

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060424\
 Data File : VX041728.D
 Acq On : 04 Jun 2024 12:21
 Operator : JC/MD
 Sample : P2657-10 10X
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3-AB-VOC

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\82X052924W.M
 Title : SW846 8260

Signal : TIC: VX041728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	694	705	722	rBV	75376	227752	4.36%	2.162%
2	5.550	722	732	750	rVB	134010	380437	7.29%	3.612%
3	5.958	789	799	809	rBV	80765	216863	4.15%	2.059%
4	6.763	922	931	948	rBV	200986	486621	9.32%	4.620%
5	8.647	1234	1240	1248	rBV	417273	659490	12.63%	6.262%
6	10.055	1465	1471	1487	rBV	449106	614798	11.78%	5.837%
7	10.299	1506	1511	1518	rBV	68897	96188	1.84%	0.913%
8	10.640	1562	1567	1580	rBV	60730	90963	1.74%	0.864%
9	11.079	1634	1639	1650	rBV	395587	511951	9.81%	4.861%
10	11.451	1696	1700	1709	rVB	52634	71583	1.37%	0.680%
11	11.750	1745	1749	1755	rBV	93877	117130	2.24%	1.112%
12	12.018	1788	1793	1800	rBV	481966	635301	12.17%	6.032%
13	12.085	1800	1804	1810	rVB	50845	64556	1.24%	0.613%
14	12.414	1851	1858	1864	rBV	114968	149549	2.86%	1.420%
15	13.774	2076	2081	2091	rBV	4373852	5220630	100.00%	49.569%
16	13.865	2092	2096	2104	rVB	68454	95196	1.82%	0.904%
17	14.634	2218	2222	2232	rVB	378680	479587	9.19%	4.554%
18	14.780	2239	2246	2254	rVB	230404	307209	5.88%	2.917%
19	15.207	2309	2316	2320	rBV	38008	52940	1.01%	0.503%
20	15.615	2376	2383	2386	rBV	32314	53334	1.02%	0.506%

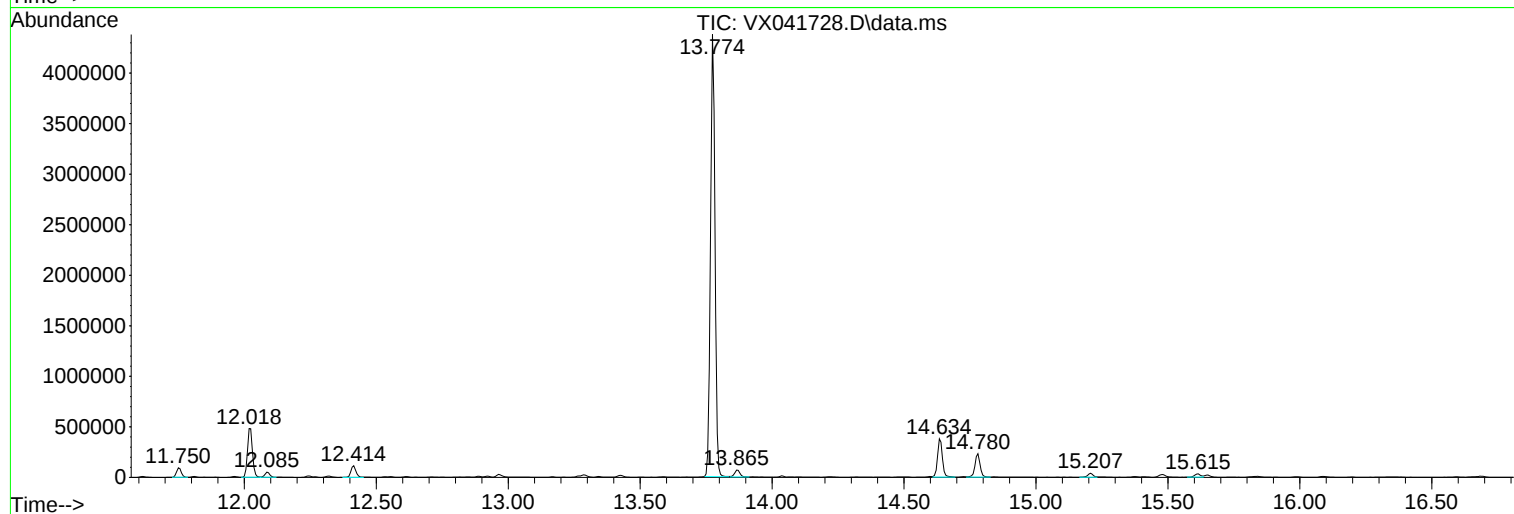
