LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	197	206	214	rBV	13021	25941	4.11%	0.431%
2	2.782	269	278	288	rBV	11693	25560	4.05%	0.424%
3	2.989	299	312	325	rBV2	62239	245201	38.83%	4.071%
4	3.111	325	332	345	rVB2	44446	107459	17.02%	1.784%
5	3.757	427	438	457	rVB	40077	107012	16.95%	1.777%
6	5.160	653	668	679	rVB9	4370	18311	2.90%	0.304%
7	5.385	692	705	721	rBV2	71389	207658	32.89%	3.448%
8	5.550	721	732	759	rVB	112566	339149	53.71%	5.631%
9	5.958	789	799	807	rBV	73041	195709	30.99%	3.250%
10	6.037	808	812	818	rVB	8824	18022	2.85%	0.299%
11	6.251	837	847	861	rVV3	67778	234961	37.21%	3.901%
12	6.361	861	865	875	rVB3	8076	21824	3.46%	0.362%
13	6.763	920	931	942	rBV	175497	427267	67.67%	7.094%
14	6.854	942	946	952	rVB5	4850	11251	1.78%	0.187%
15	7.171	992	998	1005	rBV3	9168	19575	3.10%	0.325%
16	7.360	1023	1029	1038	rVB4	3056	6922	1.10%	0.115%
17	7.562	1057	1062	1066	rVV4	4082	8777	1.39%	0.146%
18	7.775	1091	1097	1105	rVB3	6447	12852	2.04%	0.213%
19	7.885	1105	1115	1122	rBV6	5597	19049	3.02%	0.316%
20	7.982	1122	1131	1140	rVB3	19902	51328	8.13%	0.852%
21	8.110	1143	1152	1162	rBV2	36583	78566	12.44%	1.305%
22	8.214	1162	1169	1172	rBV5	3807	9619	1.52%	0.160%
23	8.305	1179	1184	1189	rBV4	7428	14376	2.28%	0.239%
24	8.427	1200	1204	1210	rVB3	6997	11489	1.82%	0.191%
25	8.507	1210	1217	1224	rVB5	10091	21656	3.43%	0.360%
26	8.647	1227	1240	1251	rBV	383333	631423	100.00%	10.484%
27	8.921	1281	1285	1289	rVV2	5364	7678	1.22%	0.127%
28	8.976	1289	1294	1299	rVB4	7411	13535	2.14%	0.225%
29	9.098	1312	1314	1319	rVB3	5360	7717	1.22%	0.128%
30	9.159	1319	1324	1335	rVB	41681	69790	11.05%	1.159%
31	9.427	1361	1368	1376	rVV4	17898	40500	6.41%	0.672%
32	9.500	1376	1380	1389	rVB3	12546	24172	3.83%	0.401%
33	9.659	1402	1406	1415	rVB4	5255	9875	1.56%	0.164%
34	9.762	1416	1423	1431	rBV4	15129	26443	4.19%	0.439%
35	10.006	1460	1463	1466	rVV2	17456	25512	4.04%	0.424%
36	10.055	1466	1471	1476	rVV	369640	498313	78.92%	8.274%

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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

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\82X102622W.M
Title : SW846 8260

37	10.104	1476	1479	1485	rVV5	7244	15604	2.47%	0.259%
38	10.153	1485	1487	1490	rVV2	6564	8178	1.30%	0.136%
39	10.195	1490	1494	1499	rVV	16951	23113	3.66%	0.384%
40	10.372	1517	1523	1528	rBV2	10172	16493	2.61%	0.274%
41	10.585	1549	1558	1564	rBV6	4318	9063	1.44%	0.150%
42	10.793	1582	1592	1593	rBV5	4610	9008	1.43%	0.150%
43	10.963	1615	1620	1625	rBV	95668	121224	19.20%	2.013%
44	11.018	1625	1629	1632	rVV3	7566	12089	1.91%	0.201%
45	11.079	1634	1639	1645	rVV	356273	453487	71.82%	7.530%
46	11.305	1673	1676	1679	rBV	8979	10734	1.70%	0.178%
47	11.616	1722	1727	1736	rVB	20635	29535	4.68%	0.490%
48	11.713	1736	1743	1746	rBV2	10623	14920	2.36%	0.248%
49	11.756	1746	1750	1754	rVB	9977	12667	2.01%	0.210%
50	11.890	1761	1772	1777	rBV4	9143	16691	2.64%	0.277%
51	12.024	1788	1794	1801	rBV	386080	485774	76.93%	8.066%
52	12.091	1801	1805	1811	rVV4	4597	8789	1.39%	0.146%
53	12.177	1816	1819	1824	rVV	12195	14201	2.25%	0.236%
54	12.250	1824	1831	1836	rVV	76390	102613	16.25%	1.704%
55	12.311	1837	1841	1851	rVV2	14360	21678	3.43%	0.360%
56	12.414	1852	1858	1863	rVB2	7767	10960	1.74%	0.182%
57	12.646	1892	1896	1900	rBV	38704	45042	7.13%	0.748%
58	12.701	1900	1905	1912	rVV	352161	447367	70.85%	7.428%
59	12.762	1912	1915	1921	rVB4	5210	7353	1.16%	0.122%
60	12.841	1921	1928	1934	rBV	13505	17144	2.72%	0.285%
61	13.036	1953	1960	1965	rVB2	10322	14273	2.26%	0.237%
62	13.134	1967	1976	1978	rBV2	12888	20086	3.18%	0.334%
63	13.170	1978	1982	1990	rVB	72909	95685	15.15%	1.589%
64	13.237	1990	1993	1997	rVB4	5131	6919	1.10%	0.115%
65	13.292	1997	2002	2007	rBV	140200	174190	27.59%	2.892%
66	13.347	2007	2011	2015	rBV2	14808	19473	3.08%	0.323%
67	13.420	2020	2023	2030	rVB2	15922	21566	3.42%	0.358%
68	13.542	2039	2043	2047	rVV	28779	40698	6.45%	0.676%
69	13.585	2047	2050	2053	rVV	9352	11713	1.86%	0.194%
70	13.640	2053	2059	2060	rVV2	22073	33417	5.29%	0.555%
71	13.664	2060	2063	2068	rVB	33082	41485	6.57%	0.689%
72	13.774	2079	2081	2091	rVB2	5300	8914	1.41%	0.148%
73	13.926	2101	2106	2110	rBV	8641	10768	1.71%	0.179%
74	14.073	2125	2130	2134	rBV	6513	8495	1.35%	0.141%
75	14.786	2242	2247	2255	rBV4	3956	6746	1.07%	0.112%

