

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050725\
 Data File : VX046073.D
 Acq On : 07 May 2025 15:26
 Operator : JC/MD
 Sample : Q1980-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3832

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046073.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.575	70	80	84	rBV6	4358	10781	2.09%	0.317%
2	5.373	693	703	720	rBV3	62105	186685	36.13%	5.486%
3	5.538	720	730	743	rVV	87515	250380	48.46%	7.358%
4	5.946	788	797	811	rBV	72261	191951	37.15%	5.641%
5	6.751	921	929	947	rBV	153887	375570	72.70%	11.036%
6	8.641	1233	1239	1251	rBV	327668	516633	100.00%	15.181%
7	10.049	1465	1470	1483	rBV	355658	473420	91.64%	13.912%
8	11.079	1633	1639	1652	rBV	273097	354588	68.63%	10.420%
9	12.018	1788	1793	1804	rBV	349006	426916	82.63%	12.545%
10	12.811	1917	1923	1929	rVB5	4818	7680	1.49%	0.226%
11	12.981	1944	1951	1956	rVB5	3436	5652	1.09%	0.166%
12	13.286	1996	2001	2007	rBV5	6027	10196	1.97%	0.300%
13	13.414	2015	2022	2024	rBV6	5493	10808	2.09%	0.318%
14	13.798	2082	2085	2089	rVB3	7967	9698	1.88%	0.285%
15	13.841	2089	2092	2094	rBV4	4484	5812	1.12%	0.171%
16	14.067	2124	2129	2132	rBV6	6210	11028	2.13%	0.324%
17	14.176	2142	2147	2150	rVV6	4280	8241	1.60%	0.242%
18	14.213	2151	2153	2157	rVB4	6370	6780	1.31%	0.199%
19	14.615	2215	2219	2221	rBV3	10243	14311	2.77%	0.421%
20	14.670	2225	2228	2231	rVV4	9372	10058	1.95%	0.296%
21	14.719	2234	2236	2238	rVV3	5703	5474	1.06%	0.161%
22	14.749	2238	2241	2244	rVV3	20086	21705	4.20%	0.638%
23	14.792	2244	2248	2252	rVB7	14958	23276	4.51%	0.684%
24	14.841	2252	2256	2261	rBV6	15937	30076	5.82%	0.884%
25	14.932	2268	2271	2272	rBV2	8690	10467	2.03%	0.308%
26	14.957	2272	2275	2282	rVB6	20385	37317	7.22%	1.097%
