

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD102021\
 Data File : VD070780.D
 Acq On : 20 Oct 2021 17:17
 Operator : VA/SY
 Sample : M4285-01
 Misc : 5.20G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 MH-EA-(1)

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82D101521S.M
 Title : SW846 8260

Signal : TIC: VD070780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.138	33	37	41	rBV4	2634	4129	1.17%	0.179%
2	2.220	46	51	54	rBV5	10981	23307	6.60%	1.012%
3	2.256	55	57	59	rVV3	4230	3865	1.09%	0.168%
4	2.308	64	66	69	rVV3	4277	4738	1.34%	0.206%
5	2.485	94	96	100	rBV5	2519	3684	1.04%	0.160%
6	2.638	117	122	127	rBV7	7408	16363	4.63%	0.710%
7	2.826	151	154	157	rBV5	6031	7473	2.11%	0.324%
8	4.973	510	519	527	rBV5	6826	20752	5.87%	0.901%
9	7.908	1010	1018	1024	rBV	50543	123795	35.03%	5.374%
10	7.973	1024	1029	1040	rVB2	85931	196062	55.49%	8.512%
11	8.326	1081	1089	1097	rBV3	68292	155027	43.87%	6.730%
12	8.861	1171	1180	1192	rVB2	120473	260071	73.60%	11.290%
13	9.132	1225	1226	1228	rVB	9950	3732	1.06%	0.162%
14	10.332	1421	1430	1438	rBV	194562	353360	100.00%	15.340%
15	11.637	1646	1652	1661	rVB	194238	335123	94.84%	14.549%
16	12.620	1813	1819	1826	rBV	133254	218650	61.88%	9.492%
17	12.931	1868	1872	1877	rVB6	5380	8151	2.31%	0.354%
18	13.261	1926	1928	1930	rVV3	3871	4063	1.15%	0.176%
19	13.561	1973	1979	1987	rVV	171465	291296	82.44%	12.646%
20	13.655	1987	1995	2002	rVV4	24645	41001	11.60%	1.780%
21	13.802	2015	2020	2022	rBV4	2422	4237	1.20%	0.184%
22	13.873	2029	2032	2034	rBV2	4090	4727	1.34%	0.205%
23	14.414	2122	2124	2127	rVB4	4177	4412	1.25%	0.192%
24	14.549	2144	2147	2154	rVB8	5810	9416	2.66%	0.409%
25	14.725	2174	2177	2179	rBV4	4512	4945	1.40%	0.215%
26	14.878	2198	2203	2210	rVB4	29286	44387	12.56%	1.927%
27	15.190	2254	2256	2257	rBV2	6797	4734	1.34%	0.206%
28	15.231	2259	2263	2268	rVB7	9628	17569	4.97%	0.763%
29	15.355	2279	2284	2287	rBV6	7988	14728	4.17%	0.639%
30	15.390	2287	2290	2295	rVB5	10766	17731	5.02%	0.770%
31	15.478	2301	2305	2307	rBV4	3792	4865	1.38%	0.211%
32	15.755	2347	2352	2357	rBV6	19353	35090	9.93%	1.523%
33	16.067	2400	2405	2409	rBV6	6698	11139	3.15%	0.484%
34	16.131	2411	2416	2418	rBV5	5843	8861	2.51%	0.385%
35	16.290	2439	2443	2445	rVB5	5547	7878	2.23%	0.342%
36	16.337	2445	2451	2458	rVB9	10404	23374	6.61%	1.015%

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ClientSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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

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37	16.408	2458	2463	2468	rVB6	3679	6706	1.90%	0.291%
38	16.702	2510	2513	2515	rBV4	2604	4047	1.15%	0.176%

