

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072524\
 Data File : VW029738.D
 Acq On : 25 Jul 2024 16:23
 Operator : SY/MD
 Sample : P3344-10
 Misc : 6.01g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BHB38

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: VW029738.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.960	8	12	26	rVB2	30064	54627	4.26%	0.631%
2	2.180	43	48	52	rBV	3691	6137	0.48%	0.071%
3	2.363	67	78	91	rBV2	39930	113778	8.87%	1.315%
4	2.582	109	114	118	rBV2	3383	6901	0.54%	0.080%
5	2.899	159	166	180	rBV	30253	89133	6.95%	1.030%
6	3.302	225	232	239	rBV4	3363	8165	0.64%	0.094%
7	3.393	242	247	259	rVV4	3819	11093	0.86%	0.128%
8	3.692	292	296	298	rVB4	514	714	0.06%	0.008%
9	3.753	304	306	309	rVV4	547	716	0.06%	0.008%
10	3.838	315	320	321	rVB5	702	818	0.06%	0.009%
11	3.863	321	324	325	rBV3	805	765	0.06%	0.009%
12	4.021	339	350	375	rBV2	66417	241609	18.83%	2.792%
13	4.265	389	390	397	rBV5	481	942	0.07%	0.011%
14	4.387	406	410	414	rBV5	982	1717	0.13%	0.020%
15	4.564	437	439	441	rBV2	701	654	0.05%	0.008%
16	4.661	453	455	461	rBV3	442	710	0.06%	0.008%
17	4.716	461	464	467	rBV3	372	637	0.05%	0.007%
18	4.765	467	472	476	rBV6	632	1115	0.09%	0.013%
19	4.917	485	497	514	rBV3	18370	78422	6.11%	0.906%
20	5.429	576	581	585	rBV7	1079	2181	0.17%	0.025%
21	5.704	622	626	628	rBV4	435	594	0.05%	0.007%
22	5.783	636	639	641	rBV4	673	912	0.07%	0.011%
23	5.948	654	666	674	rVV5	6397	20331	1.58%	0.235%
24	6.063	683	685	689	rBV3	449	648	0.05%	0.007%
25	6.563	764	767	772	rBV6	772	1283	0.10%	0.015%
26	6.801	804	806	808	rBV2	519	598	0.05%	0.007%
27	6.899	817	822	824	rBV5	876	1567	0.12%	0.018%
28	6.978	833	835	838	rBV2	467	606	0.05%	0.007%
29	7.075	843	851	866	rBV	37032	113449	8.84%	1.311%
30	7.313	888	890	892	rVB2	744	651	0.05%	0.008%
31	7.466	913	915	918	rBV3	628	755	0.06%	0.009%
32	7.545	921	928	929	rBV4	1355	2658	0.21%	0.031%
33	7.648	934	945	957	rVV	151981	378472	29.49%	4.373%
34	7.764	961	964	967	rBV4	991	1026	0.08%	0.012%
35	7.862	978	980	982	rVB3	691	599	0.05%	0.007%
36	7.911	985	988	989	rVV3	653	677	0.05%	0.008%

