LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
Sample : N2884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

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: VX028757.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	245649	201286	3.33%	0.344%
2	1.355	40	44	53	rBV	191705	222204	3.67%	0.380%
3	2.379	206	212	224	rBV	71621	123267	2.04%	0.211%
4	2.532	230	237	243	rBV	171549	311175	5.15%	0.532%
5	2.593	243	247	254	rVB	62558	103178	1.71%	0.176%
6	2.751	266	273	283	rVB	40093	74616	1.23%	0.127%
7	2.965	298	308	327	rBV2	985196	2225485	36.80%	3.803%
8	3.696	416	428	446	rBV	2254429	6047475	100.00%	10.333%
9	3.843	446	452	470	rVB2	40987	118154	1.95%	0.202%
10	4.202	500	511	524	rBV	95000	269492	4.46%	0.460%
11	4.995	631	641	655	rBV2	49926	164492	2.72%	0.281%
12	5.391	694	706	717	rBV	182509	529184	8.75%	0.904%
13	5.556	723	733	751	rVB	270722	783905	12.96%	1.339%
14	5.958	789	799	805	rBV	193090	500859	8.28%	0.856%
15	6.043	805	813	831	rVV	1041916	3017185	49.89%	5.155%
16	6.202	831	839	851	rVV3	36606	117036	1.94%	0.200%
17	6.336	851	861	879	rVB2	90656	316847	5.24%	0.541%
18	6.763	922	931	945	rBV	455031	1070577	17.70%	1.829%
19	7.208	988	1004	1013	rBV5	35281	100007	1.65%	0.171%
20	7.470	1040	1047	1052	rBV2	22571	64370	1.06%	0.110%
21	7.690	1073	1083	1092	rVB2	85393	187565	3.10%	0.320%
22	8.336	1182	1189	1198	rBV	92005	167876	2.78%	0.287%
23	8.574	1222	1228	1235	rBV	137188	240125	3.97%	0.410%
24	8.653	1235	1241	1246	rVV	1025135	1598972	26.44%	2.732%
25	8.720	1246	1252	1263	rVB	3640994	5354984	88.55%	9.150%
26	8.854	1269	1274	1281	rVB3	56936	109682	1.81%	0.187%
27	9.019	1296	1301	1305	rBV2	48818	95827	1.58%	0.164%
28	9.067	1305	1309	1315	rVV	223972	349818	5.78%	0.598%
29	9.488	1372	1378	1387	rBV	1424564	2032364	33.61%	3.473%
30	9.732	1413	1418	1427	rVB	86993	135268	2.24%	0.231%
31	9.878	1437	1442	1450	rBV	260805	354336	5.86%	0.605%
32	10.055	1464	1471	1482	rVB	1117839	1500614	24.81%	2.564%
33	10.195	1489	1494	1500	rBV	2195201	2783625	46.03%	4.756%
34	10.299	1500	1511	1522	rVV	2562456	3770090	62.34%	6.442%
35	10.415	1522	1530	1532	rVV	135987	211166	3.49%	0.361%
36	10.439	1532	1534	1542	rVV5	128191	268219	4.44%	0.458%

LSC Area Percent Report

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

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	10.652	1563	1569	1579	rVB2	1744419	3093878	51.16%	5.286%
38	10.750	1579	1585	1590	rBV3	66782	112887	1.87%	0.193%
39	10.902	1605	1610	1614	rVB	114240	152050	2.51%	0.260%
40	10.969	1614	1621	1634	rVB3	102814	221307	3.66%	0.378%
41	11.079	1634	1639	1650	rBV	839924	1159208	19.17%	1.981%
42	11.171	1650	1654	1662	rVB2	53307	80461	1.33%	0.137%
43	11.305	1672	1676	1682	rVB	60128	81826	1.35%	0.140%
44	11.378	1683	1688	1695	rBV	546016	943704	15.60%	1.612%
45	11.451	1695	1700	1704	rVV	182448	282477	4.67%	0.483%
46	11.494	1704	1707	1712	rVB4	59779	96332	1.59%	0.165%
47	11.616	1722	1727	1738	rVB2	243667	436202	7.21%	0.745%
48	11.750	1745	1749	1754	rVB	516868	632962	10.47%	1.081%
49	11.811	1754	1759	1762	rBV	359490	460605	7.62%	0.787%
50	11.847	1762	1765	1770	rVB	178992	215402	3.56%	0.368%
51	11.957	1779	1783	1788	rVB2	193630	264558	4.37%	0.452%
52	12.024	1788	1794	1801	rBV	1108108	1432831	23.69%	2.448%
53	12.085	1801	1804	1809	rVV	248997	327819	5.42%	0.560%
54	12.128	1809	1811	1822	rVB	117239	175552	2.90%	0.300%
55	12.244	1822	1830	1838	rBV2	319558	555869	9.19%	0.950%
56	12.317	1838	1842	1852	rVB3	54706	110656	1.83%	0.189%
57	12.414	1853	1858	1864	rBV	3800822	4491770	74.28%	7.675%
58	12.798	1917	1921	1927	rBV	162470	237247	3.92%	0.405%
59	12.969	1944	1949	1957	rVB5	104671	243373	4.02%	0.416%
60	13.292	1995	2002	2007	rVB4	116019	192681	3.19%	0.329%
61	13.341	2007	2010	2014	rBV	118640	150574	2.49%	0.257%
62	13.390	2014	2018	2020	rVV	59369	83432	1.38%	0.143%
63	13.426	2020	2024	2032	rVB	181018	297321	4.92%	0.508%
64	13.506	2033	2037	2042	rBV3	58137	87035	1.44%	0.149%
65	13.713	2067	2071	2073	rVV	76091	121198	2.00%	0.207%
66	13.780	2077	2082	2088	rVV	3681095	4989697	82.51%	8.526%
67	13.841	2088	2092	2094	rVV2	91035	138716	2.29%	0.237%
68	13.871	2094	2097	2101	rVB	123229	145974	2.41%	0.249%
69	14.639	2215	2223	2232	rVB	368260	498219	8.24%	0.851%
70	14.780	2240	2246	2252	rVB	279849	360694	5.96%	0.616%
71	15.206	2311	2316	2321	rVB	49537	68678	1.14%	0.117%
72	15.615	2375	2383	2386	rBV2	35059	61893	1.02%	0.106%

