

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
 Data File : VX028759.D
 Acq On : 17 May 2022 15:45
 Operator : JC/MD
 Sample : N2884-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31769

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_X\Method\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	12	rBV	293970	241049	3.16%	0.378%
2	1.355	40	44	53	rBV	214621	276744	3.63%	0.433%
3	2.379	206	212	222	rBV	190029	307475	4.04%	0.482%
4	2.538	230	238	243	rBV	100649	211745	2.78%	0.332%
5	2.593	243	247	253	rVB	75617	128717	1.69%	0.202%
6	2.751	266	273	286	rVB	42790	89728	1.18%	0.141%
7	2.965	297	308	328	rBV	1332453	2802951	36.80%	4.390%
8	3.696	415	428	453	rBV	2856603	7616692	100.00%	11.929%
9	4.196	500	510	524	rBV	139283	385912	5.07%	0.604%
10	4.556	562	569	582	rVB	65462	178550	2.34%	0.280%
11	5.001	631	642	659	rBV	51072	185693	2.44%	0.291%
12	5.391	692	706	716	rBV	182586	534178	7.01%	0.837%
13	5.556	723	733	747	rVB	278007	788138	10.35%	1.234%
14	5.958	790	799	804	rBV	188402	477868	6.27%	0.748%
15	6.043	804	813	832	rVV	1147558	3457256	45.39%	5.415%
16	6.202	832	839	852	rVV2	38663	122626	1.61%	0.192%
17	6.336	852	861	878	rVB4	98992	335825	4.41%	0.526%
18	6.763	921	931	951	rVB	459090	1088068	14.29%	1.704%
19	7.464	1039	1046	1053	rBV3	27293	86924	1.14%	0.136%
20	7.690	1073	1083	1094	rVB	108416	239213	3.14%	0.375%
21	8.336	1183	1189	1197	rBV	107232	191000	2.51%	0.299%
22	8.573	1222	1228	1234	rVV	88512	153844	2.02%	0.241%
23	8.653	1234	1241	1246	rVV	940640	1484368	19.49%	2.325%
24	8.720	1246	1252	1262	rVB	2531400	3843686	50.46%	6.020%
