

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081624\
 Data File : VW029927.D
 Acq On : 16 Aug 2024 13:35
 Operator : SY/MD
 Sample : P3504-04
 Misc : 5.00g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCXX3

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\SFAMWLM072424SMA.M
 Title : SFAM01.0

Signal : TIC: VW029927.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.174	42	47	48	rBV4	1585	2053	0.10%	0.008%
2	2.326	67	72	74	rBV	18691	30747	1.46%	0.113%
3	2.363	74	78	90	rVB	36677	94742	4.50%	0.348%
4	2.899	159	166	185	rVB	27573	83497	3.96%	0.307%
5	3.112	200	201	204	rBV3	995	806	0.04%	0.003%
6	3.289	228	230	236	rVB5	619	978	0.05%	0.004%
7	3.399	240	248	254	rVB4	2305	4769	0.23%	0.018%
8	4.039	339	353	363	rBV3	186548	689383	32.73%	2.532%
9	4.509	428	430	435	rVB4	503	682	0.03%	0.003%
10	4.600	435	445	468	rBV2	33067	124988	5.93%	0.459%
11	4.917	483	497	525	rBV2	275372	1102131	52.32%	4.049%
12	5.246	549	551	556	rVB5	855	1006	0.05%	0.004%
13	5.429	566	581	599	rBV	274874	891139	42.30%	3.274%
14	5.655	616	618	622	rVB3	486	610	0.03%	0.002%
15	5.740	627	632	633	rBV4	612	944	0.04%	0.003%
16	5.941	655	665	682	rVB3	10833	35816	1.70%	0.132%
17	6.075	682	687	689	rBV2	712	1050	0.05%	0.004%
18	6.216	697	710	728	rBV	339439	1048631	49.78%	3.852%
