

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051421\
 Data File : VX021993.D
 Acq On : 14 May 2021 14:18
 Operator : JC/MD
 Sample : M2383-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 KTW-01

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\82X050721W.M
 Title : SW846 8260

Signal : TIC: VX021993.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	693	706	720	rBV2	70679	202004	6.84%	2.638%
2	5.562	724	734	745	rBV2	91399	257310	8.71%	3.360%
3	5.964	789	800	810	rBV	77673	205511	6.96%	2.683%
4	6.769	922	932	948	rBV	173323	415297	14.06%	5.423%
5	8.653	1234	1241	1248	rBV	414258	644050	21.80%	8.409%
6	10.055	1465	1471	1480	rBV	424293	578422	19.58%	7.553%
7	10.305	1506	1512	1518	rVB	30892	43766	1.48%	0.571%
8	10.647	1562	1568	1574	rBV4	19306	31798	1.08%	0.415%
9	11.086	1634	1640	1649	rBV	387470	477544	16.16%	6.235%
10	11.756	1741	1750	1755	rBV	24769	29642	1.00%	0.387%
11	12.024	1789	1794	1801	rBV	478679	577684	19.55%	7.543%
12	12.244	1825	1830	1837	rBV	31376	37661	1.27%	0.492%
13	12.415	1853	1858	1865	rBV	176364	214095	7.25%	2.795%
14	13.427	2018	2024	2029	rVB	31600	38771	1.31%	0.506%
15	13.780	2074	2082	2092	rBV	2418380	2954246	100.00%	38.574%
16	13.872	2092	2097	2104	rVB	57074	72699	2.46%	0.949%
17	14.640	2218	2223	2231	rVB	354582	431147	14.59%	5.630%
18	14.780	2241	2246	2258	rVB	219858	280065	9.48%	3.657%
19	15.207	2308	2316	2322	rBV	36935	52405	1.77%	0.684%
20	15.481	2355	2361	2366	rBV2	21521	35392	1.20%	0.462%
21	15.615	2378	2383	2387	rBV	28623	42562	1.44%	0.556%
22	16.097	2455	2462	2468	rBV	21958	36550	1.24%	0.477%

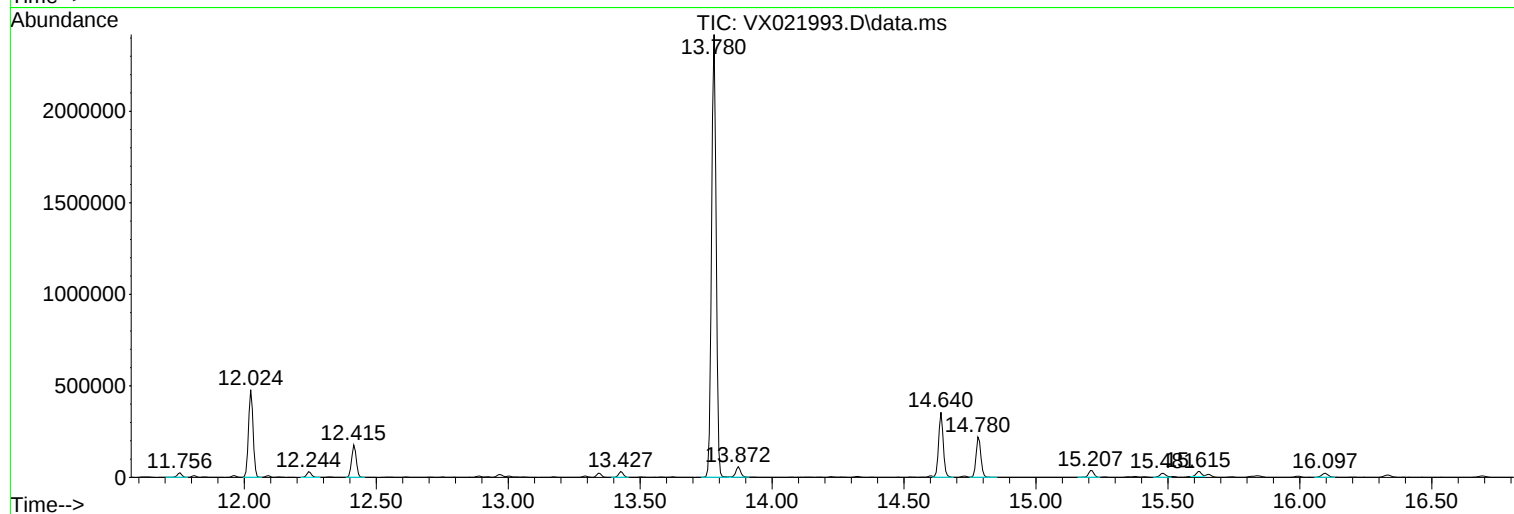
