LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

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: VX028770.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	384035	319089	3.00%	0.434%
2	1.355	40	44	53	rBV	220930	250722	2.36%	0.341%
3	2.374	206	211	224	rVB	225579	372764	3.51%	0.507%
4	2.532	229	237	243	rBV	149719	271567	2.55%	0.369%
5	2.752	266	273	284	rVB	56081	106828	1.00%	0.145%
6	2.965	297	308	325	rBV2	1833046	3986401	37.49%	5.422%
7	3.697	415	428	449	rBV	3947096	10632097	100.00%	14.462%
8	4.196	501	510	523	rBV	221194	593835	5.59%	0.808%
9	4.556	561	569	581	rVB	86052	232909	2.19%	0.317%
10	4.995	630	641	658	rBV	65103	222096	2.09%	0.302%
11	5.385	693	705	716	rBV2	207898	613212	5.77%	0.834%
12	5.556	723	733	749	rVB	320008	920531	8.66%	1.252%
13	5.958	789	799	805	rBV2	211215	574234	5.40%	0.781%
14	6.044	805	813	831	rVV	1342214	4125483	38.80%	5.611%
15	6.202	831	839	851	rVV2	48857	156086	1.47%	0.212%
16	6.336	852	861	878	rVB2	116958	397774	3.74%	0.541%
17	6.763	921	931	951	rBV	531711	1259871	11.85%	1.714%
18	7.464	1040	1046	1053	rBV3	34785	110109	1.04%	0.150%
19	7.690	1072	1083	1098	rVB	113022	257470	2.42%	0.350%
20	8.336	1182	1189	1197	rBV	119176	206240	1.94%	0.281%
21	8.574	1222	1228	1234	rBV	109263	187678	1.77%	0.255%
22	8.653	1234	1241	1246	rVV	1054405	1694394	15.94%	2.305%
23	8.720	1246	1252	1260	rVB	3030612	4521277	42.52%	6.150%
24	8.854	1269	1274	1282	rVB2	68323	134325	1.26%	0.183%
25	9.019	1296	1301	1305	rBV2	62567	125655	1.18%	0.171%
26	9.068	1305	1309	1315	rVV	306961	470755	4.43%	0.640%
27	9.488	1373	1378	1387	rVV	1442659	2048412	19.27%	2.786%
28	9.732	1413	1418	1427	rVB	135303	210256	1.98%	0.286%
29	9.878	1436	1442	1449	rBV	353151	483688	4.55%	0.658%
30	10.055	1464	1471	1482	rVB	1210224	1611393	15.16%	2.192%
31	10.195	1488	1494	1500	rBV	2785900	3574613	33.62%	4.862%
32	10.269	1501	1506	1507	rBV	225756	253083	2.38%	0.344%
33	10.299	1507	1511	1521	rVB	2707554	3789932	35.65%	5.155%
34	10.415	1521	1530	1532	rBV	209907	335218	3.15%	0.456%
35	10.653	1563	1569	1578	rVB2	2038474	3698828	34.79%	5.031%
36	10.750	1578	1585	1591	rBV4	95221	170279	1.60%	0.232%

LSC Area Percent Report

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Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

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

37	10.903	1604	1610	1614	rVB	170813	233591	2.20%	0.318%
38	10.964	1614	1620	1625	rBV2	166154	262835	2.47%	0.358%
39	11.079	1634	1639	1649	rBV	1087146	1564327	14.71%	2.128%
40	11.171	1650	1654	1661	rVB2	90449	136812	1.29%	0.186%
41	11.305	1672	1676	1683	rVB	109018	145121	1.36%	0.197%
42	11.378	1683	1688	1695	rBV	846223	1476114	13.88%	2.008%
43	11.451	1695	1700	1704	rVV	302159	446225	4.20%	0.607%
44	11.494	1704	1707	1712	rVB4	80511	120809	1.14%	0.164%
45	11.616	1722	1727	1734	rBV	368096	578445	5.44%	0.787%
46	11.756	1745	1750	1754	rVB	788964	983620	9.25%	1.338%
47	11.811	1754	1759	1762	rBV	362660	471457	4.43%	0.641%
48	11.848	1762	1765	1770	rVB2	146107	181831	1.71%	0.247%
49	11.957	1779	1783	1788	rVB2	245087	344428	3.24%	0.468%
50	12.024	1788	1794	1801	rBV	1352478	1741205	16.38%	2.368%
51	12.085	1801	1804	1809	rVV	388345	505428	4.75%	0.687%
52	12.134	1809	1812	1822	rVB	149856	227156	2.14%	0.309%
53	12.244	1822	1830	1838	rBV2	404228	649297	6.11%	0.883%
54	12.317	1838	1842	1852	rVB3	106912	192404	1.81%	0.262%
55	12.414	1852	1858	1863	rBV	3896849	4820100	45.34%	6.556%
56	12.555	1879	1881	1885	rVV2	84424	109101	1.03%	0.148%
57	12.799	1917	1921	1926	rVV	216692	269862	2.54%	0.367%
58	12.963	1944	1948	1951	rBV2	128570	162963	1.53%	0.222%
59	13.286	1997	2001	2006	rVB3	155350	215826	2.03%	0.294%
60	13.341	2006	2010	2017	rVB	121446	162660	1.53%	0.221%
61	13.426	2018	2024	2030	rVB	185667	248835	2.34%	0.338%
62	13.506	2033	2037	2046	rBV5	66779	111609	1.05%	0.152%
63	13.713	2068	2071	2076	rVB	86949	112276	1.06%	0.153%
64	13.774	2076	2081	2088	rVV	4648124	6038055	56.79%	8.213%
65	13.872	2093	2097	2103	rVB	151581	203095	1.91%	0.276%
66	14.640	2218	2223	2232	rVB	673495	855807	8.05%	1.164%
67	14.780	2241	2246	2252	rBV	483219	601408	5.66%	0.818%
68	15.207	2311	2316	2321	rVB	113267	146798	1.38%	0.200%
69	15.481	2355	2361	2371	rBV	65920	121604	1.14%	0.165%
70	15.615	2375	2383	2386	rVV2	94578	159419	1.50%	0.217%

