

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW060823\
 Data File : VW026144.D
 Acq On : 08 Jun 2023 20:18
 Operator : SY/MD
 Sample : 03101-09
 Misc : 4.24g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EZEM5

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_W\Method\SFAMWLM053023SMA.M

Title : SFAM01.0

Signal : TIC: VW026144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.143	38	42	51	rVB2	18497	34964	1.06%	0.158%
2	2.362	72	78	90	rVB	156193	372406	11.25%	1.681%
3	2.893	158	165	180	rBV	139696	393764	11.89%	1.778%
4	3.387	240	246	253	rVV2	8745	23587	0.71%	0.106%
5	3.630	285	286	288	rBV2	1530	1328	0.04%	0.006%
6	3.771	306	309	312	rVB5	1773	2119	0.06%	0.010%
7	3.850	318	322	323	rBV4	1281	1690	0.05%	0.008%
8	3.905	330	331	334	rVB3	1519	1399	0.04%	0.006%
9	4.021	338	350	360	rBV2	322209	1026416	31.00%	4.634%
10	4.118	361	366	376	rVB	74920	197864	5.98%	0.893%
11	4.368	404	407	409	rBV4	2545	3284	0.10%	0.015%
12	4.496	427	428	433	rVB5	2026	2017	0.06%	0.009%
13	4.539	433	435	438	rBV4	1574	1612	0.05%	0.007%
14	4.636	448	451	453	rVB4	1717	1715	0.05%	0.008%
15	4.667	453	456	458	rVB4	1450	1516	0.05%	0.007%
16	4.703	458	462	464	rBV5	1679	2389	0.07%	0.011%
17	4.740	464	468	472	rVB7	1626	2164	0.07%	0.010%
18	4.917	483	497	505	rBV4	16178	64524	1.95%	0.291%
19	5.118	528	530	532	rBV3	2186	2054	0.06%	0.009%
20	5.148	532	535	538	rBV5	2434	3708	0.11%	0.017%
21	5.398	573	576	579	rBV5	1952	2696	0.08%	0.012%
22	5.435	579	582	585	rBV5	1395	2425	0.07%	0.011%
23	5.465	585	587	589	rVV2	1422	1478	0.04%	0.007%
24	5.508	591	594	598	rVB5	1211	1309	0.04%	0.006%
25	5.539	598	599	604	rBV5	1549	1352	0.04%	0.006%
26	5.709	624	627	629	rBV4	1735	1541	0.05%	0.007%
27	5.746	629	633	635	rVV5	2275	3521	0.11%	0.016%
28	5.770	635	637	641	rVB4	2682	2671	0.08%	0.012%
29	5.941	658	665	667	rBV7	4579	9135	0.28%	0.041%
30	6.112	689	693	695	rBV5	1128	1393	0.04%	0.006%
31	6.160	698	701	703	rBV3	1413	1720	0.05%	0.008%
32	6.179	703	704	708	rVB4	1352	1291	0.04%	0.006%
33	6.221	708	711	714	rBV5	1264	1449	0.04%	0.007%
34	6.319	724	727	731	rVB6	923	1296	0.04%	0.006%
35	6.374	732	736	737	rVB4	1453	1451	0.04%	0.007%
36	6.429	742	745	746	rBV3	2010	1913	0.06%	0.009%

