

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072522\
 Data File : VW024080.D
 Acq On : 25 Jul 2022 20:13
 Operator : SY/VA
 Sample : N3745-07
 Misc : 5.01g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VHBLK001

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\SFAMWLM072522SMA.M
 Title : SFAM01.0

Signal : TIC: VW024080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.239	47	55	56	rBV6	11698	26923	3.51%	0.439%
2	2.343	67	72	83	rVB	121663	212872	27.72%	3.468%
3	2.873	155	159	171	rVB	69435	142661	18.58%	2.324%
4	3.684	289	292	295	rBV5	1122	1820	0.24%	0.030%
5	3.824	313	315	316	rBV2	1199	1130	0.15%	0.018%
6	4.007	334	345	360	rBV2	65069	217579	28.33%	3.545%
7	4.312	393	395	396	rBV2	1075	865	0.11%	0.014%
8	4.726	461	463	464	rVB2	1231	610	0.08%	0.010%
9	4.781	470	472	474	rBV3	920	771	0.10%	0.013%
10	4.909	484	493	509	rVB2	26391	94307	12.28%	1.536%
11	5.104	523	525	529	rBV4	959	1407	0.18%	0.023%
12	5.257	547	550	552	rBV4	1056	1259	0.16%	0.021%
13	5.281	552	554	556	rVV3	905	810	0.11%	0.013%
14	5.336	561	563	566	rBV4	1080	1106	0.14%	0.018%
15	5.726	625	627	629	rBV2	939	981	0.13%	0.016%
16	5.812	638	641	644	rBV5	1112	1962	0.26%	0.032%
17	5.927	650	660	670	rBV5	10250	33715	4.39%	0.549%
18	6.482	749	751	754	rBV4	963	878	0.11%	0.014%
19	6.513	754	756	761	rVB6	1186	1131	0.15%	0.018%
20	6.610	769	772	773	rBV3	725	657	0.09%	0.011%
