

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060424\
 Data File : VX041729.D
 Acq On : 04 Jun 2024 12:45
 Operator : JC/MD
 Sample : P2657-14 10X
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4-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: VX041729.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	695	705	721	rBV	73026	216413	3.50%	1.813%
2	5.550	722	732	747	rVB2	127563	362244	5.86%	3.035%
3	5.958	787	799	807	rBV	76750	205845	3.33%	1.724%
4	6.757	921	930	944	rBV	190863	466113	7.54%	3.905%
5	8.647	1234	1240	1248	rBV	400948	631646	10.21%	5.291%
6	8.720	1248	1252	1268	rVB	40127	69323	1.12%	0.581%
7	10.055	1465	1471	1490	rVB	413957	581823	9.41%	4.874%
8	10.299	1506	1511	1518	rBV	104411	145555	2.35%	1.219%
9	10.640	1562	1567	1584	rVB	93594	138919	2.25%	1.164%
10	11.079	1634	1639	1652	rBV	361808	482234	7.80%	4.040%
11	11.451	1695	1700	1710	rVB	74750	100794	1.63%	0.844%
12	11.750	1745	1749	1755	rBV	133323	166941	2.70%	1.398%
13	12.024	1788	1794	1800	rBV	455789	594393	9.61%	4.979%
14	12.085	1800	1804	1809	rVB	71251	89695	1.45%	0.751%
15	12.414	1852	1858	1864	rBV	229451	300804	4.86%	2.520%
16	13.774	2076	2081	2090	rVV	4993857	6185747	100.00%	51.818%
17	13.865	2092	2096	2104	rVB	85373	114737	1.85%	0.961%
18	14.633	2218	2222	2233	rVB	478017	592111	9.57%	4.960%
19	14.780	2239	2246	2254	rVB	282061	362944	5.87%	3.040%
20	15.207	2308	2316	2320	rBV	45580	63967	1.03%	0.536%
21	15.615	2373	2383	2386	rBV	38088	65133	1.05%	0.546%

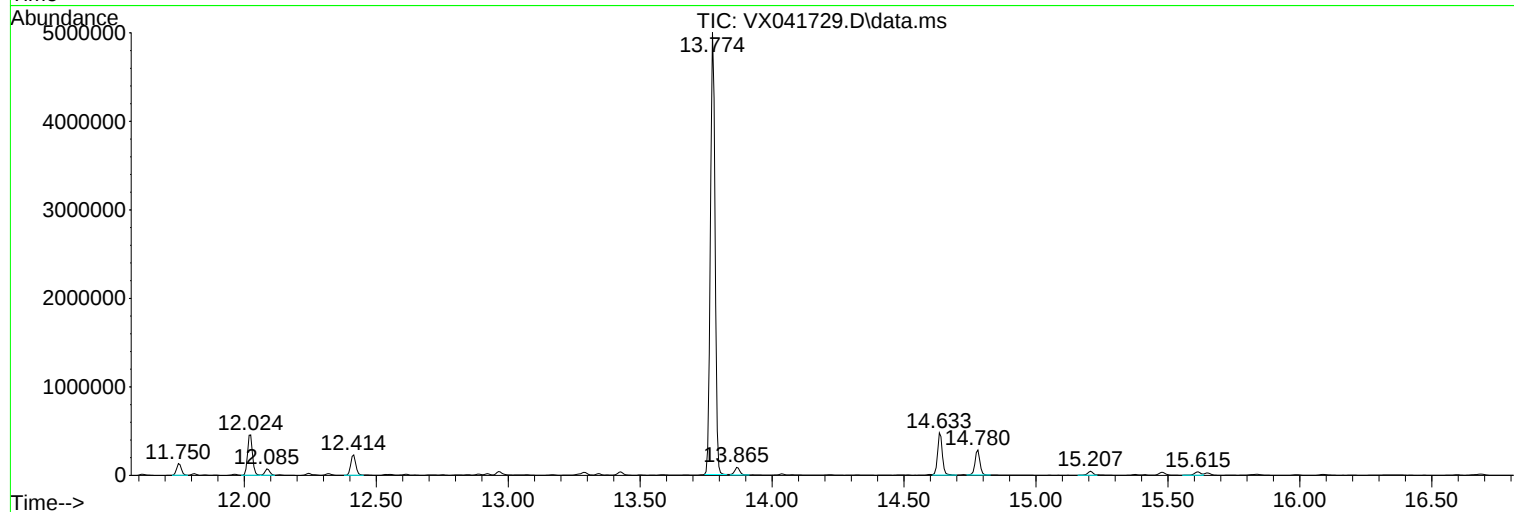
