

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
 Data File : VU048356.D
 Acq On : 29 Apr 2022 14:45
 Operator : SY/MD
 Sample : N2562-11ME
 Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW472ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	36	43	50	rBV3	12431	20985	1.22%	0.129%
2	1.597	73	80	118	rVB	96406	262602	15.22%	1.617%
3	2.128	238	245	257	rVB	46789	69280	4.02%	0.426%
4	2.530	356	370	385	rBV	252740	463278	26.85%	2.852%
5	3.044	495	530	543	rBV4	27515	77137	4.47%	0.475%
6	3.176	559	571	592	rVB	27424	63807	3.70%	0.393%
7	3.327	605	618	637	rVB4	14891	33116	1.92%	0.204%
8	3.565	683	692	693	rBV3	1295	1609	0.09%	0.010%
9	3.668	710	724	741	rVV2	30344	67786	3.93%	0.417%
10	4.411	946	955	956	rBV2	948	1245	0.07%	0.008%
11	4.507	971	985	1001	rBV3	15863	38171	2.21%	0.235%
12	4.636	1011	1025	1044	rBV	126606	401165	23.25%	2.470%
13	5.060	1139	1157	1185	rBV	289468	663276	38.45%	4.083%
14	5.362	1234	1251	1267	rBV8	20846	58780	3.41%	0.362%
15	5.446	1267	1277	1290	rVB4	6005	13566	0.79%	0.084%
16	5.578	1305	1318	1333	rBV2	14945	33785	1.96%	0.208%
17	5.716	1340	1361	1388	rBV2	676440	1725201	100.00%	10.620%
18	5.838	1393	1399	1410	rVV5	8458	15820	0.92%	0.097%
19	5.909	1412	1421	1430	rVB5	5055	8456	0.49%	0.052%
20	5.976	1430	1442	1474	rVB5	24648	63412	3.68%	0.390%
21	6.124	1474	1488	1501	rBV2	31110	59666	3.46%	0.367%
22	6.243	1510	1525	1551	rBV	594517	1169384	67.78%	7.199%
23	6.523	1603	1612	1625	rBV7	6464	13220	0.77%	0.081%
24	6.597	1627	1635	1649	rBV2	6207	11829	0.69%	0.073%
25	6.687	1649	1663	1677	rBV	379011	769093	44.58%	4.735%
26	6.851	1709	1714	1715	rBV3	2586	1827	0.11%	0.011%
27	6.976	1742	1753	1763	rVV3	8628	16298	0.94%	0.100%
28	7.070	1767	1782	1794	rBV6	6885	12861	0.75%	0.079%
29	7.227	1807	1831	1852	rVV6	12098	42168	2.44%	0.260%
30	7.304	1852	1855	1860	rVB4	751	693	0.04%	0.004%
31	7.420	1881	1891	1898	rBV5	2844	5409	0.31%	0.033%
32	7.491	1900	1913	1922	rVV5	10039	20755	1.20%	0.128%
33	7.565	1923	1936	1956	rVV2	193408	388975	22.55%	2.395%
34	7.787	2000	2005	2007	rBV5	2020	1884	0.11%	0.012%
35	7.854	2016	2026	2027	rBV	12469	15347	0.89%	0.094%
36	7.896	2028	2039	2054	rVV	776677	1451880	84.16%	8.938%

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 ALS Vial : 11 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMULM042522WMA.M
 Title : VOC Analysis

