LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
Operator : JC/MD
Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

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: VX036445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	52	rBV	830407	928621	5.28%	0.810%
2	1.745	103	108	128	rVB	13735320	17585541	100.00%	15.347%
3	1.953	136	142	157	rVB	3500001	4682726	26.63%	4.087%
4	2.215	180	185	195	rVB	235740	346289	1.97%	0.302%
5	2.337	195	205	221	rBV	922865	1811809	10.30%	1.581%
6	2.782	270	278	281	rBV	1431287	3045972	17.32%	2.658%
7	2.825	281	285	309	rVB	3903437	9117444	51.85%	7.957%
8	3.105	319	331	351	rBV	2580607	5743497	32.66%	5.013%
9	3.446	377	387	401	rBV	980169	2139409	12.17%	1.867%
10	3.733	426	434	443	rVB	187798	435281	2.48%	0.380%
11	3.837	443	451	458	rBV2	126866	319313	1.82%	0.279%
12	4.105	489	495	503	rVB	100073	251799	1.43%	0.220%
13	4.215	503	513	519	rVV	209940	607558	3.45%	0.530%
14	4.306	519	528	540	rVV	1484334	4160965	23.66%	3.631%
15	4.428	540	548	565	rVB4	67668	244436	1.39%	0.213%
16	5.135	647	664	668	rBV5	79558	335689	1.91%	0.293%
17	5.385	688	705	711	rBV4	130038	434391	2.47%	0.379%
18	5.483	711	721	731	rBV4	529204	2211625	12.58%	1.930%
19	5.623	736	744	764	rVB2	585519	2104516	11.97%	1.837%
20	5.830	764	778	791	rBV3	513191	1591592	9.05%	1.389%
21	5.958	791	799	808	rBV	108411	272040	1.55%	0.237%
22	6.159	818	832	841	rBV2	316163	1125035	6.40%	0.982%
23	6.257	841	848	857	rVV2	413062	1206722	6.86%	1.053%
24	6.360	857	865	876	rVB	318281	886422	5.04%	0.774%
25	6.610	892	906	917	rBV2	194943	489647	2.78%	0.427%
26	6.763	922	931	937	rBV	284204	734036	4.17%	0.641%
27	6.848	937	945	958	rVB3	248279	808171	4.60%	0.705%
28	7.177	990	999	1006	rBV	135712	302919	1.72%	0.264%
29	7.379	1019	1032	1044	rBV3	1095143	2814076	16.00%	2.456%
30	7.659	1072	1078	1090	rVB	233848	449070	2.55%	0.392%
31	7.988	1122	1132	1143	rVB3	112980	315881	1.80%	0.276%
32	8.104	1143	1151	1154	rBV2	210955	425498	2.42%	0.371%
33	8.141	1154	1157	1162	rVV	341177	595626	3.39%	0.520%
34	8.506	1211	1217	1226	rVB2	301690	551653	3.14%	0.481%
35	8.604	1226	1233	1236	rBV3	120527	237771	1.35%	0.208%
36	8.647	1236	1240	1248	rVB	587656	950296	5.40%	0.829%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

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

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Title : SW846 8260

37	8.842	1269	1272	1279	rVB	129865	216779	1.23%	0.189%
38	8.921	1279	1285	1290	rBV	143433	234731	1.33%	0.205%
39	9.104	1306	1315	1320	rBV2	95129	199111	1.13%	0.174%
40	9.159	1320	1324	1335	rVB	295223	508745	2.89%	0.444%
41	10.055	1467	1471	1475	rVB	582027	767214	4.36%	0.670%
42	10.146	1481	1486	1490	rVB3	132445	192638	1.10%	0.168%
43	10.195	1490	1494	1499	rVB	1270681	1571638	8.94%	1.372%
44	10.305	1507	1512	1517	rVB	361064	491528	2.80%	0.429%
45	10.963	1613	1620	1628	rVB	1125500	1403606	7.98%	1.225%
46	11.079	1635	1639	1644	rVB	481385	582443	3.31%	0.508%
47	11.305	1671	1676	1683	rVB	3411157	4059451	23.08%	3.543%
48	11.396	1685	1691	1696	rVV	483636	635620	3.61%	0.555%
49	11.451	1696	1700	1708	rVB	161305	221787	1.26%	0.194%
50	11.610	1721	1726	1734	rBV	417856	549812	3.13%	0.480%
51	11.750	1745	1749	1755	rBV	600275	700804	3.99%	0.612%
52	11.866	1763	1768	1770	rBV	265915	353005	2.01%	0.308%
53	11.890	1770	1772	1778	rVB	290430	319523	1.82%	0.279%
54	12.018	1788	1793	1799	rVB2	617335	836518	4.76%	0.730%
55	12.085	1799	1804	1809	rBV	287084	363273	2.07%	0.317%
56	12.244	1824	1830	1837	rBV2	2575154	3243735	18.45%	2.831%
57	12.311	1837	1841	1843	rBV	577689	781649	4.44%	0.682%
58	12.402	1851	1856	1861	rVB	221543	273989	1.56%	0.239%
59	12.463	1861	1866	1871	rBV	365121	431944	2.46%	0.377%
60	12.530	1872	1877	1880	rBV	227836	285729	1.62%	0.249%
61	12.615	1885	1891	1894	rBV	2760575	3394467	19.30%	2.962%
62	12.646	1894	1896	1900	rVB	452781	457855	2.60%	0.400%
63	12.701	1900	1905	1912	rBV2	1527747	2171517	12.35%	1.895%
64	12.920	1933	1941	1945	rBV	1927068	2224780	12.65%	1.942%
65	12.963	1945	1948	1953	rVV	240326	281032	1.60%	0.245%
66	13.024	1953	1958	1964	rVV4	168734	297459	1.69%	0.260%
67	13.134	1967	1976	1978	rVV3	164381	282427	1.61%	0.246%
68	13.170	1978	1982	1992	rVV	1408436	1847722	10.51%	1.613%
69	13.292	1997	2002	2008	rVV2	2539973	3517253	20.00%	3.070%
70	13.365	2012	2014	2019	rVV	168433	222526	1.27%	0.194%
71	13.420	2019	2023	2030	rVB	308630	405178	2.30%	0.354%
72	13.506	2031	2037	2040	rBV2	254804	344881	1.96%	0.301%
73	13.542	2040	2043	2046	rVV	628570	808161	4.60%	0.705%
74	13.579	2046	2049	2054	rVV3	580709	914591	5.20%	0.798%
75	13.664	2054	2063	2069	rVB2	578880	1253737	7.13%	1.094%
76	13.774	2074	2081	2090	rVB	1562950	1947113	11.07%	1.699%

