

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
 Data File : VX047445.D
 Acq On : 20 Aug 2025 16:09
 Operator : JC/MD
 Sample : Q2900-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP-01-081825

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: VX047445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.111	322	332	359	rBV	1813622	3967934	3.11%	0.580%
2	4.507	546	561	591	rBV	1525758	4597859	3.61%	0.672%
3	6.074	804	818	837	rVB2	25770073	84134924	66.00%	12.290%
4	7.135	982	992	1019	rVB	2213841	5080282	3.99%	0.742%
5	8.738	1246	1255	1261	rVB2	37608713	81715075	64.10%	11.936%
6	9.275	1337	1343	1355	rBV2	2872341	4235530	3.32%	0.619%
7	10.201	1488	1495	1501	rBV	30207850	45579340	35.75%	6.658%
8	10.311	1503	1513	1518	rBV	25590239	37927186	29.75%	5.540%
9	10.659	1563	1570	1576	rVB2	27968447	52269012	41.00%	7.635%
10	11.378	1683	1688	1691	rBV	9142964	14110267	11.07%	2.061%
11	11.451	1696	1700	1705	rVB	2511716	2946654	2.31%	0.430%
12	11.616	1721	1727	1728	rBV	1232721	1748882	1.37%	0.255%
13	11.634	1728	1730	1741	rVB	1609315	1654092	1.30%	0.242%
14	11.750	1741	1749	1754	rBV	9406058	12592710	9.88%	1.839%
15	11.811	1754	1759	1762	rVV	7003588	8974372	7.04%	1.311%
16	11.848	1762	1765	1770	rVB	1777218	2007354	1.57%	0.293%
17	12.018	1788	1793	1798	rVB2	955461	1352514	1.06%	0.198%
18	12.085	1799	1804	1808	rBV	3917485	4879539	3.83%	0.713%
19	12.134	1808	1812	1824	rVB	1578046	2000173	1.57%	0.292%
20	12.244	1824	1830	1840	rBV	15033574	19788355	15.52%	2.891%
21	12.433	1852	1861	1866	rBV2	47574559	96380197	75.61%	14.078%
22	12.750	1907	1913	1917	rVB	1210320	1618867	1.27%	0.236%
23	13.286	1993	2001	2005	rBV2	977691	1413033	1.11%	0.206%
24	13.341	2005	2010	2017	rVV	10417246	12671567	9.94%	1.851%
25	13.427	2018	2024	2030	rVV	12387616	15517234	12.17%	2.267%
26	13.500	2030	2036	2041	rVB	1104719	1448338	1.14%	0.212%
27	13.811	2076	2087	2091	rBV3	49212794	127476865	100.00%	18.621%
28	13.878	2093	2098	2104	rVB	5968556	7021864	5.51%	1.026%
29	14.640	2218	2223	2231	rVB	13293072	17063156	13.39%	2.492%
30	14.780	2241	2246	2258	rVB	9777220	12420379	9.74%	1.814%

