

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042523\
 Data File : VN077473.D
 Acq On : 25 Apr 2023 16:44
 Operator : JC\MD
 Sample : 02460-07 40X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-6

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: VN077473.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	93	99	106	rBV3	32593	60377	1.81%	0.285%
2	2.825	143	151	158	rBV3	44647	108467	3.25%	0.512%
3	3.248	215	223	239	rVB2	353659	888644	26.60%	4.194%
4	3.648	283	291	304	rVB3	41721	107687	3.22%	0.508%
5	4.419	413	422	423	rBV2	28761	47136	1.41%	0.222%
6	4.437	423	425	435	rVB5	32429	65593	1.96%	0.310%
7	5.284	555	569	574	rBV5	53541	181174	5.42%	0.855%
8	5.354	574	581	602	rVB6	91563	374602	11.21%	1.768%
9	5.825	650	661	675	rVB3	88730	289591	8.67%	1.367%
10	6.331	736	747	756	rVB4	14320	43633	1.31%	0.206%
11	7.336	908	918	936	rVB3	87261	264194	7.91%	1.247%
12	8.013	1024	1033	1043	rVB5	14983	40719	1.22%	0.192%
13	8.172	1050	1060	1065	rBV	452686	1127312	33.74%	5.320%
14	8.230	1065	1070	1081	rVV	815954	1906401	57.06%	8.996%
15	8.336	1082	1088	1098	rVB5	35063	92496	2.77%	0.436%
16	8.448	1100	1107	1113	rBV6	19995	45480	1.36%	0.215%
17	8.583	1122	1130	1143	rVB	451230	1032632	30.91%	4.873%
18	8.725	1147	1154	1159	rVV5	27209	70768	2.12%	0.334%
19	8.795	1161	1166	1172	rVV6	28845	76020	2.28%	0.359%
20	8.866	1172	1178	1185	rVB7	22546	58164	1.74%	0.274%
21	9.107	1209	1219	1233	rBV	1188890	2484738	74.37%	11.726%
22	9.607	1289	1304	1313	rBV4	51572	162560	4.87%	0.767%
23	10.107	1382	1389	1393	rBV3	19688	38050	1.14%	0.180%
24	10.571	1460	1468	1485	rBV	1764827	3340835	100.00%	15.765%
25	10.989	1532	1539	1547	rVB7	19781	53032	1.59%	0.250%
26	11.871	1678	1689	1699	rBV	1548788	2839637	85.00%	13.400%