25	8.854	1269	1274	1283	rVB3	57111	111924	1.47%	0.175%
26	9.019	1296	1301	1305	rBV2	49311	102491	1.35%	0.161%
27	9.067	1305	1309	1315	rVV	278210	421858	5.54%	0.661%
28	9.488	1373	1378	1388	rVV	1746601	2475061	32.50%	3.876%
29	9.732	1413	1418	1427	rVB	136976	208048	2.73%	0.326%
30	9.878	1436	1442	1449	rBV	400121	529705	6.95%	0.830%
31	10.055	1464	1471	1476	rBV	1263214	1628883	21.39%	2.551%
32	10.195	1488	1494	1500	rBV	2708583	3433610	45.08%	5.378%
33	10.299	1507	1511	1521	rVB	2566111	3501165	45.97%	5.483%
34	10.415	1521	1530	1532	rBV2	180829	293397	3.85%	0.460%
35	10.439	1532	1534	1537	rVB2	77790	90697	1.19%	0.142%
36	10.506	1542	1545	1552	rVB2	57081	79654	1.05%	0.125%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	10.652	1563	1569	1579	rVB2	1769673	3195026	41.95%	5.004%
38	10.750	1579	1585	1591	rBV3	81532	152427	2.00%	0.239%
39	10.902	1605	1610	1614	rVB	140359	180274	2.37%	0.282%
40	10.963	1614	1620	1630	rVB2	145084	250496	3.29%	0.392%
41	11.079	1634	1639	1650	rBV	919359	1347618	17.69%	2.111%
42	11.171	1650	1654	1663	rVB2	57527	82676	1.09%	0.129%
43	11.305	1673	1676	1683	rVB	85697	112893	1.48%	0.177%
44	11.378	1683	1688	1695	rBV	708242	1231602	16.17%	1.929%
45	11.451	1695	1700	1704	rVV	256286	367484	4.82%	0.576%
46	11.494	1704	1707	1712	rVB5	59808	97073	1.27%	0.152%
47	11.616	1722	1727	1738	rVB2	313735	543392	7.13%	0.851%
48	11.750	1745	1749	1754	rVB	637516	799168	10.49%	1.252%
49	11.811	1754	1759	1762	rBV	325960	429732	5.64%	0.673%
50	11.847	1762	1765	1770	rVB2	152301	193782	2.54%	0.303%
51	11.957	1779	1783	1788	rVB2	203610	285477	3.75%	0.447%
52	12.024	1788	1794	1798	rBV	1161600	1507206	19.79%	2.361%
