

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
 Data File : VX047446.D
 Acq On : 20 Aug 2025 16:30
 Operator : JC/MD
 Sample : Q2900-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-17B-081825

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\82X081525W.M
 Title : SW846 8260

Signal : TIC: VX047446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	44	rBV	226941	619509	15.01%	3.644%
2	5.404	698	708	725	rBV3	131479	422775	10.24%	2.487%
3	5.568	725	735	760	rVB	201035	625712	15.16%	3.680%
4	5.971	791	801	809	rBV	151801	423121	10.25%	2.489%
5	6.056	809	815	832	rVB	57368	172428	4.18%	1.014%
6	6.769	922	932	953	rBV	375619	972565	23.56%	5.721%
7	8.653	1234	1241	1248	rBV	821440	1303861	31.59%	7.669%
8	8.720	1248	1252	1267	rVB	159276	268049	6.49%	1.577%
9	10.055	1465	1471	1488	rBV	938289	1302117	31.55%	7.659%
10	10.195	1489	1494	1506	rVV	139391	188142	4.56%	1.107%
11	10.299	1506	1511	1524	rVB	113711	173912	4.21%	1.023%
12	10.653	1562	1569	1580	rBV2	89632	180387	4.37%	1.061%
13	11.079	1634	1639	1655	rBV	777672	984213	23.85%	5.789%
14	11.378	1682	1688	1690	rBV	56708	74894	1.81%	0.441%
15	11.750	1740	1749	1755	rBV	65132	83866	2.03%	0.493%
16	11.805	1755	1758	1762	rBV	32199	41547	1.01%	0.244%
17	12.018	1788	1793	1800	rBV	1109302	1333357	32.30%	7.843%
18	12.244	1824	1830	1838	rBV	78139	105297	2.55%	0.619%
19	12.408	1852	1857	1864	rBV	499341	636344	15.42%	3.743%
20	13.341	2005	2010	2017	rVB2	75881	95218	2.31%	0.560%
21	13.420	2017	2023	2029	rBV2	89460	122306	2.96%	0.719%
22	13.774	2069	2081	2092	rBV	3187301	4127507	100.00%	24.278%
23	13.865	2092	2096	2103	rVB	144636	191144	4.63%	1.124%
24	14.634	2218	2222	2232	rVB	749777	938074	22.73%	5.518%
25	14.774	2240	2245	2259	rVB	583490	767412	18.59%	4.514%
26	15.207	2310	2316	2321	rBV	56378	80756	1.96%	0.475%
27	15.475	2354	2360	2365	rBV2	50651	88599	2.15%	0.521%
28	15.609	2377	2382	2386	rBV	73343	115635	2.80%	0.680%
29	15.646	2386	2388	2396	rVB3	39988	55770	1.35%	0.328%
30	15.835	2410	2419	2431	rVB2	25389	69804	1.69%	0.411%
31	16.085	2453	2460	2470	rBV	193308	343788	8.33%	2.022%
32	16.322	2492	2499	2507	rVB	47969	92857	2.25%	0.546%

