

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
 Data File : VX036950.D
 Acq On : 11 Aug 2023 18:51
 Operator : JC/MD
 Sample : 03972-03
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 356

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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX036950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.763	586	603	618	rBV2	7537	34566	2.32%	0.222%
2	5.391	694	706	720	rBV	63903	187773	12.59%	1.205%
3	5.544	720	731	747	rVB	109102	306504	20.55%	1.968%
4	5.952	787	798	816	rBV	69806	189299	12.69%	1.215%
5	6.757	921	930	945	rBV	178718	423575	28.39%	2.719%
6	8.647	1233	1240	1249	rBV	382253	580614	38.92%	3.727%
7	10.055	1465	1471	1485	rVB	396599	540389	36.22%	3.469%
8	10.299	1503	1511	1517	rBV	27275	41536	2.78%	0.267%
9	10.860	1598	1603	1612	rBV7	7811	17316	1.16%	0.111%
10	10.945	1612	1617	1622	rVB	30851	43813	2.94%	0.281%
11	11.085	1634	1640	1650	rBV	331533	450568	30.20%	2.893%
12	11.378	1685	1688	1694	rBV2	10459	19601	1.31%	0.126%
13	11.482	1701	1705	1718	rVB3	36150	60538	4.06%	0.389%
14	11.616	1721	1727	1733	rVB6	6963	15057	1.01%	0.097%
15	11.750	1746	1749	1752	rBV2	24096	36513	2.45%	0.234%
16	11.841	1759	1764	1767	rBV3	8071	15243	1.02%	0.098%
17	11.939	1776	1780	1782	rBV2	16810	24520	1.64%	0.157%
18	11.969	1782	1785	1789	rVB2	48783	60354	4.05%	0.387%
19	12.024	1789	1794	1799	rBV	464160	590330	39.57%	3.790%
20	12.262	1826	1833	1837	rBV3	14369	38837	2.60%	0.249%
21	12.311	1837	1841	1848	rVV6	36414	75154	5.04%	0.482%
22	12.421	1855	1859	1864	rBV	133781	166059	11.13%	1.066%
23	12.463	1864	1866	1872	rVB5	24097	36974	2.48%	0.237%
24	12.555	1872	1881	1883	rBV6	26170	57480	3.85%	0.369%
25	12.732	1905	1910	1913	rBV5	14958	24379	1.63%	0.157%
26	12.817	1919	1924	1931	rVB2	86474	125930	8.44%	0.808%
27	12.890	1932	1936	1937	rBV	26439	34100	2.29%	0.219%
28	12.920	1938	1941	1945	rVV	63519	90214	6.05%	0.579%
29	12.981	1945	1951	1956	rVV4	64911	127504	8.55%	0.819%
30	13.042	1956	1961	1964	rVB5	35264	59975	4.02%	0.385%
31	13.158	1977	1980	1986	rBV4	25386	36974	2.48%	0.237%
32	13.213	1986	1989	1990	rBV2	18772	20181	1.35%	0.130%
33	13.292	1995	2002	2008	rVB6	115076	217515	14.58%	1.396%
34	13.347	2008	2011	2013	rBV3	14531	18358	1.23%	0.118%
35	13.414	2016	2022	2025	rBV7	115941	246374	16.52%	1.582%
36	13.518	2034	2039	2042	rBV4	62437	112640	7.55%	0.723%

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37	13.555	2043	2045	2047	rBV	19308	17658	1.18%	0.113%
38	13.591	2047	2051	2054	rBV4	76591	128868	8.64%	0.827%
39	13.676	2062	2065	2067	rBV4	53840	69874	4.68%	0.449%
40	13.737	2072	2075	2077	rBV2	43319	60625	4.06%	0.389%
41	13.768	2077	2080	2082	rVV	68382	76582	5.13%	0.492%
42	13.798	2082	2085	2089	rVB3	164665	187834	12.59%	1.206%
43	13.841	2089	2092	2095	rBV2	121011	162513	10.89%	1.043%
44	13.908	2100	2103	2109	rVB8	84894	161910	10.85%	1.039%
45	13.993	2114	2117	2119	rBV5	59723	83693	5.61%	0.537%
46	14.067	2125	2129	2132	rBV3	143331	204869	13.73%	1.315%
47	14.170	2143	2146	2150	rVV3	93697	135388	9.08%	0.869%
48	14.219	2150	2154	2157	rVB4	123902	165572	11.10%	1.063%
49	14.621	2216	2220	2221	rBV2	200440	276500	18.53%	1.775%
50	14.670	2225	2228	2232	rBV3	209783	277186	18.58%	1.779%
51	14.749	2238	2241	2244	rBV2	338116	400804	26.87%	2.573%
52	14.847	2253	2257	2261	rBV3	248796	397540	26.65%	2.552%
53	14.963	2268	2276	2283	rBV3	490132	1125682	75.46%	7.227%
54	15.176	2307	2311	2314	rBV5	186429	302212	20.26%	1.940%
55	15.420	2346	2351	2356	rVB	1002177	1444054	96.80%	9.271%
56	15.481	2357	2361	2368	rBV2	281943	569265	38.16%	3.655%
57	15.615	2379	2383	2386	rBV	233665	349344	23.42%	2.243%
58	15.652	2386	2389	2390	rVV	170686	219494	14.71%	1.409%
59	15.682	2391	2394	2398	rVV3	368506	616293	41.31%	3.956%
60	15.743	2399	2404	2410	rVB2	898143	1491799	100.00%	9.577%
61	15.816	2411	2416	2419	rBV	178106	365468	24.50%	2.346%
62	15.865	2421	2424	2429	rVB2	285440	445297	29.85%	2.859%
63	15.981	2440	2443	2450	rVB3	179291	335398	22.48%	2.153%
64	16.554	2533	2537	2541	rVV3	46270	73046	4.90%	0.469%
65	16.603	2542	2545	2556	rVB8	58085	134755	9.03%	0.865%
66	16.706	2557	2562	2569	rVB2	86983	170581	11.43%	1.095%

