

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
 Data File : VN077818.D
 Acq On : 23 May 2023 15:54
 Operator : JC\MD
 Sample : 02884-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 2005

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\82N051523W.M
 Title : SW846 8260

Signal : TIC: VN077818.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.089	18	23	36	rVB	487398	713891	33.03%	3.037%
2	2.324	53	63	69	rVB2	28760	74259	3.44%	0.316%
3	2.495	85	92	93	rBV3	26417	41510	1.92%	0.177%
4	2.518	93	96	103	rVB2	33197	53004	2.45%	0.225%
5	2.677	117	123	131	rBV2	21658	40483	1.87%	0.172%
6	2.818	140	147	153	rBV2	22199	47402	2.19%	0.202%
7	3.253	216	221	231	rVB5	14343	45192	2.09%	0.192%
8	4.300	392	399	406	rBV2	8268	21961	1.02%	0.093%
9	4.447	414	424	434	rBV2	26582	87650	4.06%	0.373%
10	4.736	458	473	483	rBV3	37844	126413	5.85%	0.538%
11	4.865	483	495	505	rVV4	19456	61580	2.85%	0.262%
12	5.530	592	608	627	rBV2	220056	770481	35.65%	3.278%
13	5.800	647	654	664	rVB4	8487	24410	1.13%	0.104%
