

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
 Data File : VX023043.D
 Acq On : 30 Jun 2021 18:52
 Operator : JC/MD
 Sample : M2898-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TB-01-062921

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_X\Method\82X062321W.M
 Title : SW846 8260

Signal : TIC: VX023043.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	37	rBV2	6120	11273	2.70%	0.341%
2	1.563	72	78	82	rVB4	2475	4677	1.12%	0.142%
3	5.397	696	707	718	rBV	43734	123876	29.65%	3.751%
4	5.562	723	734	746	rBV2	72624	202488	48.46%	6.131%
5	5.964	788	800	815	rBV2	57631	152384	36.47%	4.614%
6	6.769	922	932	944	rBV	128216	297859	71.28%	9.018%
7	8.653	1234	1241	1250	rBV	272577	417853	100.00%	12.651%
8	10.055	1465	1471	1484	rVB	272592	364101	87.14%	11.024%
9	11.085	1634	1640	1651	rVB	219811	278641	66.68%	8.437%
10	11.719	1740	1744	1748	rVV2	10205	12645	3.03%	0.383%
11	11.780	1752	1754	1759	rVB4	2851	4352	1.04%	0.132%
12	11.835	1759	1763	1767	rBV4	2508	4708	1.13%	0.143%
13	11.890	1767	1772	1776	rVB6	3917	5744	1.37%	0.174%
14	12.024	1789	1794	1800	rVV	275347	340793	81.56%	10.318%
15	12.152	1811	1815	1821	rBV9	2489	4516	1.08%	0.137%
16	12.317	1838	1842	1848	rBV8	3575	8145	1.95%	0.247%
17	12.475	1864	1868	1873	rVB6	4191	8141	1.95%	0.246%
18	12.555	1876	1881	1883	rVV6	3835	7562	1.81%	0.229%
19	12.585	1883	1886	1891	rVB5	6249	10423	2.49%	0.316%
20	12.689	1898	1903	1906	rBV3	7537	9213	2.20%	0.279%
21	12.823	1921	1925	1930	rVB5	7684	12258	2.93%	0.371%
22	12.896	1930	1937	1939	rBV5	8089	15461	3.70%	0.468%
23	12.988	1949	1952	1958	rVB5	6602	7884	1.89%	0.239%
24	13.213	1986	1989	1994	rVV7	3570	5938	1.42%	0.180%
25	13.298	2000	2003	2009	rVB8	8033	11473	2.75%	0.347%
26	13.390	2014	2018	2020	rBV	11722	15360	3.68%	0.465%
27	13.506	2033	2037	2042	rVB8	3062	5469	1.31%	0.166%
28	13.707	2067	2070	2073	rBV5	5698	7339	1.76%	0.222%
29	13.737	2073	2075	2079	rVB3	4997	5885	1.41%	0.178%
30	13.798	2082	2085	2089	rBV5	6563	9726	2.33%	0.294%
31	13.847	2089	2093	2099	rBV	38244	48042	11.50%	1.455%
32	13.908	2100	2103	2112	rVB8	8747	18564	4.44%	0.562%
33	13.993	2114	2117	2119	rBV4	5447	6696	1.60%	0.203%
34	14.073	2127	2130	2132	rBV4	7620	9224	2.21%	0.279%
35	14.140	2138	2141	2144	rVB3	11023	12661	3.03%	0.383%
36	14.189	2144	2149	2152	rBV	16381	22941	5.49%	0.695%

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37	14.310	2166	2169	2170	rBV2	6373	6935	1.66%	0.210%
38	14.402	2182	2184	2185	rBV	4585	4225	1.01%	0.128%
39	14.493	2197	2199	2202	rBV4	6376	8884	2.13%	0.269%
40	14.579	2212	2213	2216	rVB3	7284	4414	1.06%	0.134%
41	14.615	2216	2219	2223	rBV	100946	114433	27.39%	3.465%
42	14.725	2233	2237	2239	rBV5	10380	16383	3.92%	0.496%
43	14.756	2239	2242	2245	rVV5	12355	16113	3.86%	0.488%
44	14.798	2245	2249	2251	rVV3	19624	24774	5.93%	0.750%
45	14.847	2254	2257	2261	rVV5	18326	26289	6.29%	0.796%
46	14.938	2269	2272	2273	rBV2	9236	10585	2.53%	0.320%
47	14.963	2273	2276	2283	rVB4	35029	59479	14.23%	1.801%
48	15.213	2314	2317	2321	rVB	44510	55694	13.33%	1.686%
49	15.420	2347	2351	2356	rVB	67606	102247	24.47%	3.096%
50	15.566	2371	2375	2383	rVB	66265	106482	25.48%	3.224%
51	15.688	2391	2395	2400	rBV6	21203	40092	9.59%	1.214%
52	15.749	2400	2405	2410	rVB2	63774	105139	25.16%	3.183%
53	15.816	2413	2416	2420	rBV6	12663	19070	4.56%	0.577%
54	15.865	2421	2424	2430	rVB2	20811	34869	8.34%	1.056%
55	16.554	2533	2537	2541	rVB7	7884	13022	3.12%	0.394%
56	16.609	2544	2546	2554	rVB8	9011	17283	4.14%	0.523%
57	16.713	2558	2563	2568	rVB4	17914	32070	7.67%	0.971%

