

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071624\
 Data File : VX042338.D
 Acq On : 16 Jul 2024 13:13
 Operator : JC/MD
 Sample : P3224-05 50X
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 380AVEC-23

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\82X061824W.M
 Title : SW846 8260

Signal : TIC: VX042338.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	724	rBV2	95857	285797	9.16%	2.917%
2	5.556	724	733	754	rVB	118536	339204	10.87%	3.463%
3	5.964	791	800	808	rBV2	91633	243560	7.81%	2.486%
4	6.044	808	813	833	rVB2	22792	63178	2.02%	0.645%
5	6.769	923	932	956	rBV	191446	456360	14.62%	4.658%
6	8.653	1234	1241	1248	rBV	384256	589966	18.91%	6.022%
7	8.720	1248	1252	1263	rVB	94502	150633	4.83%	1.538%
8	10.055	1466	1471	1488	rBV	362015	489069	15.67%	4.992%
9	10.305	1506	1512	1518	rBV	119986	172104	5.52%	1.757%
10	10.646	1563	1568	1584	rVB	92670	133787	4.29%	1.366%
11	11.085	1634	1640	1651	rBV	321446	425542	13.64%	4.344%
12	11.384	1684	1689	1696	rBV	26748	48261	1.55%	0.493%
13	11.451	1696	1700	1709	rVB	53838	82413	2.64%	0.841%
14	11.756	1745	1750	1756	rVB	109618	135827	4.35%	1.386%
15	12.024	1789	1794	1801	rBV	345187	443672	14.22%	4.529%
16	12.085	1801	1804	1810	rVB	51132	69109	2.21%	0.705%
17	12.317	1838	1842	1850	rBV3	18456	31760	1.02%	0.324%
18	12.414	1850	1858	1864	rBV2	63533	98688	3.16%	1.007%
19	12.963	1945	1948	1955	rVB2	24857	38751	1.24%	0.396%
20	13.268	1992	1998	2000	rBV	28139	39416	1.26%	0.402%
21	13.286	2000	2001	2007	rVB3	29623	35396	1.13%	0.361%
22	13.426	2020	2024	2033	rVB5	18742	36268	1.16%	0.370%
23	13.774	2076	2081	2089	rVV	2499411	3120430	100.00%	31.853%
24	13.871	2090	2097	2101	rVB	45060	65355	2.09%	0.667%
25	14.640	2218	2223	2233	rVB	571977	729898	23.39%	7.451%
26	14.780	2240	2246	2254	rVB	424050	550794	17.65%	5.622%
27	15.207	2307	2316	2320	rBV	49332	72226	2.31%	0.737%
28	15.377	2336	2344	2347	rBV	37370	62405	2.00%	0.637%
29	15.408	2347	2349	2355	rVV3	22488	35078	1.12%	0.358%
30	15.481	2355	2361	2373	rVV	110419	200735	6.43%	2.049%
31	15.615	2373	2383	2386	rVV	152183	243315	7.80%	2.484%
32	15.652	2386	2389	2398	rVB	84374	128320	4.11%	1.310%
33	15.841	2411	2420	2429	rVB	35809	97954	3.14%	1.000%
34	15.987	2438	2444	2454	rVB	24359	42205	1.35%	0.431%
35	16.091	2454	2461	2469	rBV2	20562	38951	1.25%	0.398%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M