14	6.688	794	805	818	rBV3	47068	162054	7.50%	0.689%
15	7.235	891	898	907	rVB4	12969	32813	1.52%	0.140%
16	7.500	933	943	951	rBV2	8630	23495	1.09%	0.100%
17	7.741	974	984	990	rBV6	8475	23640	1.09%	0.101%
18	8.177	1047	1058	1062	rBV	298082	715470	33.10%	3.044%
19	8.229	1062	1067	1080	rVB	528901	1200645	55.55%	5.108%
20	8.612	1118	1132	1149	rBV3	622301	1934449	89.50%	8.230%
21	8.829	1161	1169	1178	rVB8	9256	30396	1.41%	0.129%
22	8.971	1186	1193	1199	rBV3	14970	32146	1.49%	0.137%
23	9.106	1207	1216	1231	rBV	752599	1576344	72.93%	6.706%
24	9.535	1278	1289	1295	rBV6	9812	27001	1.25%	0.115%
25	9.606	1295	1301	1307	rVV6	22633	54312	2.51%	0.231%
26	9.800	1327	1334	1343	rBV6	21153	52159	2.41%	0.222%
27	10.047	1370	1376	1382	rVB4	15456	27536	1.27%	0.117%
28	10.453	1438	1445	1457	rVB2	29453	60153	2.78%	0.256%
29	10.571	1457	1465	1471	rBV	1155745	2161442	100.00%	9.195%
30	10.635	1471	1476	1486	rVB	726067	1329385	61.50%	5.656%
31	11.318	1584	1592	1607	rVB	367492	792502	36.67%	3.371%
32	11.759	1663	1667	1676	rVB5	13807	27739	1.28%	0.118%
