LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 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\82X101922W.M
Title : SW846 8260

Signal : TIC: VX032346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	43	rBV	720986	914659	2.32%	0.275%
2	1.368	43	46	54	rBV	4725869	6017281	15.24%	1.807%
3	1.746	103	108	127	rVB	19629283	27467395	69.55%	8.250%
4	1.953	137	142	155	rVB	6303997	9154368	23.18%	2.750%
5	2.069	156	161	168	rVV	1625371	2219473	5.62%	0.667%
6	2.166	172	177	181	rVV	668769	997364	2.53%	0.300%
7	2.215	181	185	197	rVV	1811735	2655599	6.72%	0.798%
8	2.343	198	206	218	rVB	381130	744211	1.88%	0.224%
9	2.782	271	278	281	rVV	1180224	2603432	6.59%	0.782%
10	2.831	281	286	289	rVV	2596421	5371504	13.60%	1.613%
11	2.867	289	292	318	rVV2	1728995	4087481	10.35%	1.228%
12	3.105	318	331	349	rVB	1914781	4246049	10.75%	1.275%
13	3.318	355	366	378	rBV	332856	756105	1.91%	0.227%
14	3.446	378	387	400	rBV	789910	1747081	4.42%	0.525%
15	3.587	400	410	416	rBV	230340	593622	1.50%	0.178%
16	3.666	416	423	428	rBV	173383	427423	1.08%	0.128%
17	3.733	428	434	443	rVB	750367	1749951	4.43%	0.526%
18	3.843	443	452	458	rBV	459752	1191121	3.02%	0.358%
19	4.105	485	495	505	rVV	508382	1307208	3.31%	0.393%
20	4.215	505	513	519	rVV	166994	491739	1.25%	0.148%
21	4.312	519	529	540	rVV	3848767	10871539	27.53%	3.265%
22	4.428	540	548	563	rVB	177580	532413	1.35%	0.160%
23	5.196	664	674	690	rVB	444903	1409649	3.57%	0.423%
24	5.385	690	705	711	rBV3	116790	404608	1.02%	0.122%
25	5.483	711	721	736	rVV4	698537	3104694	7.86%	0.933%
26	5.623	737	744	765	rVB3	409653	1535900	3.89%	0.461%
27	5.830	765	778	791	rBV	355976	1073290	2.72%	0.322%
28	6.044	804	813	822	rBV	818288	2059904	5.22%	0.619%
29	6.166	823	833	837	rBV2	269811	825055	2.09%	0.248%
30	6.257	842	848	857	rVV3	549358	1617312	4.10%	0.486%
31	6.367	857	866	877	rVB2	259782	763528	1.93%	0.229%
32	6.611	895	906	914	rBV2	172747	435877	1.10%	0.131%
33	6.763	924	931	935	rBV	220973	535799	1.36%	0.161%
34	6.854	936	946	957	rVB6	419601	1571111	3.98%	0.472%
35	7.171	990	998	1007	rBV	269152	609240	1.54%	0.183%
36	7.379	1019	1032	1045	rBV4	784226	2194747	5.56%	0.659%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 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\82X101922W.M
Title : SW846 8260

37	7.659	1072	1078	1090	rVB	204007	400546	1.01%	0.120%
38	7.988	1122	1132	1144	rVB	217129	507323	1.28%	0.152%
39	8.110	1144	1152	1154	rBV	336031	635195	1.61%	0.191%
40	8.147	1154	1158	1162	rVV	544798	963463	2.44%	0.289%
41	8.507	1211	1217	1227	rVB	437800	750501	1.90%	0.225%
42	8.653	1236	1241	1247	rVB	456817	751386	1.90%	0.226%
43	8.720	1247	1252	1258	rBV	482335	751042	1.90%	0.226%
44	10.055	1467	1471	1476	rVB	443800	584703	1.48%	0.176%
45	10.207	1489	1496	1501	rVB	25745057	37451251	94.83%	11.249%
46	10.317	1506	1514	1519	rVB	27025000	39494698	100.00%	11.863%
47	10.640	1562	1567	1578	rVB	1410257	1934948	4.90%	0.581%
48	10.963	1613	1620	1626	rBV	2155934	2666086	6.75%	0.801%
49	11.085	1635	1640	1644	rBV	404213	548049	1.39%	0.165%
50	11.305	1666	1676	1682	rBV	5754604	7312583	18.52%	2.196%
51	11.402	1683	1692	1697	rVV	11117975	14658065	37.11%	4.403%
52	11.457	1697	1701	1712	rVB	5106273	6256948	15.84%	1.879%
53	11.616	1721	1727	1736	rBV	5362642	6361544	16.11%	1.911%
54	11.762	1745	1751	1756	rBV	28344353	38145926	96.58%	11.458%
55	12.024	1789	1794	1799	rVB2	610825	883444	2.24%	0.265%
56	12.091	1799	1805	1810	rBV	8914035	10675440	27.03%	3.206%
57	12.244	1825	1830	1837	rBV	8904981	12028207	30.46%	3.613%
58	12.317	1837	1842	1849	rVV3	2804706	4142430	10.49%	1.244%
59	12.408	1852	1857	1862	rBV2	430349	558491	1.41%	0.168%
60	12.463	1862	1866	1872	rVB	1168988	1389920	3.52%	0.417%
61	12.530	1872	1877	1880	rBV	2106040	3067581	7.77%	0.921%
62	12.555	1880	1881	1886	rVV	1771610	1559102	3.95%	0.468%
63	12.616	1886	1891	1894	rVV	4017640	4553144	11.53%	1.368%
64	12.646	1894	1896	1900	rVV	564056	615128	1.56%	0.185%
65	12.701	1900	1905	1917	rVB2	1744670	2591725	6.56%	0.778%
66	12.847	1924	1929	1934	rVB	975826	1232115	3.12%	0.370%
67	12.920	1934	1941	1945	rBV	1792523	2323537	5.88%	0.698%
68	12.963	1945	1948	1954	rVB	2771521	3146616	7.97%	0.945%
69	13.170	1977	1982	1986	rVB	1931582	2278946	5.77%	0.685%
70	13.292	1998	2002	2007	rVB2	3891655	5075020	12.85%	1.524%
71	13.426	2019	2024	2032	rVB	547772	723554	1.83%	0.217%
72	13.579	2046	2049	2056	rVB4	325074	591966	1.50%	0.178%
73	13.664	2060	2063	2069	rVB3	235860	410470	1.04%	0.123%
74	13.774	2076	2081	2089	rBV	4862515	6396103	16.19%	1.921%
75	14.640	2218	2223	2233	rVB	2131601	2741548	6.94%	0.823%
76	14.780	2241	2246	2257	rVB	1200267	1487445	3.77%	0.447%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 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\82X101922W.M
Title : SW846 8260

