

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
 Data File : VU048353.D
 Acq On : 29 Apr 2022 12:50
 Operator : SY/MD
 Sample : N2562-15ME
 Misc : 7.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW476ME

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: VU048353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	33	44	50	rBV3	11467	21586	1.12%	0.133%
2	1.597	73	80	117	rVB	84322	252141	13.03%	1.553%
3	1.829	122	152	153	rBV3	30688	92051	4.76%	0.567%
4	1.851	153	159	162	rBV	39429	45320	2.34%	0.279%
5	2.530	355	370	385	rBV	289468	529590	27.37%	3.263%
6	2.755	435	440	457	rVB3	2160	3954	0.20%	0.024%
7	3.038	515	528	544	rBV6	10416	27816	1.44%	0.171%
8	3.096	544	546	556	rVV6	1563	2148	0.11%	0.013%
9	3.176	557	571	588	rVV2	16289	38388	1.98%	0.237%
10	3.327	607	618	629	rVB3	2806	6151	0.32%	0.038%
11	3.668	713	724	736	rVB4	5455	11607	0.60%	0.072%
12	4.510	971	986	997	rVB5	3530	7741	0.40%	0.048%
13	4.639	1011	1026	1091	rBV2	135521	612142	31.64%	3.771%
14	5.063	1139	1158	1193	rBV	296806	754177	38.98%	4.646%
15	5.366	1236	1252	1267	rVB9	4664	13519	0.70%	0.083%
16	5.581	1308	1319	1328	rVB7	2943	5783	0.30%	0.036%
17	5.716	1341	1361	1391	rBV2	770806	1934911	100.00%	11.921%
18	5.829	1394	1396	1410	rVB6	2351	3371	0.17%	0.021%
19	5.977	1429	1442	1461	rBV2	17199	43417	2.24%	0.267%
20	6.124	1472	1488	1497	rBV4	6361	12903	0.67%	0.079%
21	6.247	1511	1526	1558	rVB	414445	867732	44.85%	5.346%
22	6.523	1603	1612	1623	rBV8	5631	11358	0.59%	0.070%
23	6.600	1626	1636	1648	rBV5	6391	13760	0.71%	0.085%
24	6.690	1648	1664	1695	rBV	406516	892414	46.12%	5.498%
25	6.970	1745	1751	1766	rVB8	2094	3853	0.20%	0.024%
26	7.063	1770	1780	1790	rBV7	3240	6650	0.34%	0.041%
27	7.221	1807	1829	1849	rBV8	10014	38409	1.99%	0.237%
28	7.468	1897	1906	1908	rBV4	2747	3332	0.17%	0.021%
29	7.491	1908	1913	1923	rVB6	4133	6039	0.31%	0.037%
30	7.568	1923	1937	1958	rBV	206671	430372	22.24%	2.651%
31	7.784	1995	2004	2015	rBV7	1464	3085	0.16%	0.019%
32	7.896	2020	2039	2056	rVV	840599	1599769	82.68%	9.856%
33	7.970	2057	2062	2088	rVB3	23454	61882	3.20%	0.381%
34	8.124	2103	2110	2117	rBV4	6539	10196	0.53%	0.063%
35	8.182	2117	2128	2156	rVB	132848	302424	15.63%	1.863%
36	8.362	2171	2184	2194	rBV8	2350	5546	0.29%	0.034%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

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

37	8.536	2232	2238	2246	rVB6	1933	2433	0.13%	0.015%
38	8.665	2253	2278	2302	rBV	512444	1240256	64.10%	7.641%
39	8.800	2312	2320	2327	rBV7	2754	4307	0.22%	0.027%
40	8.864	2335	2340	2347	rVB5	2619	3821	0.20%	0.024%
41	8.925	2348	2359	2367	rBV4	9945	18258	0.94%	0.112%
42	9.066	2393	2403	2411	rBV7	2532	4350	0.22%	0.027%
43	9.118	2414	2419	2425	rVB4	2249	2558	0.13%	0.016%
44	9.163	2425	2433	2441	rBV5	5893	10155	0.52%	0.063%
45	9.211	2441	2448	2457	rVB2	5577	9549	0.49%	0.059%
46	9.333	2475	2486	2496	rBV3	5981	9869	0.51%	0.061%
47	9.423	2499	2514	2536	rBV	551946	1131388	58.47%	6.970%
48	9.575	2550	2561	2572	rVB	6310	11753	0.61%	0.072%
49	9.668	2576	2590	2591	rVV5	3393	5573	0.29%	0.034%
50	9.700	2591	2600	2607	rVV6	8846	19739	1.02%	0.122%
51	9.745	2607	2614	2629	rVB4	14378	25201	1.30%	0.155%
52	9.877	2646	2655	2667	rBV4	2608	4751	0.25%	0.029%
53	10.025	2689	2701	2717	rBV4	4058	11345	0.59%	0.070%
54	10.115	2718	2729	2741	rBV9	3954	7961	0.41%	0.049%
55	10.250	2758	2771	2784	rBV5	12930	25105	1.30%	0.155%
56	10.356	2795	2804	2809	rBV9	3474	6315	0.33%	0.039%
57	10.394	2809	2816	2828	rVB2	12063	20761	1.07%	0.128%
58	10.465	2828	2838	2852	rVB10	2188	5235	0.27%	0.032%
59	10.555	2852	2866	2875	rBV10	4727	11499	0.59%	0.071%
60	10.623	2879	2887	2892	rVV5	5227	7566	0.39%	0.047%
61	10.655	2893	2897	2910	rVB6	4187	8204	0.42%	0.051%
62	10.767	2918	2932	2959	rVB	739218	1230029	63.57%	7.578%
63	10.902	2969	2974	2982	rBV7	1617	1791	0.09%	0.011%
64	10.944	2982	2987	2989	rBV6	2247	1986	0.10%	0.012%
65	11.015	3002	3009	3013	rBV8	2131	3182	0.16%	0.020%
66	11.063	3017	3024	3030	rVV9	5128	7913	0.41%	0.049%
67	11.115	3031	3040	3056	rVB2	38126	67428	3.48%	0.415%
68	11.198	3056	3066	3074	rVB9	2679	5161	0.27%	0.032%
69	11.311	3088	3101	3113	rBV9	4744	11376	0.59%	0.070%
70	11.375	3113	3121	3126	rBV7	3922	6138	0.32%	0.038%
71	11.417	3126	3134	3142	rVV3	24673	34359	1.78%	0.212%
72	11.465	3142	3149	3173	rVB7	12275	35082	1.81%	0.216%
73	11.574	3173	3183	3187	rBV6	4366	7388	0.38%	0.046%
74	11.639	3198	3203	3214	rVB10	7151	12266	0.63%	0.076%
75	11.697	3216	3221	3223	rBV4	3802	3669	0.19%	0.023%
76	11.816	3246	3258	3272	rBV	718085	1154620	59.67%	7.113%

