LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

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\82X072522W.M
Title : SW846 8260

Signal : TIC: VX030310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	16	25	31	rBV2	15198	35383	2.87%	0.458%
2	1.301	31	35	41	rVV	9283	21697	1.76%	0.281%
3	1.746	104	108	116	rVB	27272	39309	3.18%	0.509%
4	2.380	209	212	222	rVB	8049	13991	1.13%	0.181%
5	2.544	230	239	245	rBV	16514	31874	2.58%	0.413%
6	2.782	269	278	283	rBV	32925	74937	6.07%	0.971%
7	2.867	288	292	298	rVV2	9197	21021	1.70%	0.272%
8	2.947	301	305	313	rVB	6010	12741	1.03%	0.165%
9	3.105	322	331	340	rVB2	17872	40955	3.32%	0.531%
10	3.733	427	434	442	rBV5	5013	12450	1.01%	0.161%
11	3.837	444	451	461	rVB6	4886	12915	1.05%	0.167%
12	4.215	507	513	523	rVB4	5477	14433	1.17%	0.187%
13	5.391	692	706	715	rBV2	135804	401636	32.52%	5.204%
14	5.477	715	720	725	rVB3	12832	28867	2.34%	0.374%
15	5.556	725	733	743	rBV	135772	376022	30.45%	4.872%
16	5.842	772	780	790	rBV7	4807	15657	1.27%	0.203%
17	5.964	790	800	809	rVV	165952	440178	35.64%	5.703%
18	6.044	809	813	827	rVV	12814	36160	2.93%	0.469%
19	6.251	839	847	857	rVV3	20396	66141	5.36%	0.857%
20	6.361	857	865	875	rVB6	8258	24597	1.99%	0.319%
21	6.769	922	932	942	rBV	253541	591934	47.93%	7.669%
22	7.367	1020	1030	1043	rBV7	14381	42868	3.47%	0.555%
23	7.879	1112	1114	1122	rVV5	6132	12886	1.04%	0.167%
24	7.988	1124	1132	1139	rVB2	19534	42172	3.41%	0.546%
25	8.110	1142	1152	1163	rBV4	41041	102306	8.28%	1.326%
26	8.433	1200	1205	1210	rVB	12695	21913	1.77%	0.284%
27	8.513	1212	1218	1225	rVB5	13922	28235	2.29%	0.366%
28	8.653	1225	1241	1251	rBV	791069	1234999	100.00%	16.001%
29	8.970	1288	1293	1299	rVB5	10632	22366	1.81%	0.290%
30	9.104	1311	1315	1320	rVB4	8009	12409	1.00%	0.161%
31	9.165	1320	1325	1329	rBV2	8721	13654	1.11%	0.177%
32	9.452	1364	1372	1377	rBV5	6433	16958	1.37%	0.220%
33	10.055	1466	1471	1477	rBV	560231	767242	62.12%	9.941%
34	10.963	1615	1620	1626	rBV	87528	111851	9.06%	1.449%
35	11.085	1634	1640	1646	rBV	587872	755619	61.18%	9.790%
36	11.305	1670	1676	1683	rVB	108922	140640	11.39%	1.822%

LSC Area Percent Report

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Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

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\82X072522W.M
Title : SW846 8260

37	11.616	1719	1727	1732	rBV2	11997	18570	1.50%	0.241%
38	11.866	1764	1768	1770	rBV	17295	21485	1.74%	0.278%
39	11.890	1770	1772	1778	rVB	18453	21760	1.76%	0.282%
40	12.024	1788	1794	1802	rBV	752003	897559	72.68%	11.629%
41	12.244	1824	1830	1836	rBV2	226741	296358	24.00%	3.840%
42	12.317	1838	1842	1844	rBV2	10412	13007	1.05%	0.169%
43	12.408	1852	1857	1861	rBV	26652	32825	2.66%	0.425%
44	12.616	1882	1891	1894	rBV	37382	47109	3.81%	0.610%
45	12.646	1894	1896	1901	rVV3	14235	19361	1.57%	0.251%
46	12.701	1901	1905	1912	rVB	109147	146759	11.88%	1.902%
47	12.841	1925	1928	1933	rVB2	12291	16104	1.30%	0.209%
48	12.920	1933	1941	1947	rBV	89623	125776	10.18%	1.630%
49	13.030	1955	1959	1964	rVB3	10288	16046	1.30%	0.208%
50	13.140	1973	1977	1979	rBV2	21230	25747	2.08%	0.334%
51	13.170	1979	1982	1985	rVV	30885	33432	2.71%	0.433%
52	13.292	1997	2002	2008	rVV2	54797	75225	6.09%	0.975%
53	13.548	2040	2044	2046	rBV2	13559	17045	1.38%	0.221%
54	13.585	2046	2050	2053	rVB3	11926	15018	1.22%	0.195%
55	13.664	2061	2063	2074	rVB3	11172	16031	1.30%	0.208%
56	13.798	2079	2085	2090	rVV9	6012	13957	1.13%	0.181%
57	13.853	2090	2094	2099	rVV2	19729	24749	2.00%	0.321%
58	13.926	2099	2106	2110	rVV2	20838	31569	2.56%	0.409%
59	14.213	2148	2153	2160	rBV5	7084	14694	1.19%	0.190%
60	14.323	2163	2171	2176	rBV	13232	19605	1.59%	0.254%
61	14.640	2220	2223	2226	rVV2	11068	14434	1.17%	0.187%
62	14.780	2241	2246	2252	rBV	52798	74112	6.00%	0.960%
63	15.810	2410	2415	2419	rBV5	6777	12361	1.00%	0.160%
64	15.993	2439	2445	2450	rBV2	10779	18324	1.48%	0.237%

