

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD032921\
 Data File : VD068708.D
 Acq On : 29 Mar 2021 19:53
 Operator : VA/SY
 Sample : M1828-04
 Misc : 6.96G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 FS-SB14(5-6)

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\82D031921S.M
 Title : SW846 8260

Signal : TIC: VD068708.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.144	35	38	42	rBV3	1876	3373	1.99%	0.205%
2	2.215	47	50	51	rBV2	3294	2651	1.57%	0.161%
3	2.232	51	53	56	rVV3	3549	4616	2.73%	0.281%
4	2.268	57	59	62	rVB4	3684	3643	2.15%	0.222%
5	2.320	65	68	72	rBV6	2837	4263	2.52%	0.259%
6	2.356	72	74	75	rBV2	2318	2077	1.23%	0.126%
7	2.632	117	121	127	rVB5	6136	11773	6.96%	0.716%
8	2.691	128	131	140	rVB5	7563	16606	9.82%	1.010%
9	2.779	140	146	148	rBV3	2413	4156	2.46%	0.253%
10	4.156	377	380	382	rBV2	2084	2400	1.42%	0.146%
11	4.326	408	409	414	rVB2	1460	2141	1.27%	0.130%
12	7.167	888	892	893	rBV3	2132	2867	1.69%	0.174%
13	7.367	920	926	927	rBV3	2233	3546	2.10%	0.216%
14	7.520	948	952	953	rBV3	1983	2140	1.27%	0.130%
15	7.550	953	957	959	rVB5	2754	3675	2.17%	0.224%
16	7.573	959	961	964	rBV3	3620	4660	2.75%	0.283%
17	7.767	992	994	997	rVB3	2350	2436	1.44%	0.148%
18	7.803	997	1000	1001	rBV3	3210	3852	2.28%	0.234%
19	7.914	1013	1019	1024	rBV2	15400	33400	19.75%	2.031%
20	7.985	1024	1031	1040	rVV3	30766	74515	44.05%	4.532%
21	8.067	1043	1045	1048	rVB4	3203	3456	2.04%	0.210%
22	8.255	1073	1077	1078	rBV4	3616	3577	2.11%	0.218%
23	8.338	1084	1091	1099	rVB2	25894	54356	32.13%	3.306%
24	8.432	1104	1107	1108	rBV3	3398	3756	2.22%	0.228%
25	8.497	1117	1118	1120	rVB2	3836	2091	1.24%	0.127%
26	8.597	1133	1135	1137	rBV3	4963	3902	2.31%	0.237%
27	8.820	1171	1173	1174	rBV2	4179	2627	1.55%	0.160%
28	8.867	1174	1181	1189	rBV	57600	121316	71.72%	7.378%
29	8.973	1197	1199	1200	rBV2	3848	3092	1.83%	0.188%
30	9.020	1205	1207	1208	rBV2	4628	2351	1.39%	0.143%
31	9.120	1222	1224	1225	rBV2	5082	3396	2.01%	0.207%
32	10.344	1426	1432	1437	rBV	80232	145758	86.17%	8.865%
33	11.643	1649	1653	1659	rVB	79874	126875	75.00%	7.716%
34	12.626	1817	1820	1825	rVB	72287	116133	68.65%	7.063%
35	13.402	1950	1952	1953	rBV2	16587	9846	5.82%	0.599%
36	13.573	1976	1981	1987	rBV	103310	169156	100.00%	10.288%

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37	13.820	2018	2023	2034	rVB6	49566	140243	82.91%	8.529%
38	14.396	2117	2121	2126	rBV7	9126	19585	11.58%	1.191%
39	14.502	2137	2139	2140	rBV2	4269	3308	1.96%	0.201%
40	14.679	2167	2169	2171	rBV3	4062	4053	2.40%	0.246%
41	14.743	2176	2180	2185	rVV7	9308	18272	10.80%	1.111%
42	14.820	2190	2193	2196	rVV5	8874	15243	9.01%	0.927%
43	14.867	2196	2201	2205	rVB7	21341	39560	23.39%	2.406%
44	14.949	2212	2215	2217	rBV4	4814	4965	2.94%	0.302%
45	15.237	2260	2264	2267	rBV6	6327	9309	5.50%	0.566%
46	15.290	2268	2273	2279	rVB8	14317	29828	17.63%	1.814%
47	15.355	2279	2284	2290	rBV3	28138	48577	28.72%	2.954%
48	15.420	2292	2295	2296	rBV3	7732	8245	4.87%	0.501%
49	15.590	2319	2324	2332	rVB3	30017	52018	30.75%	3.164%
50	15.661	2334	2336	2338	rBV3	5481	5565	3.29%	0.338%
51	15.767	2350	2354	2362	rVB10	13096	25676	15.18%	1.562%
52	15.908	2373	2378	2380	rBV6	4343	7310	4.32%	0.445%
53	16.137	2413	2417	2421	rBV6	10860	17123	10.12%	1.041%
54	16.184	2422	2425	2427	rBV4	8637	10941	6.47%	0.665%
55	16.267	2435	2439	2444	rVB7	16266	27473	16.24%	1.671%
56	16.337	2446	2451	2458	rVB4	35304	67335	39.81%	4.095%
57	16.508	2478	2480	2481	rBV2	4440	3513	2.08%	0.214%
58	16.549	2481	2487	2492	rVV3	54246	104823	61.97%	6.375%
59	16.667	2501	2507	2509	rBV6	11672	20777	12.28%	1.264%

