

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060424\
 Data File : VX041727.D
 Acq On : 04 Jun 2024 11:58
 Operator : JC/MD
 Sample : P2657-18
 Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 5-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: VX041727.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	695	706	722	rBV2	71233	219676	4.94%	2.213%
2	5.543	722	731	747	rVB	136095	385204	8.66%	3.880%
3	5.958	789	799	808	rBV	77246	216373	4.86%	2.179%
4	6.757	920	930	948	rBV	204293	490989	11.04%	4.945%
5	8.647	1234	1240	1248	rBV	417617	666799	14.99%	6.716%
6	8.720	1248	1252	1275	rVB	25265	52147	1.17%	0.525%
7	10.055	1465	1471	1490	rBV	445614	618988	13.91%	6.234%
8	10.299	1505	1511	1518	rBV	68621	97783	2.20%	0.985%
9	10.640	1562	1567	1578	rBV	61268	93372	2.10%	0.940%
10	11.085	1634	1640	1653	rBV	379745	514549	11.57%	5.183%
11	11.451	1695	1700	1711	rVB	57693	82453	1.85%	0.830%
12	11.750	1745	1749	1755	rBV	89036	114253	2.57%	1.151%
13	12.024	1788	1794	1800	rBV	526992	660318	14.84%	6.651%
14	12.085	1800	1804	1810	rVB	52533	69793	1.57%	0.703%
15	12.414	1849	1858	1864	rBV	124807	164019	3.69%	1.652%
16	13.286	1991	2001	2007	rBV3	26760	48359	1.09%	0.487%
17	13.774	2076	2081	2089	rBV	3558066	4448938	100.00%	44.810%
18	13.865	2092	2096	2104	rVB	53154	76395	1.72%	0.769%
19	14.633	2218	2222	2233	rVB	357605	450204	10.12%	4.534%
20	14.780	2239	2246	2254	rVB	233588	301643	6.78%	3.038%
21	15.206	2308	2316	2321	rBV	34242	48827	1.10%	0.492%
22	15.481	2355	2361	2374	rVB2	27841	48758	1.10%	0.491%
