

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
 Data File : VU055906.D
 Acq On : 26 Oct 2023 15:36
 Operator : MD/SY
 Sample : 04961-14ME
 Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0LJ1ME

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055906.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.477	49	58	66	rBV3	17419	39455	0.76%	0.159%
2	1.595	88	95	121	rVB	220853	359761	6.89%	1.453%
3	1.872	176	181	201	rVB	51237	87222	1.67%	0.352%
4	2.541	377	389	415	rBV	423286	745227	14.26%	3.009%
5	2.766	451	459	460	rBV3	2172	2207	0.04%	0.009%
6	2.862	483	489	492	rBV3	568	629	0.01%	0.003%
7	2.927	507	509	512	rBV3	715	548	0.01%	0.002%
8	3.036	530	543	549	rBV3	7588	14855	0.28%	0.060%
9	3.174	572	586	603	rBV	24010	58060	1.11%	0.234%
10	3.293	620	623	624	rBV3	746	416	0.01%	0.002%
11	3.332	628	635	637	rBV5	1339	1572	0.03%	0.006%
12	3.467	673	677	681	rVB2	373	361	0.01%	0.001%
13	3.666	734	739	740	rBV2	1754	1258	0.02%	0.005%
14	3.859	794	799	801	rBV	374	319	0.01%	0.001%
15	3.930	818	821	825	rBV3	459	402	0.01%	0.002%
16	4.145	884	888	891	rVV	580	421	0.01%	0.002%
17	4.280	923	930	934	rBV	322	353	0.01%	0.001%
18	4.502	995	999	1000	rBV	677	472	0.01%	0.002%
19	4.531	1006	1008	1014	rVB2	894	664	0.01%	0.003%
20	4.628	1023	1038	1086	rBV2	124827	450829	8.63%	1.820%
21	4.859	1108	1110	1113	rBV2	486	348	0.01%	0.001%
22	5.055	1153	1171	1206	rBV	377231	897591	17.18%	3.624%
23	5.328	1239	1256	1262	rBV7	5722	14535	0.28%	0.059%
24	5.451	1291	1294	1298	rBV4	518	334	0.01%	0.001%
25	5.515	1312	1314	1321	rVB3	542	424	0.01%	0.002%
26	5.714	1354	1376	1410	rBV2	874754	2287311	43.77%	9.235%
27	5.869	1421	1424	1427	rVB3	1024	755	0.01%	0.003%
28	5.888	1427	1430	1438	rVB3	728	854	0.02%	0.003%
29	5.920	1438	1440	1447	rVB3	557	443	0.01%	0.002%
30	5.975	1447	1457	1469	rBV6	4678	11107	0.21%	0.045%
31	6.123	1496	1503	1505	rBV4	1709	1798	0.03%	0.007%
32	6.161	1512	1515	1519	rVB3	845	518	0.01%	0.002%
33	6.242	1523	1540	1571	rBV	615566	1252053	23.96%	5.055%
34	6.537	1617	1632	1644	rBV2	61352	122610	2.35%	0.495%
35	6.685	1664	1678	1711	rBV	493690	1005281	19.24%	4.059%
36	6.801	1712	1714	1718	rVB2	1351	696	0.01%	0.003%

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 ALS Vial : 16 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 E0LJ1ME

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\SFAMULM101023WMA.M
 Title : VOC Analysis

