LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036443.D
Acq On : 06 Jul 2023 18:39
Operator : JC/MD
Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

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\82X062323W.M
Title : SW846 8260

Signal : TIC: VX036443.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	43	46	52	rBV	478657	515120	5.67%	0.609%
2	1.746	103	108	128	rVB	6993806	9089225	100.00%	10.747%
3	1.953	136	142	157	rVB	1592694	2129167	23.43%	2.517%
4	2.215	180	185	193	rVB	120100	173560	1.91%	0.205%
5	2.337	193	205	222	rVB	549088	1090444	12.00%	1.289%
6	2.782	270	278	281	rBV	818451	1747501	19.23%	2.066%
7	2.825	281	285	307	rVB	2227699	5407914	59.50%	6.394%
8	3.105	320	331	345	rBV	1584461	3540391	38.95%	4.186%
9	3.446	378	387	399	rBV	485638	1057267	11.63%	1.250%
10	3.733	427	434	442	rVB	118036	272764	3.00%	0.323%
11	3.837	442	451	459	rBV	77881	200290	2.20%	0.237%
12	4.105	490	495	504	rVB2	62246	150890	1.66%	0.178%
13	4.215	504	513	519	rVV2	86357	242730	2.67%	0.287%
14	4.306	519	528	540	rVV	956154	2692084	29.62%	3.183%
15	4.428	540	548	564	rVB3	39730	142677	1.57%	0.169%
16	5.135	646	664	669	rBV5	52442	223535	2.46%	0.264%
17	5.385	689	705	712	rBV3	115728	375089	4.13%	0.443%
18	5.477	712	720	729	rBV5	321930	1255862	13.82%	1.485%
19	5.623	738	744	766	rVB	276346	940274	10.34%	1.112%
20	5.830	766	778	791	rBV5	299746	957590	10.54%	1.132%
21	5.958	791	799	808	rBV	110358	281115	3.09%	0.332%
22	6.165	819	833	841	rBV2	195948	708088	7.79%	0.837%
23	6.257	842	848	857	rVV2	248190	707314	7.78%	0.836%
24	6.361	857	865	878	rVB2	190198	531678	5.85%	0.629%
25	6.610	891	906	916	rBV2	102573	258099	2.84%	0.305%
26	6.763	922	931	938	rBV	283556	712920	7.84%	0.843%
27	6.848	939	945	955	rVB4	129014	382853	4.21%	0.453%
28	7.171	991	998	1006	rVB2	74165	165122	1.82%	0.195%
29	7.379	1020	1032	1043	rBV3	578233	1528390	16.82%	1.807%
30	7.659	1071	1078	1087	rVB	137490	271318	2.99%	0.321%
31	7.775	1090	1097	1104	rVB3	45960	95158	1.05%	0.113%
32	7.860	1104	1111	1112	rBV2	56279	101290	1.11%	0.120%
33	7.885	1112	1115	1122	rVV2	66477	125017	1.38%	0.148%
34	7.988	1122	1132	1143	rVB2	62367	180941	1.99%	0.214%
35	8.110	1143	1152	1154	rBV2	112703	231406	2.55%	0.274%
36	8.147	1154	1158	1162	rVV	242442	415603	4.57%	0.491%

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Instrument :
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ClientSampleId :
MW-6

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\82X062323W.M
Title : SW846 8260

37	8.189	1162	1165	1175	rVB4	42621	93321	1.03%	0.110%
38	8.433	1200	1205	1210	rBV2	69623	121345	1.34%	0.143%
39	8.506	1211	1217	1226	rVB2	244988	437801	4.82%	0.518%
40	8.604	1226	1233	1235	rBV2	81392	136073	1.50%	0.161%
41	8.647	1235	1240	1249	rVB	563547	934803	10.28%	1.105%
42	8.842	1265	1272	1280	rVB2	114717	232776	2.56%	0.275%
43	8.927	1280	1286	1290	rVV	85941	144479	1.59%	0.171%
44	9.104	1306	1315	1320	rBV2	70753	140474	1.55%	0.166%
45	9.165	1320	1325	1335	rVB	190877	324508	3.57%	0.384%
46	9.451	1364	1372	1377	rBV4	57084	170350	1.87%	0.201%
47	9.500	1377	1380	1386	rVV3	57899	112971	1.24%	0.134%
48	10.025	1460	1466	1467	rBV2	87914	123380	1.36%	0.146%
49	10.055	1467	1471	1476	rVB	583221	752130	8.27%	0.889%
50	10.146	1481	1486	1489	rVV2	127144	198958	2.19%	0.235%
51	10.195	1489	1494	1499	rVB	1237758	1528320	16.81%	1.807%
52	10.305	1507	1512	1517	rVB	461848	606372	6.67%	0.717%
53	10.963	1613	1620	1627	rVB	1306855	1597729	17.58%	1.889%
54	11.079	1635	1639	1644	rVB	459427	568188	6.25%	0.672%
55	11.305	1660	1676	1685	rBV	3711832	4508388	49.60%	5.331%
56	11.396	1685	1691	1696	rVV	686347	877860	9.66%	1.038%
57	11.451	1696	1700	1707	rVB	293181	386982	4.26%	0.458%
58	11.610	1721	1726	1735	rBV	498078	645138	7.10%	0.763%
59	11.750	1745	1749	1755	rBV	965126	1140680	12.55%	1.349%
60	11.866	1763	1768	1770	rBV	255769	342358	3.77%	0.405%
61	11.890	1770	1772	1778	rVB	283183	313610	3.45%	0.371%
62	11.969	1778	1785	1788	rBV	83917	102615	1.13%	0.121%
63	12.024	1788	1794	1800	rVB2	580307	800387	8.81%	0.946%
64	12.085	1800	1804	1809	rBV	392330	480697	5.29%	0.568%
65	12.244	1824	1830	1837	rBV2	3258702	4019793	44.23%	4.753%
66	12.311	1837	1841	1851	rVB2	582252	1147405	12.62%	1.357%
67	12.402	1851	1856	1861	rVB	242752	292499	3.22%	0.346%
68	12.463	1861	1866	1872	rBV	190354	216529	2.38%	0.256%
69	12.530	1872	1877	1885	rBV	251600	370953	4.08%	0.439%
70	12.616	1885	1891	1894	rBV	2310643	2892072	31.82%	3.419%
71	12.646	1894	1896	1900	rVB	499959	498659	5.49%	0.590%
72	12.701	1900	1905	1912	rBV	1638387	2261688	24.88%	2.674%
73	12.841	1923	1928	1933	rVB2	109523	160800	1.77%	0.190%
74	12.920	1933	1941	1945	rBV	1817446	2167630	23.85%	2.563%
75	12.963	1945	1948	1953	rVB	343783	399809	4.40%	0.473%
76	13.024	1953	1958	1964	rBV3	152494	268362	2.95%	0.317%