53	12.085	1801	1804	1809	rVV	333660	423348	5.56%	0.663%
54	12.134	1809	1812	1818	rVB	136465	174756	2.29%	0.274%
55	12.244	1822	1830	1838	rBV2	344347	546166	7.17%	0.855%
56	12.317	1838	1842	1851	rVB3	80833	141950	1.86%	0.222%
57	12.414	1852	1858	1863	rBV	4040739	4850290	63.68%	7.596%
58	12.554	1879	1881	1885	rVV2	71354	97512	1.28%	0.153%
59	12.615	1888	1891	1894	rVB	76794	89048	1.17%	0.139%
60	12.713	1901	1907	1911	rBV4	40160	85252	1.12%	0.134%
61	12.798	1917	1921	1925	rBV	167667	203233	2.67%	0.318%
62	12.847	1925	1929	1933	rVB	102269	116679	1.53%	0.183%
63	12.963	1945	1948	1951	rBV2	120844	164329	2.16%	0.257%
64	12.993	1951	1953	1957	rVB	81510	81677	1.07%	0.128%
65	13.286	1997	2001	2006	rVB2	166427	222543	2.92%	0.349%
66	13.341	2006	2010	2018	rVB	126565	171198	2.25%	0.268%
67	13.426	2018	2024	2030	rBV	177833	235049	3.09%	0.368%
68	13.506	2033	2037	2042	rBV2	52895	79242	1.04%	0.124%
69	13.713	2068	2071	2076	rVB	67804	90956	1.19%	0.142%
70	13.780	2076	2082	2088	rBV	4097493	5373450	70.55%	8.416%
71	13.871	2093	2097	2103	rVB	133818	182499	2.40%	0.286%
72	14.639	2218	2223	2233	rVB	586624	747390	9.81%	1.171%
73	14.780	2241	2246	2252	rBV	427361	521589	6.85%	0.817%
74	15.206	2310	2316	2323	rVB	94482	126233	1.66%	0.198%
75	15.475	2355	2360	2371	rVB	59246	106152	1.39%	0.166%
76	15.615	2375	2383	2386	rVV	83989	138528	1.82%	0.217%

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Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Title : SW846 8260

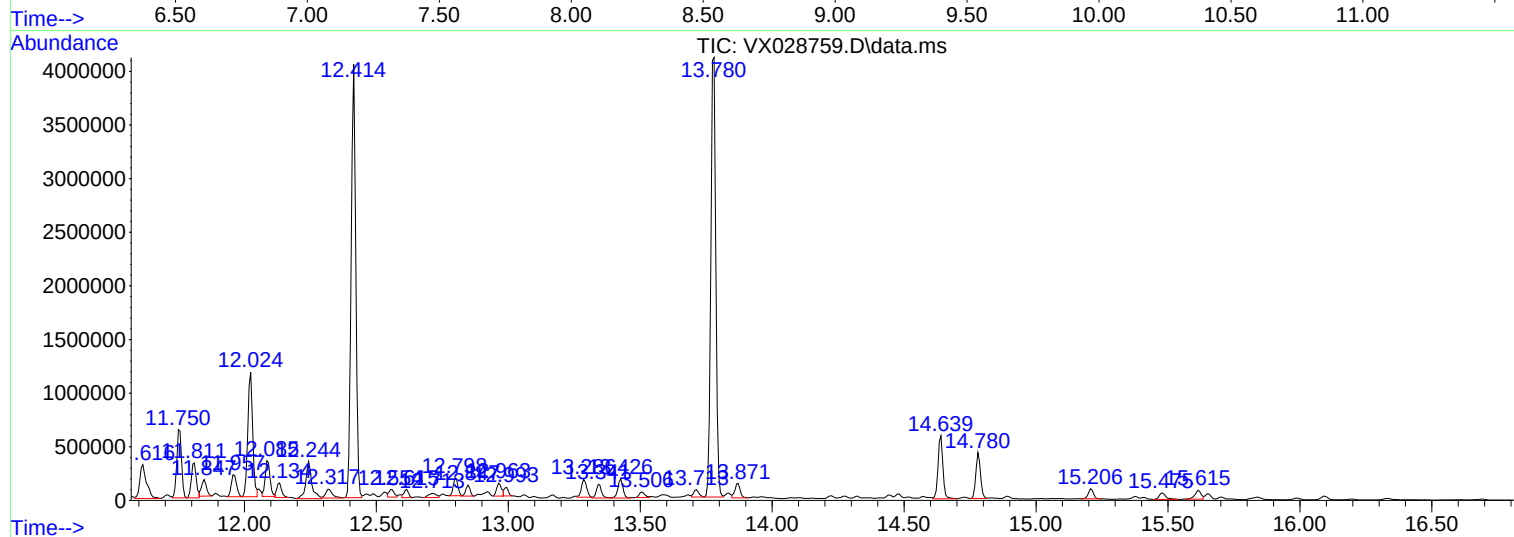
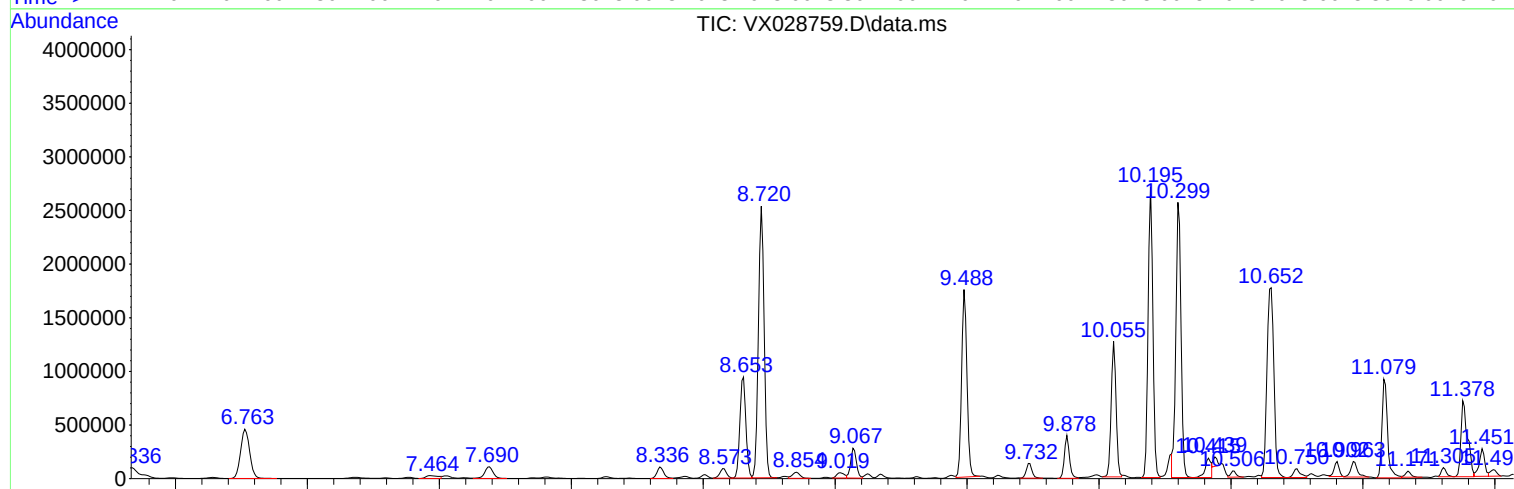