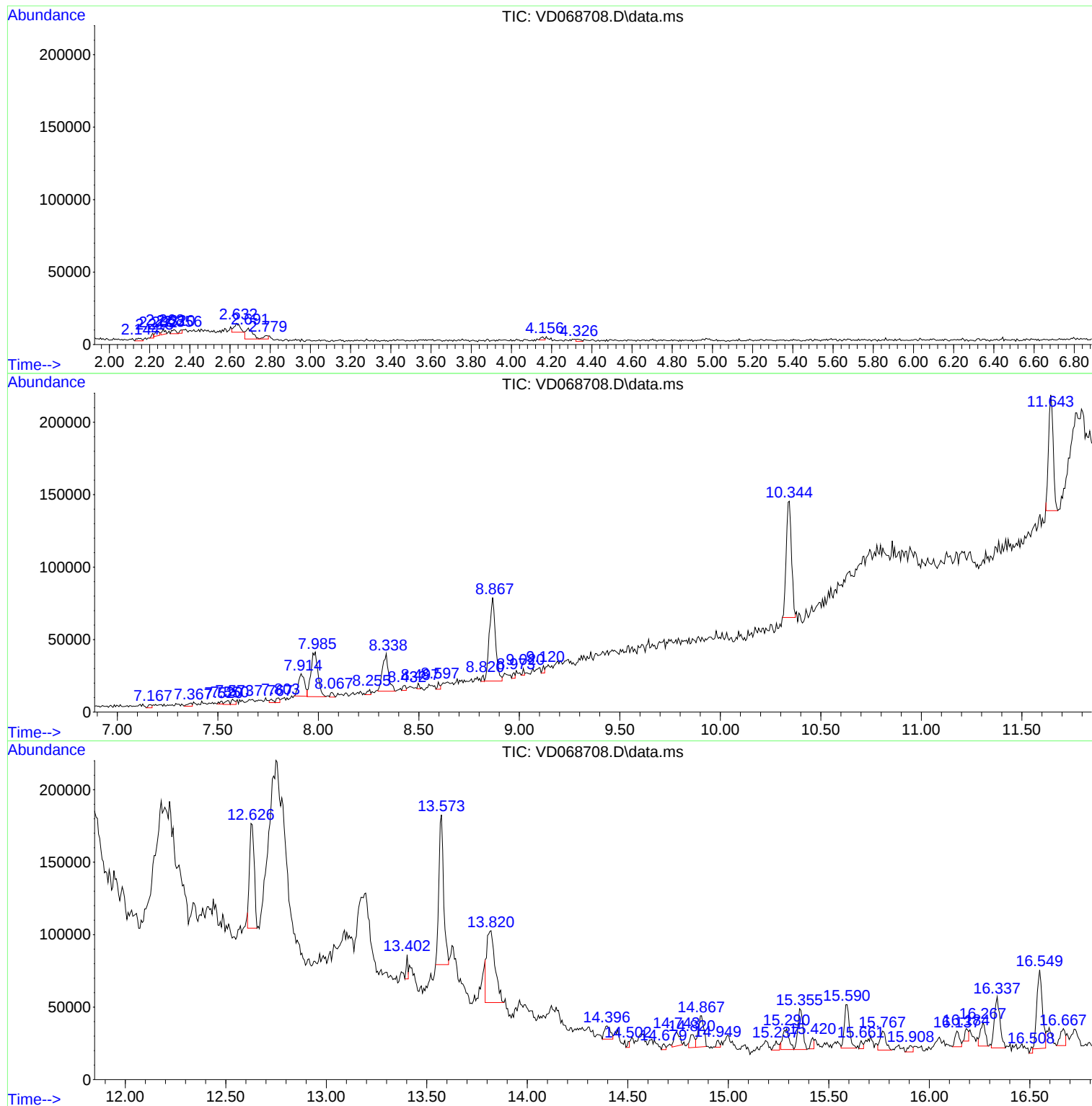
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :
FS-SB14(5-6)

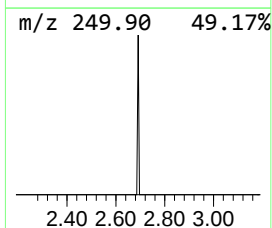
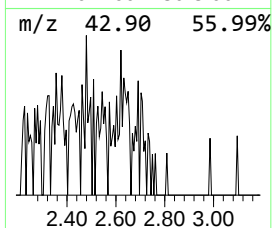
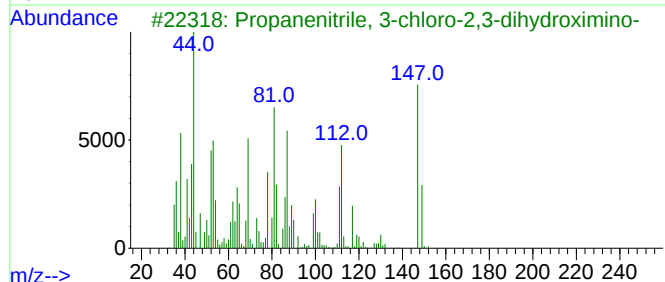
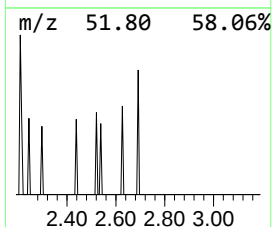
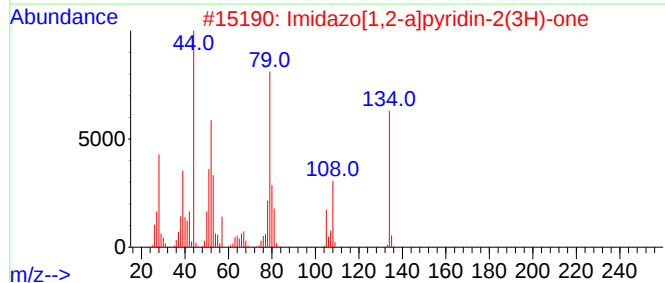
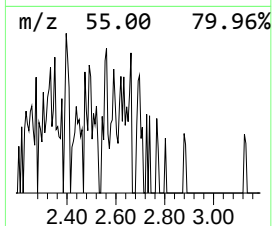
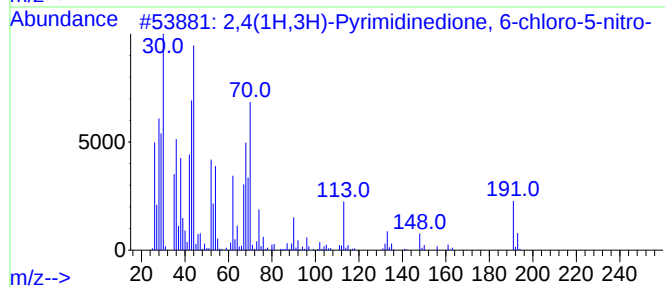
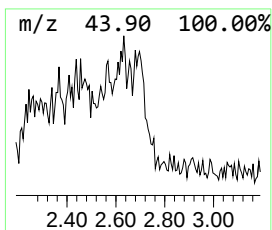
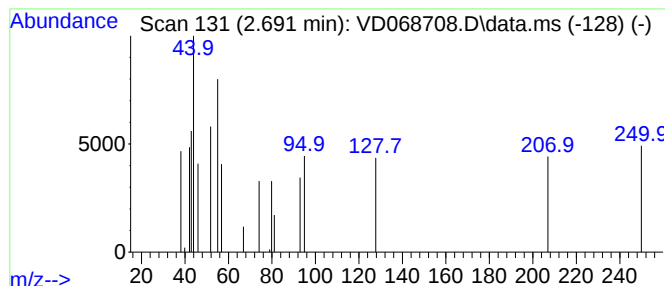
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031921S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.691 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.691	11.14 ug/l	16606	Pentafluorobenzene	7.985

