

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
 Data File : VU050468.D
 Acq On : 26 Aug 2022 19:36
 Operator : SY/MD
 Sample : N4322-05ME
 Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY165ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050468.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	38	43	48	rBV3	4216	4947	0.15%	0.024%
2	1.511	49	53	66	rVB2	3958	5605	0.17%	0.028%
3	1.591	70	78	86	rBV	197923	267169	8.27%	1.318%
4	1.877	162	167	174	rBV	70395	87190	2.70%	0.430%
5	2.520	353	367	387	rBV	667175	1084267	33.56%	5.349%
6	2.626	395	400	401	rBV3	688	602	0.02%	0.003%
7	2.742	432	436	438	rBV3	383	312	0.01%	0.002%
8	2.929	489	494	496	rBV2	577	594	0.02%	0.003%
9	3.025	514	524	536	rBV2	10664	20839	0.64%	0.103%
10	3.179	556	572	595	rBV2	23190	59904	1.85%	0.296%
11	3.430	648	650	655	rVB2	256	210	0.01%	0.001%
12	3.459	655	659	662	rBV2	195	200	0.01%	0.001%
13	3.523	675	679	680	rBV2	323	224	0.01%	0.001%
14	3.642	712	716	717	rBV2	420	238	0.01%	0.001%
15	3.662	717	722	725	rBV2	621	686	0.02%	0.003%
16	3.816	765	770	773	rVV2	395	314	0.01%	0.002%
17	4.118	861	864	869	rVB2	279	266	0.01%	0.001%
18	4.340	924	933	946	rBV2	691	1521	0.05%	0.008%
19	4.642	1014	1027	1089	rBV	248027	873169	27.02%	4.308%
20	5.060	1138	1157	1186	rBV	541893	1247542	38.61%	6.155%
21	5.292	1218	1229	1234	rBV2	1485	2385	0.07%	0.012%
22	5.356	1245	1249	1250	rBV	605	361	0.01%	0.002%
23	5.716	1340	1361	1399	rBV2	1292468	3231121	100.00%	15.941%
24	5.980	1432	1443	1465	rBV5	11367	28974	0.90%	0.143%
25	6.089	1472	1477	1479	rVB2	258	210	0.01%	0.001%
26	6.105	1479	1482	1485	rVB3	409	288	0.01%	0.001%
27	6.134	1488	1491	1495	rBV2	347	322	0.01%	0.002%
28	6.247	1511	1526	1550	rBV	288990	579050	17.92%	2.857%
29	6.391	1568	1571	1573	rBV3	365	197	0.01%	0.001%
30	6.459	1586	1592	1595	rBV3	326	349	0.01%	0.002%
31	6.536	1603	1616	1628	rBV7	12715	26175	0.81%	0.129%
32	6.607	1628	1638	1648	rBV5	4915	10256	0.32%	0.051%
33	6.690	1648	1664	1692	rVB	714131	1450247	44.88%	7.155%
34	6.797	1695	1697	1698	rBV	863	346	0.01%	0.002%
35	6.899	1724	1729	1730	rBV	281	195	0.01%	0.001%
36	6.977	1747	1753	1754	rBV2	411	291	0.01%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

37	7.221	1814	1829	1844	rVV7	5069	14084	0.44%	0.069%
38	7.494	1906	1914	1922	rBV4	1806	2596	0.08%	0.013%
39	7.565	1922	1936	1956	rBV	333561	634419	19.63%	3.130%
40	7.700	1974	1978	1981	rBV3	650	574	0.02%	0.003%
41	7.793	2004	2007	2011	rVV	520	401	0.01%	0.002%
42	7.896	2025	2039	2060	rBV	1369249	2432655	75.29%	12.002%
43	8.073	2091	2094	2098	rVB4	549	473	0.01%	0.002%
44	8.124	2104	2110	2117	rBV8	2732	4294	0.13%	0.021%
45	8.182	2117	2128	2153	rVB	219259	426171	13.19%	2.103%
46	8.301	2162	2165	2168	rVB3	353	209	0.01%	0.001%
47	8.317	2168	2170	2173	rBV	255	196	0.01%	0.001%
48	8.346	2175	2179	2180	rBV2	683	428	0.01%	0.002%
49	8.417	2197	2201	2204	rBV3	309	230	0.01%	0.001%
50	8.552	2231	2243	2258	rBV2	142324	245990	7.61%	1.214%
51	8.658	2258	2276	2304	rBV	774738	1911085	59.15%	9.429%
52	8.922	2349	2358	2369	rBV7	4440	8485	0.26%	0.042%
53	9.060	2398	2401	2402	rBV3	932	543	0.02%	0.003%
54	9.118	2410	2419	2425	rBV7	1456	2052	0.06%	0.010%
55	9.173	2425	2436	2441	rVV8	2265	4233	0.13%	0.021%
56	9.211	2444	2448	2460	rVB3	3867	5460	0.17%	0.027%
57	9.282	2467	2470	2472	rBV3	330	227	0.01%	0.001%
58	9.337	2478	2487	2497	rBV6	3809	6539	0.20%	0.032%
59	9.420	2498	2513	2535	rBV	374225	705247	21.83%	3.479%
60	9.558	2552	2556	2557	rBV4	513	329	0.01%	0.002%
61	9.578	2560	2562	2566	rVB	531	323	0.01%	0.002%
62	9.613	2566	2573	2579	rBV3	612	744	0.02%	0.004%
63	9.655	2581	2586	2591	rBV5	1096	1155	0.04%	0.006%
64	9.742	2604	2613	2623	rVB5	7816	11877	0.37%	0.059%
65	9.870	2647	2653	2654	rBV4	1074	1030	0.03%	0.005%
66	9.931	2669	2672	2676	rVV2	263	228	0.01%	0.001%
67	9.964	2676	2682	2684	rVV3	559	540	0.02%	0.003%
68	10.012	2691	2697	2699	rBV3	1712	1562	0.05%	0.008%
69	10.115	2720	2729	2730	rBV4	1335	1413	0.04%	0.007%
70	10.211	2755	2759	2760	rBV2	347	219	0.01%	0.001%
71	10.253	2761	2772	2783	rVB4	7985	12891	0.40%	0.064%
72	10.314	2783	2791	2792	rBV4	1615	1536	0.05%	0.008%
73	10.394	2809	2816	2828	rVB4	10226	16429	0.51%	0.081%
74	10.456	2830	2835	2837	rBV6	898	981	0.03%	0.005%
75	10.555	2854	2866	2875	rBV9	4342	9207	0.28%	0.045%
76	10.623	2882	2887	2893	rBV3	5124	5879	0.18%	0.029%