Sum of corrected areas: 73519627

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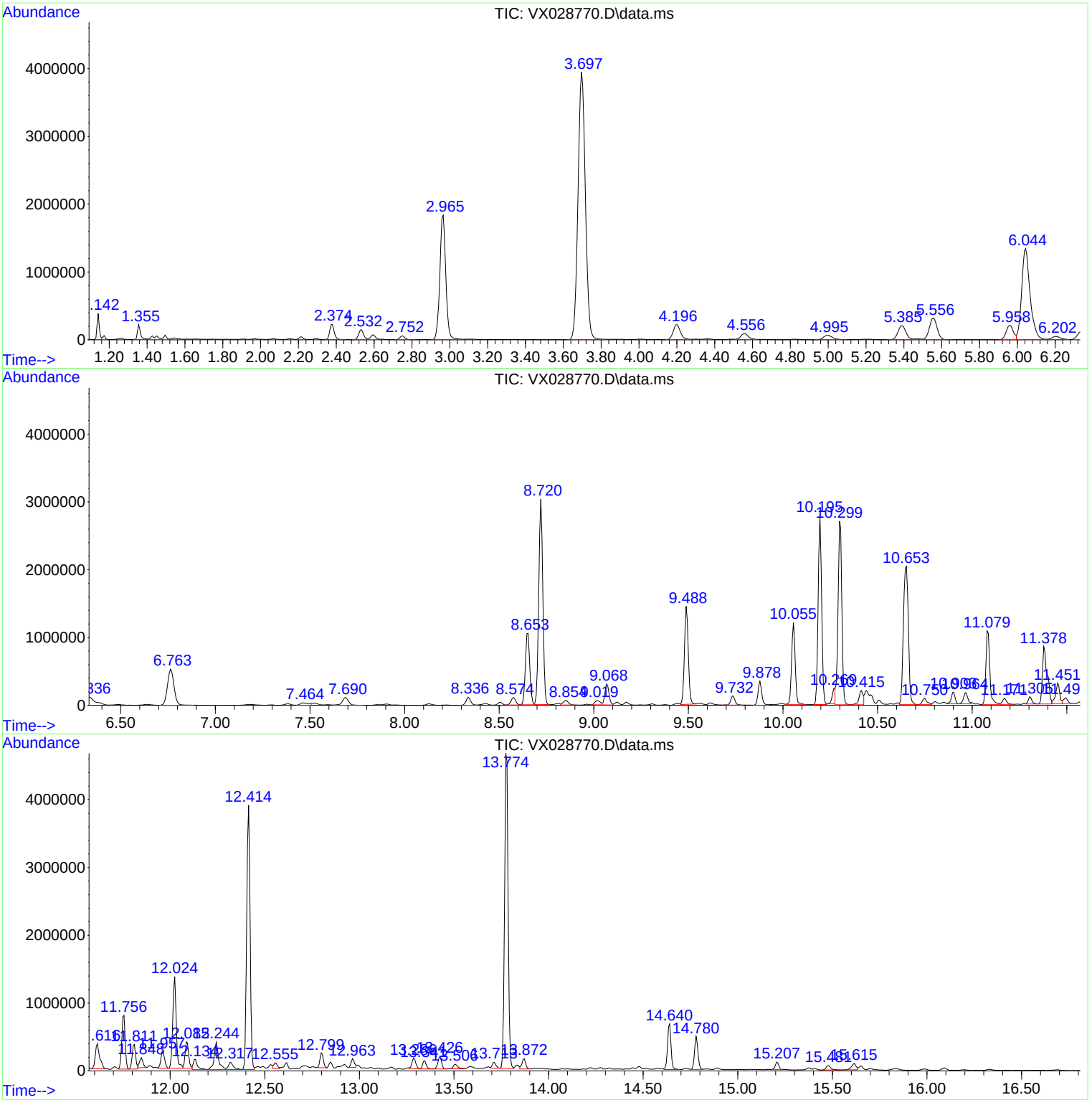
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

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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Data File : VX028770.D
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ClientSampleId :
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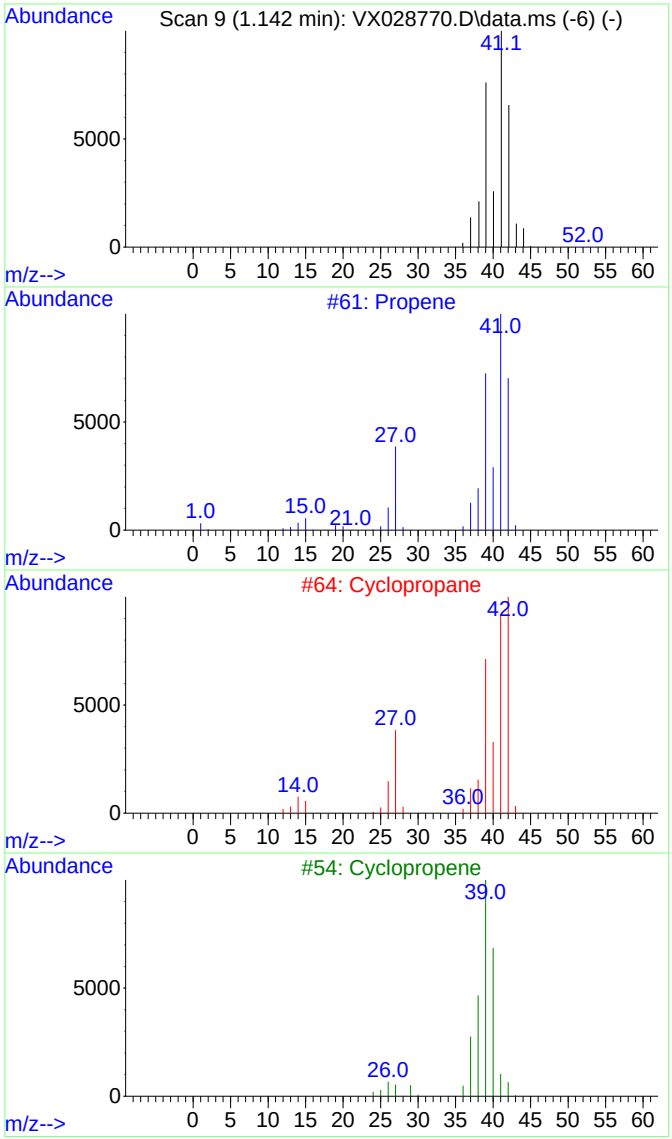
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

