LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-06

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\82X042021W.M
Title : SW846 8260

Signal : TIC: VX021774.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.349	35	43	44	rBV3	5408	14598	1.84%	0.191%
2	1.587	76	82	87	rVB7	6876	11859	1.49%	0.155%
3	2.825	278	285	289	rBV2	11447	25669	3.23%	0.336%
4	2.904	296	298	312	rVB6	3743	10733	1.35%	0.140%
5	3.154	331	339	346	rBV3	8391	20781	2.62%	0.272%
6	4.282	514	524	532	rBV2	13562	41427	5.22%	0.542%
7	4.367	532	538	550	rVB2	11089	33097	4.17%	0.433%
8	5.196	663	674	676	rBV7	3897	9131	1.15%	0.119%
9	5.464	706	718	727	rBV	95144	270076	34.01%	3.533%
10	5.629	734	745	752	rBV	152695	442575	55.74%	5.790%
11	5.696	752	756	769	rVB	43764	117677	14.82%	1.539%
12	5.903	782	790	798	rBV7	3580	10384	1.31%	0.136%
13	6.031	801	811	819	rBV	90350	241604	30.43%	3.161%
14	6.111	819	824	833	rVV2	17686	46957	5.91%	0.614%
15	6.233	836	844	845	rVV4	5161	10169	1.28%	0.133%
16	6.318	845	858	869	rVV	92008	288735	36.36%	3.777%
17	6.422	869	875	889	rVB6	5879	17399	2.19%	0.228%
18	6.830	929	942	951	rBV	238090	564595	71.11%	7.386%
19	7.421	1030	1039	1049	rVB6	12271	38666	4.87%	0.506%
20	7.549	1054	1060	1066	rVV2	8115	16532	2.08%	0.216%
21	7.610	1066	1070	1074	rVV4	8342	17525	2.21%	0.229%
22	7.659	1074	1078	1083	rVV	8477	17638	2.22%	0.231%
23	7.824	1099	1105	1111	rVB5	4651	9601	1.21%	0.126%
24	8.037	1131	1140	1148	rVB	76377	151126	19.03%	1.977%
25	8.159	1150	1160	1169	rBV	110691	229544	28.91%	3.003%
26	8.549	1219	1224	1233	rVB6	7928	16578	2.09%	0.217%
27	8.696	1236	1248	1257	rBV	485597	794006	100.00%	10.387%
28	9.147	1314	1322	1326	rVB2	6167	10674	1.34%	0.140%
29	9.202	1326	1331	1335	rBV	11178	17403	2.19%	0.228%
30	9.549	1383	1388	1394	rVB7	4024	8007	1.01%	0.105%
31	10.092	1467	1477	1487	rBV	436525	610207	76.85%	7.983%
32	10.232	1496	1500	1505	rBV	9953	13060	1.64%	0.171%
33	10.342	1510	1518	1523	rVB	9581	17241	2.17%	0.226%
34	11.000	1620	1626	1632	rBV	160645	203031	25.57%	2.656%
35	11.122	1640	1646	1651	rBV	336491	446460	56.23%	5.841%
36	11.341	1677	1682	1691	rVB	315346	377763	47.58%	4.942%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
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Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-06

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\82X042021W.M
Title : SW846 8260

37	11.652	1728	1733	1737	rVB	13645	17378	2.19%	0.227%
38	11.786	1752	1755	1760	rVB	7314	9317	1.17%	0.122%
39	11.902	1770	1774	1776	rBV	36227	43825	5.52%	0.573%
40	11.927	1776	1778	1782	rVB	32263	34645	4.36%	0.453%
41	12.061	1794	1800	1808	rBV	406904	502054	63.23%	6.568%
42	12.213	1821	1825	1831	rBV2	6109	8187	1.03%	0.107%
43	12.280	1831	1836	1843	rVV	392590	485119	61.10%	6.346%
44	12.353	1843	1848	1856	rVB2	58017	87292	10.99%	1.142%
45	12.439	1858	1862	1867	rBV	33816	44437	5.60%	0.581%
46	12.512	1867	1874	1879	rVB2	13859	21894	2.76%	0.286%
47	12.652	1890	1897	1900	rBV	215159	260996	32.87%	3.414%
48	12.683	1900	1902	1906	rVV	17512	19207	2.42%	0.251%
49	12.737	1906	1911	1919	rVV2	117791	173231	21.82%	2.266%
50	12.878	1928	1934	1938	rVB2	5989	9440	1.19%	0.123%
51	12.957	1938	1947	1953	rBV	138749	179915	22.66%	2.354%
52	13.061	1959	1964	1970	rVB2	11858	18266	2.30%	0.239%
53	13.152	1972	1979	1981	rBV2	11901	17553	2.21%	0.230%
54	13.207	1985	1988	1995	rVV	33888	45261	5.70%	0.592%
55	13.298	1995	2003	2004	rVV3	8236	15877	2.00%	0.208%
56	13.329	2004	2008	2014	rVV3	39185	59298	7.47%	0.776%
57	13.408	2018	2021	2026	rVV	8897	14183	1.79%	0.186%
58	13.463	2026	2030	2034	rVB2	9563	12754	1.61%	0.167%
59	13.585	2046	2050	2052	rVV	14545	20576	2.59%	0.269%
60	13.615	2052	2055	2059	rVV	22773	29659	3.74%	0.388%
61	13.676	2059	2065	2068	rVV2	11252	22522	2.84%	0.295%
62	13.713	2068	2071	2075	rVB2	14249	19078	2.40%	0.250%
63	13.817	2080	2088	2097	rBV	113216	145587	18.34%	1.905%
64	13.963	2105	2112	2117	rBV6	5575	8531	1.07%	0.112%
65	14.115	2131	2137	2141	rBV	10158	14344	1.81%	0.188%
66	14.262	2155	2161	2170	rBV3	8446	17049	2.15%	0.223%
67	14.359	2170	2177	2182	rVV	21379	28400	3.58%	0.372%
68	14.414	2182	2186	2190	rVB2	6882	9527	1.20%	0.125%
69	14.640	2215	2223	2226	rBV3	4842	8501	1.07%	0.111%
70	14.822	2246	2253	2262	rBV	30455	41895	5.28%	0.548%
71	16.389	2502	2510	2515	rBV	13647	25874	3.26%	0.338%