Title : SW846 8260

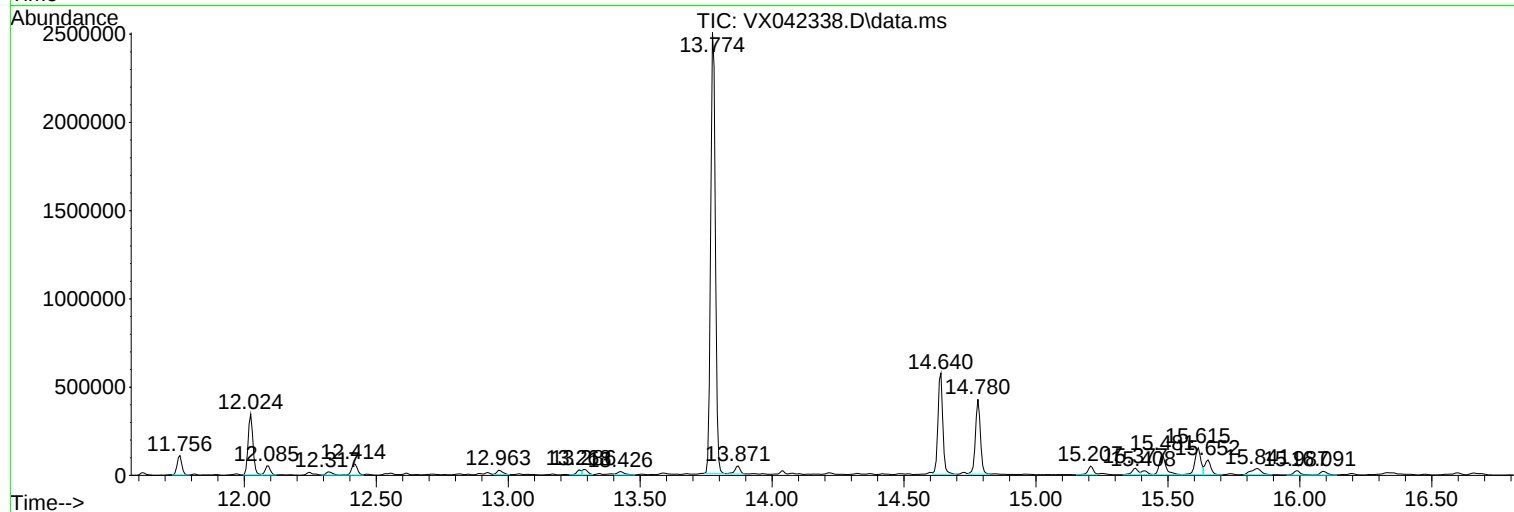
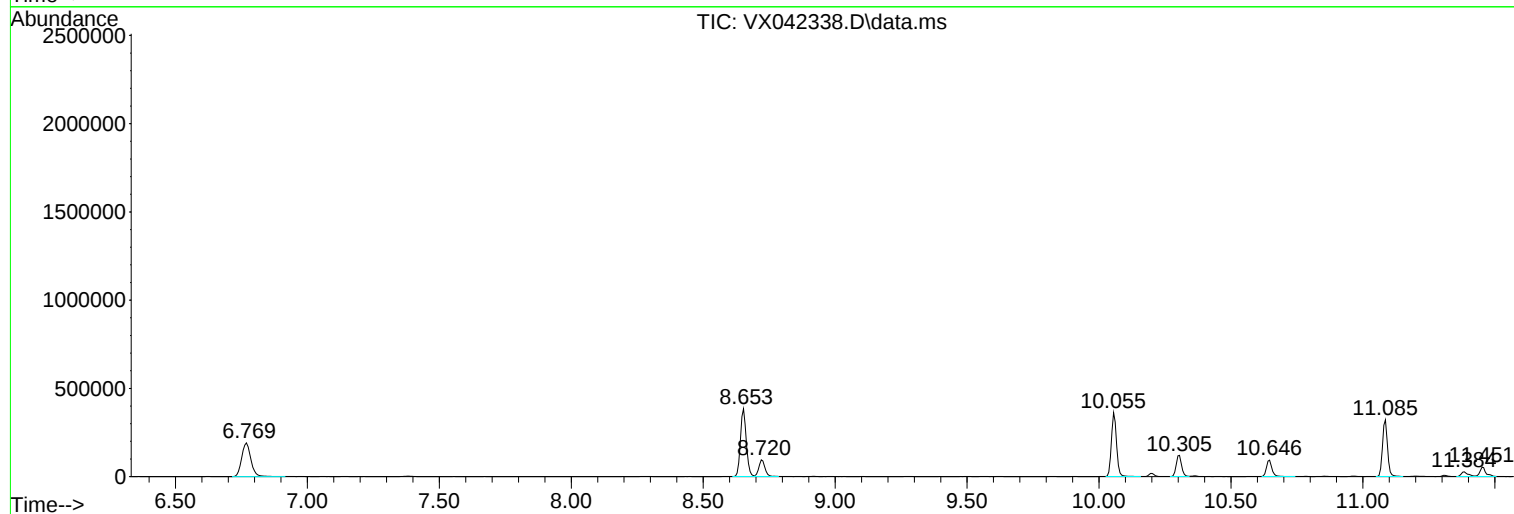
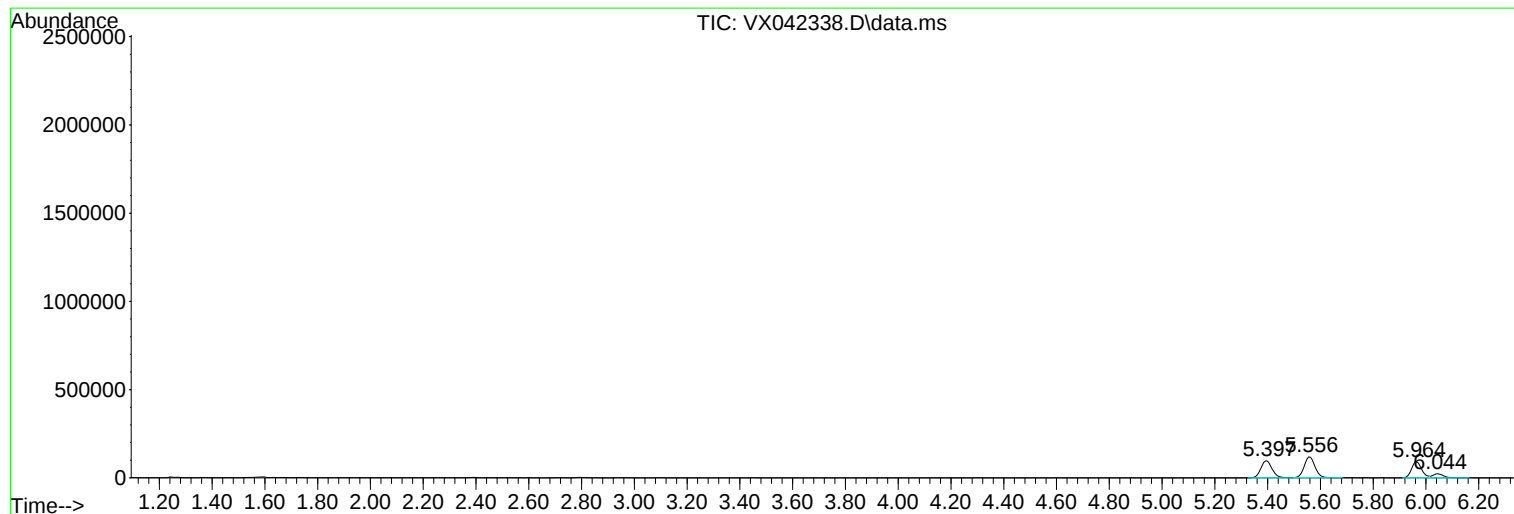
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