Sum of corrected areas: 7718038

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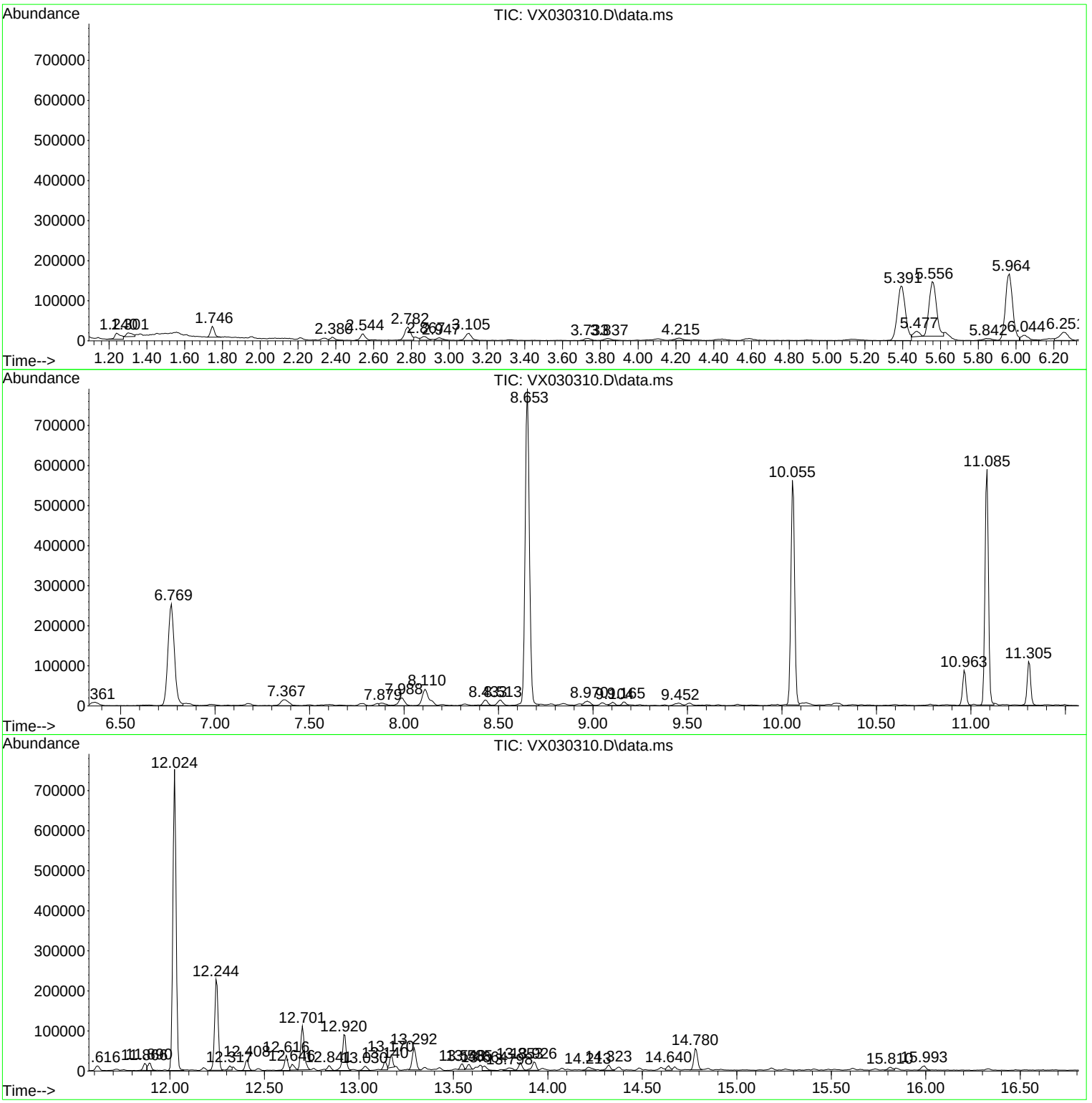
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

