LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

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\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033077.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	52	rVV	316320	366413	3.29%	0.359%
2	1.752	104	109	123	rVB	499971	651917	5.85%	0.640%
3	1.965	138	144	155	rVB2	265199	554597	4.98%	0.544%
4	2.069	155	161	170	rVV	240833	346591	3.11%	0.340%
5	2.166	171	177	181	rVV	153001	223378	2.01%	0.219%
6	2.215	181	185	199	rVB	407214	623759	5.60%	0.612%
7	2.751	259	273	281	rBV2	181017	462034	4.15%	0.453%
8	2.867	288	292	304	rVB2	235888	538842	4.84%	0.529%
9	2.989	304	312	324	rVV	101738	402312	3.61%	0.395%
10	3.111	324	332	345	rVB2	160712	402360	3.61%	0.395%
11	3.318	357	366	378	rBV	49191	117122	1.05%	0.115%
12	3.733	428	434	444	rVB3	135800	347334	3.12%	0.341%
13	3.843	444	452	457	rBV	78413	193124	1.73%	0.189%
14	4.105	486	495	507	rBV	95732	247162	2.22%	0.242%
15	4.306	518	528	539	rVV	292833	832822	7.48%	0.817%
16	4.428	539	548	561	rVB2	44098	130266	1.17%	0.128%
17	5.196	663	674	692	rVB	111090	342008	3.07%	0.336%
18	5.385	692	705	712	rBV	72974	226472	2.03%	0.222%
19	5.470	712	719	726	rVV	113920	319891	2.87%	0.314%
20	5.556	726	733	742	rVB	120570	326366	2.93%	0.320%
21	5.958	790	799	803	rBV	71577	177277	1.59%	0.174%
22	6.044	803	813	825	rVB	4180122	10919018	98.05%	10.711%
23	6.202	826	839	845	rBV2	89189	292554	2.63%	0.287%
24	6.361	857	865	877	rVB6	37985	125352	1.13%	0.123%
25	6.763	923	931	938	rBV	225606	584906	5.25%	0.574%
26	7.171	990	998	1009	rVB2	72265	168577	1.51%	0.165%
27	7.379	1020	1032	1046	rBV4	162970	429898	3.86%	0.422%
28	8.141	1153	1157	1162	rVB	176364	284969	2.56%	0.280%
29	8.507	1210	1217	1227	rVB2	130661	232166	2.08%	0.228%
30	8.647	1235	1240	1246	rVB	345656	537023	4.82%	0.527%
31	8.720	1246	1252	1259	rBV	669244	1019423	9.15%	1.000%
32	9.458	1364	1373	1377	rBV3	62294	121219	1.09%	0.119%
33	10.055	1461	1471	1476	rBV	484367	663253	5.96%	0.651%
34	10.195	1488	1494	1500	rBV	8226648	10663949	95.76%	10.461%
35	10.305	1506	1512	1518	rVB	8564429	11135925	100.00%	10.924%
36	10.646	1562	1568	1578	rVB	5257798	6923606	62.17%	6.792%

LSC Area Percent Report

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Instrument :
MSVOA_X
ClientSampleId :
DUP112122

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Title : SW846 8260

37	10.963	1614	1620	1626	rBV	677019	839255	7.54%	0.823%
38	11.079	1634	1639	1645	rBV	330107	416602	3.74%	0.409%
39	11.305	1668	1676	1683	rBV	1727076	2038647	18.31%	2.000%
40	11.378	1683	1688	1690	rVV	1530805	2123624	19.07%	2.083%
41	11.396	1690	1691	1696	rVV	1885680	1906370	17.12%	1.870%
42	11.451	1696	1700	1706	rVB	1571936	1870503	16.80%	1.835%
43	11.610	1721	1726	1736	rBV	2049302	2631637	23.63%	2.582%
44	11.756	1744	1750	1755	rVB	7729430	9337319	83.85%	9.160%
45	11.969	1779	1785	1789	rBV	95917	121183	1.09%	0.119%
46	12.024	1789	1794	1798	rVV2	562388	763587	6.86%	0.749%
47	12.085	1798	1804	1809	rVB	2602185	3176987	28.53%	3.117%
48	12.244	1824	1830	1838	rBV	3514162	4638684	41.66%	4.551%
49	12.317	1838	1842	1852	rVB3	619148	917506	8.24%	0.900%
50	12.408	1852	1857	1862	rBV2	275326	370501	3.33%	0.363%
51	12.463	1862	1866	1872	rVB	256030	297634	2.67%	0.292%
52	12.530	1872	1877	1879	rBV	461557	563875	5.06%	0.553%
53	12.555	1879	1881	1885	rVB	343622	364182	3.27%	0.357%
54	12.616	1885	1891	1894	rBV	919986	1161762	10.43%	1.140%
55	12.646	1894	1896	1900	rVB	223787	225899	2.03%	0.222%
56	12.701	1900	1905	1913	rBV2	673851	981279	8.81%	0.963%
57	12.847	1924	1929	1934	rVB2	240604	297384	2.67%	0.292%
58	12.920	1934	1941	1944	rBV	589516	697991	6.27%	0.685%
59	12.963	1944	1948	1954	rVB	679360	797208	7.16%	0.782%
60	13.024	1954	1958	1964	rBV3	52357	115651	1.04%	0.113%
61	13.170	1978	1982	1986	rVB	639400	738280	6.63%	0.724%
62	13.292	1997	2002	2007	rVB2	1466074	1884042	16.92%	1.848%
63	13.341	2007	2010	2013	rBV3	102788	111723	1.00%	0.110%
64	13.420	2018	2023	2032	rVB	422219	544235	4.89%	0.534%
65	13.542	2040	2043	2046	rBV	126856	149869	1.35%	0.147%
66	13.585	2046	2050	2055	rVB3	139226	210669	1.89%	0.207%
67	13.664	2060	2063	2069	rVB2	161778	250172	2.25%	0.245%
68	13.774	2074	2081	2090	rBV	2990958	3797394	34.10%	3.725%
69	13.865	2090	2096	2100	rBV2	91679	152065	1.37%	0.149%
70	13.926	2100	2106	2110	rBV2	102178	134162	1.20%	0.132%
71	14.073	2125	2130	2138	rBV	112317	164695	1.48%	0.162%
72	14.225	2149	2155	2163	rVB4	156395	314123	2.82%	0.308%
73	14.371	2176	2179	2184	rVB	91949	112088	1.01%	0.110%
74	14.481	2192	2197	2202	rBV2	108181	149239	1.34%	0.146%
75	14.640	2210	2223	2233	rBV	1449795	1921243	17.25%	1.885%
76	14.780	2241	2246	2255	rBV	1103199	1378166	12.38%	1.352%

