

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
 Data File : VX035444.D
 Acq On : 01 May 2023 16:41
 Operator : JC/MD
 Sample : 02522-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-1A

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	26	31	41	rBV3	8588	25926	2.33%	0.325%
2	5.385	692	705	720	rBV2	123408	359081	32.22%	4.499%
3	5.550	720	732	750	rVB	224449	635396	57.02%	7.961%
4	5.958	786	799	808	rBV	138203	358895	32.21%	4.497%
5	6.038	808	812	830	rVB4	10089	27618	2.48%	0.346%
6	6.763	921	931	946	rBV	343758	825811	74.11%	10.347%
7	8.580	1223	1229	1234	rBV	17667	29480	2.65%	0.369%
8	8.647	1234	1240	1250	rVV	733272	1114300	100.00%	13.961%
9	10.055	1465	1471	1486	rBV	734192	994361	89.24%	12.459%
10	10.305	1504	1512	1516	rBV2	8702	13511	1.21%	0.169%
11	11.079	1634	1639	1650	rBV	615727	798727	71.68%	10.008%
12	11.616	1722	1727	1732	rBV2	7951	11388	1.02%	0.143%
13	11.756	1745	1750	1756	rVB	27975	36948	3.32%	0.463%
14	12.024	1788	1794	1801	rBV	787634	1009230	90.57%	12.645%
15	12.085	1801	1804	1810	rVB	8555	13044	1.17%	0.163%
16	12.244	1822	1830	1833	rBV4	26960	49955	4.48%	0.626%
17	12.317	1839	1842	1853	rVB7	16108	35844	3.22%	0.449%
18	12.616	1886	1891	1894	rBV3	9948	14972	1.34%	0.188%
19	12.695	1901	1904	1912	rVB	11026	18064	1.62%	0.226%
20	12.853	1915	1930	1933	rBV4	38294	128122	11.50%	1.605%
21	13.170	1978	1982	1987	rVB3	13211	19488	1.75%	0.244%
22	13.286	1993	2001	2006	rBV7	18945	48370	4.34%	0.606%
23	13.426	2020	2024	2034	rVB4	26462	55239	4.96%	0.692%
24	13.579	2047	2049	2059	rVB7	7922	17410	1.56%	0.218%
25	13.774	2072	2081	2089	rBV	204305	289633	25.99%	3.629%
26	14.640	2215	2223	2232	rVB	161895	237582	21.32%	2.977%
