LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

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\82X022322W.M
Title : SW846 8260

Signal : TIC: VX027252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	44	rBV	44578	76351	18.00%	2.325%
2	2.788	271	279	282	rBV2	3683	8348	1.97%	0.254%
3	2.831	282	286	296	rVB2	5888	12036	2.84%	0.367%
4	3.111	323	332	345	rBV2	9269	23521	5.55%	0.716%
5	3.764	430	439	447	rBV3	2698	7149	1.69%	0.218%
6	4.215	505	513	522	rBV3	2743	7725	1.82%	0.235%
7	5.391	695	706	719	rBV	48668	140681	33.17%	4.284%
8	5.562	719	734	754	rVB	83084	260675	61.47%	7.938%
9	5.830	768	778	787	rBV4	4139	11626	2.74%	0.354%
10	5.964	789	800	812	rBV	50496	135474	31.95%	4.126%
11	6.172	821	834	839	rBV3	2437	7718	1.82%	0.235%
12	6.257	839	848	859	rVV2	17015	52181	12.31%	1.589%
13	6.763	923	931	942	rBV	136158	309802	73.06%	9.435%
14	7.379	1023	1032	1042	rBV4	7007	18116	4.27%	0.552%
15	7.501	1046	1052	1057	rBV2	2593	4576	1.08%	0.139%
16	7.562	1057	1062	1066	rBV2	2353	4721	1.11%	0.144%
17	7.988	1123	1132	1140	rVB	14674	29805	7.03%	0.908%
18	8.110	1143	1152	1160	rBV	23250	47229	11.14%	1.438%
19	8.190	1160	1165	1170	rVB2	3136	5408	1.28%	0.165%
20	8.653	1228	1241	1249	rBV	265683	424062	100.00%	12.914%
21	8.964	1287	1292	1301	rVB5	5206	11219	2.65%	0.342%
22	9.049	1301	1306	1311	rBV4	2948	5312	1.25%	0.162%
23	10.055	1465	1471	1480	rBV	279862	366733	86.48%	11.168%
24	10.195	1490	1494	1501	rVB	4171	5126	1.21%	0.156%
25	10.305	1509	1512	1517	rVB	4134	5243	1.24%	0.160%
26	11.085	1634	1640	1646	rBV	217708	282556	66.63%	8.605%
27	11.305	1673	1676	1681	rVB	8509	10399	2.45%	0.317%
28	11.384	1684	1689	1690	rBV	28443	37382	8.82%	1.138%
29	11.451	1696	1700	1707	rVB	26863	33744	7.96%	1.028%
30	11.616	1722	1727	1731	rBV	15697	19439	4.58%	0.592%
31	11.756	1745	1750	1758	rVB	45428	55940	13.19%	1.704%
32	11.975	1781	1786	1789	rBV	6012	7190	1.70%	0.219%
33	12.024	1789	1794	1799	rVV	294570	362719	85.53%	11.046%
34	12.091	1802	1805	1812	rVB	7339	9309	2.20%	0.283%
35	12.250	1826	1831	1833	rBV	21814	30900	7.29%	0.941%
36	12.268	1833	1834	1838	rVV	21585	19573	4.62%	0.596%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

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\82X022322W.M
Title : SW846 8260

37	12.317	1838	1842	1852	rVB2	45243	65100	15.35%	1.983%
38	12.463	1862	1866	1872	rVB	14250	17441	4.11%	0.531%
39	12.530	1872	1877	1880	rBV	21354	31781	7.49%	0.968%
40	12.555	1880	1881	1886	rVB	19469	17002	4.01%	0.518%
41	12.616	1886	1891	1895	rBV	43704	52835	12.46%	1.609%
42	12.701	1901	1905	1915	rBV2	14500	27795	6.55%	0.846%
43	12.847	1925	1929	1934	rVB2	10609	13203	3.11%	0.402%
44	12.920	1934	1941	1945	rBV	21538	28512	6.72%	0.868%
45	12.963	1945	1948	1955	rVB	34872	40427	9.53%	1.231%
46	13.024	1955	1958	1960	rBV2	3785	5002	1.18%	0.152%
47	13.170	1978	1982	1986	rVB2	13716	15565	3.67%	0.474%
48	13.256	1992	1996	1998	rBV2	3713	5194	1.22%	0.158%
49	13.292	1998	2002	2012	rVV2	30431	43620	10.29%	1.328%
50	13.426	2019	2024	2031	rVB2	3998	5453	1.29%	0.166%
51	13.548	2040	2044	2047	rBV	6390	8768	2.07%	0.267%
52	13.585	2047	2050	2056	rVB4	7938	12950	3.05%	0.394%
53	13.664	2061	2063	2069	rVB2	7184	10030	2.37%	0.305%
54	13.926	2100	2106	2110	rBV2	3489	4778	1.13%	0.146%
55	14.079	2126	2131	2137	rVB	4757	5446	1.28%	0.166%
56	14.219	2149	2154	2160	rBV3	4281	7434	1.75%	0.226%
57	14.640	2216	2223	2228	rBV	7483	9671	2.28%	0.295%
58	14.780	2242	2246	2255	rBV	4484	5700	1.34%	0.174%