37	7.970	2055	2062	2086	rVB	86968	182936	10.60%	1.126%
38	8.127	2105	2111	2118	rVB2	17424	23987	1.39%	0.148%
39	8.182	2118	2128	2155	rVB2	119355	287289	16.65%	1.769%
40	8.369	2174	2186	2194	rVB10	4507	8605	0.50%	0.053%
41	8.539	2233	2239	2245	rVB4	1133	1239	0.07%	0.008%
42	8.661	2259	2277	2304	rBV	524988	1135267	65.80%	6.989%
43	8.803	2314	2321	2331	rVB6	7345	12910	0.75%	0.079%
44	8.864	2333	2340	2349	rVB3	12493	21147	1.23%	0.130%
45	8.925	2349	2359	2369	rBV8	5210	10649	0.62%	0.066%
46	9.073	2396	2405	2413	rVV6	3727	5896	0.34%	0.036%
47	9.121	2413	2420	2426	rVV5	1901	2693	0.16%	0.017%
48	9.166	2426	2434	2441	rVV7	4212	6894	0.40%	0.042%
49	9.211	2442	2448	2457	rVB4	5070	8154	0.47%	0.050%
50	9.336	2478	2487	2495	rVB3	4993	7742	0.45%	0.048%
51	9.423	2500	2514	2536	rBV	793967	1603721	92.96%	9.872%
52	9.574	2550	2561	2576	rVB2	42759	76679	4.44%	0.472%
53	9.697	2576	2599	2609	rBV	49705	107886	6.25%	0.664%
54	9.867	2646	2652	2653	rBV4	879	721	0.04%	0.004%
55	9.886	2656	2658	2665	rVB2	898	802	0.05%	0.005%
56	10.031	2691	2703	2711	rBV6	2733	6352	0.37%	0.039%
57	10.108	2716	2727	2741	rVV2	20845	39385	2.28%	0.242%
58	10.246	2757	2770	2773	rBV6	3652	6283	0.36%	0.039%
59	10.359	2797	2805	2812	rBV6	6465	11446	0.66%	0.070%
60	10.491	2833	2846	2855	rBV2	7387	12717	0.74%	0.078%
61	10.626	2879	2888	2891	rVV5	949	1321	0.08%	0.008%
62	10.671	2896	2902	2916	rVB7	2882	6070	0.35%	0.037%
63	10.767	2918	2932	2956	rBV	694928	1137723	65.95%	7.004%
64	10.912	2968	2977	2988	rBV2	12382	19829	1.15%	0.122%
65	11.005	2998	3006	3021	rBV	13527	30547	1.77%	0.188%
66	11.098	3028	3035	3038	rBV2	6692	9392	0.54%	0.058%
67	11.253	3077	3083	3086	rBV4	783	701	0.04%	0.004%
68	11.298	3086	3097	3114	rVB2	8331	15454	0.90%	0.095%
69	11.420	3128	3135	3140	rBV6	1731	2121	0.12%	0.013%
70	11.475	3140	3152	3163	rBV	37626	61327	3.55%	0.378%
71	11.581	3177	3185	3189	rBV5	1101	1768	0.10%	0.011%
72	11.648	3200	3206	3214	rVB	4113	5960	0.35%	0.037%
73	11.706	3216	3224	3232	rBV9	3123	6389	0.37%	0.039%
74	11.819	3244	3259	3275	rBV	1059253	1691674	98.06%	10.414%
75	11.899	3278	3284	3294	rVB	13230	20578	1.19%	0.127%
76	12.102	3340	3347	3350	rBV5	3552	4759	0.28%	0.029%

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 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW472ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMULM042522WMA.M
 Title : VOC Analysis

77	12.198	3364	3377	3397	rVB	911974	1494497	86.63%	9.200%
78	12.275	3397	3401	3403	rBV4	950	803	0.05%	0.005%
79	12.330	3411	3418	3425	rVB6	5500	7859	0.46%	0.048%
80	12.378	3429	3433	3446	rVB5	3788	6923	0.40%	0.043%
81	12.468	3451	3461	3466	rBV3	4673	7534	0.44%	0.046%
82	12.574	3488	3494	3501	rVB3	5189	7070	0.41%	0.044%
83	12.687	3523	3529	3537	rBV6	3317	5838	0.34%	0.036%
84	12.770	3551	3555	3558	rBV3	1143	1089	0.06%	0.007%
85	12.883	3583	3590	3593	rBV3	3503	4336	0.25%	0.027%
86	13.031	3628	3636	3649	rVB4	4796	9200	0.53%	0.057%
87	13.111	3656	3661	3662	rBV3	892	795	0.05%	0.005%
88	13.253	3701	3705	3706	rBV2	1364	888	0.05%	0.005%
89	13.561	3798	3801	3805	rBV3	759	716	0.04%	0.004%
90	13.593	3807	3811	3816	rVV8	1287	1458	0.08%	0.009%
91	13.687	3838	3840	3846	rVB5	1098	838	0.05%	0.005%
92	13.729	3849	3853	3855	rBV3	1362	1072	0.06%	0.007%
93	13.841	3878	3888	3898	rBV9	4881	9657	0.56%	0.059%
94	13.944	3914	3920	3931	rVB7	2928	4804	0.28%	0.030%
95	14.095	3961	3967	3974	rBV3	4145	5879	0.34%	0.036%
96	14.452	4072	4078	4084	rBV6	4189	5116	0.30%	0.031%
97	14.732	4162	4165	4170	rBV4	1016	774	0.04%	0.005%
98	14.809	4187	4189	4196	rBV7	1546	1101	0.06%	0.007%
99	14.937	4224	4229	4235	rBV6	2366	2662	0.15%	0.016%
100	15.024	4252	4256	4262	rBV7	2459	2648	0.15%	0.016%