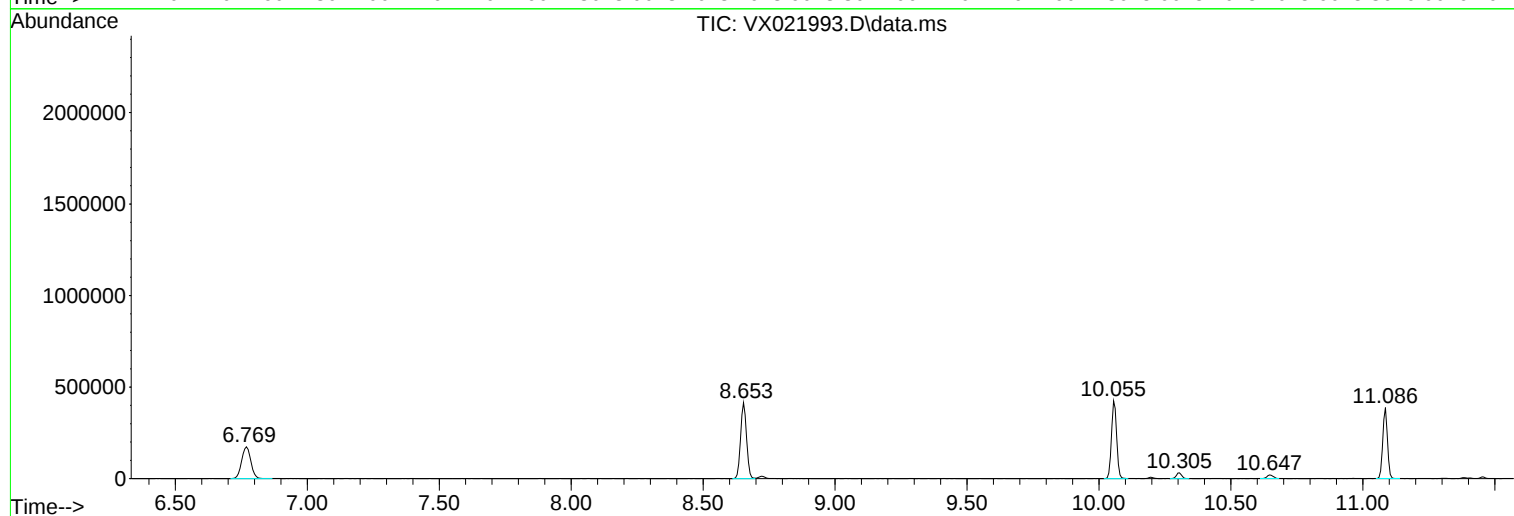
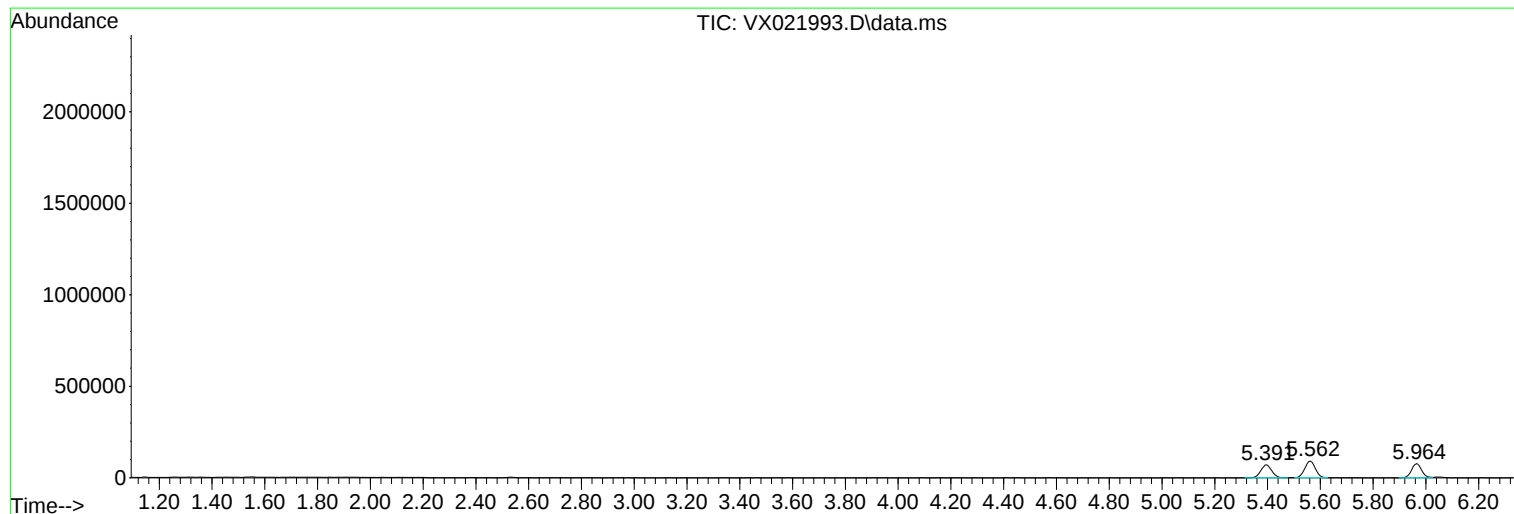
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

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



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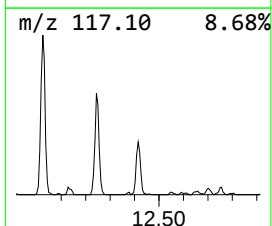
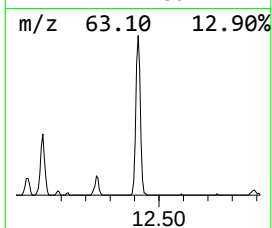
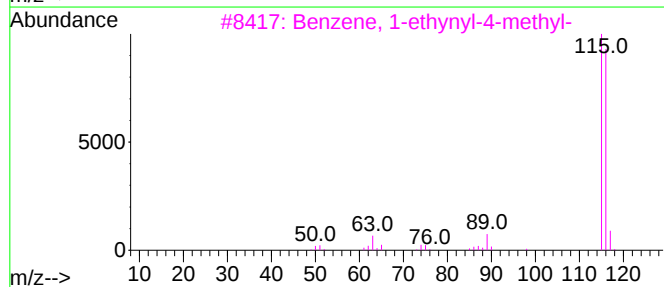
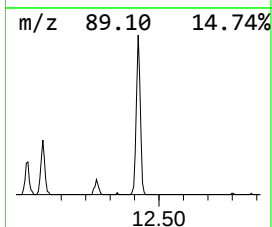
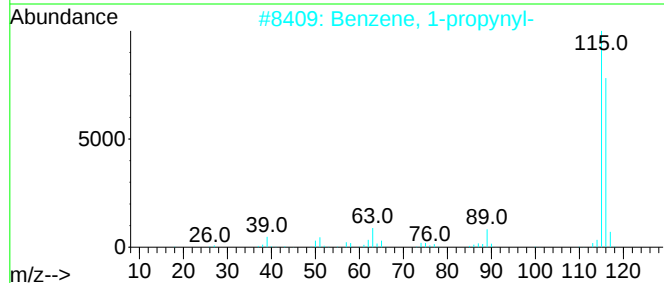
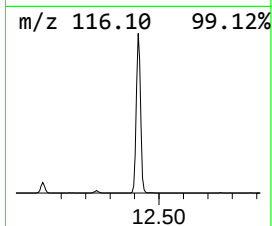
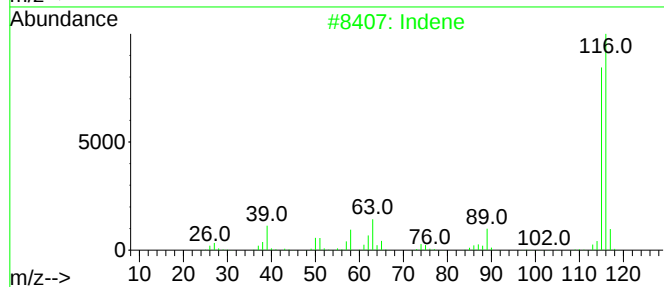
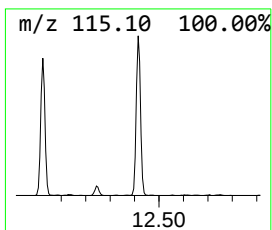
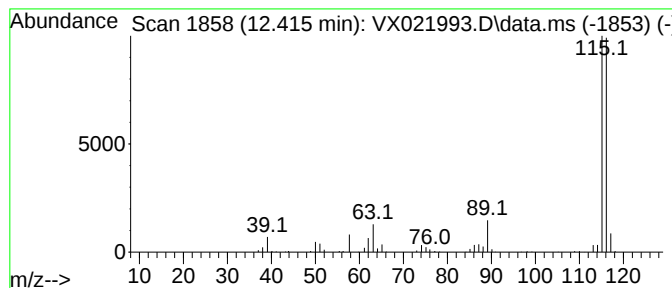
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

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

Peak Number 1 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	18.53 ug/l	214095	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	96
