

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
 Data File : VU043073.D
 Acq On : 14 Apr 2021 00:15
 Operator : SY/MD
 Sample : M1978-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 W-2

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: VU043073.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	37	46	60	rBV	11272	22758	2.76%	0.418%
2	1.607	73	83	90	rBV6	5188	11322	1.37%	0.208%
3	2.633	390	402	417	rBV2	7609	14903	1.81%	0.274%
4	4.443	953	965	980	rVB4	5130	12407	1.51%	0.228%
5	4.674	1022	1037	1049	rBV2	5816	12845	1.56%	0.236%
6	5.298	1215	1231	1244	rBV	129228	272028	33.00%	5.002%
7	5.382	1244	1257	1272	rVV	205659	417975	50.70%	7.686%
8	5.469	1272	1284	1298	rVB4	14816	34545	4.19%	0.635%
9	5.600	1314	1325	1335	rBV4	5958	11520	1.40%	0.212%
10	5.710	1343	1359	1376	rBV	142298	293328	35.58%	5.394%
11	5.858	1395	1405	1409	rBV6	8023	14141	1.72%	0.260%
12	5.909	1410	1421	1439	rVV2	36254	86920	10.54%	1.598%
13	6.256	1514	1529	1547	rBV	302696	562521	68.24%	10.344%
14	6.552	1611	1621	1631	rVB4	6843	11978	1.45%	0.220%
15	6.745	1671	1681	1694	rBV6	5385	12684	1.54%	0.233%
16	6.870	1711	1720	1731	rBV6	4659	8723	1.06%	0.160%
17	7.263	1826	1842	1855	rVB3	22821	47411	5.75%	0.872%
18	7.388	1866	1881	1891	rBV2	30619	58565	7.10%	1.077%
19	7.906	2014	2042	2058	rVV	468131	824359	100.00%	15.158%
20	8.375	2173	2188	2196	rBV4	9781	19156	2.32%	0.352%
21	8.562	2236	2246	2256	rVB3	18520	29609	3.59%	0.544%
22	8.796	2300	2319	2335	rBV9	10496	25568	3.10%	0.470%
23	9.423	2498	2514	2531	rBV	438120	709027	86.01%	13.038%
24	10.639	2879	2892	2909	rBV	361383	582331	70.64%	10.708%
25	11.652	3200	3207	3213	rVV4	5679	8824	1.07%	0.162%
26	11.819	3246	3259	3275	rBV	458678	717927	87.09%	13.201%
27	12.105	3329	3348	3361	rBV	39635	62040	7.53%	1.141%
28	12.192	3364	3375	3391	rVB2	13705	21709	2.63%	0.399%
29	12.308	3402	3411	3421	rBV3	8125	11554	1.40%	0.212%
30	12.398	3429	3439	3449	rBV3	16627	26404	3.20%	0.486%
31	12.716	3523	3538	3548	rBV6	13089	23917	2.90%	0.440%
32	12.873	3566	3587	3591	rBV5	11325	23366	2.83%	0.430%
33	12.947	3602	3610	3618	rBV4	10739	16372	1.99%	0.301%
34	13.118	3653	3663	3675	rVB3	26276	47394	5.75%	0.871%
35	13.234	3687	3699	3704	rBV2	18109	29241	3.55%	0.538%
36	13.333	3719	3730	3739	rBV3	12840	18462	2.24%	0.339%

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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	13.391	3739	3748	3759	rVB5	10105	15729	1.91%	0.289%
38	13.472	3759	3773	3784	rBV5	6490	11998	1.46%	0.221%
39	13.590	3799	3810	3821	rVB5	7150	12516	1.52%	0.230%
40	13.758	3852	3862	3873	rBV10	4588	10439	1.27%	0.192%
41	13.893	3894	3904	3906	rVV3	18984	26057	3.16%	0.479%
42	13.918	3907	3912	3922	rVB	34850	50349	6.11%	0.926%
43	14.066	3951	3958	3966	rBV2	6653	9542	1.16%	0.175%
44	14.304	4017	4032	4040	rBV4	10891	20304	2.46%	0.373%
45	14.356	4040	4048	4059	rVB4	8736	13986	1.70%	0.257%
46	14.690	4140	4152	4158	rBV5	10266	21123	2.56%	0.388%
47	14.816	4181	4191	4203	rBV2	42655	66002	8.01%	1.214%
48	14.883	4203	4212	4224	rVB3	29803	48378	5.87%	0.890%
49	15.034	4246	4259	4268	rBV4	6419	11757	1.43%	0.216%
50	15.201	4303	4311	4326	rVB7	7882	16266	1.97%	0.299%