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

37	8.142	1024	1026	1028	rBV3	870	975	0.08%	0.011%
38	8.276	1037	1048	1066	rBV2	276262	861362	67.12%	9.952%
39	8.581	1092	1098	1104	rVV7	943	1839	0.14%	0.021%
40	8.691	1111	1116	1129	rVB7	1685	6121	0.48%	0.071%
41	8.843	1131	1141	1154	rBV	441881	868510	67.68%	10.035%
42	9.026	1169	1171	1173	rBV3	879	967	0.08%	0.011%
43	9.081	1173	1180	1186	rVB9	2895	7257	0.57%	0.084%
44	9.166	1192	1194	1195	rBV2	688	582	0.05%	0.007%
45	9.270	1202	1211	1222	rBV	216448	444140	34.61%	5.132%
46	9.416	1230	1235	1241	rVB4	3839	6886	0.54%	0.080%
47	9.660	1267	1275	1283	rBV7	2214	6040	0.47%	0.070%
48	10.032	1329	1336	1347	rBV	102755	190438	14.84%	2.200%
49	10.203	1360	1364	1366	rBV4	550	666	0.05%	0.008%
50	10.319	1376	1383	1391	rVV	350511	625042	48.70%	7.222%
51	10.380	1391	1393	1400	rVB2	4771	8821	0.69%	0.102%
52	10.502	1407	1413	1419	rBV8	1686	3733	0.29%	0.043%
53	10.575	1419	1425	1438	rVV	67594	121262	9.45%	1.401%
54	10.697	1440	1445	1452	rVB2	6339	11053	0.86%	0.128%
55	10.855	1466	1471	1476	rBV9	2579	6196	0.48%	0.072%
56	10.922	1476	1482	1497	rVV	143355	247018	19.25%	2.854%
57	11.069	1500	1506	1518	rVV	70738	120238	9.37%	1.389%
58	11.404	1559	1561	1564	rBV4	648	794	0.06%	0.009%
59	11.629	1564	1598	1609	rBV	666067	1283344	100.00%	14.828%
60	11.831	1627	1631	1637	rBV5	2745	4816	0.38%	0.056%
61	11.910	1642	1644	1647	rVB4	768	786	0.06%	0.009%
62	11.959	1647	1652	1654	rBV4	626	666	0.05%	0.008%
63	12.166	1682	1686	1690	rVV6	2077	3294	0.26%	0.038%
64	12.245	1697	1699	1703	rVB5	991	982	0.08%	0.011%
65	12.337	1708	1714	1720	rBV3	7493	13320	1.04%	0.154%
66	12.446	1731	1732	1736	rVB3	720	737	0.06%	0.009%
67	12.483	1736	1738	1740	rBV3	656	705	0.05%	0.008%
68	12.599	1752	1757	1762	rVB	7252	11478	0.89%	0.133%
69	12.690	1764	1772	1780	rBV	199490	325964	25.40%	3.766%
70	12.794	1788	1789	1792	rVB3	765	594	0.05%	0.007%
71	12.843	1794	1797	1798	rBV3	622	590	0.05%	0.007%
72	12.891	1802	1805	1808	rBV4	1096	1606	0.13%	0.019%
73	12.928	1809	1811	1813	rBV3	676	613	0.05%	0.007%
74	13.099	1837	1839	1844	rVB5	751	1120	0.09%	0.013%
75	13.251	1859	1864	1867	rBV5	1579	2257	0.18%	0.026%
76	13.391	1882	1887	1897	rVV2	17867	29777	2.32%	0.344%

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 Title : SFAM01.0

77	13.556	1907	1914	1921	rBV	618117	1002267	78.10%	11.580%
78	13.647	1924	1929	1943	rVB5	29630	94387	7.35%	1.091%
79	13.849	1955	1962	1969	rBV	383324	632130	49.26%	7.304%
80	14.062	1992	1997	2003	rVB2	12660	22192	1.73%	0.256%
81	14.178	2005	2016	2033	rVB5	22278	79658	6.21%	0.920%
82	14.318	2033	2039	2048	rBV	30023	49172	3.83%	0.568%
83	14.458	2050	2062	2074	rBV2	106324	326938	25.48%	3.777%
84	14.714	2096	2104	2111	rBV2	4675	11993	0.93%	0.139%
85	14.830	2120	2123	2127	rBV6	922	1136	0.09%	0.013%
86	14.861	2127	2128	2133	rVV5	745	1126	0.09%	0.013%
87	14.958	2137	2144	2145	rBV7	1630	2422	0.19%	0.028%
88	15.098	2164	2167	2172	rVB6	1844	2665	0.21%	0.031%
89	15.172	2175	2179	2188	rVV10	3410	9905	0.77%	0.114%
90	15.239	2188	2190	2193	rVB4	1499	1668	0.13%	0.019%
91	15.312	2199	2202	2206	rBV5	1249	2008	0.16%	0.023%
92	15.476	2222	2229	2234	rBV	7532	14889	1.16%	0.172%
93	15.537	2235	2239	2247	rVB4	4617	8311	0.65%	0.096%
94	15.647	2255	2257	2261	rBV3	1142	1275	0.10%	0.015%
95	15.714	2265	2268	2274	rVB7	1326	2378	0.19%	0.027%
96	15.842	2283	2289	2295	rBV4	5863	10506	0.82%	0.121%
97	16.080	2325	2328	2332	rBV6	1098	1724	0.13%	0.020%
98	16.202	2346	2348	2349	rBV2	1038	684	0.05%	0.008%
99	16.482	2390	2394	2402	rVB7	2830	6270	0.49%	0.072%
100	16.574	2407	2409	2412	rBV3	719	947	0.07%	0.011%

