

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051321\
 Data File : VX021971.D
 Acq On : 13 May 2021 16:43
 Operator : JC/MD
 Sample : M2383-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP-02-05122021

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: VX021971.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	695	707	720	rBV	68228	198559	7.05%	2.672%
2	5.562	720	734	748	rVB	90886	258967	9.19%	3.485%
3	5.964	789	800	810	rBV2	76275	200454	7.12%	2.698%
4	6.769	922	932	941	rBV	168913	409465	14.54%	5.511%
5	8.653	1234	1241	1248	rBV	411851	630196	22.37%	8.482%
6	10.055	1466	1471	1478	rBV	425529	576207	20.45%	7.755%
7	10.305	1506	1512	1517	rBV	30140	40690	1.44%	0.548%
8	10.646	1563	1568	1574	rVB3	18088	28639	1.02%	0.385%
9	11.085	1634	1640	1650	rBV	380952	471065	16.72%	6.340%
10	11.756	1744	1750	1755	rBV	25230	29905	1.06%	0.402%
11	12.024	1789	1794	1801	rBV	460896	576304	20.46%	7.757%
12	12.244	1825	1830	1837	rVB	27015	35878	1.27%	0.483%
13	12.414	1853	1858	1864	rBV	150058	182723	6.49%	2.459%
14	13.426	2019	2024	2030	rBV	25605	33956	1.21%	0.457%
15	13.780	2074	2082	2090	rBV	2307358	2816956	100.00%	37.914%
16	13.871	2092	2097	2103	rVB	54040	69525	2.47%	0.936%
17	14.640	2219	2223	2232	rVB	343961	423101	15.02%	5.695%
18	14.780	2241	2246	2255	rVB	206463	274092	9.73%	3.689%
19	15.207	2308	2316	2322	rBV	38203	53560	1.90%	0.721%
20	15.481	2355	2361	2365	rBV2	20981	33728	1.20%	0.454%
21	15.615	2372	2383	2387	rBV	31225	55528	1.97%	0.747%
22	16.097	2456	2462	2468	rVB2	17865	30402	1.08%	0.409%

