

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD091824\
 Data File : VD079864.D
 Acq On : 18 Sep 2024 15:17
 Operator : RP/MD
 Sample : P4083-13
 Misc : 5.32G/10ml/MSVOA_D/SOIL/A
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 A4EL3

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\SFAMDLM091024SMA.M

Title : SFAM01.0

Signal : TIC: VD079864.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	13	27	44	rBV	2734487	4227807	100.00%	51.068%
2	1.893	49	52	55	rVB2	8493	10594	0.25%	0.128%
3	2.022	73	74	79	rVB2	1199	995	0.02%	0.012%
4	2.081	79	84	86	rBV3	1170	2030	0.05%	0.025%
5	2.105	86	88	91	rBV2	2142	2721	0.06%	0.033%
6	2.152	94	96	97	rBV2	1805	1646	0.04%	0.020%
7	2.169	97	99	101	rVB	1787	1195	0.03%	0.014%
8	2.275	110	117	127	rBV	151771	229115	5.42%	2.768%
9	2.493	152	154	156	rBV2	1730	1976	0.05%	0.024%
10	2.540	159	162	163	rBV	3436	4001	0.09%	0.048%
11	2.758	197	199	200	rVB	2046	1021	0.02%	0.012%
12	2.805	200	207	214	rBV	109972	209229	4.95%	2.527%
13	2.993	237	239	242	rVB2	1284	1220	0.03%	0.015%
14	3.028	242	245	247	rBV	1771	1997	0.05%	0.024%
15	3.069	250	252	253	rBV2	1660	880	0.02%	0.011%
16	3.246	280	282	285	rBV	569	695	0.02%	0.008%
17	3.311	289	293	299	rVB3	2010	3199	0.08%	0.039%
18	3.381	304	305	309	rVB	1166	904	0.02%	0.011%
19	3.422	309	312	314	rBV2	717	935	0.02%	0.011%
20	3.916	386	396	406	rBV	85149	227393	5.38%	2.747%
21	4.022	406	414	426	rVB2	11170	32997	0.78%	0.399%
22	4.246	449	452	453	rBV2	1051	818	0.02%	0.010%
23	4.269	453	456	458	rVV2	1789	1624	0.04%	0.020%
24	4.740	535	536	539	rVV2	837	786	0.02%	0.009%
25	4.769	539	541	542	rVV	1187	934	0.02%	0.011%
26	4.805	542	547	554	rVV4	3774	9092	0.22%	0.110%
27	4.899	561	563	564	rVV	998	868	0.02%	0.010%
28	4.987	574	578	581	rBV	579	681	0.02%	0.008%
29	5.216	615	617	620	rVB2	1008	688	0.02%	0.008%
30	5.428	649	653	654	rVB	1124	1003	0.02%	0.012%
31	5.446	654	656	659	rBV2	715	901	0.02%	0.011%
32	5.840	721	723	725	rBV	865	635	0.02%	0.008%
33	6.228	785	789	793	rBV2	492	877	0.02%	0.011%
34	6.987	910	918	927	rVV2	12303	33757	0.80%	0.408%
35	7.075	929	933	936	rBV5	3285	5346	0.13%	0.065%
36	7.316	972	974	978	rVV	567	720	0.02%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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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\SFAMDLM091024SMA.M
 Title : SFAM01.0