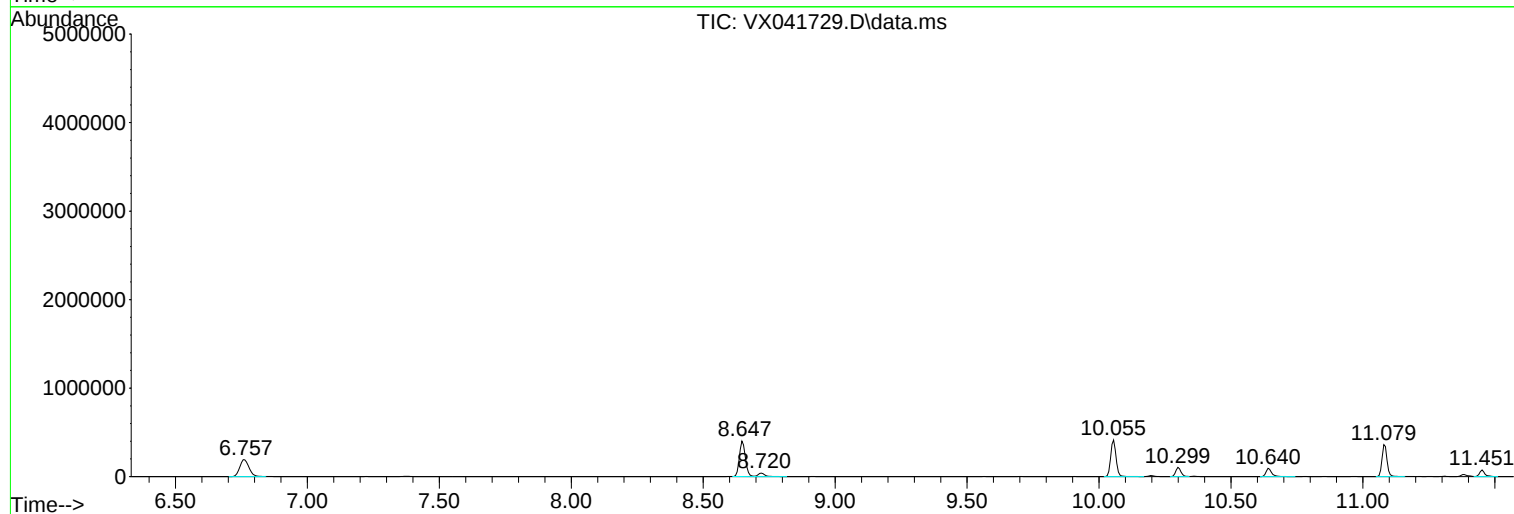
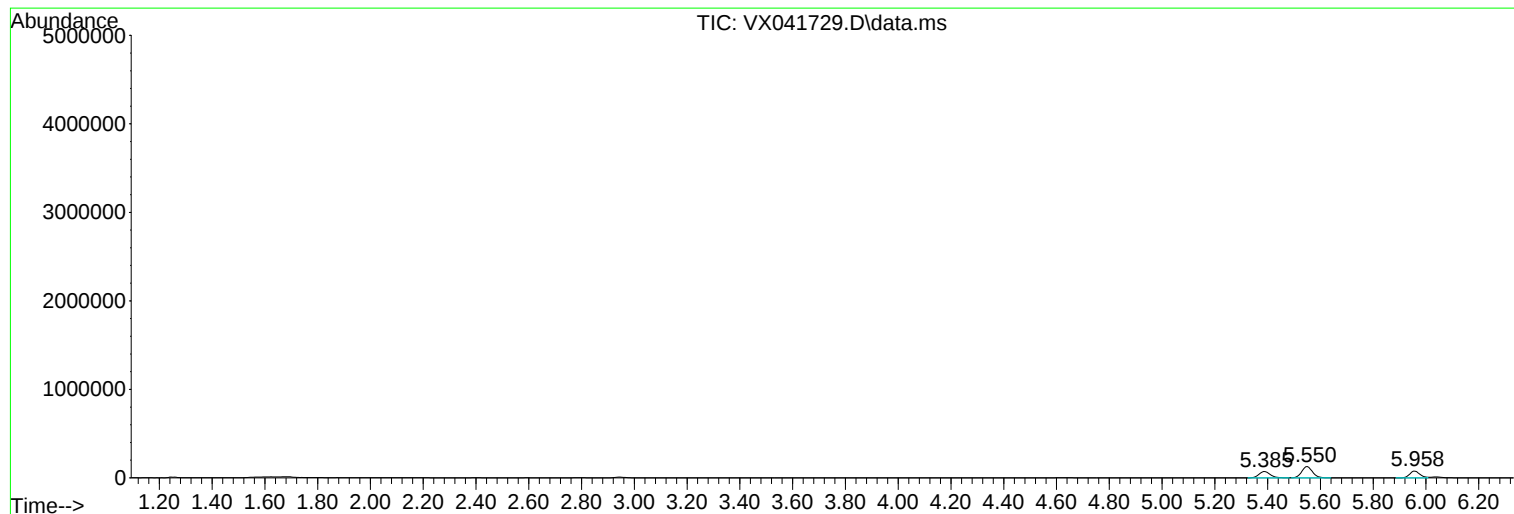
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4-AB-VOC

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



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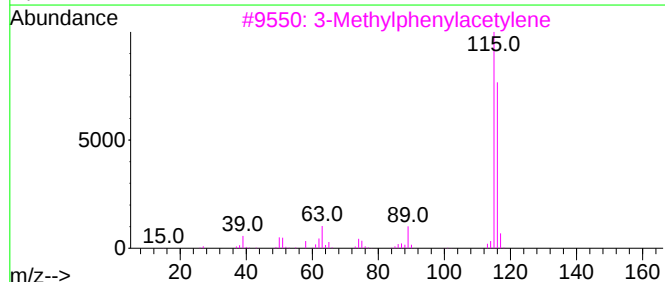
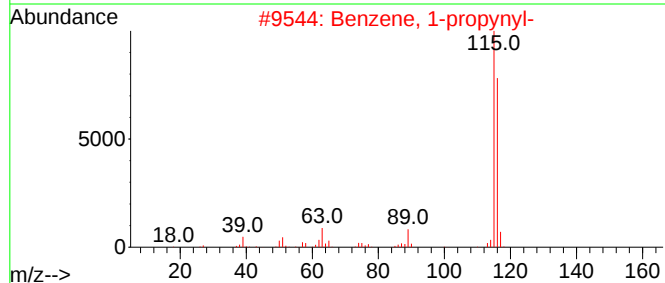
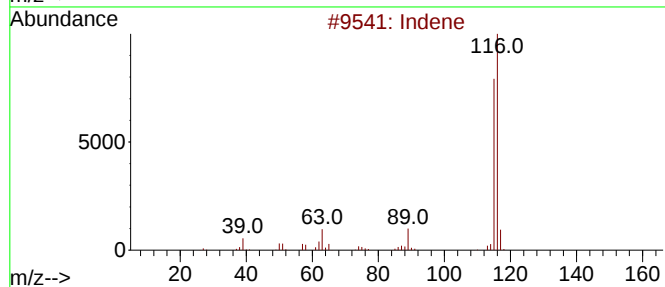
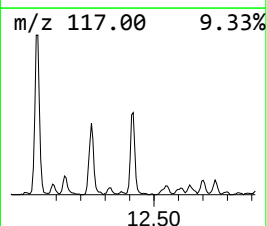
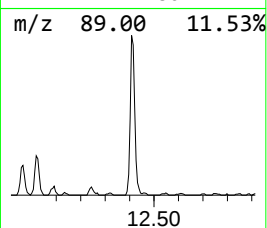
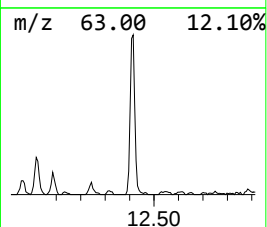
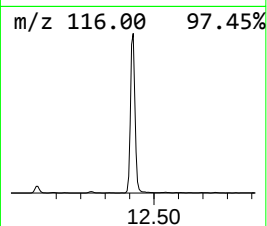
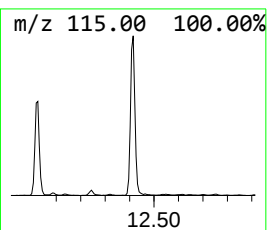
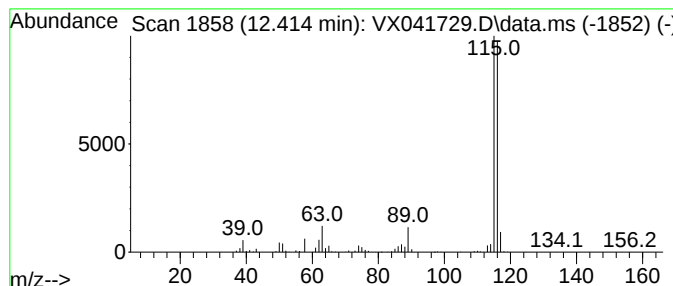
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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.