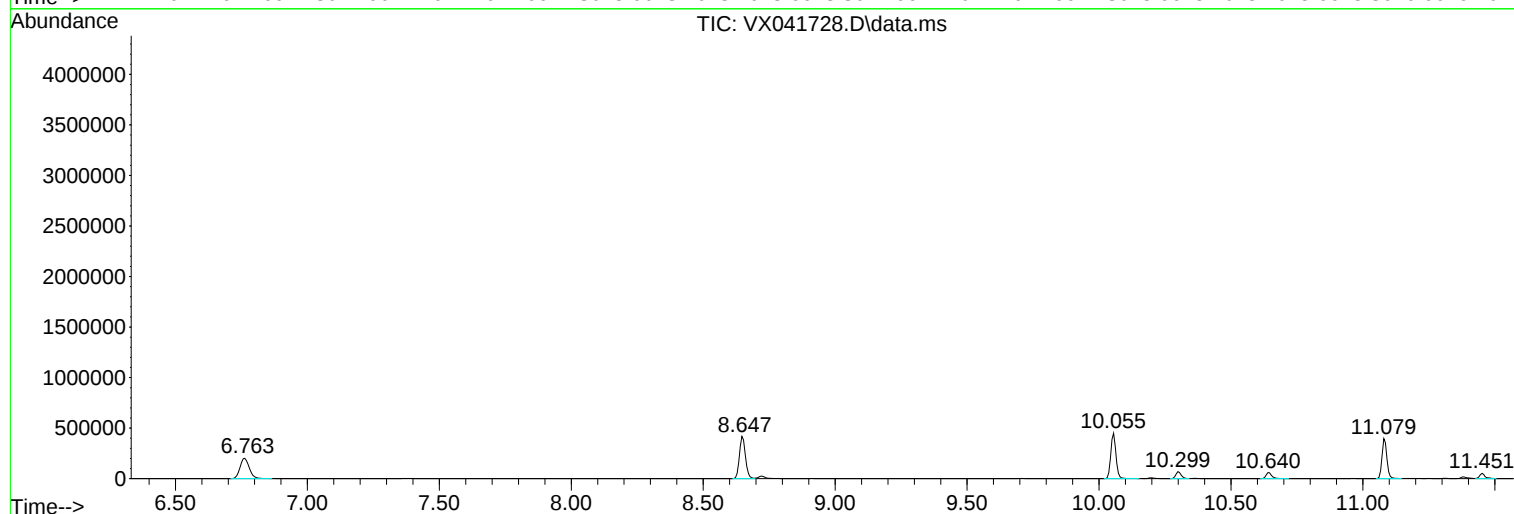
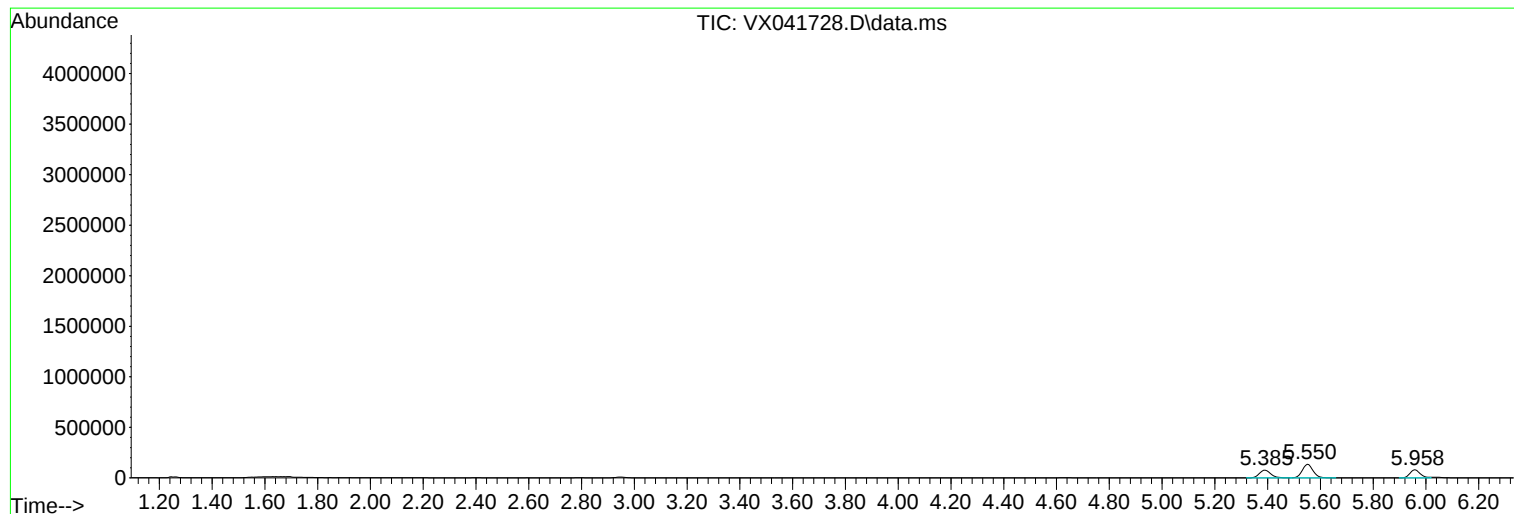
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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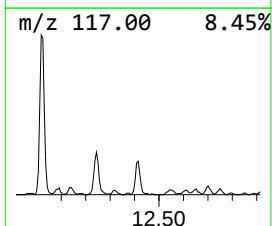
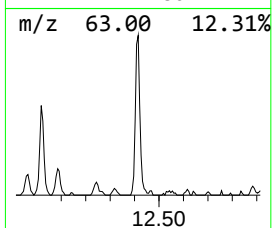
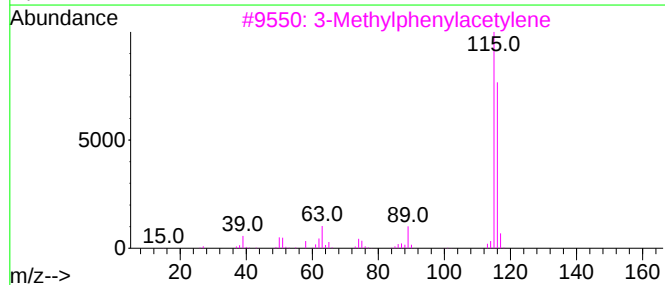
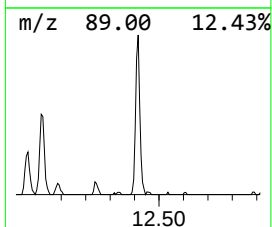
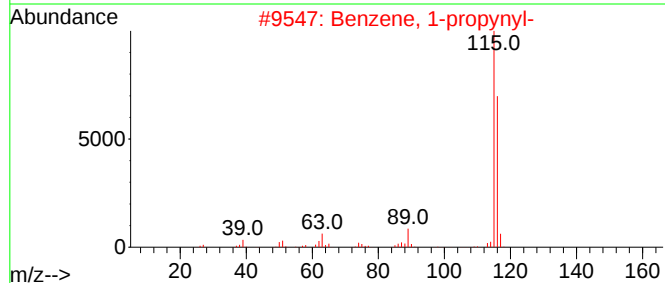
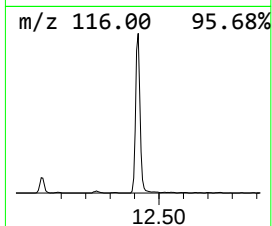
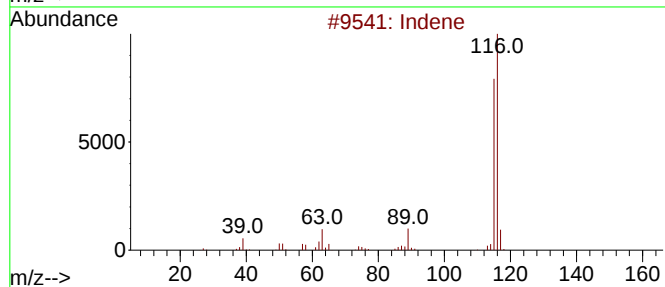
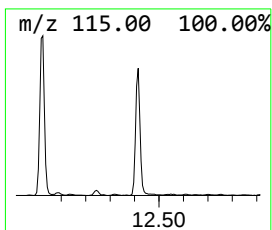
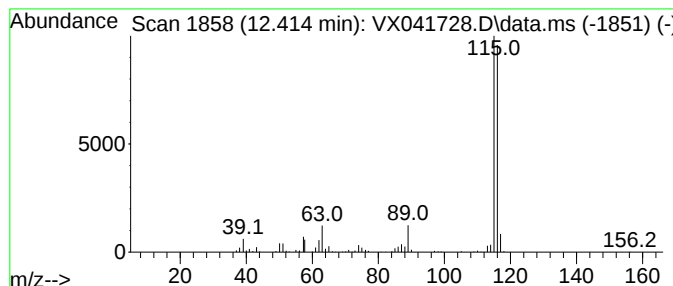
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 2 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	11.77 ug/l	149549	1,4-Dichlorobenzene-d4	12.024

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