37	6.939	1755	1757	1762	rVV2	478	372	0.01%	0.002%
38	7.013	1775	1780	1785	rBV3	404	457	0.01%	0.002%
39	7.045	1785	1790	1792	rBV3	780	714	0.01%	0.003%
40	7.116	1811	1812	1820	rVB2	625	420	0.01%	0.002%
41	7.190	1820	1835	1836	rBV4	5376	5914	0.11%	0.024%
42	7.328	1875	1878	1881	rBV3	713	529	0.01%	0.002%
43	7.415	1903	1905	1909	rBV	660	514	0.01%	0.002%
44	7.463	1917	1920	1922	rBV2	522	334	0.01%	0.001%
45	7.492	1922	1929	1937	rBV5	2788	4277	0.08%	0.017%
46	7.563	1938	1951	1975	rBV	262389	516537	9.89%	2.086%
47	7.701	1990	1994	1998	rBV6	1596	1762	0.03%	0.007%
48	7.788	2013	2021	2034	rVB7	5378	9115	0.17%	0.037%
49	7.894	2040	2054	2073	rBV	1025413	1874382	35.87%	7.568%
50	8.068	2105	2108	2110	rBV3	743	503	0.01%	0.002%
51	8.129	2119	2127	2131	rBV7	3929	5873	0.11%	0.024%
52	8.180	2132	2143	2171	rVB	163865	359076	6.87%	1.450%
53	8.296	2176	2179	2184	rVB4	514	382	0.01%	0.002%
54	8.338	2184	2192	2194	rBV5	1200	1544	0.03%	0.006%
55	8.399	2208	2211	2216	rBV3	701	651	0.01%	0.003%
56	8.431	2216	2221	2222	rBV2	688	544	0.01%	0.002%
57	8.479	2230	2236	2239	rVB4	1028	948	0.02%	0.004%
58	8.547	2243	2257	2276	rBV	3005618	5225280	100.00%	21.098%
59	8.647	2277	2288	2319	rVB	577086	1182207	22.62%	4.773%
60	8.920	2364	2373	2385	rBV10	4011	9105	0.17%	0.037%
61	9.055	2411	2415	2418	rBV4	1469	1277	0.02%	0.005%
62	9.116	2428	2434	2441	rVB5	3450	4187	0.08%	0.017%
63	9.171	2441	2451	2455	rBV7	5290	9187	0.18%	0.037%
64	9.209	2457	2463	2478	rVB3	11477	20034	0.38%	0.081%
65	9.270	2479	2482	2483	rBV2	772	344	0.01%	0.001%
66	9.332	2490	2501	2515	rBV3	11547	19498	0.37%	0.079%
67	9.418	2515	2528	2560	rBV	871684	1650857	31.59%	6.666%
68	9.563	2566	2573	2574	rBV6	2244	2144	0.04%	0.009%
69	9.653	2592	2601	2603	rBV7	1917	2326	0.04%	0.009%
70	9.698	2609	2615	2621	rBV5	5355	8945	0.17%	0.036%
71	9.743	2623	2629	2644	rVB4	21564	34589	0.66%	0.140%
72	9.868	2661	2668	2677	rVB4	2926	4349	0.08%	0.018%
73	9.910	2679	2681	2683	rBV	567	330	0.01%	0.001%
74	9.952	2686	2694	2704	rBV7	2228	4058	0.08%	0.016%
75	10.013	2706	2713	2727	rBV7	6321	12392	0.24%	0.050%
76	10.119	2733	2746	2758	rBV9	7733	19602	0.38%	0.079%

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Instrument :
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 ClientSampleId :
 E0LJ1ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

77	10.196	2768	2770	2771	rBV2	908	376	0.01%	0.002%
78	10.248	2777	2786	2797	rVB3	20728	34844	0.67%	0.141%
79	10.309	2802	2805	2807	rBV3	2313	1734	0.03%	0.007%
80	10.393	2823	2831	2844	rVB2	30184	48732	0.93%	0.197%
81	10.553	2868	2881	2891	rBV5	15961	36680	0.70%	0.148%
82	10.621	2897	2902	2908	rBV2	14203	17680	0.34%	0.071%
83	10.759	2927	2945	2976	rBV	794505	1313830	25.14%	5.305%
84	11.003	3018	3021	3022	rBV3	1620	1059	0.02%	0.004%
85	11.058	3030	3038	3045	rBV7	12707	23465	0.45%	0.095%
86	11.113	3046	3055	3070	rVB2	82353	135689	2.60%	0.548%
87	11.309	3110	3116	3128	rBV8	9345	13270	0.25%	0.054%
88	11.370	3130	3135	3140	rBV7	7811	10392	0.20%	0.042%
89	11.415	3141	3149	3157	rVB2	54688	75151	1.44%	0.303%
90	11.569	3191	3197	3203	rBV9	5404	8227	0.16%	0.033%
91	11.814	3262	3273	3286	rBV	1058245	1719866	32.91%	6.944%
92	12.000	3325	3331	3349	rVB4	25726	46900	0.90%	0.189%
93	12.193	3378	3391	3406	rBV	1111289	1828217	34.99%	7.382%
94	12.325	3424	3432	3442	rVB	187340	259977	4.98%	1.050%
95	12.663	3529	3537	3548	rBV4	28931	47387	0.91%	0.191%
96	13.003	3637	3643	3649	rBV3	21025	28579	0.55%	0.115%
97	13.129	3677	3682	3692	rVB3	26425	35509	0.68%	0.143%
98	13.428	3767	3775	3799	rVB	219847	375998	7.20%	1.518%
99	13.582	3815	3823	3831	rBV	105484	158838	3.04%	0.641%
100	14.447	4085	4092	4100	rVB	146772	187043	3.58%	0.755%