37	7.440	993	995	998	rVB	1061	642	0.02%	0.008%
38	7.569	1007	1017	1031	rVV2	105980	271402	6.42%	3.278%
39	7.704	1038	1040	1042	rVB	1039	673	0.02%	0.008%
40	7.746	1045	1047	1050	rVB	774	729	0.02%	0.009%
41	7.969	1081	1085	1087	rVB2	551	727	0.02%	0.009%
42	8.063	1097	1101	1104	rBV	872	1589	0.04%	0.019%
43	8.204	1115	1125	1139	rVV2	203438	604879	14.31%	7.306%
44	8.298	1139	1141	1142	rVV	1063	659	0.02%	0.008%
45	8.457	1166	1168	1169	rBV	829	660	0.02%	0.008%
46	8.569	1185	1187	1188	rBV	1083	746	0.02%	0.009%
47	8.646	1198	1200	1204	rVB2	1245	1325	0.03%	0.016%
48	8.693	1204	1208	1210	rBV2	593	702	0.02%	0.008%
49	8.781	1212	1223	1232	rVV	215576	446333	10.56%	5.391%
50	8.846	1232	1234	1238	rVB3	1119	1391	0.03%	0.017%
51	8.875	1238	1239	1243	rBV	668	648	0.02%	0.008%
52	8.916	1244	1246	1249	rVB2	906	734	0.02%	0.009%
53	8.951	1249	1252	1253	rBV	1069	815	0.02%	0.010%
54	9.016	1261	1263	1265	rVB	1385	879	0.02%	0.011%
55	9.046	1265	1268	1269	rBV	874	751	0.02%	0.009%
56	9.210	1286	1296	1306	rBV2	133111	289325	6.84%	3.495%
57	9.281	1306	1308	1310	rVV2	853	905	0.02%	0.011%
58	9.393	1325	1327	1328	rVV	1002	662	0.02%	0.008%
59	9.428	1330	1333	1334	rVB	1053	769	0.02%	0.009%
60	9.469	1338	1340	1342	rVB	1248	1042	0.02%	0.013%
61	9.493	1342	1344	1347	rBV2	1070	1274	0.03%	0.015%
62	9.575	1356	1358	1359	rBV	1017	722	0.02%	0.009%
63	9.598	1359	1362	1363	rVB	1247	1160	0.03%	0.014%
64	9.616	1363	1365	1366	rVB	1398	834	0.02%	0.010%
65	9.628	1366	1367	1371	rBV3	1299	1824	0.04%	0.022%
66	9.657	1371	1372	1375	rVV2	793	698	0.02%	0.008%
67	9.693	1377	1378	1382	rVV2	1205	1451	0.03%	0.018%
68	9.728	1382	1384	1385	rVB3	1213	752	0.02%	0.009%
69	9.740	1385	1386	1391	rBV2	1079	1441	0.03%	0.017%
70	9.781	1391	1393	1394	rBV2	1230	789	0.02%	0.010%
71	9.910	1413	1415	1417	rBV2	1376	1257	0.03%	0.015%
72	9.981	1417	1427	1436	rBV	66311	126154	2.98%	1.524%
73	10.075	1441	1443	1444	rVV	1506	1005	0.02%	0.012%
74	10.175	1457	1460	1461	rVB2	1545	1295	0.03%	0.016%
75	10.187	1461	1462	1465	rBV2	1313	986	0.02%	0.012%
76	10.269	1467	1476	1484	rBV	207406	376226	8.90%	4.544%

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MSVOA_D
ClientSampleId :
A4EL3

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.M
Title : SFAM01.0

77	10.328	1485	1486	1489	rVB	2637	1400	0.03%	0.017%
78	10.410	1498	1500	1501	rBV	1005	732	0.02%	0.009%
79	10.469	1509	1510	1513	rVB	1748	1314	0.03%	0.016%
80	10.522	1513	1519	1529	rBV2	41841	79186	1.87%	0.956%
81	10.587	1529	1530	1535	rVB3	2252	2689	0.06%	0.032%
82	10.622	1535	1536	1537	rBV	2078	1277	0.03%	0.015%
83	10.663	1540	1543	1546	rVV3	4101	5660	0.13%	0.068%
84	10.692	1546	1548	1549	rVB2	1423	966	0.02%	0.012%
85	10.787	1562	1564	1566	rBV2	1826	1773	0.04%	0.021%
86	10.810	1566	1568	1571	rVB3	1625	1254	0.03%	0.015%
87	10.875	1571	1579	1586	rBV	49063	92288	2.18%	1.115%
88	11.151	1622	1626	1628	rBV5	3077	4021	0.10%	0.049%
89	11.481	1680	1682	1683	rBV2	2580	1543	0.04%	0.019%
90	11.581	1691	1699	1706	rBV	201926	358654	8.48%	4.332%
91	12.069	1780	1782	1785	rBV4	4454	3852	0.09%	0.047%
92	12.398	1834	1838	1841	rBV6	6627	11100	0.26%	0.134%
93	12.645	1874	1880	1887	rBV2	56816	104503	2.47%	1.262%
94	12.734	1890	1895	1902	rVB3	35844	63367	1.50%	0.765%
95	13.516	2023	2028	2034	rVB	88763	146474	3.46%	1.769%
96	13.810	2074	2078	2087	rVB3	56669	104393	2.47%	1.261%
97	14.345	2165	2169	2172	rBV5	17390	26657	0.63%	0.322%
98	14.810	2246	2248	2254	rVB5	19722	29702	0.70%	0.359%
99	15.298	2328	2331	2338	rVB3	38936	62754	1.48%	0.758%
100	16.498	2534	2535	2537	rBV2	8330	5032	0.12%	0.061%