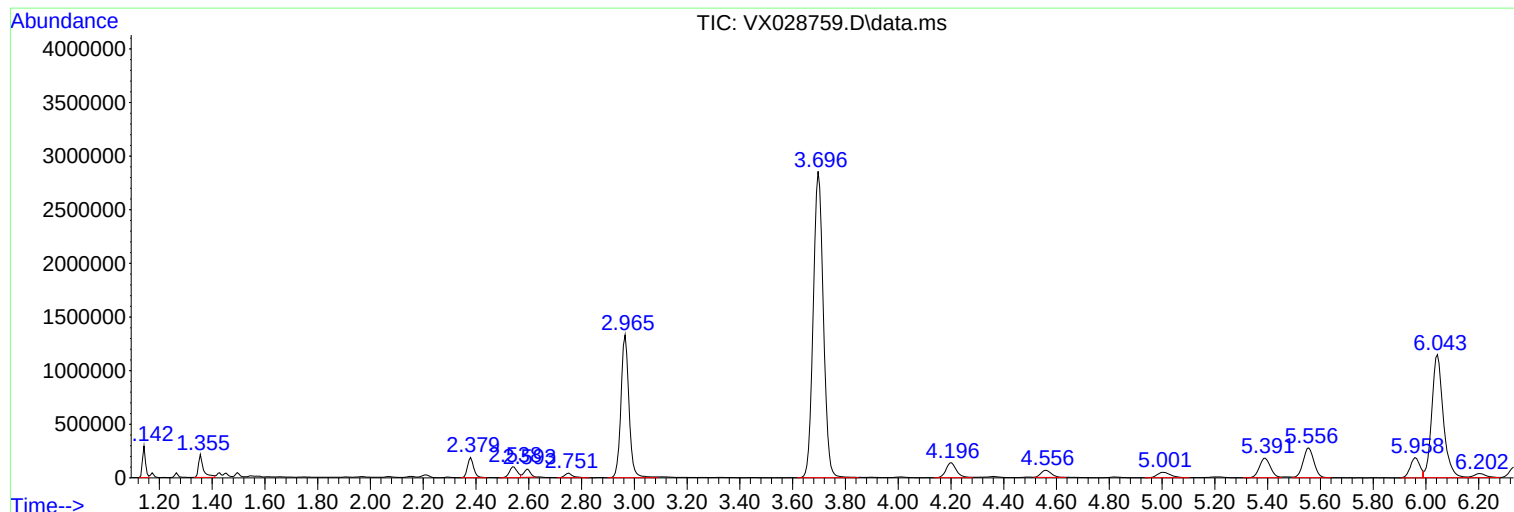
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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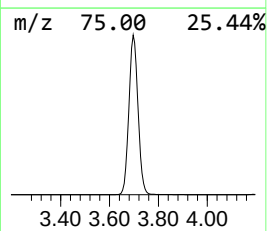
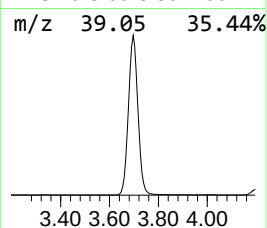
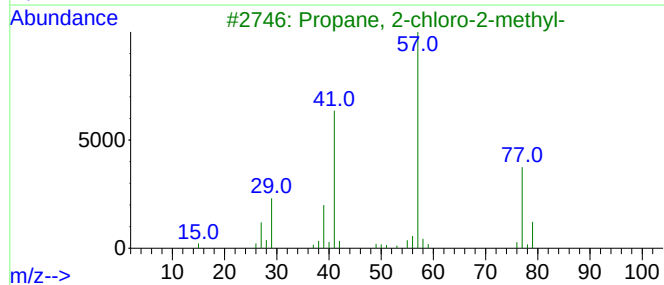
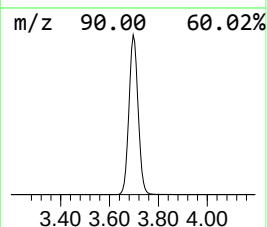
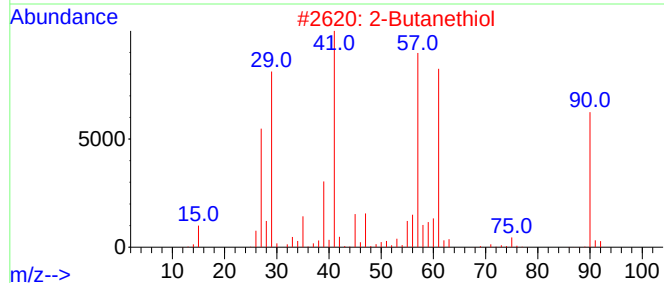
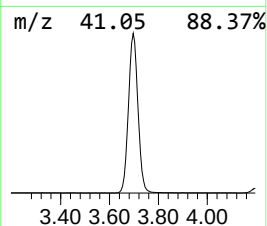
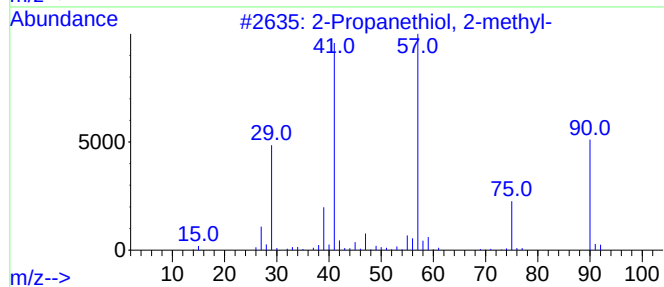
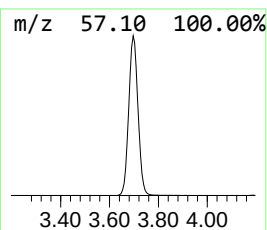
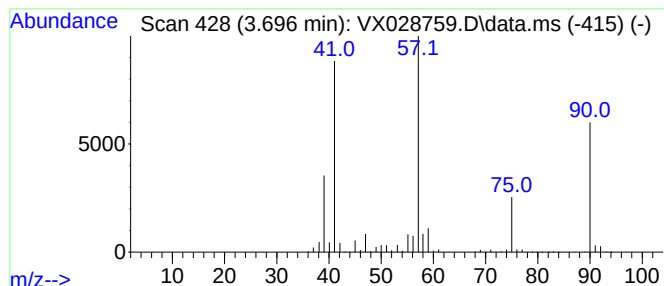
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	483.21 ug/l	7616690	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	91
2	2-Butanethiol			90	C4H10S	000513-53-1	42
3	Propane, 2-chloro-2-methyl-			92	C4H9Cl	000507-20-0	22
4	Ethynyl tert-butyl sulfoxide			130	C6H10OS	041463-34-7	16
5	Propane, 2-bromo-2-methyl-			136	C4H9Br	000507-19-7	14



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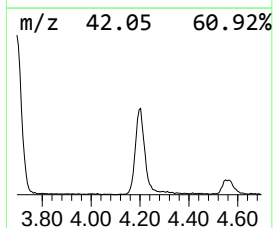
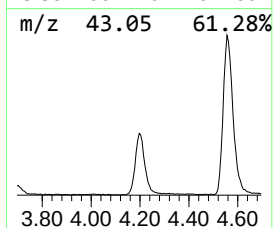
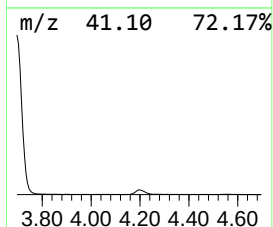
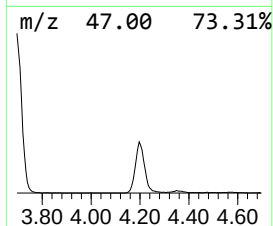
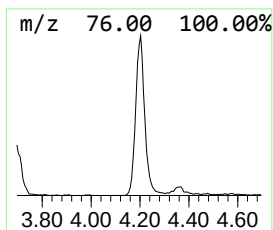
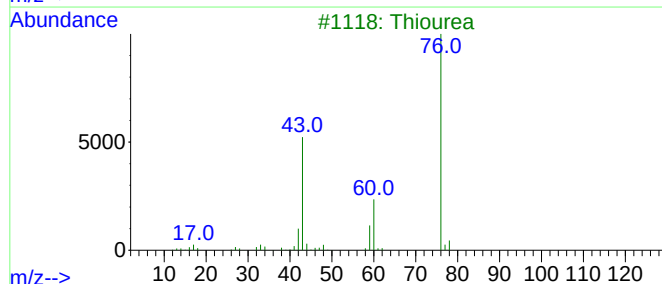
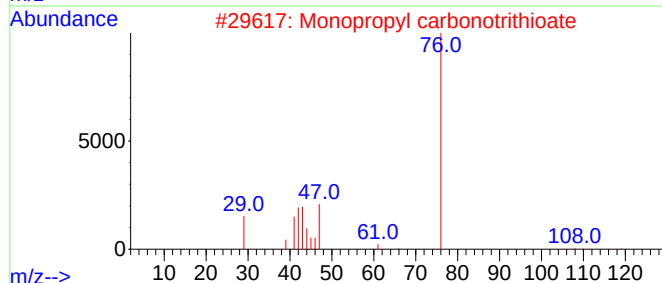
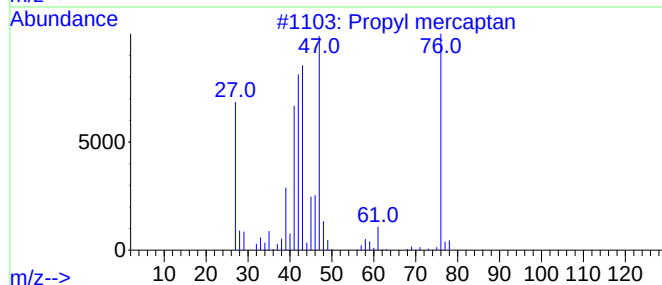
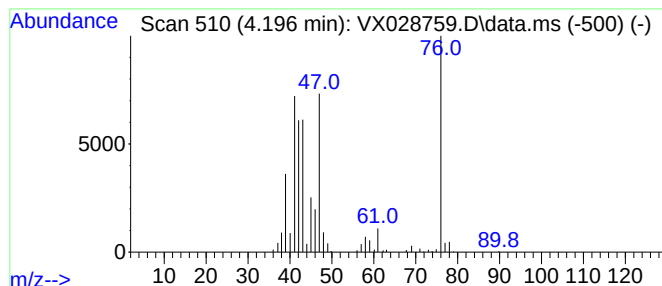
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propyl mercaptan Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.196	24.48 ug/l	385912	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propyl mercaptan	76	C3H8S	000107-03-9	97
2			Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	74