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Peak Location: TOP

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 Title : VOC Analysis

77	10.764	2911	2931	2957	rBV	1092993	1840654	56.97%	9.081%
78	10.976	2995	2997	3006	rVB4	1175	1417	0.04%	0.007%
79	11.015	3007	3009	3011	rBV2	536	282	0.01%	0.001%
80	11.066	3016	3025	3031	rVV9	4264	7423	0.23%	0.037%
81	11.115	3032	3040	3058	rVB2	30605	49293	1.53%	0.243%
82	11.179	3058	3060	3061	rBV	578	269	0.01%	0.001%
83	11.253	3078	3083	3091	rVB4	1044	1092	0.03%	0.005%
84	11.311	3095	3101	3113	rBV8	3438	5456	0.17%	0.027%
85	11.382	3116	3123	3126	rBV6	2786	3481	0.11%	0.017%
86	11.417	3127	3134	3141	rVV2	18964	25061	0.78%	0.124%
87	11.574	3173	3183	3187	rBV5	3225	4576	0.14%	0.023%
88	11.710	3216	3225	3231	rBV10	3679	6733	0.21%	0.033%
89	11.816	3247	3258	3271	rBV	359712	566904	17.55%	2.797%
90	12.086	3337	3342	3343	rBV4	1574	1302	0.04%	0.006%
91	12.198	3364	3377	3404	rBV	1179281	1928581	59.69%	9.515%
92	12.327	3410	3417	3428	rVB	56652	79012	2.45%	0.390%
93	12.664	3516	3522	3530	rVB7	7329	11032	0.34%	0.054%
94	12.928	3598	3604	3623	rVB7	10927	33881	1.05%	0.167%
95	13.009	3623	3629	3635	rBV9	5780	8040	0.25%	0.040%
96	13.047	3637	3641	3651	rVB10	7222	10512	0.33%	0.052%
97	13.433	3753	3761	3784	rVB2	53232	94959	2.94%	0.468%
98	13.587	3801	3809	3819	rBV	33294	52477	1.62%	0.259%
99	14.452	4070	4078	4087	rBV2	42045	57892	1.79%	0.286%
100	16.295	4645	4651	4659	rVB3	14609	18965	0.59%	0.094%

