LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023017.D
Acq On : 29 Jun 2021 20:38
Operator : JC/MD
Sample : M2875-11
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\82X062321W.M
Title : SW846 8260

Signal : TIC: VX023017.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	323	333	345	rBV3	64257	170701	6.04%	1.158%
2	4.312	520	529	541	rVB	48823	137648	4.87%	0.934%
3	5.196	667	674	685	rVB5	9531	31620	1.12%	0.214%
4	5.397	695	707	713	rBV	42837	126629	4.48%	0.859%
5	5.483	713	721	728	rVV5	33505	113534	4.02%	0.770%
6	5.562	728	734	741	rVB2	46403	120784	4.27%	0.819%
7	5.836	768	779	791	rBV2	39791	119484	4.23%	0.810%
8	5.964	791	800	806	rBV	55949	148978	5.27%	1.010%
9	6.050	806	814	825	rVB	302719	783488	27.71%	5.314%
10	6.178	825	835	836	rBV2	27862	68618	2.43%	0.465%
11	6.263	844	849	855	rVB2	35748	82195	2.91%	0.557%
12	6.342	855	862	878	rVB5	69698	253105	8.95%	1.717%
13	6.610	894	906	916	rBV5	12742	32951	1.17%	0.223%
14	6.769	922	932	939	rBV	125642	320589	11.34%	2.174%
15	6.848	941	945	958	rVB3	50557	141849	5.02%	0.962%
16	7.068	974	981	991	rVV3	16741	38948	1.38%	0.264%
17	7.177	991	999	1007	rVB2	27379	59271	2.10%	0.402%
18	7.385	1020	1033	1044	rBV3	148381	404458	14.30%	2.743%
19	7.665	1072	1079	1090	rVB	35993	72546	2.57%	0.492%
20	7.860	1104	1111	1112	rBV	28704	45239	1.60%	0.307%
21	7.885	1113	1115	1123	rVB3	31276	53299	1.88%	0.361%
22	7.988	1123	1132	1144	rVB3	33045	91129	3.22%	0.618%
23	8.110	1144	1152	1156	rBV2	52126	115950	4.10%	0.786%
24	8.147	1156	1158	1162	rVB	35976	44631	1.58%	0.303%
25	8.317	1181	1186	1192	rVB5	15772	33459	1.18%	0.227%
26	8.506	1212	1217	1227	rVB3	86460	181590	6.42%	1.232%
27	8.610	1227	1234	1236	rBV2	39988	74549	2.64%	0.506%
28	8.653	1236	1241	1248	rVB	268358	424912	15.03%	2.882%
29	8.726	1248	1253	1258	rBV2	15396	30562	1.08%	0.207%
30	8.823	1265	1269	1272	rBV3	16623	28741	1.02%	0.195%
31	8.927	1280	1286	1290	rBV2	21845	40268	1.42%	0.273%
32	8.976	1290	1294	1301	rVB3	31584	55193	1.95%	0.374%
33	9.104	1308	1315	1320	rVV	36100	61621	2.18%	0.418%
34	9.165	1320	1325	1336	rVB	81347	136202	4.82%	0.924%
35	9.433	1365	1369	1371	rBV	22468	30501	1.08%	0.207%
36	9.506	1377	1381	1387	rVB4	31549	64281	2.27%	0.436%

LSC Area Percent Report

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Title : SW846 8260

37	9.567	1387	1391	1395	rBV	27789	38431	1.36%	0.261%
38	9.762	1417	1423	1429	rBV4	24603	42733	1.51%	0.290%
39	10.055	1467	1471	1476	rBV	242724	317508	11.23%	2.153%
40	10.128	1481	1483	1491	rVB2	24389	52545	1.86%	0.356%
41	10.305	1505	1512	1518	rVB	182338	261542	9.25%	1.774%
42	10.646	1563	1568	1572	rVB	24944	32328	1.14%	0.219%
43	10.963	1615	1620	1629	rVB	211729	263916	9.33%	1.790%
44	11.085	1635	1640	1644	rBV	187005	236739	8.37%	1.606%
45	11.305	1672	1676	1683	rVB	222652	279688	9.89%	1.897%
46	11.402	1683	1692	1696	rVV	58427	80698	2.85%	0.547%
47	11.616	1721	1727	1735	rVB	301464	368055	13.02%	2.496%
48	11.866	1763	1768	1770	rBV	39429	49818	1.76%	0.338%
49	11.890	1770	1772	1778	rVB	50357	62031	2.19%	0.421%
50	12.024	1789	1794	1799	rBV	239155	303162	10.72%	2.056%
51	12.091	1801	1805	1813	rVB	55726	71150	2.52%	0.483%
52	12.244	1825	1830	1837	rBV2	2209722	2827626	100.00%	19.178%
53	12.317	1837	1842	1849	rVV2	136393	203667	7.20%	1.381%
54	12.408	1853	1857	1862	rVB2	57431	77591	2.74%	0.526%
55	12.469	1862	1867	1874	rBV2	99827	140064	4.95%	0.950%
56	12.615	1885	1891	1894	rBV	540837	638959	22.60%	4.334%
57	12.646	1894	1896	1900	rVV	169897	187365	6.63%	1.271%
58	12.701	1900	1905	1913	rVB	685420	910612	32.20%	6.176%
59	12.841	1923	1928	1933	rVB3	24119	33410	1.18%	0.227%
60	12.926	1937	1942	1946	rVV	319357	402210	14.22%	2.728%
61	12.969	1946	1949	1954	rVV4	21869	32620	1.15%	0.221%
62	13.030	1954	1959	1967	rVB2	37009	58481	2.07%	0.397%
63	13.140	1967	1977	1978	rBV3	27031	46484	1.64%	0.315%
64	13.170	1978	1982	1991	rVV	326440	394820	13.96%	2.678%
65	13.262	1991	1997	1998	rVV4	22244	28714	1.02%	0.195%
66	13.292	1998	2002	2008	rVV2	525396	707846	25.03%	4.801%
67	13.347	2008	2011	2013	rVV3	35304	45748	1.62%	0.310%
68	13.371	2013	2015	2020	rVV	22423	29414	1.04%	0.199%
69	13.426	2020	2024	2031	rVB	55810	72731	2.57%	0.493%
70	13.506	2031	2037	2040	rBV2	20183	29339	1.04%	0.199%
71	13.548	2040	2044	2047	rVV	80760	115123	4.07%	0.781%
72	13.585	2047	2050	2054	rVV2	56096	79895	2.83%	0.542%
73	13.646	2054	2060	2061	rVV2	48767	75883	2.68%	0.515%
74	13.664	2061	2063	2070	rVB2	66378	97360	3.44%	0.660%
75	13.780	2075	2082	2090	rBV	87203	122400	4.33%	0.830%
76	13.926	2100	2106	2110	rBV2	26387	35638	1.26%	0.242%