Sum of corrected areas: 58526413

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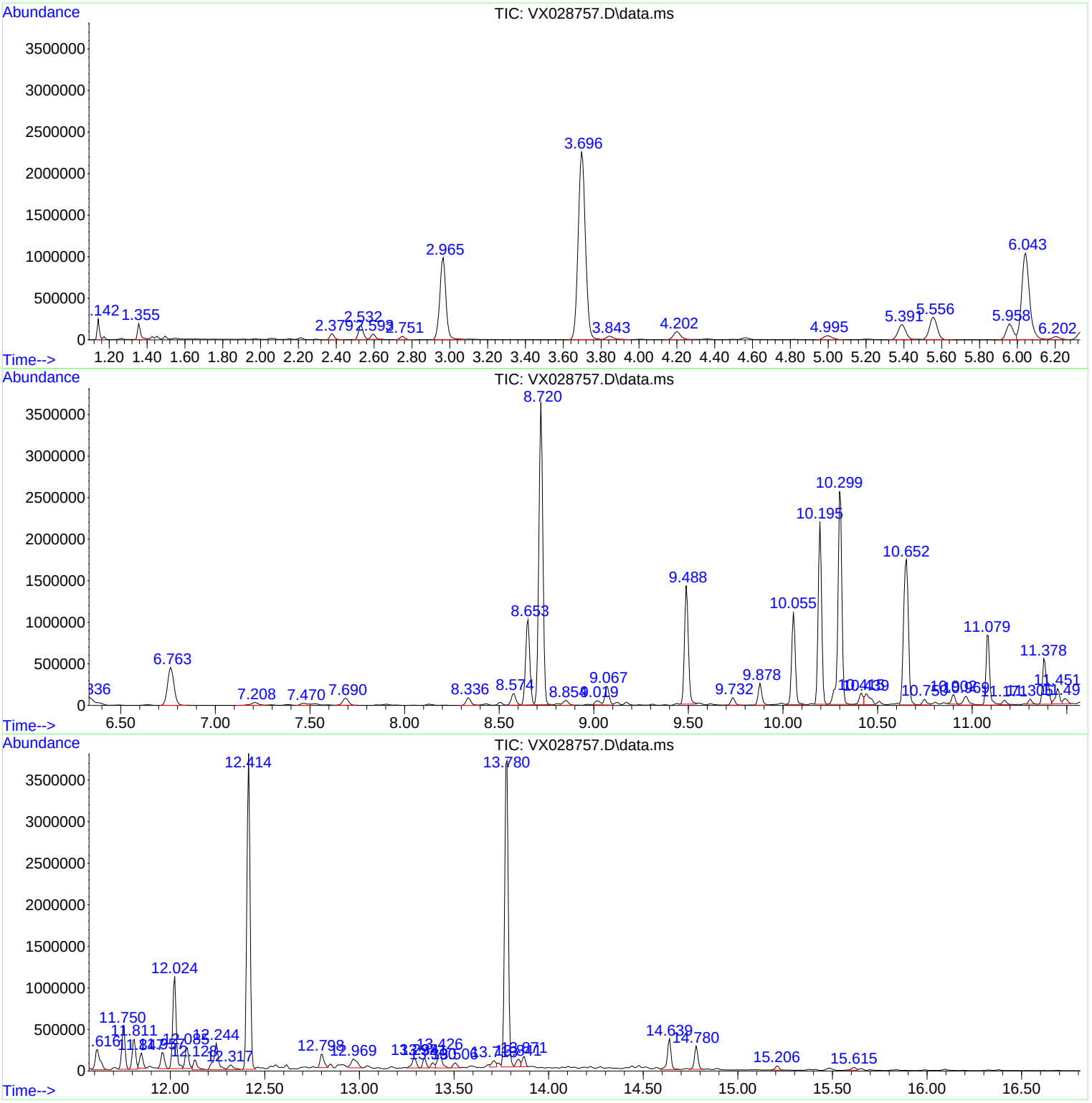
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

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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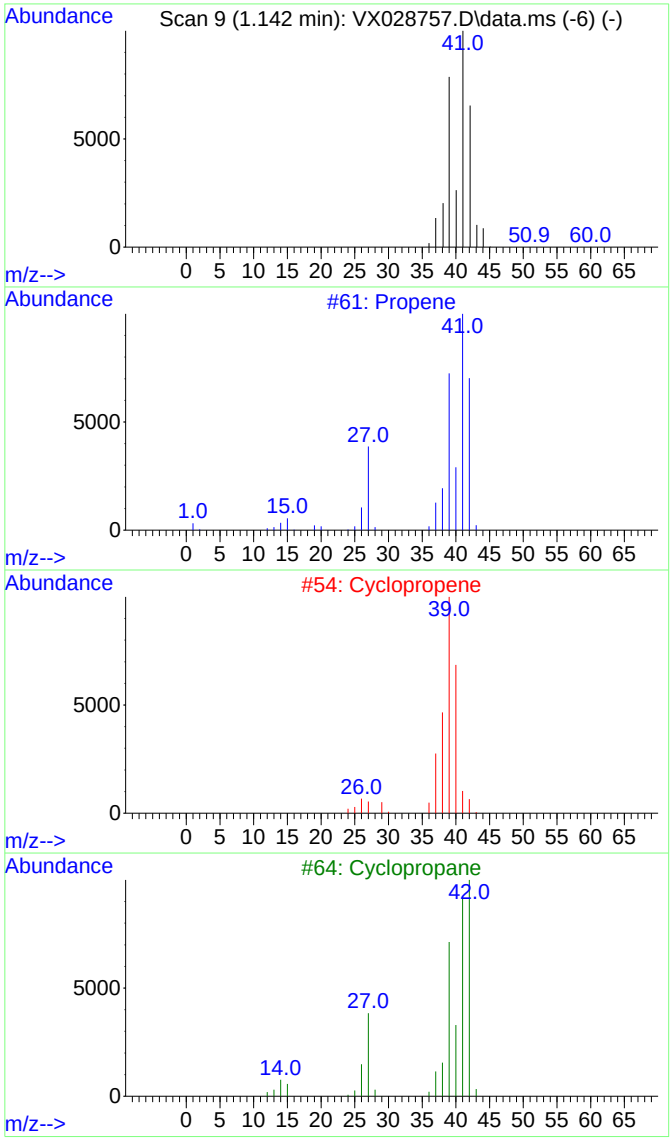
Quant Title : SW846 8260