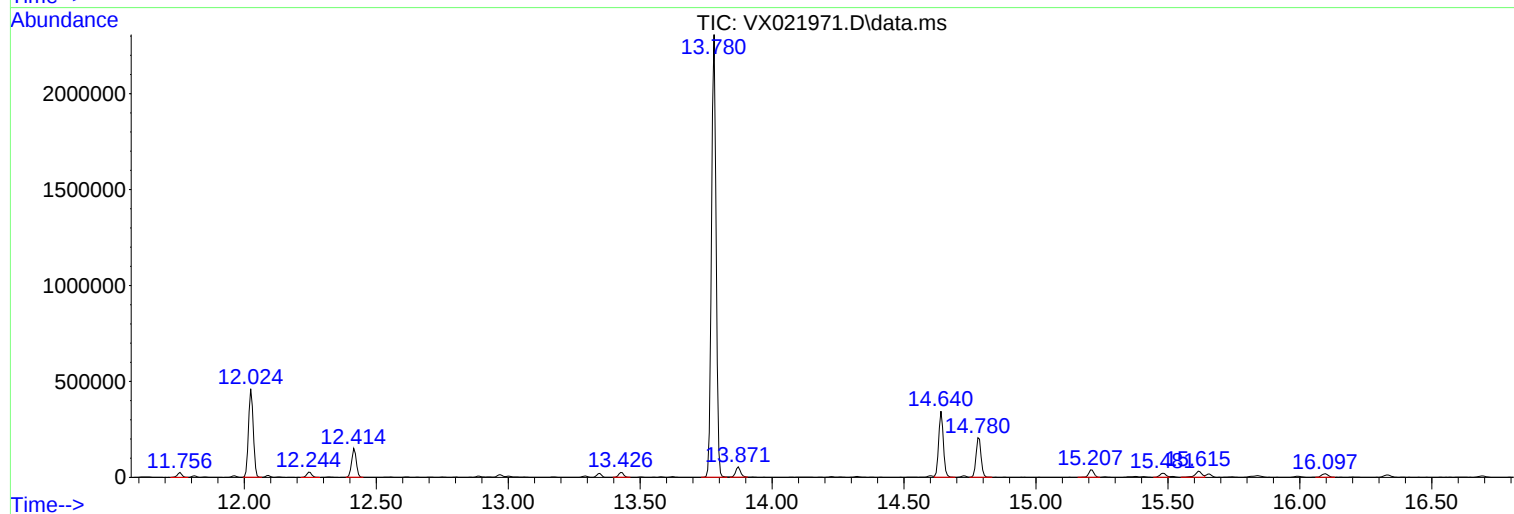
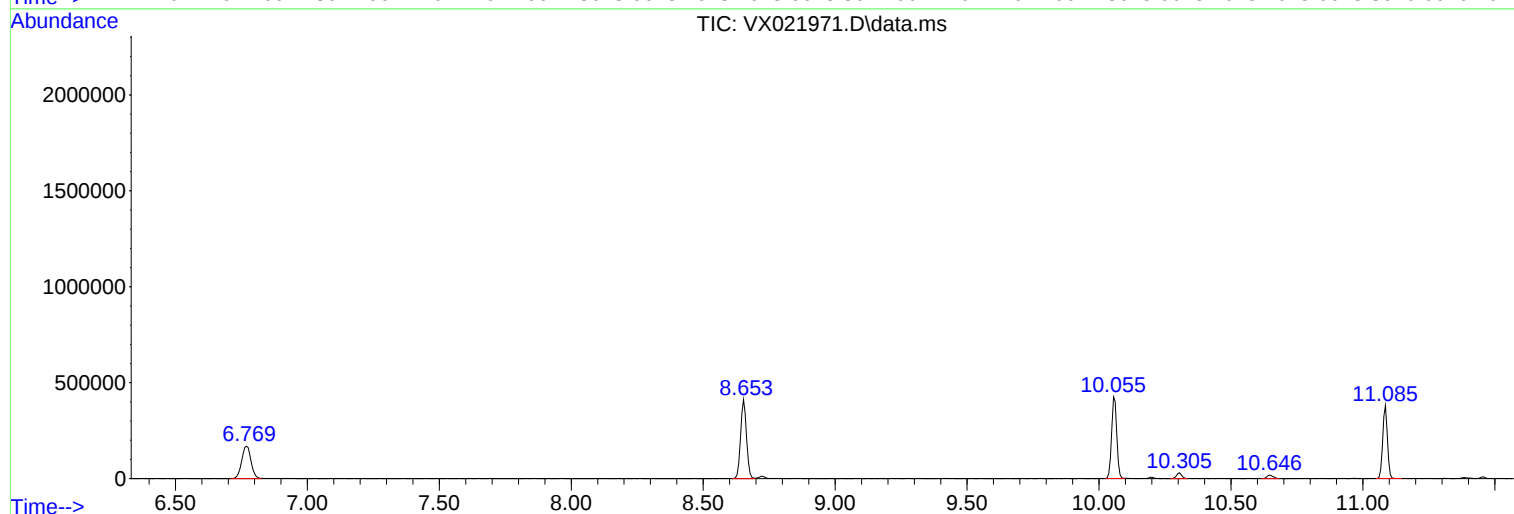
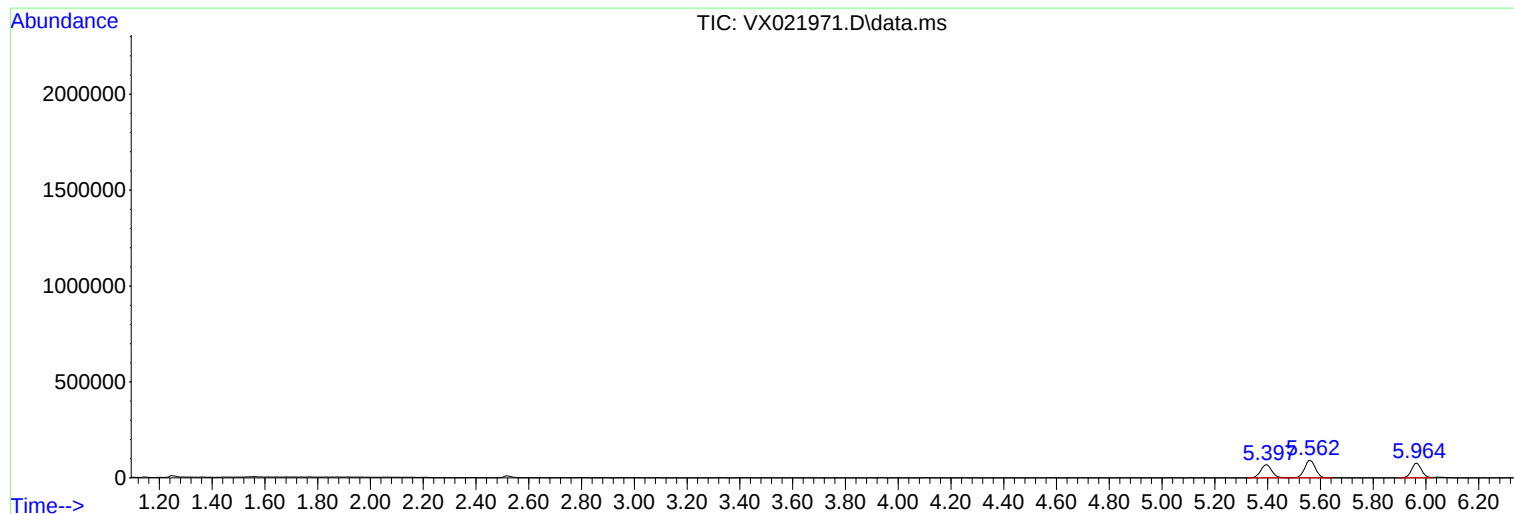
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Quant Title : SW846 8260

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



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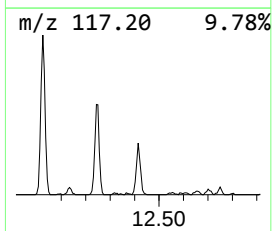
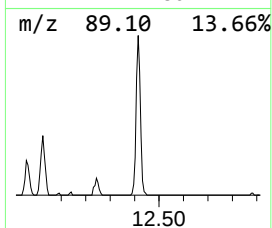
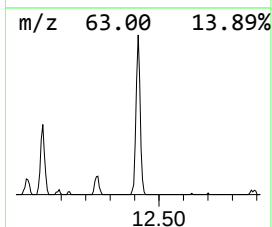
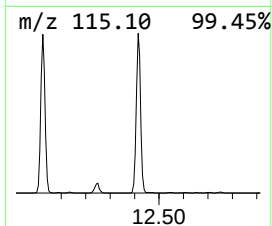
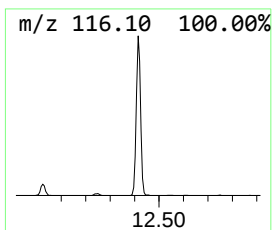
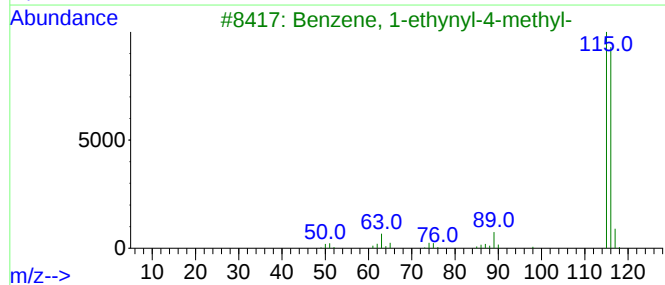
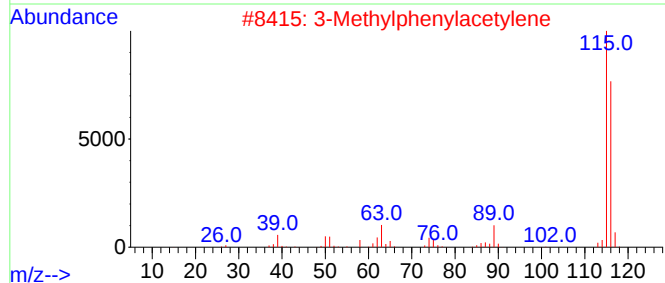
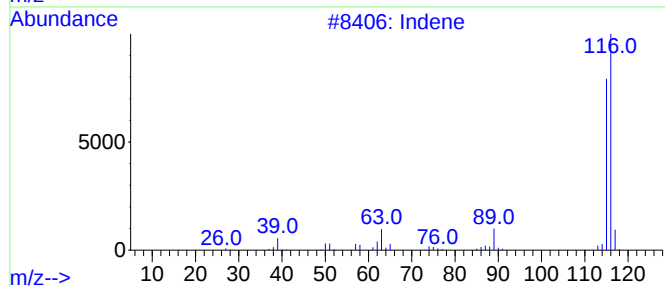
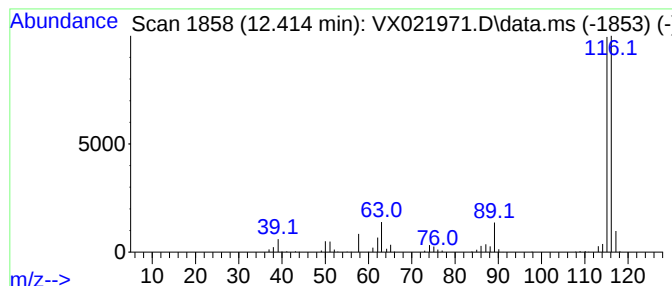
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

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.