27	11.966	1699	1705	1714	rVB	88736	155689	4.66%	0.735%
28	12.083	1716	1725	1732	rBV2	28531	56918	1.70%	0.269%
29	12.701	1822	1830	1836	rVB	68047	115984	3.47%	0.547%
30	12.854	1847	1856	1868	rBV	1131579	1964422	58.80%	9.270%
31	13.036	1880	1887	1895	rVB	153341	272162	8.15%	1.284%
32	13.136	1895	1904	1908	rBV2	28970	53339	1.60%	0.252%
33	13.342	1932	1939	1945	rVB	22435	35933	1.08%	0.170%
34	13.489	1958	1964	1971	rVB2	34379	59069	1.77%	0.279%
35	13.795	2009	2016	2027	rVB	1292094	2203772	65.96%	10.400%
36	13.960	2038	2044	2046	rBV4	34181	54148	1.62%	0.256%

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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
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37	14.001	2046	2051	2056	rVB	91770	142182	4.26%	0.671%
38	14.336	2103	2108	2114	rVB2	36270	54557	1.63%	0.257%
39	14.448	2123	2127	2133	rVB2	67508	116939	3.50%	0.552%
40	14.930	2202	2209	2217	rVB4	25486	46500	1.39%	0.219%
41	15.054	2222	2230	2236	rBV3	31324	59295	1.77%	0.280%

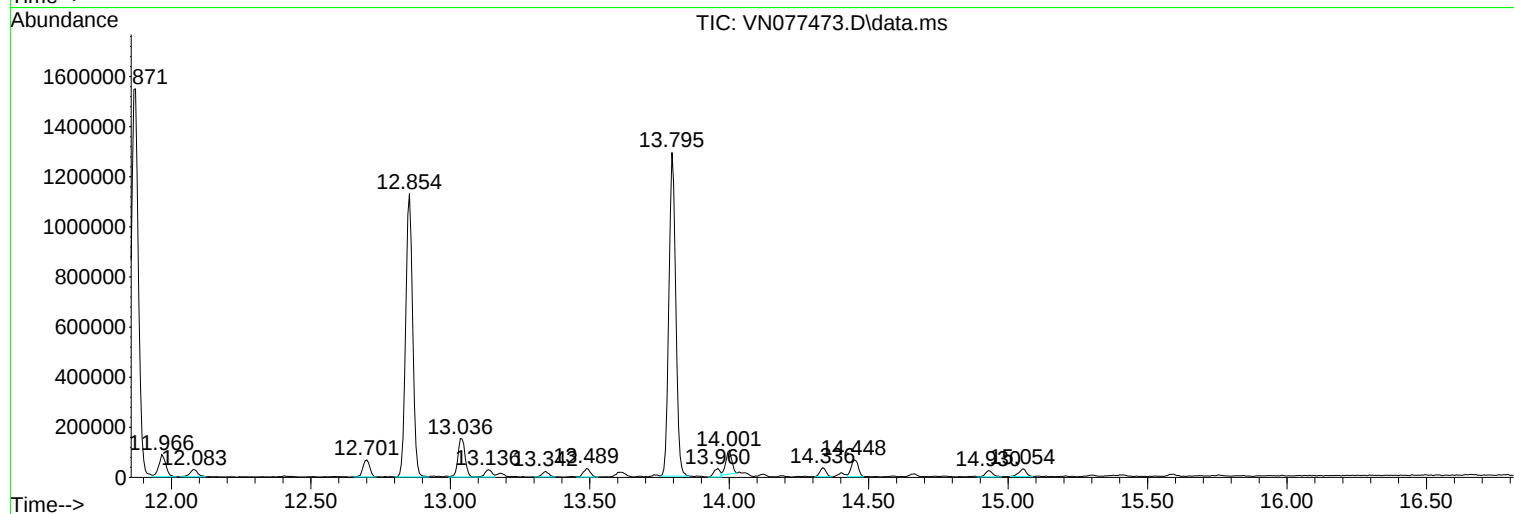
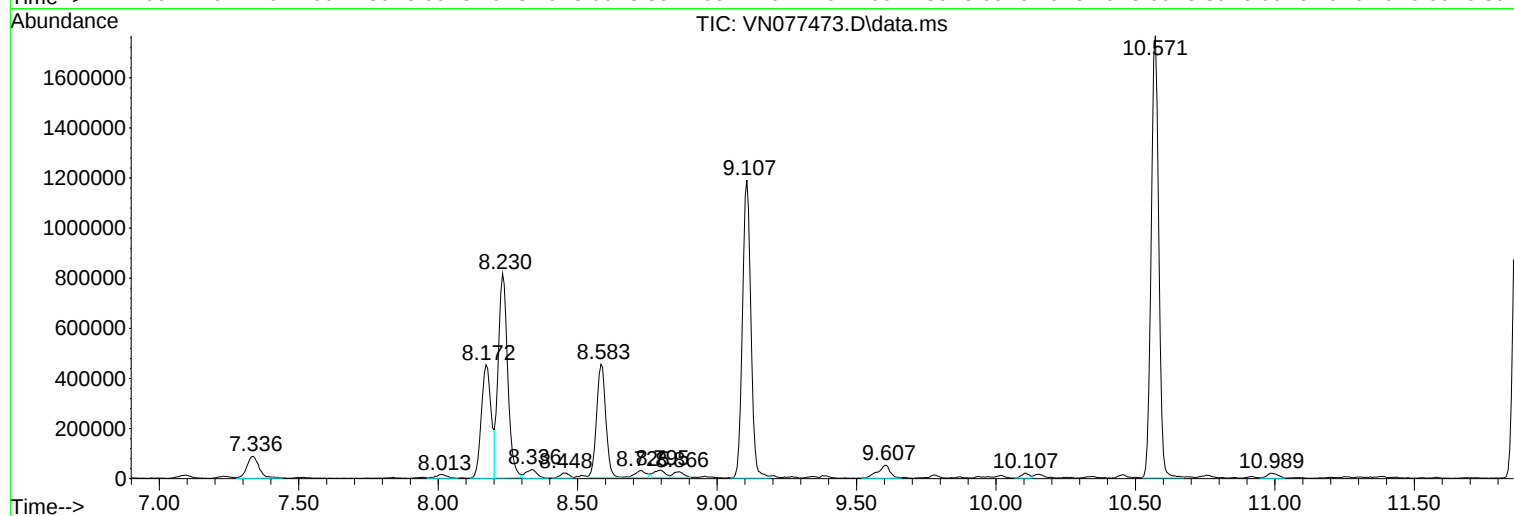
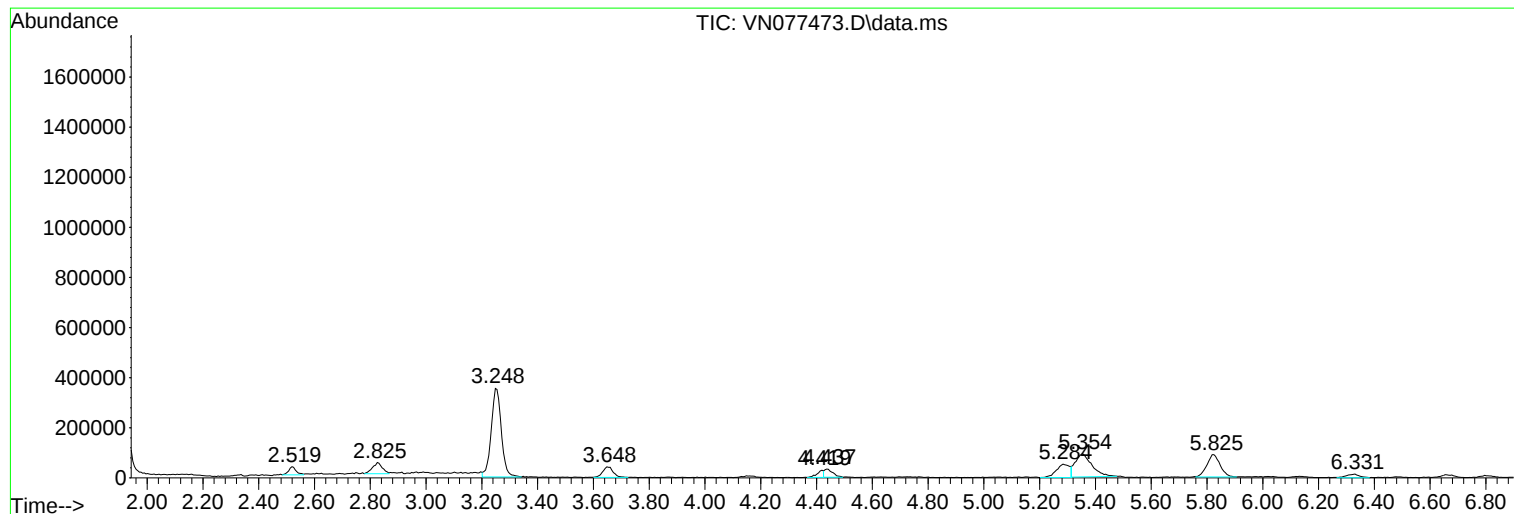
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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



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MW-6

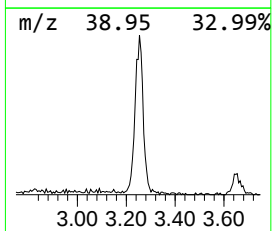
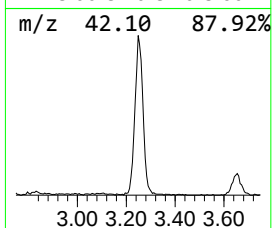
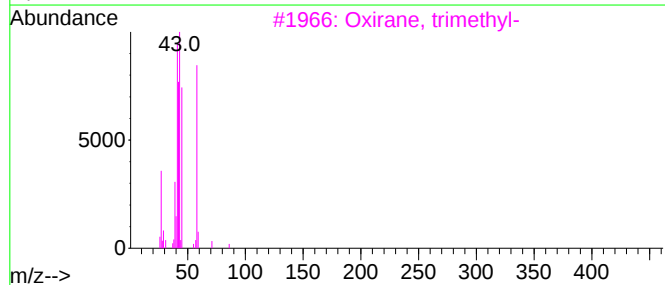
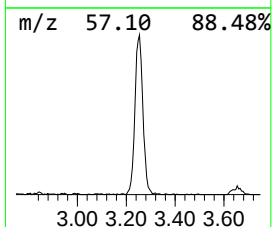
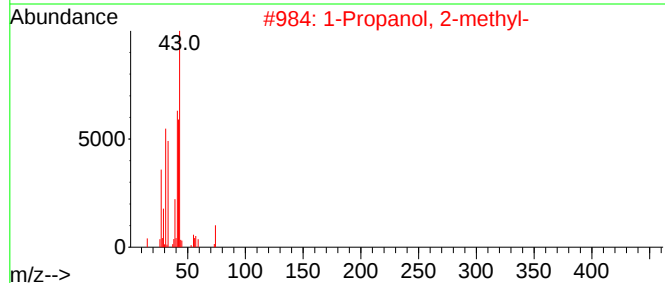
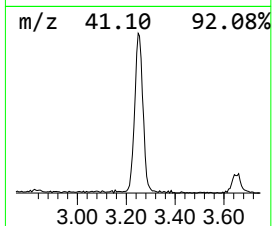
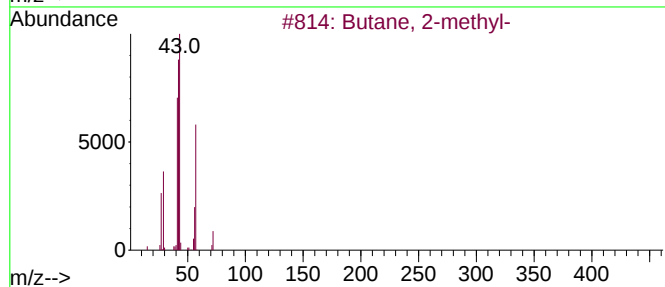
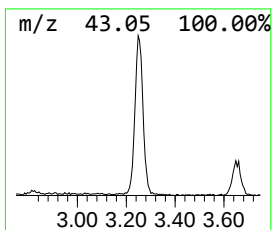
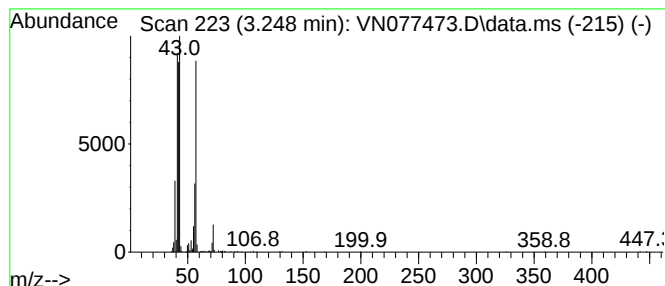
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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.