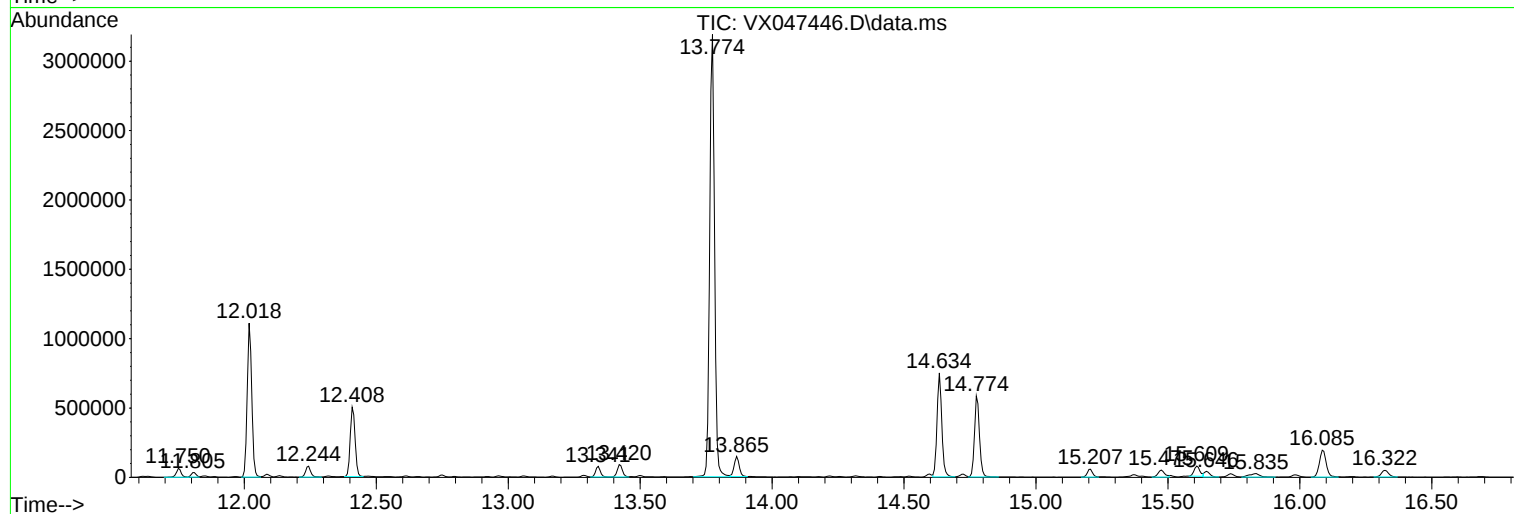
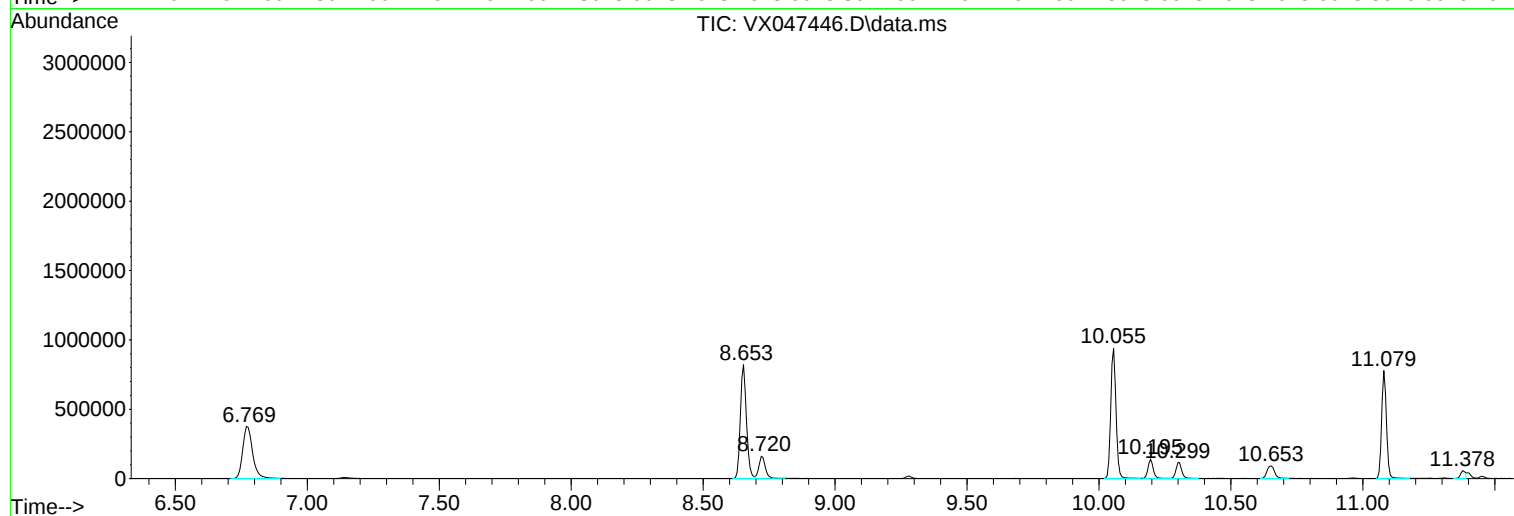
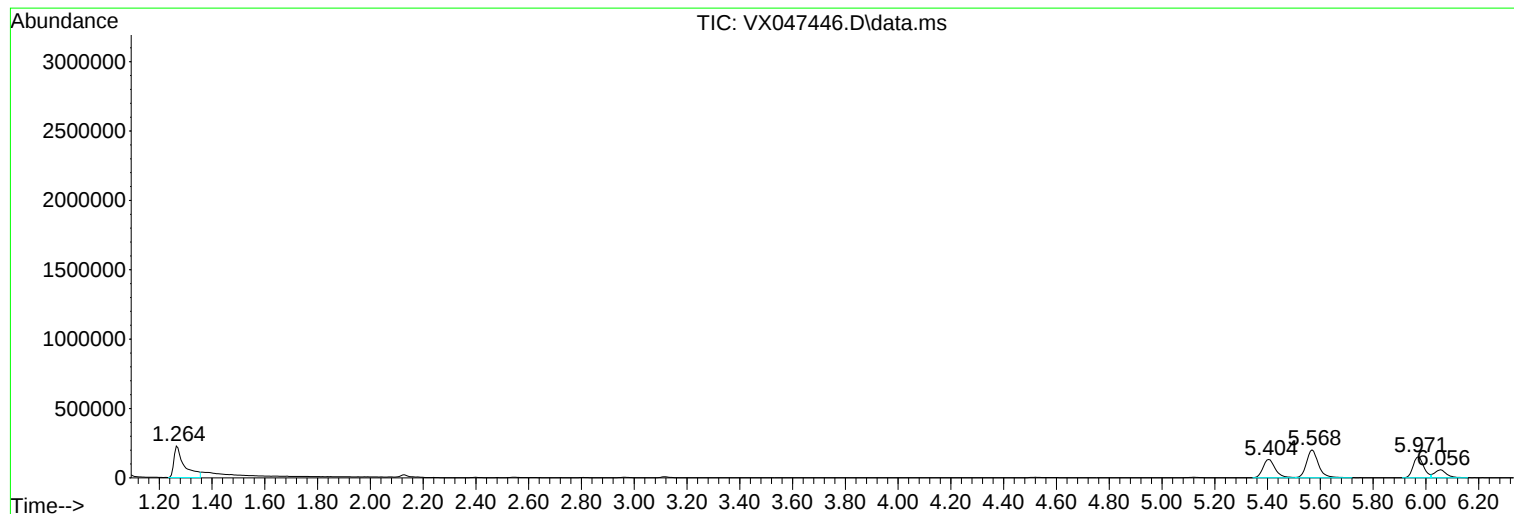
Sum of corrected areas: 17000966