19	6.350	730	732	735	rVV3	514	593	0.03%	0.002%
20	6.386	735	738	744	rVB4	555	924	0.04%	0.003%
21	6.831	807	811	814	rBV3	544	953	0.05%	0.004%
22	6.917	820	825	827	rBV4	813	1130	0.05%	0.004%
23	7.081	843	852	855	rBV	20638	49565	2.35%	0.182%
24	7.167	858	866	884	rVB	144188	413539	19.63%	1.519%
25	7.673	934	949	966	rBV2	582752	1638151	77.77%	6.018%
26	7.788	966	968	973	rVB5	873	1168	0.06%	0.004%
27	7.874	976	982	989	rVB3	4199	9658	0.46%	0.035%
28	7.947	991	994	996	rBV4	723	828	0.04%	0.003%
29	7.971	996	998	1000	rVB2	864	718	0.03%	0.003%
30	8.069	1003	1014	1028	rBV	91920	228166	10.83%	0.838%
31	8.276	1036	1048	1049	rBV	223724	383818	18.22%	1.410%
32	8.325	1050	1056	1076	rVB	839127	1958027	92.95%	7.193%
33	8.557	1088	1094	1096	rBV6	1377	2666	0.13%	0.010%
34	8.697	1109	1117	1118	rBV5	1799	2935	0.14%	0.011%
35	8.843	1132	1141	1150	rBV	239344	475820	22.59%	1.748%
36	9.093	1173	1182	1194	rBV	901109	1750721	83.11%	6.431%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
 Title : SFAM01.0

37	9.276	1203	1212	1219	rBV	146906	309906	14.71%	1.138%
38	9.367	1219	1227	1242	rVB	321321	643646	30.56%	2.364%
39	9.691	1268	1280	1290	rBV	20047	41284	1.96%	0.152%
40	9.806	1297	1299	1304	rVB4	657	950	0.05%	0.003%
