

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121823\
 Data File : VD077957.D
 Acq On : 18 Dec 2023 19:41
 Operator : RP/MD
 Sample : 05808-19
 Misc : 4.03G/10ml/MSVOA_D/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 C0B15

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_D\Method\SFAMDLM112923SMA.M
 Title : SFAM01.0

Signal : TIC: VD077957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	14	27	41	rBV	891621	1347845	100.00%	15.137%
2	1.993	67	69	72	rVB2	1205	1029	0.08%	0.012%
3	2.069	76	82	83	rBV	3767	3814	0.28%	0.043%
4	2.146	91	95	96	rBV	2805	3522	0.26%	0.040%
5	2.275	112	117	124	rBV	189000	282239	20.94%	3.170%
6	2.805	201	207	217	rVB	164787	303749	22.54%	3.411%
7	3.287	287	289	290	rBV	1762	1220	0.09%	0.014%
8	3.305	290	292	293	rVV2	2035	1059	0.08%	0.012%
9	3.375	303	304	307	rBV2	1049	997	0.07%	0.011%
10	3.634	346	348	351	rBV2	1159	1802	0.13%	0.020%
11	3.758	365	369	370	rBV3	1147	1209	0.09%	0.014%
12	3.805	375	377	379	rBV2	1127	1122	0.08%	0.013%
13	3.846	381	384	386	rBV2	1880	1595	0.12%	0.018%
14	3.922	386	397	408	rVV	129388	346091	25.68%	3.887%
15	4.022	408	414	427	rVV	12550	36941	2.74%	0.415%
16	4.181	439	441	447	rVB3	1375	2132	0.16%	0.024%
17	4.363	468	472	473	rBV2	1353	1757	0.13%	0.020%
18	4.552	498	504	505	rBV2	2556	2647	0.20%	0.030%
19	4.805	542	547	554	rVB5	4894	11034	0.82%	0.124%
20	4.857	554	556	557	rBV2	1277	1090	0.08%	0.012%
21	4.946	569	571	574	rVB2	2053	1173	0.09%	0.013%
22	4.987	577	578	583	rBV2	1096	1420	0.11%	0.016%
23	5.134	602	603	608	rVB2	2791	2594	0.19%	0.029%
24	5.234	617	620	623	rBV2	695	1060	0.08%	0.012%
25	5.405	647	649	653	rBV	1127	1329	0.10%	0.015%
26	5.534	668	671	674	rBV2	1146	1515	0.11%	0.017%
27	5.687	693	697	698	rVB3	1927	1861	0.14%	0.021%
28	5.899	731	733	737	rBV3	952	1466	0.11%	0.016%
29	6.069	759	762	765	rVB2	1311	1621	0.12%	0.018%
30	6.663	861	863	865	rBV2	1466	1191	0.09%	0.013%
31	6.757	877	879	880	rBV2	1302	1123	0.08%	0.013%
32	6.769	880	881	883	rBV2	1073	1036	0.08%	0.012%
33	6.987	908	918	925	rBV2	33283	94420	7.01%	1.060%
34	7.316	971	974	976	rBV2	1085	1125	0.08%	0.013%
35	7.446	994	996	997	rVB2	2123	1143	0.08%	0.013%
36	7.569	1006	1017	1029	rBV2	184253	479678	35.59%	5.387%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM112923SMA.M
 Title : SFAM01.0