Sum of corrected areas: 7644200

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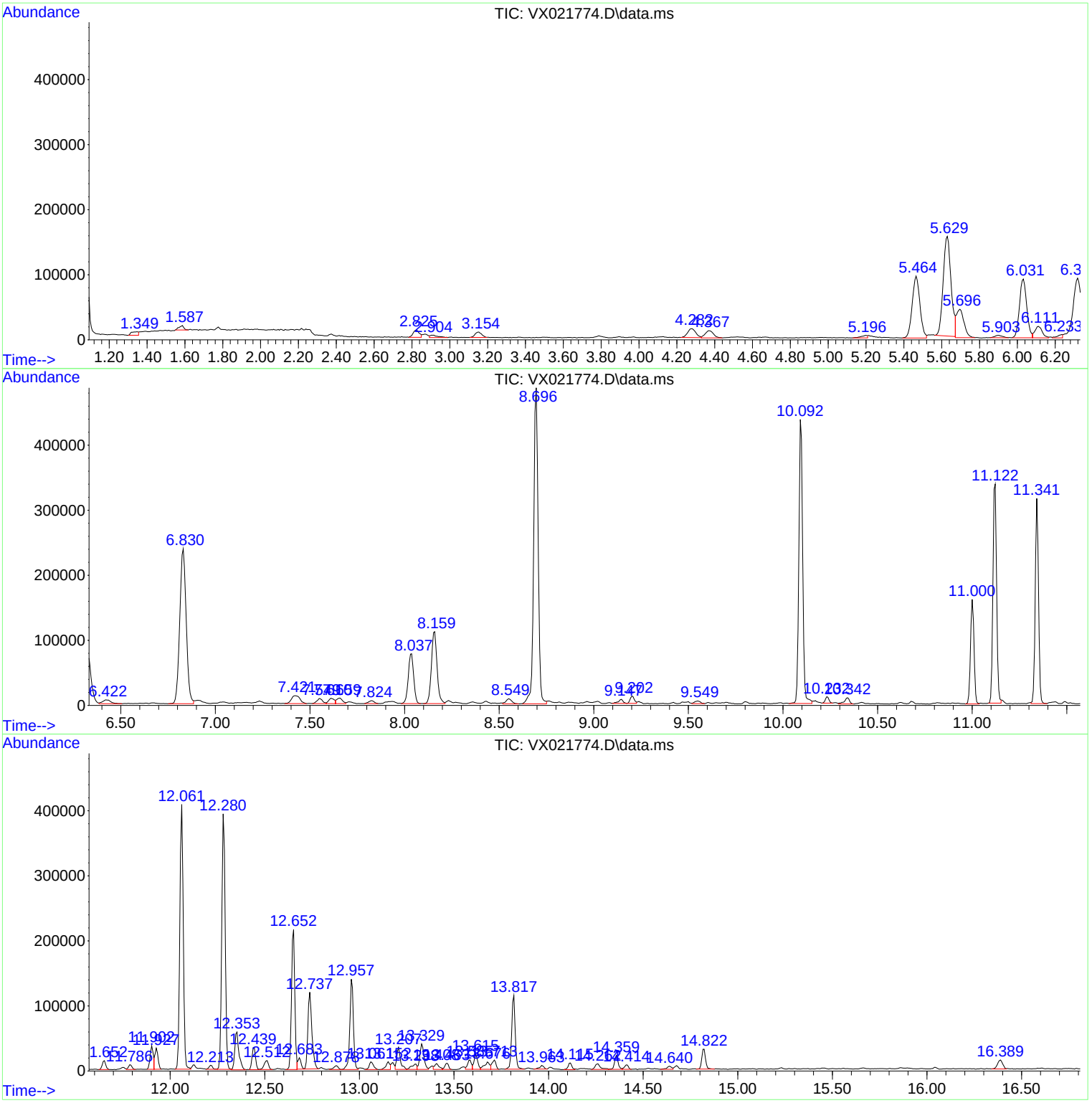
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
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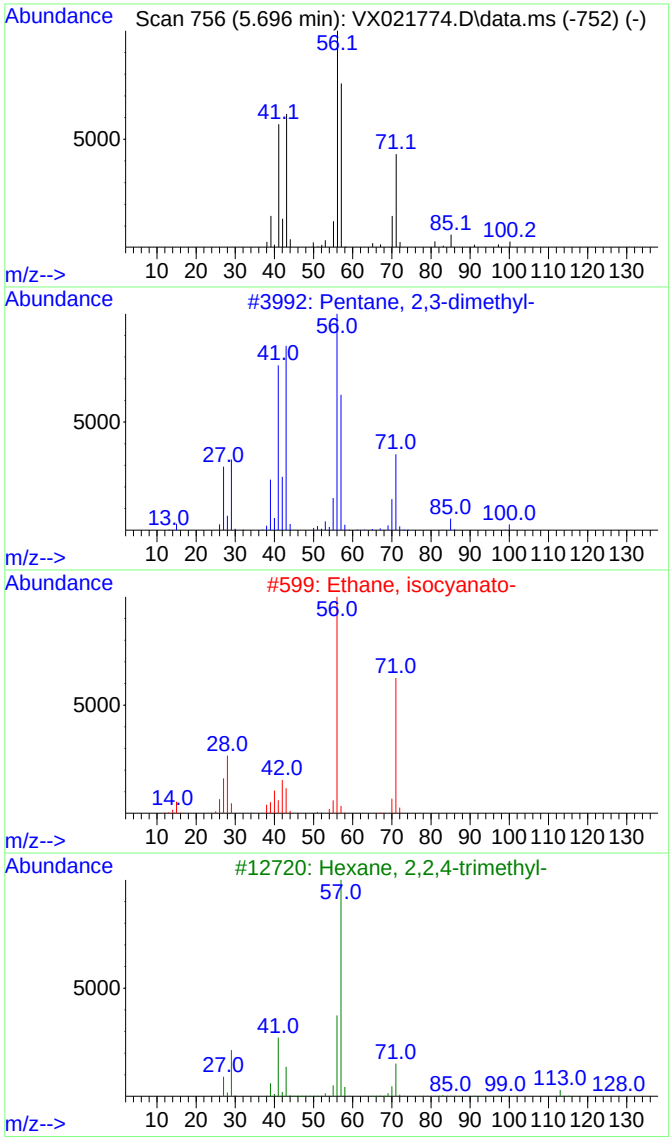
Quant Title : SW846 8260