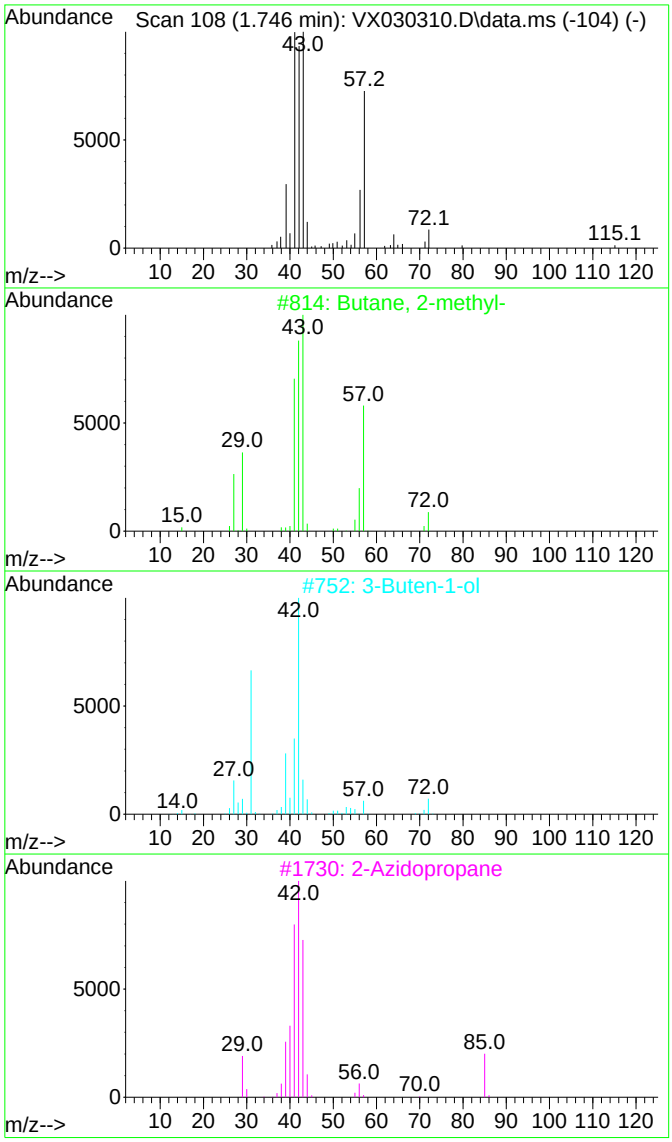
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

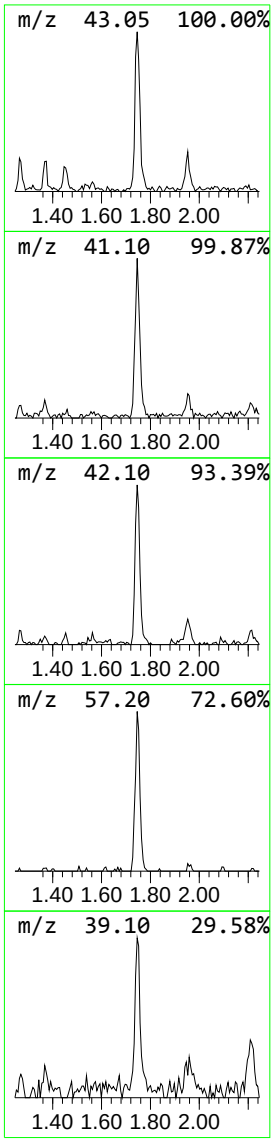
****

Peak Number 1 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	5.23 ug/l	39309	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	2-Azidopropane	85	C3H7N3	000691-57-6	36
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5	Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

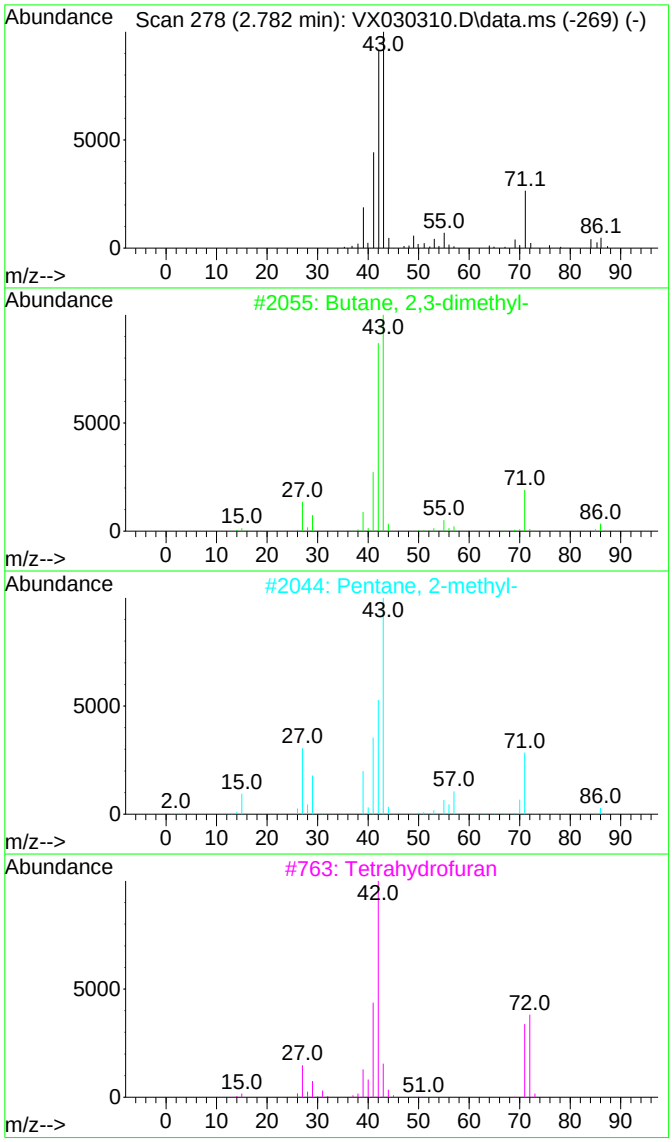
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