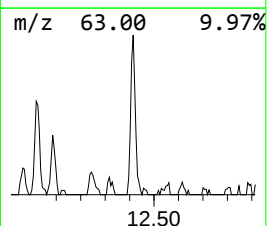
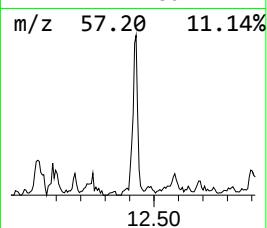
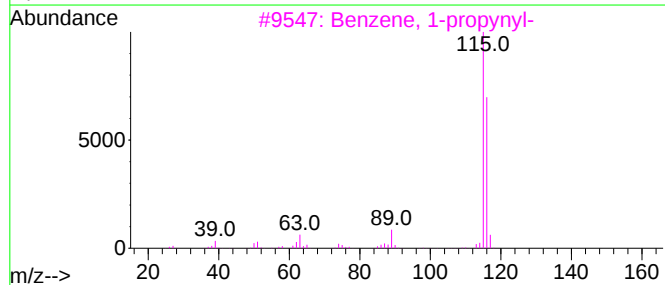
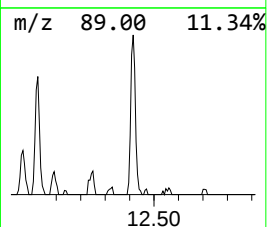
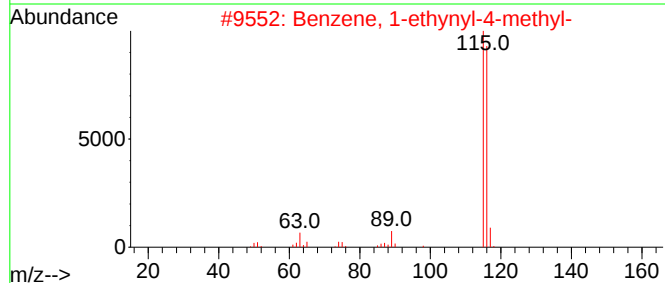
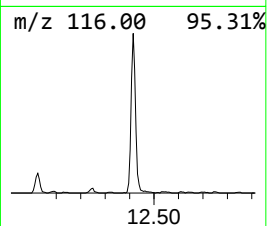
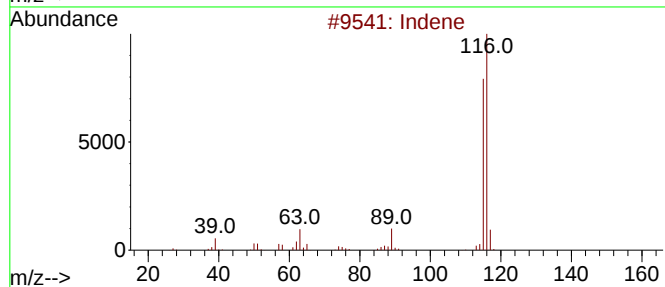
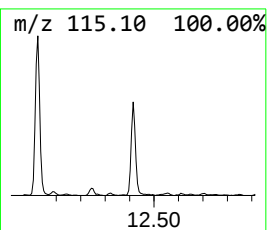
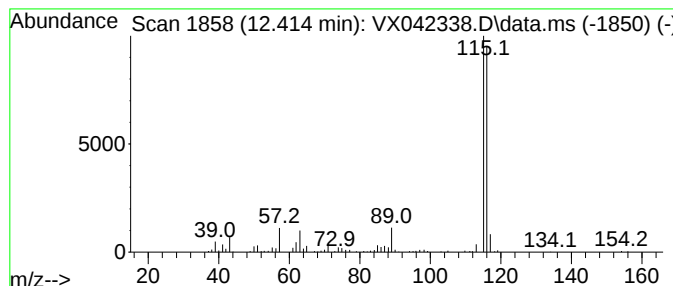
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 2 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	11.12 ug/l	98688	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	94
2			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	90
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	80



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Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