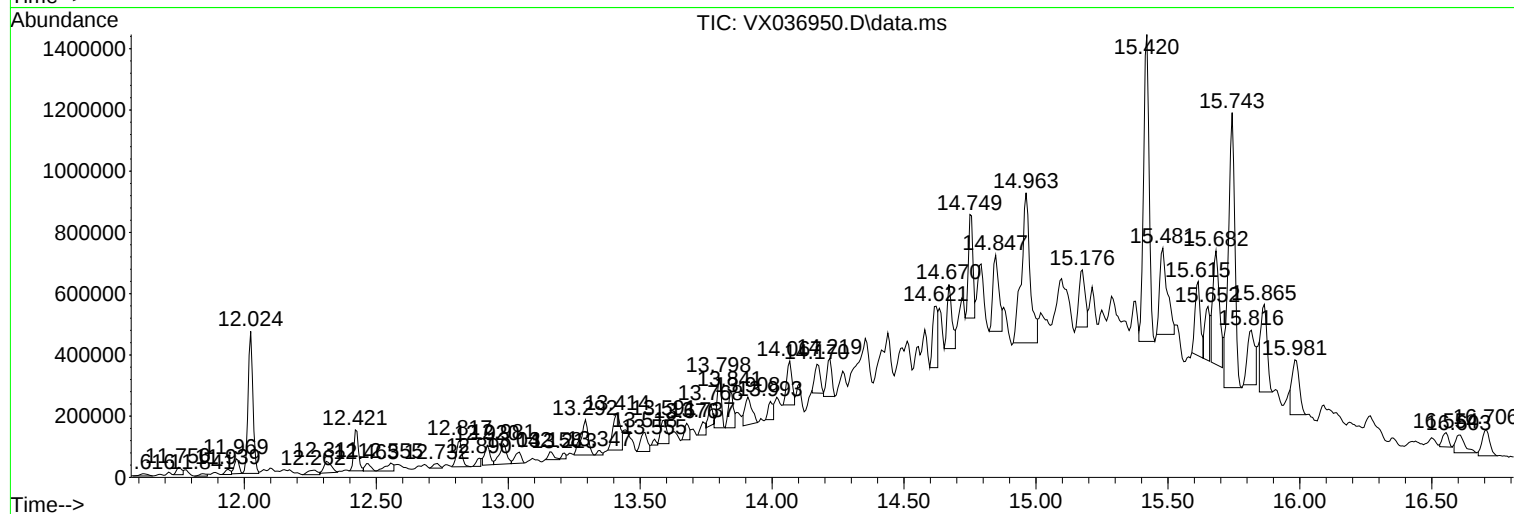
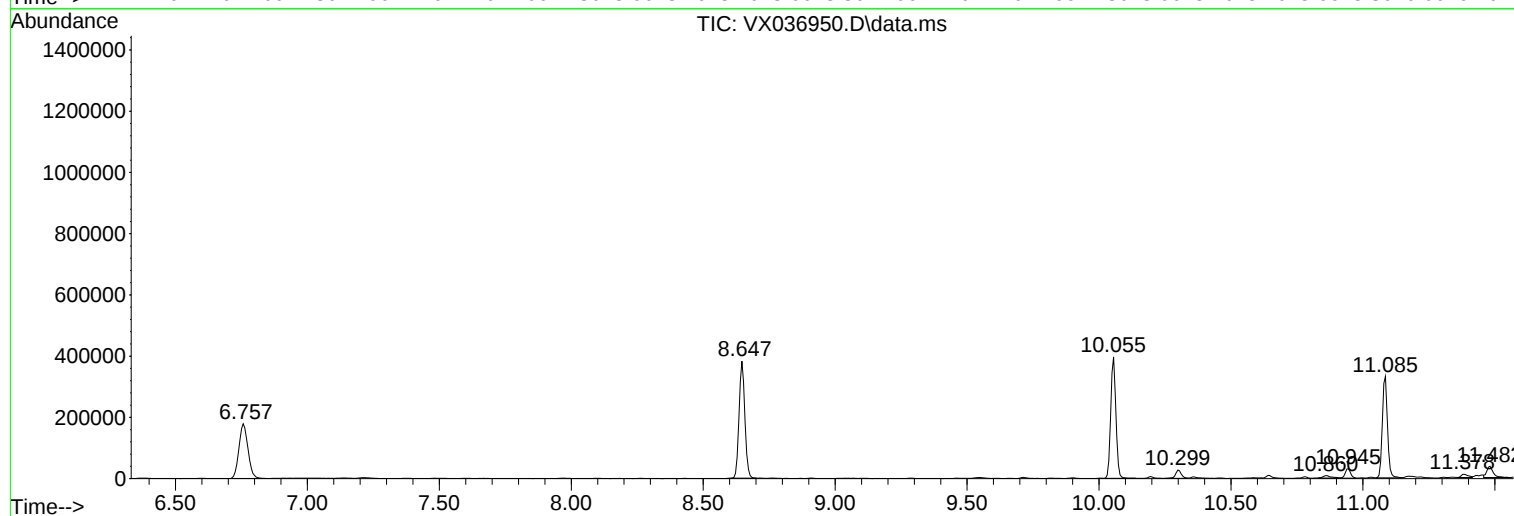
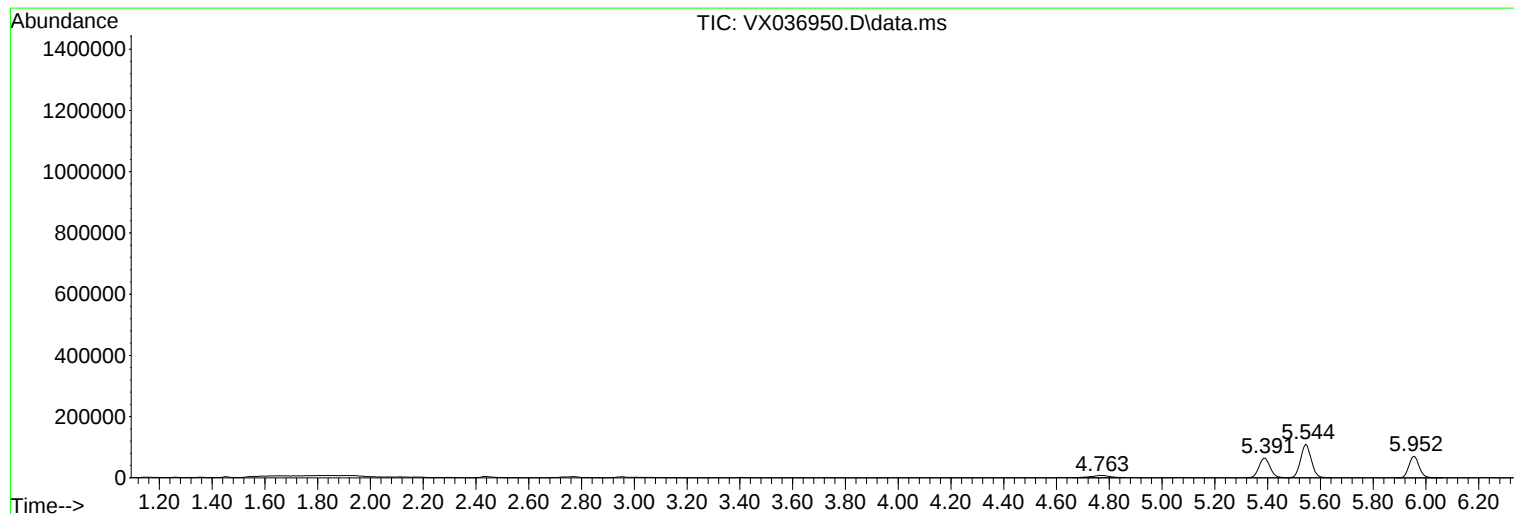
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