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

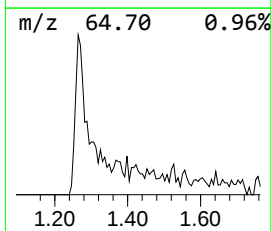
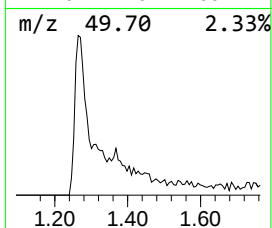
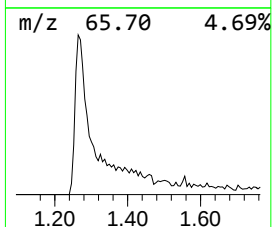
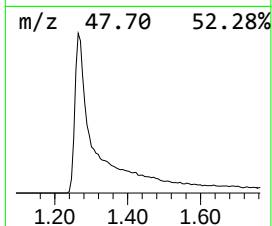
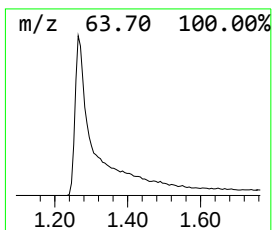
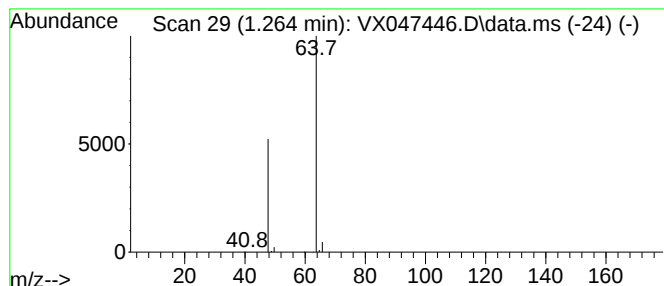
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	49.50 ug/l	619509	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