27	14.780	2239	2246	2253	rBV	157596	209441	18.80%	2.624%
28	15.207	2307	2316	2321	rBV	24728	43388	3.89%	0.544%
29	15.377	2339	2344	2348	rBV	35969	57363	5.15%	0.719%
30	15.481	2355	2361	2366	rBV2	38314	66523	5.97%	0.833%
31	15.615	2378	2383	2387	rBV	57665	92004	8.26%	1.153%
32	15.652	2387	2389	2397	rVB	27858	38269	3.43%	0.479%
33	15.841	2411	2420	2429	rVB2	23289	63693	5.72%	0.798%
34	15.987	2437	2444	2451	rBV3	20198	38491	3.45%	0.482%
35	16.091	2456	2461	2467	rVB2	11688	18968	1.70%	0.238%
36	16.200	2474	2479	2485	rVB6	8225	15618	1.40%	0.196%

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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\82X042523W.M
Title : SW846 8260

37	16.328	2492	2500	2512	rBV3	59780	128890	11.57%	1.615%
38	16.603	2541	2545	2549	rVB6	7978	14121	1.27%	0.177%
39	16.664	2550	2555	2566	rVB6	10803	26080	2.34%	0.327%

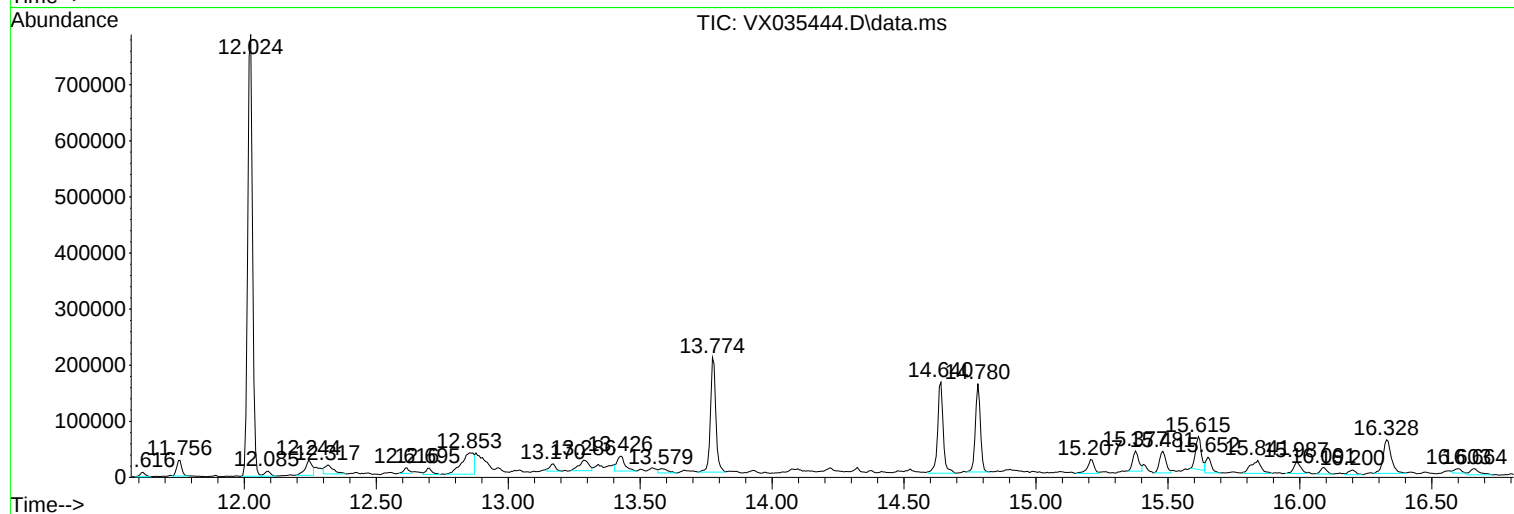
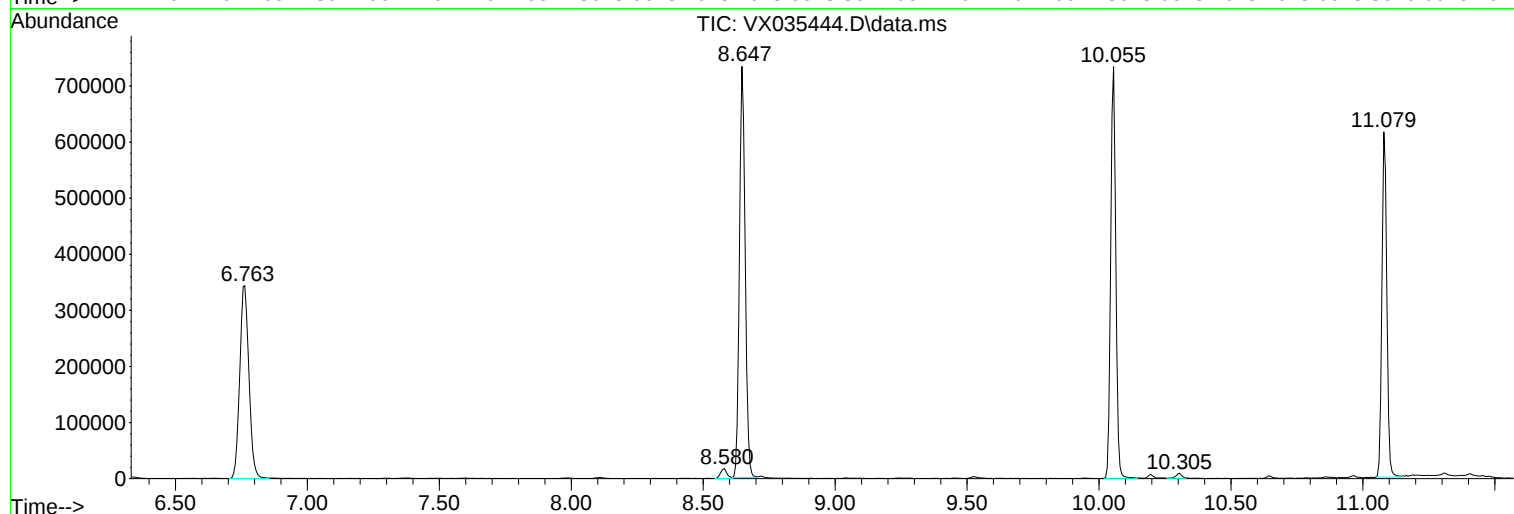
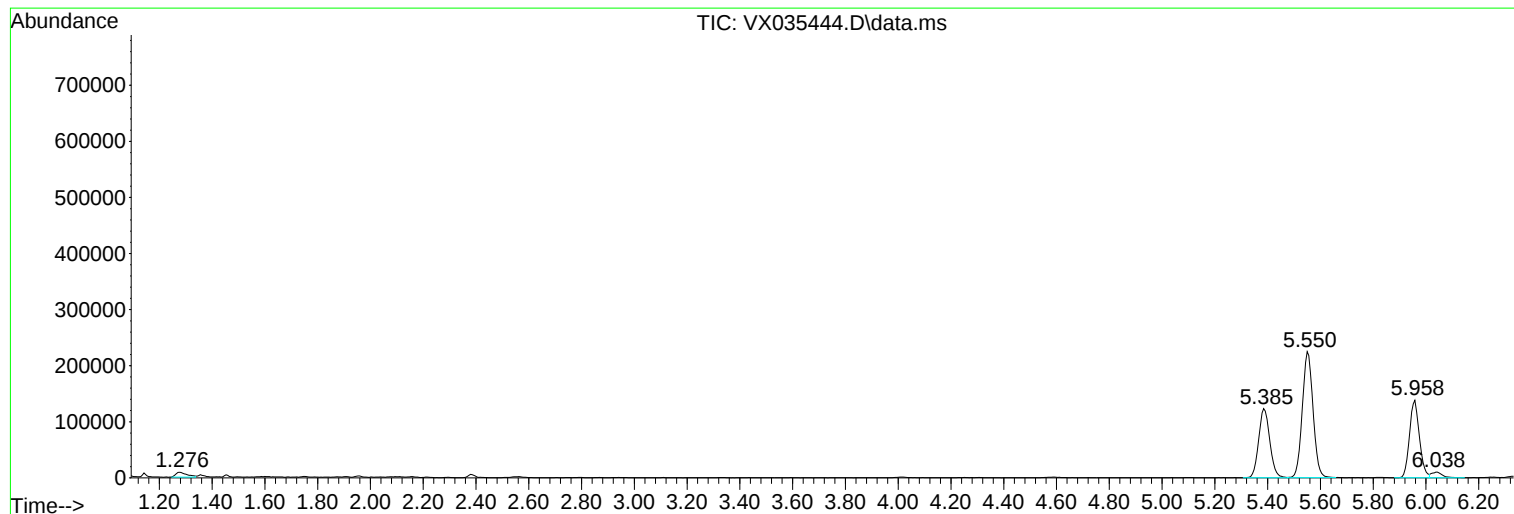
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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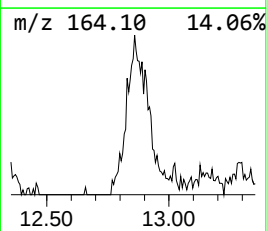
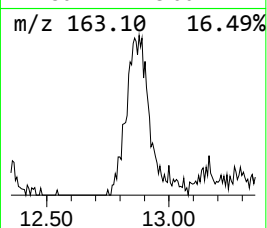
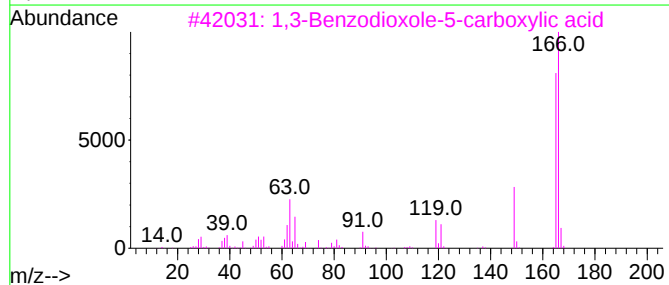
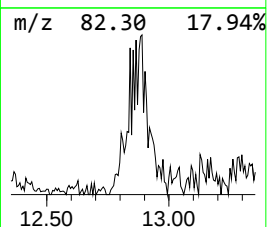
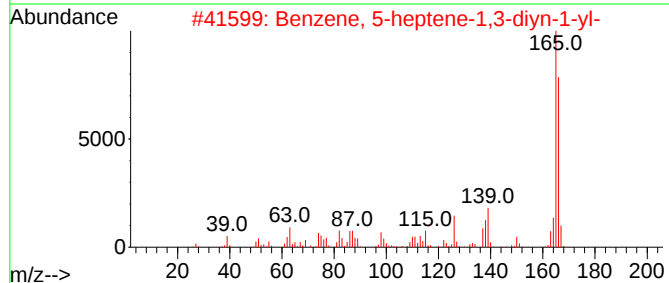
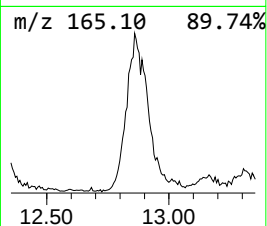
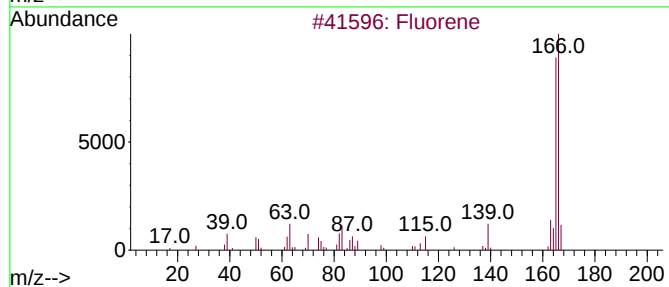
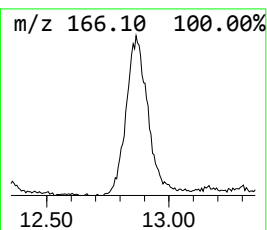
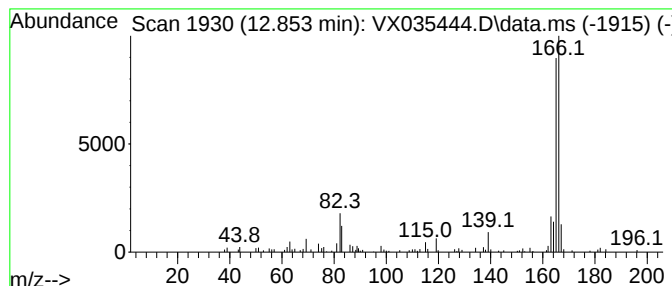
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.853	6.35 ug/l	128122	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluorene	166	C13H10	000086-73-7	90
2			Benzene, 5-heptene-1,3-diyn-1-yl-	166	C13H10	013678-98-3	72
