

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW121924\
 Data File : VW031408.D
 Acq On : 20 Dec 2024 01:44
 Operator : SY/MD
 Sample : P5333-11
 Misc : 9.63g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 E2913

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\SFAMWLM121324SMA.M
 Title : SFAM01.0

Signal : TIC: VW031408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.192	42	50	51	rBV5	5424	12314	0.55%	0.074%
2	2.356	71	77	93	rBV	180262	404123	17.96%	2.427%
3	2.899	158	166	180	rBV	125874	364052	16.18%	2.186%
4	4.015	339	349	369	rBV	313376	909779	40.44%	5.463%
5	4.191	376	378	379	rBV2	2186	1647	0.07%	0.010%
6	4.258	387	389	392	rVB4	1215	1434	0.06%	0.009%
7	4.386	406	410	412	rVB3	1229	1648	0.07%	0.010%
8	4.417	412	415	416	rBV3	980	1121	0.05%	0.007%
9	4.484	424	426	428	rBV3	936	903	0.04%	0.005%
10	4.600	440	445	446	rBV4	1148	1055	0.05%	0.006%
11	4.618	446	448	451	rBV4	1325	1932	0.09%	0.012%
12	4.899	492	494	497	rVV4	847	1113	0.05%	0.007%
13	5.082	523	524	526	rBV2	932	859	0.04%	0.005%
14	5.222	546	547	550	rBV2	815	918	0.04%	0.006%
15	5.429	578	581	582	rBV2	1163	937	0.04%	0.006%
16	5.466	585	587	590	rVB2	1298	1129	0.05%	0.007%
17	5.612	608	611	615	rBV5	657	904	0.04%	0.005%
18	5.795	640	641	645	rVB4	964	788	0.04%	0.005%
19	5.837	647	648	654	rBV4	884	1624	0.07%	0.010%
20	5.947	657	666	671	rBV8	4883	13571	0.60%	0.081%
21	6.283	718	721	724	rVB4	925	1073	0.05%	0.006%
22	6.319	724	727	730	rBV5	657	882	0.04%	0.005%
23	6.453	746	749	750	rBV2	885	794	0.04%	0.005%
24	6.575	765	769	771	rBV3	1135	1182	0.05%	0.007%
25	6.624	774	777	780	rBV5	867	1050	0.05%	0.006%
26	6.715	790	792	793	rBV2	807	762	0.03%	0.005%
27	6.935	826	828	832	rBV4	706	971	0.04%	0.006%
28	7.099	847	855	859	rBV	17618	48049	2.14%	0.289%
29	7.398	900	904	905	rBV4	762	754	0.03%	0.005%
30	7.471	914	916	920	rVB4	645	780	0.03%	0.005%
31	7.532	923	926	928	rBV4	829	1151	0.05%	0.007%
32	7.563	928	931	932	rVV3	930	961	0.04%	0.006%
33	7.648	935	945	962	rVV	425978	1029072	45.74%	6.180%
34	7.916	986	989	990	rBV2	1000	1152	0.05%	0.007%
35	8.014	1002	1005	1006	rVV3	763	833	0.04%	0.005%
36	8.032	1006	1008	1012	rVV5	1040	1125	0.05%	0.007%