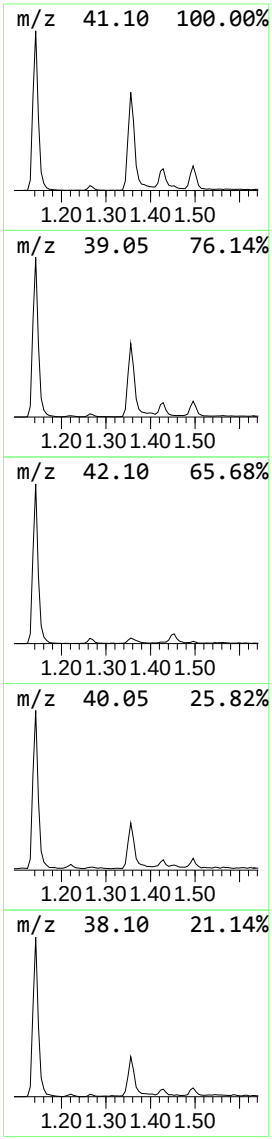
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	17.33 ug/l	319089	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Cyclopropane	42	C3H6	000075-19-4	9
3	Cyclopropene	40	C3H4	002781-85-3	9
4	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4
5	4-Amino-1-butanol	89	C4H11NO	013325-10-5	1





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

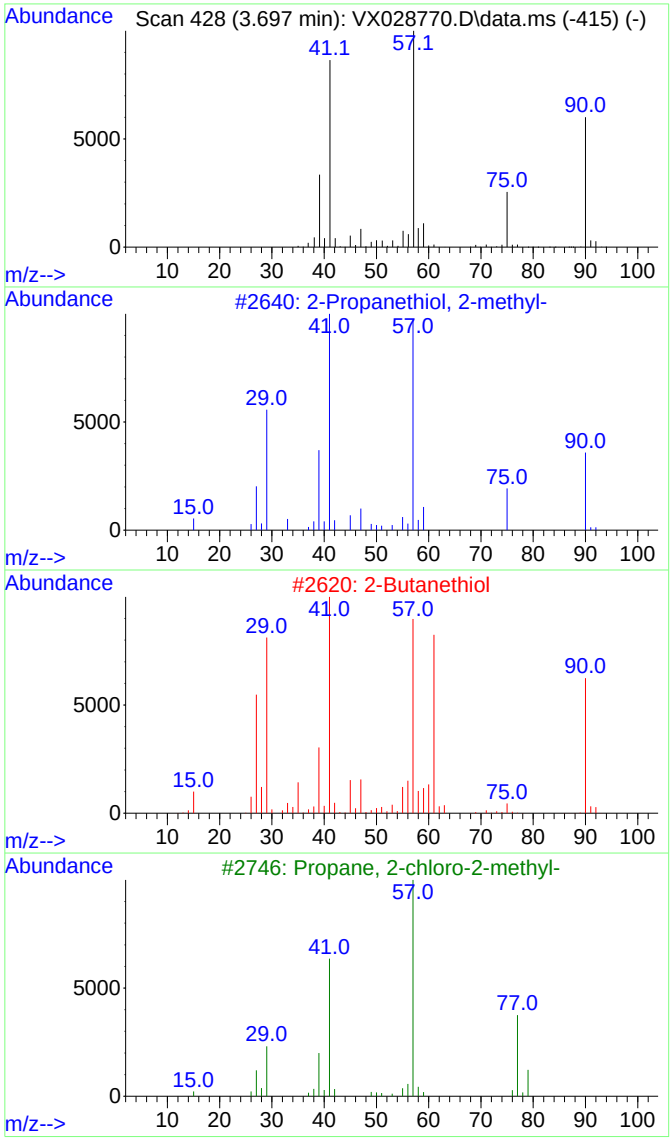
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

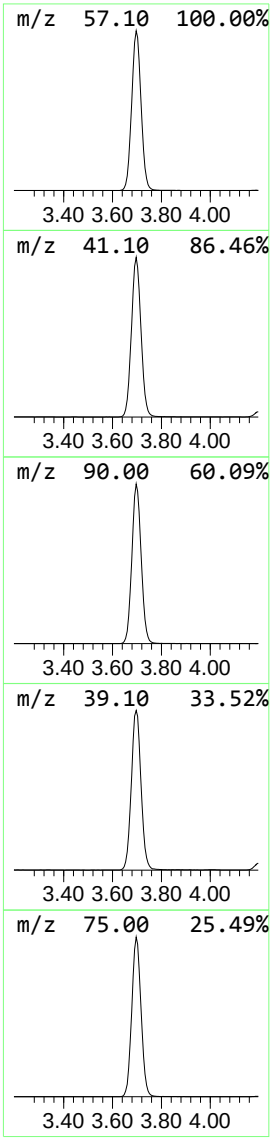
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.697	577.50 ug/l	10632100	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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Data File : VX028770.D
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

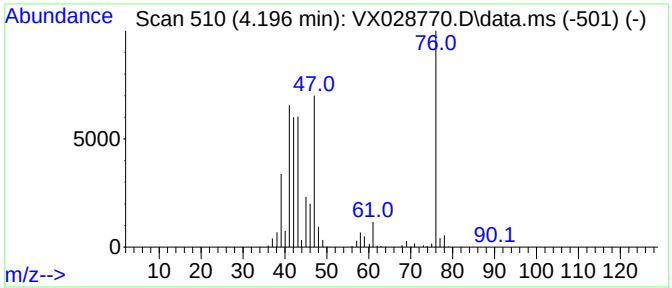
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