41	9.904	1312	1315	1318	rVB5	613	809	0.04%	0.003%
42	9.934	1318	1320	1321	rBV2	626	594	0.03%	0.002%
43	10.069	1337	1342	1350	rVB	547910	995479	47.26%	3.657%
44	10.142	1350	1354	1358	rVV	14784	24105	1.14%	0.089%
45	10.209	1358	1365	1376	rVB	454365	801209	38.04%	2.943%
46	10.319	1376	1383	1391	rVB	304167	538316	25.56%	1.977%
47	10.605	1419	1430	1440	rBV	575350	1061915	50.41%	3.901%
48	10.703	1440	1446	1452	rVB	36982	67603	3.21%	0.248%
49	10.782	1452	1459	1467	rBV	404942	705894	33.51%	2.593%
50	10.922	1476	1482	1489	rBV	76031	132029	6.27%	0.485%
51	11.062	1499	1505	1513	rVB3	12012	21873	1.04%	0.080%
52	11.172	1519	1523	1526	rBV5	2797	4236	0.20%	0.016%
53	11.233	1526	1533	1541	rVV	167874	293836	13.95%	1.079%
54	11.398	1557	1560	1562	rBV3	904	1089	0.05%	0.004%
55	11.434	1564	1566	1573	rVB5	2402	3237	0.15%	0.012%
56	11.544	1577	1584	1588	rBV6	1290	2730	0.13%	0.010%
57	11.629	1589	1598	1606	rBV	346885	577217	27.40%	2.120%
58	11.727	1608	1614	1620	rVB6	4764	8625	0.41%	0.032%
59	11.782	1620	1623	1624	rBV3	526	603	0.03%	0.002%
60	11.830	1624	1631	1651	rVV	929572	1637096	77.72%	6.014%
61	12.160	1677	1685	1694	rBV	1321167	2106496	100.00%	7.738%
62	12.239	1694	1698	1709	rVV2	5083	10655	0.51%	0.039%
63	12.349	1709	1716	1724	rVB	65196	120040	5.70%	0.441%