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	83
5			1-indanol trifluoroacetate ester	230	C11H9F3O2	1000376-43-6	74



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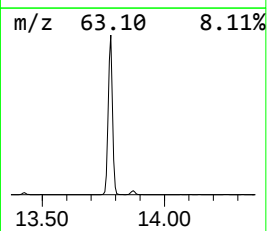
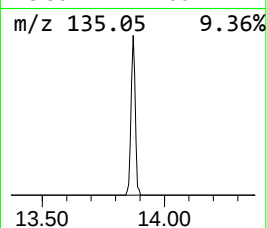
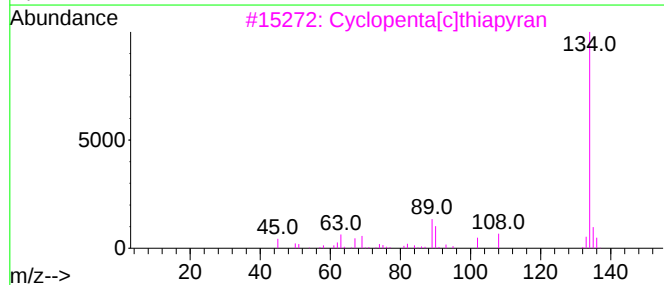
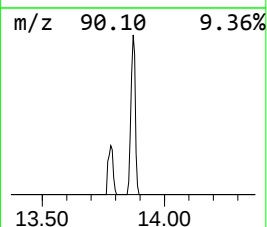
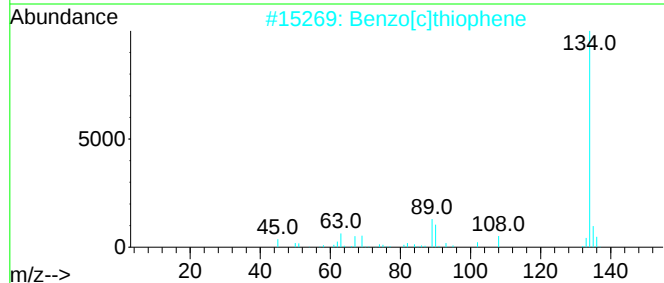
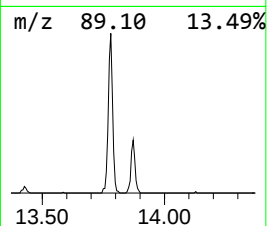
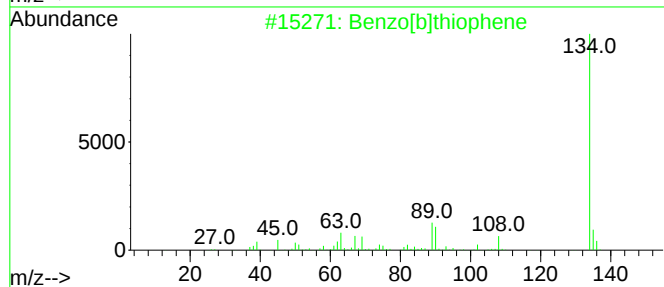
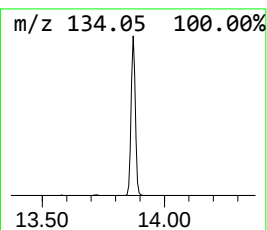
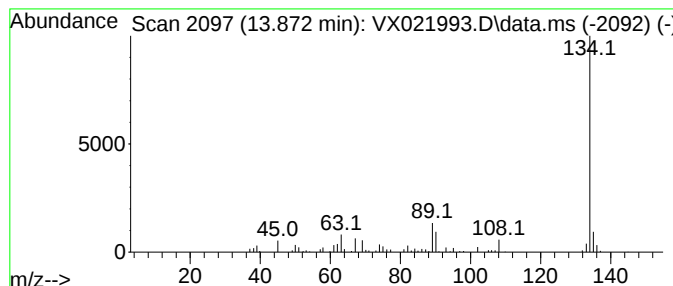
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzo[b]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.872	6.29 ug/l	72699	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4			2H-Benzimidazol-2-one, 1,3-dihydro-	134	C7H6N2O	000615-16-7	53