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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

77	11.873	3273	3276	3282	rVV5	8576	10451	0.54%	0.064%
78	11.912	3282	3288	3296	rVB6	8974	12768	0.66%	0.079%
79	11.996	3302	3314	3326	rVB10	10688	27615	1.43%	0.170%
80	12.086	3335	3342	3344	rBV4	2985	3403	0.18%	0.021%
81	12.198	3364	3377	3393	rBV	931125	1502386	77.65%	9.256%
82	12.330	3409	3418	3429	rBV	83552	118972	6.15%	0.733%
83	12.500	3459	3471	3475	rBV	4893	11739	0.61%	0.072%
84	12.664	3517	3522	3531	rVB4	11699	17268	0.89%	0.106%
85	12.767	3551	3554	3557	rBV4	2076	1789	0.09%	0.011%
86	12.951	3588	3611	3623	rBV8	17071	59925	3.10%	0.369%
87	13.005	3623	3628	3634	rVV6	7349	10312	0.53%	0.064%
88	13.050	3635	3642	3650	rVB6	12771	20035	1.04%	0.123%
89	13.134	3661	3668	3679	rVB5	10634	17293	0.89%	0.107%
90	13.356	3731	3737	3748	rBV10	6450	9996	0.52%	0.062%
91	13.433	3752	3761	3784	rVB2	108471	181945	9.40%	1.121%
92	13.587	3801	3809	3831	rBV2	49815	93586	4.84%	0.577%
93	13.732	3848	3854	3859	rBV9	3347	5121	0.26%	0.032%
94	13.999	3933	3937	3944	rVB5	15581	17713	0.92%	0.109%
95	14.092	3962	3966	3970	rBV4	7961	8759	0.45%	0.054%
96	14.192	3986	3997	4008	rBV5	23533	43215	2.23%	0.266%
97	14.452	4069	4078	4086	rBV	83633	117526	6.07%	0.724%
98	14.571	4110	4115	4122	rVB6	10825	13827	0.71%	0.085%
99	15.211	4306	4314	4326	rBV9	11276	19480	1.01%	0.120%
100	15.401	4367	4373	4391	rVB	24040	40486	2.09%	0.249%

