

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044500.D
 Acq On : 26 Dec 2024 11:30
 Operator : JC/MD
 Sample : P5333-07ME
 Misc : 3.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2910ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	33	rVB	4911	4894	0.47%	0.062%
2	1.368	42	46	63	rVB	85555	164637	15.95%	2.073%
3	1.630	69	89	90	rBV	52393	142106	13.77%	1.789%
4	2.288	190	197	210	rBV	207024	344404	33.37%	4.336%
5	2.538	233	238	242	rVB3	621	725	0.07%	0.009%
6	2.605	247	249	250	rVB2	592	355	0.03%	0.004%
7	2.660	255	258	259	rBV	444	491	0.05%	0.006%
8	2.727	263	269	272	rBV6	1120	2267	0.22%	0.029%
9	2.764	273	275	276	rBV2	543	374	0.04%	0.005%
10	2.837	285	287	292	rVB2	470	759	0.07%	0.010%
11	2.953	297	306	311	rBV2	3897	10540	1.02%	0.133%
12	3.050	321	322	324	rVB2	681	347	0.03%	0.004%
13	3.081	324	327	330	rBV2	444	458	0.04%	0.006%
14	3.203	344	347	348	rBV	637	472	0.05%	0.006%
15	3.276	356	359	362	rBV3	379	540	0.05%	0.007%
16	3.367	372	374	377	rVB	644	433	0.04%	0.005%
17	3.416	379	382	383	rBV	602	647	0.06%	0.008%
18	3.520	398	399	402	rVB	695	366	0.04%	0.005%
19	3.544	402	403	405	rBV2	463	379	0.04%	0.005%
20	3.678	423	425	429	rVB3	313	357	0.03%	0.004%
21	3.757	435	438	439	rVB2	489	355	0.03%	0.004%
22	3.782	439	442	444	rBV	342	468	0.05%	0.006%
23	3.843	450	452	455	rVB2	572	588	0.06%	0.007%
24	3.898	455	461	463	rBV4	503	1051	0.10%	0.013%
25	4.483	549	557	576	rBV	35569	152918	14.81%	1.925%
26	4.867	617	620	621	rBV2	764	719	0.07%	0.009%
27	4.916	625	628	629	rBV2	556	479	0.05%	0.006%
28	4.952	633	634	636	rBV2	458	342	0.03%	0.004%
29	5.050	636	650	668	rBV2	126370	412458	39.96%	5.193%
30	5.471	717	719	721	rBV3	338	373	0.04%	0.005%
31	5.531	727	729	731	rBV2	614	789	0.08%	0.010%
32	5.592	738	739	742	rBV3	445	474	0.05%	0.006%
33	5.672	750	752	754	rVB2	466	413	0.04%	0.005%
34	5.824	774	777	779	rBV3	525	635	0.06%	0.008%
35	5.958	788	799	819	rBV2	350290	1032231	100.00%	12.996%
36	6.153	829	831	835	rVB3	796	1077	0.10%	0.014%

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 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2910ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