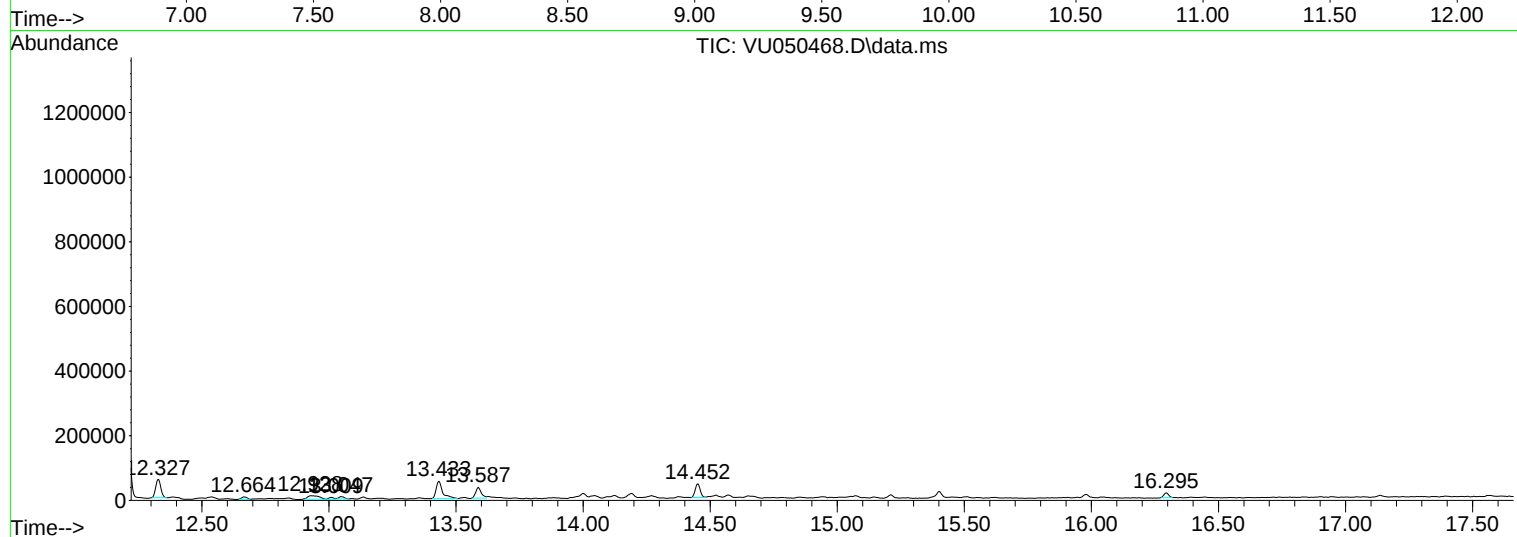
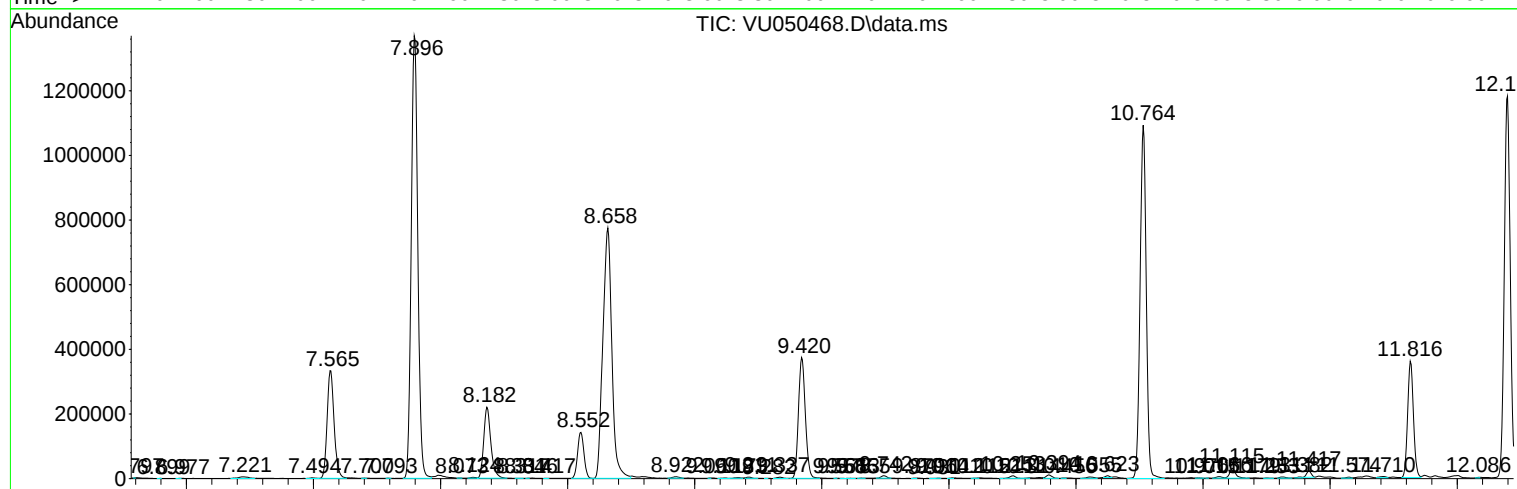
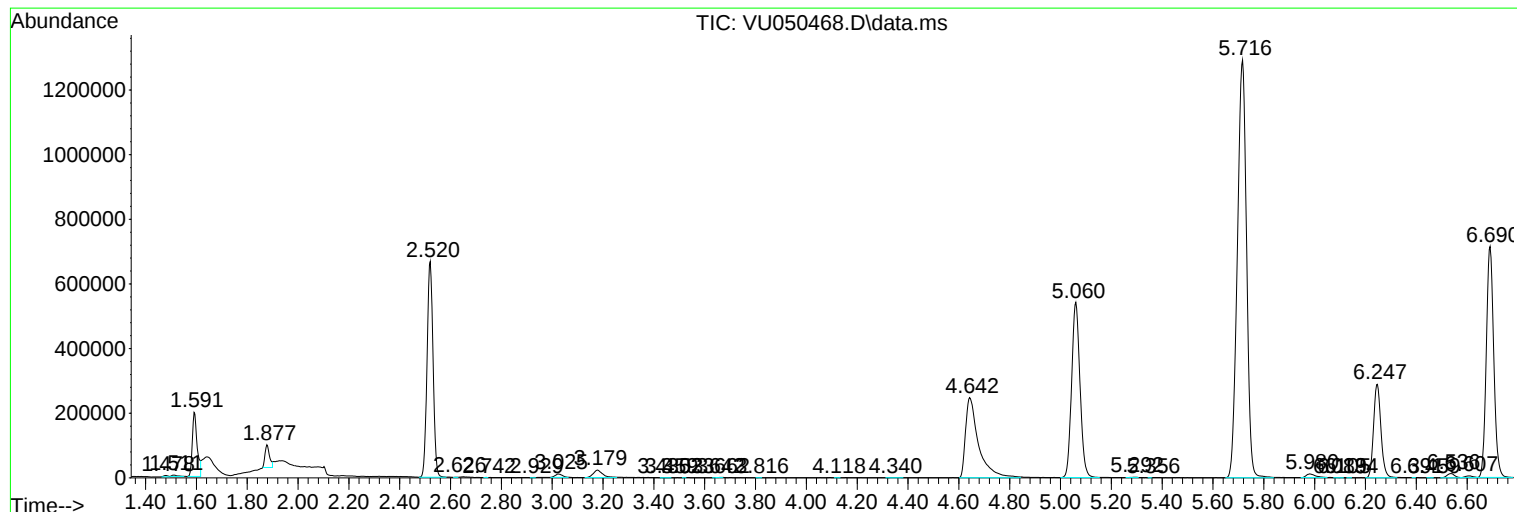
Sum of corrected areas: 20268794