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4(1H,3H)-Pyrimidinedione, 6-ch...	191	C4H2ClN3O4	006630-30-4	40		
2	Imidazo[1,2-a]pyridin-2(3H)-one	134	C7H6N2O	003999-06-2	12		
3	Propanenitrile, 3-chloro-2,3-dih...	147	C3H2ClN3O2	139912-33-7	9		
4	3-Pentanone, dimethylhydrazone	128	C7H16N2	016795-73-6	5		
5	3-(Ethyl-hydrazono)-butan-2-one	128	C6H12N2O	1000194-94-0	5		



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Instrument :
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ClientSampleId :
FS-SB14(5-6)

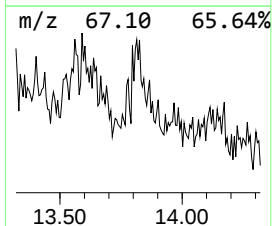
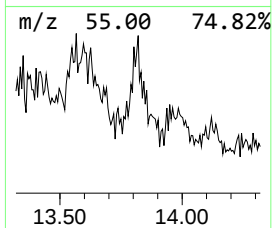
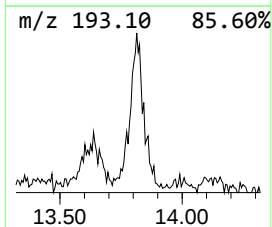
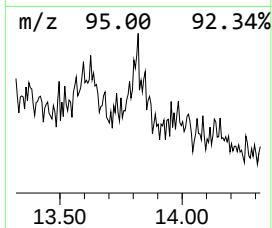
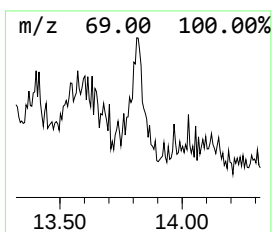
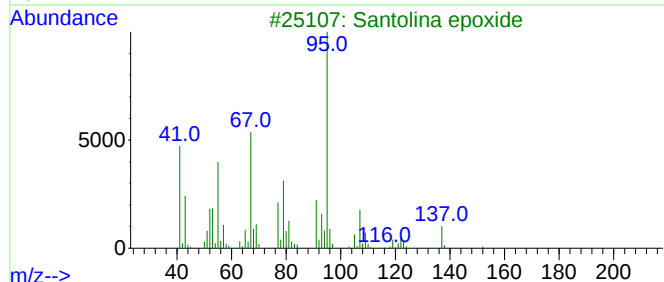
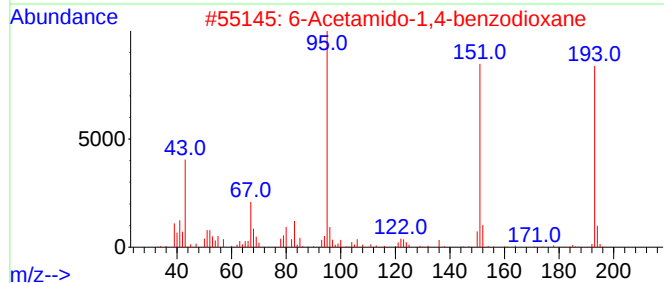
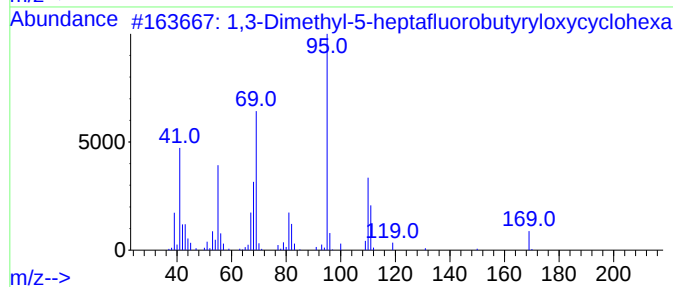
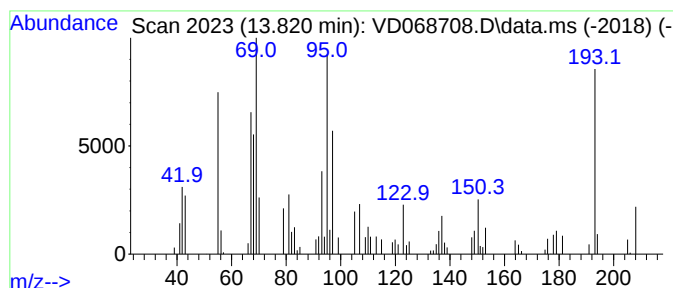
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031921S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.820 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.820	41.45 ug/l	140243	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-5-heptafluorobutyry...	324	C12H15F7O2	1000216-63-8	27
2			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	27
3			Santolina epoxide	152	C10H16O	060485-45-2	15
4			Bornyl acetate	196	C12H20O2	000076-49-3	14
5			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	196	C12H20O2	005655-61-8	14