23	15.615	2374	2383	2386	rBV	34054	58664	1.32%	0.591%

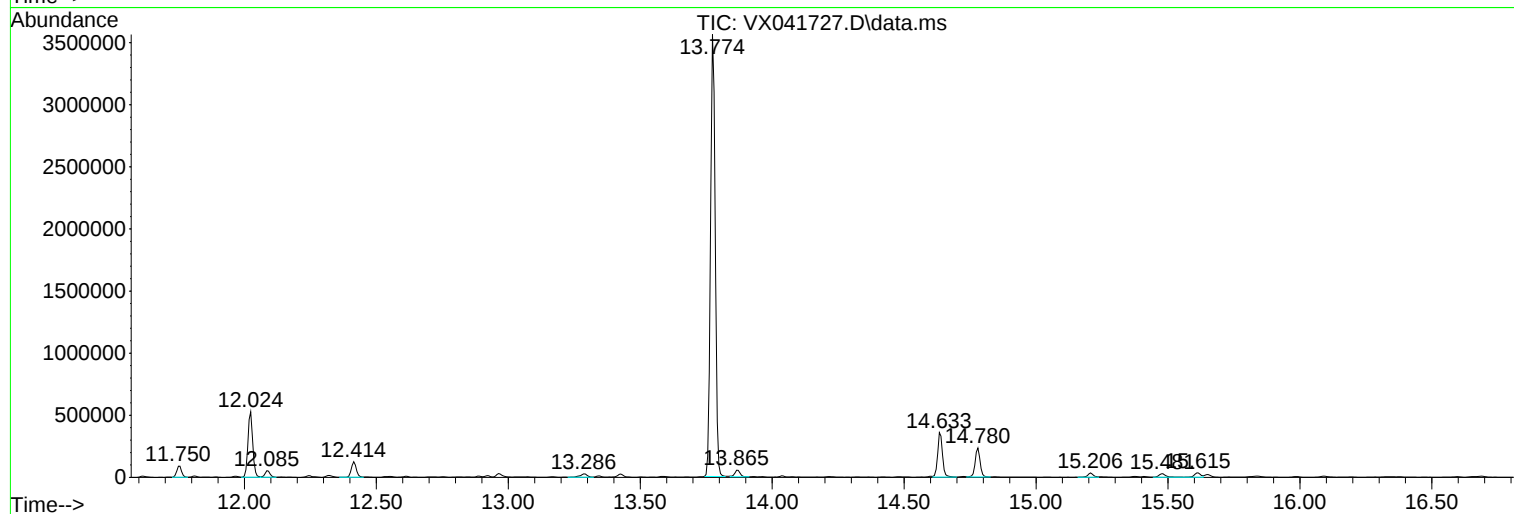
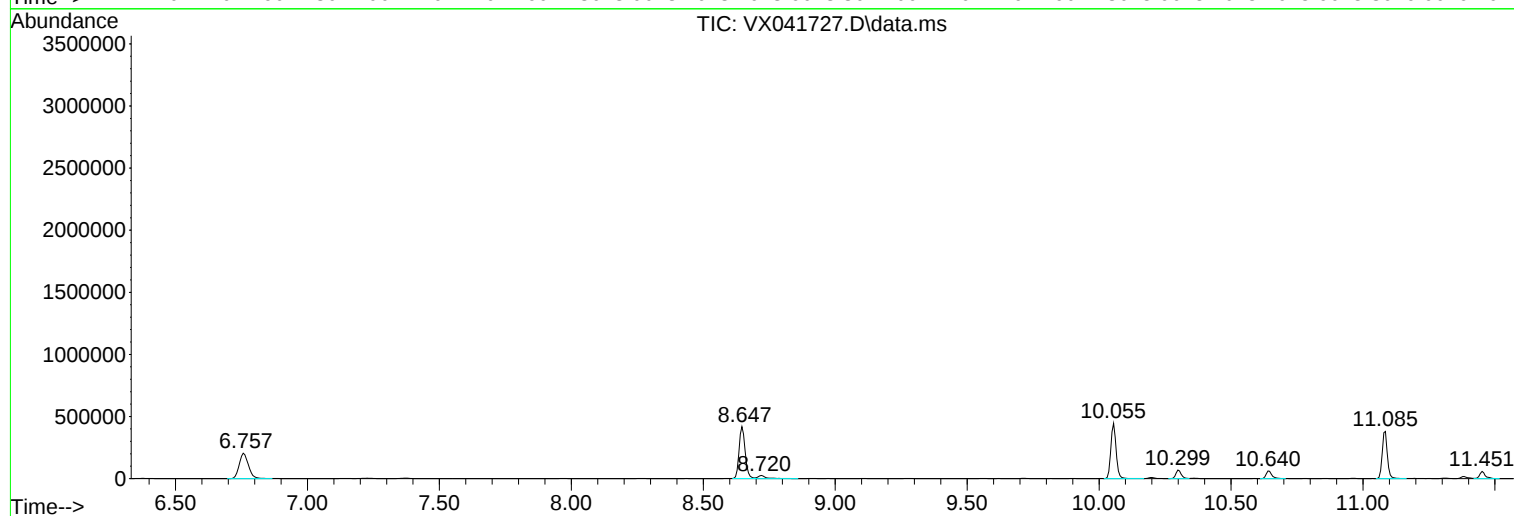
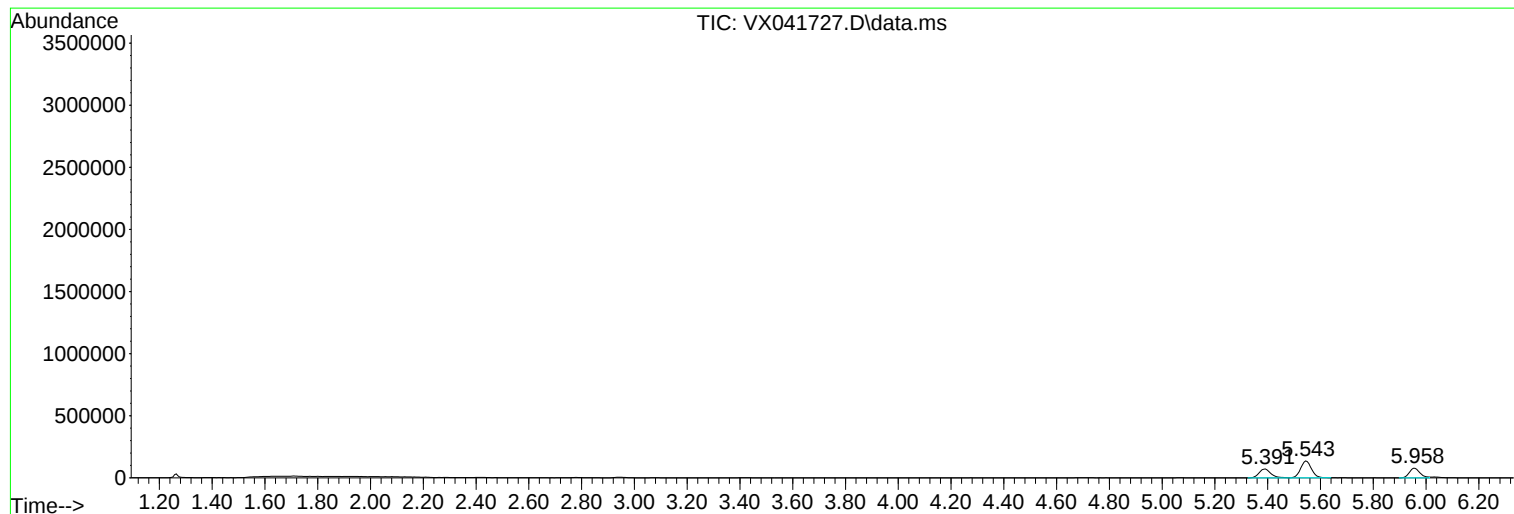
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
5-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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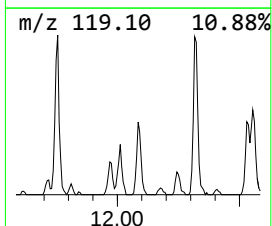
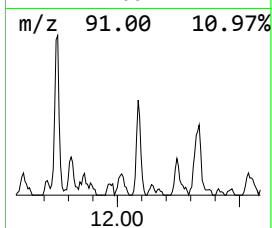
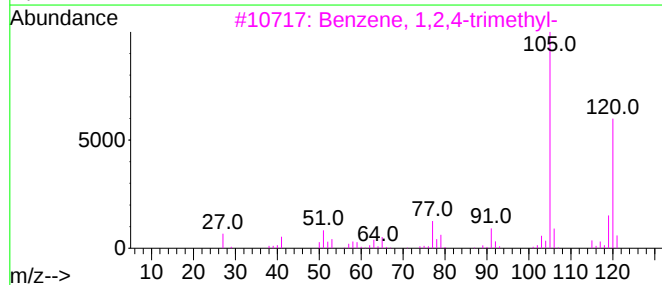
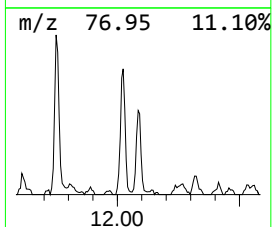
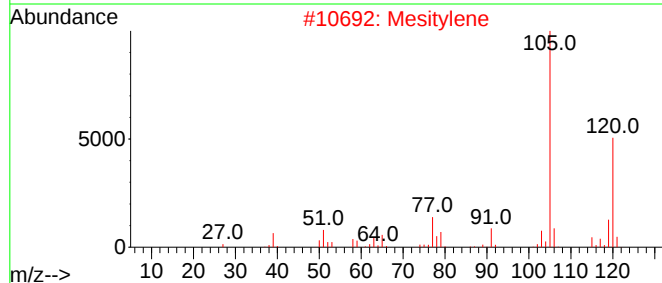
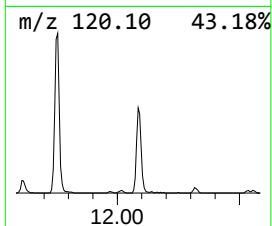
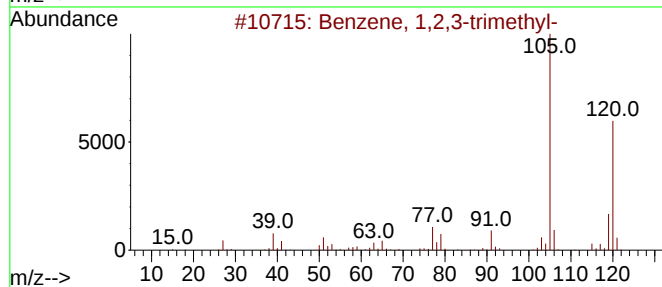
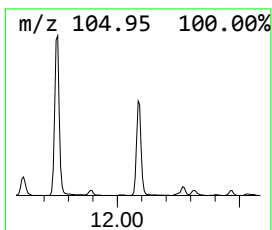
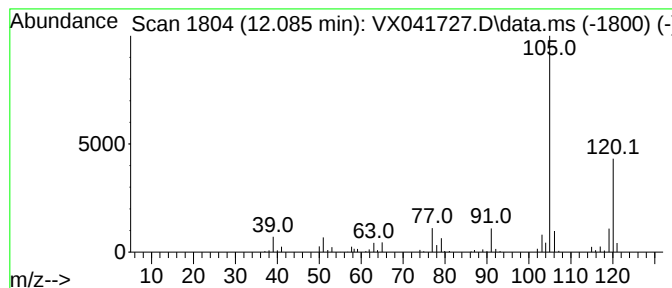