LSC Area Percent Report

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Title : SW846 8260

77	15.377	2336	2344	2347	rBV	73136	114464	1.03%	0.112%
78	15.475	2353	2360	2366	rBV	198090	318825	2.86%	0.313%
79	15.615	2374	2383	2386	rBV	282709	448456	4.03%	0.440%
80	15.652	2386	2389	2396	rVB	178838	252039	2.26%	0.247%
81	15.834	2409	2419	2431	rVB	77937	202535	1.82%	0.199%

Sum of corrected areas: 101937639

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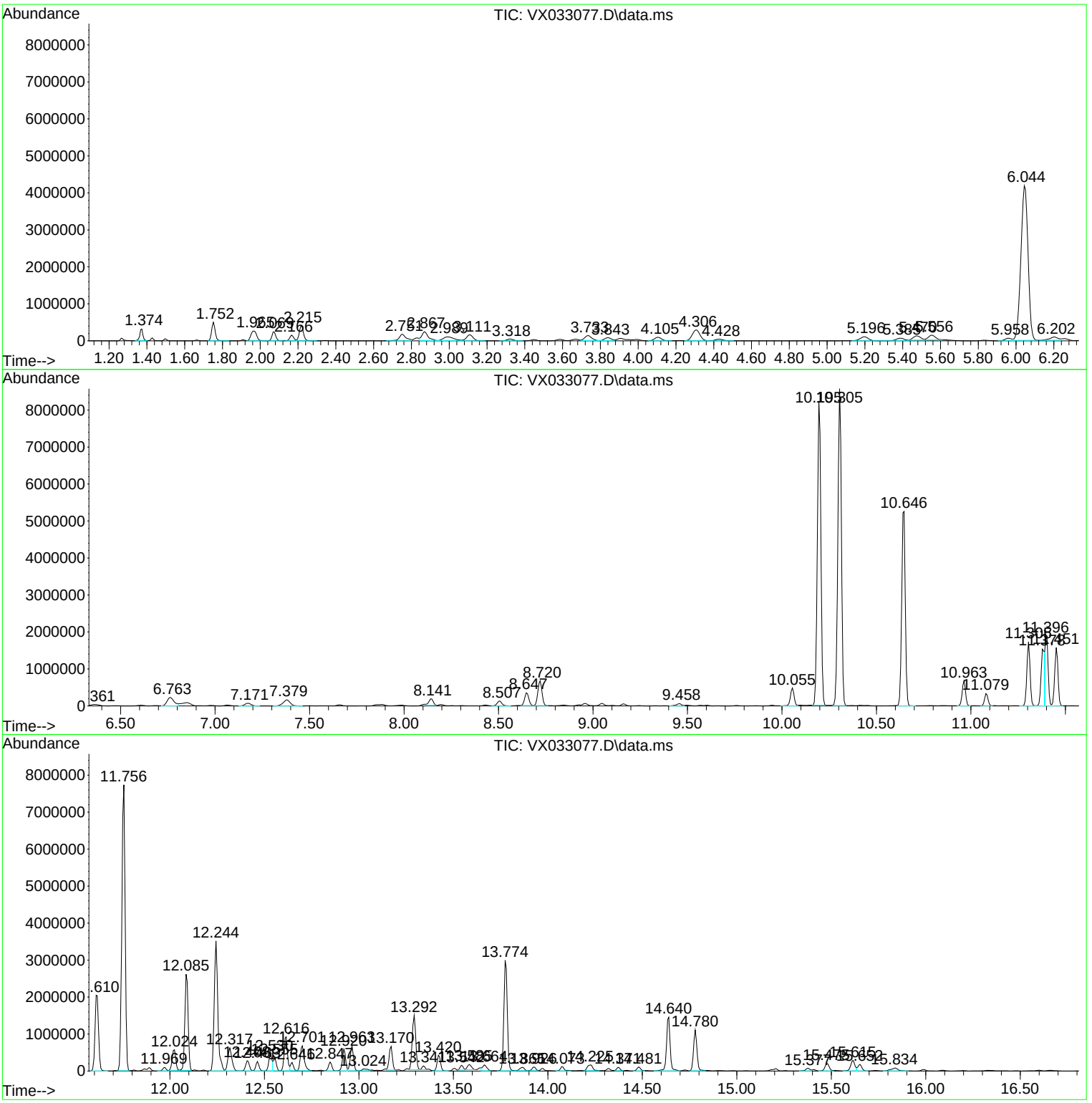
Instrument :
MSVOA_X
ClientSampleId :
DUP112122