3			Thiourea	76	CH4N2S	000062-56-6	40
4			Ethane, fluoro-	48	C2H5F	000353-36-6	9
5			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9



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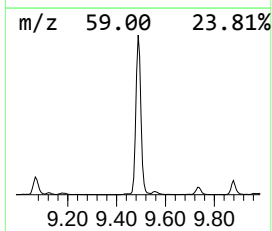
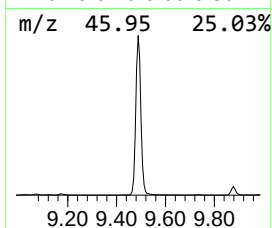
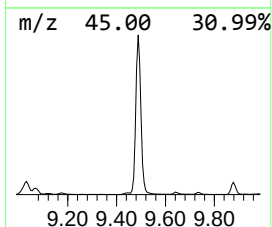
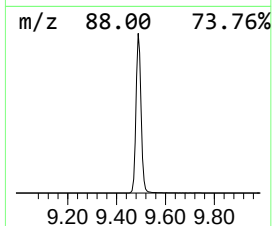
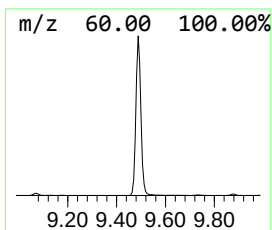
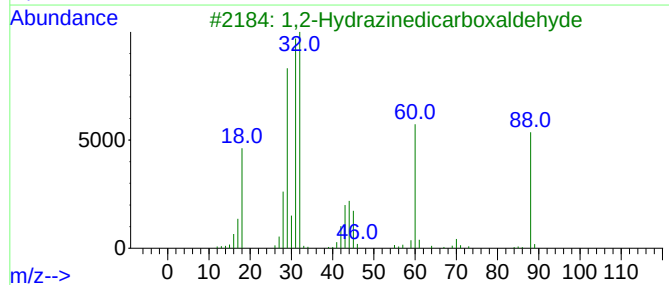
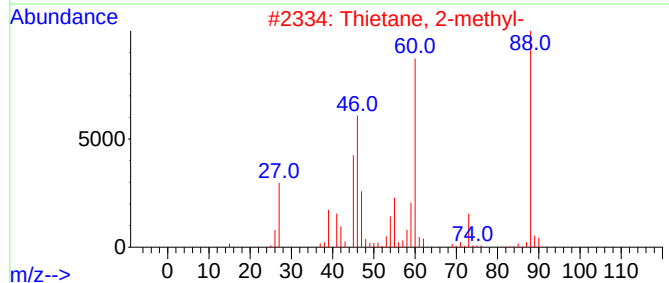
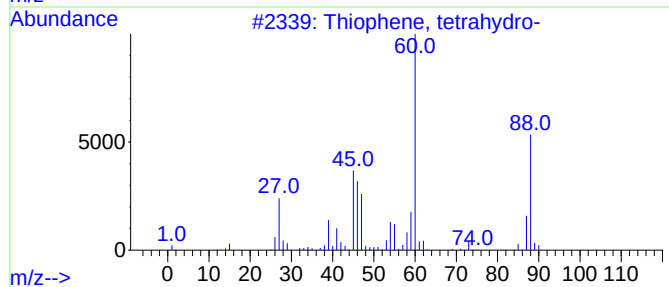
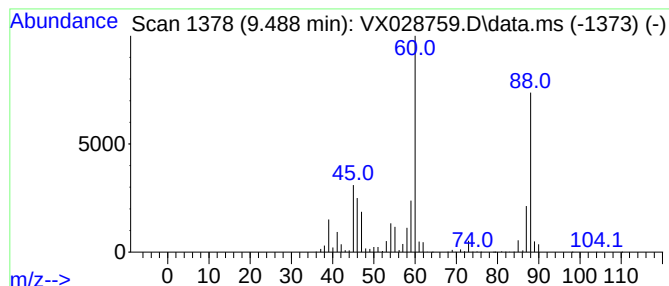
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	75.97 ug/l	2475060	Chlorobenzene-d5	10.055

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	74
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	53
4			Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	35



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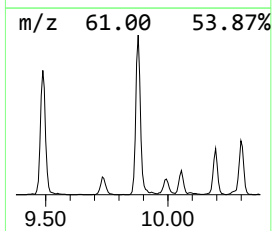
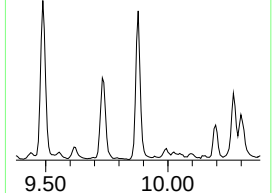
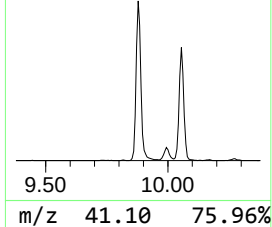
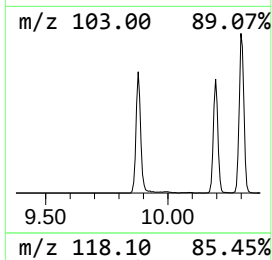
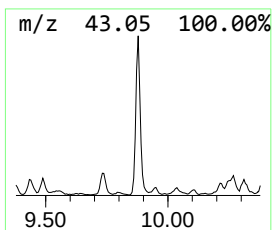
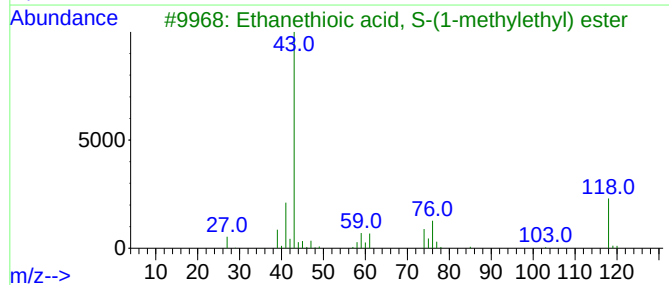
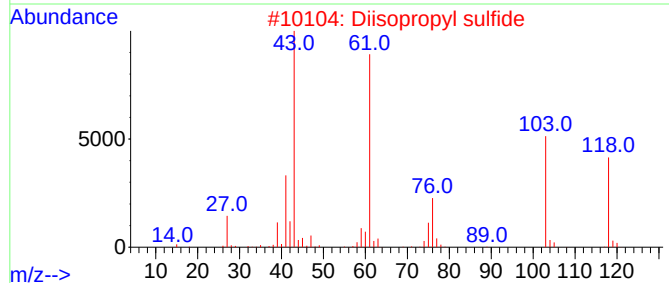
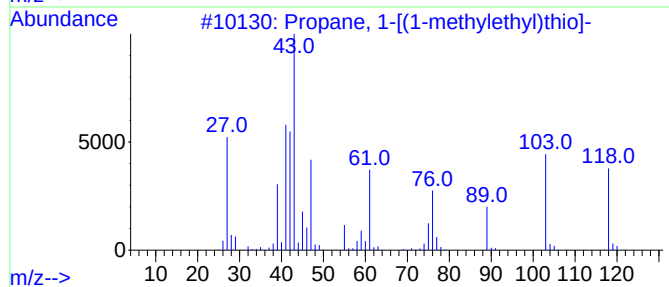
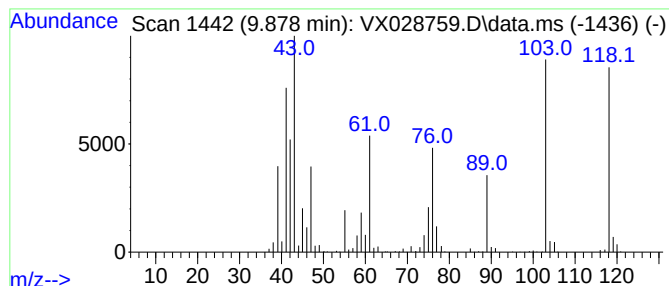
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Quant Title : SW846 8260

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

Peak Number 4 Propane, 1-[(1-methylethyl)... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.878	16.26 ug/l	529705	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-[(1-methylethyl)thio]-	118	C6H14S	005008-73-1	96