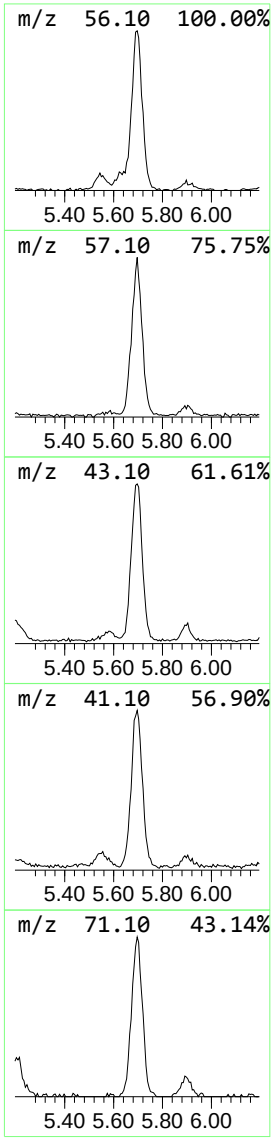
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.696	13.29 ug/l	117677	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Ethane, isocyanato-	71	C3H5NO	000109-90-0	59
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50
4	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	45
5	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

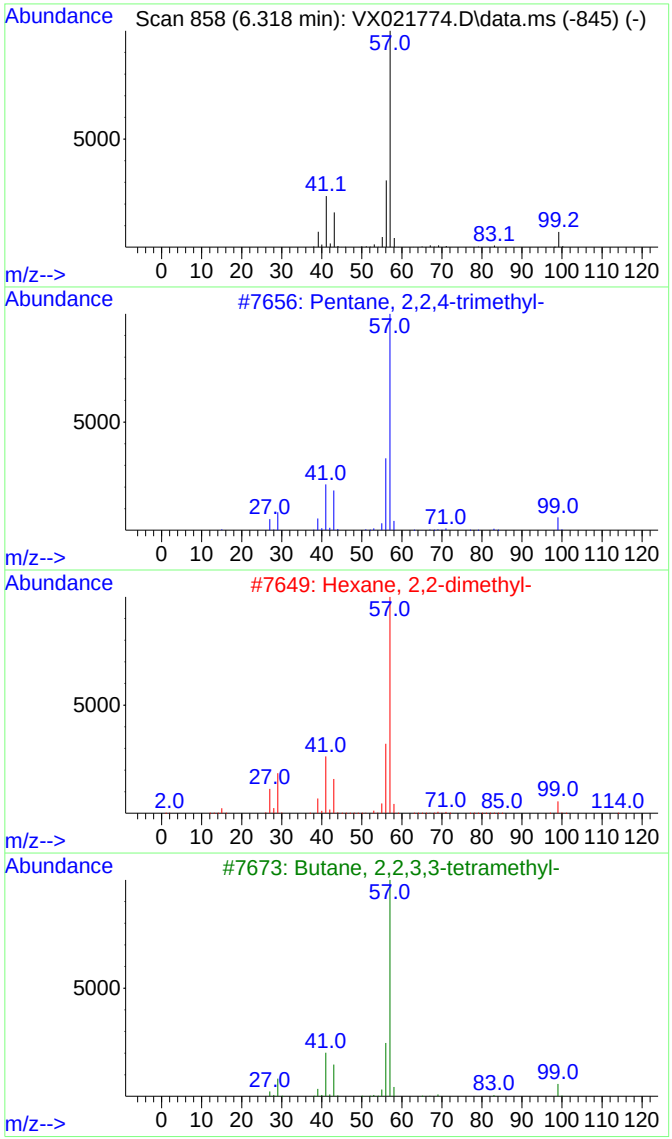
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