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ClientSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Title : SW846 8260

77	13.134	1967	1976	1978	rVV3	159250	256677	2.82%	0.303%
78	13.170	1978	1982	1992	rVB	1451717	1896927	20.87%	2.243%
79	13.256	1992	1996	1997	rBV2	113814	123815	1.36%	0.146%
80	13.292	1997	2002	2008	rVV2	2416736	3261584	35.88%	3.856%
81	13.371	2012	2015	2020	rVV	126007	173215	1.91%	0.205%
82	13.420	2020	2023	2030	rVB	189277	246017	2.71%	0.291%
83	13.506	2032	2037	2039	rBV2	200482	248389	2.73%	0.294%
84	13.542	2039	2043	2046	rVV	496022	672799	7.40%	0.795%
85	13.579	2046	2049	2054	rVV2	449300	727609	8.01%	0.860%
86	13.640	2054	2059	2060	rVV2	239121	343667	3.78%	0.406%
87	13.664	2060	2063	2070	rVB2	464605	687560	7.56%	0.813%
88	13.774	2074	2081	2090	rBV	411590	599142	6.59%	0.708%
89	13.926	2099	2106	2110	rBV2	205533	304133	3.35%	0.360%
90	13.969	2110	2113	2117	rVB	140393	161923	1.78%	0.191%
91	14.073	2126	2130	2137	rBV	343621	432494	4.76%	0.511%
92	14.213	2148	2153	2163	rBV	263064	443835	4.88%	0.525%
93	14.323	2167	2171	2175	rVV	141779	196321	2.16%	0.232%
94	14.371	2175	2179	2184	rVB	196939	235021	2.59%	0.278%
95	14.633	2218	2222	2233	rVB	1003238	1303719	14.34%	1.541%
96	14.780	2241	2246	2255	rVB	649729	841915	9.26%	0.995%

Sum of corrected areas: 84576340

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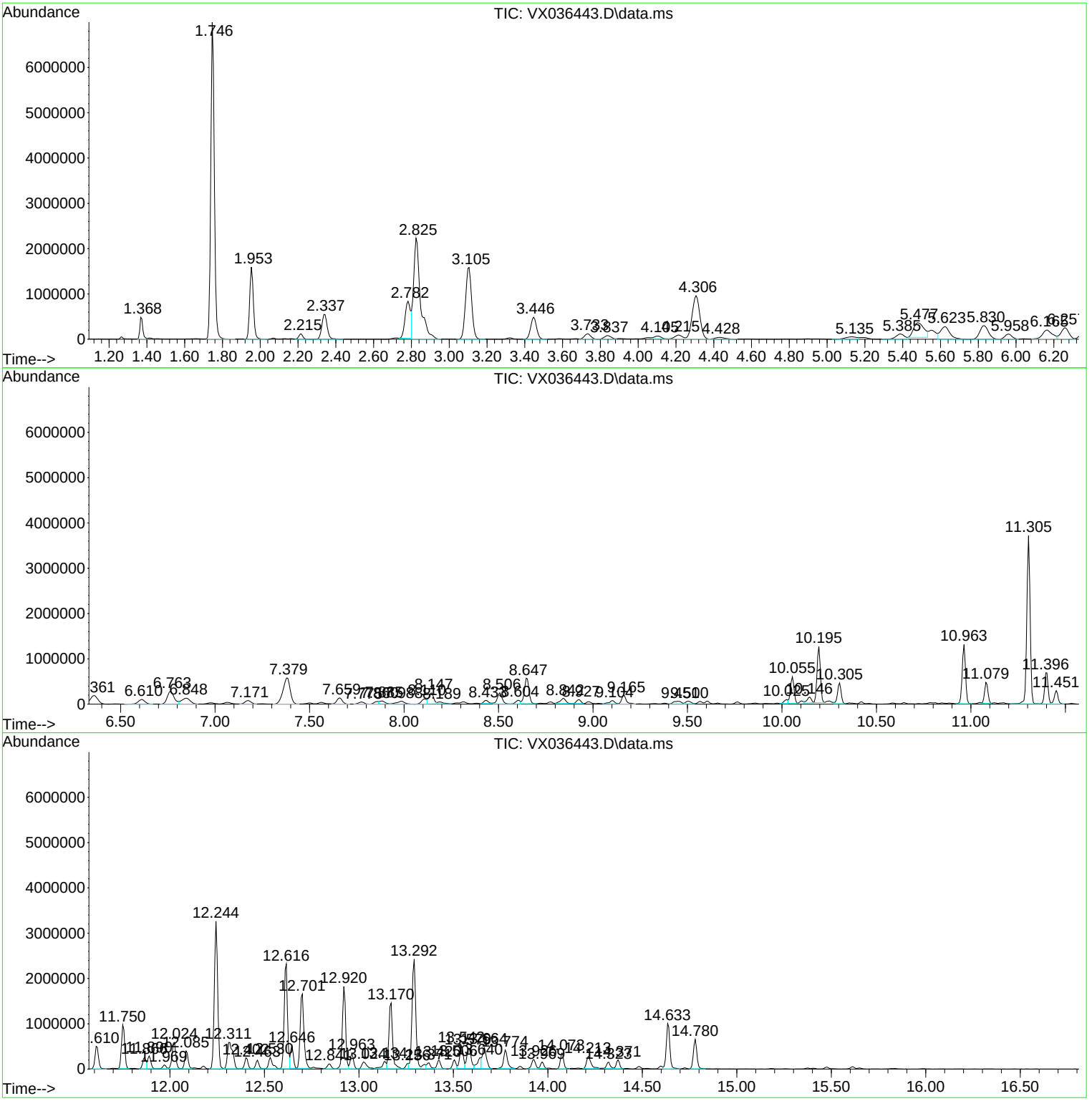
Instrument :
MSVOA_X
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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



