

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102725\
 Data File : VN088107.D
 Acq On : 27 Oct 2025 12:50
 Operator : JC\MD
 Sample : Q3454-01 5X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 101625

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_N\methods\82N102325W.M
 Title : SW846 8260

Signal : TIC: VN088107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.147	1041	1053	1058	rBV2	242966	587741	2.07%	0.993%
2	8.206	1058	1063	1077	rVB	333303	746963	2.63%	1.262%
3	8.583	1110	1127	1144	rBV3	645794	1985882	6.98%	3.354%
4	9.083	1202	1212	1224	rBV	619915	1273637	4.48%	2.151%
5	10.547	1453	1461	1466	rBV	935870	1741146	6.12%	2.941%
6	10.606	1466	1471	1484	rVB	1165918	2181946	7.67%	3.685%
7	11.841	1674	1681	1692	rBV	864069	1615765	5.68%	2.729%
8	11.941	1692	1698	1705	rVV	527243	919182	3.23%	1.552%
9	12.041	1705	1715	1729	rBV2	835747	1944250	6.84%	3.284%
10	12.165	1729	1736	1756	rBV4	128442	542330	1.91%	0.916%
11	12.382	1766	1773	1786	rVB3	748246	1629067	5.73%	2.751%
12	12.829	1842	1849	1857	rVB	676348	1196475	4.21%	2.021%
13	13.459	1949	1956	1961	rBV	412156	715706	2.52%	1.209%
14	13.688	1988	1995	2002	rBV	336723	630866	2.22%	1.066%
15	13.771	2002	2009	2017	rVV2	948089	1981804	6.97%	3.347%
16	13.971	2036	2043	2054	rBV	858812	1469325	5.17%	2.482%
17	14.153	2066	2074	2082	rBV	3754491	6501224	22.86%	10.981%
18	14.612	2137	2152	2158	rBV6	112333	384028	1.35%	0.649%
19	14.700	2163	2167	2175	rVB	129304	294621	1.04%	0.498%
20	15.182	2242	2249	2258	rVB	180565	353548	1.24%	0.597%
21	15.612	2310	2322	2333	rBV	14765069	28433997	100.00%	48.025%
22	15.712	2333	2339	2350	rVB	447295	950042	3.34%	1.605%
23	16.747	2507	2515	2522	rBV	486940	1127272	3.96%	1.904%