Sum of corrected areas: 3283695

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
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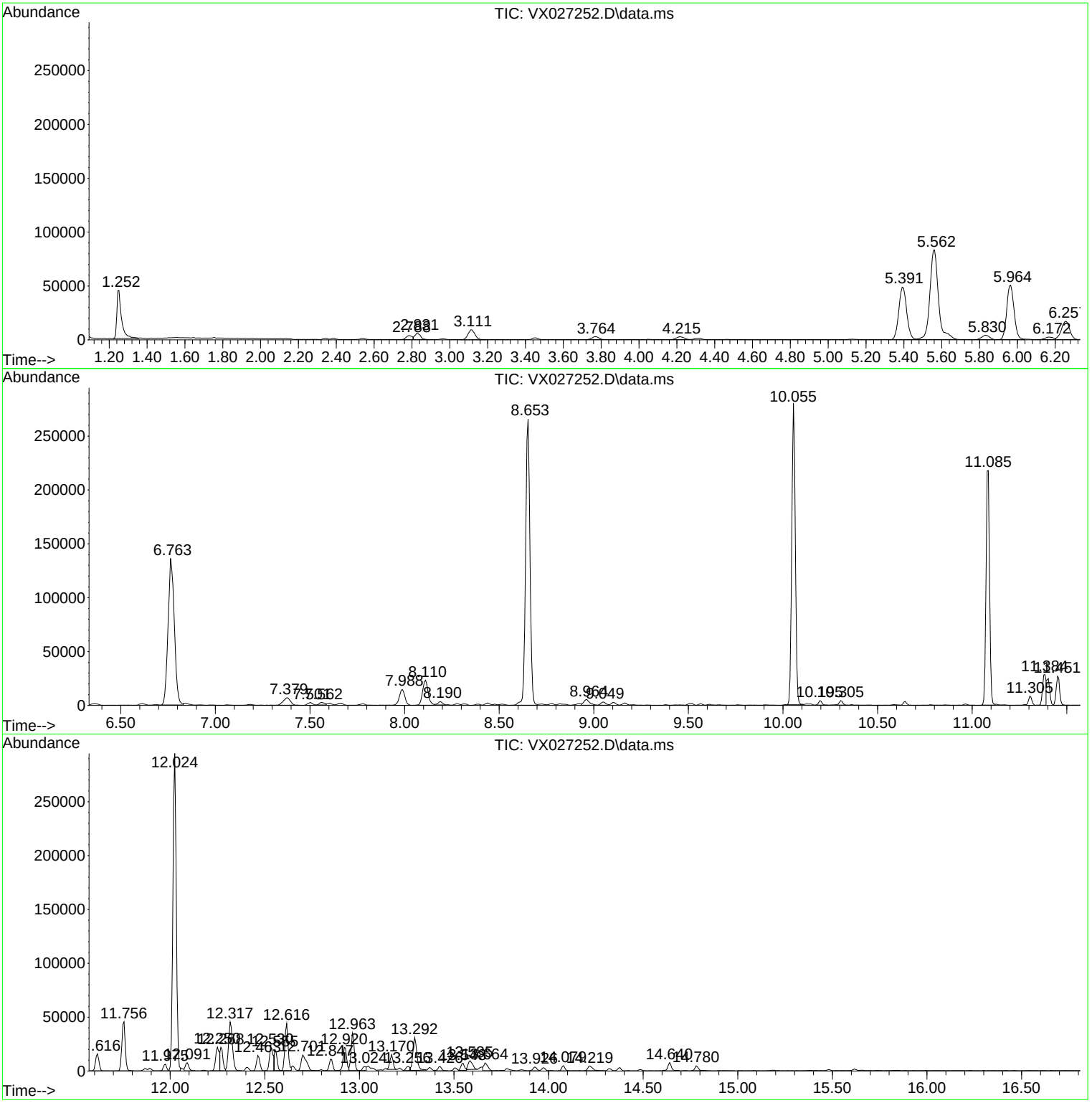
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
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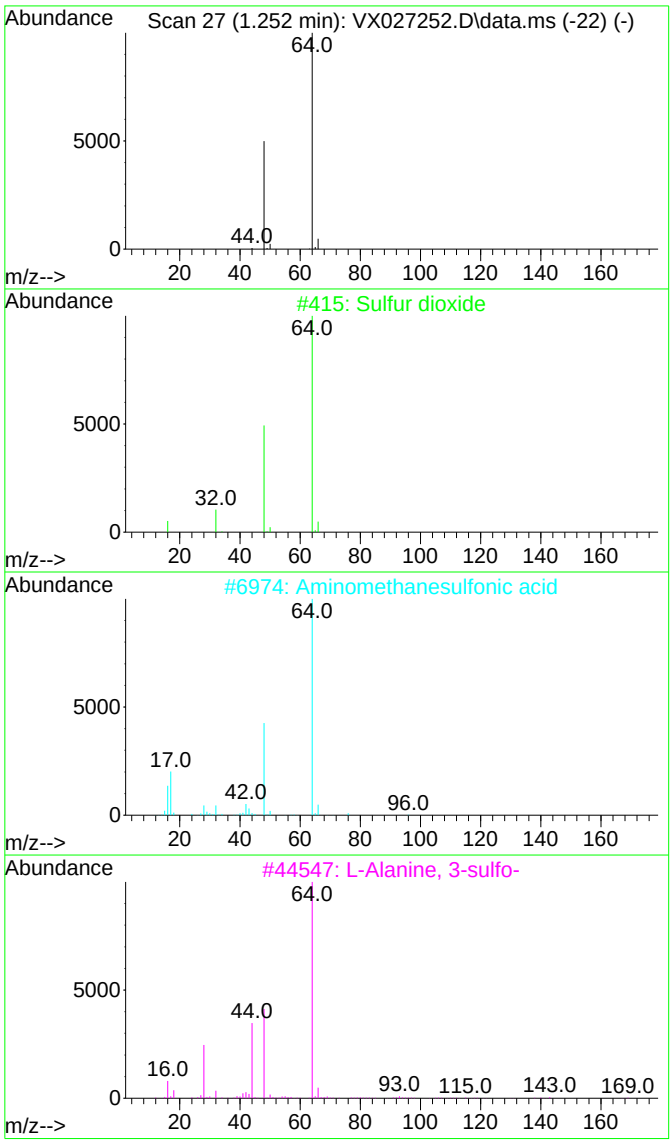
Quant Title : SW846 8260