27	15.213	2314	2317	2320	rVB4	14391	17378	3.36%	0.511%
28	15.371	2340	2343	2346	rBV5	8872	14092	2.73%	0.414%
29	15.414	2346	2350	2356	rVB2	61676	87808	17.00%	2.580%
30	15.481	2357	2361	2367	rBV6	18751	42756	8.28%	1.256%
31	15.615	2379	2383	2385	rBV2	16035	24034	4.65%	0.706%
32	15.737	2399	2403	2409	rVB3	61768	100378	19.43%	2.950%
33	16.085	2456	2460	2466	rBV7	17928	38541	7.46%	1.133%
34	16.706	2557	2562	2567	rVB2	34215	62566	12.11%	1.839%

Sum of corrected areas: 3403056

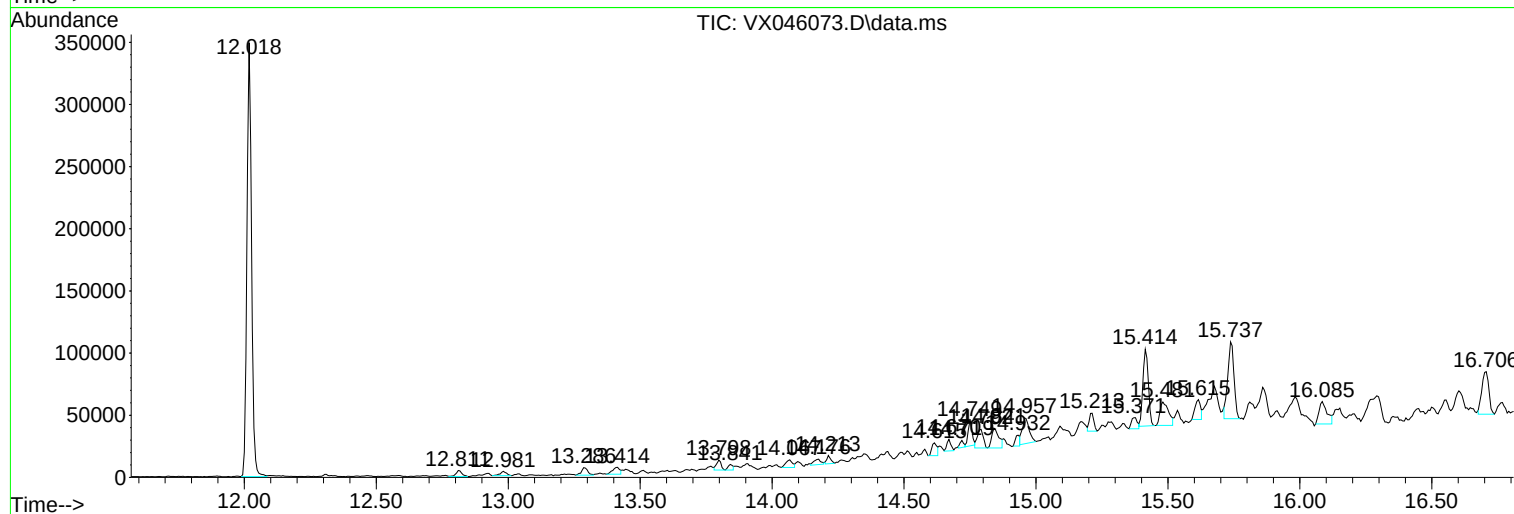
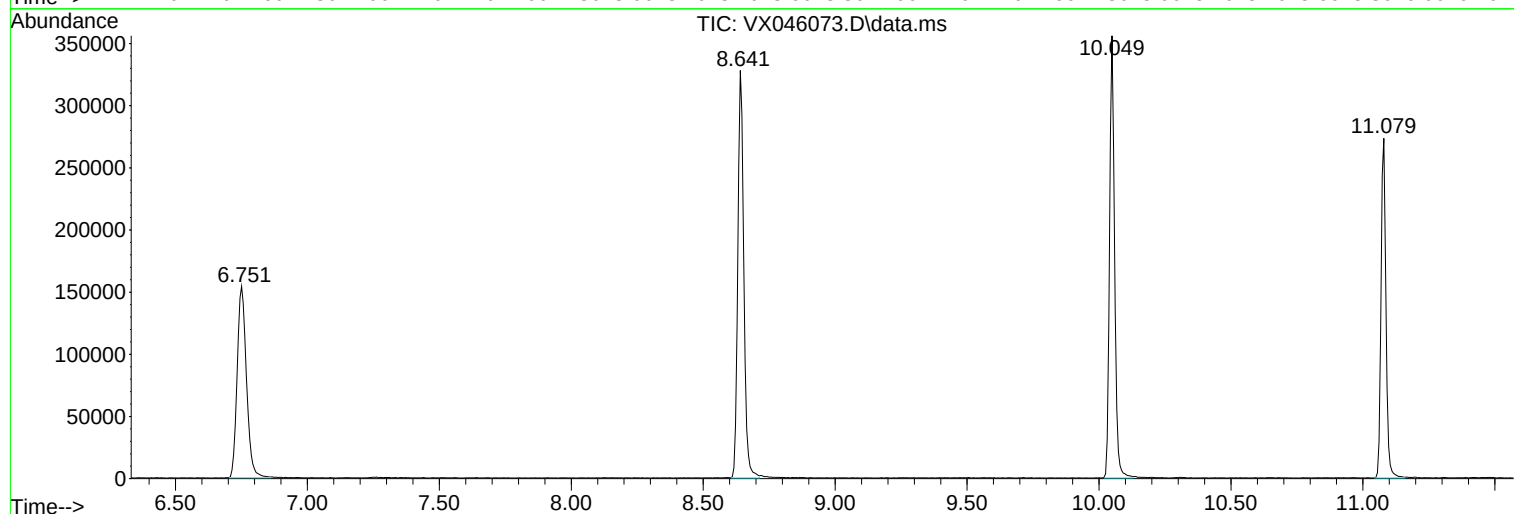
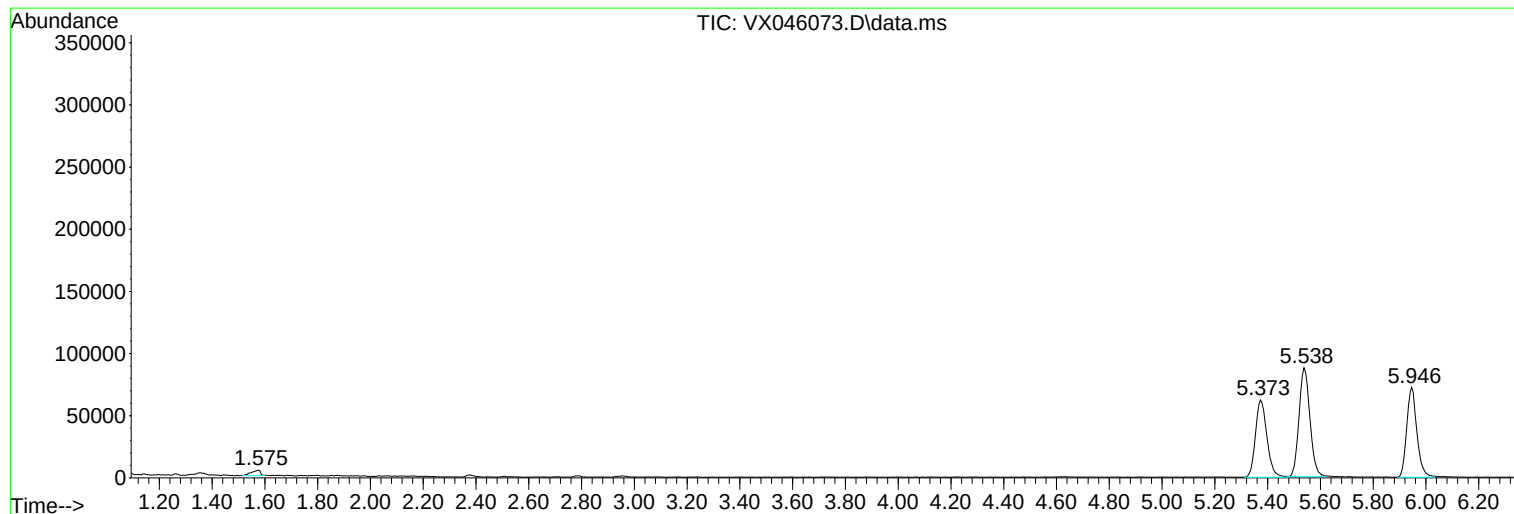
Instrument :
MSVOA_X
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Quant Title : SW846 8260

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



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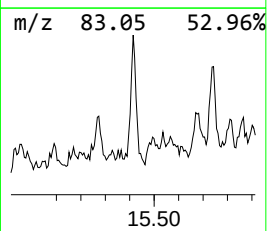