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Integrator: RTE

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 Title : SFAM01.0

37	8.148	1025	1027	1030	rVB4	679	824	0.04%	0.005%
38	8.276	1037	1048	1065	rBV2	761473	2249756	100.00%	13.510%
39	8.691	1110	1116	1117	rBV5	1572	3186	0.14%	0.019%
40	8.837	1131	1140	1152	rVV	1008425	2010831	89.38%	12.075%
41	9.075	1173	1179	1189	rVB9	2828	9074	0.40%	0.054%
42	9.154	1189	1192	1195	rBV5	953	1411	0.06%	0.008%
43	9.270	1201	1211	1221	rBV	543190	1113555	49.50%	6.687%
44	9.575	1259	1261	1262	rBV2	812	748	0.03%	0.004%
45	9.636	1268	1271	1273	rBV5	822	1062	0.05%	0.006%
46	9.666	1273	1276	1278	rVB3	753	855	0.04%	0.005%
47	9.703	1278	1282	1284	rBV5	684	853	0.04%	0.005%
48	9.806	1297	1299	1303	rVB4	882	768	0.03%	0.005%
49	10.032	1328	1336	1346	rBV	143986	266484	11.85%	1.600%
50	10.215	1363	1366	1369	rBV4	1003	1575	0.07%	0.009%
51	10.318	1375	1383	1391	rBV	985960	1761005	78.28%	10.575%
52	10.507	1412	1414	1416	rVB3	1741	1479	0.07%	0.009%
53	10.574	1416	1425	1433	rBV	81185	151164	6.72%	0.908%
54	10.696	1440	1445	1452	rVB2	14275	24230	1.08%	0.146%
55	10.855	1466	1471	1475	rBV7	1237	2732	0.12%	0.016%
56	10.928	1475	1483	1495	rBV2	68887	155198	6.90%	0.932%
57	11.160	1519	1521	1523	rBV3	937	764	0.03%	0.005%
58	11.324	1545	1548	1554	rBV5	968	1628	0.07%	0.010%
59	11.465	1570	1571	1575	rBV4	682	759	0.03%	0.005%
60	11.538	1580	1583	1585	rVB4	819	938	0.04%	0.006%
61	11.629	1587	1598	1611	rBV	1043129	1804422	80.21%	10.836%
62	11.830	1625	1631	1643	rVB	11053	24927	1.11%	0.150%
63	12.160	1675	1685	1693	rBV	72024	123413	5.49%	0.741%
64	12.361	1713	1718	1725	rVB5	8452	16241	0.72%	0.098%
65	12.458	1727	1734	1744	rBV	60273	105912	4.71%	0.636%
66	12.605	1750	1758	1764	rVB	15845	30085	1.34%	0.181%
67	12.690	1764	1772	1779	rBV	276977	502951	22.36%	3.020%
68	12.757	1779	1783	1787	rVV	107342	173277	7.70%	1.041%
69	12.800	1787	1790	1795	rVV	47821	71651	3.18%	0.430%
70	12.861	1795	1800	1804	rVV	208336	328711	14.61%	1.974%
71	12.940	1808	1813	1821	rVB	151886	243888	10.84%	1.465%
72	13.019	1821	1826	1832	rVB2	11302	19816	0.88%	0.119%
73	13.098	1832	1839	1846	rBV	128428	206451	9.18%	1.240%
74	13.184	1850	1853	1855	rBV3	2636	3108	0.14%	0.019%
75	13.245	1856	1863	1876	rVB	300025	486325	21.62%	2.920%
76	13.379	1878	1885	1886	rBV6	5047	9552	0.42%	0.057%

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 Title : SFAM01.0

77	13.434	1892	1894	1897	rBV	4467	5006	0.22%	0.030%
78	13.550	1907	1913	1925	rBV2	575806	1054406	46.87%	6.332%
79	13.708	1935	1939	1942	rBV2	12342	19217	0.85%	0.115%
80	13.751	1942	1946	1948	rVV3	15624	26794	1.19%	0.161%
81	13.781	1948	1951	1955	rVV3	20621	35865	1.59%	0.215%
82	13.848	1955	1962	1973	rVB	410462	680076	30.23%	4.084%
83	14.007	1981	1988	1990	rBV3	10556	20013	0.89%	0.120%
84	14.190	2013	2018	2024	rBV8	5588	11832	0.53%	0.071%
85	14.281	2031	2033	2034	rBV2	887	751	0.03%	0.005%
86	14.336	2036	2042	2045	rVV7	3274	5764	0.26%	0.035%
87	14.458	2058	2062	2065	rVB5	2437	3259	0.14%	0.020%
88	14.519	2065	2072	2081	rVB5	6514	14891	0.66%	0.089%
89	14.641	2090	2092	2096	rVB5	1000	1113	0.05%	0.007%
90	14.690	2097	2100	2101	rBV3	1562	1588	0.07%	0.010%
91	14.714	2101	2104	2111	rVB3	6325	8307	0.37%	0.050%
92	14.769	2111	2113	2114	rBV2	888	880	0.04%	0.005%
93	14.939	2139	2141	2145	rVB5	838	858	0.04%	0.005%
94	15.080	2162	2164	2166	rBV3	869	919	0.04%	0.006%
95	15.196	2180	2183	2185	rBV3	3002	3744	0.17%	0.022%
96	15.360	2206	2210	2219	rVB2	7579	15960	0.71%	0.096%
97	15.476	2224	2229	2235	rVV2	6748	13267	0.59%	0.080%
98	15.933	2300	2304	2306	rBV5	842	1120	0.05%	0.007%
99	16.025	2318	2319	2320	rBV	1342	792	0.04%	0.005%
100	16.634	2415	2419	2421	rBV5	1588	2351	0.10%	0.014%

