

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051421\
 Data File : VX021992.D
 Acq On : 14 May 2021 13:54
 Operator : JC/MD
 Sample : M2383-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP-02-05112021

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: VX021992.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.397	696	707	721	rBV2	68574	197649	7.32%	2.717%
2	5.562	721	734	746	rBV2	91766	256748	9.51%	3.529%
3	5.971	790	801	809	rBV2	75496	198999	7.37%	2.735%
4	6.769	922	932	942	rBV	173790	416446	15.42%	5.724%
5	8.653	1234	1241	1248	rBV	405613	632724	23.43%	8.697%
6	10.055	1466	1471	1485	rVB	422975	583744	21.62%	8.024%
7	10.305	1506	1512	1519	rVB	27576	40101	1.48%	0.551%
8	10.647	1563	1568	1576	rVB3	17984	28685	1.06%	0.394%
9	11.085	1634	1640	1653	rVB	389842	476660	17.65%	6.552%
10	11.756	1744	1750	1755	rBV	23060	27893	1.03%	0.383%
11	12.024	1789	1794	1801	rBV	492368	584365	21.64%	8.033%
12	12.244	1823	1830	1839	rBV	25756	33691	1.25%	0.463%
13	12.414	1853	1858	1863	rBV	153772	181374	6.72%	2.493%
14	13.427	2018	2024	2029	rBV	26686	33745	1.25%	0.464%
15	13.780	2074	2082	2090	rBV	2218030	2700467	100.00%	37.121%
16	13.872	2090	2097	2104	rVB	49783	65624	2.43%	0.902%
17	14.640	2218	2223	2232	rVB	329424	403256	14.93%	5.543%
18	14.780	2241	2246	2257	rVB	193058	255962	9.48%	3.518%
19	15.207	2309	2316	2322	rBV	35084	48017	1.78%	0.660%
20	15.481	2356	2361	2365	rBV	19778	30184	1.12%	0.415%
21	15.615	2371	2383	2387	rBV	28825	51464	1.91%	0.707%
22	16.097	2455	2462	2469	rBV	17171	27053	1.00%	0.372%

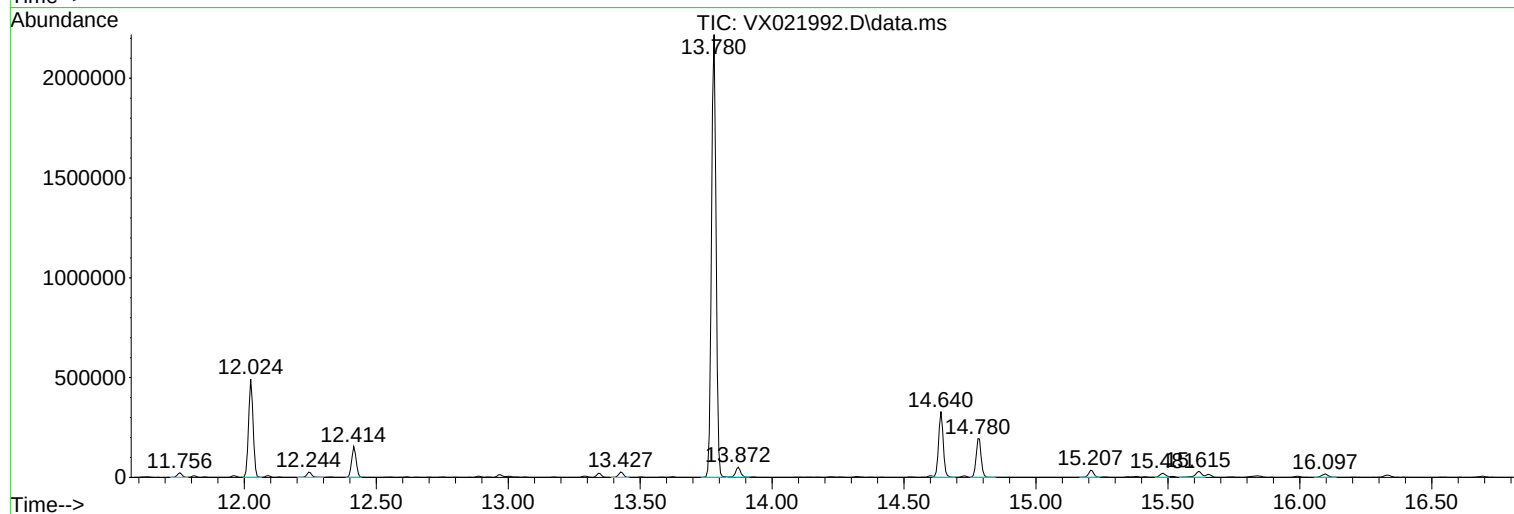
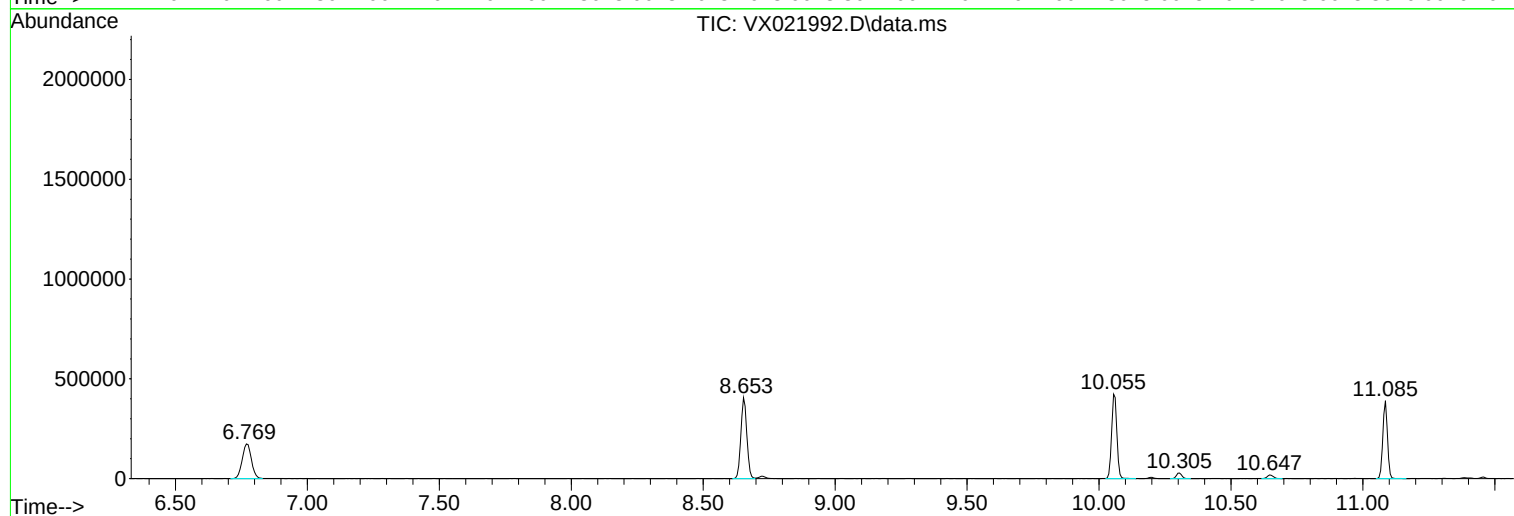