33	11.870	1676	1686	1696	rBV	1011469	1863656	86.22%	7.928%
34	11.970	1696	1703	1709	rVV	196233	359606	16.64%	1.530%
35	12.076	1709	1721	1729	rVV	488985	1013597	46.89%	4.312%
36	12.147	1729	1733	1734	rVV3	15709	21819	1.01%	0.093%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
 Data File : VN077818.D
 Acq On : 23 May 2023 15:54
 Operator : JC\MD
 Sample : 02884-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 2005

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\82N051523W.M
 Title : SW846 8260

37	12.206	1738	1743	1754	rVB3	60277	122245	5.66%	0.520%
38	12.412	1765	1778	1789	rBV3	356284	744825	34.46%	3.169%
39	12.500	1789	1793	1798	rVB5	17855	30905	1.43%	0.131%
40	12.647	1812	1818	1823	rVV2	48672	105823	4.90%	0.450%
41	12.700	1823	1827	1834	rVB3	64544	122705	5.68%	0.522%
42	12.853	1845	1853	1860	rBV	793955	1429924	66.16%	6.083%
43	13.047	1880	1886	1891	rBV2	43666	92604	4.28%	0.394%
44	13.106	1891	1896	1900	rVV	122276	217766	10.08%	0.926%
45	13.176	1904	1908	1915	rVB	93590	168743	7.81%	0.718%