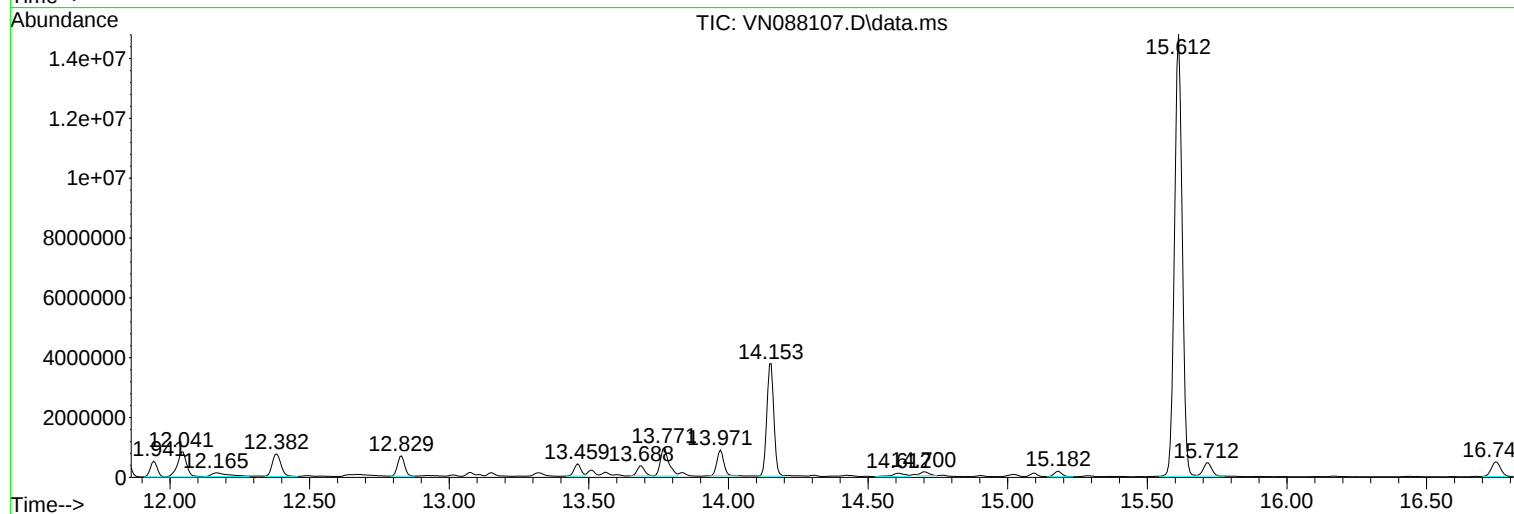
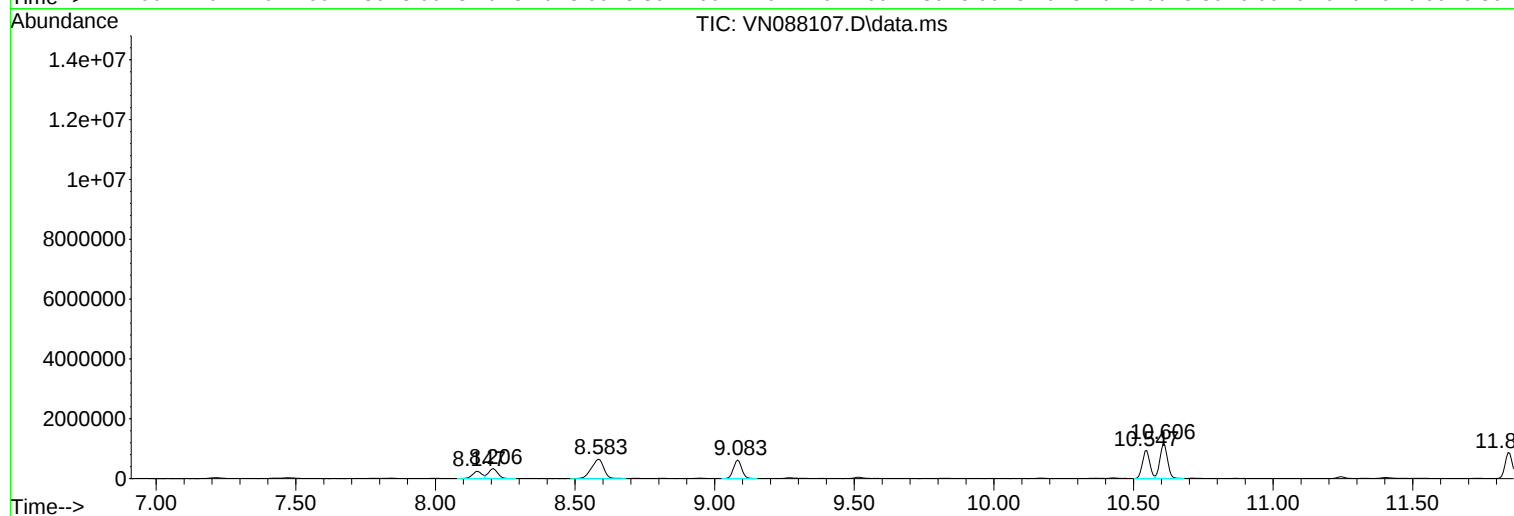
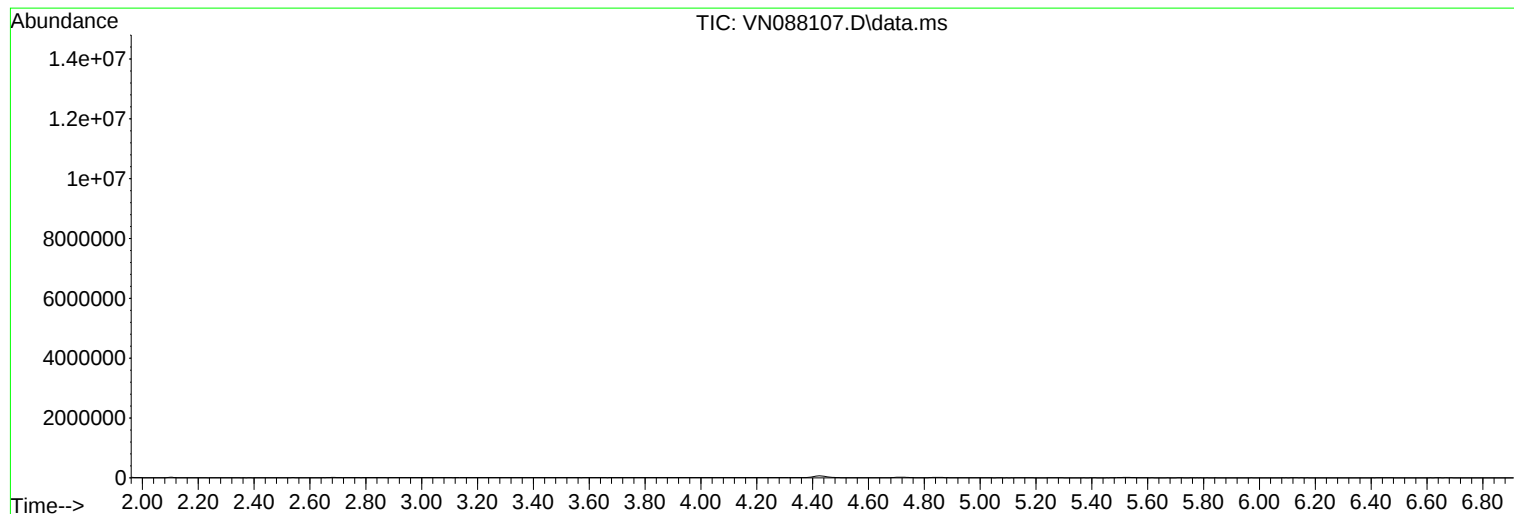
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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