21	6.629	773	775	777	rBV3	814	702	0.09%	0.011%
22	6.653	777	779	781	rVB3	1232	864	0.11%	0.014%
23	6.860	811	813	816	rBV3	1051	1240	0.16%	0.020%
24	6.976	828	832	833	rBV4	1164	1236	0.16%	0.020%
25	7.080	842	849	858	rBV2	24171	67185	8.75%	1.095%
26	7.311	884	887	888	rBV3	1378	949	0.12%	0.015%
27	7.647	932	942	953	rBV	136491	338167	44.03%	5.509%
28	7.915	985	986	987	rBV2	963	631	0.08%	0.010%
29	7.951	987	992	997	rVB8	3383	7773	1.01%	0.127%
30	8.031	1002	1005	1007	rBV4	895	1091	0.14%	0.018%
31	8.134	1019	1022	1024	rBV3	610	742	0.10%	0.012%
32	8.275	1033	1045	1060	rBV2	249703	767977	100.00%	12.511%
33	8.756	1120	1124	1125	rBV3	854	1035	0.13%	0.017%
34	8.842	1130	1138	1148	rVV	239958	471846	61.44%	7.687%
35	9.085	1172	1178	1183	rBV8	3654	8018	1.04%	0.131%
36	9.274	1200	1209	1217	rBV	175306	363169	47.29%	5.916%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SFAMWLM072522SMA.M
 Title : SFAM01.0

37	9.494	1241	1245	1246	rBV4	1037	1317	0.17%	0.021%
38	9.567	1256	1257	1260	rVB3	1063	828	0.11%	0.013%
39	9.610	1260	1264	1265	rBV4	1875	2252	0.29%	0.037%
40	9.762	1285	1289	1292	rBV5	1332	2808	0.37%	0.046%
41	9.847	1302	1303	1305	rBV2	769	627	0.08%	0.010%
42	9.878	1306	1308	1310	rVB2	1321	951	0.12%	0.015%
43	9.945	1317	1319	1321	rBV3	1241	1260	0.16%	0.021%
44	10.030	1326	1333	1346	rVV	83294	162163	21.12%	2.642%
45	10.213	1359	1363	1368	rBV8	2107	4771	0.62%	0.078%