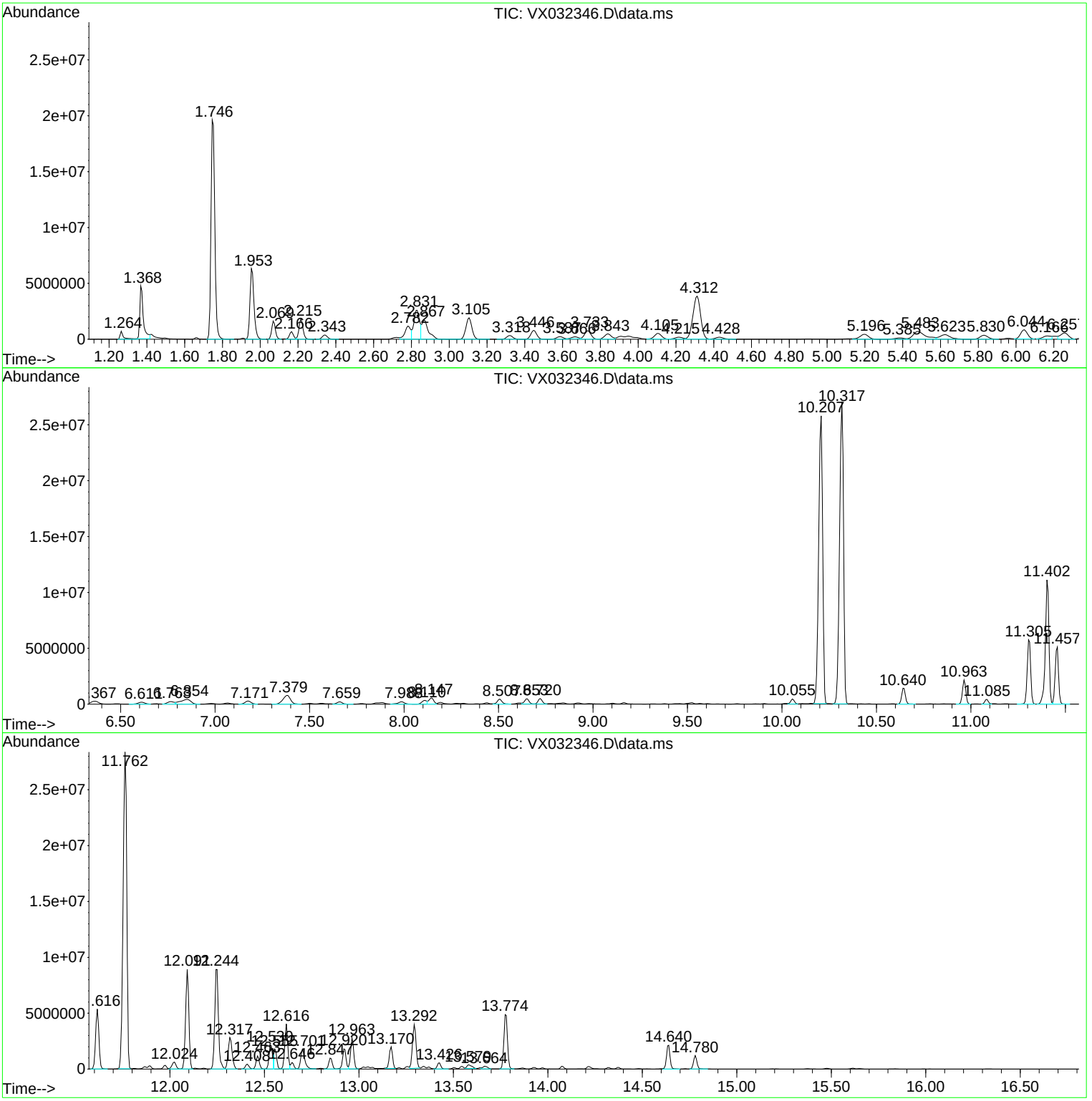
Sum of corrected areas: 332933921

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

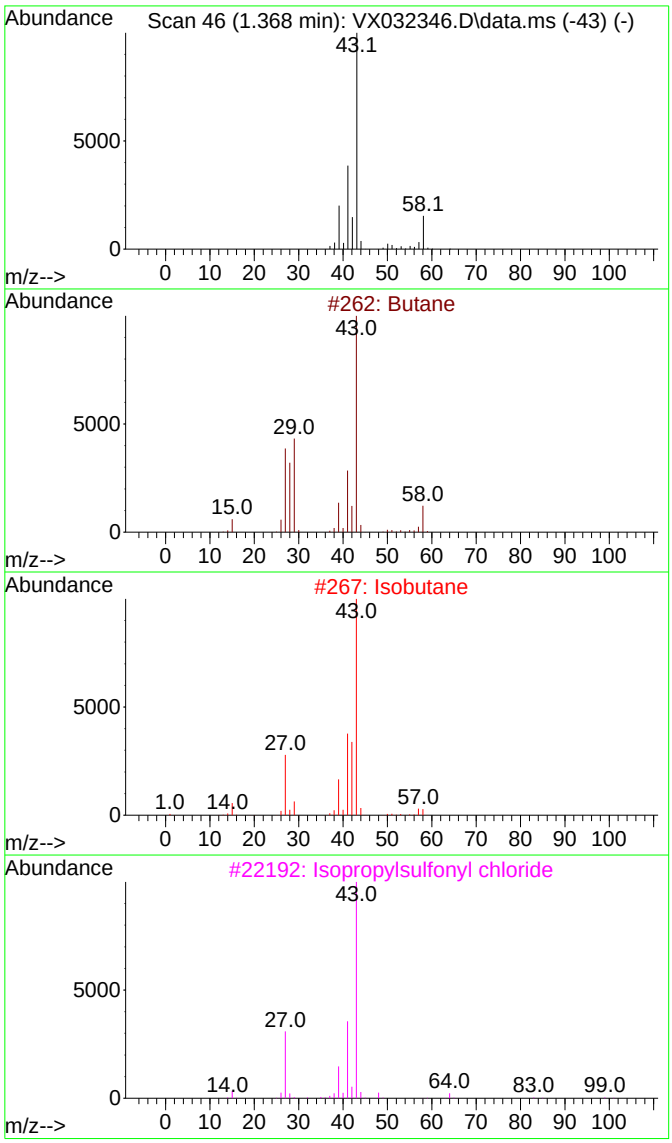
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

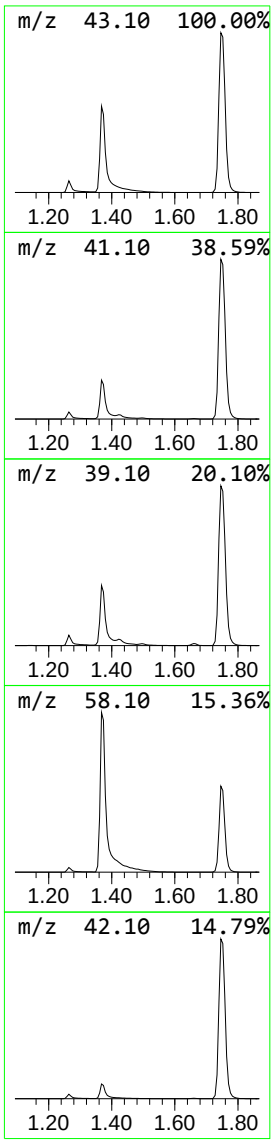