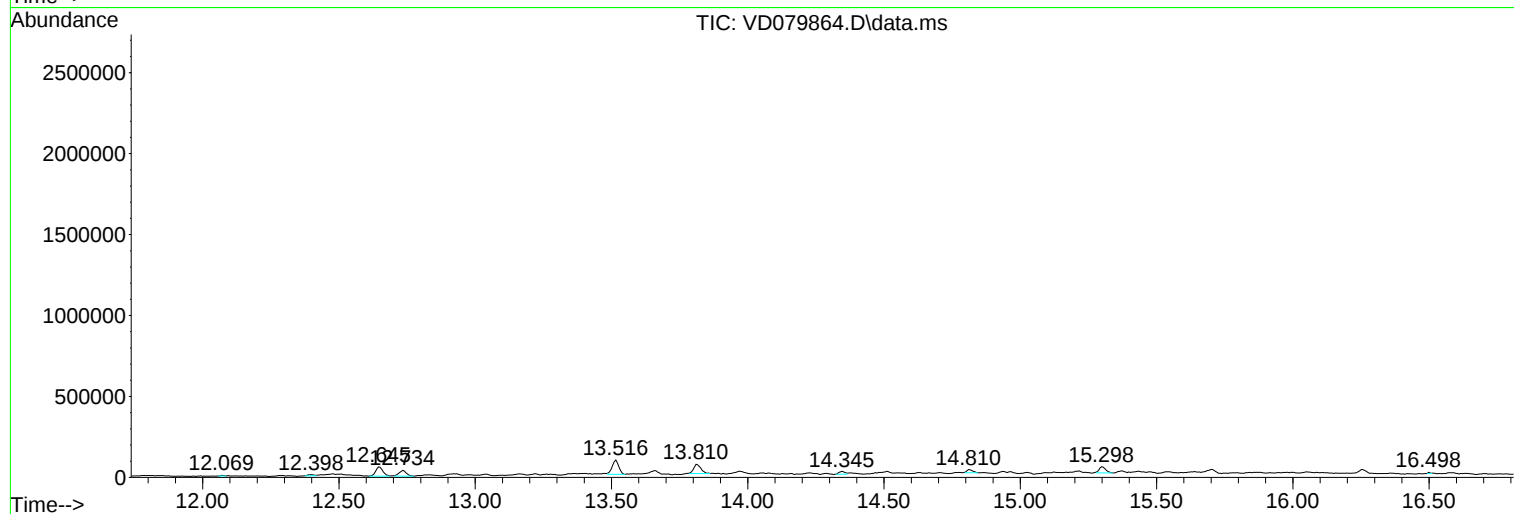
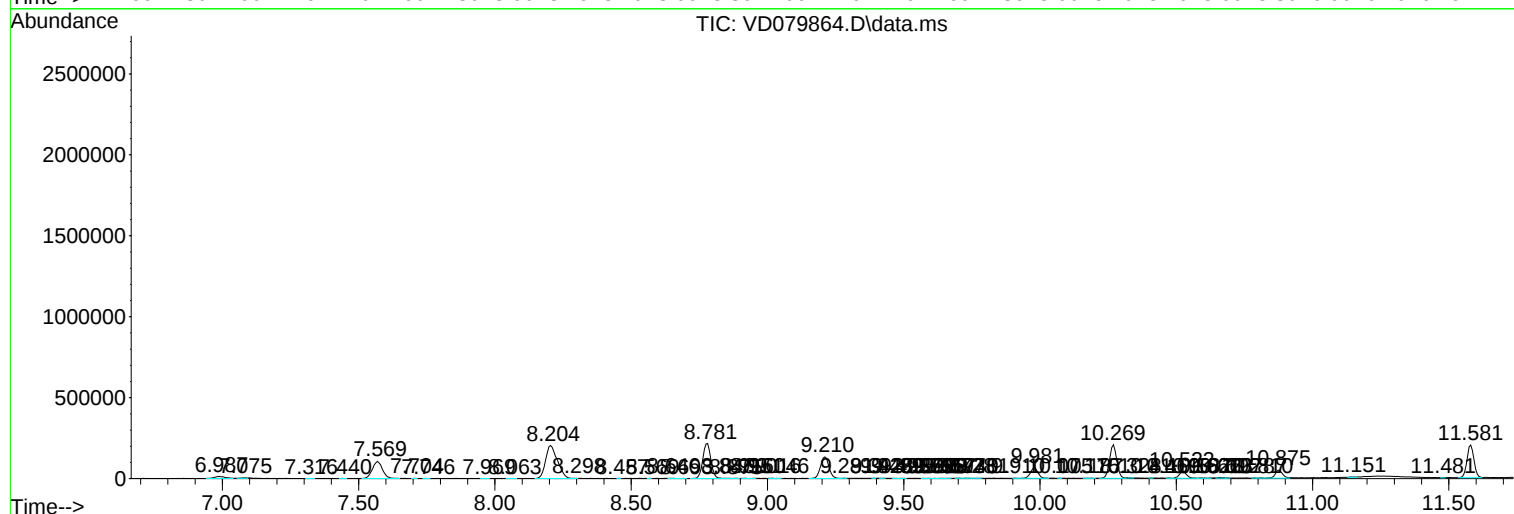