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	5.28 ug/l	69793	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Mesitylene	120	C9H12	000108-67-8	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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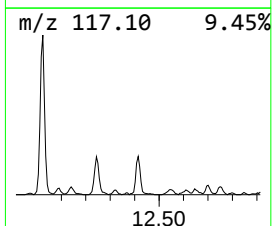
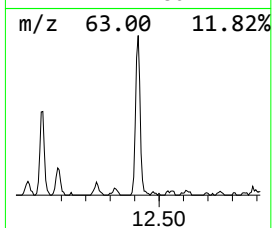
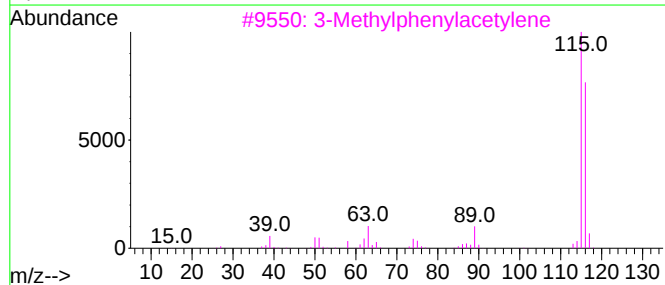
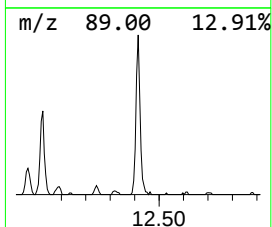
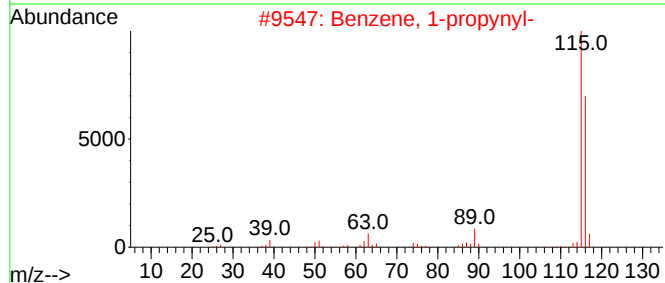
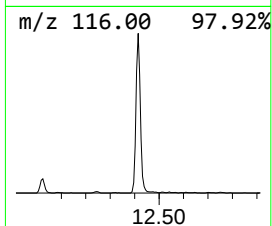
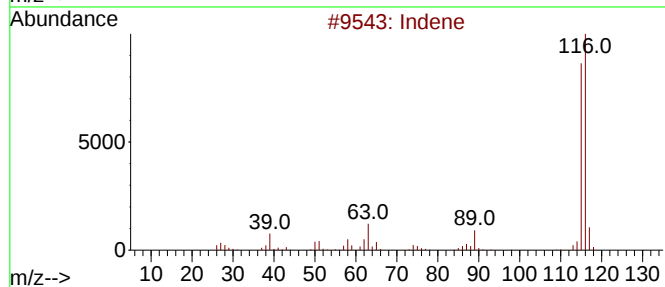
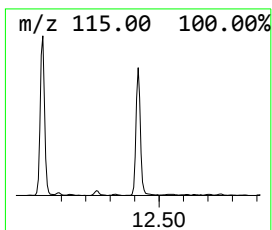
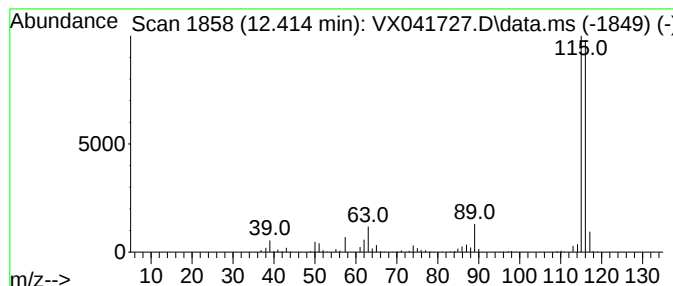
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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	12.42 ug/l	164019	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	95