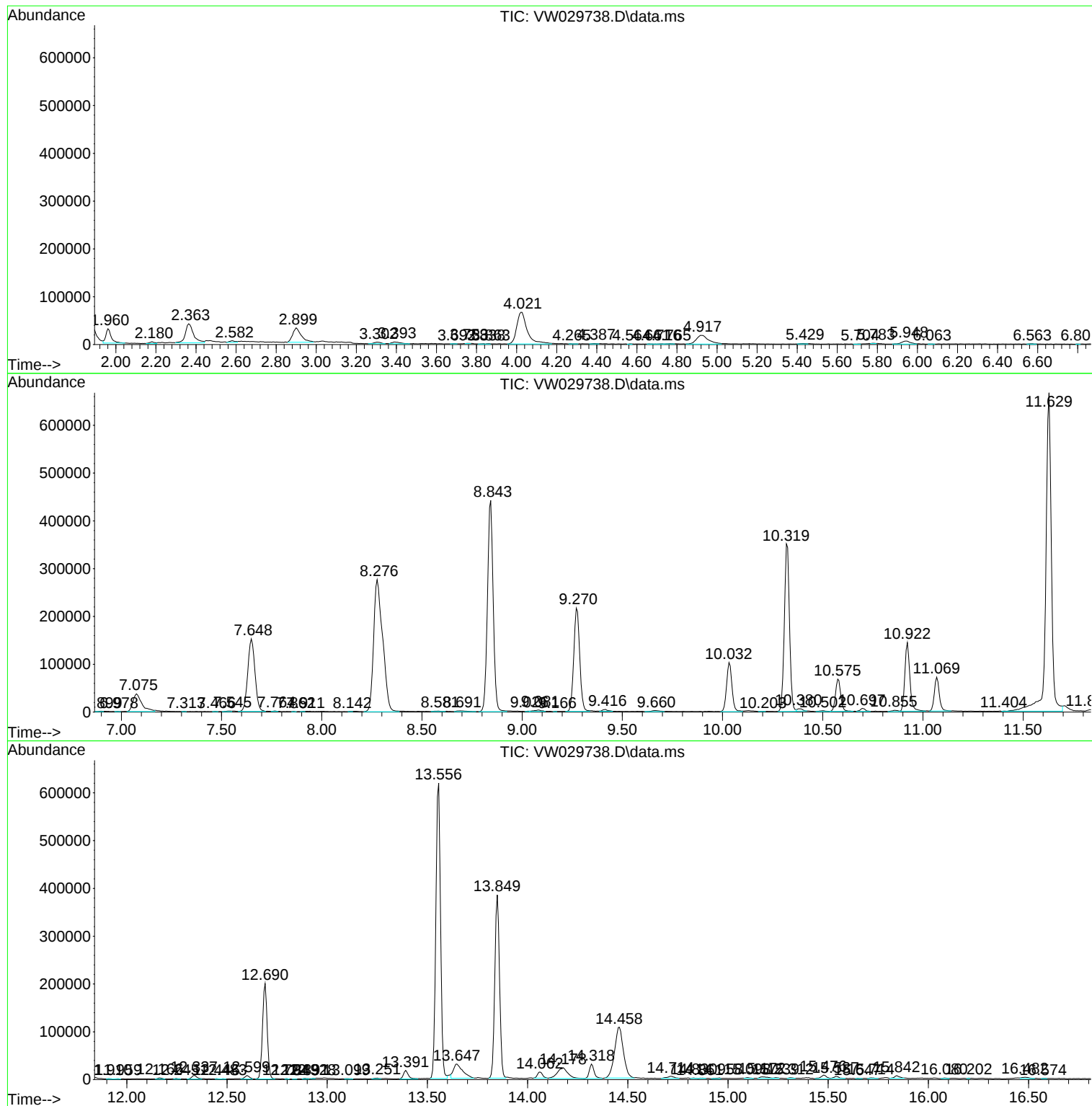
Sum of corrected areas: 8654900

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Instrument :
MSVOA_W
ClientSampleId :
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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072524\
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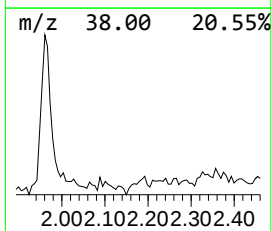
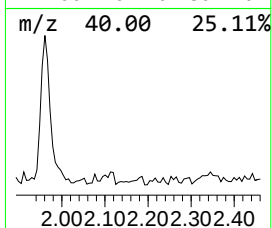
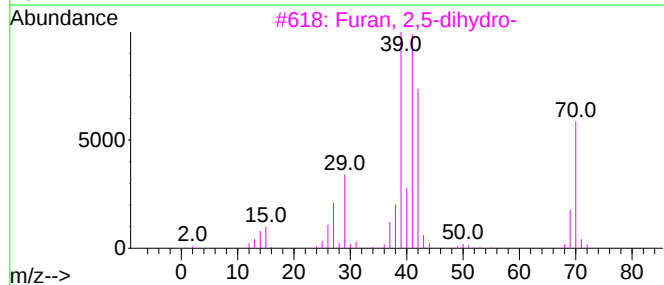
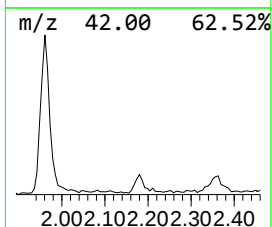
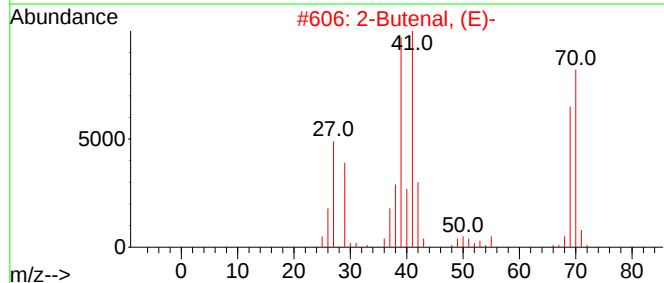