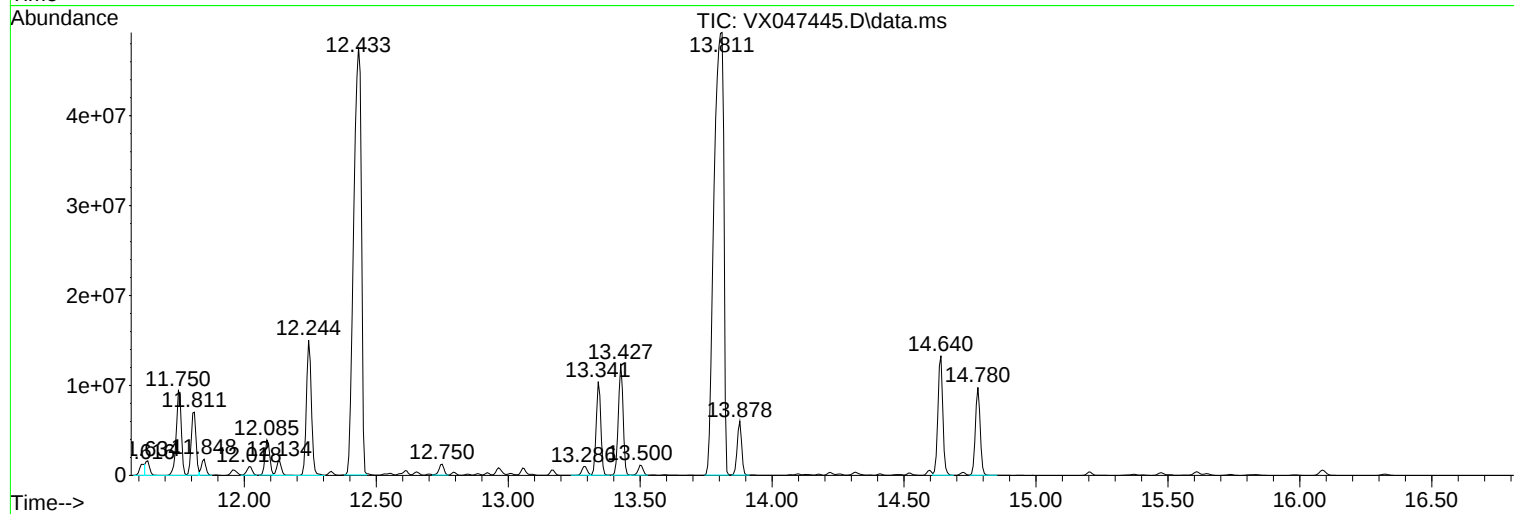
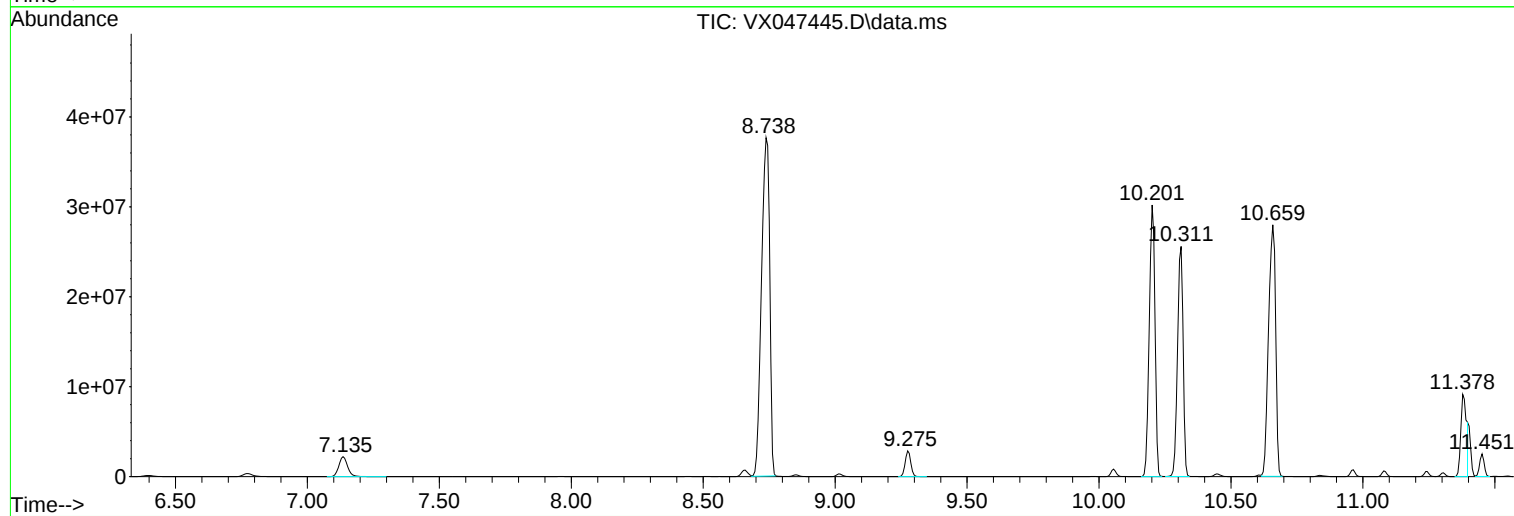
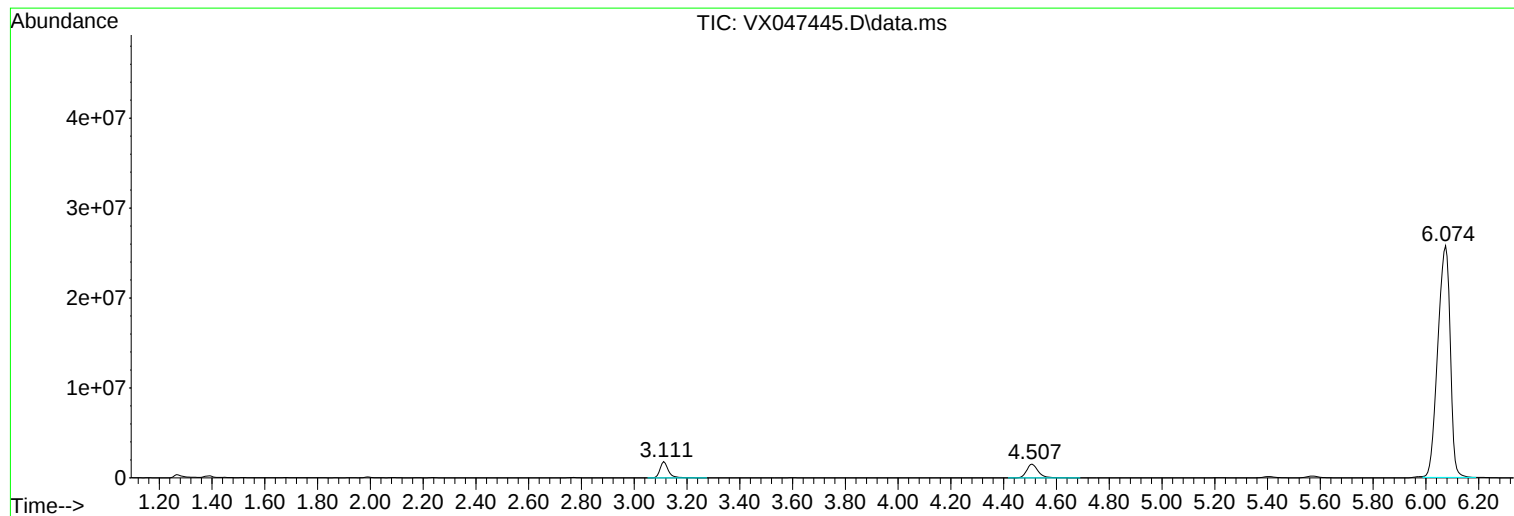
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Instrument :
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ClientSampleId :
DUP-01-081825