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

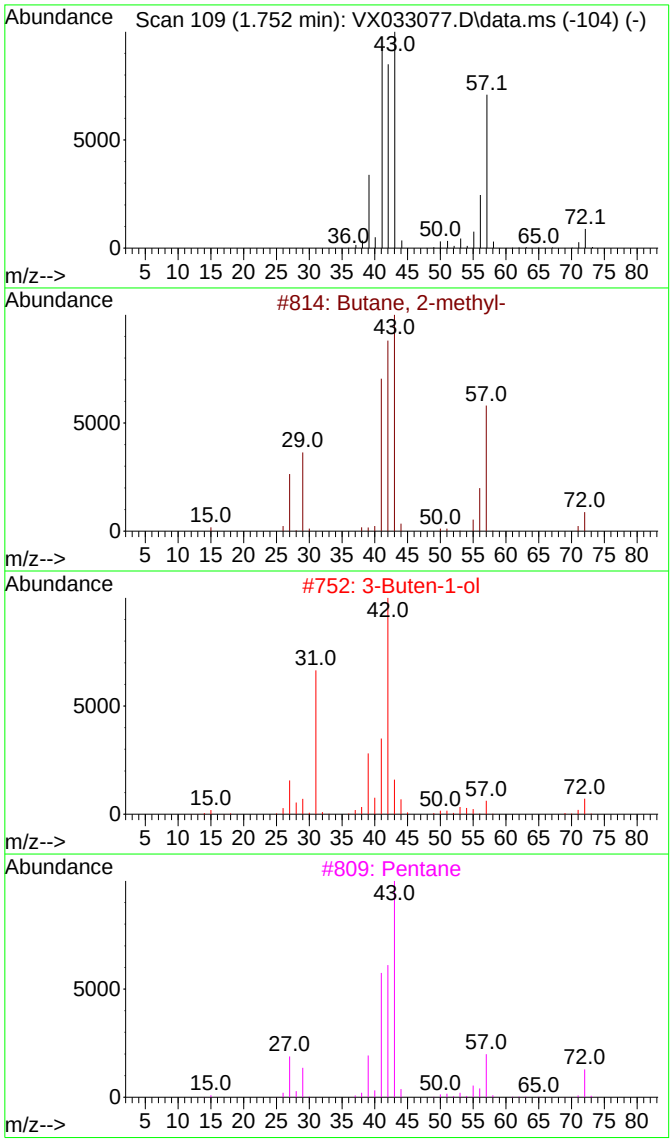
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

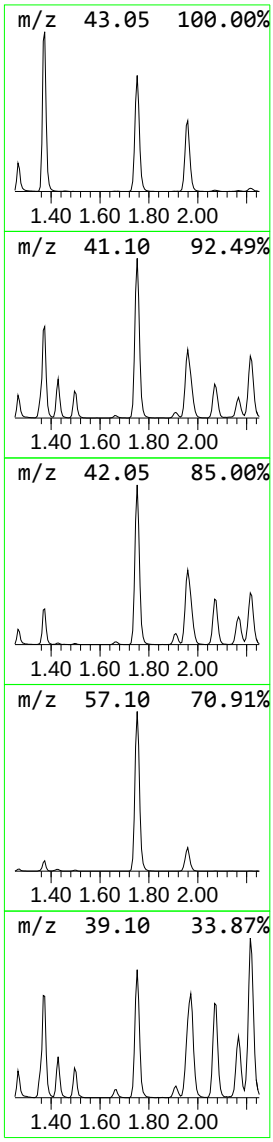
****

Peak Number 1 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	99.88 ug/l	651917	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Azetidine	57	C3H7N	000503-29-7	9
5	1-Butene	56	C4H8	000106-98-9	9





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Operator : JC/MD
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

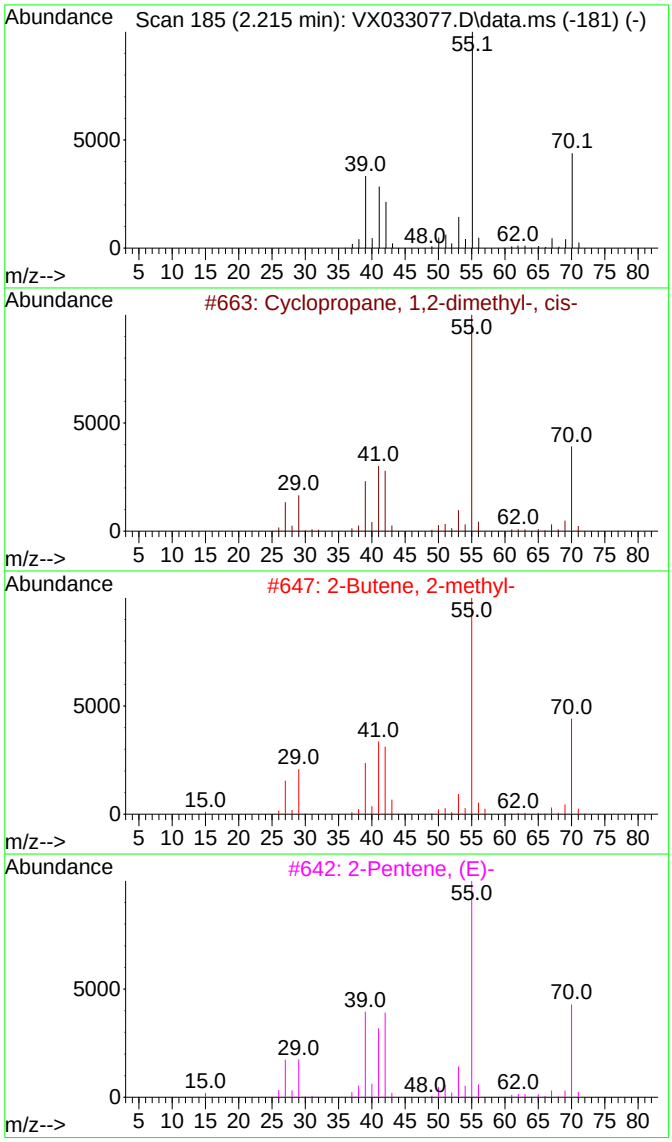
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

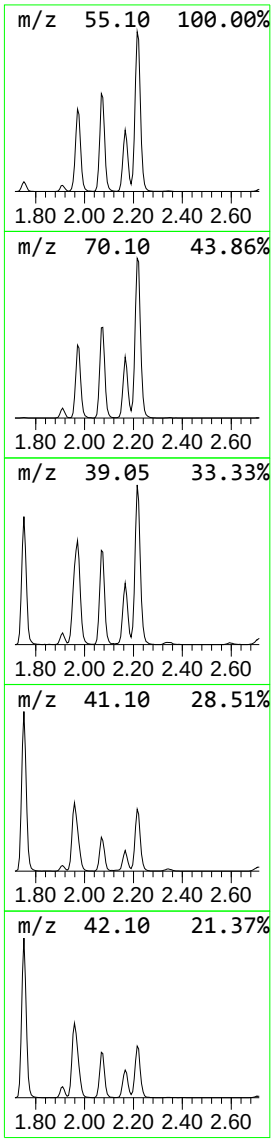
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopropane, 1,2-dimethyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	95.56 ug/l	623759	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3	2-Pentene, (E)-	70	C5H10	000646-04-8	87
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