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	195.89 ug/l	6017280	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	86
2	Isobutane	58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

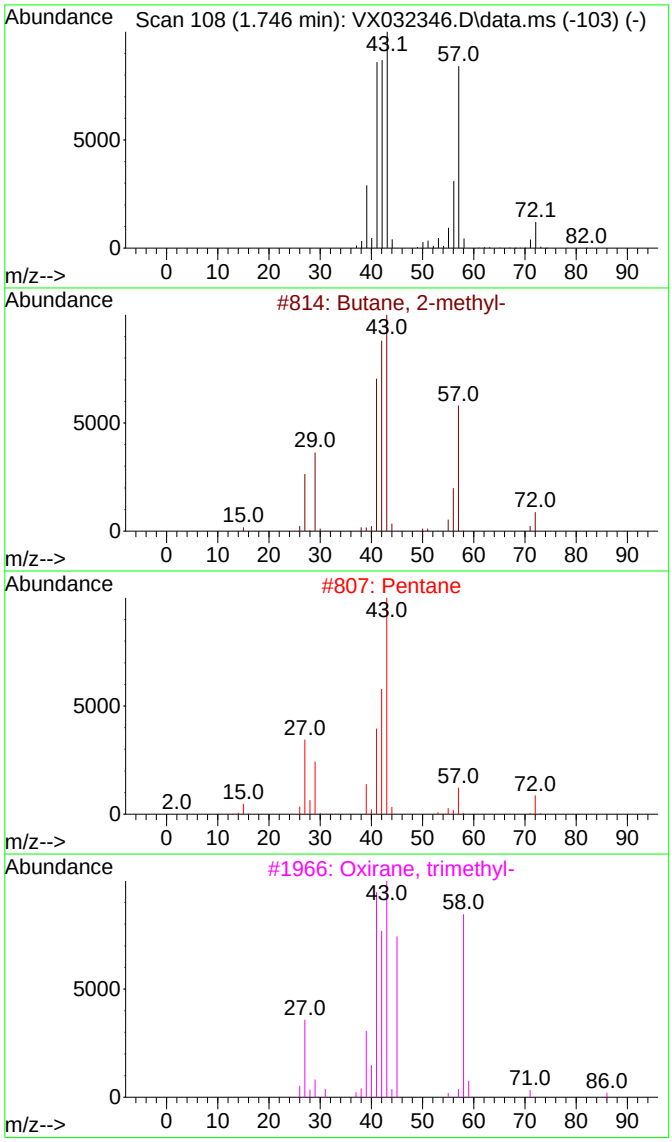
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