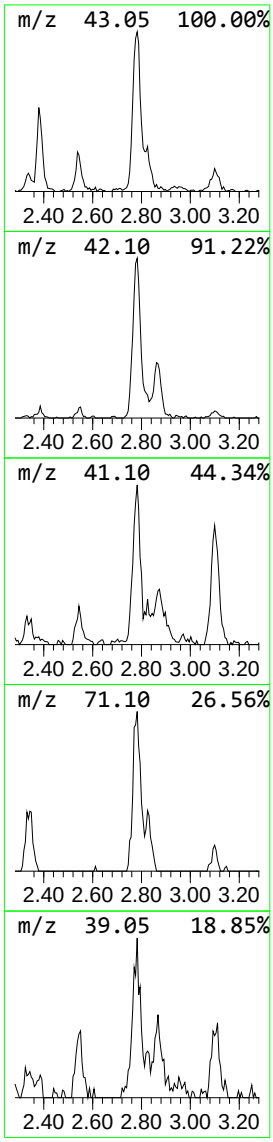
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	9.96 ug/l	74937	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	43
3	Tetrahydrofuran	72	C4H8O	000109-99-9	36
4	Pentane	72	C5H12	000109-66-0	33
5	Dichloroacetic acid, pentyl ester	198	C7H12Cl2O2	037079-03-1	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

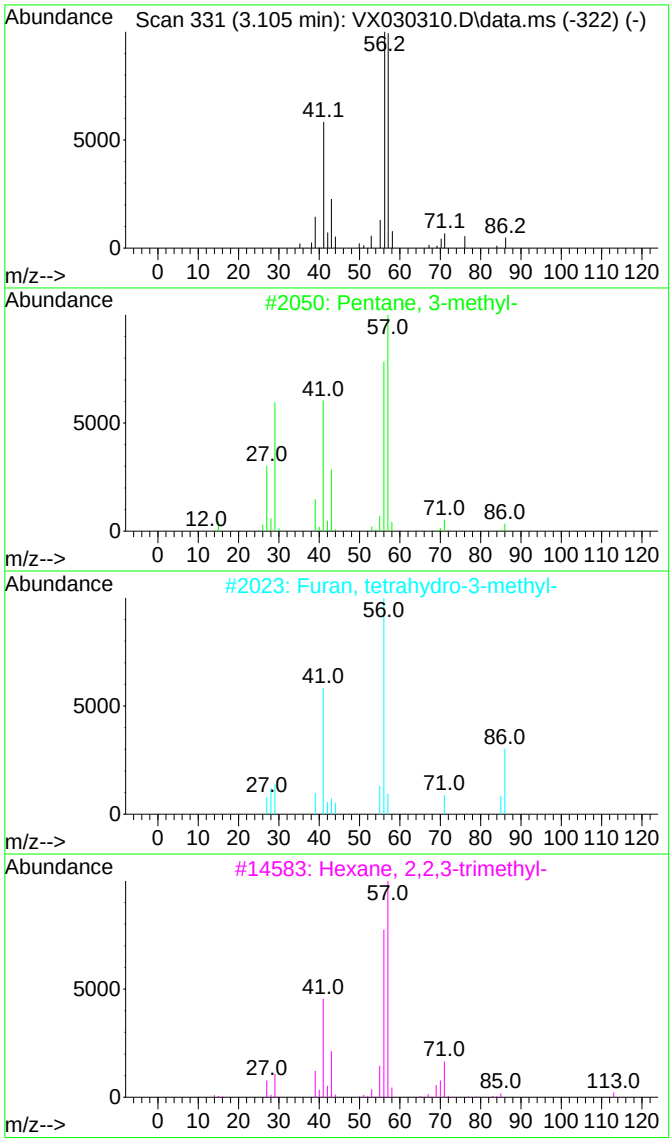
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