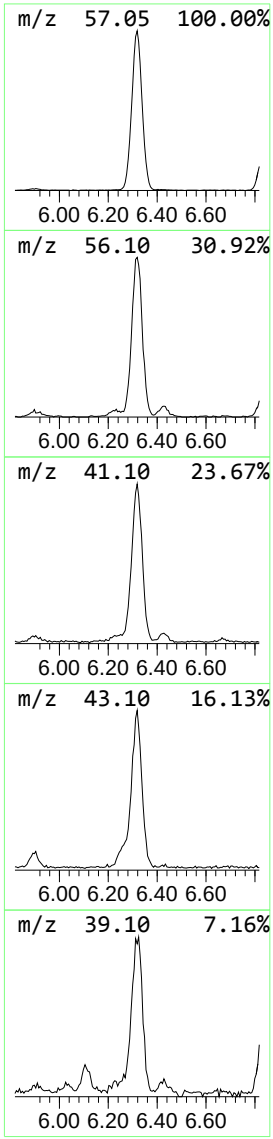
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.318	25.57 ug/l	288735	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
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Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

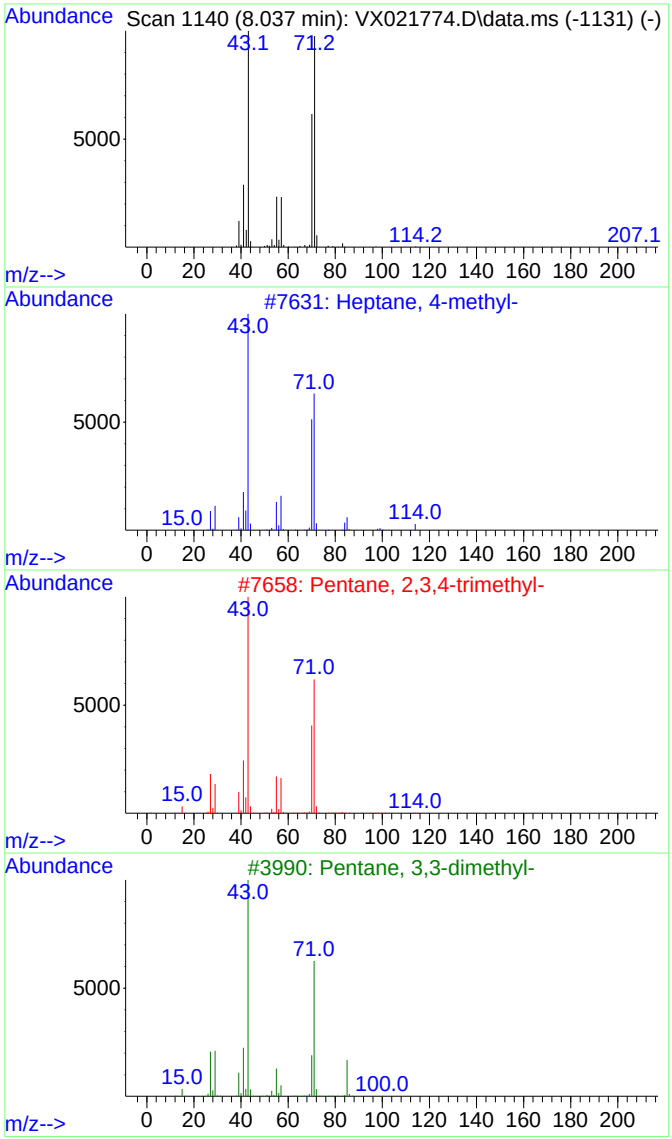
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

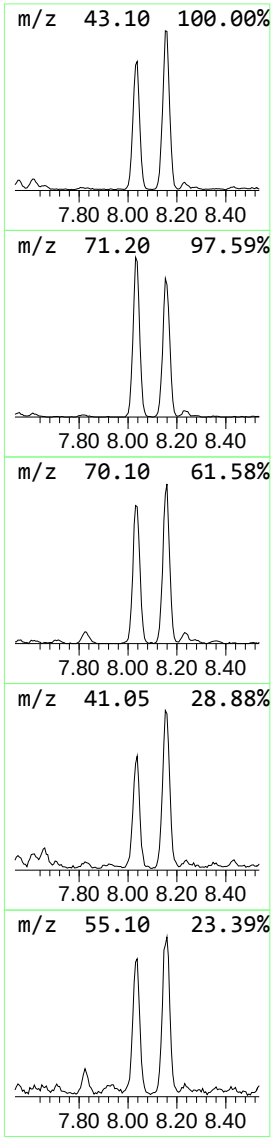
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.037	13.38 ug/l	151126	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	80
3	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72
4	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	64
5	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