LSC Area Percent Report

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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

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

77	13.926	2099	2106	2110	rBV2	253492	370207	2.11%	0.323%
78	13.969	2110	2113	2117	rVB2	194503	221120	1.26%	0.193%
79	14.073	2125	2130	2136	rBV	439600	532818	3.03%	0.465%
80	14.213	2148	2153	2163	rBV	338398	588447	3.35%	0.514%
81	14.322	2167	2171	2176	rVV	153006	238032	1.35%	0.208%
82	14.371	2176	2179	2183	rVB	233601	274399	1.56%	0.239%
83	14.633	2218	2222	2233	rVB	1257843	1676269	9.53%	1.463%
84	14.780	2241	2246	2255	rBV	628837	822441	4.68%	0.718%

Sum of corrected areas: 114583040

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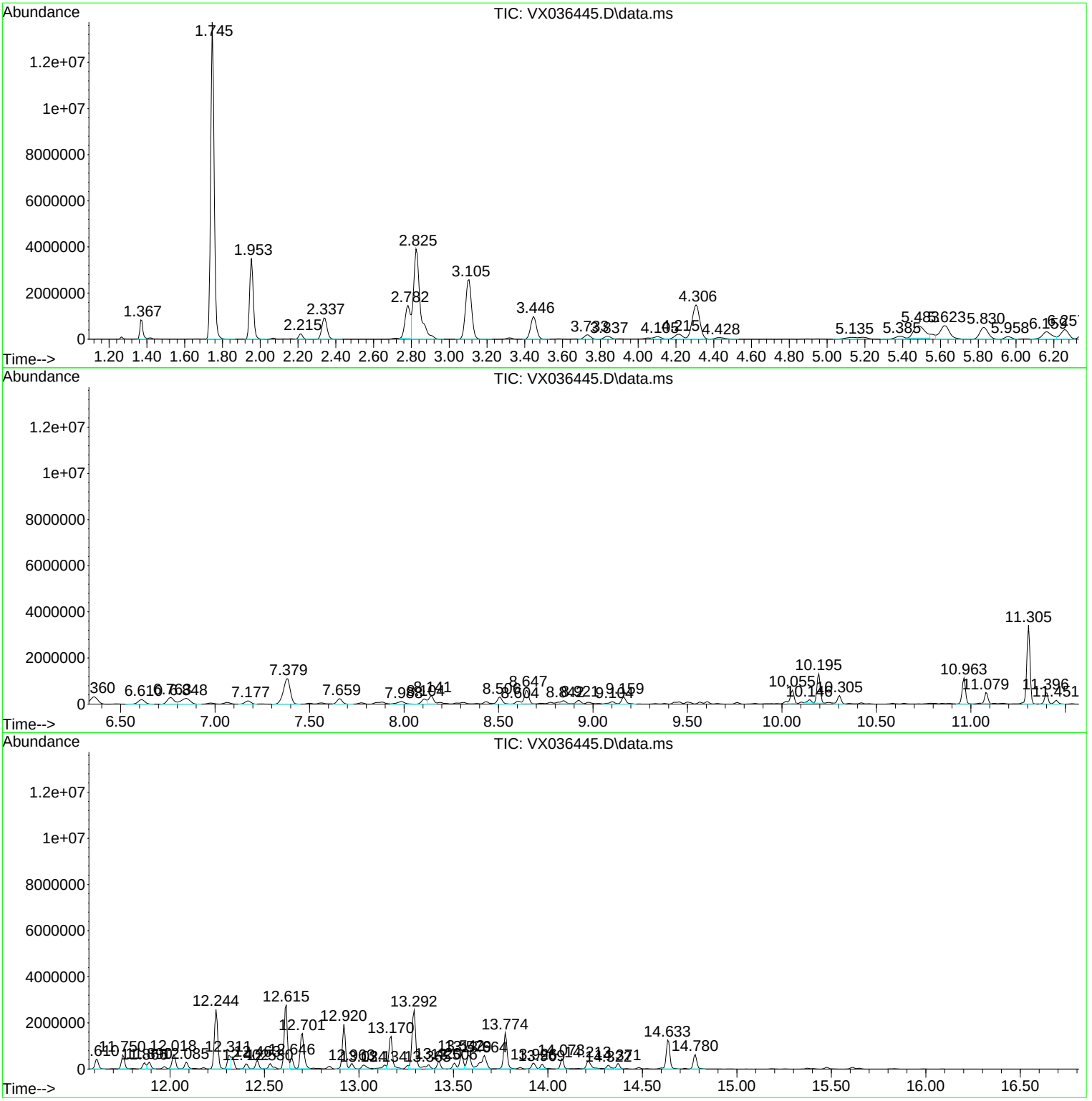
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