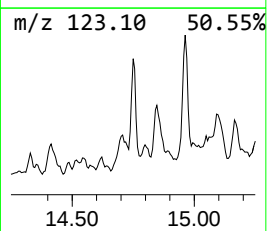
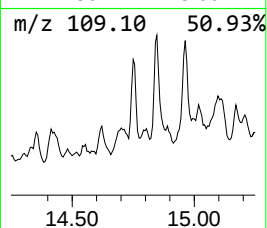
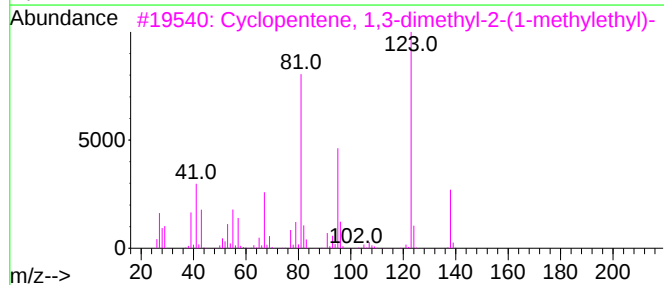
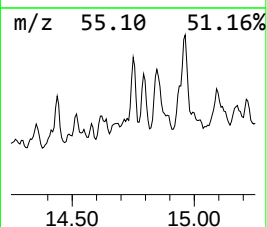
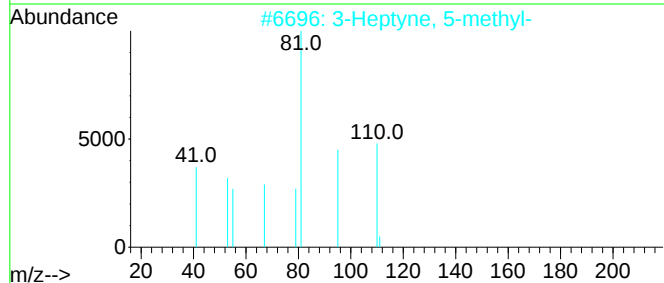
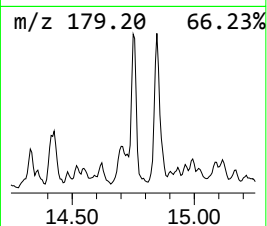
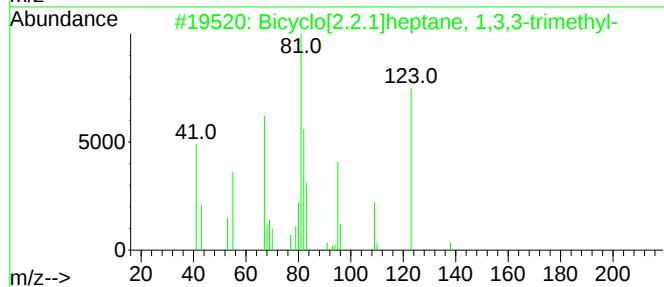
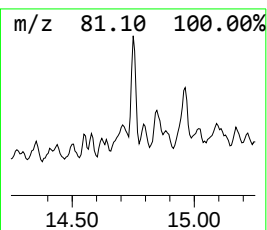
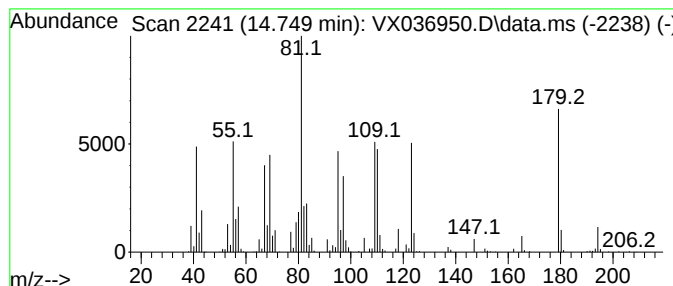
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Bicyclo[2.2.1]heptane, 1,3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.749	33.95 ug/l	400804	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	55
2			3-Heptyne, 5-methyl-	110	C8H14	061228-09-9	43
3			Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	38
4			2-Ethylcyclohexanol, heptafluoro...	324	C12H15F7O2	959079-92-6	38
5			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	38



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ClientSampleId :
356

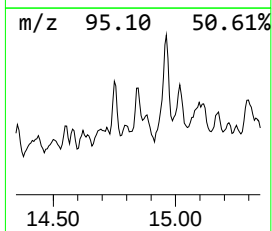
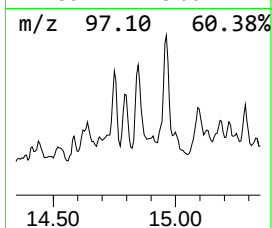
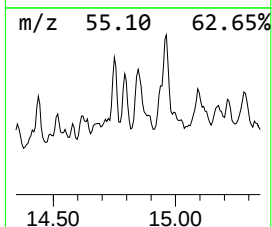
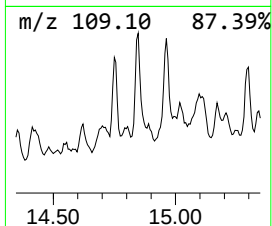
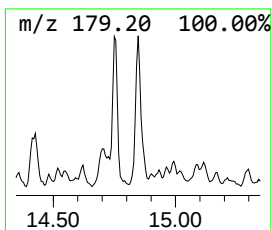
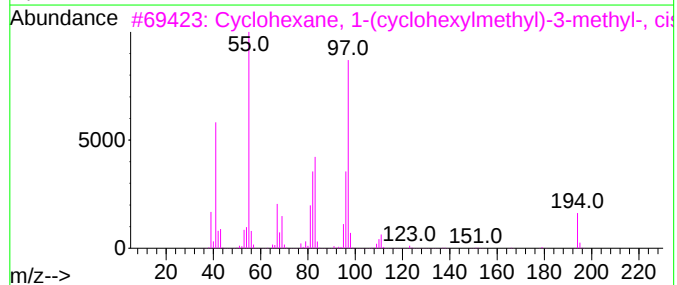
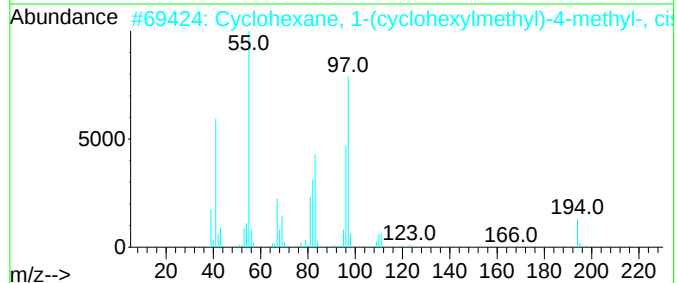
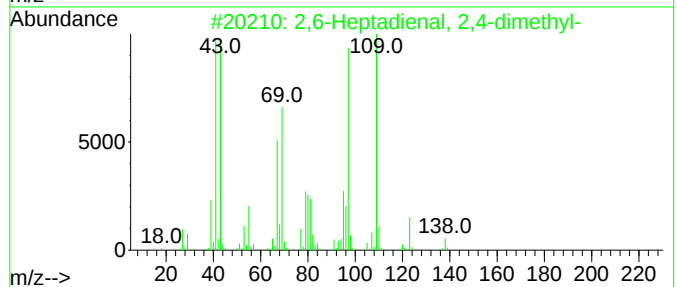
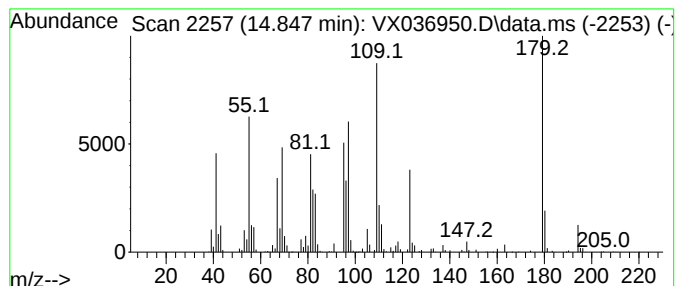
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown14.847 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	33.67 ug/l	397540	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
2			Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-97-1	25
3			Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-96-0	15
4			Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-95-9	15
5			1,4-Bis[.alpha.-methoxyethyl]ben...	194	C12H18O2	129770-42-9	14