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Sample : N5614-02
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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
MW-16S

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
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Title : SW846 8260

Sum of corrected areas: 6022647

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
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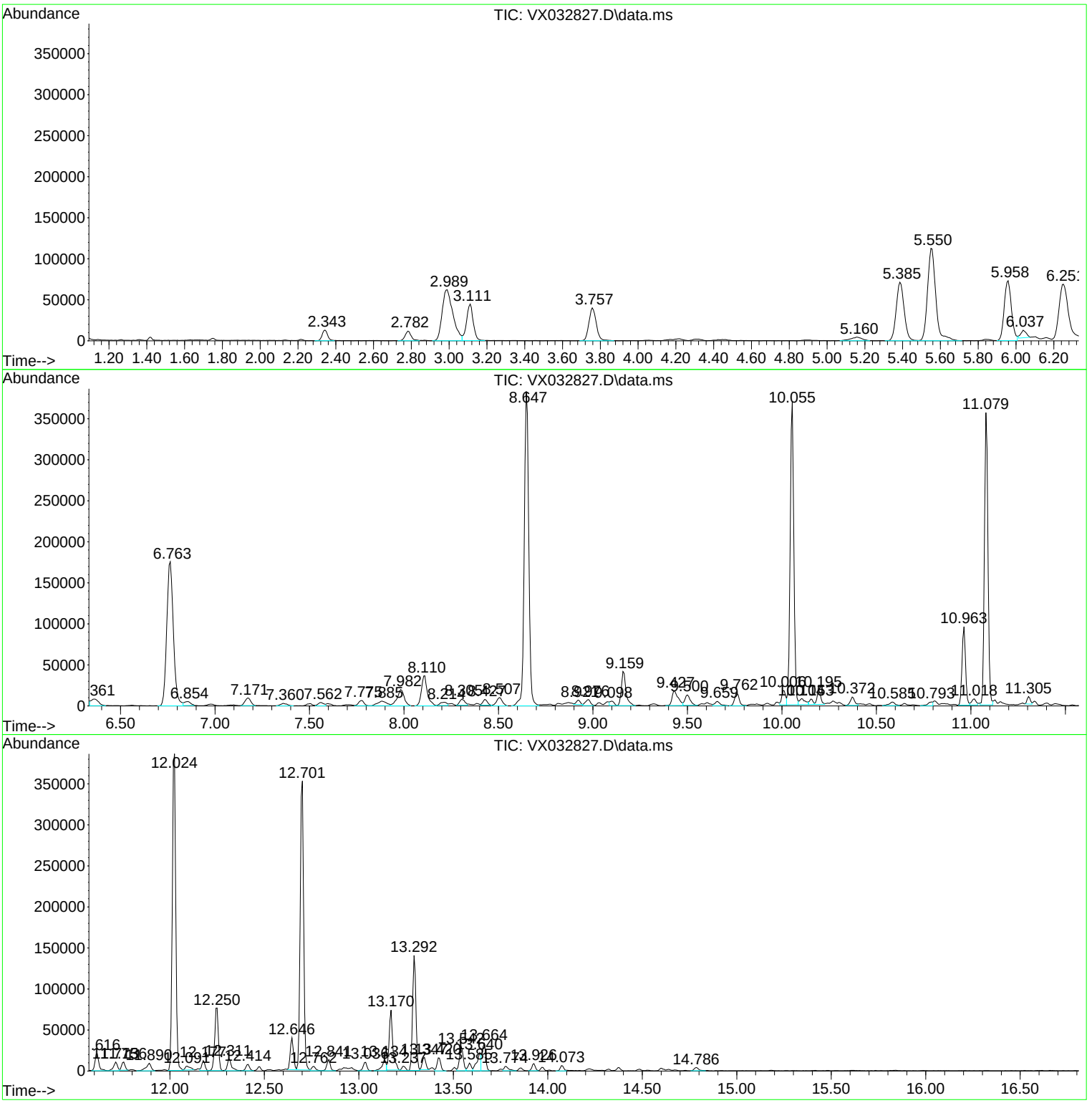
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

