LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

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\82U052622W.M
Title : SW846 8260

Signal : TIC: VU048697.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.494	36	48	54	rBV2	11209	22227	1.82%	0.201%
2	1.996	196	204	216	rVB	40243	56202	4.60%	0.509%
3	2.205	262	269	281	rVB3	7788	12996	1.06%	0.118%
4	2.758	427	441	460	rBV	8727	19463	1.59%	0.176%
5	3.044	514	530	534	rBV5	15054	30603	2.50%	0.277%
6	3.083	535	542	553	rVB2	26741	51000	4.17%	0.462%
7	3.362	612	629	657	rVB	105129	241335	19.74%	2.186%
8	4.433	947	962	977	rBV5	9712	25912	2.12%	0.235%
9	4.530	977	992	1008	rVB4	16187	38648	3.16%	0.350%
10	5.134	1166	1180	1191	rBV7	6239	14289	1.17%	0.129%
11	5.292	1213	1229	1242	rBV2	215375	461082	37.72%	4.177%
12	5.375	1242	1255	1271	rVV	324800	686719	56.18%	6.221%
13	5.462	1271	1282	1300	rVB4	33723	82465	6.75%	0.747%
14	5.591	1305	1322	1334	rBV5	25616	59318	4.85%	0.537%
15	5.703	1344	1357	1370	rBV2	213963	435029	35.59%	3.941%
16	5.777	1370	1380	1391	rVB	45116	86763	7.10%	0.786%
17	5.848	1392	1402	1409	rBV5	20940	42423	3.47%	0.384%
18	5.909	1410	1421	1422	rBV2	36013	58757	4.81%	0.532%
19	6.250	1512	1527	1564	rBV	431435	871493	71.29%	7.895%
20	6.555	1612	1622	1636	rVB	8299	19300	1.58%	0.175%
21	6.742	1667	1680	1681	rBV3	28538	40446	3.31%	0.366%
22	6.867	1710	1719	1730	rBV3	8275	14170	1.16%	0.128%
23	7.076	1767	1784	1794	rVB7	8885	19047	1.56%	0.173%
24	7.166	1798	1812	1827	rBV7	13113	38723	3.17%	0.351%
25	7.256	1827	1840	1855	rVB4	31543	70276	5.75%	0.637%
26	7.382	1855	1879	1891	rBV3	40743	94240	7.71%	0.854%
27	7.465	1901	1905	1918	rVB4	10335	16668	1.36%	0.151%
28	7.539	1918	1928	1937	rBV8	6200	12811	1.05%	0.116%
29	7.626	1947	1955	1969	rBV4	19312	39593	3.24%	0.359%
30	7.755	1985	1995	2013	rVB8	16087	42350	3.46%	0.384%
31	7.899	2015	2040	2059	rBV	651098	1178958	96.45%	10.680%
32	8.034	2071	2082	2088	rBV10	10029	22426	1.83%	0.203%
33	8.102	2097	2103	2115	rVB8	9457	17791	1.46%	0.161%
34	8.169	2116	2124	2137	rVB9	8185	19239	1.57%	0.174%
35	8.247	2137	2148	2164	rVB9	16308	42208	3.45%	0.382%
36	8.369	2164	2186	2192	rBV4	21459	44820	3.67%	0.406%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

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\82U052622W.M
Title : SW846 8260