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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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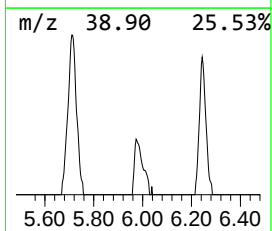
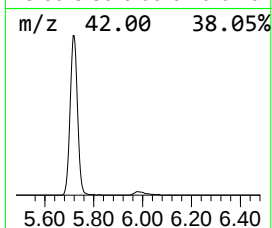
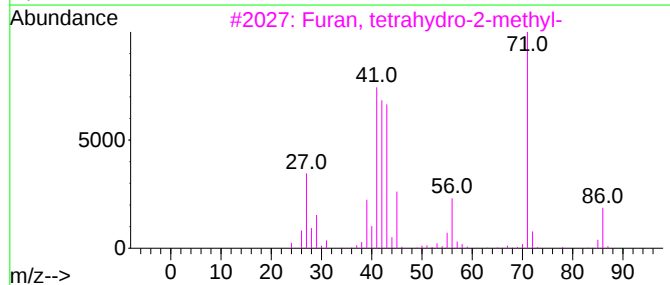
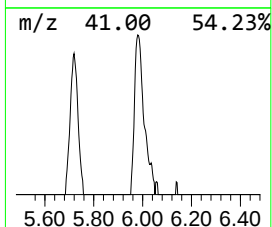
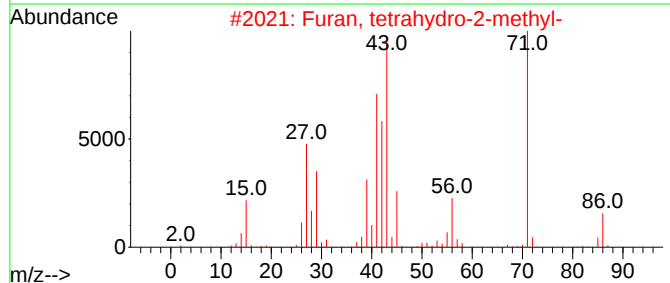
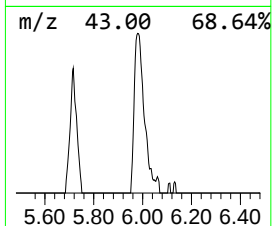
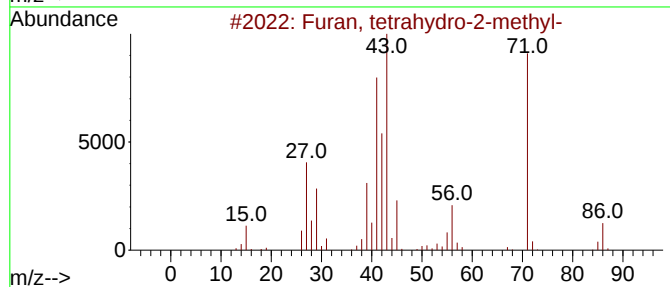
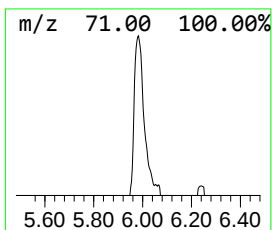
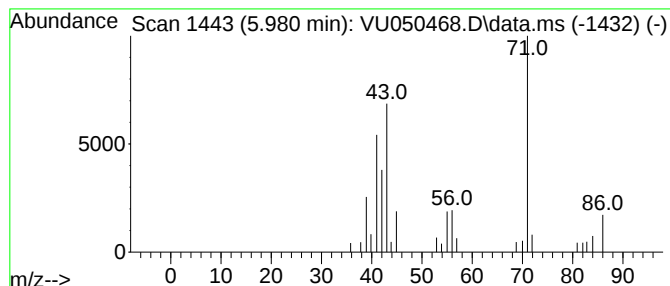
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Furan, tetrahydro-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.980	2.50 ug/L	28974	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	87
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	87
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	86
4			Pyrrolidine	71	C4H9N	000123-75-1	40
5			Oxirane, butyl-	100	C6H12O	001436-34-6	40



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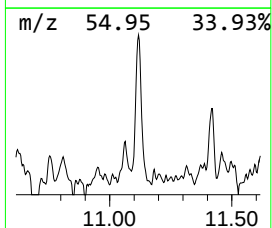
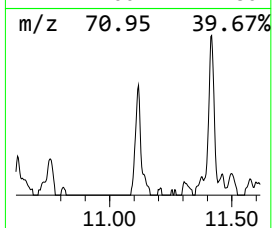
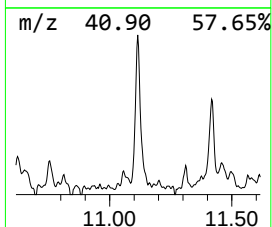
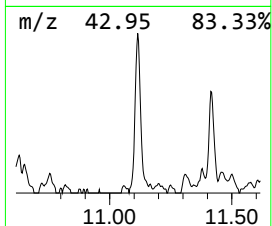
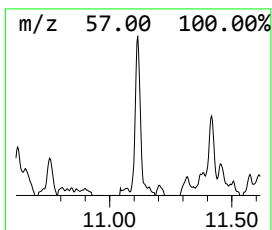
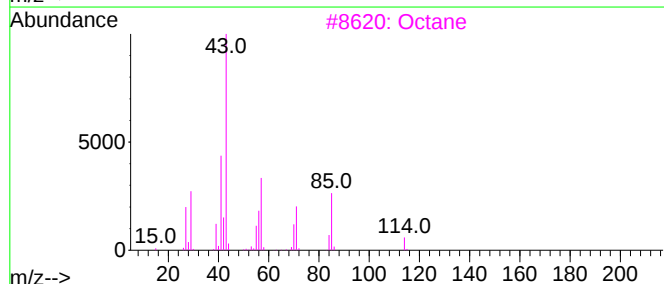
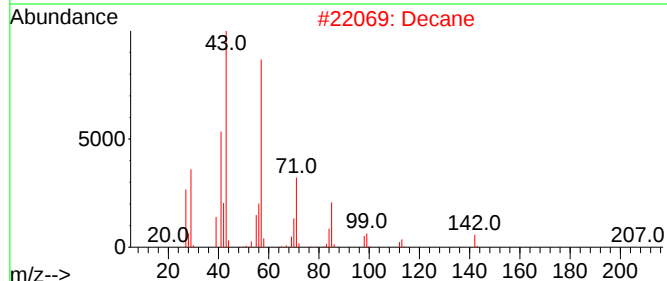
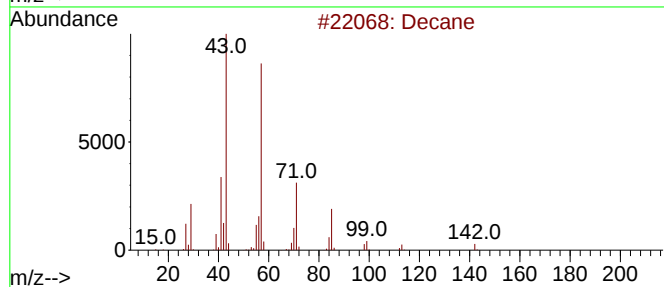
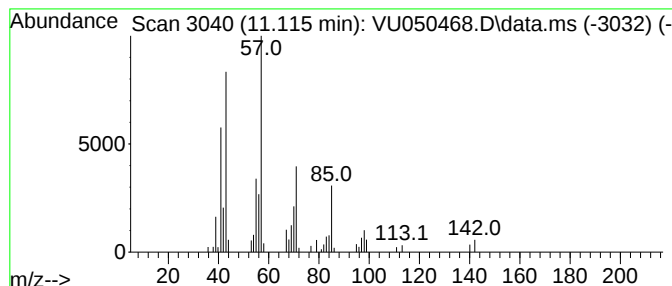
Instrument :
MSVOA_U
ClientSampleId :
EY165ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.115	4.35 ug/L	49293	1,4-Dichlorobenzene-d4		11.816	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane		142	C10H22	000124-18-5	87
2	Decane		142	C10H22	000124-18-5	64
3	Octane		114	C8H18	000111-65-9	53
4	Undecane		156	C11H24	001120-21-4	53
5	Undecane, 3-methyl-		170	C12H26	001002-43-3	50