12.414	25.30 ug/l	300804	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	91
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	86



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ClientSampleId :
4-AB-VOC

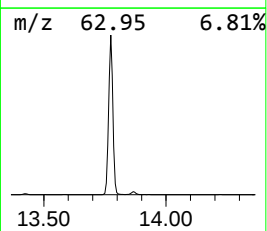
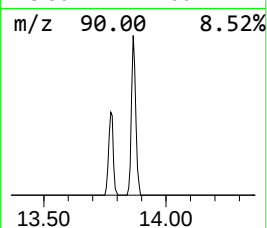
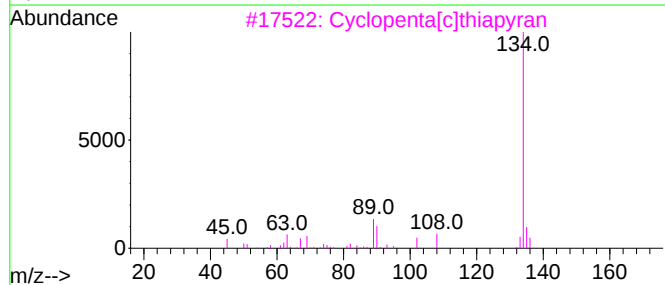
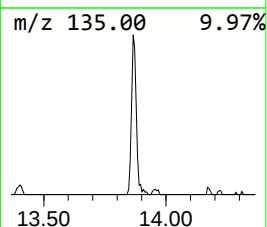
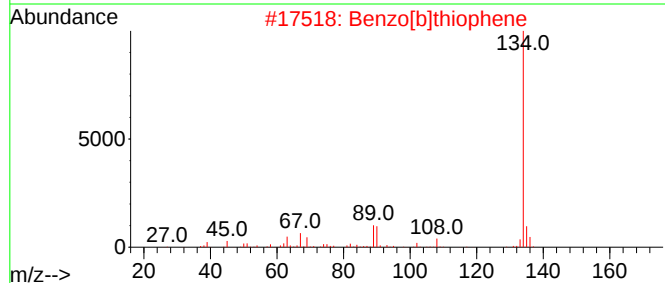
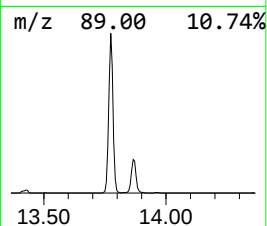
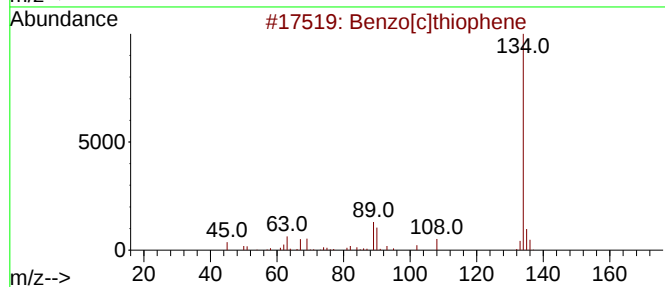
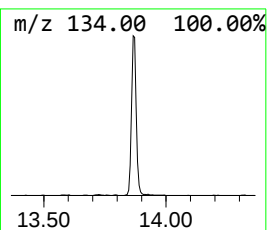
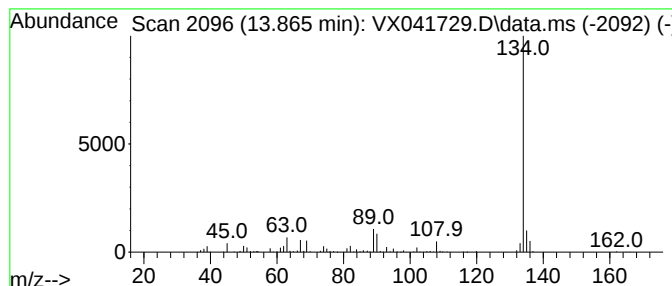
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzo[c]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.865	9.65 ug/l	114737	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	95