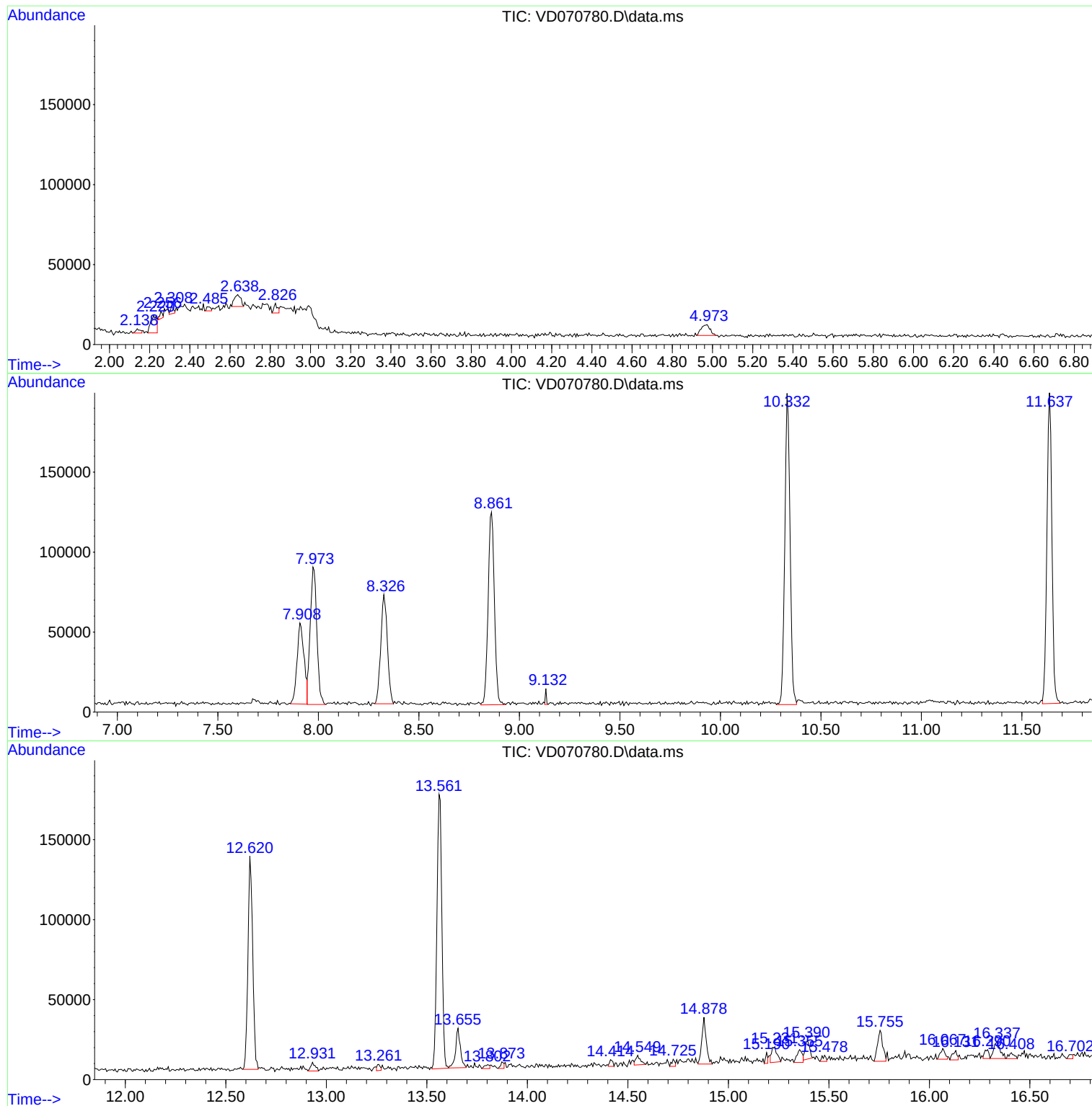
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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