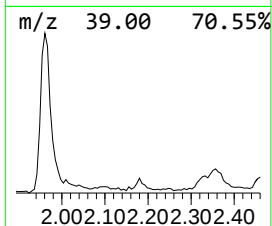
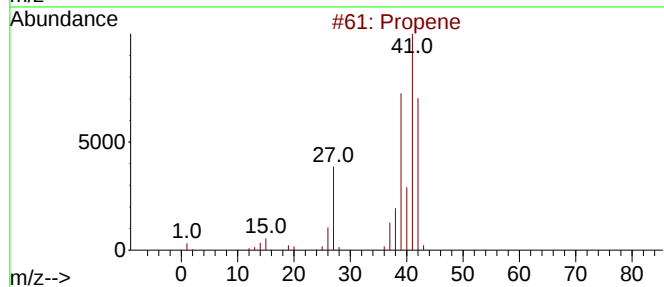
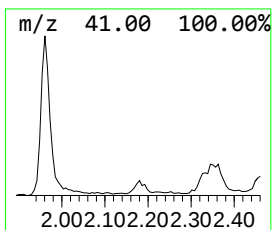
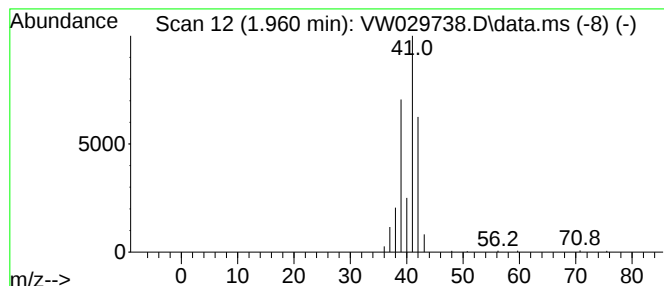
Instrument :
MSVOA_W
ClientSampleId :
BHB38

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.960	1.57 ug/L	54627	1,4-Difluorobenzene	8.843	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	2-Butenal, (E)-	70	C4H6O	000123-73-9	72
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	50
4	2-Butenal	70	C4H6O	004170-30-3	50
5	Cyclopropane	42	C3H6	000075-19-4	47