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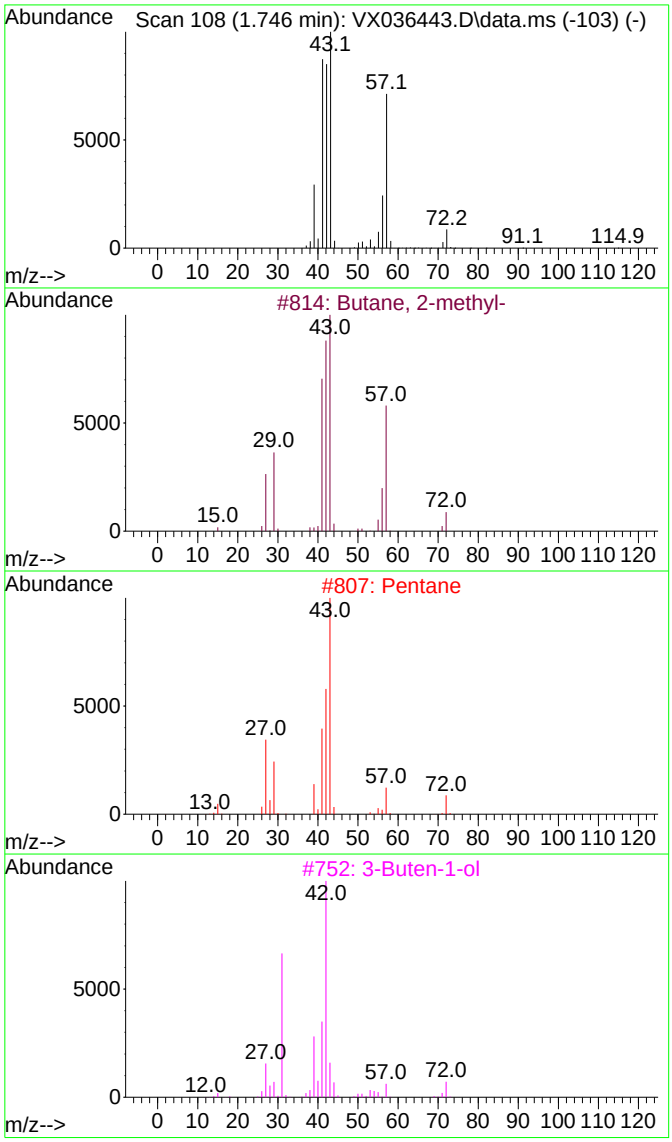
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

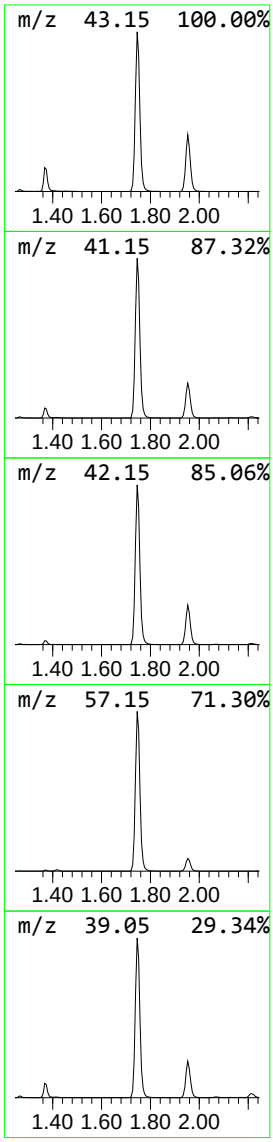
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	483.33 ug/l	9089230	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	45
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	10
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

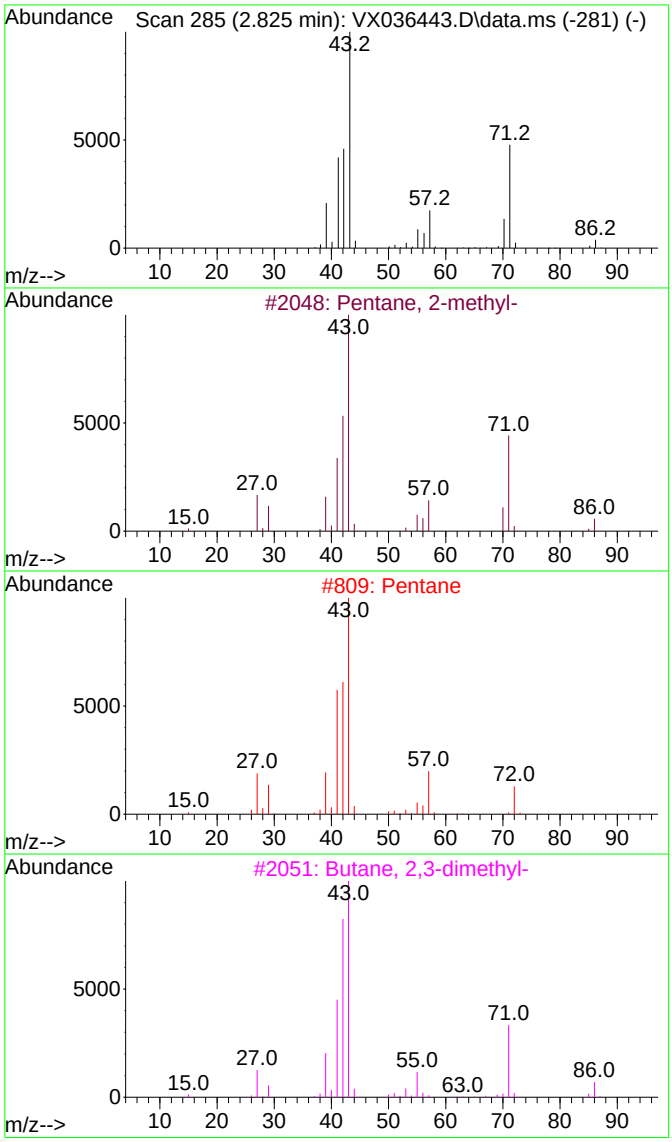
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