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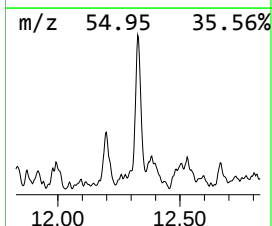
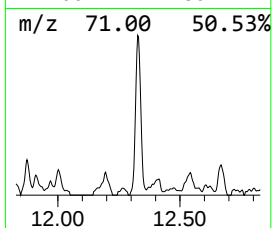
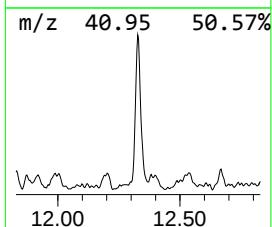
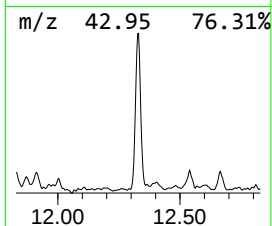
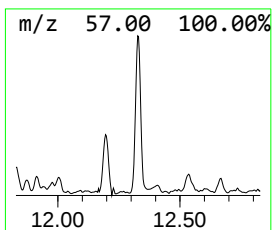
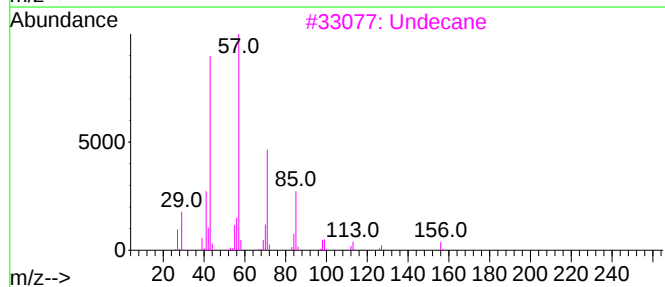
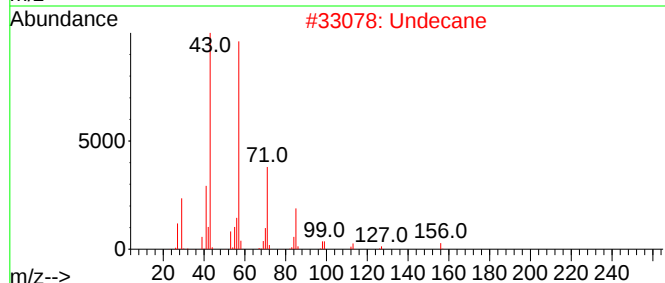
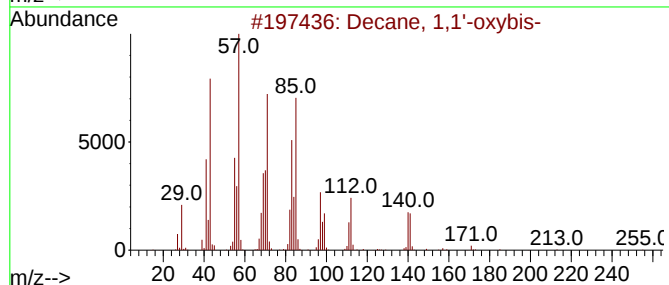
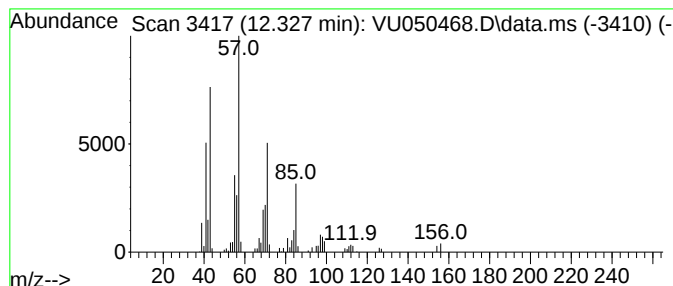
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Quant Title : VOC Analysis