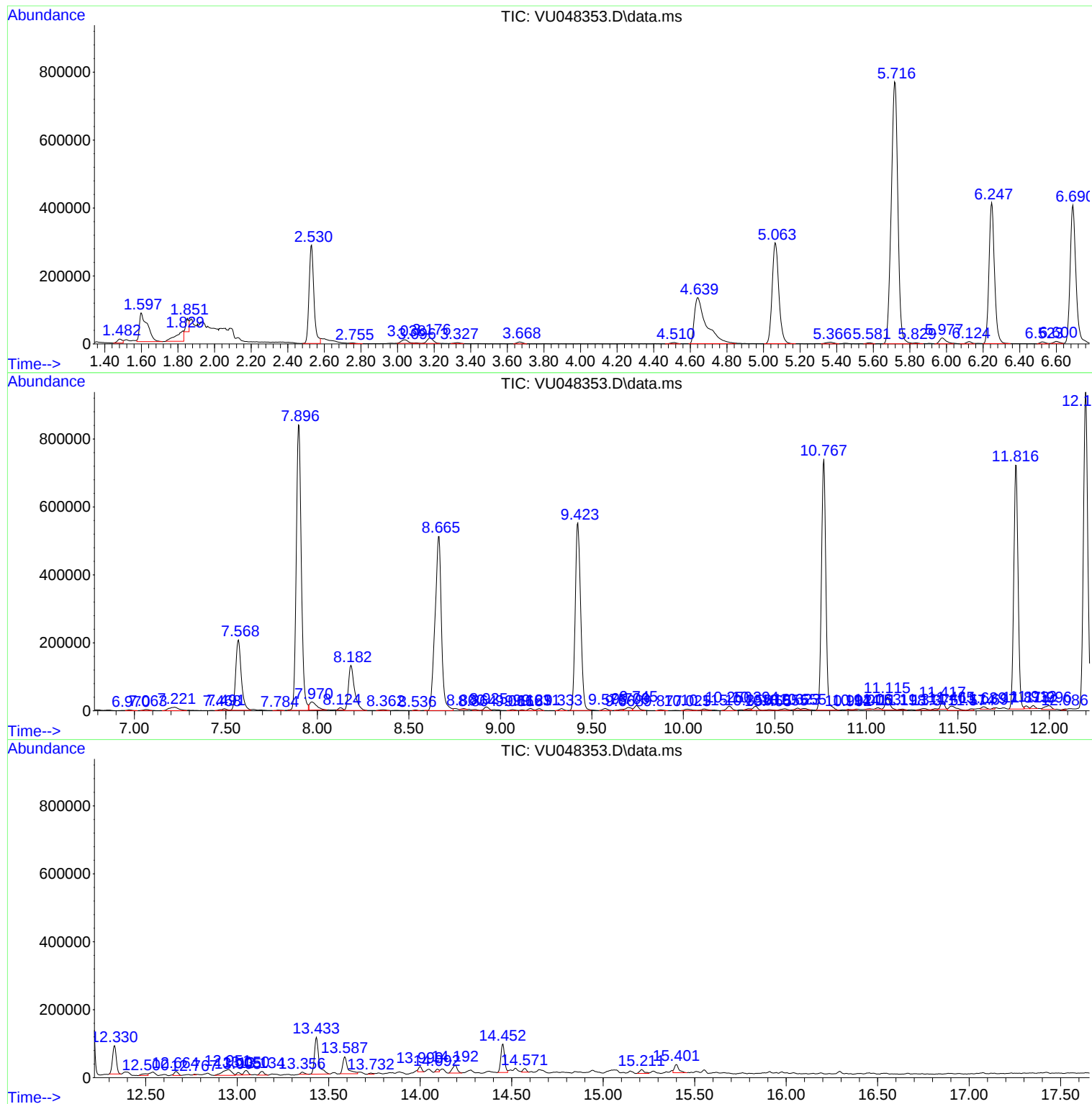
Sum of corrected areas: 16231487

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW476ME

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



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW476ME

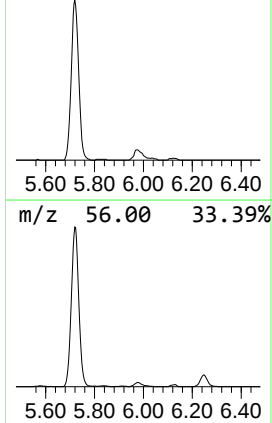
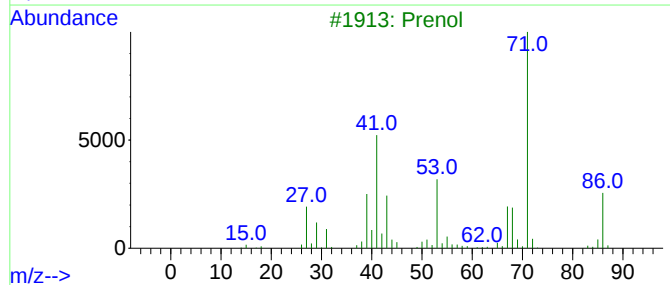
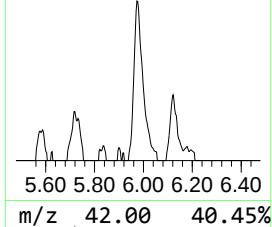
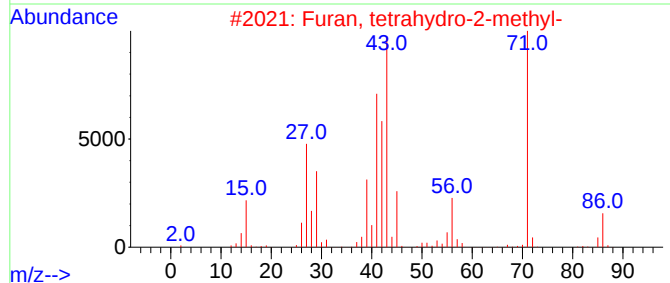
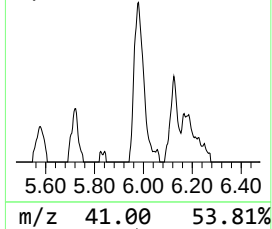
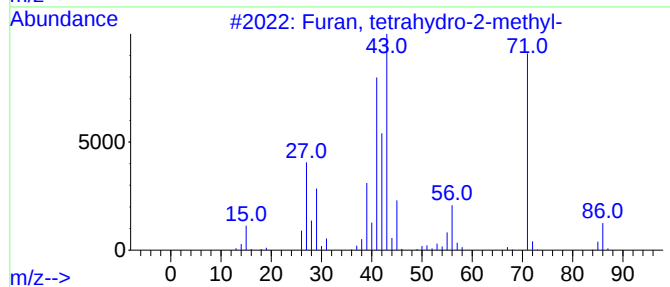
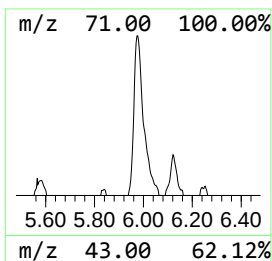
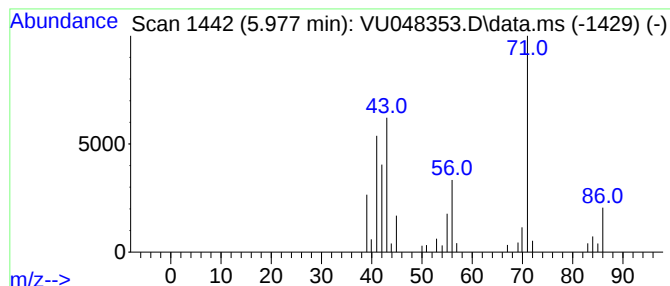
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Furan, tetrahydro-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.977	2.50 ug/L	43417	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	64
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	64
3			Prenol	86	C5H10O	000556-82-1	46
4			Oxirane, propyl-	86	C5H10O	001003-14-1	38
5			Pyrrolidine	71	C4H9N	000123-75-1	38



