

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW012825\
 Data File : VW031622.D
 Acq On : 28 Jan 2025 16:41
 Operator : SY/MD
 Sample : Q1190-15RE
 Misc : 9.45g/10mL/MSVOA_W/SOIL/B
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A44T4RE

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.M
 Title : SFAM01.0

Signal : TIC: VW031622.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.954	9	11	16	rVB2	6751	7154	0.28%	0.040%
2	2.168	40	46	48	rBV2	4155	8395	0.33%	0.047%
3	2.198	49	51	52	rBV2	2227	1807	0.07%	0.010%
4	2.363	71	78	95	rBV	105949	322694	12.55%	1.825%
5	2.893	158	165	181	rVB	93671	274397	10.67%	1.552%
6	3.381	237	245	255	rBV	29990	68739	2.67%	0.389%
7	3.551	271	273	280	rBV5	677	1161	0.05%	0.007%
8	3.844	317	321	322	rBV3	772	1059	0.04%	0.006%
9	3.881	326	327	330	rBV3	569	684	0.03%	0.004%
10	4.009	336	348	363	rBV2	260346	914172	35.56%	5.171%
11	4.685	452	459	466	rBV4	3175	8495	0.33%	0.048%
12	4.905	490	495	497	rBV4	1365	2252	0.09%	0.013%
13	5.216	542	546	547	rBV2	774	739	0.03%	0.004%
14	5.393	572	575	576	rBV2	763	864	0.03%	0.005%
15	5.417	576	579	580	rVV3	1073	1253	0.05%	0.007%
16	5.429	580	581	584	rVV3	1083	1259	0.05%	0.007%
17	5.563	602	603	607	rVB2	617	713	0.03%	0.004%
18	5.710	623	627	628	rBV4	475	641	0.02%	0.004%
19	5.783	629	639	640	rBV2	5648	10525	0.41%	0.060%
20	5.935	655	664	676	rVB3	6093	19789	0.77%	0.112%
21	6.118	690	694	699	rBV7	707	1184	0.05%	0.007%
22	6.283	717	721	723	rBV3	428	691	0.03%	0.004%
23	6.356	731	733	737	rBV4	411	571	0.02%	0.003%
24	6.453	747	749	754	rVB3	620	759	0.03%	0.004%
25	6.563	766	767	770	rBV2	655	700	0.03%	0.004%
26	6.606	770	774	775	rBV2	699	722	0.03%	0.004%
27	6.898	810	822	833	rBV2	20311	63671	2.48%	0.360%
28	7.081	844	852	876	rBV	95482	323184	12.57%	1.828%
29	7.404	901	905	907	rVB2	585	697	0.03%	0.004%
30	7.642	934	944	956	rBV	437040	1085056	42.21%	6.137%
31	7.953	989	995	997	rBV5	1142	2067	0.08%	0.012%
32	8.270	1037	1047	1064	rBV2	868083	2570701	100.00%	14.540%
33	8.557	1082	1094	1104	rBV2	10625	32471	1.26%	0.184%
34	8.703	1110	1118	1128	rBV	26423	61222	2.38%	0.346%
35	8.837	1131	1140	1159	rBV2	918900	1884138	73.29%	10.657%
36	9.087	1170	1181	1195	rVB	45958	104019	4.05%	0.588%

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Integrator: RTE

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Stop Thrs : 0

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Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.M
 Title : SFAM01.0