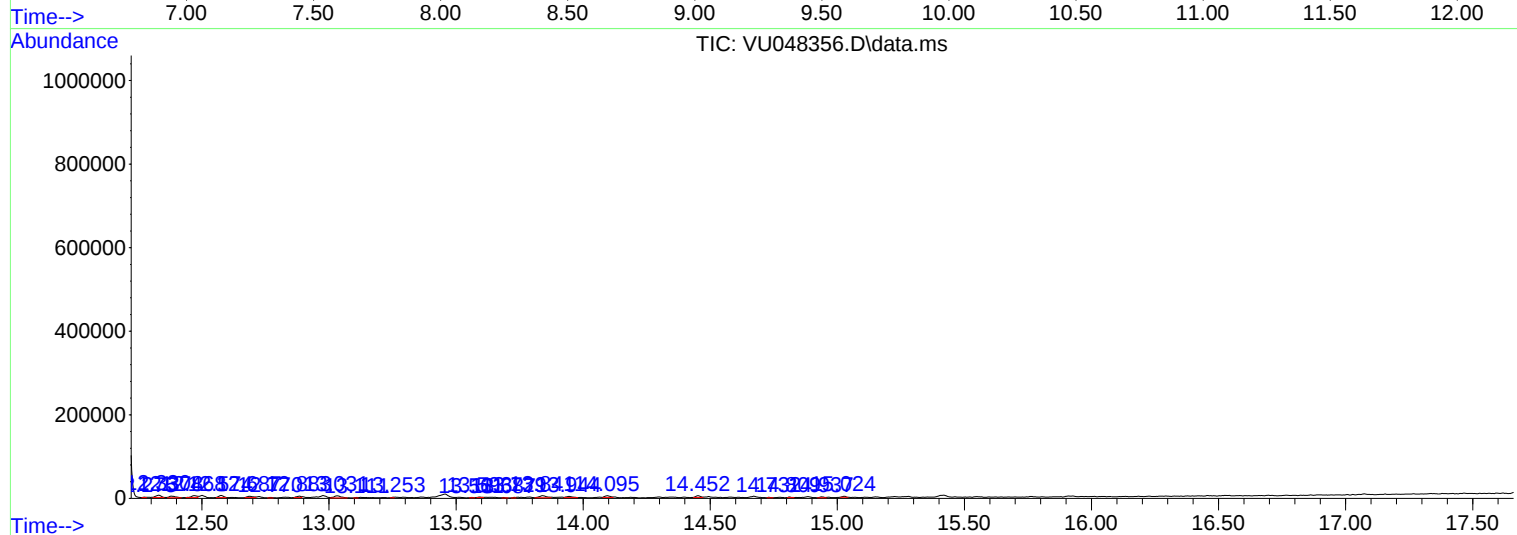
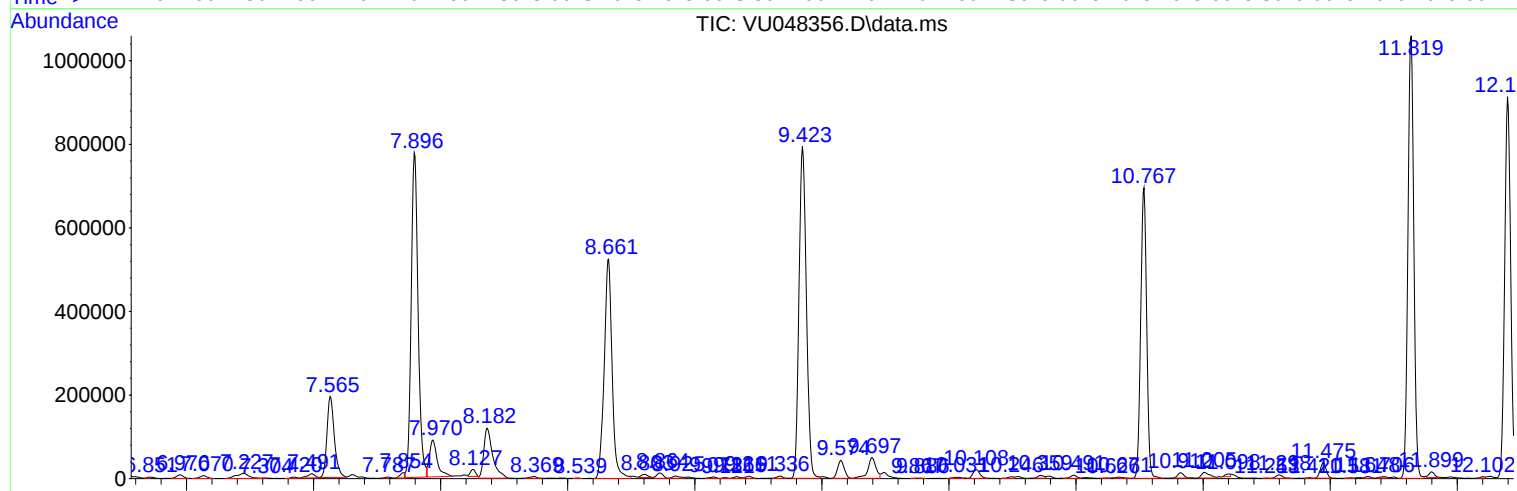
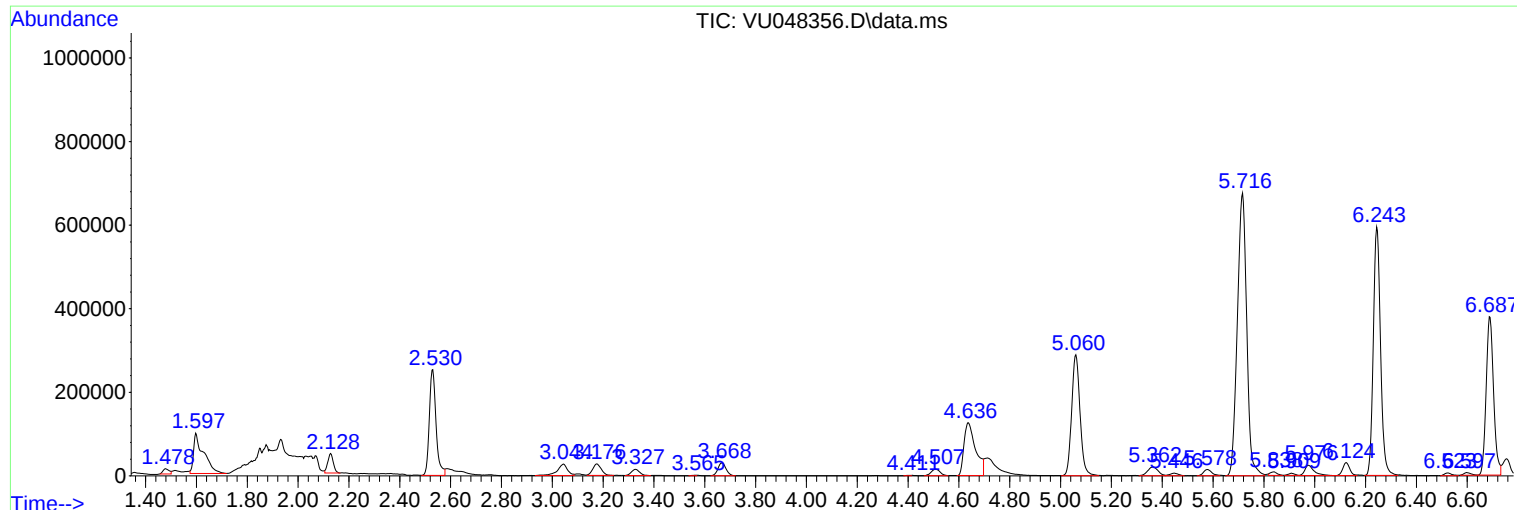
Sum of corrected areas: 16244336

