LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034813.D
Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	40	46	52	rBV	32969	40077	2.59%	0.203%
2	1.752	103	109	117	rBV	168008	219631	14.19%	1.113%
3	1.959	138	143	152	rVB	73022	109311	7.06%	0.554%
4	2.215	181	185	192	rVB2	14490	22895	1.48%	0.116%
5	2.343	200	206	209	rBV2	10990	20315	1.31%	0.103%
6	2.380	209	212	220	rVB	12449	21243	1.37%	0.108%
7	2.782	271	278	281	rBV	37237	74790	4.83%	0.379%
8	2.825	281	285	290	rVB	59033	102689	6.63%	0.521%
9	3.099	320	330	342	rBV	88665	201254	13.00%	1.020%
10	3.319	359	366	379	rBV3	10365	28801	1.86%	0.146%
11	3.447	379	387	397	rVB	26048	58688	3.79%	0.297%
12	3.672	416	424	429	rBV3	8389	20319	1.31%	0.103%
13	4.306	518	528	540	rVB2	102267	292921	18.92%	1.485%
14	4.818	601	612	622	rBV3	12523	40539	2.62%	0.205%
15	5.190	667	673	683	rVB6	5999	20677	1.34%	0.105%
16	5.385	693	705	713	rBV	170339	500812	32.35%	2.539%
17	5.471	713	719	725	rVV3	67099	215543	13.92%	1.093%
18	5.550	725	732	764	rVB2	298978	950225	61.37%	4.817%
19	5.830	767	778	789	rBV4	31752	103829	6.71%	0.526%
20	5.952	789	798	812	rBV	200382	534841	34.55%	2.711%
21	6.159	820	832	842	rBV6	30808	109988	7.10%	0.558%
22	6.257	842	848	856	rVV3	29672	79873	5.16%	0.405%
23	6.355	856	864	877	rVB3	31086	87875	5.68%	0.445%
24	6.605	898	905	915	rBV6	6812	20092	1.30%	0.102%
25	6.757	921	930	943	rBV	467220	1140106	73.64%	5.779%
26	7.379	1019	1032	1043	rVB2	131690	325285	21.01%	1.649%
27	7.659	1070	1078	1085	rVB2	15989	32347	2.09%	0.164%
28	7.775	1090	1097	1103	rVB3	13400	25342	1.64%	0.128%
29	7.958	1121	1127	1141	rVB4	12408	32266	2.08%	0.164%
30	8.318	1175	1186	1193	rBV7	9690	26071	1.68%	0.132%
31	8.433	1200	1205	1212	rBV	23664	43968	2.84%	0.223%
32	8.507	1212	1217	1224	rVB4	19993	38544	2.49%	0.195%
33	8.598	1224	1232	1234	rBV3	32160	63265	4.09%	0.321%
34	8.647	1234	1240	1247	rVV	997301	1548230	100.00%	7.848%
35	8.720	1247	1252	1257	rVV	86720	144511	9.33%	0.733%
36	8.769	1257	1260	1263	rVV3	15612	27414	1.77%	0.139%

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ClientSampleId :
MW-3

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\82X031023W.M
Title : SW846 8260

37	8.811	1263	1267	1270	rVV3	15831	30179	1.95%	0.153%
38	8.976	1289	1294	1301	rVB	26659	44182	2.85%	0.224%
39	9.098	1305	1314	1320	rBV2	18239	34049	2.20%	0.173%
40	9.159	1320	1324	1329	rBV	13722	21368	1.38%	0.108%
41	9.439	1364	1370	1376	rBV3	12979	31786	2.05%	0.161%
42	9.531	1376	1385	1396	rVV	117644	250551	16.18%	1.270%
43	9.616	1396	1399	1403	rVV2	16179	25526	1.65%	0.129%
44	9.830	1428	1434	1443	rBV10	7825	21267	1.37%	0.108%
45	10.055	1463	1471	1479	rBV	947838	1321610	85.36%	6.699%
46	10.189	1487	1493	1499	rVV3	76998	159564	10.31%	0.809%
47	10.299	1503	1511	1518	rVB	638375	892234	57.63%	4.523%
48	10.586	1552	1558	1562	rVV7	7853	19834	1.28%	0.101%
49	10.640	1562	1567	1579	rVB	431476	563428	36.39%	2.856%
50	10.775	1583	1589	1594	rBV3	13353	22410	1.45%	0.114%
51	10.890	1604	1608	1614	rVB2	21898	32312	2.09%	0.164%
52	10.964	1614	1620	1630	rVB	78678	105831	6.84%	0.536%
53	11.079	1634	1639	1645	rBV	812712	1013598	65.47%	5.138%
54	11.305	1670	1676	1683	rVV	102103	135512	8.75%	0.687%
55	11.378	1683	1688	1696	rVV	282854	493332	31.86%	2.501%
56	11.451	1696	1700	1709	rVB	117990	151051	9.76%	0.766%
57	11.610	1721	1726	1733	rVB	293670	382012	24.67%	1.936%
58	11.750	1744	1749	1756	rBV	632219	757365	48.92%	3.839%
59	11.866	1761	1768	1770	rBV	14912	24475	1.58%	0.124%
60	11.890	1770	1772	1781	rVB3	20493	34873	2.25%	0.177%
61	11.969	1781	1785	1788	rBV	37890	45691	2.95%	0.232%
62	12.018	1788	1793	1800	rVV	965569	1237561	79.93%	6.273%
63	12.085	1800	1804	1810	rVB	244783	291140	18.80%	1.476%
64	12.244	1823	1830	1832	rBV2	137116	181668	11.73%	0.921%
65	12.268	1832	1834	1837	rVB	88711	89850	5.80%	0.455%
66	12.311	1837	1841	1850	rVB4	106171	186163	12.02%	0.944%
67	12.408	1850	1857	1862	rBV2	22531	32768	2.12%	0.166%
68	12.463	1862	1866	1871	rVB	41960	52215	3.37%	0.265%
69	12.530	1871	1877	1879	rBV	105912	128755	8.32%	0.653%
70	12.555	1879	1881	1885	rVB	60219	65234	4.21%	0.331%
71	12.610	1885	1890	1894	rBV	276977	340906	22.02%	1.728%
72	12.646	1894	1896	1900	rVB	35505	37535	2.42%	0.190%
73	12.701	1900	1905	1913	rBV2	244216	380222	24.56%	1.927%
74	12.805	1917	1922	1925	rBV2	37524	55222	3.57%	0.280%
75	12.847	1925	1929	1934	rVB2	58627	80380	5.19%	0.407%
76	12.920	1934	1941	1945	rBV	177838	217932	14.08%	1.105%