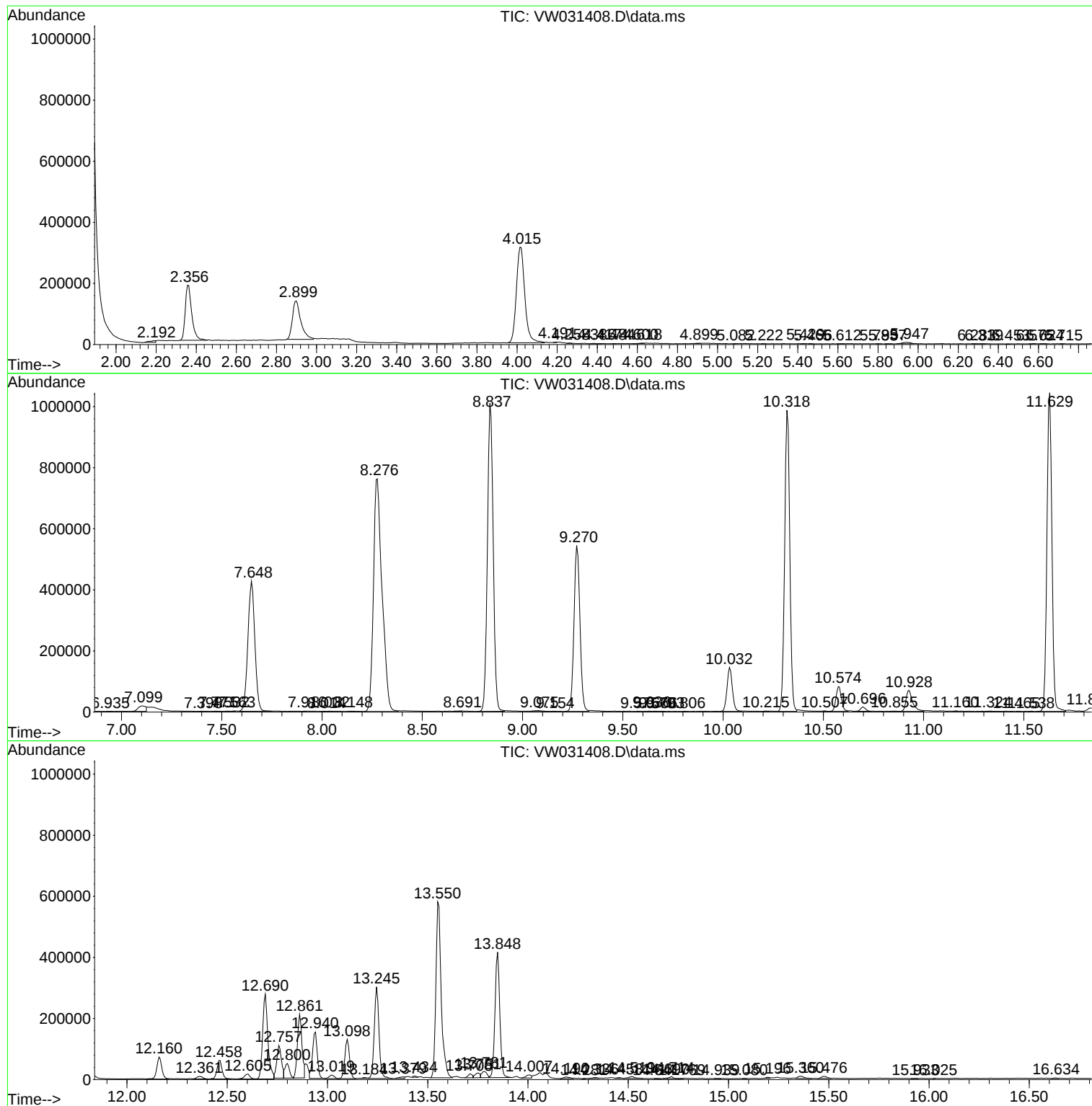
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM121324SMA.M
Quant Title : SFAM01.0