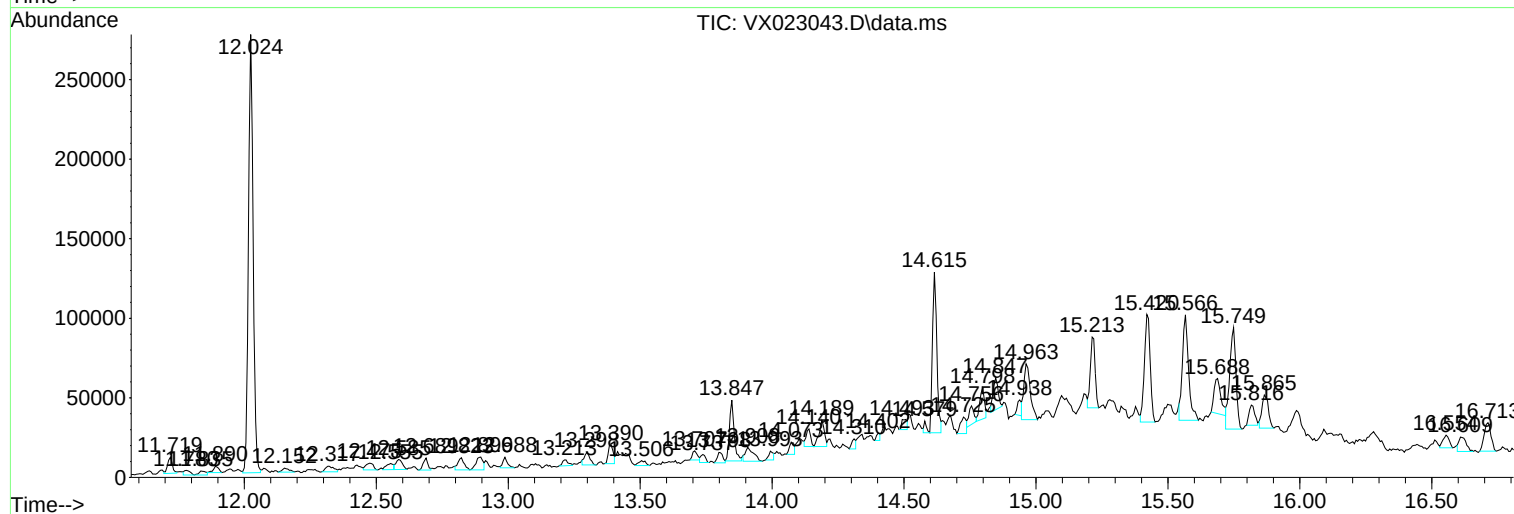
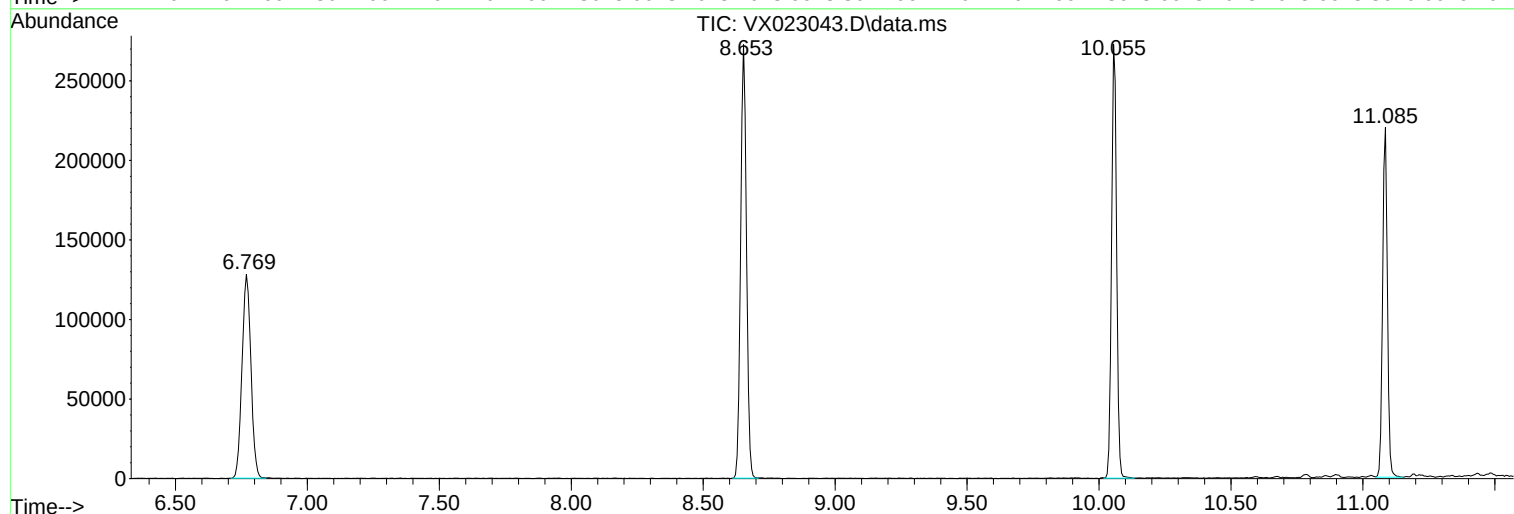
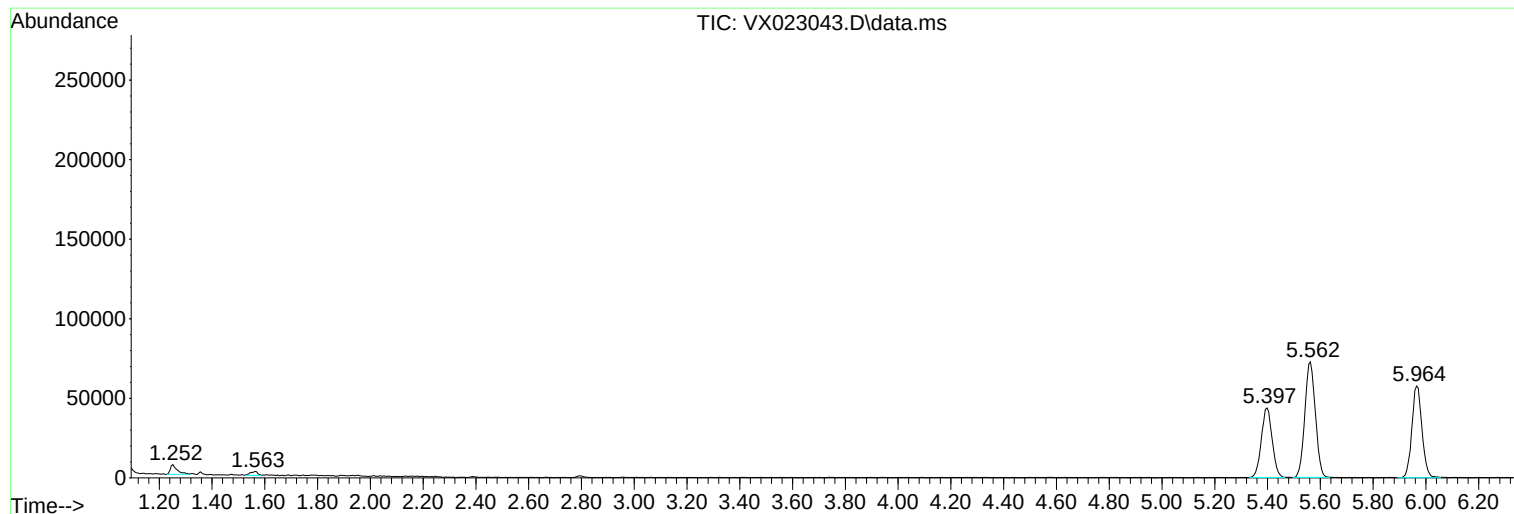
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Quant Title : SW846 8260