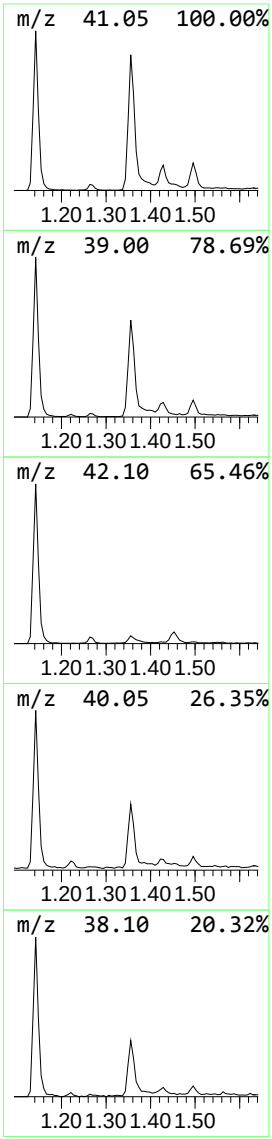
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	12.84 ug/l	201286	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Cyclopropene	40	C3H4	002781-85-3	10
3	Cyclopropane	42	C3H6	000075-19-4	9
4	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4
5	Acetonitrile	41	C2H3N	000075-05-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
Sample : N2884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

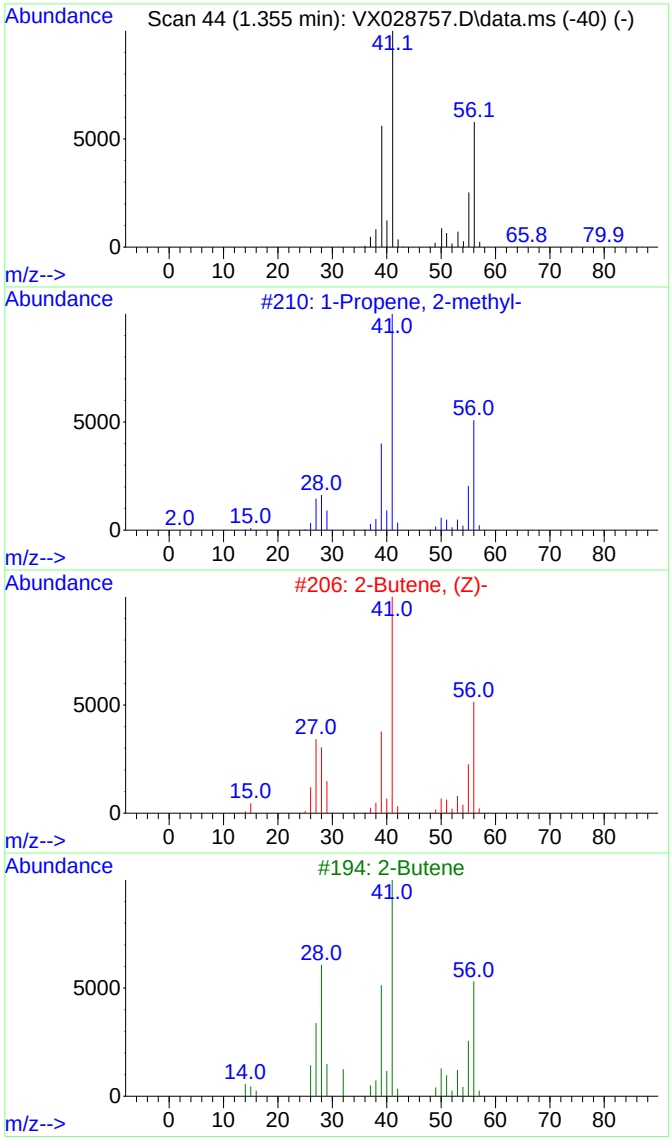
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

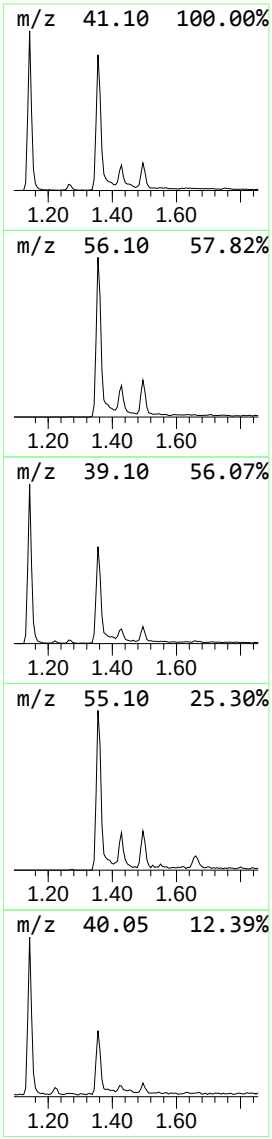
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.355	14.17 ug/l	222204	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2	2-Butene, (Z)-	56	C4H8	000590-18-1	80
3	2-Butene	56	C4H8	000107-01-7	80
4	1-Butene	56	C4H8	000106-98-9	52
5	Cyclobutane	56	C4H8	000287-23-0	52





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Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