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 Title : SFAM01.0

37	6.606	772	774	775	rBV2	1923	1454	0.04%	0.007%
38	6.904	820	823	824	rBV3	1986	1347	0.04%	0.006%
39	6.990	830	837	838	rBV7	1935	2822	0.09%	0.013%
40	7.075	842	851	860	rBV	110679	334733	10.11%	1.511%
41	7.544	927	928	934	rVB6	1658	1660	0.05%	0.007%
42	7.648	934	945	957	rBV	559125	1353151	40.86%	6.110%
43	7.819	971	973	976	rBV4	1469	1586	0.05%	0.007%
44	7.855	976	979	982	rBV5	1314	1327	0.04%	0.006%
45	7.935	990	992	993	rBV2	1854	1529	0.05%	0.007%
46	8.148	1024	1027	1031	rVV6	2138	3079	0.09%	0.014%
47	8.276	1037	1048	1065	rBV2	1102089	3311407	100.00%	14.951%
48	8.416	1069	1071	1073	rVV3	1756	1507	0.05%	0.007%
49	8.532	1087	1090	1093	rBV5	1948	2824	0.09%	0.013%
50	8.575	1093	1097	1098	rVV4	998	1651	0.05%	0.007%
51	8.697	1110	1117	1123	rBV4	3143	9380	0.28%	0.042%
52	8.843	1131	1141	1157	rBV	1080307	2185710	66.01%	9.869%
53	8.995	1163	1166	1170	rVB6	1955	2774	0.08%	0.013%
54	9.075	1176	1179	1186	rVB8	4963	8203	0.25%	0.037%
55	9.154	1191	1192	1196	rBV4	1548	1750	0.05%	0.008%
56	9.270	1203	1211	1221	rBV	785338	1606114	48.50%	7.252%
57	9.514	1249	1251	1254	rVB4	1957	2293	0.07%	0.010%
58	9.550	1254	1257	1258	rBV2	1271	1323	0.04%	0.006%
59	9.605	1263	1266	1268	rBV4	1768	1856	0.06%	0.008%
60	9.666	1270	1276	1284	rBV4	7499	15468	0.47%	0.070%
61	9.745	1287	1289	1297	rVB9	3894	6838	0.21%	0.031%
62	9.806	1297	1299	1302	rBV4	2114	2215	0.07%	0.010%
63	9.843	1302	1305	1307	rBV4	1953	2782	0.08%	0.013%
64	9.959	1320	1324	1327	rBV6	1941	2916	0.09%	0.013%
65	10.032	1327	1336	1344	rBV	317903	576830	17.42%	2.604%
66	10.318	1375	1383	1391	rBV	1365753	2427254	73.30%	10.959%
67	10.501	1409	1413	1418	rVB8	4190	7315	0.22%	0.033%
68	10.574	1418	1425	1436	rBV	204746	360449	10.89%	1.627%
69	10.745	1451	1453	1455	rBV3	1406	1494	0.05%	0.007%
70	10.849	1465	1470	1475	rVB8	6678	12451	0.38%	0.056%
71	10.922	1475	1482	1496	rBV	385609	727562	21.97%	3.285%
72	11.093	1507	1510	1518	rVB10	2955	7043	0.21%	0.032%
73	11.172	1520	1523	1527	rVV5	5285	8146	0.25%	0.037%
74	11.227	1528	1532	1538	rVB5	8425	13925	0.42%	0.063%
75	11.336	1548	1550	1554	rVB4	5088	4792	0.14%	0.022%
76	11.507	1573	1578	1584	rBV4	4608	11254	0.34%	0.051%

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77	11.629	1590	1598	1608	rBV	1329327	2203007	66.53%	9.947%
78	11.727	1611	1614	1617	rBV2	5354	7929	0.24%	0.036%
79	11.873	1634	1638	1642	rVB3	12861	20560	0.62%	0.093%
80	11.916	1642	1645	1649	rVB4	11671	18188	0.55%	0.082%
81	11.970	1651	1654	1658	rBV5	4132	8210	0.25%	0.037%
82	12.056	1664	1668	1673	rVB6	7319	14700	0.44%	0.066%
83	12.135	1673	1681	1692	rBV5	34827	102168	3.09%	0.461%
84	12.251	1696	1700	1704	rVB	37044	55193	1.67%	0.249%
85	12.361	1704	1718	1726	rBV4	59442	205458	6.20%	0.928%
86	12.586	1752	1755	1757	rBV	11703	14964	0.45%	0.068%
87	12.690	1765	1772	1779	rBV	561885	940625	28.41%	4.247%
88	12.775	1783	1786	1793	rVB3	46748	79440	2.40%	0.359%
89	12.854	1794	1799	1804	rBV5	20381	45005	1.36%	0.203%
90	12.940	1805	1813	1818	rBV5	58382	148430	4.48%	0.670%
91	13.074	1832	1835	1839	rBV3	20955	26584	0.80%	0.120%
92	13.123	1839	1843	1846	rBV3	26037	40171	1.21%	0.181%
93	13.159	1846	1849	1851	rBV2	25124	33152	1.00%	0.150%
94	13.287	1867	1870	1875	rBV3	25031	38201	1.15%	0.172%
95	13.556	1908	1914	1920	rBV	884439	1435331	43.35%	6.481%
96	13.848	1956	1962	1971	rBV	735225	1321429	39.91%	5.966%
97	14.379	2046	2049	2054	rVB4	33611	47925	1.45%	0.216%
98	14.494	2065	2068	2073	rBV3	17242	29320	0.89%	0.132%
99	15.323	2199	2204	2211	rVB	32698	58810	1.78%	0.266%
100	16.275	2356	2360	2369	rVB2	24563	47489	1.43%	0.214%