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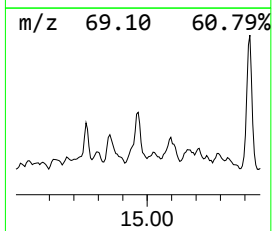
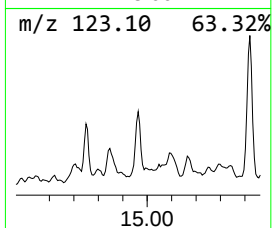
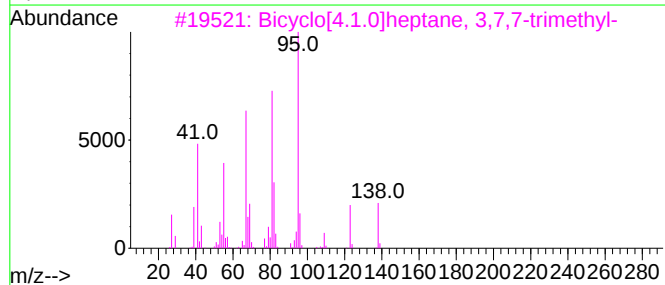
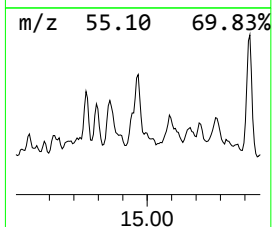
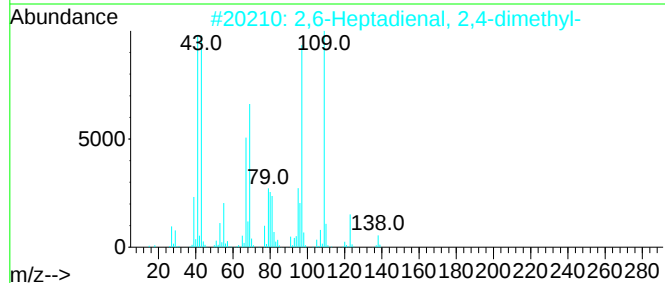
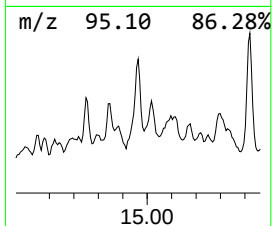
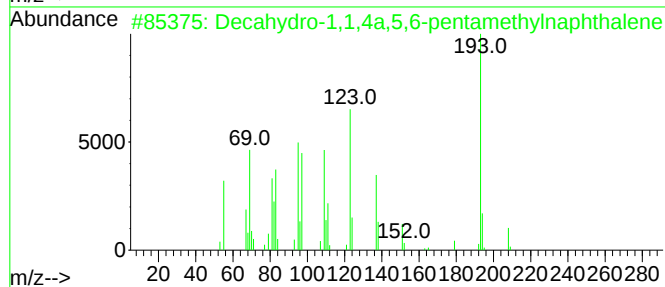
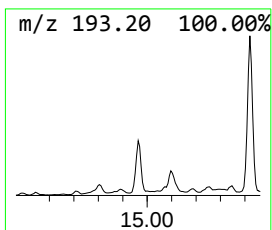
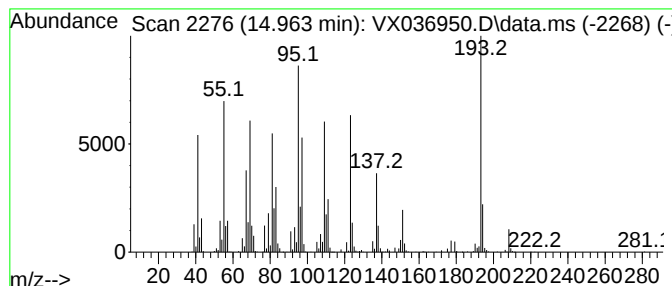
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	95.34 ug/l	1125680	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	96
2			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	25
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25
5			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	18



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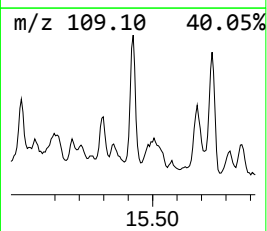
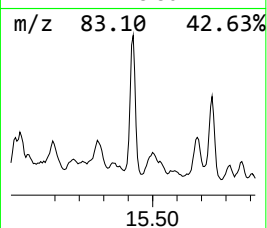
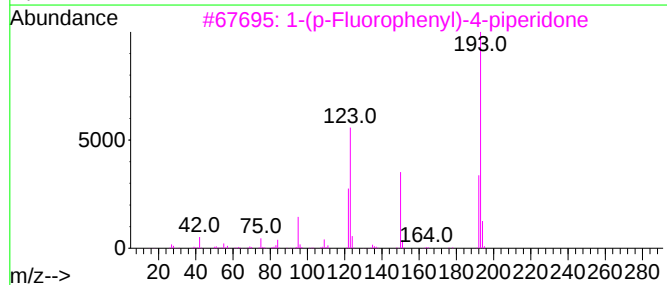
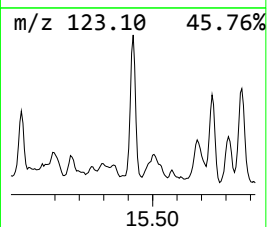
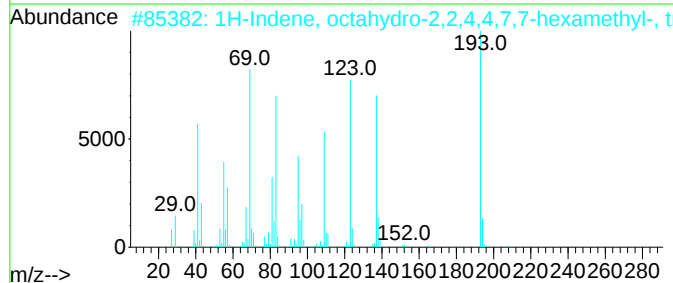
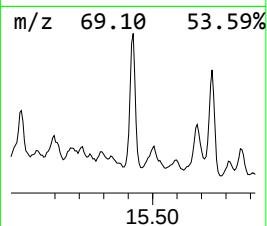
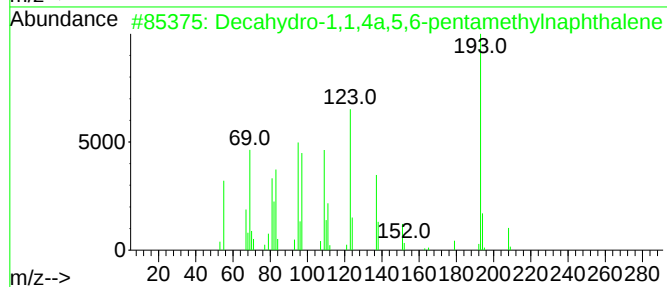
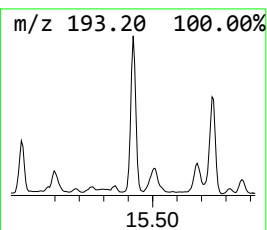
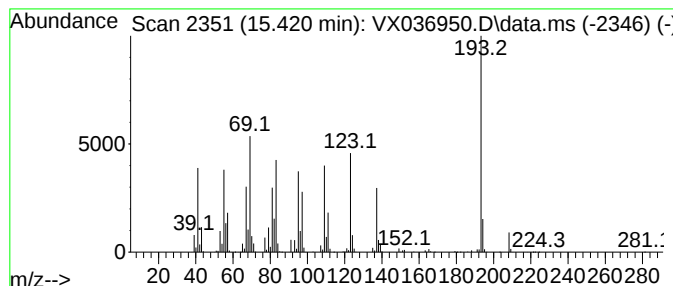
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Quant Title : SW846 8260