37	9.270	1201	1211	1220	rBV	620002	1253605	48.77%	7.091%
38	9.404	1226	1233	1245	rVB	142902	275044	10.70%	1.556%
39	9.544	1254	1256	1262	rVB4	897	1149	0.04%	0.006%
40	9.666	1270	1276	1286	rVB8	2815	7347	0.29%	0.042%
41	9.745	1286	1289	1294	rVB5	665	1144	0.04%	0.006%
42	9.825	1300	1302	1305	rVB3	603	571	0.02%	0.003%
43	9.886	1310	1312	1314	rBV2	684	546	0.02%	0.003%
44	10.032	1326	1336	1349	rBV	236512	426851	16.60%	2.414%
45	10.129	1349	1352	1358	rVB4	2344	4243	0.17%	0.024%
46	10.190	1358	1362	1364	rBV4	587	539	0.02%	0.003%
47	10.209	1364	1365	1368	rVB3	839	634	0.02%	0.004%
48	10.318	1372	1383	1391	rBV	965126	1744902	67.88%	9.869%
49	10.501	1405	1413	1418	rVB6	5651	12758	0.50%	0.072%
50	10.575	1418	1425	1431	rBV	111917	196678	7.65%	1.112%
51	10.629	1431	1434	1440	rVV4	10706	21480	0.84%	0.121%
52	10.696	1440	1445	1452	rVB	15175	28565	1.11%	0.162%
53	10.861	1466	1472	1476	rVV3	8880	16082	0.63%	0.091%
54	10.922	1476	1482	1497	rVB	299990	512421	19.93%	2.898%
55	11.068	1498	1506	1520	rBV	1255911	2066563	80.39%	11.689%
56	11.276	1538	1540	1544	rVB3	819	855	0.03%	0.005%
57	11.568	1583	1588	1590	rBV5	1841	3184	0.12%	0.018%
58	11.629	1590	1598	1607	rVV	743761	1276566	49.66%	7.220%
59	11.745	1613	1617	1623	rVB4	5320	9862	0.38%	0.056%
60	11.843	1627	1633	1644	rVV4	8741	27669	1.08%	0.156%
61	11.940	1645	1649	1660	rVB5	10822	20924	0.81%	0.118%
62	12.019	1660	1662	1663	rBV2	619	550	0.02%	0.003%
63	12.160	1682	1685	1688	rBV4	2132	3592	0.14%	0.020%
64	12.239	1694	1698	1703	rVB2	4072	6021	0.23%	0.034%
65	12.336	1703	1714	1724	rBV	79236	141107	5.49%	0.798%
66	12.507	1739	1742	1746	rVB	2119	2693	0.10%	0.015%
67	12.599	1752	1757	1764	rVB	46778	74513	2.90%	0.421%
68	12.690	1764	1772	1780	rVB	348770	585857	22.79%	3.314%
69	12.928	1797	1811	1821	rBV3	12784	34534	1.34%	0.195%
70	13.037	1824	1829	1835	rBV4	6727	12975	0.50%	0.073%
71	13.098	1835	1839	1843	rVV7	5249	9837	0.38%	0.056%
72	13.153	1843	1848	1853	rVB2	18792	31908	1.24%	0.180%
73	13.391	1879	1887	1897	rBV	56847	99821	3.88%	0.565%
74	13.489	1902	1903	1906	rVV3	1822	1767	0.07%	0.010%
75	13.550	1907	1913	1923	rVV	268474	440527	17.14%	2.492%
76	13.647	1924	1929	1935	rVB4	6104	11423	0.44%	0.065%

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 Title : SFAM01.0

77	13.745	1943	1945	1948	rVB4	923	895	0.03%	0.005%
78	13.787	1949	1952	1954	rBV3	2647	3442	0.13%	0.019%
79	13.848	1955	1962	1975	rVB	213581	370250	14.40%	2.094%
80	13.976	1980	1983	1985	rBV4	1544	1822	0.07%	0.010%
81	14.013	1985	1989	1992	rVV5	2581	4849	0.19%	0.027%
82	14.062	1992	1997	2007	rVB2	27958	58426	2.27%	0.330%
83	14.318	2034	2039	2050	rBV2	27580	49538	1.93%	0.280%
84	14.488	2065	2067	2069	rBV2	860	815	0.03%	0.005%
85	14.616	2085	2088	2089	rBV3	2068	1838	0.07%	0.010%
86	14.775	2112	2114	2117	rBV4	508	762	0.03%	0.004%
87	14.946	2137	2142	2146	rBV7	3993	7396	0.29%	0.042%
88	15.135	2169	2173	2175	rVB4	1213	1548	0.06%	0.009%
89	15.171	2175	2179	2185	rBV7	3414	7486	0.29%	0.042%
90	15.330	2203	2205	2207	rBV3	1436	1455	0.06%	0.008%
91	15.354	2207	2209	2210	rVV2	878	765	0.03%	0.004%
92	15.476	2224	2229	2236	rVB2	5631	10020	0.39%	0.057%
93	15.848	2286	2290	2293	rBV6	2273	4078	0.16%	0.023%
94	15.952	2303	2307	2310	rBV4	1693	2612	0.10%	0.015%
95	16.195	2345	2347	2348	rBV	1004	782	0.03%	0.004%
96	16.348	2369	2372	2373	rVB3	775	743	0.03%	0.004%
97	16.366	2373	2375	2379	rBV4	826	1138	0.04%	0.006%
98	16.452	2388	2389	2391	rBV2	897	633	0.02%	0.004%
99	16.482	2391	2394	2400	rVB7	1520	1972	0.08%	0.011%
100	16.555	2405	2406	2409	rBV2	1043	770	0.03%	0.004%