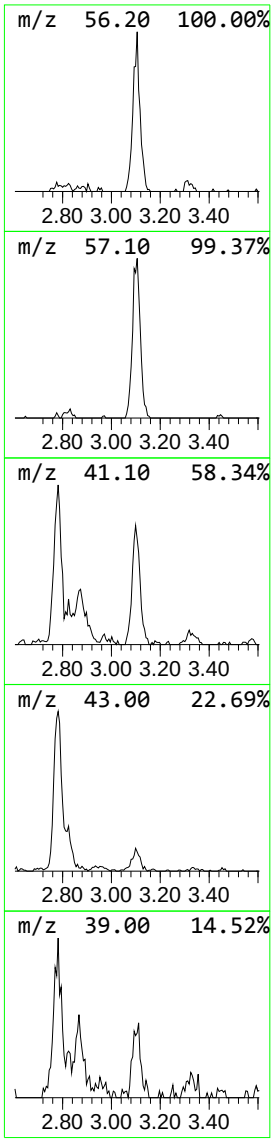
****

Peak Number 3 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	5.45 ug/l	40955	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	59
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	56
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	40
5	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

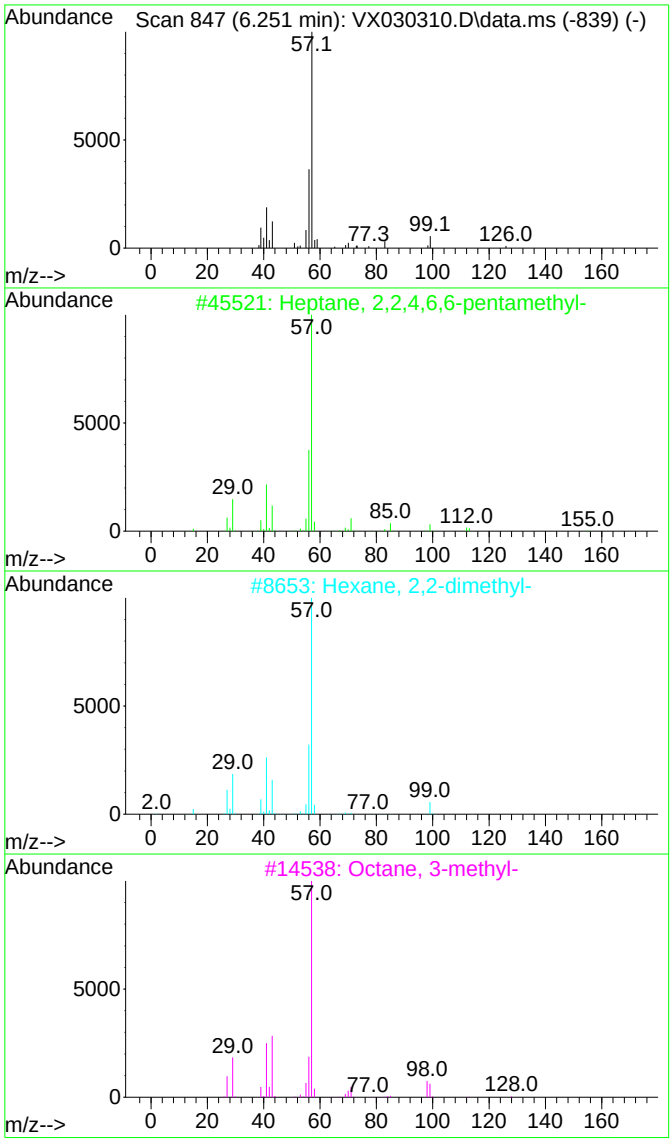
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

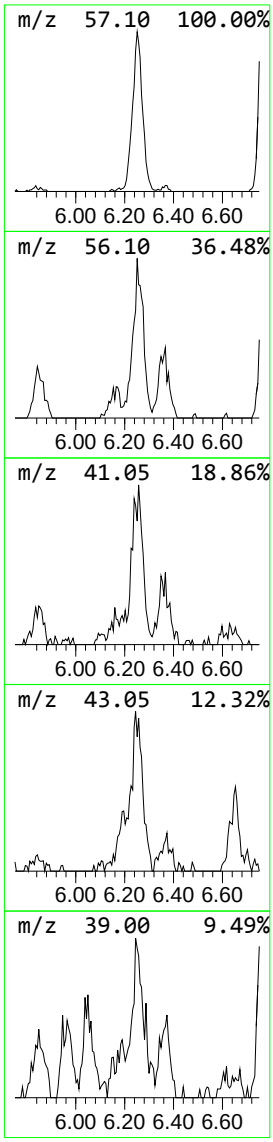
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptane, 2,2,4,6,6-pentamet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	5.59 ug/l	66141	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	50
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	50
3	Octane, 3-methyl-	128	C9H20	002216-33-3	50
4	Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	45
5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