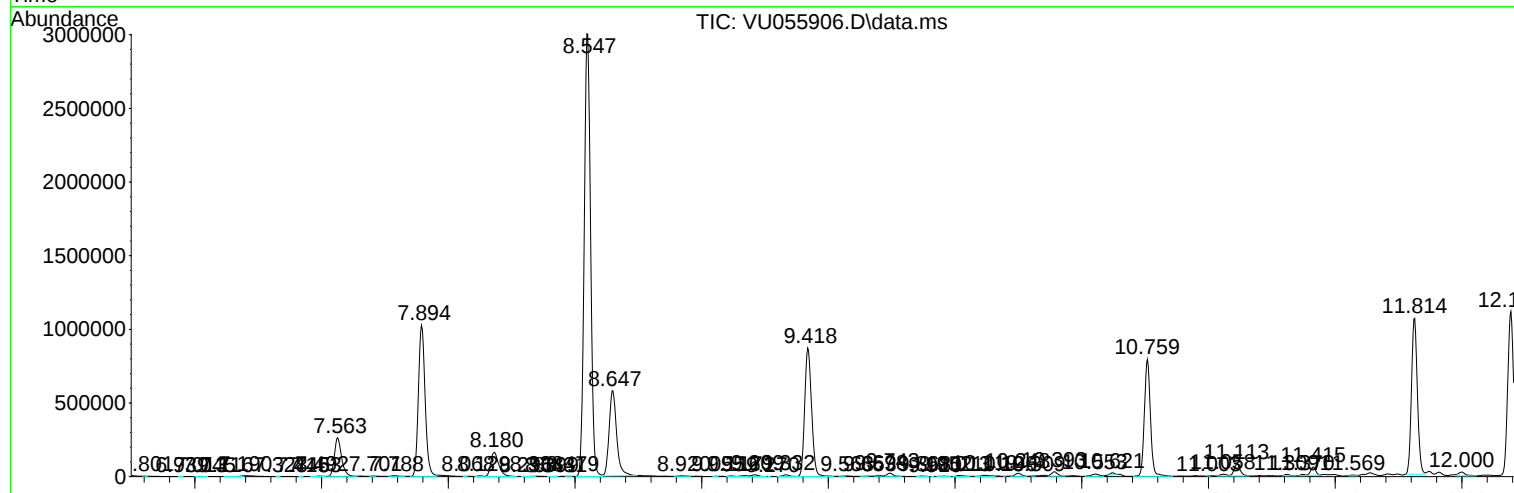
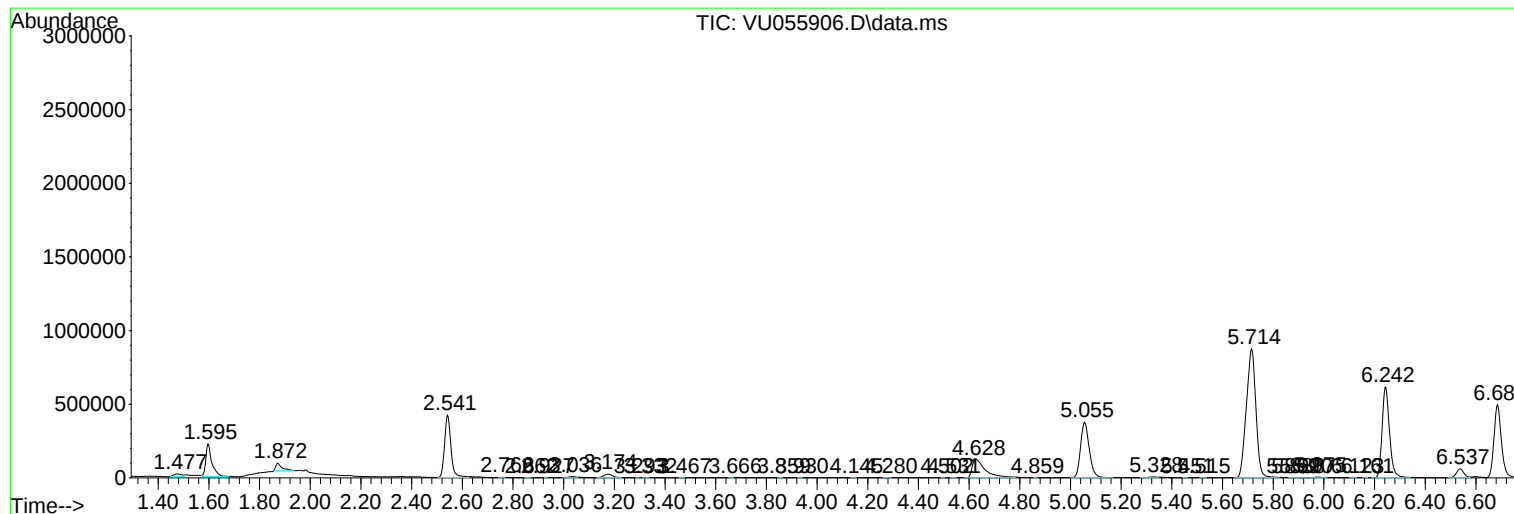
Sum of corrected areas: 24766691