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW472ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW472ME

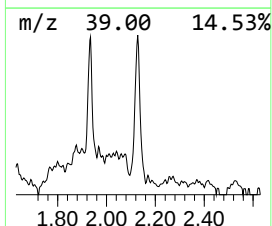
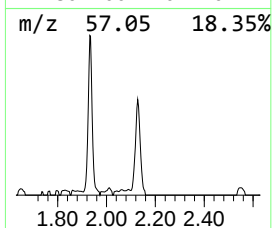
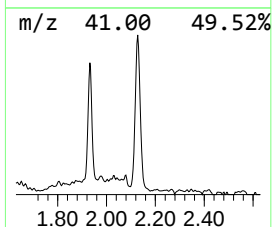
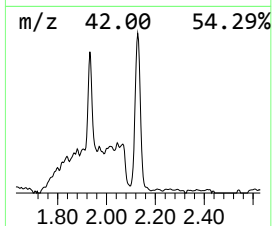
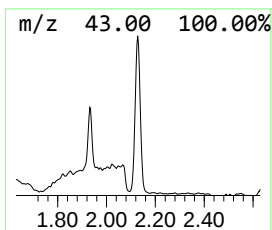
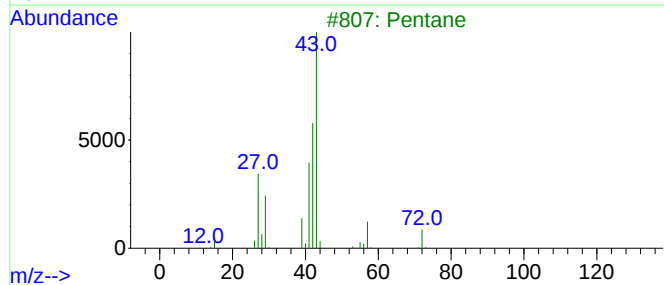
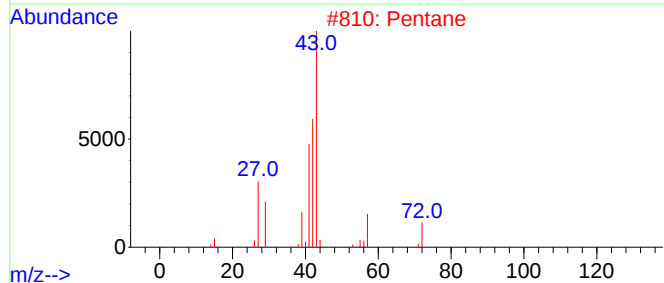
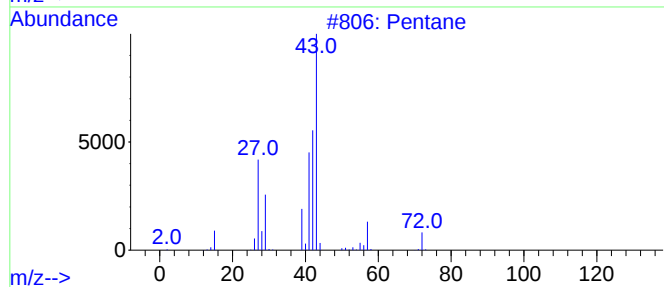
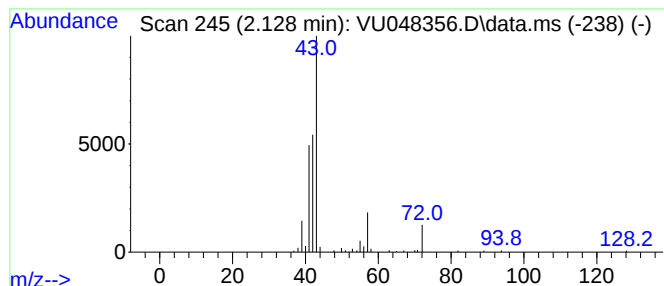
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	2.96 ug/L	69280	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	86
2	Pentane			72	C5H12	000109-66-0	86
3	Pentane			72	C5H12	000109-66-0	80
4	Pentane			72	C5H12	000109-66-0	72
5	Butane, 2,3-dimethyl-			86	C6H14	000079-29-8	25