37	6.190	835	837	839	rBV3	362	445	0.04%	0.006%
38	6.367	862	866	872	rVV5	1026	2325	0.23%	0.029%
39	6.580	898	901	903	rBV3	273	362	0.04%	0.005%
40	6.611	903	906	908	rBV3	438	635	0.06%	0.008%
41	6.757	921	930	944	rBV	244871	608204	58.92%	7.658%
42	7.056	978	979	982	rBV3	547	449	0.04%	0.006%
43	7.110	982	988	995	rBV9	2941	9071	0.88%	0.114%
44	7.208	1001	1004	1006	rBV3	1160	1593	0.15%	0.020%
45	7.299	1011	1019	1035	rVB	201356	456993	44.27%	5.754%
46	7.525	1054	1056	1057	rBV2	473	380	0.04%	0.005%
47	7.592	1066	1067	1069	rVB	644	429	0.04%	0.005%
48	7.616	1069	1071	1072	rBV	410	391	0.04%	0.005%
49	7.891	1114	1116	1118	rVB3	538	415	0.04%	0.005%
50	7.921	1118	1121	1122	rBV2	425	480	0.05%	0.006%
51	7.946	1122	1125	1129	rVV5	914	1772	0.17%	0.022%
52	8.116	1151	1153	1155	rVB2	529	406	0.04%	0.005%
53	8.159	1158	1160	1165	rBV4	650	902	0.09%	0.011%
54	8.220	1168	1170	1172	rBV3	431	406	0.04%	0.005%
55	8.275	1173	1179	1181	rBV5	1561	2811	0.27%	0.035%
56	8.324	1181	1187	1201	rVV	121493	206836	20.04%	2.604%
57	8.476	1210	1212	1213	rVB2	1020	561	0.05%	0.007%
58	8.507	1215	1217	1219	rBV2	444	381	0.04%	0.005%
59	8.586	1226	1230	1233	rBV4	924	1457	0.14%	0.018%
60	8.647	1233	1240	1253	rBV	505893	840372	81.41%	10.581%
61	8.848	1271	1273	1275	rVB3	721	353	0.03%	0.004%
62	8.909	1278	1283	1285	rBV3	3662	5971	0.58%	0.075%
63	8.952	1285	1290	1305	rVB	80962	136094	13.18%	1.713%
64	9.104	1312	1315	1317	rBV4	933	1251	0.12%	0.016%
65	9.287	1342	1345	1348	rVB4	1116	1574	0.15%	0.020%
66	9.354	1354	1356	1357	rBV2	534	404	0.04%	0.005%
67	9.391	1357	1362	1377	rVV	186511	348120	33.73%	4.383%
68	9.616	1395	1399	1405	rVB4	5036	7656	0.74%	0.096%
69	9.701	1411	1413	1417	rVB5	1516	1681	0.16%	0.021%
70	9.756	1417	1422	1425	rBV5	1642	2580	0.25%	0.032%
71	9.817	1428	1432	1436	rBV6	2026	3698	0.36%	0.047%
72	9.897	1442	1445	1450	rVB4	3658	5276	0.51%	0.066%
73	10.006	1459	1463	1465	rBV4	2586	3442	0.33%	0.043%
74	10.049	1465	1470	1485	rVB	520806	730624	70.78%	9.199%
75	10.268	1504	1506	1508	rBV3	1273	1271	0.12%	0.016%
76	10.360	1517	1521	1527	rVB3	13740	17583	1.70%	0.221%

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 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2910ME

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_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	10.451	1533	1536	1540	rVB3	2262	3140	0.30%	0.040%
78	10.774	1582	1589	1593	rBV3	8110	12529	1.21%	0.158%
79	10.890	1605	1608	1614	rVB2	7635	10497	1.02%	0.132%
80	10.939	1614	1616	1618	rBV2	1380	1508	0.15%	0.019%
81	11.189	1651	1657	1669	rBV	328551	451604	43.75%	5.686%
82	11.317	1675	1678	1679	rBV2	1665	1761	0.17%	0.022%
83	11.433	1693	1697	1699	rBV4	3148	4365	0.42%	0.055%
84	11.476	1700	1704	1709	rVB	35550	40010	3.88%	0.504%
85	11.713	1739	1743	1746	rBV	16219	18333	1.78%	0.231%
86	11.829	1758	1762	1763	rBV3	1285	1590	0.15%	0.020%
87	12.018	1788	1793	1800	rBV	576243	745368	72.21%	9.385%
88	12.317	1837	1842	1850	rBV	584506	742543	71.94%	9.349%
89	12.420	1855	1859	1863	rVV	53003	57190	5.54%	0.720%
90	12.683	1898	1902	1905	rBV4	4564	6307	0.61%	0.079%
91	12.884	1932	1935	1943	rBV7	6726	14330	1.39%	0.180%
92	13.036	1956	1960	1963	rBV5	3770	5897	0.57%	0.074%
93	13.134	1973	1976	1982	rBV5	5724	7953	0.77%	0.100%
94	13.268	1994	1998	2001	rBV	37289	47483	4.60%	0.598%
95	13.384	2013	2017	2020	rBV	14270	17171	1.66%	0.216%
96	14.036	2121	2124	2128	rVB	28461	28986	2.81%	0.365%
97	14.615	2215	2219	2221	rBV4	5792	8116	0.79%	0.102%
98	14.749	2239	2241	2244	rVB	8894	9980	0.97%	0.126%
99	14.877	2259	2262	2267	rVB	12845	14202	1.38%	0.179%
100	15.127	2301	2303	2307	rBV3	4171	5052	0.49%	0.064%