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Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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Operator : MD/SY
Sample : 04961-14ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

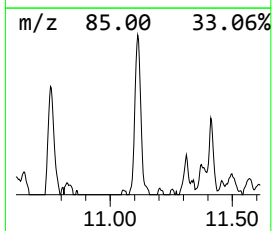
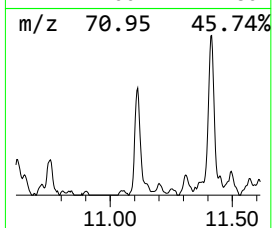
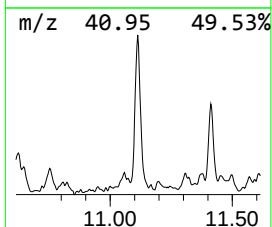
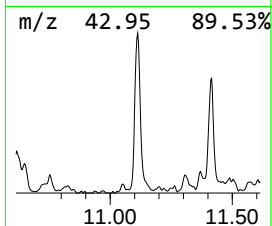
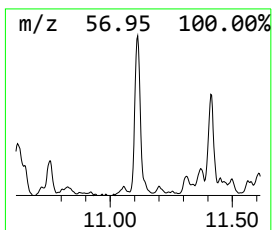
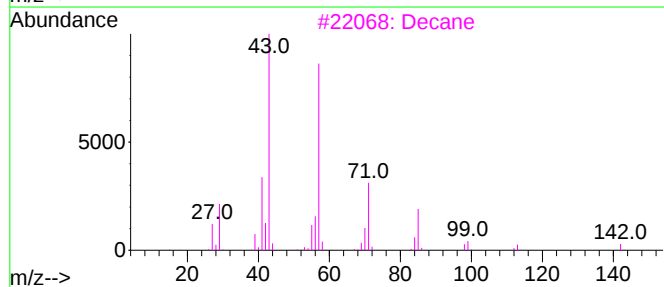
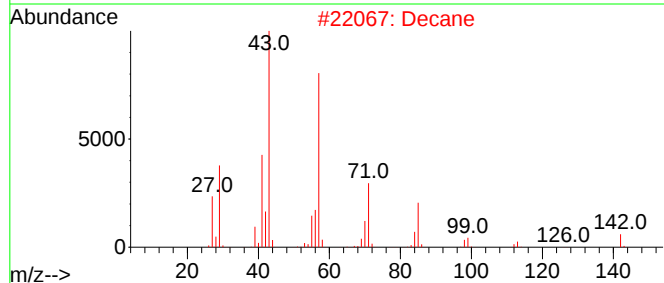
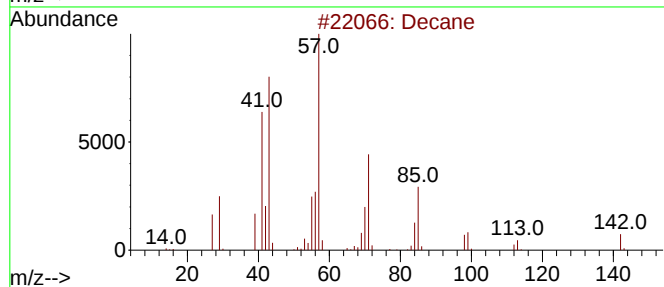
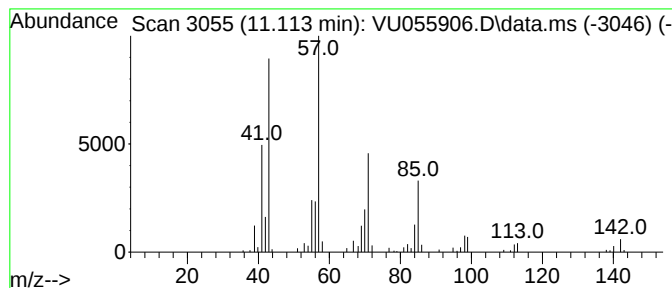
Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.113	3.94 ug/L	135689	1,4-Dichlorobenzene-d4		11.814	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane		142	C10H22	000124-18-5	97
2	Decane		142	C10H22	000124-18-5	95
3	Decane		142	C10H22	000124-18-5	90
4	Carbonic acid, prop-1-en-2-yl tr...		284	C17H32O3	1000382-90-8	78
5	Decane		142	C10H22	000124-18-5	70