3.248	23.31 ug/l	888644	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	36
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4			Pentane	72	C5H12	000109-66-0	28
5			3-Buten-1-ol	72	C4H8O	000627-27-0	25



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

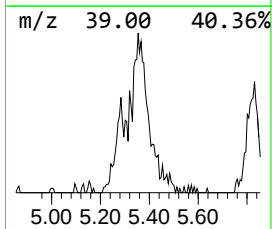
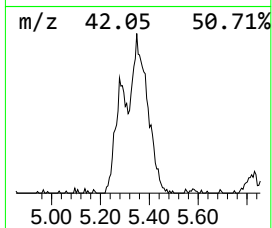
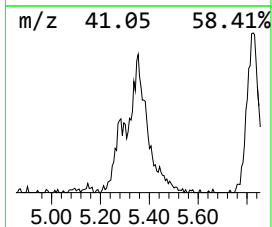
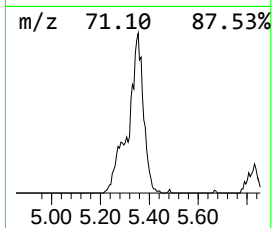
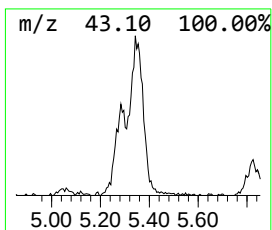
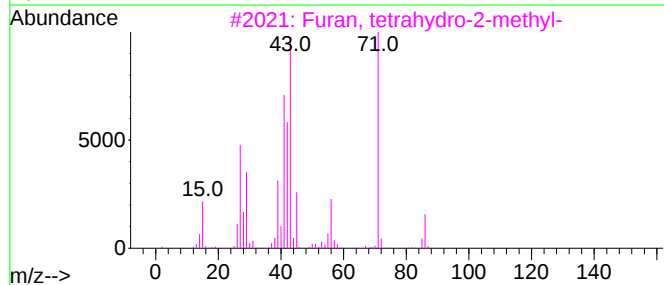
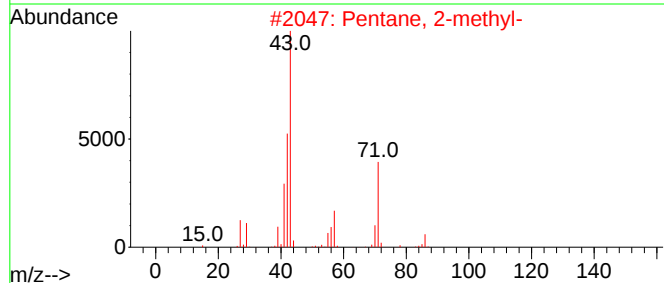
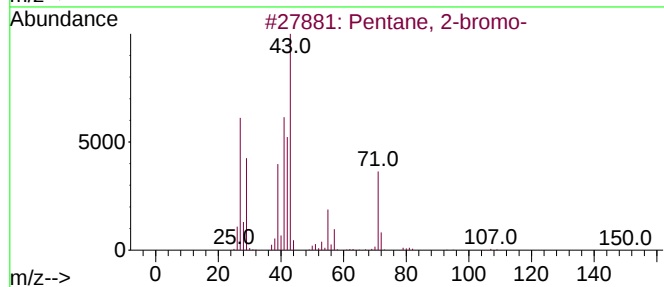
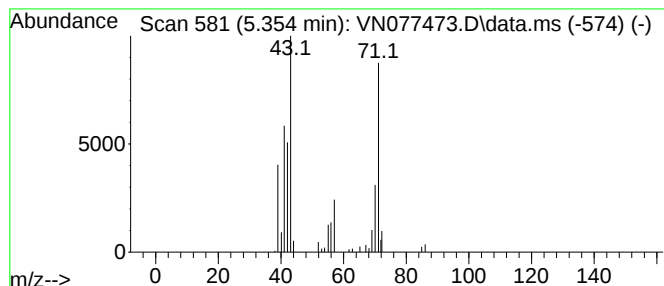
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.354	9.82 ug/l	374602	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	64
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	59
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	38
4			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	32
