

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW052522\
 Data File : VW023325.D
 Acq On : 25 May 2022 16:48
 Operator : SY/VA
 Sample : N2995-20
 Misc : 5.06g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GBGS1

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\SFAMWLM050222SMA.M
 Title : SFAM01.0

Signal : TIC: VW023325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.160	36	42	47	rBV	7746	15284	1.65%	0.183%
2	2.221	47	52	53	rBV5	4520	5629	0.61%	0.068%
3	2.349	68	73	82	rBV	75351	126967	13.75%	1.523%
4	2.879	155	160	171	rVB	48643	107600	11.65%	1.290%
5	3.294	226	228	229	rBV2	1456	1430	0.15%	0.017%
6	3.343	234	236	238	rVV3	1289	1328	0.14%	0.016%
7	3.373	238	241	242	rVV3	1196	1252	0.14%	0.015%
8	3.391	242	244	247	rVB4	1253	1197	0.13%	0.014%
9	3.544	261	269	272	rBV6	2663	6309	0.68%	0.076%
10	3.599	276	278	282	rVB4	1368	1372	0.15%	0.016%
11	3.763	303	305	308	rVB4	1200	1245	0.13%	0.015%
12	3.806	308	312	316	rBV6	1193	2242	0.24%	0.027%
13	3.879	319	324	327	rBV6	1035	1543	0.17%	0.019%
14	4.019	337	347	359	rBV	79377	244856	26.51%	2.936%
15	4.294	390	392	397	rVB6	962	1542	0.17%	0.018%
16	4.367	401	404	407	rBV4	708	1081	0.12%	0.013%
17	4.410	407	411	412	rBV4	1034	1387	0.15%	0.017%
18	4.562	431	436	440	rVB7	985	2199	0.24%	0.026%
19	4.611	440	444	446	rBV3	821	1246	0.13%	0.015%
20	4.666	451	453	455	rBV4	1064	1438	0.16%	0.017%
21	4.781	469	472	476	rBV5	1337	2422	0.26%	0.029%
22	4.867	481	486	487	rBV4	918	1212	0.13%	0.015%
23	4.922	487	495	505	rVV3	6529	21762	2.36%	0.261%
24	5.031	511	513	516	rBV4	1371	1794	0.19%	0.022%
25	5.111	523	526	527	rBV3	1099	1075	0.12%	0.013%
26	5.245	545	548	552	rBV6	1476	1763	0.19%	0.021%
27	5.306	556	558	562	rBV4	894	1516	0.16%	0.018%
28	5.458	581	583	586	rBV3	870	1083	0.12%	0.013%
29	5.793	635	638	639	rBV3	986	1146	0.12%	0.014%
30	5.897	652	655	656	rBV3	1626	1673	0.18%	0.020%
31	5.934	656	661	662	rBV4	3486	5396	0.58%	0.065%
32	6.208	703	706	709	rBV5	939	1268	0.14%	0.015%
33	6.525	756	758	760	rVB	1328	1116	0.12%	0.013%
34	6.555	760	763	768	rBV5	740	1189	0.13%	0.014%
35	6.629	772	775	778	rVB3	1535	1778	0.19%	0.021%
36	6.659	778	780	783	rBV4	1299	1664	0.18%	0.020%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
 Title : SFAM01.0