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Instrument :
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ClientSampleId :
EW476ME

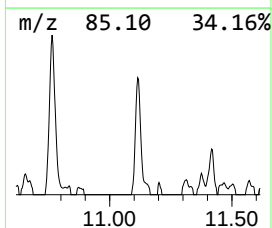
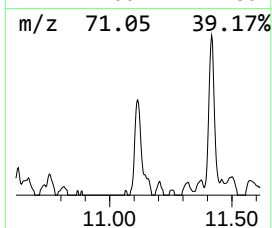
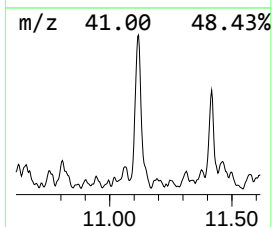
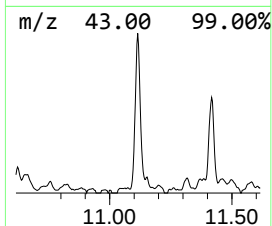
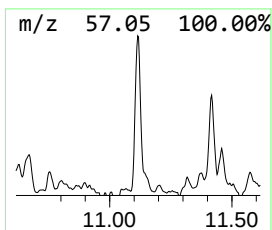
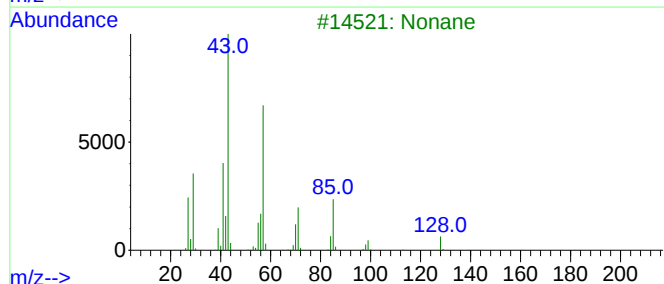
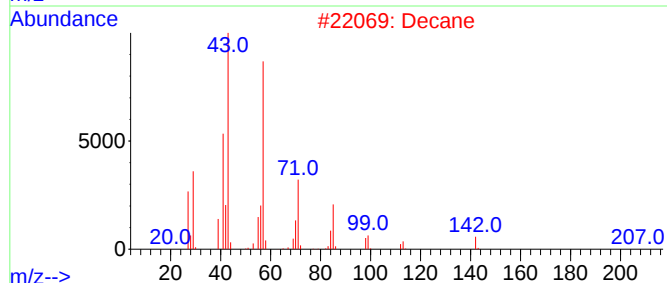
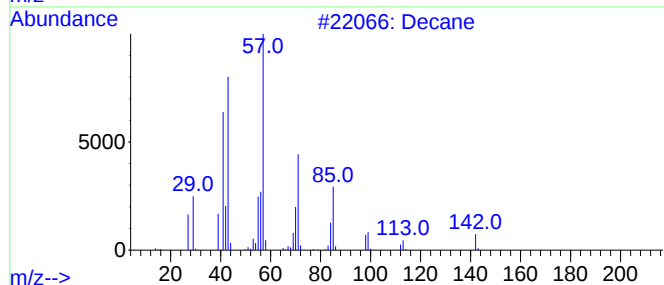
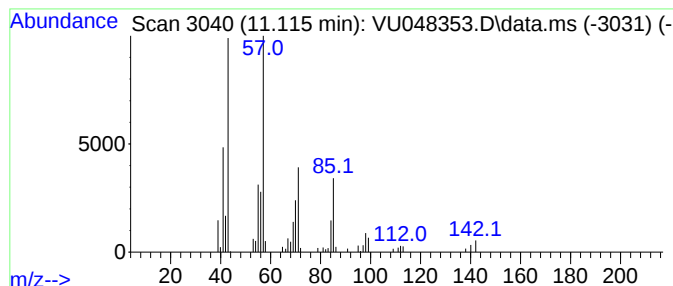
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	2.92 ug/L	67428	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	90
2			Decane	142	C10H22	000124-18-5	83
3			Nonane	128	C9H20	000111-84-2	72
4			Decane	142	C10H22	000124-18-5	64
5			Octane	114	C8H18	000111-65-9	64