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	45



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
4-AB-VOC

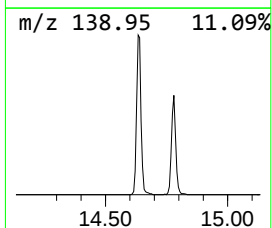
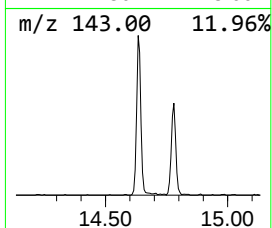
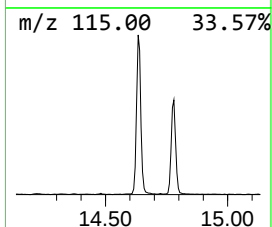
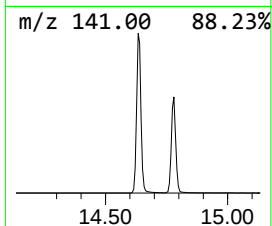
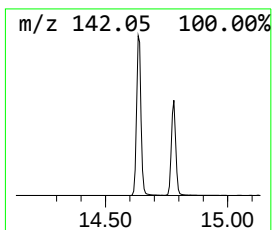
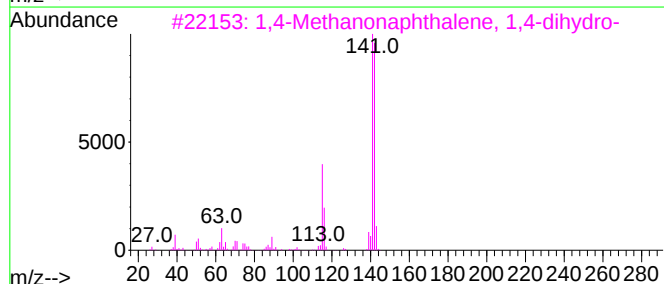
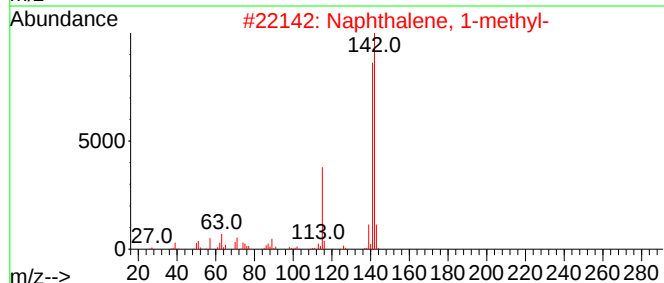
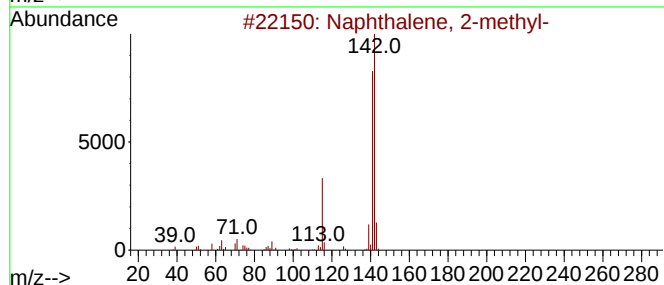
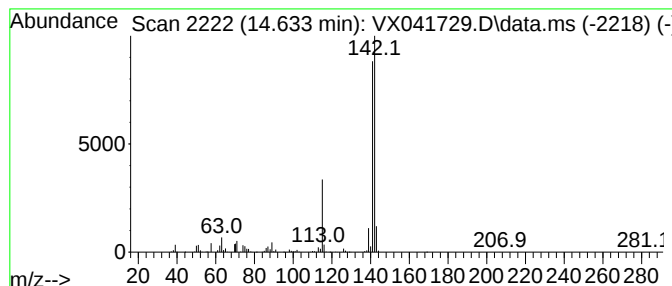
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	49.81 ug/l	592111	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	64



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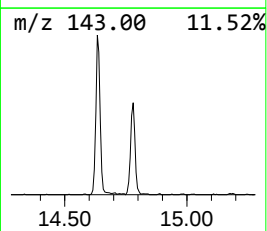
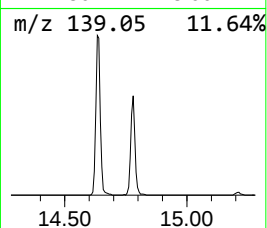
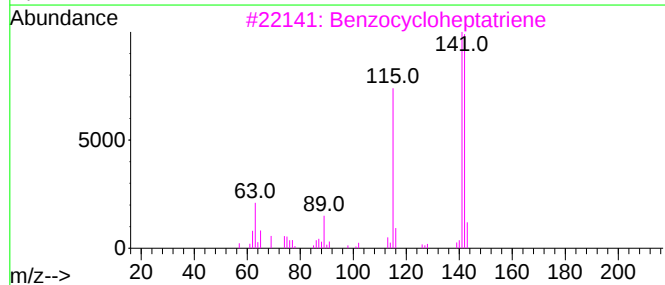
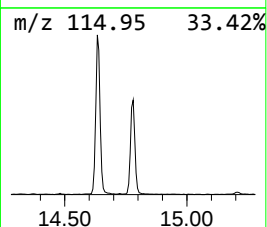