5			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	25



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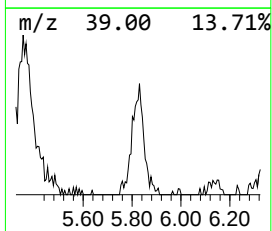
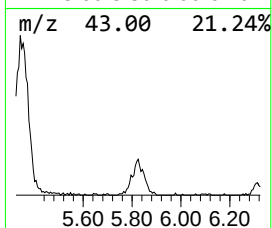
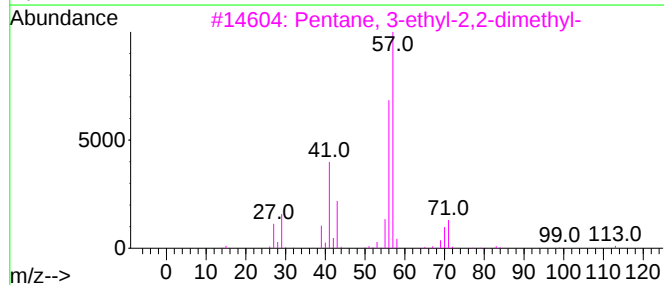
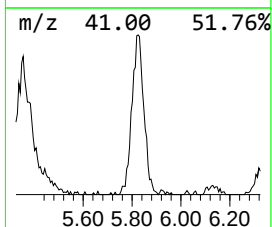
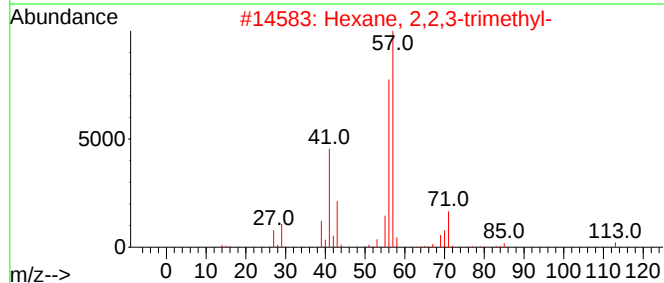
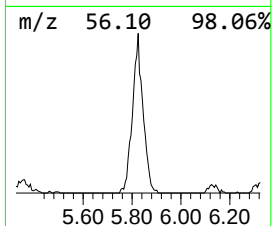
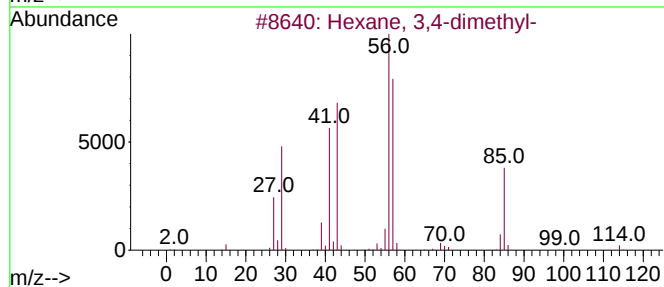
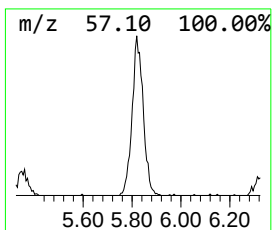
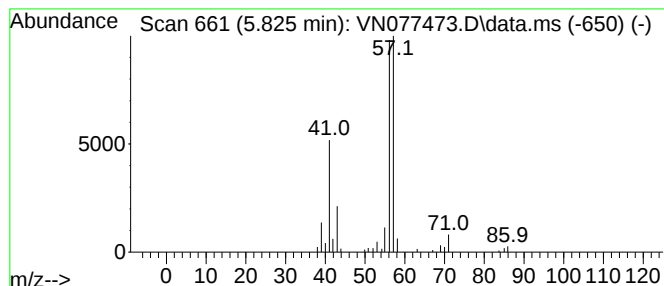
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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

Peak Number 3 Hexane, 3,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.825	7.60 ug/l	289591	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	78
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	74
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	64
5			2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	64