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

Peak Number 5 Decane, 1,1'-oxybis- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	6.97 ug/L	79012	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	83
2			Undecane	156	C11H24	001120-21-4	80
3			Undecane	156	C11H24	001120-21-4	72
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	64
5			Nonane	128	C9H20	000111-84-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050468.D
Acq On : 26 Aug 2022 19:36
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

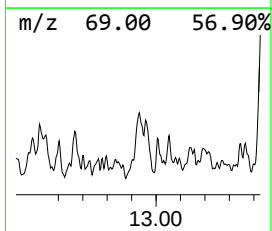
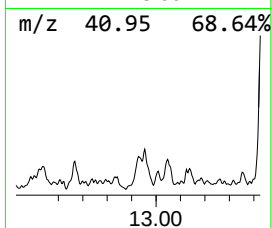
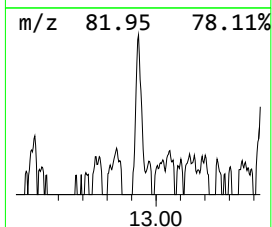
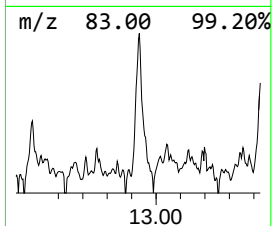
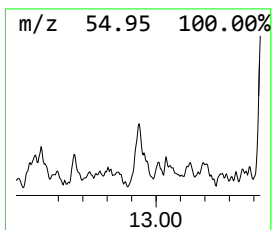
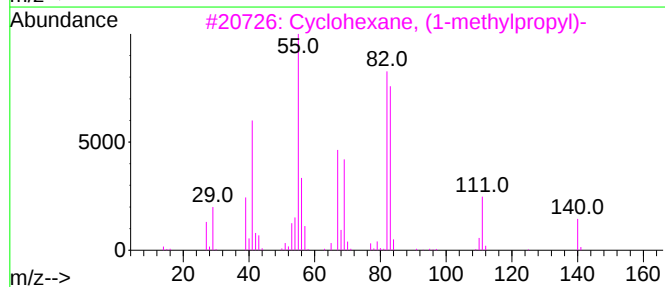
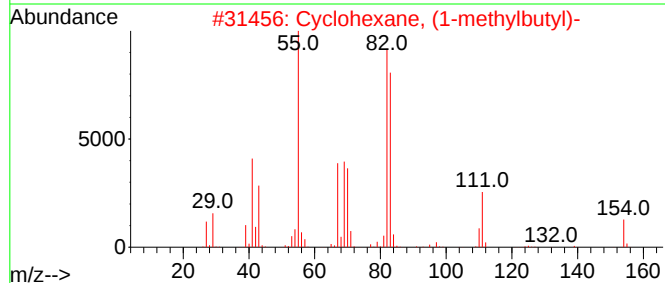
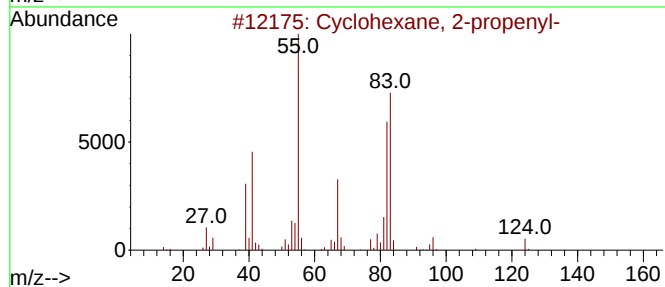
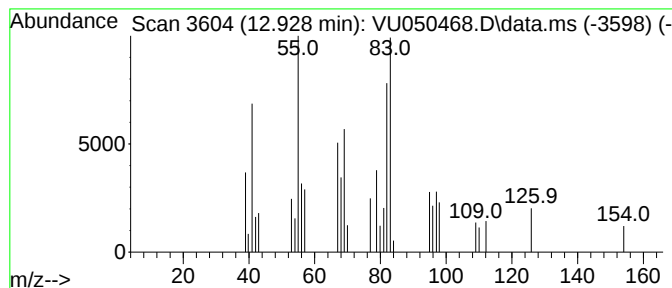
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Quant Title : VOC Analysis

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

Peak Number 6 Cyclohexane, 2-propenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.928	2.99 ug/L	33881	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	50
2			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	49
3			Cyclohexane, (1-methylpropyl)-	140	C10H20	007058-01-7	47
4			13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	38
5			3-Hexyne	82	C6H10	000928-49-4	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050468.D
Acq On : 26 Aug 2022 19:36
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