37	8.411	2193	2199	2210	rVB2	23263	37862	3.10%	0.343%
38	8.488	2215	2223	2235	rVB2	14526	25674	2.10%	0.233%
39	8.555	2235	2244	2254	rBV3	18149	29870	2.44%	0.271%
40	8.716	2281	2294	2309	rBV	51619	98207	8.03%	0.890%
41	8.806	2309	2322	2333	rVB10	11400	30793	2.52%	0.279%
42	9.079	2390	2407	2424	rBV10	9650	29650	2.43%	0.269%
43	9.272	2456	2467	2478	rBV3	12327	23246	1.90%	0.211%
44	9.337	2478	2487	2499	rVB10	8616	16267	1.33%	0.147%
45	9.417	2499	2512	2533	rBV	653189	1118920	91.53%	10.136%
46	9.571	2551	2560	2570	rBV2	38784	63039	5.16%	0.571%
47	9.693	2589	2598	2610	rVB10	9451	22606	1.85%	0.205%
48	10.484	2833	2844	2853	rBV3	13868	21122	1.73%	0.191%
49	10.632	2877	2890	2917	rBV	587435	967948	79.18%	8.768%
50	10.906	2967	2975	2992	rVB2	14064	27339	2.24%	0.248%
51	11.291	3084	3095	3108	rBV2	37612	62048	5.08%	0.562%
52	11.417	3119	3134	3145	rBV2	4614	12255	1.00%	0.111%
53	11.610	3183	3194	3199	rBV3	9007	13878	1.14%	0.126%
54	11.645	3199	3205	3212	rVB3	10442	15142	1.24%	0.137%
55	11.812	3244	3257	3278	rBV	756421	1222402	100.00%	11.073%
56	12.098	3331	3346	3359	rVV2	368674	604820	49.48%	5.479%
57	12.185	3362	3373	3390	rVB2	48550	85850	7.02%	0.778%
58	12.304	3400	3410	3422	rBV3	19270	31358	2.57%	0.284%
59	12.385	3423	3435	3449	rVB5	38393	75811	6.20%	0.687%
60	12.571	3480	3493	3500	rBV	65653	101488	8.30%	0.919%
61	12.613	3500	3506	3516	rVV	29121	43159	3.53%	0.391%
62	12.680	3516	3527	3546	rVV	279561	488648	39.97%	4.426%
63	12.864	3577	3584	3596	rVB2	11980	19652	1.61%	0.178%
64	12.973	3599	3618	3630	rVV	89898	144166	11.79%	1.306%
65	13.108	3651	3660	3672	rVB4	26423	45213	3.70%	0.410%
66	13.253	3692	3705	3710	rBV5	16330	27427	2.24%	0.248%
67	13.295	3710	3718	3726	rVV	58156	82140	6.72%	0.744%
68	13.455	3761	3768	3781	rBV5	17381	27829	2.28%	0.252%
69	13.523	3781	3789	3795	rVV8	16033	27356	2.24%	0.248%
70	13.561	3796	3801	3814	rVV	15660	25146	2.06%	0.228%
71	13.626	3814	3821	3833	rVB9	7983	13643	1.12%	0.124%
72	13.738	3846	3856	3861	rBV5	8603	14859	1.22%	0.135%
73	13.786	3861	3871	3879	rVV2	52219	86312	7.06%	0.782%
74	13.838	3879	3887	3895	rVB4	23329	35009	2.86%	0.317%
75	13.912	3895	3910	3915	rBV3	25851	47877	3.92%	0.434%
76	14.089	3947	3965	3988	rBV2	24324	51510	4.21%	0.467%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

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\82U052622W.M
Title : SW846 8260

77	14.285	4017	4026	4037	rBV6	10674	16844	1.38%	0.153%
78	14.487	4080	4089	4098	rBV	16646	24063	1.97%	0.218%
79	14.876	4203	4210	4220	rVB4	8207	12746	1.04%	0.115%
80	15.413	4367	4377	4387	rBV2	22549	38194	3.12%	0.346%