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

Peak Number 4 unknown15.420 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	122.31 ug/l	1444050	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	74
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	47
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
4			Iminostilbene	193	C14H11N	000256-96-2	32
5			1H-Pyrazole, 3,5-bis(1,1-dimethy...	208	C13H24N2	125281-21-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

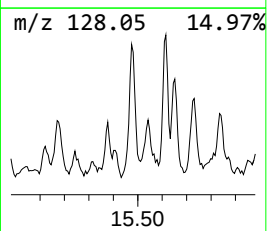
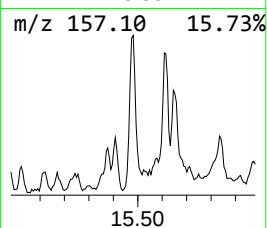
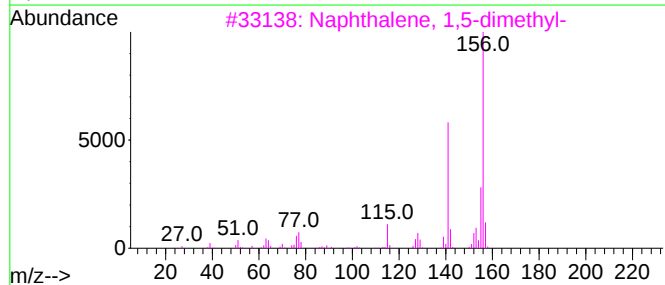
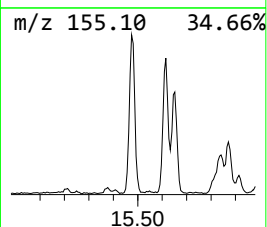
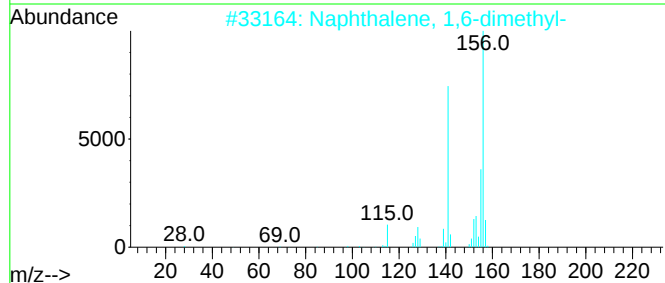
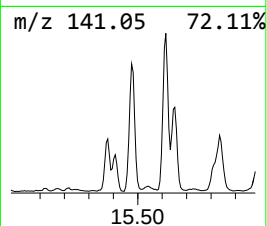
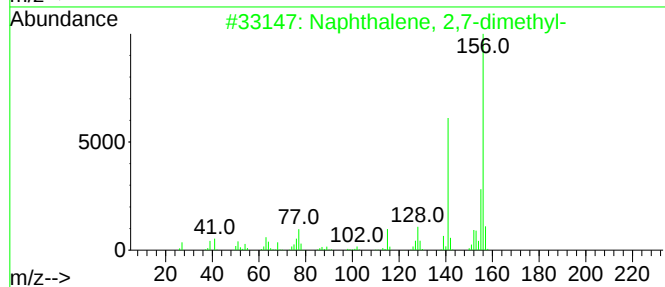
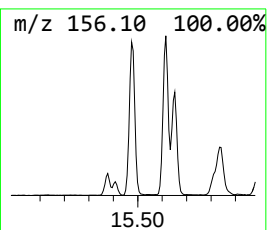
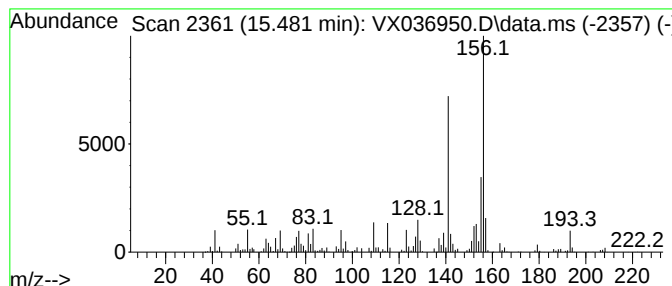
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	48.22 ug/l	569265	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