Sum of corrected areas: 7942490

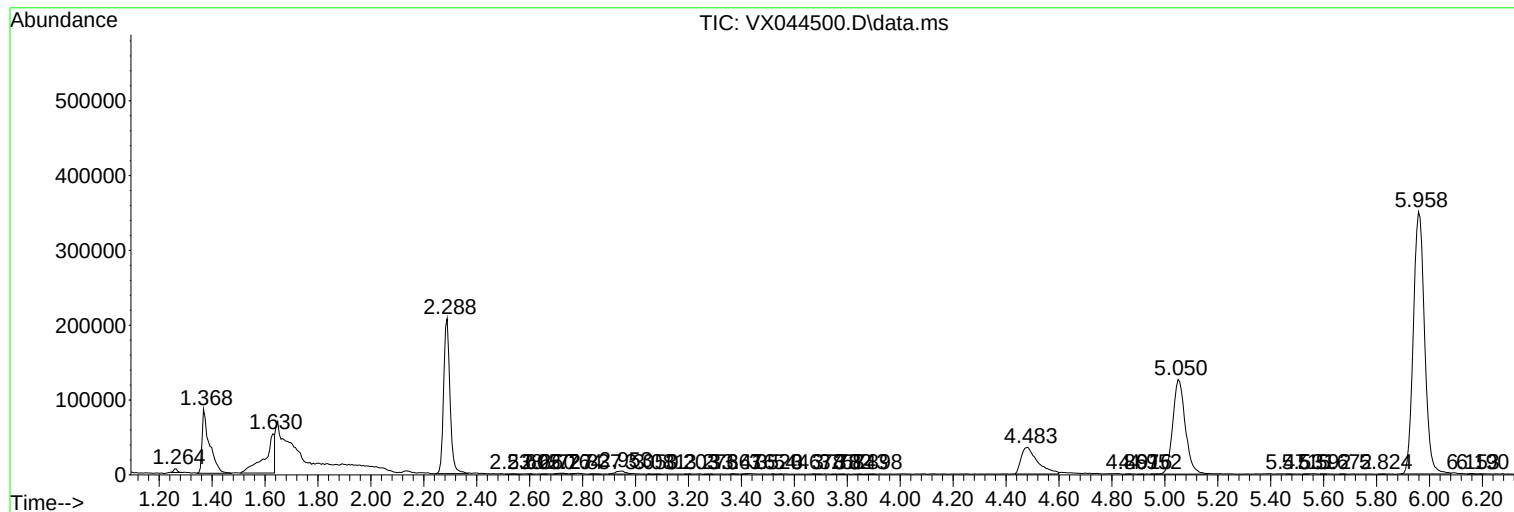
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
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Misc : 3.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2910ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
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Sample : P5333-07ME
Misc : 3.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2910ME