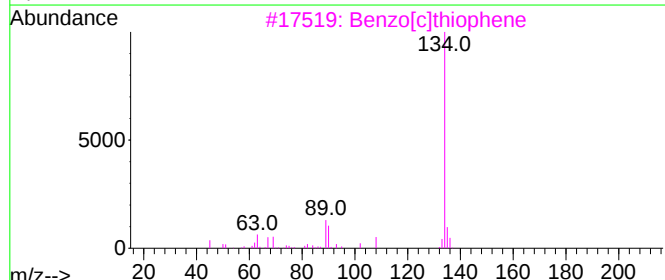
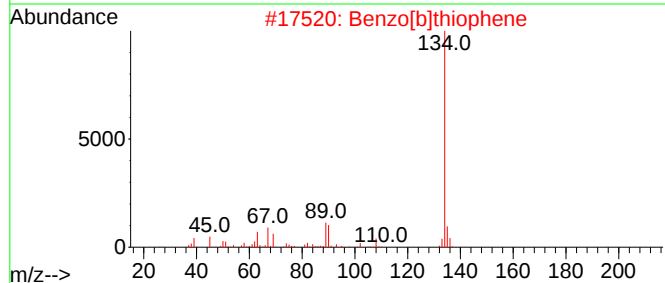
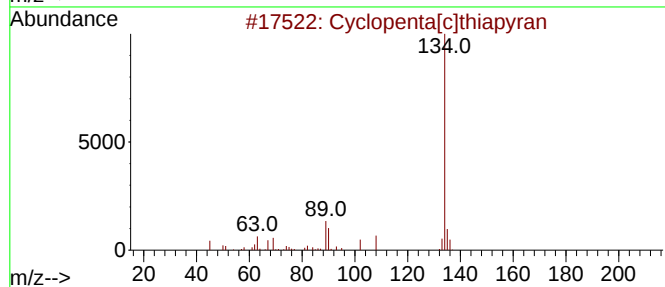
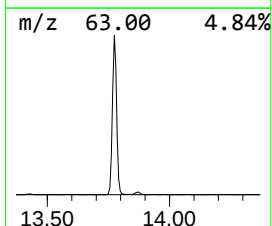
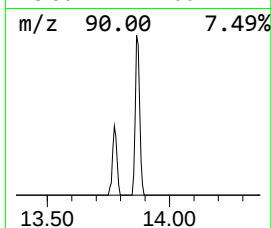
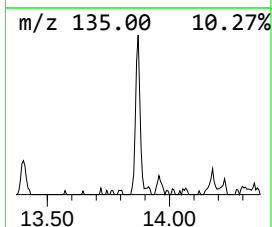
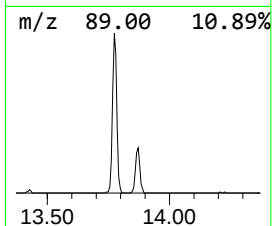
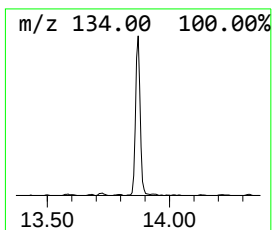
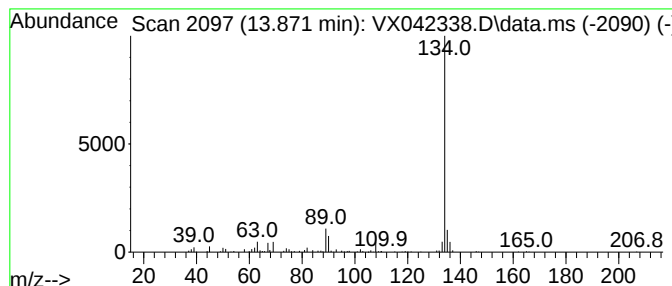
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopenta[c]thiapyran Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	7.37 ug/l	65355	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	91
3			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
4			3-Deazaadenine	134	C6H6N4	006811-77-4	50
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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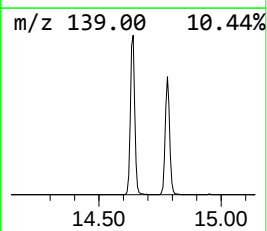
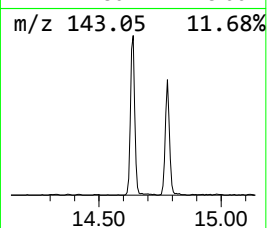
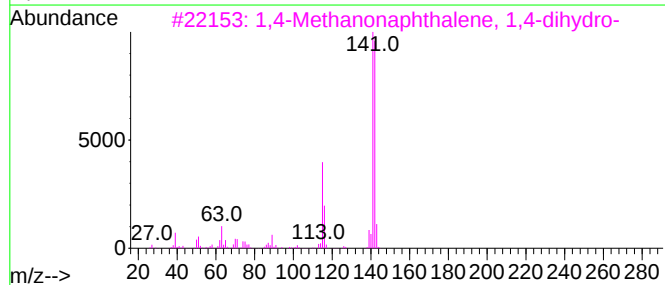
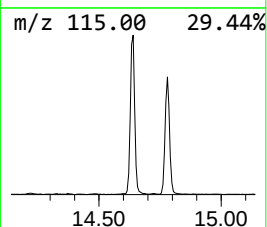
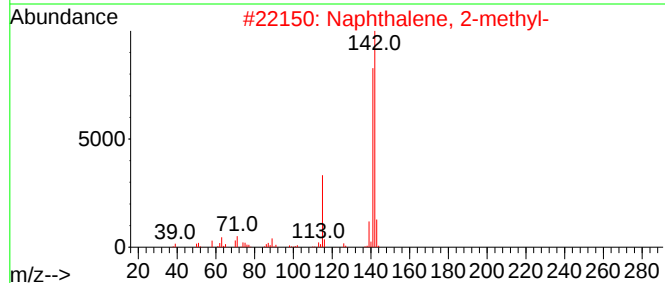
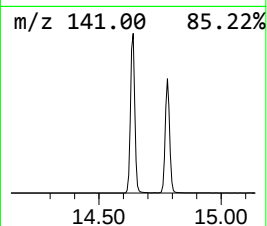
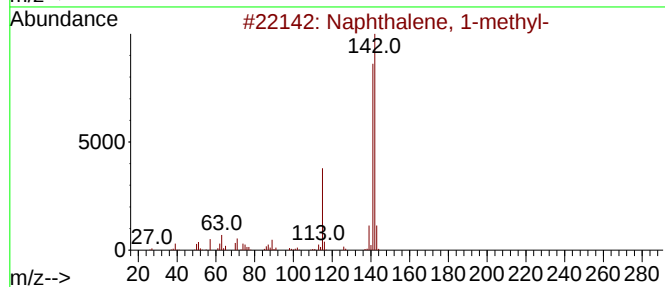
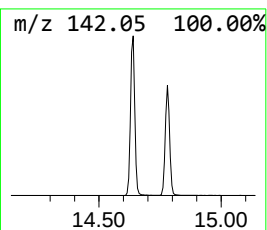
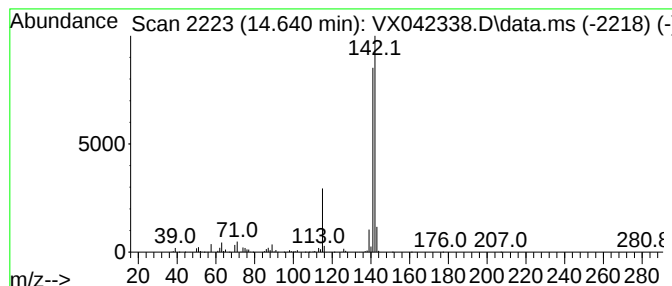
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	82.26 ug/l	729898	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	78