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



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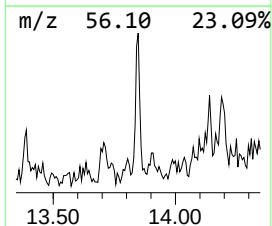
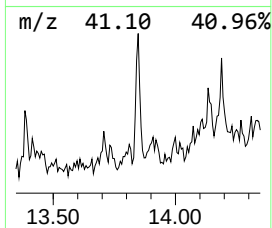
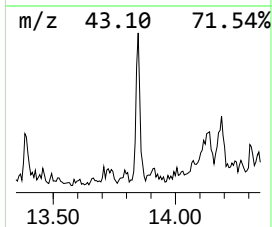
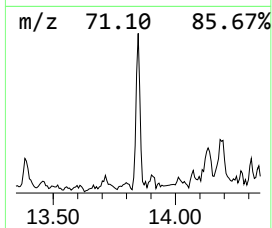
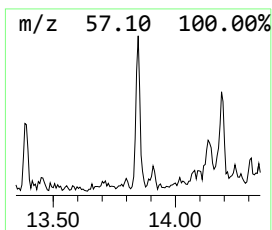
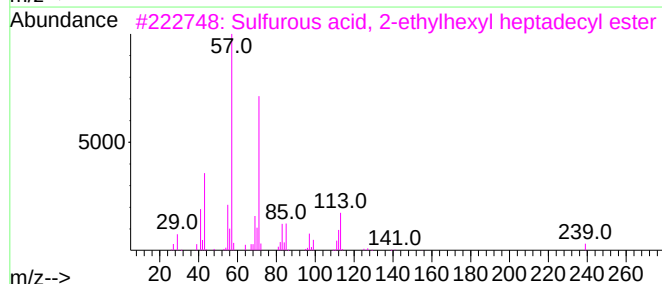
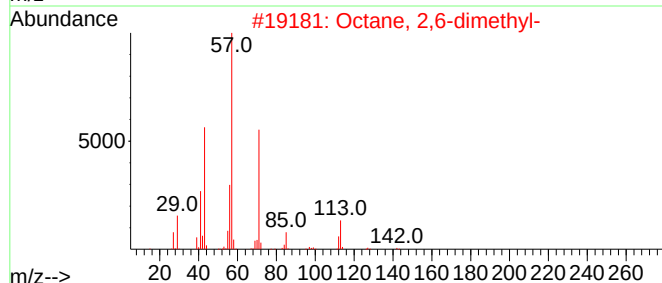
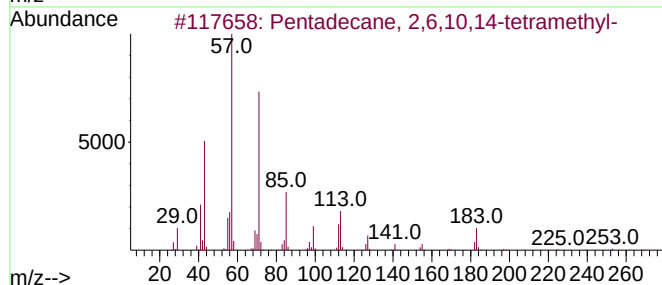
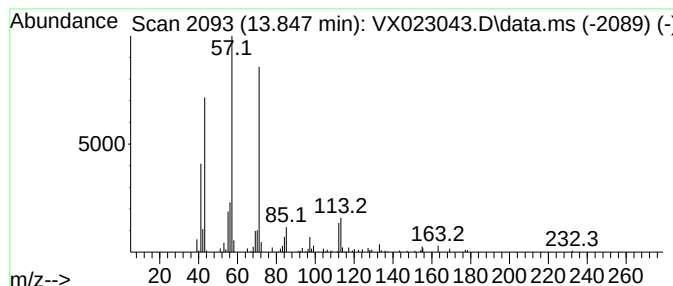
Instrument :
MSVOA_X
ClientSampleId :
TB-01-062921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentadecane, 2,6,10,14-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.847	7.05 ug/l	48042	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	86
3	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	80
4	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	64
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64



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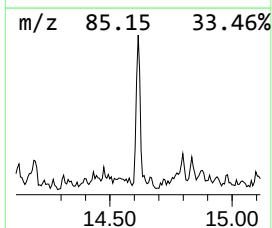
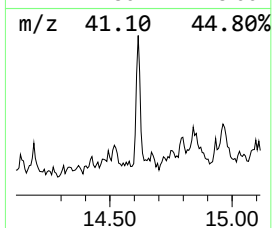
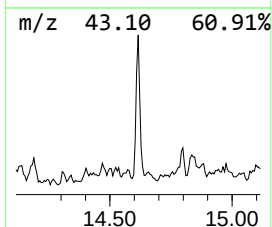
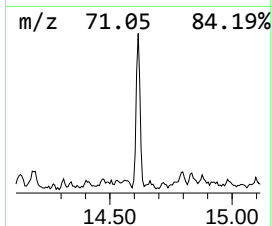
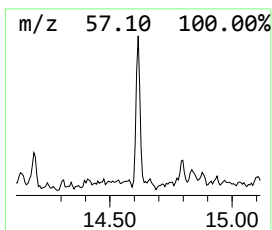
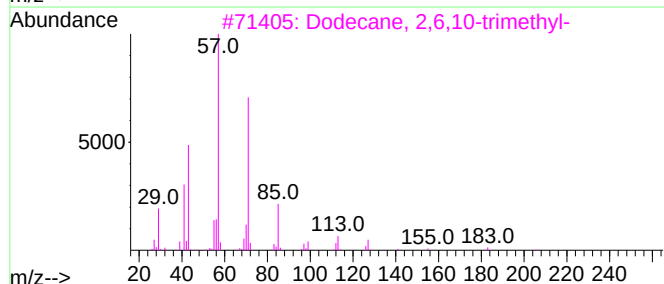
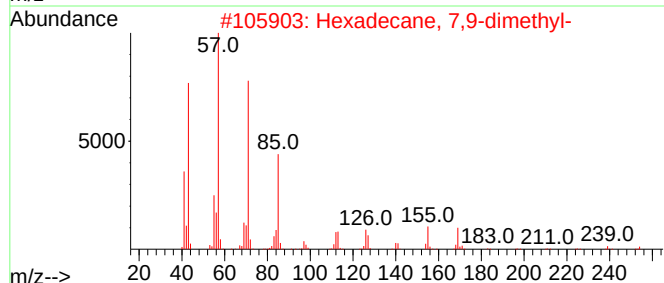
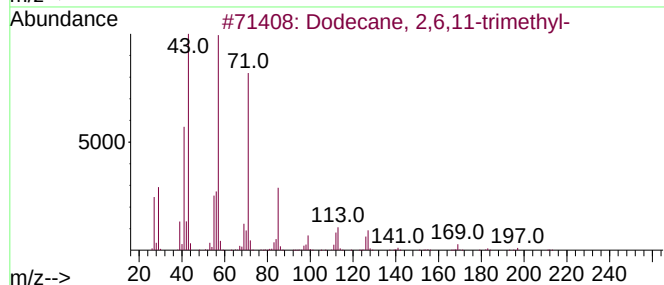
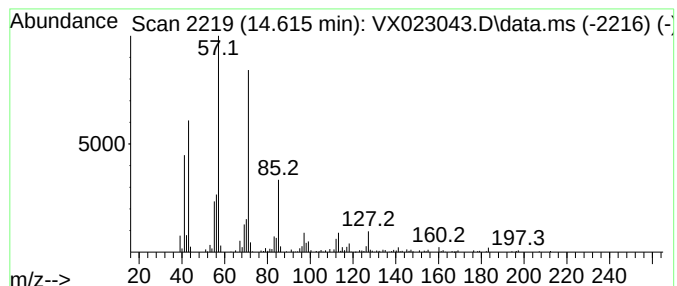
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 2 Dodecane, 2,6,11-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	16.79 ug/l	114433	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	91
2			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	72
3			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
4			Nonane, 3-methyl-	142	C10H22	005911-04-6	64
5			Heptacosane	380	C27H56	000593-49-7	59