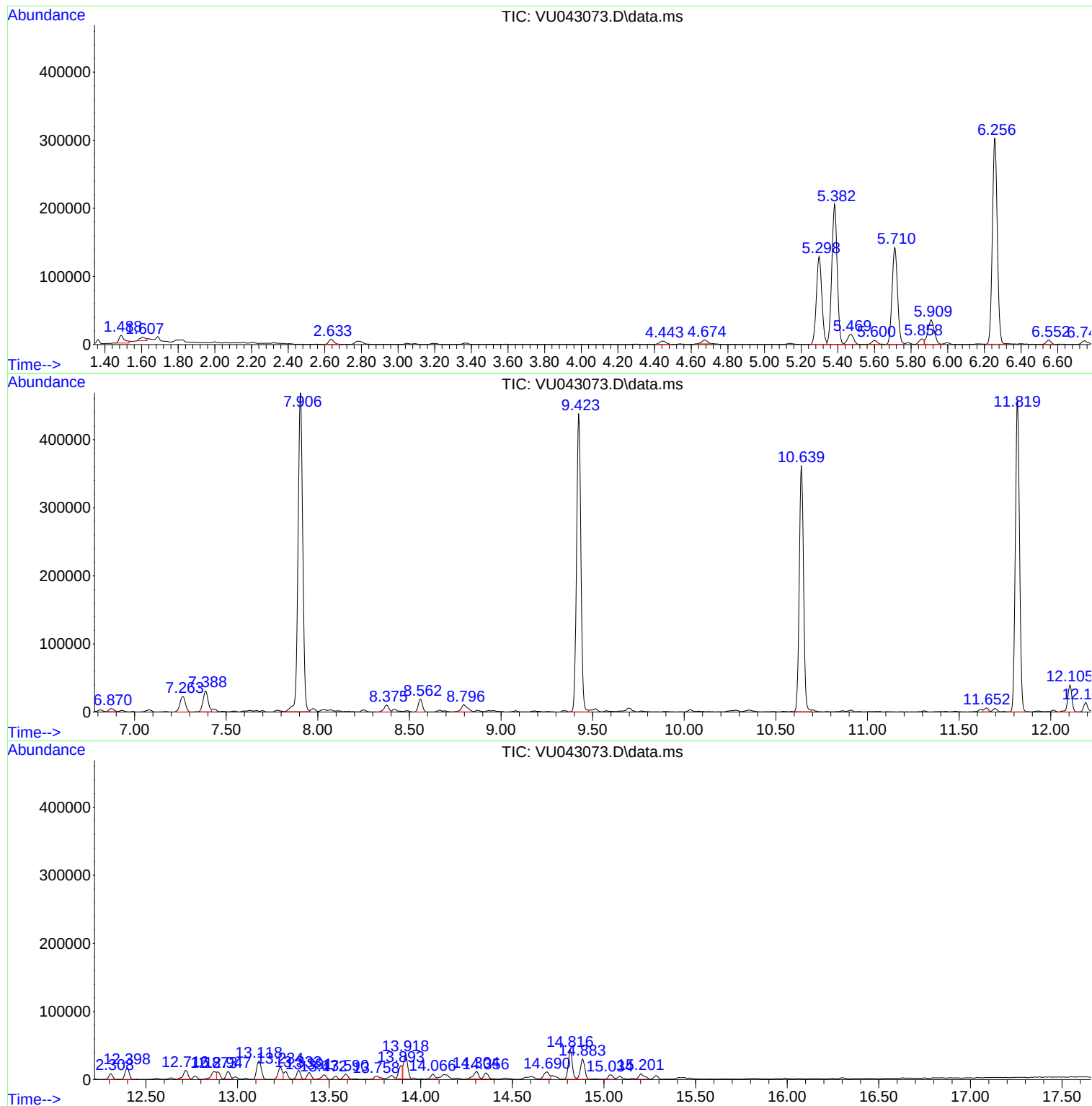
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Instrument :
MSVOA_U
ClientSampled :
W-2