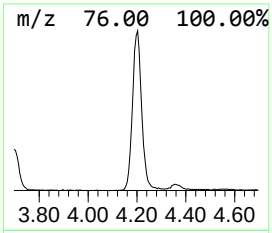
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

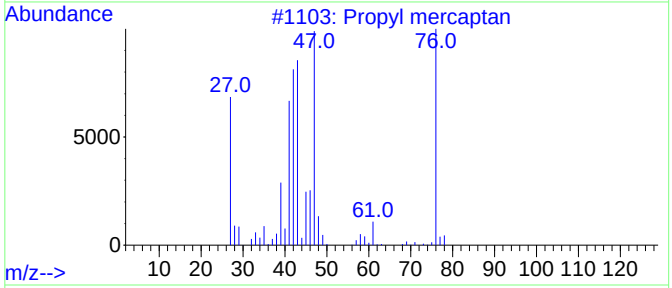
****
Peak Number 3 Propyl mercaptan Concentration Rank 5

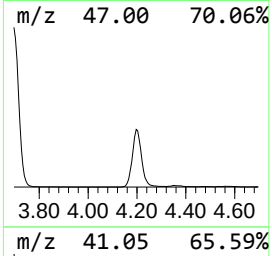
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.196	32.26 ug/l	593835	Pentafluorobenzene	5.556

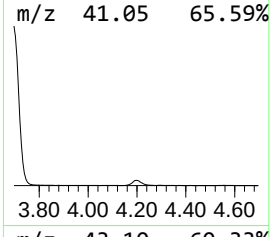
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	97
2	Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	74
3	Thiourea	76	CH4N2S	000062-56-6	53
4	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9
5	Isopropyl phosphine	76	C3H9P	004538-29-8	7

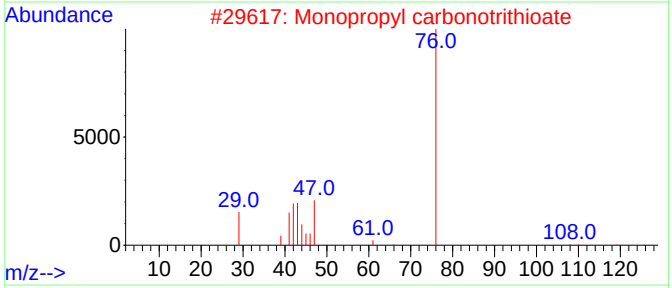


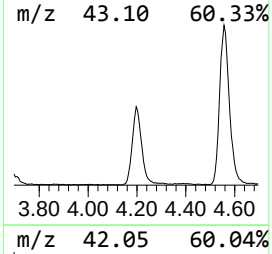


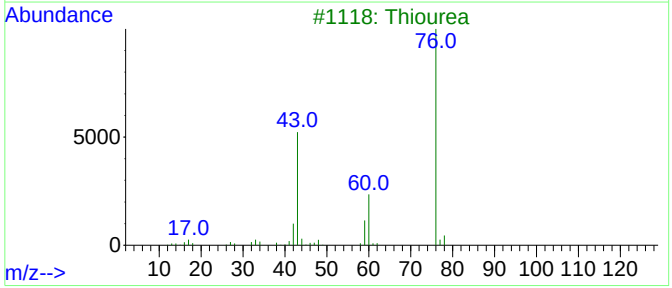


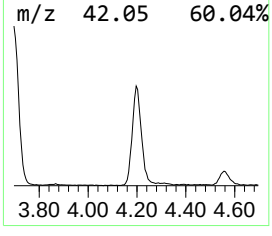












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Instrument :
MSVOA_X
ClientSampleId :
31770

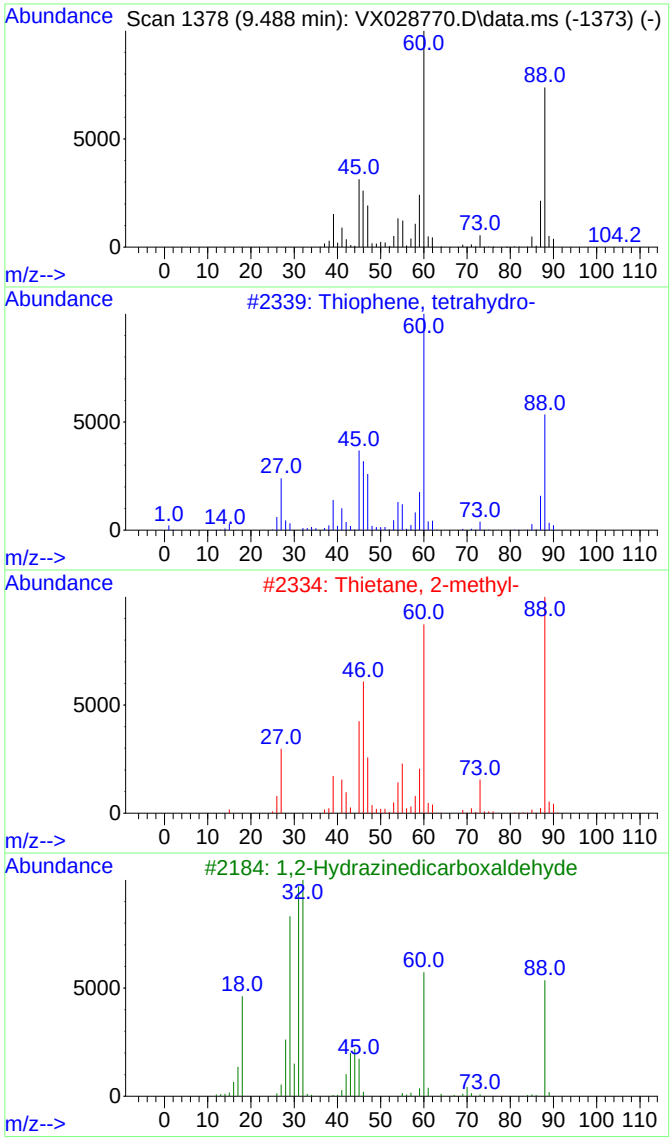
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