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Instrument :
MSVOA_U
ClientSampleId :
EW472ME

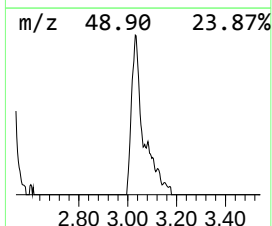
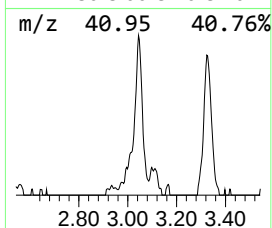
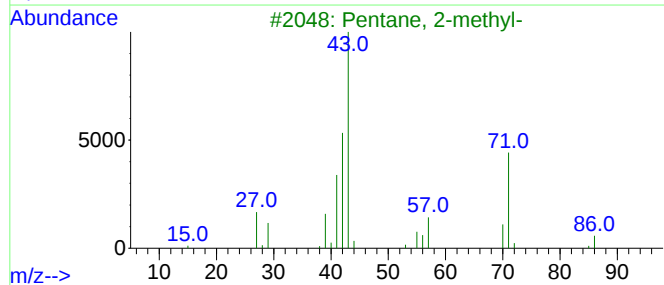
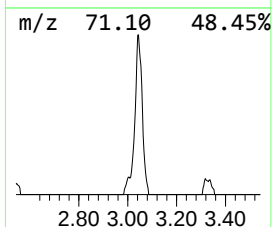
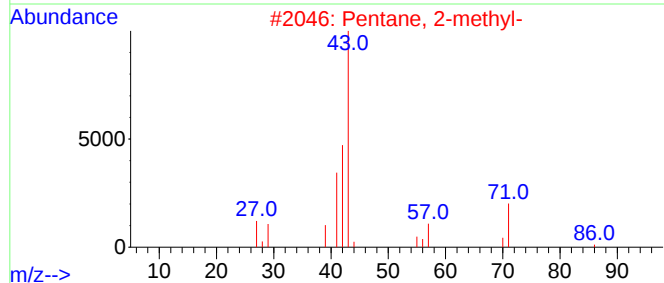
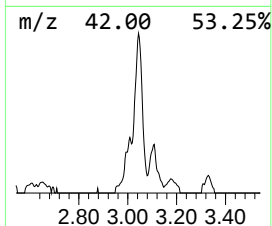
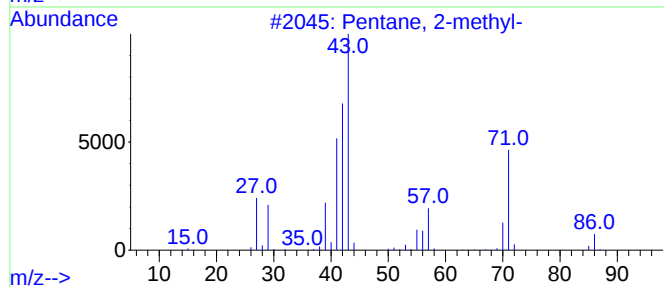
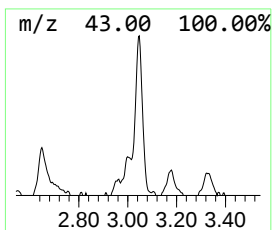
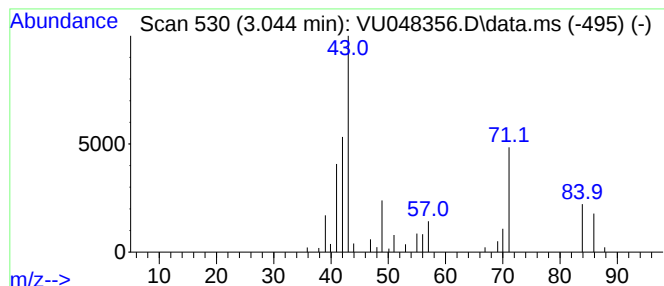
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.044	3.30 ug/L	77137	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	32
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	32