46	10.323	1373	1381	1388	rBV	371657	638327	83.12%	10.399%
47	10.579	1416	1423	1431	rBV	59413	110745	14.42%	1.804%
48	10.658	1435	1436	1439	rBV3	997	1076	0.14%	0.018%
49	10.853	1464	1468	1473	rBV6	3211	6051	0.79%	0.099%
50	10.920	1473	1479	1492	rBV	107325	195164	25.41%	3.179%
51	11.457	1564	1567	1571	rVB6	803	1254	0.16%	0.020%
52	11.554	1580	1583	1588	rVB7	1374	2145	0.28%	0.035%
53	11.628	1588	1595	1605	rBV	382270	652962	85.02%	10.637%
54	11.835	1626	1629	1633	rVB5	2877	4589	0.60%	0.075%
55	11.975	1649	1652	1656	rBV4	1168	1405	0.18%	0.023%
56	12.073	1667	1668	1670	rBV2	1045	642	0.08%	0.010%
57	12.128	1675	1677	1679	rVV3	724	644	0.08%	0.010%
58	12.170	1679	1684	1691	rVB6	5663	12414	1.62%	0.202%
59	12.396	1719	1721	1722	rBV2	1163	727	0.09%	0.012%
60	12.463	1727	1732	1736	rVV4	4289	7581	0.99%	0.124%
61	12.688	1762	1769	1777	rBV	173248	289120	37.65%	4.710%
62	12.841	1792	1794	1797	rVB4	1064	808	0.11%	0.013%
63	12.865	1797	1798	1801	rBV3	809	620	0.08%	0.010%
64	12.938	1805	1810	1816	rVV6	5017	9631	1.25%	0.157%
65	13.012	1820	1822	1825	rVB3	1993	1720	0.22%	0.028%
66	13.060	1828	1830	1832	rVB3	819	728	0.09%	0.012%
67	13.079	1832	1833	1835	rBV2	1035	777	0.10%	0.013%
68	13.213	1853	1855	1856	rBV2	1116	1107	0.14%	0.018%
69	13.243	1856	1860	1867	rVV5	4031	9492	1.24%	0.155%
70	13.304	1867	1870	1871	rVB2	1027	946	0.12%	0.015%
71	13.371	1876	1881	1884	rBV6	1172	1823	0.24%	0.030%