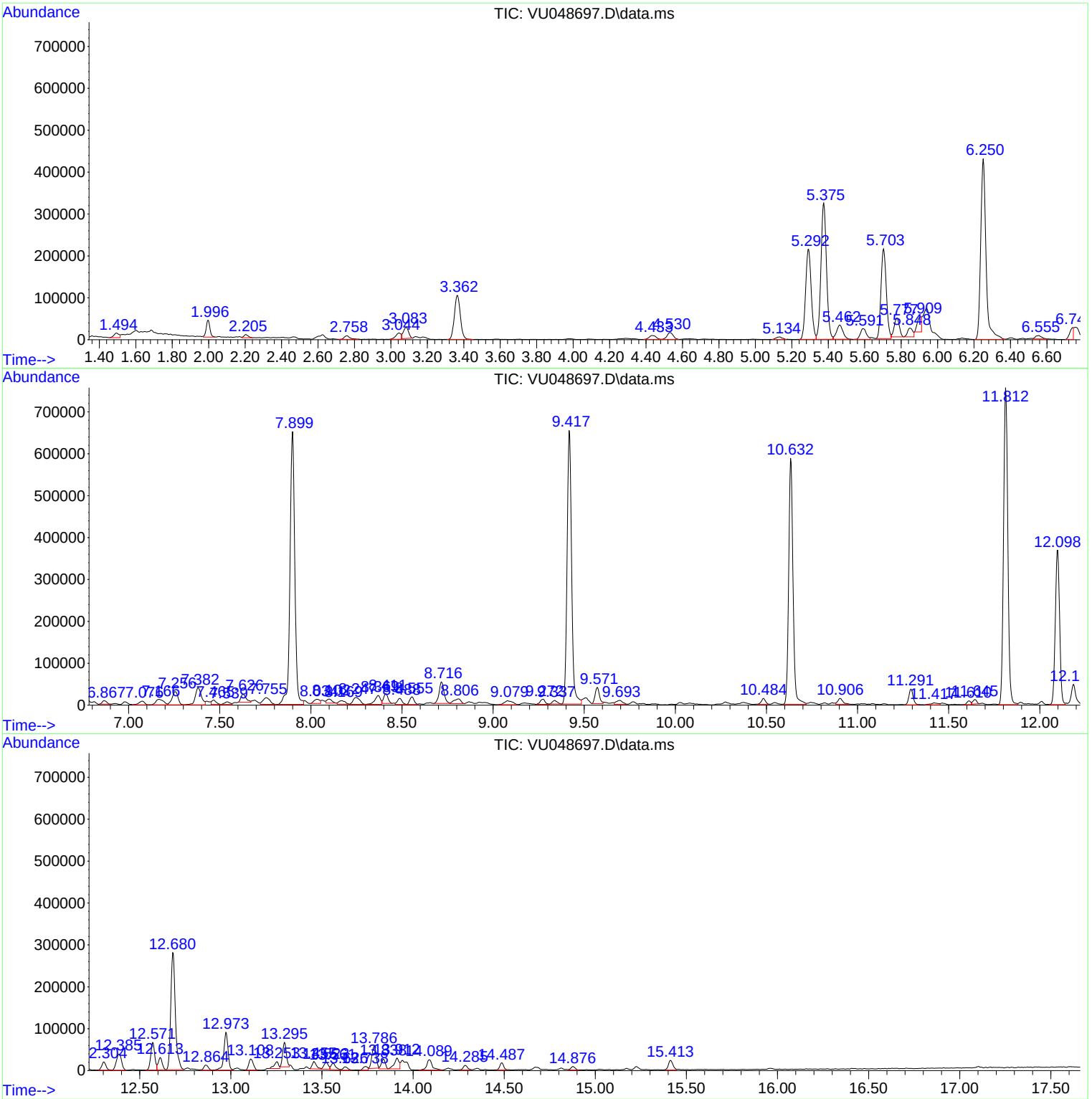
Sum of corrected areas: 11039178

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

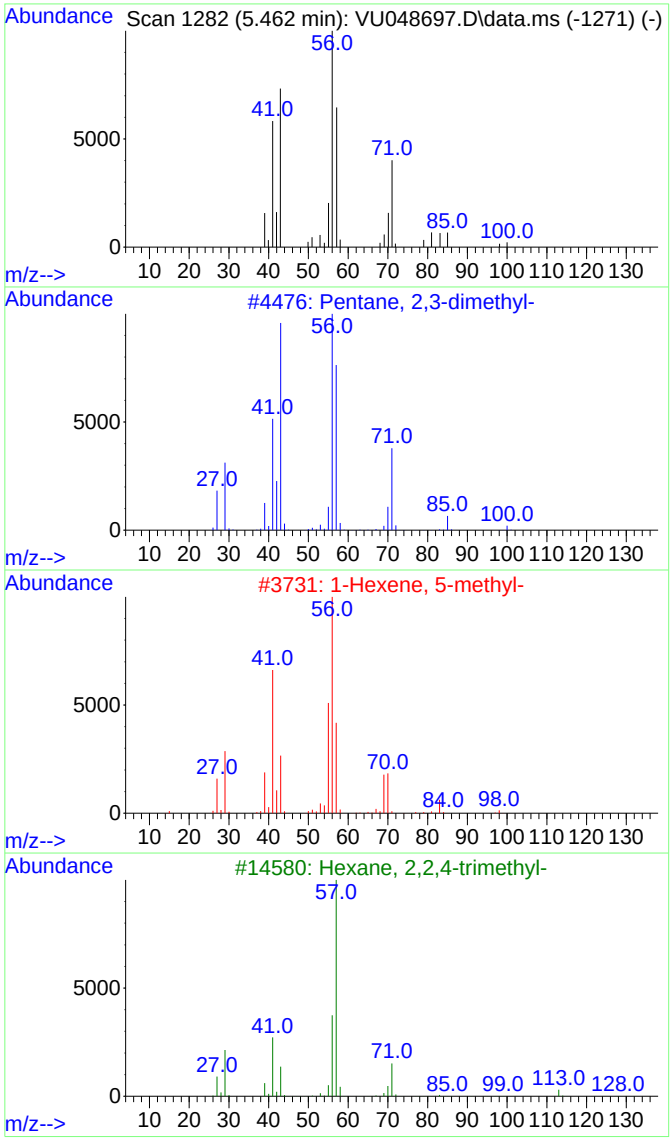
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