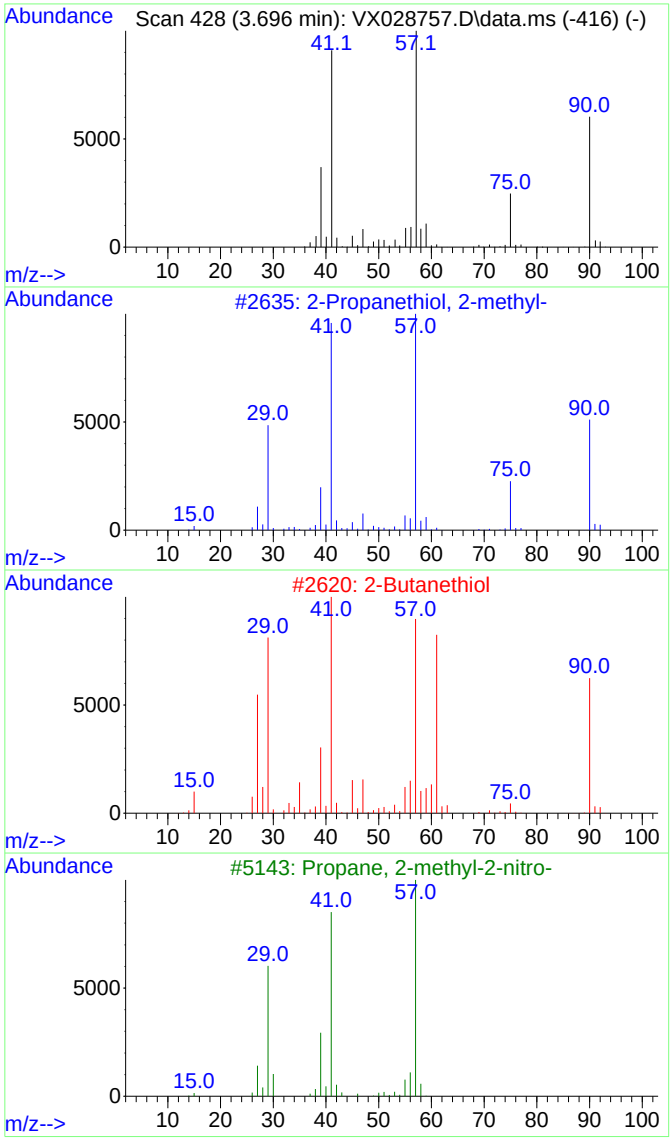
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

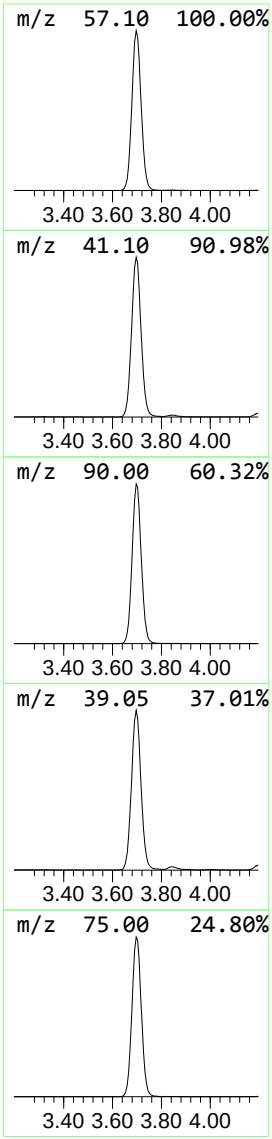
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	385.73 ug/l	6047480	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	52
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
4	Propane, 2-chloro-2-methyl-	92	C4H9Cl	000507-20-0	16
5	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	16





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ALS Vial : 11 Sample Multiplier: 1

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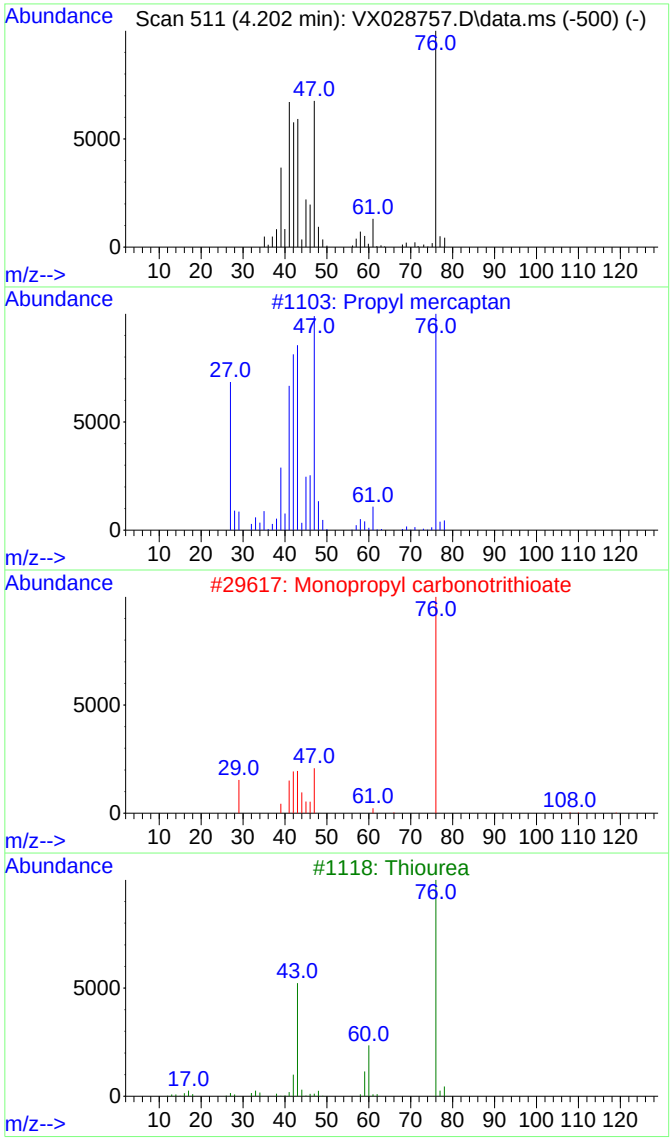
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