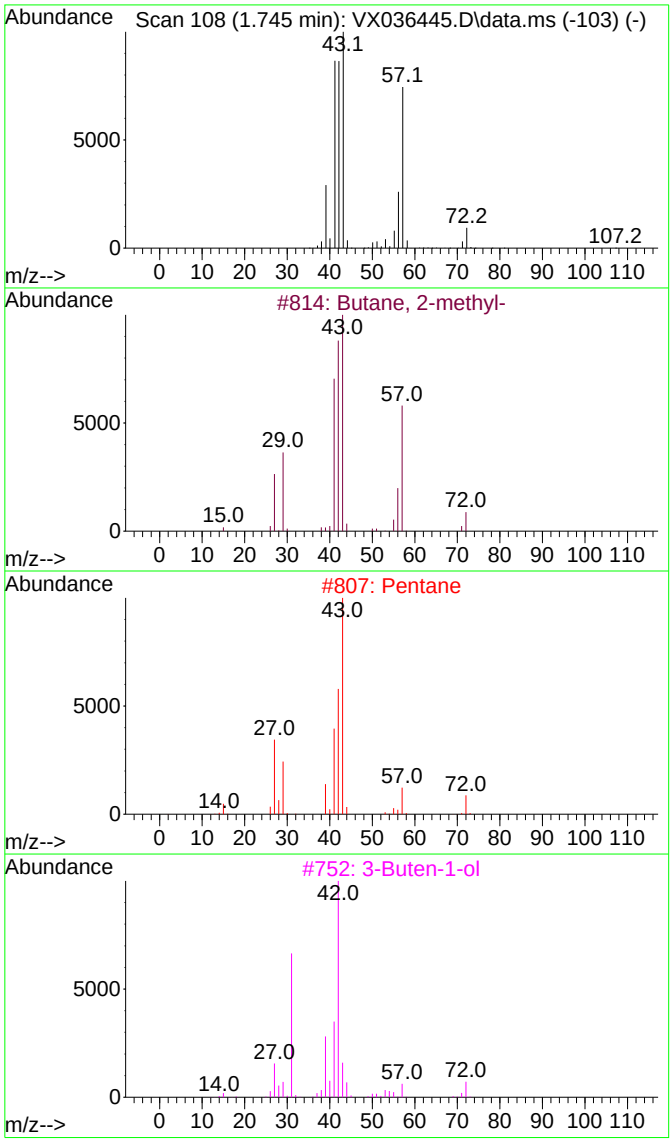
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

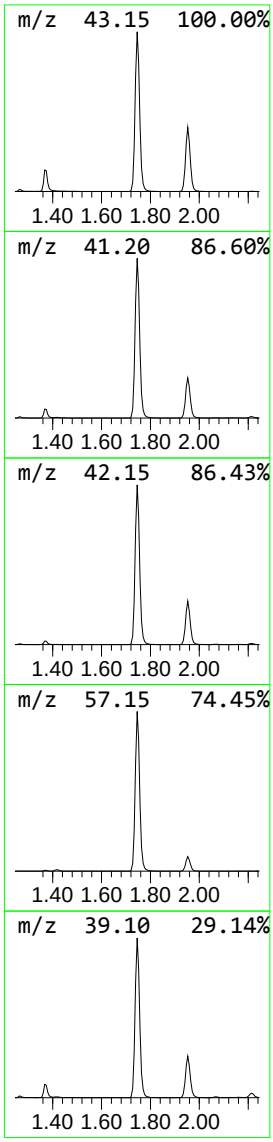
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	417.81 ug/l	17585500	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Pentane	72	C5H12	000109-66-0	42
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





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Data File : VX036445.D
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

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

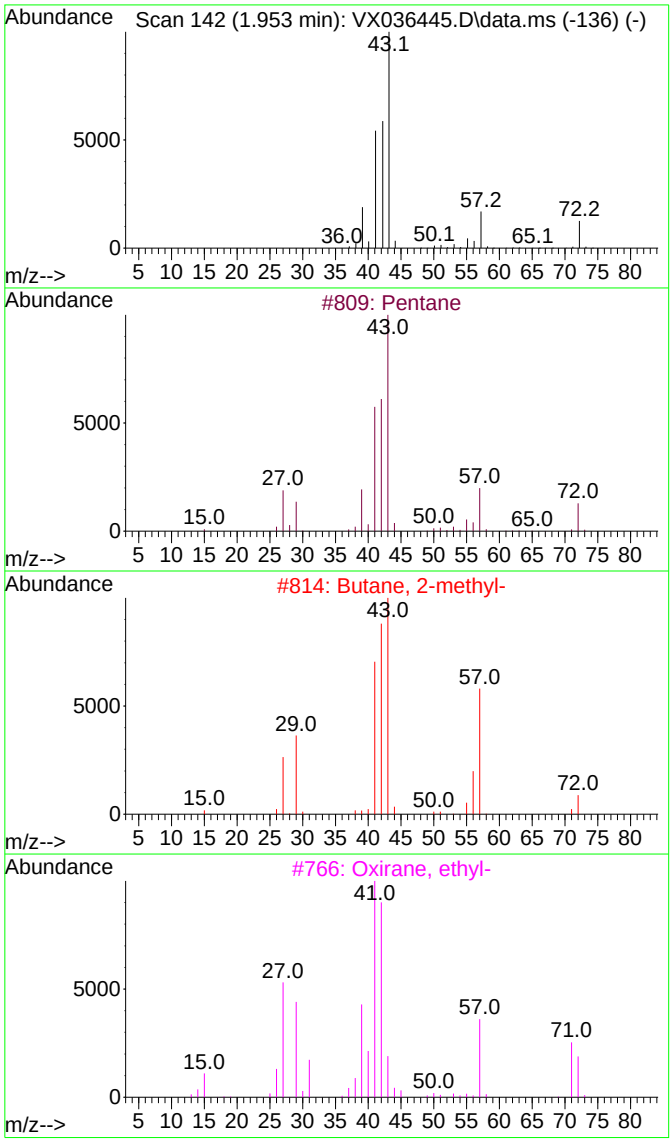
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

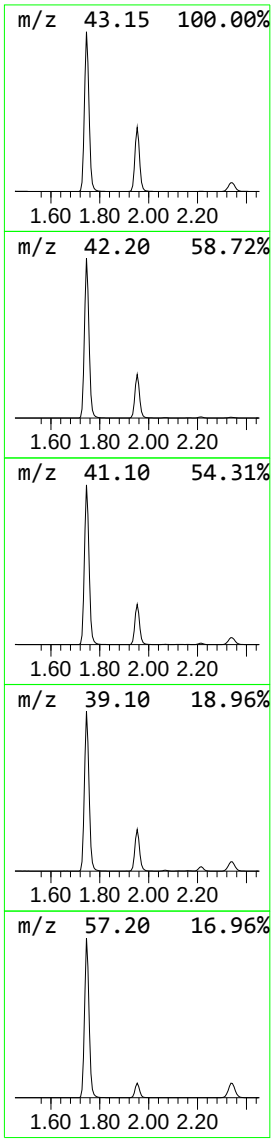
****

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	111.25 ug/l	4682730	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	59
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	53
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