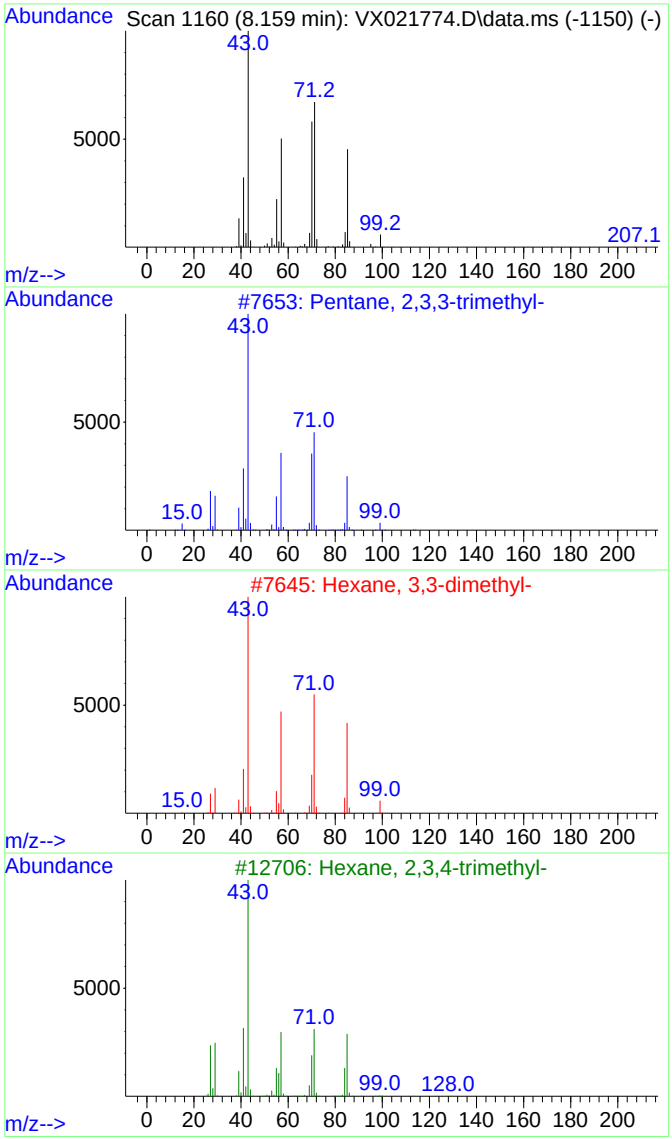
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

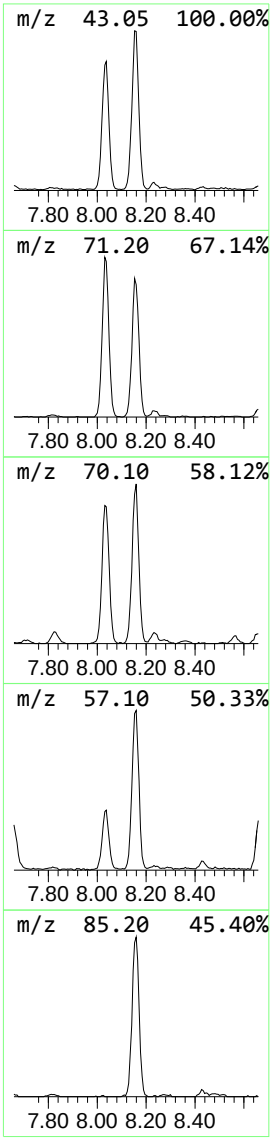
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.159	20.33 ug/l	229544	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

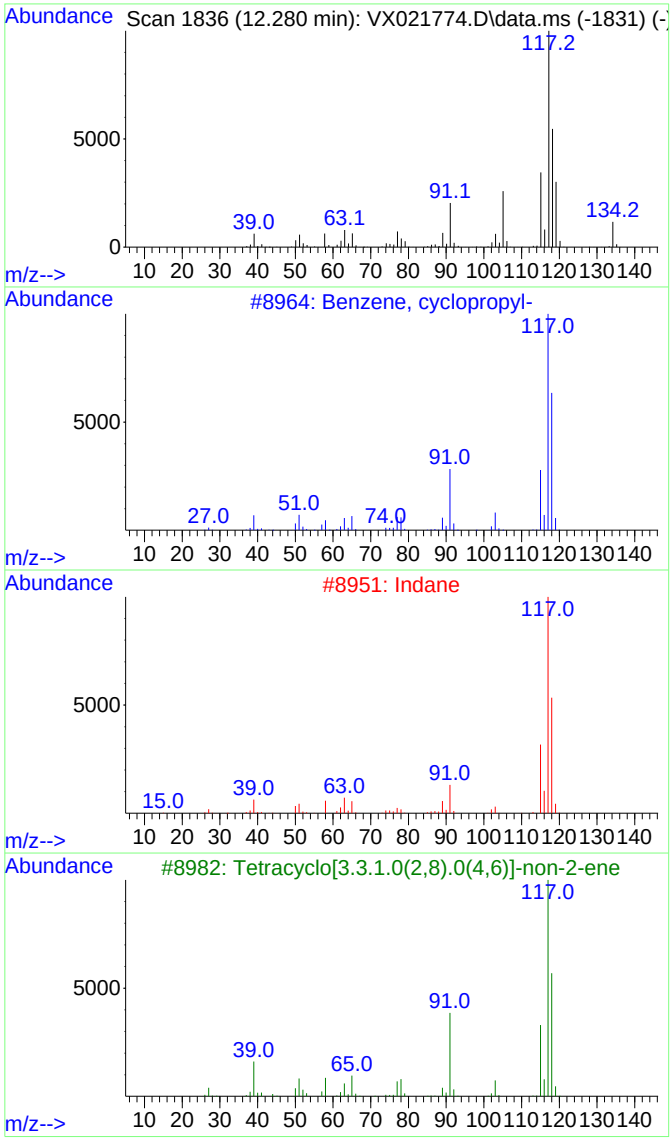
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