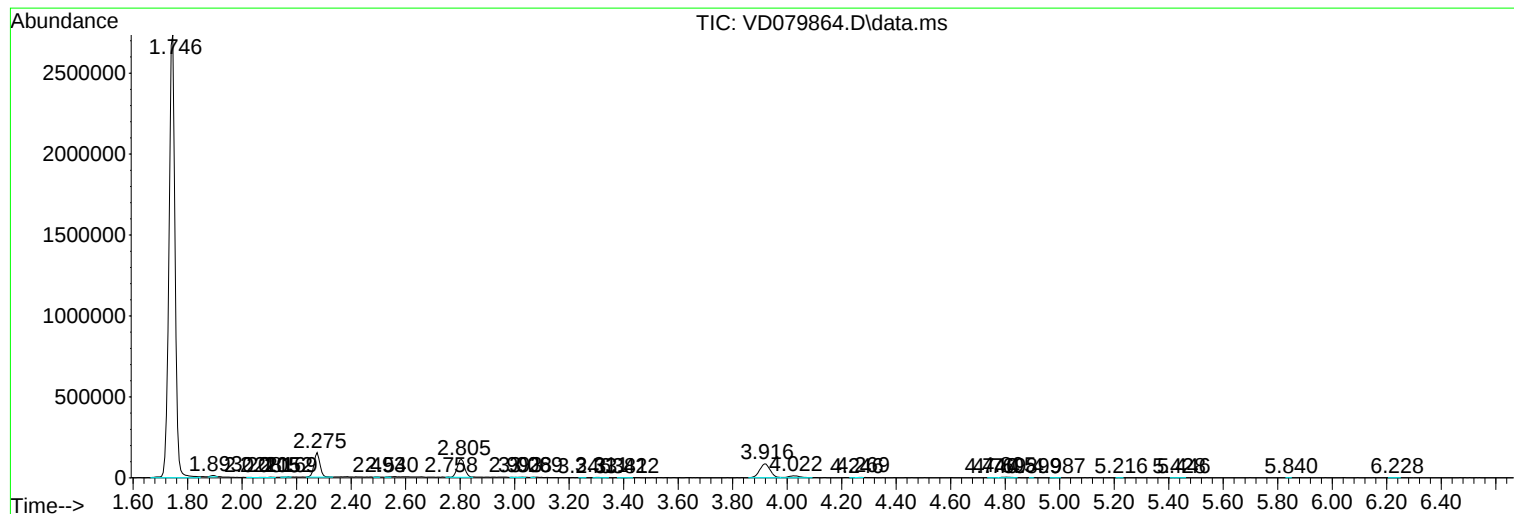
Sum of corrected areas: 8278726