37	6.708	785	788	789	rVB3	1160	1116	0.12%	0.013%
38	7.080	840	849	856	rBV	50217	140828	15.25%	1.689%
39	7.250	871	877	878	rBV2	6613	10352	1.12%	0.124%
40	7.531	922	923	925	rVV2	1607	1319	0.14%	0.016%
41	7.647	933	942	954	rVB	169246	406232	43.98%	4.872%
42	7.866	975	978	980	rBV4	907	1160	0.13%	0.014%
43	7.891	980	982	986	rVB4	1191	1239	0.13%	0.015%
44	7.933	986	989	991	rBV4	1266	1696	0.18%	0.020%
45	8.189	1028	1031	1034	rVB5	1690	1986	0.22%	0.024%
46	8.275	1034	1045	1059	rBV2	292933	923631	100.00%	11.076%
47	8.372	1059	1061	1064	rVB3	1182	1458	0.16%	0.017%
48	8.470	1075	1077	1082	rVB6	1627	1779	0.19%	0.021%
49	8.573	1092	1094	1097	rBV4	922	1232	0.13%	0.015%
50	8.842	1126	1138	1149	rBV	297544	585487	63.39%	7.021%
51	8.921	1149	1151	1152	rVV2	1428	1116	0.12%	0.013%
52	9.274	1199	1209	1219	rBV	218011	446592	48.35%	5.356%
53	9.665	1266	1273	1276	rBV8	1947	4079	0.44%	0.049%
54	9.872	1305	1307	1310	rVB5	1667	1246	0.13%	0.015%
55	9.927	1310	1316	1317	rBV5	1318	1742	0.19%	0.021%
56	10.037	1327	1334	1343	rBV	111340	205781	22.28%	2.468%
57	10.146	1351	1352	1357	rVB5	1726	1826	0.20%	0.022%
58	10.323	1371	1381	1388	rBV	406586	725537	78.55%	8.701%
59	10.384	1388	1391	1398	rVB3	6394	11342	1.23%	0.136%
60	10.579	1416	1423	1431	rBV	83253	139830	15.14%	1.677%
61	10.701	1437	1443	1450	rVB2	33453	60875	6.59%	0.730%
62	10.921	1472	1479	1488	rBV	192825	341444	36.97%	4.095%
63	11.073	1499	1504	1508	rVB6	4830	8765	0.95%	0.105%
64	11.286	1535	1539	1541	rVB3	1161	1158	0.13%	0.014%
65	11.335	1543	1547	1551	rVB6	1721	2848	0.31%	0.034%
66	11.408	1551	1559	1563	rBV6	4778	12231	1.32%	0.147%
67	11.506	1572	1575	1582	rBV4	5056	8747	0.95%	0.105%
68	11.628	1585	1595	1604	rBV	461482	781562	84.62%	9.373%
69	11.841	1623	1630	1632	rBV7	12567	20339	2.20%	0.244%
70	12.012	1652	1658	1660	rBV5	3962	7559	0.82%	0.091%
71	12.061	1662	1666	1672	rVB2	10727	16751	1.81%	0.201%
72	12.134	1672	1678	1684	rBV4	24259	49921	5.40%	0.599%
73	12.183	1684	1686	1690	rVB4	7038	7788	0.84%	0.093%
74	12.250	1693	1697	1702	rVB	31315	47823	5.18%	0.574%
75	12.329	1702	1710	1713	rBV6	17930	48148	5.21%	0.577%
76	12.603	1749	1755	1761	rVB2	274693	446521	48.34%	5.355%

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 Title : SFAM01.0

77	12.689	1764	1769	1776	rVB	272775	440837	47.73%	5.287%
78	12.774	1781	1783	1790	rVB4	17540	29048	3.14%	0.348%
79	12.859	1791	1797	1799	rBV6	7962	16117	1.74%	0.193%
80	12.932	1804	1809	1816	rBV5	22450	46903	5.08%	0.562%
81	13.073	1829	1832	1836	rBV6	8202	11021	1.19%	0.132%
82	13.121	1836	1840	1843	rBV5	5968	7642	0.83%	0.092%
83	13.158	1844	1846	1850	rVB5	4998	7090	0.77%	0.085%
84	13.377	1878	1882	1883	rBV4	3208	4345	0.47%	0.052%
85	13.554	1903	1911	1918	rBV	509876	806083	87.27%	9.667%
86	13.646	1922	1926	1932	rVB4	9975	17452	1.89%	0.209%
87	13.853	1949	1960	1968	rBV	441784	755790	81.83%	9.064%
88	13.999	1982	1984	1985	rBV2	1856	1329	0.14%	0.016%
89	14.066	1989	1995	2001	rVV	47260	78780	8.53%	0.945%
90	14.207	2011	2018	2021	rBV9	3146	8340	0.90%	0.100%
91	14.322	2032	2037	2043	rBV3	19611	30554	3.31%	0.366%
92	14.719	2098	2102	2105	rVB6	2518	4217	0.46%	0.051%
93	14.786	2111	2113	2115	rBV2	2485	2231	0.24%	0.027%
94	14.962	2140	2142	2146	rBV5	2455	3581	0.39%	0.043%
95	14.993	2146	2147	2149	rBV2	2099	1684	0.18%	0.020%
96	16.023	2314	2316	2321	rBV6	1406	1979	0.21%	0.024%
97	16.139	2332	2335	2337	rBV4	1495	2051	0.22%	0.025%
98	16.438	2383	2384	2386	rBV2	1334	1348	0.15%	0.016%
99	16.590	2406	2409	2411	rBV4	1681	1719	0.19%	0.021%
100	16.615	2411	2413	2417	rBV5	1714	2459	0.27%	0.029%