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

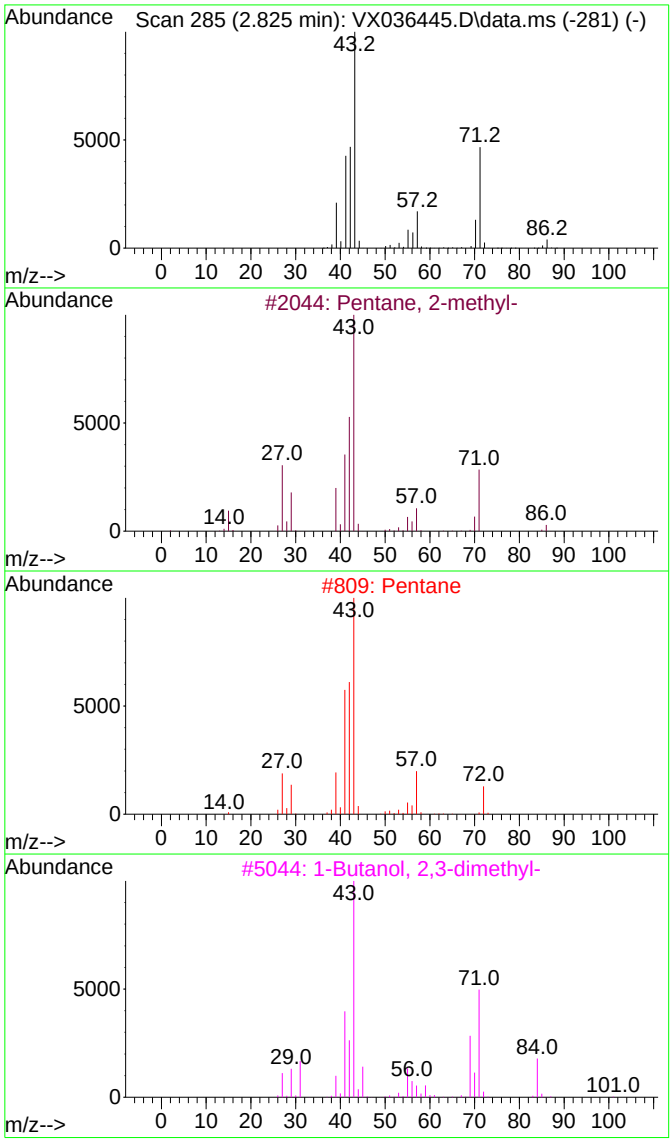
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

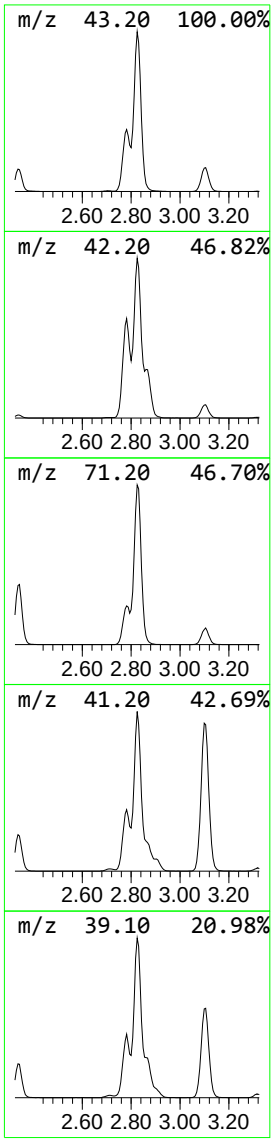
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	216.62 ug/l	9117440	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Pentane	72	C5H12	000109-66-0	46
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

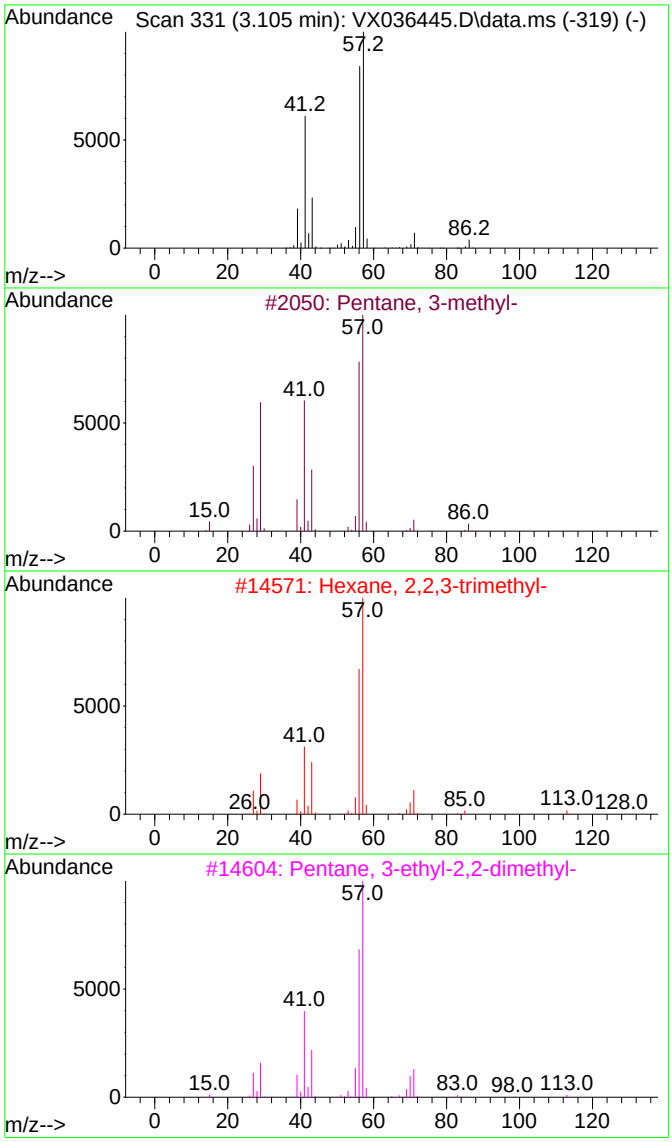
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