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW476ME

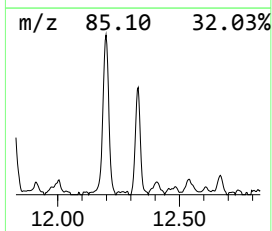
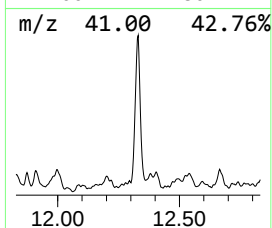
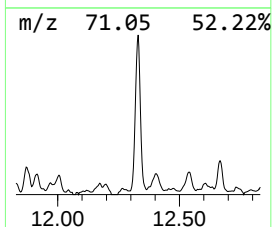
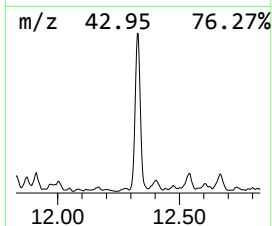
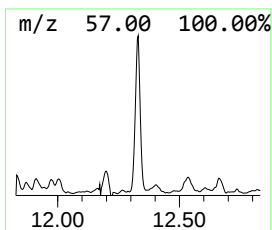
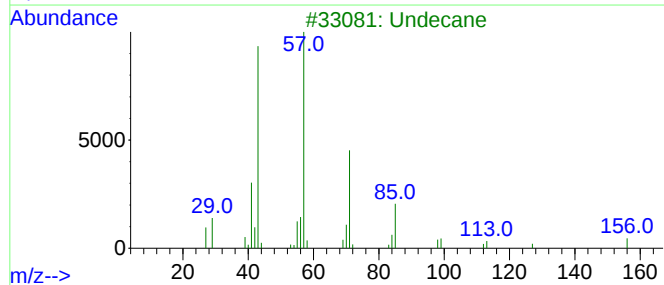
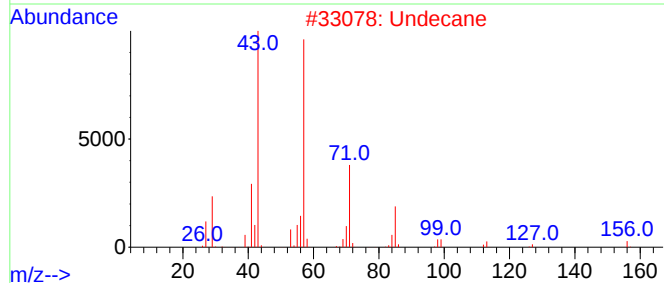
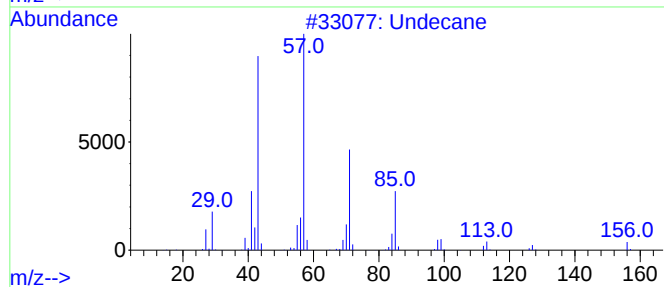
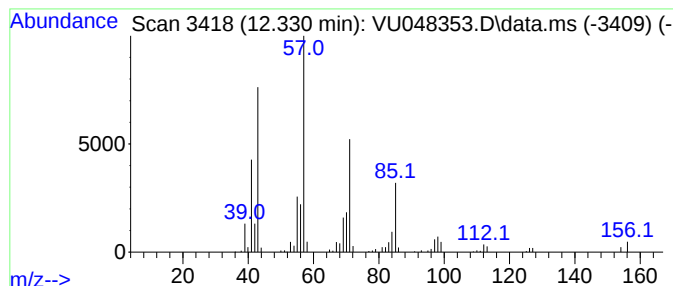
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	5.15 ug/L	118972	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	87
2	Undecane			156	C11H24	001120-21-4	74
3	Undecane			156	C11H24	001120-21-4	68
4	Undecane			156	C11H24	001120-21-4	68
5	Decane, 3,8-dimethyl-			170	C12H26	017312-55-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048353.D
Acq On : 29 Apr 2022 12:50
Operator : SY/MD
Sample : N2562-15ME
Misc : 7.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW476ME

