LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

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_U\Method\82U041221W.M
Title : SW846 8260

Signal : TIC: VU043072.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	39	46	55	rBV2	9777	18162	2.24%	0.257%
2	2.636	386	403	421	rBV2	8829	18172	2.24%	0.257%
3	2.797	437	453	475	rBV2	7241	22190	2.74%	0.314%
4	3.047	517	531	540	rBV4	4772	10238	1.26%	0.145%
5	3.369	619	631	645	rVB2	8031	16436	2.03%	0.233%
6	4.443	950	965	980	rVB3	13127	33717	4.16%	0.477%
7	5.298	1215	1231	1244	rBV2	129162	277091	34.21%	3.923%
8	5.382	1244	1257	1271	rVV	210203	433751	53.56%	6.141%
9	5.469	1271	1284	1301	rVB2	37128	83562	10.32%	1.183%
10	5.600	1312	1325	1339	rBV4	8604	19703	2.43%	0.279%
11	5.710	1345	1359	1378	rBV	146528	296900	36.66%	4.203%
12	5.858	1393	1405	1408	rBV3	16500	26968	3.33%	0.382%
13	5.909	1409	1421	1439	rVV	129417	303877	37.52%	4.302%
14	5.996	1439	1448	1459	rVB5	4151	8195	1.01%	0.116%
15	6.256	1513	1529	1549	rBV	309693	577242	71.27%	8.172%
16	6.745	1669	1681	1692	rBV5	10743	23312	2.88%	0.330%
17	6.816	1694	1703	1711	rVV3	12506	23726	2.93%	0.336%
18	6.874	1711	1721	1731	rVV3	20650	38683	4.78%	0.548%
19	6.932	1731	1739	1749	rVB3	5817	10839	1.34%	0.153%
20	7.079	1771	1785	1796	rBV6	10952	22846	2.82%	0.323%
21	7.263	1823	1842	1859	rVB3	70727	142915	17.65%	2.023%
22	7.385	1868	1880	1890	rBV2	77229	153077	18.90%	2.167%
23	7.433	1891	1895	1905	rVB2	16554	23556	2.91%	0.333%
24	7.549	1922	1931	1939	rVB2	7375	11257	1.39%	0.159%
25	7.665	1961	1967	1974	rBV4	7525	10021	1.24%	0.142%
26	7.777	1992	2002	2013	rBV3	6102	11113	1.37%	0.157%
27	7.864	2013	2029	2030	rBV4	17492	33166	4.10%	0.470%
28	7.906	2031	2042	2057	rVB	468732	809892	100.00%	11.466%
29	8.028	2071	2080	2088	rBV6	7964	15730	1.94%	0.223%
30	8.253	2137	2150	2165	rVB5	7205	15704	1.94%	0.222%
31	8.375	2168	2188	2196	rBV4	18721	38759	4.79%	0.549%
32	8.665	2261	2278	2284	rBV8	5128	11440	1.41%	0.162%
33	8.796	2313	2319	2335	rVB8	9655	25187	3.11%	0.357%
34	9.343	2478	2489	2500	rBV4	7394	15188	1.88%	0.215%
35	9.423	2501	2514	2529	rBV	434526	712073	87.92%	10.081%
36	9.697	2589	2599	2615	rVB7	9918	23656	2.92%	0.335%

LSC Area Percent Report

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Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

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_U\Method\82U041221W.M
Title : SW846 8260

37	10.034	2695	2704	2712	rBV6	5579	9336	1.15%	0.132%
38	10.491	2837	2846	2854	rBV2	10355	15894	1.96%	0.225%
39	10.639	2880	2892	2907	rBV	365592	592908	73.21%	8.394%
40	10.912	2965	2977	2987	rVB	11496	20985	2.59%	0.297%
41	11.616	3180	3196	3201	rBV2	16839	27523	3.40%	0.390%
42	11.648	3201	3206	3215	rVB	17808	26226	3.24%	0.371%
43	11.819	3247	3259	3275	rBV	450013	719586	88.85%	10.188%
44	12.105	3338	3348	3362	rVB3	103026	162343	20.05%	2.298%
45	12.192	3362	3375	3395	rVB3	26291	54260	6.70%	0.768%
46	12.311	3402	3412	3421	rBV3	18557	28155	3.48%	0.399%
47	12.398	3426	3439	3452	rVB3	18198	30971	3.82%	0.438%
48	12.578	3480	3495	3502	rBV2	14005	22891	2.83%	0.324%
49	12.623	3502	3509	3521	rVB7	7541	12355	1.53%	0.175%
50	12.713	3521	3537	3548	rBV7	26239	63955	7.90%	0.905%
51	12.870	3577	3586	3590	rBV4	9812	14175	1.75%	0.201%
52	12.980	3602	3620	3633	rBV2	51905	97114	11.99%	1.375%
53	13.115	3651	3662	3676	rBV3	40401	70712	8.73%	1.001%
54	13.234	3683	3699	3702	rBV4	19521	31963	3.95%	0.453%
55	13.333	3724	3730	3740	rVB2	10720	15257	1.88%	0.216%
56	13.391	3740	3748	3753	rBV5	6122	9799	1.21%	0.139%
57	13.462	3762	3770	3787	rVB2	53147	94841	11.71%	1.343%
58	13.568	3796	3803	3818	rVV4	22405	43050	5.32%	0.609%
59	13.639	3818	3825	3835	rVB3	6221	11199	1.38%	0.159%
60	13.745	3848	3858	3866	rBV4	13360	25774	3.18%	0.365%
61	13.793	3866	3873	3879	rVB2	7868	10700	1.32%	0.151%
62	13.841	3879	3888	3897	rBV3	53548	79592	9.83%	1.127%
63	13.889	3897	3903	3904	rBV2	13531	11180	1.38%	0.158%
64	13.918	3906	3912	3918	rVV	21409	26665	3.29%	0.378%
65	14.066	3950	3958	3965	rBV2	5841	8665	1.07%	0.123%
66	14.127	3971	3977	3992	rVB8	6491	13792	1.70%	0.195%
67	14.201	3992	4000	4012	rVB8	6991	13053	1.61%	0.185%
68	14.295	4012	4029	4040	rBV6	29733	60538	7.47%	0.857%
69	14.352	4040	4047	4057	rVV3	16444	24578	3.03%	0.348%
70	14.494	4083	4091	4102	rVB2	21371	34003	4.20%	0.481%
71	14.674	4136	4147	4159	rBV3	49436	92652	11.44%	1.312%
72	14.815	4182	4191	4201	rBV2	37267	58053	7.17%	0.822%
73	14.883	4203	4212	4223	rVB3	34550	56329	6.96%	0.797%
74	14.944	4223	4231	4240	rBV6	5384	8168	1.01%	0.116%
75	15.034	4249	4259	4268	rBV4	10497	19052	2.35%	0.270%
76	15.211	4304	4314	4328	rVV4	7884	17148	2.12%	0.243%