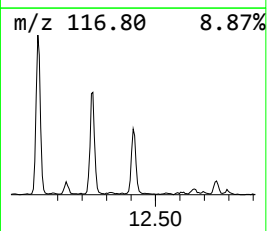
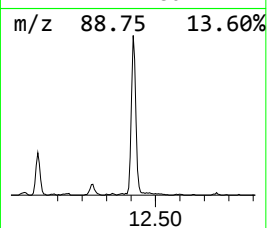
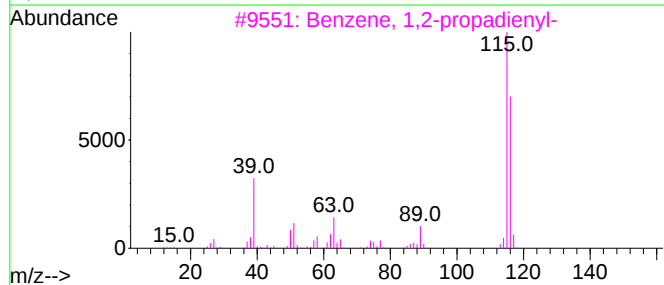
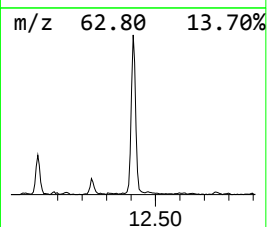
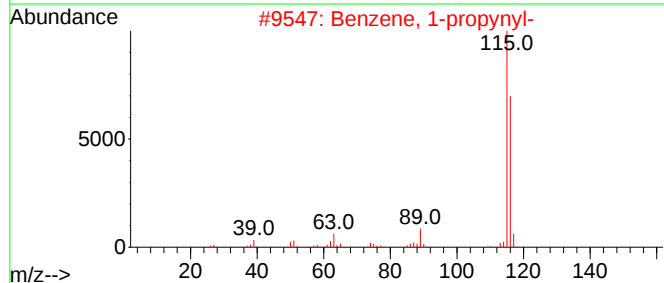
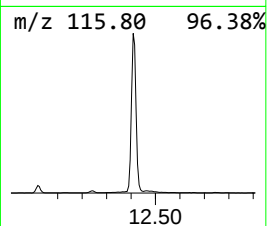
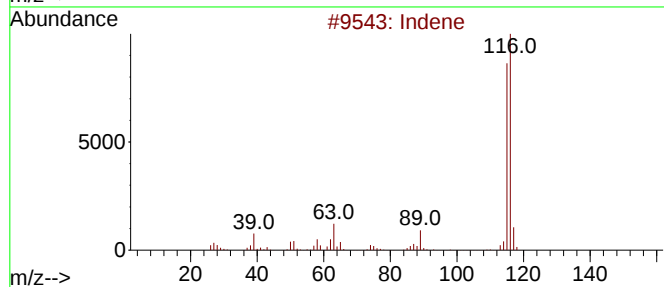
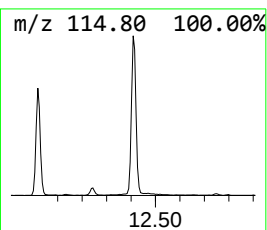
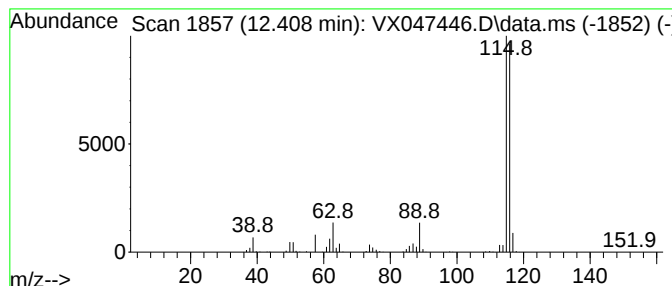
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 2 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.408	23.86 ug/l	636344	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			3-Methylphenylacetylene	116	C9H8	000766-82-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