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW472ME

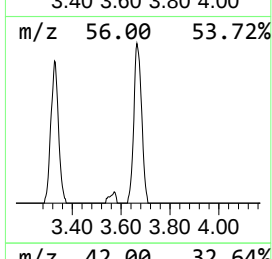
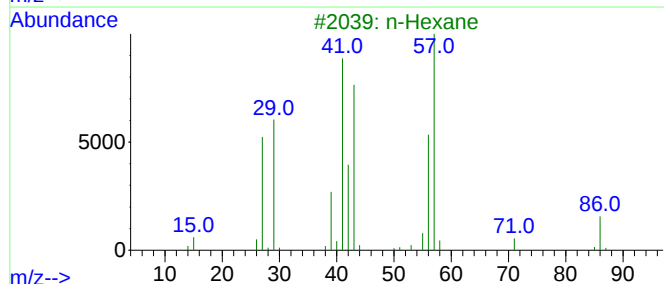
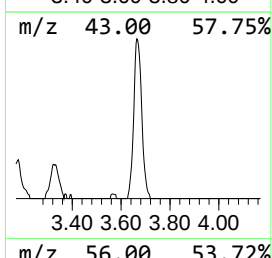
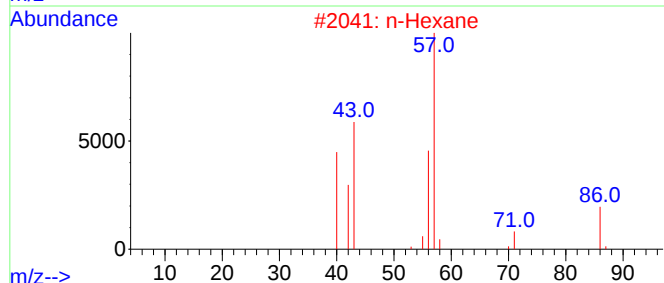
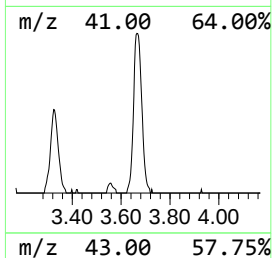
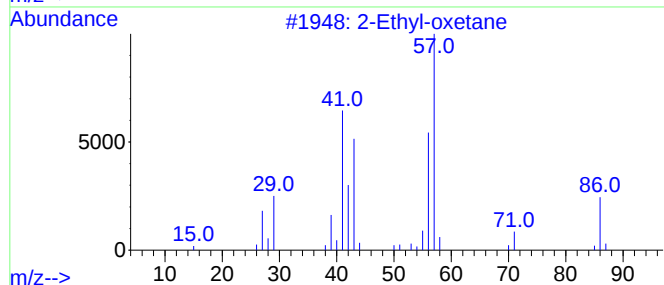
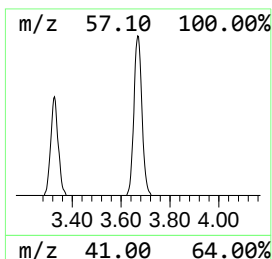
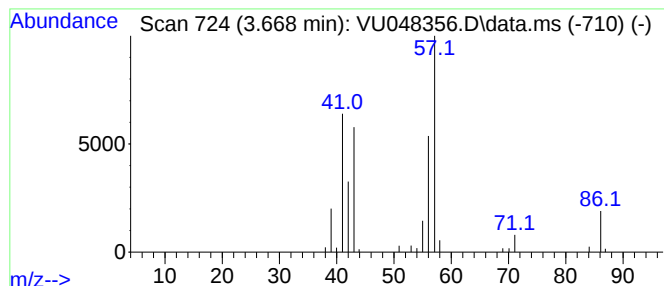
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Quant Title : VOC Analysis