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77	14.079	2126	2131	2137	rBV	32577	39894	1.41%	0.271%
78	14.219	2149	2154	2166	rBV4	23787	50157	1.77%	0.340%
79	14.780	2240	2246	2251	rBV	46877	60176	2.13%	0.408%

Sum of corrected areas: 14744094

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Instrument :
MSVOA_X
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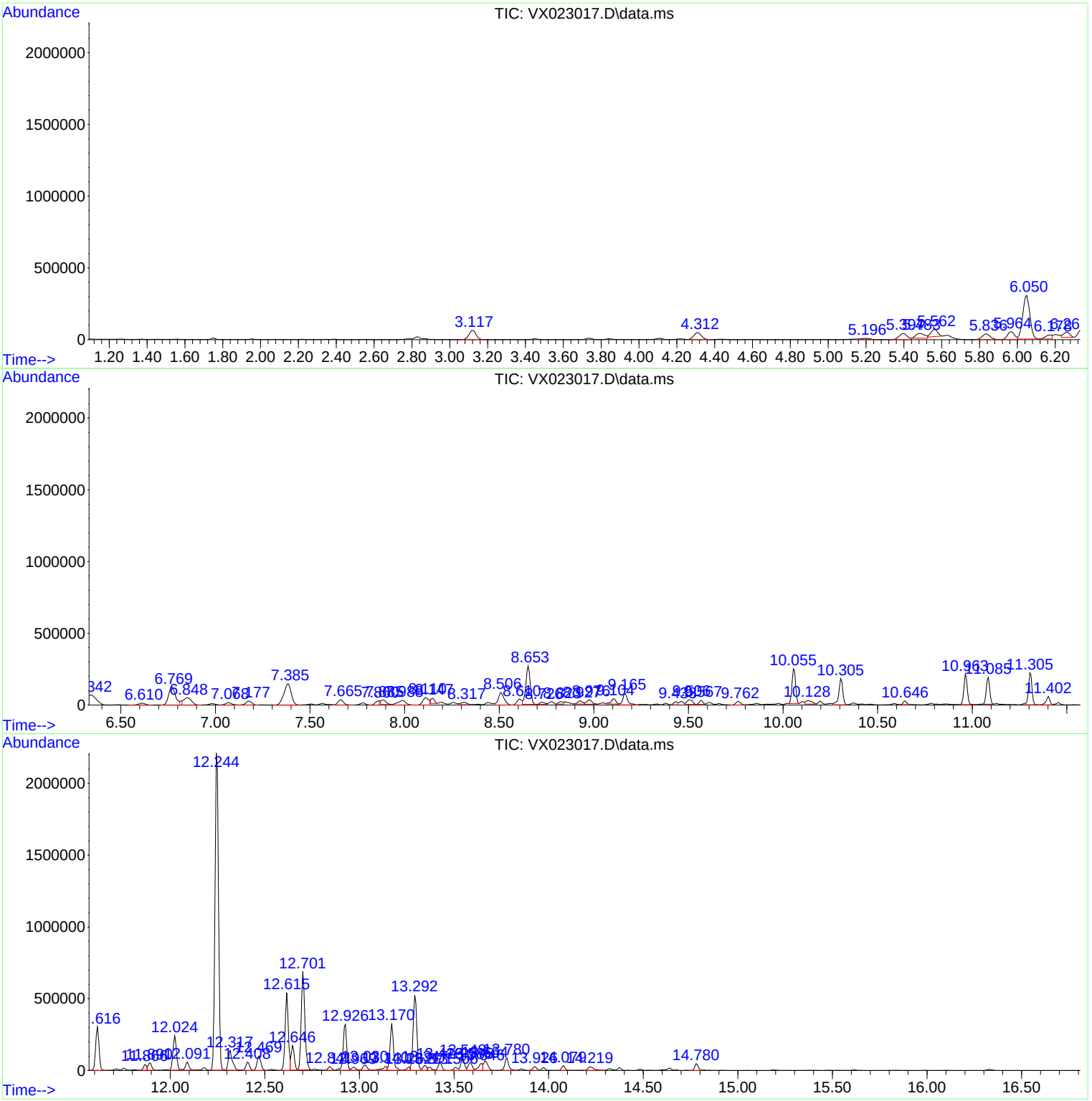
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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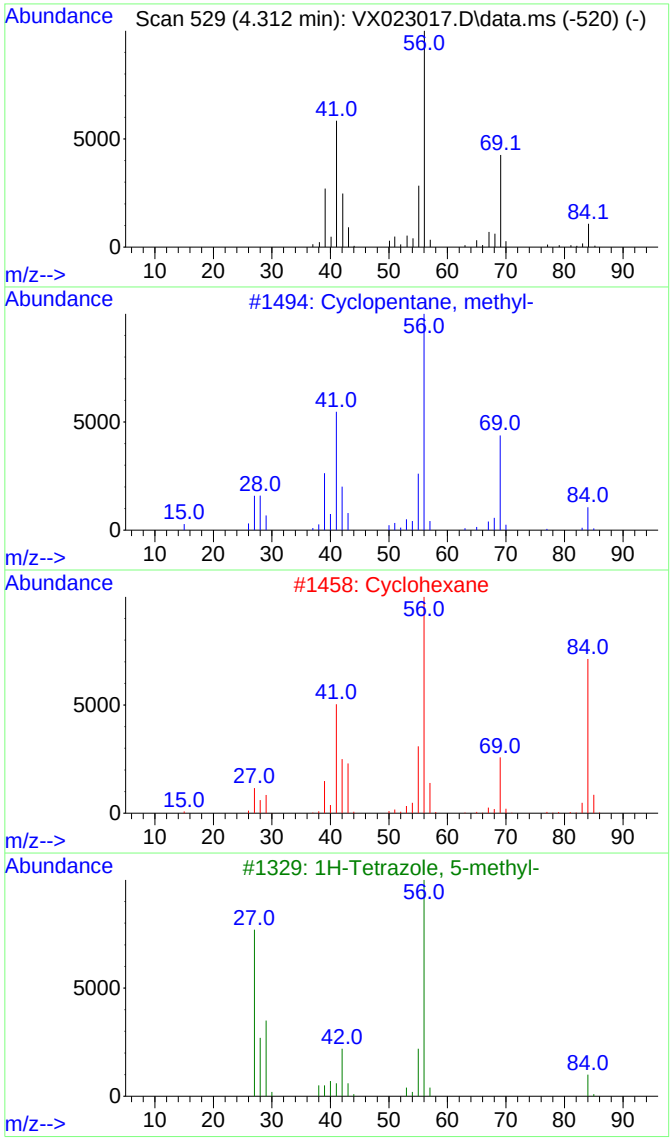
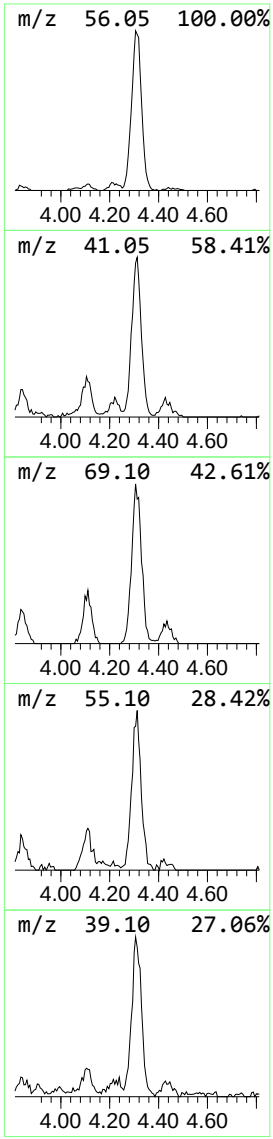
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	56.98 ug/l	137648	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	56
5	Cyclobutane	56	C4H8	000287-23-0	50