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Instrument :
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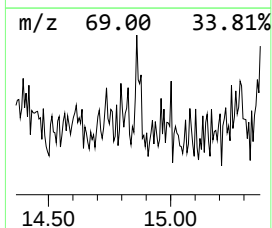
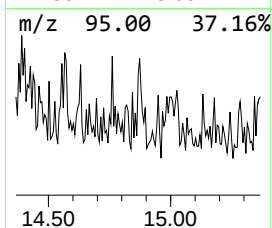
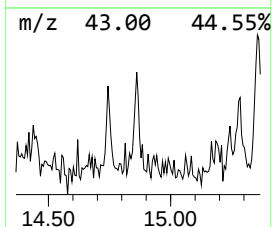
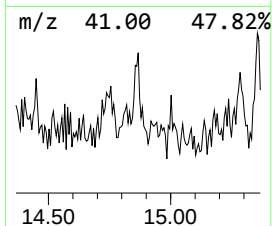
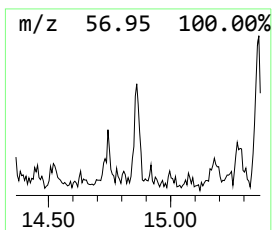
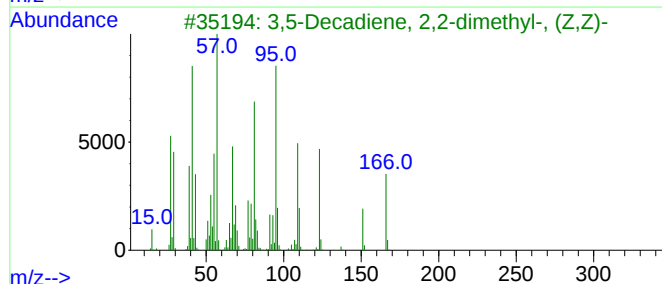
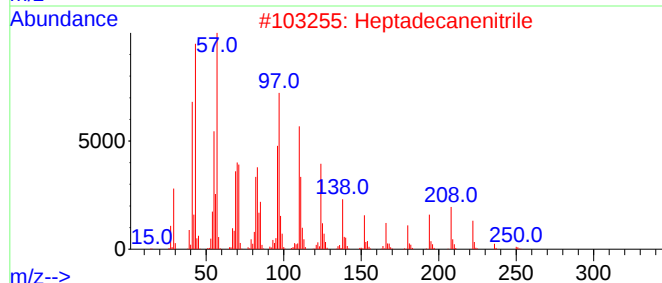
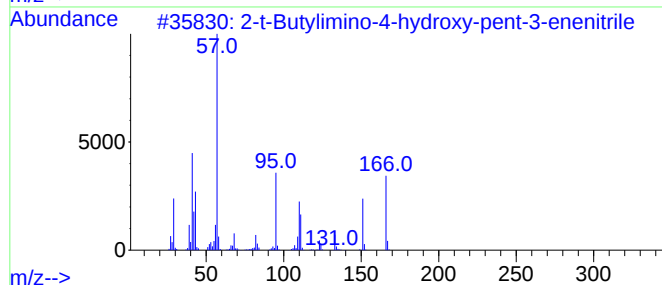
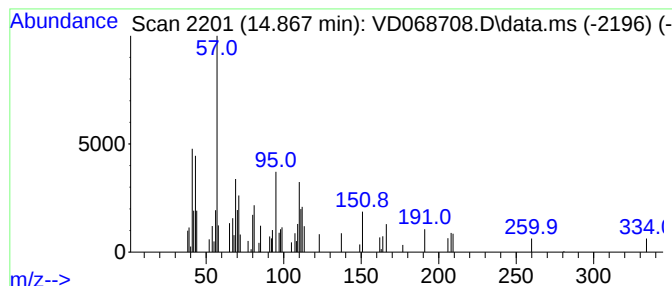
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031921S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.867 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.867	11.69 ug/l	39560	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-t-Butylimino-4-hydroxy-pent-3-enitrile	166	C9H14N2O	1000186-22-1	43		
2	Heptadecanenitrile	251	C17H33N	005399-02-0	25		
3	3,5-Decadiene, 2,2-dimethyl-, (Z,Z)-	166	C12H22	055638-50-1	10		
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	9		
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	9		