12.414	15.85 ug/l	182723	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



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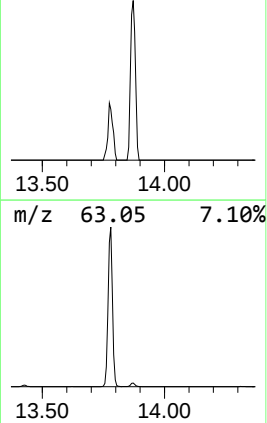
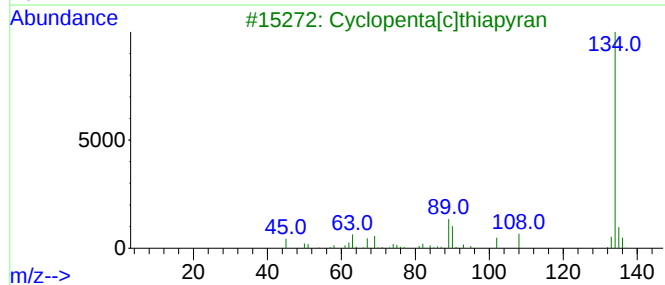
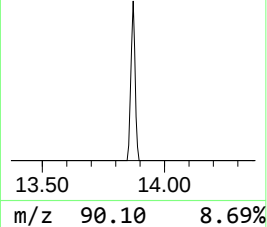
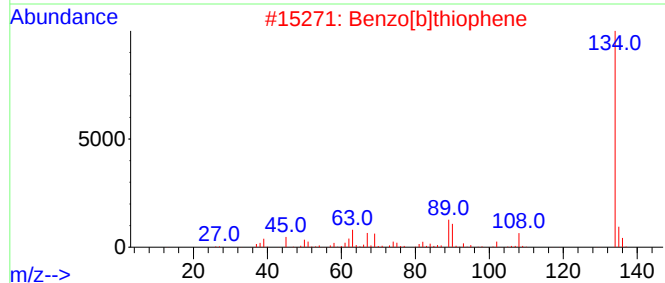
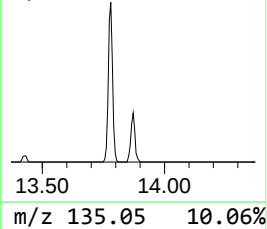
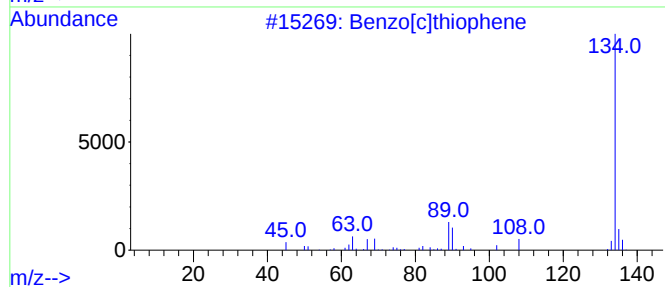
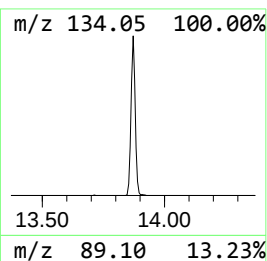
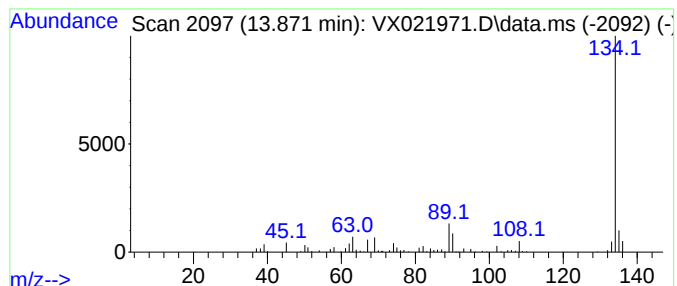
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050721W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzo[c]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	6.03 ug/l	69525	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4			[1]Benzo[h]thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	56