37	7.675	1033	1035	1037	rVB3	1184	985	0.07%	0.011%
38	7.993	1087	1089	1091	rBV2	803	994	0.07%	0.011%
39	8.204	1114	1125	1139	rBV2	362392	1082411	80.31%	12.156%
40	8.351	1149	1150	1152	rBV2	2265	1313	0.10%	0.015%
41	8.469	1168	1170	1171	rBV	2196	1376	0.10%	0.015%
42	8.569	1185	1187	1189	rVV	1201	1162	0.09%	0.013%
43	8.640	1193	1199	1208	rVB2	9808	22590	1.68%	0.254%
44	8.781	1213	1223	1235	rBV	329853	691214	51.28%	7.763%
45	8.904	1242	1244	1246	rBV	1314	1731	0.13%	0.019%
46	9.210	1287	1296	1306	rVV2	243124	515015	38.21%	5.784%
47	9.346	1314	1319	1326	rVB3	15407	29006	2.15%	0.326%
48	9.481	1339	1342	1344	rBV2	1496	1608	0.12%	0.018%
49	9.504	1344	1346	1349	rVB3	1279	1302	0.10%	0.015%
50	9.545	1351	1353	1358	rVV4	1233	2043	0.15%	0.023%
51	9.681	1374	1376	1380	rVB	870	1006	0.07%	0.011%
52	9.740	1385	1386	1390	rVV2	1320	1319	0.10%	0.015%
53	9.981	1419	1427	1439	rVB2	136545	252264	18.72%	2.833%
54	10.269	1466	1476	1487	rBV	431291	785680	58.29%	8.823%
55	10.528	1512	1520	1527	rBV	82815	152986	11.35%	1.718%
56	10.663	1535	1543	1551	rBV2	92119	175901	13.05%	1.975%
57	10.875	1573	1579	1587	rVV	137097	244959	18.17%	2.751%
58	10.951	1591	1592	1595	rBV3	1722	1827	0.14%	0.021%
59	10.975	1595	1596	1597	rVV	2115	1291	0.10%	0.014%
60	11.022	1598	1604	1612	rVV2	88432	154105	11.43%	1.731%
61	11.104	1616	1618	1620	rVB2	1685	1383	0.10%	0.016%
62	11.404	1665	1669	1671	rVV2	1523	1590	0.12%	0.018%
63	11.528	1688	1690	1692	rBV2	1972	2048	0.15%	0.023%
64	11.581	1692	1699	1708	rBV	386336	648063	48.08%	7.278%
65	11.675	1713	1715	1717	rVV	1844	1728	0.13%	0.019%
66	11.722	1720	1723	1727	rBV3	1207	1352	0.10%	0.015%
67	11.792	1730	1735	1742	rVB6	6354	12895	0.96%	0.145%
68	11.845	1742	1744	1746	rBV2	1460	1265	0.09%	0.014%
69	11.945	1759	1761	1764	rBV2	1318	1757	0.13%	0.020%
70	11.975	1764	1766	1772	rVB5	3140	4856	0.36%	0.055%
71	12.034	1774	1776	1778	rBV	1769	1172	0.09%	0.013%
72	12.116	1787	1790	1796	rVB5	3542	6375	0.47%	0.072%
73	12.234	1807	1810	1812	rBV2	953	1326	0.10%	0.015%
74	12.298	1817	1821	1827	rVB5	7339	13785	1.02%	0.155%
75	12.581	1861	1869	1875	rBV	86777	142851	10.60%	1.604%
76	12.651	1875	1881	1889	rVV	170717	282764	20.98%	3.176%

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77	12.745	1893	1897	1899	rBV2	1939	1808	0.13%	0.020%
78	12.945	1928	1931	1933	rBV2	1021	1231	0.09%	0.014%
79	13.069	1950	1952	1954	rVB2	1528	1231	0.09%	0.014%
80	13.116	1956	1960	1966	rVV4	6821	11487	0.85%	0.129%
81	13.181	1966	1971	1975	rVB	4612	7986	0.59%	0.090%
82	13.363	1997	2002	2008	rBV5	8915	15544	1.15%	0.175%
83	13.469	2018	2020	2022	rBV	1261	1010	0.07%	0.011%
84	13.516	2022	2028	2036	rVV	184862	309795	22.98%	3.479%
85	13.722	2061	2063	2067	rBV3	1204	1175	0.09%	0.013%
86	13.816	2072	2079	2088	rBV	160664	273599	20.30%	3.073%
87	13.928	2096	2098	2104	rBV5	1518	2066	0.15%	0.023%
88	14.051	2113	2119	2125	rBV	36971	54972	4.08%	0.617%
89	14.292	2157	2160	2167	rVB4	5461	8092	0.60%	0.091%
90	14.586	2208	2210	2212	rBV2	996	1159	0.09%	0.013%
91	15.098	2294	2297	2299	rBV3	1262	1360	0.10%	0.015%
92	15.216	2315	2317	2319	rBV2	1447	1012	0.08%	0.011%
93	15.345	2335	2339	2341	rBV3	1789	2577	0.19%	0.029%
94	15.475	2358	2361	2362	rBV2	4361	4155	0.31%	0.047%
95	16.186	2480	2482	2485	rVB2	1709	1320	0.10%	0.015%
96	16.522	2537	2539	2540	rVB	2270	1076	0.08%	0.012%
97	16.539	2540	2542	2545	rVV	1297	1128	0.08%	0.013%
98	16.586	2548	2550	2552	rVB2	1652	1253	0.09%	0.014%
99	16.686	2565	2567	2571	rBV2	1495	2131	0.16%	0.024%
100	16.722	2571	2573	2575	rVV2	1960	1305	0.10%	0.015%