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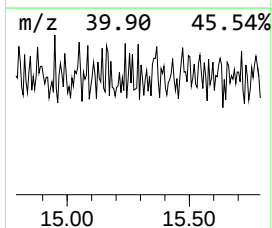
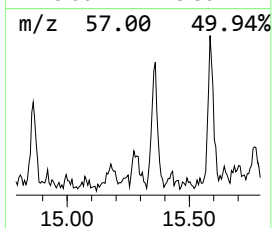
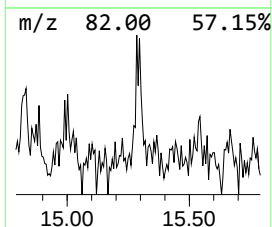
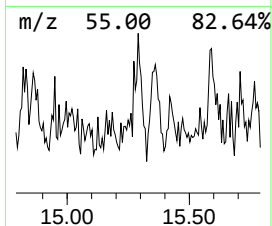
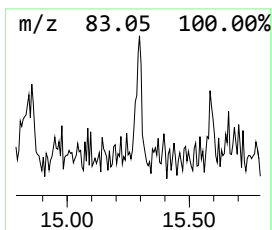
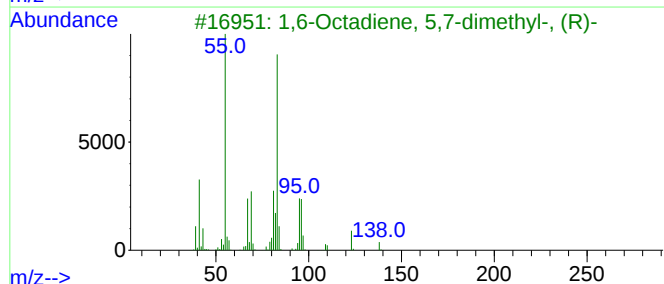
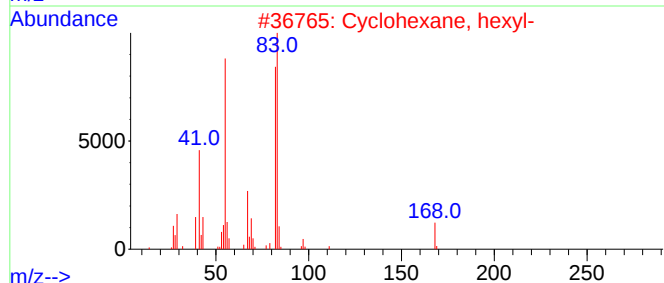
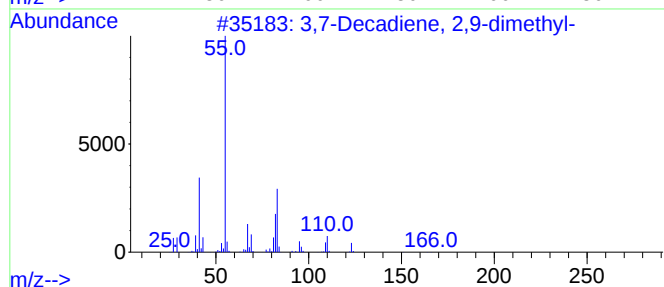
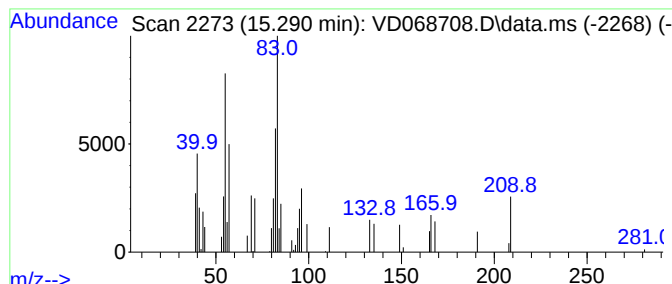
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031921S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3,7-Decadiene, 2,9-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.290	8.82 ug/l	29828	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,7-Decadiene, 2,9-dimethyl-	166	C12H22	074630-13-0	47
2			Cyclohexane, hexyl-	168	C12H24	004292-75-5	43
3			1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	43
4			Sulfurous acid, dicyclohexyl ester	246	C12H22O3S	006214-17-1	38
5			4-Methylthiomorpholine-1,1-dioxide	149	C5H11NO2S	025343-91-3	38



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FS-SB14(5-6)

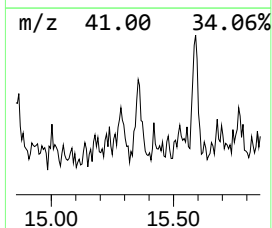
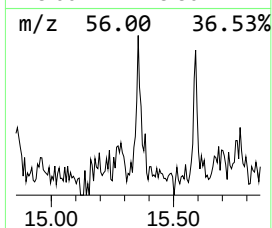
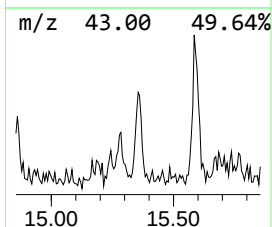
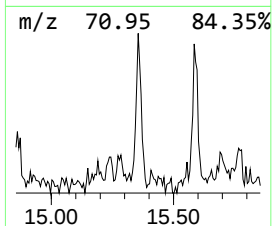
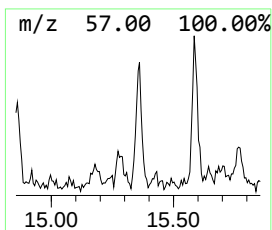
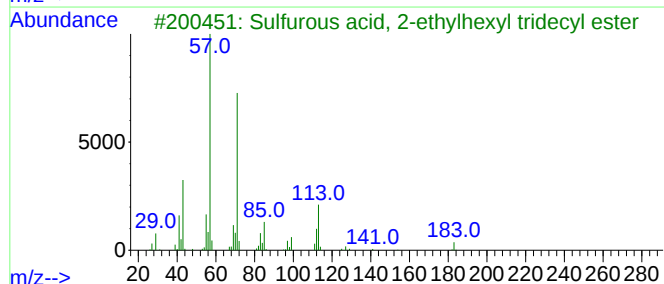
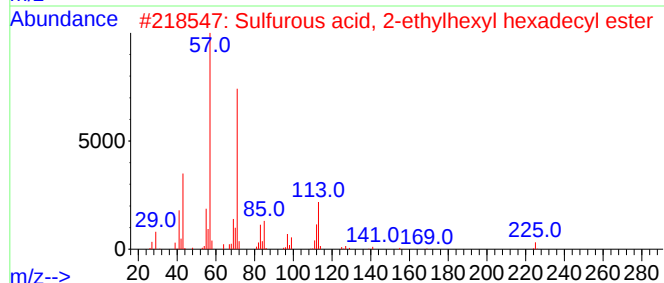
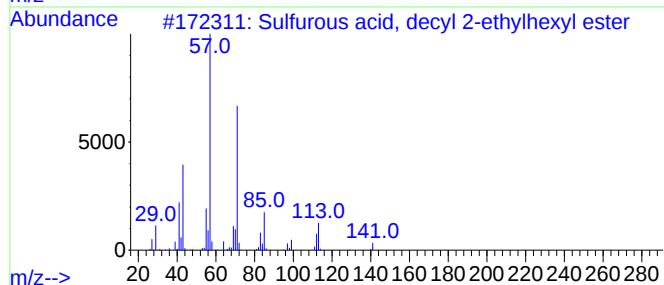
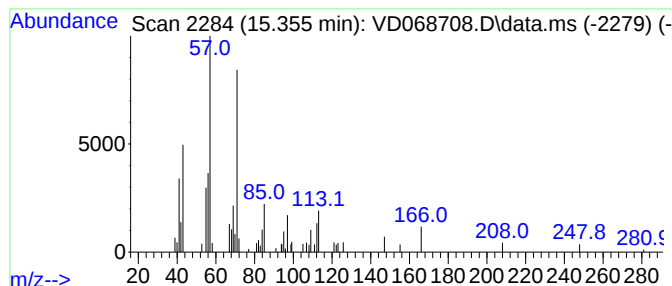
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, decyl 2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.355	14.36 ug/l	48577	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59
2			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	53
3			Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	53
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	53
5			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD032921\
Data File : VD068708.D
Acq On : 29 Mar 2021 19:53
Operator : VA/SY
Sample : M1828-04
Misc : 6.96G/5.00ml/MSVOA_D/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
FS-SB14(5-6)