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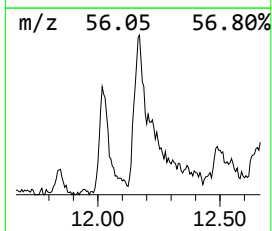
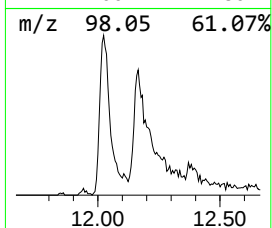
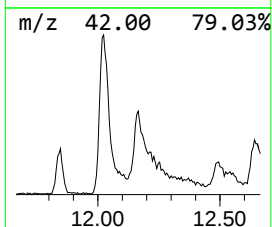
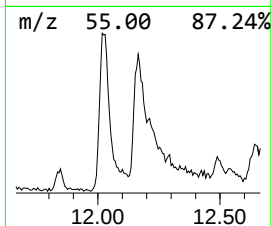
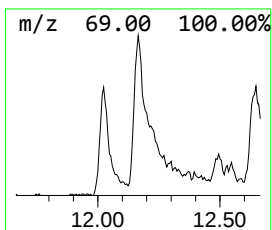
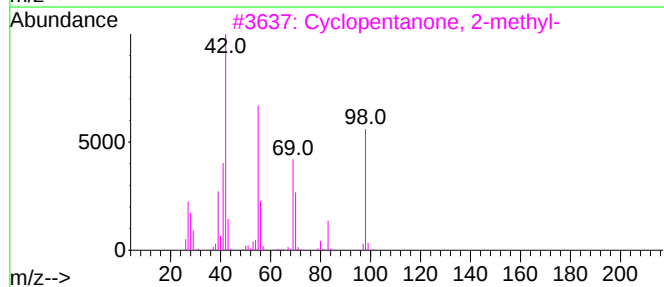
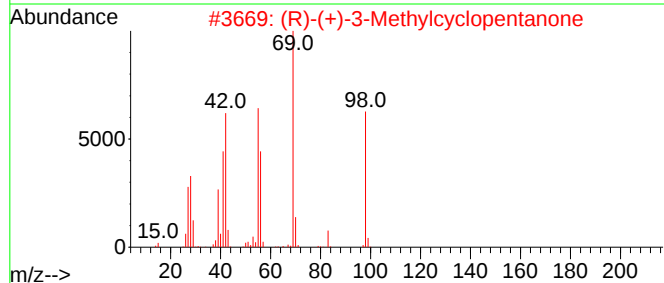
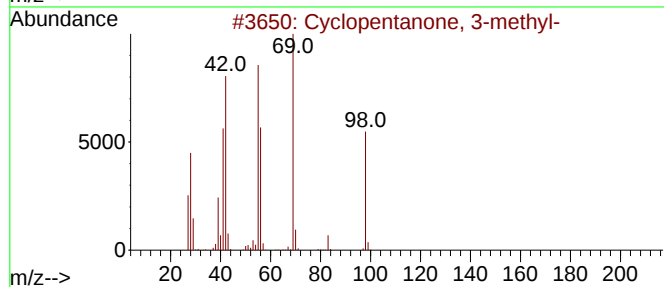
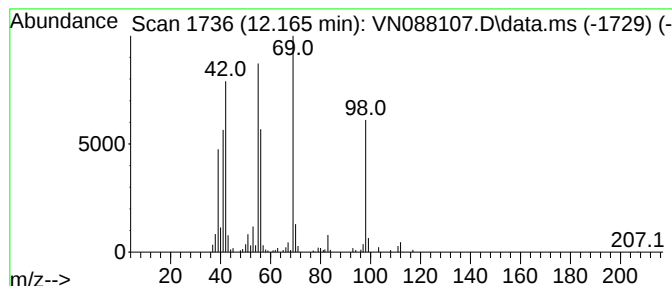
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Quant Title : SW846 8260