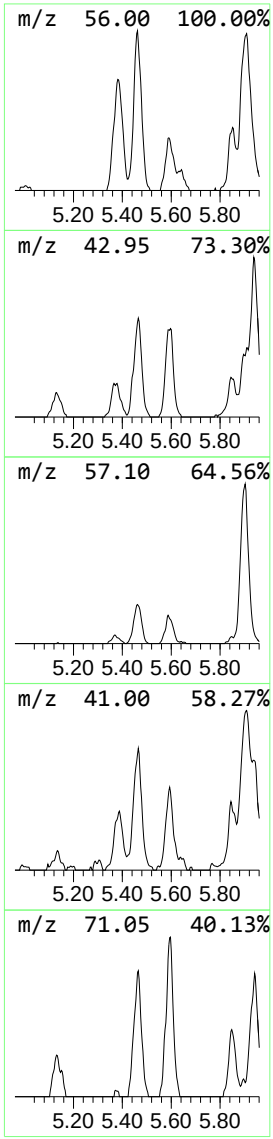
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.462	6.00 ug/l	82465	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	43
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

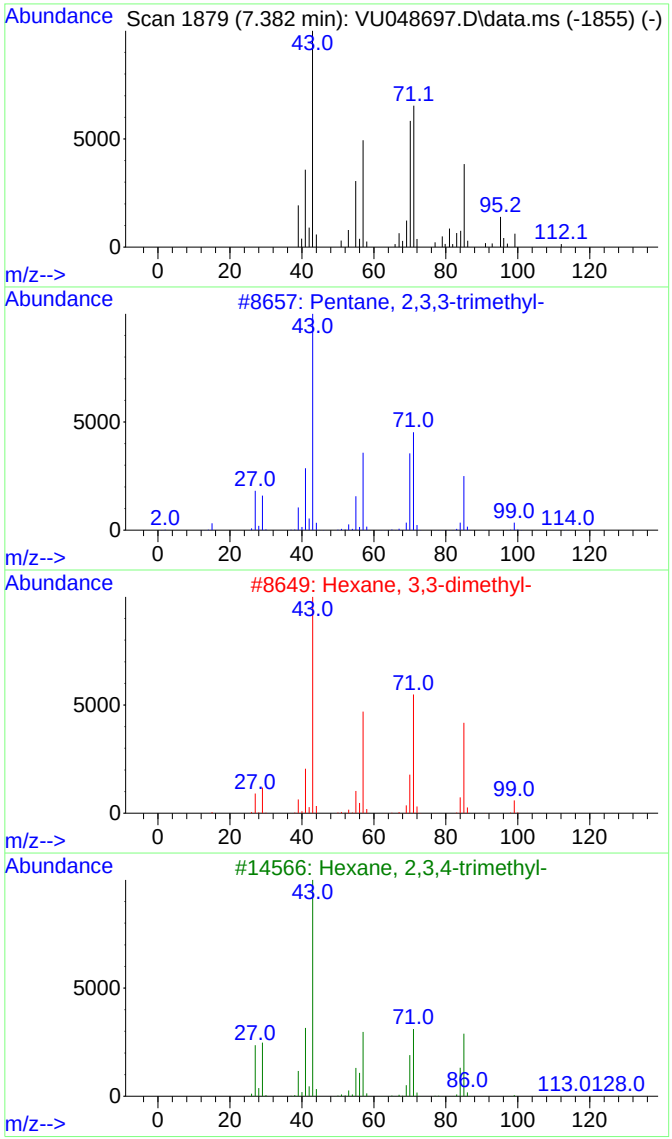
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