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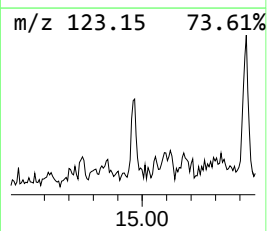
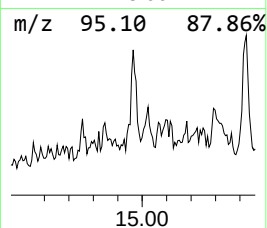
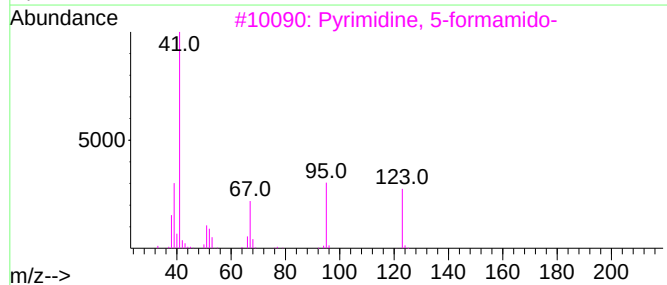
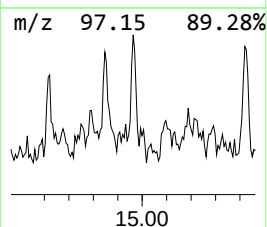
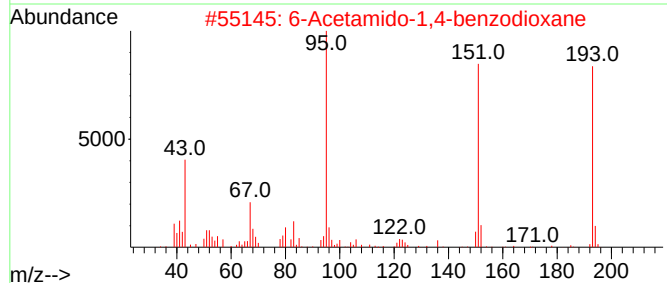
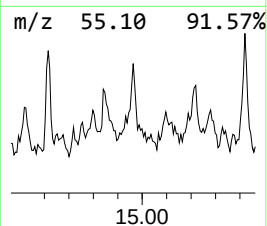
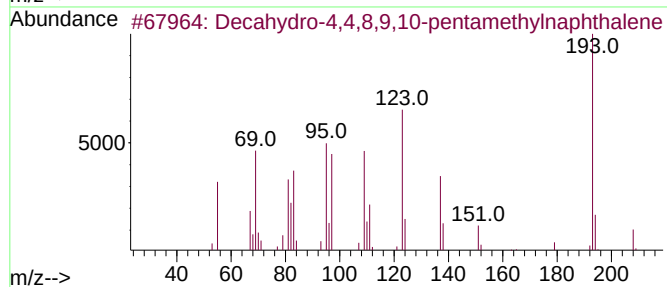
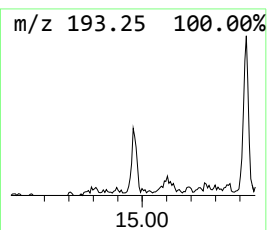
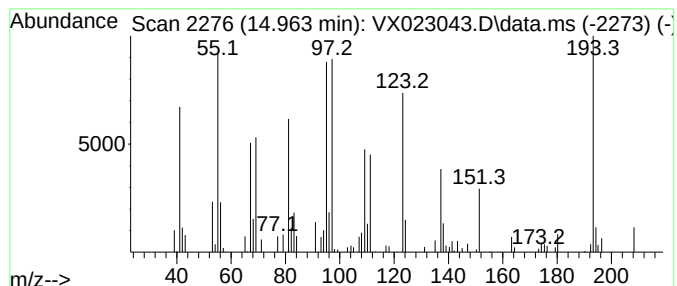
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Decahydro-4,4,8,9,10-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	8.73 ug/l	59479	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	76
2			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	27
3			Pyrimidine, 5-formamido-	123	C5H5N3O	056621-84-2	18
4			2-Anthracenamine	193	C14H11N	000613-13-8	14
5			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	14