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ALS Vial : 37 Sample Multiplier: 1

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ClientSampleId :
MW-3

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

77	12.963	1945	1948	1954	rVB	87570	104179	6.73%	0.528%
78	13.024	1954	1958	1960	rBV2	28227	41794	2.70%	0.212%
79	13.134	1972	1976	1978	rBV	23484	27466	1.77%	0.139%
80	13.170	1978	1982	1992	rVB	147707	217248	14.03%	1.101%
81	13.256	1992	1996	1997	rBV2	25755	28694	1.85%	0.145%
82	13.292	1997	2002	2008	rVV2	337238	464683	30.01%	2.355%
83	13.372	2012	2015	2019	rVV	23131	26759	1.73%	0.136%
84	13.420	2019	2023	2031	rVB	54458	75054	4.85%	0.380%
85	13.506	2031	2037	2040	rBV2	37062	52837	3.41%	0.268%
86	13.542	2040	2043	2046	rVV	77955	104460	6.75%	0.529%
87	13.585	2046	2050	2056	rVV6	78077	154834	10.00%	0.785%
88	13.640	2056	2059	2060	rVV	51745	61632	3.98%	0.312%
89	13.664	2060	2063	2068	rVV2	96572	143874	9.29%	0.729%
90	13.713	2068	2071	2075	rVV	16142	22193	1.43%	0.112%
91	13.774	2075	2081	2088	rVV	303928	390106	25.20%	1.977%
92	13.865	2088	2096	2100	rVV3	35758	64549	4.17%	0.327%
93	13.926	2100	2106	2110	rVV2	28286	40027	2.59%	0.203%
94	13.969	2110	2113	2117	rVB	30492	34380	2.22%	0.174%
95	14.073	2126	2130	2135	rBV	46863	59003	3.81%	0.299%
96	14.213	2148	2153	2162	rBV2	40549	73443	4.74%	0.372%
97	14.371	2175	2179	2183	rVB	34176	39948	2.58%	0.202%
98	14.597	2210	2216	2219	rBV2	14739	22898	1.48%	0.116%
99	14.634	2219	2222	2233	rVB	63674	91493	5.91%	0.464%
100	14.780	2241	2246	2254	rBV2	51184	70402	4.55%	0.357%