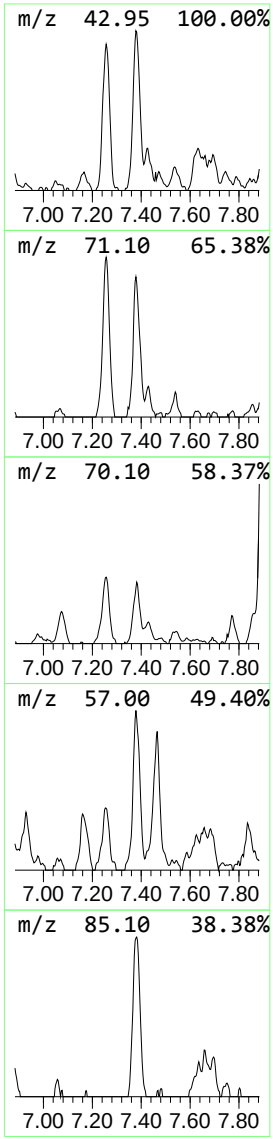
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.382	5.41 ug/l	94240	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
4	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	50
5	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

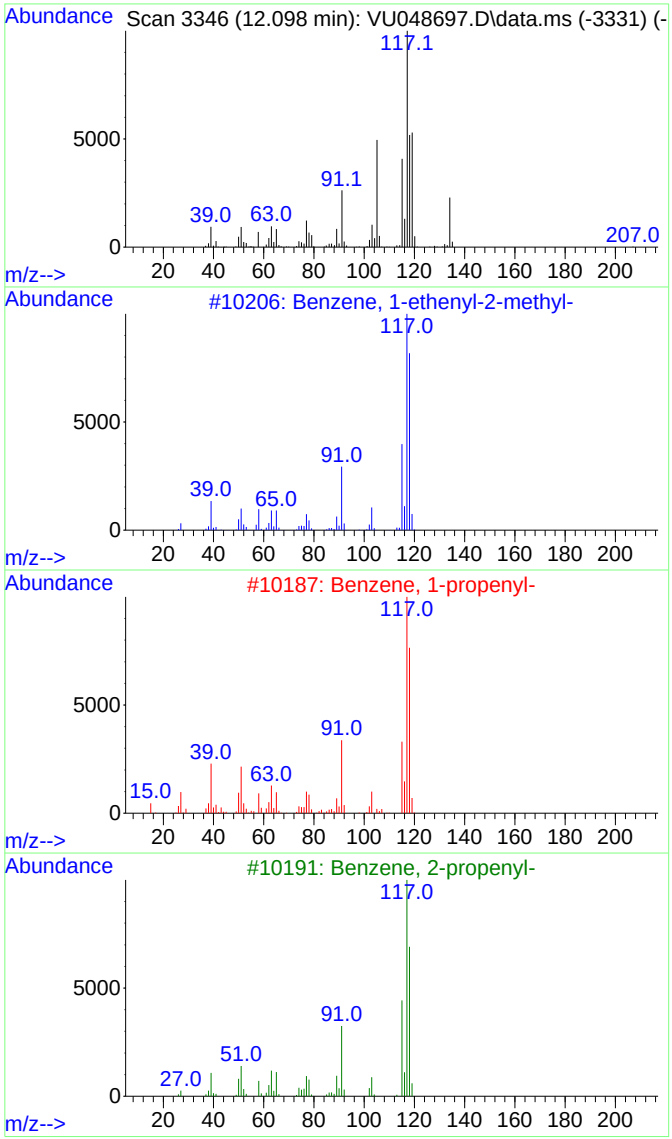
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