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

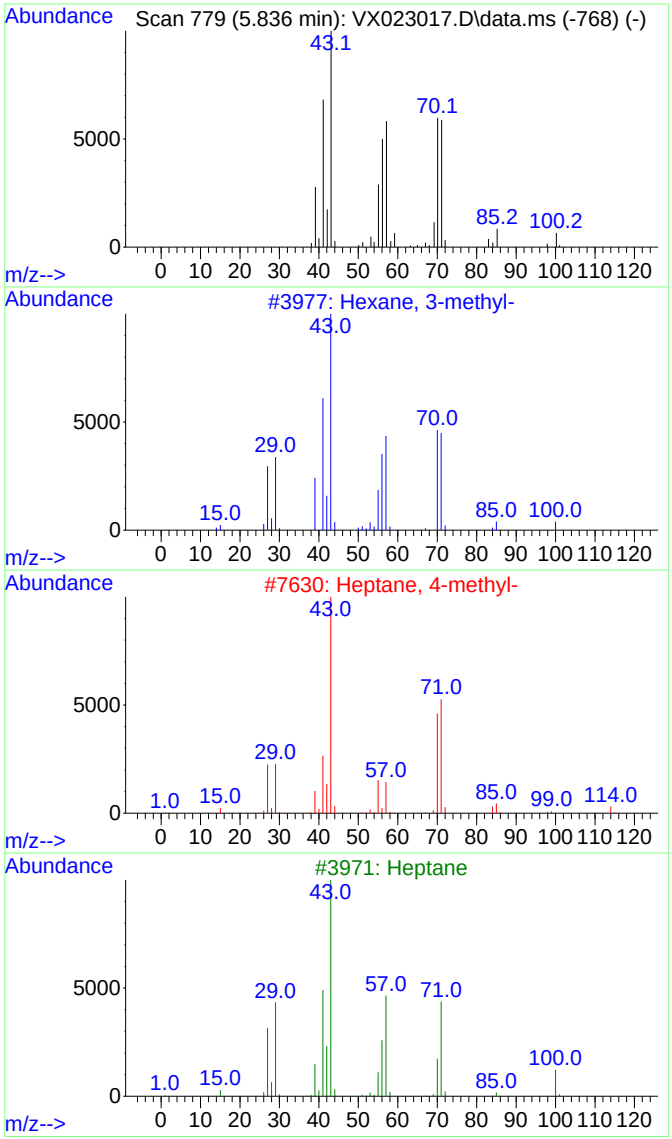
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

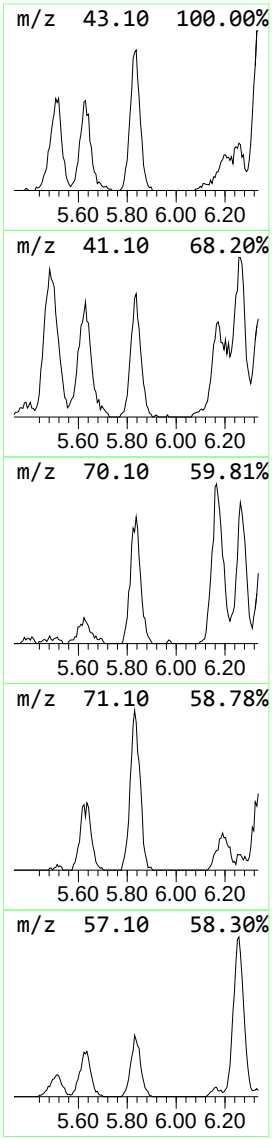
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	49.46 ug/l	119484	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	93
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
3	Heptane	100	C7H16	000142-82-5	52
4	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	50
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	50