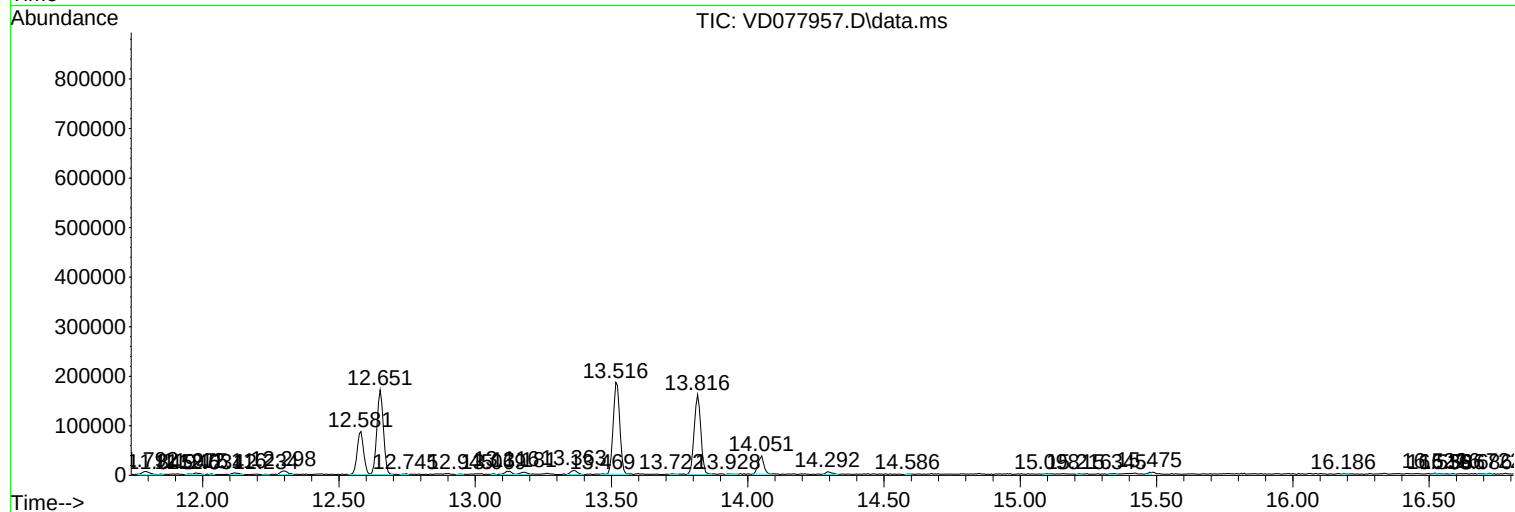
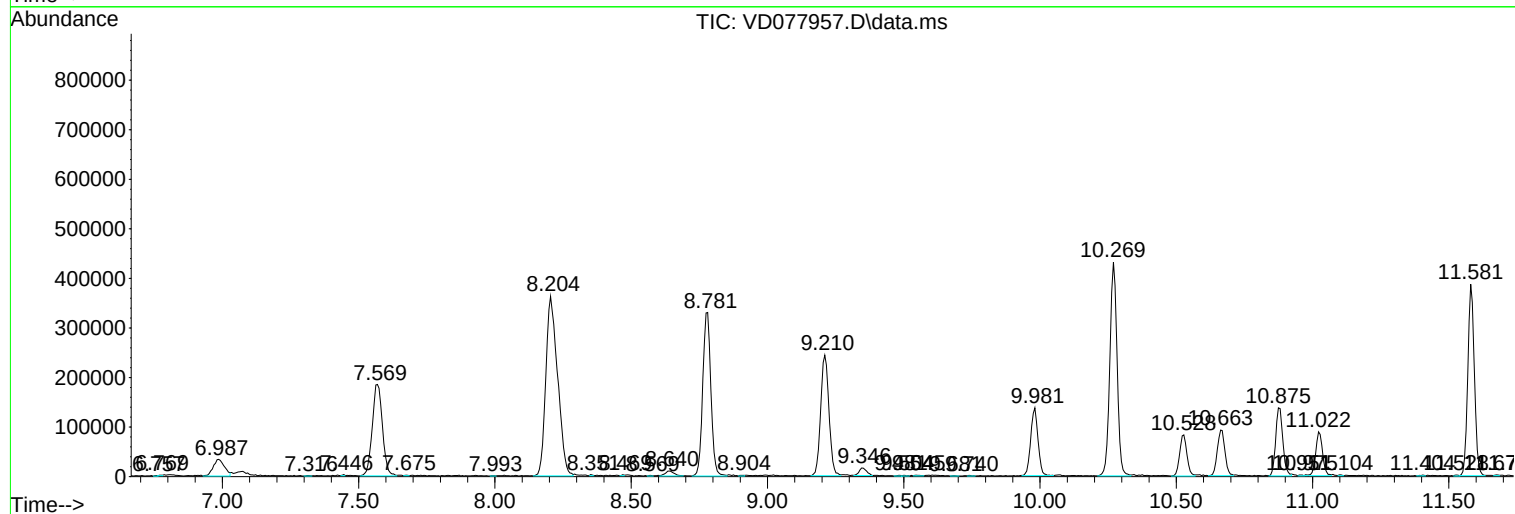