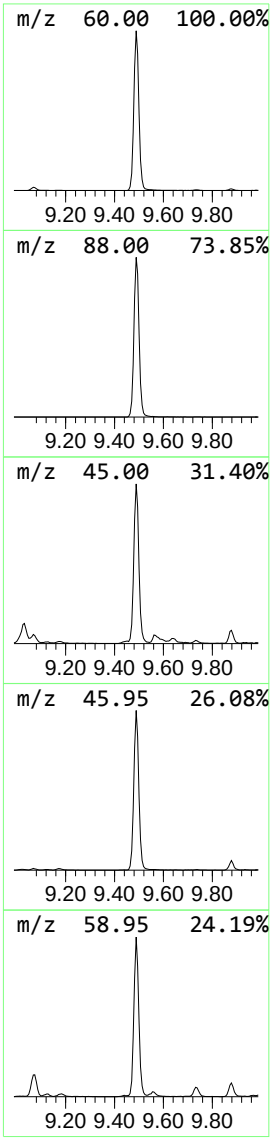
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	63.56 ug/l	2048410	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	83
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	38





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MSVOA_X
ClientSampleId :
31770

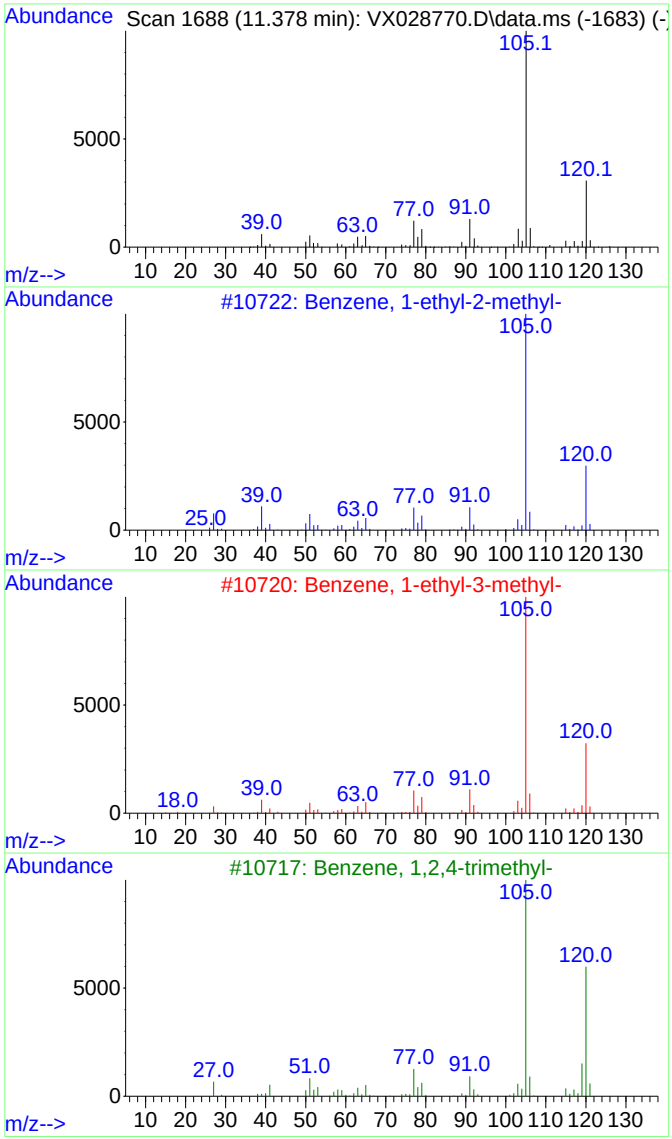
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

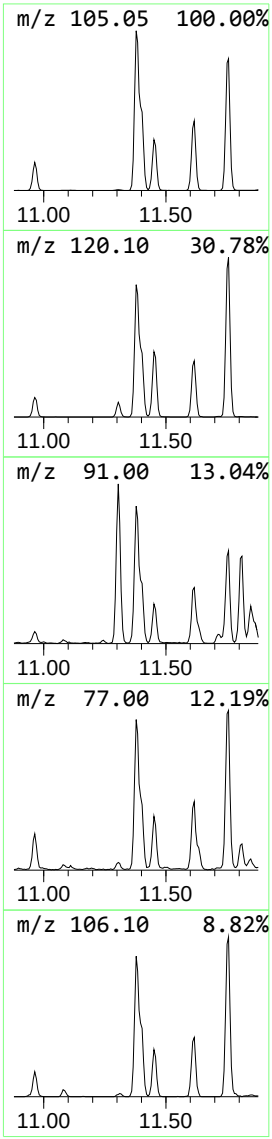
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	42.39 ug/l	1476110	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	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