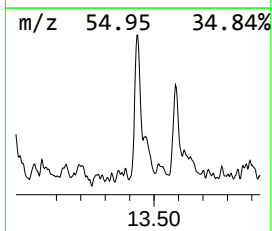
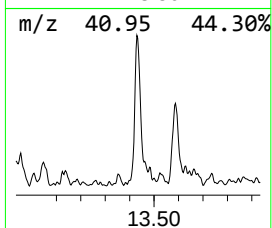
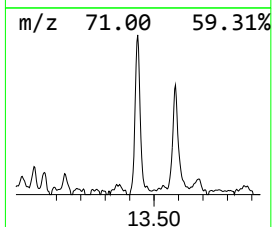
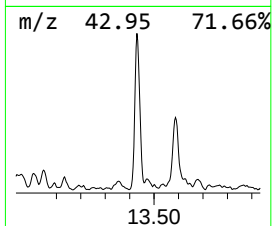
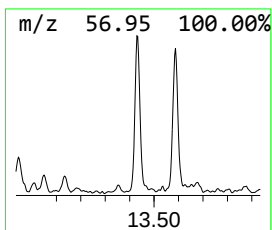
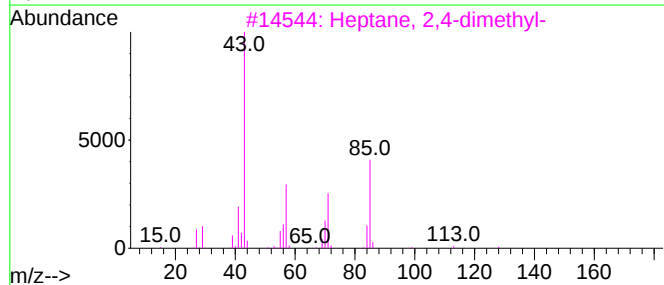
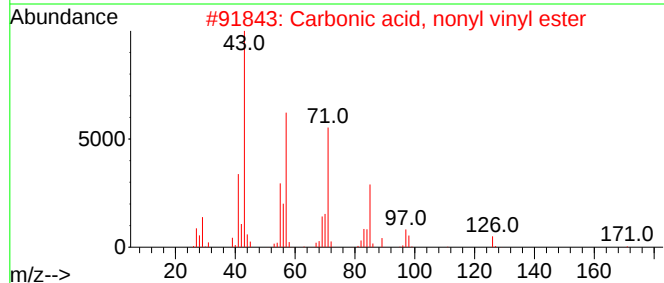
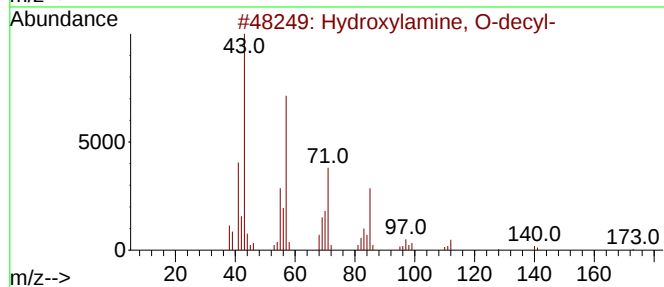
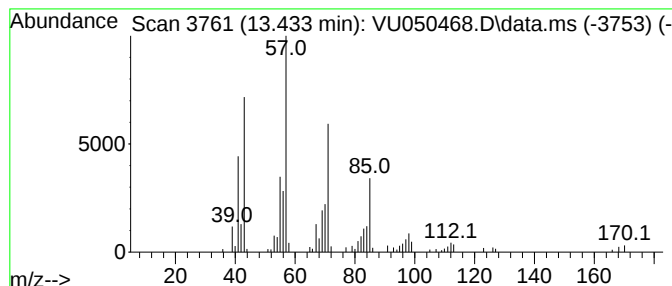
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Quant Title : VOC Analysis

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

Peak Number 7 Hydroxylamine, O-decyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	8.38 ug/L	94959	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	72
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	59
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
4			Undecane	156	C11H24	001120-21-4	59
5			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050468.D
Acq On : 26 Aug 2022 19:36
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

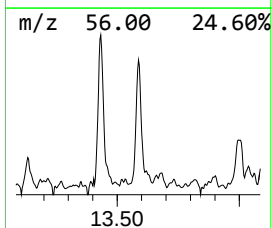
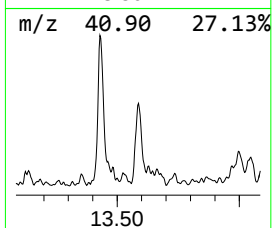
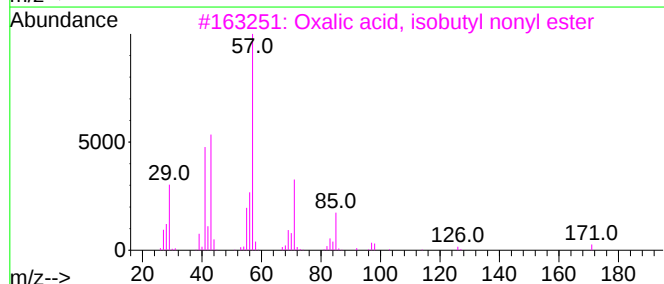
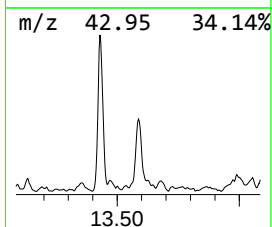
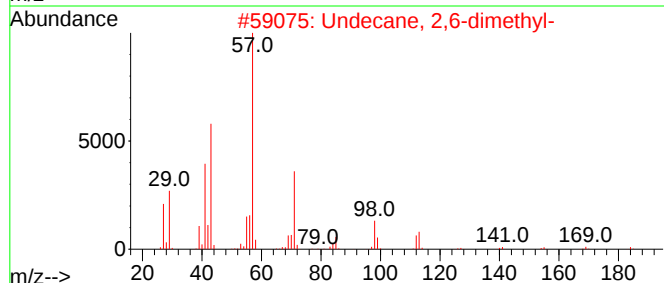
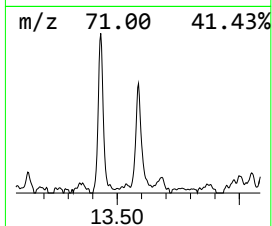
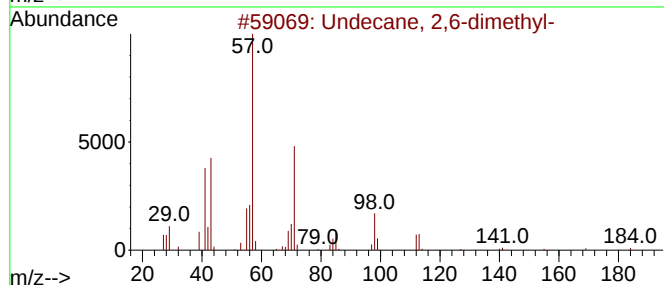
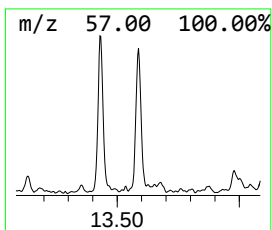
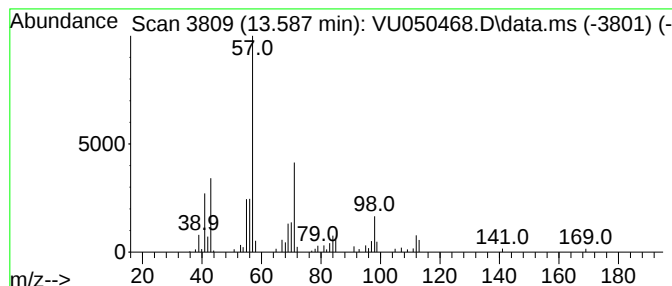
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Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	4.63 ug/L	52477	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	78
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
3			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59
4			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	59
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050468.D
Acq On : 26 Aug 2022 19:36
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