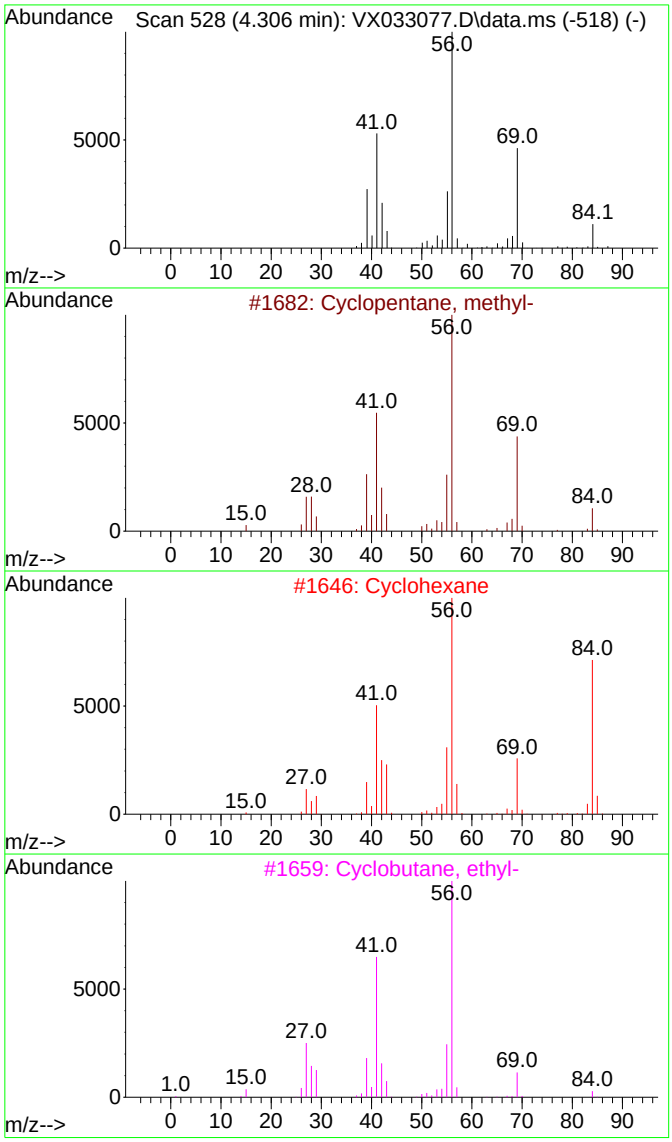
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

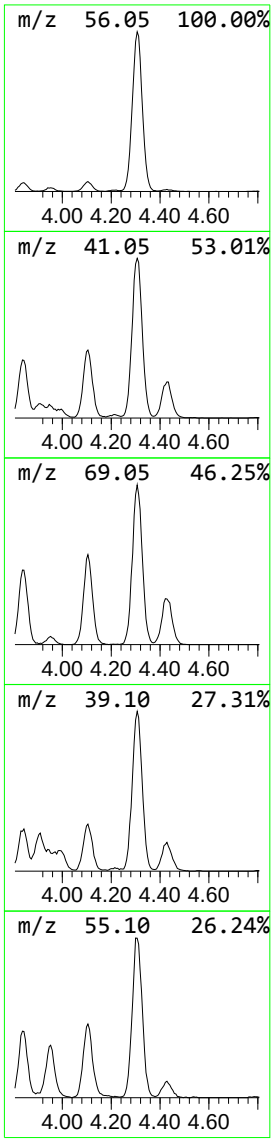
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	127.59 ug/l	832822	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72





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Instrument :
MSVOA_X
ClientSampleId :
DUP112122

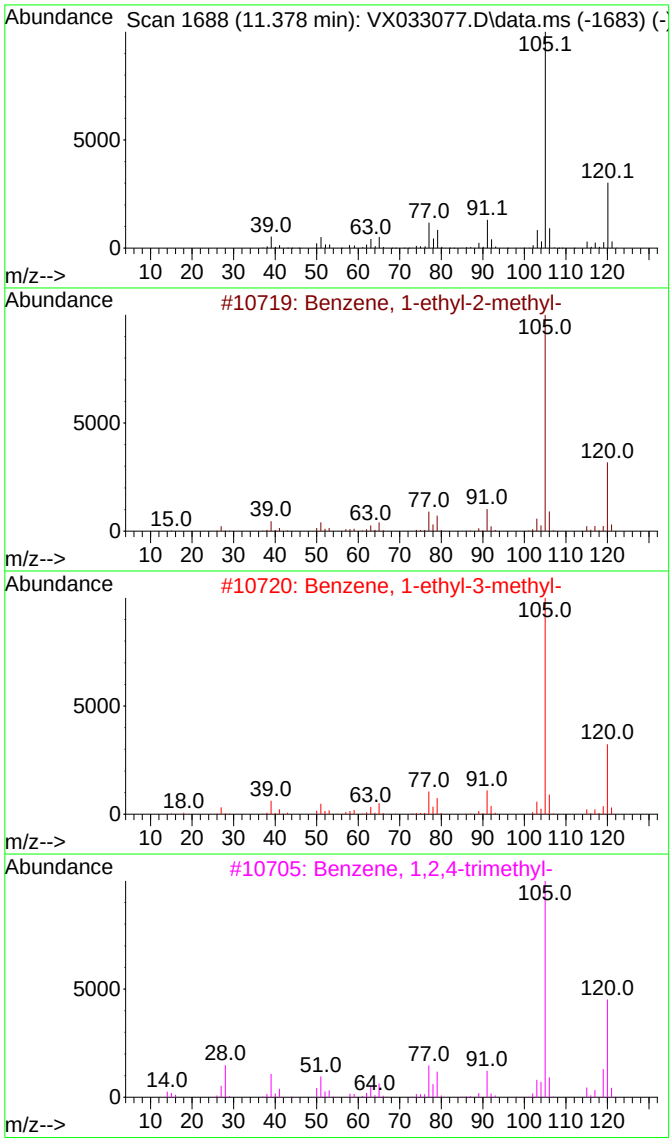
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