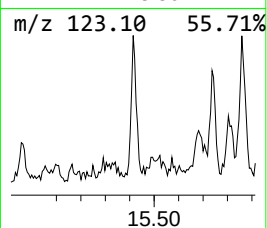
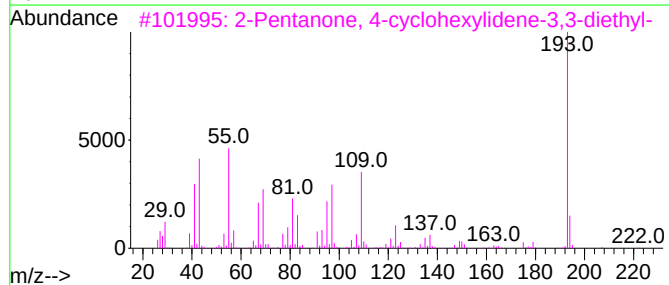
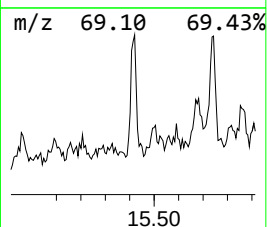
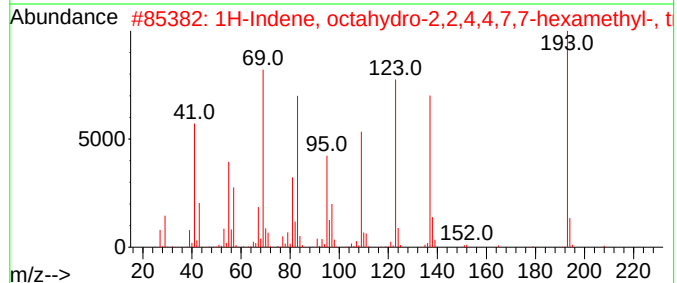
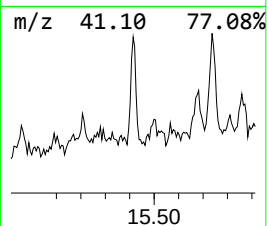
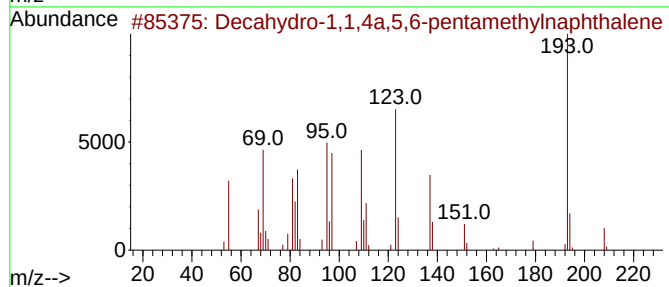
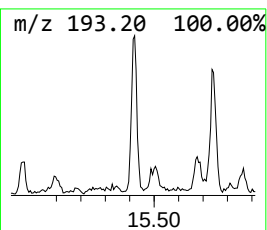
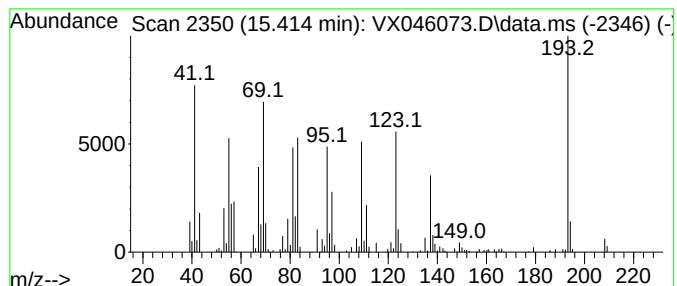
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown15.414 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	10.28 ug/l	87808	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35
4			2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	25
5			1-Methyl-3-(trifluoromethyl)-1H...	193	C7H10F3N3	1000511-73-1	22



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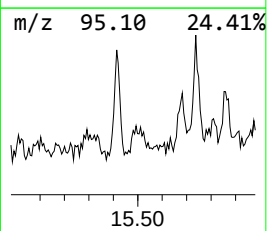
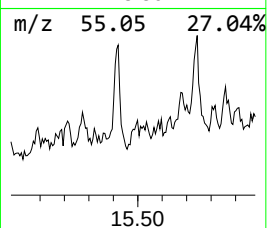
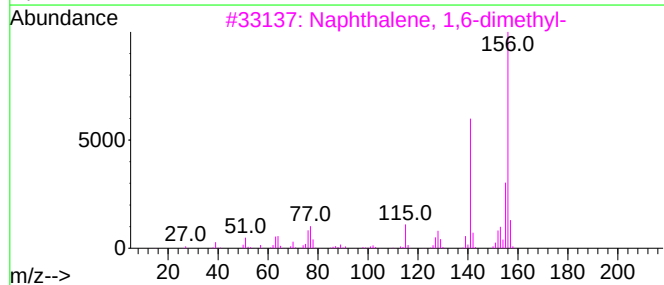
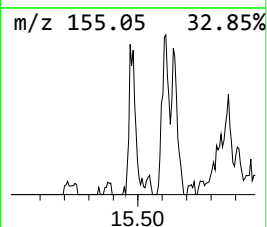