2			Diisopropyl sulfide	118	C6H14S	000625-80-9	52
3			Ethanethioic acid, S-(1-methylet...	118	C5H10OS	000926-73-8	35
4			Ethanethioic acid, S-propyl ester	118	C5H10OS	002307-10-0	35
5			Acetamide, N-(aminothioxomethyl)-	118	C3H6N2OS	000591-08-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31769

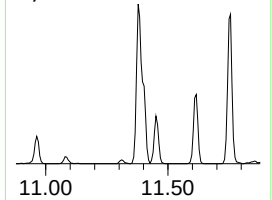
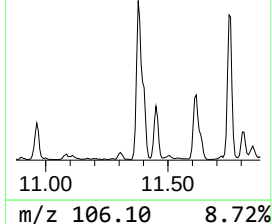
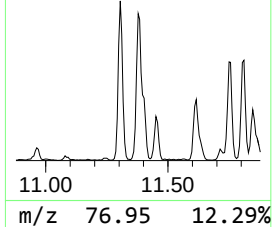
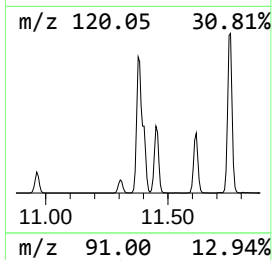
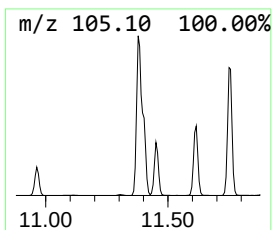
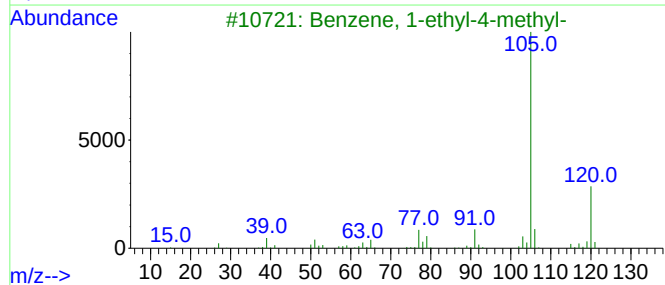
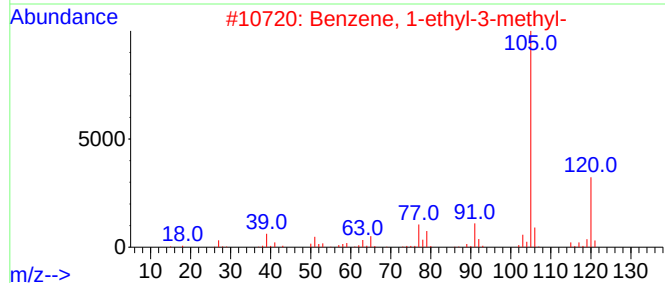
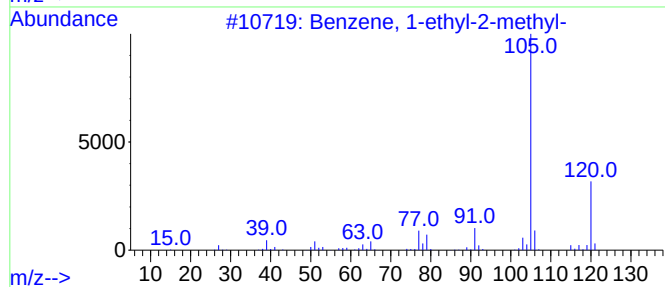
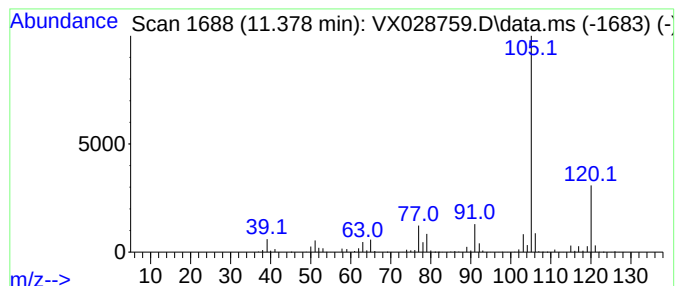
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	40.86 ug/l	1231600	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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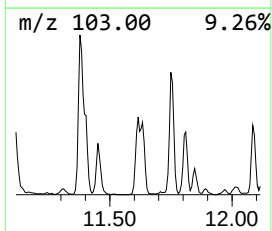
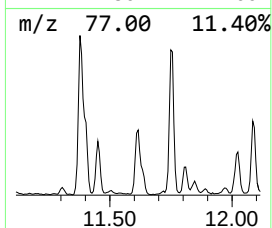
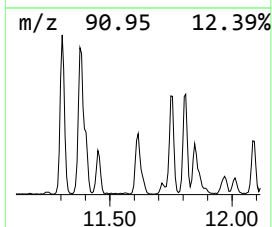
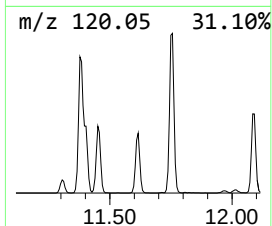
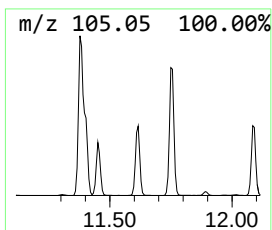
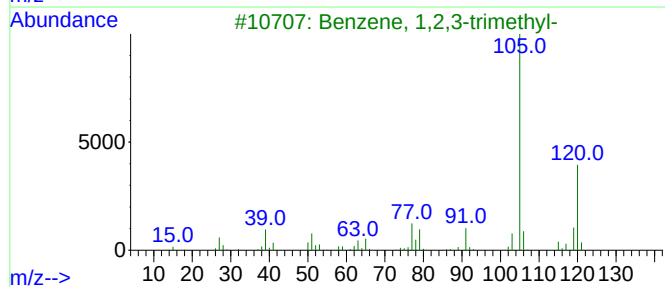
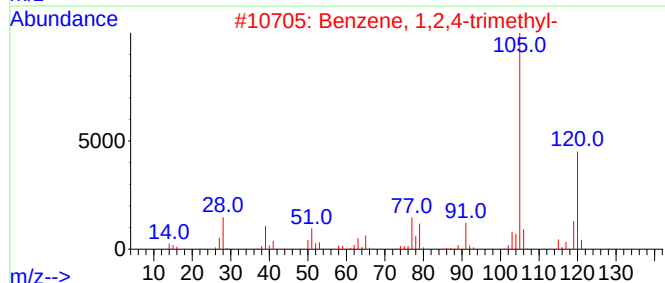
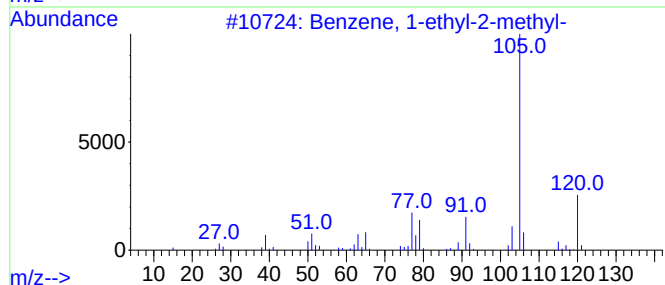
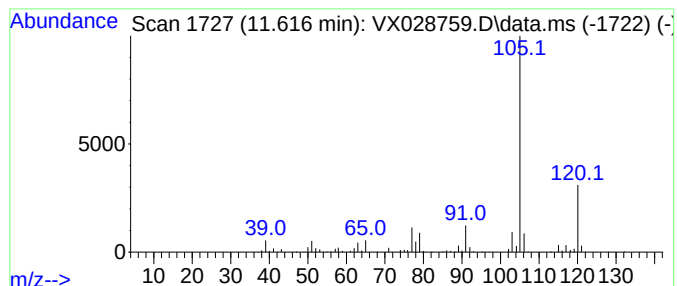
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	18.03 ug/l	543392	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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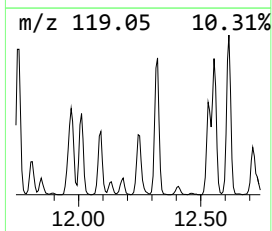
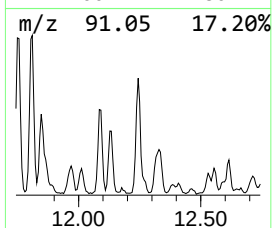
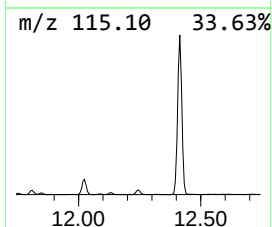
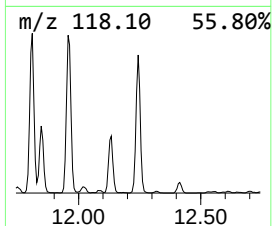