Sum of corrected areas: 19728124

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MSVOA_X
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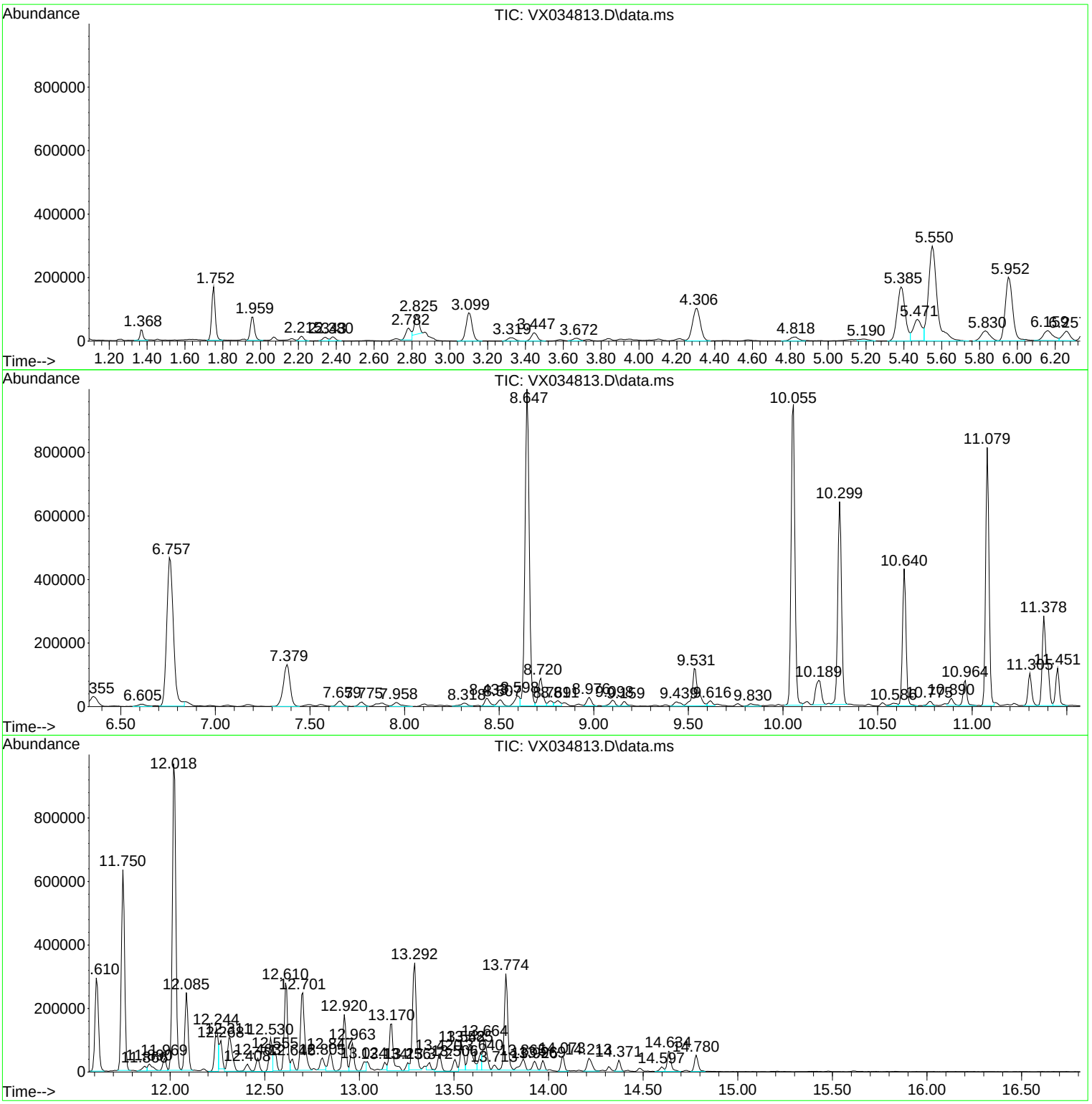
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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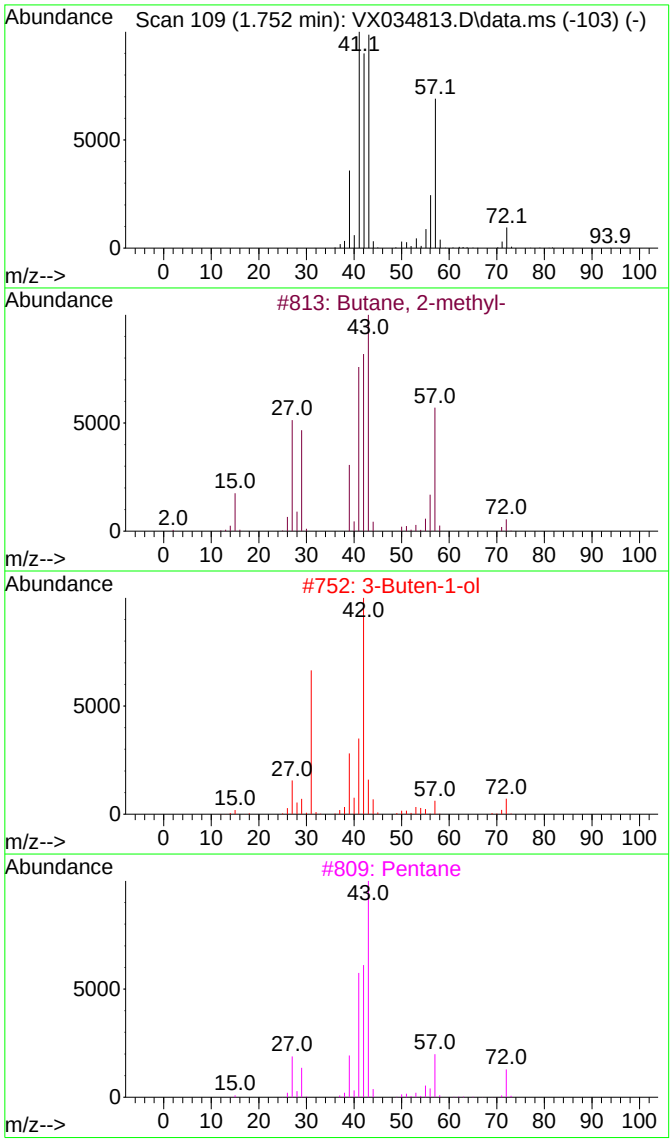
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

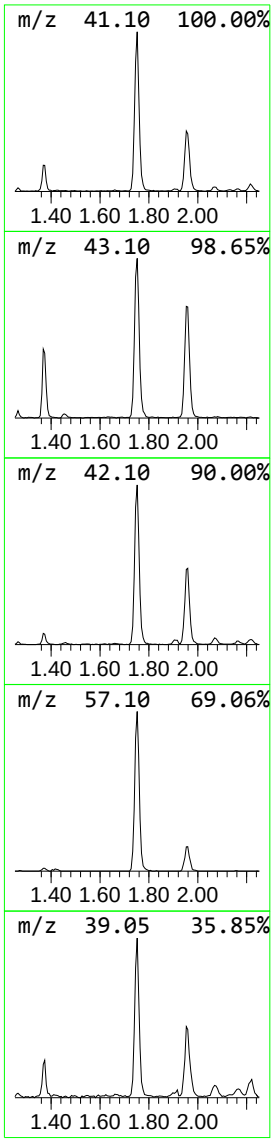
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	11.56 ug/l	219631	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	42
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	14