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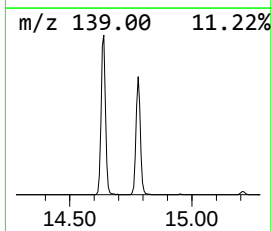
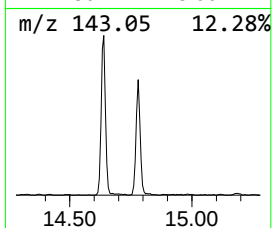
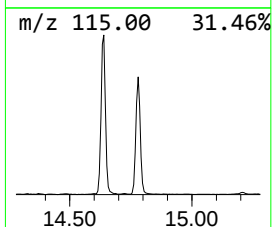
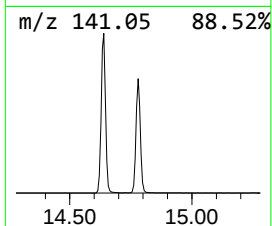
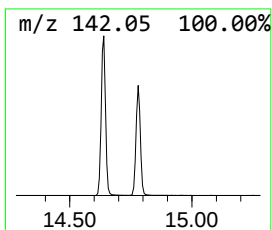
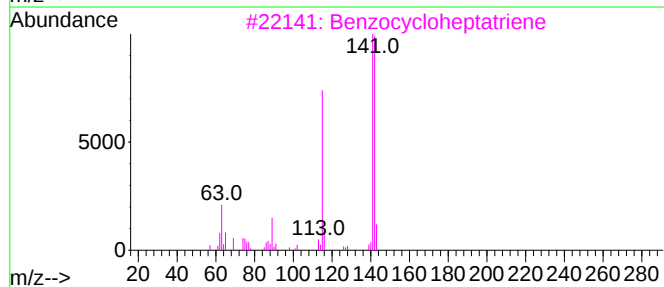
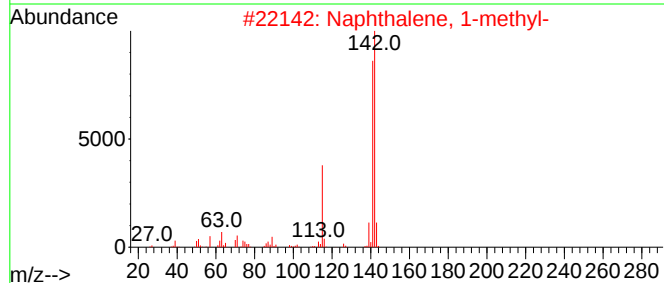
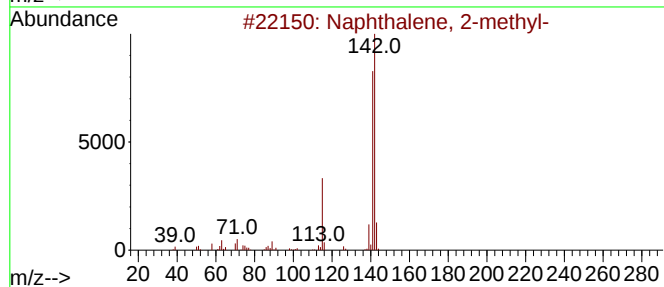
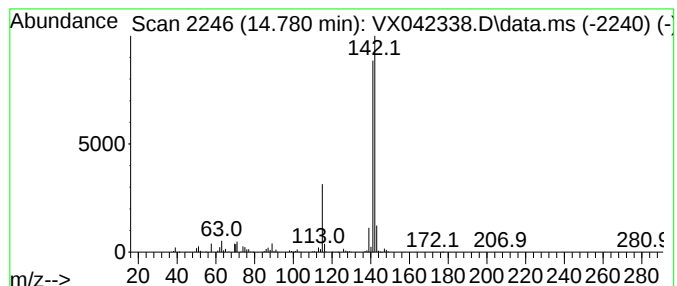
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Quant Title : SW846 8260

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	62.07 ug/l	550794	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



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Instrument :
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ClientSampleId :
380AVEC-23

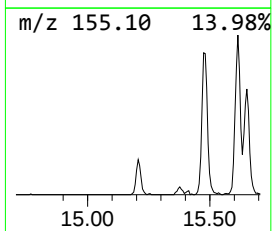
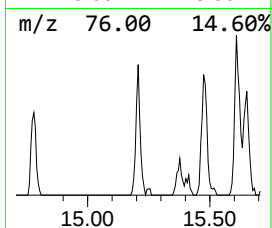
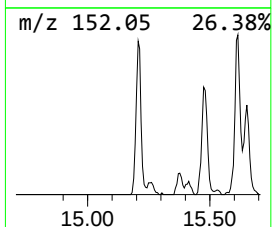
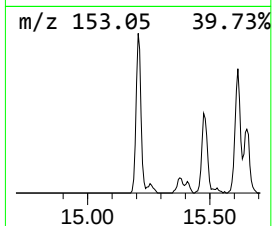
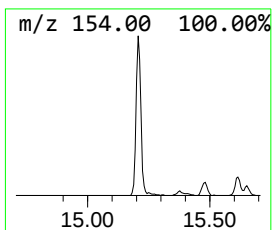
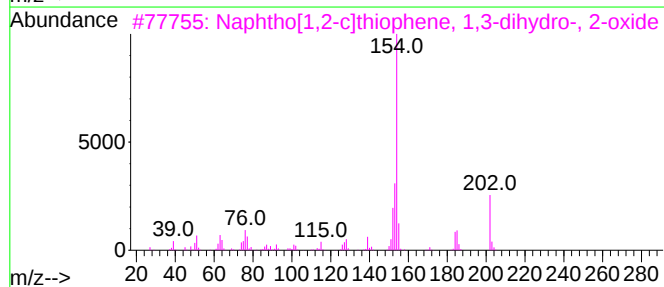
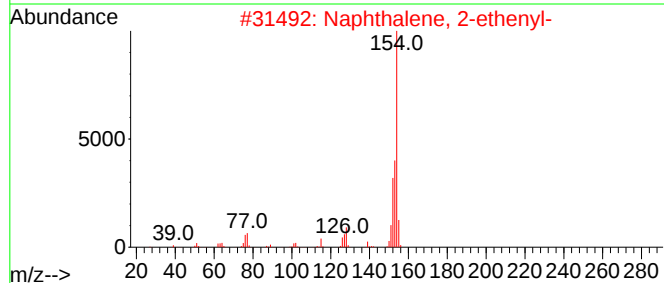
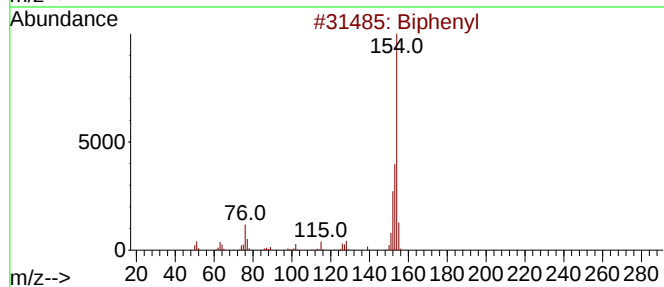
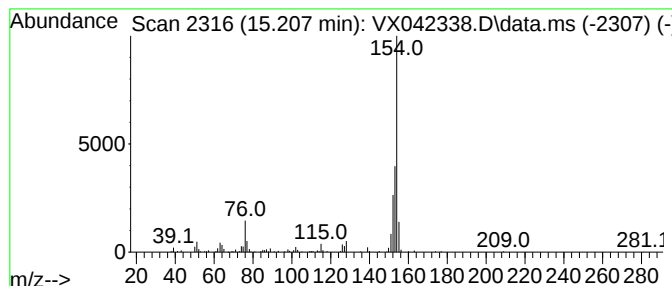
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2-ethenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	8.14 ug/l	72226	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	C12H100S	031739-49-8	74
4			3-Quinolincarbonitrile	154	C10H6N2	034846-64-5	49
5			6-Cyanoquinoline	154	C10H6N2	023395-72-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071624\
Data File : VX042338.D
Acq On : 16 Jul 2024 13:13
Operator : JC/MD
Sample : P3224-05 50X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

