

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
 Data File : VX038458.D
 Acq On : 24 Oct 2023 16:18
 Operator : JC/MD
 Sample : 05022-01
 Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 OILY-DEBRIS

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\82X100523W.M
 Title : SW846 8260

Signal : TIC: VX038458.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.569	68	79	80	rBV4	13744	35719	3.78%	0.601%
2	5.391	695	706	721	rBV	94485	275340	29.11%	4.629%
3	5.544	721	731	748	rVB	159084	457432	48.37%	7.690%
4	5.958	788	799	812	rBV	104533	278055	29.40%	4.675%
5	6.757	919	930	943	rBV	252821	616039	65.14%	10.357%
6	8.647	1233	1240	1256	rBV	544056	861566	91.10%	14.484%
7	10.055	1465	1471	1489	rBV	556537	810913	85.75%	13.633%
8	11.085	1634	1640	1652	rBV	504193	662783	70.08%	11.143%
9	12.024	1789	1794	1804	rBV	767283	945708	100.00%	15.899%
10	12.262	1825	1833	1837	rBV6	3268	10580	1.12%	0.178%
11	13.292	1999	2002	2008	rVB6	7609	11896	1.26%	0.200%
12	13.414	2014	2022	2025	rBV6	8575	20270	2.14%	0.341%
13	13.591	2047	2051	2055	rBV3	9656	13906	1.47%	0.234%
14	13.798	2082	2085	2089	rVB5	11383	14638	1.55%	0.246%
15	13.841	2089	2092	2095	rBV4	8415	11848	1.25%	0.199%
16	13.920	2100	2105	2109	rVB6	7934	17704	1.87%	0.298%
17	14.067	2126	2129	2132	rVB4	7551	9856	1.04%	0.166%
18	14.170	2142	2146	2150	rBV5	14719	18391	1.94%	0.309%
19	14.225	2151	2155	2157	rBV5	12362	17023	1.80%	0.286%
20	14.256	2157	2160	2164	rVV3	15243	20778	2.20%	0.349%
21	14.439	2187	2190	2195	rVB3	15244	19217	2.03%	0.323%
22	14.579	2210	2213	2216	rVB5	9261	11465	1.21%	0.193%
23	14.615	2216	2219	2222	rBV4	13811	22797	2.41%	0.383%
24	14.749	2238	2241	2244	rBV4	28290	36117	3.82%	0.607%
25	14.792	2245	2248	2253	rVV6	18811	26985	2.85%	0.454%
26	14.847	2253	2257	2267	rVB9	21724	57329	6.06%	0.964%