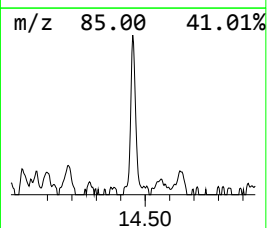
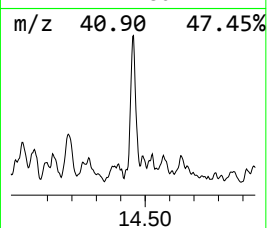
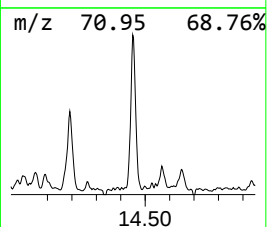
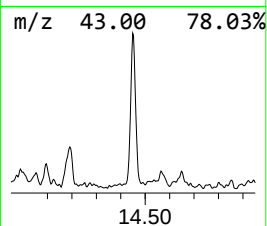
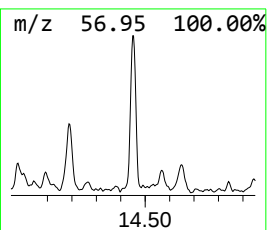
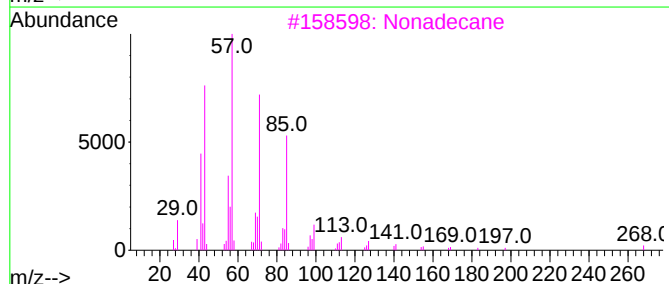
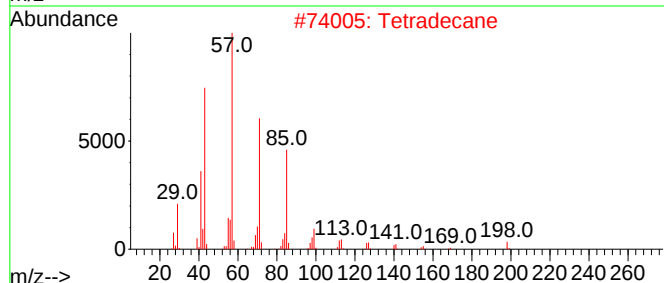
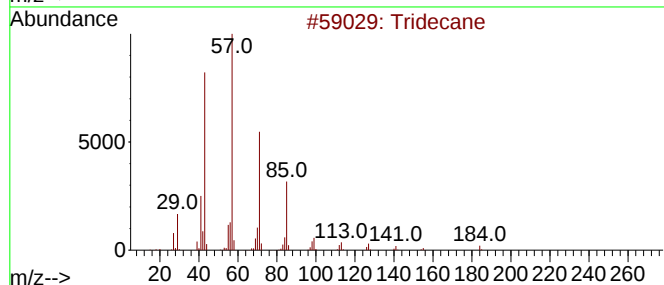
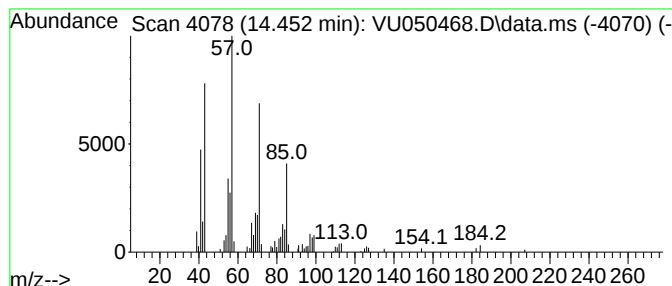
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Quant Title : VOC Analysis

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.452	5.11 ug/L	57892	1,4-Dichlorobenzene-d4	11.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	90
2		Tetradecane	198	C14H30	000629-59-4	86
3		Nonadecane	268	C19H40	000629-92-5	86
4		Tetradecane	198	C14H30	000629-59-4	86
5		Tridecane	184	C13H28	000629-50-5	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050468.D
Acq On : 26 Aug 2022 19:36
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Furan, tetrahyd...	5.980	2.5	ug/L	28974	1	6.247	579050	50.0
(DEL) Alkane: S...	11.115	4.3	ug/L	49293	3	11.816	566904	50.0
Decane, 1,1'-ox...	12.327	7.0	ug/L	79012	3	11.816	566904	50.0
Cyclohexane, 2-...	12.928	3.0	ug/L	33881	3	11.816	566904	50.0
Hydroxylamine, ...	13.433	8.4	ug/L	94959	3	11.816	566904	50.0
(DEL) Alkane: S...	13.587	4.6	ug/L	52477	3	11.816	566904	50.0
(DEL) Alkane: S...	14.452	5.1	ug/L	57892	3	11.816	566904	50.0