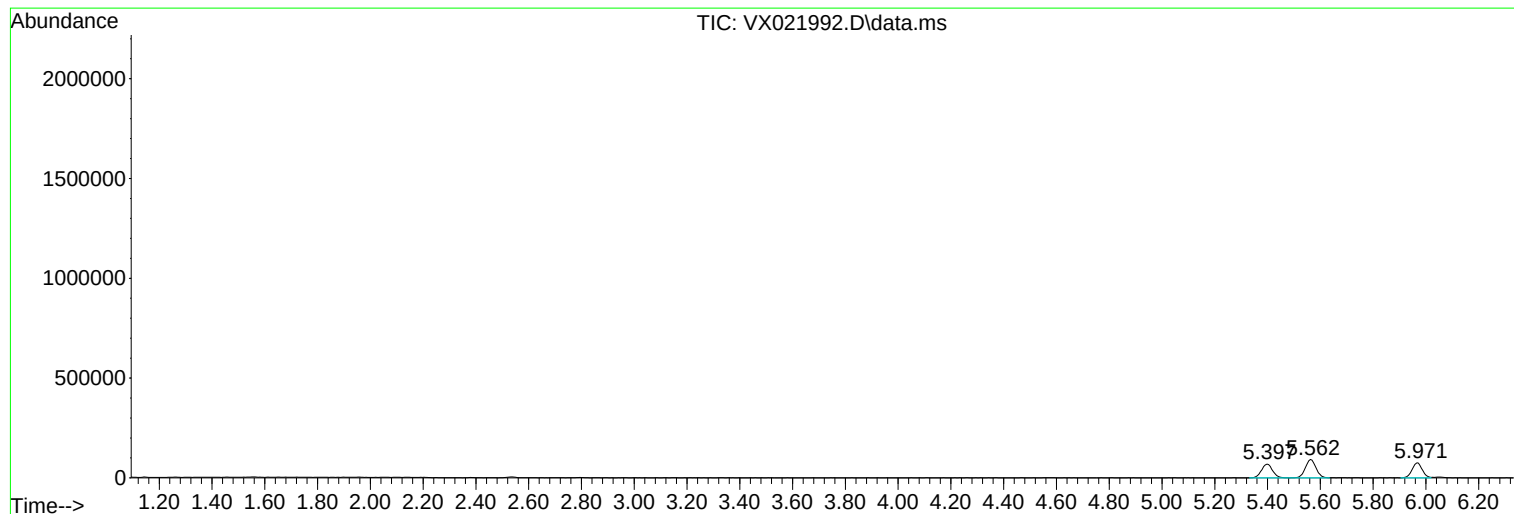
Sum of corrected areas: 7274851

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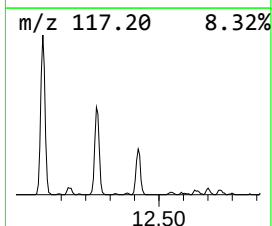
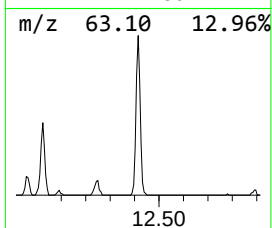
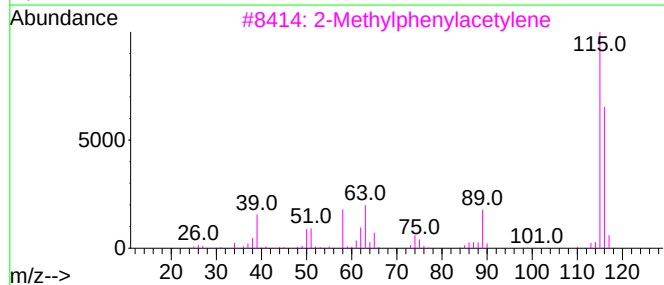
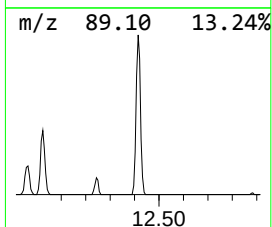
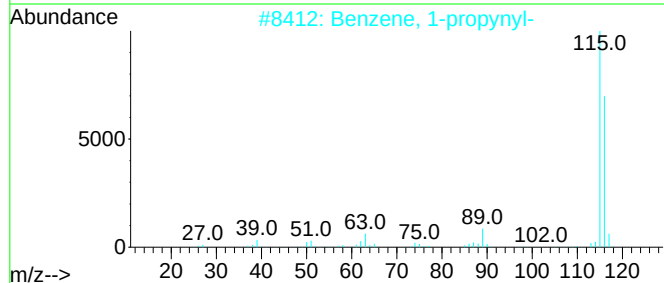
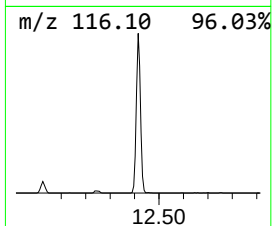
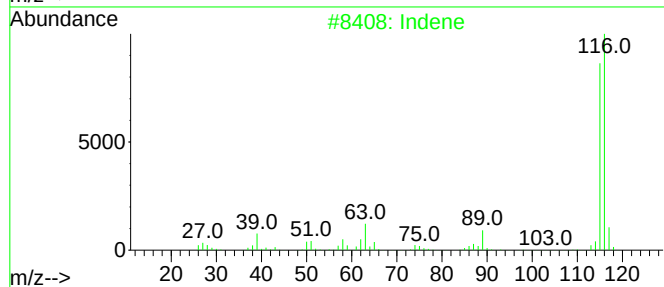
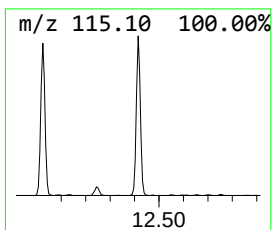
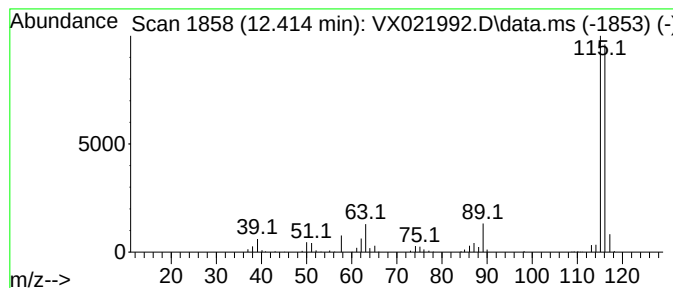
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

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	15.52 ug/l	181374	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			2-Methylphenylacetylene	116	C9H8	000766-47-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



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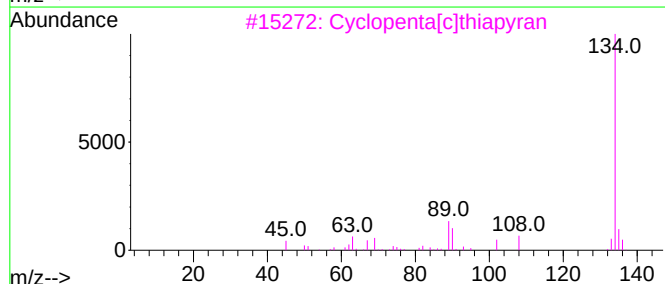