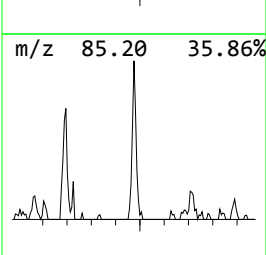
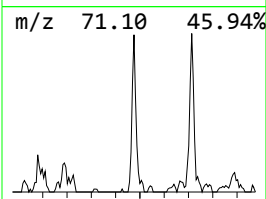
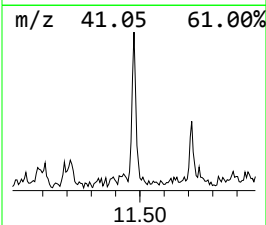
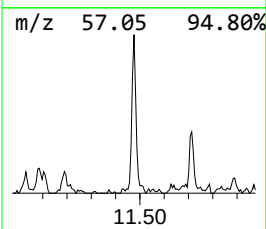
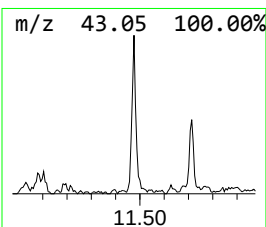
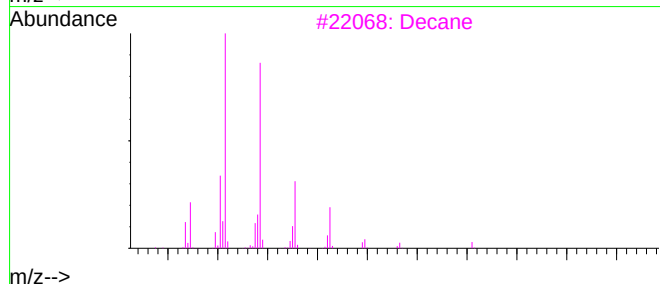
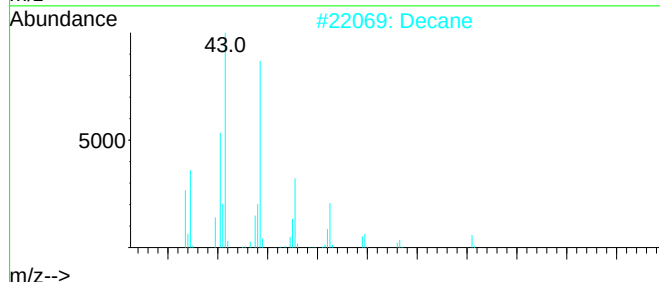
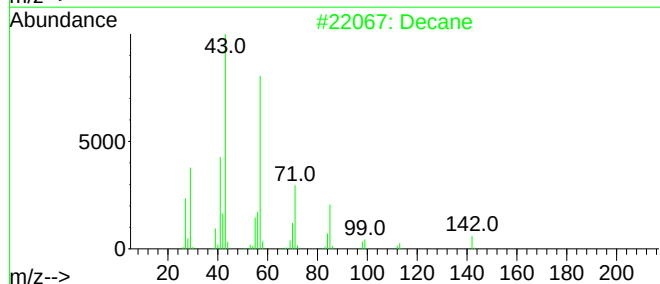
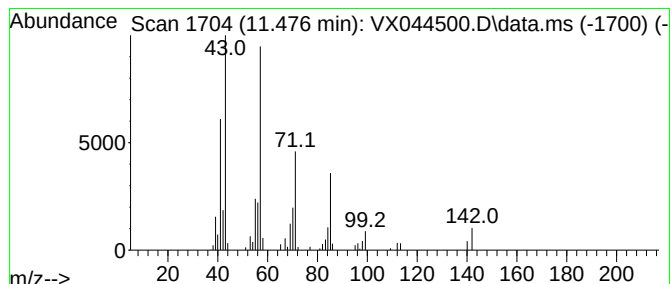
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.476	2.68 ug/L	40010	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	91
2	Decane	142	C10H22	000124-18-5	90
3	Decane	142	C10H22	000124-18-5	87
4	Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	78
5	Decane	142	C10H22	000124-18-5	64



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Operator : JC/MD
Sample : P5333-07ME
Misc : 3.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2910ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