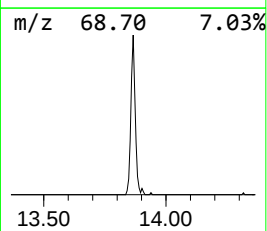
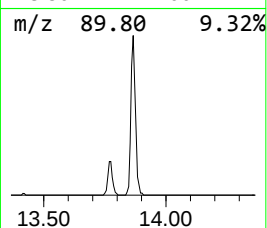
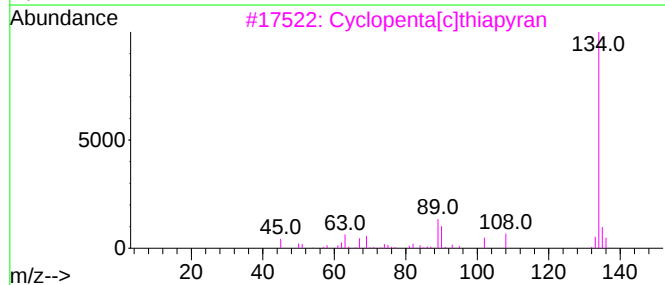
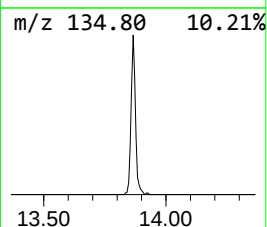
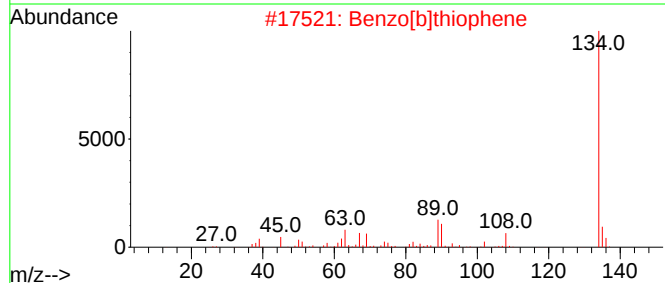
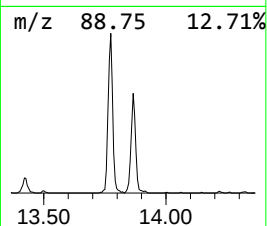
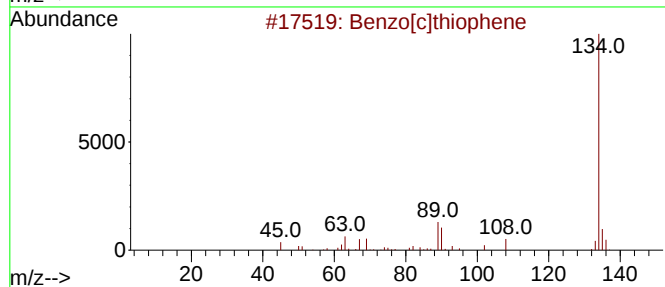
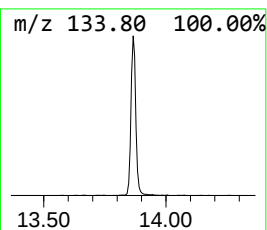
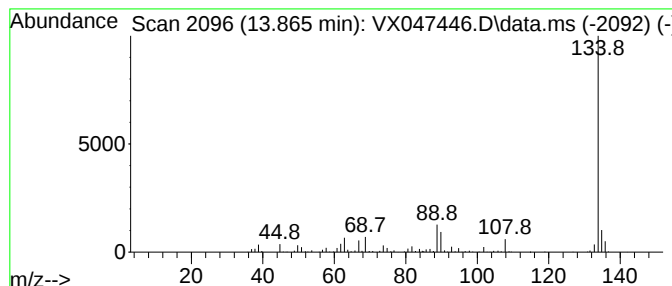
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzo[c]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.866	7.17 ug/l	191144	1,4-Dichlorobenzene-d4	12.018

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	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	90
4			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	64
5			[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