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	94
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
5-AB-VOC

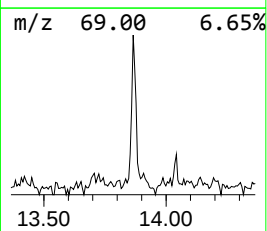
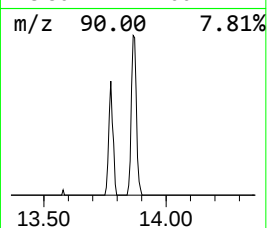
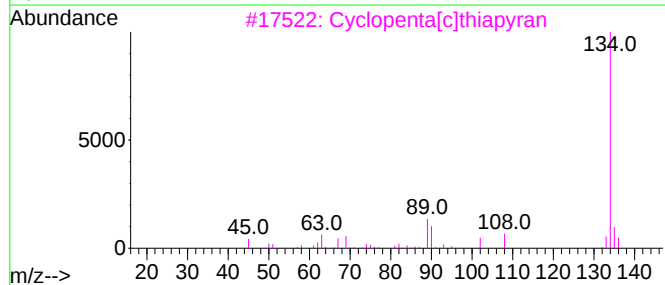
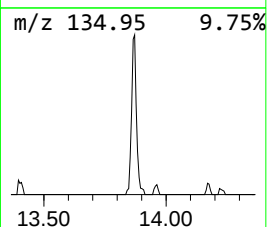
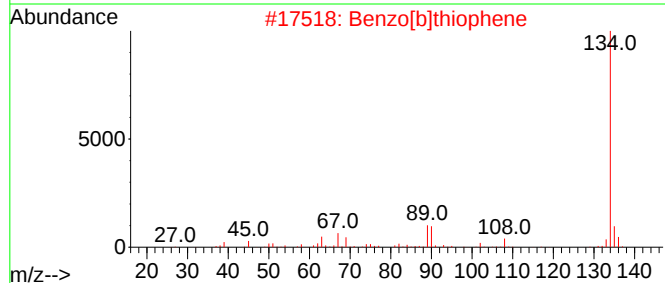
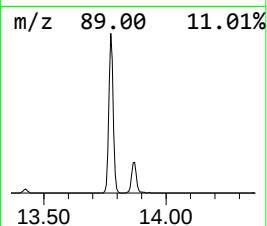
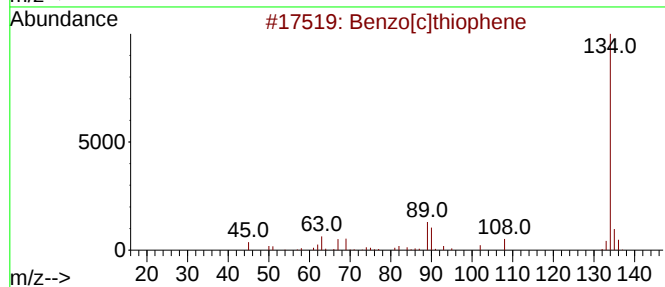
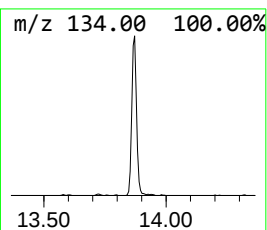
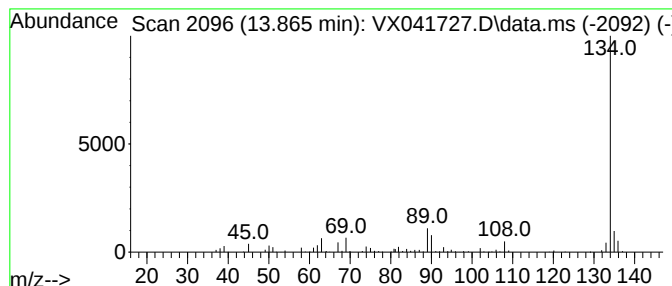
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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	5.78 ug/l	76395	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			5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	45
5			3-Deazaadenine	134	C6H6N4	006811-77-4	45