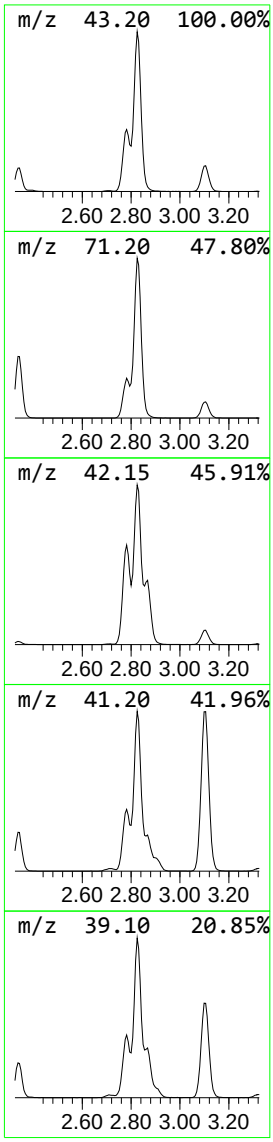
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	287.57 ug/l	5407910	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Pentane	72	C5H12	000109-66-0	46
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
4	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40
5	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38





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Instrument :
MSVOA_X
ClientSampleId :
MW-6

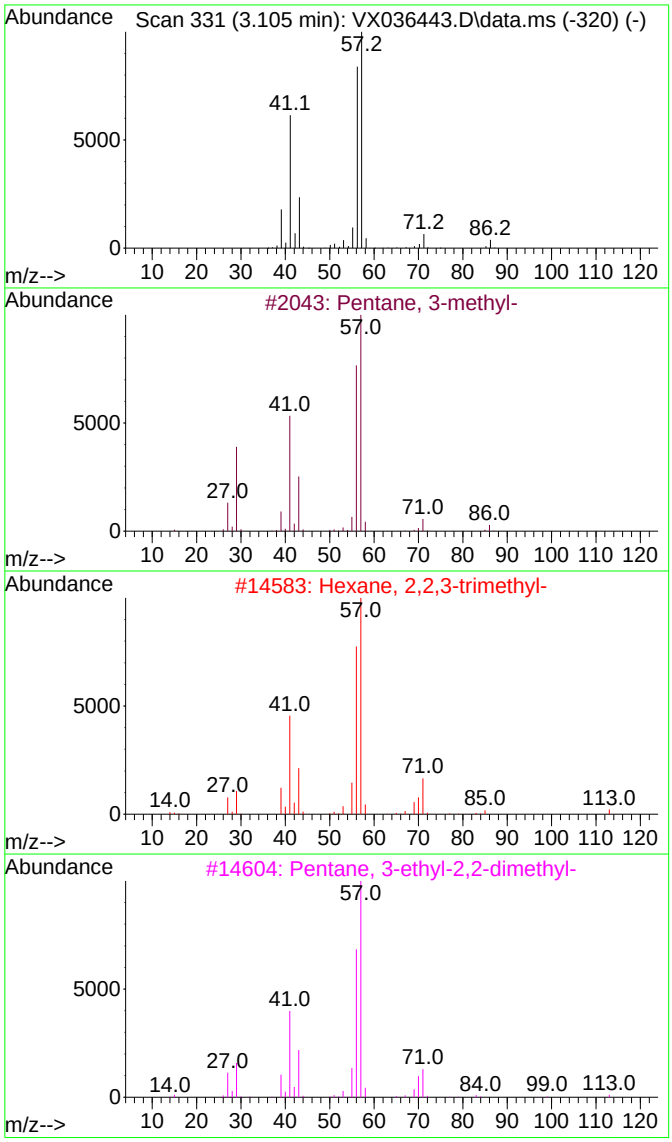
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

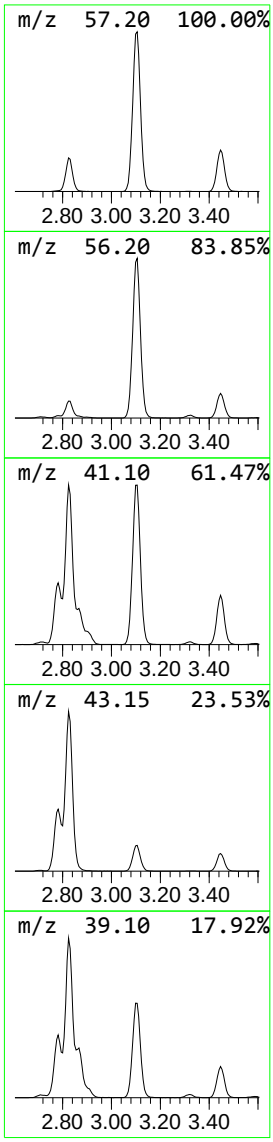
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	188.26 ug/l	3540390	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40





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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

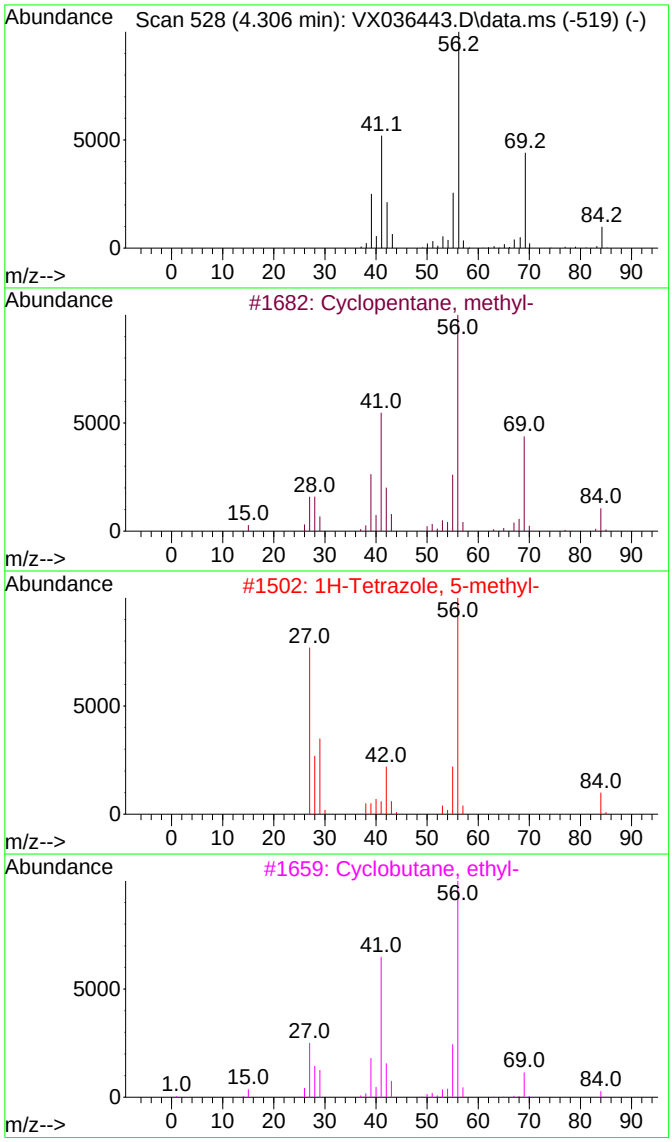
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