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Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

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_U\Method\82U041221W.M
Title : SW846 8260

77	15.407	4367	4375	4381	rBV6	5908	9497	1.17%	0.134%

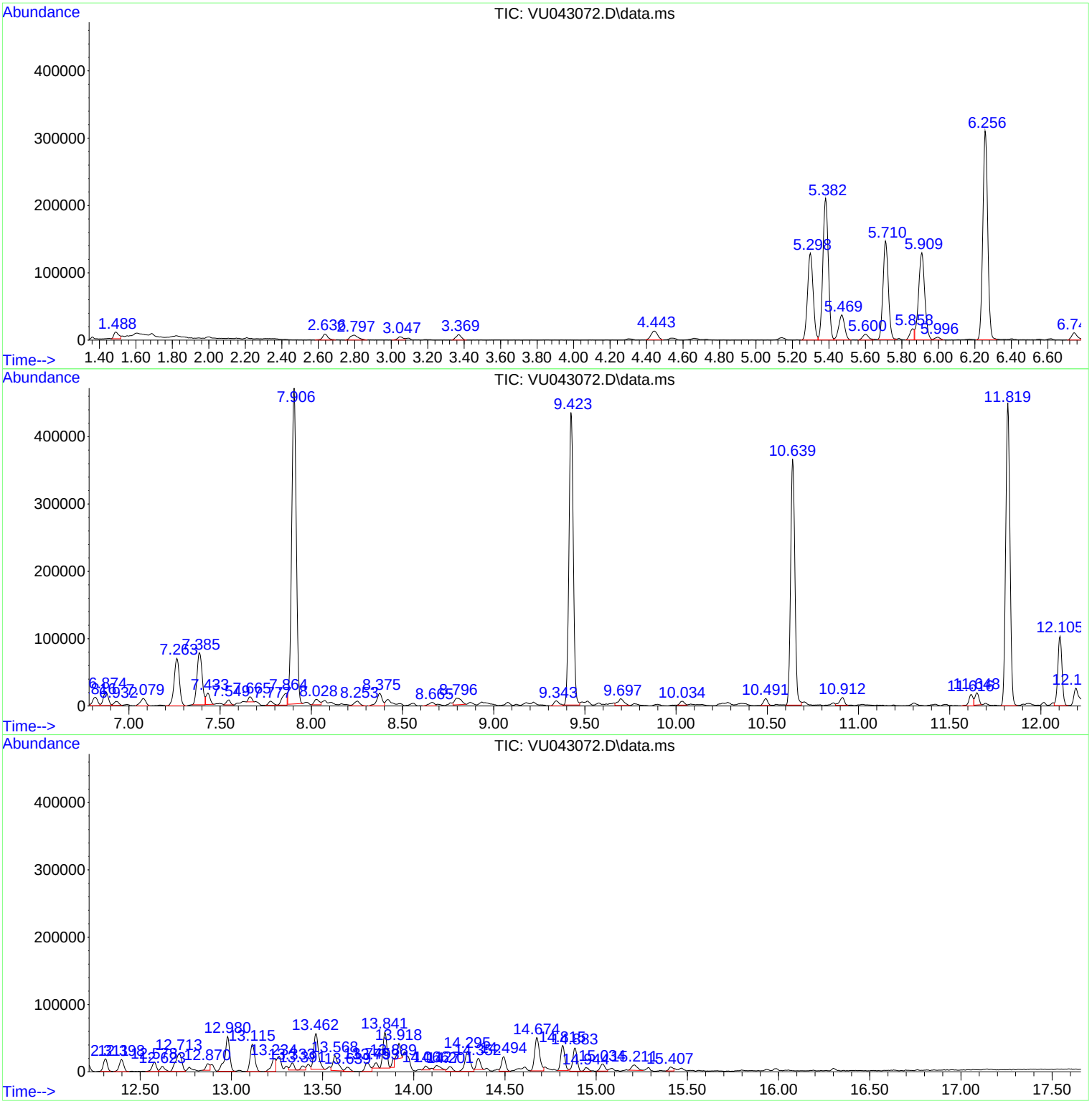
Sum of corrected areas: 7063281

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
W-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