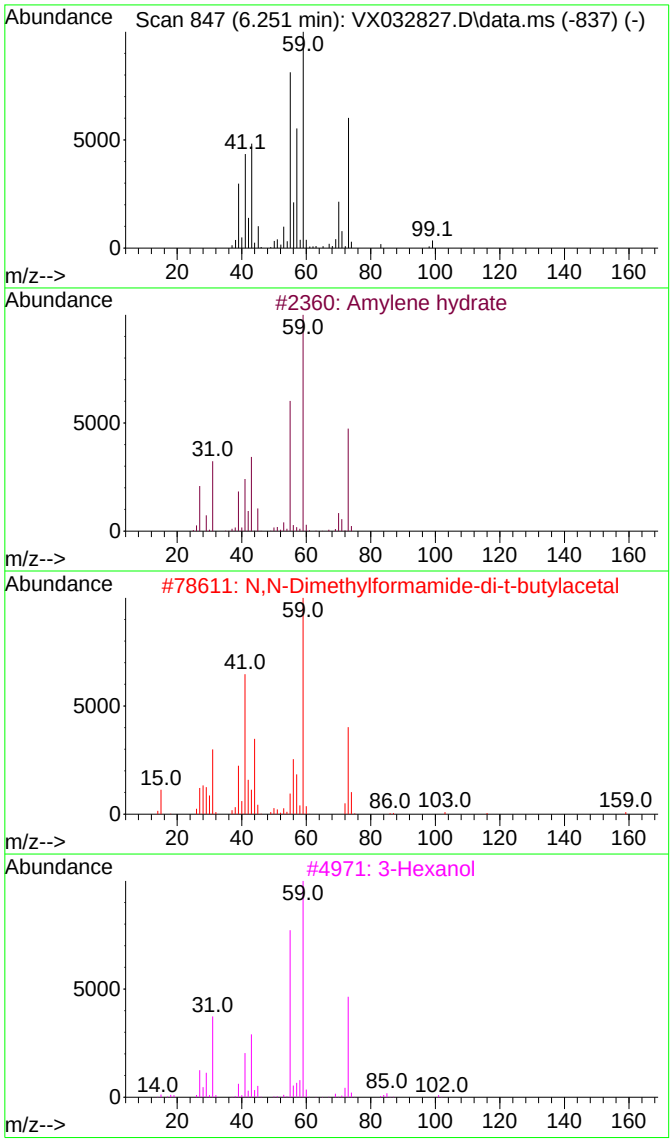
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

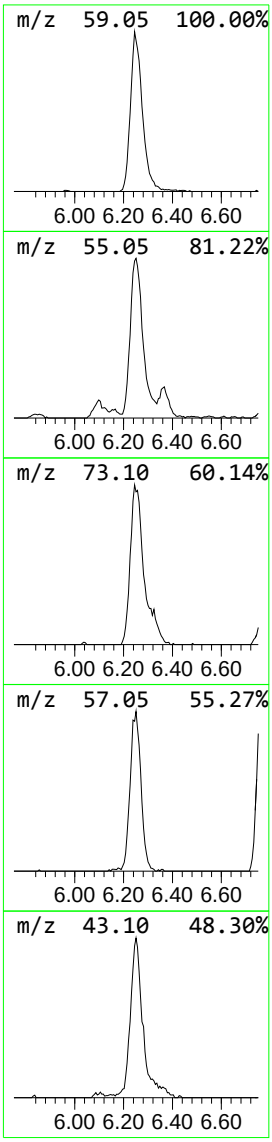
****

Peak Number 1 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	27.50 ug/l	234961	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	53
2	N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	42
3	3-Hexanol	102	C6H14O	000623-37-0	42
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40
5	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