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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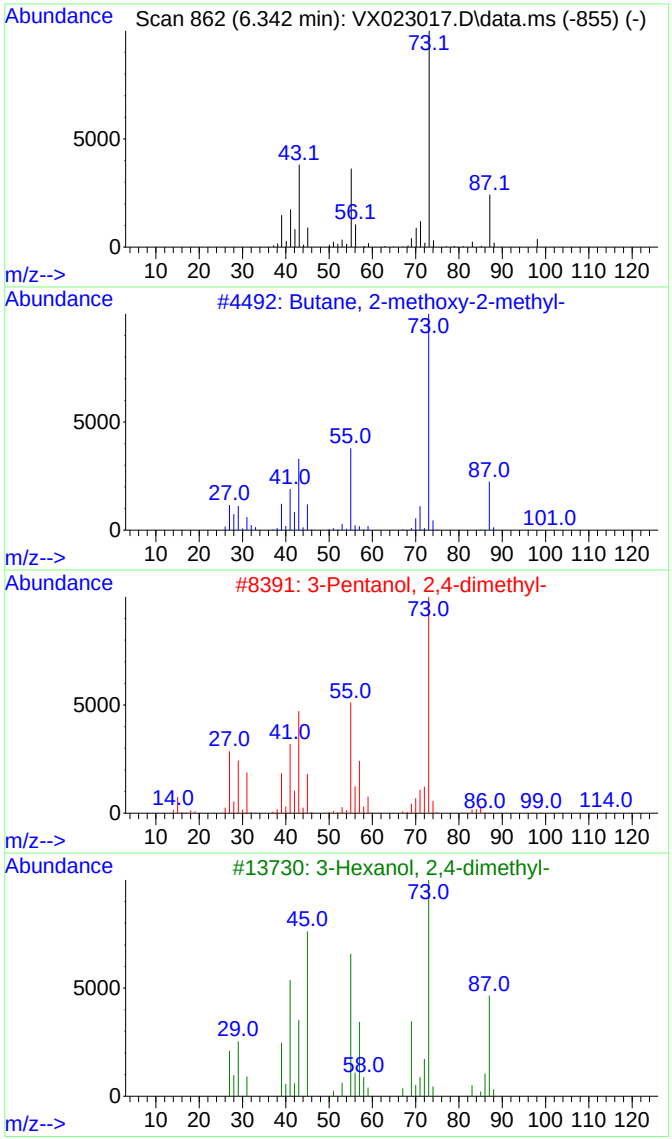
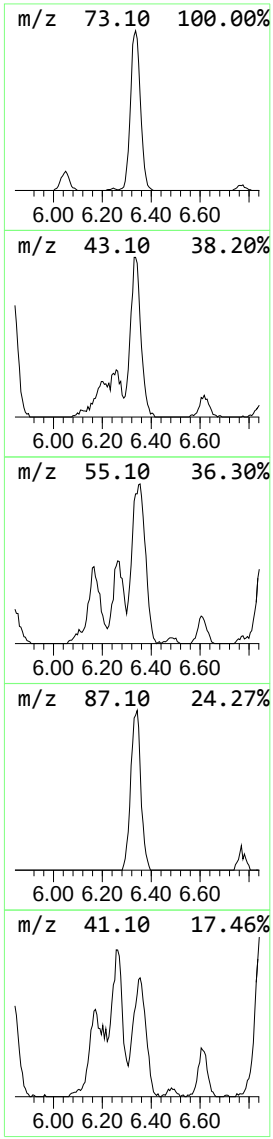
****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.342	39.48 ug/l	253105	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	47
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	28
4	Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	12
5	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9





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MSVOA_X
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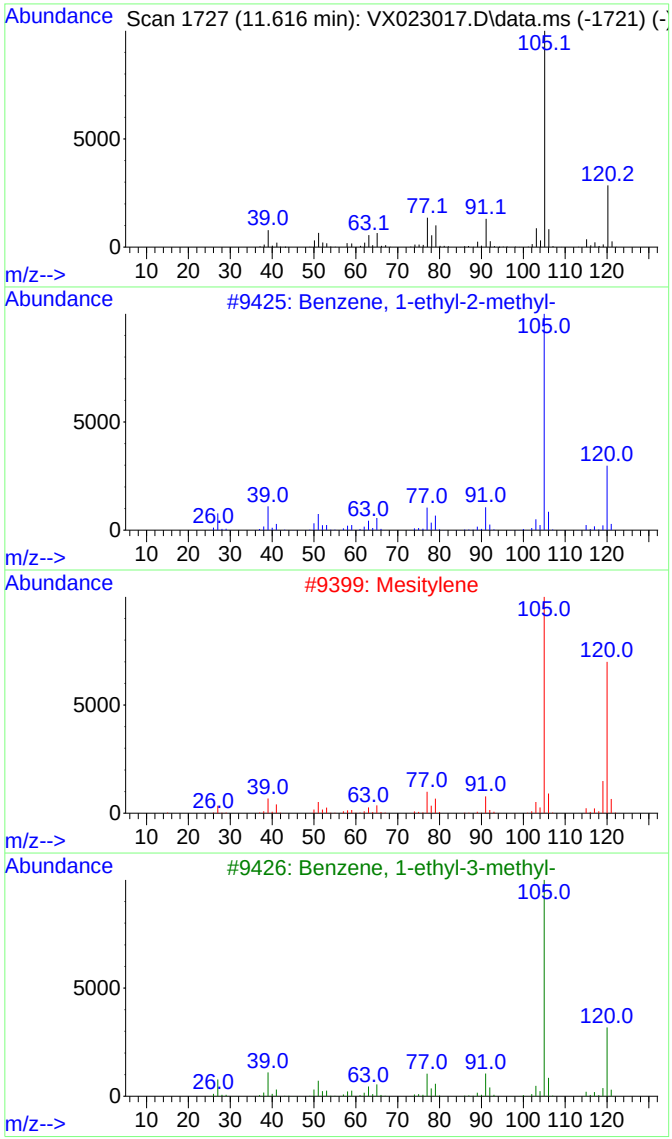
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