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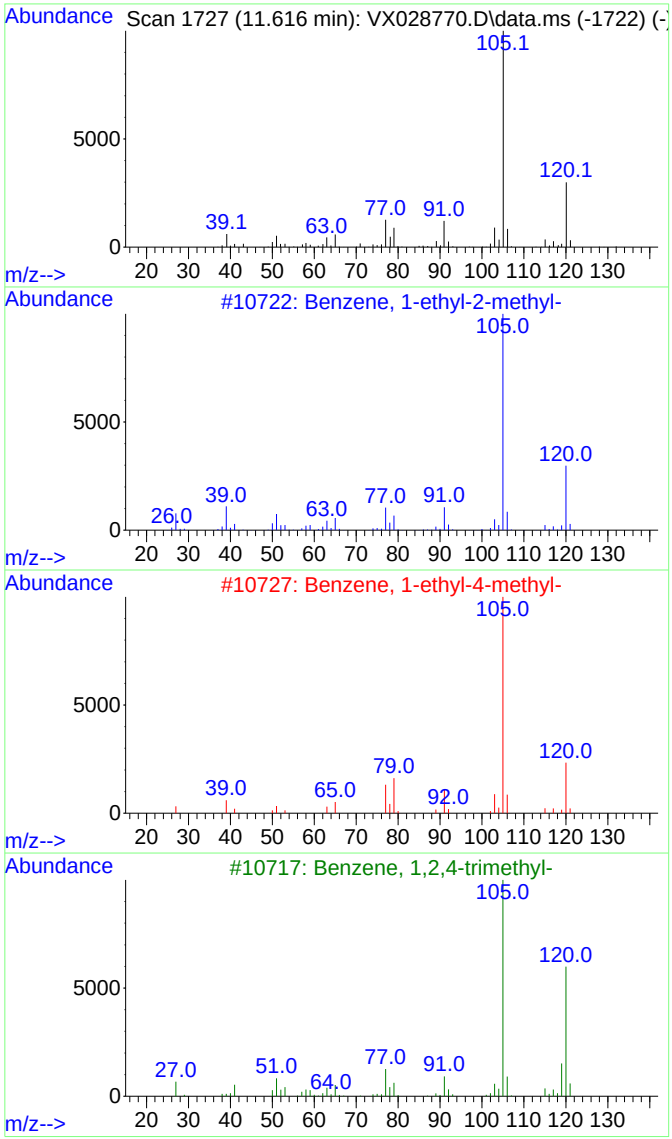
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

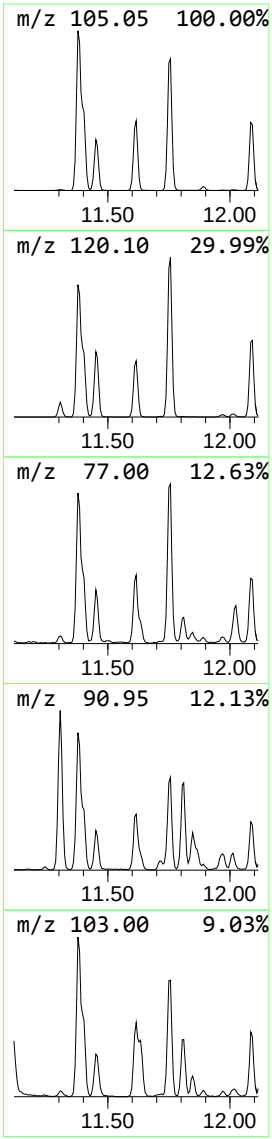
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	16.61 ug/l	578445	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-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

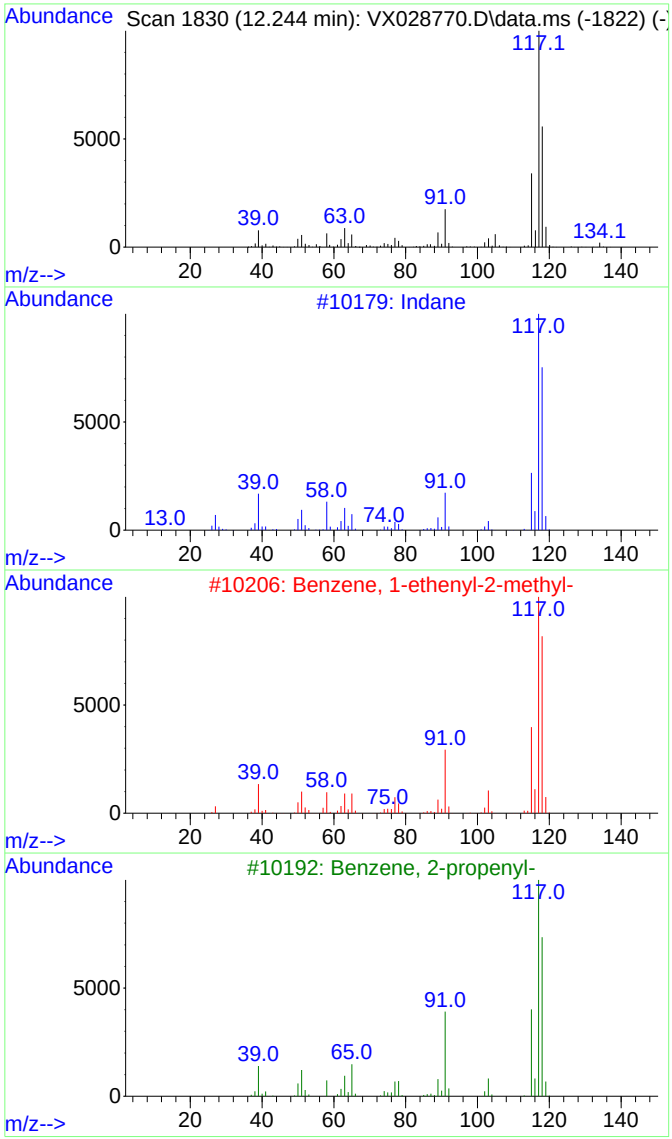
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

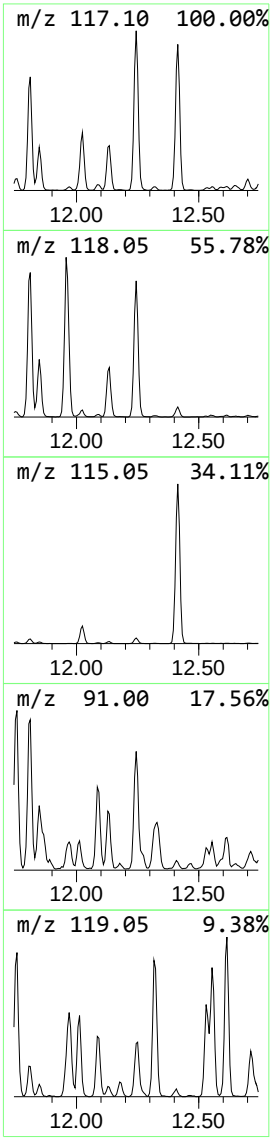
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	18.65 ug/l	649297	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	74
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