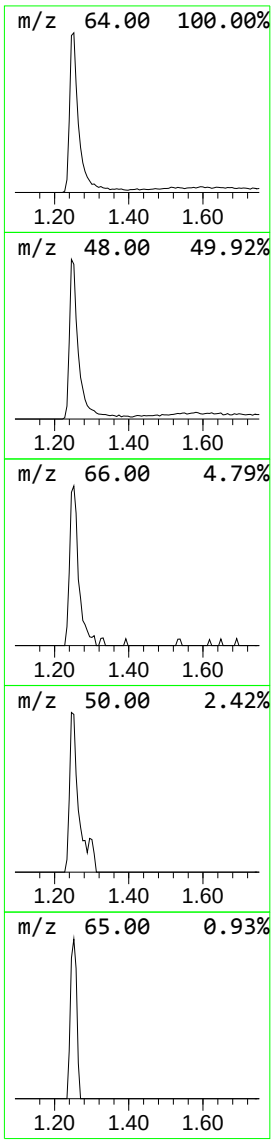
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	14.64 ug/l	76351	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

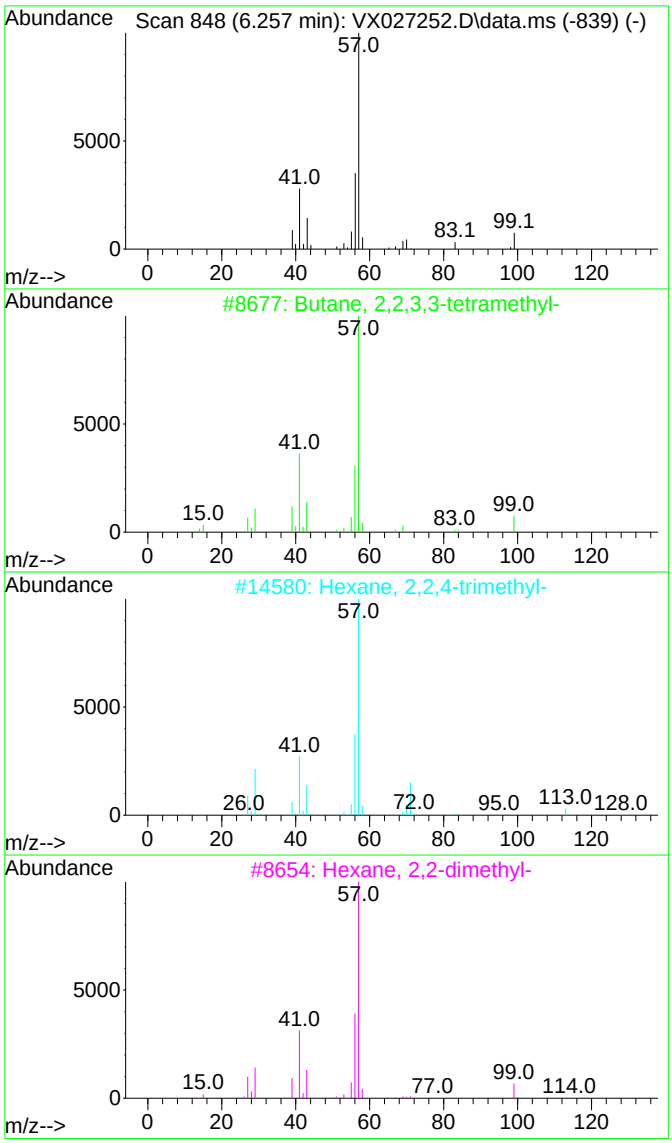
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