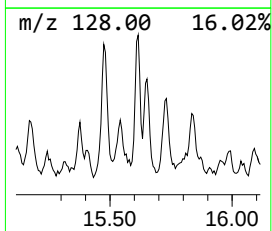
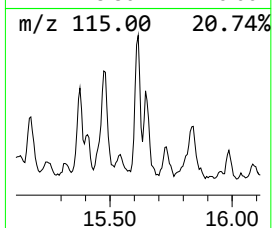
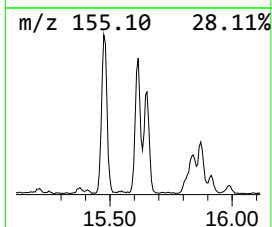
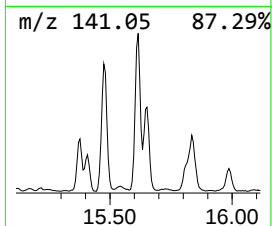
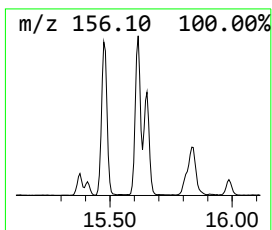
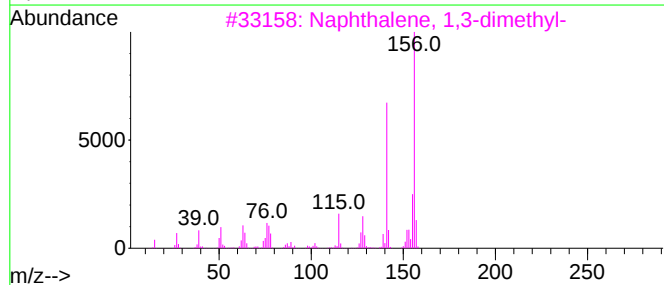
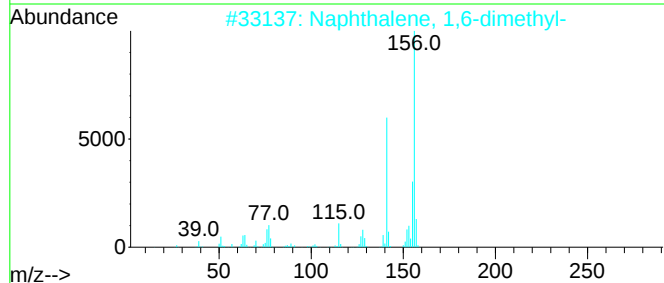
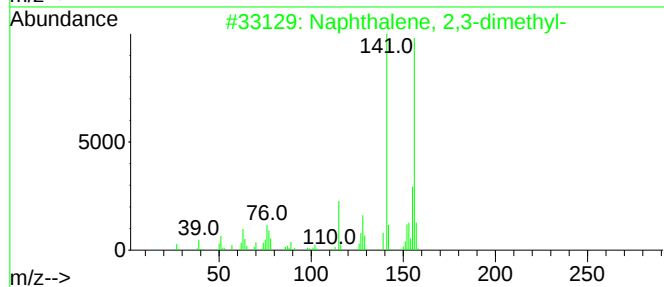
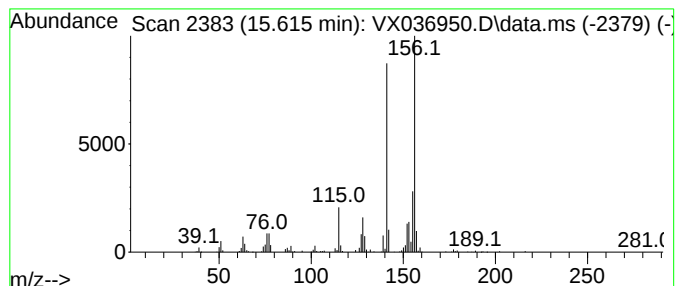
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	29.59 ug/l	349344	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

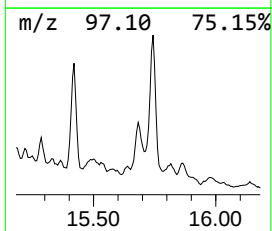
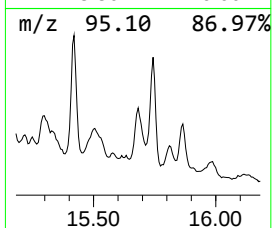
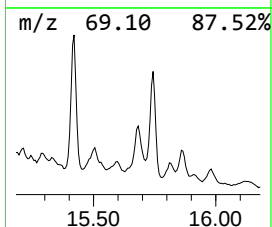
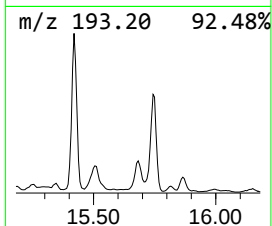
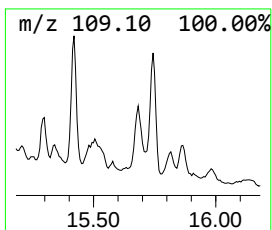
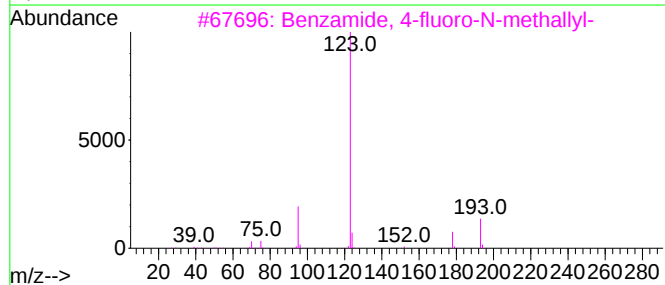
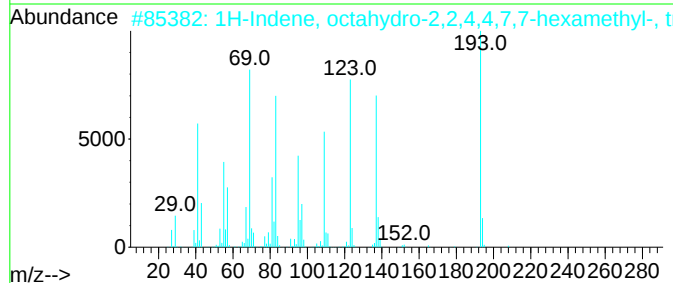
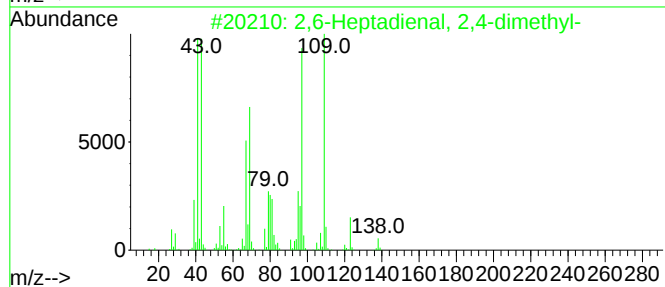
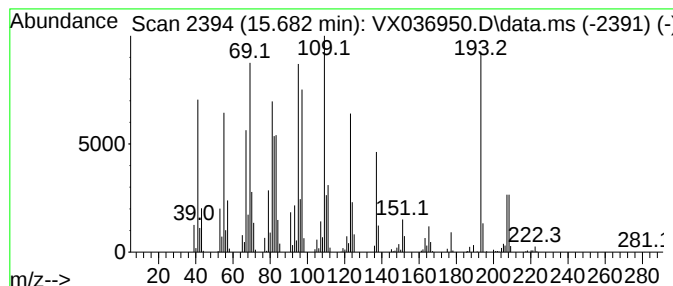
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Quant Title : SW846 8260