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
A4EL3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.M
Quant Title : SFAM01.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD091824\
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Misc : 5.32G/10ml/MSVOA_D/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

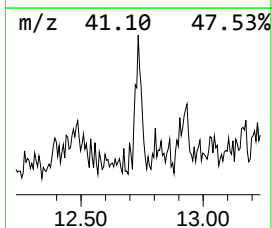
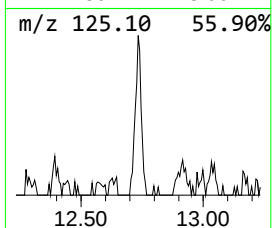
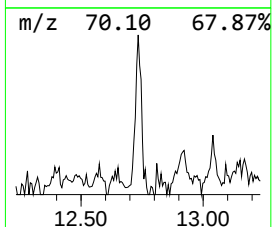
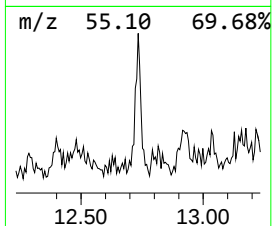
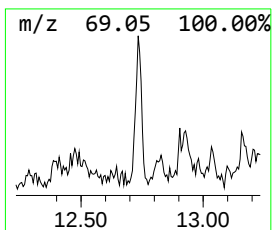
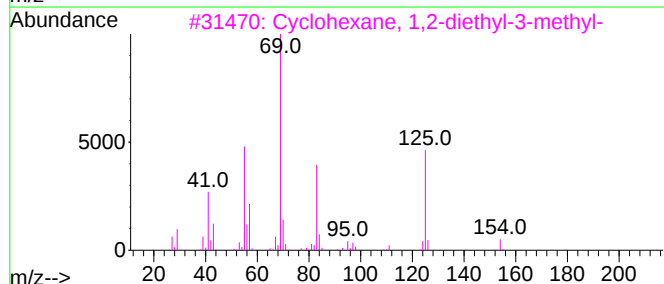
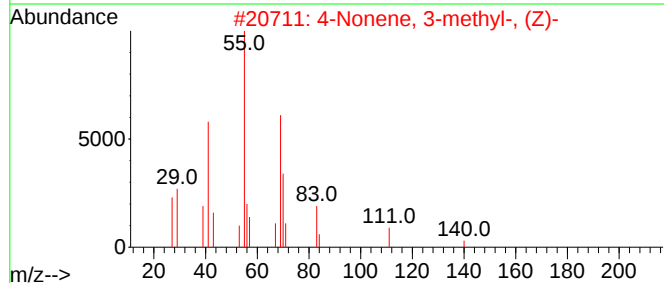
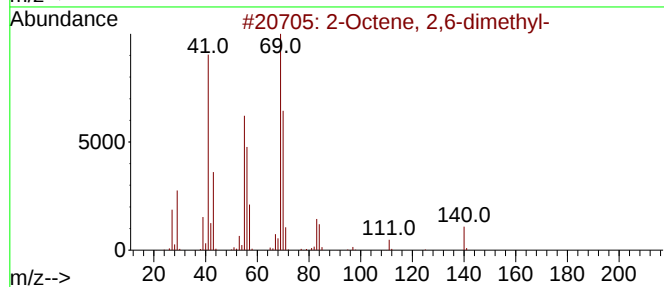
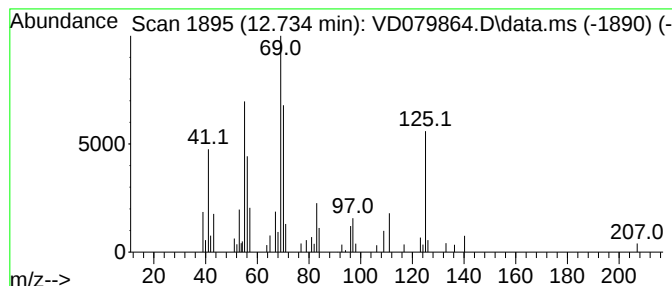
Instrument :
MSVOA_D
ClientSampleId :
A4EL3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.734	10.82 ug/L	63367	1,4-Dichlorobenzene-d4		13.516	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Octene, 2,6-dimethyl-		140	C10H20	004057-42-5	62
2	4-Nonene, 3-methyl-, (Z)-		140	C10H20	063830-69-3	52
3	Cyclohexane, 1,2-diethyl-3-methyl-		154	C11H22	061141-80-8	47
4	3-Undecene, 2-methyl-, (Z)-		168	C12H24	074630-48-1	47
5	Cyclohexane, 1,1,2,3-tetramethyl-		140	C10H20	006783-92-2	46