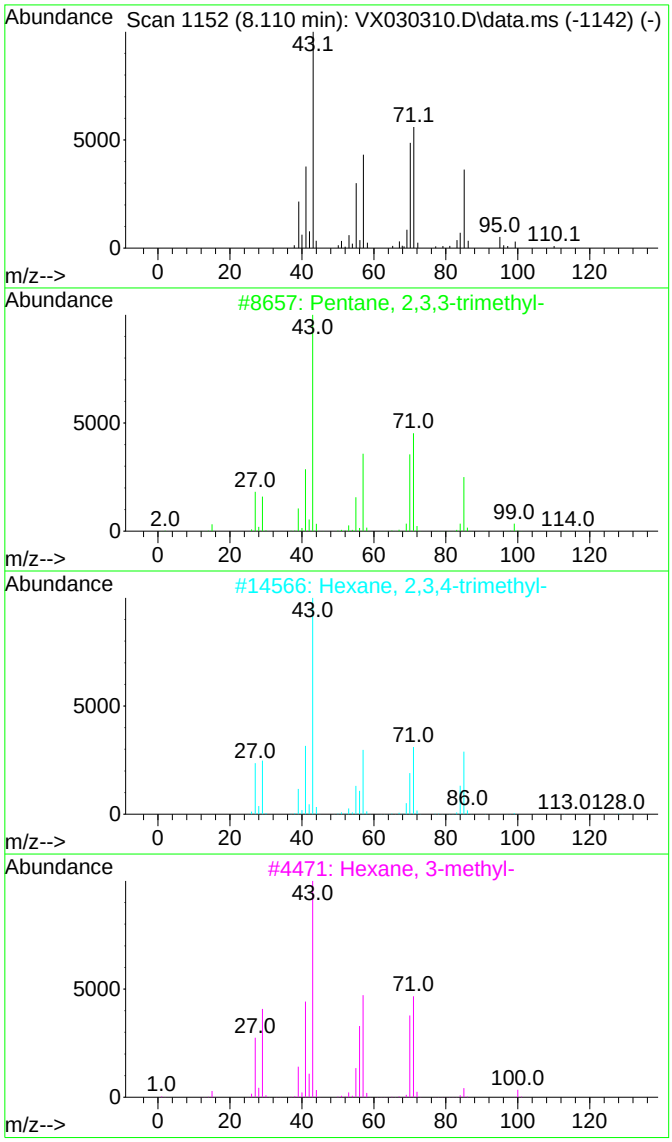
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

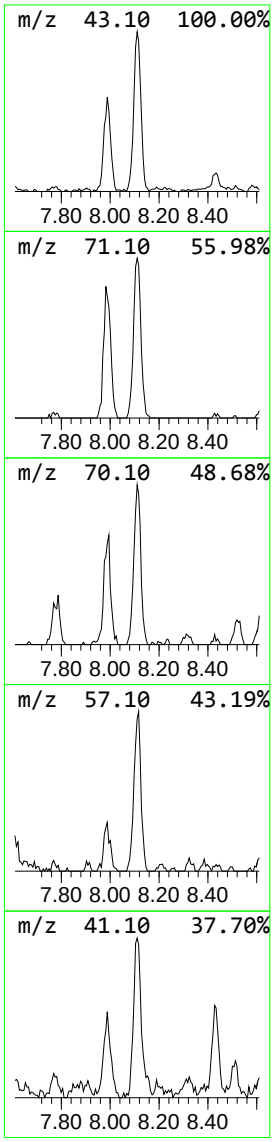
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	8.64 ug/l	102306	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
4	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	50
5	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	45





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

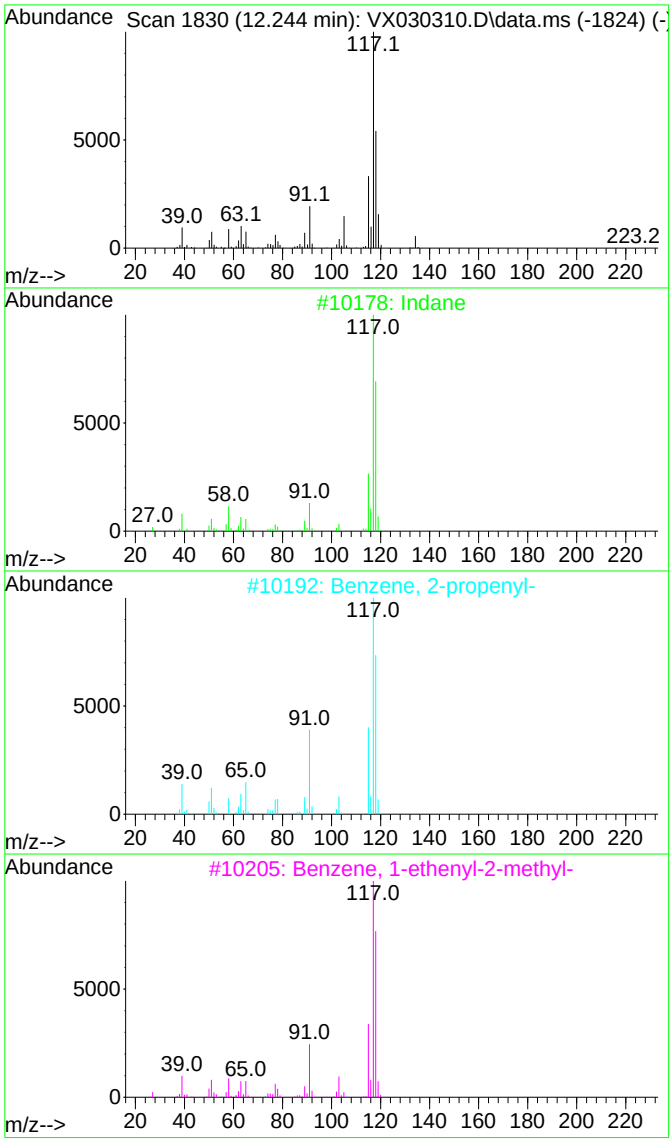
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