46	13.347	1931	1937	1945	rVB2	80540	177059	8.19%	0.753%
47	13.488	1955	1961	1966	rVV	229435	378668	17.52%	1.611%
48	13.535	1966	1969	1974	rVV2	63998	95878	4.44%	0.408%
49	13.588	1974	1978	1984	rVV2	32983	51405	2.38%	0.219%
50	13.717	1996	2000	2006	rVB4	33560	62160	2.88%	0.264%
51	13.800	2006	2014	2023	rBV2	883607	1718843	79.52%	7.312%
52	14.000	2043	2048	2062	rVB5	54120	170992	7.91%	0.727%
53	14.182	2072	2079	2086	rVB	363128	600681	27.79%	2.555%
54	14.247	2086	2090	2094	rBV6	19659	34793	1.61%	0.148%
55	14.341	2101	2106	2111	rVB2	17658	33108	1.53%	0.141%
56	14.453	2120	2125	2132	rBV8	21378	54241	2.51%	0.231%
57	14.582	2144	2147	2151	rVB4	14635	21726	1.01%	0.092%
58	14.800	2178	2184	2192	rVB4	18598	47214	2.18%	0.201%
59	15.041	2220	2225	2233	rBV3	34553	81279	3.76%	0.346%
60	15.123	2233	2239	2246	rVB5	21930	45304	2.10%	0.193%
61	15.217	2248	2255	2263	rBV4	36628	69647	3.22%	0.296%
62	15.500	2296	2303	2309	rBV8	19517	40190	1.86%	0.171%
63	15.647	2321	2328	2339	rVB	599104	1156714	53.52%	4.921%

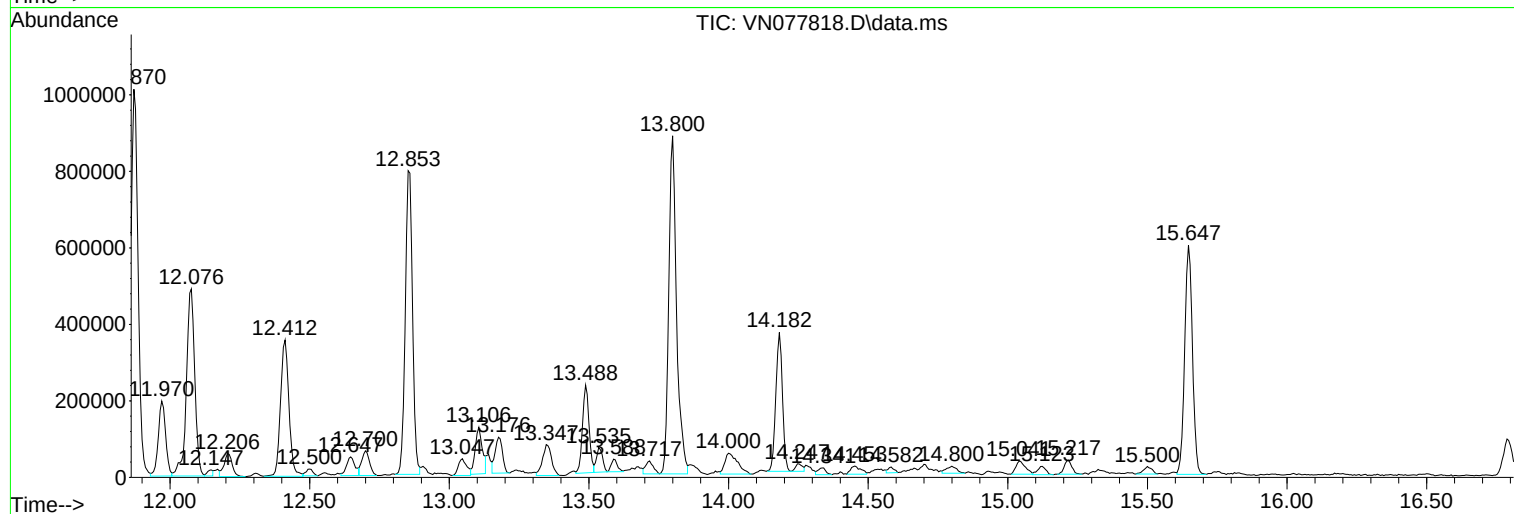