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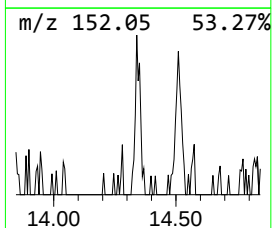
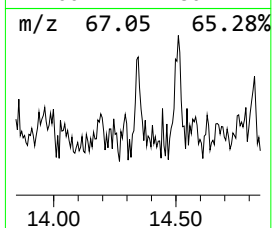
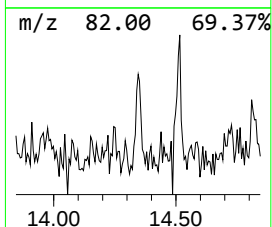
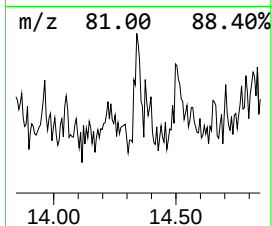
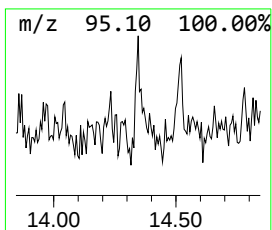
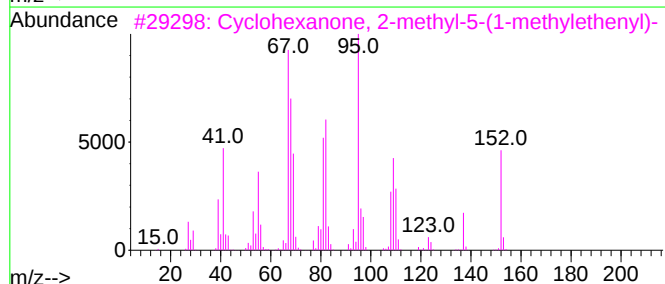
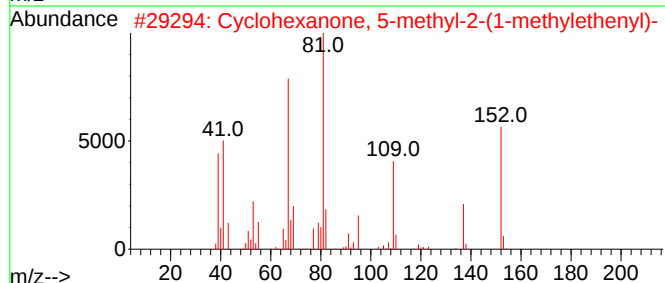
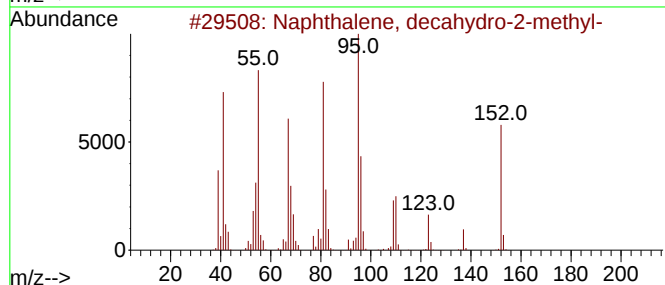
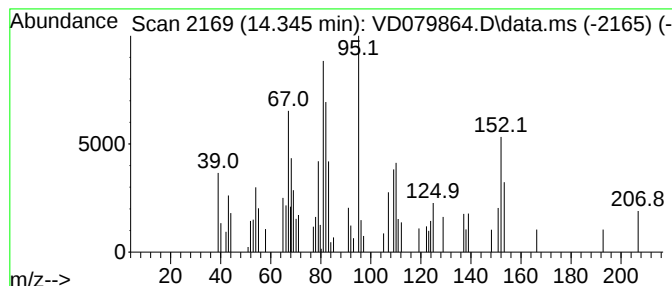
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	4.55 ug/L	26657	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	46
2			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	42
3			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	42
4			1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	41
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	38