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



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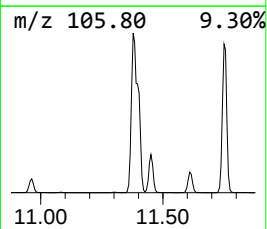
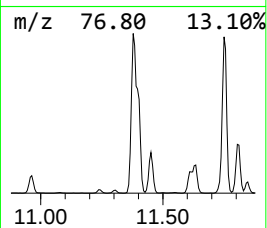
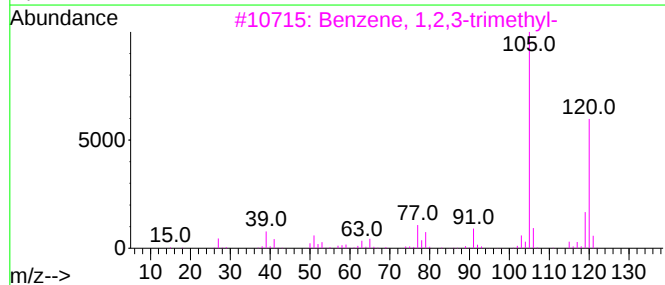
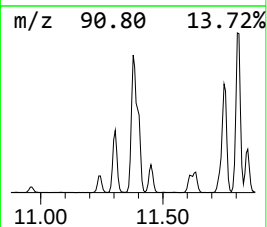
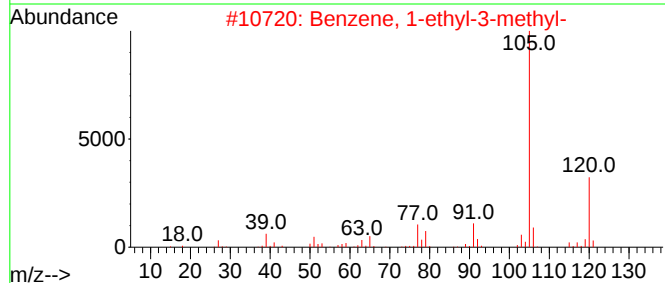
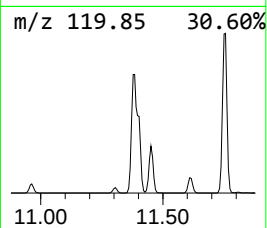
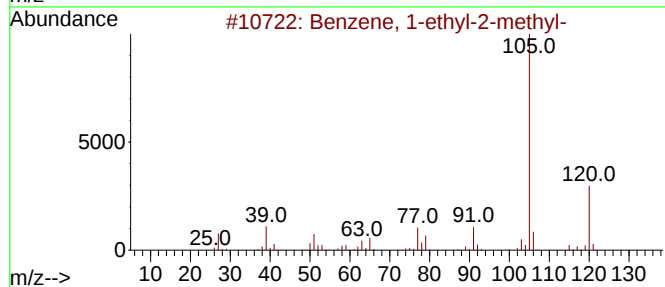
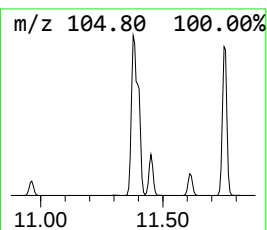
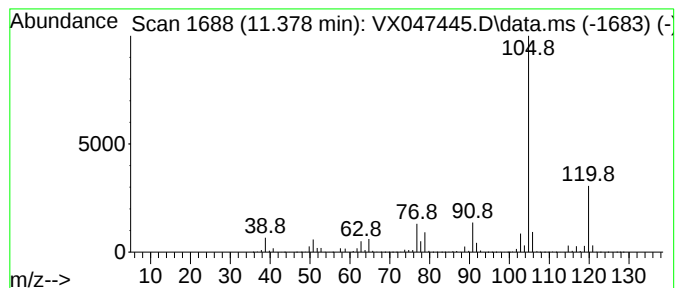
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	521.63 ug/l	14110300	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01-081825

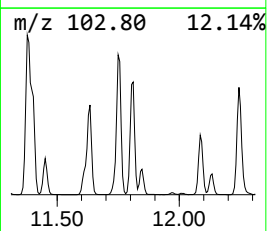
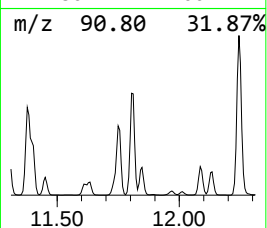
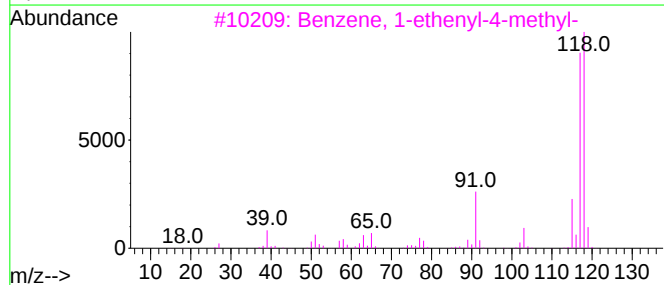
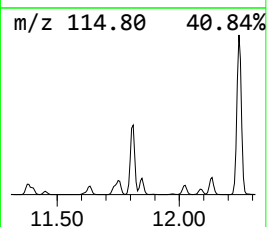
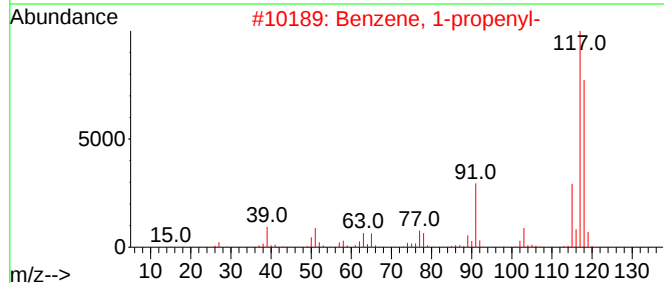
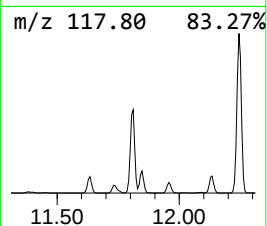
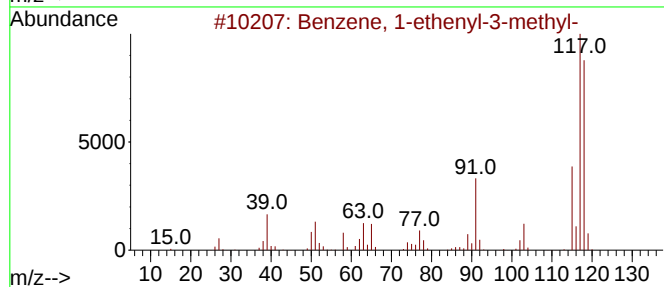
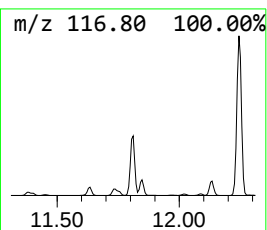
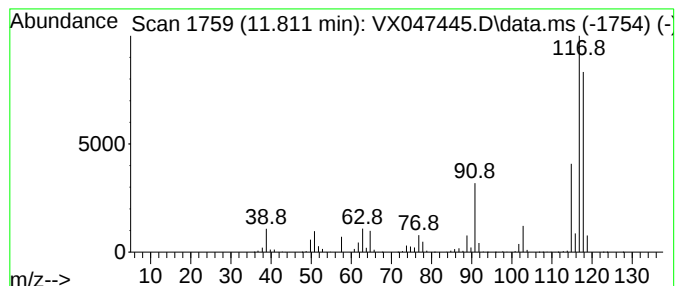
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethenyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.811	331.77 ug/l	8974370	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	96
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	95
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	95
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	94