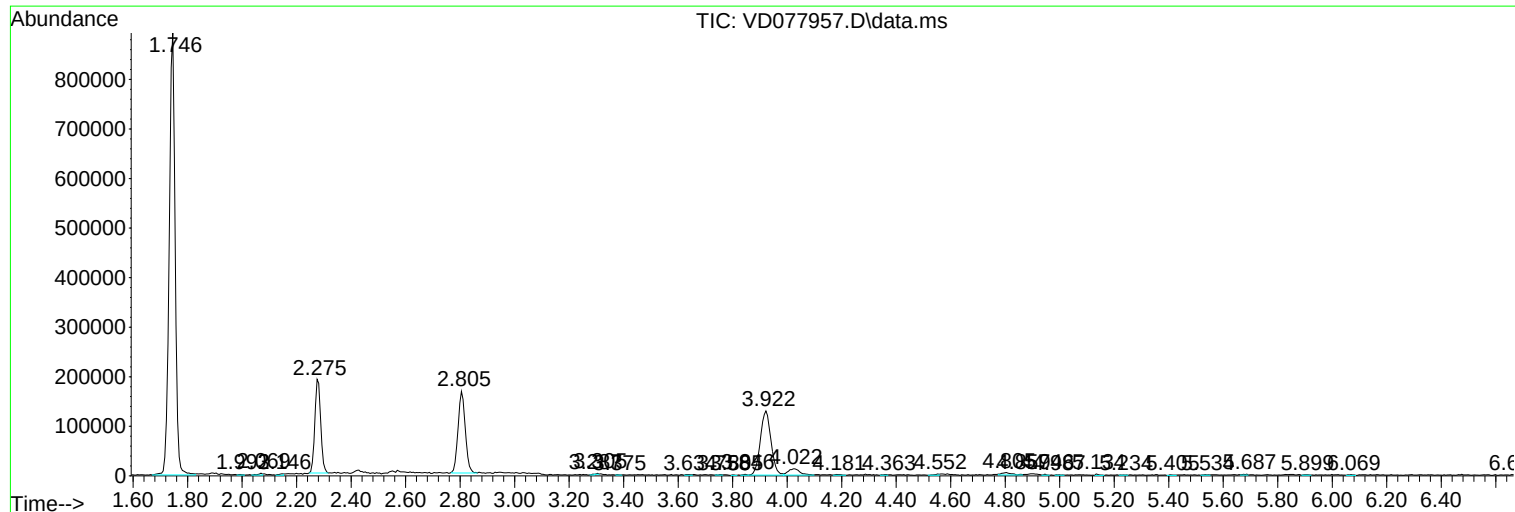
Sum of corrected areas: 8904419