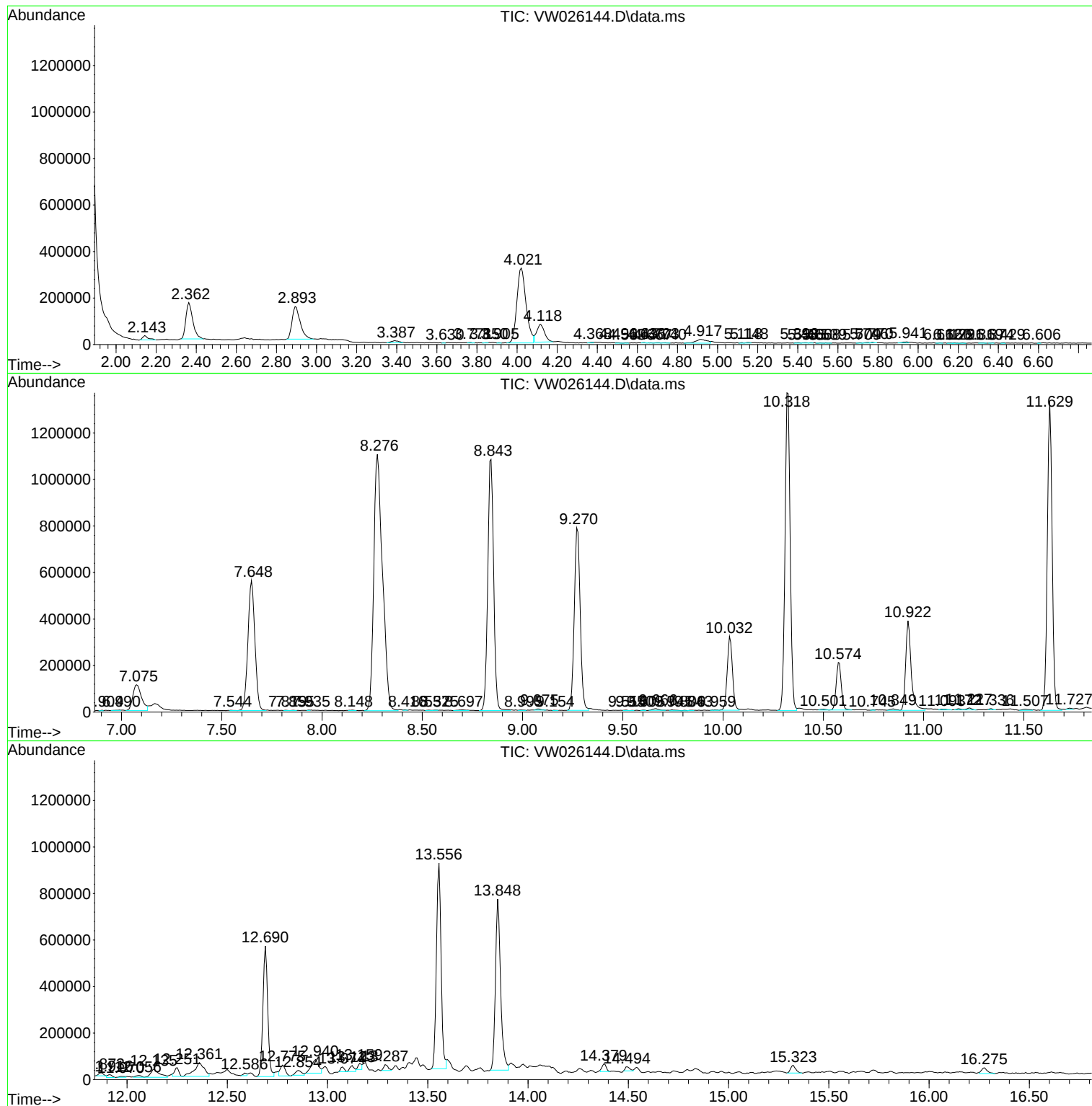
Sum of corrected areas: 22147664

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM053023SMA.M
Quant Title : SFAM01.0