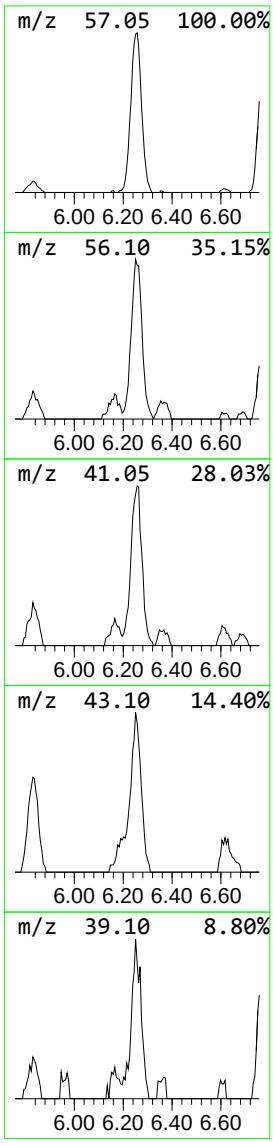
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	8.42 ug/l	52181	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53
5	2-Pentene, 5-butoxy-, (E)-	142	C9H18O	054004-23-8	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

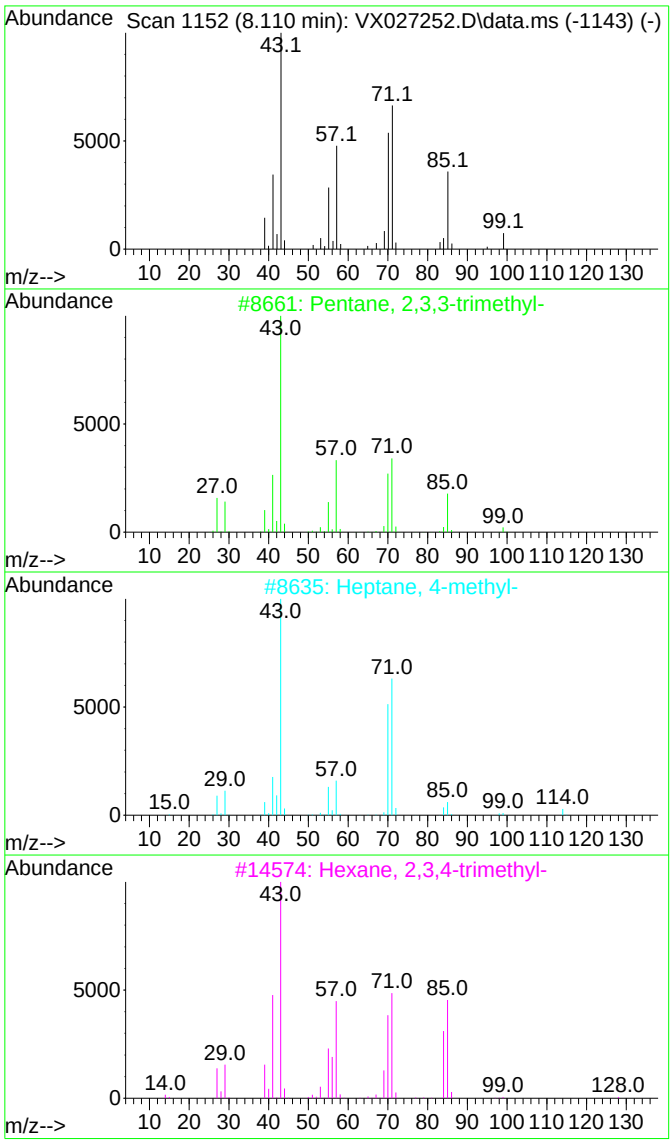
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

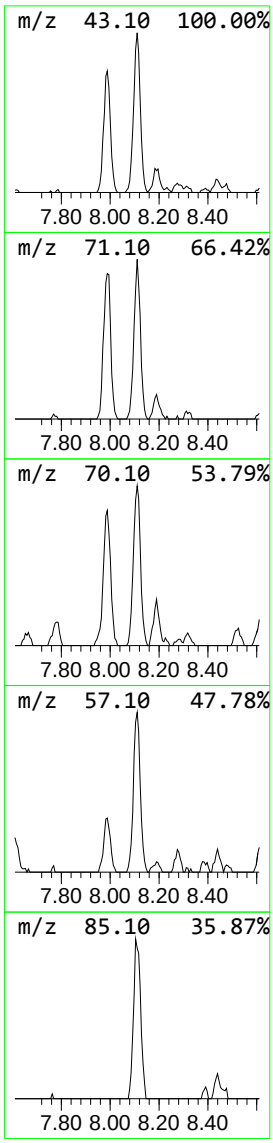
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	7.62 ug/l	47229	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