Sum of corrected areas: 17679987

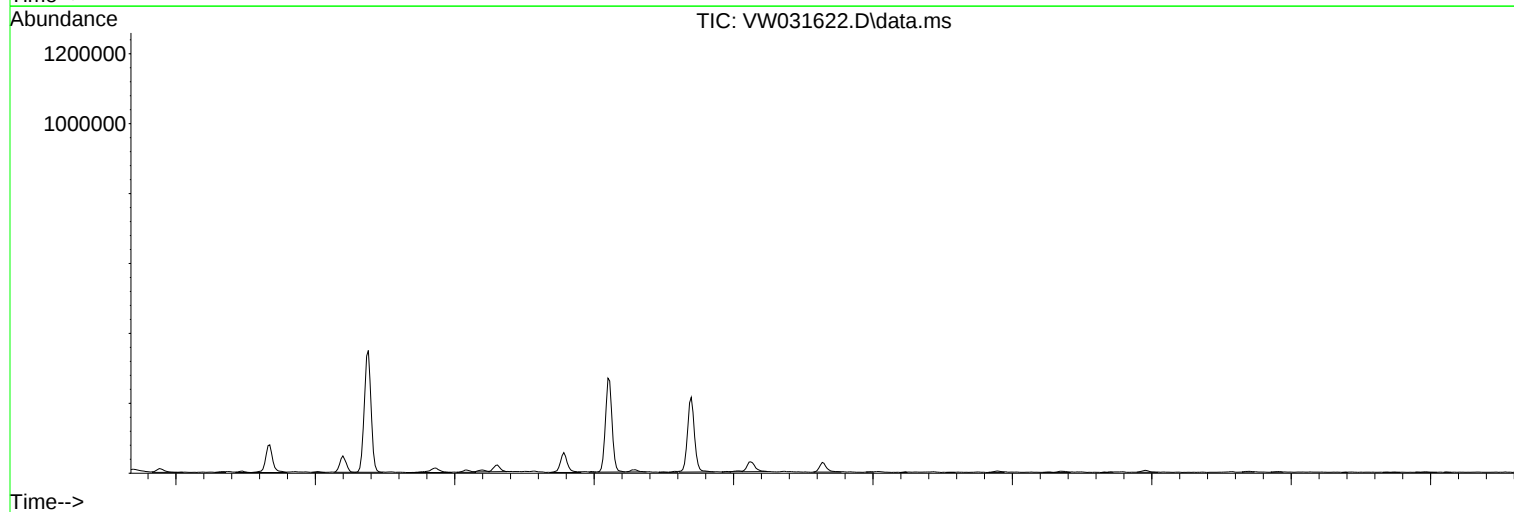
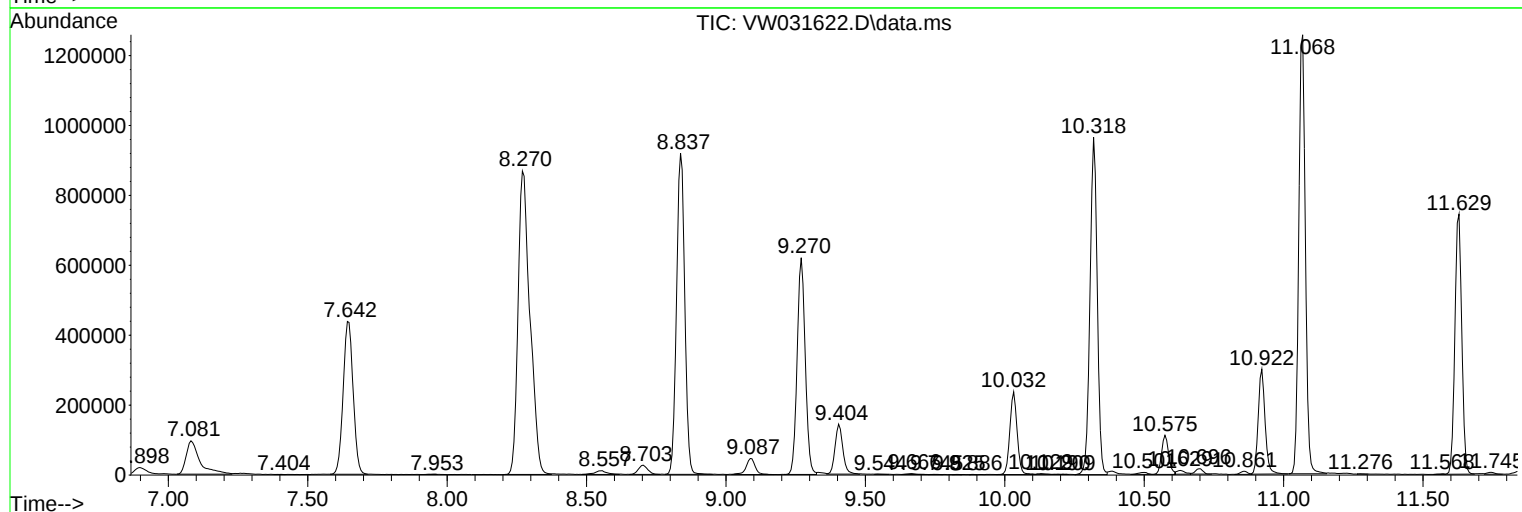