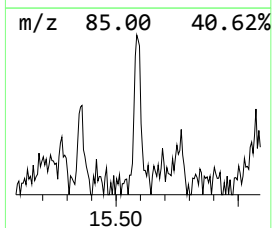
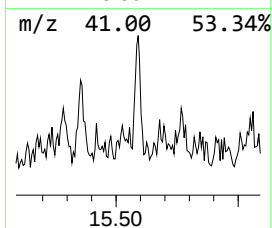
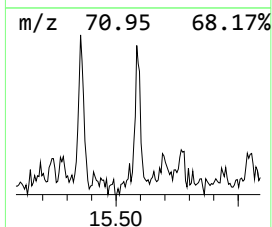
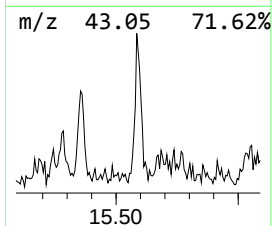
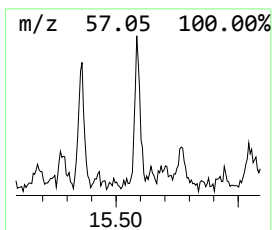
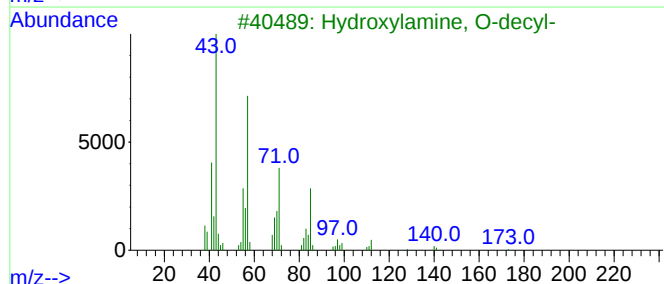
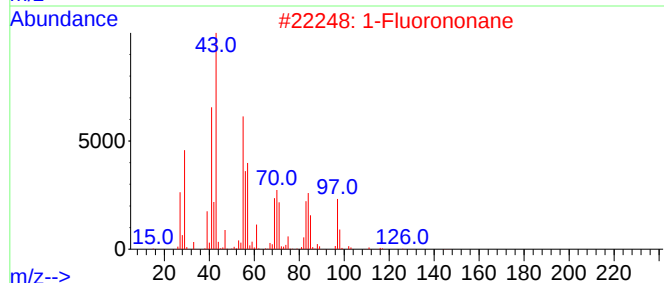
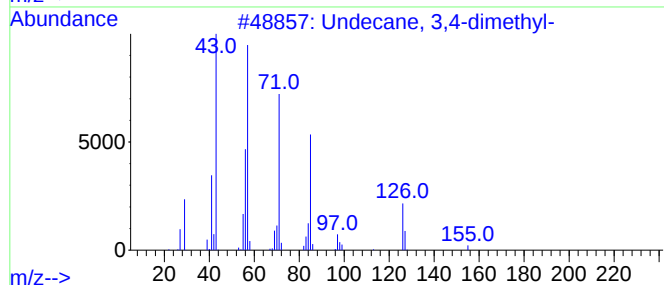
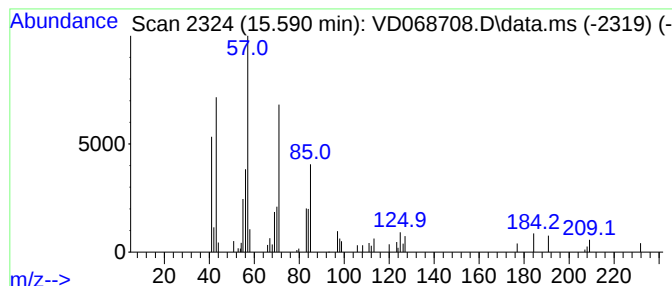
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Undecane, 3,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.590	15.38 ug/l	52018	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	53
2			1-Fluorononane	146	C9H19F	000463-18-3	47
3			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	47
4			Tridecane	184	C13H28	000629-50-5	45
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD032921\
Data File : VD068708.D
Acq On : 29 Mar 2021 19:53
Operator : VA/SY
Sample : M1828-04
Misc : 6.96G/5.00ml/MSVOA_D/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
FS-SB14(5-6)