72	13.463	1894	1896	1898	rBV3	854	696	0.09%	0.011%
73	13.493	1898	1901	1905	rVV5	5119	8382	1.09%	0.137%
74	13.554	1905	1911	1922	rVB	376566	609810	79.40%	9.934%
75	13.652	1924	1927	1930	rVV5	1792	2232	0.29%	0.036%
76	13.707	1934	1936	1938	rBV3	1013	808	0.11%	0.013%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072522SMA.M
 Title : SFAM01.0

77	13.853	1952	1960	1968	rBV	341978	564977	73.57%	9.204%
78	14.054	1991	1993	1995	rBV3	1725	1963	0.26%	0.032%
79	14.133	2004	2006	2010	rVB4	885	921	0.12%	0.015%
80	14.170	2010	2012	2013	rBV2	1158	832	0.11%	0.014%
81	14.322	2035	2037	2040	rBV4	1547	1609	0.21%	0.026%
82	14.353	2040	2042	2043	rVB2	1164	676	0.09%	0.011%
83	14.389	2046	2048	2053	rBV6	940	1611	0.21%	0.026%
84	14.627	2083	2087	2093	rVB7	4366	7819	1.02%	0.127%
85	14.682	2093	2096	2097	rBV2	965	839	0.11%	0.014%
86	14.712	2097	2101	2102	rBV4	1207	1667	0.22%	0.027%
87	14.767	2107	2110	2113	rBV4	1242	1796	0.23%	0.029%
88	14.920	2133	2135	2137	rBV3	1072	1105	0.14%	0.018%
89	15.060	2156	2158	2159	rBV2	969	862	0.11%	0.014%
90	15.127	2165	2169	2174	rVB7	2866	4708	0.61%	0.077%
91	15.359	2203	2207	2213	rBV5	2527	5129	0.67%	0.084%
92	15.548	2234	2238	2242	rBV6	3253	5710	0.74%	0.093%
93	15.816	2280	2282	2285	rVB4	879	1020	0.13%	0.017%
94	16.102	2326	2329	2330	rBV3	869	1050	0.14%	0.017%
95	16.194	2342	2344	2347	rBV4	1202	1537	0.20%	0.025%
96	16.304	2359	2362	2364	rBV3	997	1420	0.18%	0.023%