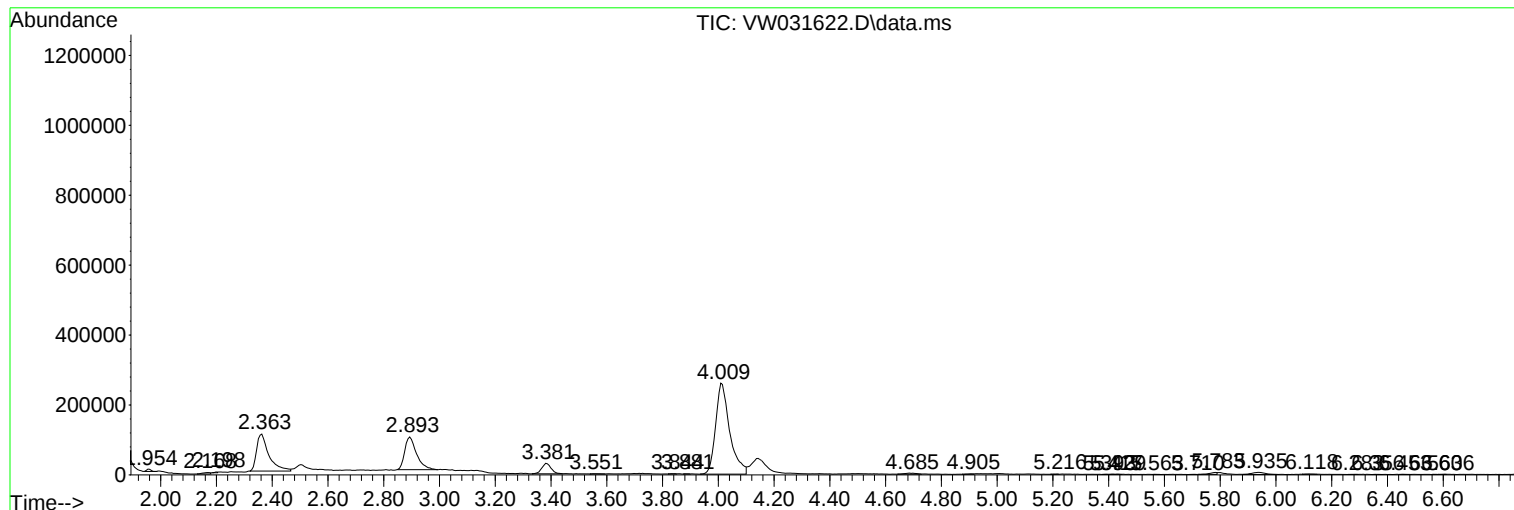
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.M
Quant Title : SFAM01.0