27	14.963	2273	2276	2284	rVB2	32459	46535	4.92%	0.782%
28	15.414	2346	2350	2355	rVB	103456	147272	15.57%	2.476%
29	15.682	2390	2394	2398	rBV5	38823	69555	7.35%	1.169%
30	15.743	2400	2404	2409	rVB	115826	179070	18.94%	3.010%
31	15.865	2420	2424	2431	rBV5	39574	80782	8.54%	1.358%
32	16.706	2557	2562	2567	rVB2	72573	140637	14.87%	2.364%

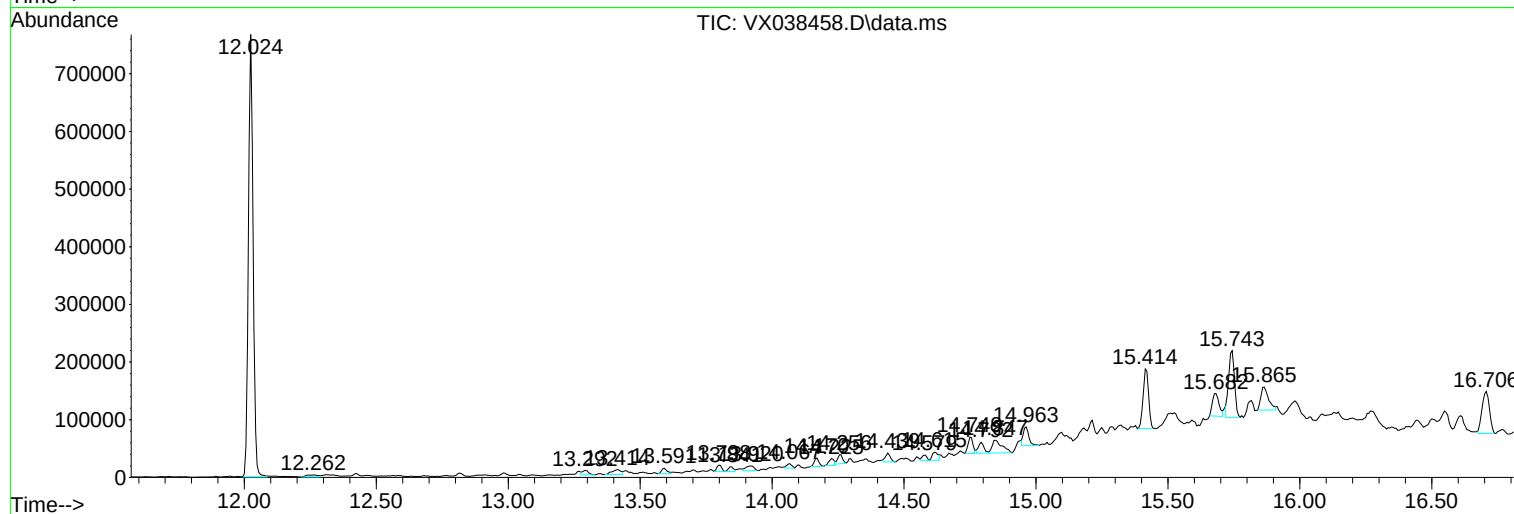
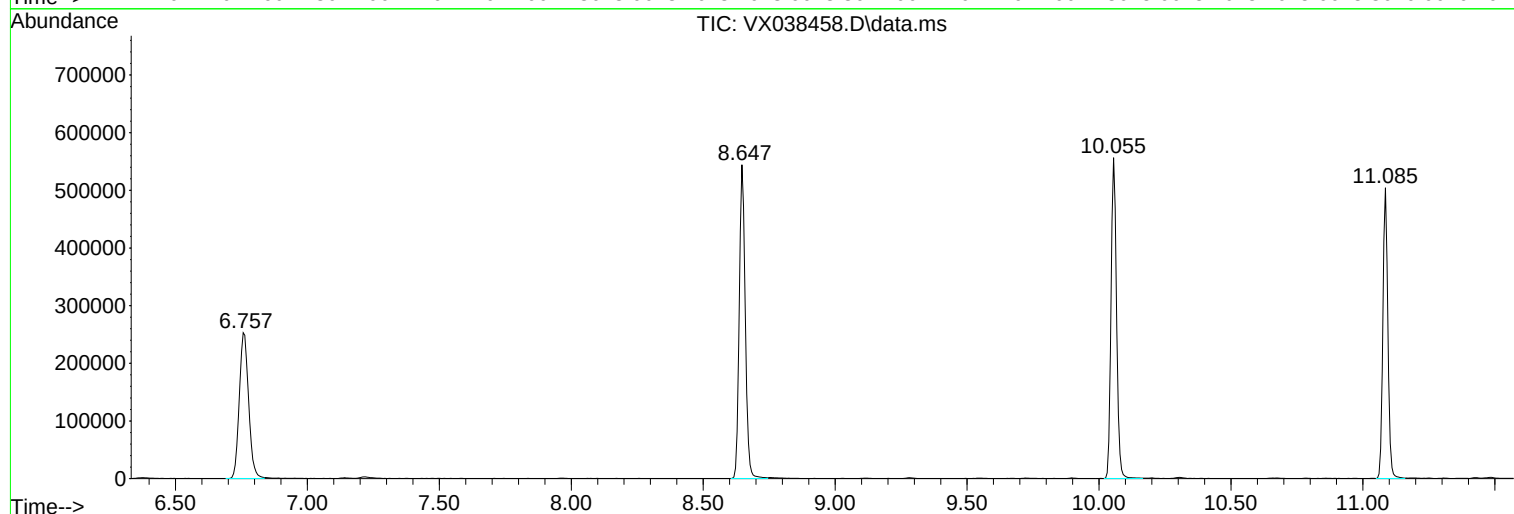
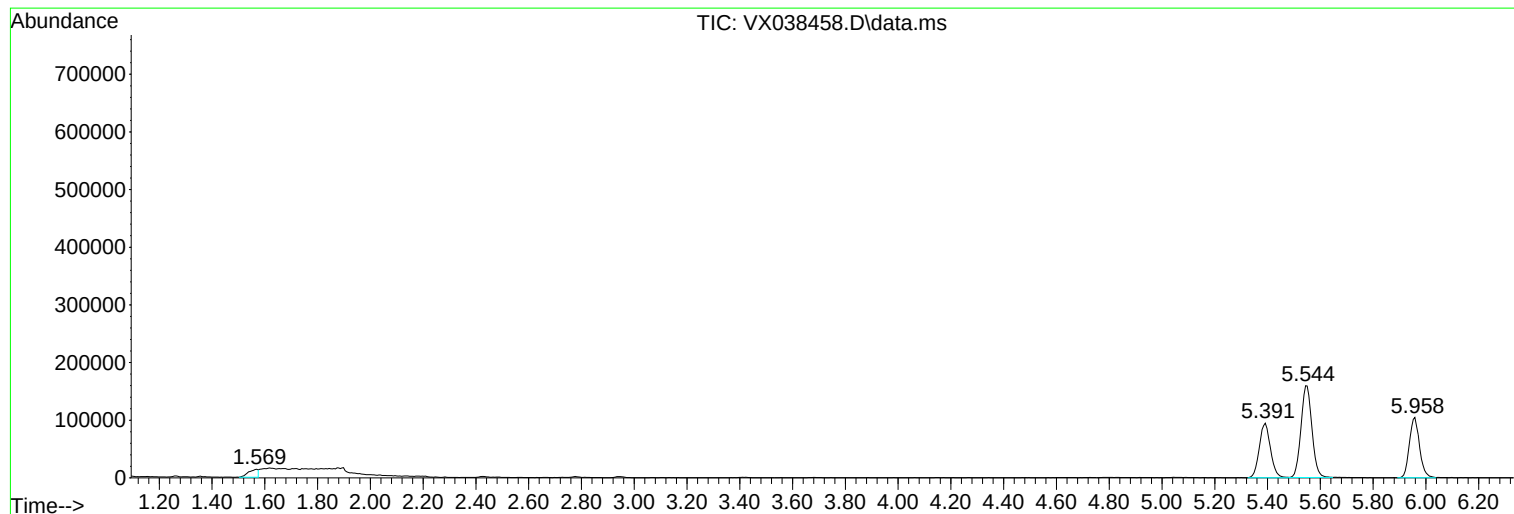
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Instrument :
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OILY-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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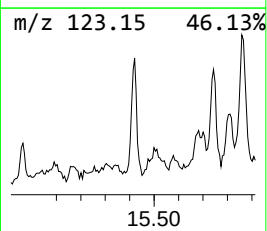
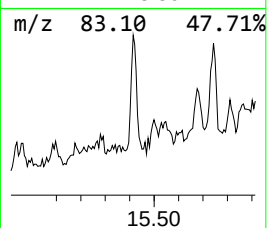
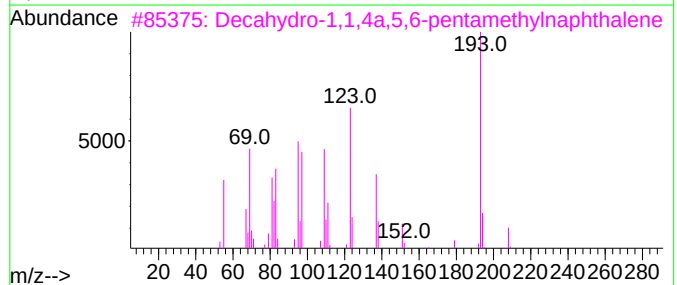
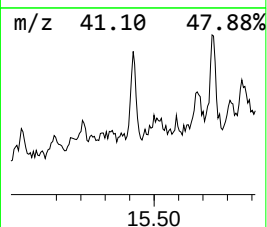