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



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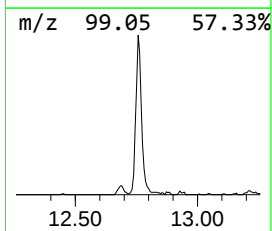
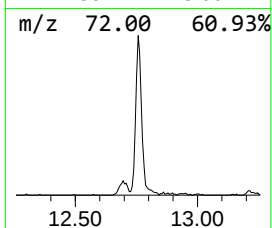
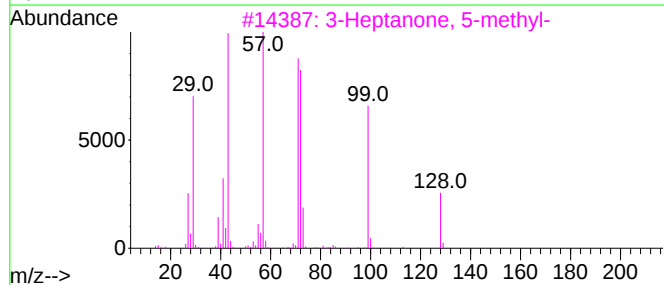
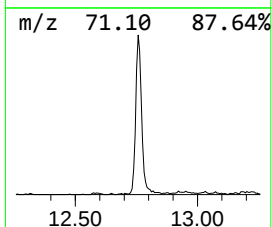
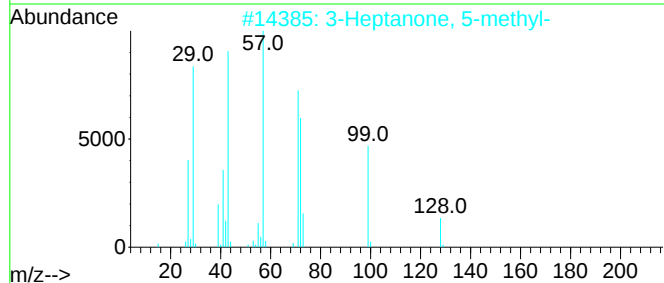
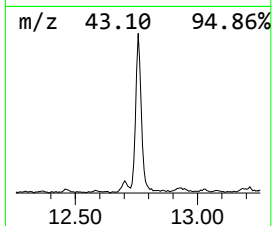
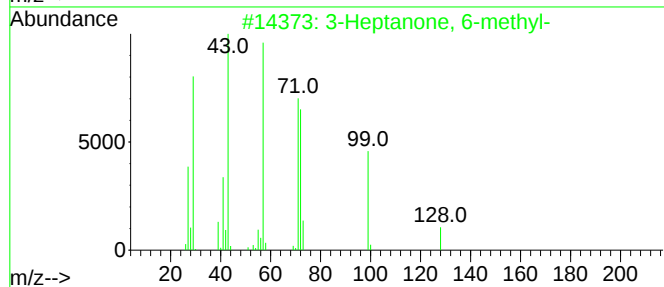
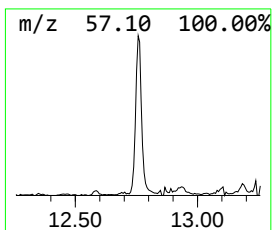
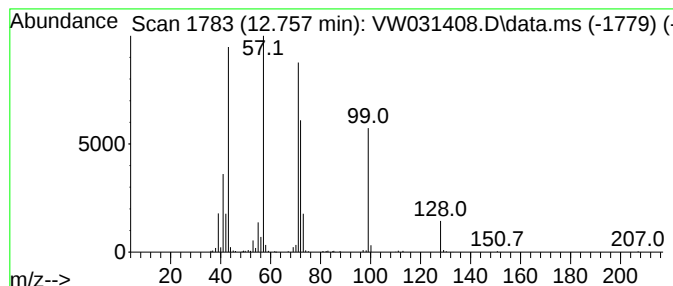
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM121324SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 3-Heptanone, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	4.11 ug/L	173277	1,4-Dichlorobenzene-d4	13.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	95
2		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	94
3		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	91
4		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	91
5		Ethyl amylketone	128	C8H16O	020616-93-7	87