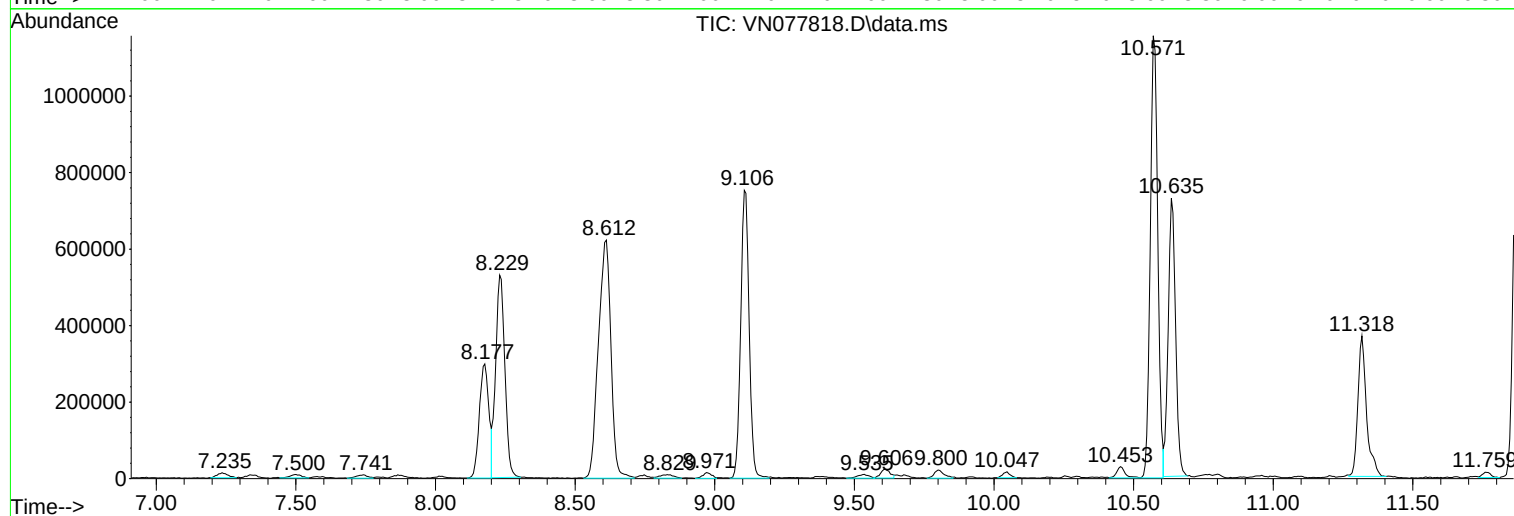
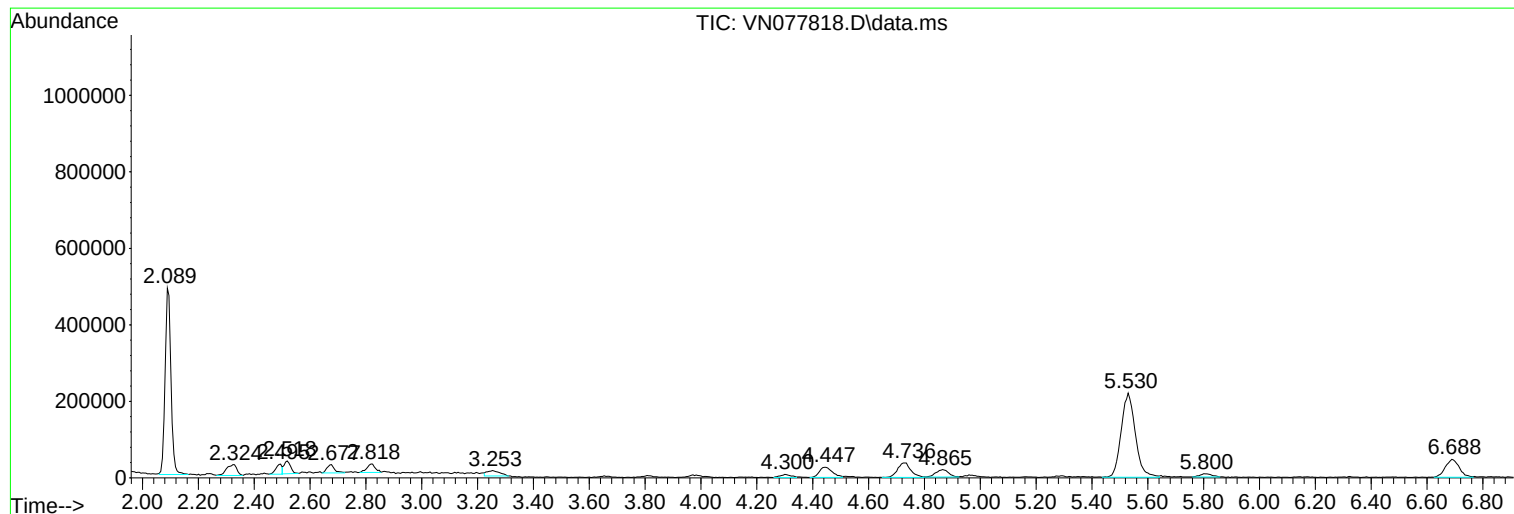
Sum of corrected areas: 23506037

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

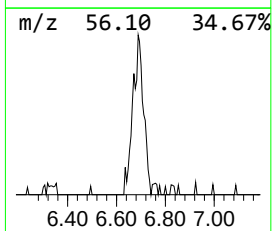
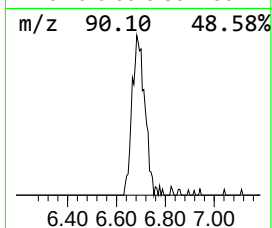
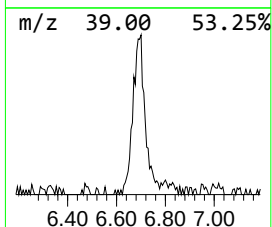
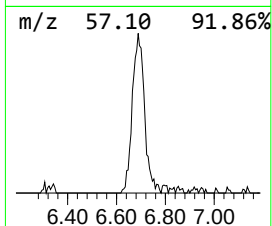
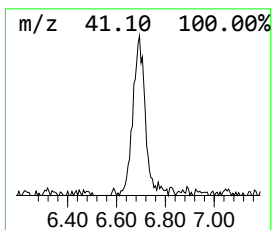
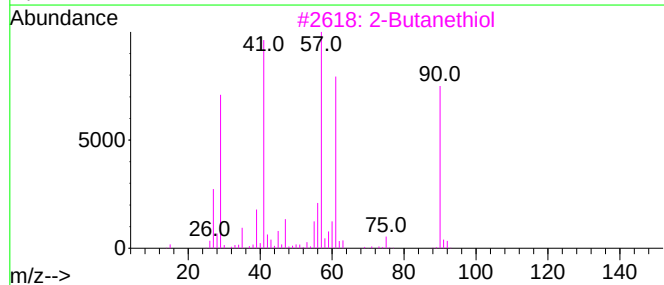
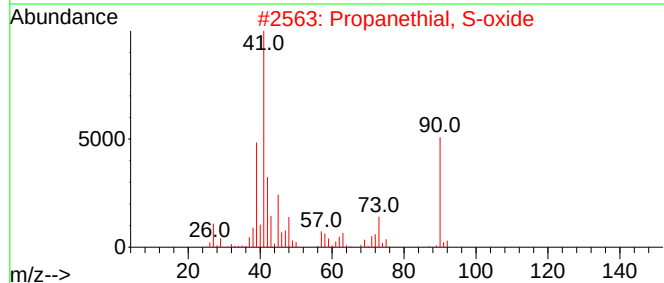
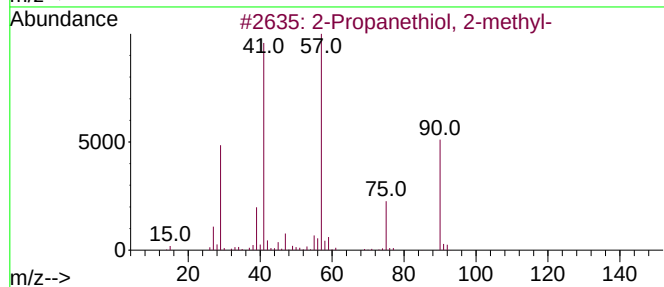
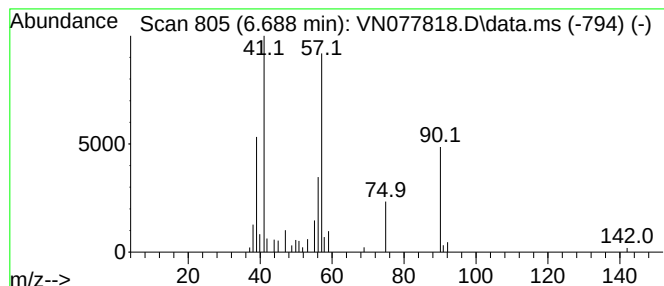
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.688	6.75 ug/l	162054	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	62
2			Propanethial, S-oxide	90	C3H6OS	032157-29-2	47
3			2-Butanethiol	90	C4H10S	000513-53-1	46
4			Acetoacetic acid, 1,3-dithio-, S...	190	C8H14OS2	020383-06-6	42
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

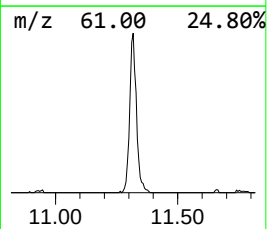
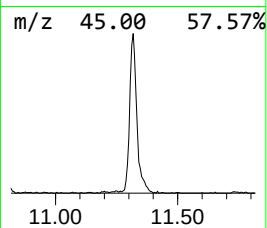
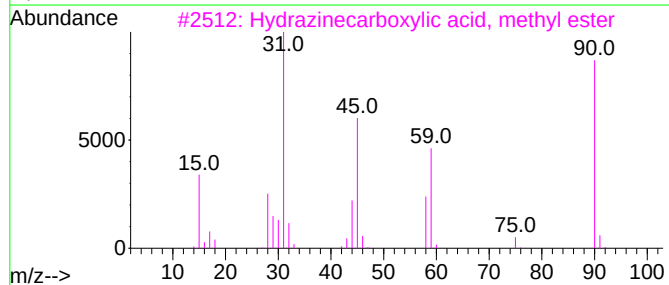
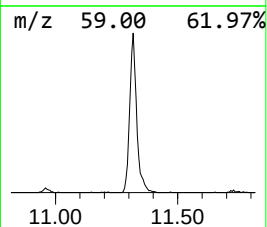