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Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

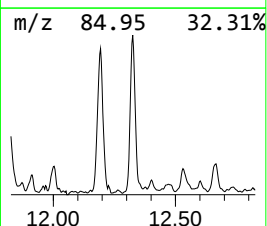
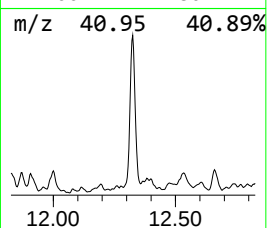
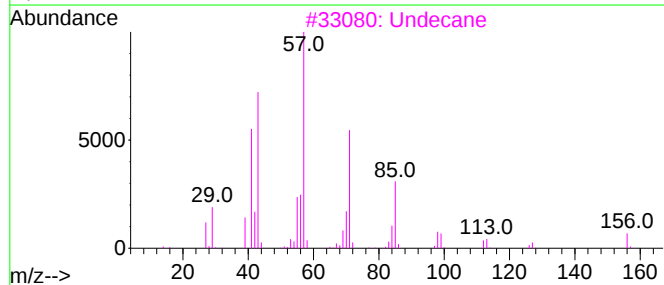
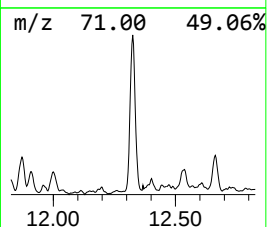
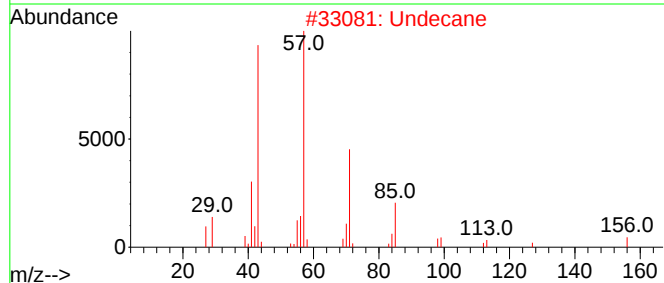
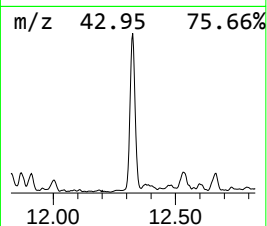
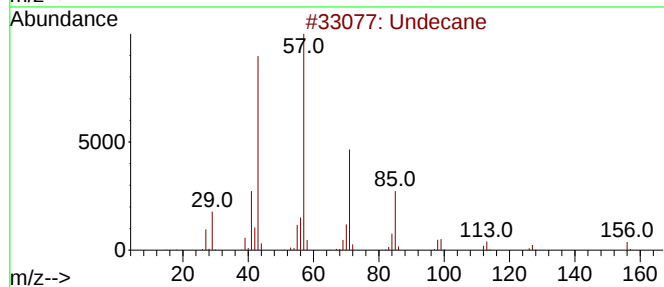
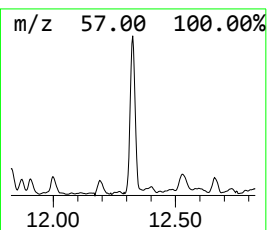
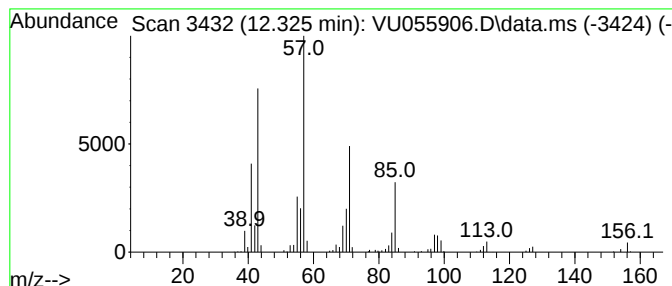
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.325	7.56 ug/L	259977	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	90
2	Undecane			156	C11H24	001120-21-4	90
3	Undecane			156	C11H24	001120-21-4	87
4	Undecane			156	C11H24	001120-21-4	81
5	Undecane			156	C11H24	001120-21-4	76