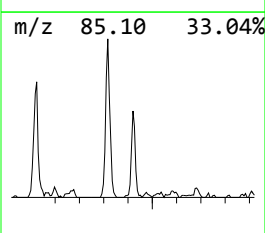
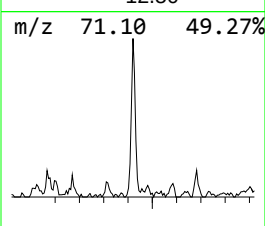
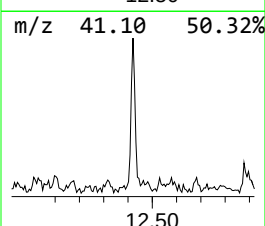
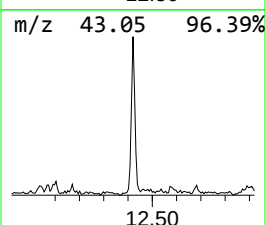
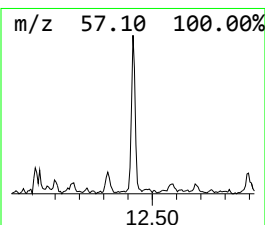
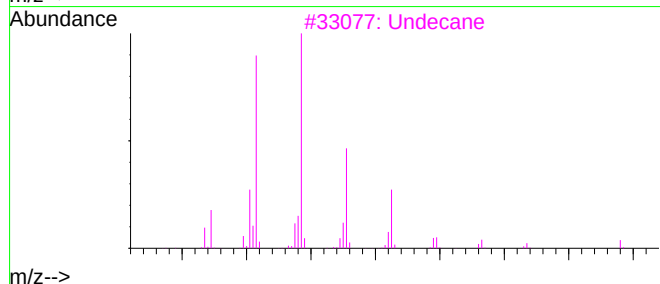
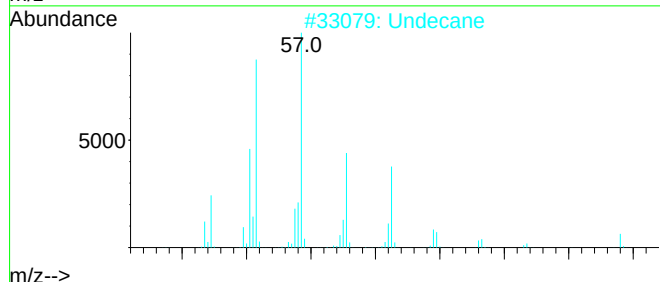
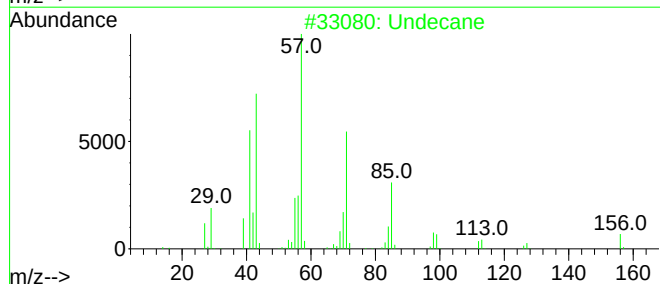
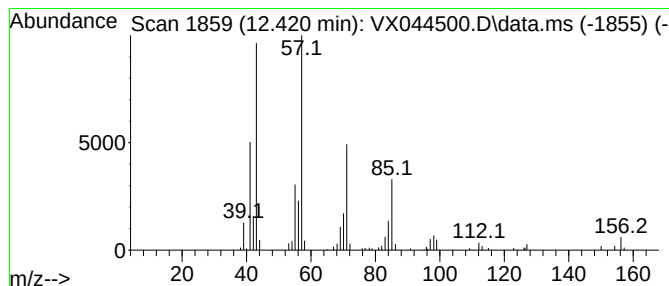
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	3.84 ug/L	57190	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Undecane	156	C11H24	001120-21-4	87
3	Undecane	156	C11H24	001120-21-4	83
4	Undecane	156	C11H24	001120-21-4	80
5	Undecane	156	C11H24	001120-21-4	74



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Sample : P5333-07ME
Misc : 3.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2910ME