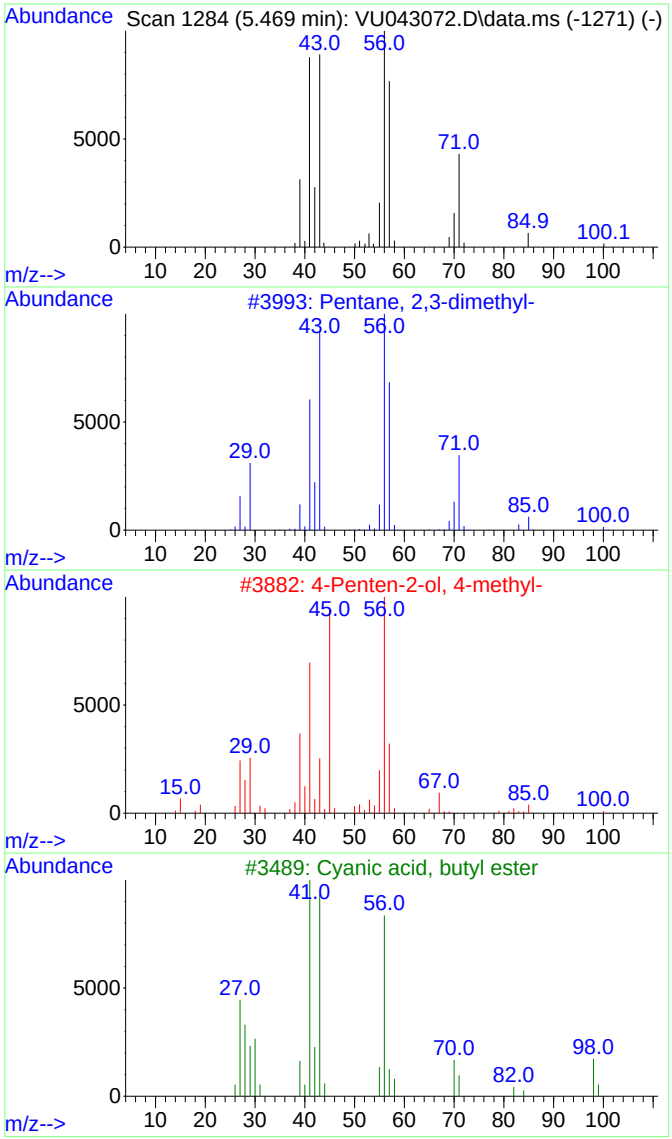
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

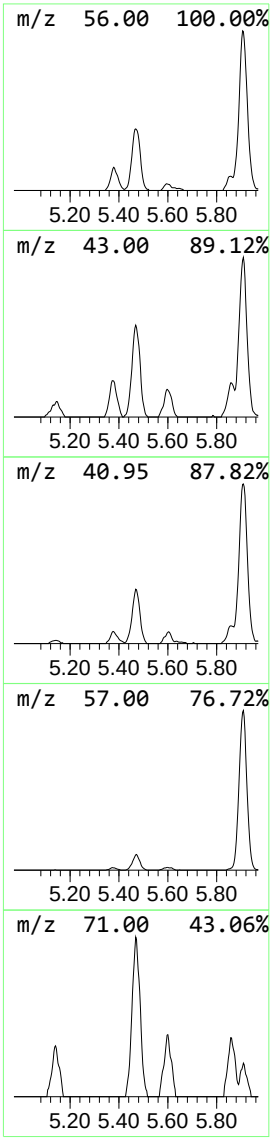
****

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.469	9.63 ug/l	83562	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	38
3	Cyanic acid, butyl ester	99	C5H9NO	001768-24-7	38
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37
5	Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

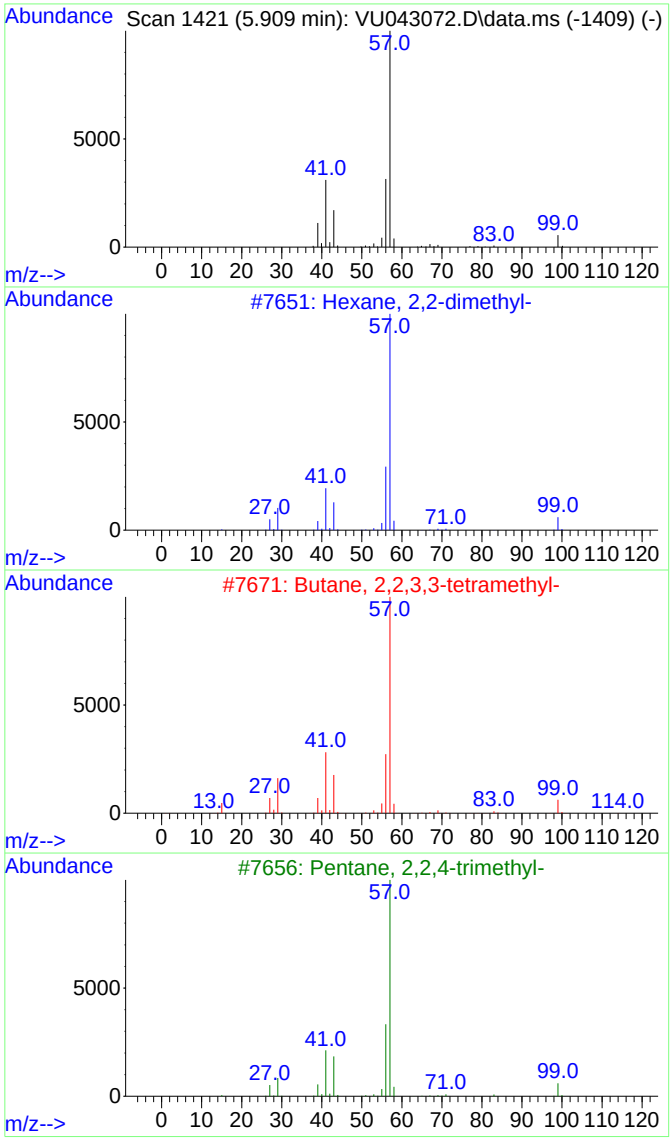
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