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

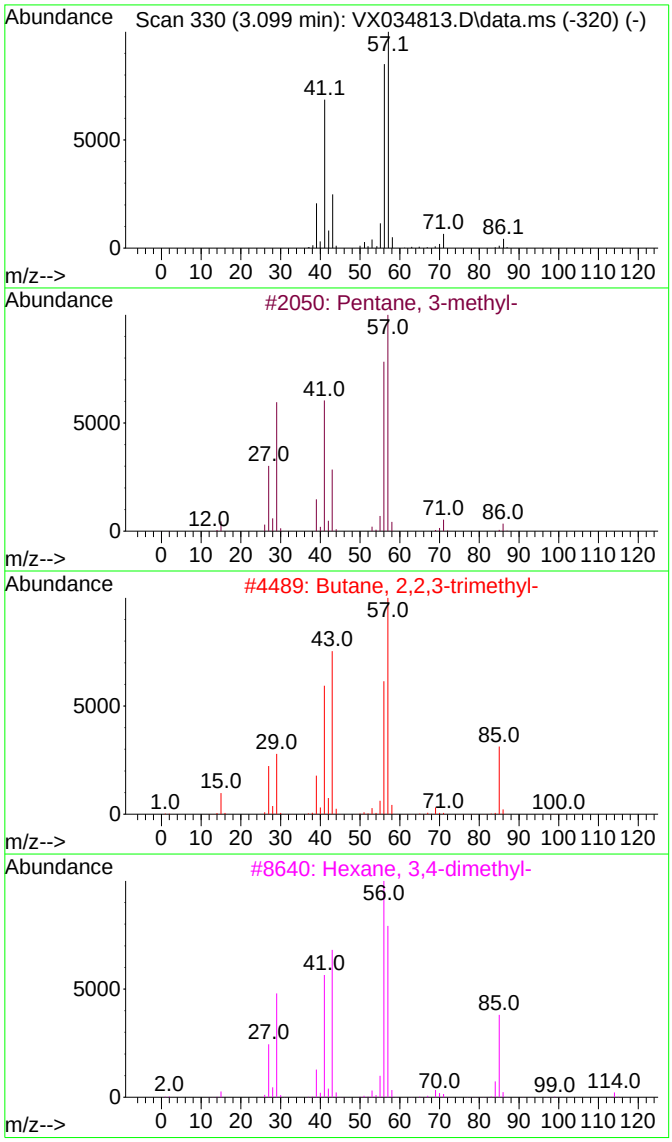
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

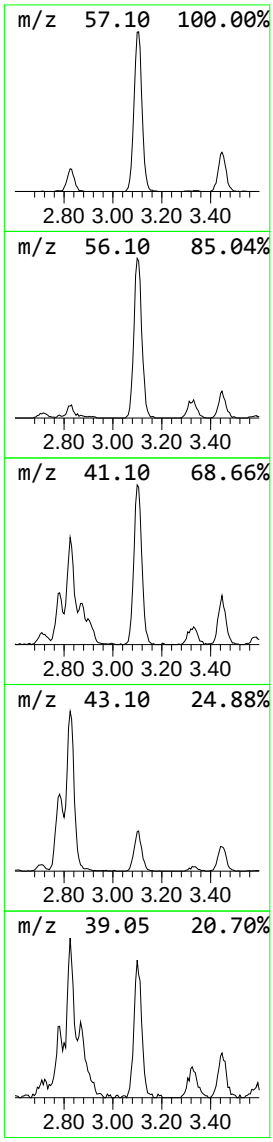
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.099	10.59 ug/l	201254	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	43
4	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40
5	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	40





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MSVOA_X
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MW-3

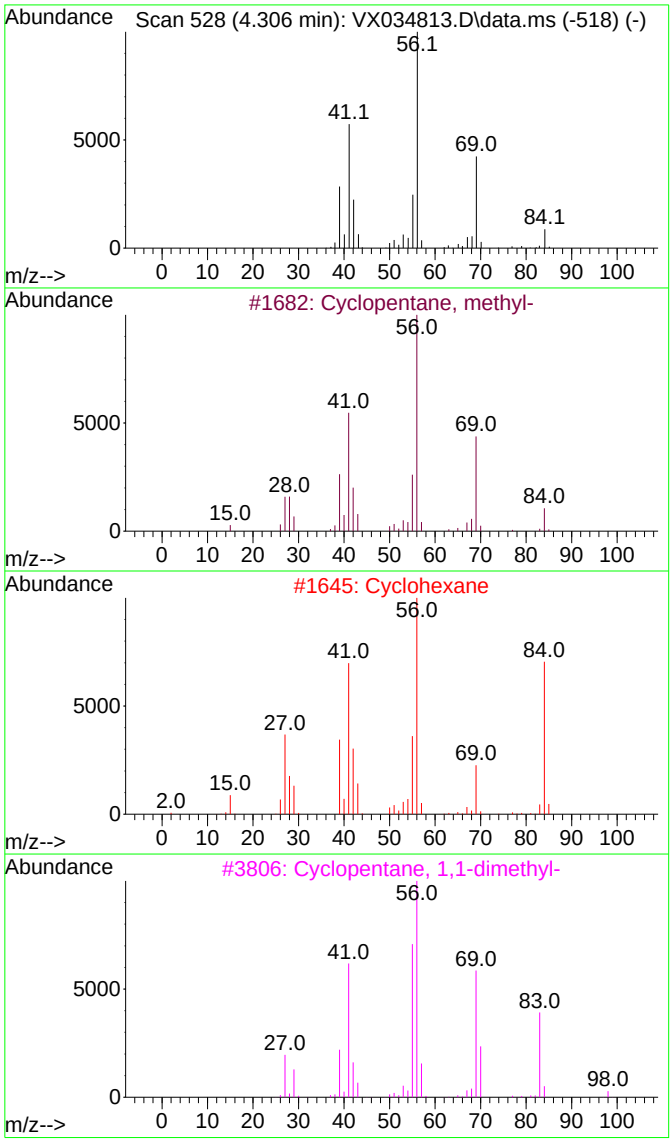
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

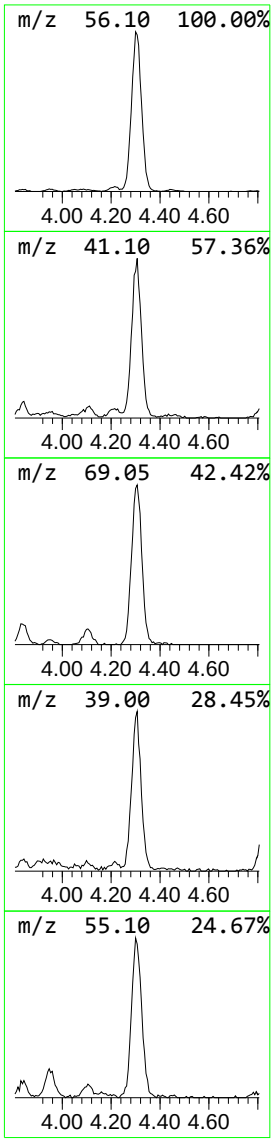
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	15.41 ug/l	292921	Pentafluorobenzene	5.550