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
5-AB-VOC

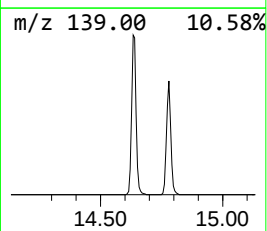
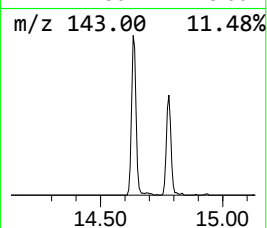
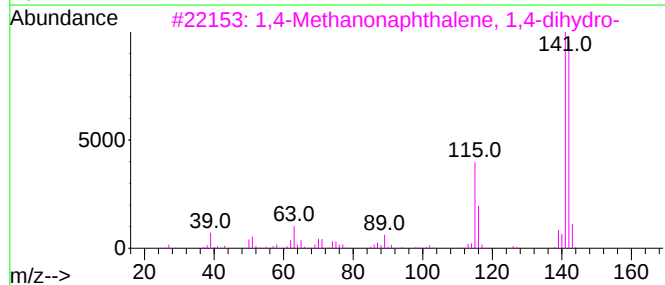
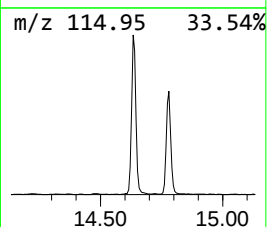
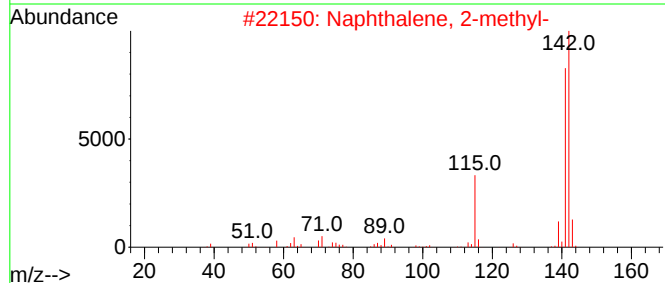
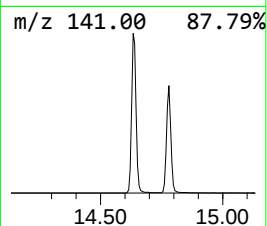
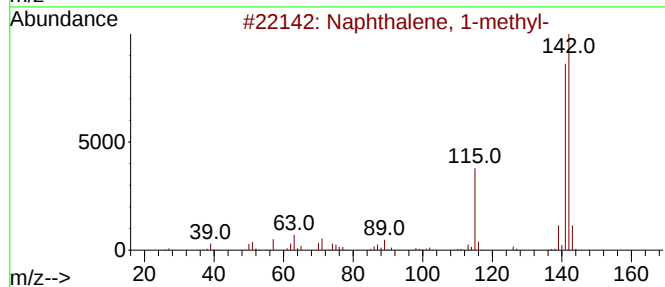
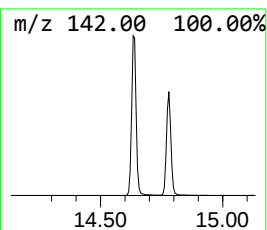
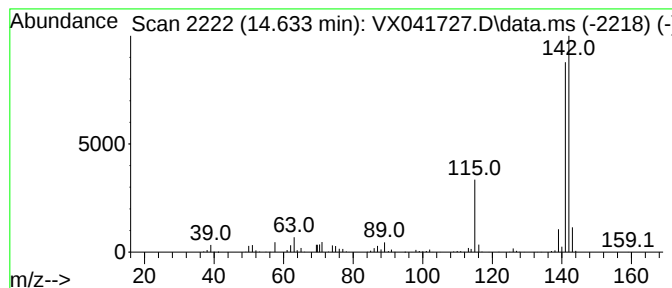
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	34.09 ug/l	450204	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	64



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ALS Vial : 7 Sample Multiplier: 1

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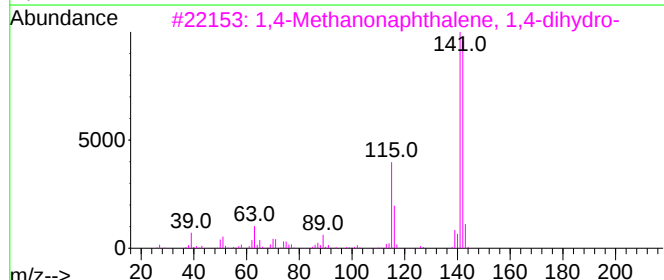
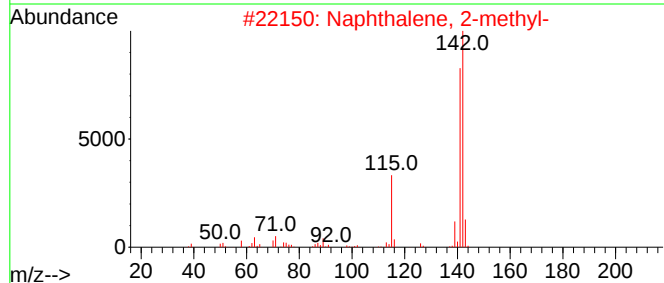