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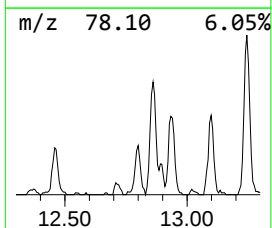
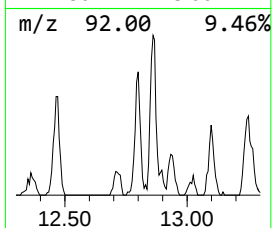
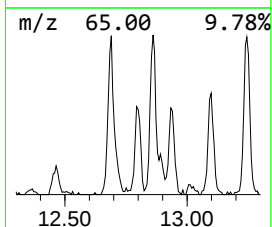
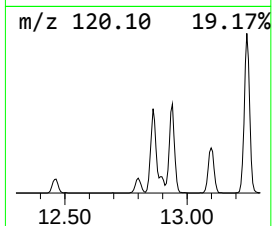
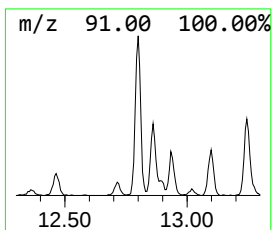
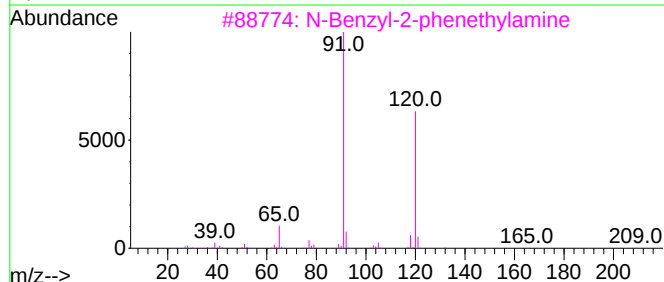
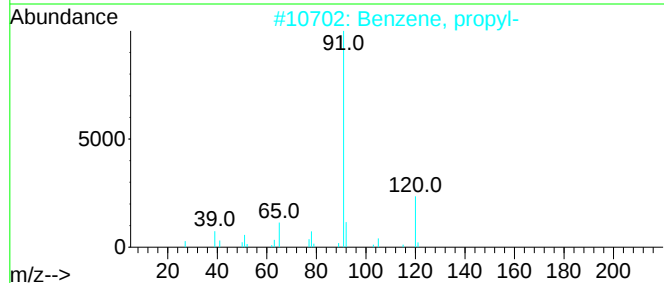
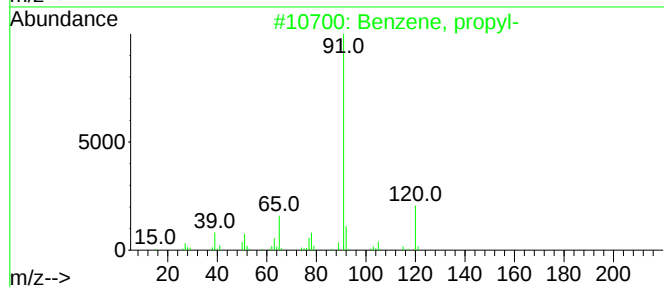
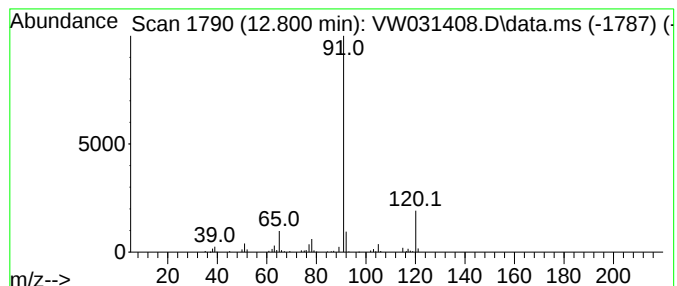
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM121324SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Benzene, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.800	1.70 ug/L	71651	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	90
2			Benzene, propyl-	120	C9H12	000103-65-1	90
3			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	78
4			Benzene, propyl-	120	C9H12	000103-65-1	76
5			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	53