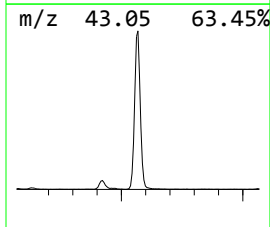
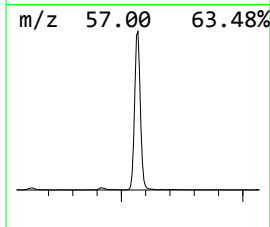
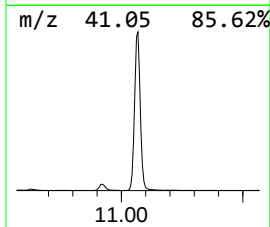
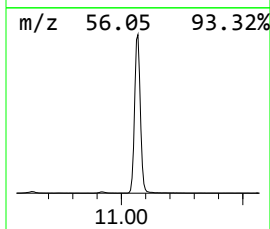
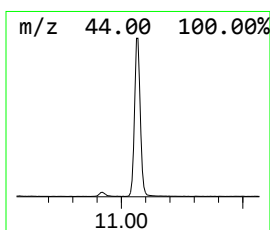
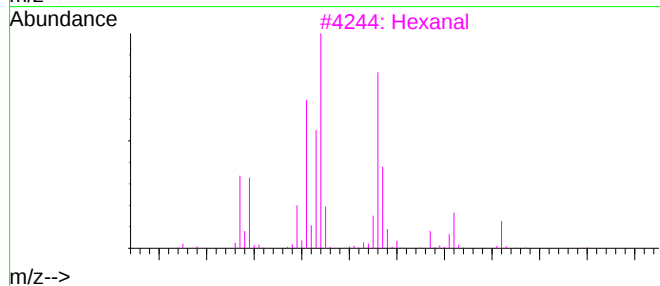
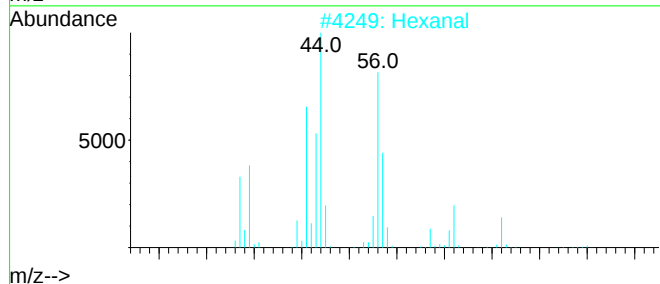
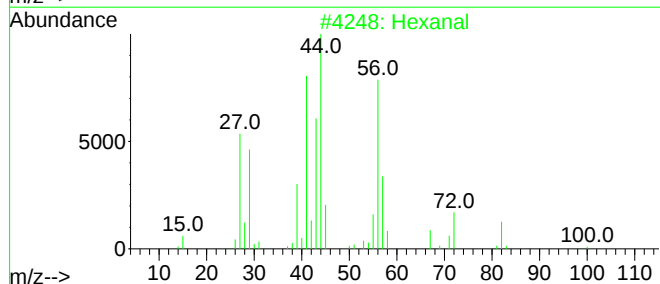
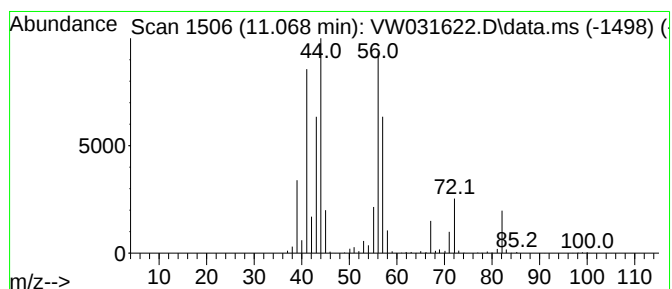
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.068	40.47 ug/L	2066560	Chlorobenzene-d5	11.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Hexanal	100	C6H12O	000066-25-1	90
3	Hexanal	100	C6H12O	000066-25-1	86
4	Hexanal	100	C6H12O	000066-25-1	81
5	Hexanal	100	C6H12O	000066-25-1	78