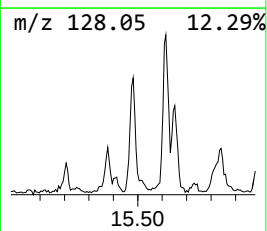
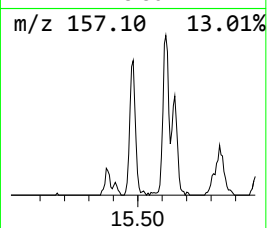
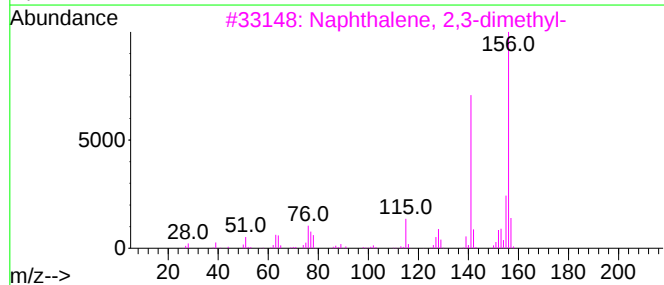
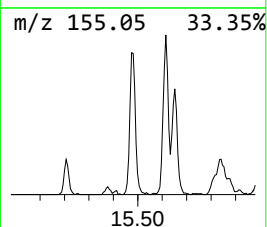
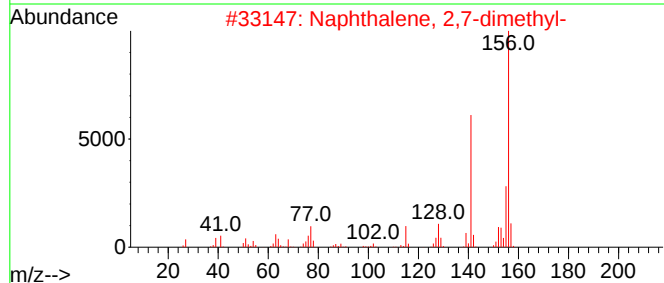
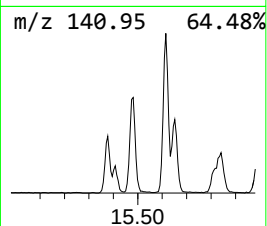
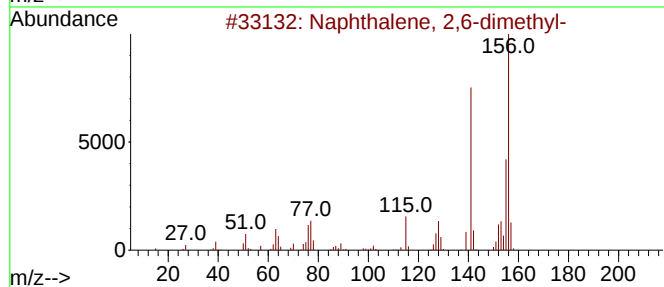
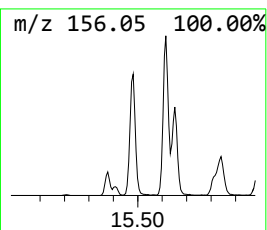
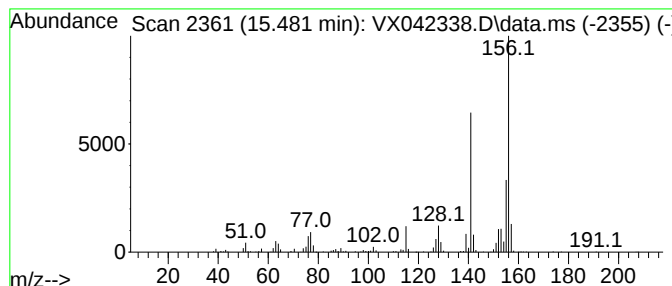
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	22.62 ug/l	200735	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071624\
Data File : VX042338.D
Acq On : 16 Jul 2024 13:13
Operator : JC/MD
Sample : P3224-05 50X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