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	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56





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MSVOA_X
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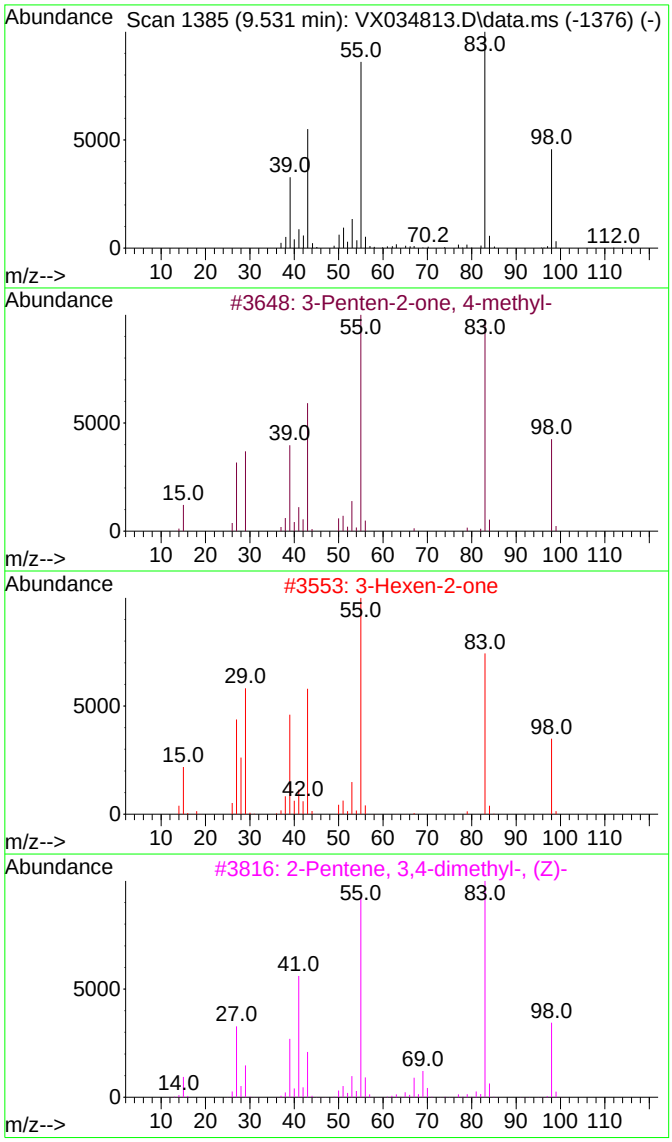
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

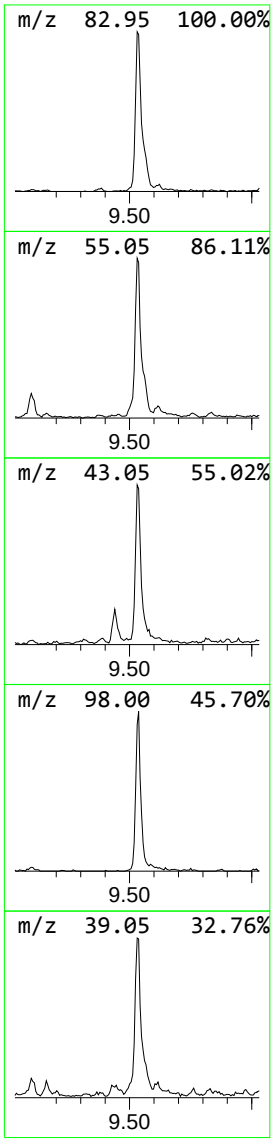
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.531	9.48 ug/l	250551	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	78





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Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

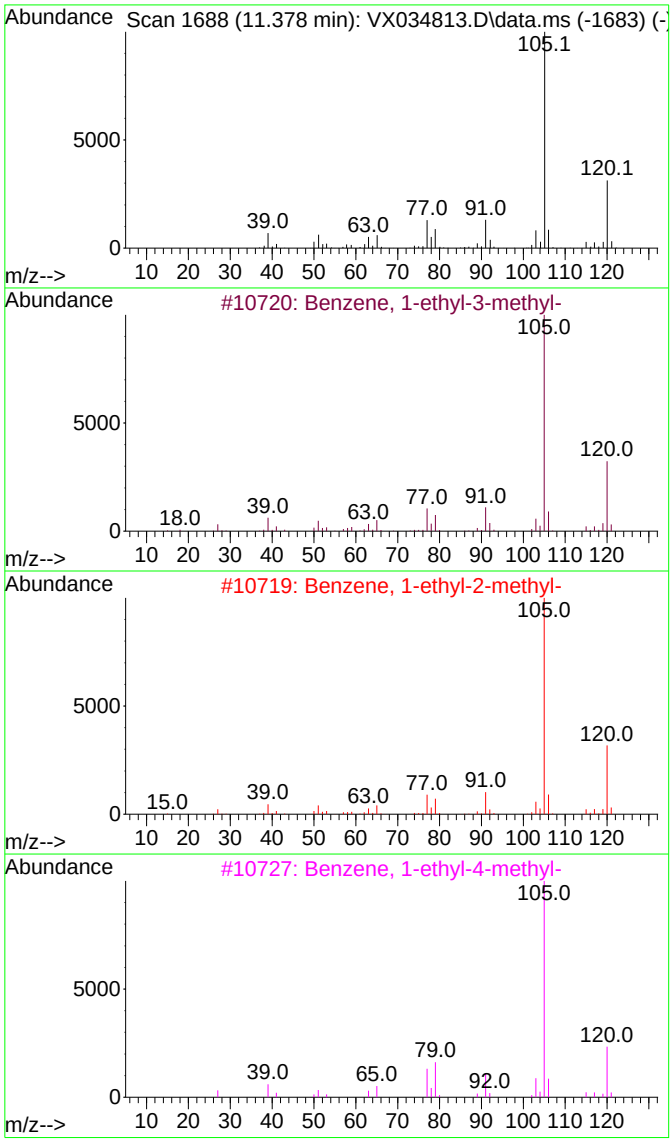
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