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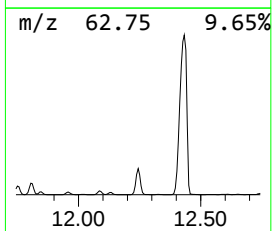
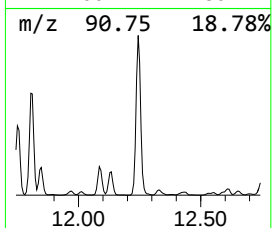
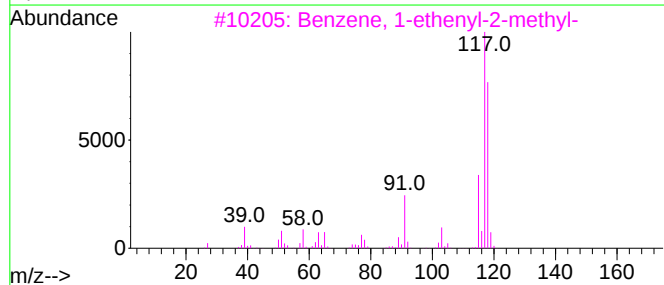
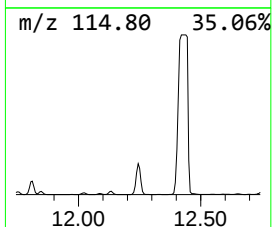
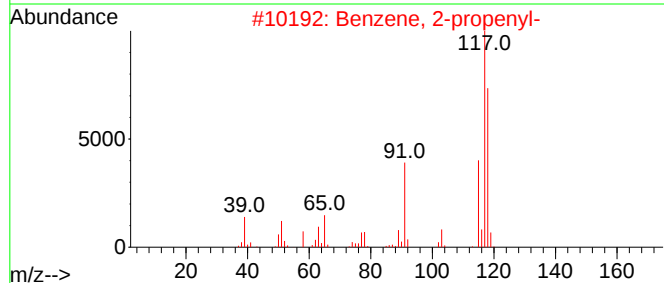
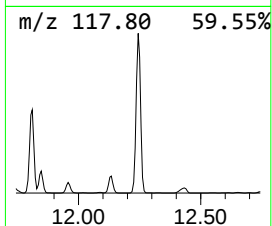
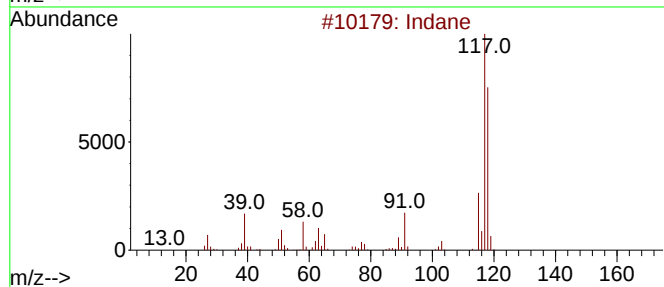
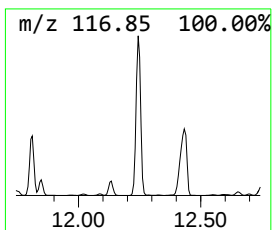
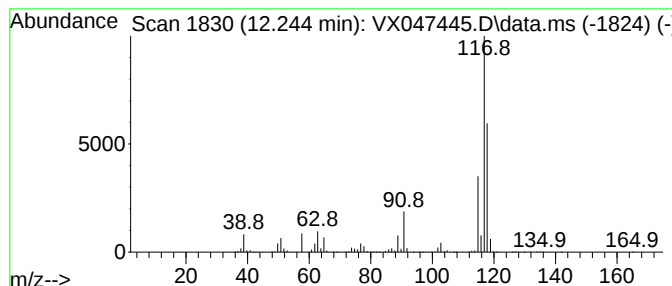
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	731.54 ug/l	19788400	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	68
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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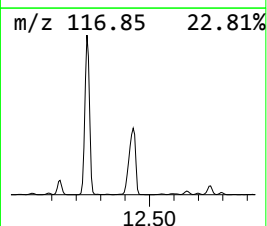
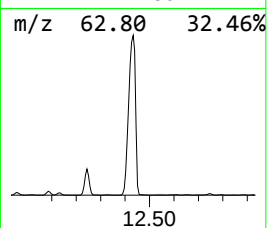
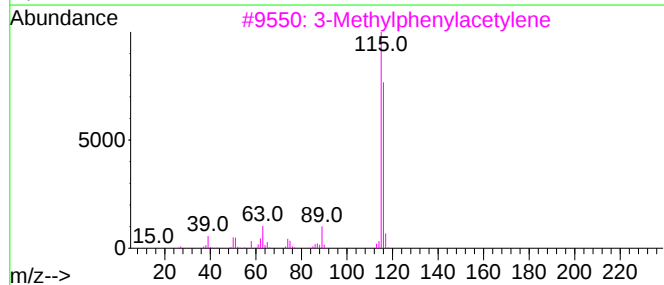
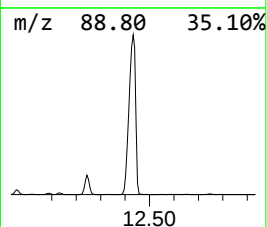
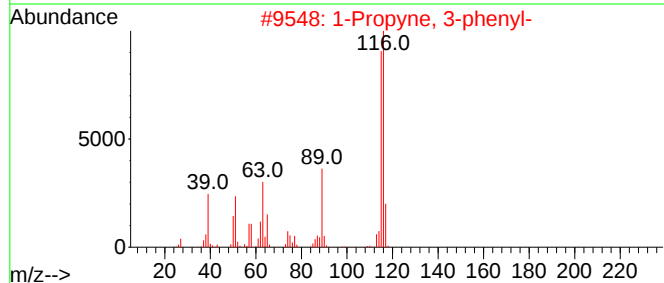
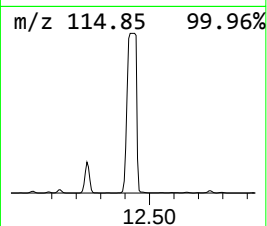
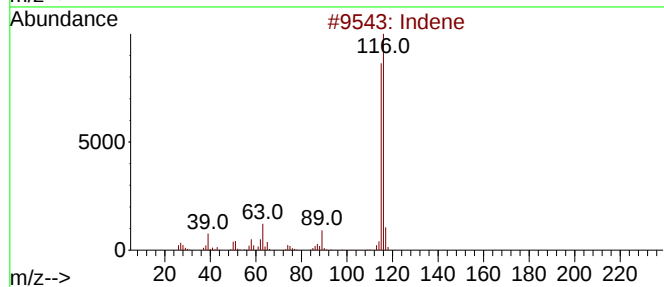
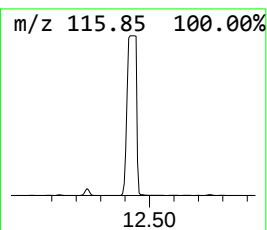
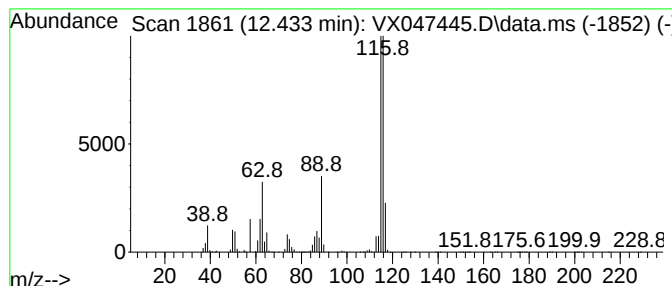
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Quant Title : SW846 8260