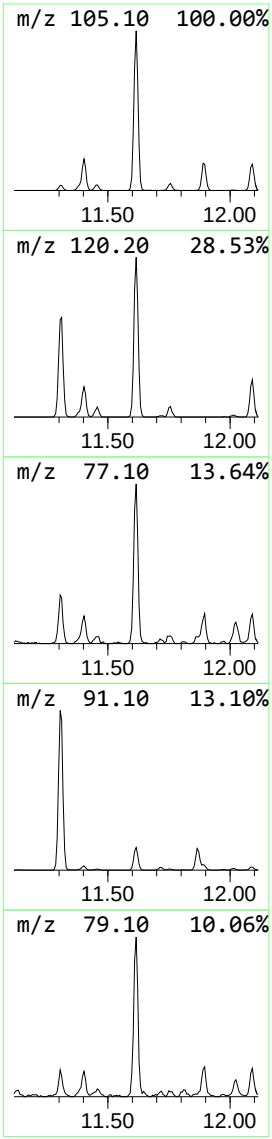
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	60.70 ug/l	368055	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	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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MSVOA_X
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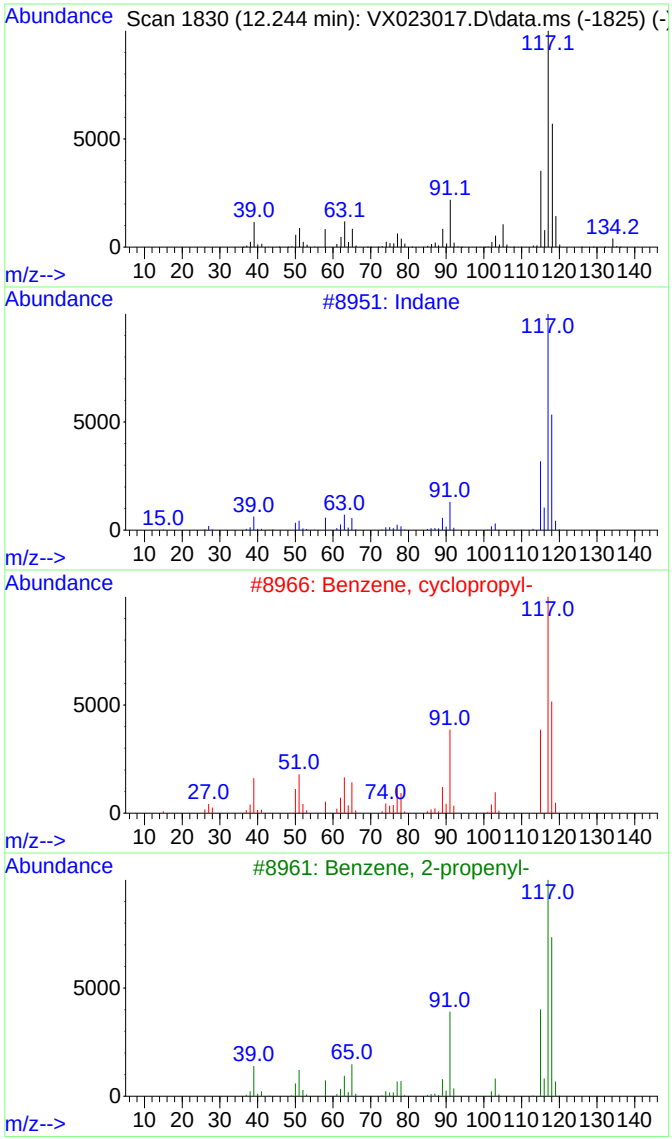
Quant Title : SW846 8260

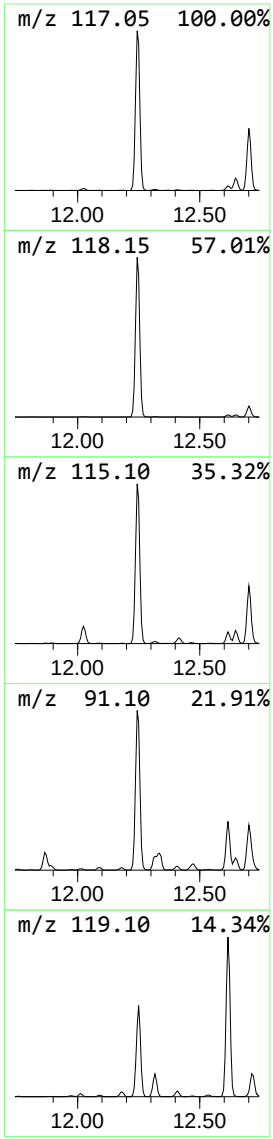
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	466.36 ug/l	2827630	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	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	55





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

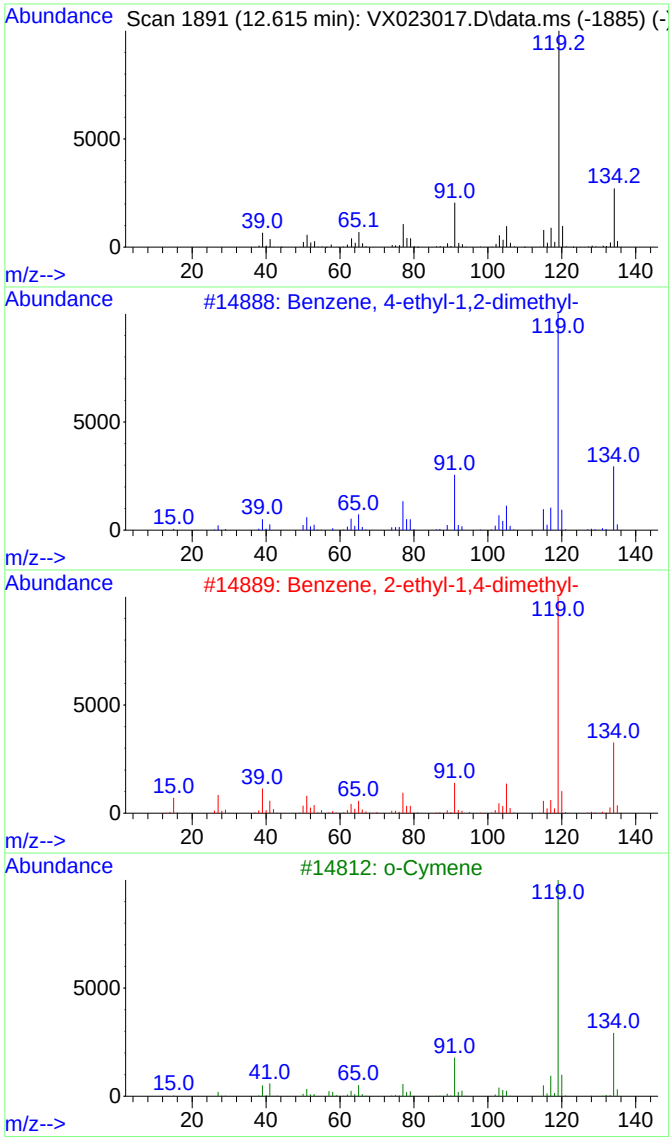
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