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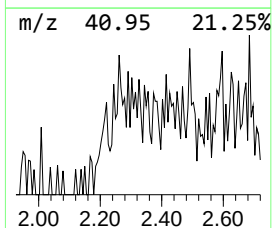
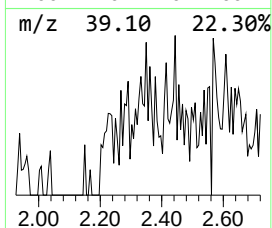
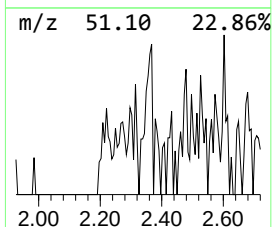
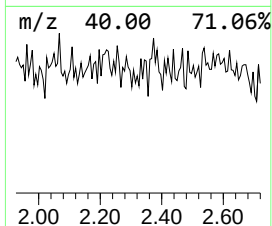
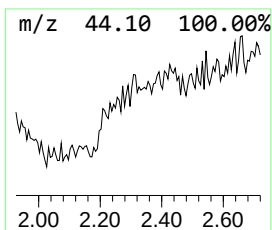
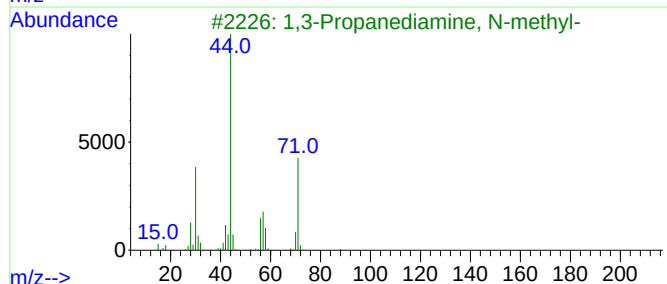
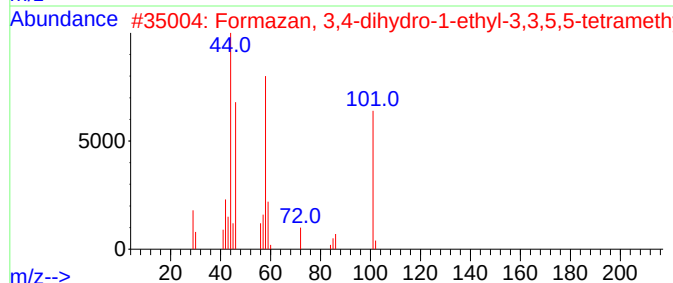
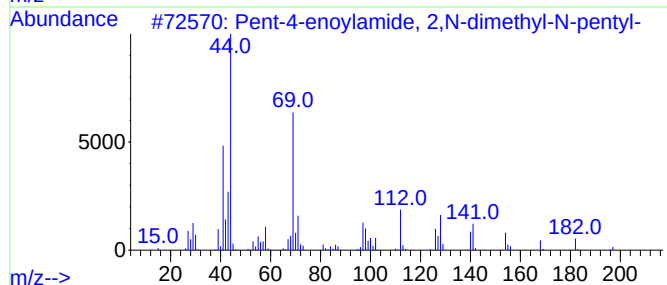
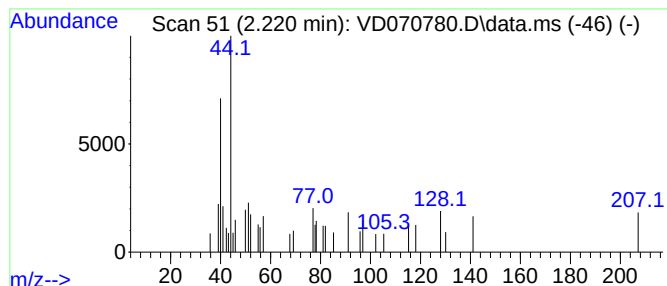
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.220 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.220	5.94 ug/l	23307	Pentafluorobenzene	7.973

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pent-4-enoylamide, 2,N-dimethyl-...	197	C12H23NO	1010437-40-0	33
2			Formazan, 3,4-dihydro-1-ethyl-3,...	158	C7H18N4	1000298-97-1	23
3			1,3-Propanediamine, N-methyl-	88	C4H12N2	006291-84-5	17
4			N-(3-Methylaminopropyl)-N-methyl...	130	C6H14N2O	1000288-73-4	9
5			MDMA methylene homolog	207	C12H17NO2	1010386-32-2	9