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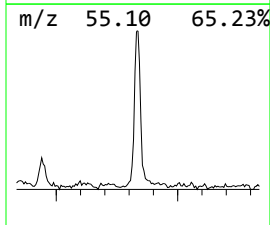
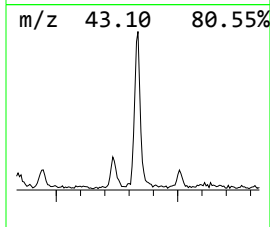
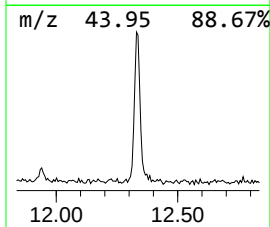
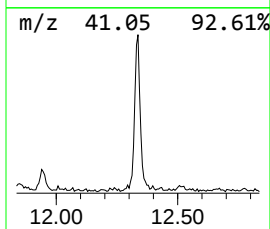
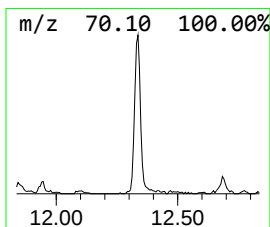
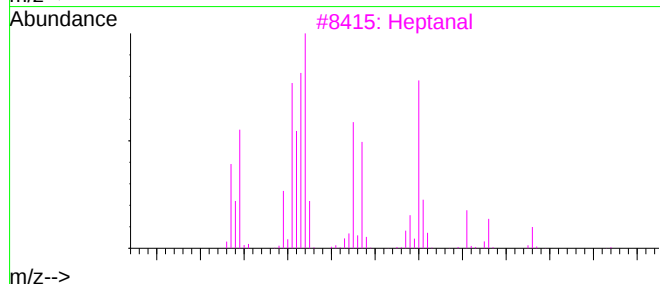
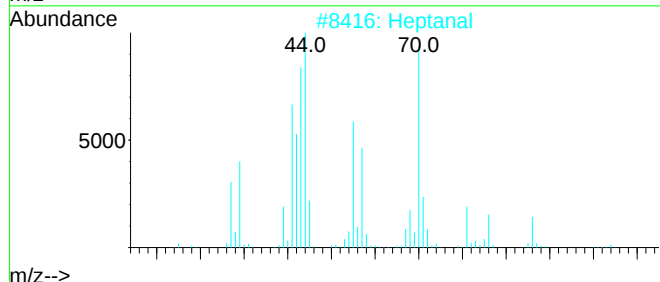
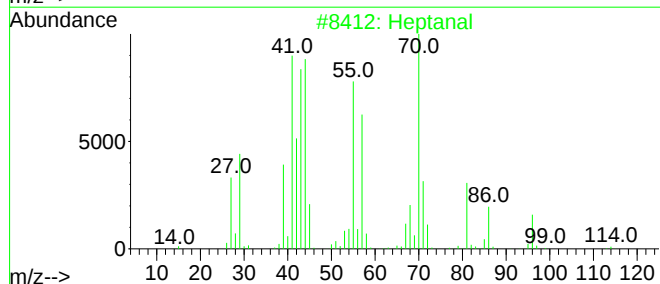
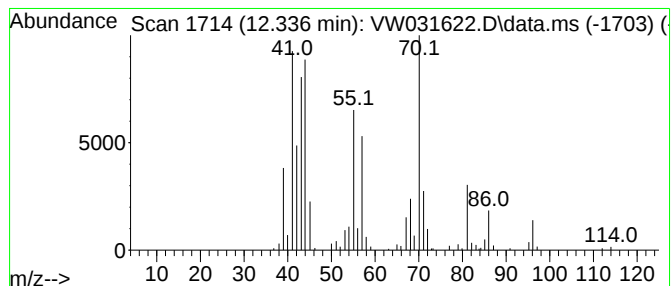
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.336	2.76 ug/L	141107	Chlorobenzene-d5		11.629	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptanal		114	C7H14O	000111-71-7	96
2	Heptanal		114	C7H14O	000111-71-7	96
3	Heptanal		114	C7H14O	000111-71-7	80
4	1-Butanamine, 3-methyl-		87	C5H13N	000107-85-7	45
5	Heptanal		114	C7H14O	000111-71-7	38