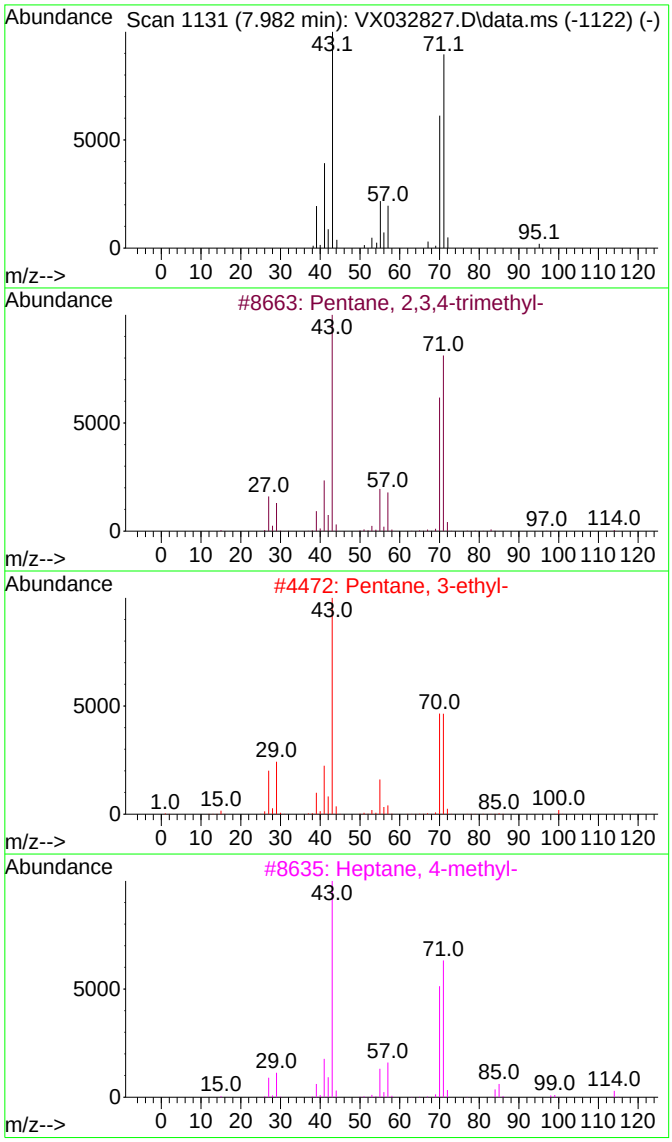
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

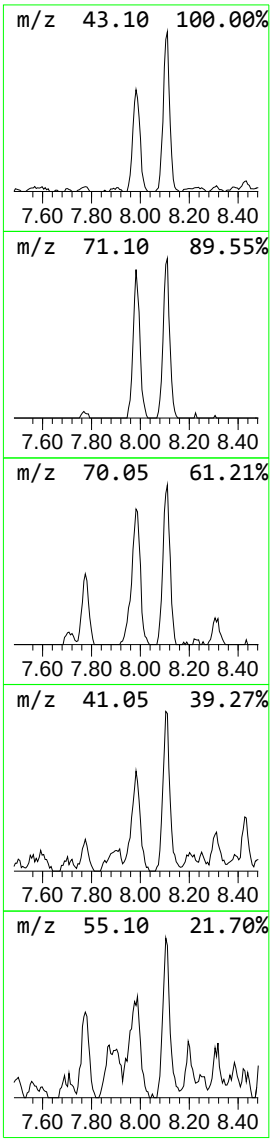
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	6.01 ug/l	51328	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	78
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

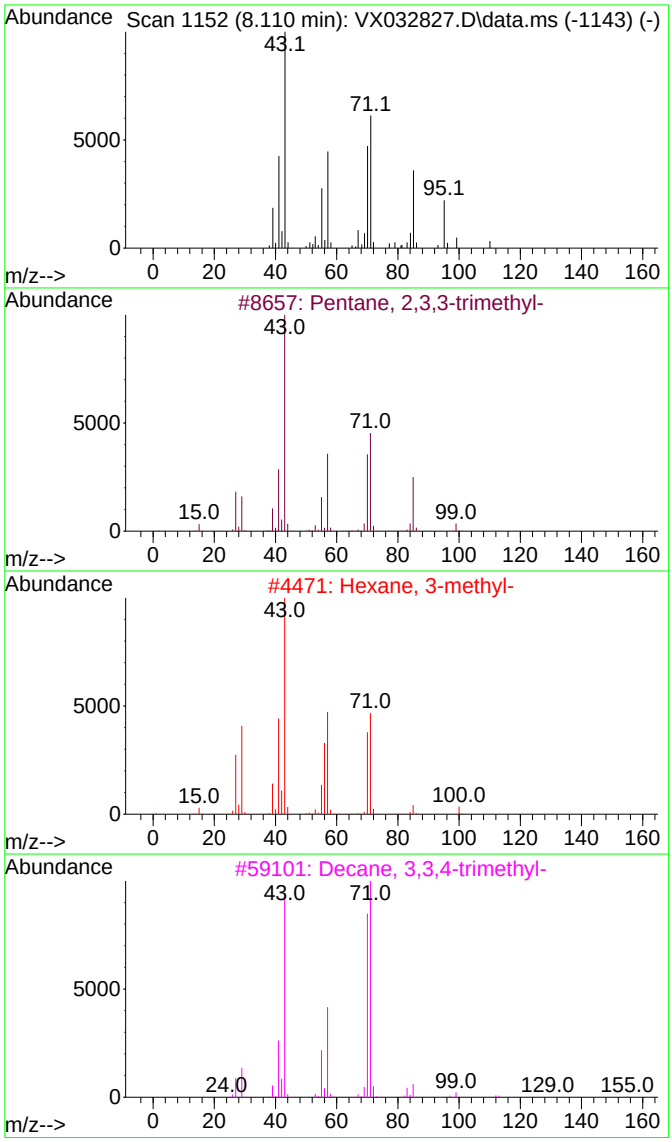
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