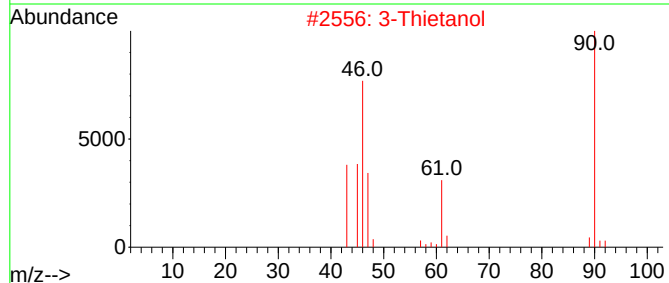
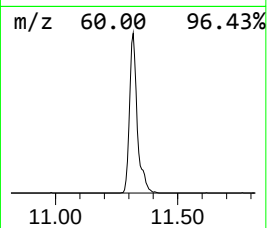
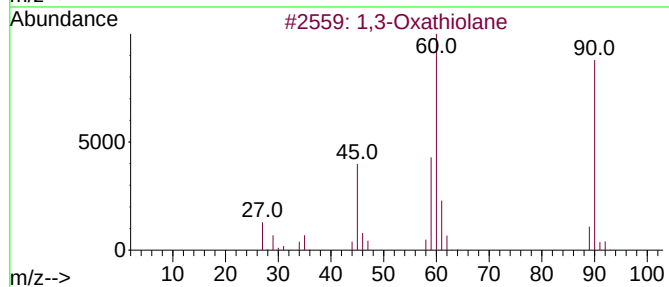
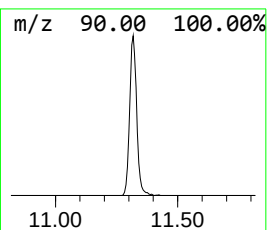
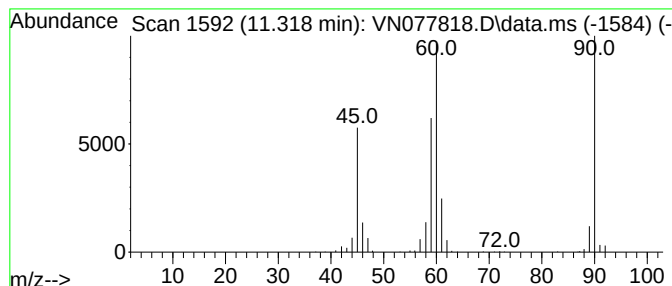
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 3 1,3-Oxathiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.318	21.26 ug/l	792502	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Oxathiolane	90	C3H6OS	002094-97-5	90
2			3-Thietanol	90	C3H6OS	010304-16-2	42
3			Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38
4			(S)-Methyl 2,3-dihydroxypropanoate	120	C4H8O4	010303-88-5	33
5			Ethylvinyl sulfide	88	C4H8S	000627-50-9	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

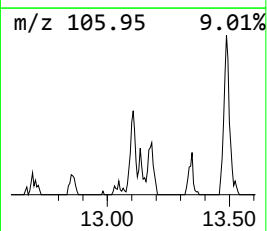
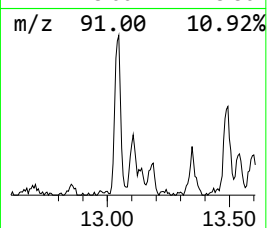
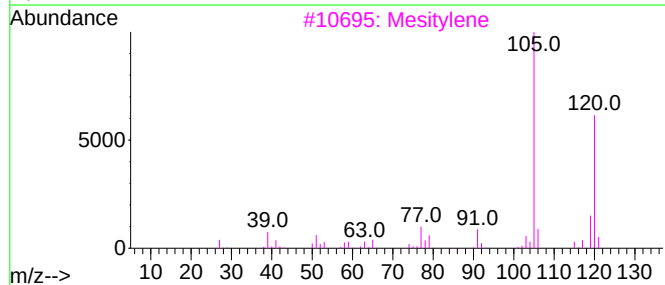
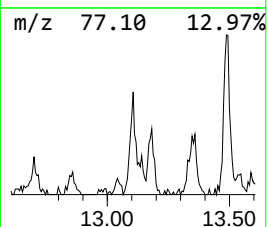
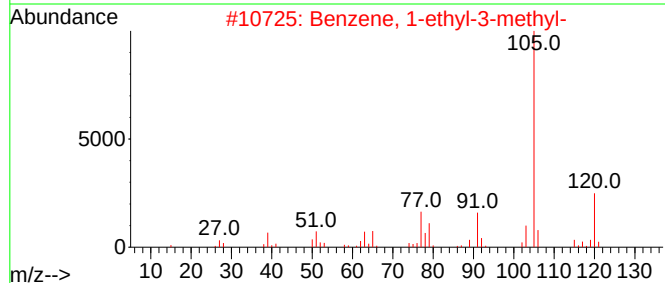
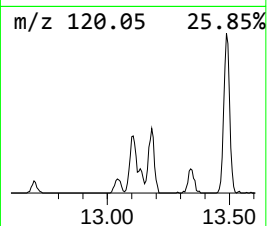
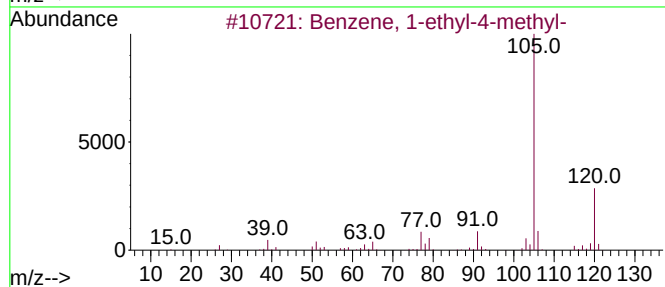
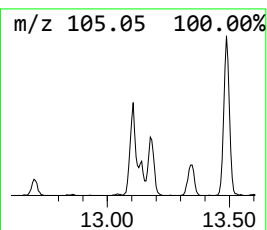