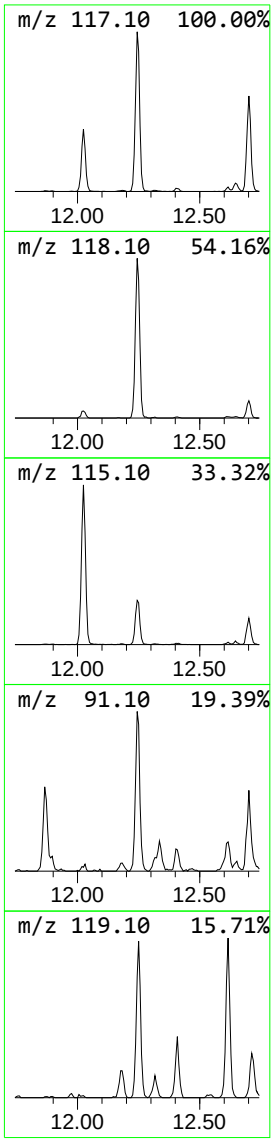
****

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	16.51 ug/l	296358	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
5	Indan, 1-methyl-	132	C10H12	000767-58-8	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

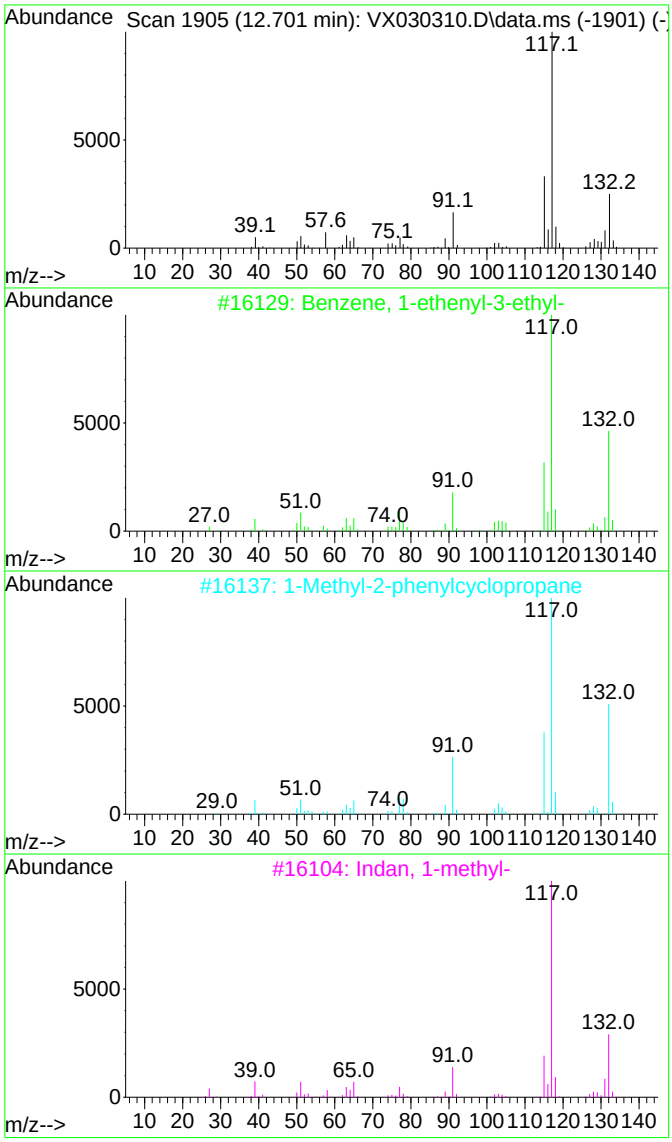
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

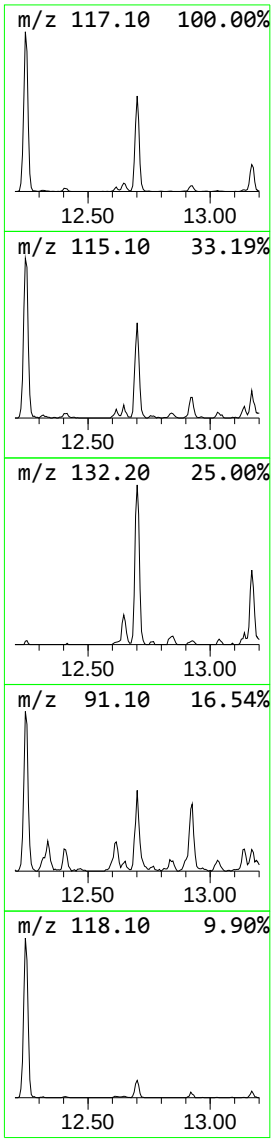
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	8.18 ug/l	146759	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
3	Indan, 1-methyl-	132	C10H12	000767-58-8	90
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87