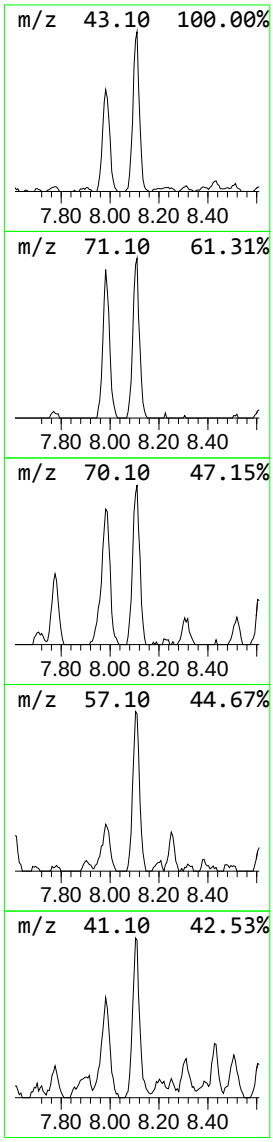
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	9.19 ug/l	78566	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	53
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	50
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50





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MSVOA_X
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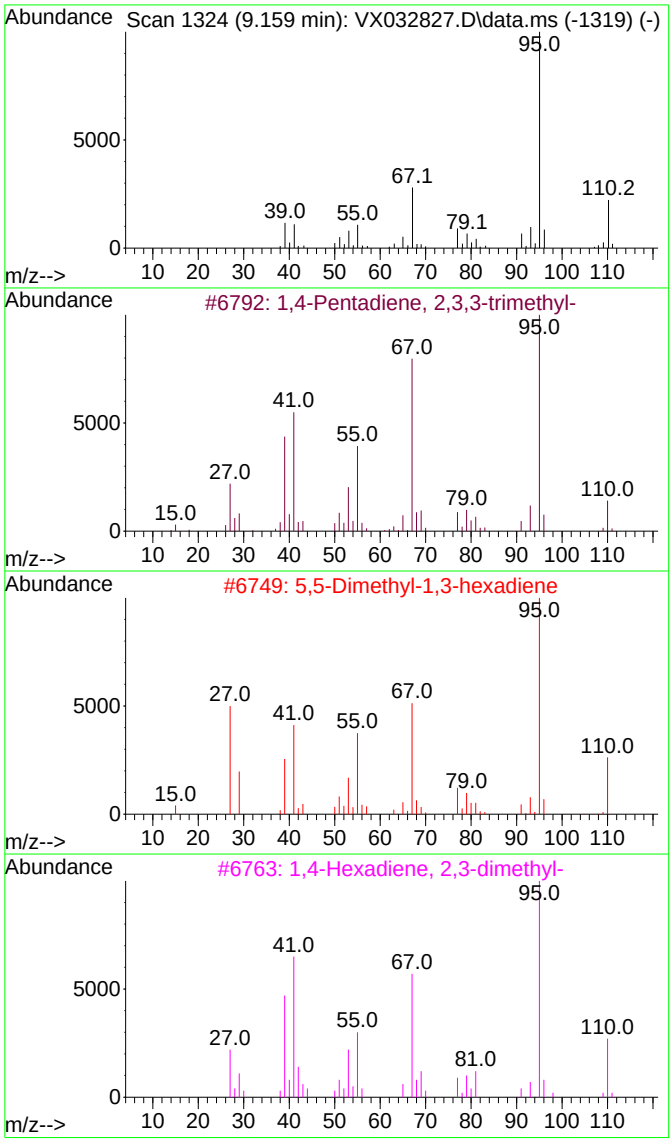
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

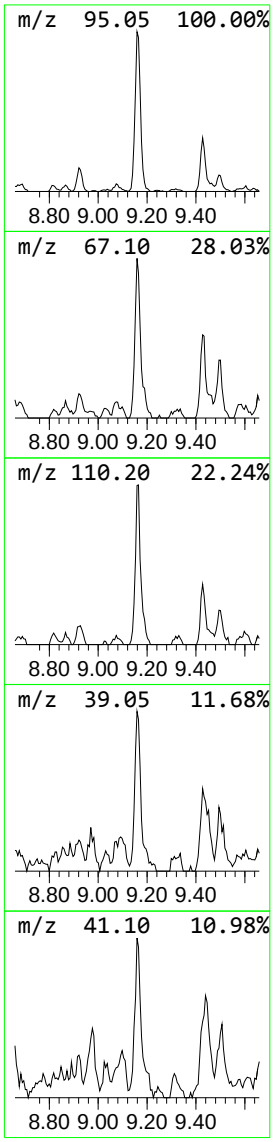
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.159	7.00 ug/l	69790	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	90
2	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	87
3	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	86
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	83
5	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	81