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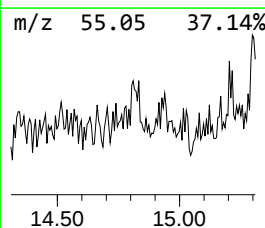
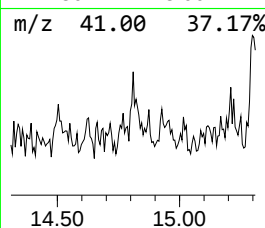
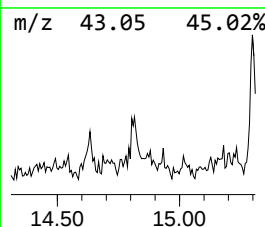
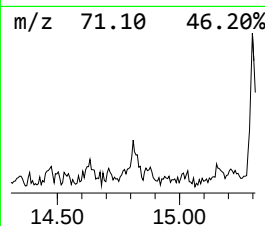
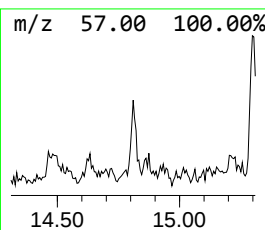
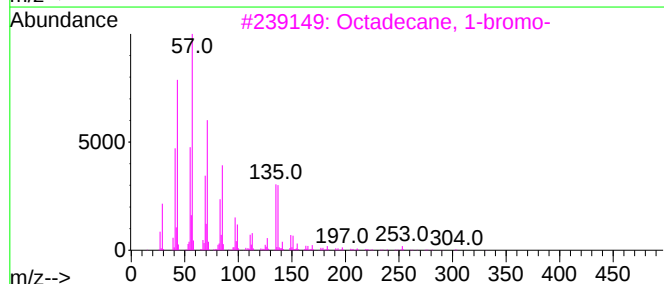
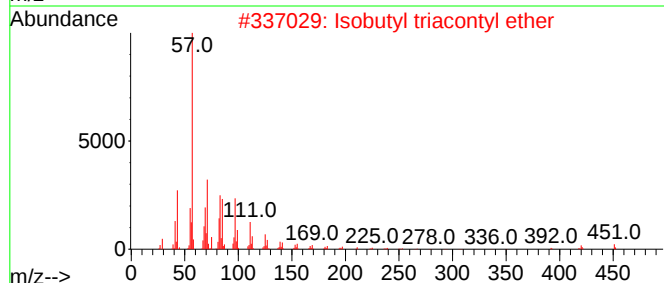
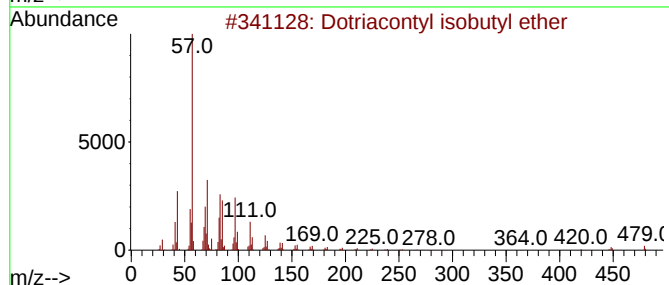
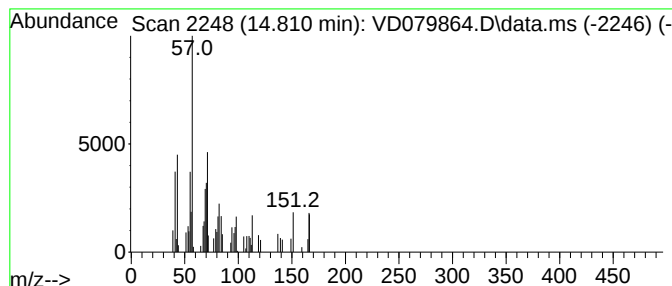
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	5.07 ug/L	29702	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontyl isobutyl ether	523	C36H74O	1010406-33-6	32
2			Isobutyl triacontyl ether	495	C34H70O	1000406-33-5	32
3			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	25
4			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	22
5			Ether, 6-methylheptyl vinyl	156	C10H20O	010573-35-0	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD091824\
Data File : VD079864.D
Acq On : 18 Sep 2024 15:17
Operator : RP/MD
Sample : P4083-13
Misc : 5.32G/10ml/MSVOA_D/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
A4EL3