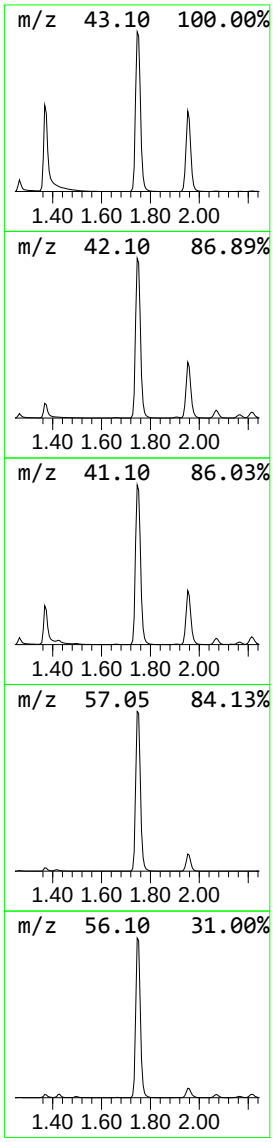
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	894.18 ug/l	27467400	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	42
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
4	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

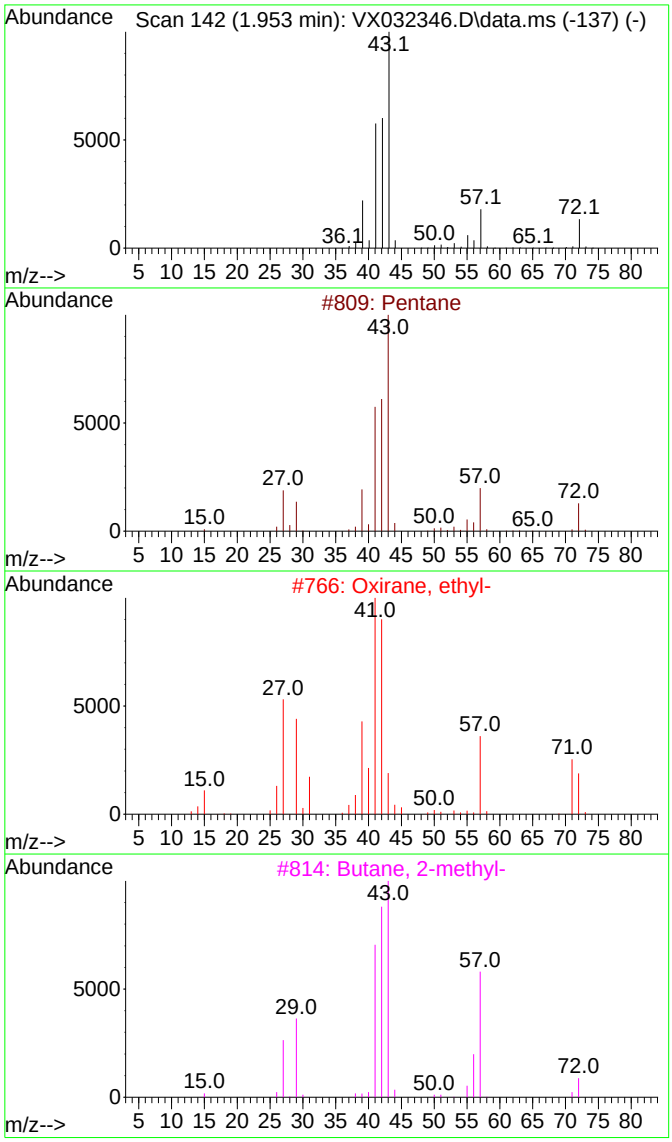
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

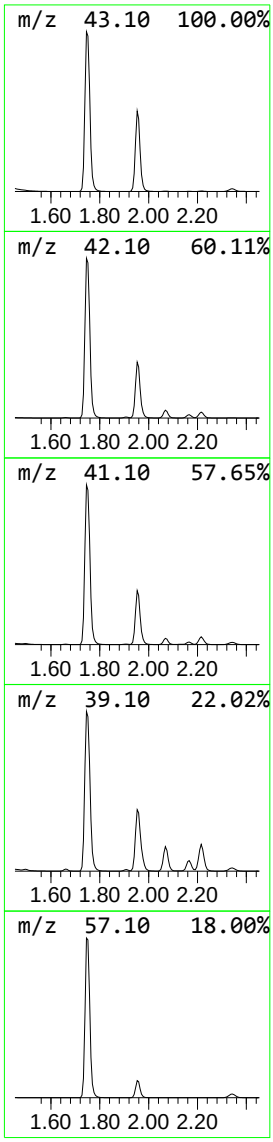
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	298.01 ug/l	9154370	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Butane, 2-methyl-	72	C5H12	000078-78-4	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