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM112923SMA.M
Quant Title : SFAM01.0

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



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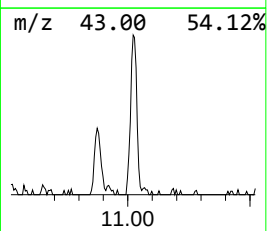
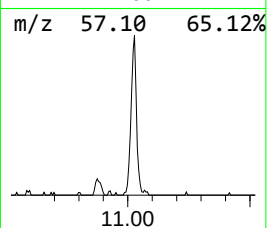
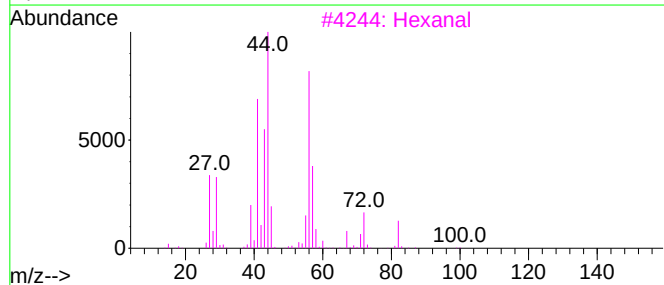
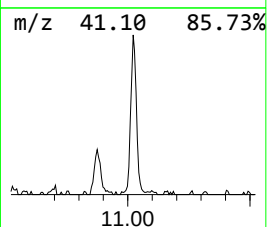
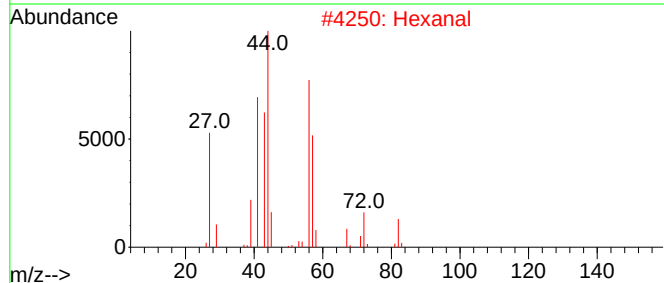
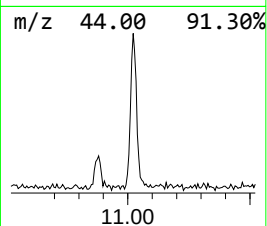
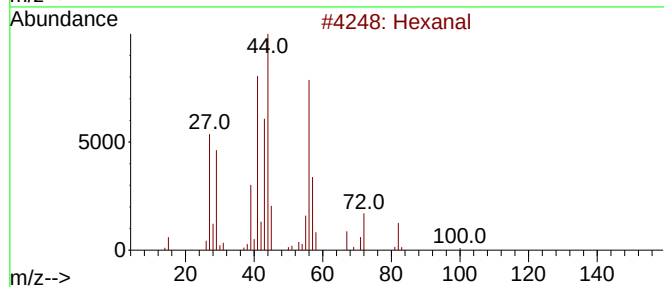
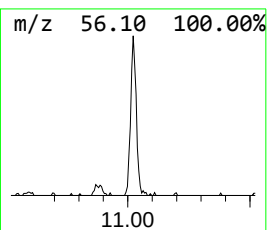
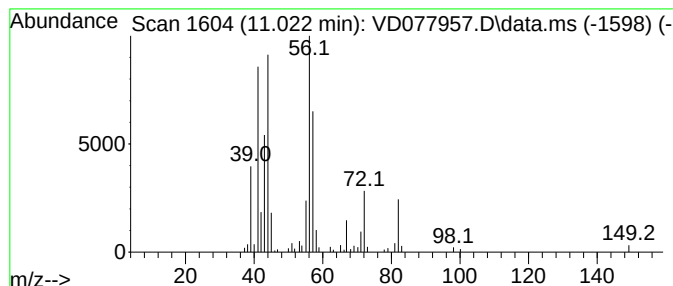
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM112923SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.022	5.94 ug/L	154105	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	87
2	Hexanal			100	C6H12O	000066-25-1	80
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	64