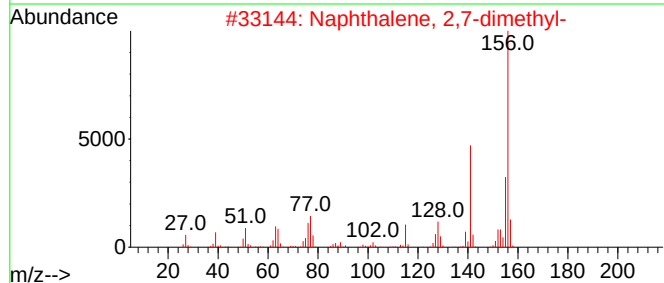
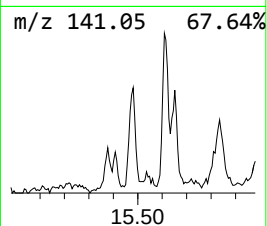
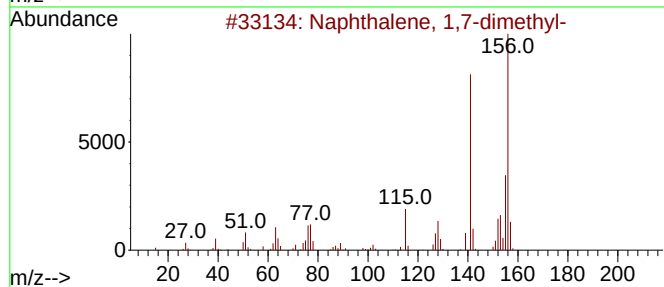
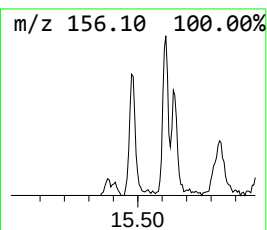
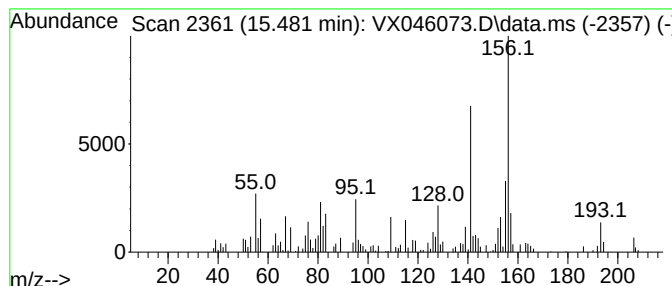
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 1,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	5.01 ug/l	42756	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	86
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	81
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	76
4			1,4-benzenedicarbonitrile, 2,5-d...	156	C10H8N2	1000404-33-1	76
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	70



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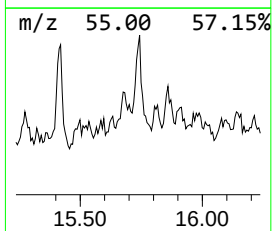
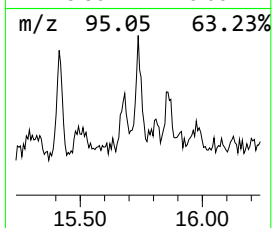
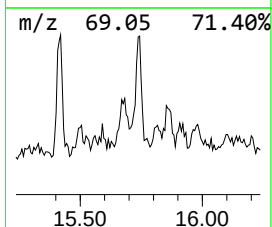
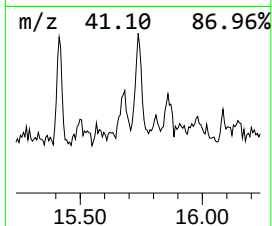