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Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

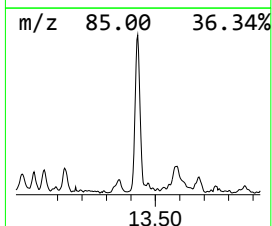
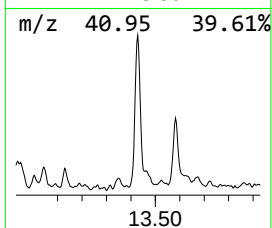
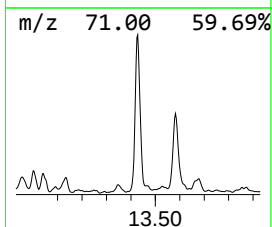
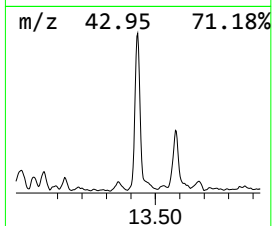
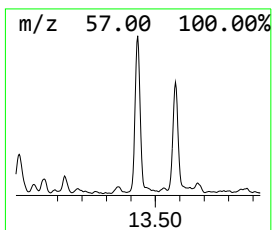
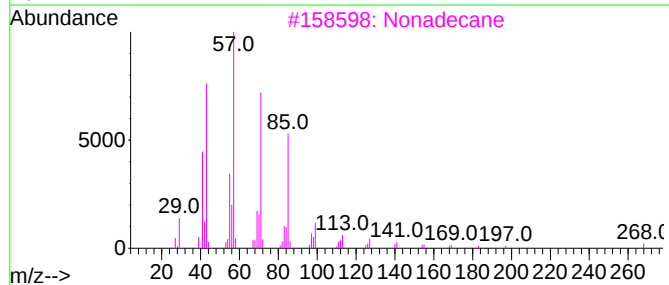
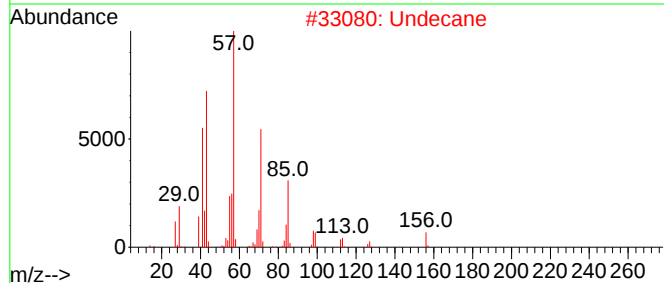
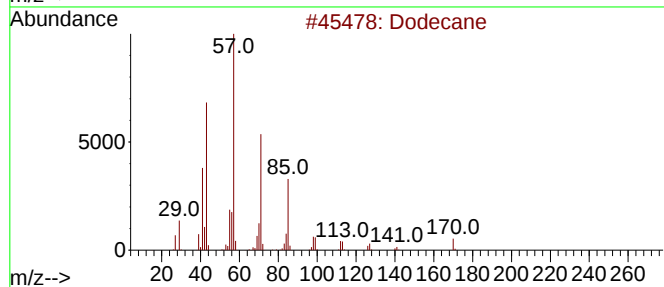
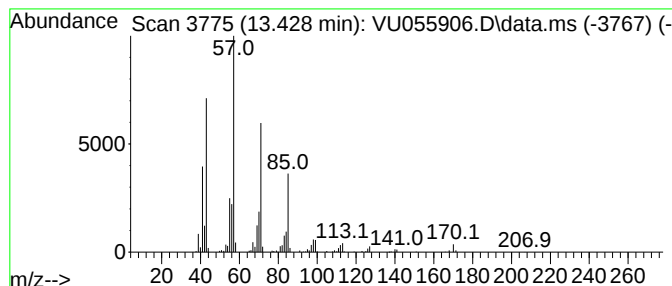
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.428	10.93 ug/L	375998	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	90
2			Undecane	156	C11H24	001120-21-4	83
3			Nonadecane	268	C19H40	000629-92-5	72
4			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	72
5			Decane	142	C10H22	000124-18-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
Data File : VU055906.D
Acq On : 26 Oct 2023 15:36
Operator : MD/SY
Sample : 04961-14ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