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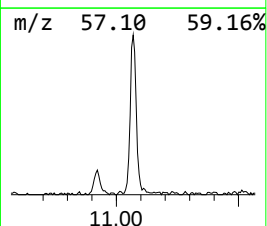
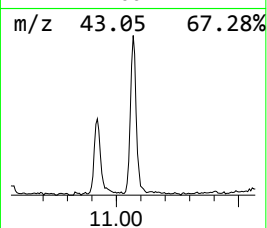
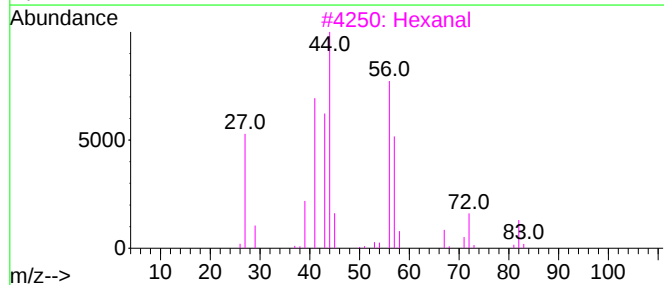
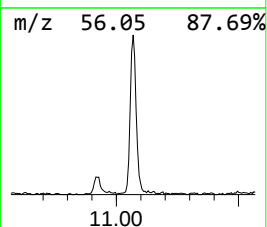
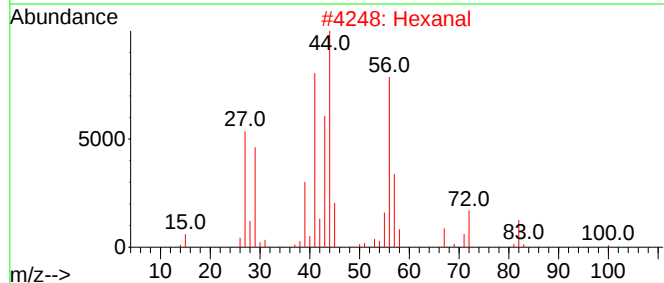
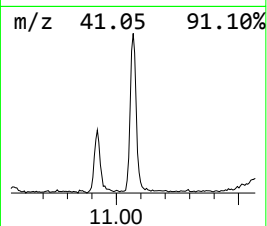
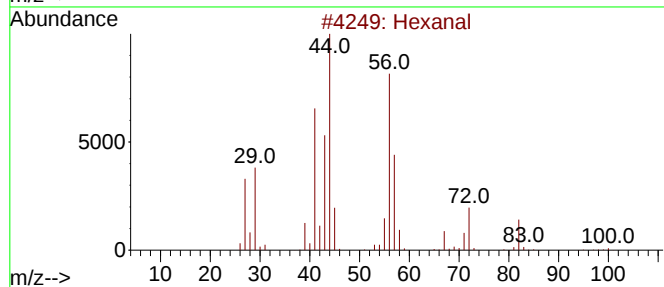
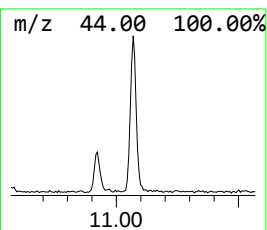
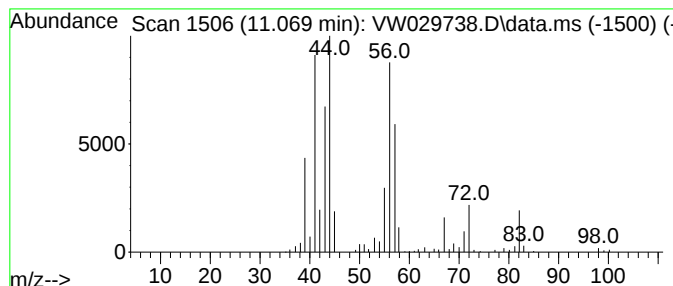
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	2.34 ug/L	120238	Chlorobenzene-d5	11.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	93
2	Hexanal			100	C6H12O	000066-25-1	76
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	64



