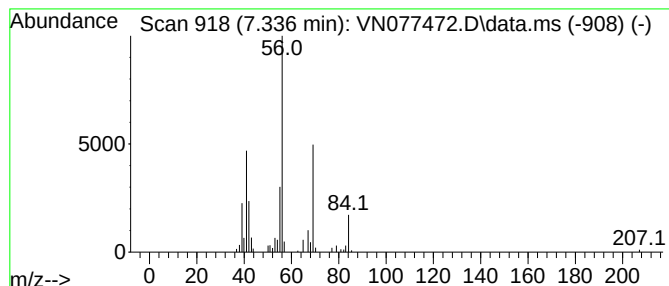
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.336	6.73 ug/l	239565	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclohexane	84	C6H12	000110-82-7	80
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	58
5			Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042523\
Data File : VN077472.D
Acq On : 25 Apr 2023 16:20
Operator : JC\MD
Sample : 02460-06 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

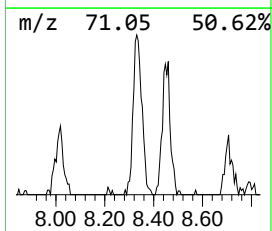
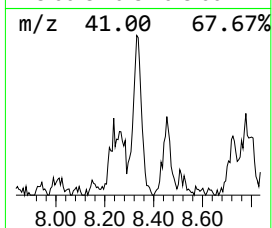
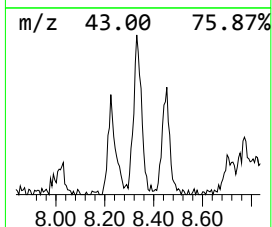
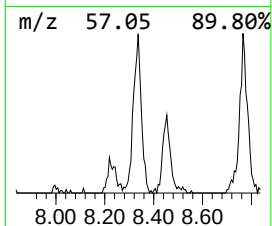
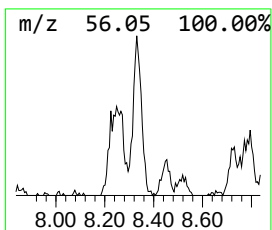
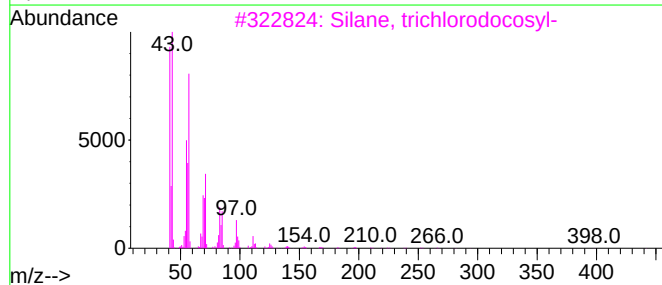
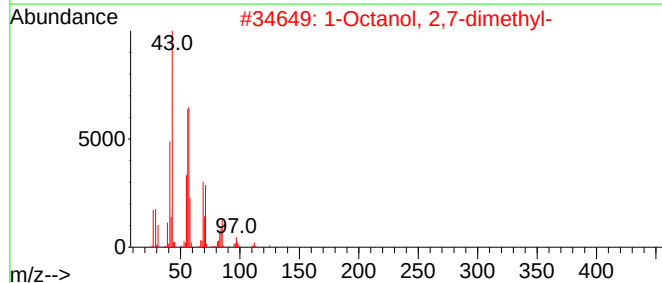
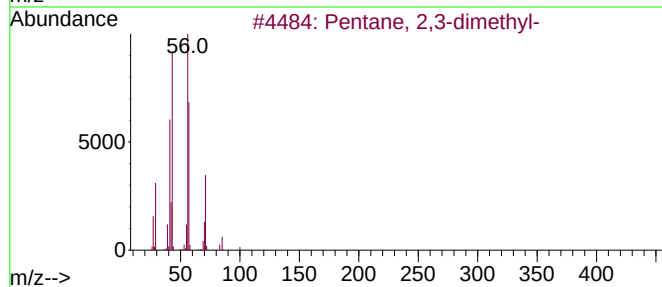
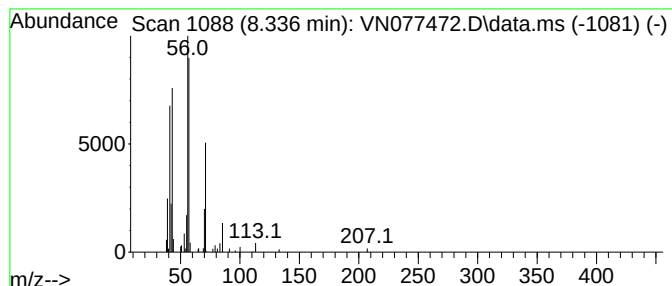
Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.336	5.55 ug/l	197568	Pentafluorobenzene	8.230	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	74
2	1-Octanol, 2,7-dimethyl-	158	C10H22O	015250-22-3	64
3	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	50
4	Hexyl octyl ether	214	C14H30O	017071-54-4	45
5	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042523\
Data File : VN077472.D
Acq On : 25 Apr 2023 16:20
Operator : JC\MD
Sample : 02460-06 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.254	24.2	ug/l	861795	1	8.230	1780060	50.0
Butane, 2,3-dim...	5.295	5.9	ug/l	211335	1	8.230	1780060	50.0
Pentane, 2-bromo-	5.354	10.9	ug/l	386873	1	8.230	1780060	50.0
Pentane, 3-methyl-	5.819	9.5	ug/l	339745	1	8.230	1780060	50.0
Cyclopentane, m...	7.336	6.7	ug/l	239565	1	8.230	1780060	50.0
Pentane, 2,3-di...	8.336	5.5	ug/l	197568	1	8.230	1780060	50.0