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

Peak Number 4 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	3563.00 ug/l	96380200	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	90
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	80
5	Benzene, 1-propynyl-	116	C9H8	000673-32-5	64



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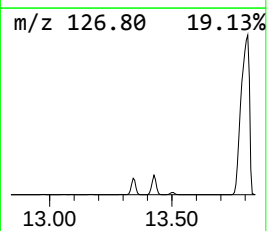
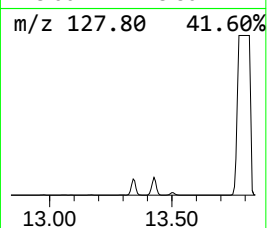
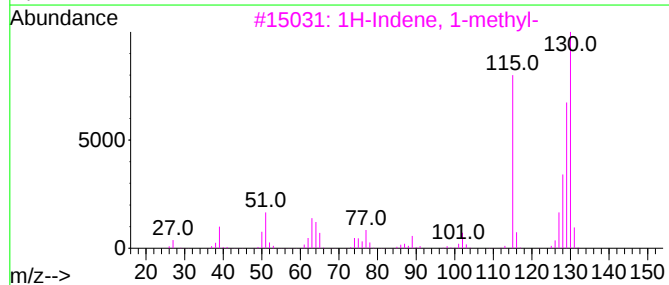
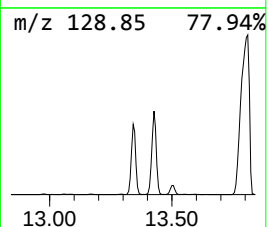
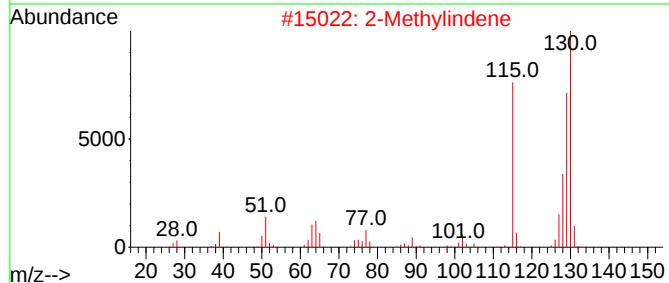
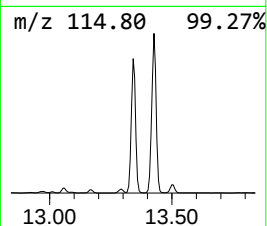
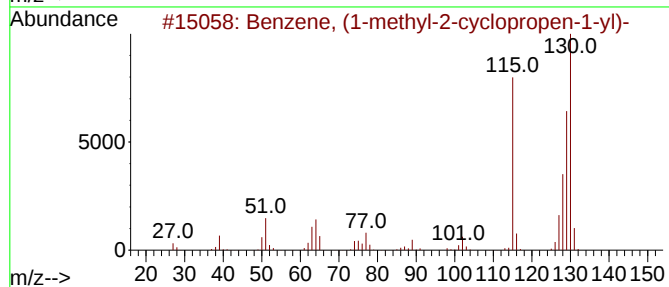
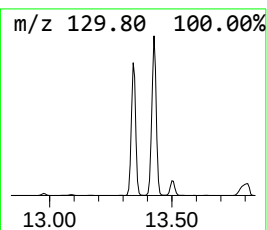
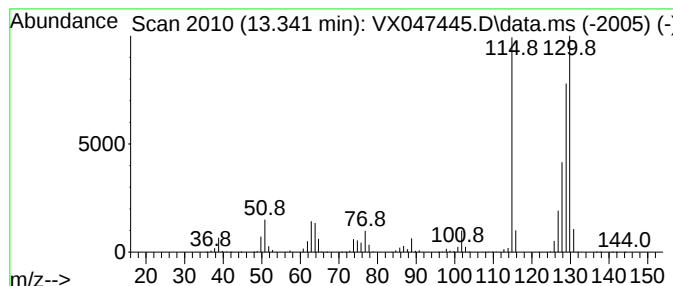
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081525W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, (1-methyl-2-cyclop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	468.44 ug/l	12671600	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	97
2			2-Methylindene	130	C10H10	002177-47-1	97
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
5			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95