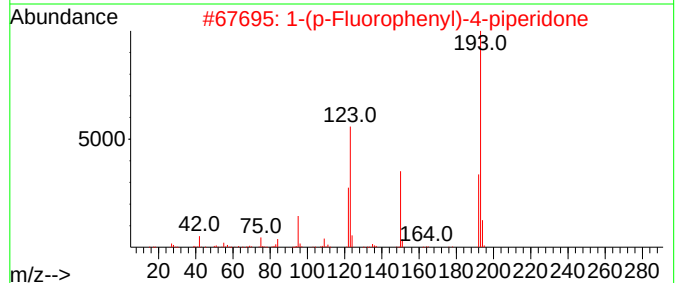
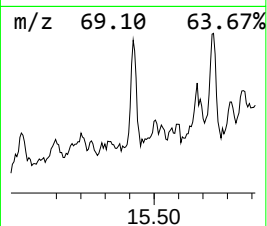
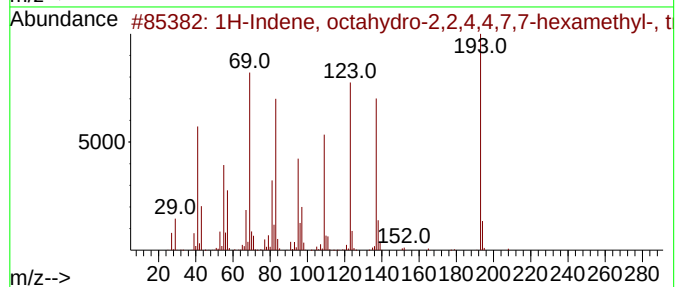
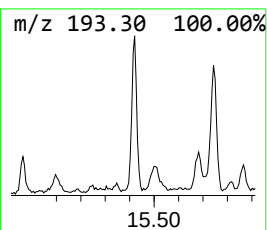
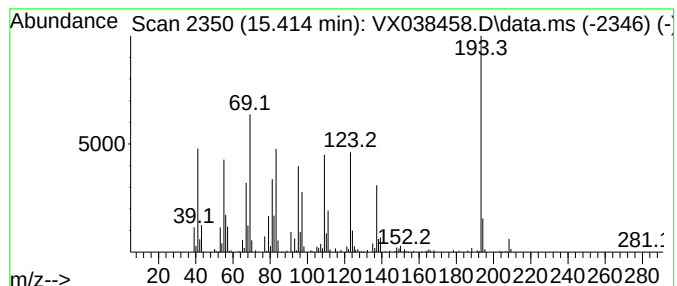
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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	7.79 ug/l	147272	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
4			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	25
5			2-Anthracenamine	193	C14H11N	000613-13-8	22



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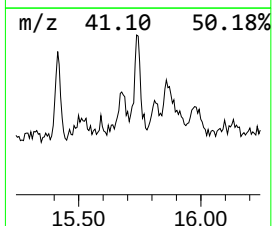
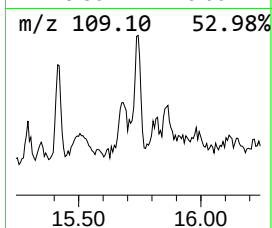
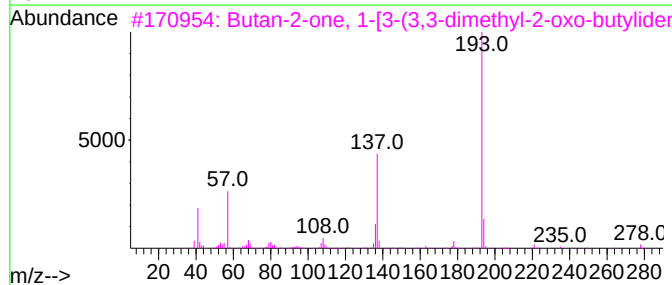
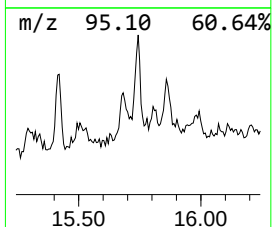
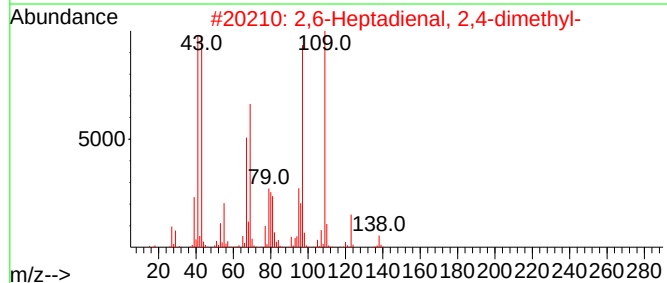
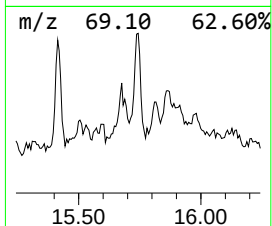
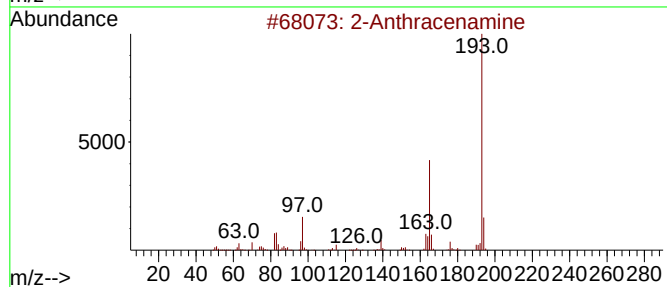
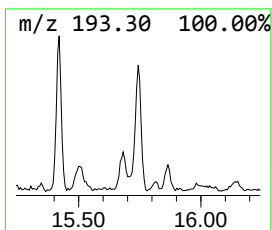