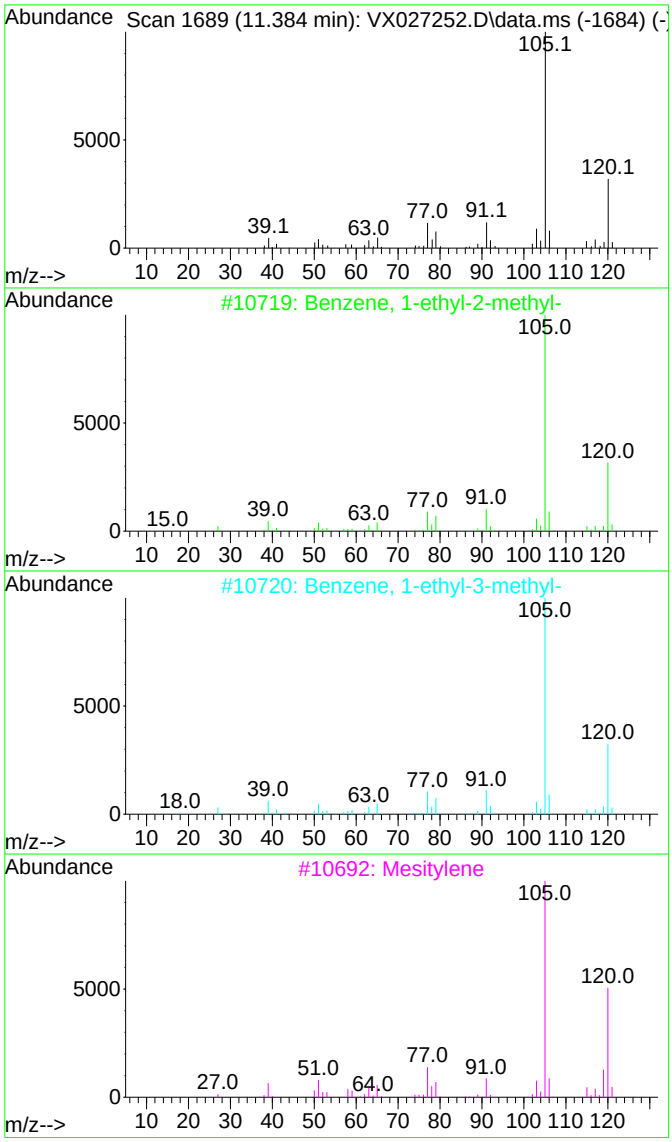
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

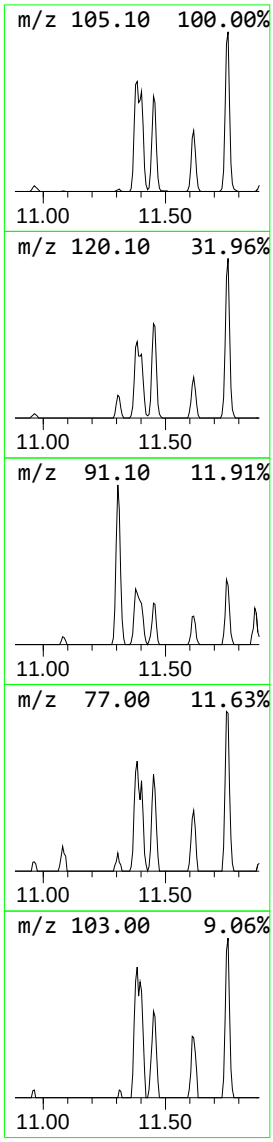
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	5.15 ug/l	37382	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	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