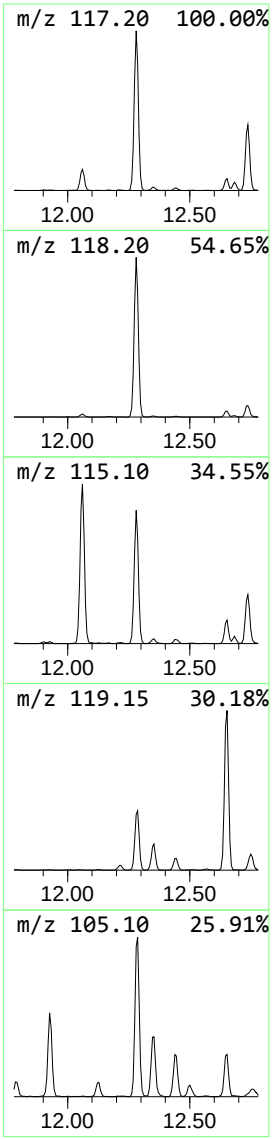
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.280	48.31 ug/l	485119	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
2	Indane	118	C9H10	000496-11-7	64
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	58





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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

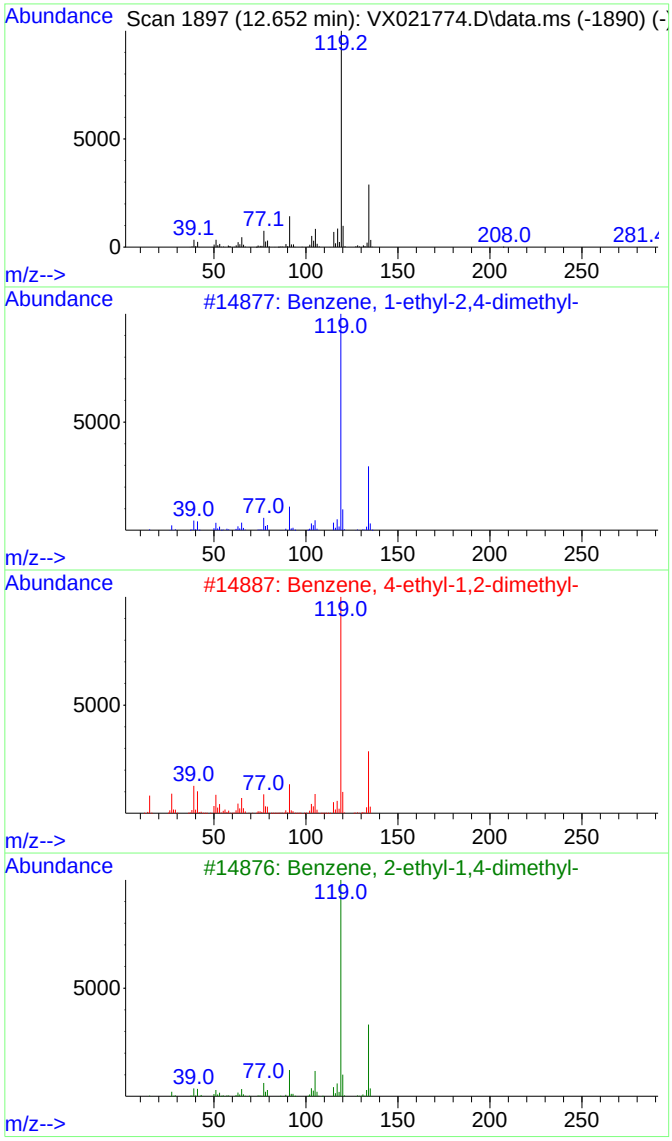
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

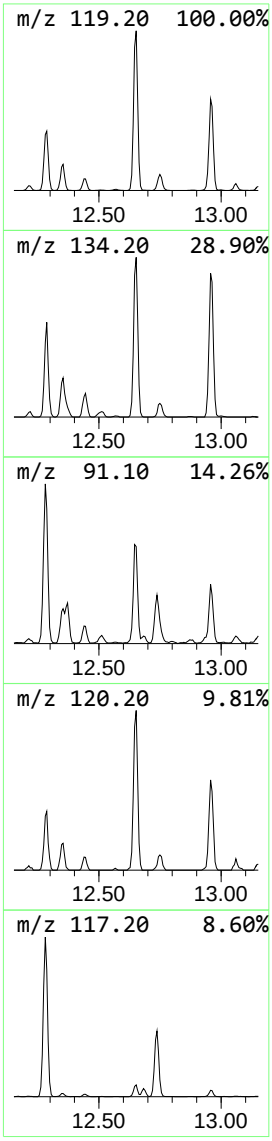
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.652	25.99 ug/l	260996	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