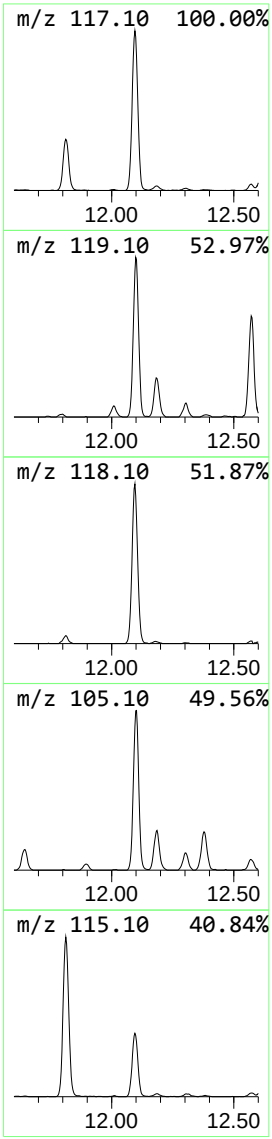
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethenyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.099	24.74 ug/l	604820	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	80
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	55
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
4	Indane	118	C9H10	000496-11-7	50
5	Deltacyclene	118	C9H10	007785-10-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

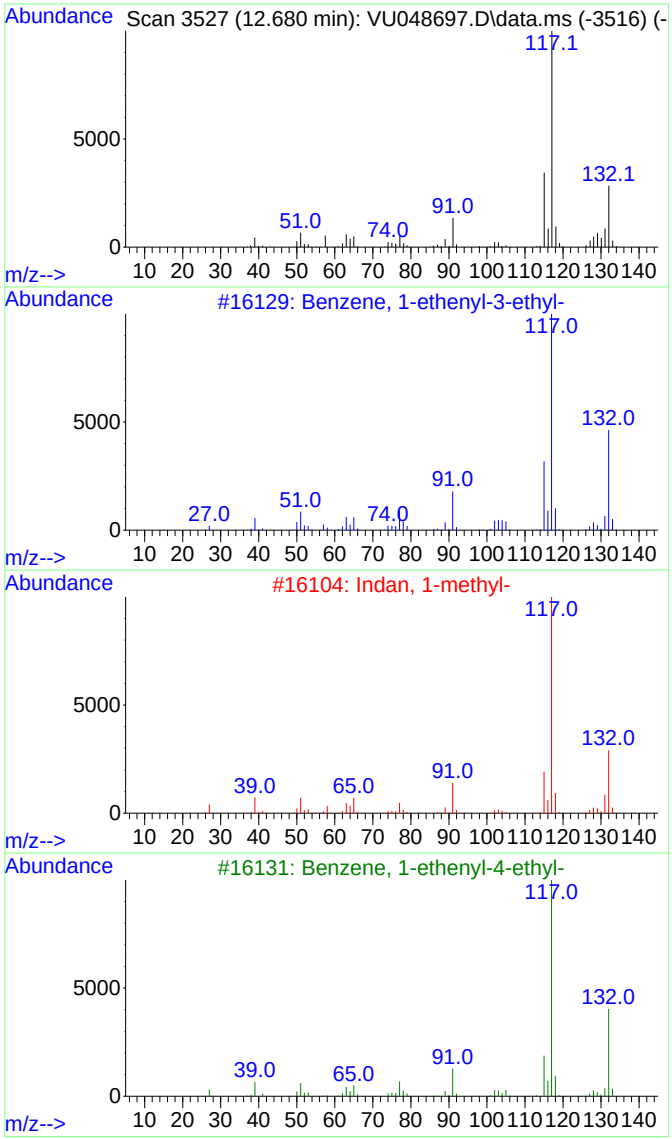
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

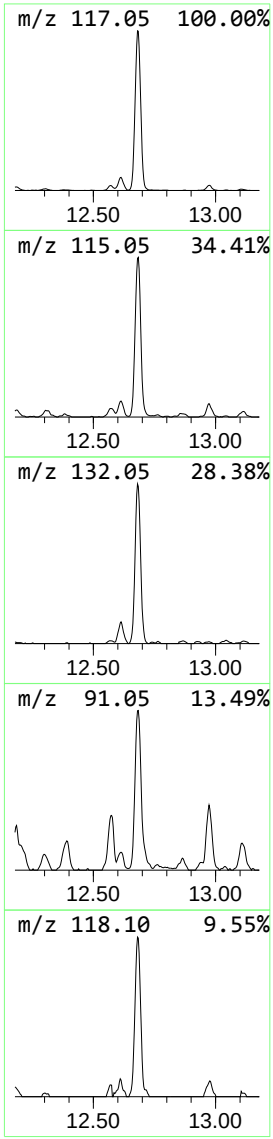
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	19.99 ug/l	488648	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