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

Peak Number 4 2-Ethyl-oxetane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.668	2.90 ug/L	67786	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	91
2			n-Hexane	86	C6H14	000110-54-3	86
3			n-Hexane	86	C6H14	000110-54-3	83
4			n-Hexane	86	C6H14	000110-54-3	83
5			n-Hexane	86	C6H14	000110-54-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048356.D
Acq On : 29 Apr 2022 14:45
Operator : SY/MD
Sample : N2562-11ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW472ME

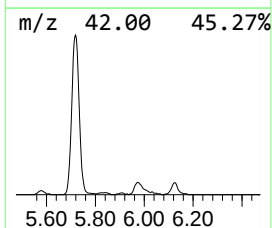
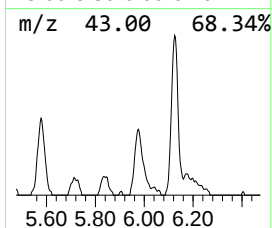
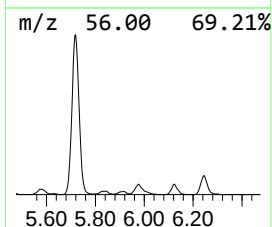
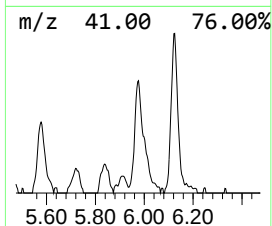
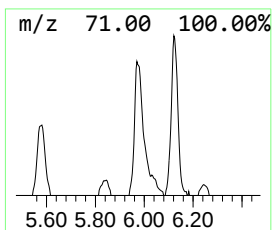
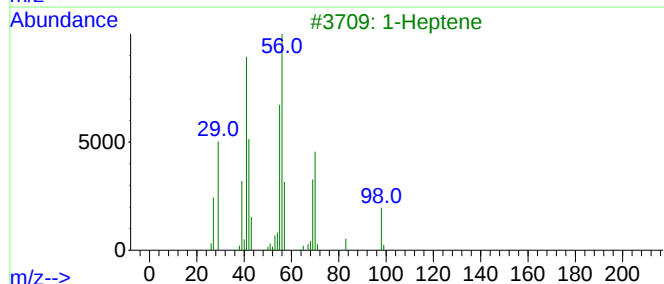
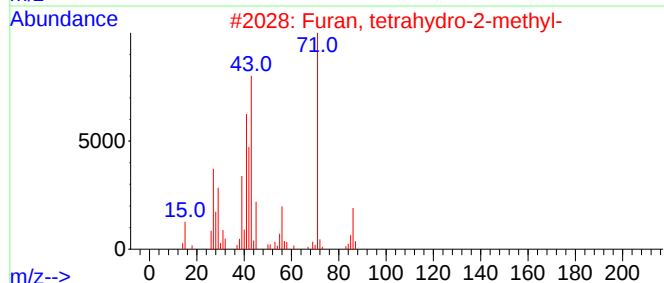
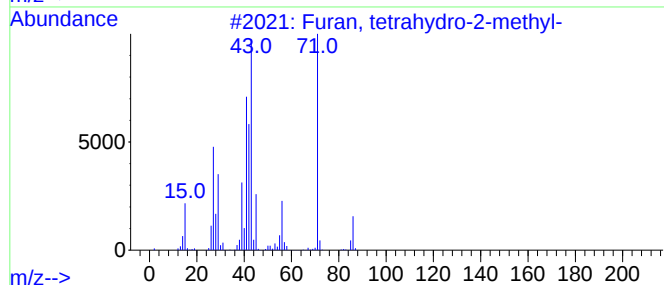
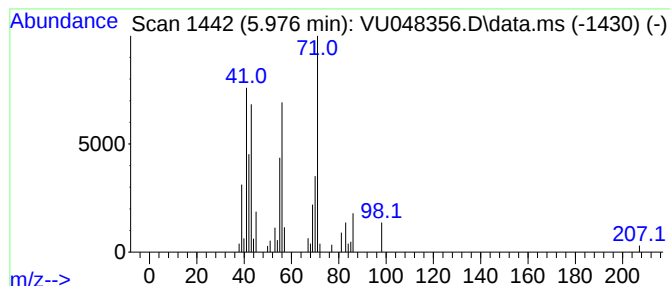
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Quant Title : VOC Analysis

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

Peak Number 5 Furan, tetrahydro-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.976	2.71 ug/L	63412	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	52
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	52
3			1-Heptene	98	C7H14	000592-76-7	50
4			1-Heptene	98	C7H14	000592-76-7	46
5			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048356.D
Acq On : 29 Apr 2022 14:45
Operator : SY/MD
Sample : N2562-11ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