3			1,3-Benzodioxole-5-carboxylic acid	166	C8H6O4	000094-53-1	59
4			Benzaldehyde, 3,4-dimethoxy-	166	C9H10O3	000120-14-9	59
5			Fluorene-9-methanol	196	C14H12O	024324-17-2	53



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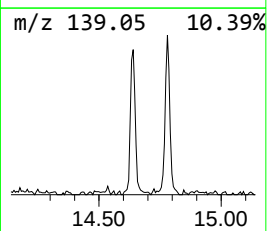
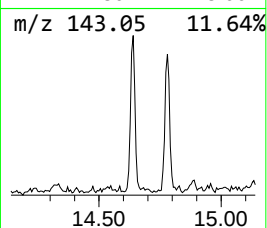
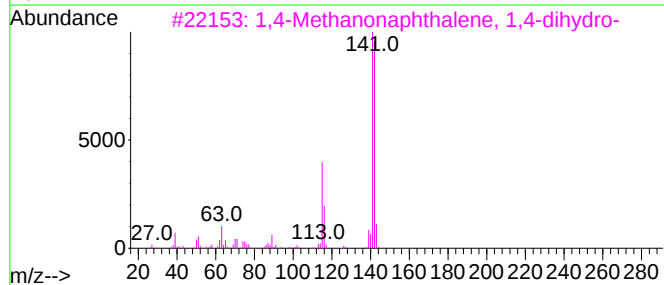
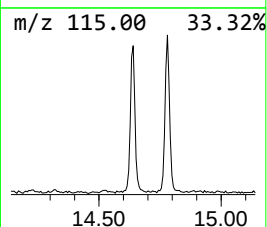
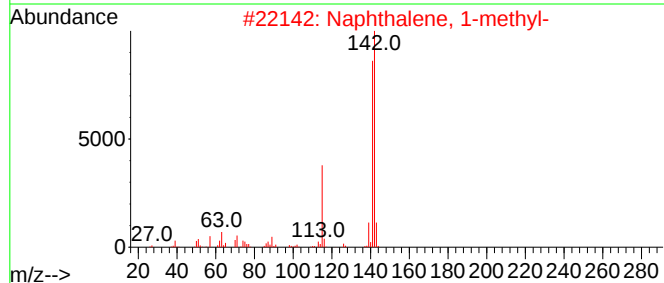
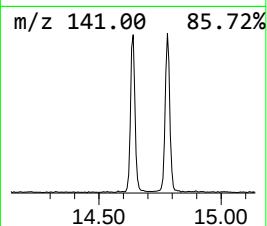
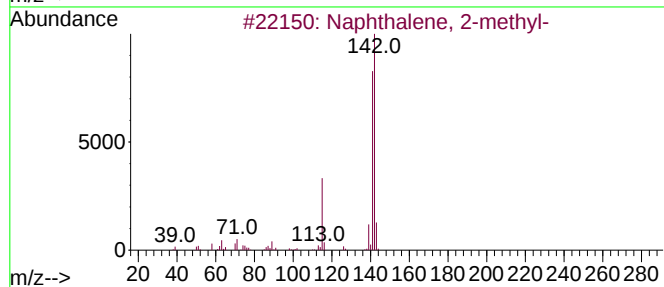
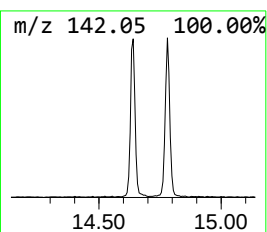
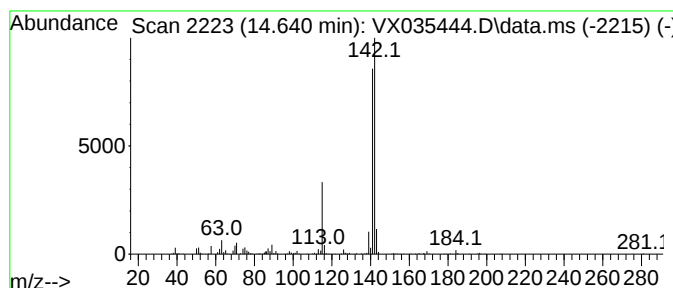
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	11.77 ug/l	237582	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1A

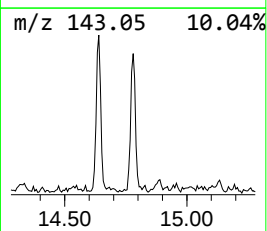
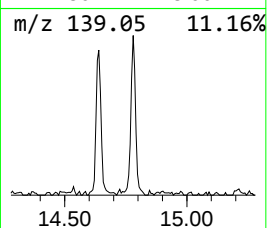
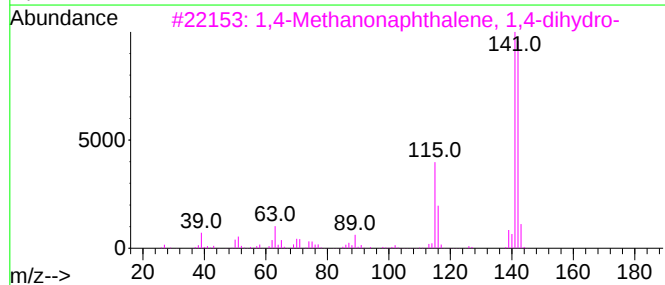