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Instrument :
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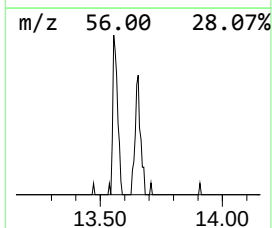
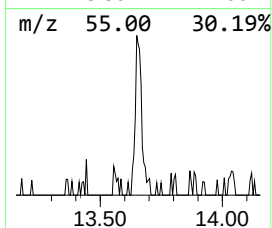
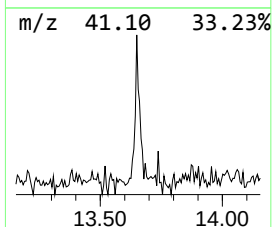
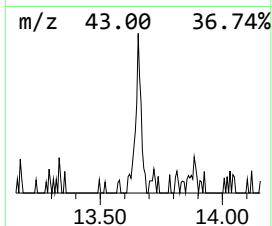
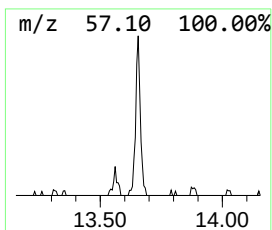
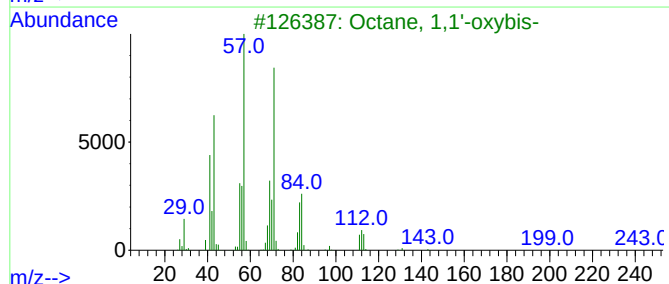
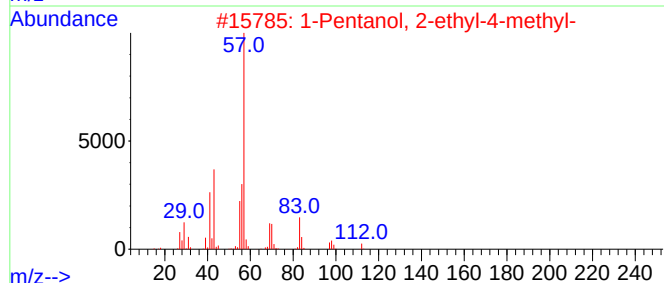
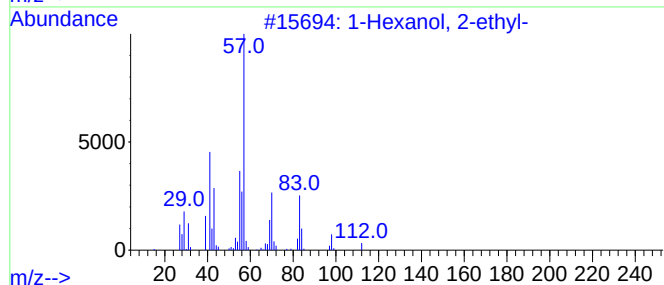
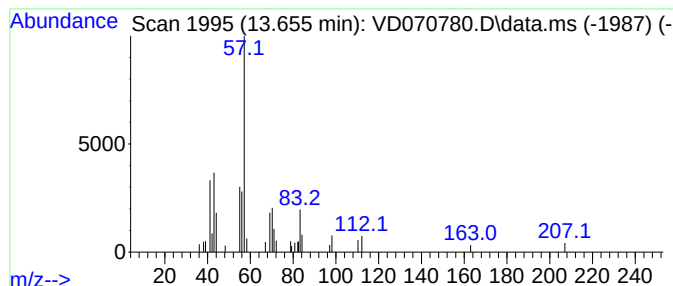
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.655	7.04 ug/l	41001	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50
4			Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