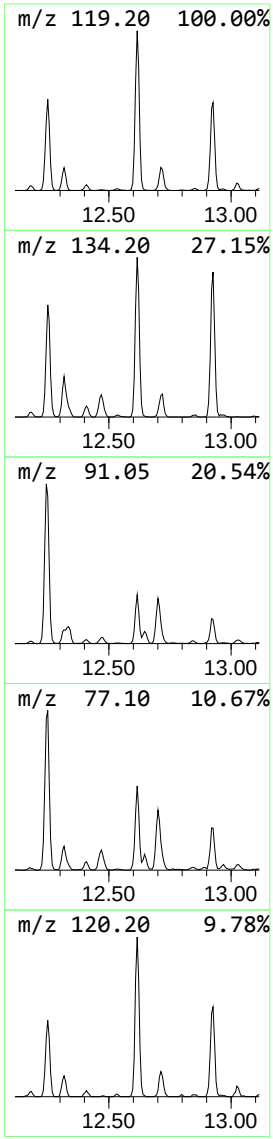
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.615	105.38 ug/l	638959	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	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	p-Cymene	134	C10H14	000099-87-6	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023017.D
Acq On : 29 Jun 2021 20:38
Operator : JC/MD
Sample : M2875-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

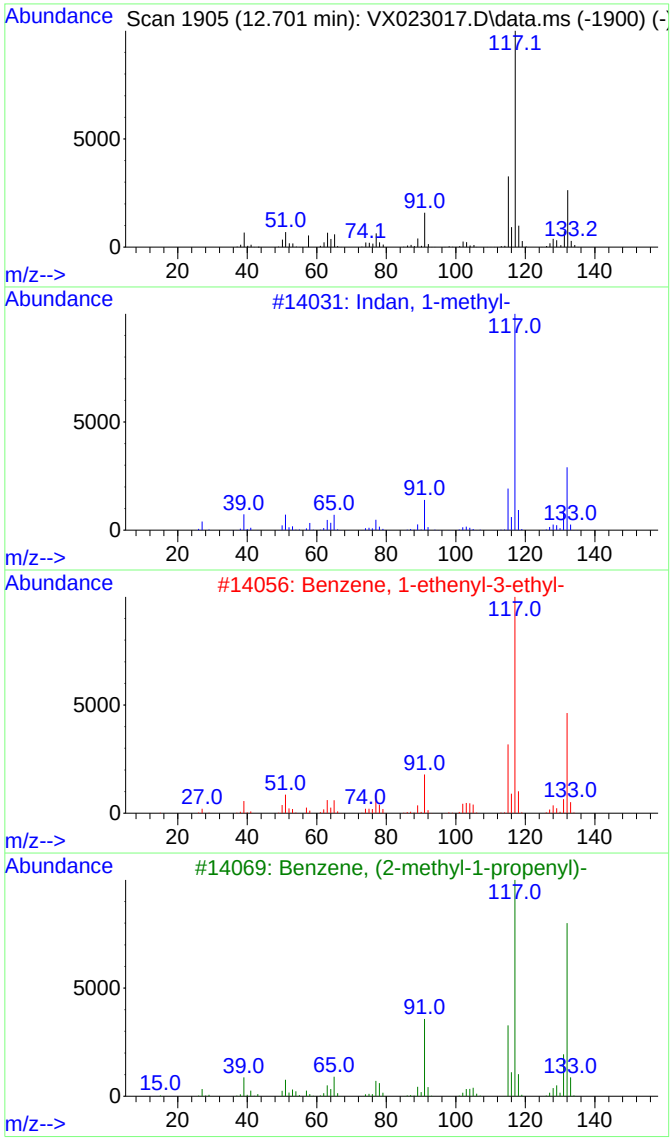
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

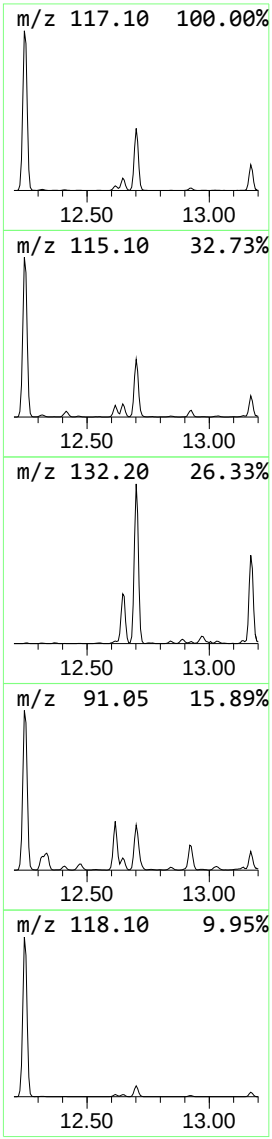
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indan, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	150.19 ug/l	910612	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	91
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
5	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023017.D
Acq On : 29 Jun 2021 20:38
Operator : JC/MD
Sample : M2875-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