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MSVOA_X
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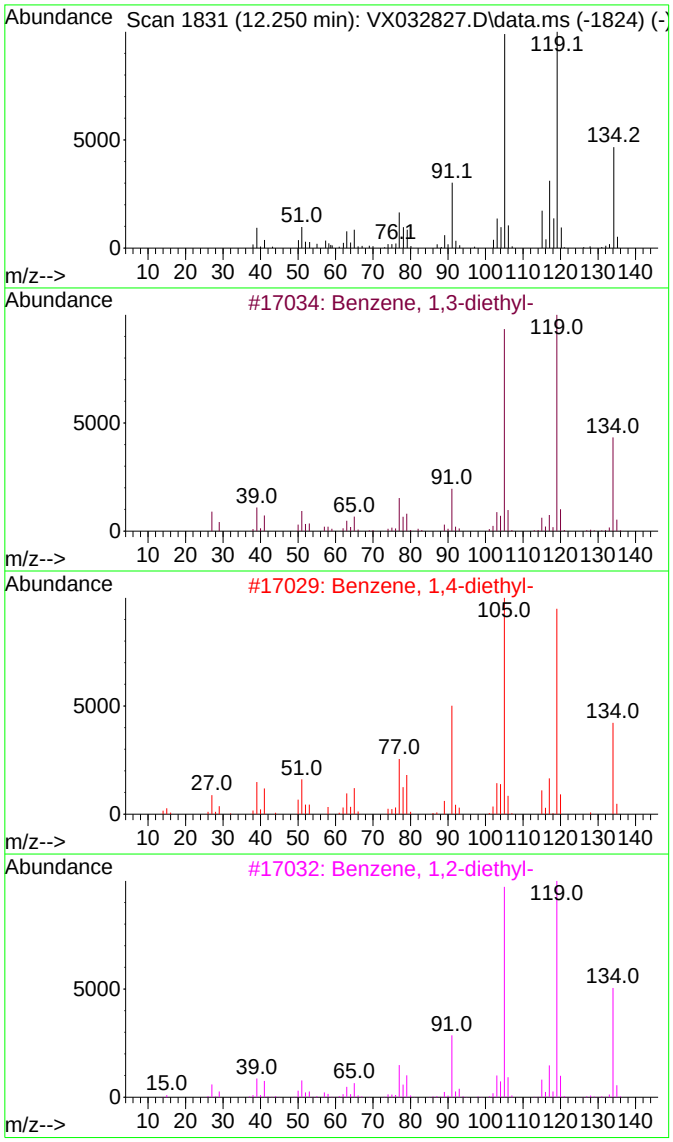
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

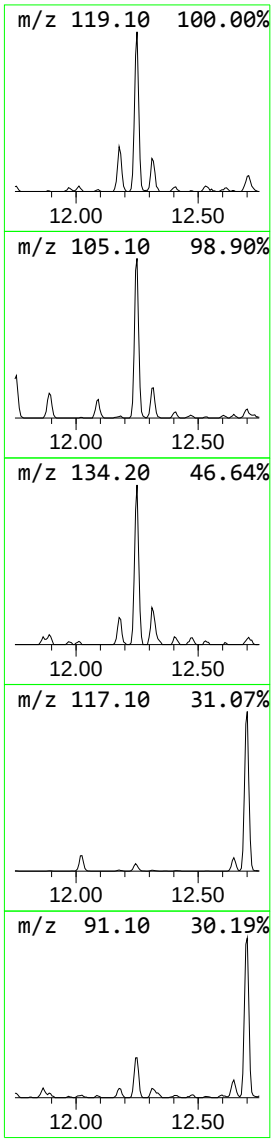
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,3-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	10.56 ug/l	102613	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	94
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
4	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	87
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	83





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Data File : VX032827.D
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

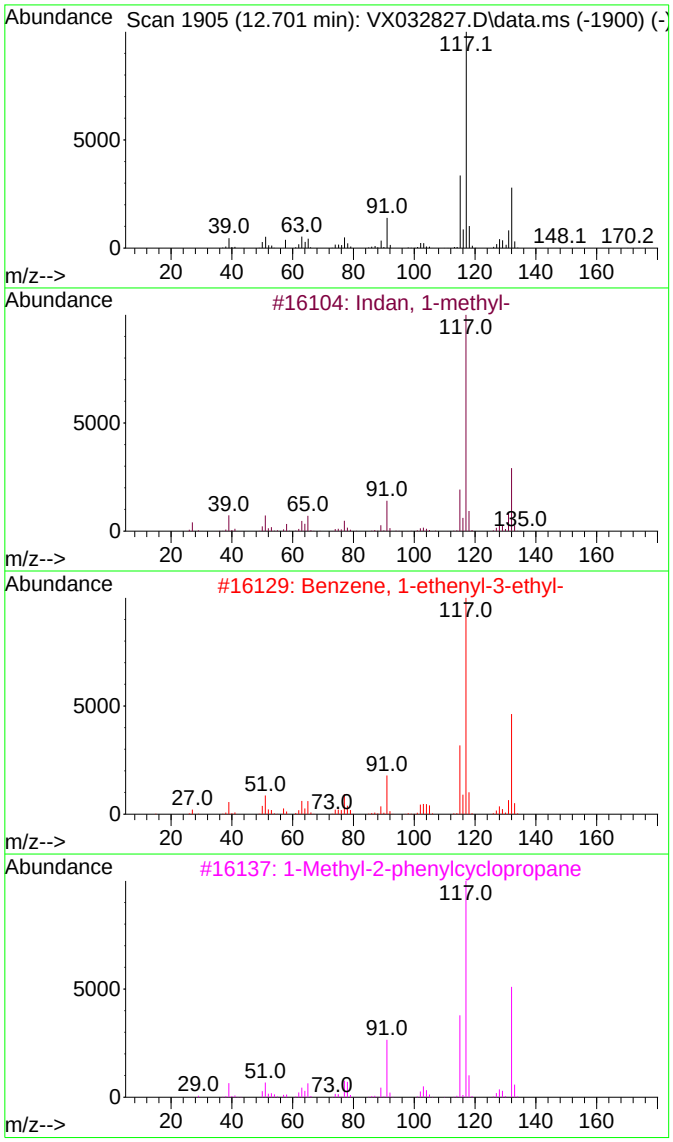
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