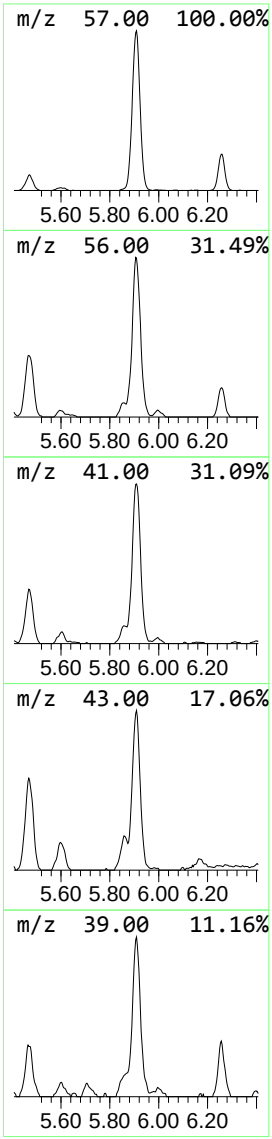
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.909	26.32 ug/l	303877	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
W-1

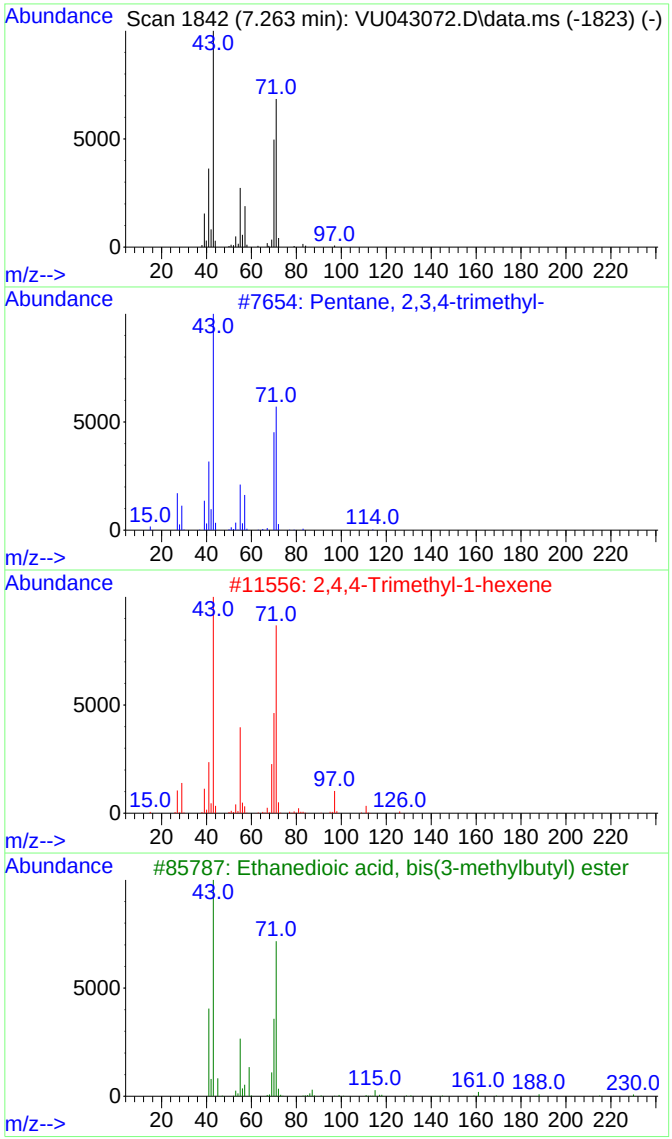
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

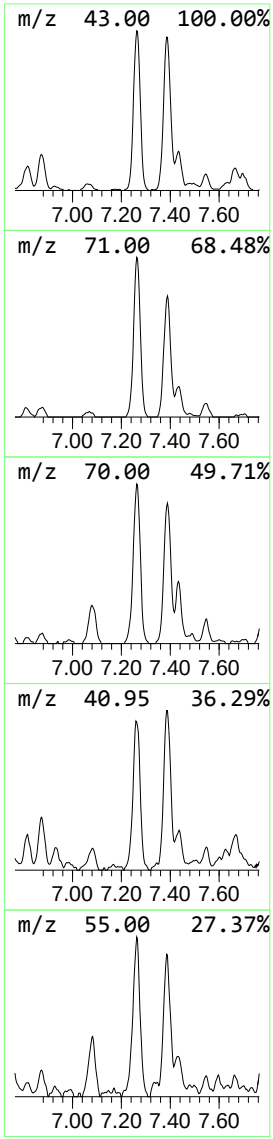
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.263	12.38 ug/l	142915	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72
3	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
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Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