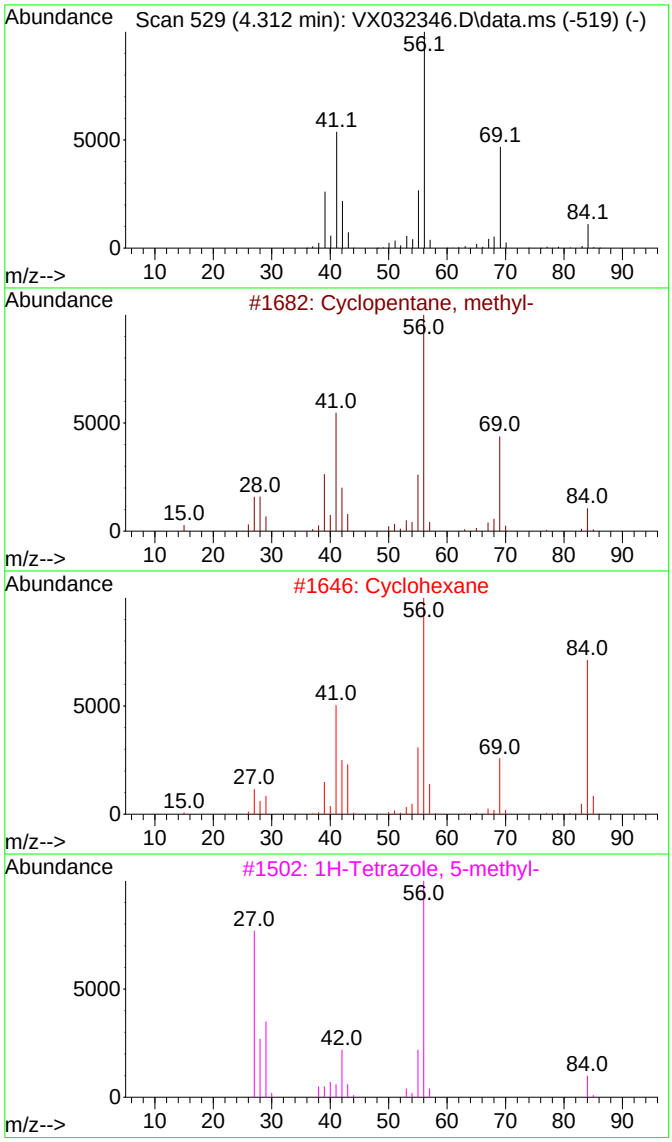
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

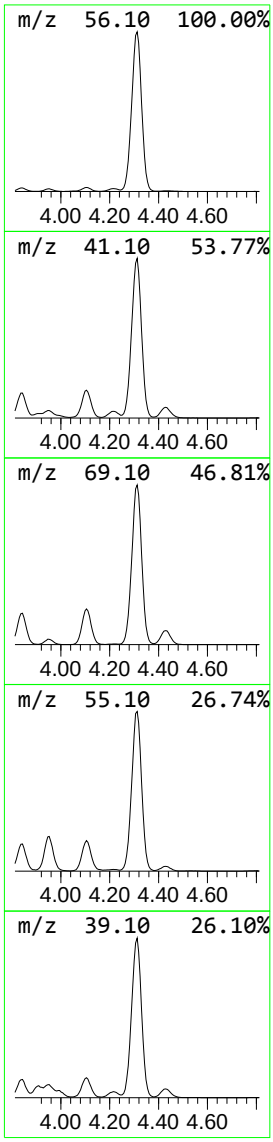
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	353.91 ug/l	10871500	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	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

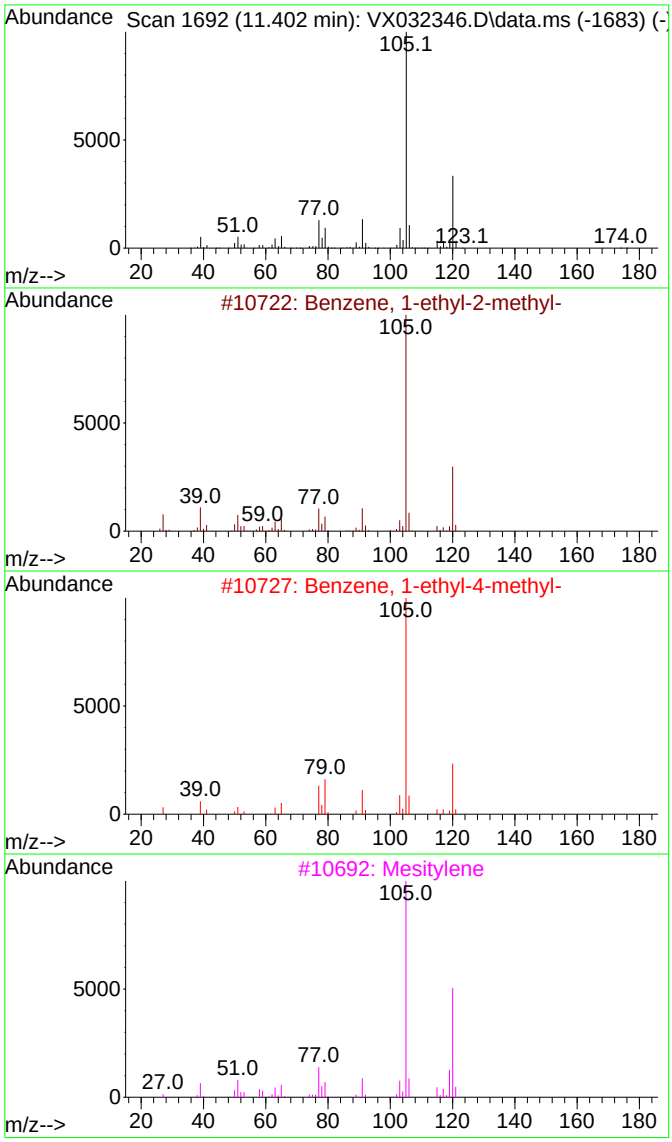
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