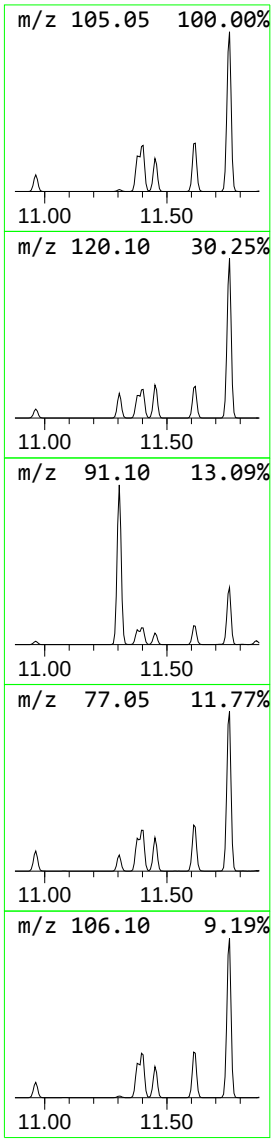
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	139.06 ug/l	2123620	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	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

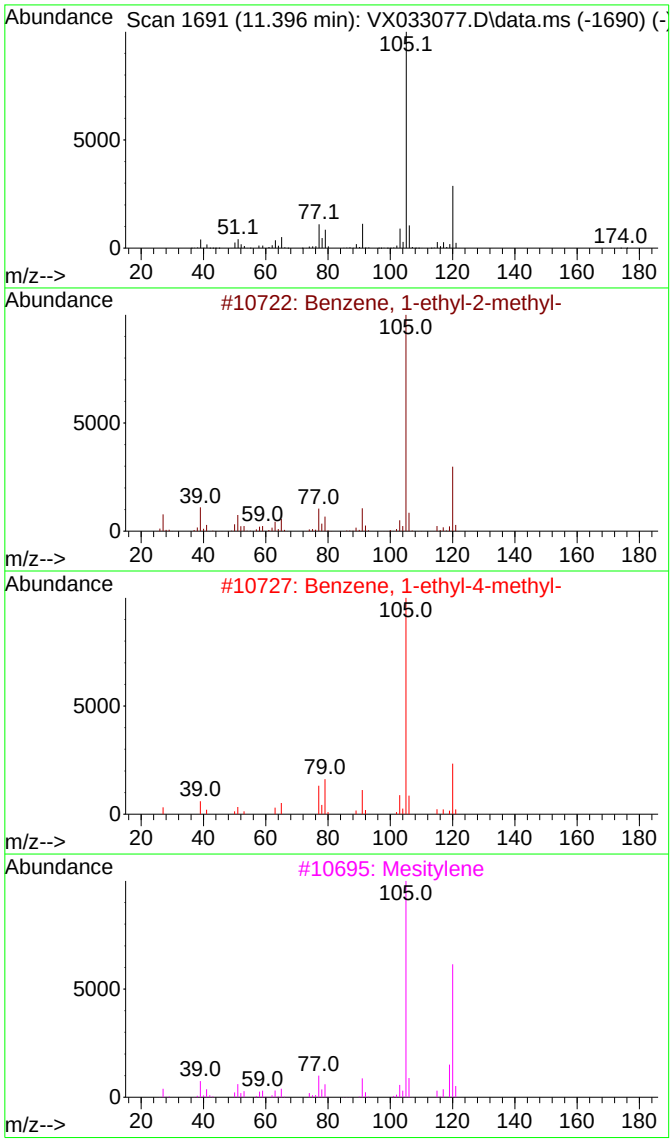
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

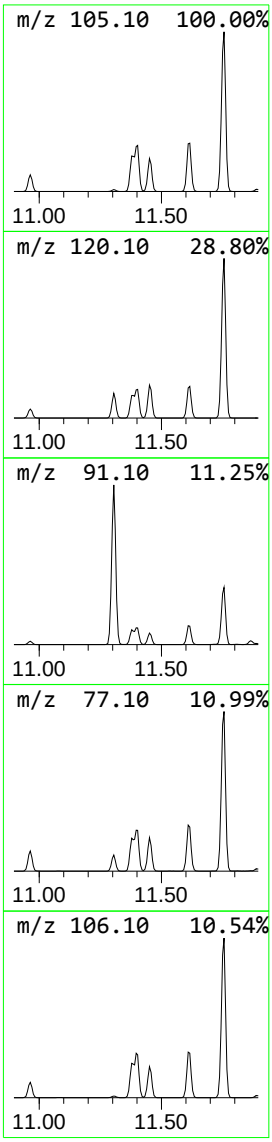
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.396	124.83 ug/l	1906370	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	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