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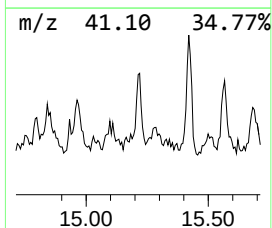
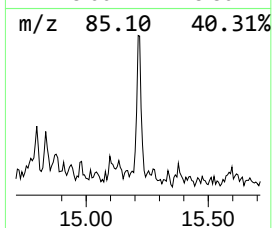
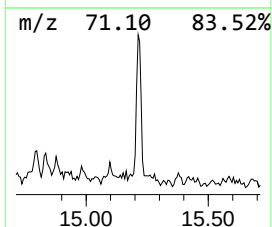
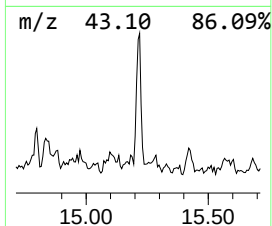
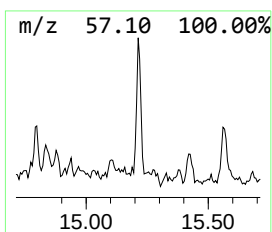
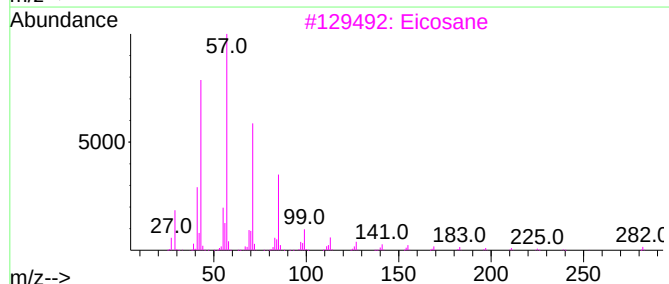
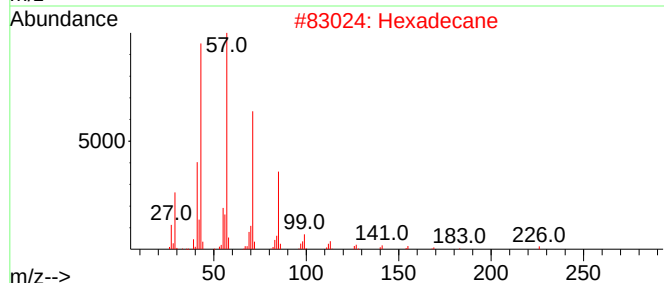
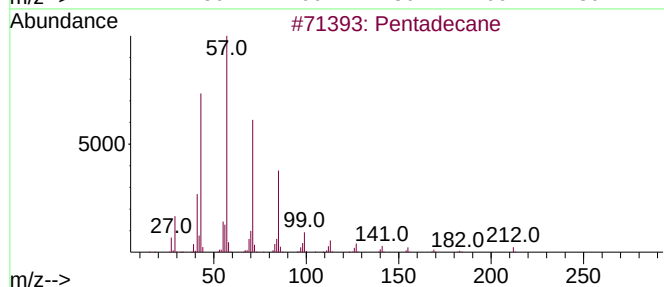
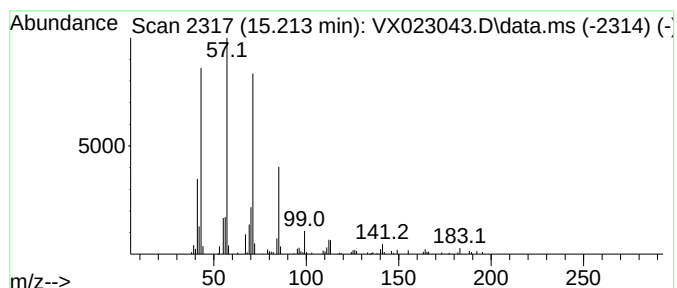
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.213	8.17 ug/l	55694	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	86
2			Hexadecane	226	C16H34	000544-76-3	80
3			Eicosane	282	C20H42	000112-95-8	80
4			Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78
5			Octacosane	394	C28H58	000630-02-4	72



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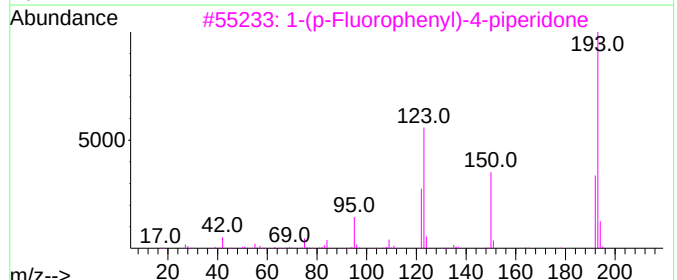
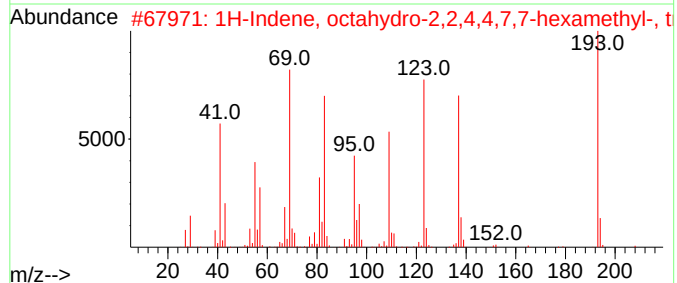
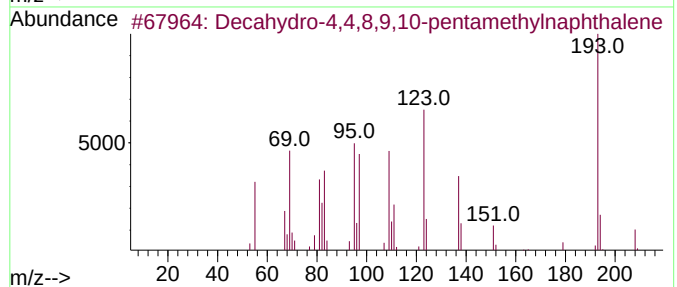
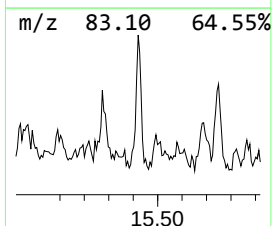
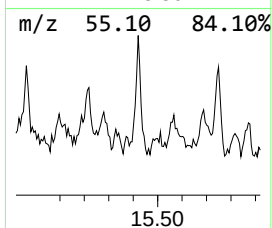
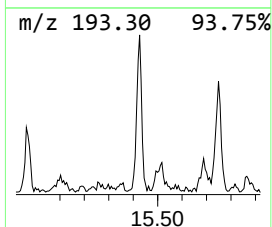
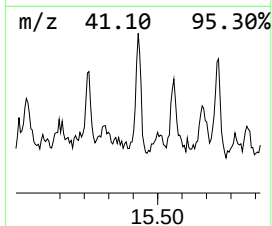
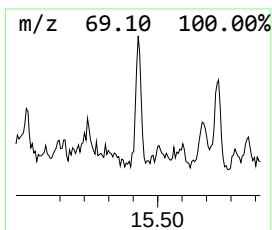
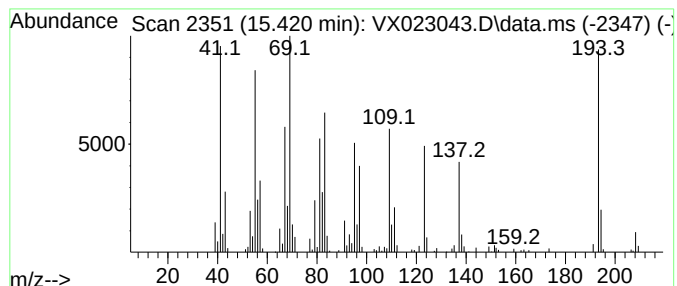
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 5 1H-Indene, octahydro-2,2,4,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	15.00 ug/l	102247	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	60
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	59
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
4			1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	14
5			Citronellol	156	C10H20O	000106-22-9	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
Data File : VX023043.D
Acq On : 30 Jun 2021 18:52
Operator : JC/MD
Sample : M2898-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TB-01-062921