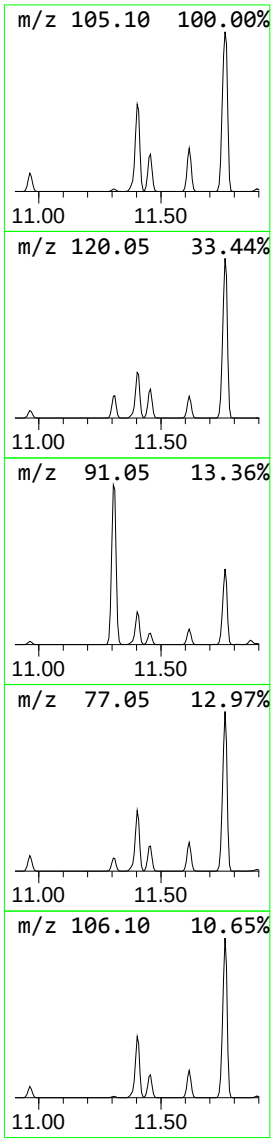
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.402	829.60 ug/l	14658100	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-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

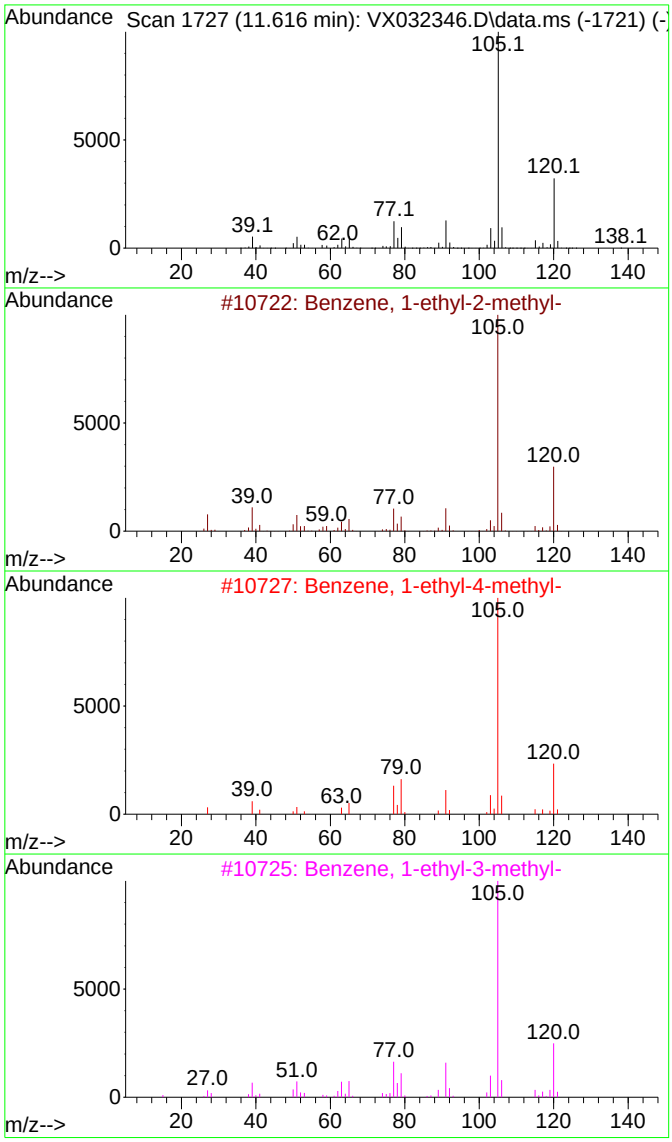
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

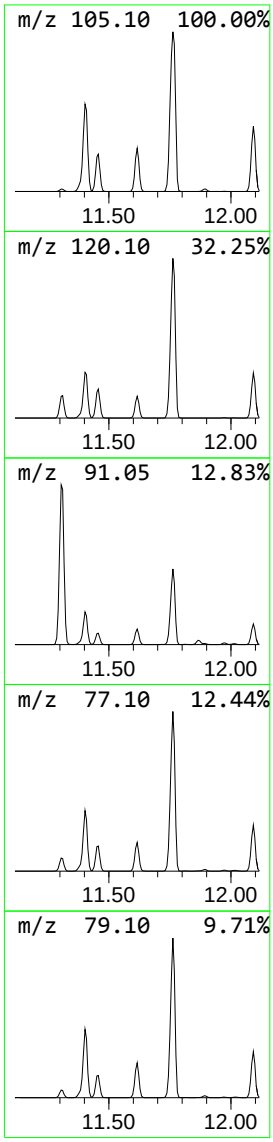
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	360.04 ug/l	6361540	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-ethyl-3-methyl-	120	C9H12	000620-14-4	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\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