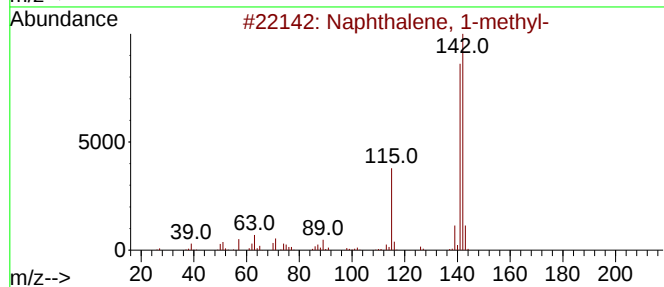
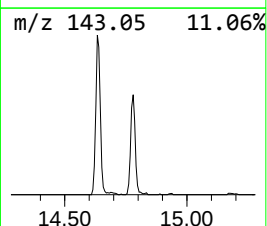
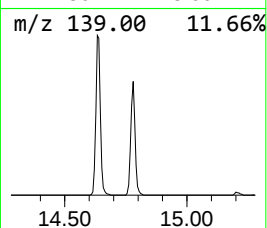
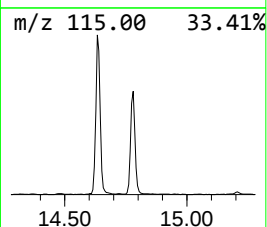
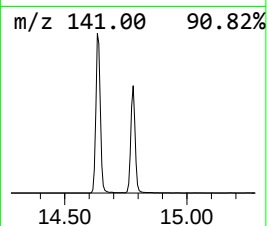
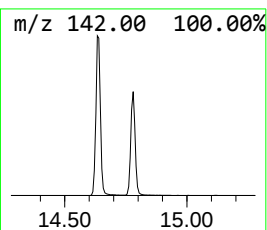
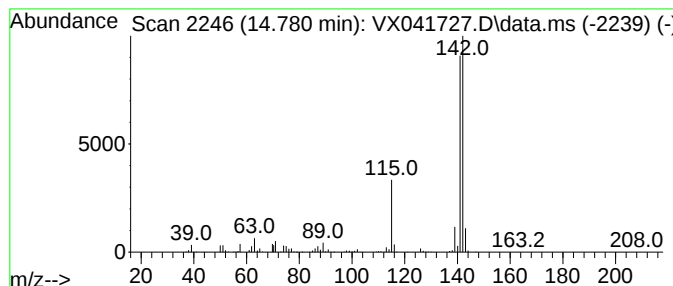
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	22.84 ug/l	301643	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	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,2,3-...	12.085	5.3	ug/l	69793	4	12.024	660318	50.0
Indene	12.414	12.4	ug/l	164019	4	12.024	660318	50.0
Benzo[c]thiophene	13.865	5.8	ug/l	76395	4	12.024	660318	50.0
Naphthalene, 1-...	14.633	34.1	ug/l	450204	4	12.024	660318	50.0
1,4-Methanonaph...	14.780	22.8	ug/l	301643	4	12.024	660318	50.0