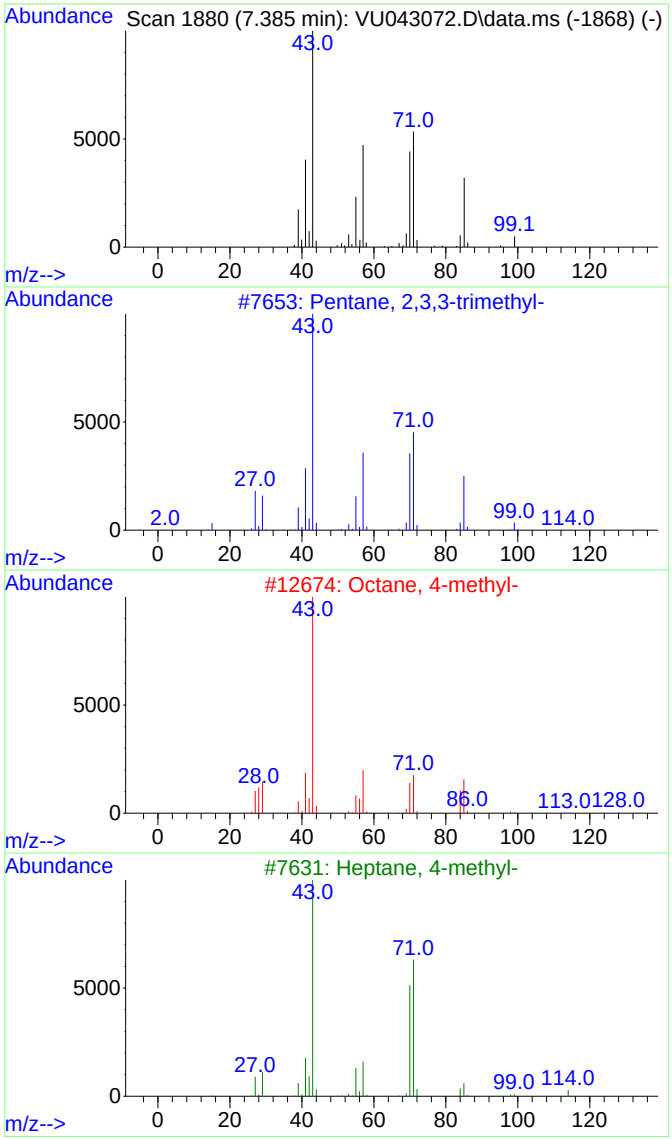
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

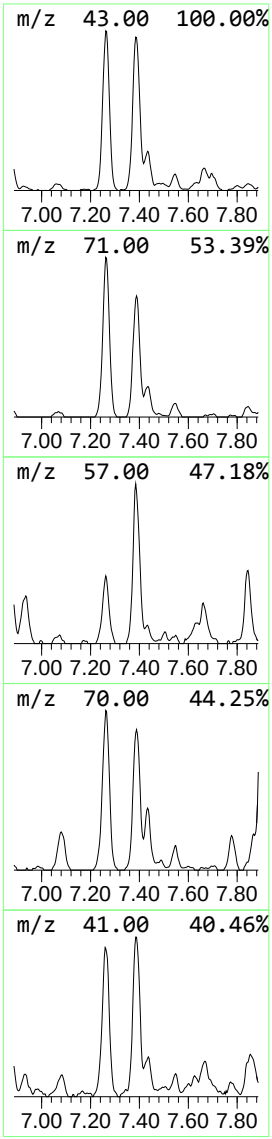
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.385	13.26 ug/l	153077	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Octane, 4-methyl-	128	C9H20	002216-34-4	78
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59





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Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

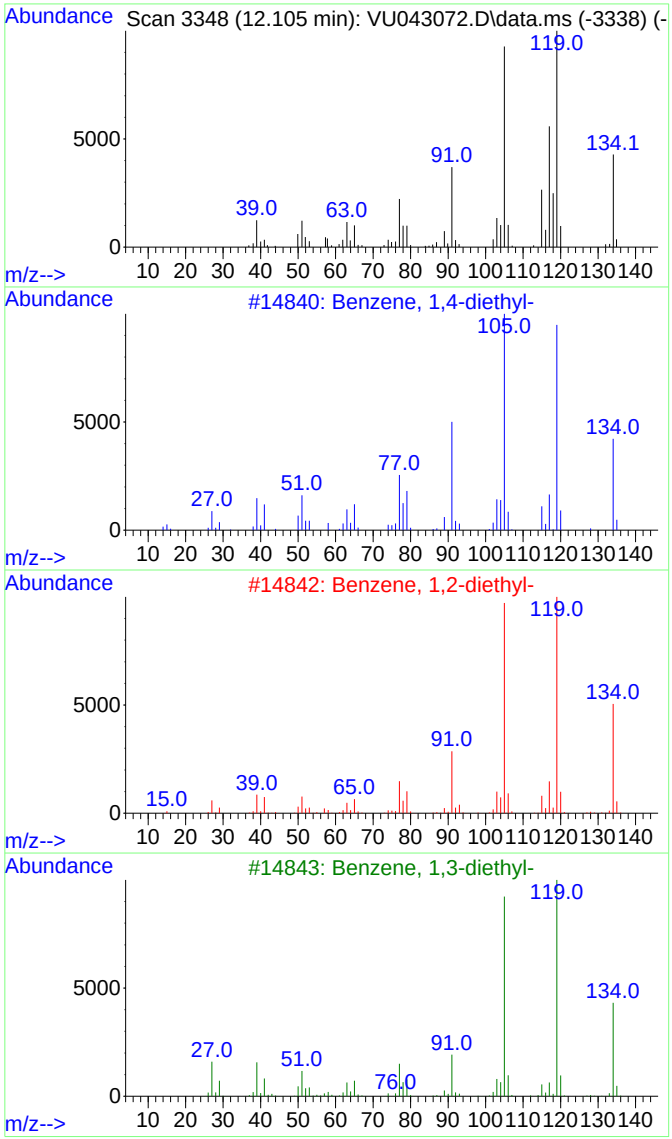
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