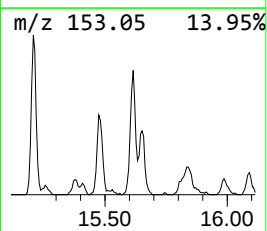
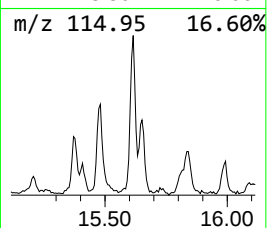
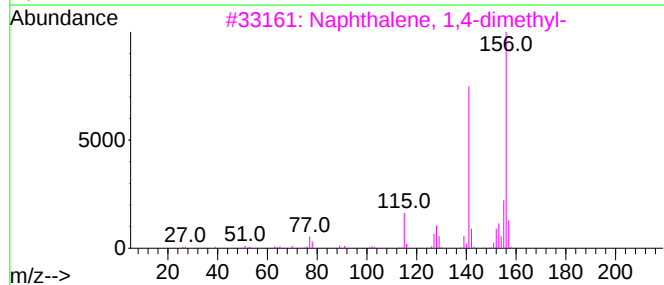
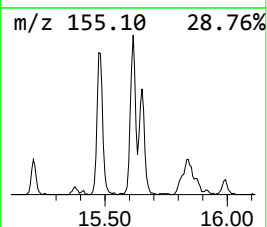
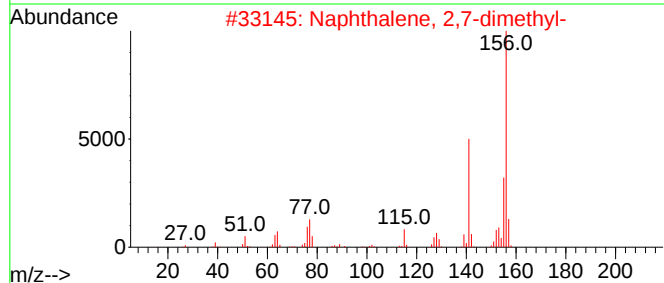
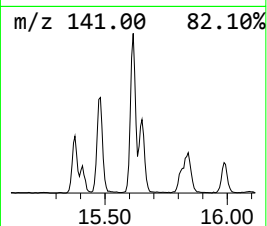
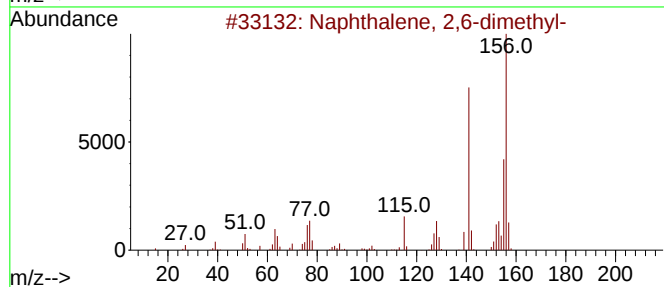
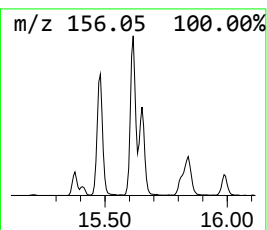
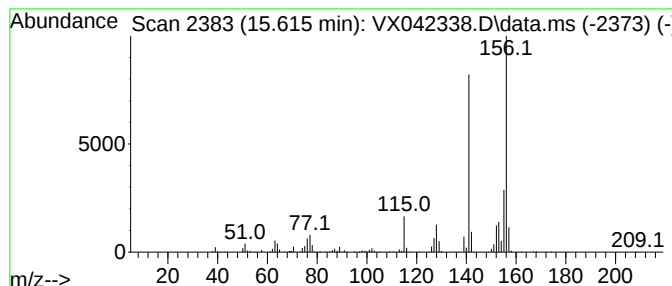
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	27.42 ug/l	243315	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071624\
Data File : VX042338.D
Acq On : 16 Jul 2024 13:13
Operator : JC/MD
Sample : P3224-05 50X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

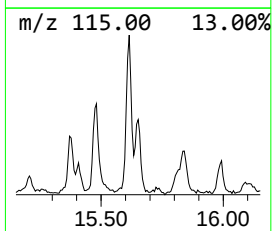
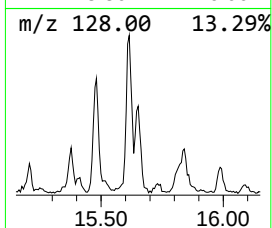
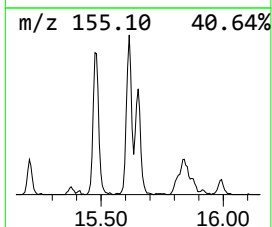
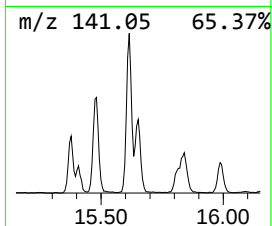
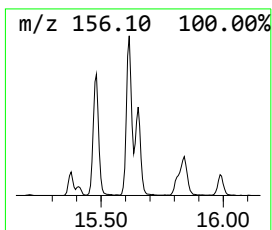
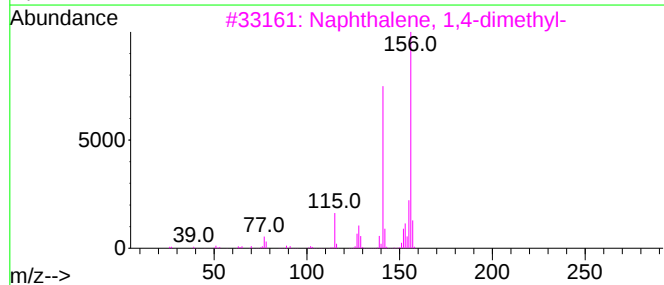
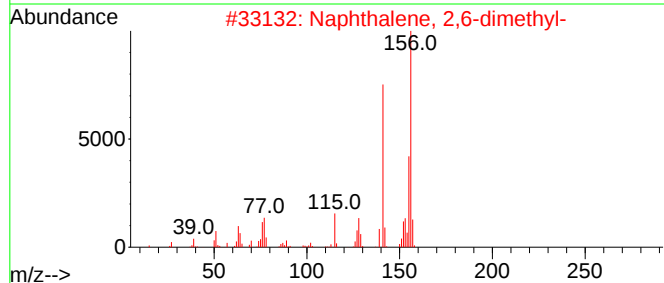
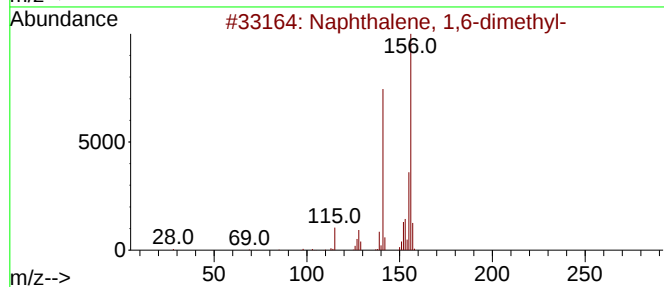
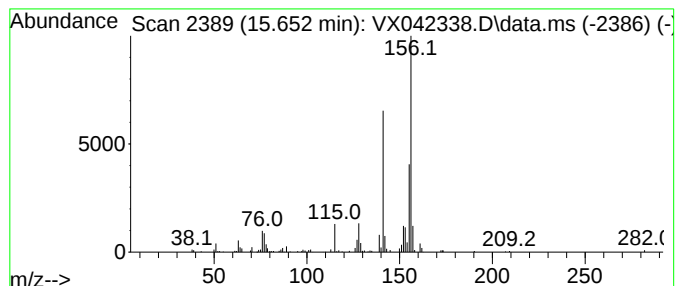
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	14.46 ug/l	128320	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	96
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071624\
Data File : VX042338.D
Acq On : 16 Jul 2024 13:13
Operator : JC/MD
Sample : P3224-05 50X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