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



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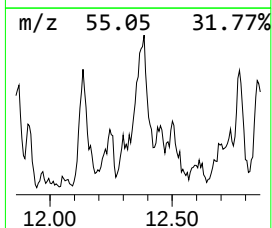
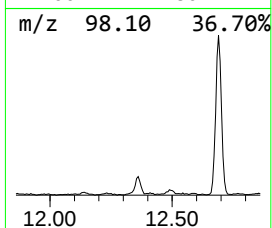
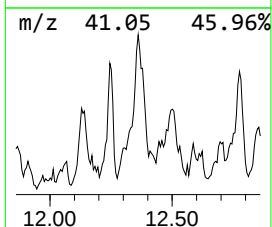
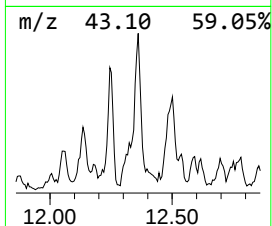
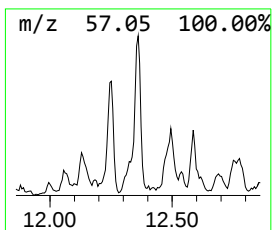
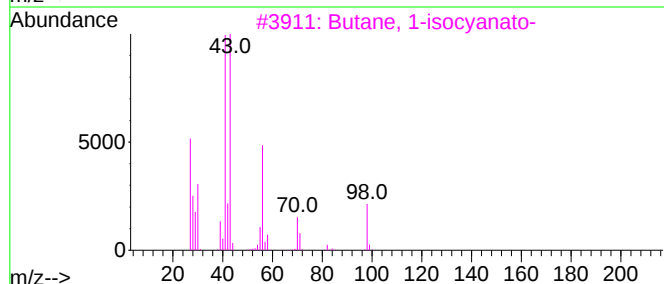
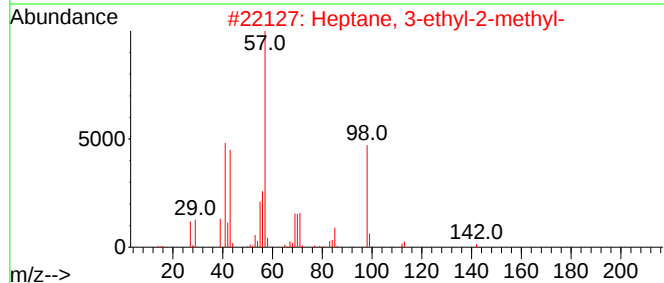
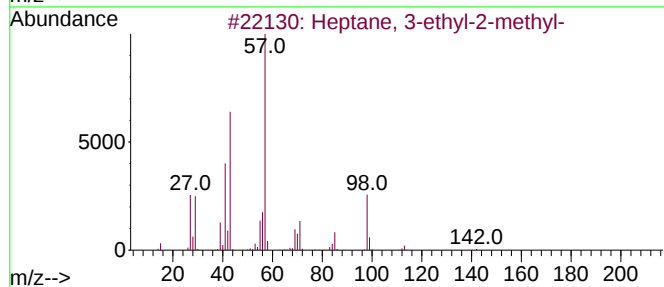
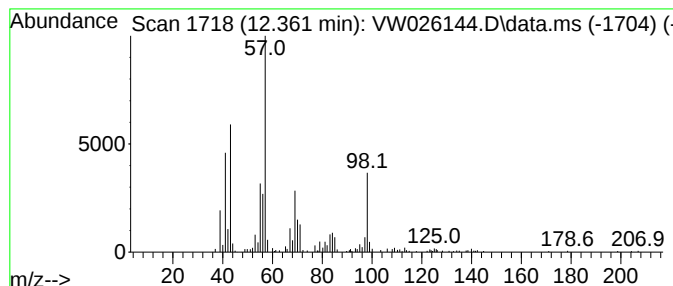
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM053023SMA.M
Quant Title : SFAM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.361	2.33 ug/L	205458	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	58
2			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	58
3			Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	50
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	47
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	47