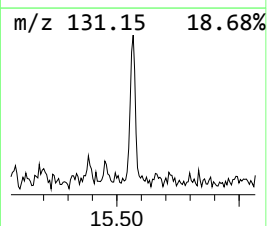
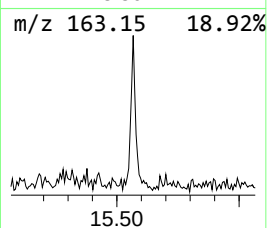
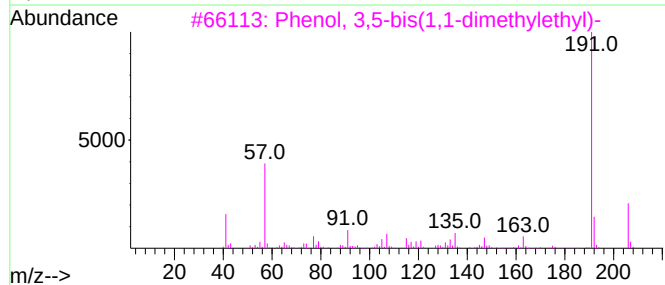
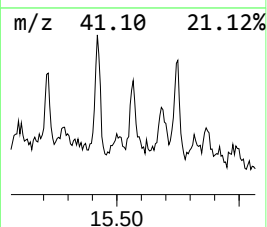
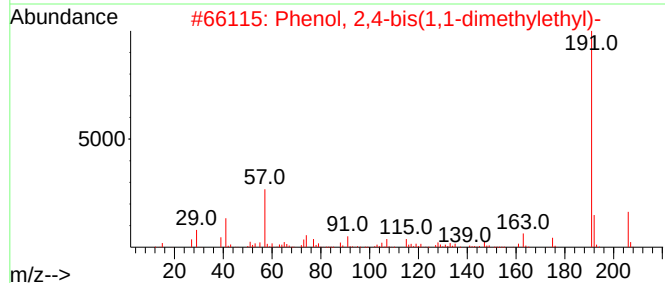
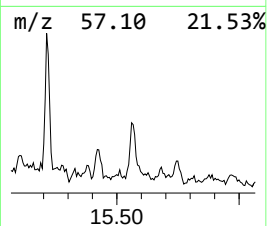
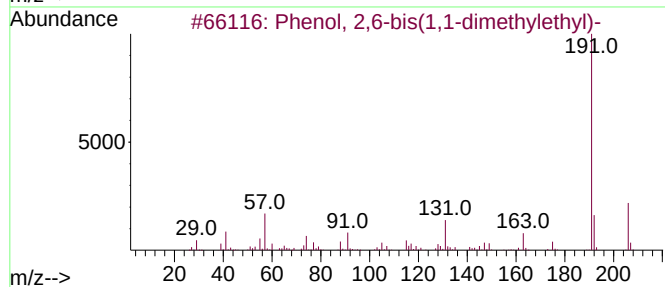
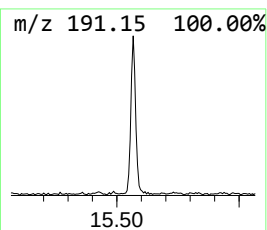
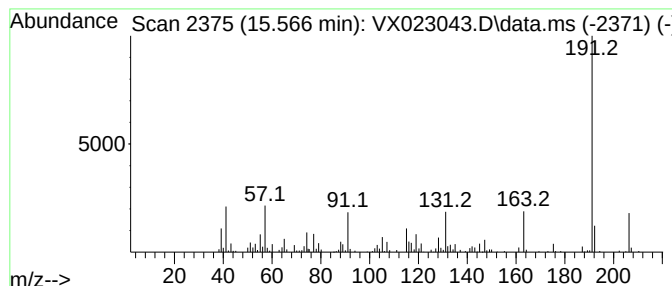
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Quant Title : SW846 8260

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

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.566	15.62 ug/l	106482	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2			Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	81
3			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	74
4			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	74
5			2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
Data File : VX023043.D
Acq On : 30 Jun 2021 18:52
Operator : JC/MD
Sample : M2898-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