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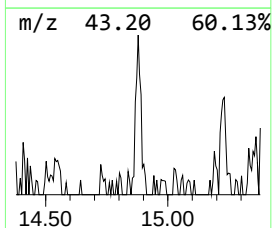
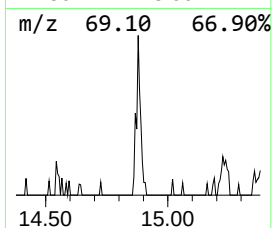
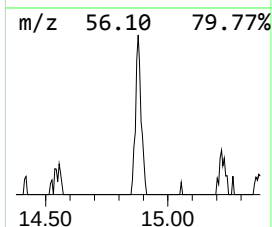
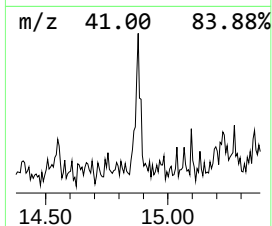
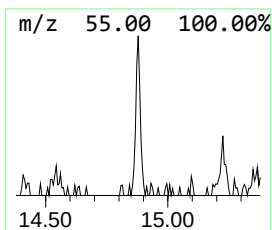
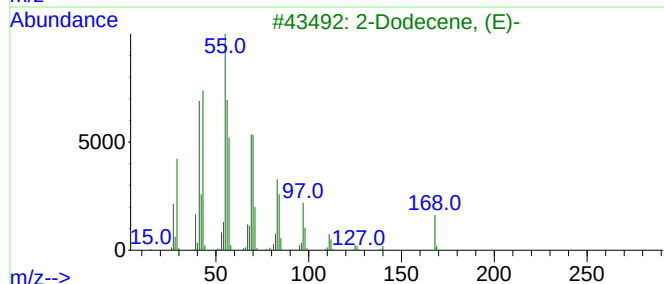
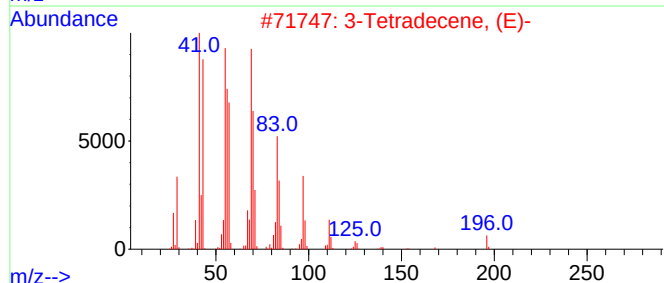
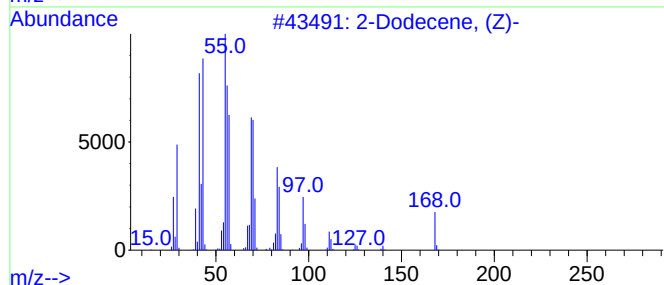
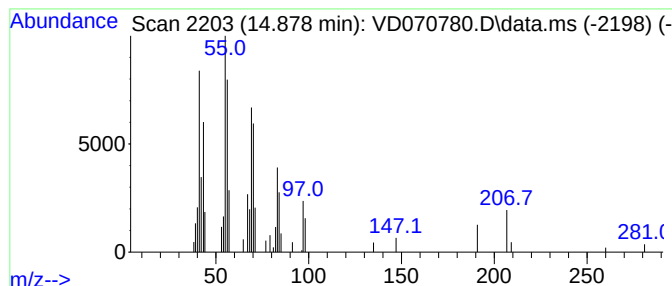
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Dodecene, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.878	7.62 ug/l	44387	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Dodecene, (Z)-	168	C12H24	007206-26-0	80
2			3-Tetradecene, (E)-	196	C14H28	041446-68-8	80
3			2-Dodecene, (E)-	168	C12H24	007206-13-5	80
4			3-Tetradecene, (Z)-	196	C14H28	041446-67-7	80
5			Acetic acid, trifluoro-, nonyl e...	240	C11H19F3O2	030767-14-7	80