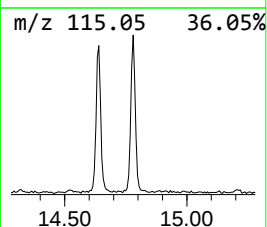
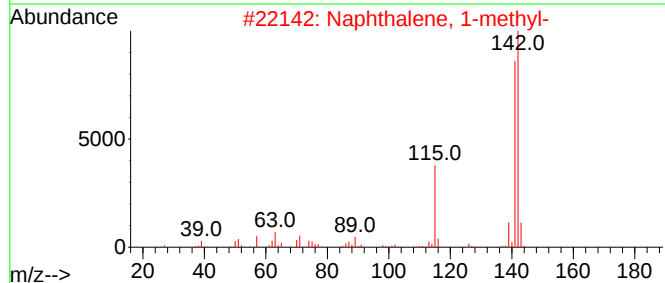
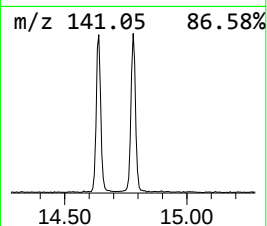
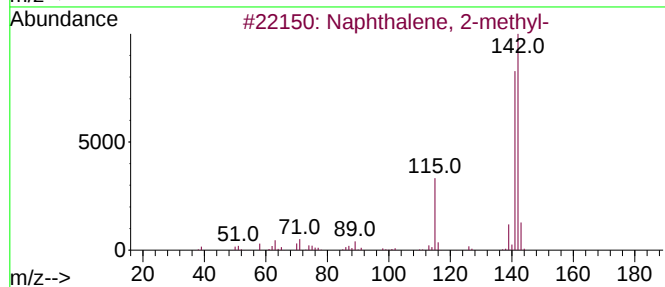
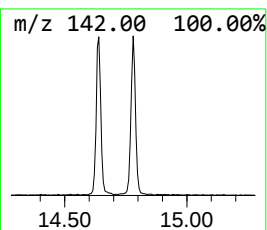
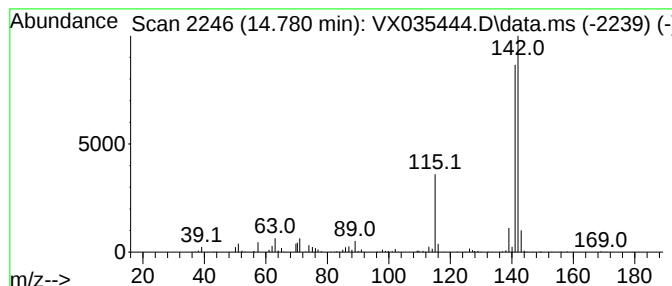
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	10.38 ug/l	209441	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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Instrument :
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ClientSampleId :
MW-1A

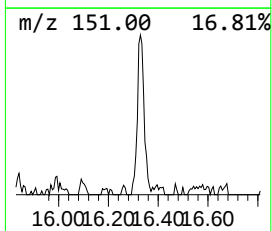
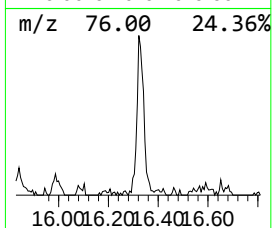
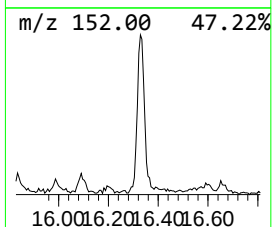
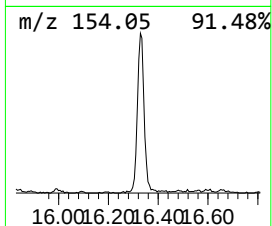
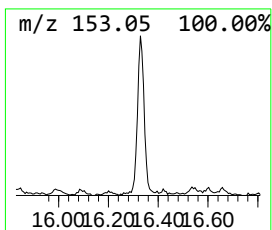
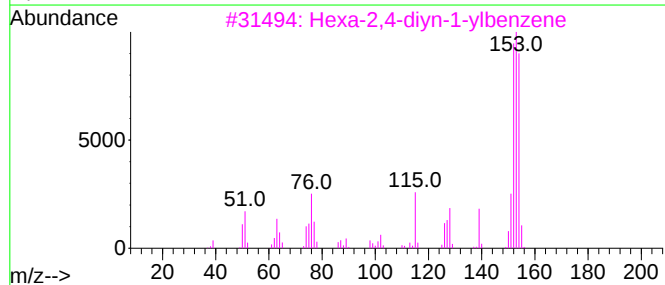
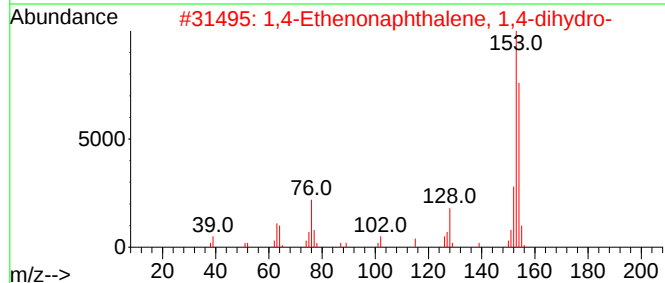
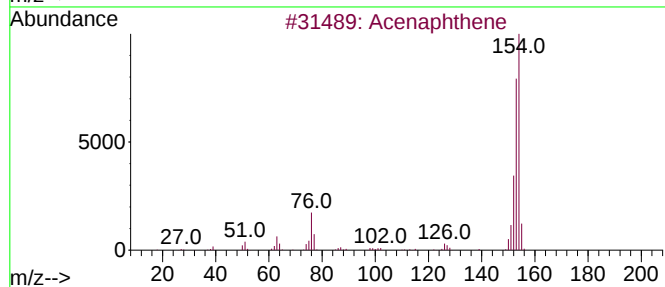