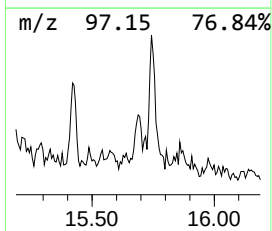
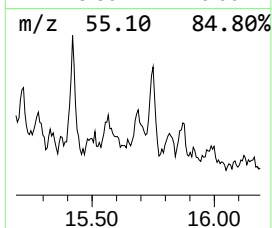
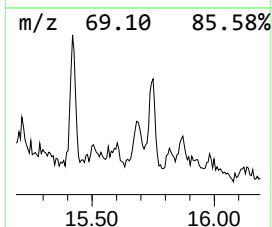
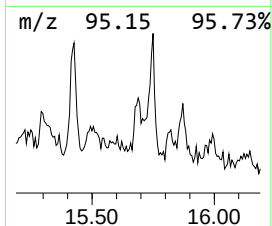
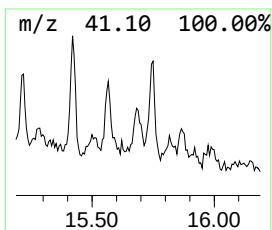
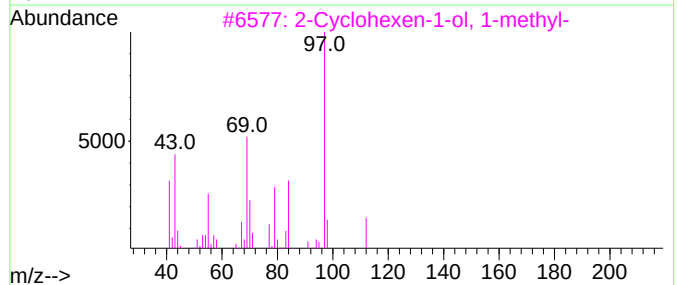
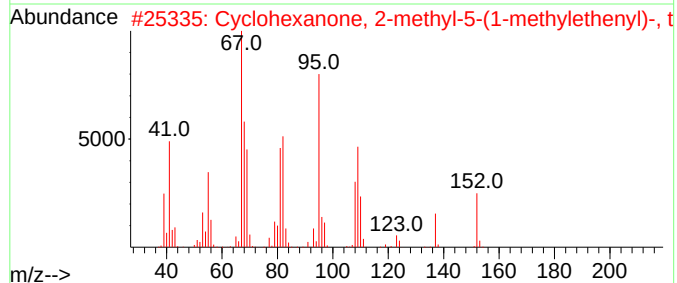
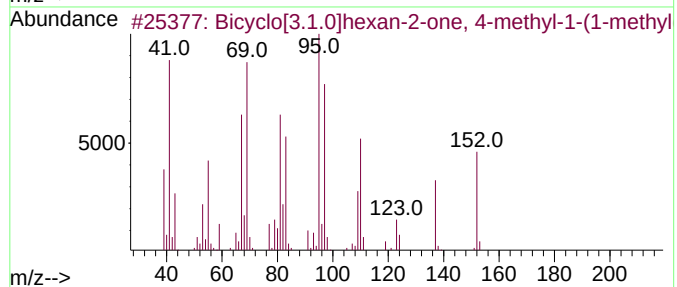
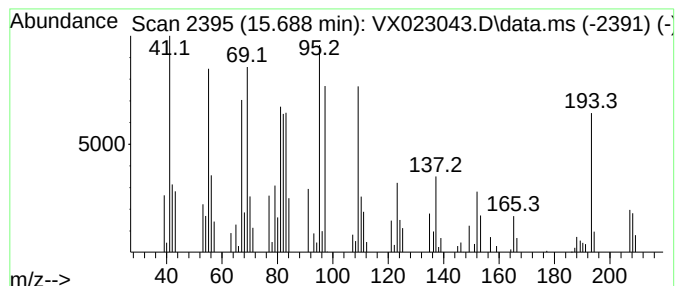
Instrument :
MSVOA_X
ClientSampleId :
TB-01-062921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 7 Bicyclo[3.1.0]hexan-2-one, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.688	5.88 ug/l	40092	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexan-2-one, 4-met...		152	C10H16O	002506-61-8	52
2	Cyclohexanone, 2-methyl-5-(1-met...		152	C10H16O	005948-04-9	38
3	2-Cyclohexen-1-ol, 1-methyl-		112	C7H12O	023758-27-2	25
4	Naphthalene, decahydro-1,4a-dime...		208	C15H28	030824-81-8	25
5	7-Tetradecanol		214	C14H30O	003981-79-1	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
Data File : VX023043.D
Acq On : 30 Jun 2021 18:52
Operator : JC/MD
Sample : M2898-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TB-01-062921

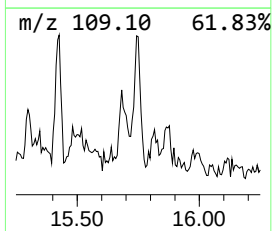
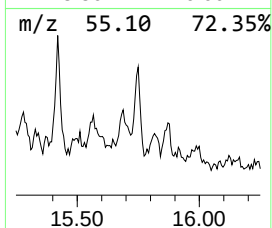
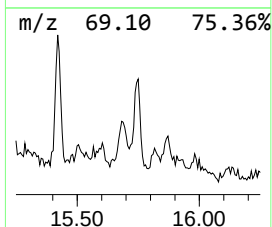
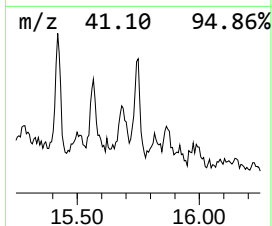
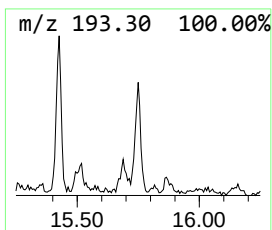
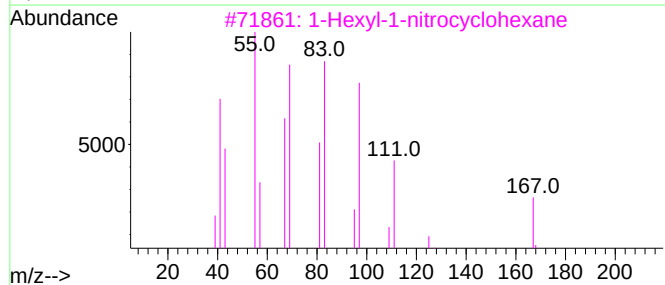
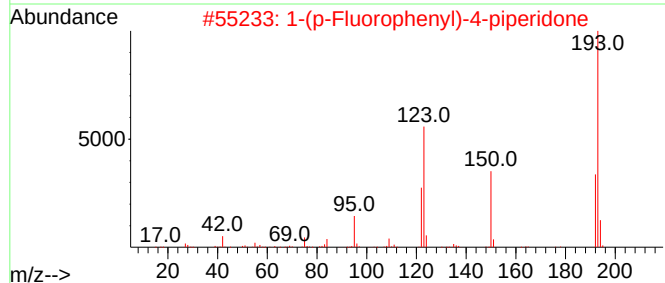
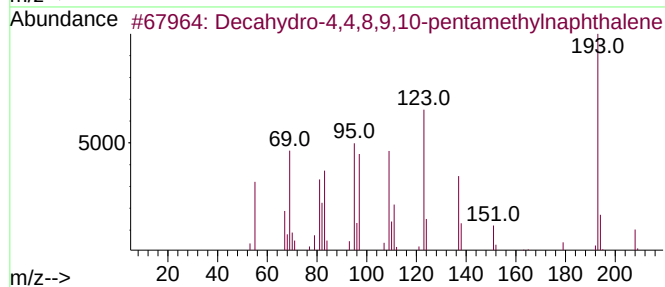
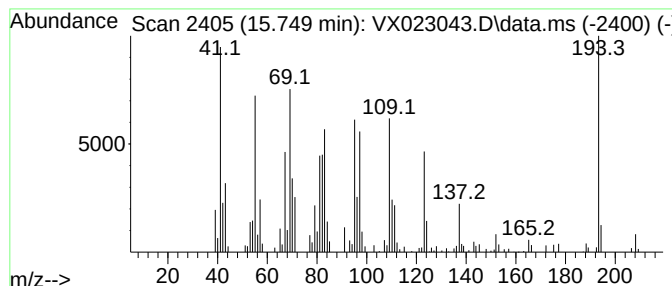
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.749 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.749	15.43 ug/l	105139	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	35
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
3			1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	27
4			Phosphetane, 1-chloro-2,2,3,4,4-...	194	C8H16ClOP	029276-11-7	27
5			Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
Data File : VX023043.D
Acq On : 30 Jun 2021 18:52
Operator : JC/MD
Sample : M2898-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TB-01-062921