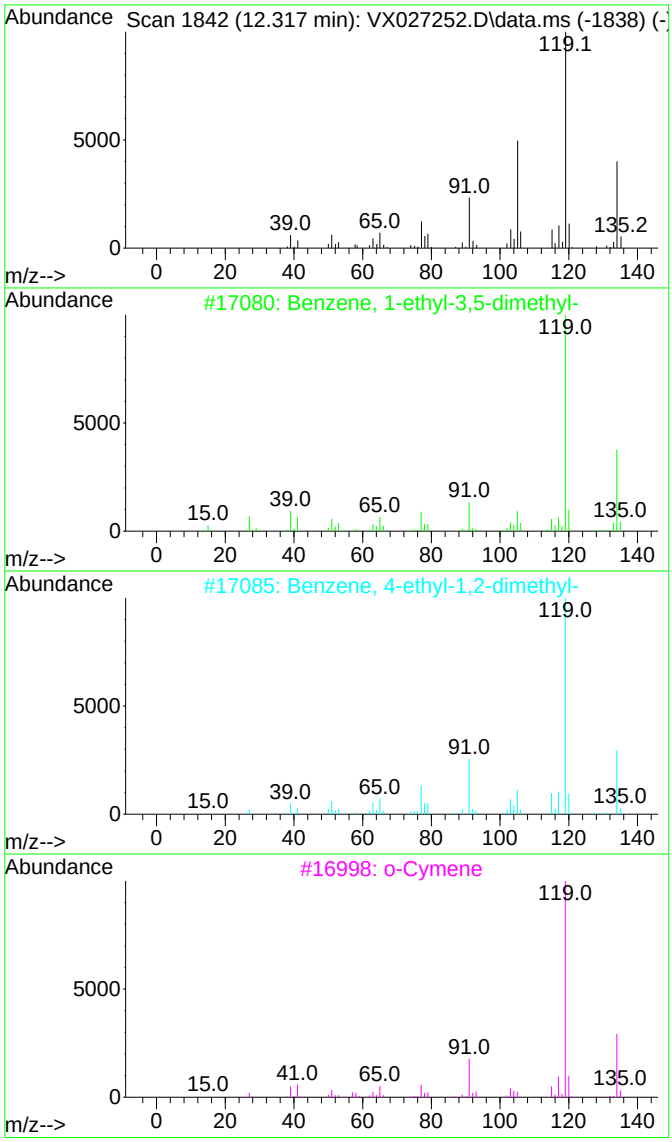
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

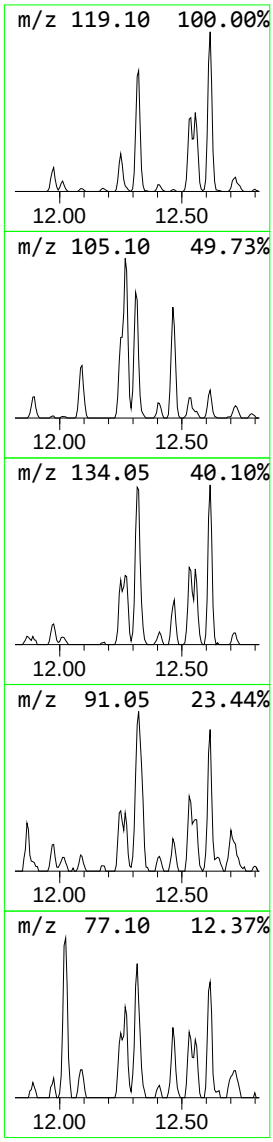
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	8.97 ug/l	65100	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	95
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
3	o-Cymene	134	C10H14	000527-84-4	94
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
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Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

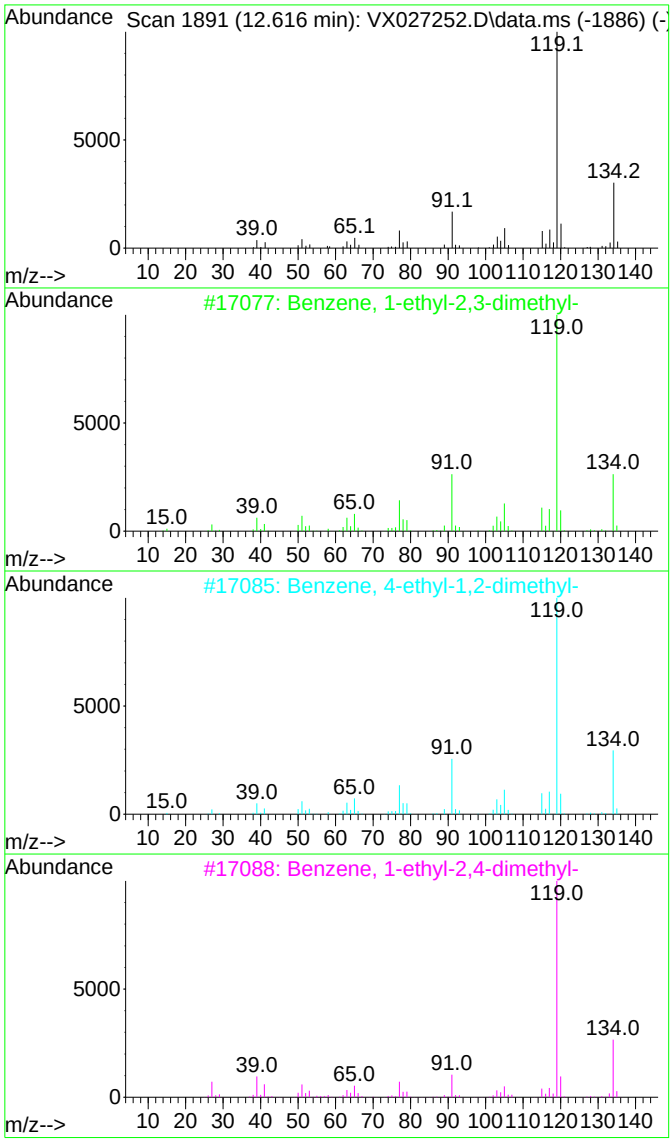
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