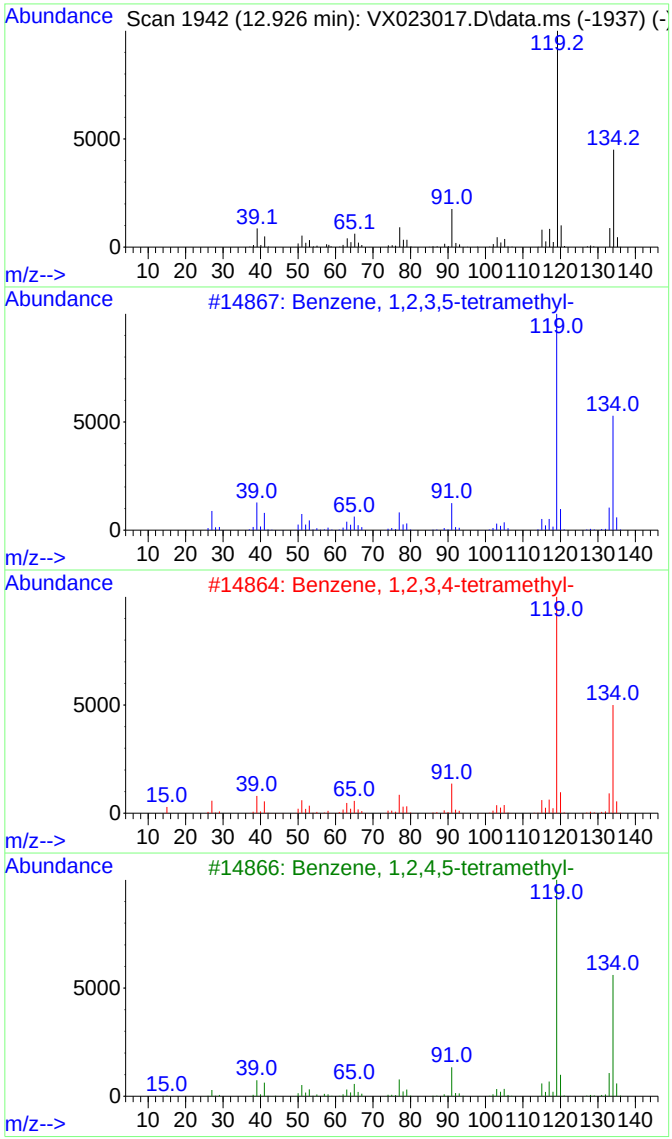
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

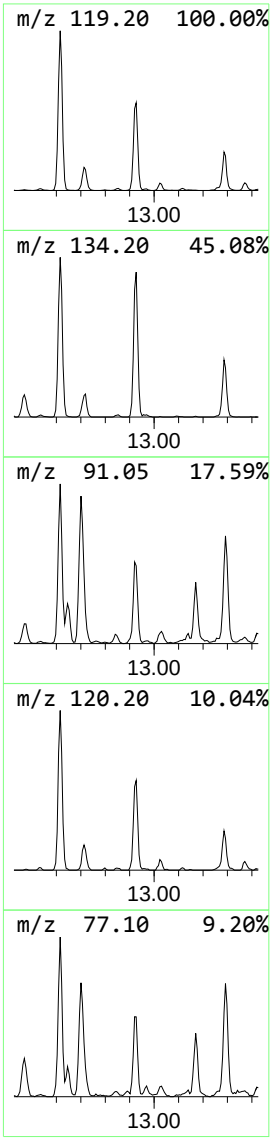
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.926	66.34 ug/l	402210	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
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\VX062921\
Data File : VX023017.D
Acq On : 29 Jun 2021 20:38
Operator : JC/MD
Sample : M2875-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

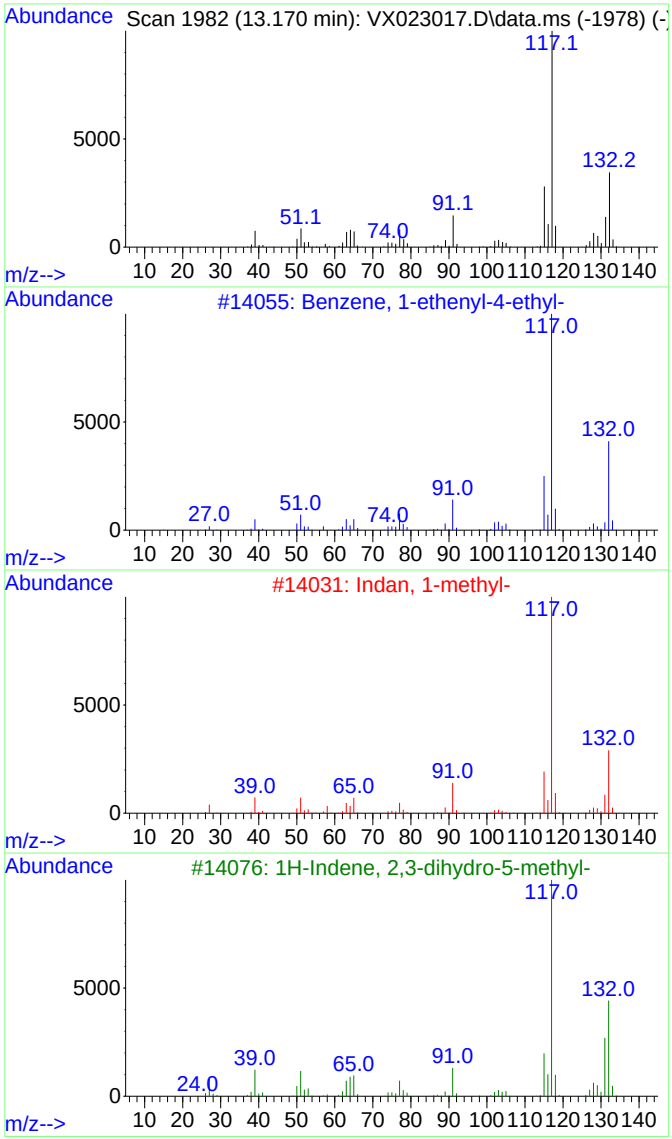
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