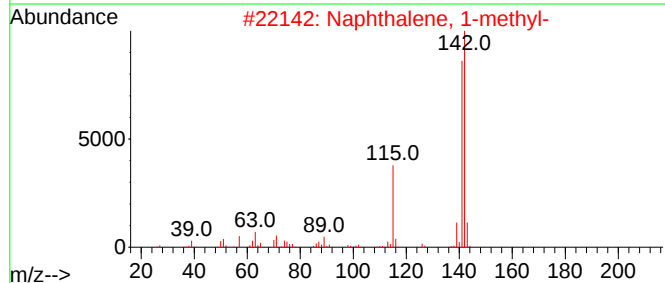
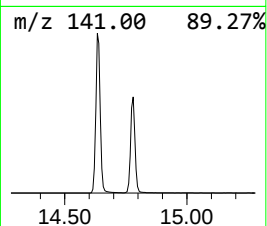
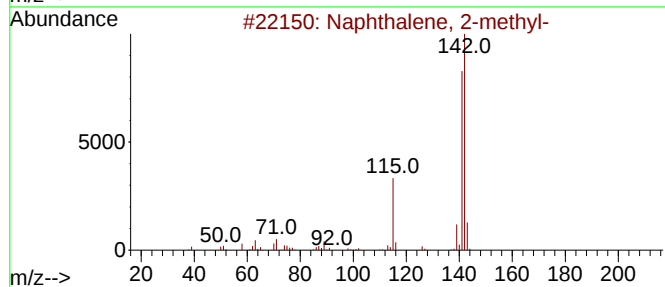
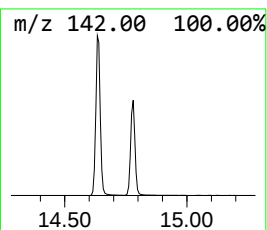
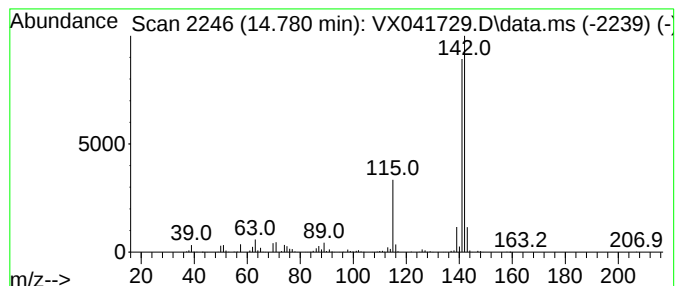
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	30.53 ug/l	362944	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			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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MSVOA_X
ClientSampleId :
4-AB-VOC

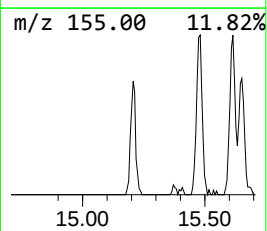
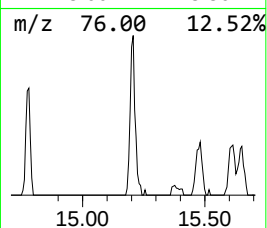
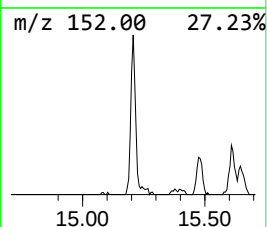
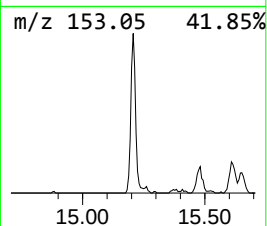
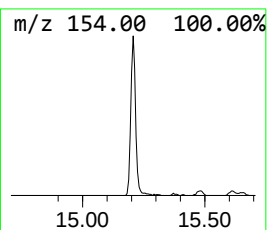
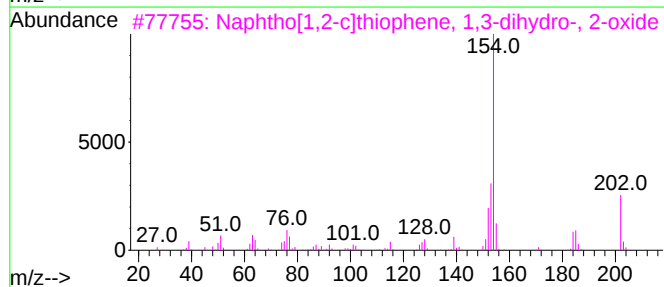
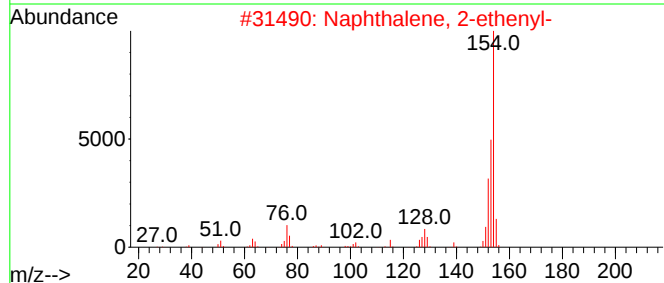
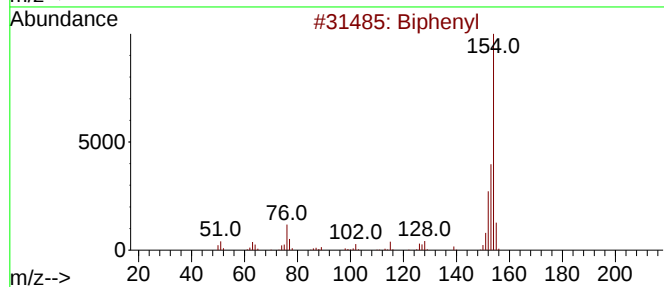