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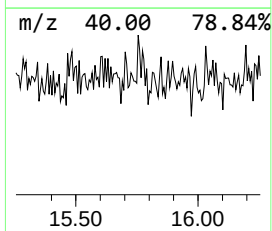
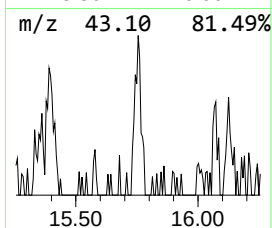
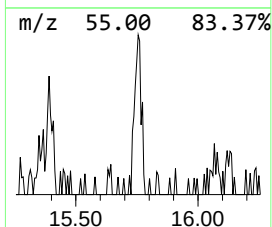
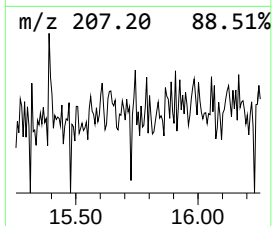
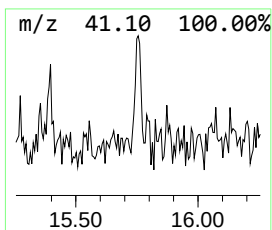
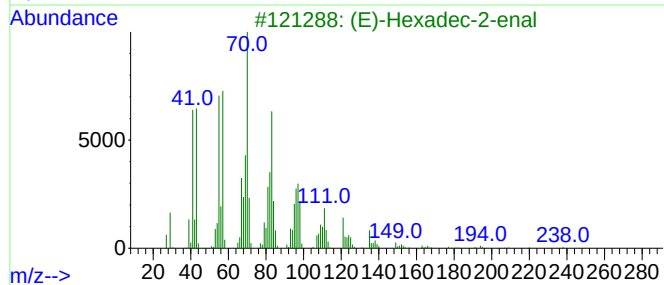
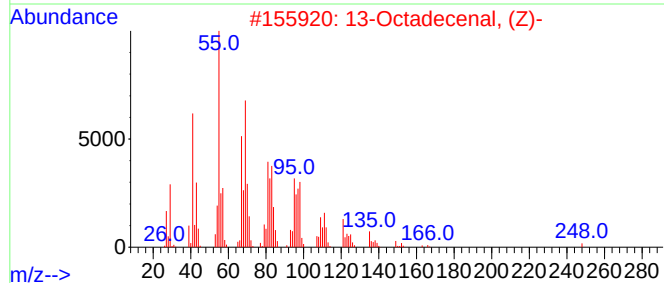
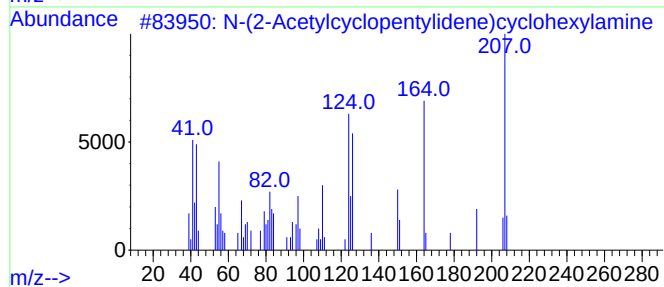
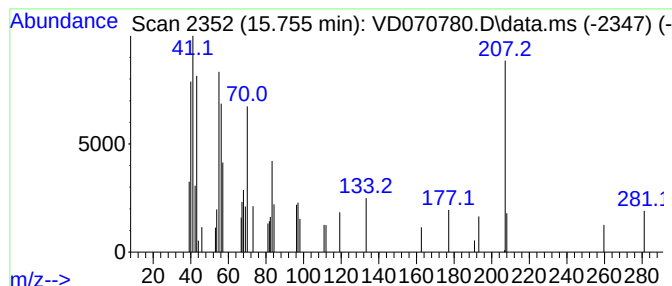
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.755 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.755	6.02 ug/l	35090	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(2-Acetylcyclopentylidene)cycl...	207	C13H21NO	1000100-48-5	43
2			13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	25
3			(E)-Hexadec-2-enal	238	C16H30O	022644-96-8	22
4			cis-Vaccenic acid	282	C18H34O2	000506-17-2	22
5			9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	22



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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
unknown2.220	2.220	5.9	ug/l	23307	1	7.973	196062	50.0
1-Hexanol, 2-et...	13.655	7.0	ug/l	41001	4	13.561	291296	50.0
2-Dodecene, (Z)-	14.878	7.6	ug/l	44387	4	13.561	291296	50.0
unknown15.755	15.755	6.0	ug/l	35090	4	13.561	291296	50.0