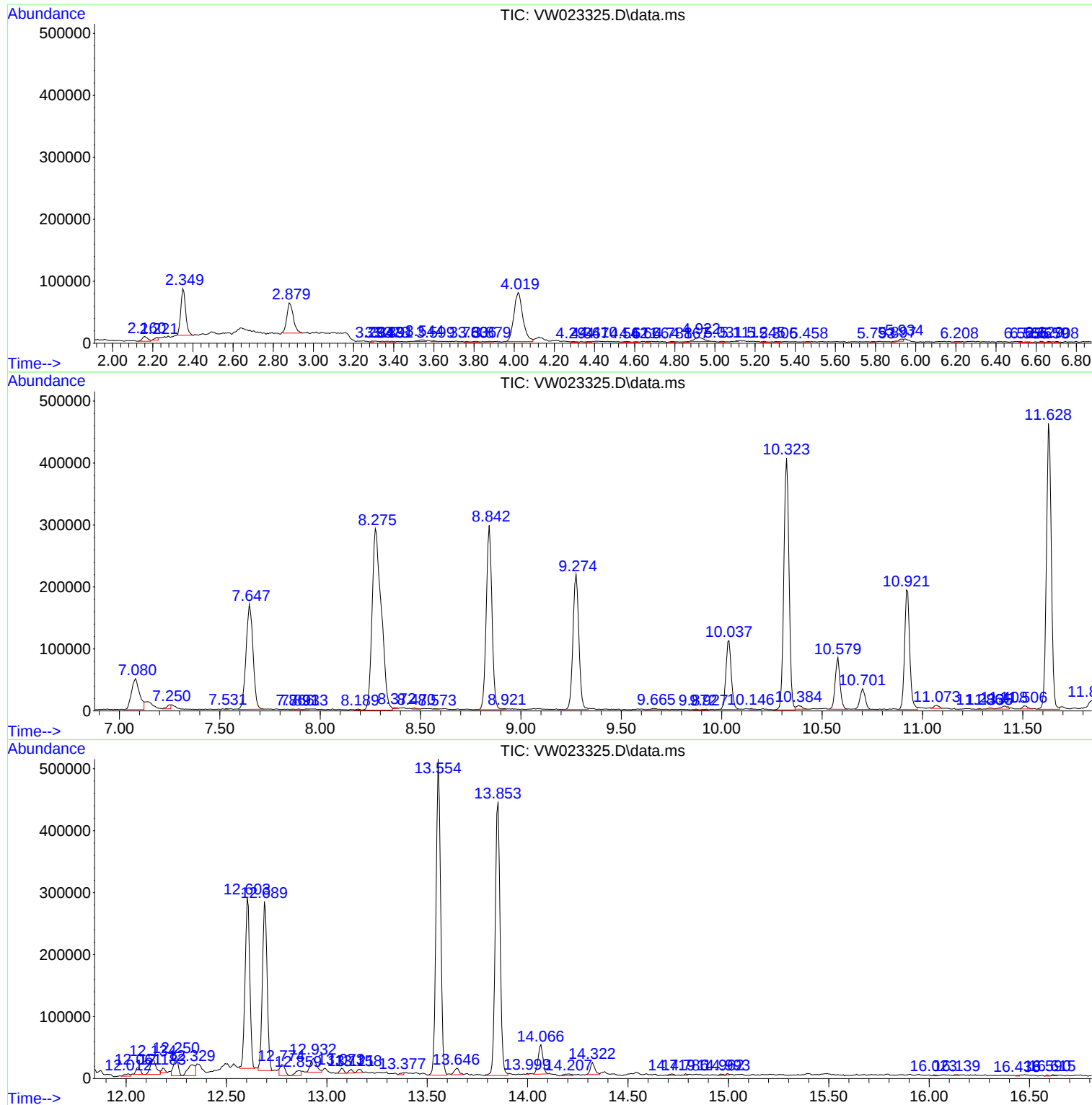
Sum of corrected areas: 8338690

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Instrument :
MSVOA_W
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GBGS1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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