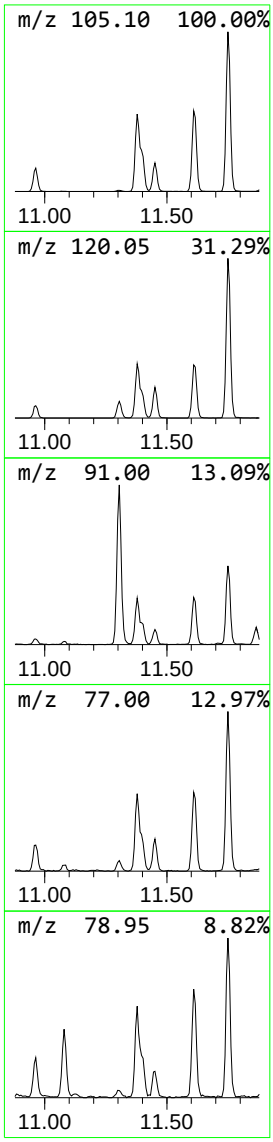
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	19.93 ug/l	493332	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034813.D
Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

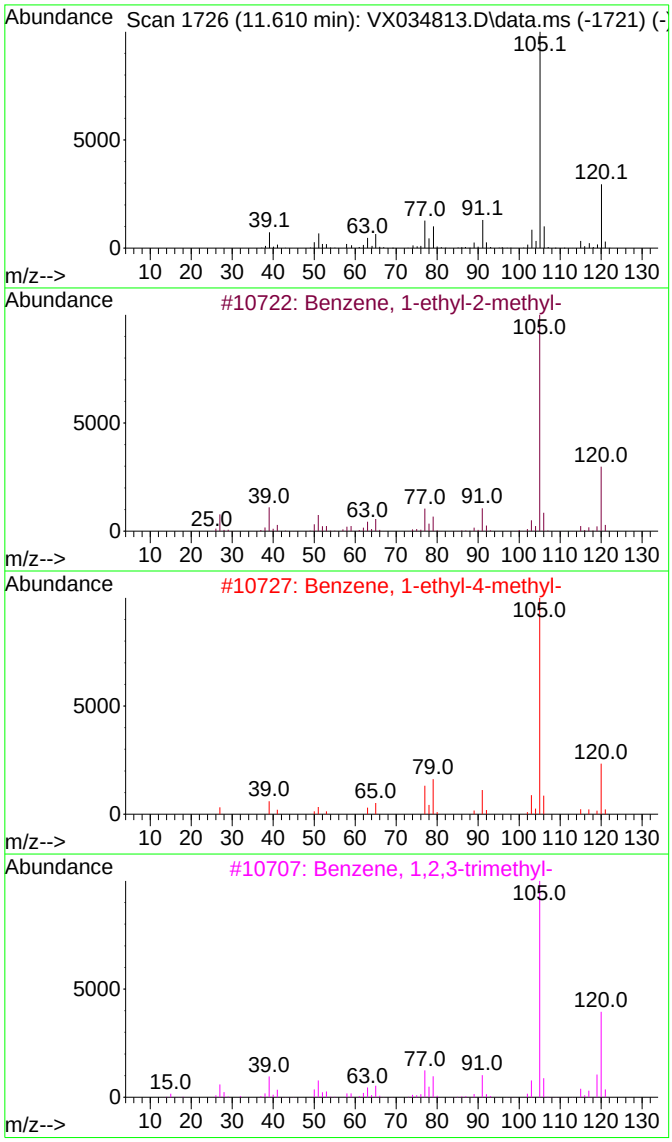
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

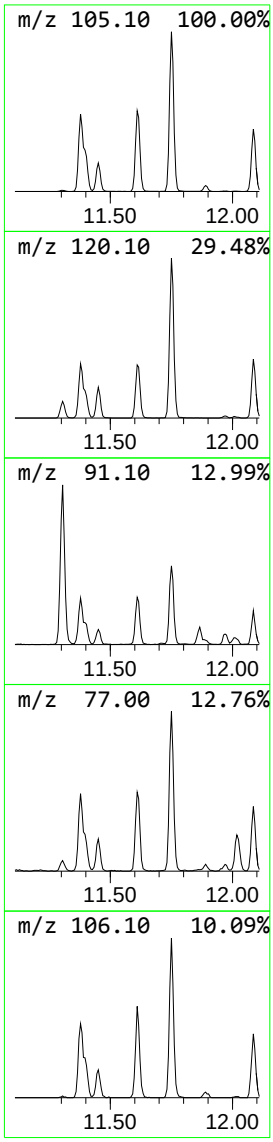
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	15.43 ug/l	382012	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	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\VX032823\
Data File : VX034813.D
Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