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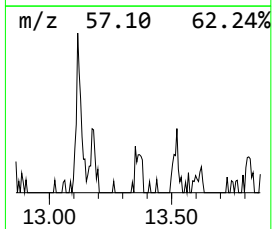
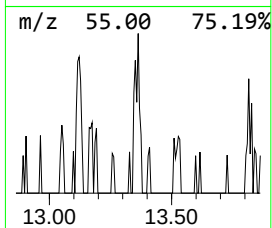
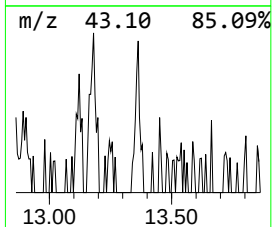
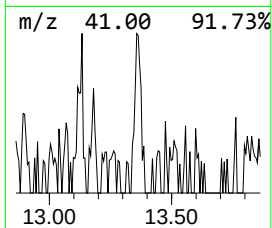
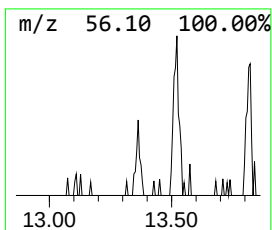
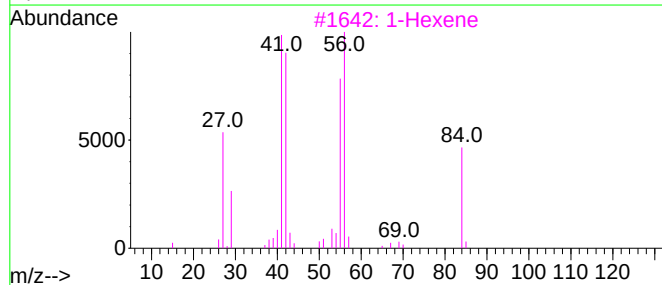
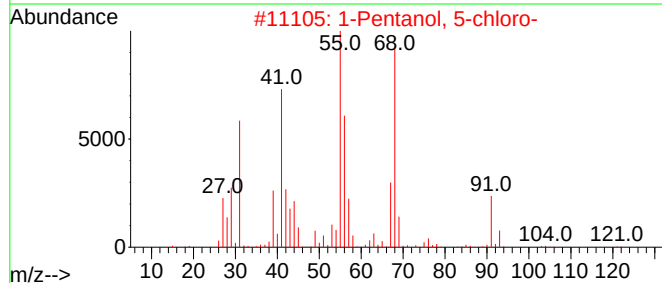
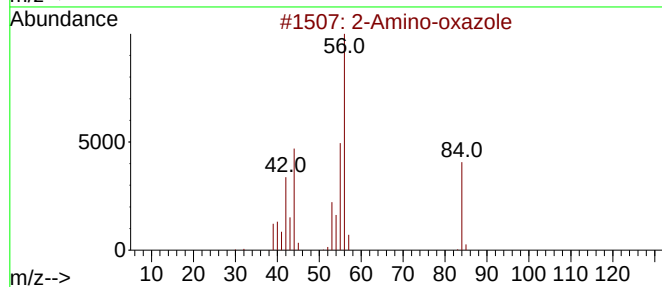
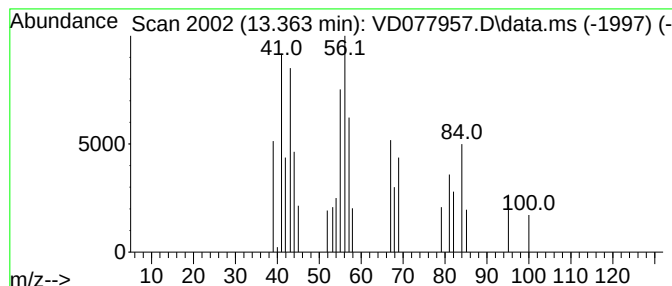
Instrument :
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ClientSampleId :
COB15

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Quant Title : SFAM01.0

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

Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.363	1.25 ug/L	15544	1,4-Dichlorobenzene-d4		13.516	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Amino-oxazole		84	C3H4N2O	004570-45-0	38
2	1-Pentanol, 5-chloro-		122	C5H11ClO	005259-98-3	32
3	1-Hexene		84	C6H12	000592-41-6	30
4	Cyanic acid, propyl ester		85	C4H7NO	001768-36-1	27
5	1-Octanol		130	C8H18O	000111-87-5	27



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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	11.022	5.9	ug/L	154105	2	11.581	648063	25.0
unknown-01	13.363	1.3	ug/L	15544	3	13.516	309795	25.0