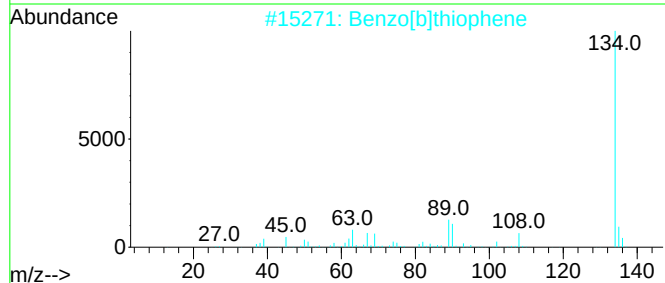
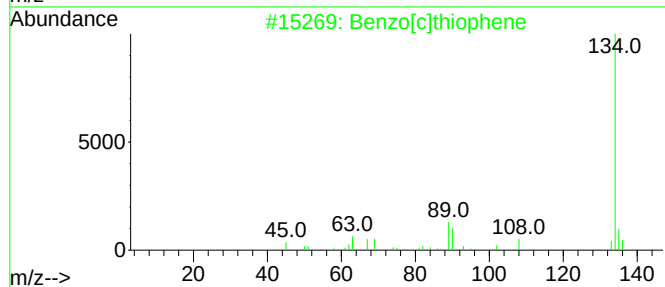
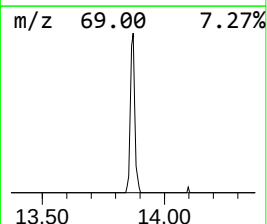
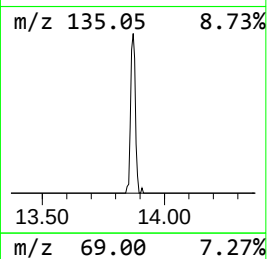
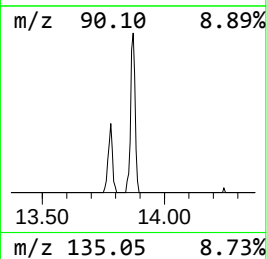
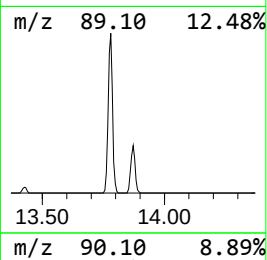
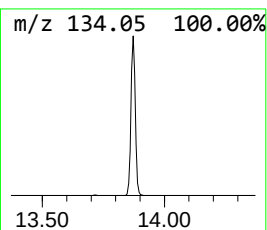
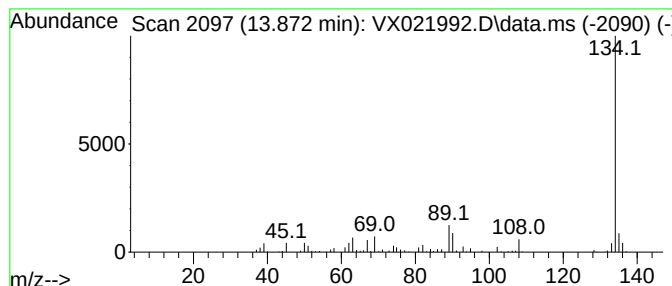
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Quant Title : SW846 8260

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

Peak Number 2 Benzo[c]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	5.61 ug/l	65624	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			2H-Benzimidazol-2-one, 1,3-dihydro-	134	C7H6N2O	000615-16-7	42
5			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	39