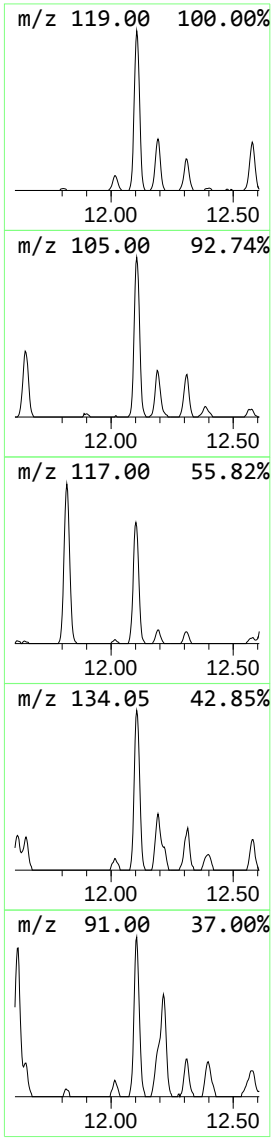
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	11.28 ug/l	162343	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	76
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	70
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	58
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
W-1

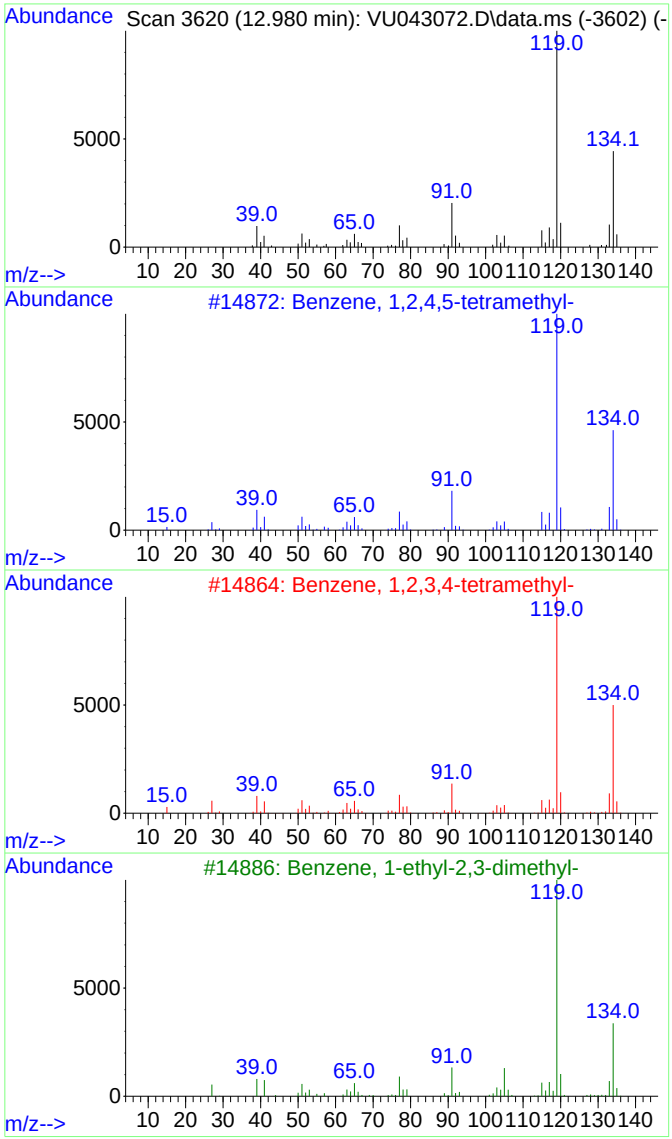
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

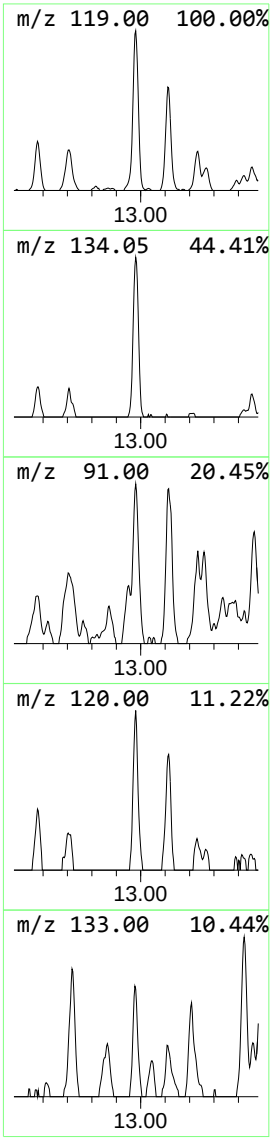
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	6.75 ug/l	97114	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91





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Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
W-1