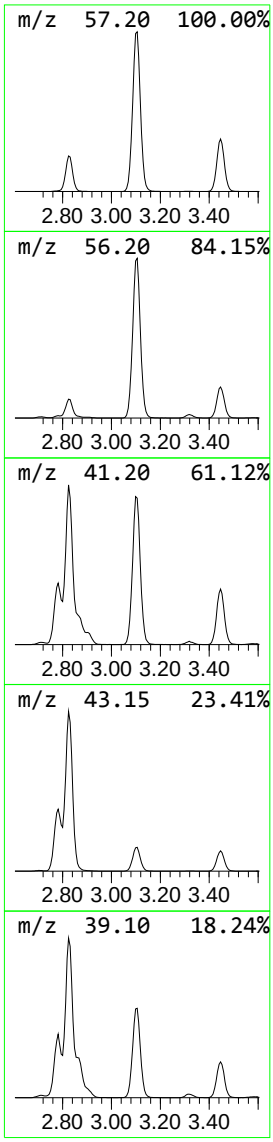
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	136.46 ug/l	5743500	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	64
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40
5	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
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Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

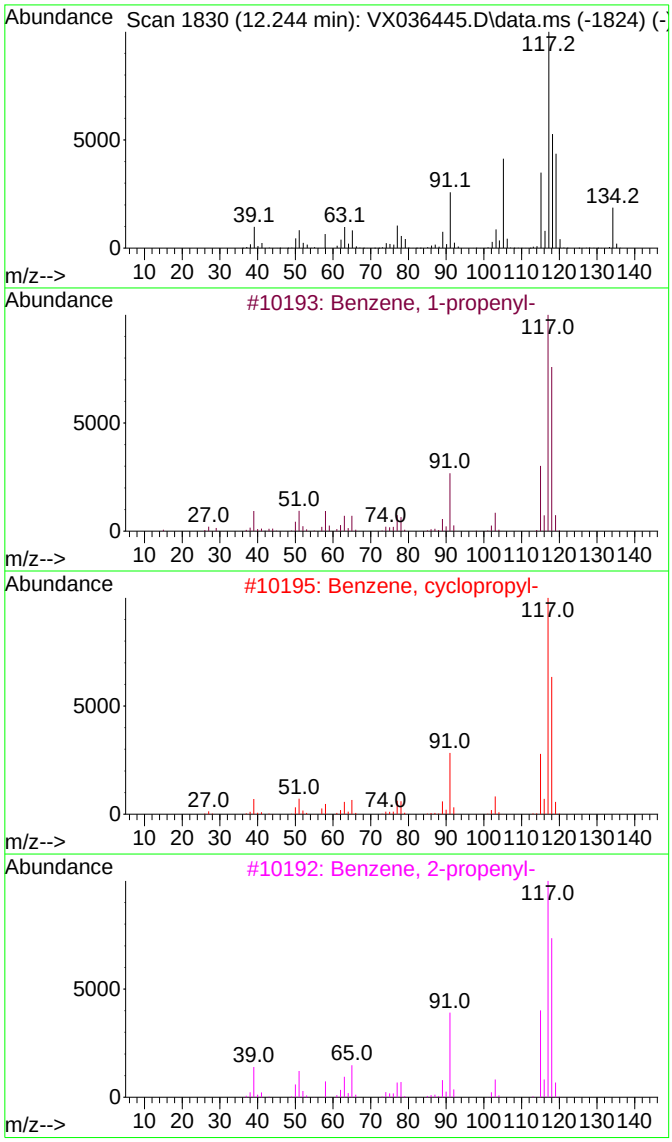
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

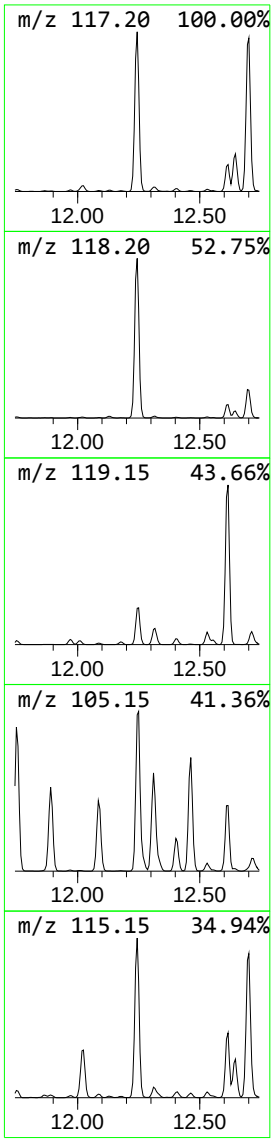
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	193.88 ug/l	3243740	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	91
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5	Deltacyclene	118	C9H10	007785-10-6	55





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Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