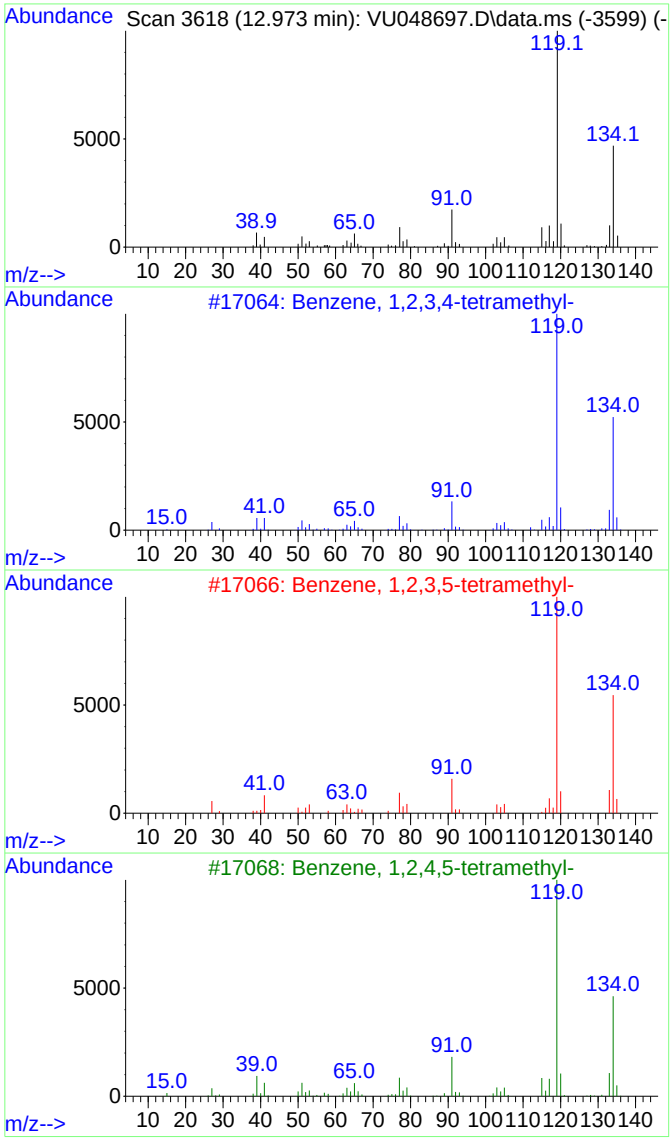
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

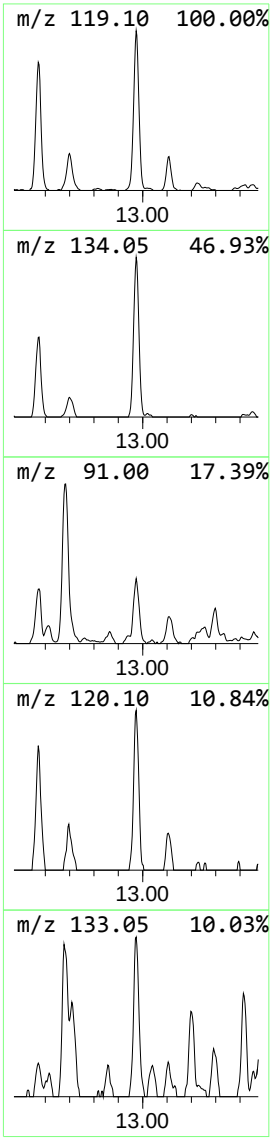
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.973	5.90 ug/l	144166	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048697.D
Acq On : 27 May 2022 16:38
Operator : SY/MD
Sample : N3056-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-05

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.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
Pentane, 2,3-di...	5.462	6.0	ug/l	82465	1	5.375	686719	50.0
Pentane, 2,3,3-...	7.382	5.4	ug/l	94240	2	6.250	871493	50.0
Benzene, 1-ethe...	12.099	24.7	ug/l	604820	4	11.812	1222400	50.0
Benzene, 1-ethe...	12.680	20.0	ug/l	488648	4	11.812	1222400	50.0
Benzene, 1,2,3,...	12.973	5.9	ug/l	144166	4	11.812	1222400	50.0