64	12.458	1728	1734	1739	rBV3	4185	7756	0.37%	0.028%
65	12.513	1739	1743	1751	rVB4	1986	3267	0.16%	0.012%
66	12.599	1751	1757	1764	rVB3	25755	47669	2.26%	0.175%
67	12.708	1764	1775	1780	rBV2	335916	732930	34.79%	2.692%
68	12.763	1780	1784	1797	rVB	429225	698951	33.18%	2.568%
69	12.867	1797	1801	1802	rBV3	1239	1540	0.07%	0.006%
70	12.928	1807	1811	1819	rVB2	6737	11509	0.55%	0.042%
71	13.031	1825	1828	1831	rBV4	1079	1468	0.07%	0.005%
72	13.245	1852	1863	1867	rBV6	10271	22455	1.07%	0.082%
73	13.391	1882	1887	1892	rBV5	3164	5351	0.25%	0.020%
74	13.495	1894	1904	1909	rBV	618983	993025	47.14%	3.648%
75	13.568	1909	1916	1925	rVB2	695639	1544053	73.30%	5.672%
76	13.848	1955	1962	1975	rVB	260277	422421	20.05%	1.552%

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 Title : SFAM01.0

77	14.013	1985	1989	1992	rBV6	1522	2669	0.13%	0.010%
78	14.062	1992	1997	2005	rVB2	8463	17663	0.84%	0.065%
79	14.214	2019	2022	2032	rVB3	2940	4728	0.22%	0.017%
80	14.318	2034	2039	2048	rVB7	7482	13392	0.64%	0.049%
81	14.476	2058	2065	2076	rBV2	43520	79793	3.79%	0.293%
82	14.617	2084	2088	2093	rBV4	3399	5356	0.25%	0.020%
83	14.677	2096	2098	2100	rBV3	629	681	0.03%	0.003%
84	14.726	2102	2106	2111	rBV7	1285	2671	0.13%	0.010%
85	14.866	2123	2129	2136	rVB9	1139	2893	0.14%	0.011%