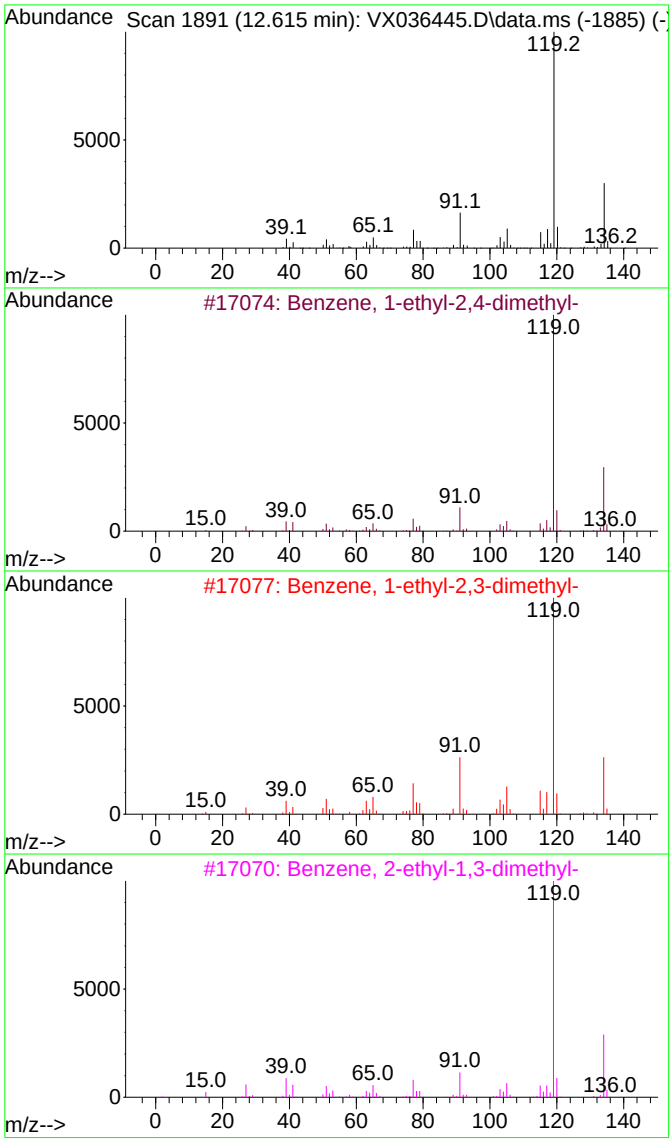
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

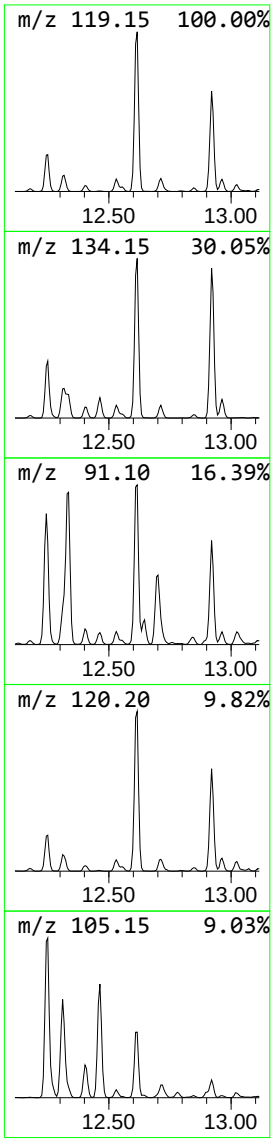
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	202.89 ug/l	3394470	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5	o-Cymene	134	C10H14	000527-84-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
Operator : JC/MD
Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

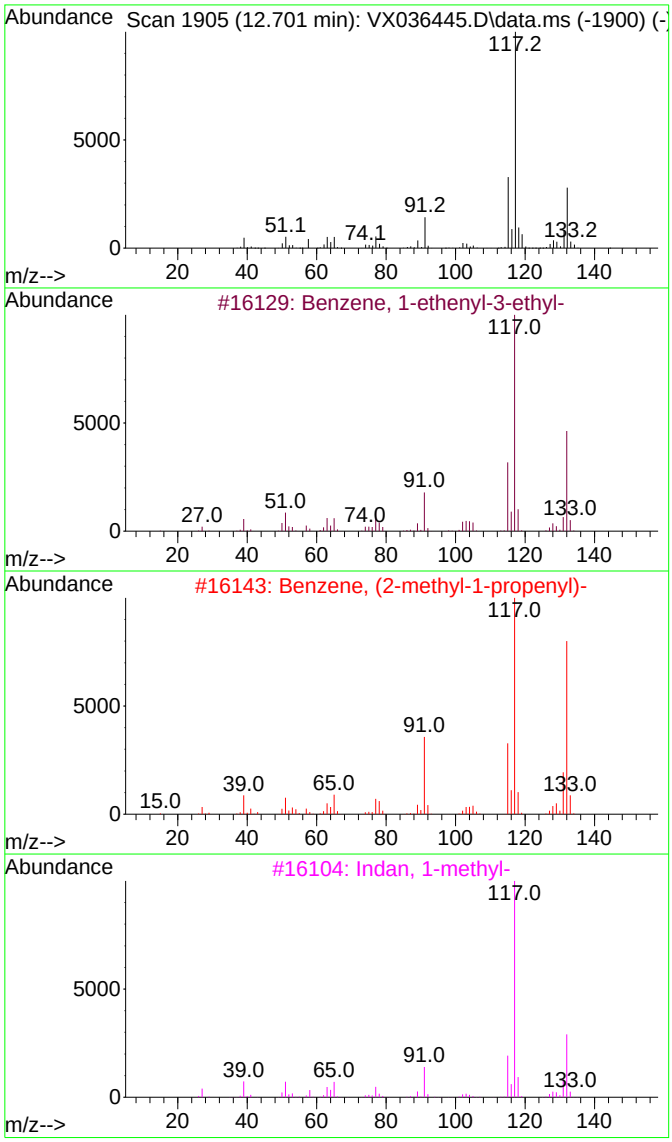
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

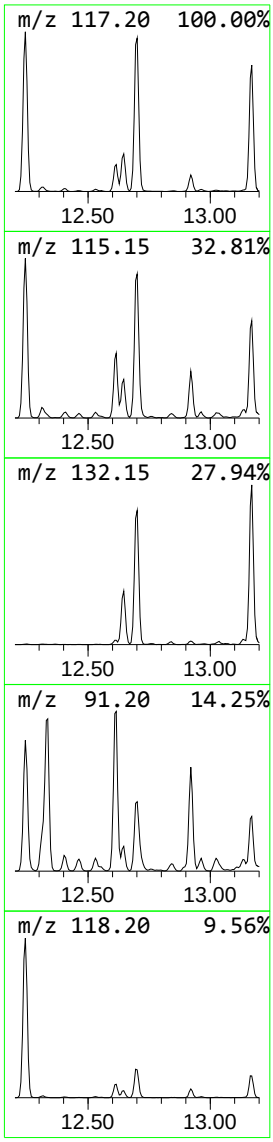
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	129.79 ug/l	2171520	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	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
Operator : JC/MD
Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