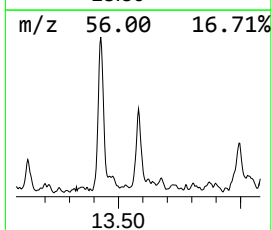
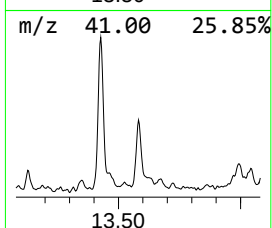
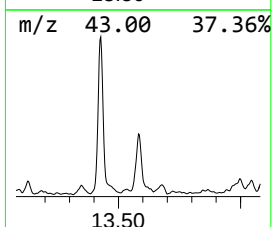
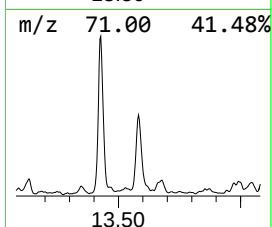
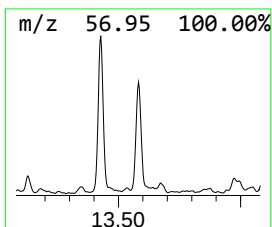
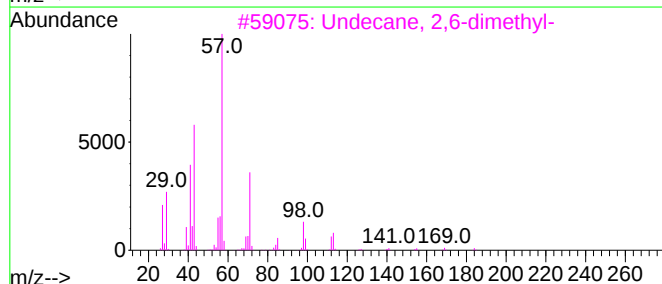
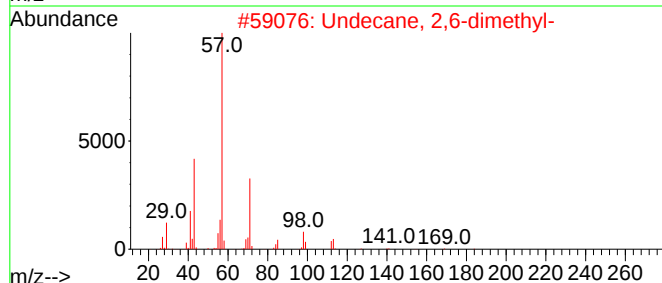
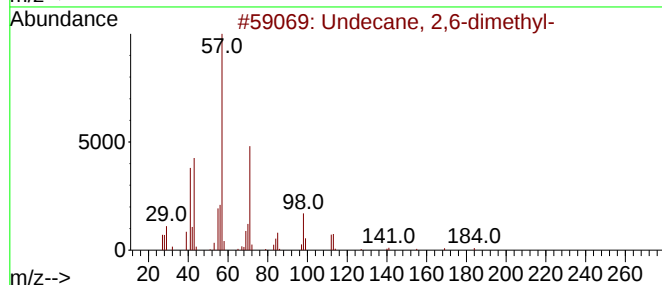
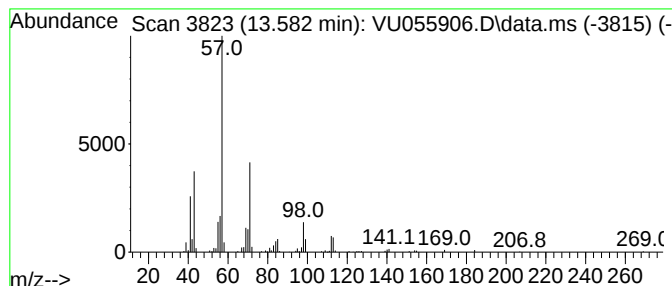
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.582	4.62 ug/L	158838	1,4-Dichlorobenzene-d4	11.814

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	94
2		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	94
3		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
4		Dodecane, 6-methyl-	184	C13H28	006044-71-9	90
5		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
Data File : VU055906.D
Acq On : 26 Oct 2023 15:36
Operator : MD/SY
Sample : 04961-14ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