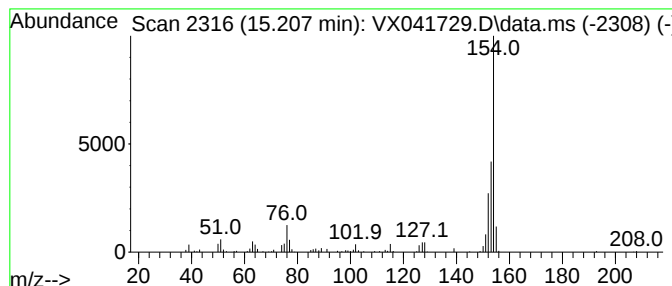
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 6 Biphenyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	5.38 ug/l	63967	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	95
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
3			Naphtho[1,2-c]thiophene, 1,3-dih...	202	C12H10S	031739-49-8	50
4			Acenaphthene	154	C12H10	000083-32-9	47
5			6-Cyanoquinoline	154	C10H6N2	023395-72-4	43



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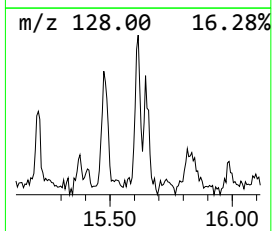
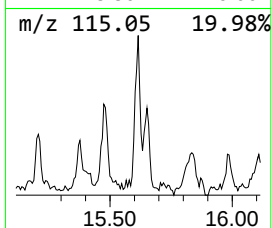
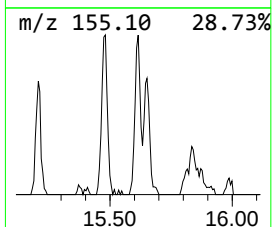
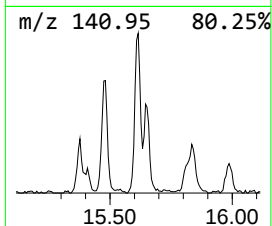
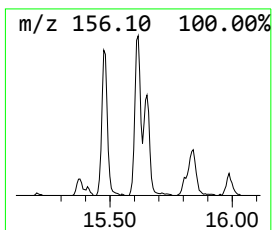
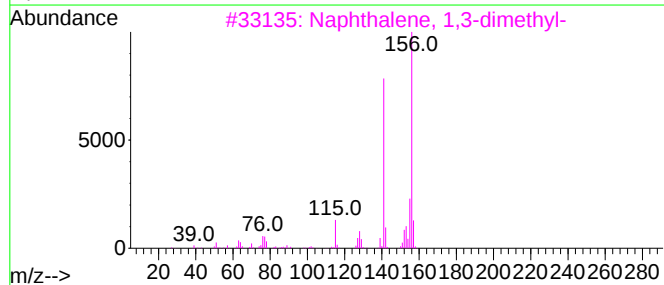
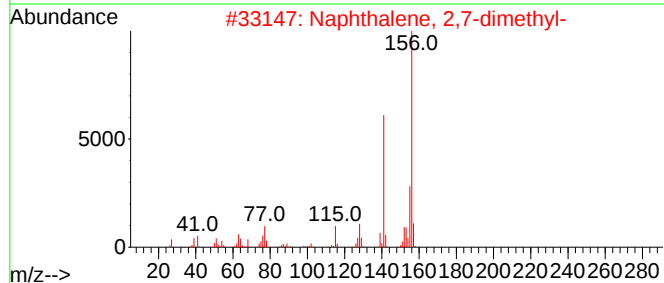
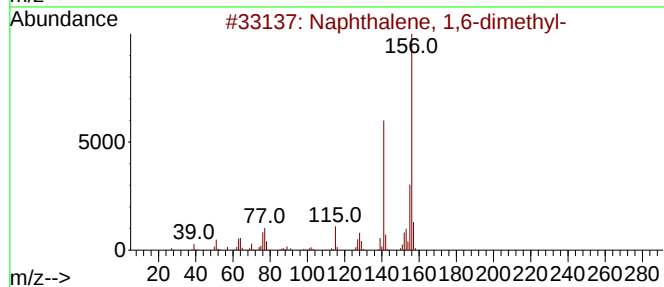