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50



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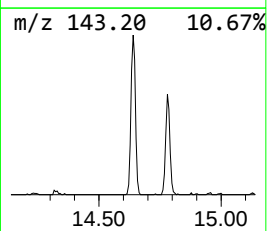
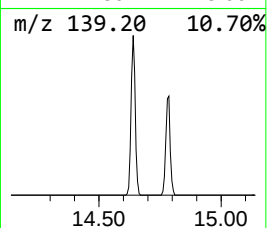
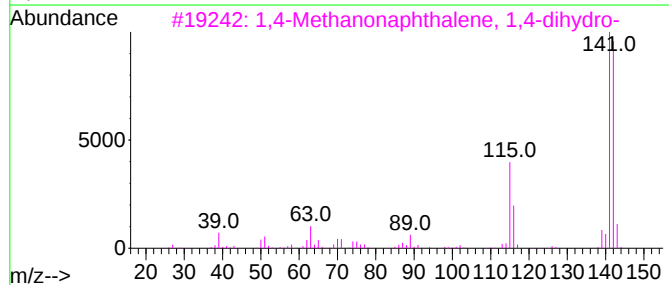
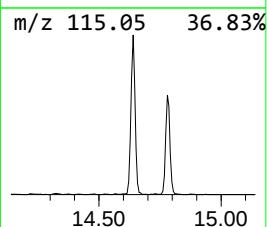
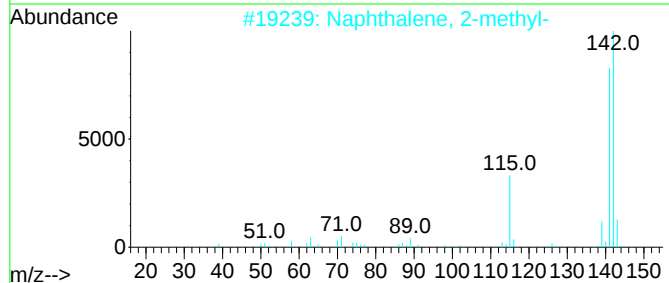
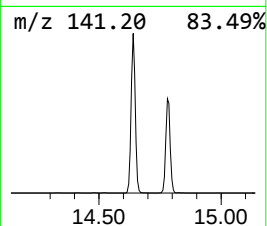
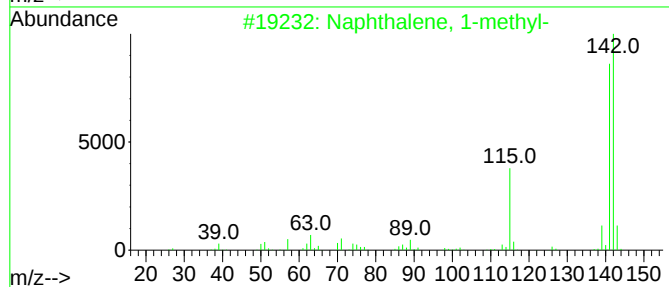
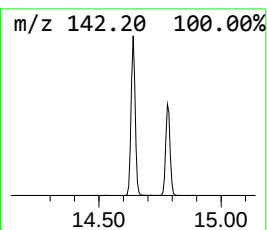
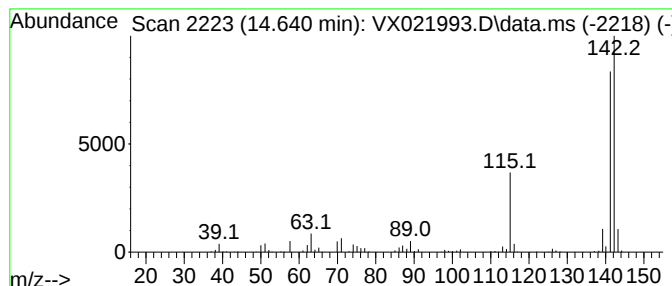
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	37.32 ug/l	431147	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	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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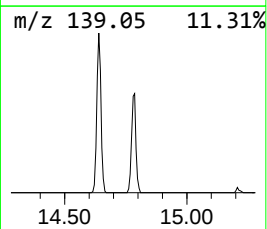