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ClientSampleId :
DUP-01-081825

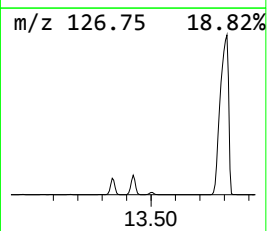
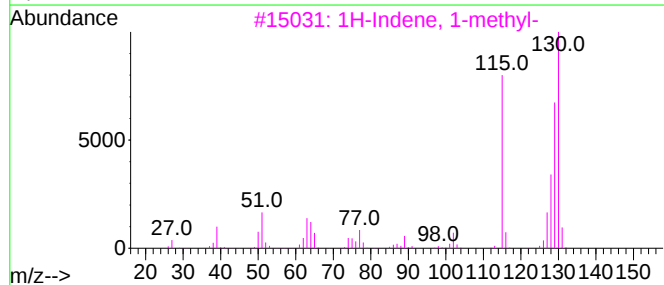
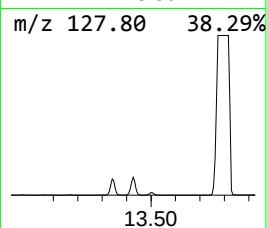
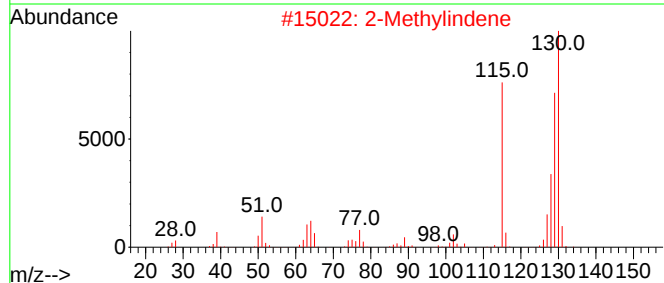
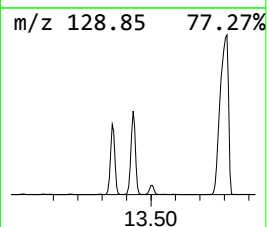
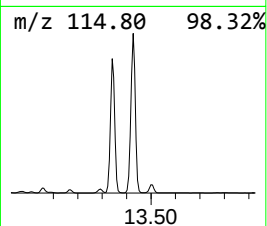
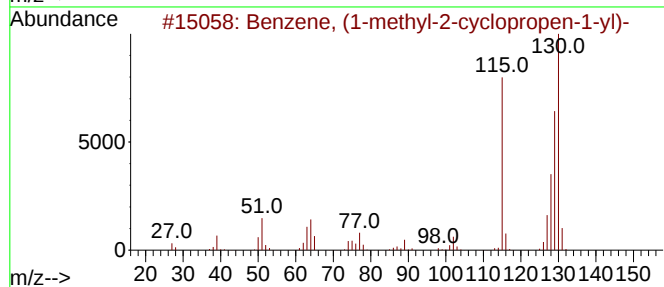
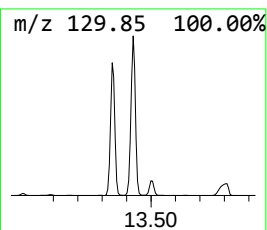
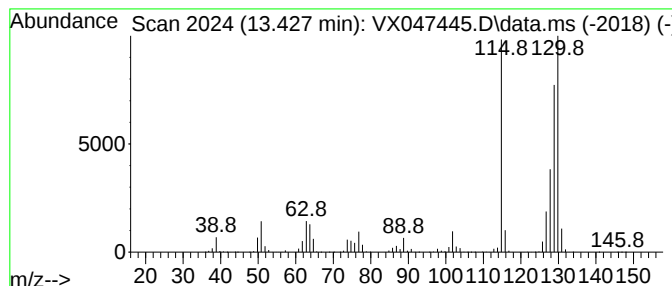
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Quant Title : SW846 8260

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

Peak Number 6 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	573.64 ug/l	15517200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	97
2			2-Methylindene	130	C10H10	002177-47-1	97
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
5			Benzene, 1-butylnyl-	130	C10H10	000622-76-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047445.D
Acq On : 20 Aug 2025 16:09
Operator : JC/MD
Sample : Q2900-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01-081825