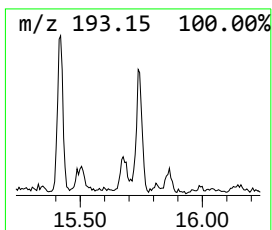
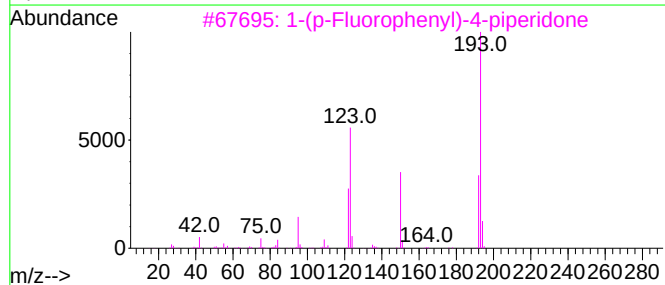
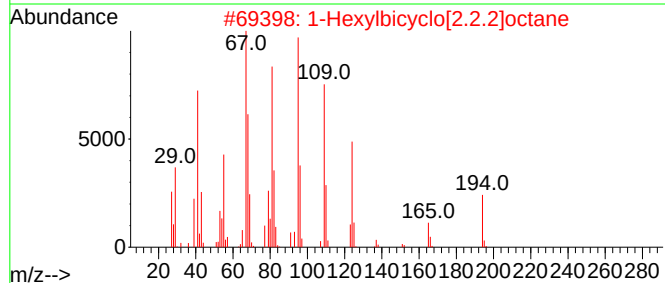
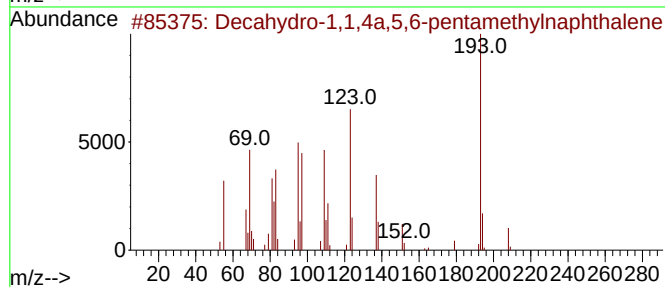
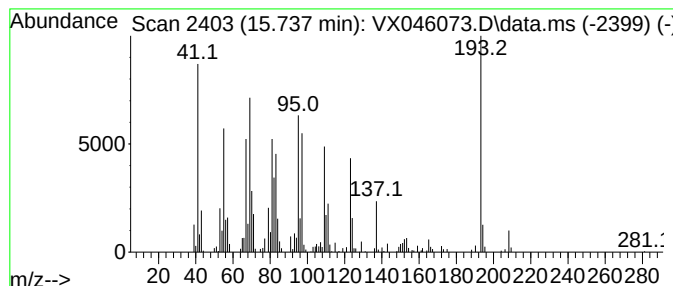
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.737	11.76 ug/l	100378	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	81
2			1-Hexylbicyclo[2.2.2]octane	194	C14H26	1000435-94-2	41
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
4			3-Oxatricyclo[4.1.1.0(2,4)]octan...	152	C10H16O	001686-14-2	22
5			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	22



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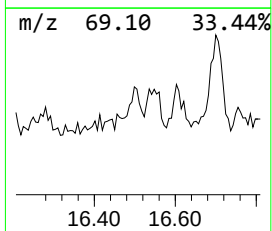
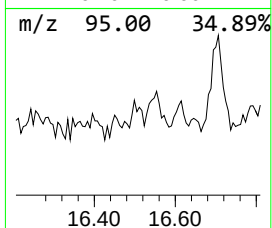
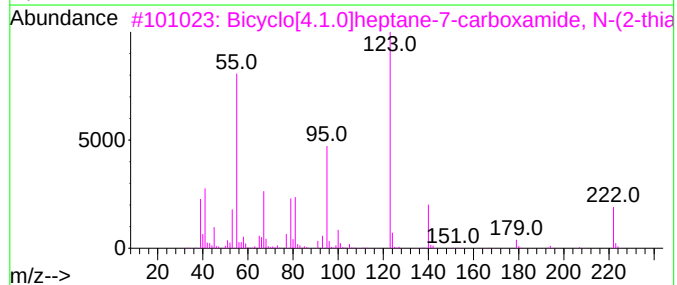
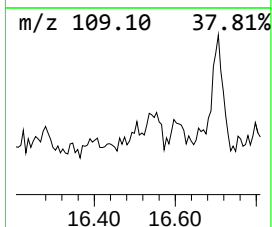
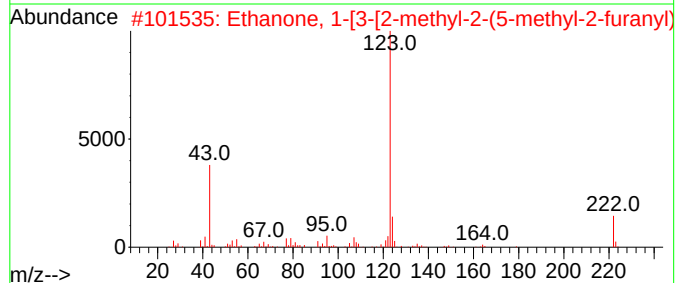