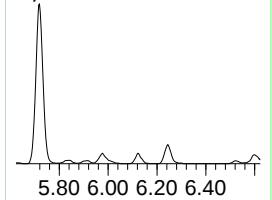
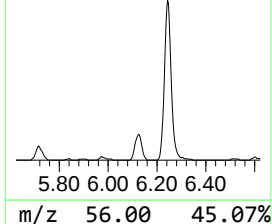
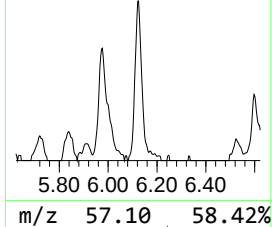
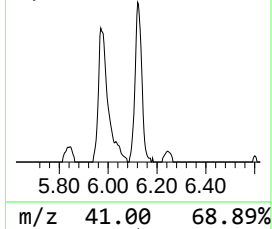
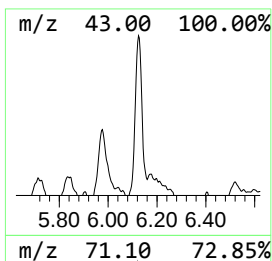
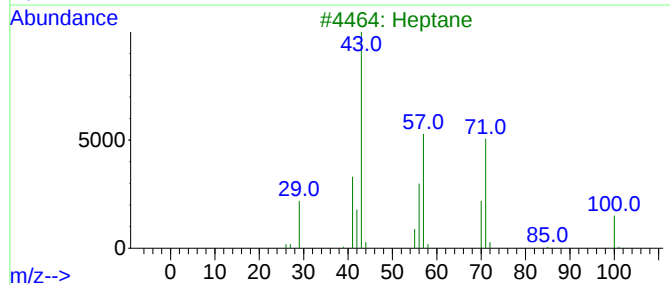
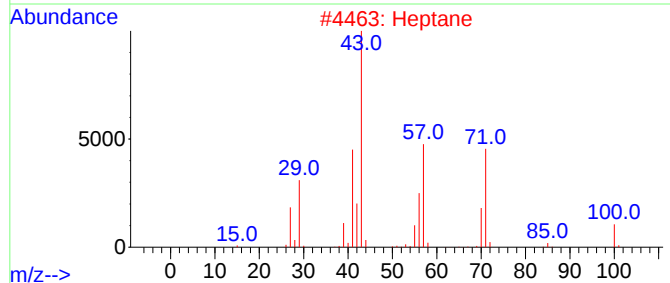
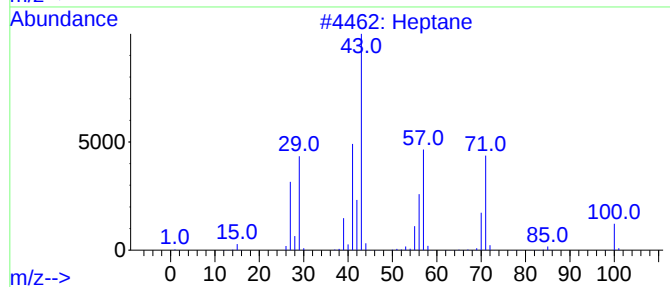
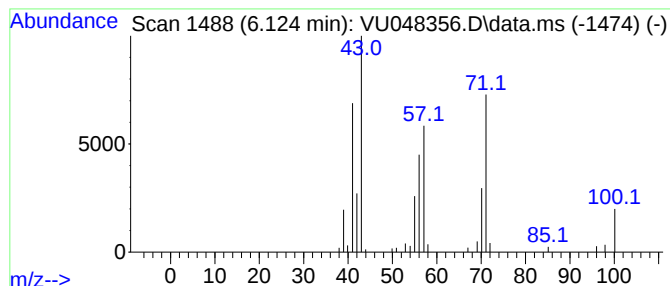
Instrument :
MSVOA_U
ClientSampleId :
EW472ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.124	2.55 ug/L	59666	1,4-Difluorobenzene	6.243	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	87
2	Heptane	100	C7H16	000142-82-5	78
3	Heptane	100	C7H16	000142-82-5	72
4	Heptane	100	C7H16	000142-82-5	64
5	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048356.D
Acq On : 29 Apr 2022 14:45
Operator : SY/MD
Sample : N2562-11ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW472ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.128	3.0	ug/L	69280	1	6.243	1169380	50.0
(DEL) Alkane: S...	3.044	3.3	ug/L	77137	1	6.243	1169380	50.0
2-Ethyl-oxetane	3.668	2.9	ug/L	67786	1	6.243	1169380	50.0
Furan, tetrahyd...	5.976	2.7	ug/L	63412	1	6.243	1169380	50.0
(DEL) Alkane: S...	6.124	2.5	ug/L	59666	1	6.243	1169380	50.0