97	16.547	2400	2402	2403	rBV2	1356	845	0.11%	0.014%
98	16.700	2426	2427	2431	rVB3	1501	1344	0.18%	0.022%
99	16.743	2432	2434	2437	rVB4	793	701	0.09%	0.011%
100	16.773	2437	2439	2440	rBV2	809	723	0.09%	0.012%

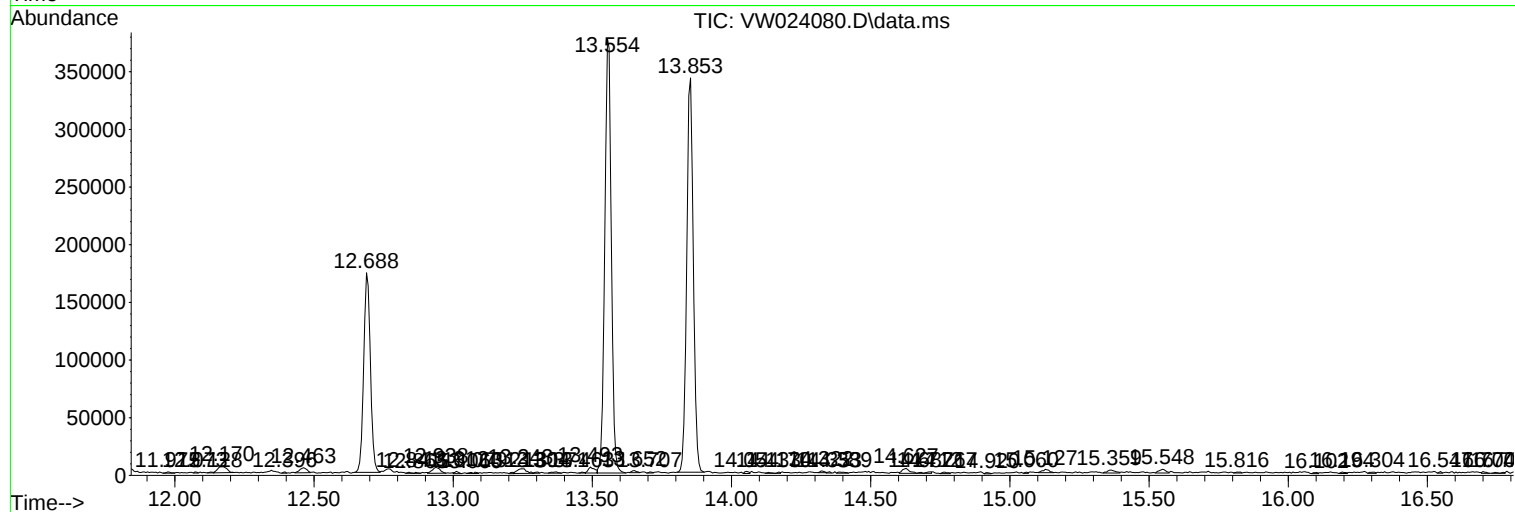
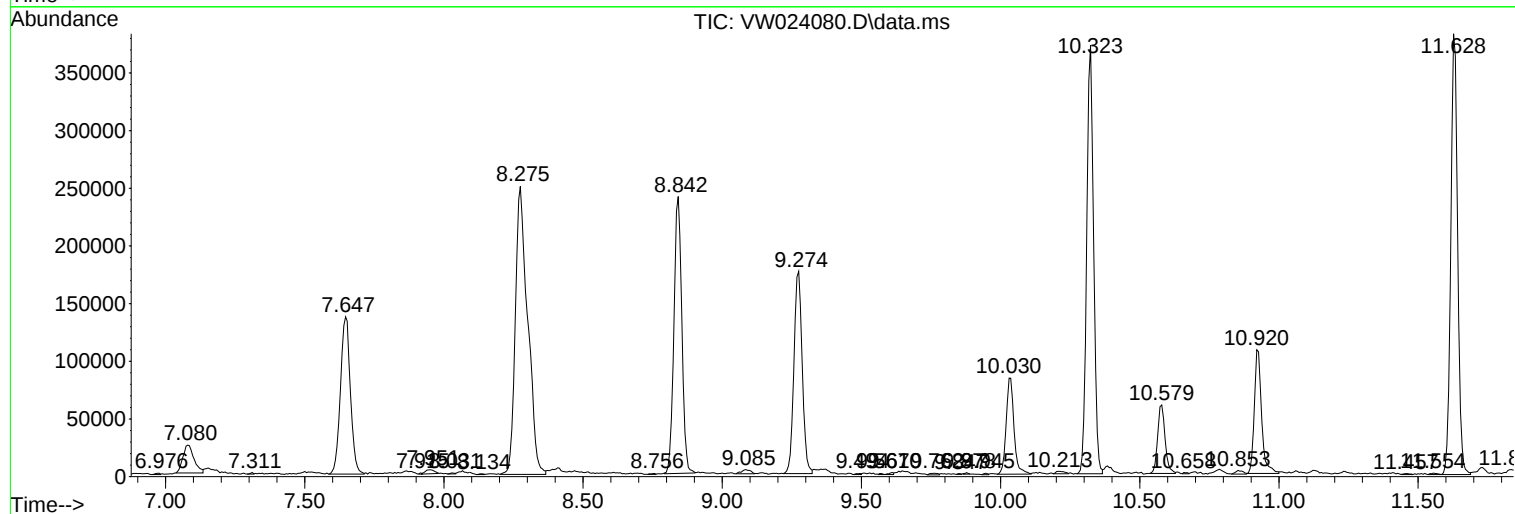
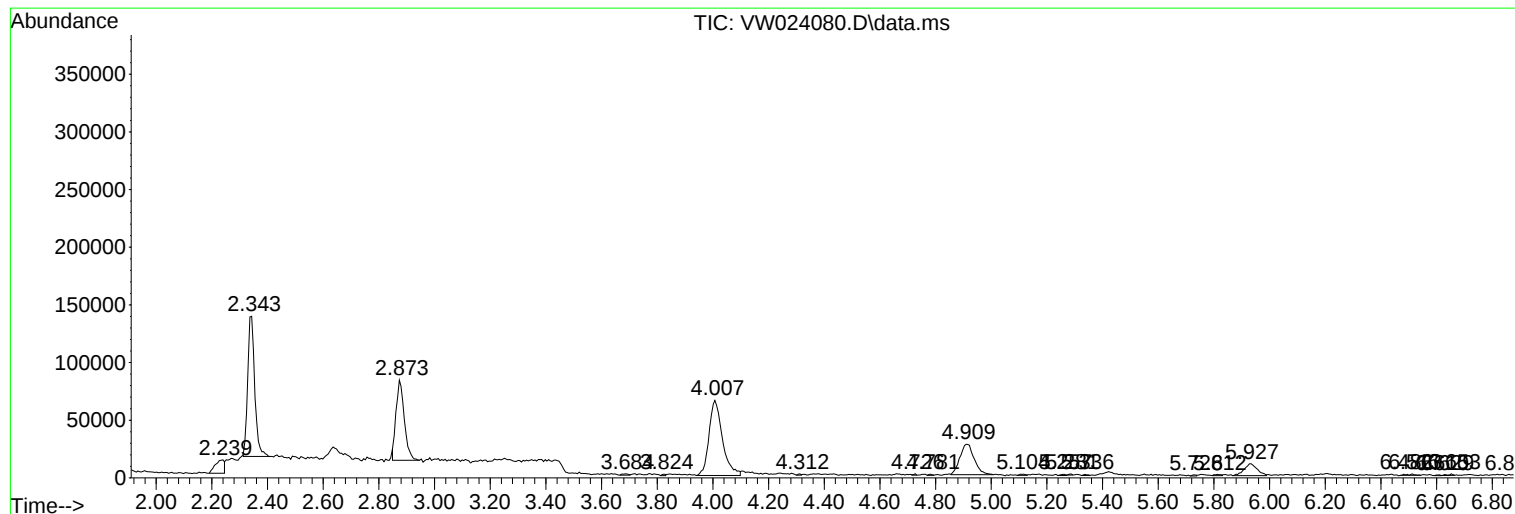
Sum of corrected areas: 6138336

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072522SMA.M
Quant Title : SFAM01.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072522\
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Instrument :
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ClientSampleId :
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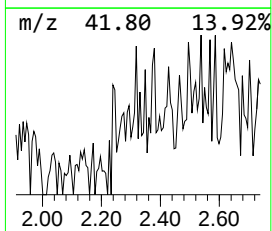
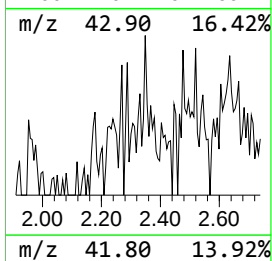
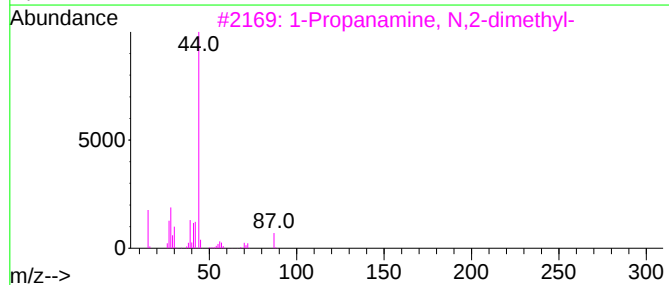
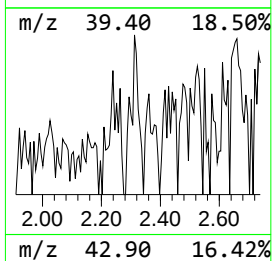
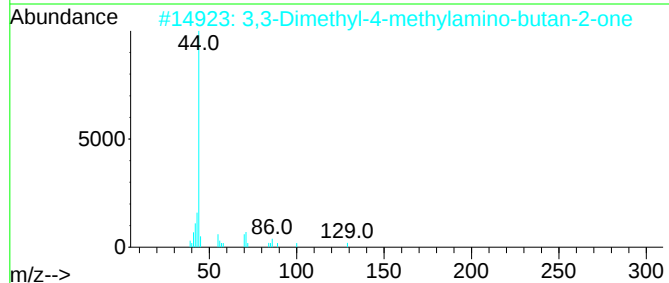
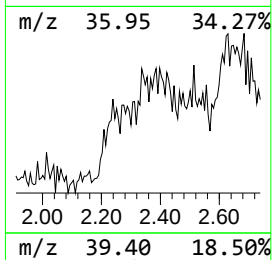
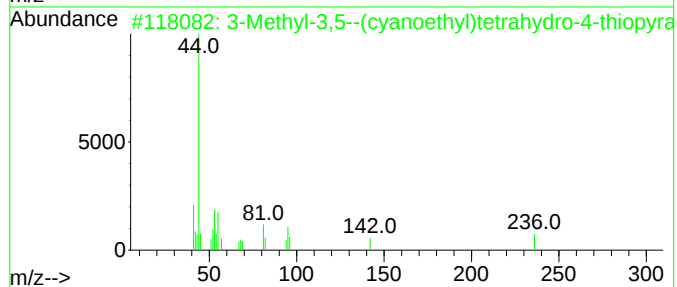
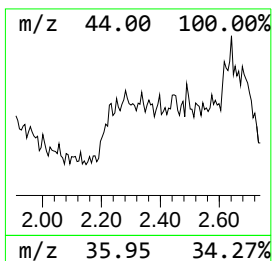
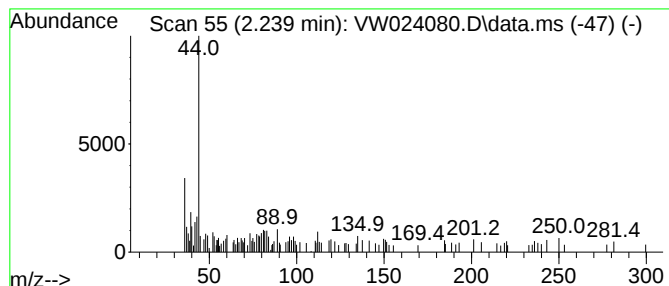
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072522SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 3-Methyl-3,5--(cyanoethyl)t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.239	1.43 ug/L	26923	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-3,5--(cyanoethyl)tetrah...	236	C12H16N2OS	1000140-32-3	70