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Instrument :
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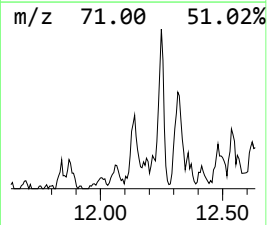
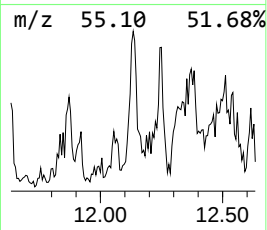
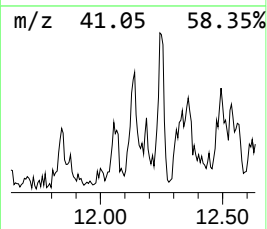
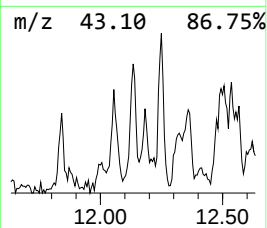
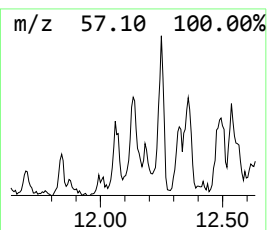
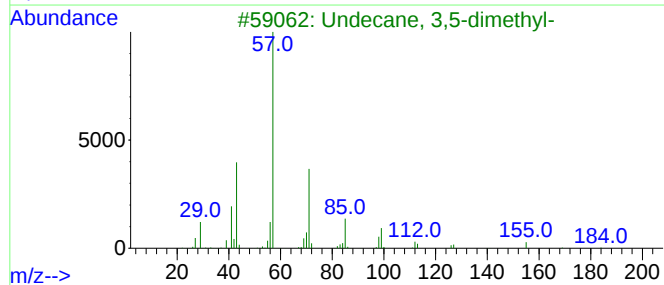
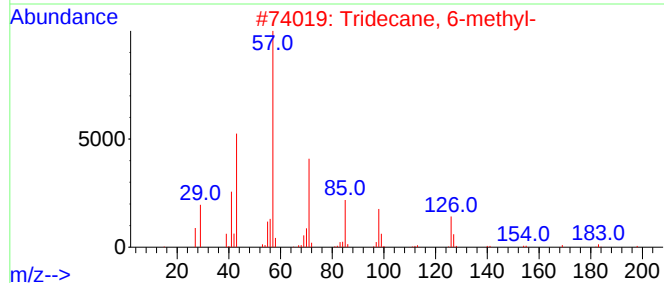
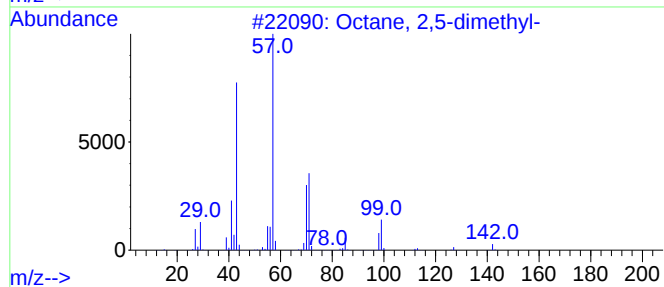
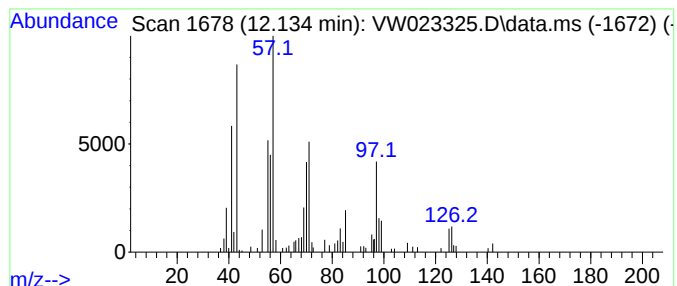
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.134	1.60 ug/L	49921	Chlorobenzene-d5	11.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,5-dimethyl-		142	C10H22		015869-89-3	43
2	Tridecane, 6-methyl-		198	C14H30		013287-21-3	35
3	Undecane, 3,5-dimethyl-		184	C13H28		017312-81-1	22
4	Butane, 2,2-dimethyl-		86	C6H14		000075-83-2	22
5	Oxalic acid, allyl nonyl ester		256	C14H24O4		1000309-23-7	22



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ALS Vial : 1 Sample Multiplier: 1