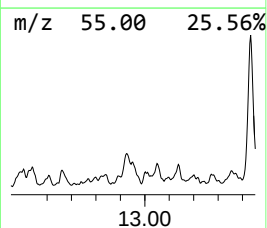
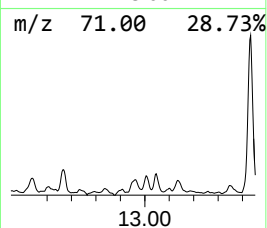
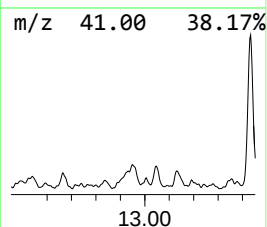
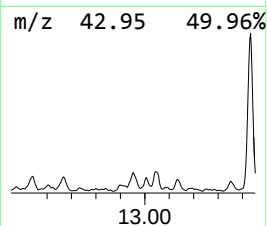
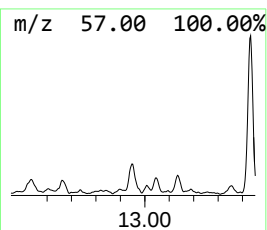
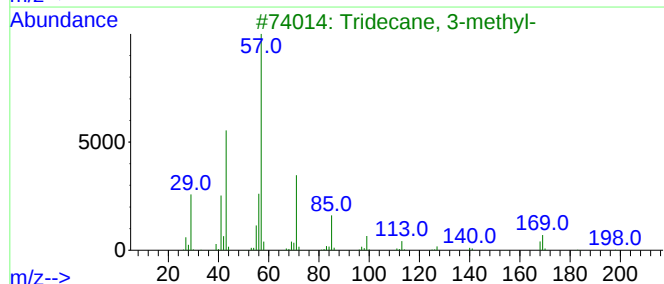
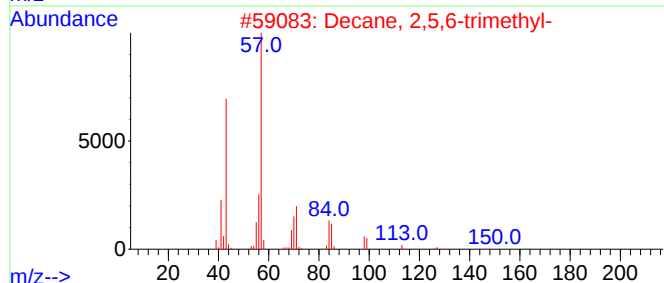
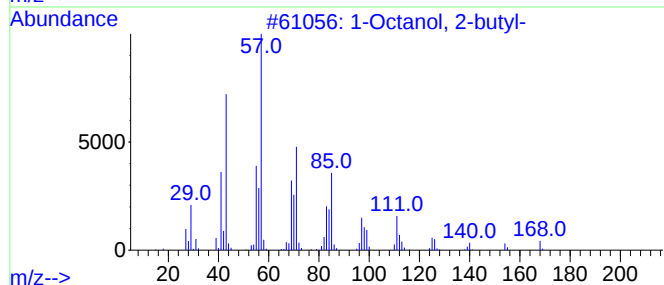
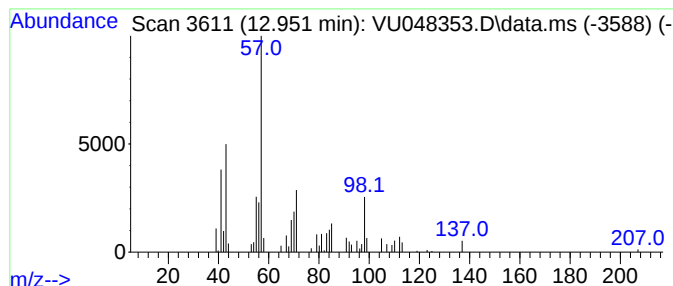
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Quant Title : VOC Analysis

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

Peak Number 5 1-Octanol, 2-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	2.60 ug/L	59925	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	50
2			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	50
3			Tridecane, 3-methyl-	198	C14H30	006418-41-3	50
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	49
5			Octane, 4,5-dipropyl-	198	C14H30	020905-05-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048353.D
Acq On : 29 Apr 2022 12:50
Operator : SY/MD
Sample : N2562-15ME
Misc : 7.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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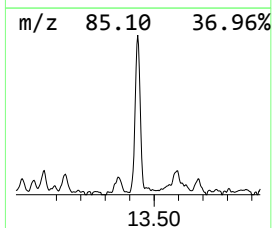
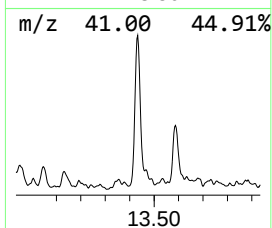
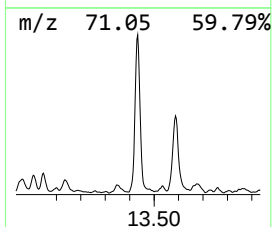
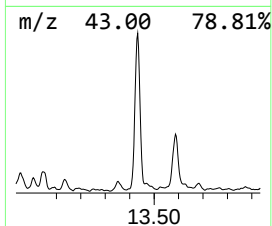
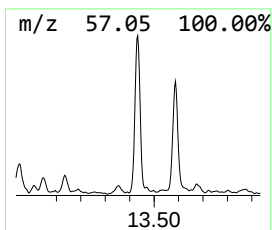
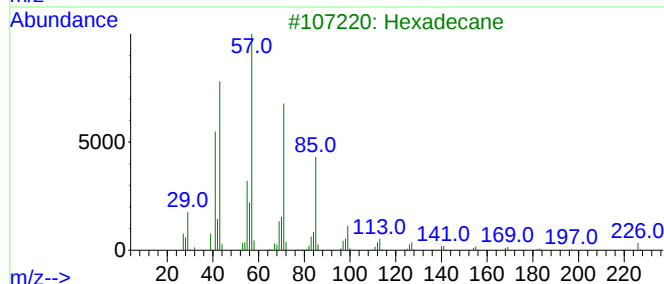
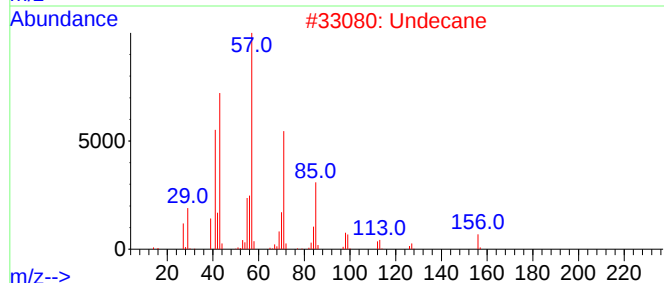
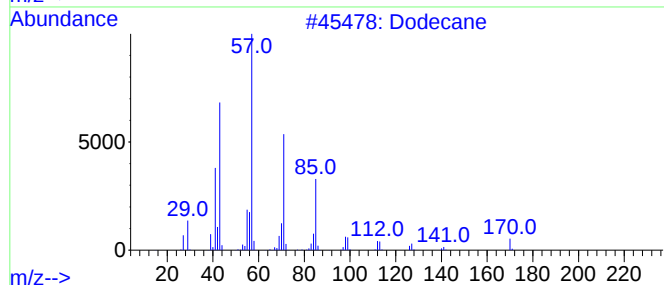
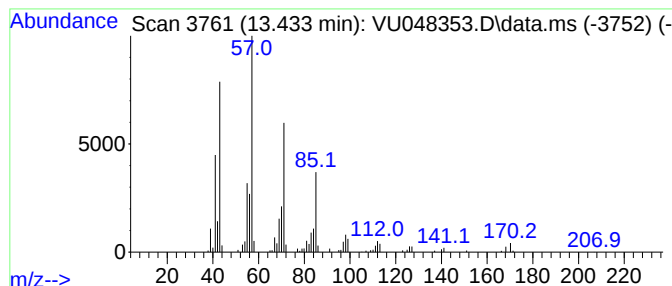
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	7.88 ug/L	181945	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Undecane	156	C11H24	001120-21-4	90
3			Hexadecane	226	C16H34	000544-76-3	80
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	72
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048353.D
Acq On : 29 Apr 2022 12:50
Operator : SY/MD
Sample : N2562-15ME
Misc : 7.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW476ME