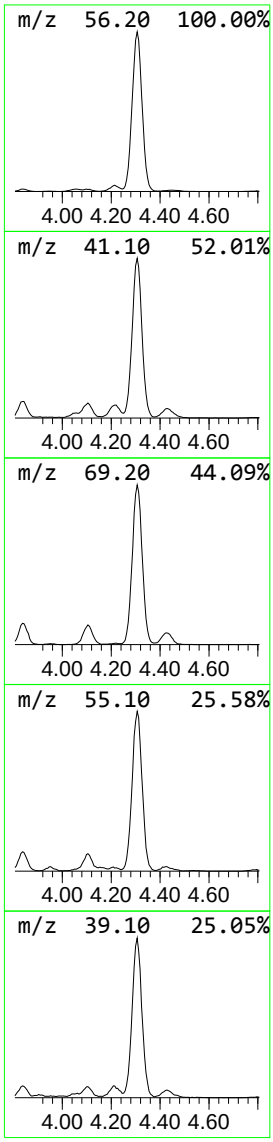
****

Peak Number 4 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	143.15 ug/l	2692080	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclohexane	84	C6H12	000110-82-7	56
5	Cyclobutane	56	C4H8	000287-23-0	53





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

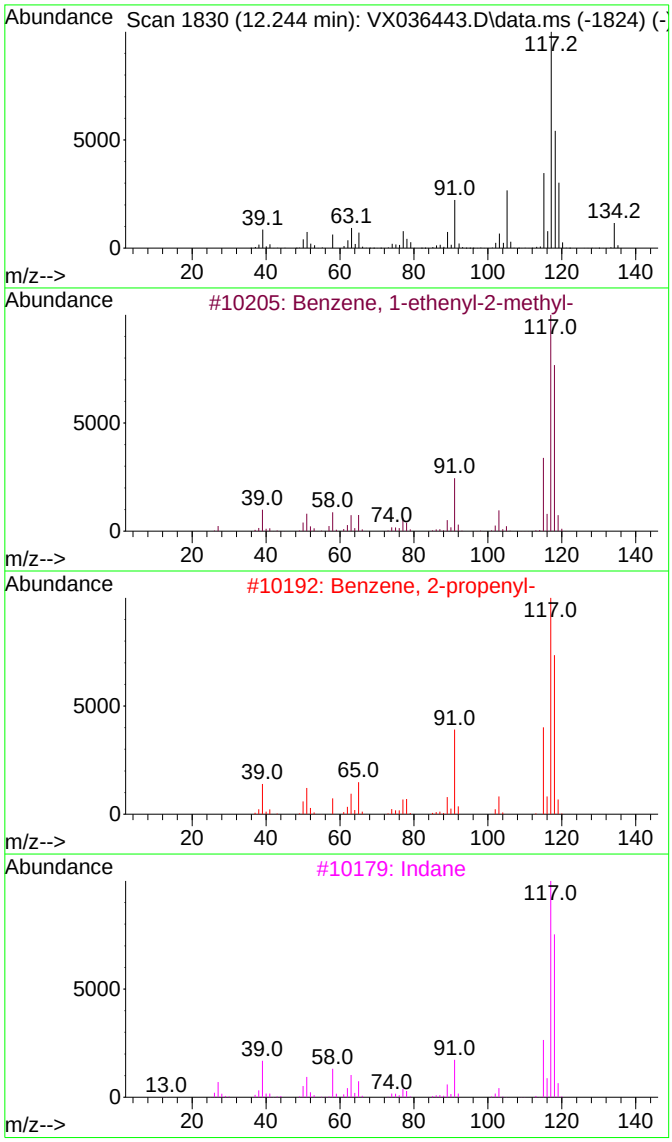
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

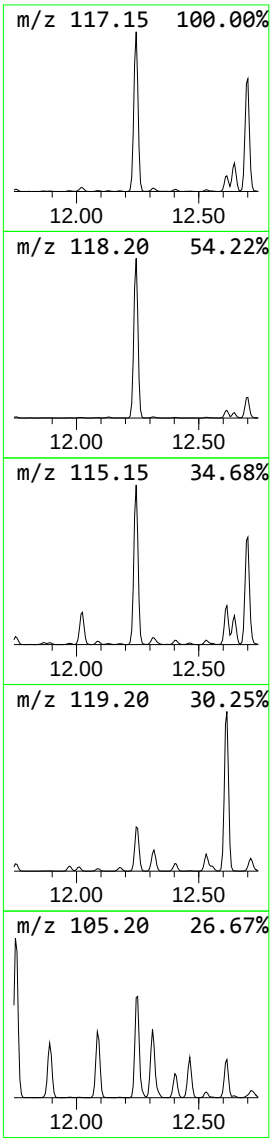
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	251.12 ug/l	4019790	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	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Indane	118	C9H10	000496-11-7	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	50





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Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