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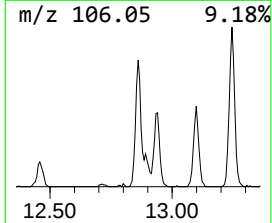
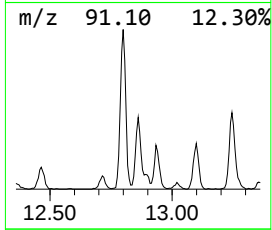
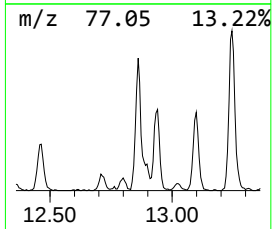
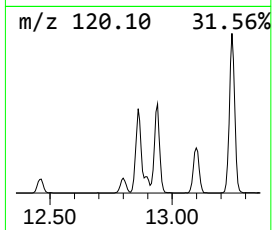
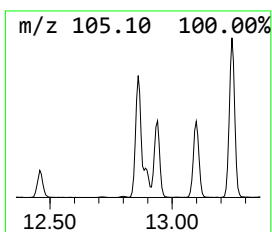
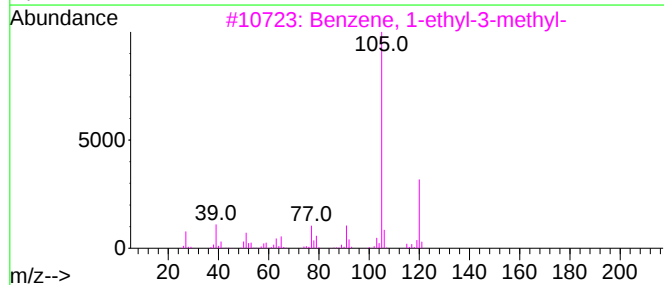
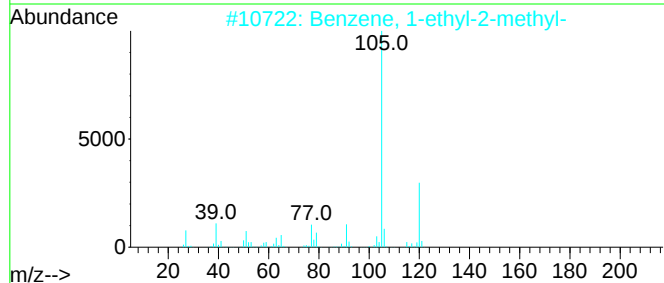
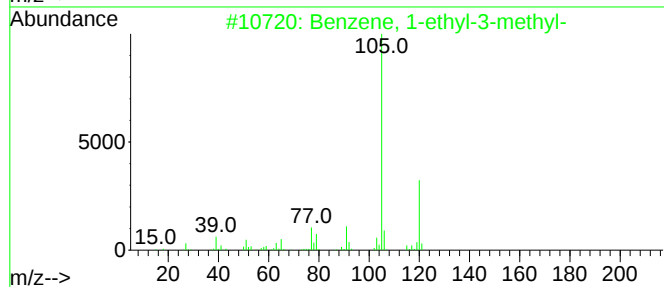
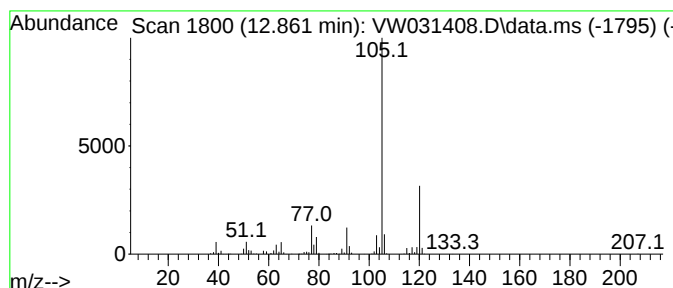
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Quant Title : SFAM01.0

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

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.861	7.79 ug/L	328711	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW121924\
Data File : VW031408.D
Acq On : 20 Dec 2024 01:44
Operator : SY/MD
Sample : P5333-11
Misc : 9.63g/10mL/MSVOA_W/SOIL/A
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E2913