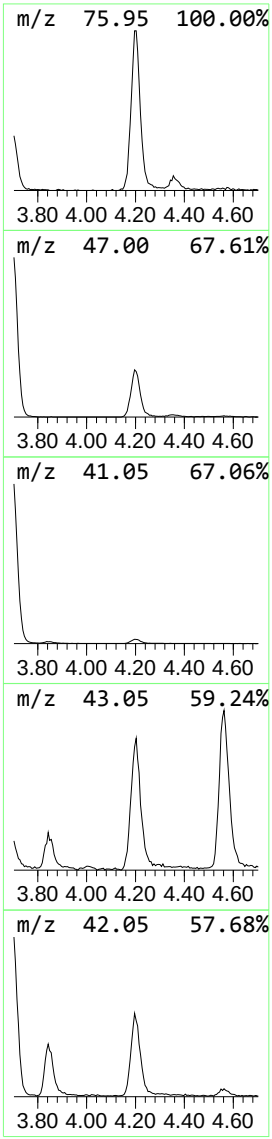
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propyl mercaptan Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.202	17.19 ug/l	269492	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	95
2	Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	74
3	Thiourea	76	CH4N2S	000062-56-6	36
4	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9
5	Nitric acid, butyl ester	119	C4H9NO3	000928-45-0	9





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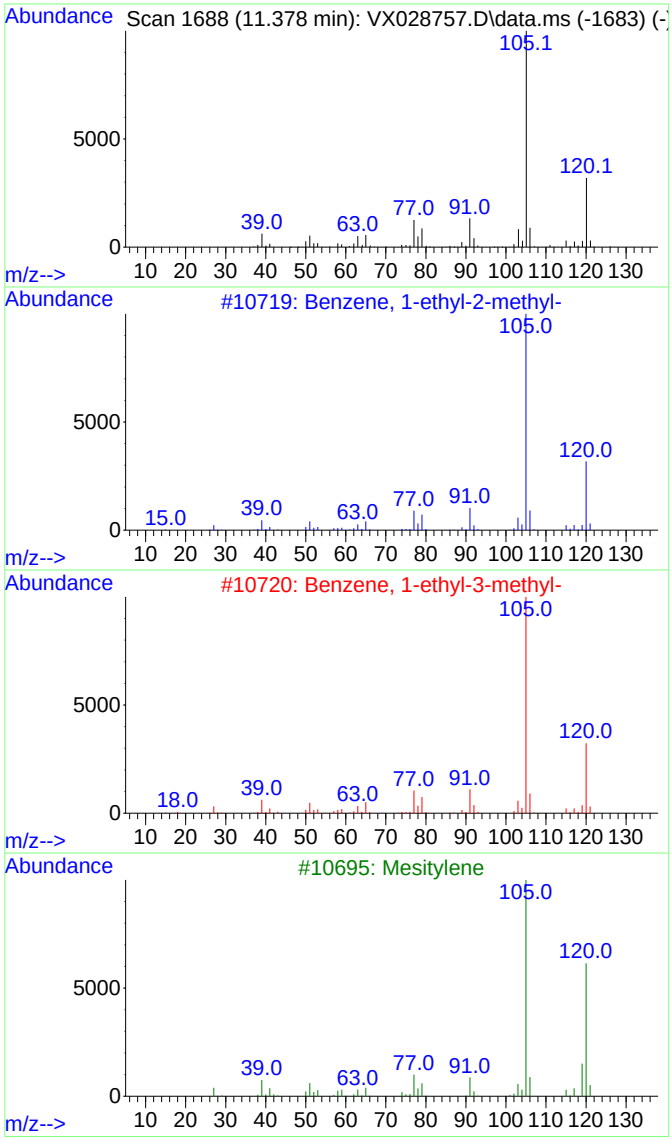
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

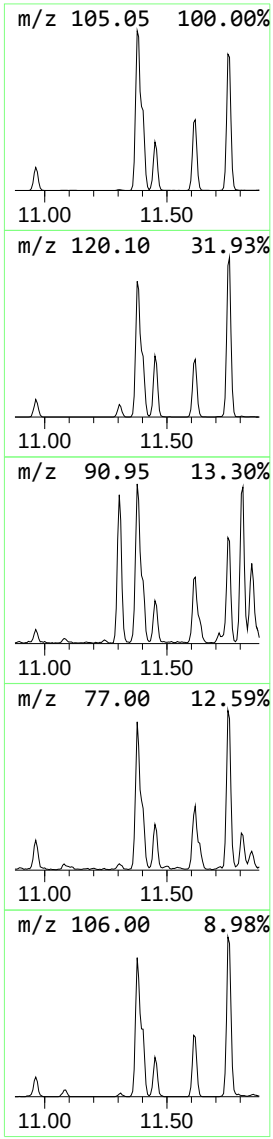
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	32.93 ug/l	943704	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	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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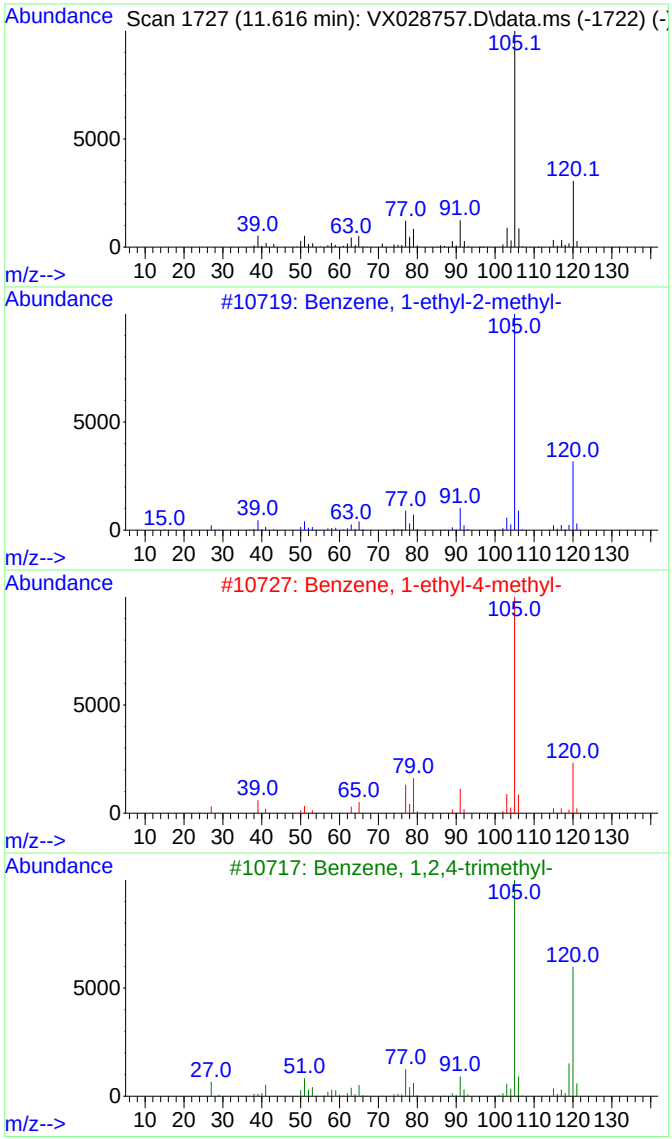
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