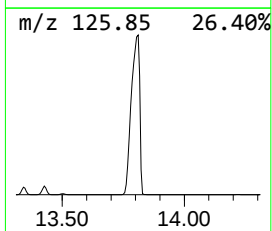
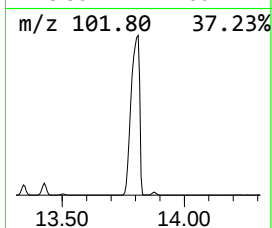
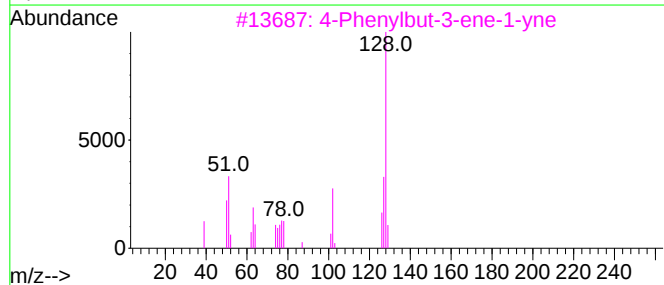
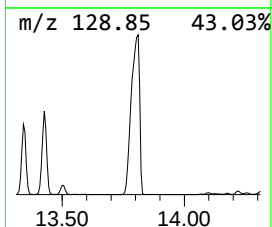
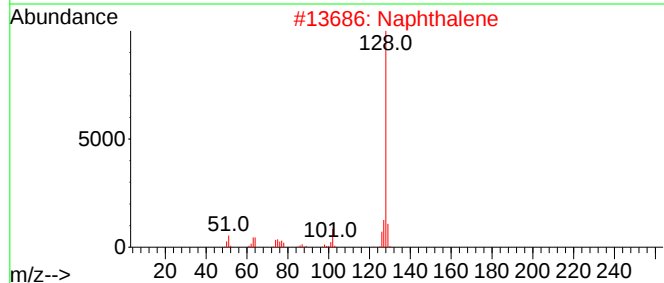
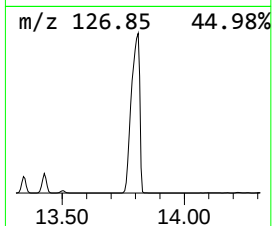
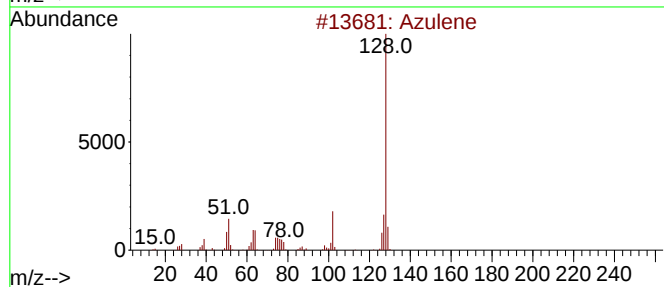
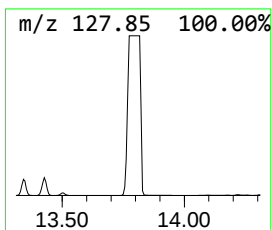
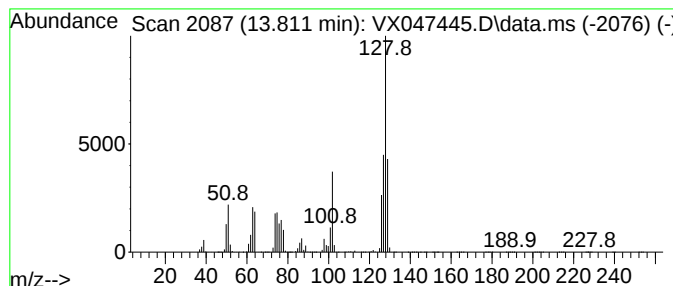
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Quant Title : SW846 8260

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

Peak Number 7 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.811	4712.59 ug/l	127477000	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	93
2			Naphthalene	128	C10H8	000091-20-3	93
3			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	90
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	47
5			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047445.D
Acq On : 20 Aug 2025 16:09
Operator : JC/MD
Sample : Q2900-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01-081825

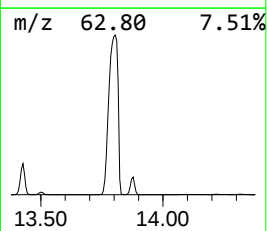
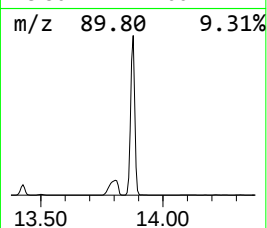
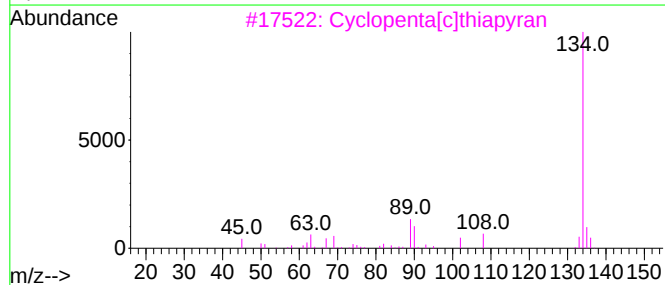
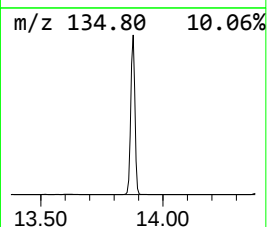
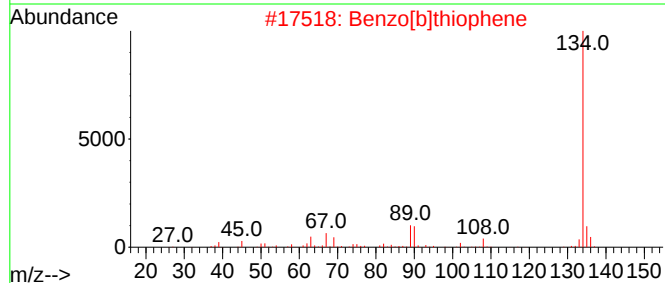
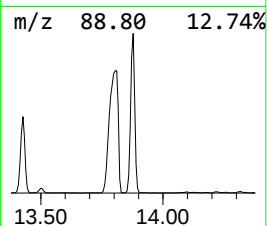
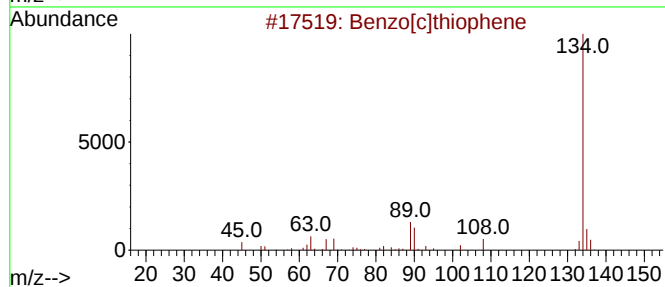
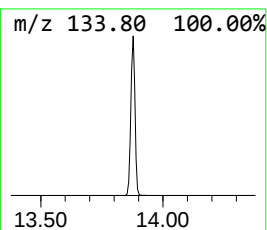
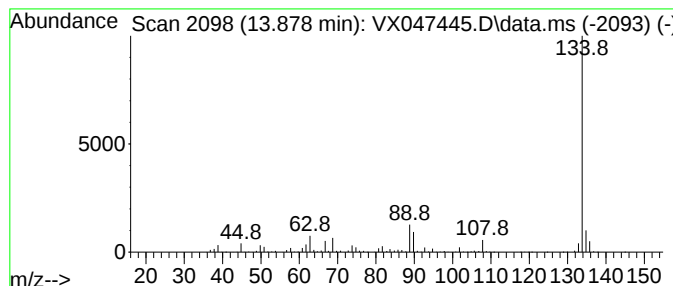
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[c]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.878	259.59 ug/l	7021860	1,4-Dichlorobenzene-d4	12.024