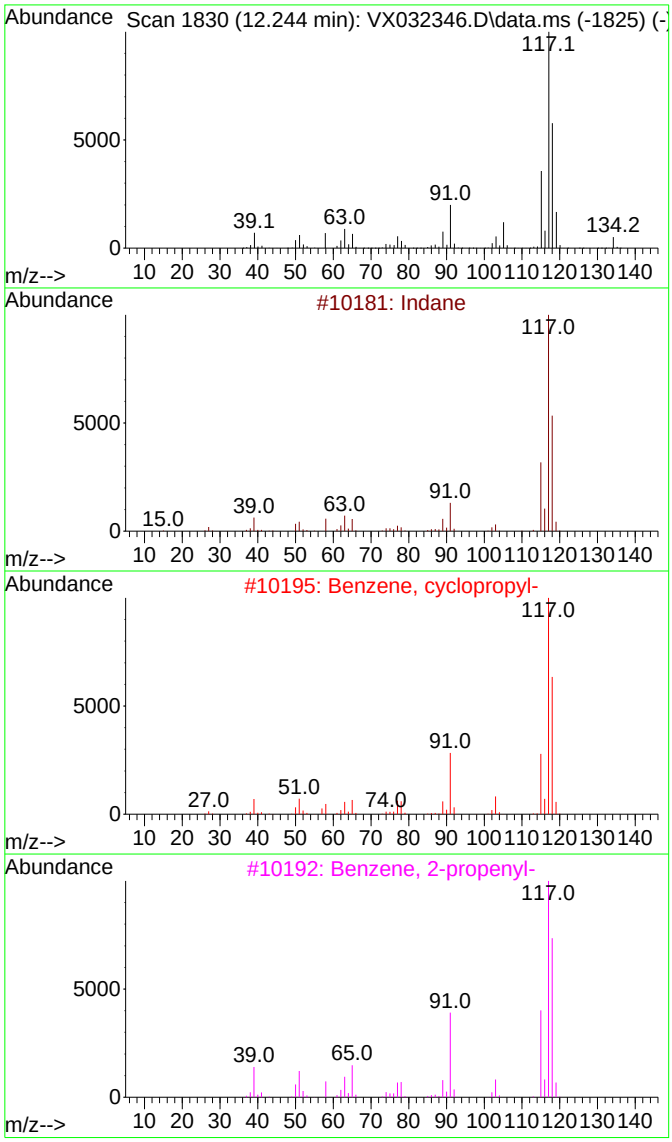
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

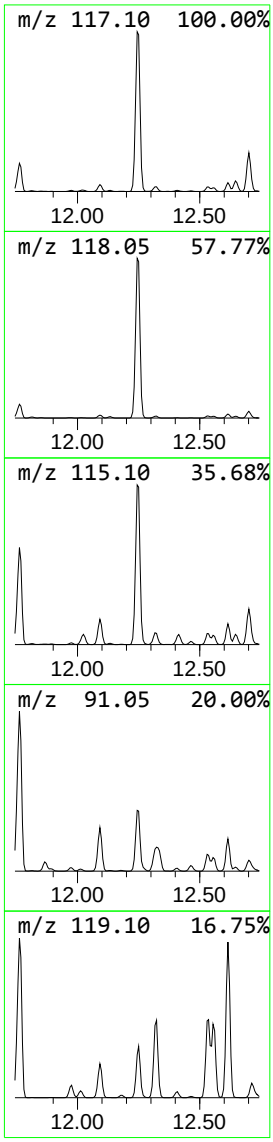
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	680.76 ug/l	12028200	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4	Deltacyclene	118	C9H10	007785-10-6	58
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

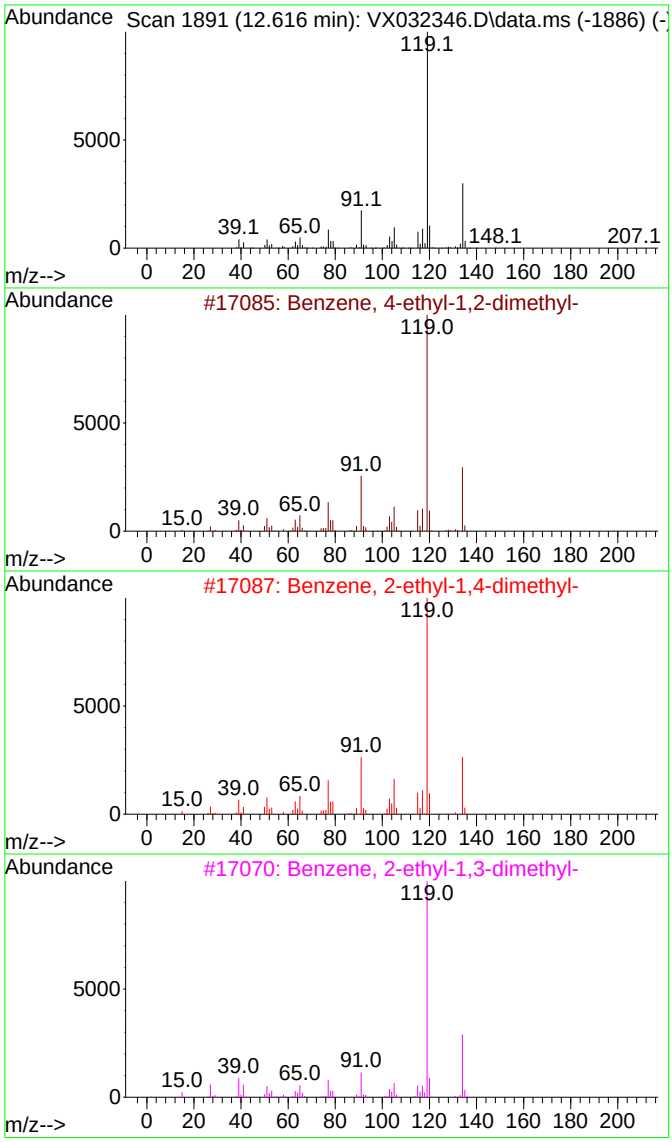
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