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



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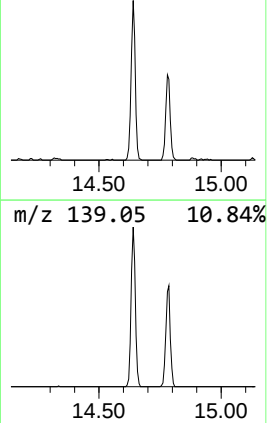
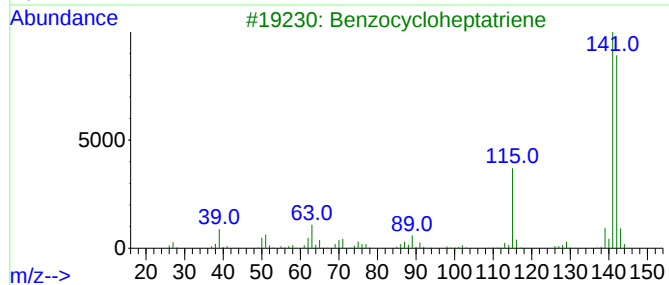
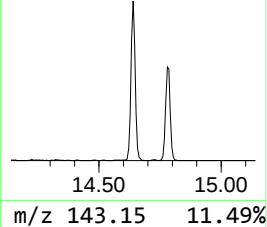
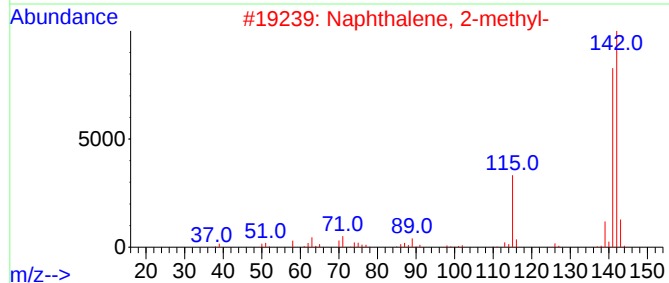
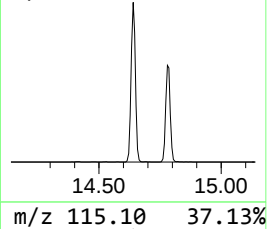
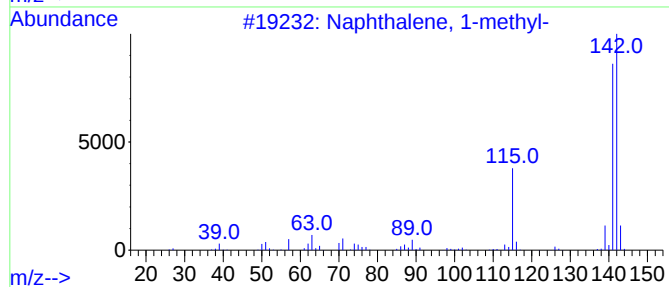
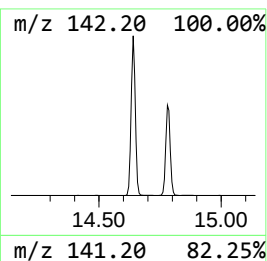
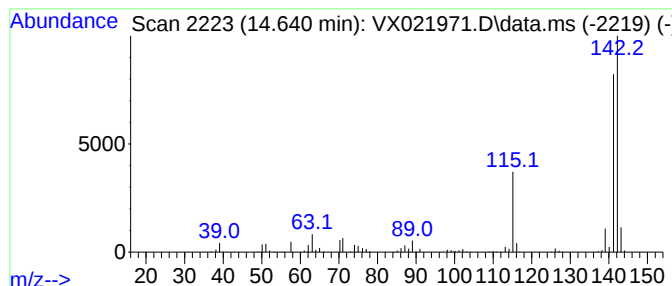
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Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	36.71 ug/l	423101	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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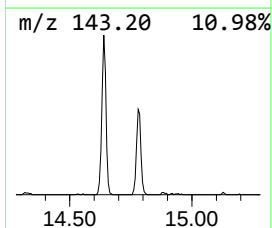