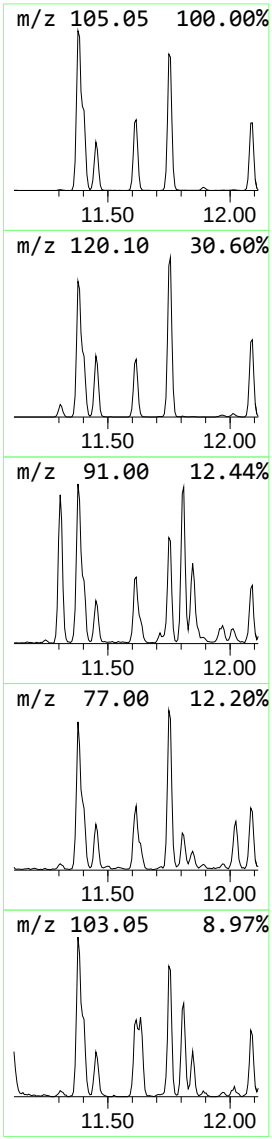
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	15.22 ug/l	436202	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
Sample : N2884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

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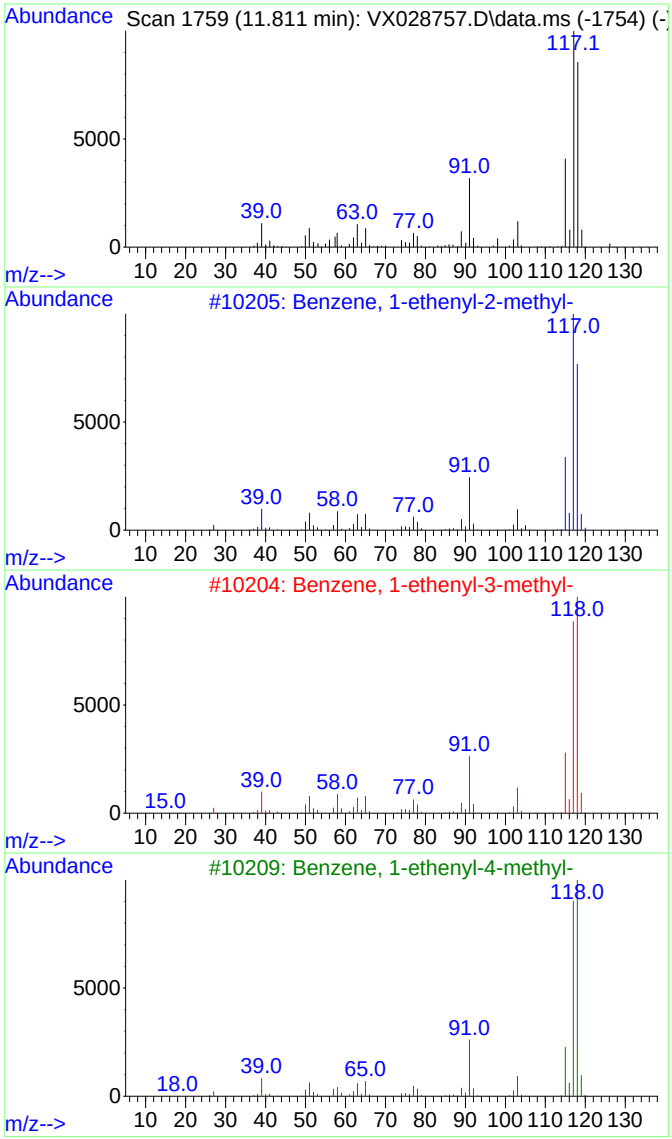
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

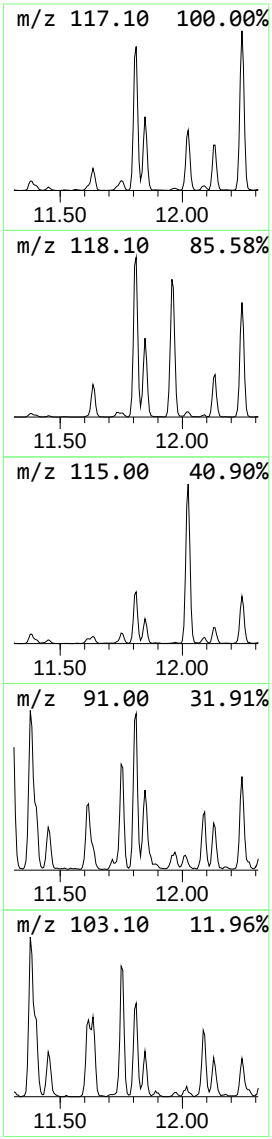
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.811	16.07 ug/l	460605	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
2	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	94
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	94
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	91
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
Sample : N2884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