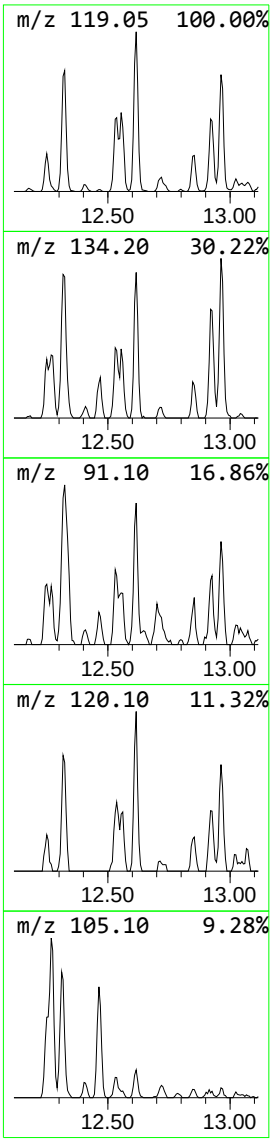
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	7.28 ug/l	52835	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5	o-Cymene	134	C10H14	000527-84-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

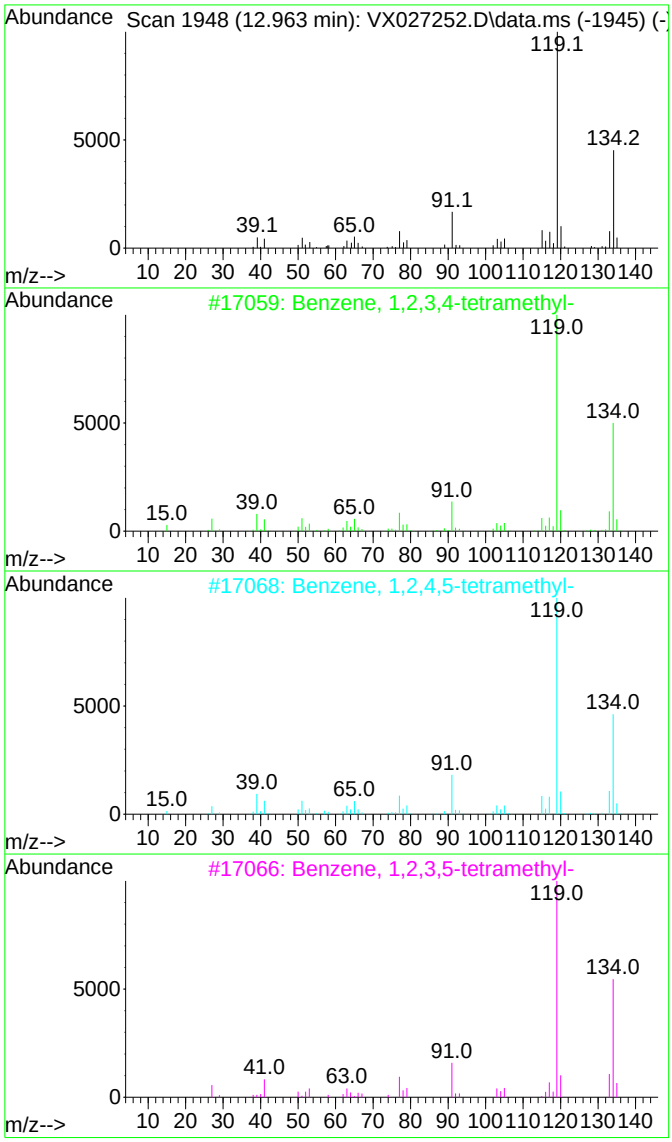
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

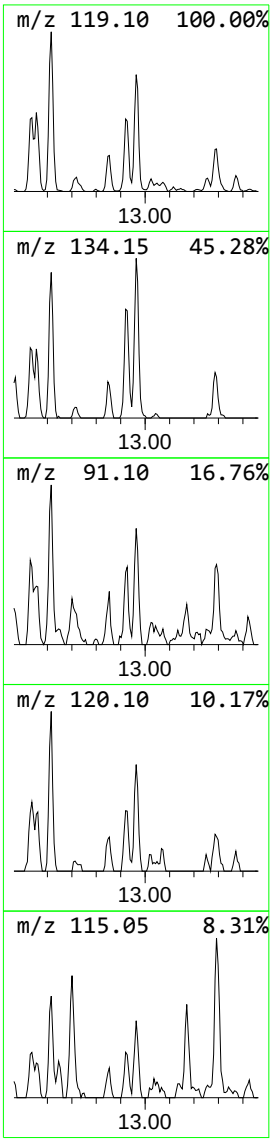
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	5.57 ug/l	40427	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