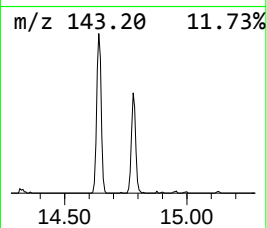
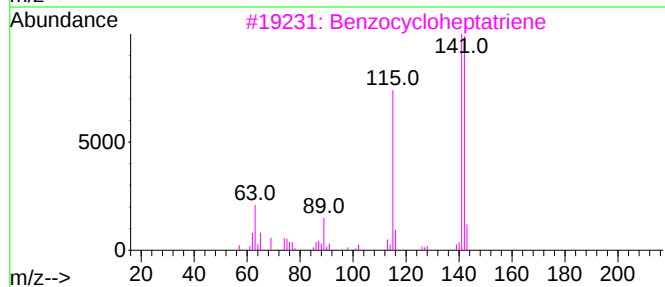
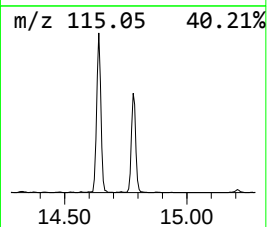
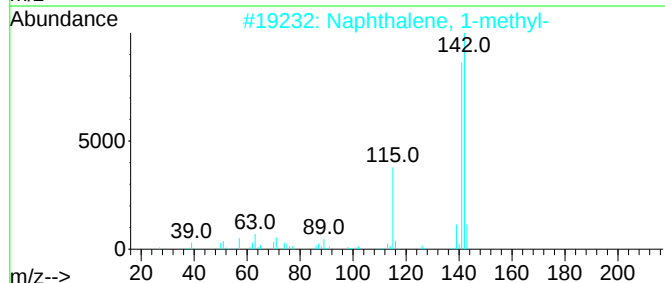
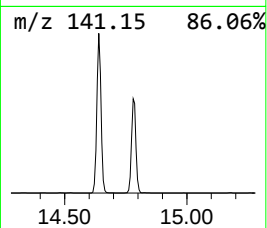
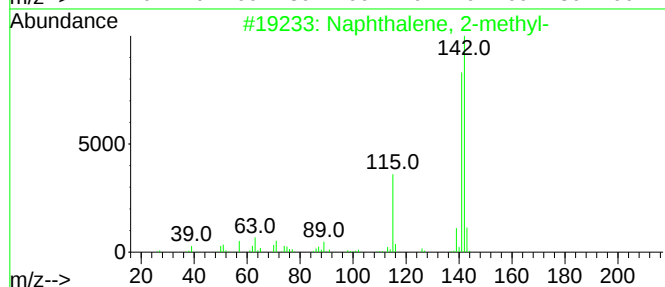
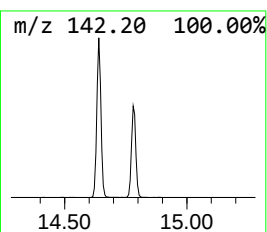
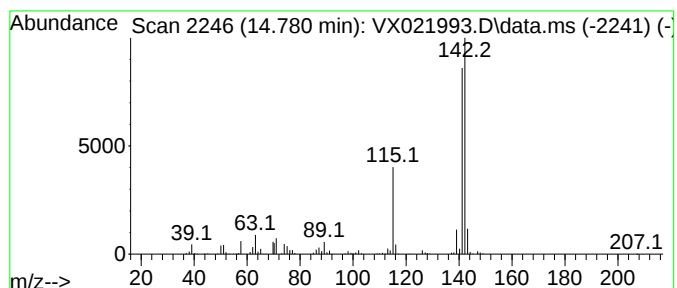
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	24.24 ug/l	280065	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			Benzocycloheptatriene	142	C11H10	000264-09-5	93
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indene	12.415	18.5	ug/l	214095	4	12.024	577684	50.0
Benzo[b]thiophene	13.872	6.3	ug/l	72699	4	12.024	577684	50.0
Naphthalene, 1-...	14.640	37.3	ug/l	431147	4	12.024	577684	50.0
Benzocyclohepta...	14.780	24.2	ug/l	280065	4	12.024	577684	50.0