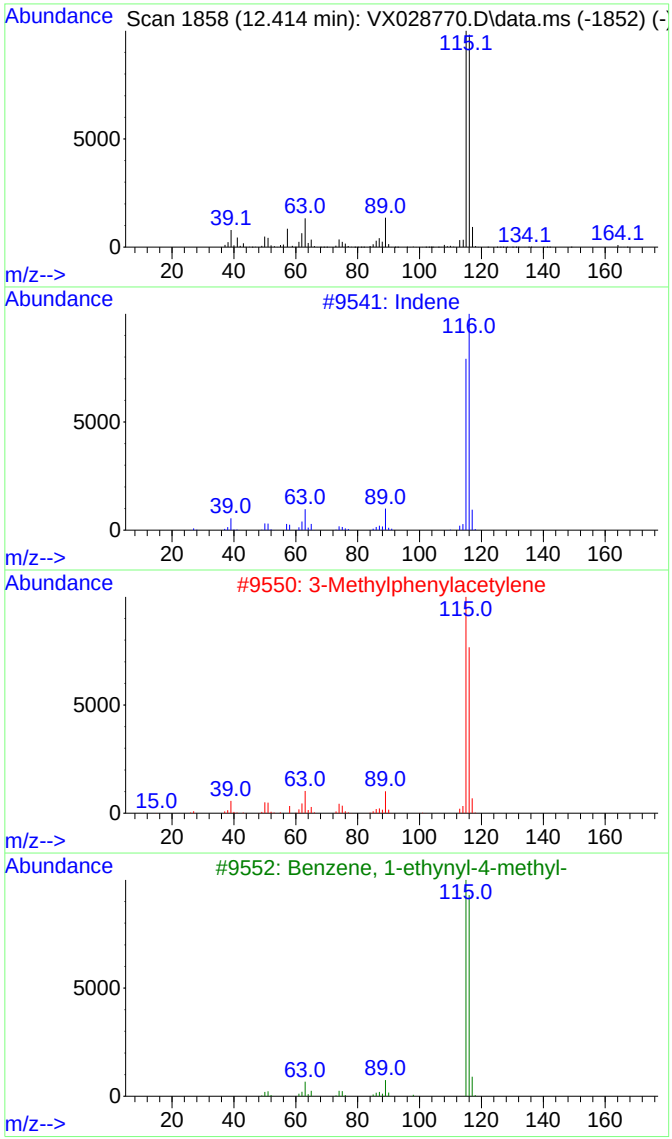
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

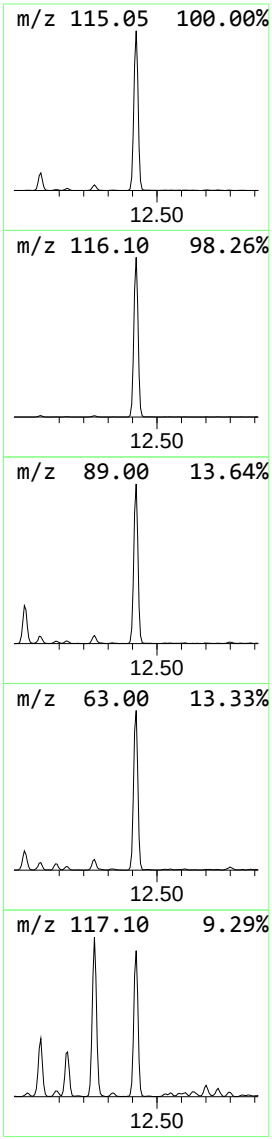
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	138.41 ug/l	4820100	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	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

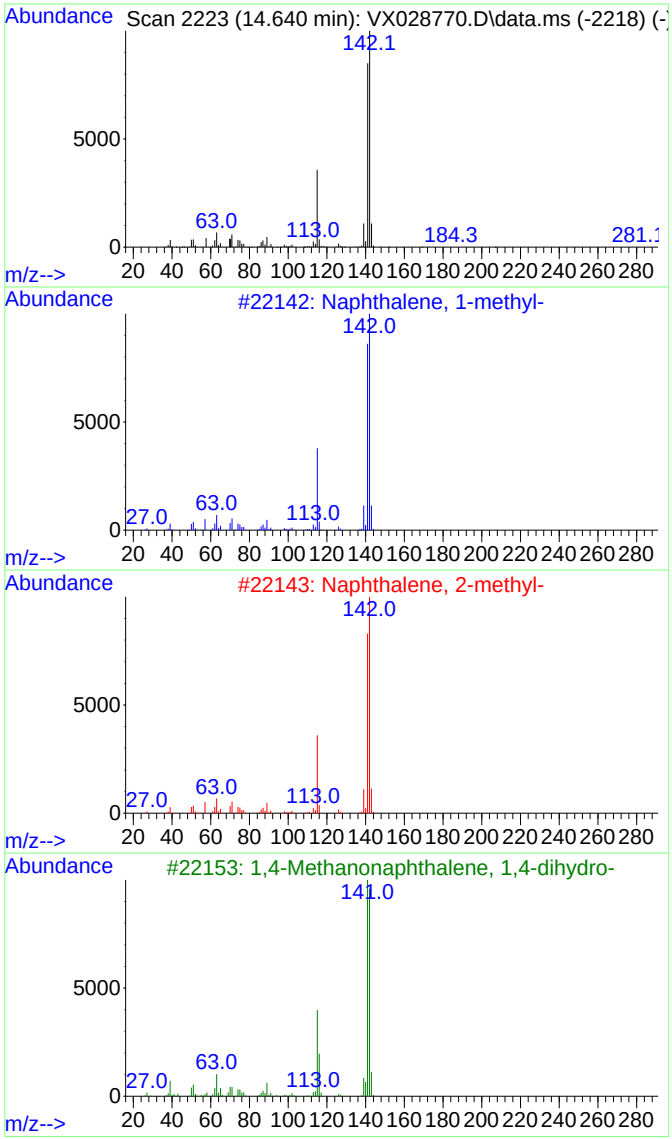
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