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



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Sample : M1978-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
W-2

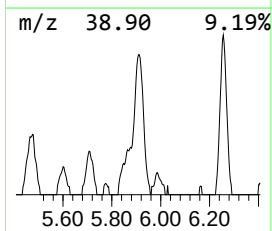
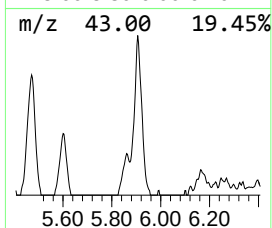
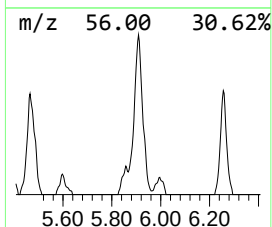
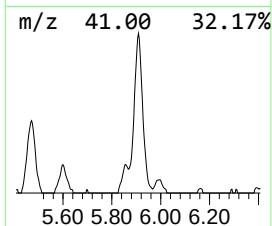
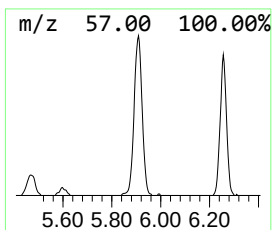
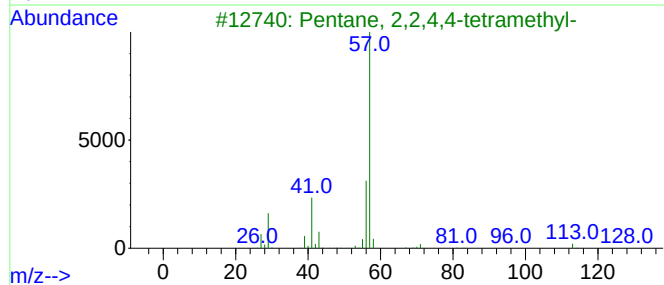
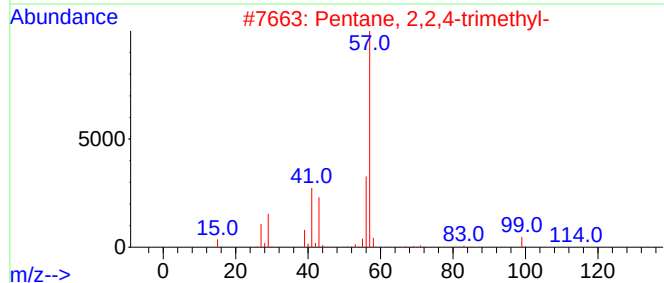
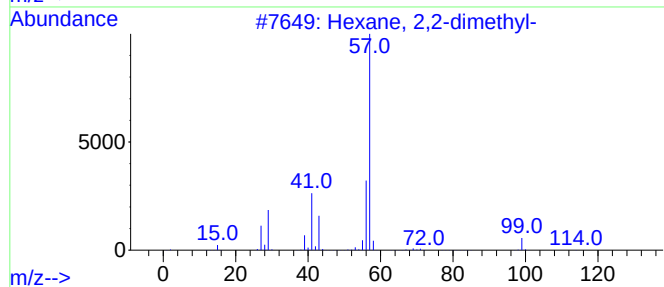
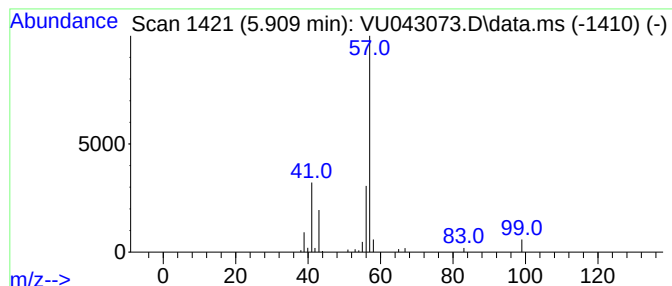
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.909	7.73 ug/l	86920	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
4			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	56
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45