86	14.921	2136	2138	2140	rBV3	574	757	0.04%	0.003%
87	15.068	2157	2162	2164	rBV3	2254	2978	0.14%	0.011%
88	15.129	2164	2172	2178	rBV	204379	355153	16.86%	1.305%
89	15.360	2201	2210	2218	rBV	624316	1077664	51.16%	3.959%
90	15.543	2237	2240	2247	rVB8	2047	4077	0.19%	0.015%
91	15.635	2253	2255	2259	rBV4	922	1154	0.05%	0.004%
92	15.671	2259	2261	2265	rBV4	710	919	0.04%	0.003%
93	15.842	2284	2289	2292	rBV7	1964	3544	0.17%	0.013%
94	15.958	2302	2308	2313	rVB5	2084	3780	0.18%	0.014%
95	16.092	2326	2330	2334	rBV7	1025	1370	0.07%	0.005%
96	16.128	2334	2336	2340	rVB5	946	1063	0.05%	0.004%
97	16.208	2347	2349	2352	rBV2	434	584	0.03%	0.002%
98	16.403	2377	2381	2384	rVB5	619	689	0.03%	0.003%
99	16.445	2384	2388	2391	rBV5	655	1059	0.05%	0.004%
100	16.708	2428	2431	2433	rVB3	665	643	0.03%	0.002%

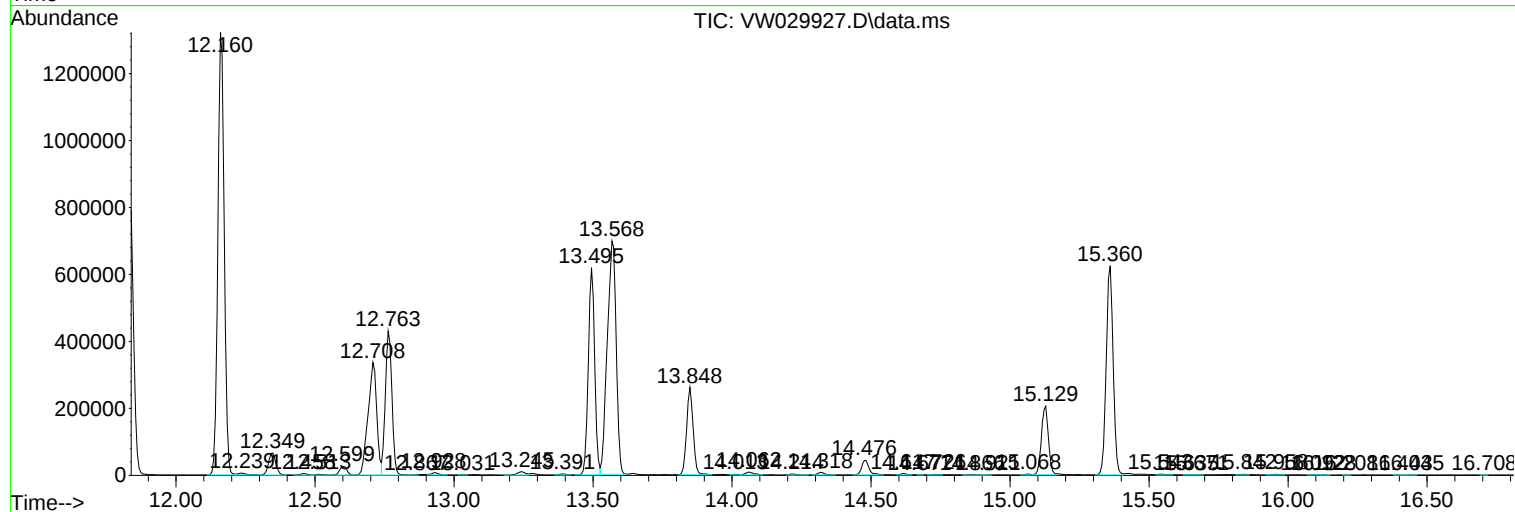
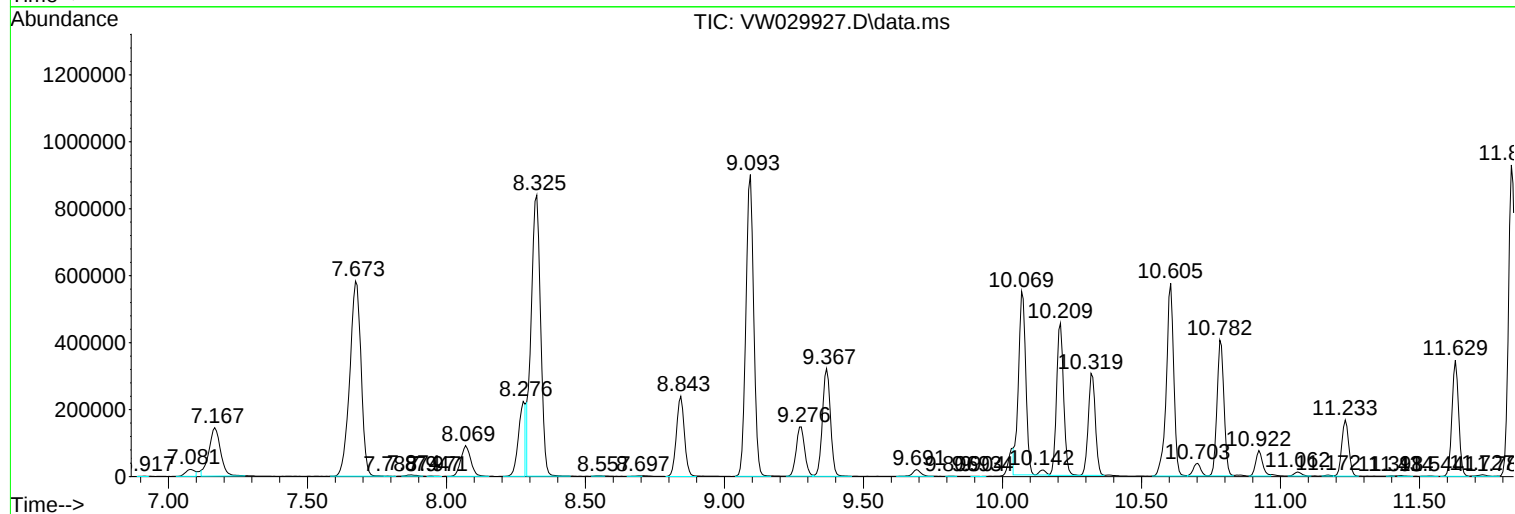
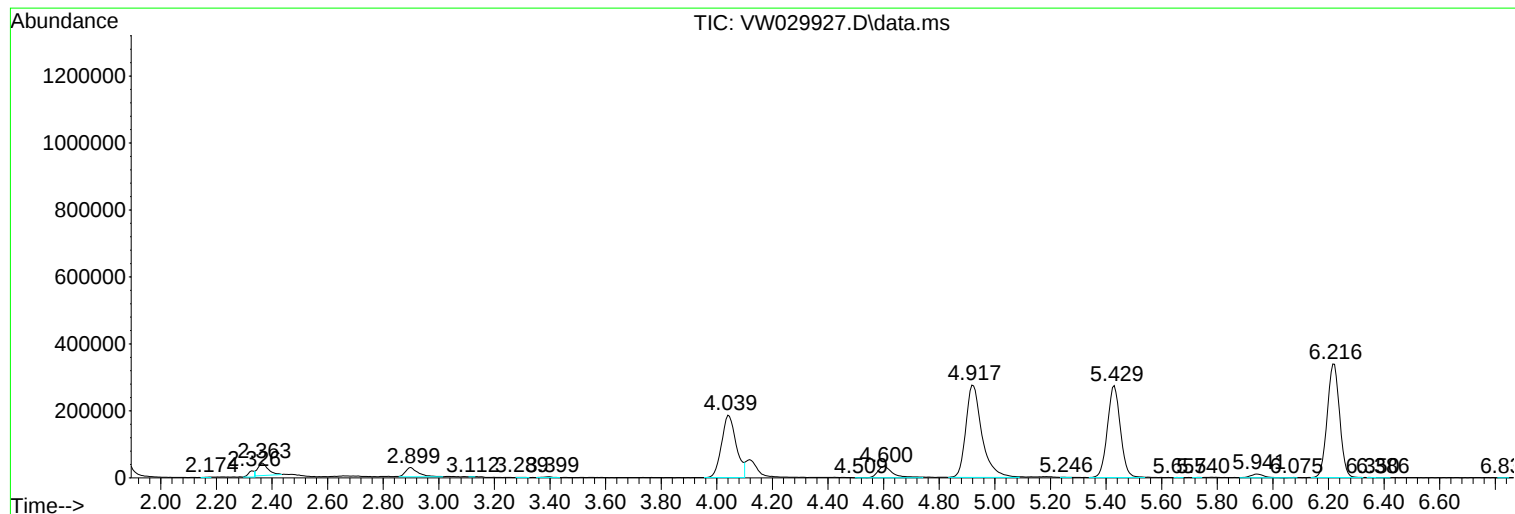
Sum of corrected areas: 27222499

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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



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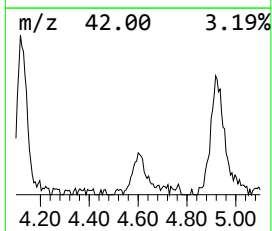
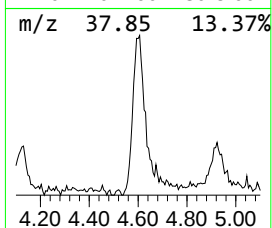
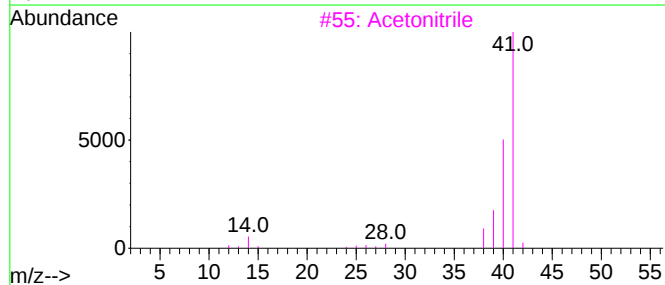