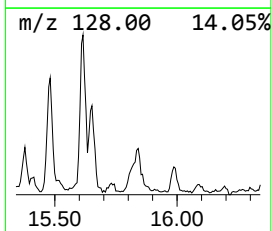
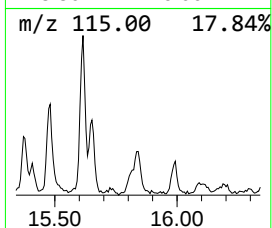
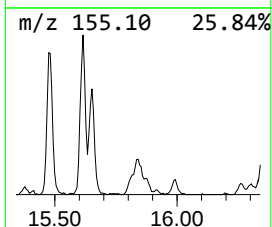
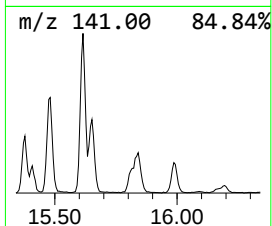
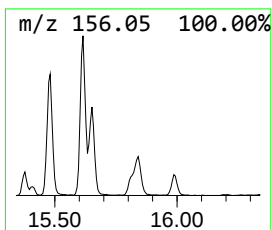
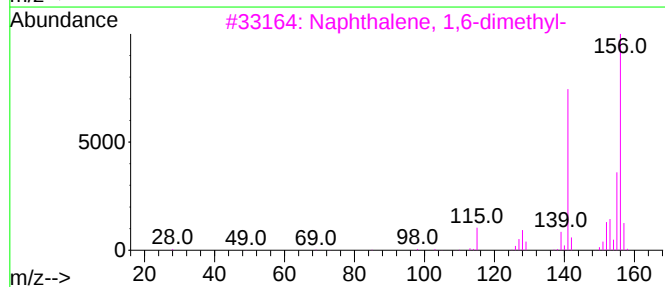
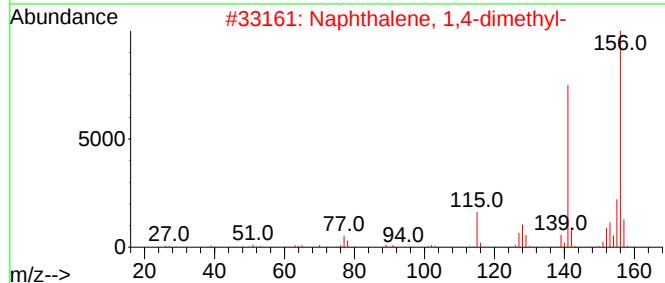
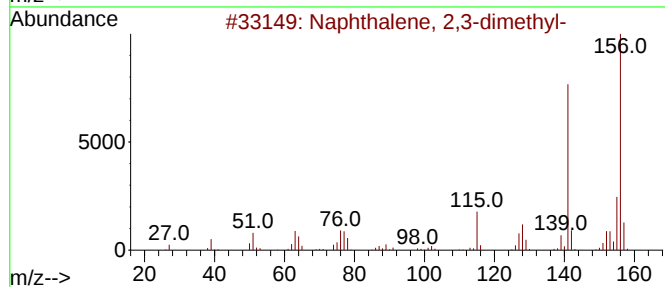
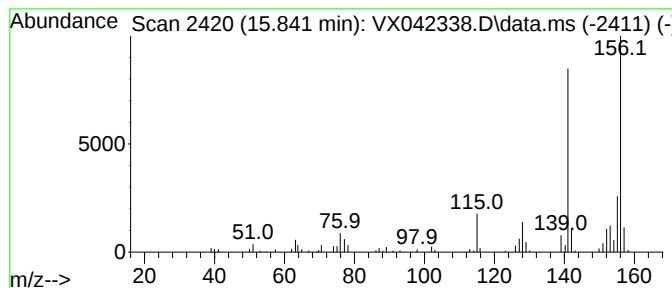
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	11.04 ug/l	97954	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071624\
Data File : VX042338.D
Acq On : 16 Jul 2024 13:13
Operator : JC/MD
Sample : P3224-05 50X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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Cyclopenta[c]th...	13.871	7.4	ug/l	65355	4	12.024	443672	50.0
1,4-Methanonaph...	14.640	82.3	ug/l	729898	4	12.024	443672	50.0
Benzocyclohepta...	14.780	62.1	ug/l	550794	4	12.024	443672	50.0
Naphthalene, 2-...	15.207	8.1	ug/l	72226	4	12.024	443672	50.0
Naphthalene, 2,...	15.481	22.6	ug/l	200735	4	12.024	443672	50.0
Naphthalene, 2,...	15.615	27.4	ug/l	243315	4	12.024	443672	50.0
Naphthalene, 1,...	15.652	14.5	ug/l	128320	4	12.024	443672	50.0
Naphthalene, 2,...	15.841	11.0	ug/l	97954	4	12.024	443672	50.0