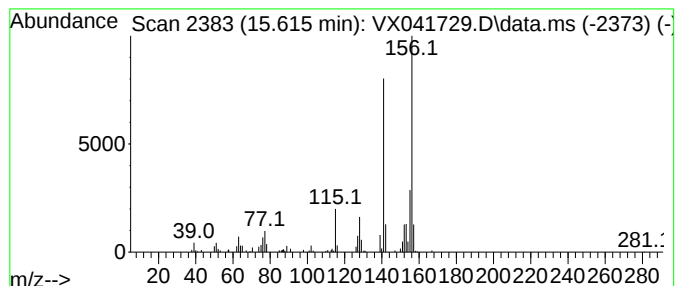
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	5.48 ug/l	65133	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	95
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060424\
Data File : VX041729.D
Acq On : 04 Jun 2024 12:45
Operator : JC/MD
Sample : P2657-14 10X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4-AB-VOC

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indene	12.414	25.3	ug/l	300804	4	12.024	594393	50.0
Benzo[c]thiophene	13.865	9.7	ug/l	114737	4	12.024	594393	50.0
Naphthalene, 1-...	14.633	49.8	ug/l	592111	4	12.024	594393	50.0
Benzocyclohepta...	14.780	30.5	ug/l	362944	4	12.024	594393	50.0
Biphenyl	15.207	5.4	ug/l	63967	4	12.024	594393	50.0
Naphthalene, 1,...	15.615	5.5	ug/l	65133	4	12.024	594393	50.0