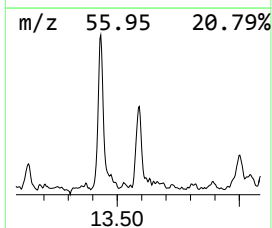
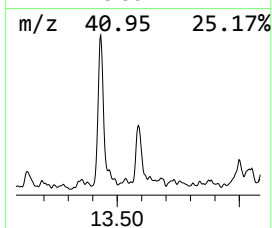
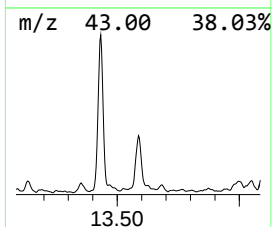
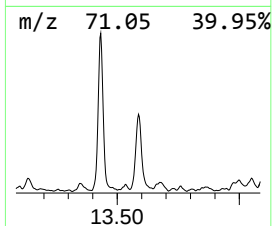
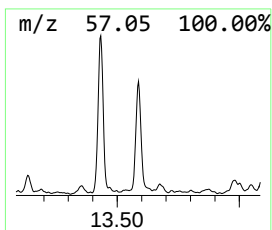
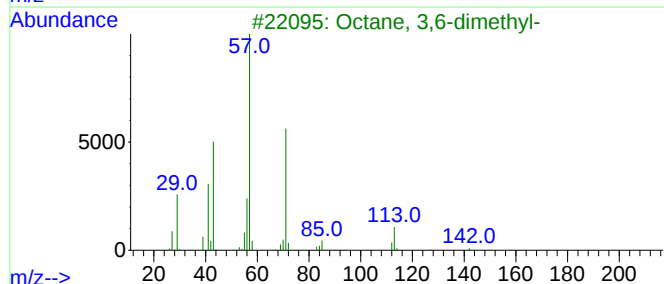
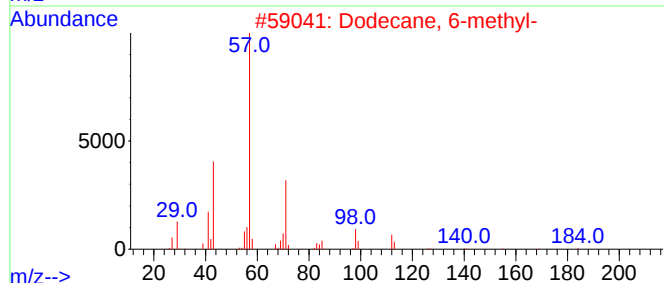
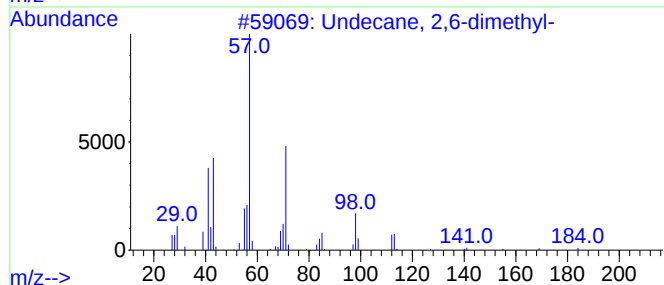
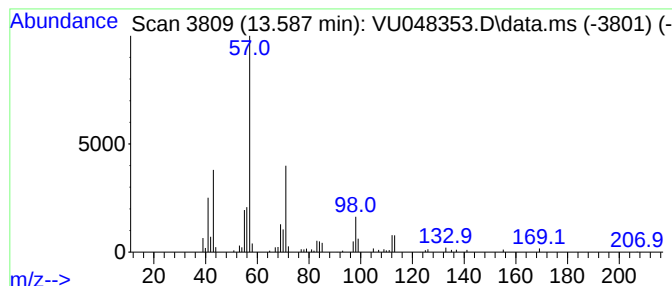
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	4.05 ug/L	93586	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	78
2			Dodecane, 6-methyl-	184	C13H28	006044-71-9	64
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59
4			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
Data File : VU048353.D
Acq On : 29 Apr 2022 12:50
Operator : SY/MD
Sample : N2562-15ME
Misc : 7.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW476ME