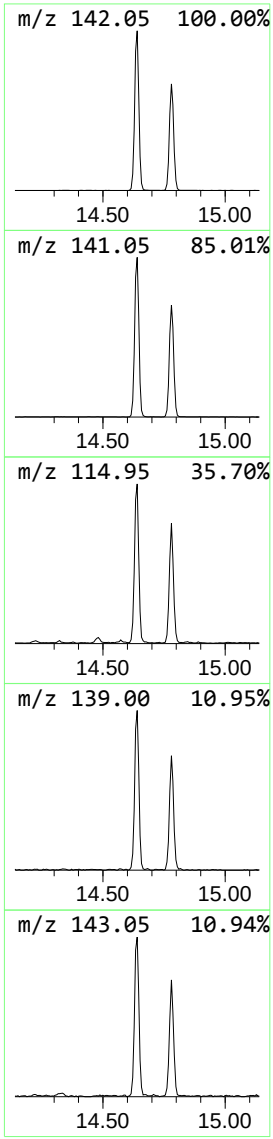
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	24.58 ug/l	855807	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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

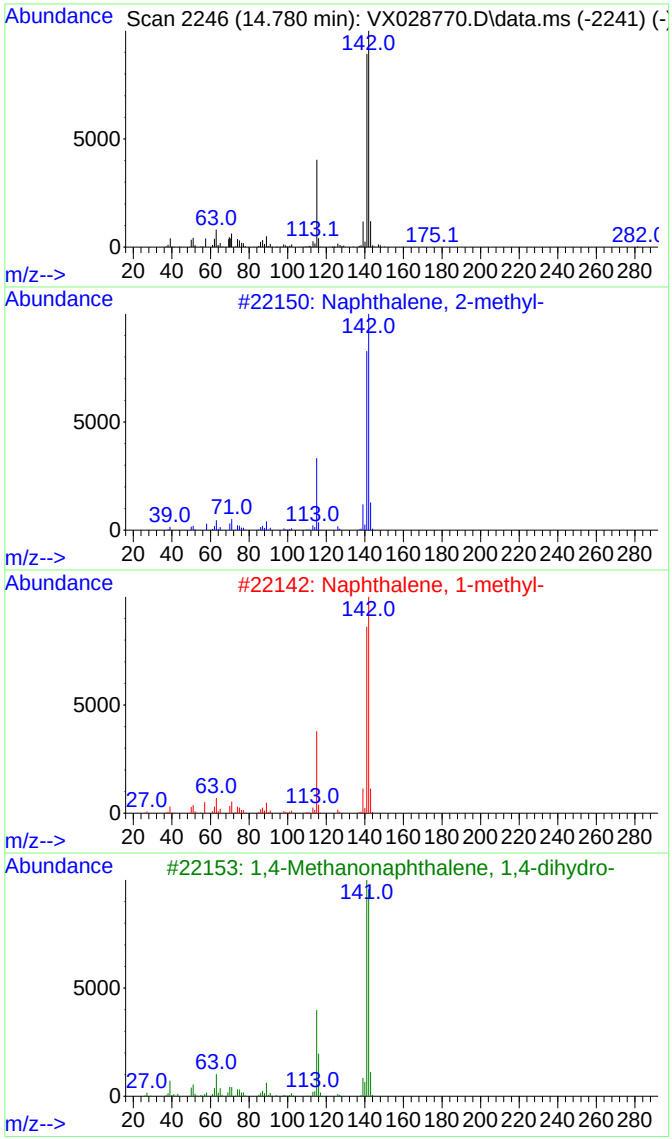
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

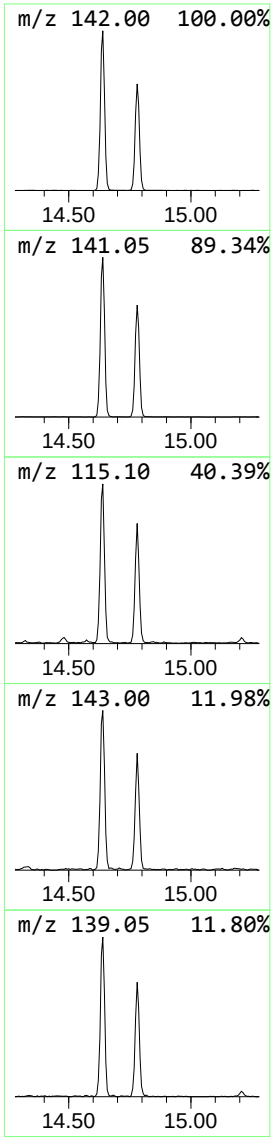
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	17.27 ug/l	601408	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	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028770.D
Acq On : 17 May 2022 20:02
Operator : JC/MD
Sample : N2884-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31770

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propene	1.142	17.3	ug/l	319089	1	5.556	920531	50.0
2-Propanethiol,...	3.697	577.5	ug/l	10632100	1	5.556	920531	50.0
Propyl mercaptan	4.196	32.3	ug/l	593835	1	5.556	920531	50.0
Thiophene, tetr...	9.488	63.6	ug/l	2048410	3	10.055	1611390	50.0
Benzene, 1-ethy...	11.378	42.4	ug/l	1476110	4	12.024	1741210	50.0
Benzene, 1-ethy...	11.616	16.6	ug/l	578445	4	12.024	1741210	50.0
Indane	12.244	18.6	ug/l	649297	4	12.024	1741210	50.0
Indene	12.415	138.4	ug/l	4820100	4	12.024	1741210	50.0
Naphthalene, 1-...	14.640	24.6	ug/l	855807	4	12.024	1741210	50.0
1,4-Methanonaph...	14.780	17.3	ug/l	601408	4	12.024	1741210	50.0