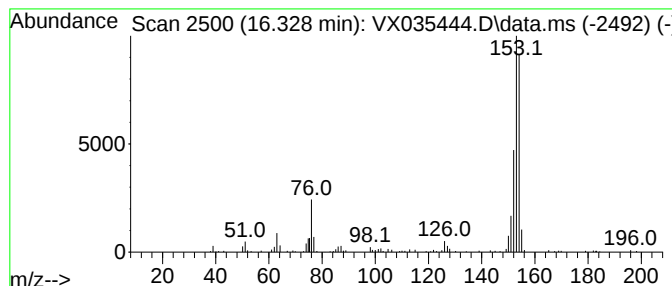
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Quant Title : SW846 8260

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

Peak Number 4 Acenaphthene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	6.39 ug/l	128890	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	76
2			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	72
3			Hexa-2,4-diyne-1-ylbenzene	154	C12H10	000520-74-1	59
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	42



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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
Fluorene	12.853	6.3	ug/l	128122	4	12.024	1009230	50.0
1,4-Methanonaph...	14.640	11.8	ug/l	237582	4	12.024	1009230	50.0
Benzocyclohepta...	14.780	10.4	ug/l	209441	4	12.024	1009230	50.0
Acenaphthene	16.328	6.4	ug/l	128890	4	12.024	1009230	50.0