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ClientSampleId :
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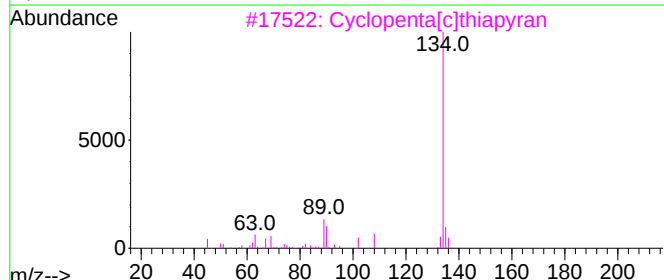
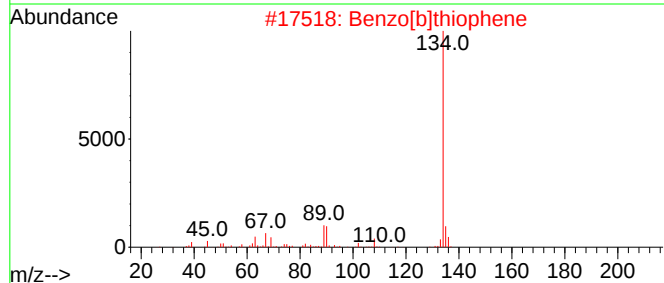
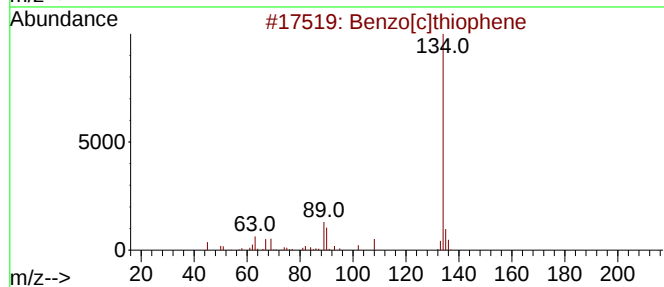
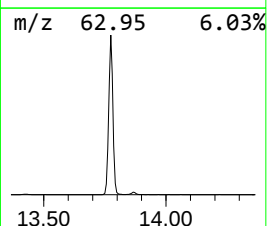
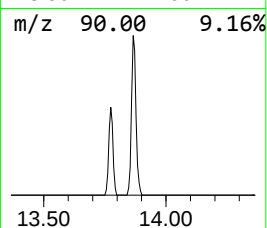
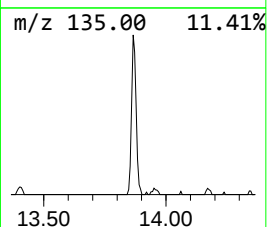
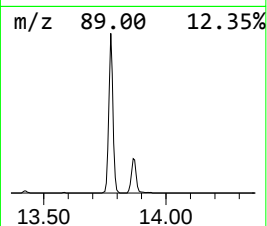
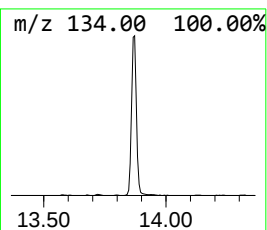
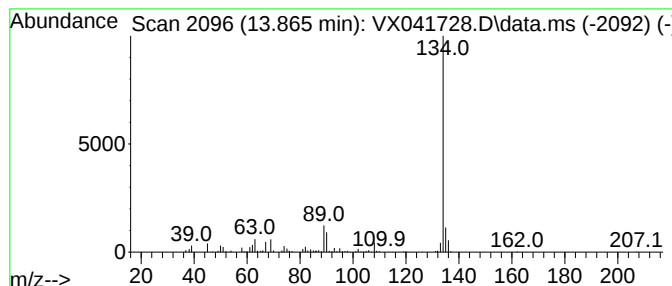
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzo[c]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.865	7.49 ug/l	95196	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5			3-Deazaadenine	134	C6H6N4	006811-77-4	59