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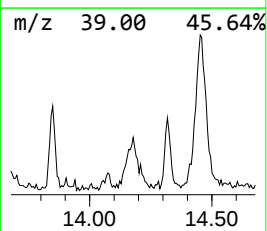
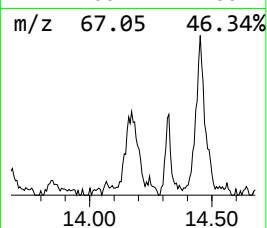
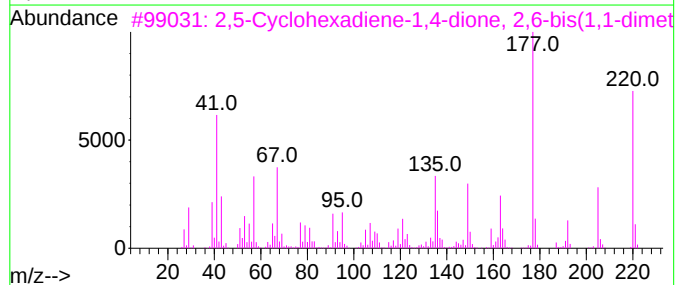
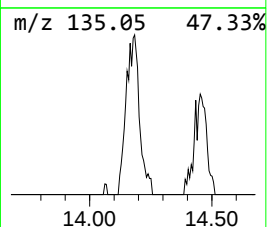
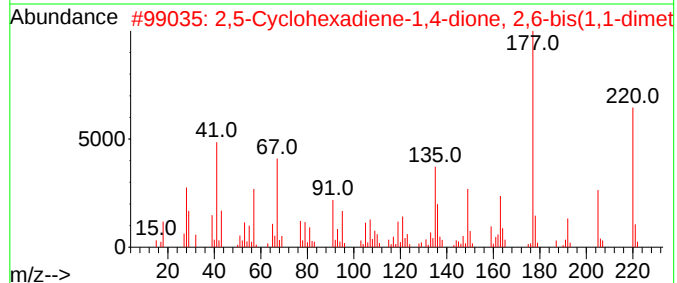
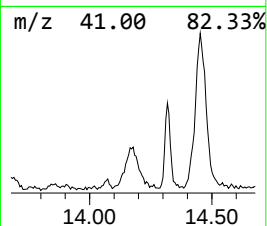
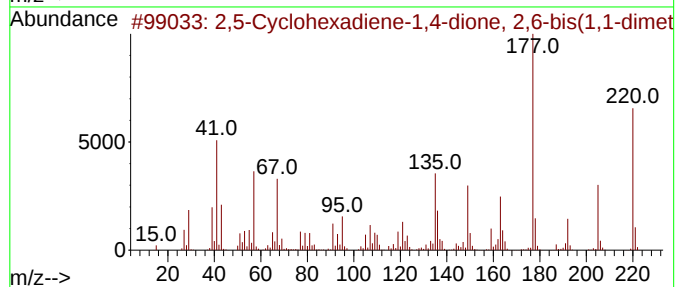
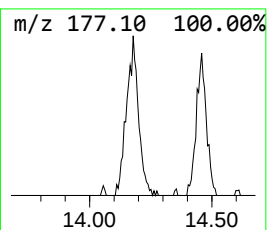
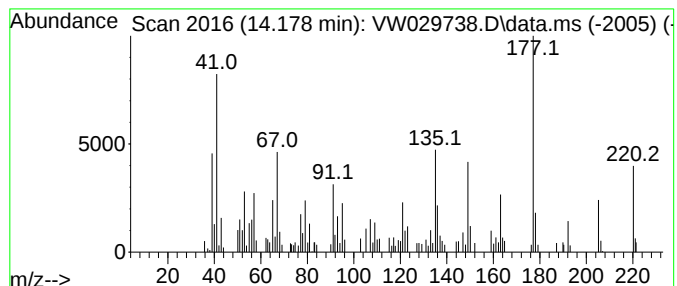
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.178	1.99 ug/L	79658	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
4			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
5			2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072524\
Data File : VW029738.D
Acq On : 25 Jul 2024 16:23
Operator : SY/MD
Sample : P3344-10
Misc : 6.01g/10mL/MSVOA_W/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
BHB38