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

Peak Number 7 2,6-Heptadienal, 2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.682	52.20 ug/l	616293	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	50
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
3			Benzamide, 4-fluoro-N-methallyl-	193	C11H12FNO	1000340-31-9	30
4			1-Cyclohexanol, 2-(3-methyl-1,3-...	208	C14H24O	1000196-01-6	27
5			1H-Pyrazole, 1-methyl-4-(4,4,5,5...	208	C10H17BN2O2	1000319-69-0	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

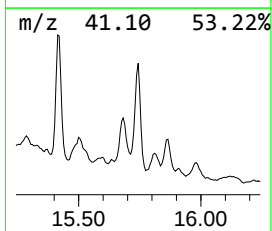
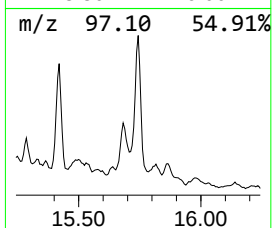
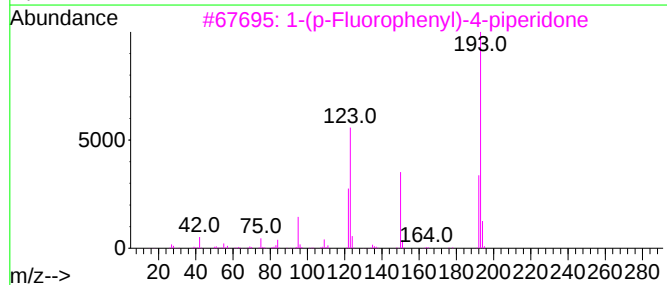
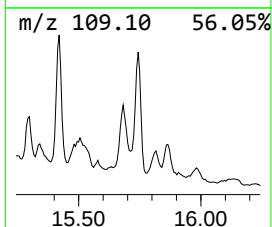
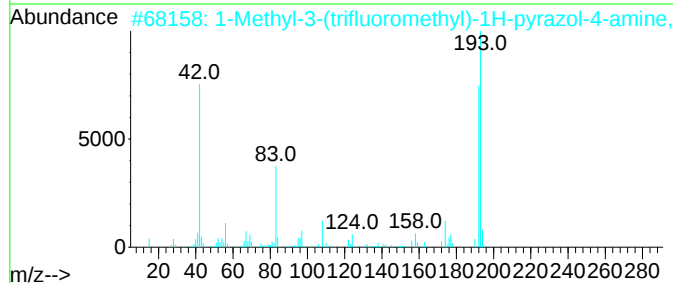
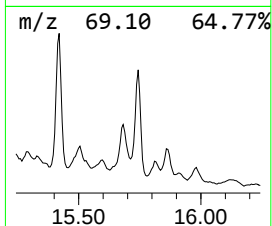
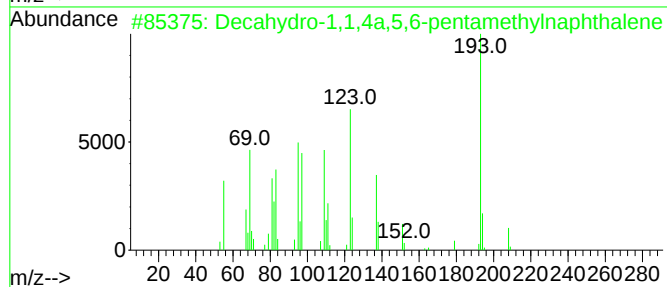
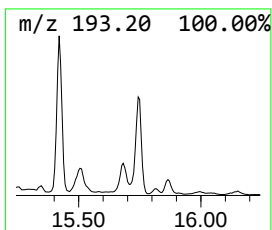
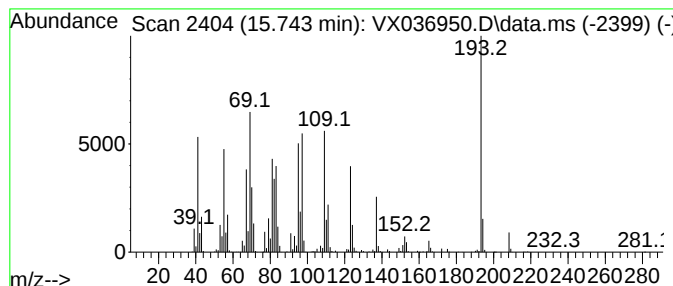
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.743 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	126.35 ug/l	1491800	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	87
2			1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	27
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
4			2-Phenylindolizine	193	C14H11N	025379-20-8	27
5			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

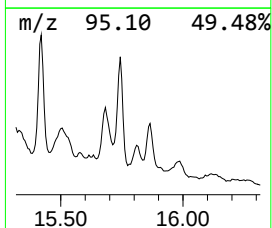
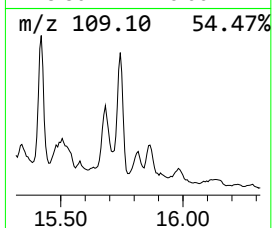
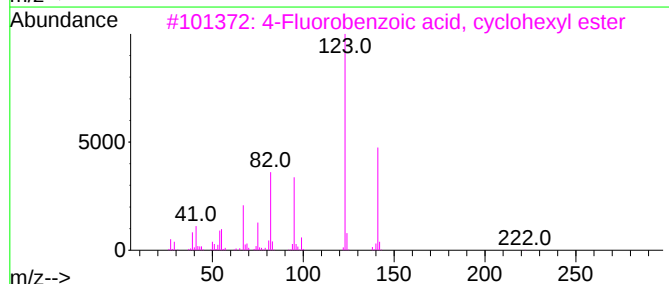
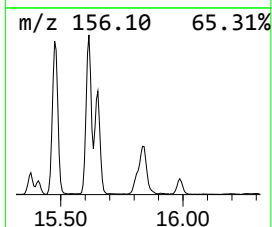
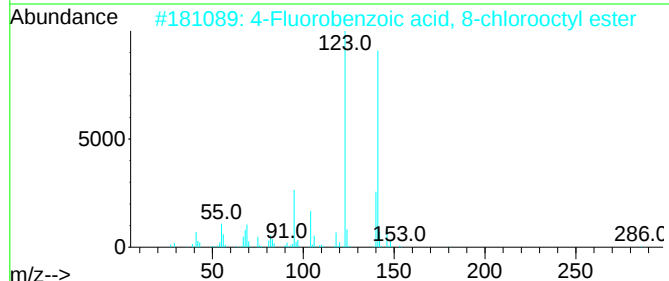
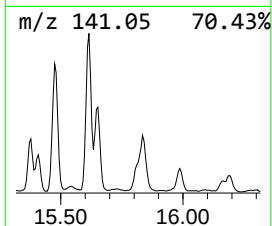
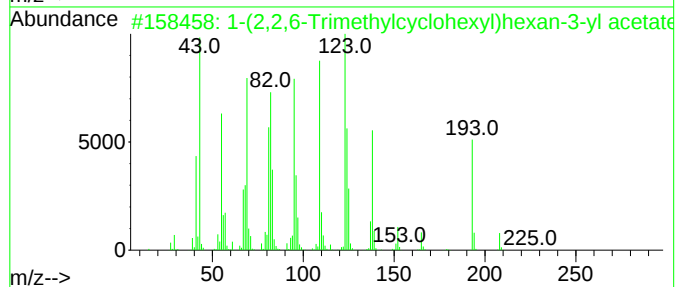
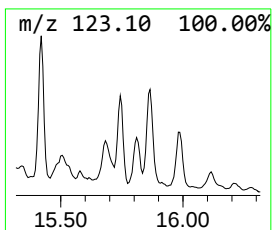
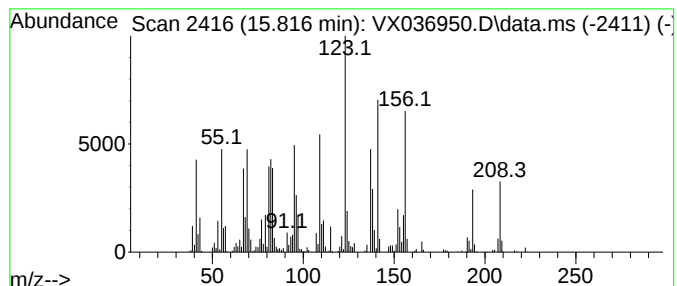
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.816 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.816	30.95 ug/l	365468	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2,2,6-Trimethylcyclohexyl)hex...	268	C17H32O2	1000498-96-1	35
2			4-Fluorobenzoic acid, 8-chlorooc...	286	C15H20ClF02	1000355-67-9	35
3			4-Fluorobenzoic acid, cyclohexyl...	222	C13H15F02	090172-17-1	35
4			2-Fluorobenzoic acid, tridecyl e...	322	C20H31F02	1000279-04-1	35
5			2-Cyclopenten-1-one, 2,3,4,5-tet...	138	C9H14O	054458-61-6	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