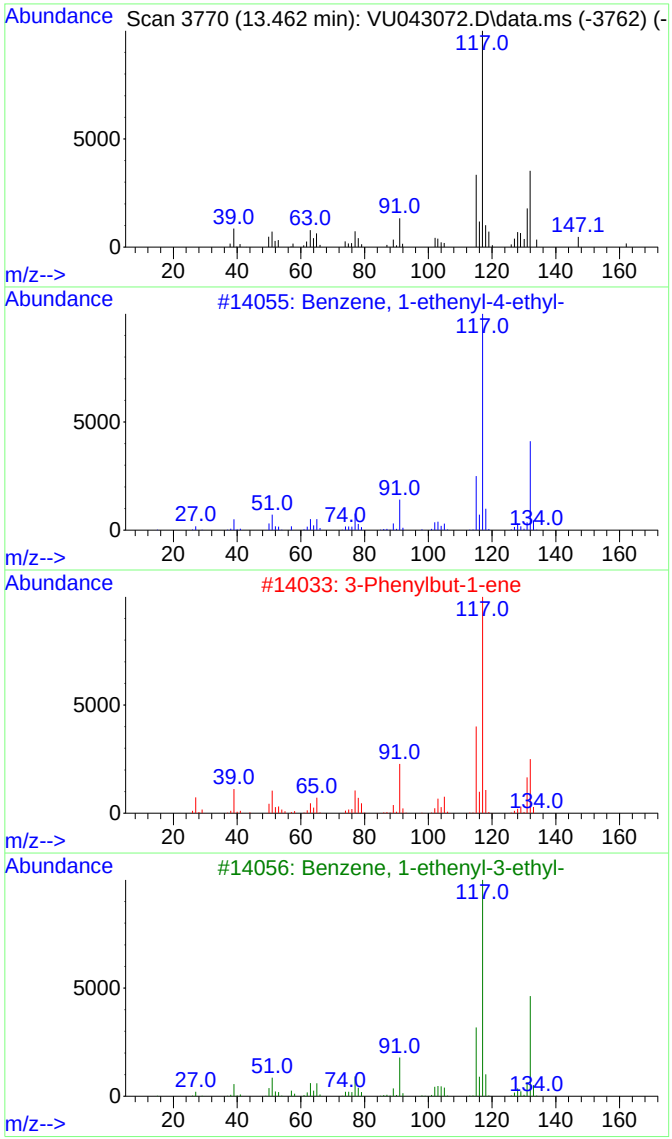
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

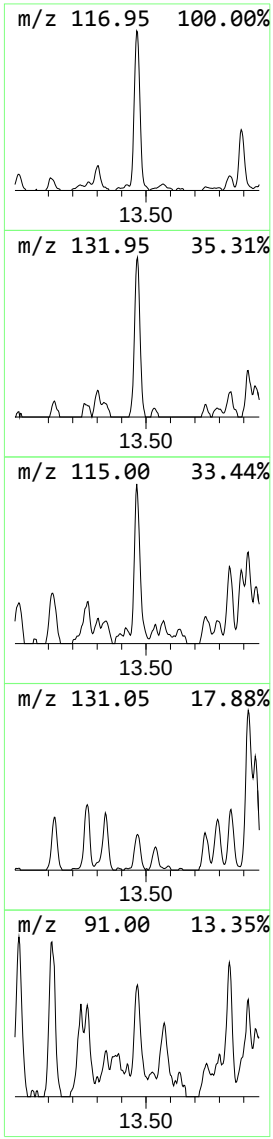
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.462	6.59 ug/l	94841	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

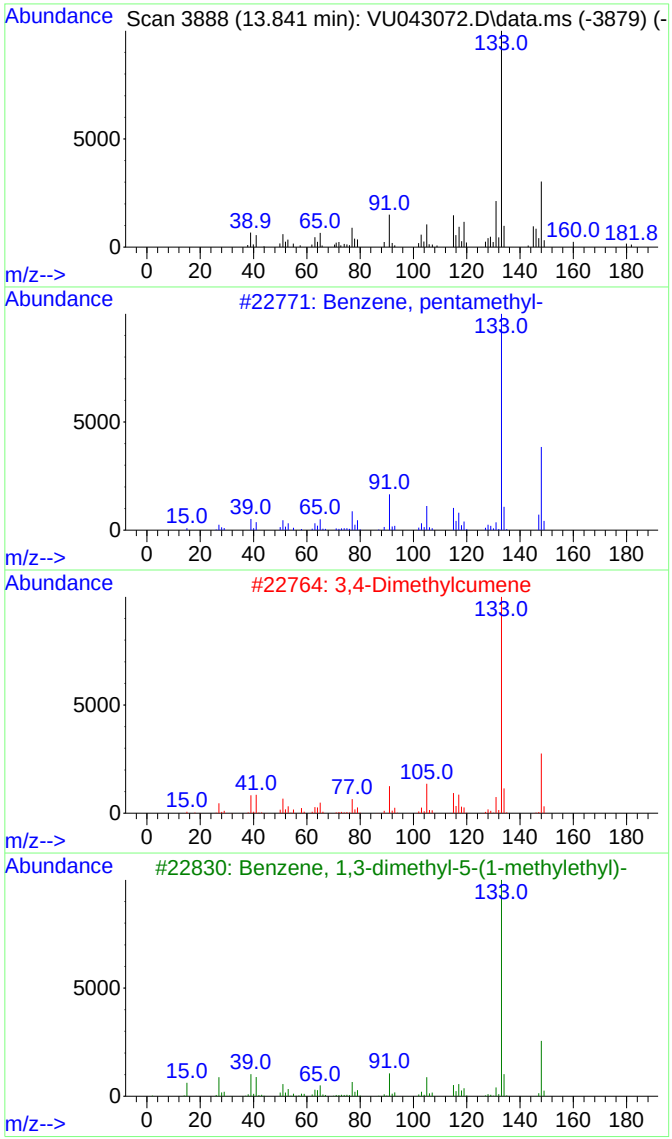
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