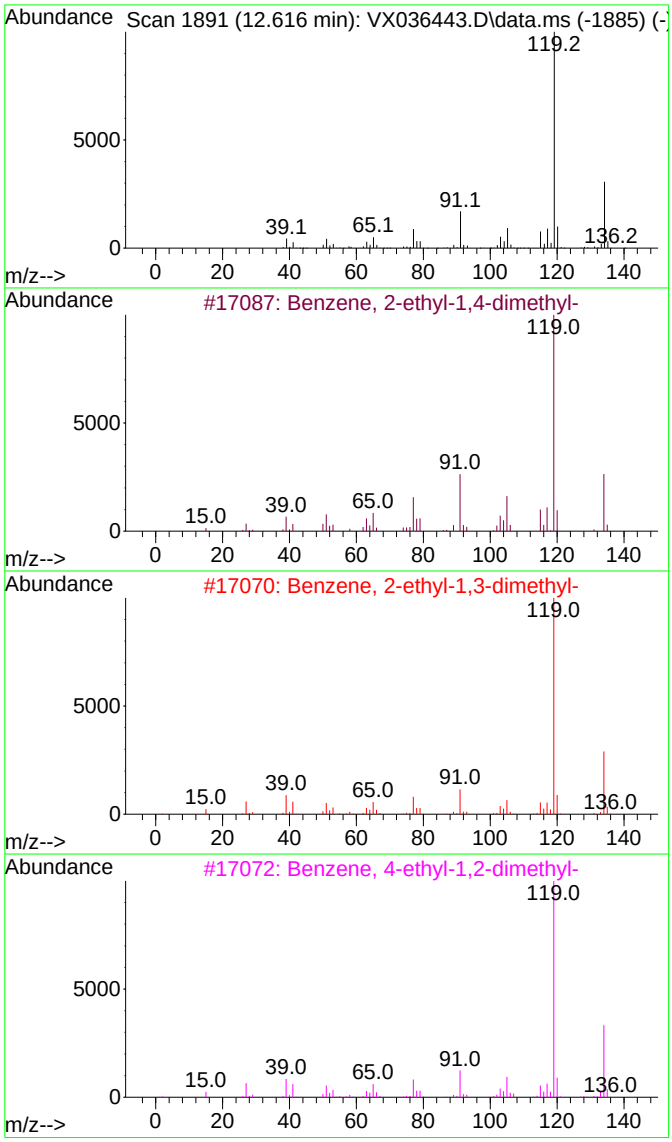
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

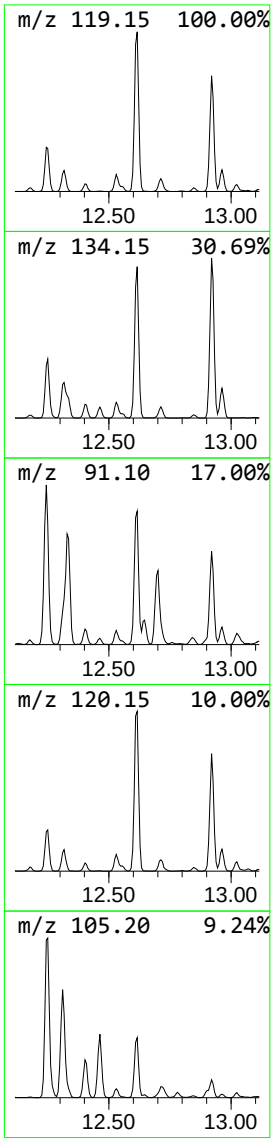
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	180.67 ug/l	2892070	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, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5	o-Cymene	134	C10H14	000527-84-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036443.D
Acq On : 06 Jul 2023 18:39
Operator : JC/MD
Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

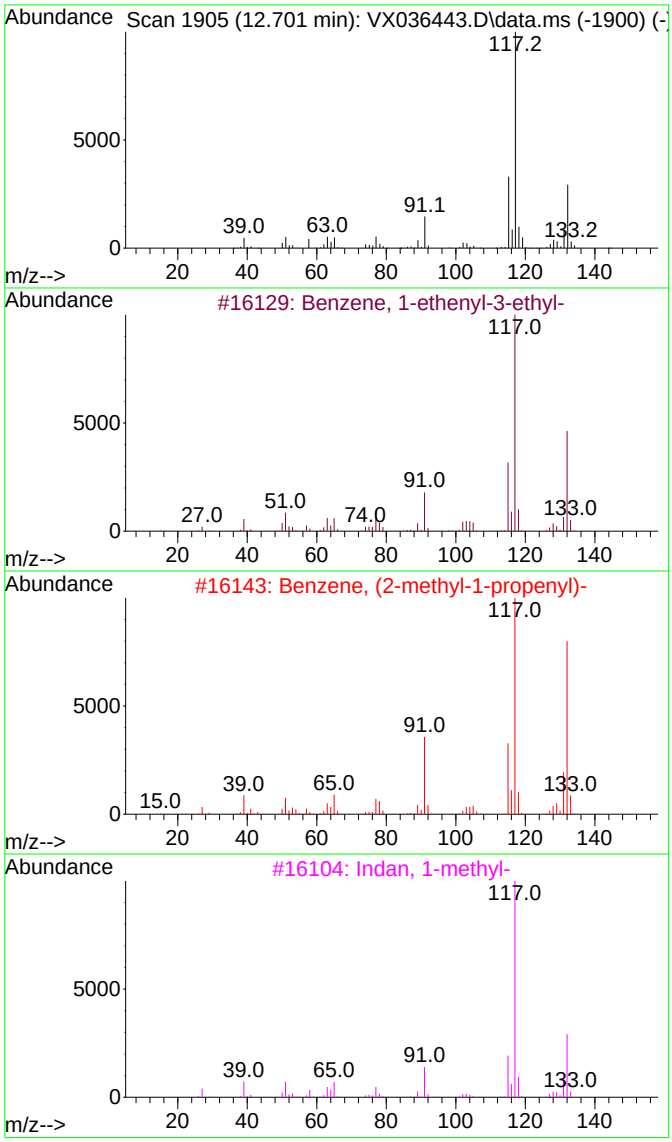
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

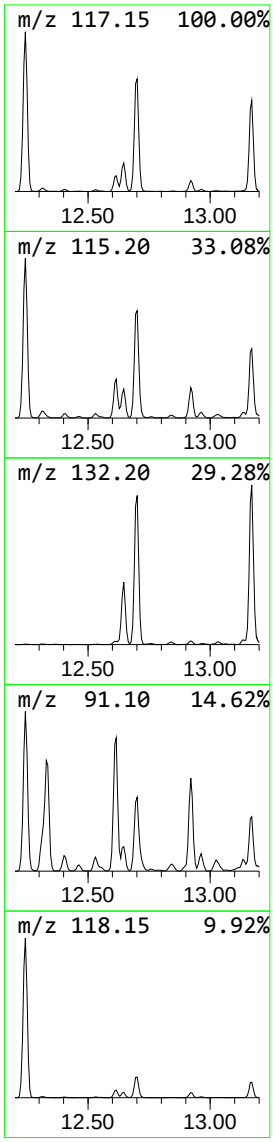
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	141.29 ug/l	2261690	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	90
2	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036443.D
Acq On : 06 Jul 2023 18:39
Operator : JC/MD
Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