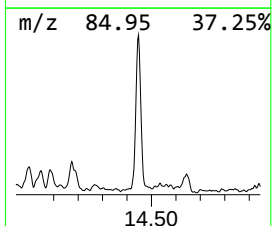
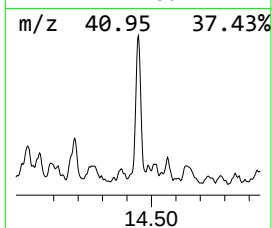
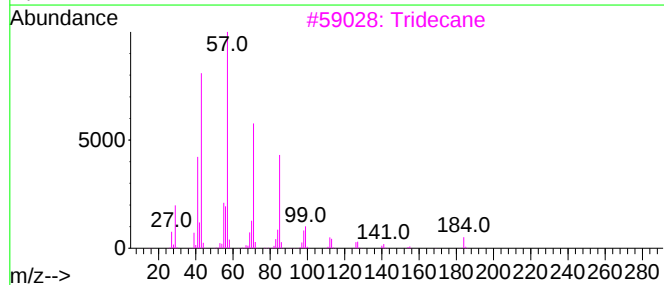
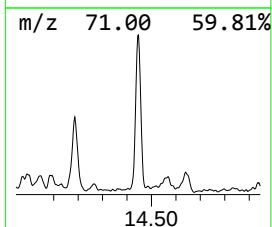
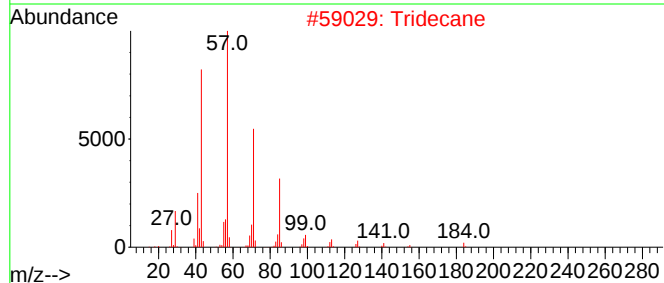
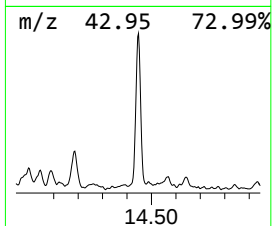
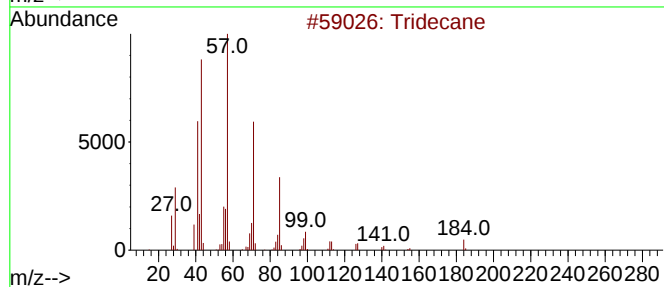
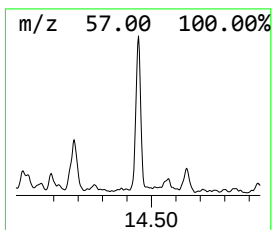
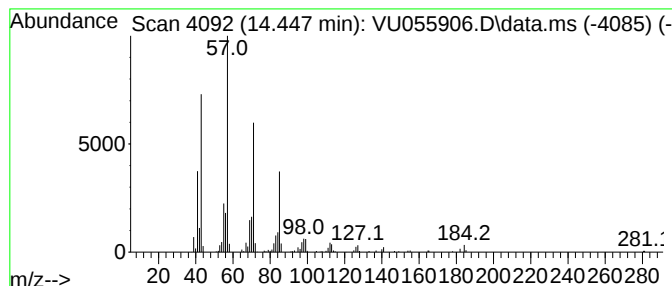
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	5.44 ug/L	187043	1,4-Dichlorobenzene-d4	11.814

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	95
2		Tridecane	184	C13H28	000629-50-5	95
3		Tridecane	184	C13H28	000629-50-5	93
4		Tridecane	184	C13H28	000629-50-5	91
5		Tridecane	184	C13H28	000629-50-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
Data File : VU055906.D
Acq On : 26 Oct 2023 15:36
Operator : MD/SY
Sample : 04961-14ME
Misc : 5.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

							--Internal Standard--			
TIC Top	Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc	
(DEL)	Alkane: S...	11.113	3.9	ug/L	135689	3	11.814	1719870	50.0	
(DEL)	Alkane: S...	12.325	7.6	ug/L	259977	3	11.814	1719870	50.0	
(DEL)	Alkane: S...	13.428	10.9	ug/L	375998	3	11.814	1719870	50.0	
(DEL)	Alkane: S...	13.582	4.6	ug/L	158838	3	11.814	1719870	50.0	
(DEL)	Alkane: S...	14.447	5.4	ug/L	187043	3	11.814	1719870	50.0	