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Instrument :
MSVOA_X
ClientSampleId :
3-AB-VOC

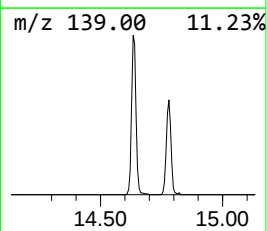
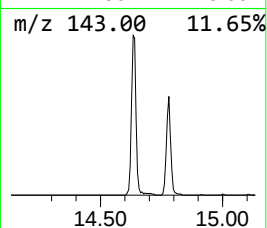
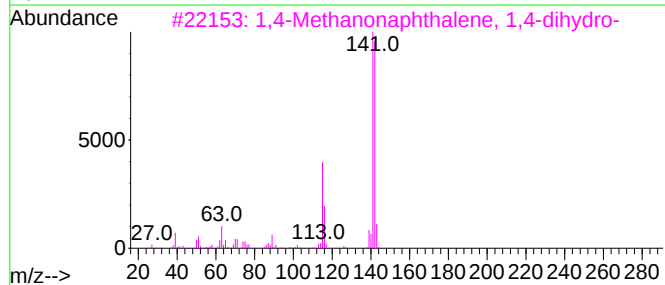
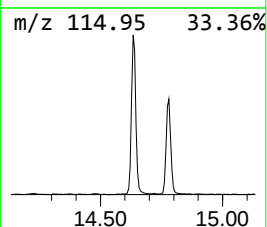
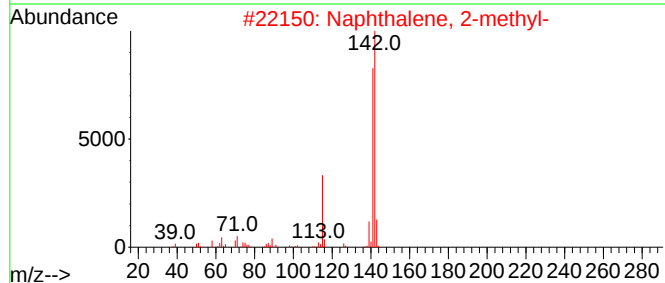
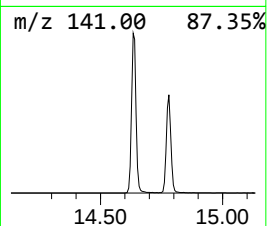
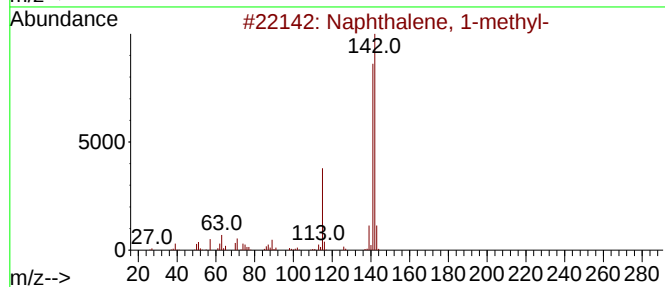
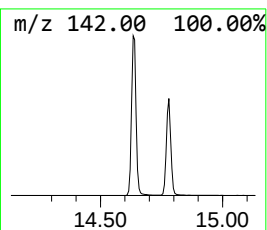
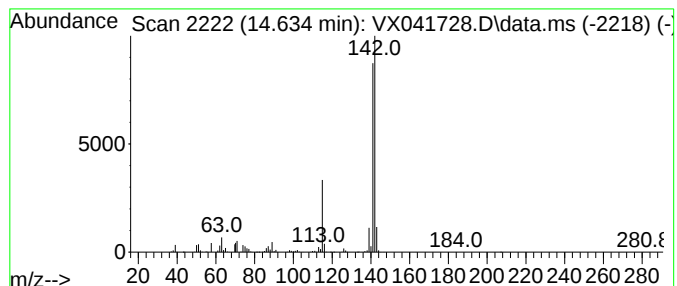
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	37.74 ug/l	479587	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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50



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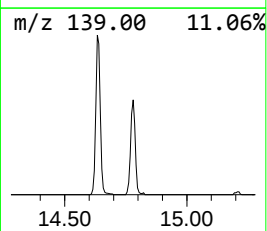