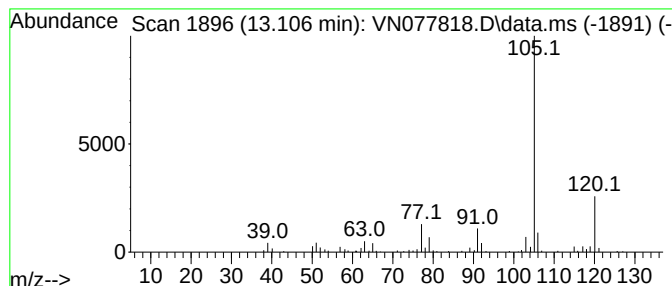
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.106	6.33 ug/l	217766	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

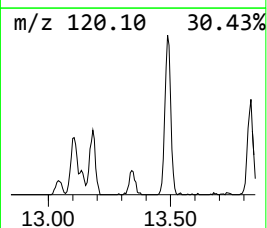
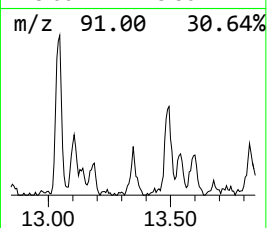
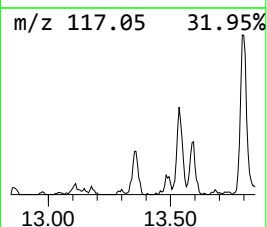
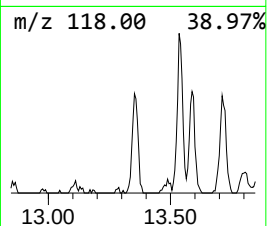
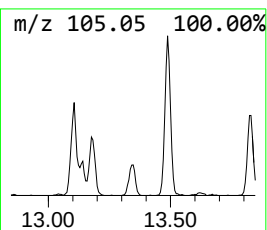
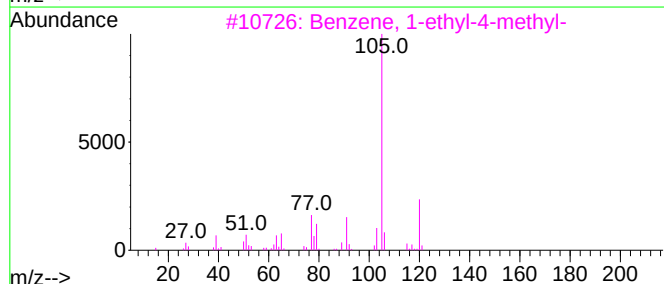
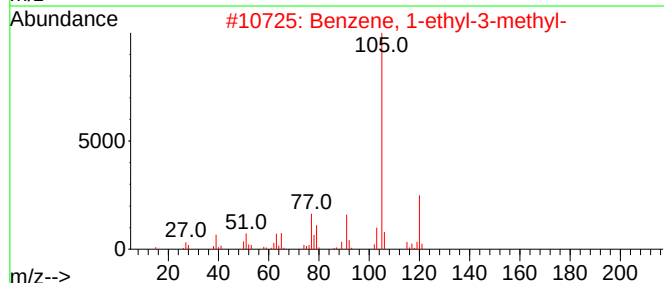
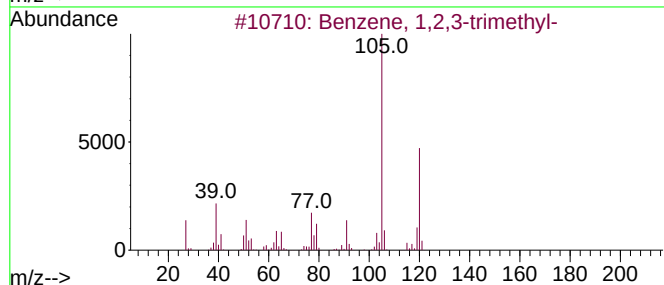
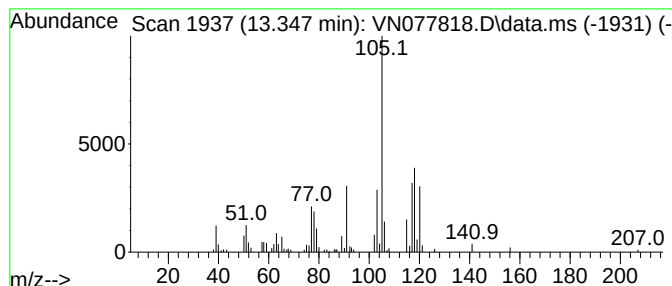
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.347 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.347	5.15 ug/l	177059	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	45
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	43
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	43
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	38
5			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

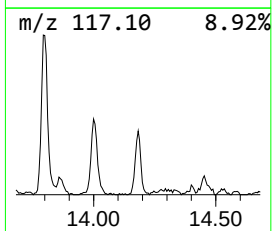
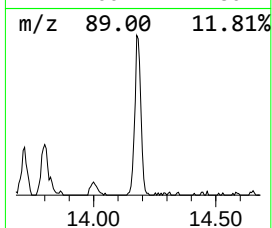