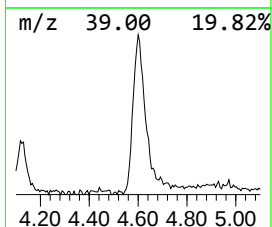
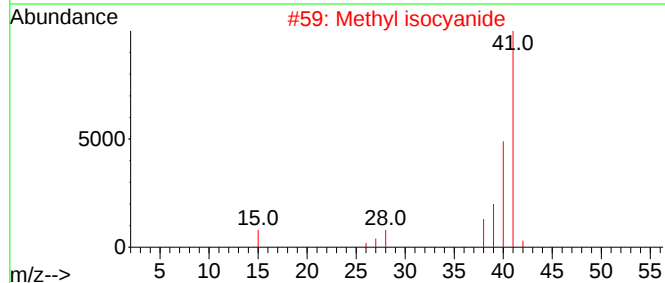
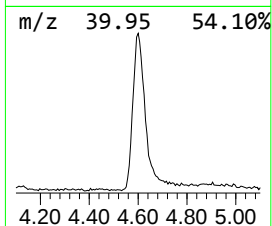
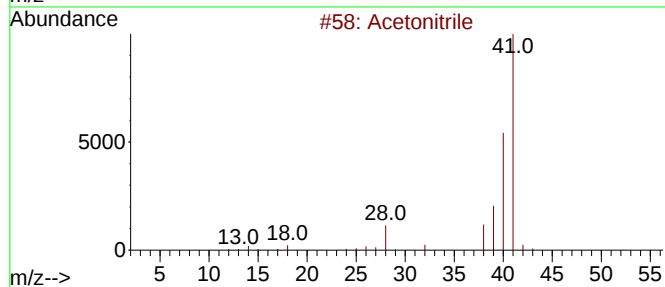
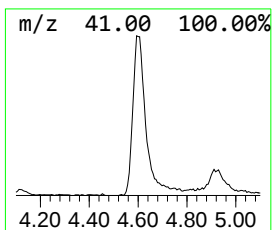
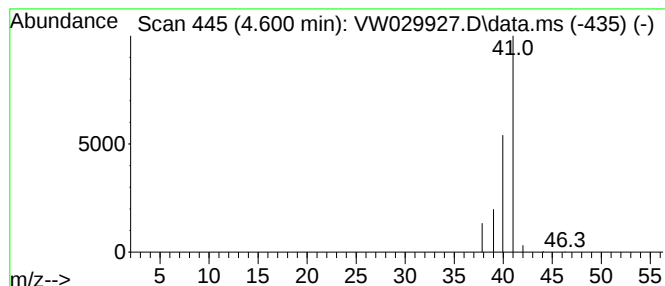
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Acetonitrile Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.600	6.57 ug/L	124988	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile	41	C2H3N	000075-05-8	64
2			Methyl isocyanide	41	C2H3N	000593-75-9	64
3			Acetonitrile	41	C2H3N	000075-05-8	64
4			Acetonitrile	41	C2H3N	000075-05-8	64
5			Acetonitrile	41	C2H3N	000075-05-8	5



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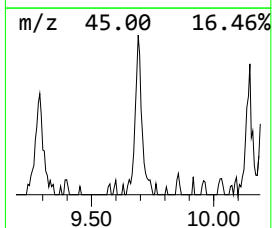
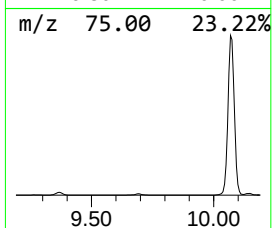
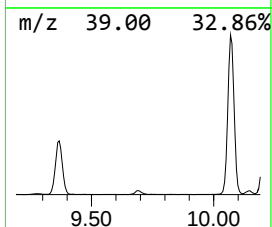
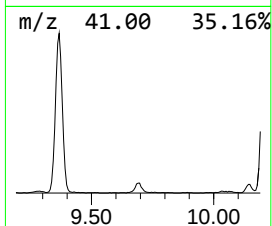
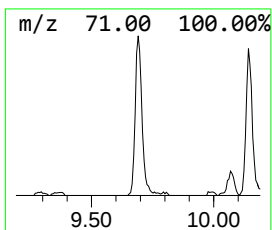
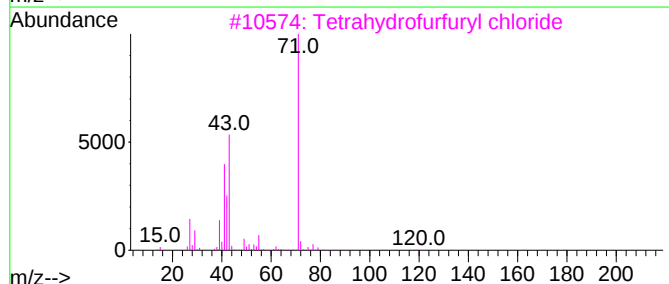
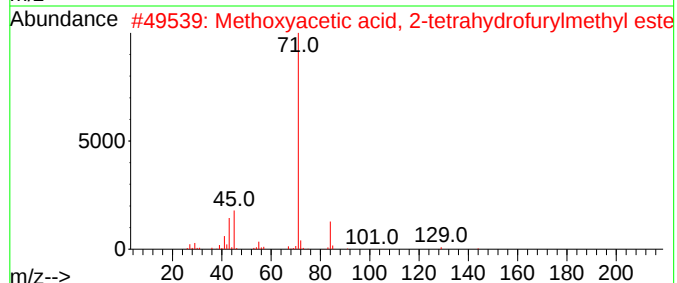
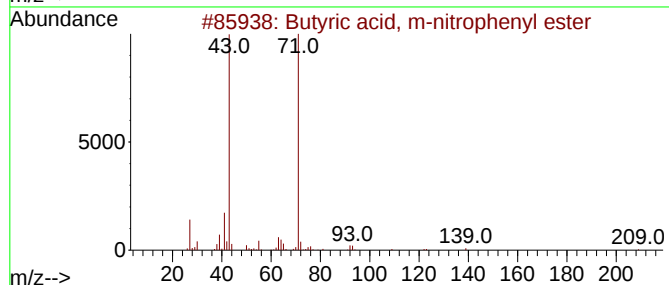
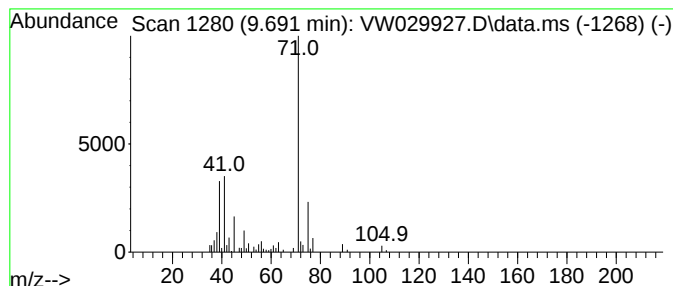
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.691	2.17 ug/L	41284	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyric acid, m-nitrophenyl ester	209	C10H11NO4	014617-97-1	38