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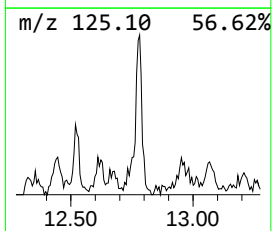
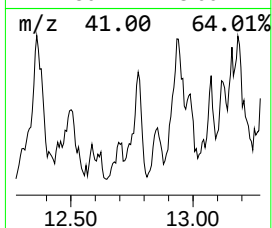
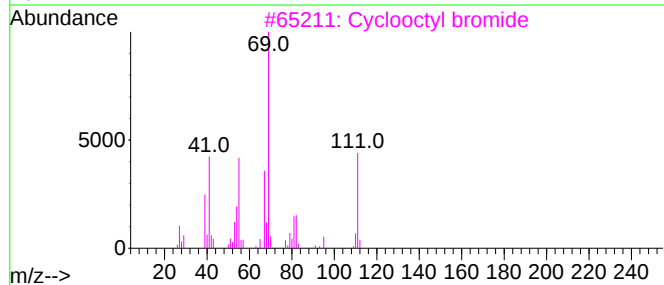
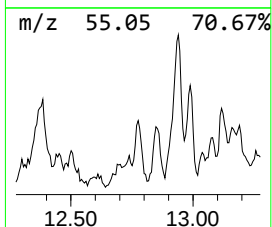
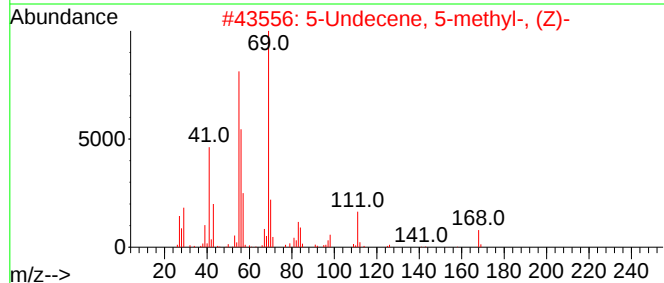
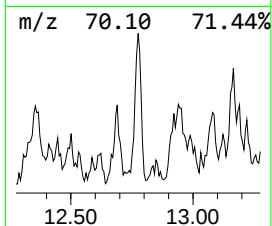
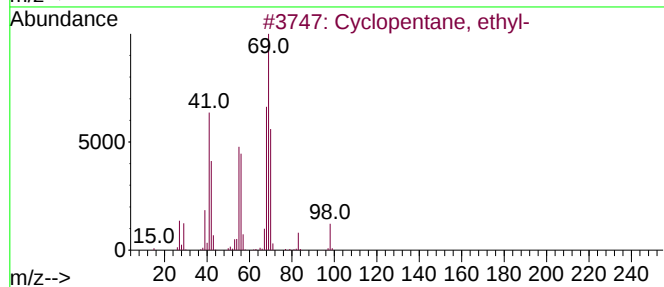
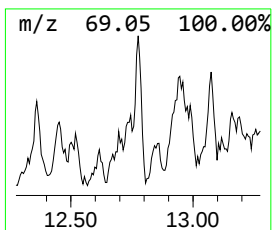
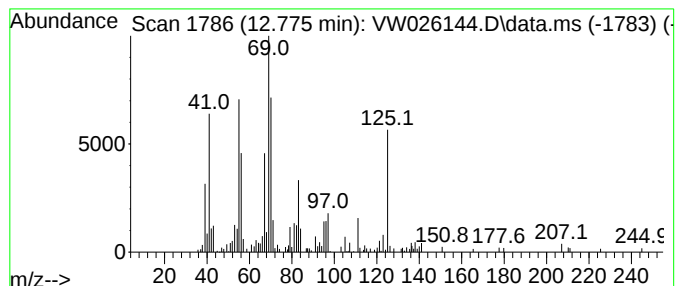
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM053023SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Cyclic12.775 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	1.38 ug/L	79440	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, ethyl-	98	C7H14	001640-89-7	47
2			5-Undecene, 5-methyl-, (Z)-	168	C12H24	057024-93-8	38
3			Cyclooctyl bromide	190	C8H15Br	001556-09-8	35
4			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	35
5			Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	27