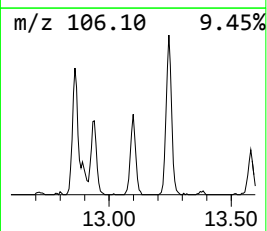
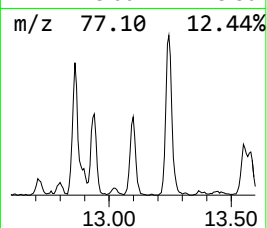
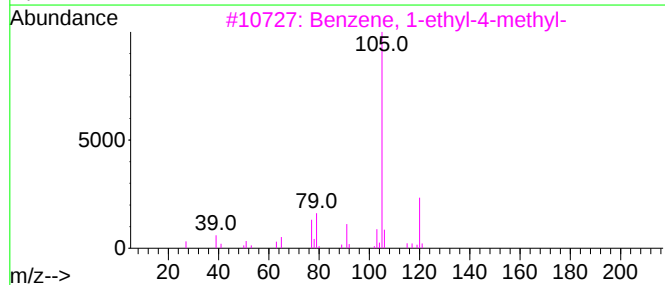
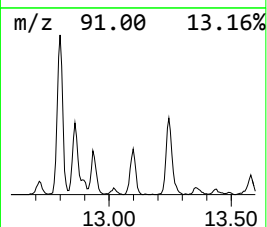
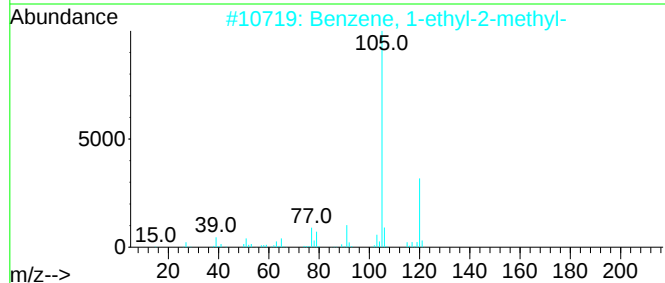
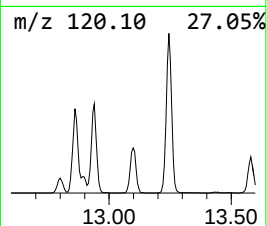
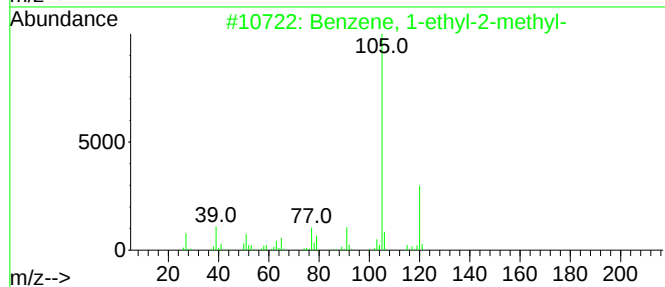
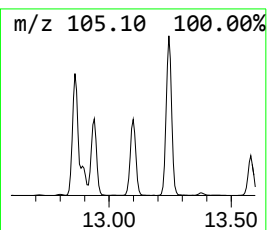
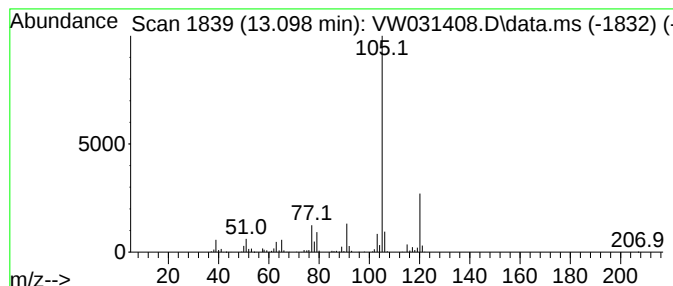
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Quant Title : SFAM01.0

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	4.89 ug/L	206451	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW121924\
Data File : VW031408.D
Acq On : 20 Dec 2024 01:44
Operator : SY/MD
Sample : P5333-11
Misc : 9.63g/10mL/MSVOA_W/SOIL/A
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E2913

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM121324SMA.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
3-Heptanone, 6-...	12.757	4.1	ug/L	173277	3	13.550	1054410	25.0
Benzene, propyl-	12.800	1.7	ug/L	71651	3	13.550	1054410	25.0
Benzene, 1-ethy...	12.861	7.8	ug/L	328711	3	13.550	1054410	25.0
Benzene, 1-ethy...	13.098	4.9	ug/L	206451	3	13.550	1054410	25.0