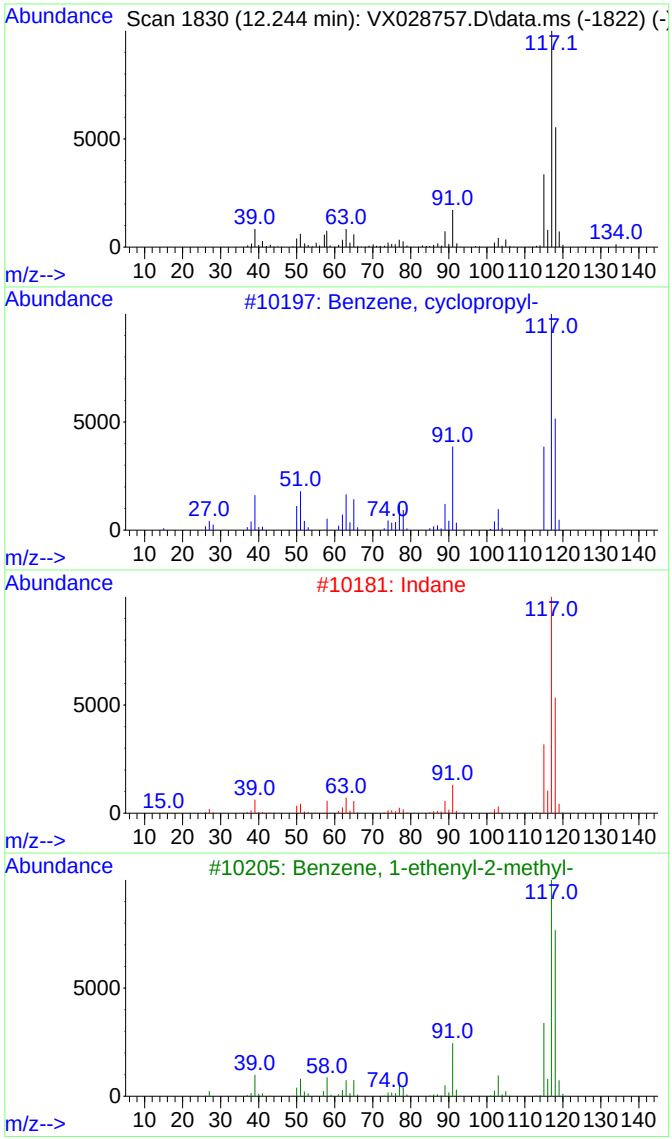
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

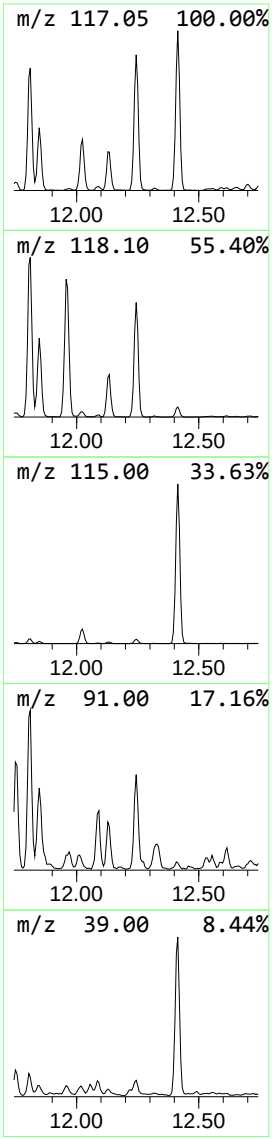
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	19.40 ug/l	555869	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
2	Indane	118	C9H10	000496-11-7	91
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
Sample : N2884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

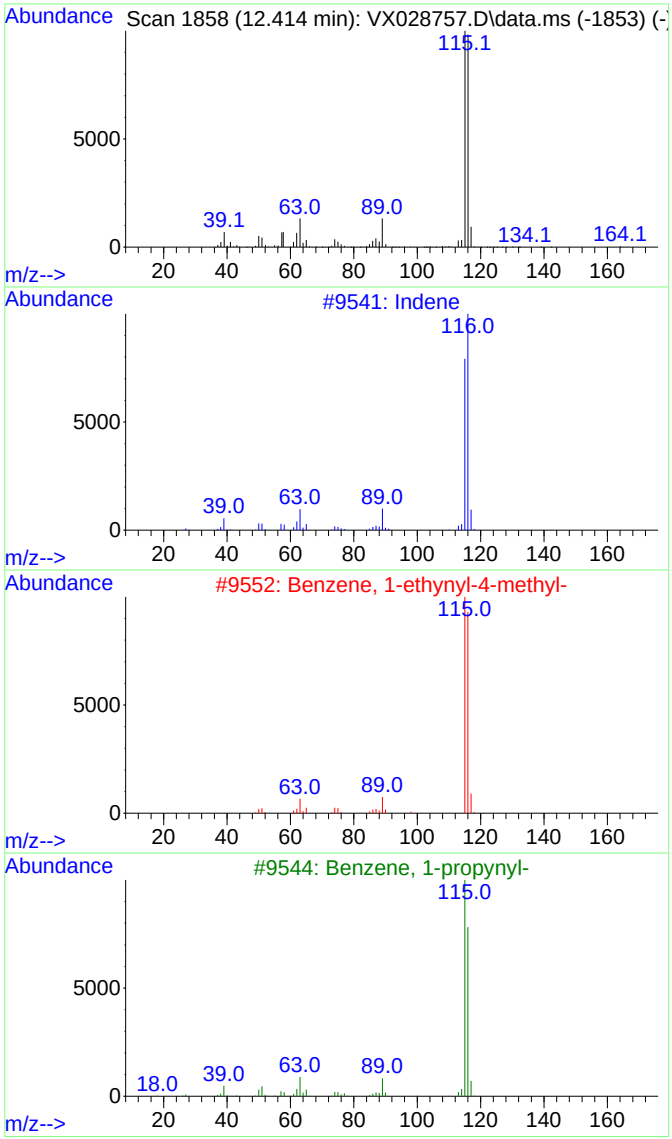
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