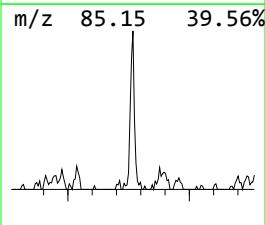
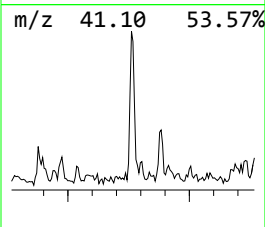
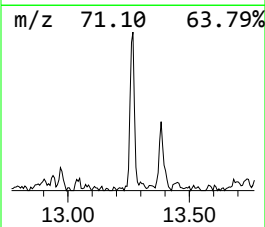
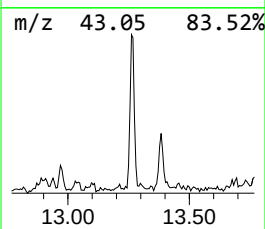
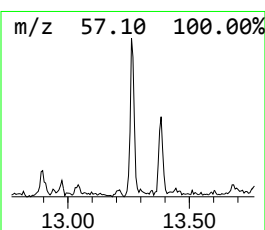
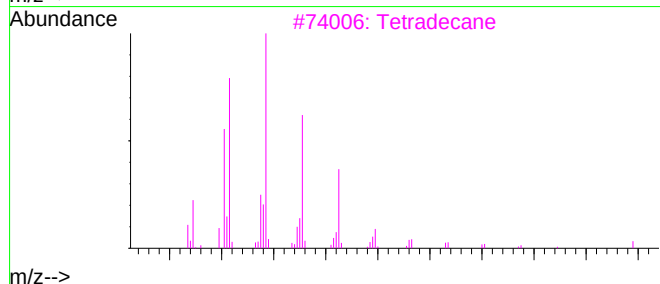
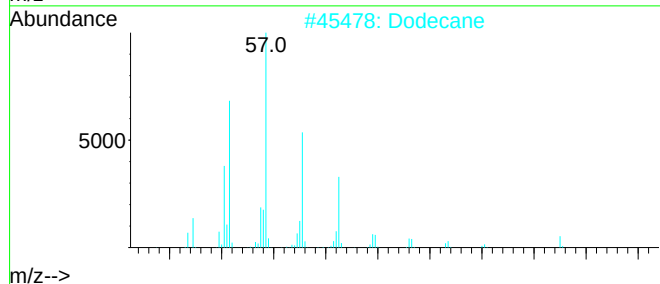
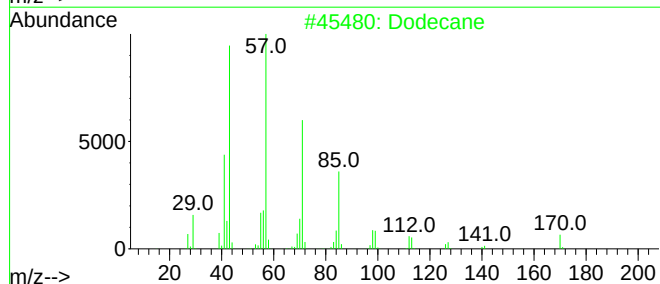
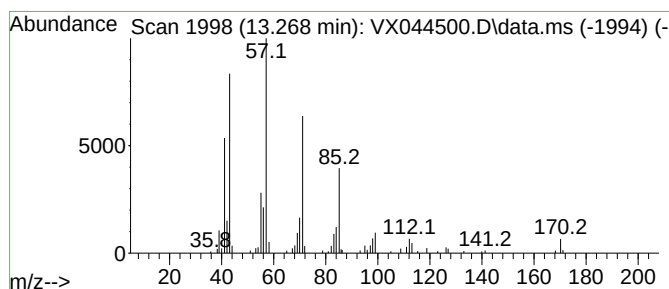
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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.	
13.268	3.19 ug/L	47483	1,4-Dichlorobenzene-d4		12.018	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane		170	C12H26	000112-40-3	95
2	Dodecane		170	C12H26	000112-40-3	94
3	Tetradecane		198	C14H30	000629-59-4	91
4	Dodecane		170	C12H26	000112-40-3	90
5	Hexadecane		226	C16H34	000544-76-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044500.D
Acq On : 26 Dec 2024 11:30
Operator : JC/MD
Sample : P5333-07ME
Misc : 3.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2910ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.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...	11.476	2.7	ug/L	40010	3	12.018	745368	50.0
(DEL) Alkane: S...	12.421	3.8	ug/L	57190	3	12.018	745368	50.0
(DEL) Alkane: S...	13.268	3.2	ug/L	47483	3	12.018	745368	50.0