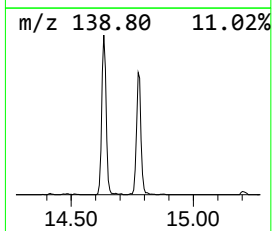
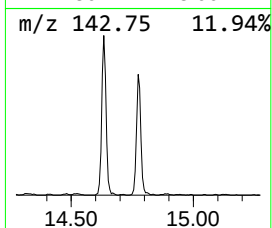
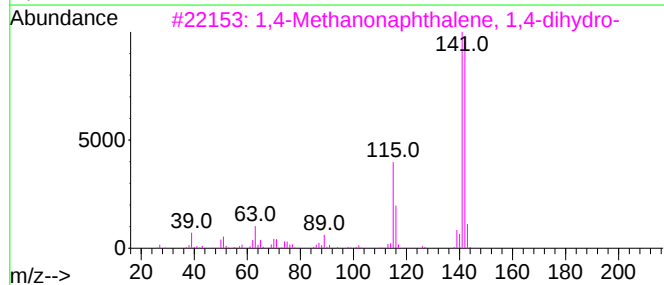
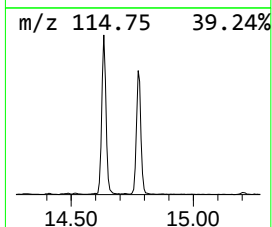
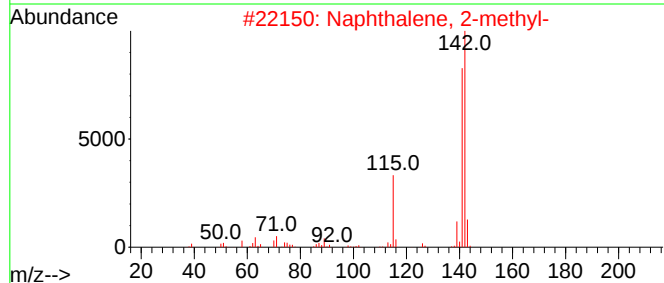
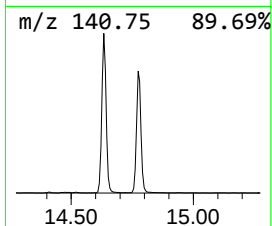
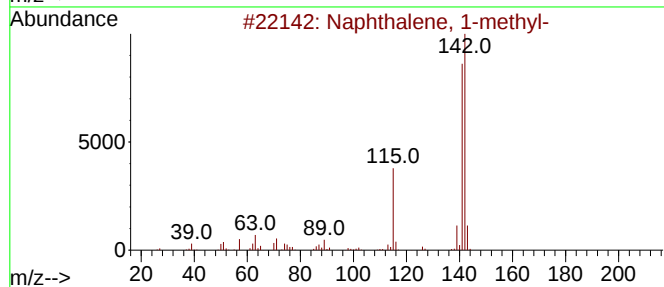
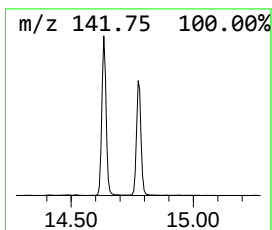
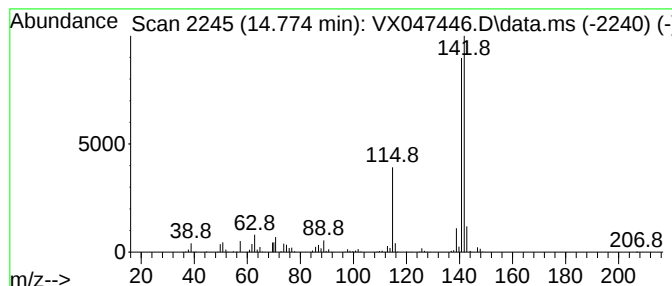
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	28.78 ug/l	767412	1,4-Dichlorobenzene-d4	12.018

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	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