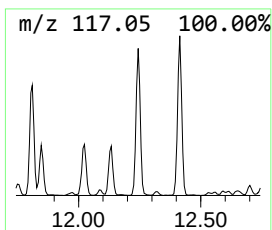
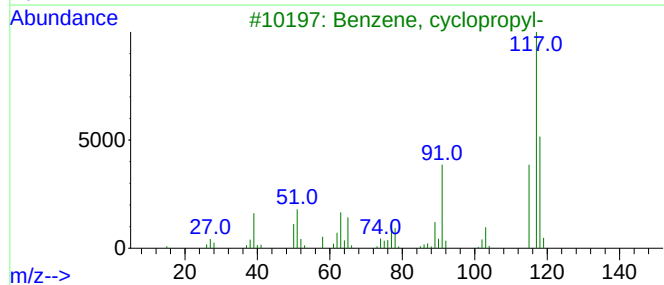
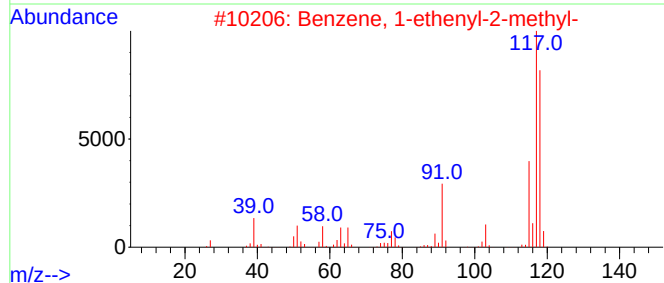
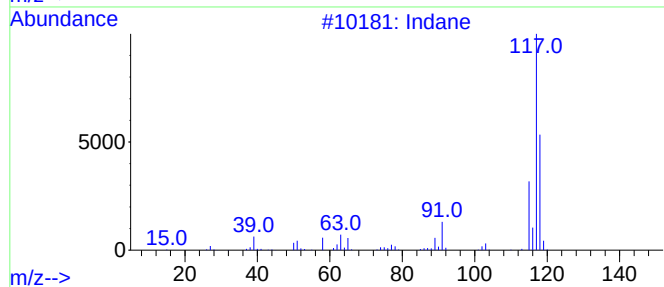
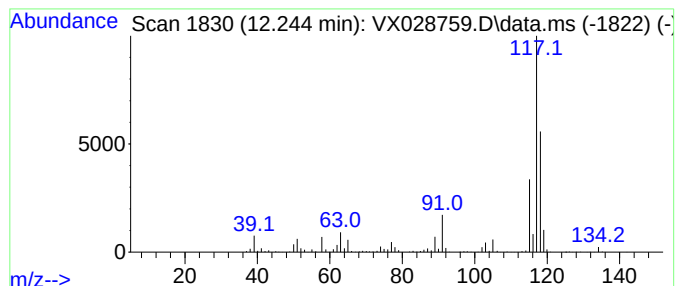
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	18.12 ug/l	546166	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	90
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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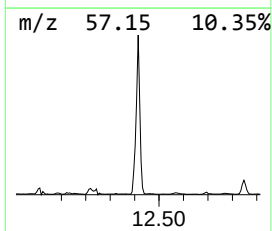
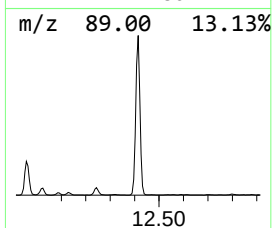
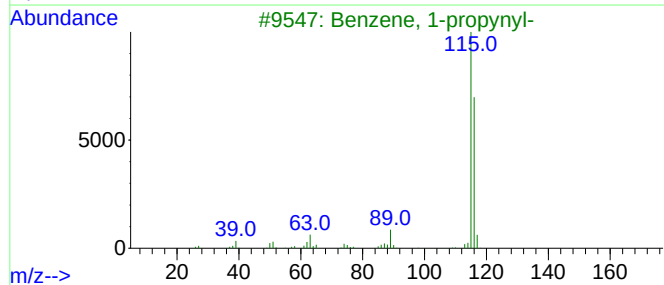
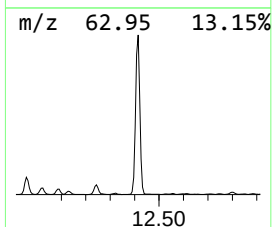
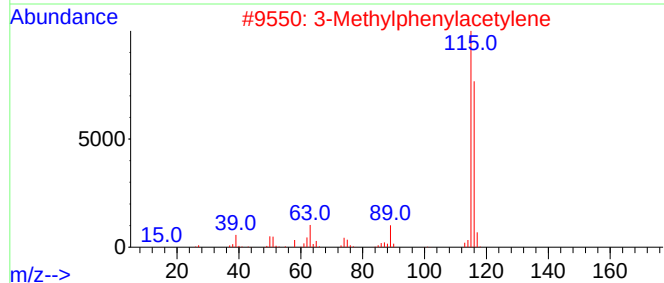
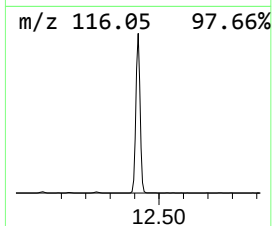
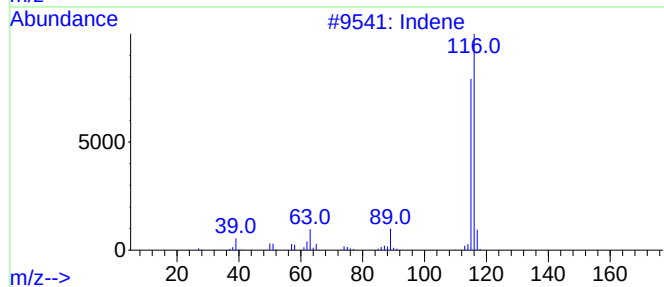
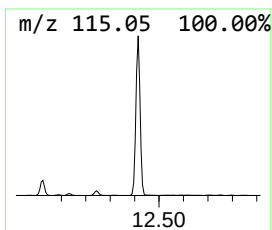
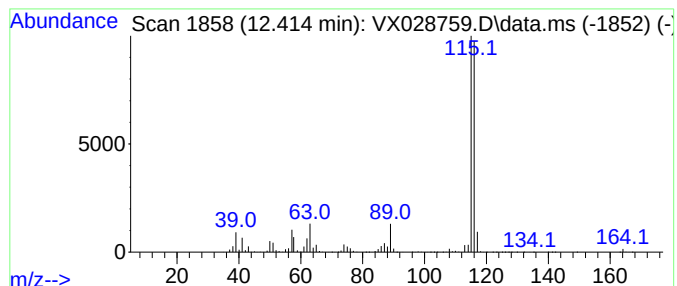
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Quant Title : SW846 8260

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

Peak Number 8 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	160.90 ug/l	4850290	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	94
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	93
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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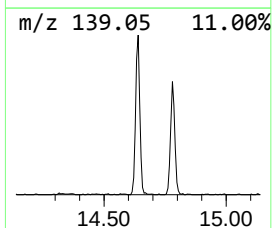
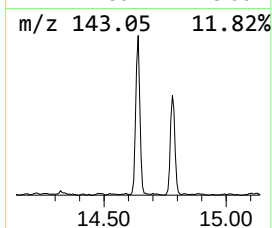
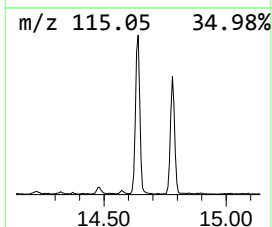
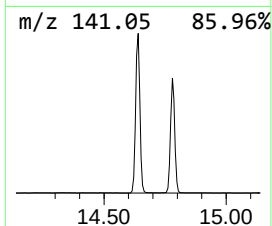
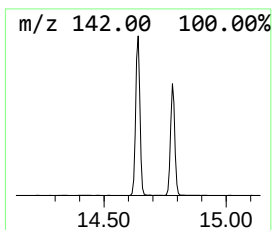
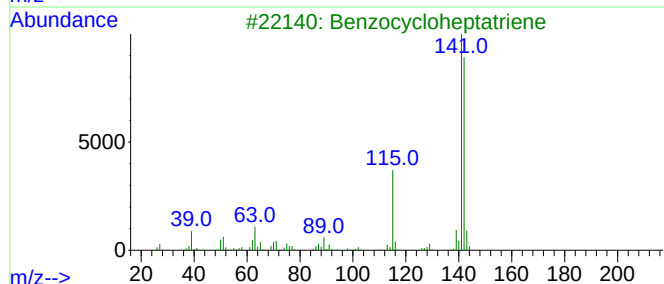
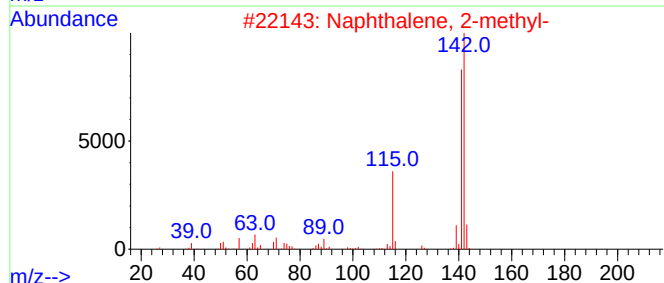
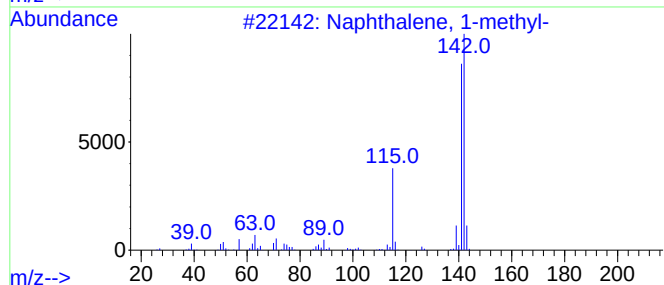
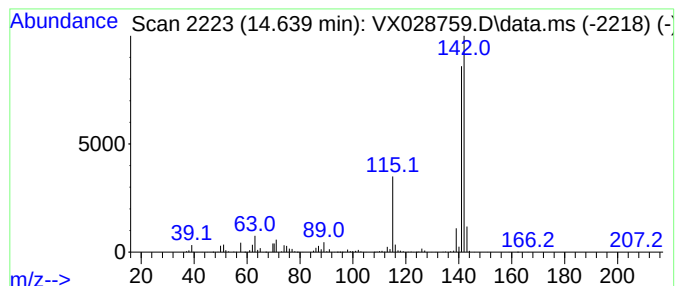