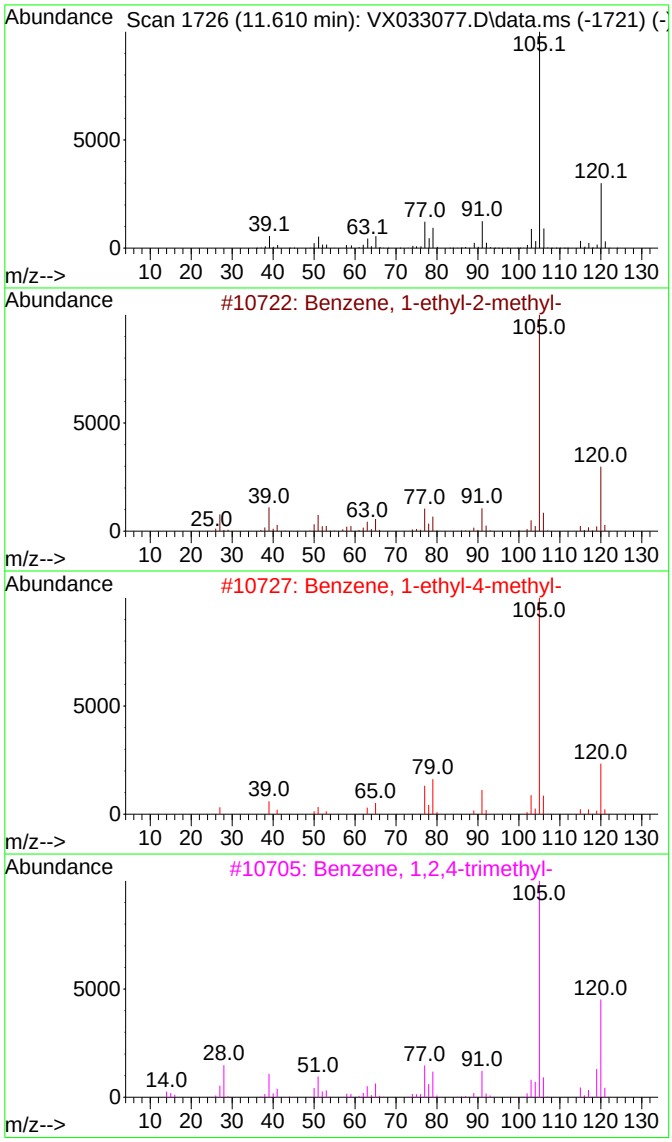
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

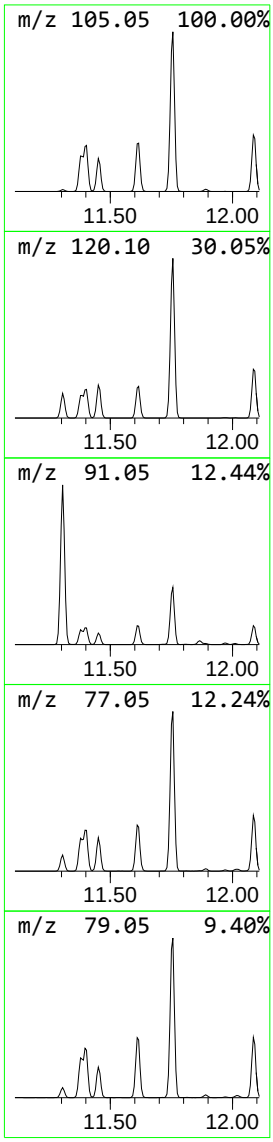
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	172.32 ug/l	2631640	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	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

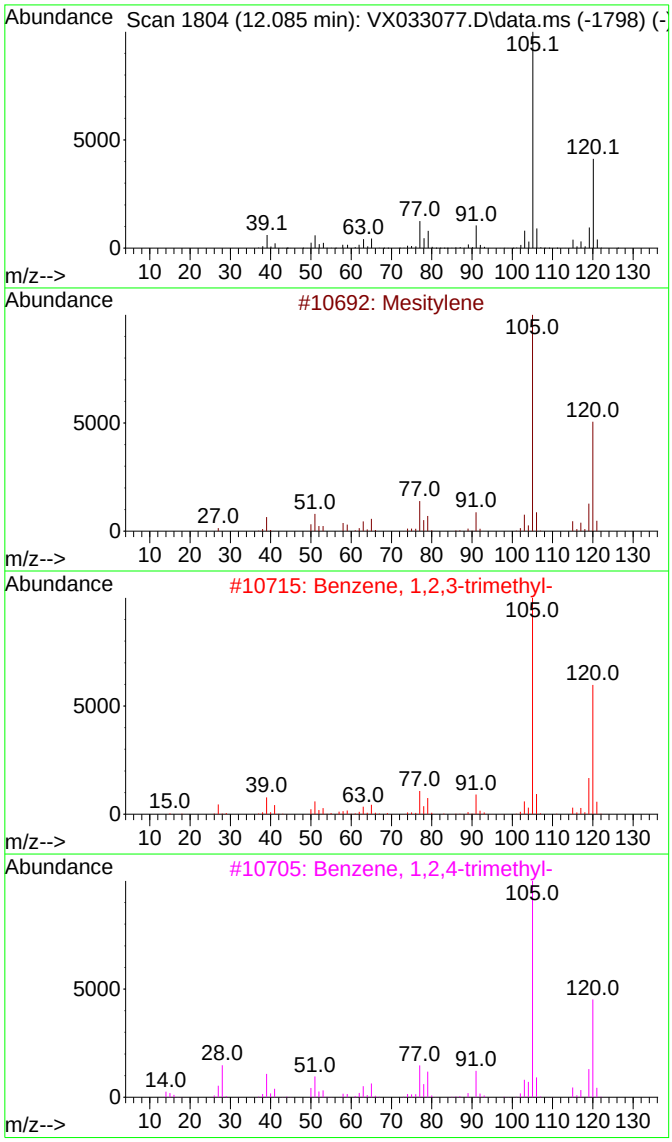
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

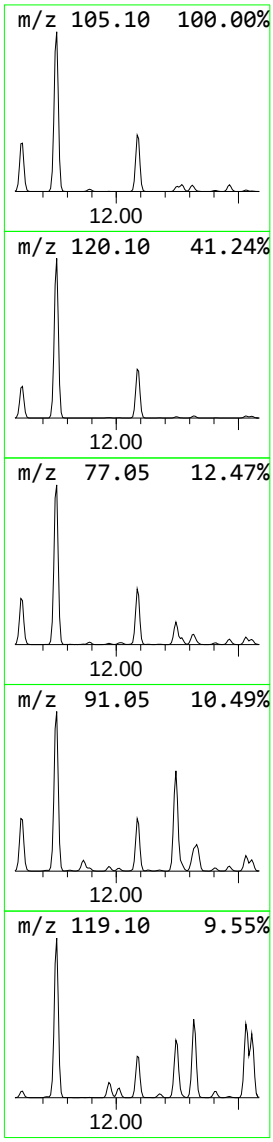
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	208.03 ug/l	3176990	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