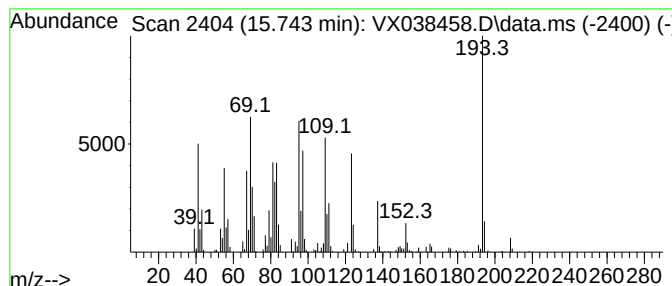
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown15.743 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	9.47 ug/l	179070	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Anthracenamine			193	C14H11N	000613-13-8	27
2	2,6-Heptadienal, 2,4-dimethyl-			138	C9H14O	085136-08-9	20
3	Butan-2-one, 1-[3-(3,3-dimethyl-...			278	C16H26N2O2	1000303-34-2	14
4	[1,1'-Biphenyl]-4-acetonitrile			193	C14H11N	031603-77-7	14
5	trans-4a-Methyl-decahydronaphtha...			152	C11H20	002547-27-5	11



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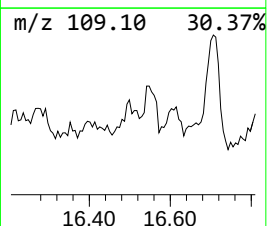
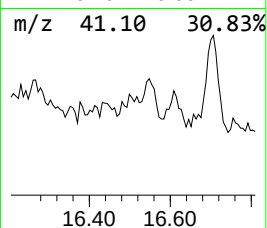
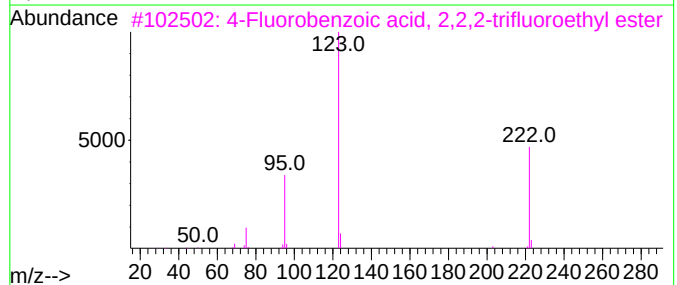
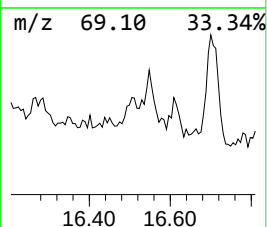
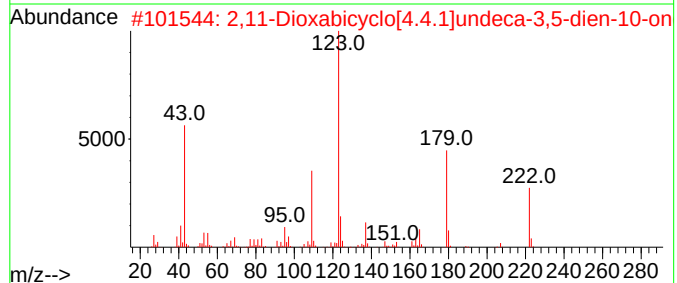
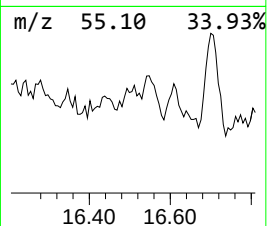
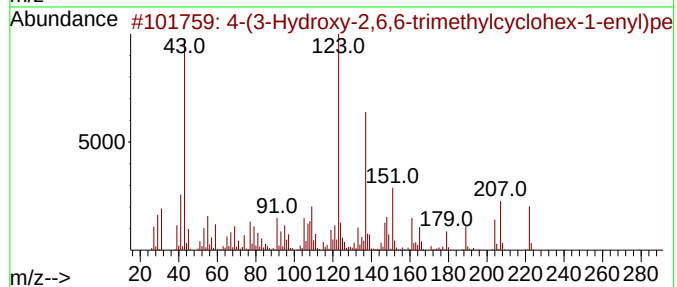