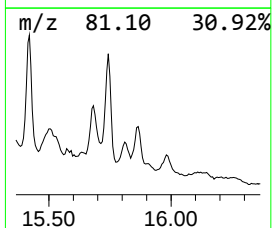
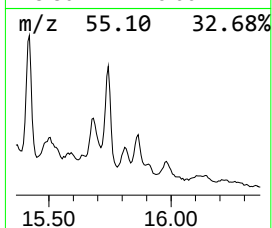
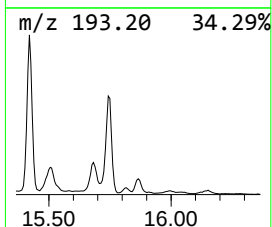
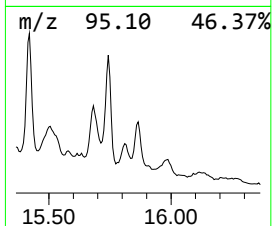
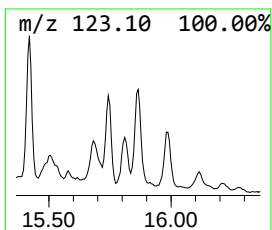
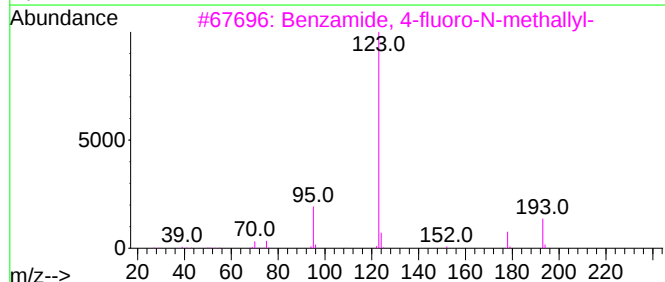
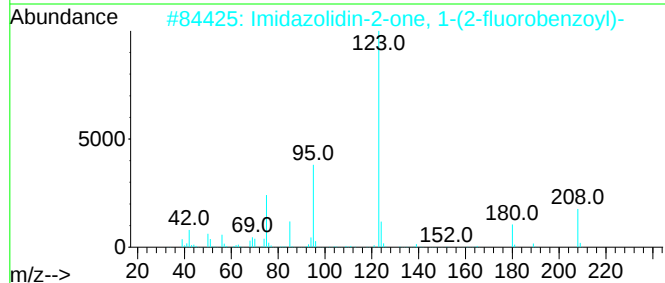
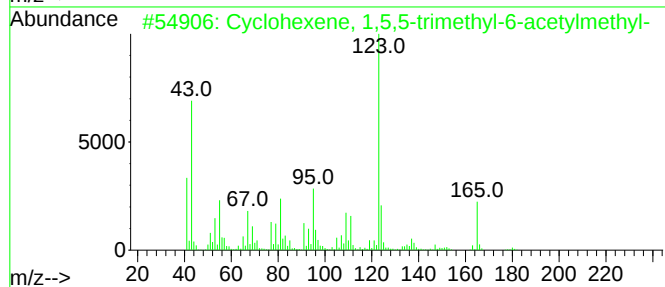
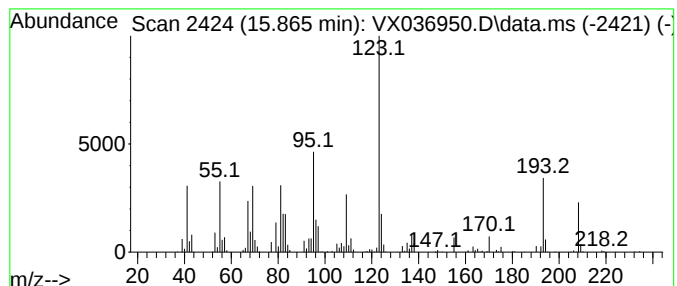
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexene, 1,5,5-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.865	37.72 ug/l	445297	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	59
2			Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1010310-62-2	58
3			Benzamide, 4-fluoro-N-methallyl-	193	C11H12FNO	1000340-31-9	53
4			3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	47
5			Benzoic acid, 4-fluoro-, N'-(5,...	248	C13H13FN2O2	1000350-57-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036950.D
Acq On : 11 Aug 2023 18:51
Operator : JC/MD
Sample : 03972-03
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Bicyclo[2.2.1]h...	14.749	34.0	ug/l	400804	4	12.024	590330	50.0
unknown14.847	14.847	33.7	ug/l	397540	4	12.024	590330	50.0
Decahydro-1,1,4...	14.963	95.3	ug/l	1125680	4	12.024	590330	50.0
unknown15.420	15.420	122.3	ug/l	1444050	4	12.024	590330	50.0
Naphthalene, 2,...	15.481	48.2	ug/l	569265	4	12.024	590330	50.0
Naphthalene, 2,...	15.615	29.6	ug/l	349344	4	12.024	590330	50.0
2,6-Heptadienal...	15.682	52.2	ug/l	616293	4	12.024	590330	50.0
unknown15.743	15.743	126.3	ug/l	1491800	4	12.024	590330	50.0
unknown15.816	15.816	30.9	ug/l	365468	4	12.024	590330	50.0
Cyclohexene, 1,...	15.865	37.7	ug/l	445297	4	12.024	590330	50.0