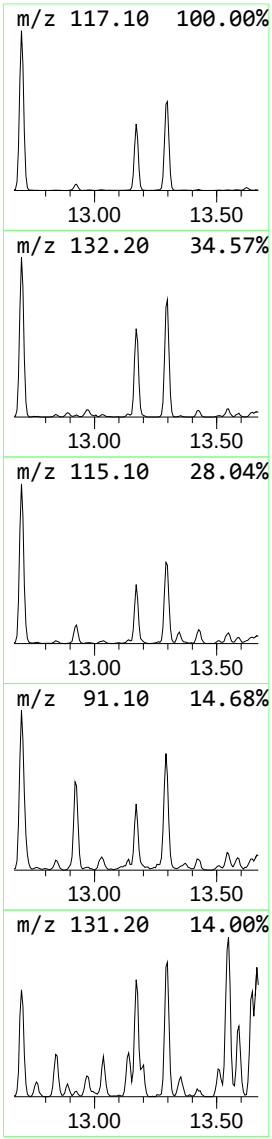
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	65.12 ug/l	394820	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	Indan, 1-methyl-	132	C10H12	000767-58-8	91
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023017.D
Acq On : 29 Jun 2021 20:38
Operator : JC/MD
Sample : M2875-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5

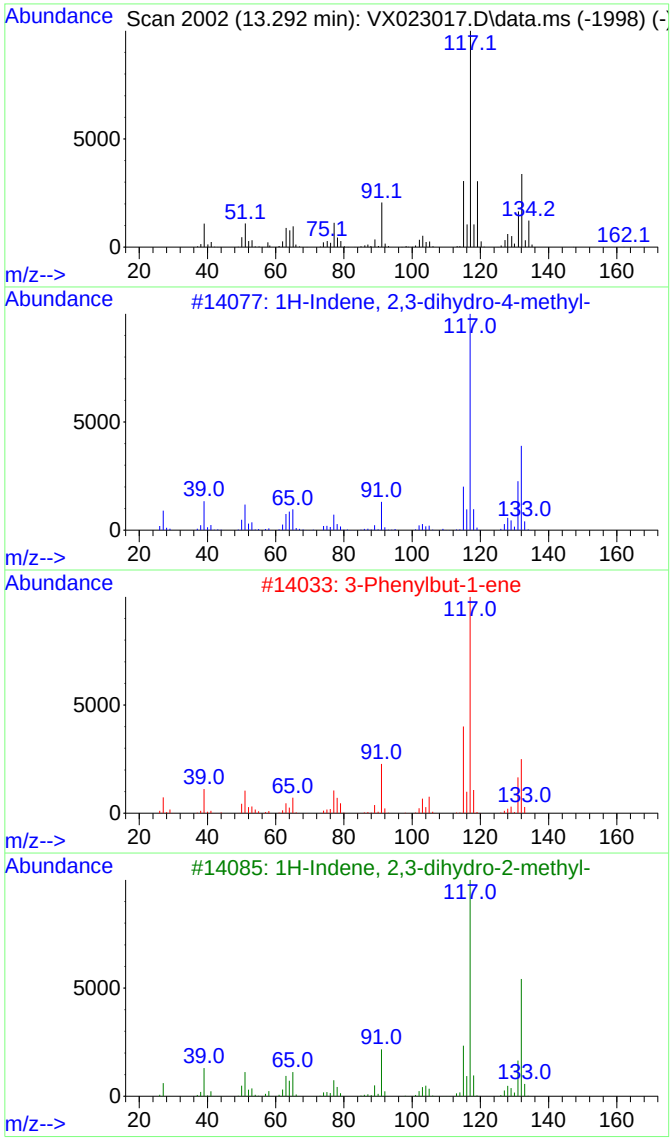
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

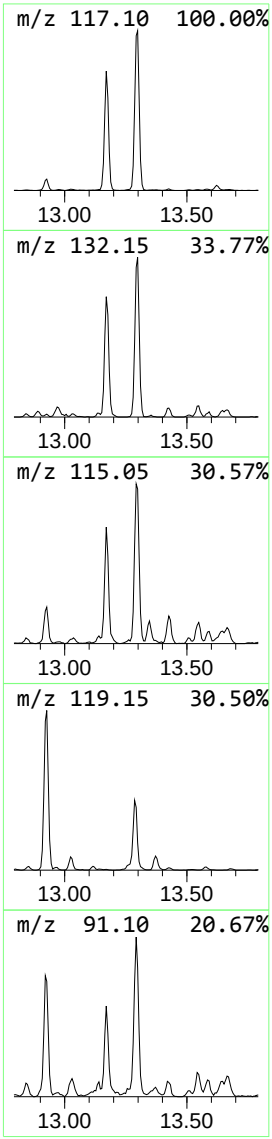
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	116.74 ug/l	707846	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
3	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	81
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5	Indan, 1-methyl-	132	C10H12	000767-58-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023017.D
Acq On : 29 Jun 2021 20:38
Operator : JC/MD
Sample : M2875-11
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\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, m...	4.312	57.0	ug/l	137648	1	5.562	120784	50.0
Hexane, 3-methyl-	5.836	49.5	ug/l	119484	1	5.562	120784	50.0
Butane, 2-metho...	6.342	39.5	ug/l	253105	2	6.769	320589	50.0
Benzene, 1-ethy...	11.616	60.7	ug/l	368055	4	12.024	303162	50.0
Indane	12.243	466.4	ug/l	2827630	4	12.024	303162	50.0
Benzene, 4-ethy...	12.615	105.4	ug/l	638959	4	12.024	303162	50.0
Indan, 1-methyl-	12.701	150.2	ug/l	910612	4	12.024	303162	50.0
Benzene, 1,2,3,...	12.926	66.3	ug/l	402210	4	12.024	303162	50.0
Benzene, 1-ethe...	13.170	65.1	ug/l	394820	4	12.024	303162	50.0
1H-Indene, 2,3-...	13.292	116.7	ug/l	707846	4	12.024	303162	50.0