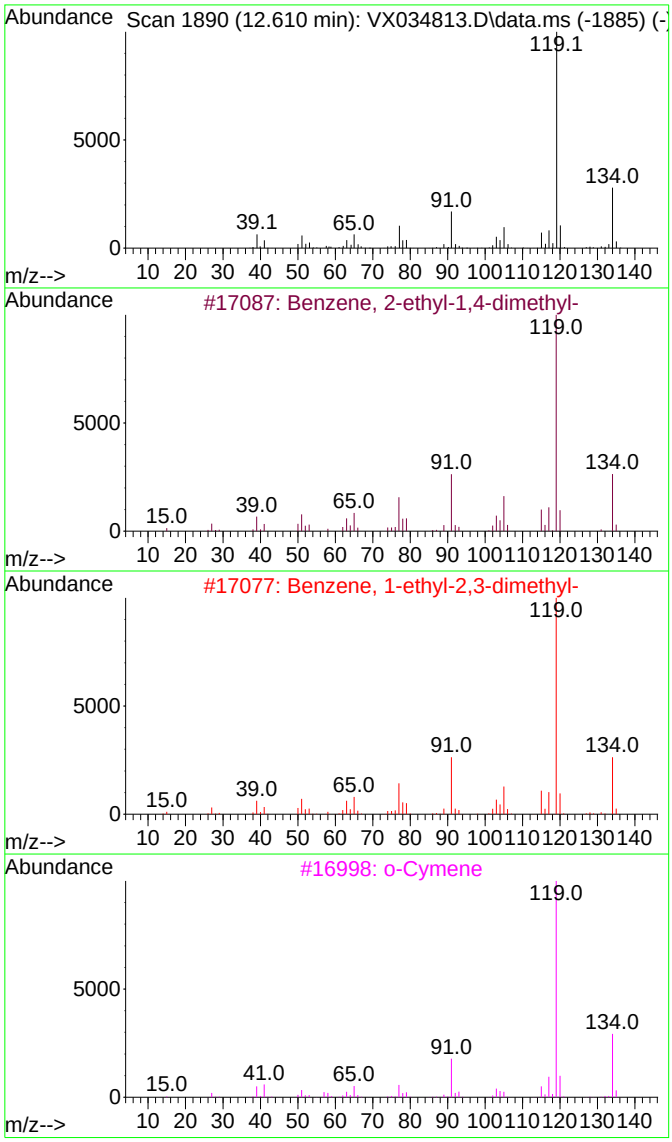
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

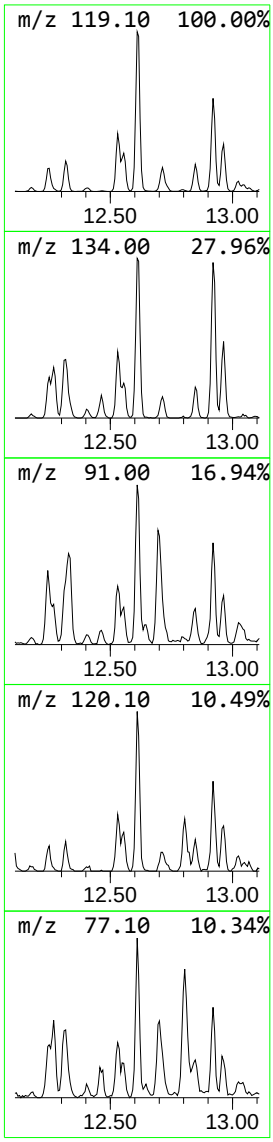
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	13.77 ug/l	340906	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	p-Cymene	134	C10H14	000099-87-6	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034813.D
Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

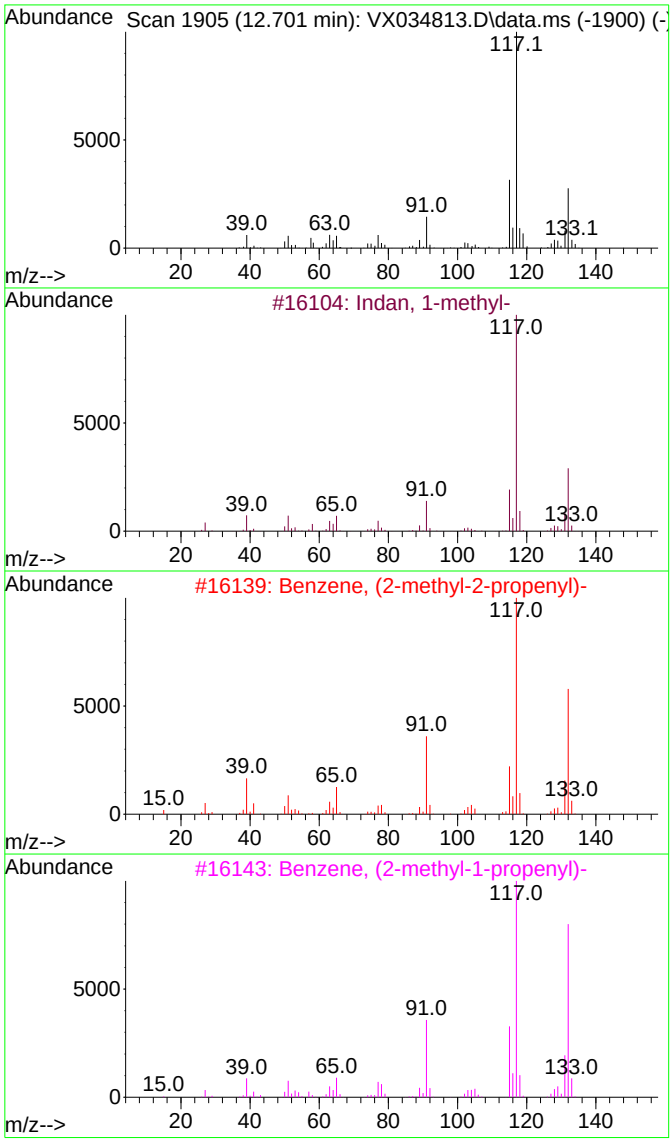
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