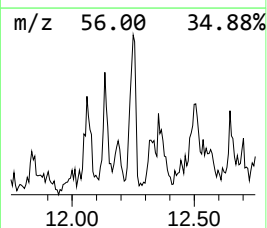
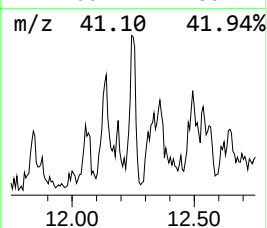
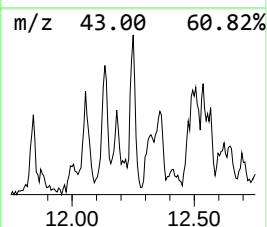
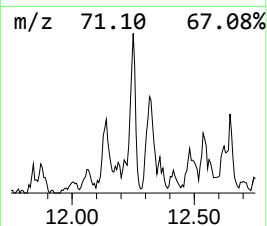
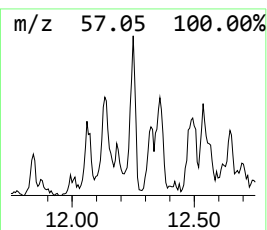
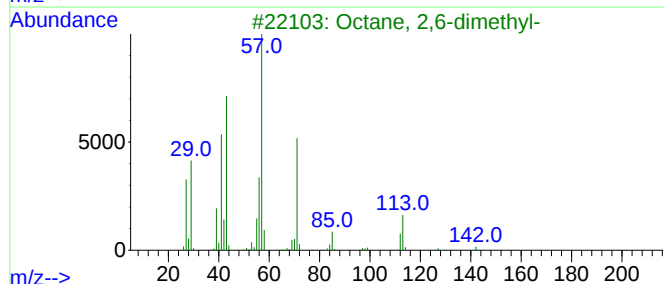
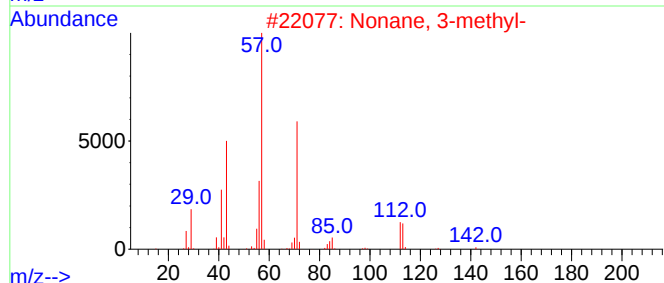
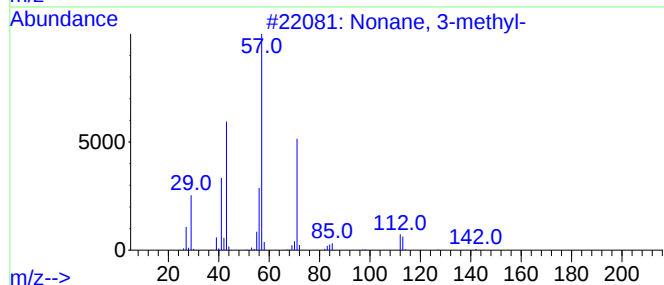
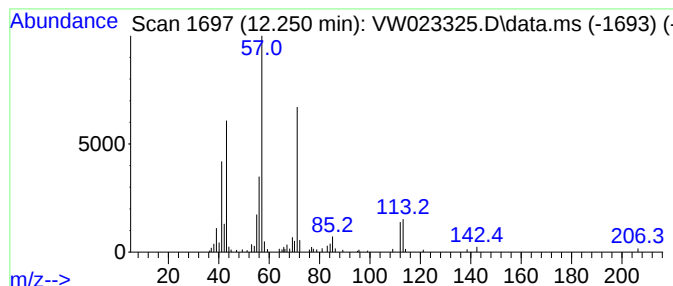
Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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.	
12.250	1.53 ug/L	47823	Chlorobenzene-d5		11.628	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-		142	C10H22	005911-04-6	91
2	Nonane, 3-methyl-		142	C10H22	005911-04-6	91
3	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	91
4	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	86
5	Octane, 3,6-dimethyl-		142	C10H22	015869-94-0	64