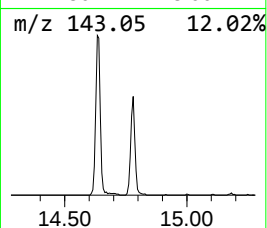
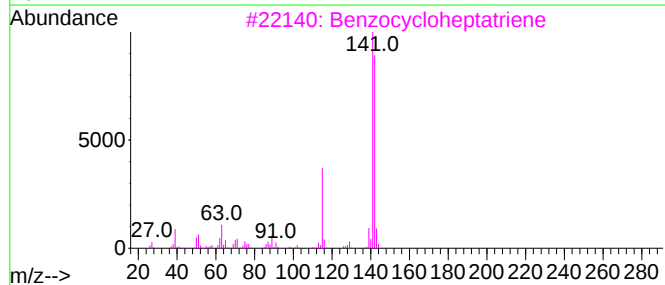
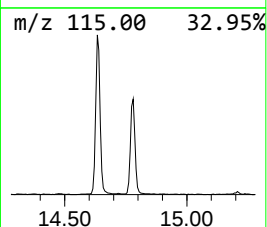
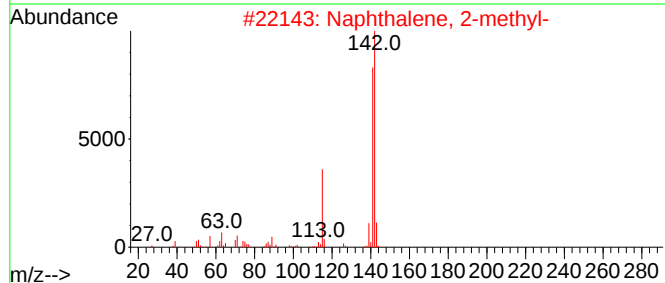
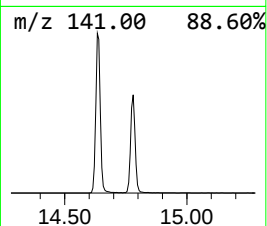
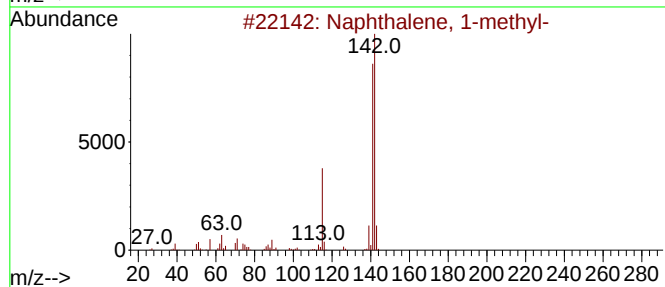
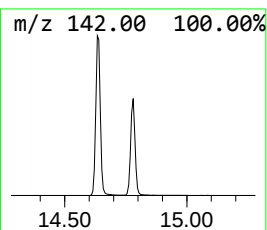
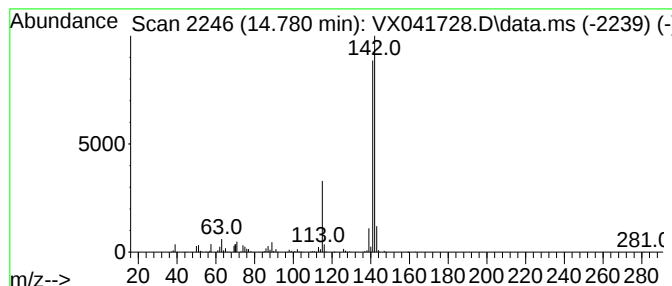
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	24.18 ug/l	307209	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	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indene	12.415	11.8	ug/l	149549	4	12.024	635301	50.0
Benzo[c]thiophene	13.865	7.5	ug/l	95196	4	12.024	635301	50.0
Naphthalene, 1-...	14.634	37.7	ug/l	479587	4	12.024	635301	50.0
1,4-Methanonaph...	14.780	24.2	ug/l	307209	4	12.024	635301	50.0