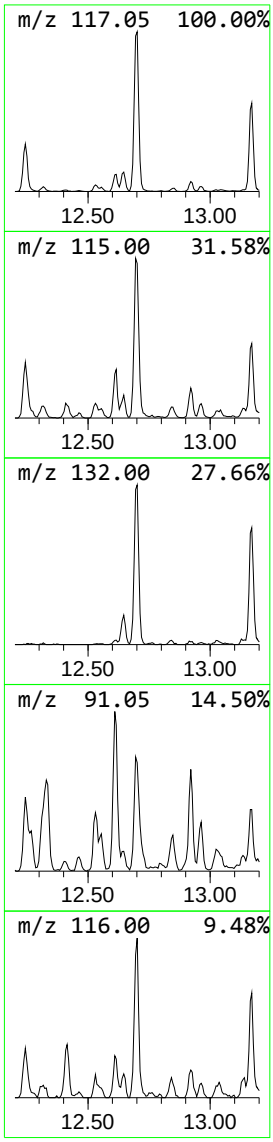
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	15.36 ug/l	380222	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	91
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034813.D
Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

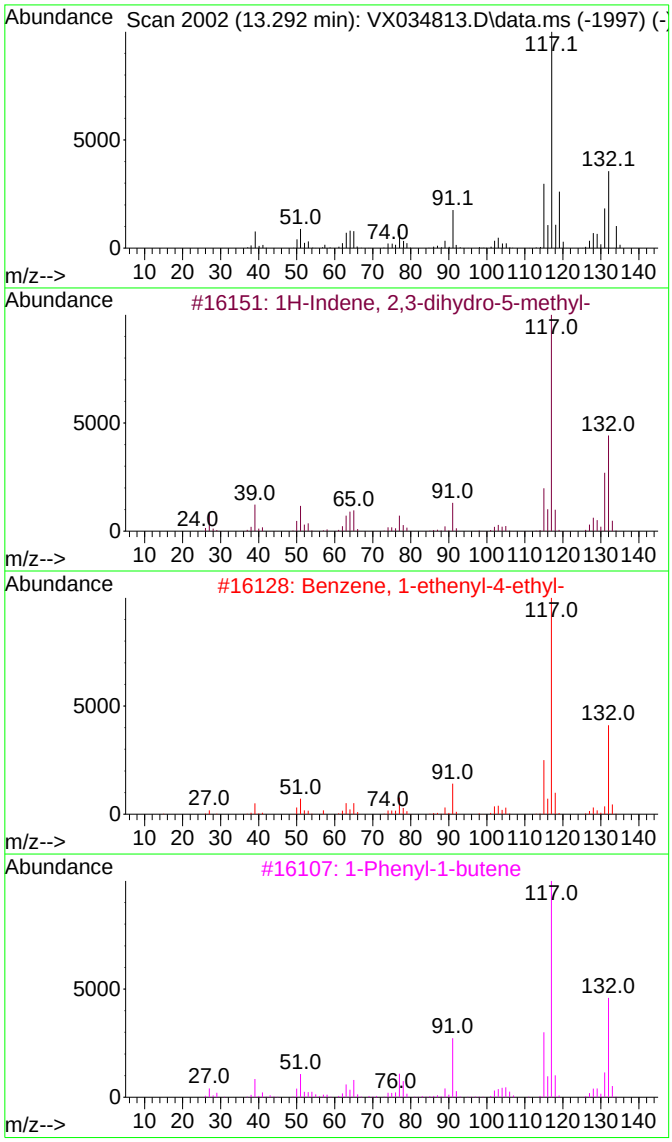
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

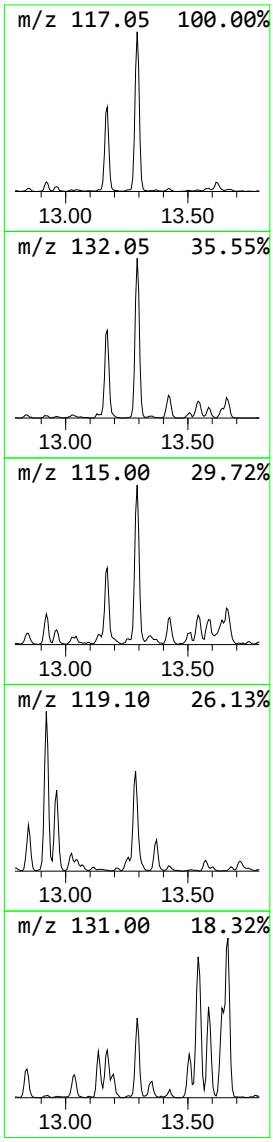
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	18.77 ug/l	464683	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
4	Indan, 1-methyl-	132	C10H12	000767-58-8	81
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034813.D
Acq On : 28 Mar 2023 23:01
Operator : JC/MD
Sample : 02084-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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	11.6	ug/l	219631	1	5.550	950225	50.0
Pentane, 3-methyl-	3.099	10.6	ug/l	201254	1	5.550	950225	50.0
Cyclopentane, m...	4.306	15.4	ug/l	292921	1	5.550	950225	50.0
3-Penten-2-one,...	9.531	9.5	ug/l	250551	3	10.055	1321610	50.0
Benzene, 1-ethy...	11.378	19.9	ug/l	493332	4	12.024	1237560	50.0
Benzene, 1-ethy...	11.610	15.4	ug/l	382012	4	12.024	1237560	50.0
Benzene, 2-ethy...	12.610	13.8	ug/l	340906	4	12.024	1237560	50.0
Indan, 1-methyl-	12.701	15.4	ug/l	380222	4	12.024	1237560	50.0
1H-Indene, 2,3-...	13.292	18.8	ug/l	464683	4	12.024	1237560	50.0