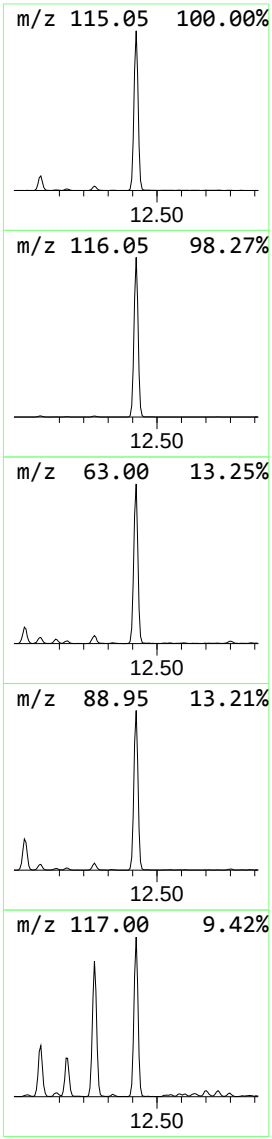
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	156.75 ug/l	4491770	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
Sample : N2884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31767

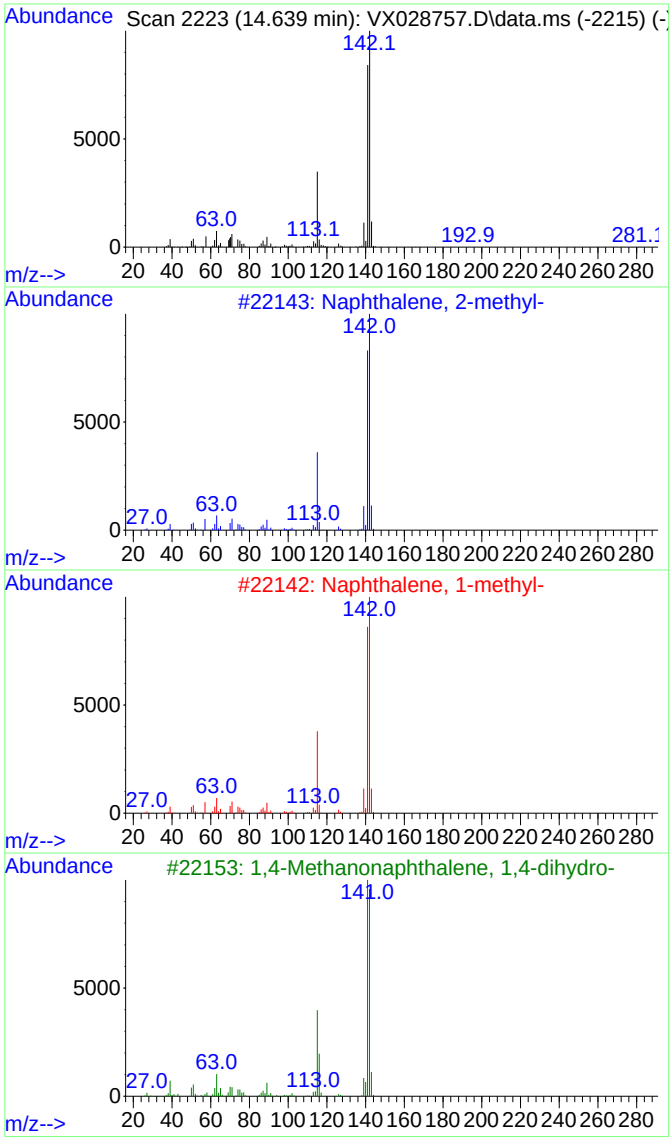
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

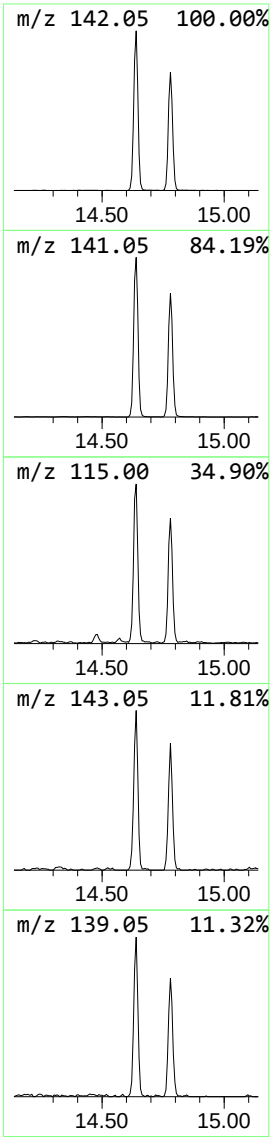
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	17.39 ug/l	498219	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	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028757.D
Acq On : 17 May 2022 14:58
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
31767

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	12.8	ug/l	201286	1	5.556	783905	50.0
1-Propene, 2-me...	1.355	14.2	ug/l	222204	1	5.556	783905	50.0
2-Propanethiol,...	3.696	385.7	ug/l	6047480	1	5.556	783905	50.0
Propyl mercaptan	4.202	17.2	ug/l	269492	1	5.556	783905	50.0
Benzene, 1-ethy...	11.378	32.9	ug/l	943704	4	12.024	1432830	50.0
Benzene, 1-ethy...	11.616	15.2	ug/l	436202	4	12.024	1432830	50.0
Benzene, 1-ethe...	11.811	16.1	ug/l	460605	4	12.024	1432830	50.0
Benzene, cyclop...	12.244	19.4	ug/l	555869	4	12.024	1432830	50.0
Indene	12.414	156.8	ug/l	4491770	4	12.024	1432830	50.0
Naphthalene, 1-...	14.640	17.4	ug/l	498219	4	12.024	1432830	50.0