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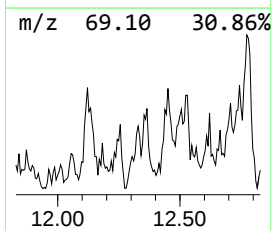
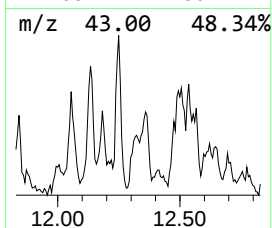
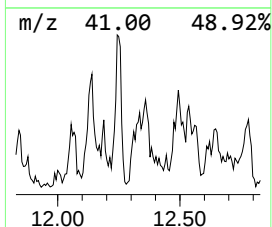
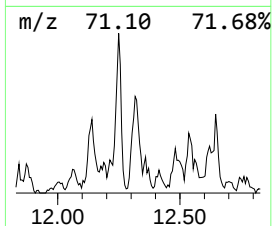
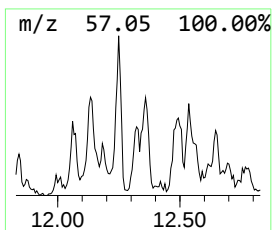
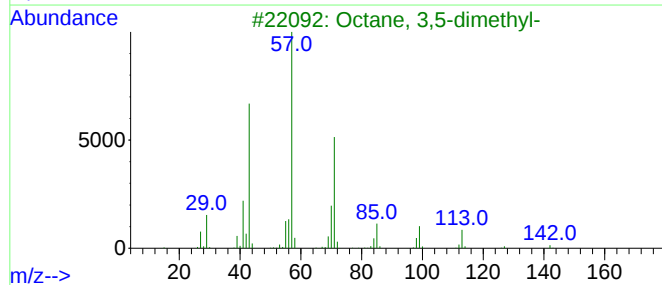
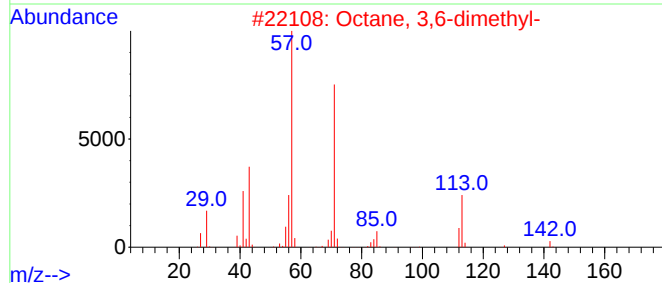
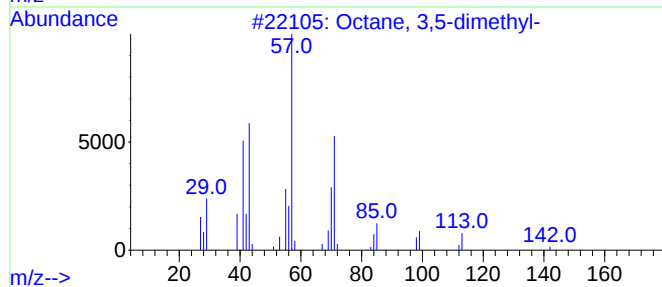
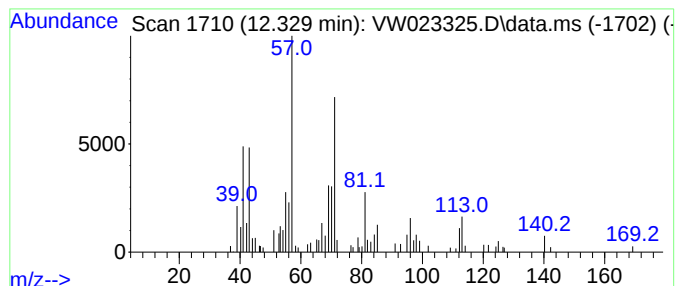
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.329	1.54 ug/L	48148	Chlorobenzene-d5	11.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	68
2			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	58
3			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	52
4			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	47
5			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW052522\
Data File : VW023325.D
Acq On : 25 May 2022 16:48
Operator : SY/VA
Sample : N2995-20
Misc : 5.06g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GBGS1