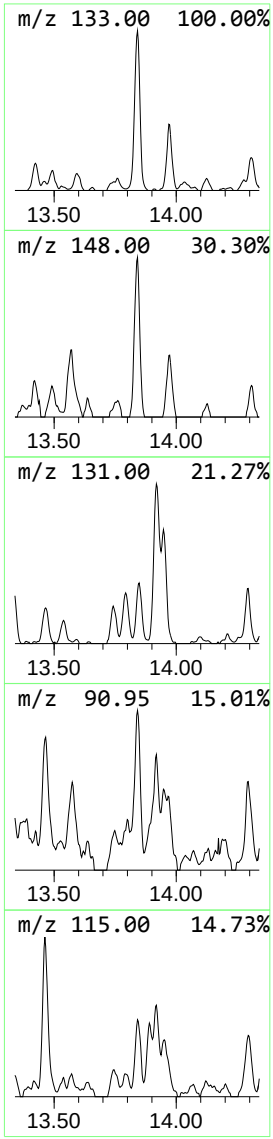
****

Peak Number 8 Benzene, pentamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	5.53 ug/l	79592	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, pentamethyl-	148	C11H16	000700-12-9	76
2	3,4-Dimethylcumene	148	C11H16	1000370-34-1	76
3	Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	68
4	Benzene, 1-(1,1-dimethylethyl)-3...	148	C11H16	001075-38-3	62
5	Benzene, 2,4-dimethyl-1-(1-methy...	148	C11H16	004706-89-2	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

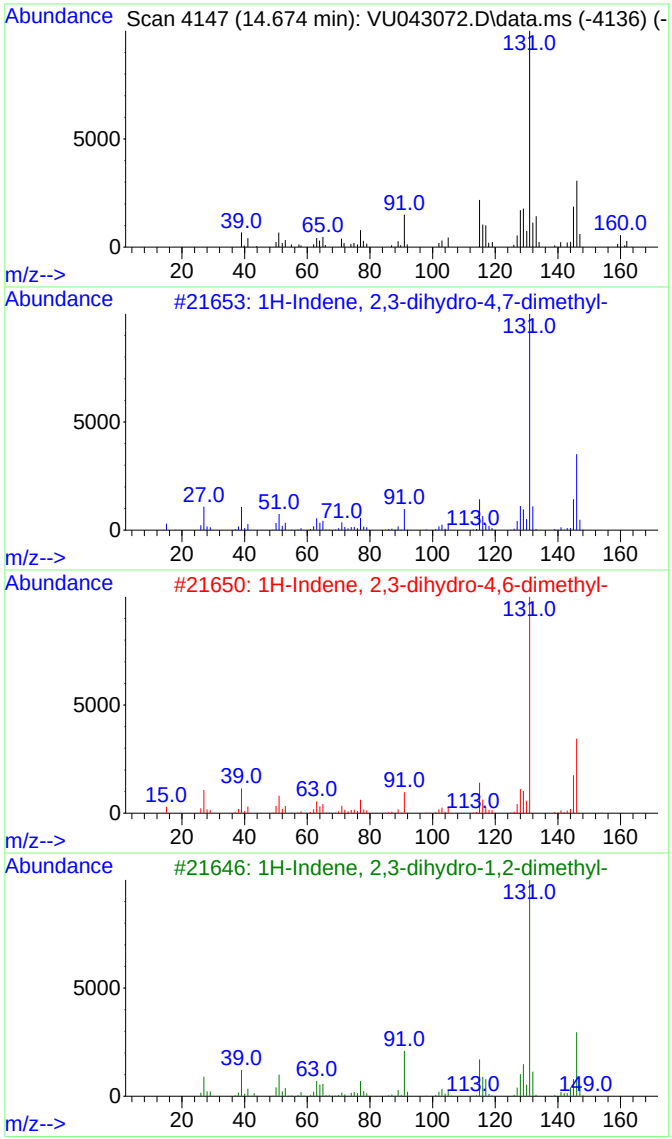
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

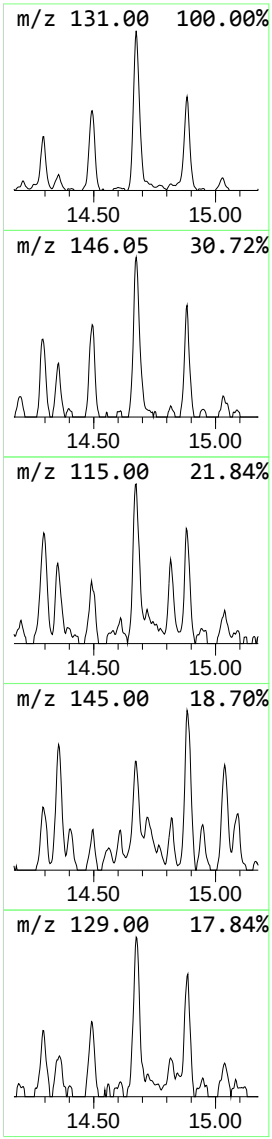
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.674	6.44 ug/l	92652	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	93
2	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	87
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87
4	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	86
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043072.D
Acq On : 13 Apr 2021 23:52
Operator : SY/MD
Sample : M1978-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : W-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.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...	5.469	9.6	ug/l	83562	1	5.382	433751	50.0
Hexane, 2,2-dim...	5.909	26.3	ug/l	303877	2	6.256	577242	50.0
Pentane, 2,3,4-...	7.263	12.4	ug/l	142915	2	6.256	577242	50.0
Pentane, 2,3,3-...	7.385	13.3	ug/l	153077	2	6.256	577242	50.0
Benzene, 1,4-di...	12.105	11.3	ug/l	162343	4	11.819	719586	50.0
Benzene, 1,2,4,...	12.980	6.8	ug/l	97114	4	11.819	719586	50.0
Benzene, 1-ethe...	13.462	6.6	ug/l	94841	4	11.819	719586	50.0
Benzene, pentam...	13.841	5.5	ug/l	79592	4	11.819	719586	50.0
1H-Indene, 2,3-...	14.674	6.4	ug/l	92652	4	11.819	719586	50.0