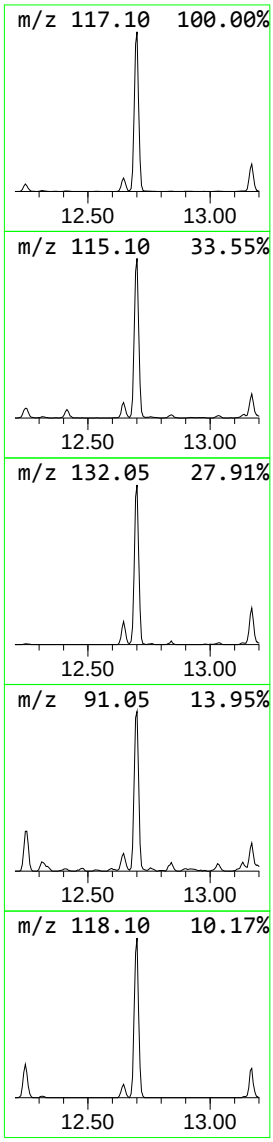
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indan, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	46.05 ug/l	447367	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, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

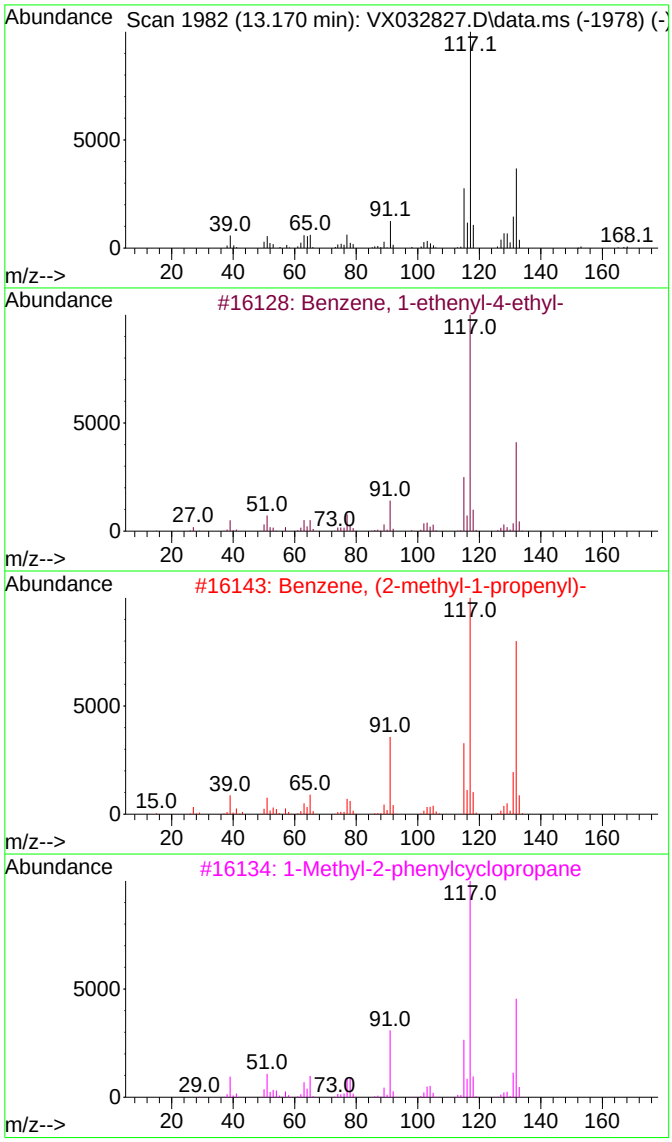
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

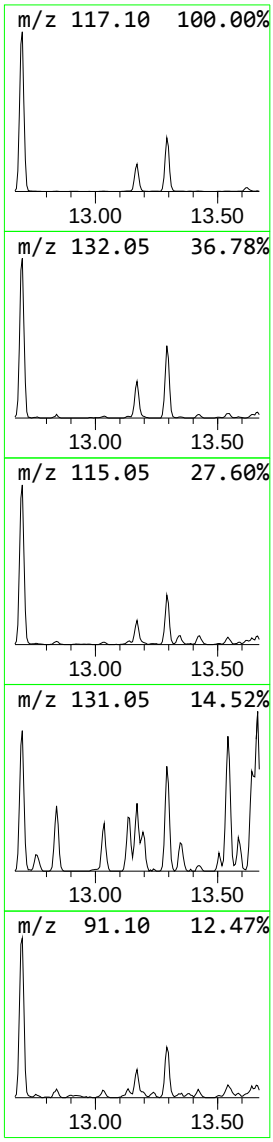
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	9.85 ug/l	95685	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	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