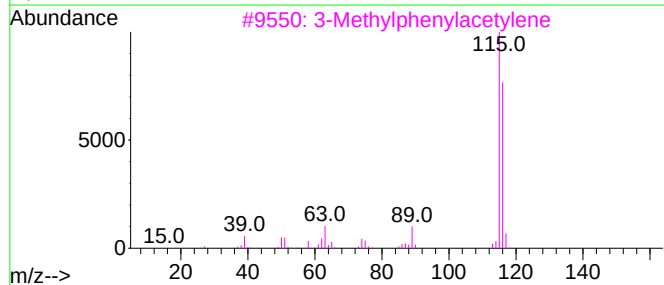
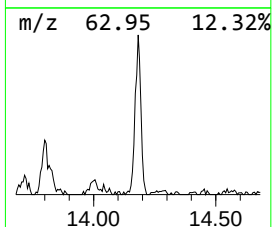
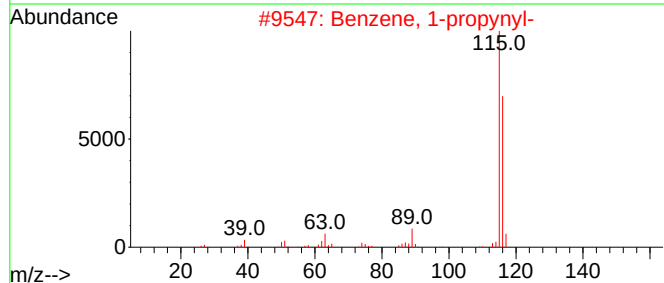
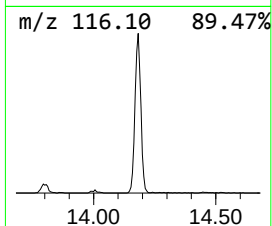
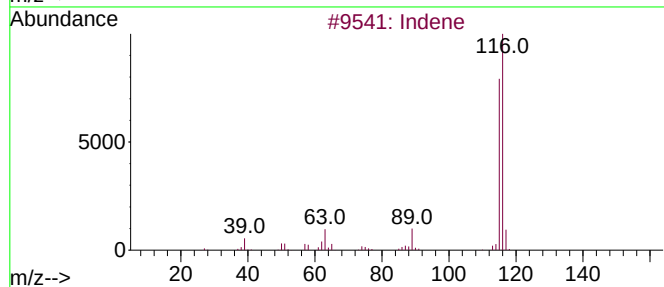
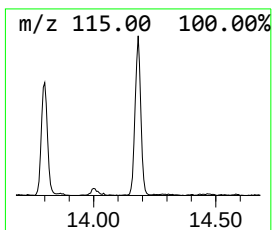
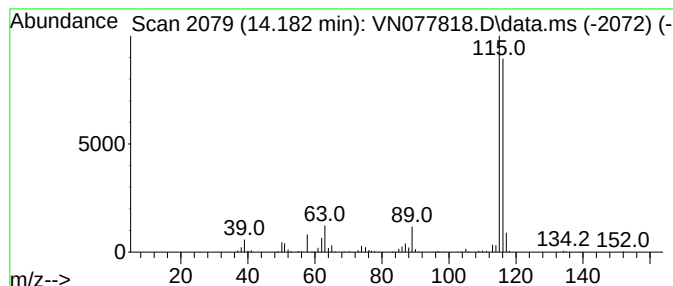
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 6 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	17.47 ug/l	600681	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052323\
Data File : VN077818.D
Acq On : 23 May 2023 15:54
Operator : JC\MD
Sample : 02884-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2005

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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
2-Propanethiol,...	6.688	6.8	ug/l	162054	1	8.235	1200650	50.0
1,3-Oxathiolane	11.318	21.3	ug/l	792502	3	11.870	1863660	50.0
Benzene, 1-ethy...	13.106	6.3	ug/l	217766	4	13.800	1718840	50.0
unknown13.347	13.347	5.2	ug/l	177059	4	13.800	1718840	50.0
Indene	14.182	17.5	ug/l	600681	4	13.800	1718840	50.0