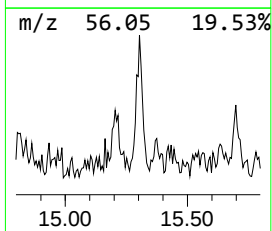
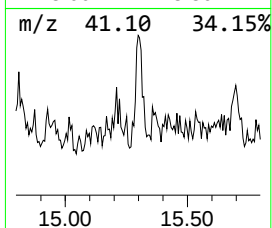
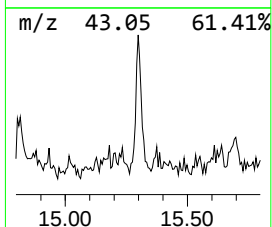
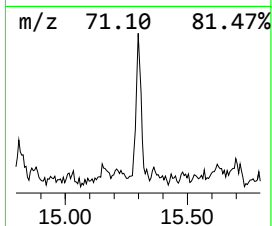
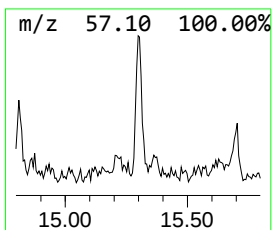
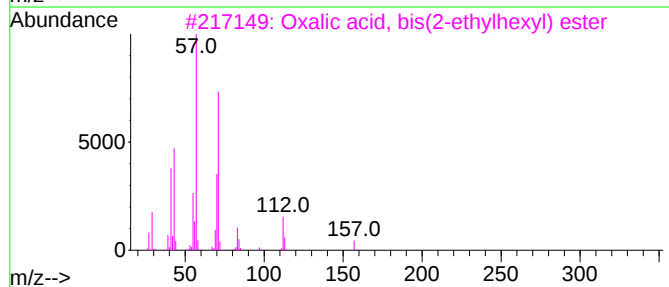
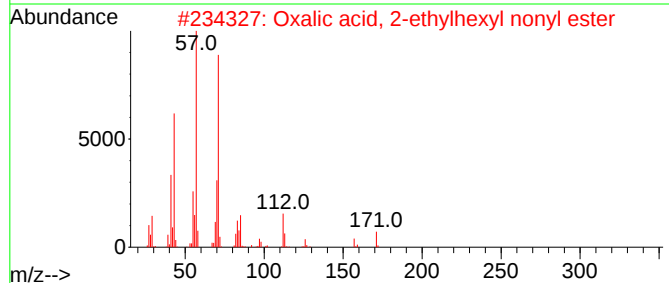
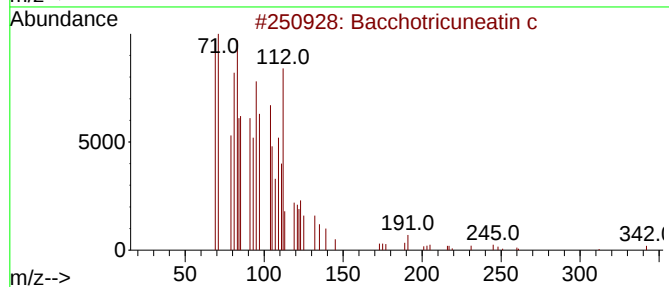
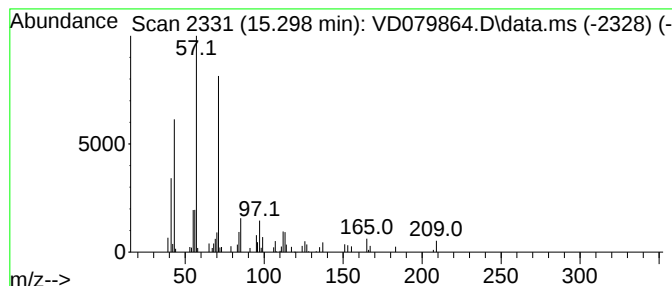
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.M
Quant Title : SFAM01.0

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

Peak Number 6 Bacchotricuneatin c Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	10.71 ug/L	62754	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bacchotricuneatin c	342	C20H22O5	066563-30-2	80
2			Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	72
3			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	64
4			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59
5			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD091824\
Data File : VD079864.D
Acq On : 18 Sep 2024 15:17
Operator : RP/MD
Sample : P4083-13
Misc : 5.32G/10ml/MSVOA_D/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
A4EL3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM091024SMA.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...	12.734	10.8	ug/L	63367	3	13.516	146474	25.0
unknown-01	14.345	4.5	ug/L	26657	3	13.516	146474	25.0
unknown-02	14.810	5.1	ug/L	29702	3	13.516	146474	25.0
Bacchotricuneat...	15.298	10.7	ug/L	62754	3	13.516	146474	25.0