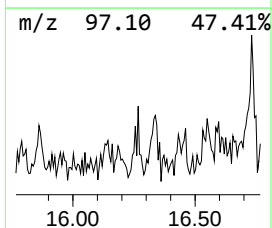
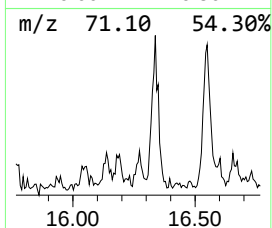
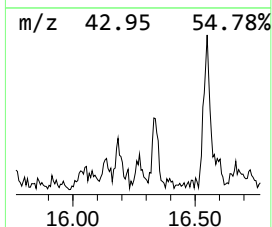
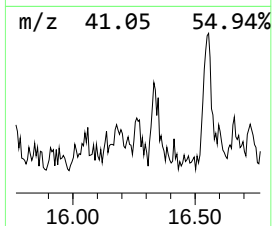
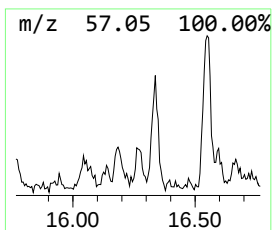
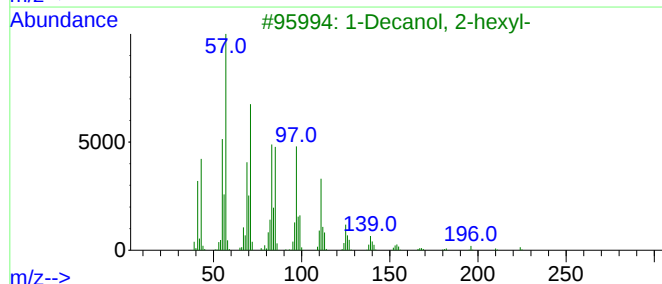
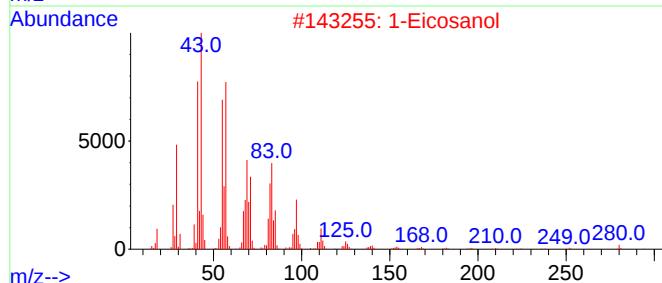
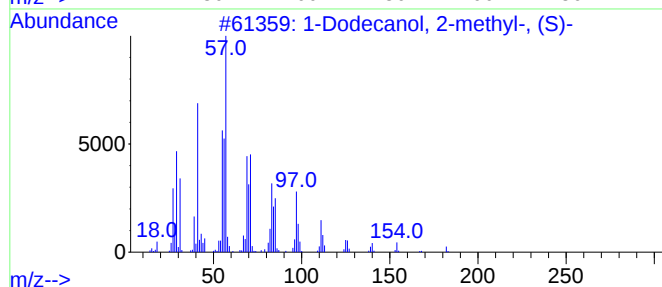
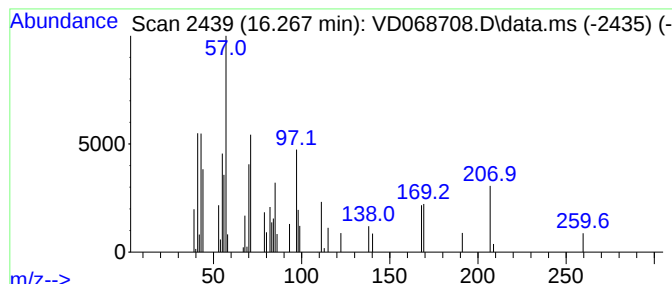
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Dodecanol, 2-methyl-, (S)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.267	8.12 ug/l	27473	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanol, 2-methyl-, (S)-	200	C13H28O	057289-26-6	50
2			1-Eicosanol	298	C20H42O	000629-96-9	47
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
4			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	38
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD032921\
Data File : VD068708.D
Acq On : 29 Mar 2021 19:53
Operator : VA/SY
Sample : M1828-04
Misc : 6.96G/5.00ml/MSVOA_D/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
FS-SB14(5-6)

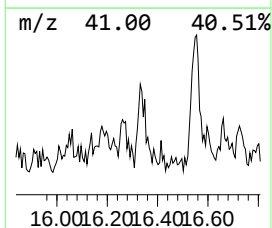
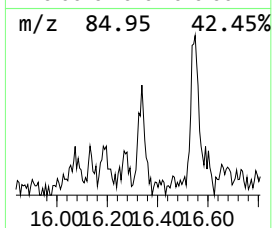
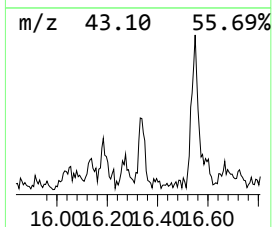
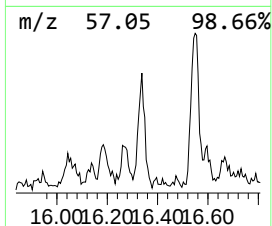
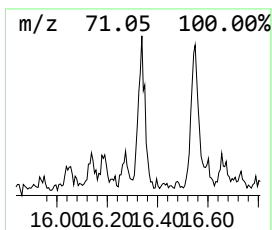
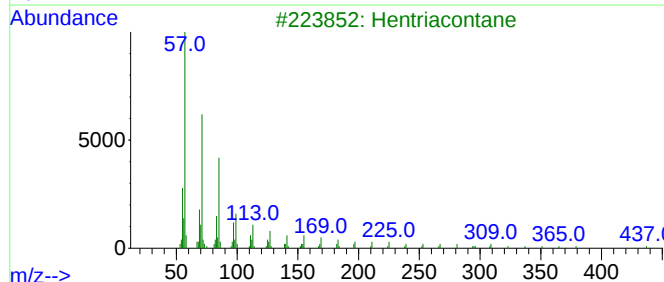
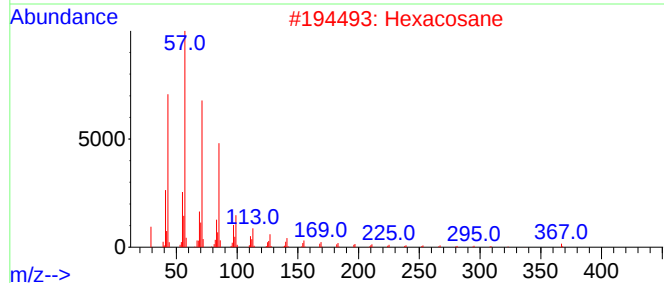
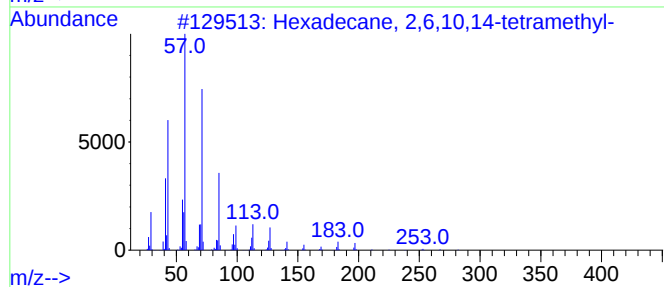
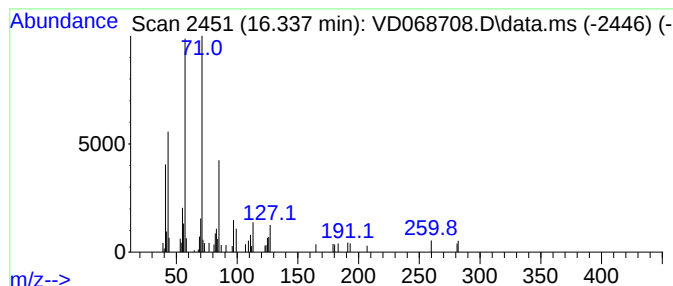
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.337	19.90 ug/l	67335	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
2			Hexacosane	366	C26H54	000630-01-3	58
3			Hentriacontane	437	C31H64	000630-04-6	58
4			5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	53
5			Sulfurous acid, pentyl tridecyl ...	334	C18H38O3S	1000309-14-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD032921\
Data File : VD068708.D
Acq On : 29 Mar 2021 19:53
Operator : VA/SY
Sample : M1828-04
Misc : 6.96G/5.00ml/MSVOA_D/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
FS-SB14(5-6)