2			Methoxyacetic acid, 2-tetrahydro...	174	C8H14O4	1000282-41-3	33
3			Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	28
4			Hexanoic acid, 2-tetrahydrofuryl...	200	C11H20O3	002217-34-7	25
5			2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	25



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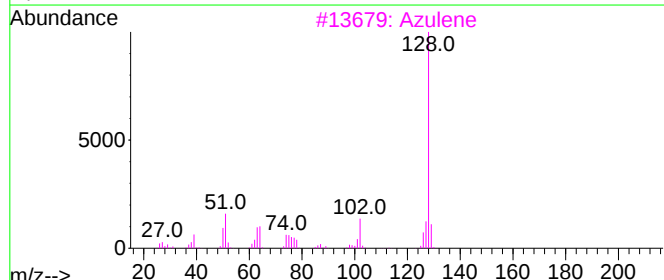
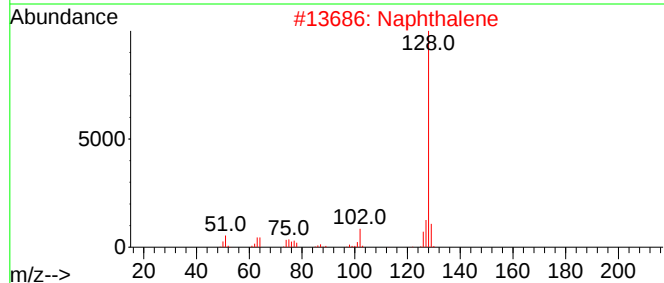
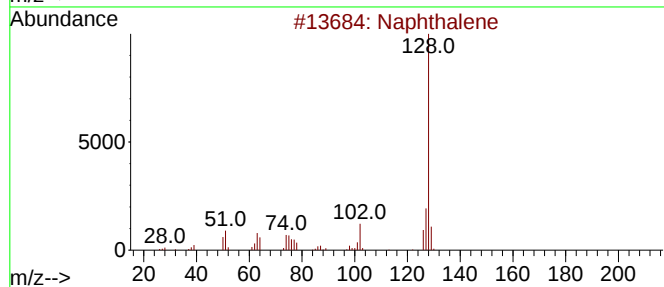
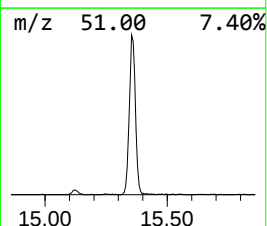
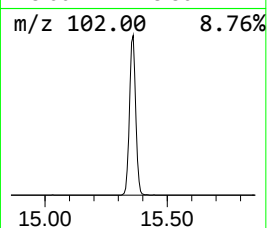
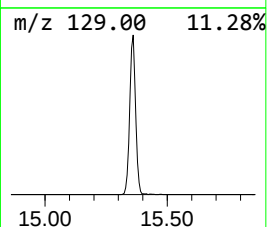
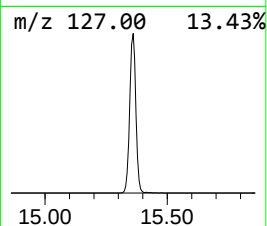
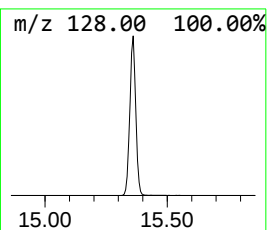
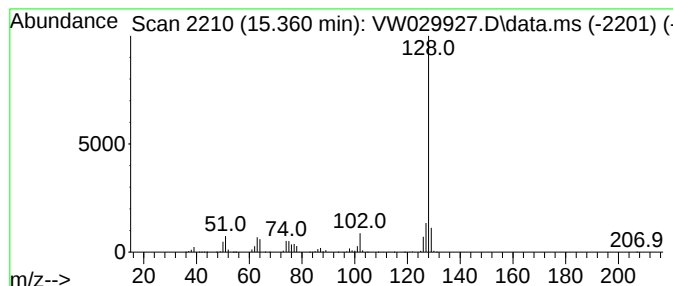
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.360	17.45 ug/L	1077660	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081624\
Data File : VW029927.D
Acq On : 16 Aug 2024 13:35
Operator : SY/MD
Sample : P3504-04
Misc : 5.00g/10mL/MSVOA_W/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCXX3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.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
Acetonitrile	4.600	6.6	ug/L	124988	1	8.843	475820	25.0
unknown-01	9.691	2.2	ug/L	41284	1	8.843	475820	25.0
Azulene	15.360	17.4	ug/L	1077660	3	13.556	1544050	25.0