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	94
4			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	56
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047445.D
Acq On : 20 Aug 2025 16:09
Operator : JC/MD
Sample : Q2900-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01-081825

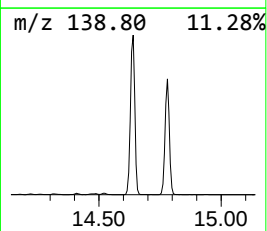
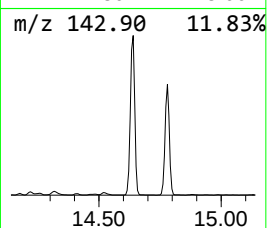
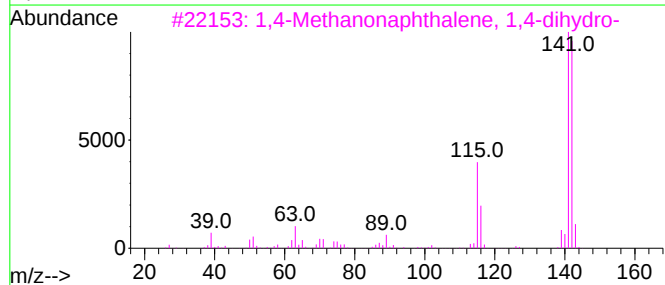
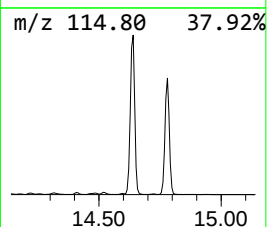
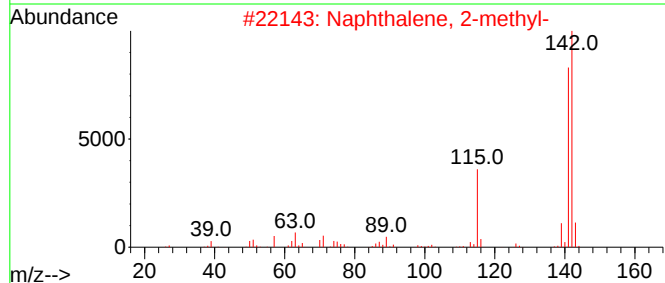
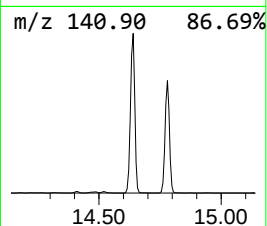
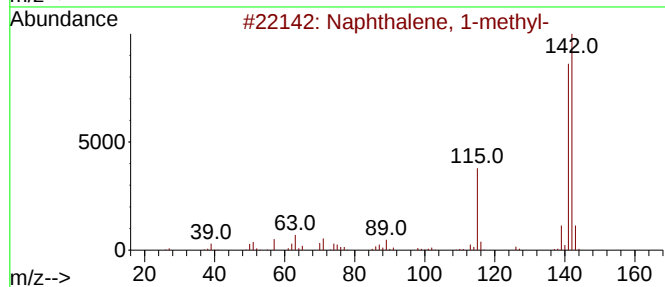
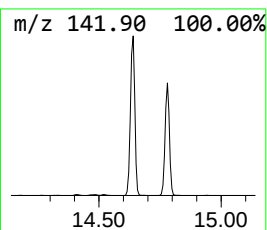
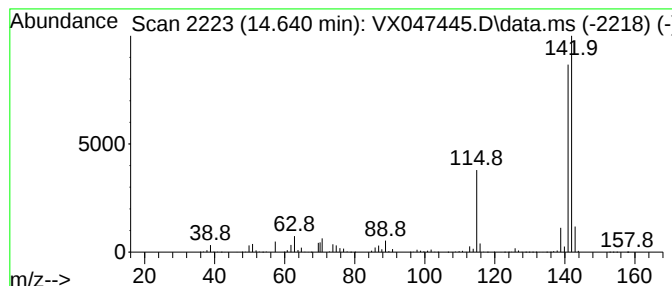
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	630.79 ug/l	17063200	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	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082025\
Data File : VX047445.D
Acq On : 20 Aug 2025 16:09
Operator : JC/MD
Sample : Q2900-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-01-081825

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
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Benzene, 1-ethe...	11.811	331.8	ug/l	8974370	4	12.024	1352510	50.0
Indane	12.244	731.5	ug/l	19788400	4	12.024	1352510	50.0
Indene	12.433	3563.0	ug/l	96380200	4	12.024	1352510	50.0
Benzene, (1-met...	13.341	468.4	ug/l	12671600	4	12.024	1352510	50.0
2-Methylindene	13.427	573.6	ug/l	15517200	4	12.024	1352510	50.0
Azulene	13.811	4712.6	ug/l	127477000	4	12.024	1352510	50.0
Benzo[c]thiophene	13.878	259.6	ug/l	7021860	4	12.024	1352510	50.0
Naphthalene, 1-...	14.640	630.8	ug/l	17063200	4	12.024	1352510	50.0