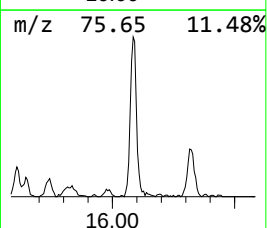
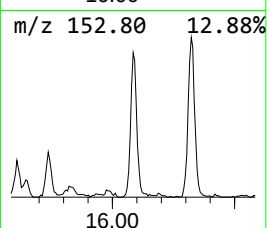
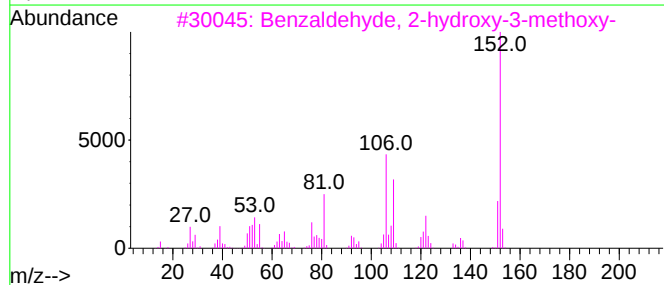
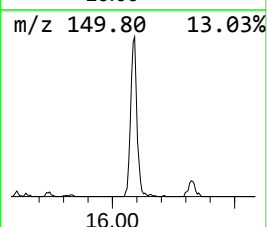
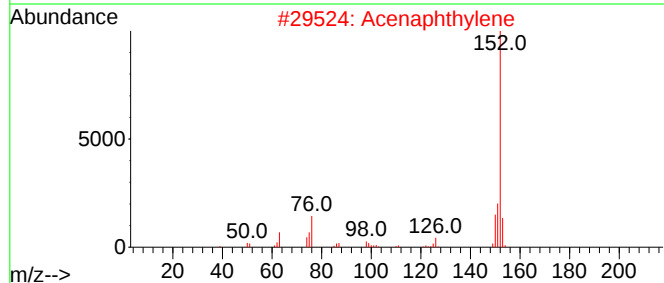
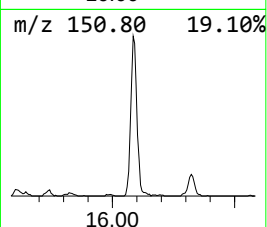
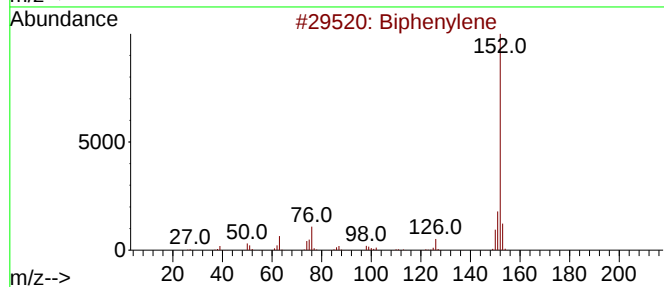
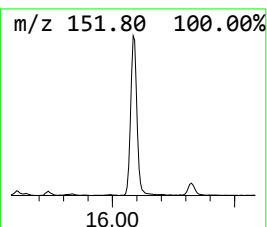
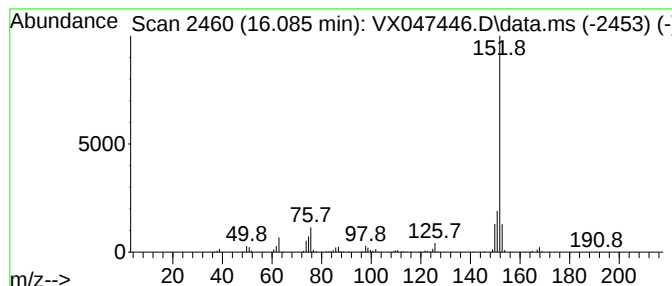
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 7 Biphenylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.085	12.89 ug/l	343788	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenylene	152	C12H8	000259-79-0	97
2			Acenaphthylene	152	C12H8	000208-96-8	95
3			Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	50
4			5,6-Dihydro-4-methylthieno(2,3-d...	152	C7H8N2S	092204-06-3	45
5			Benzaldehyde, 2-hydroxy-5-methoxy-	152	C8H8O3	000672-13-9	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047446.D
Acq On : 20 Aug 2025 16:30
Operator : JC/MD
Sample : Q2900-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17B-081825

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.264	49.5	ug/l	619509	1	5.568	625712	50.0
Indene	12.408	23.9	ug/l	636344	4	12.018	1333360	50.0
Benzo[c]thiophene	13.866	7.2	ug/l	191144	4	12.018	1333360	50.0
Naphthalene, 1-...	14.774	28.8	ug/l	767412	4	12.018	1333360	50.0
Biphenylene	16.085	12.9	ug/l	343788	4	12.018	1333360	50.0