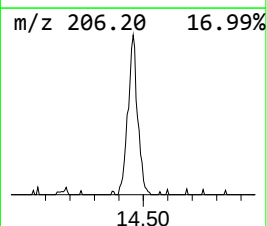
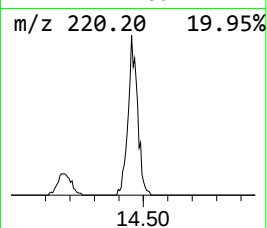
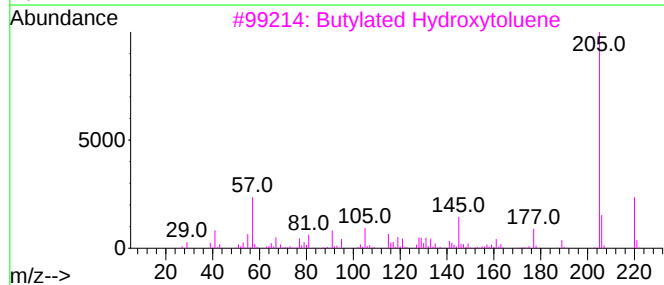
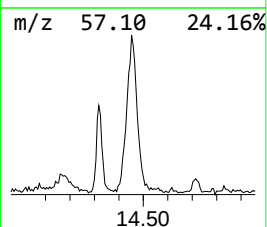
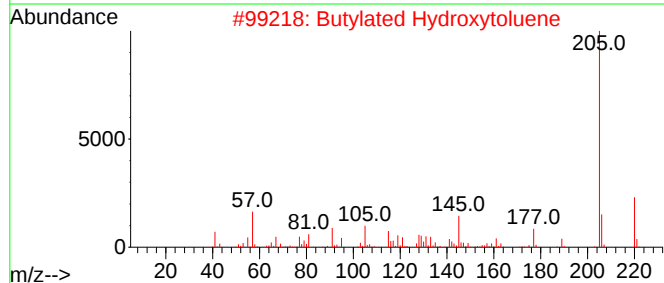
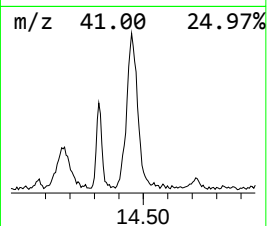
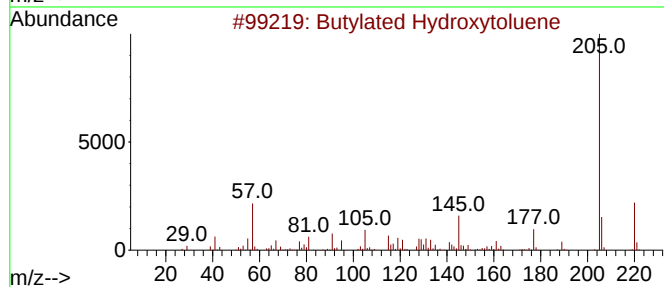
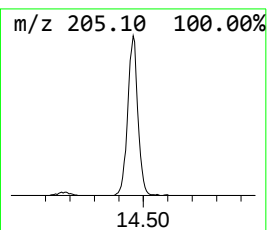
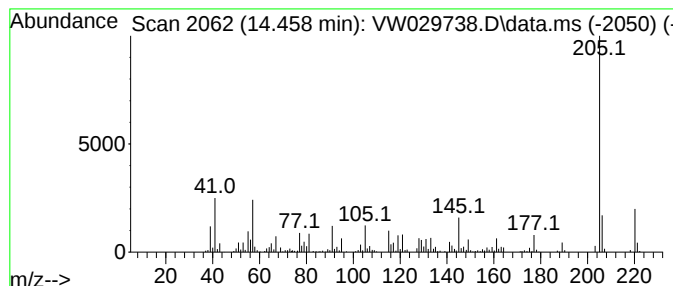
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Quant Title : SFAM01.0

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.458	8.15 ug/L	326938	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072524\
Data File : VW029738.D
Acq On : 25 Jul 2024 16:23
Operator : SY/MD
Sample : P3344-10
Misc : 6.01g/10mL/MSVOA_W/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
BHB38

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
(DEL) Alkane: S...	1.960	1.6	ug/L	54627	1	8.843	868510	25.0
Hexanal	11.069	2.3	ug/L	120238	2	11.630	1283340	25.0
unknown-01	13.647	2.4	ug/L	94387	3	13.556	1002270	25.0
2,5-Cyclohexadi...	14.178	2.0	ug/L	79658	3	13.556	1002270	25.0
Butylated Hydro...	14.458	8.2	ug/L	326938	3	13.556	1002270	25.0