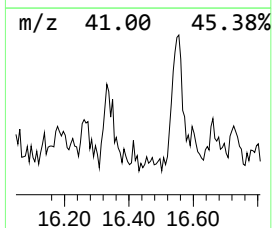
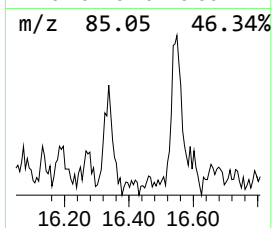
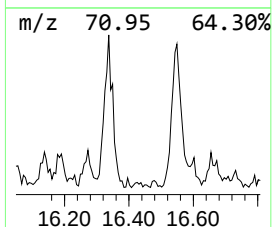
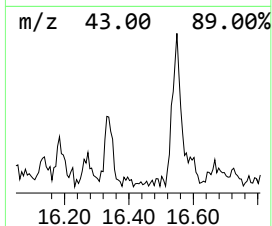
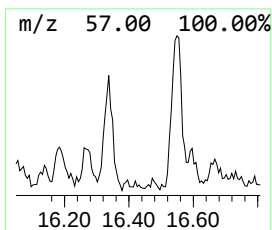
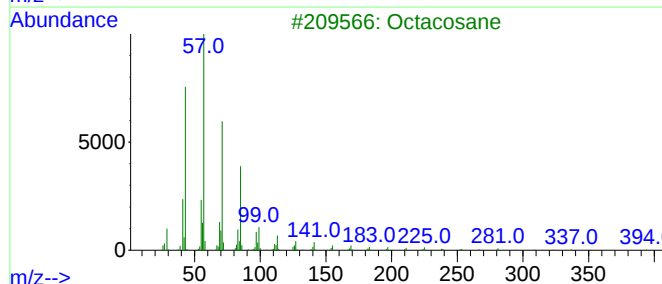
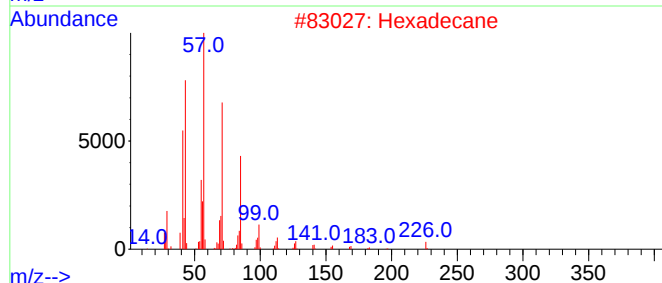
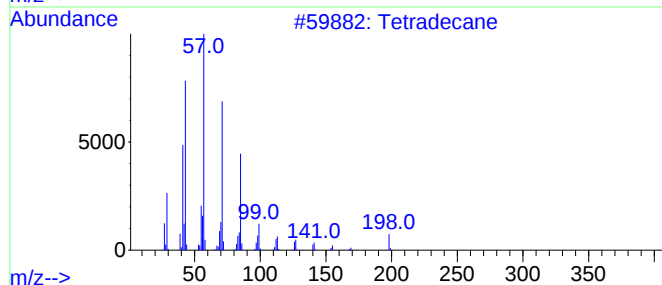
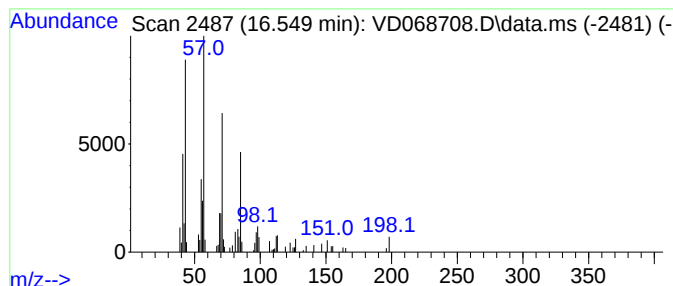
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.549	30.98 ug/l	104823	1,4-Dichlorobenzene-d4	13.573

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	90
2		Hexadecane	226	C16H34	000544-76-3	72
3		Octacosane	394	C28H58	000630-02-4	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD032921\
Data File : VD068708.D
Acq On : 29 Mar 2021 19:53
Operator : VA/SY
Sample : M1828-04
Misc : 6.96G/5.00ml/MSVOA_D/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
FS-SB14(5-6)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031921S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown13.820	13.820	41.5	ug/l	140243	4	13.573	169156	50.0
unknown14.867	14.867	11.7	ug/l	39560	4	13.573	169156	50.0
3,7-Decadiene, ...	15.290	8.8	ug/l	29828	4	13.573	169156	50.0
Sulfurous acid, ...	15.355	14.4	ug/l	48577	4	13.573	169156	50.0
Undecane, 3,4-d...	15.590	15.4	ug/l	52018	4	13.573	169156	50.0
1-Dodecanol, 2-...	16.267	8.1	ug/l	27473	4	13.573	169156	50.0
Hexadecane, 2,6...	16.337	19.9	ug/l	67335	4	13.573	169156	50.0
Tetradecane	16.549	31.0	ug/l	104823	4	13.573	169156	50.0