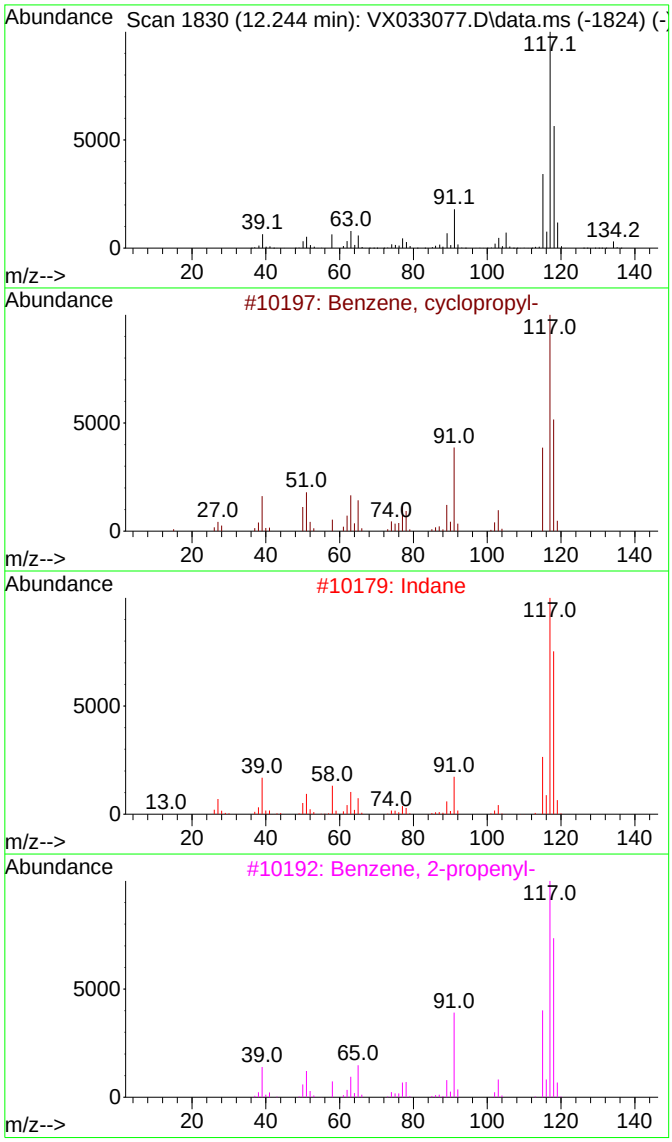
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

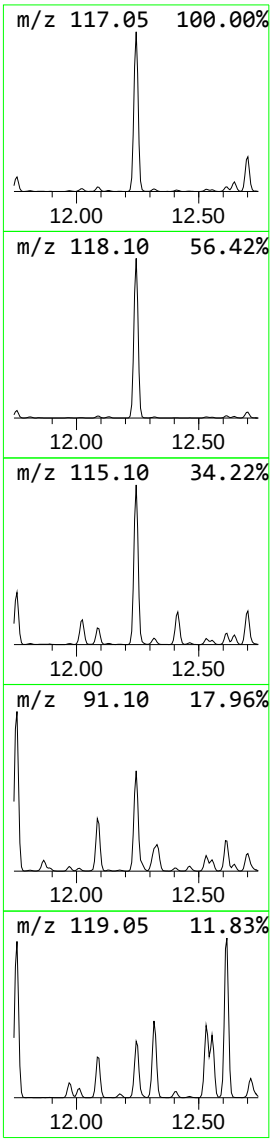
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	303.74 ug/l	4638680	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2	Indane	118	C9H10	000496-11-7	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4	Deltacyclene	118	C9H10	007785-10-6	64
5	Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

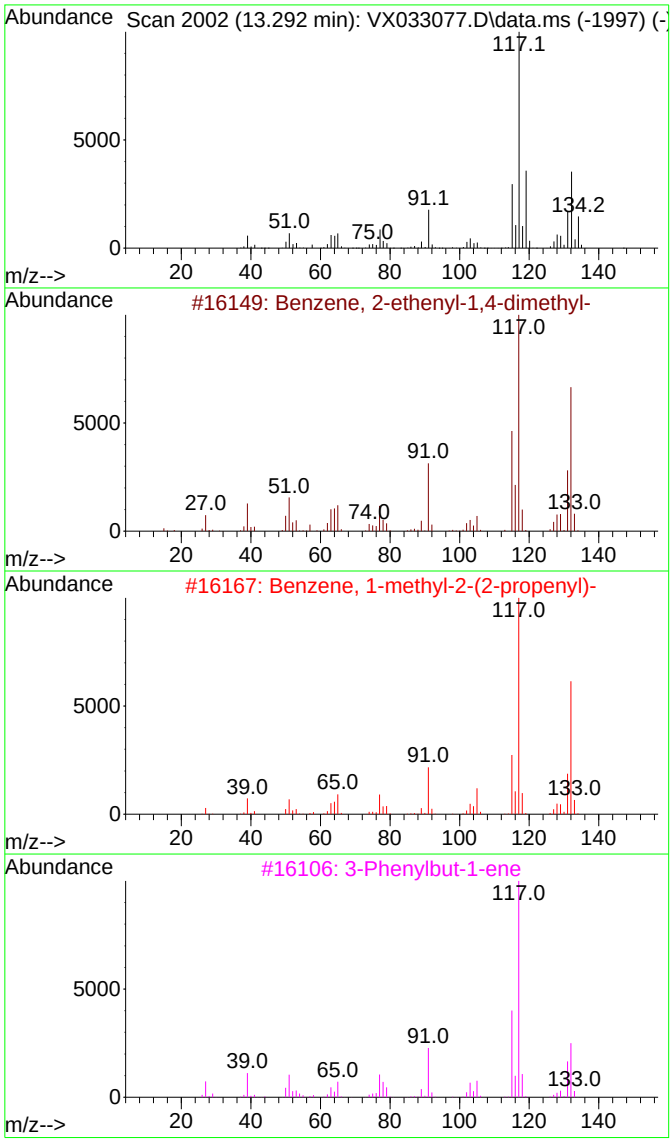
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