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Instrument :
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ClientSampleId :
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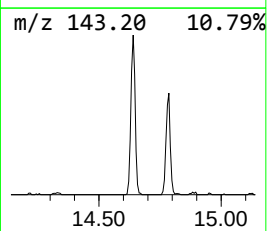
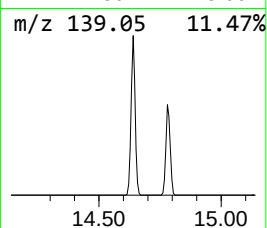
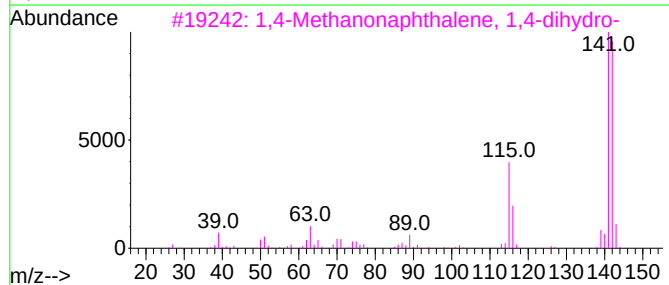
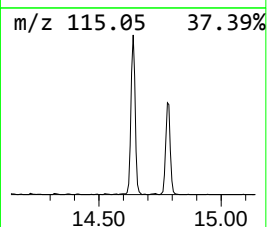
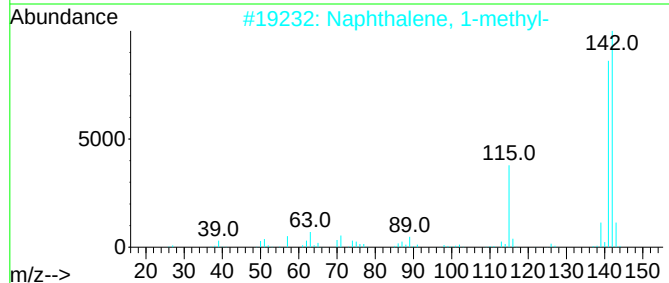
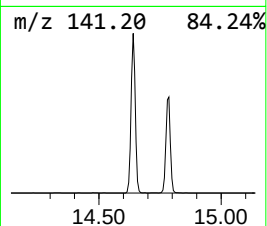
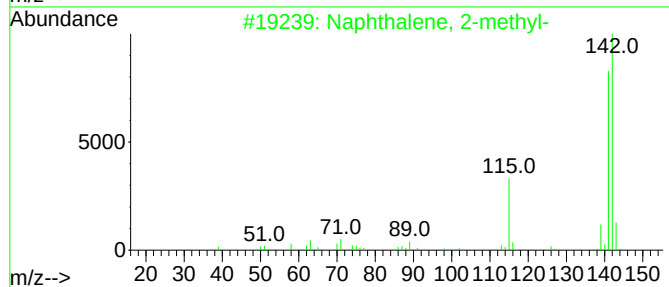
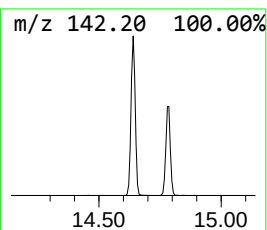
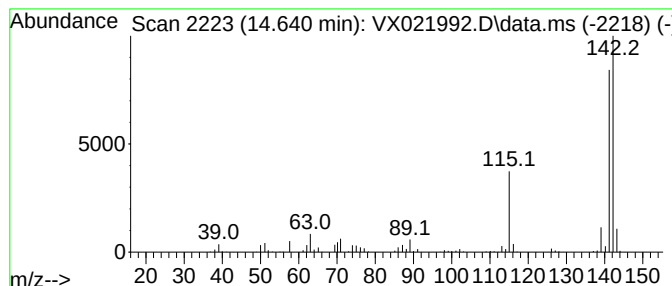
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Quant Title : SW846 8260

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	34.50 ug/l	403256	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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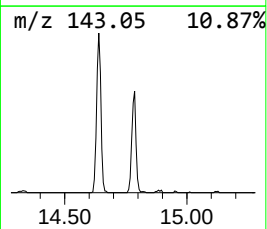