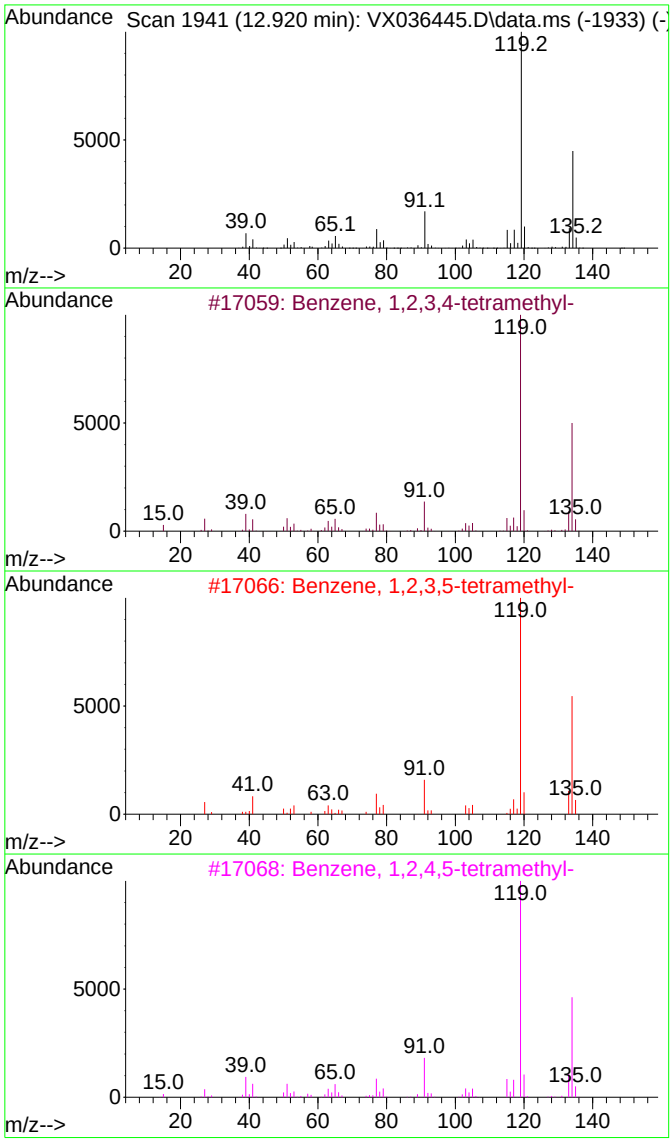
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

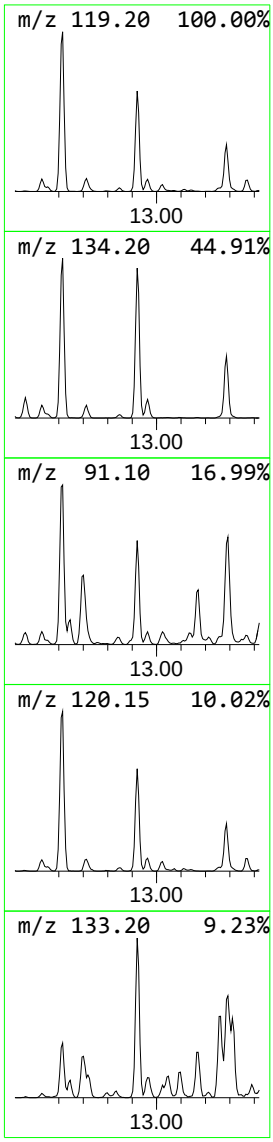
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	132.98 ug/l	2224780	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, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
Operator : JC/MD
Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

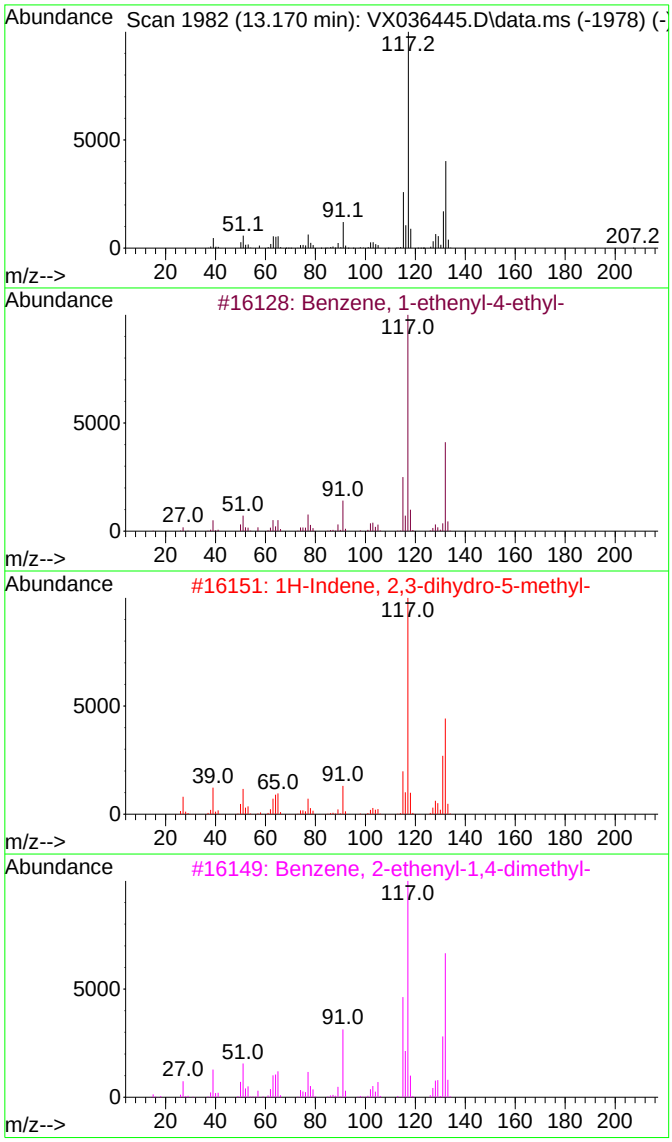
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