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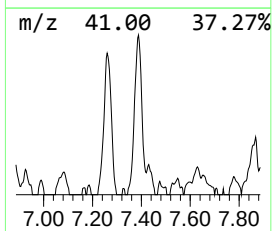
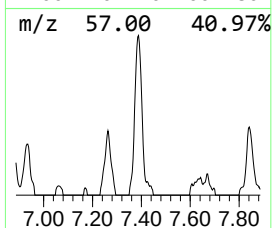
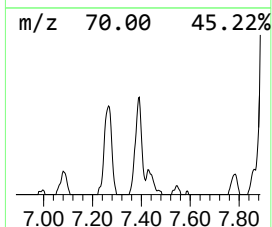
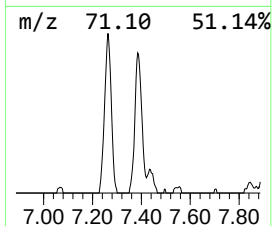
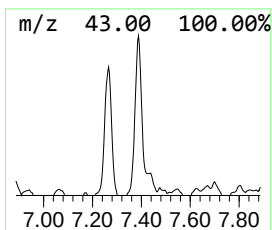
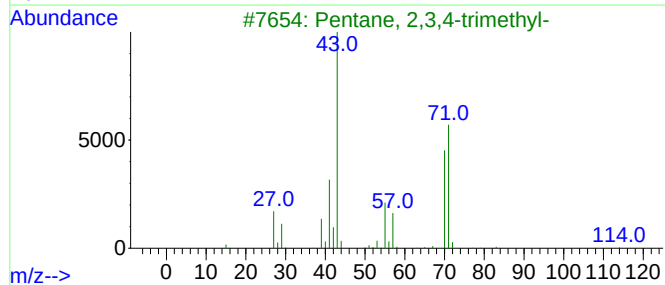
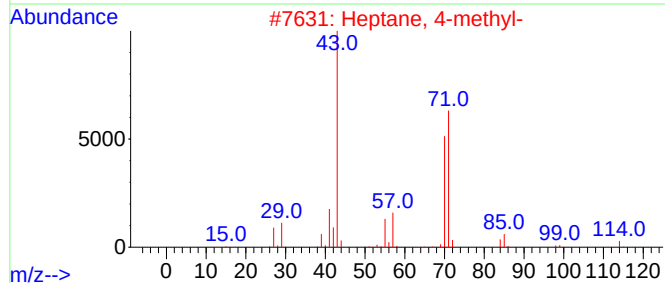
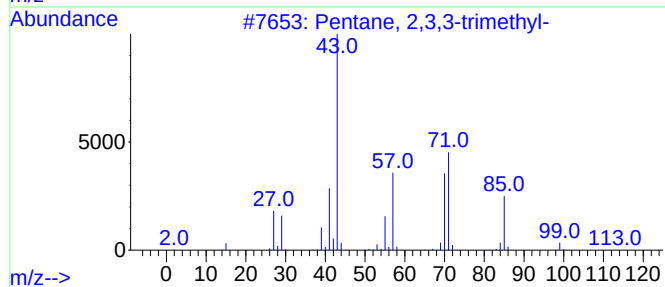
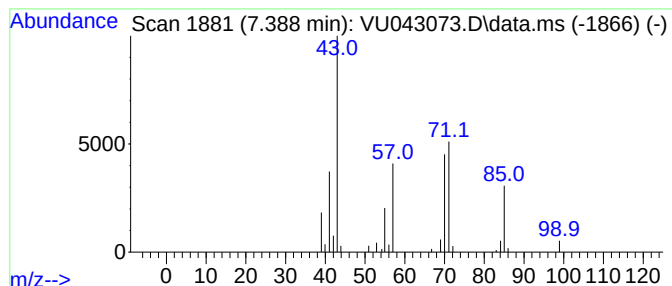
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.388	5.21 ug/l	58565	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 2,2-dim...	5.909	7.7	ug/l	86920	2	6.256	562521	50.0
Pentane, 2,3,3-...	7.388	5.2	ug/l	58565	2	6.256	562521	50.0