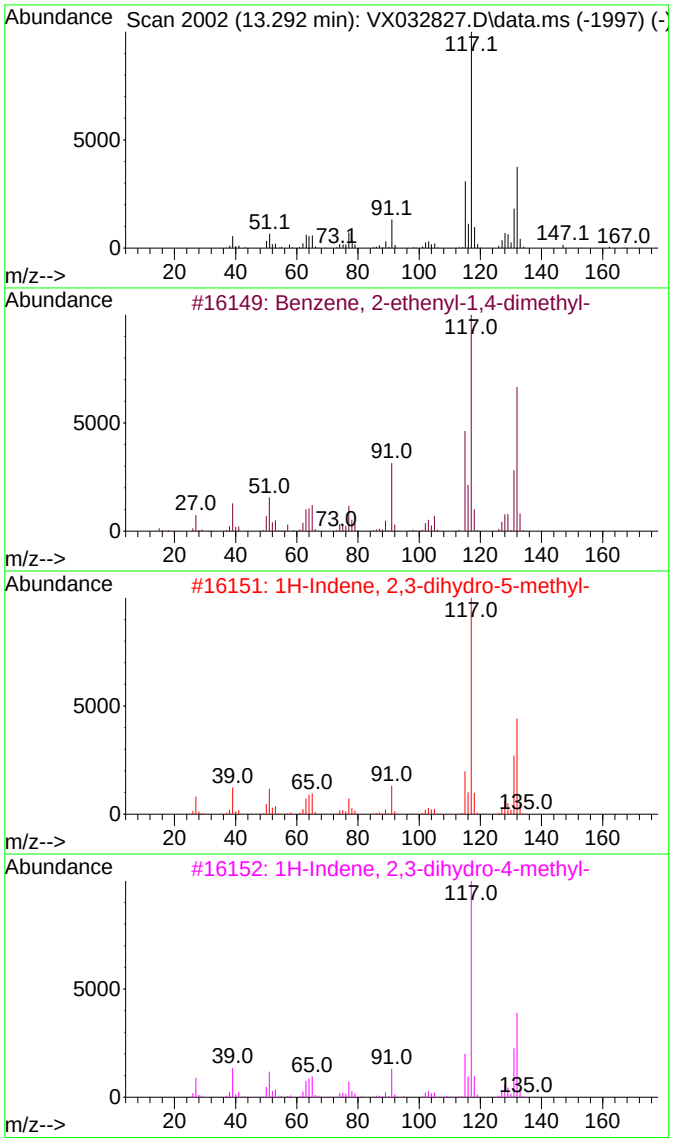
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

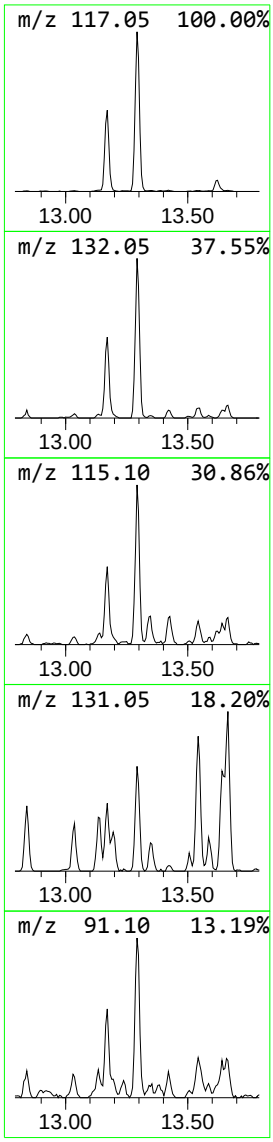
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.93 ug/l	174190	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	92
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032827.D
Acq On : 15 Nov 2022 16:58
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
Amylene hydrate	6.251	27.5	ug/l	234961	2	6.763	427267	50.0
Pentane, 2,3,4-...	7.982	6.0	ug/l	51328	2	6.763	427267	50.0
Pentane, 2,3,3-...	8.110	9.2	ug/l	78566	2	6.763	427267	50.0
1,4-Pentadiene,...	9.159	7.0	ug/l	69790	3	10.055	498313	50.0
Benzene, 1,3-di...	12.250	10.6	ug/l	102613	4	12.024	485774	50.0
Indan, 1-methyl-	12.701	46.0	ug/l	447367	4	12.024	485774	50.0
Benzene, 1-ethe...	13.170	9.8	ug/l	95685	4	12.024	485774	50.0
Benzene, 2-ethe...	13.292	17.9	ug/l	174190	4	12.024	485774	50.0