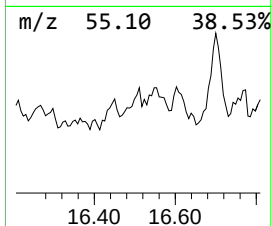
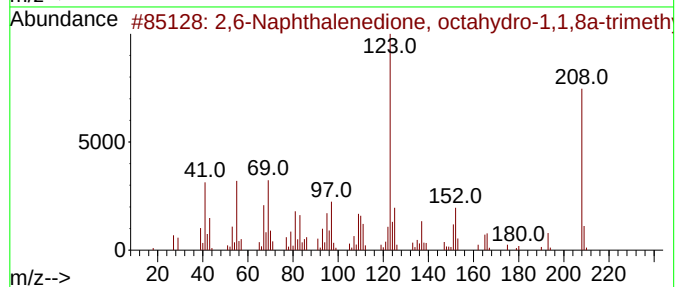
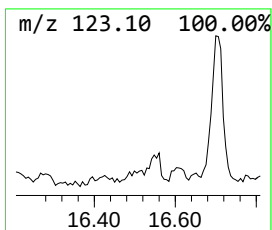
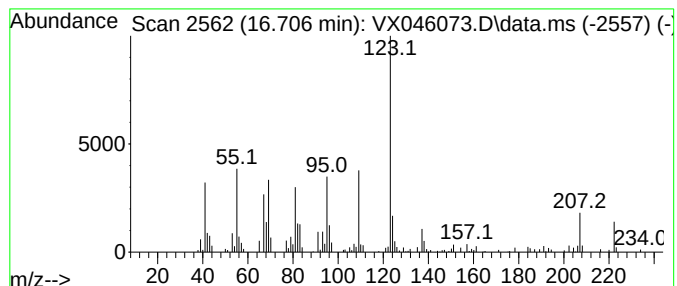
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Peak Number 4 2,6-Naphthalenedione, octah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.706	7.33 ug/l	62566	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-17-5	59
2			Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	55
3			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	53
4			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	52
5			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown15.414	15.414	10.3	ug/l	87808	4	12.018	426916	50.0
Naphthalene, 1,...	15.481	5.0	ug/l	42756	4	12.018	426916	50.0
Decahydro-1,1,4...	15.737	11.8	ug/l	100378	4	12.018	426916	50.0
2,6-Naphthalene...	16.706	7.3	ug/l	62566	4	12.018	426916	50.0