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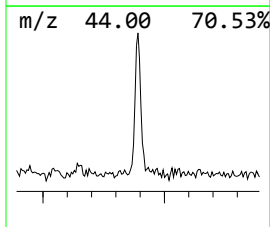
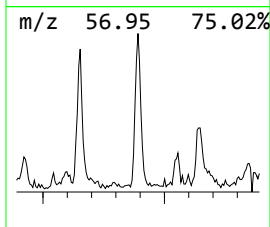
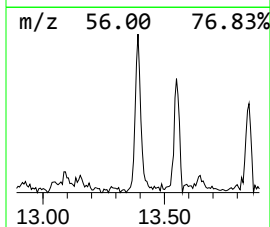
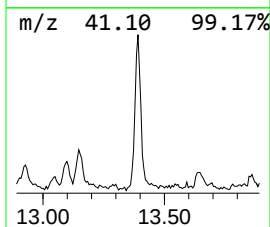
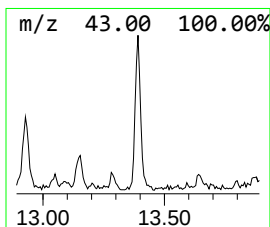
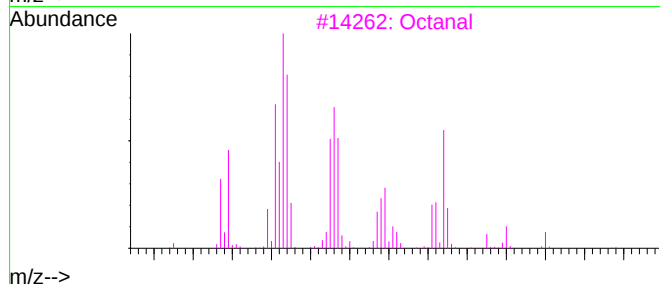
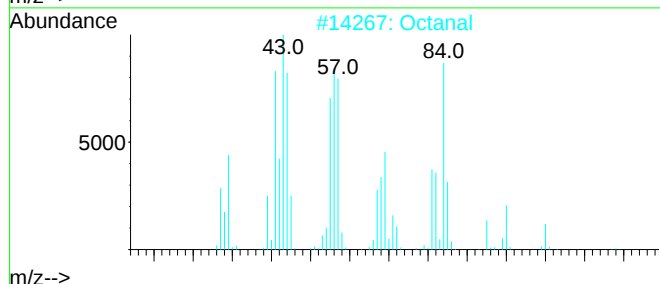
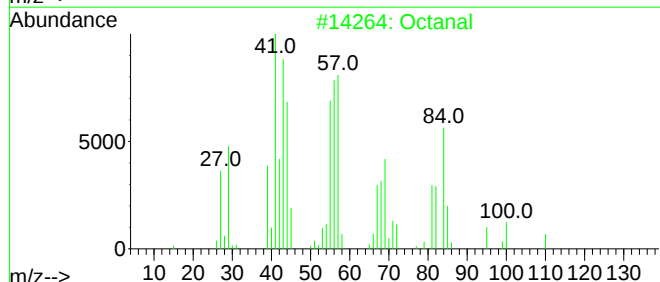
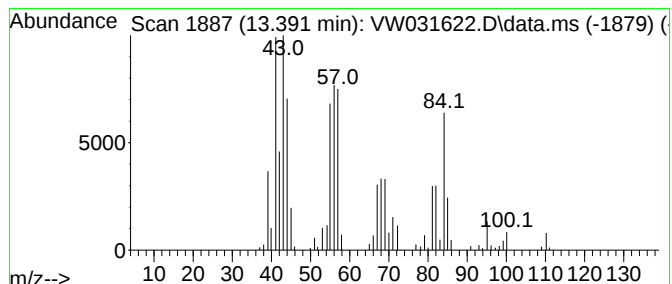
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.391	5.66 ug/L	99821	1,4-Dichlorobenzene-d4		13.550	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octanal		128	C8H16O	000124-13-0	91
2	Octanal		128	C8H16O	000124-13-0	86
3	Octanal		128	C8H16O	000124-13-0	86
4	1-Hexene		84	C6H12	000592-41-6	43
5	1-Pentene, 2-methyl-		84	C6H12	000763-29-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW012825\
Data File : VW031622.D
Acq On : 28 Jan 2025 16:41
Operator : SY/MD
Sample : Q1190-15RE
Misc : 9.45g/10mL/MSVOA_W/SOIL/B
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A44T4RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011025SMA.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
Hexanal	11.068	40.5	ug/L	2066560	2	11.629	1276570	25.0
Heptanal	12.336	2.8	ug/L	141107	2	11.629	1276570	25.0
Octanal	13.391	5.7	ug/L	99821	3	13.550	440527	25.0