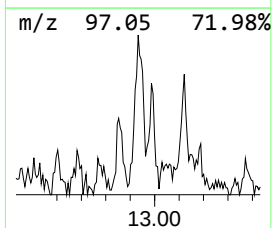
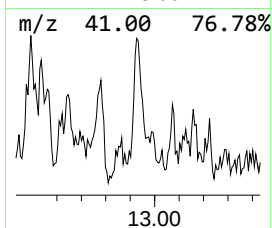
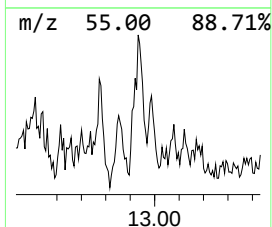
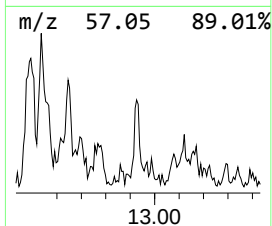
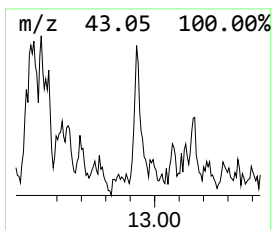
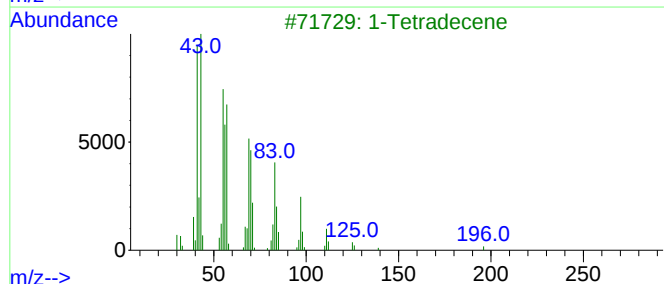
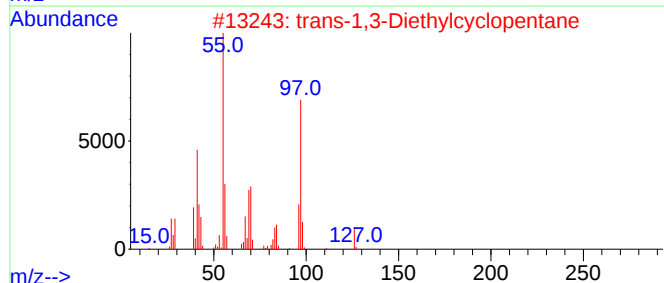
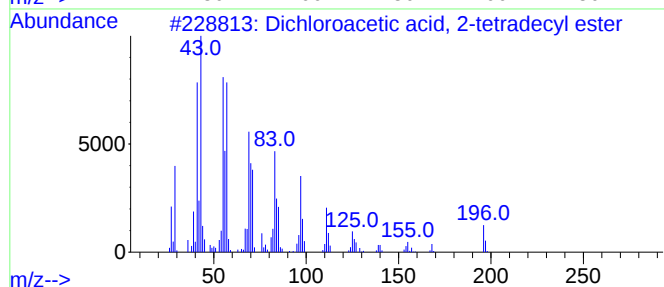
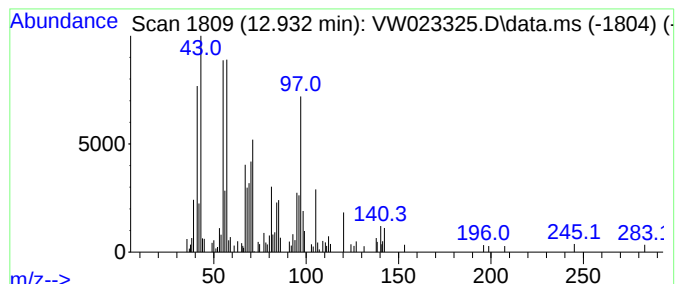
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Quant Title : SFAM01.0

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

Peak Number 7 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.932	1.45 ug/L	46903	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, 2-tetradecy...	324	C16H30Cl2O2	1000280-64-4	43
2			trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	38
3			1-Tetradecene	196	C14H28	001120-36-1	30
4			Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	27
5			Cyclotetradecane	196	C14H28	000295-17-0	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW052522\
Data File : VW023325.D
Acq On : 25 May 2022 16:48
Operator : SY/VA
Sample : N2995-20
Misc : 5.06g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GBGS1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.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...	12.134	1.6	ug/L	49921	2	11.628	781562	25.0
(DEL) Alkane: S...	12.250	1.5	ug/L	47823	2	11.628	781562	25.0
(DEL) Alkane: S...	12.329	1.5	ug/L	48148	2	11.628	781562	25.0
unknown-01	12.932	1.5	ug/L	46903	3	13.554	806083	25.0