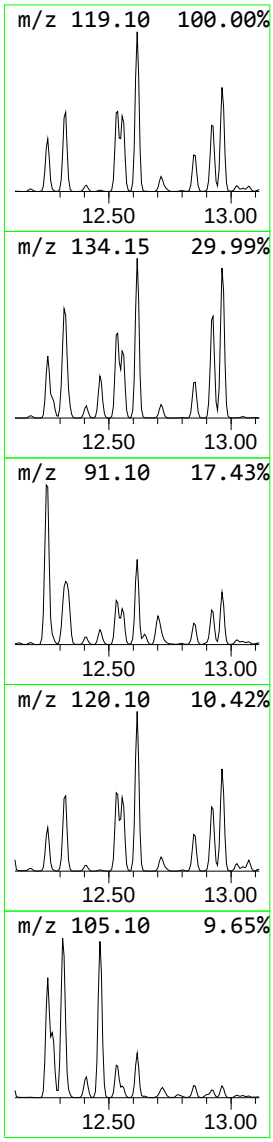
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	257.69 ug/l	4553140	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	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\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

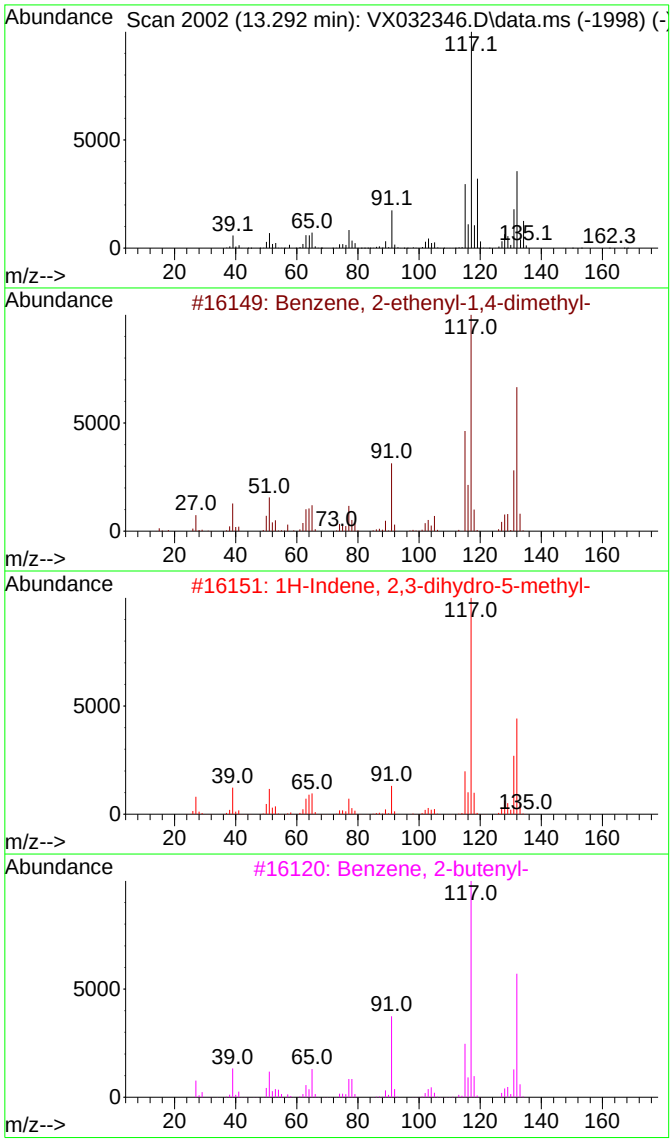
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

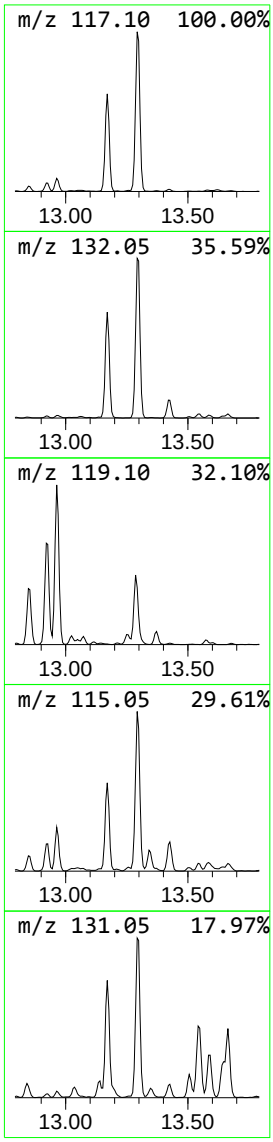
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	287.23 ug/l	5075020	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	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102422\
Data File : VX032346.D
Acq On : 24 Oct 2022 17:30
Operator : JC/MD
Sample : N5260-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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	1.368	195.9	ug/l	6017280	1	5.556	1535900	50.0
Butane, 2-methyl-	1.746	894.2	ug/l	27467400	1	5.556	1535900	50.0
Pentane	1.953	298.0	ug/l	9154370	1	5.556	1535900	50.0
Cyclopentane, m...	4.312	353.9	ug/l	10871500	1	5.556	1535900	50.0
Benzene, 1-ethy...	11.402	829.6	ug/l	14658100	4	12.024	883444	50.0
Benzene, 1-ethy...	11.616	360.0	ug/l	6361540	4	12.024	883444	50.0
Indane	12.244	680.8	ug/l	12028200	4	12.024	883444	50.0
Benzene, 4-ethy...	12.616	257.7	ug/l	4553140	4	12.024	883444	50.0
Benzene, 2-ethe...	13.292	287.2	ug/l	5075020	4	12.024	883444	50.0