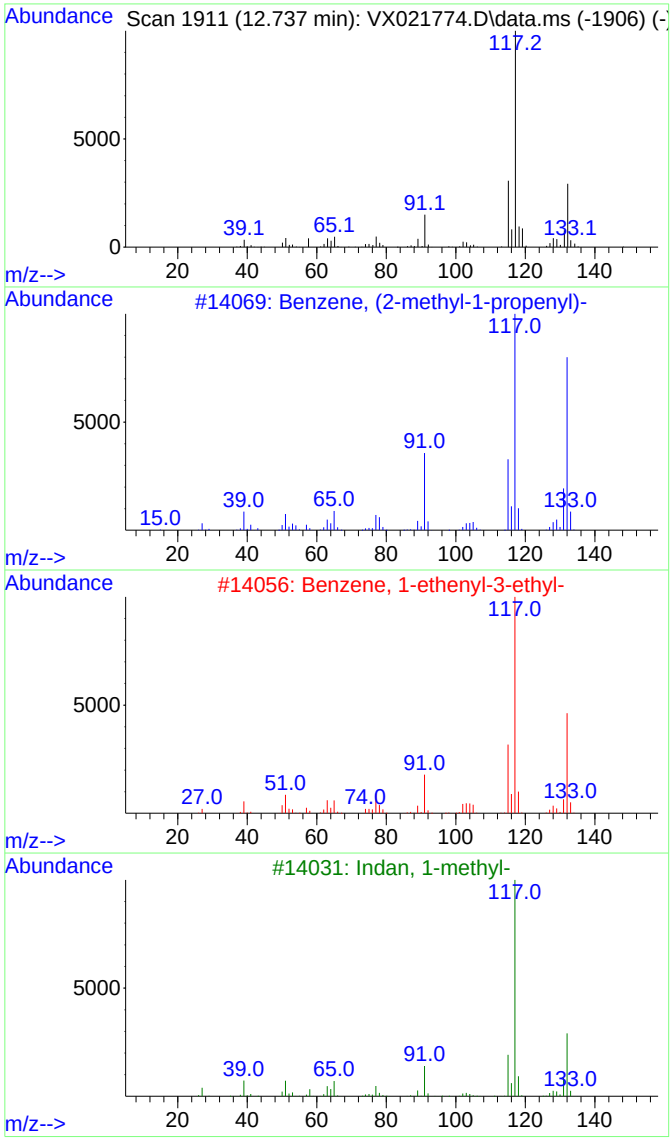
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

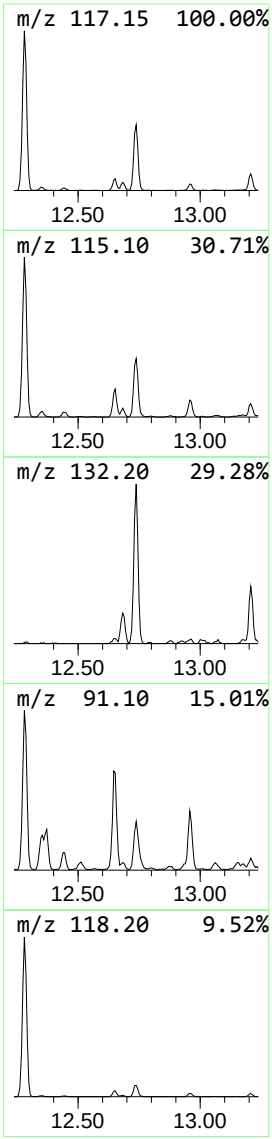
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.738	17.25 ug/l	173231	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

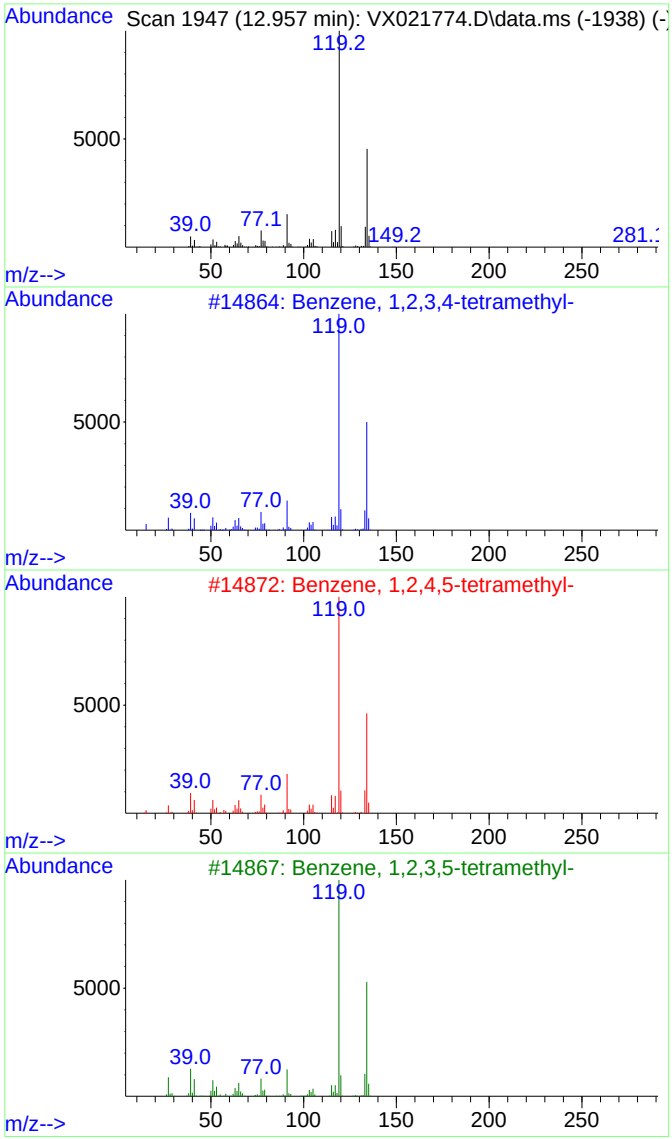
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