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MW-6

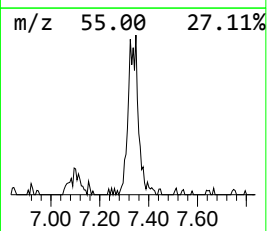
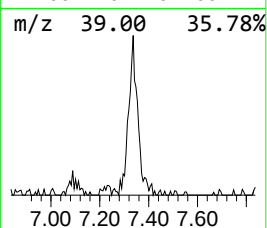
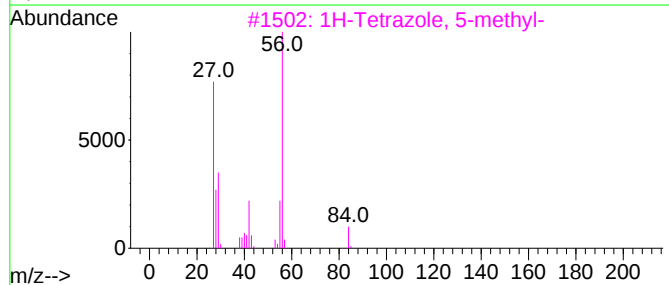
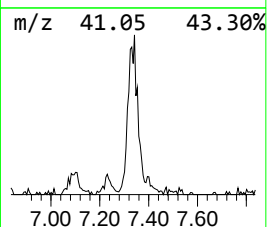
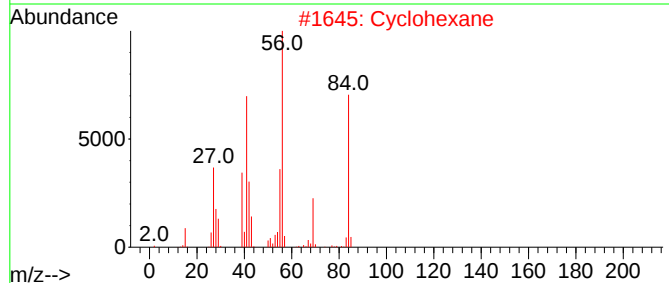
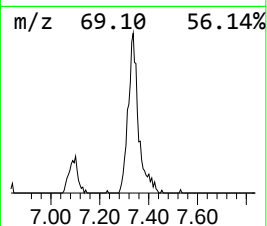
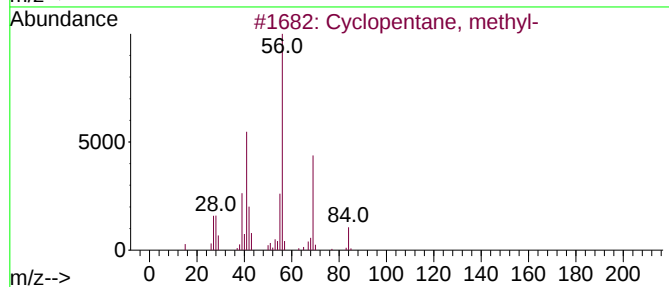
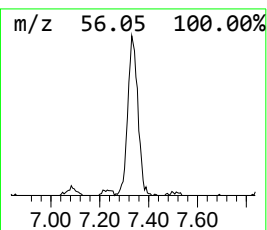
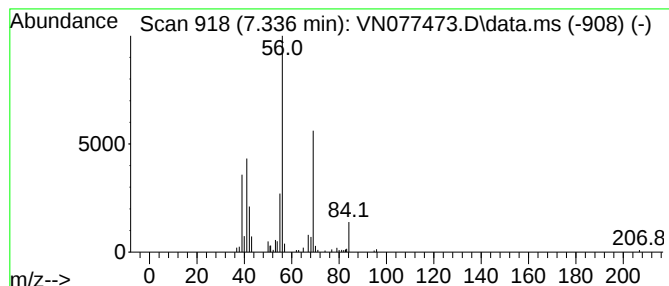
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.336	6.93 ug/l	264194	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclohexane	84	C6H12	000110-82-7	86
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	56
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.248	23.3	ug/l	888644	1	8.230	1906400	50.0
Pentane, 2-bromo-	5.354	9.8	ug/l	374602	1	8.230	1906400	50.0
Hexane, 3,4-dim...	5.825	7.6	ug/l	289591	1	8.230	1906400	50.0
Cyclopentane, m...	7.336	6.9	ug/l	264194	1	8.230	1906400	50.0