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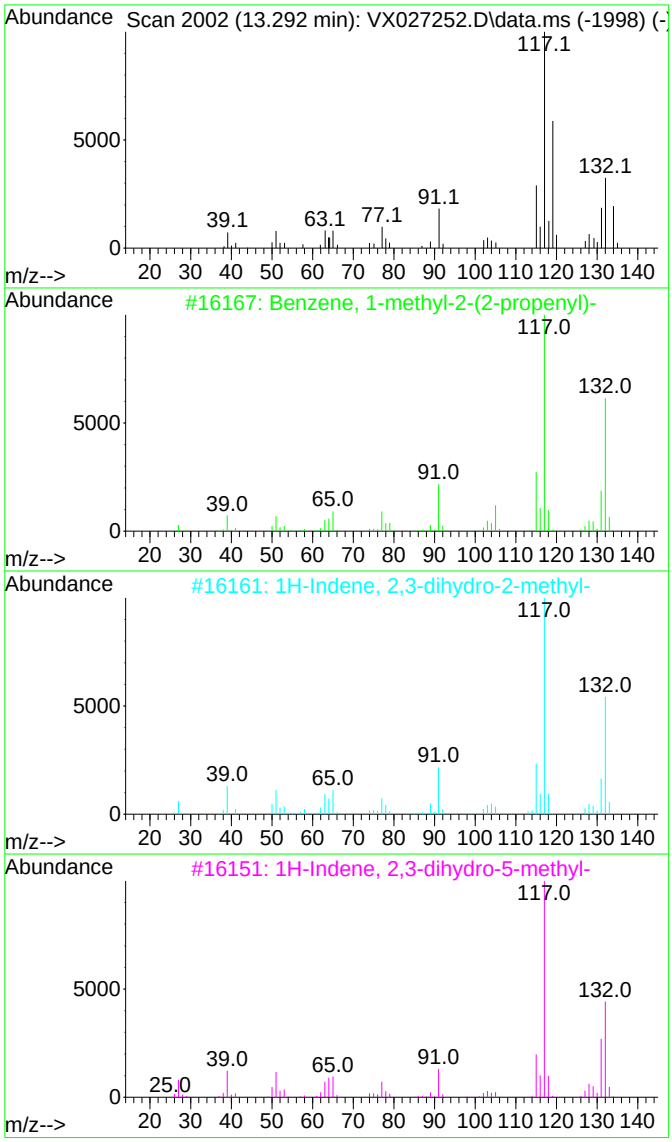
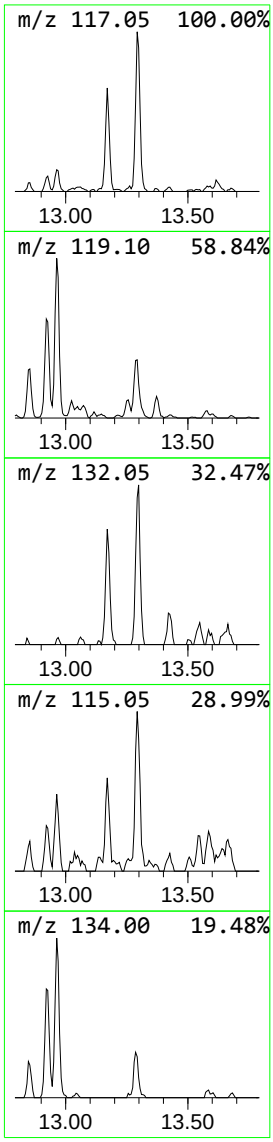
Peak Number 8 Benzene, 1-methyl-2-(2-prop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.01 ug/l	43620	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	70
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	64
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	64
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027252.D
Acq On : 01 Mar 2022 16:40
Operator : JC/MD
Sample : N1688-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-33

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.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
Sulfur dioxide	1.252	14.6	ug/l	76351	1	5.562	260675	50.0
Butane, 2,2,3,3...	6.257	8.4	ug/l	52181	2	6.763	309802	50.0
Pentane, 2,3,3-...	8.110	7.6	ug/l	47229	2	6.763	309802	50.0
Benzene, 1-ethy...	11.384	5.2	ug/l	37382	4	12.024	362719	50.0
Benzene, 1-ethy...	12.317	9.0	ug/l	65100	4	12.024	362719	50.0
Benzene, 1-ethy...	12.616	7.3	ug/l	52835	4	12.024	362719	50.0
Benzene, 1,2,3,...	12.963	5.6	ug/l	40427	4	12.024	362719	50.0
Benzene, 1-meth...	13.292	6.0	ug/l	43620	4	12.024	362719	50.0