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	24.79 ug/l	747390	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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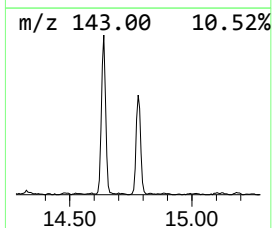
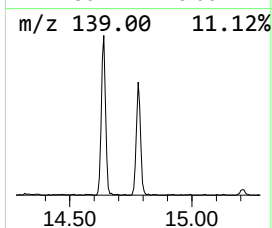
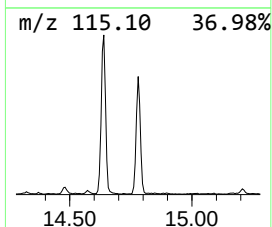
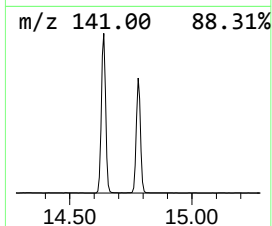
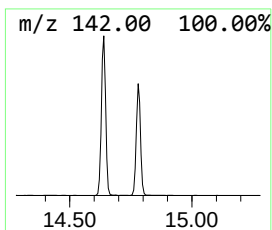
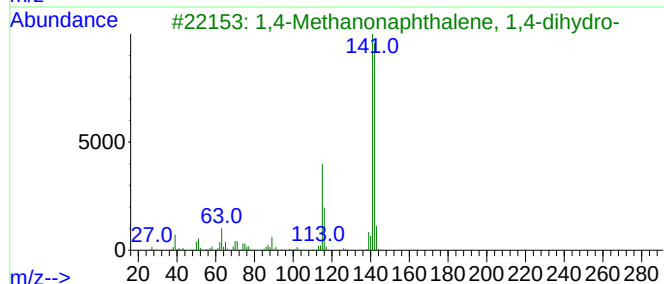
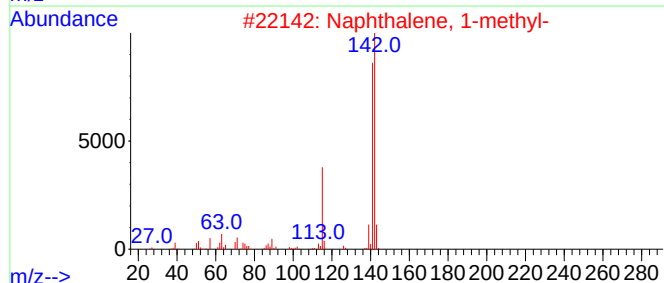
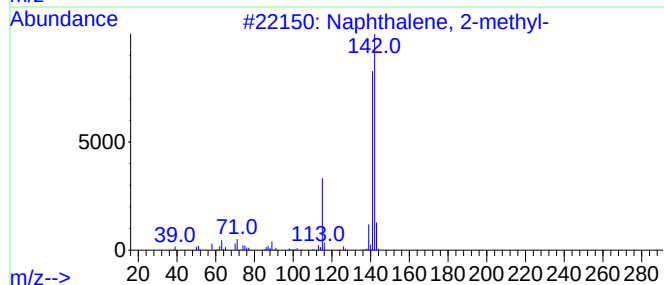
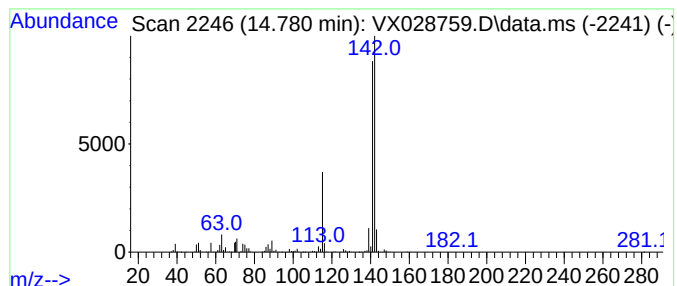
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	17.30 ug/l	521589	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4		Benzocycloheptatriene	142	C11H10	000264-09-5	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028759.D
Acq On : 17 May 2022 15:45
Operator : JC/MD
Sample : N2884-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31769

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
2-Propanethiol,...	3.696	483.2	ug/l	7616690	1	5.556	788138	50.0
Propyl mercaptan	4.196	24.5	ug/l	385912	1	5.556	788138	50.0
Thiophene, tetr...	9.488	76.0	ug/l	2475060	3	10.055	1628880	50.0
Propane, 1-[(1-...	9.878	16.3	ug/l	529705	3	10.055	1628880	50.0
Benzene, 1-ethy...	11.378	40.9	ug/l	1231600	4	12.024	1507210	50.0
Benzene, 1,2,4-...	11.616	18.0	ug/l	543392	4	12.024	1507210	50.0
Indane	12.244	18.1	ug/l	546166	4	12.024	1507210	50.0
Indene	12.414	160.9	ug/l	4850290	4	12.024	1507210	50.0
Naphthalene, 1-...	14.640	24.8	ug/l	747390	4	12.024	1507210	50.0
1,4-Methanonaph...	14.780	17.3	ug/l	521589	4	12.024	1507210	50.0