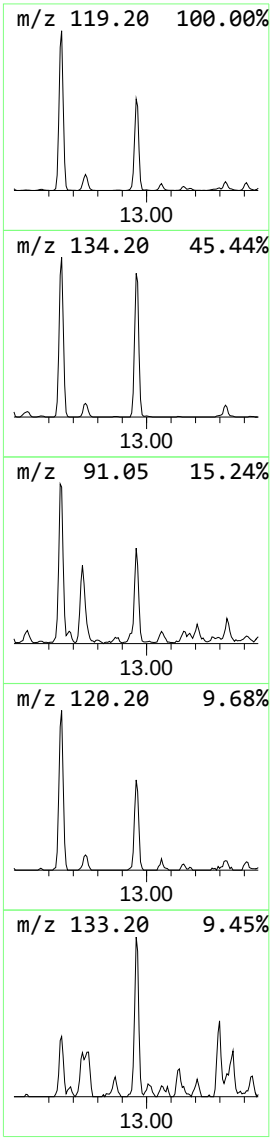
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.957	17.92 ug/l	179915	1,4-Dichlorobenzene-d4	12.061

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	97
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

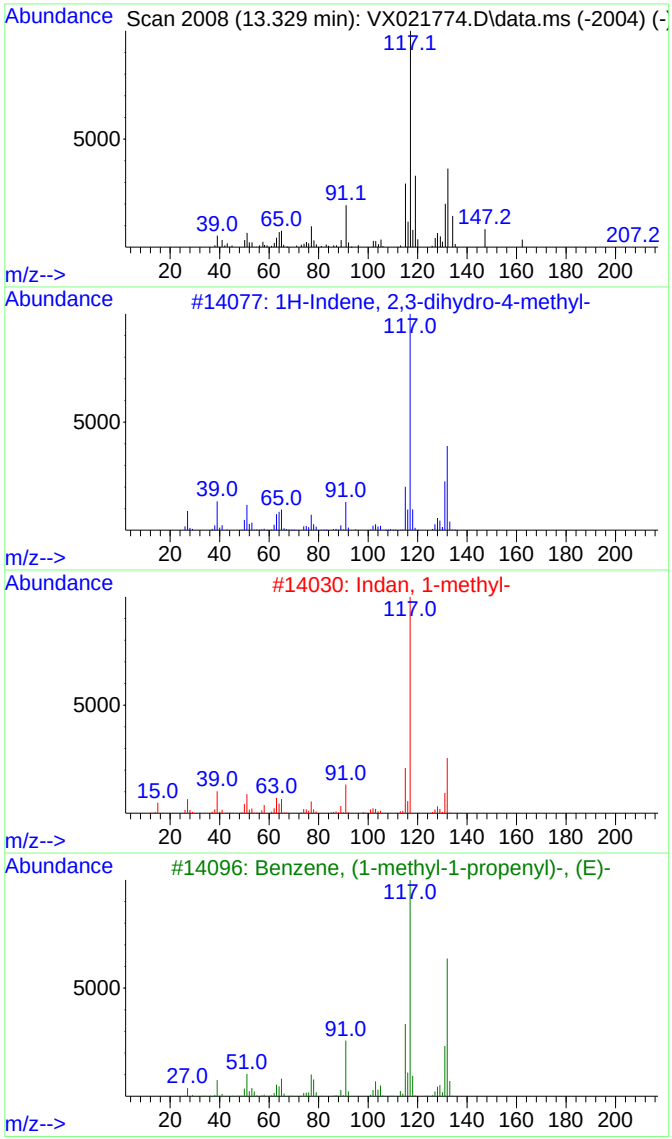
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

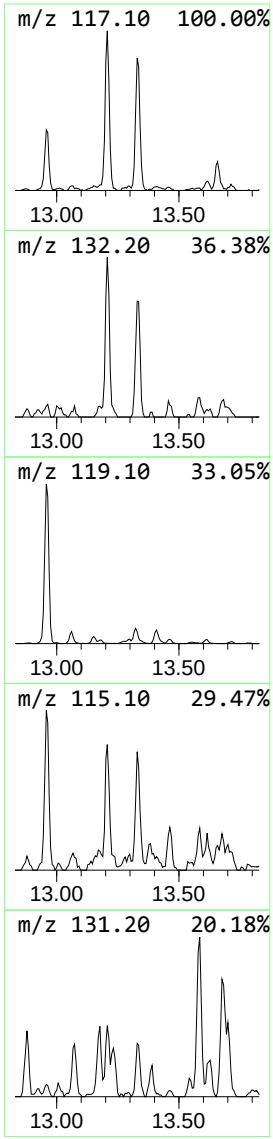
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.329	5.91 ug/l	59298	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
2	Indan, 1-methyl-	132	C10H12	000767-58-8	70
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	68
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042021\
Data File : VX021774.D
Acq On : 20 Apr 2021 23:22
Operator : JC/MD
Sample : M2079-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.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
Pentane, 2,3-di...	5.696	13.3	ug/l	117677	1	5.629	442575	50.0
Pentane, 2,2,4-...	6.318	25.6	ug/l	288735	2	6.830	564595	50.0
Heptane, 4-methyl-	8.037	13.4	ug/l	151126	2	6.830	564595	50.0
Pentane, 2,3,3-...	8.159	20.3	ug/l	229544	2	6.830	564595	50.0
Benzene, cyclop...	12.280	48.3	ug/l	485119	4	12.061	502054	50.0
Benzene, 1-ethy...	12.652	26.0	ug/l	260996	4	12.061	502054	50.0
Benzene, (2-met...	12.738	17.3	ug/l	173231	4	12.061	502054	50.0
Benzene, 1,2,3,...	12.957	17.9	ug/l	179915	4	12.061	502054	50.0
1H-Indene, 2,3-...	13.329	5.9	ug/l	59298	4	12.061	502054	50.0