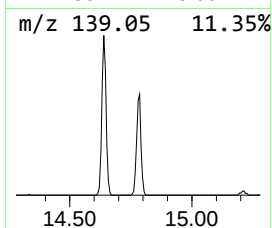
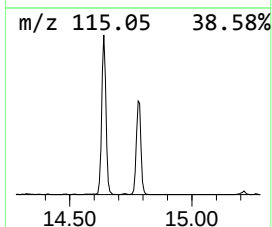
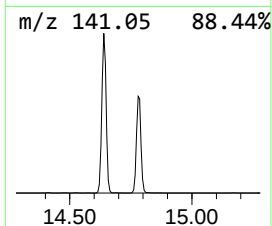
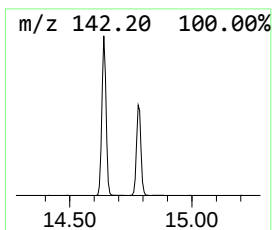
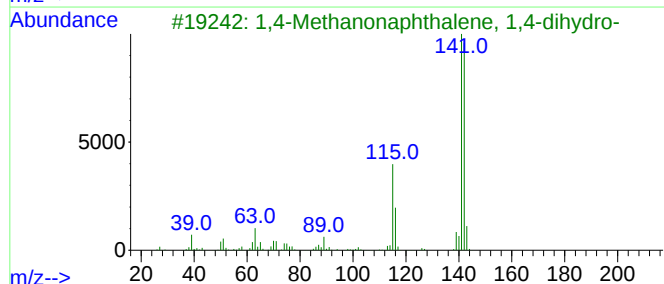
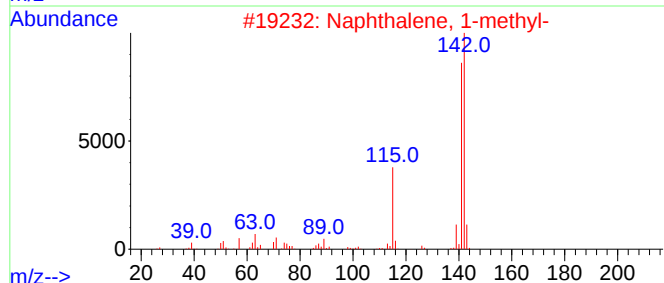
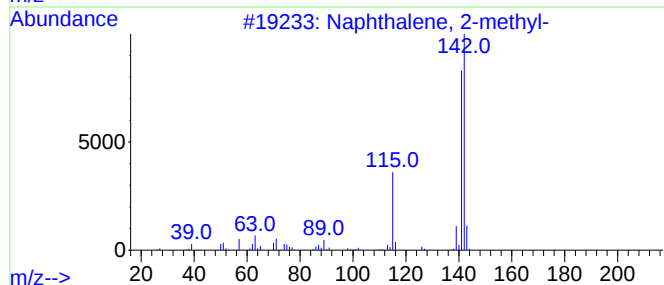
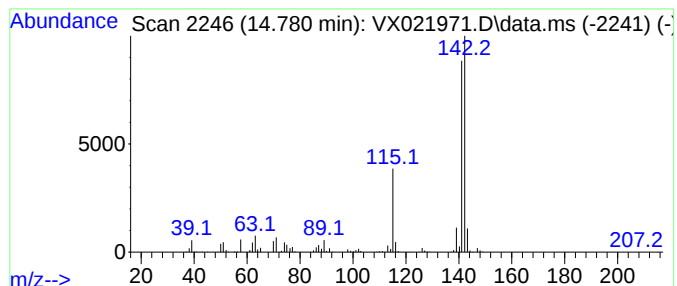
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	23.78 ug/l	274092	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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indene	12.414	15.9	ug/l	182723	4	12.024	576304	50.0
Benzo[c]thiophene	13.871	6.0	ug/l	69525	4	12.024	576304	50.0
Naphthalene, 1-...	14.640	36.7	ug/l	423101	4	12.024	576304	50.0
1,4-Methanonaph...	14.780	23.8	ug/l	274092	4	12.024	576304	50.0