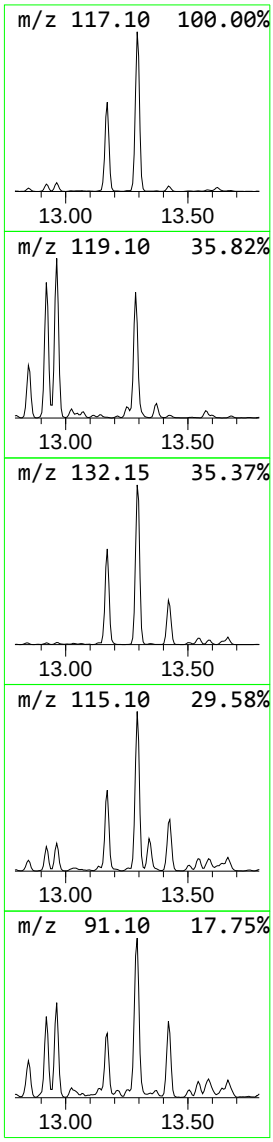
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	123.37 ug/l	1884040	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87





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Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

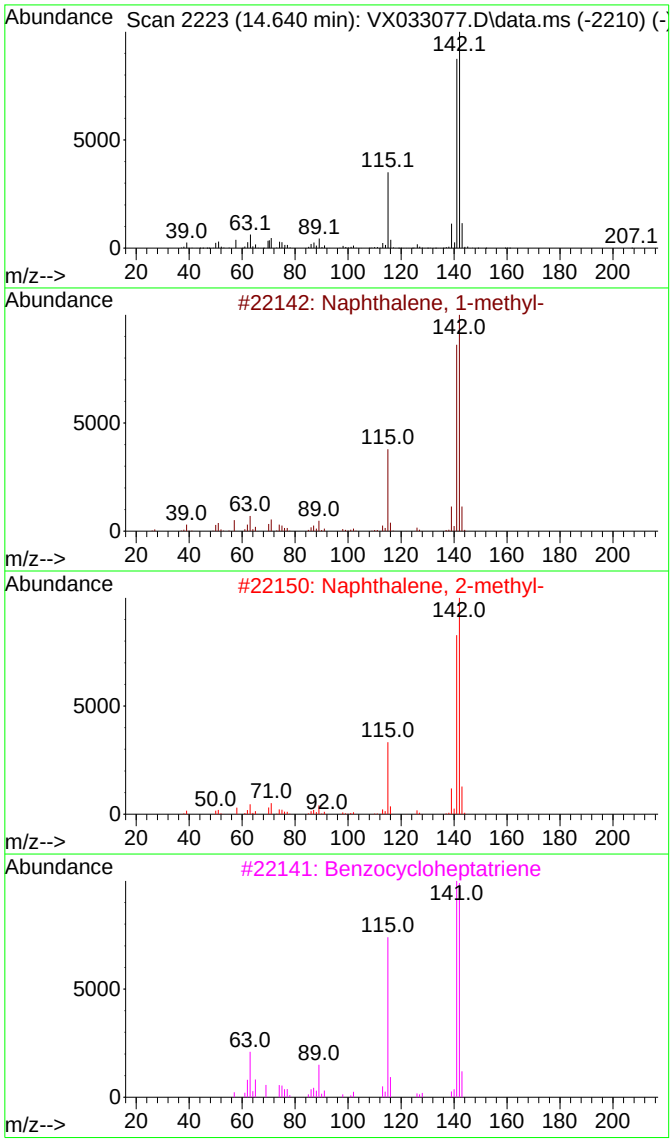
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

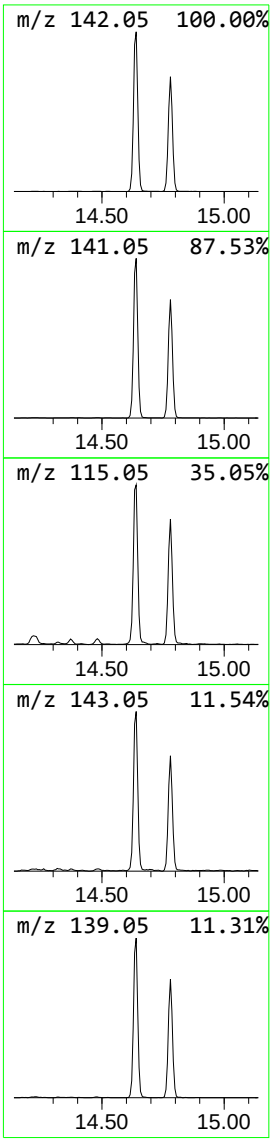
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzocycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	125.80 ug/l	1921240	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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033077.D
Acq On : 25 Nov 2022 18:46
Operator : JC/MD
Sample : N5747-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP112122

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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-	1.752	99.9	ug/l	651917	1	5.556	326366	50.0
Cyclopropane, 1...	2.215	95.6	ug/l	623759	1	5.556	326366	50.0
Cyclopentane, m...	4.306	127.6	ug/l	832822	1	5.556	326366	50.0
Benzene, 1-ethy...	11.378	139.1	ug/l	2123620	4	12.024	763587	50.0
Benzene, 1-ethy...	11.396	124.8	ug/l	1906370	4	12.024	763587	50.0
Benzene, 1-ethy...	11.610	172.3	ug/l	2631640	4	12.024	763587	50.0
Benzene, 1,2,3-...	12.085	208.0	ug/l	3176990	4	12.024	763587	50.0
Benzene, cyclop...	12.244	303.7	ug/l	4638680	4	12.024	763587	50.0
Benzene, 2-ethe...	13.292	123.4	ug/l	1884040	4	12.024	763587	50.0
Benzocyclohepta...	14.640	125.8	ug/l	1921240	4	12.024	763587	50.0