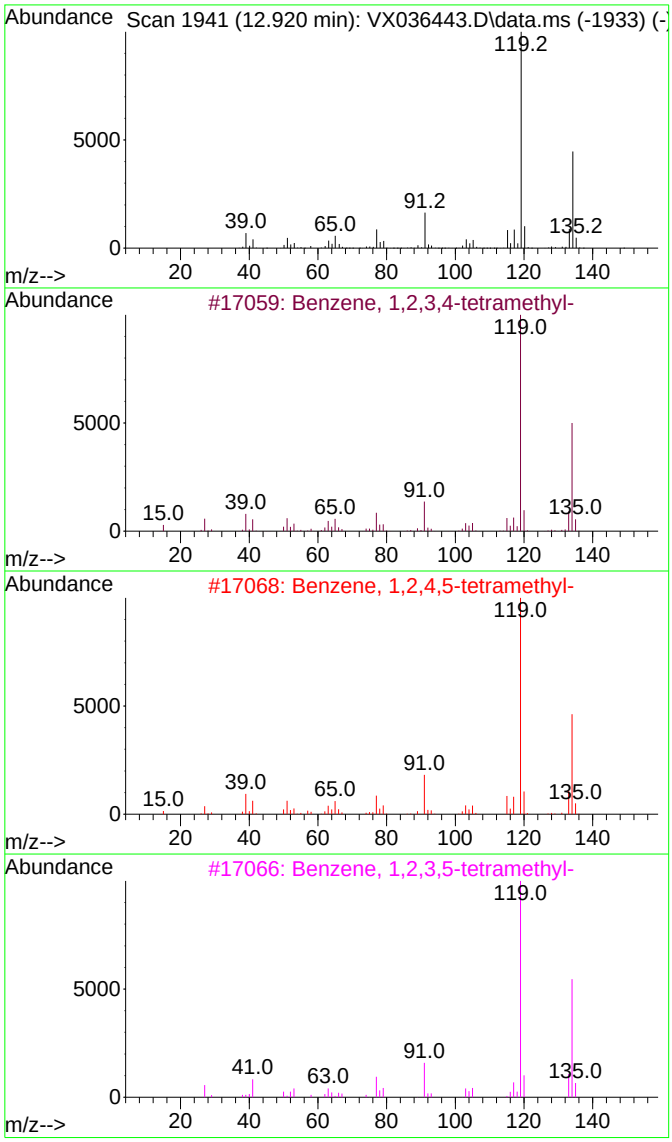
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

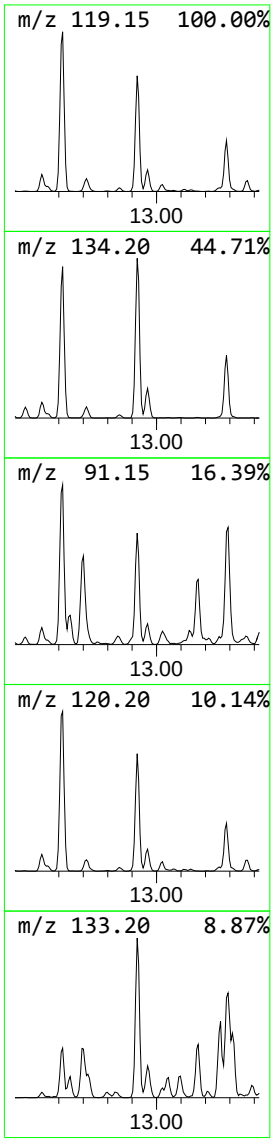
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	135.41 ug/l	2167630	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	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036443.D
Acq On : 06 Jul 2023 18:39
Operator : JC/MD
Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

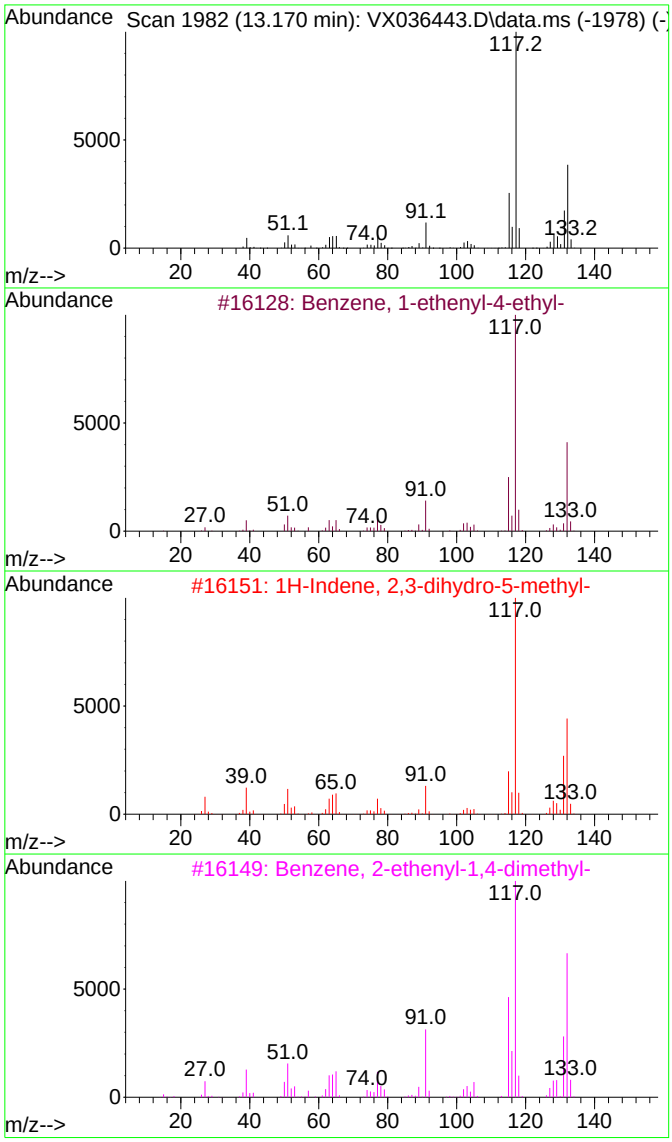
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