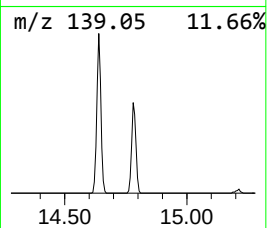
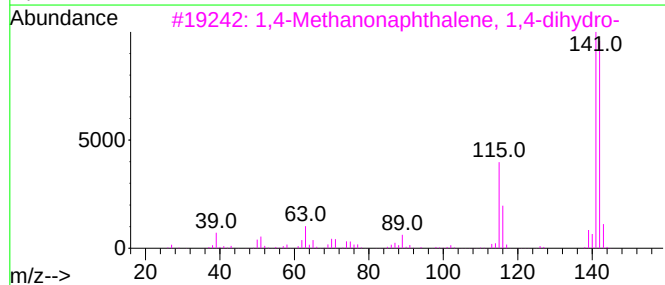
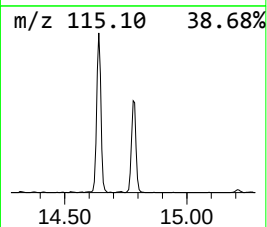
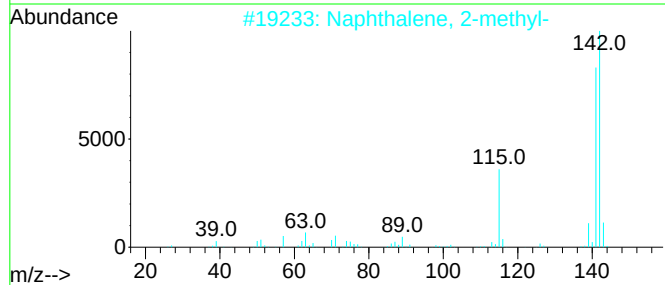
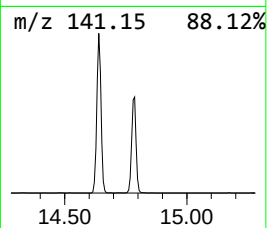
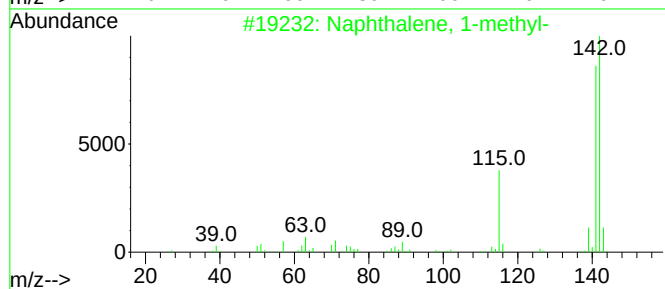
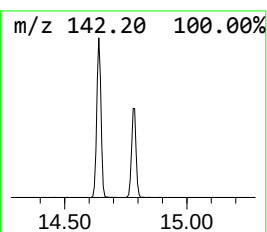
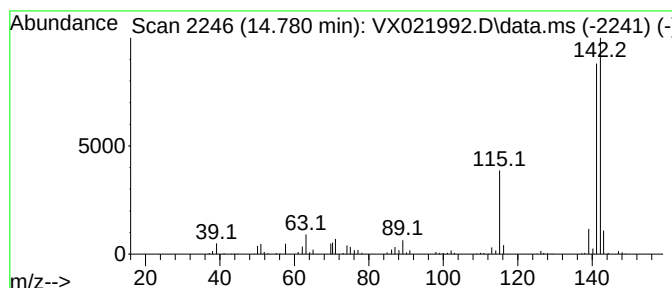
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Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	21.90 ug/l	255962	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	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indene	12.415	15.5	ug/l	181374	4	12.024	584365	50.0
Benzo[c]thiophene	13.871	5.6	ug/l	65624	4	12.024	584365	50.0
Naphthalene, 1-...	14.640	34.5	ug/l	403256	4	12.024	584365	50.0
1,4-Methanonaph...	14.780	21.9	ug/l	255962	4	12.024	584365	50.0