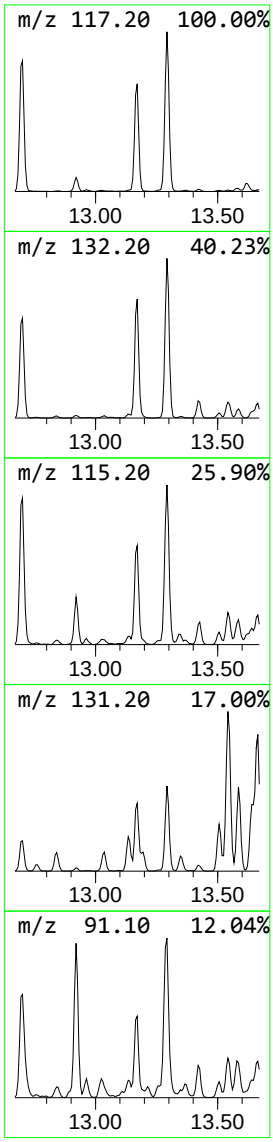
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	110.44 ug/l	1847720	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	Indan, 1-methyl-	132	C10H12	000767-58-8	91
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
Operator : JC/MD
Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

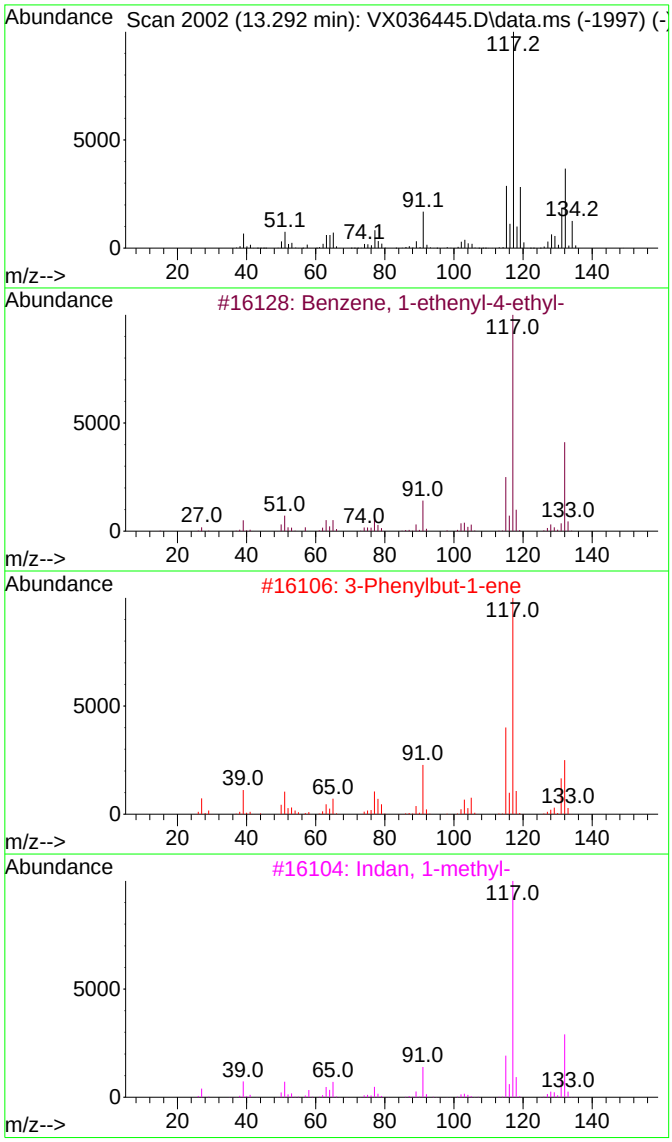
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

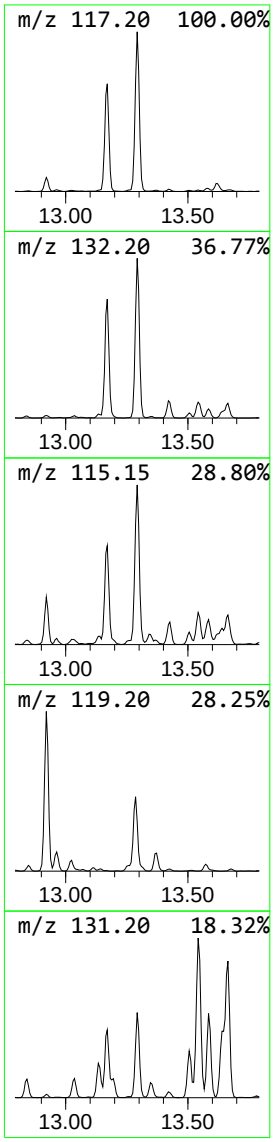
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3-Phenylbut-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	210.23 ug/l	3517250	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	89
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3	Indan, 1-methyl-	132	C10H12	000767-58-8	81
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	81
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070623\
Data File : VX036445.D
Acq On : 06 Jul 2023 19:27
Operator : JC/MD
Sample : 03500-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

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-	1.745	417.8	ug/l	17585500	1	5.556	2104520	50.0
Pentane	1.953	111.3	ug/l	4682730	1	5.556	2104520	50.0
Pentane, 2-methyl-	2.825	216.6	ug/l	9117440	1	5.556	2104520	50.0
Pentane, 3-methyl-	3.105	136.5	ug/l	5743500	1	5.556	2104520	50.0
Benzene, 1-prop...	12.244	193.9	ug/l	3243740	4	12.024	836518	50.0
Benzene, 1-ethy...	12.616	202.9	ug/l	3394470	4	12.024	836518	50.0
Benzene, 1-ethe...	12.701	129.8	ug/l	2171520	4	12.024	836518	50.0
Benzene, 1,2,3,...	12.920	133.0	ug/l	2224780	4	12.024	836518	50.0
Benzene, 1-ethe...	13.170	110.4	ug/l	1847720	4	12.024	836518	50.0
3-Phenylbut-1-ene	13.292	210.2	ug/l	3517250	4	12.024	836518	50.0