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Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

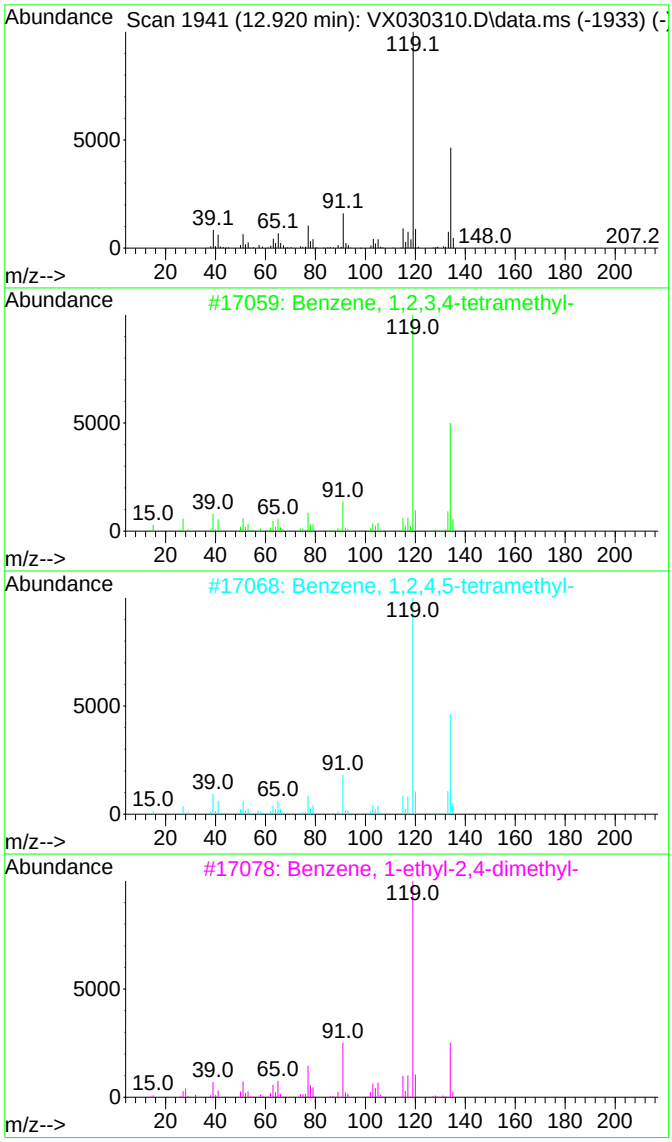
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

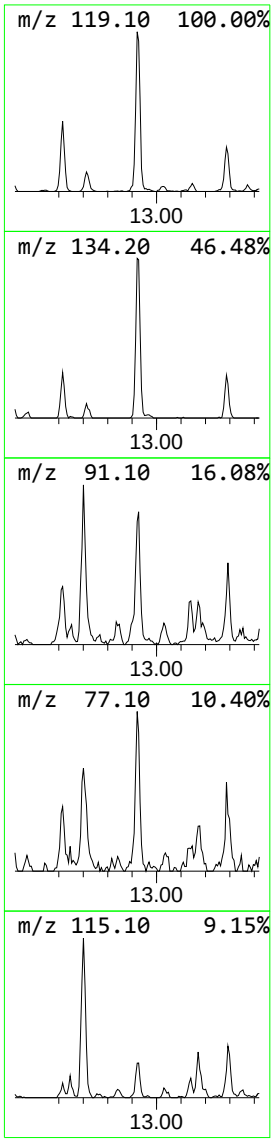
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	7.01 ug/l	125776	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-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030310.D
Acq On : 29 Jul 2022 18:06
Operator : JC/MD
Sample : N3861-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21RR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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
Butane, 2-methyl-	1.746	5.2	ug/l	39309	1	5.562	376022	50.0
Butane, 2,3-dim...	2.782	10.0	ug/l	74937	1	5.562	376022	50.0
Pentane, 3-methyl-	3.105	5.5	ug/l	40955	1	5.562	376022	50.0
Heptane, 2,2,4,...	6.251	5.6	ug/l	66141	2	6.769	591934	50.0
Pentane, 2,3,3-...	8.110	8.6	ug/l	102306	2	6.769	591934	50.0
Indane	12.244	16.5	ug/l	296358	4	12.024	897559	50.0
Benzene, 1-ethe...	12.701	8.2	ug/l	146759	4	12.024	897559	50.0
Benzene, 1,2,3,...	12.920	7.0	ug/l	125776	4	12.024	897559	50.0