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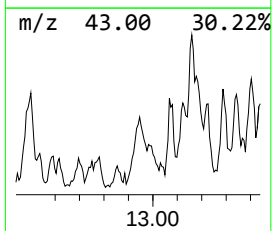
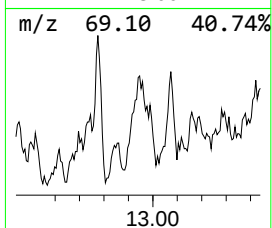
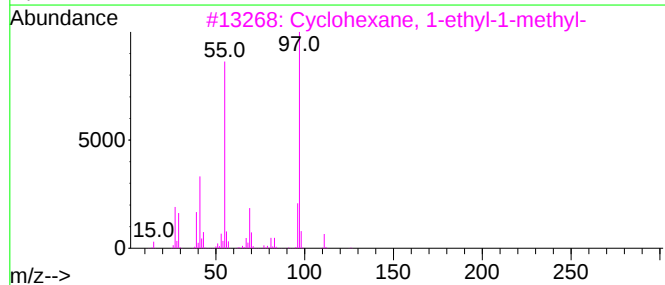
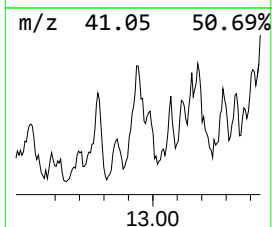
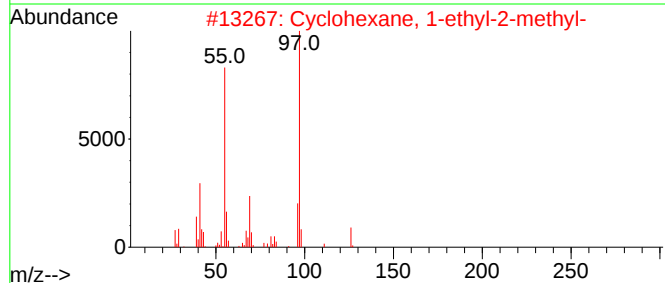
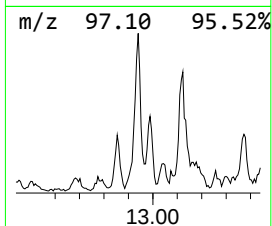
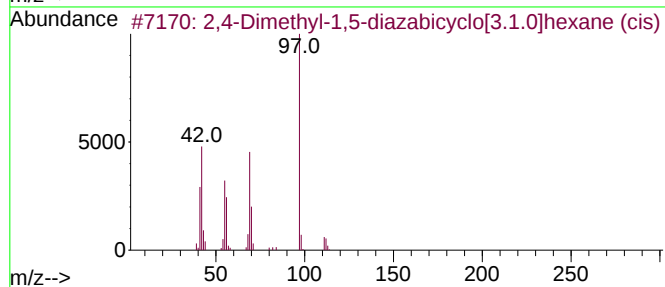
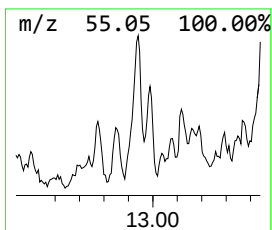
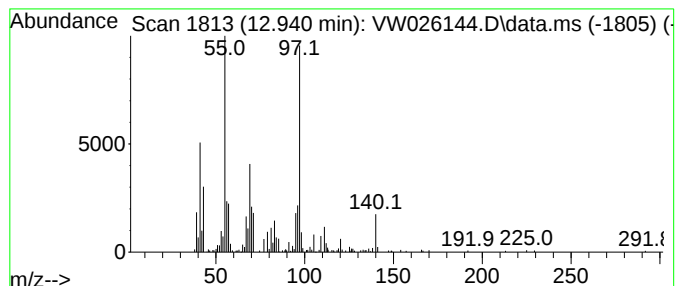
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Quant Title : SFAM01.0

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

Peak Number 4 2,4-Dimethyl-1,5-diazabicyc... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.940	2.59 ug/L	148430	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	64
2			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	59
3			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	59
4			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	49
5			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW060823\
Data File : VW026144.D
Acq On : 08 Jun 2023 20:18
Operator : SY/MD
Sample : 03101-09
Misc : 4.24g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EZEM5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM053023SMA.M
Quant Title : SFAM01.0

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...	12.361	2.3	ug/L	205458	2	11.629	2203010	25.0
(DEL) Alkane: C...	12.775	1.4	ug/L	79440	3	13.556	1435330	25.0
2,4-Dimethyl-1,...	12.940	2.6	ug/L	148430	3	13.556	1435330	25.0