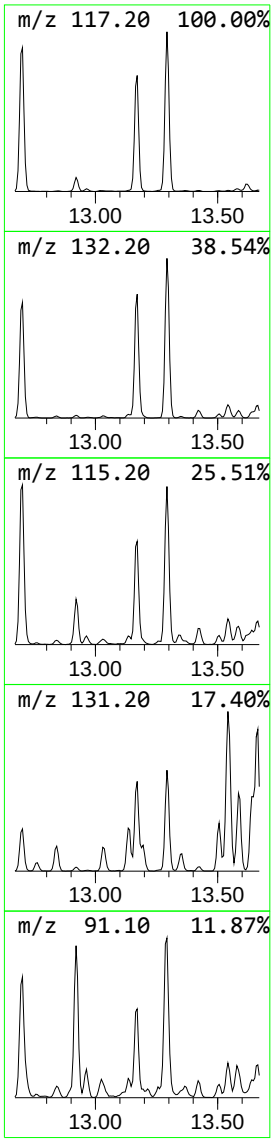
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	118.50 ug/l	1896930	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	Indan, 1-methyl-	132	C10H12	000767-58-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036443.D
Acq On : 06 Jul 2023 18:39
Operator : JC/MD
Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

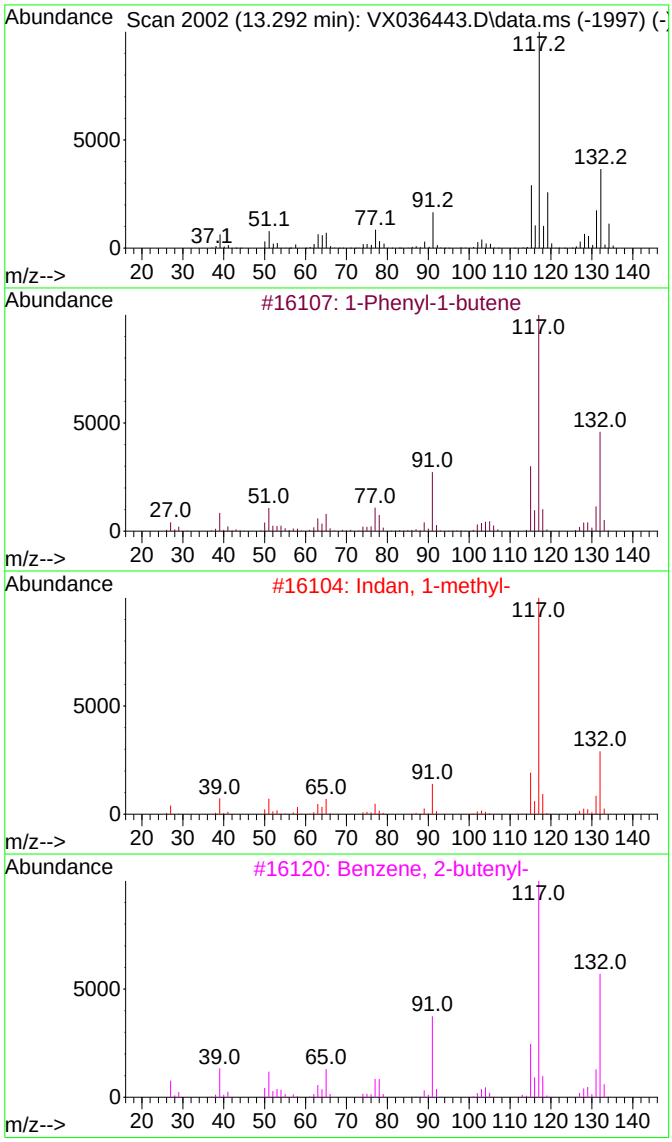
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

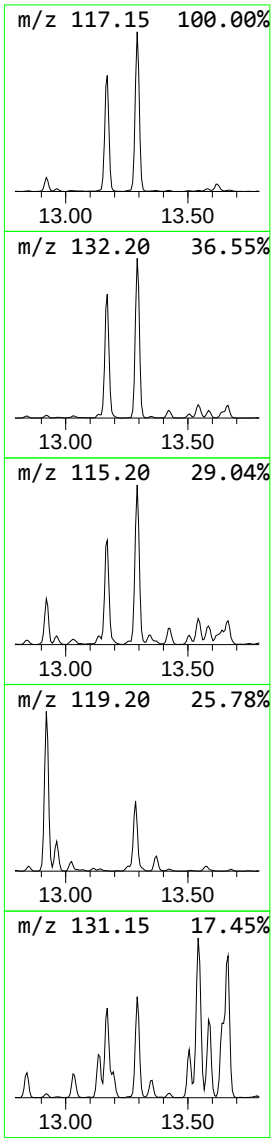
****

Peak Number 10 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	203.75 ug/l	3261580	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2	Indan, 1-methyl-	132	C10H12	000767-58-8	81
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	81
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036443.D
Acq On : 06 Jul 2023 18:39
Operator : JC/MD
Sample : 03500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.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	483.3	ug/l	9089230	1	5.556	940274	50.0
Pentane, 2-methyl-	2.825	287.6	ug/l	5407910	1	5.556	940274	50.0
Pentane, 3-methyl-	3.105	188.3	ug/l	3540390	1	5.556	940274	50.0
Cyclopentane, m...	4.306	143.2	ug/l	2692080	1	5.556	940274	50.0
Benzene, 1-ethe...	12.244	251.1	ug/l	4019790	4	12.024	800387	50.0
Benzene, 2-ethy...	12.616	180.7	ug/l	2892070	4	12.024	800387	50.0
Benzene, 1-ethe...	12.701	141.3	ug/l	2261690	4	12.024	800387	50.0
Benzene, 1,2,3,...	12.920	135.4	ug/l	2167630	4	12.024	800387	50.0
Benzene, 1-ethe...	13.170	118.5	ug/l	1896930	4	12.024	800387	50.0
1-Phenyl-1-butene	13.292	203.8	ug/l	3261580	4	12.024	800387	50.0