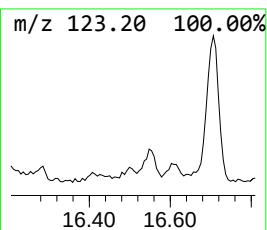
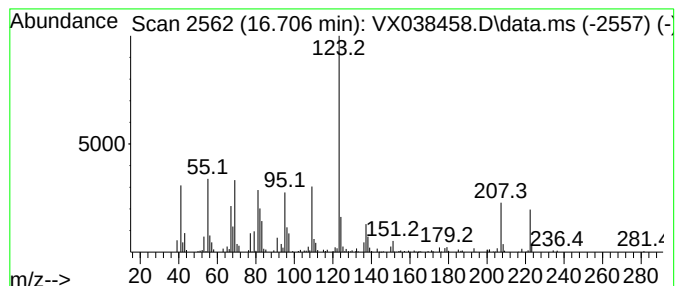
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Quant Title : SW846 8260

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

Peak Number 3 4-(3-Hydroxy-2,6,6-trimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.706	7.44 ug/l	140637	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(3-Hydroxy-2,6,6-trimethylcycl...	222	C14H22O2	097306-57-5	59
2			2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
3			4-Fluorobenzoic acid, 2,2,2-trif...	222	C9H6F4O2	1000325-53-2	47
4			.beta.-Chloro-para-fluoropropiop...	186	C9H8ClFO	000347-93-3	43
5			4(1H)-Pyrimidinone, 6-(1-methyle...	180	C9H12N2O2	1000503-76-7	43



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown15.743	15.743	9.5	ug/l	179070	4	12.024	945708	50.0
4-(3-Hydroxy-2,...	16.706	7.4	ug/l	140637	4	12.024	945708	50.0