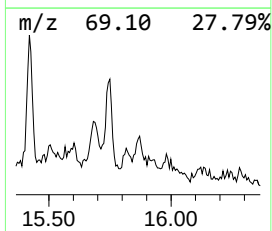
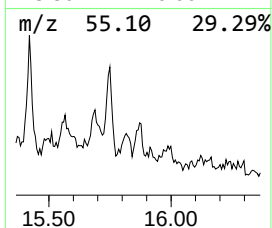
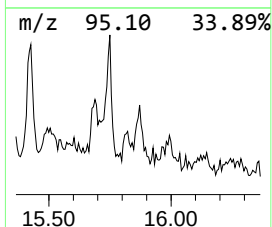
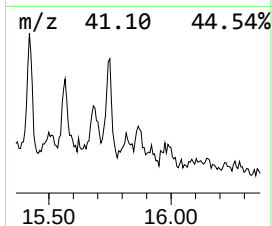
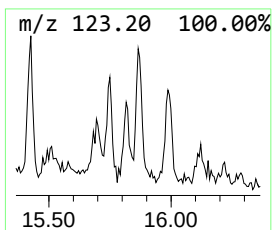
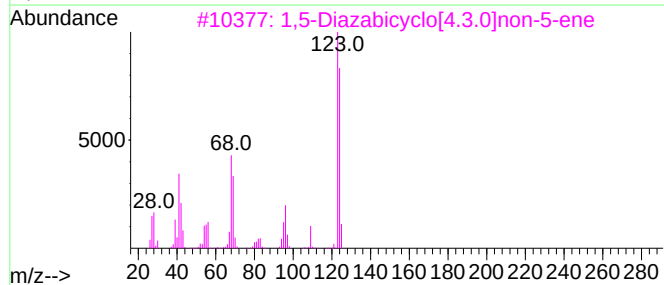
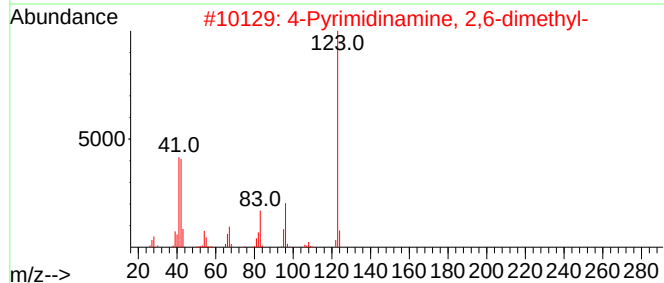
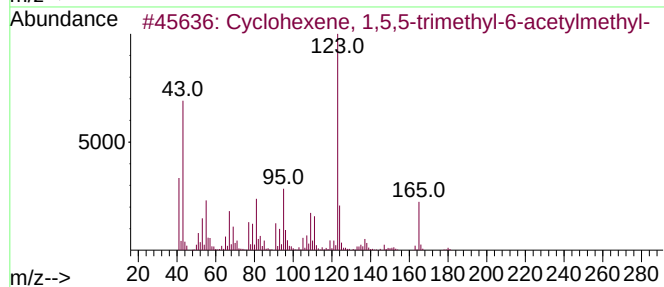
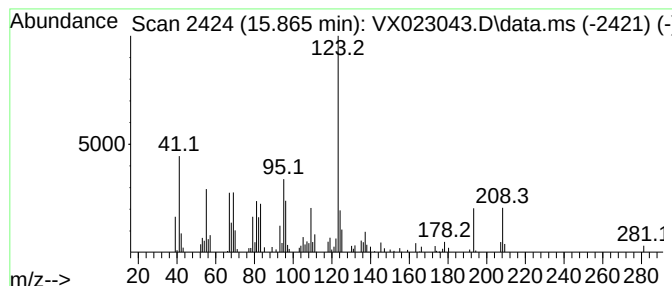
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexene, 1,5,5-trimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.865	5.12 ug/l	34869	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	52
2			4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	43
3			1,5-Diazabicyclo[4.3.0]non-5-ene	124	C7H12N2	003001-72-7	43
4			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	38
5			Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
Data File : VX023043.D
Acq On : 30 Jun 2021 18:52
Operator : JC/MD
Sample : M2898-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TB-01-062921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.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
Pentadecane, 2,...	13.847	7.0	ug/l	48042	4	12.024	340793	50.0
Dodecane, 2,6,1...	14.615	16.8	ug/l	114433	4	12.024	340793	50.0
Decahydro-4,4,8...	14.963	8.7	ug/l	59479	4	12.024	340793	50.0
Pentadecane	15.213	8.2	ug/l	55694	4	12.024	340793	50.0
1H-Indene, octa...	15.420	15.0	ug/l	102247	4	12.024	340793	50.0
Phenol, 2,6-bis...	15.566	15.6	ug/l	106482	4	12.024	340793	50.0
Bicyclo[3.1.0]h...	15.688	5.9	ug/l	40092	4	12.024	340793	50.0
unknown15.749	15.749	15.4	ug/l	105139	4	12.024	340793	50.0
Cyclohexene, 1,...	15.865	5.1	ug/l	34869	4	12.024	340793	50.0