2			3,3-Dimethyl-4-methylamino-butan...	129	C7H15NO	123528-99-4	52
3			1-Propanamine, N,2-dimethyl-	87	C5H13N	000625-43-4	43
4			Isobutyramide, N-methyl-N-hexyl-	185	C11H23NO	1010421-21-5	43
5			Histidine, 1,N-dimethyl-4-nitro-	228	C8H12N4O4	1000129-55-1	40



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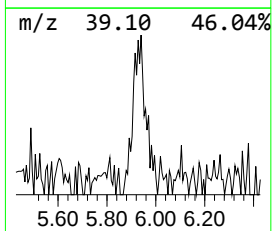
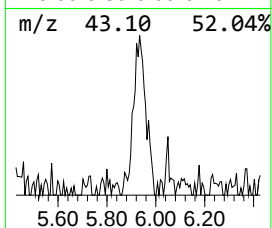
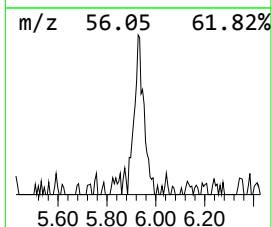
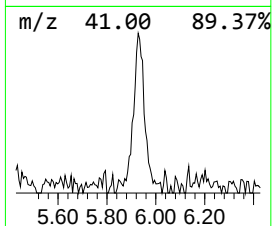
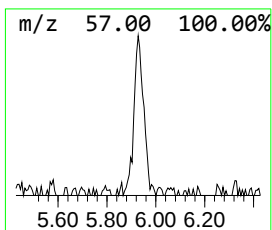
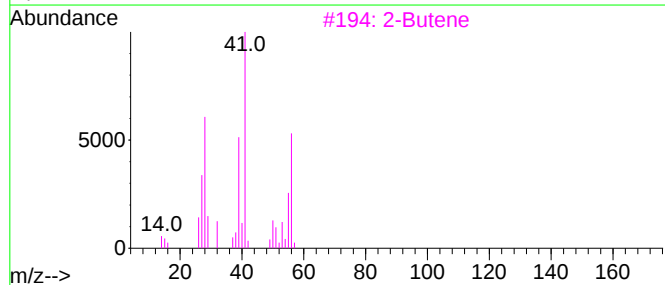
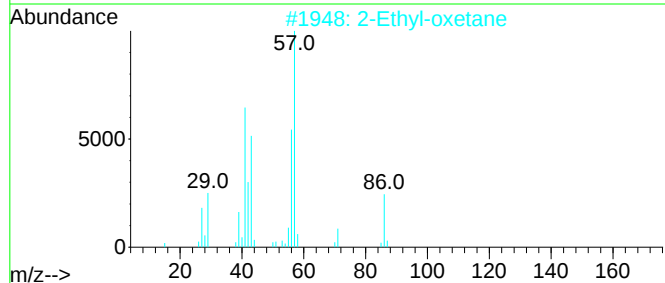
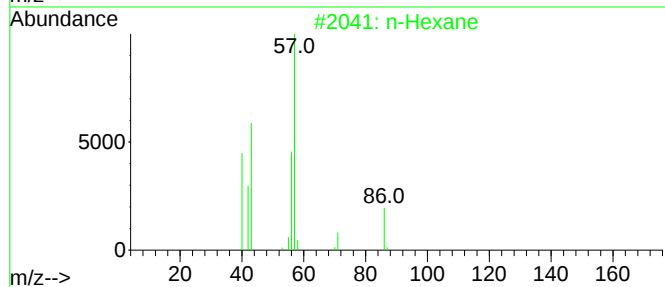
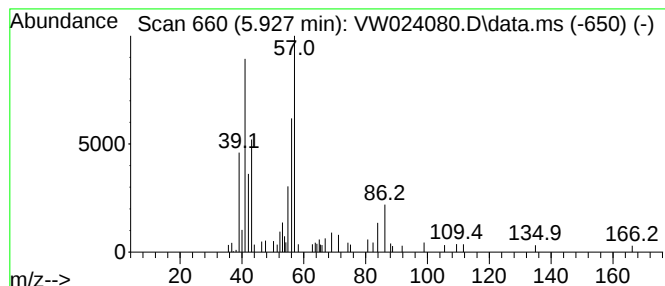
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072522SMA.M
Quant Title : SFAM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.927	1.79 ug/L	33715	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexane	86	C6H14	000110-54-3	64
2		2-Ethyl-oxetane	86	C5H10O	1010386-40-2	47
3		2-Butene	56	C4H8	000107-01-7	38
4		Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	38
5		1,3-Cyclopentanedione, 4-butyl-	154	C9H14O2	054244-72-3	37



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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
3-Methyl-3,5--(...	2.239	1.4	ug/L	26923	1	8.842	471846	25.0
(DEL) Alkane: S...	5.927	1.8	ug/L	33715	1	8.842	471846	25.0