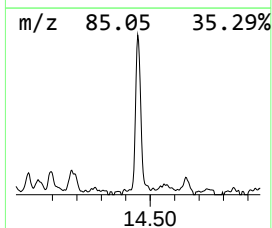
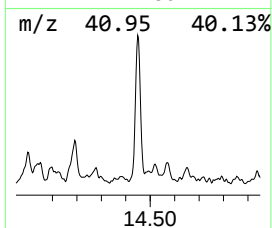
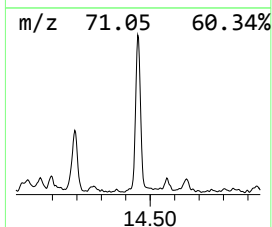
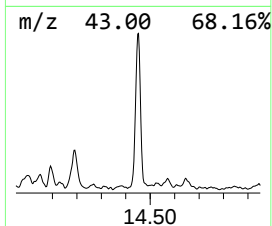
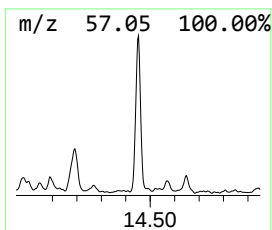
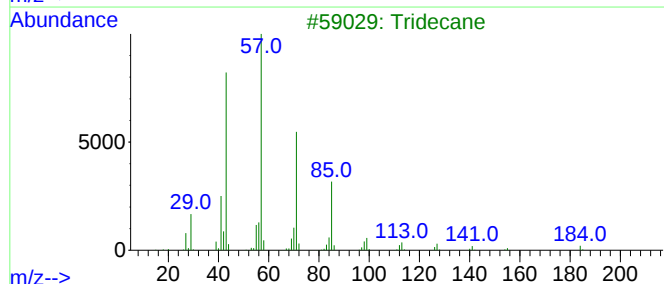
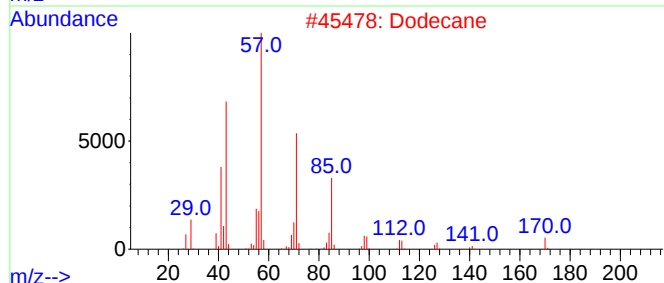
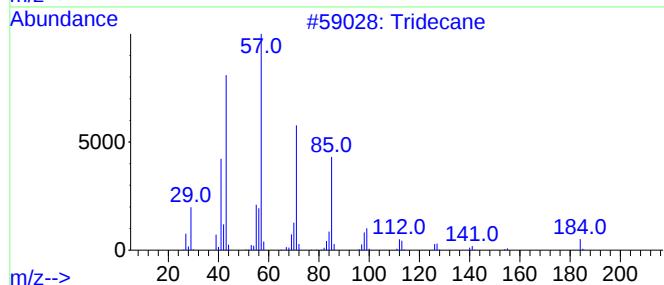
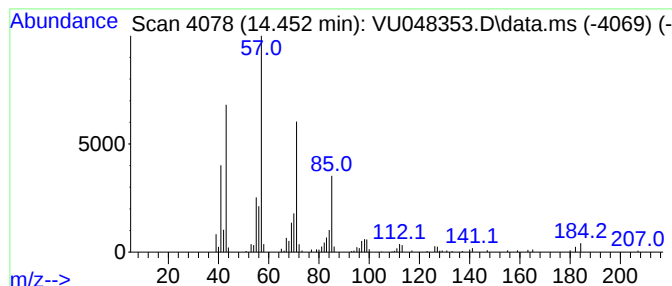
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Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.452	5.09 ug/L	117526	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	91
2			Dodecane	170	C12H26	000112-40-3	86
3			Tridecane	184	C13H28	000629-50-5	80
4			Nonadecane	268	C19H40	000629-92-5	80
5			Nonane	128	C9H20	000111-84-2	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
 Data File : VU048353.D
 Acq On : 29 Apr 2022 12:50
 Operator : SY/MD
 Sample : N2562-15ME
 Misc : 7.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW476ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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...	5.977	2.5	ug/L	43417	1	6.247	867732	50.0
(DEL) Alkane: S...	11.115	2.9	ug/L	67428	3	11.819	1154620	50.0
(DEL) Alkane: S...	12.330	5.2	ug/L	118972	3	11.819	1154620	50.0
1-Octanol, 2-bu...	12.951	2.6	ug/L	59925	3	11.819	1154620	50.0
(DEL) Alkane: S...	13.433	7.9	ug/L	181945	3	11.819	1154620	50.0
(DEL) Alkane: S...	13.587	4.0	ug/L	93586	3	11.819	1154620	50.0
(DEL) Alkane: S...	14.452	5.1	ug/L	117526	3	11.819	1154620	50.0