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

Peak Number 1 Cyclopentanone, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.165	16.78 ug/l	542330	Chlorobenzene-d5	11.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	87
2			(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	87
3			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	46
4			3-Hexene, 2-methyl-, (Z)-	98	C7H14	015840-60-5	43
5			3-Heptene	98	C7H14	000592-78-9	38



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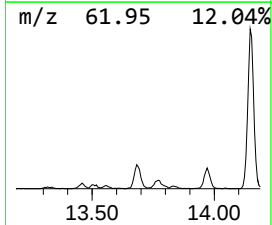
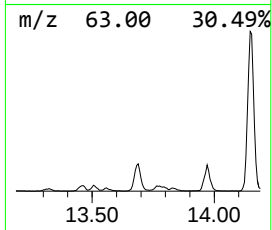
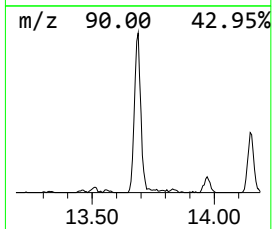
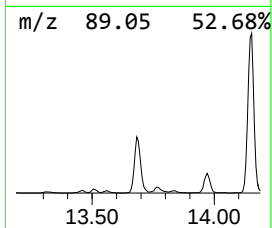
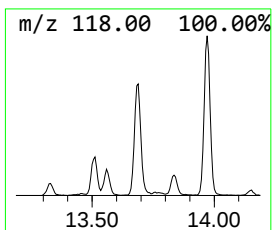
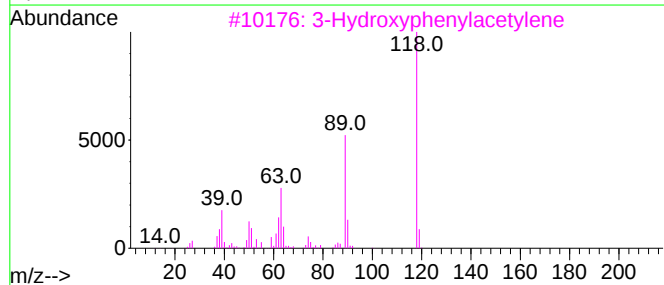
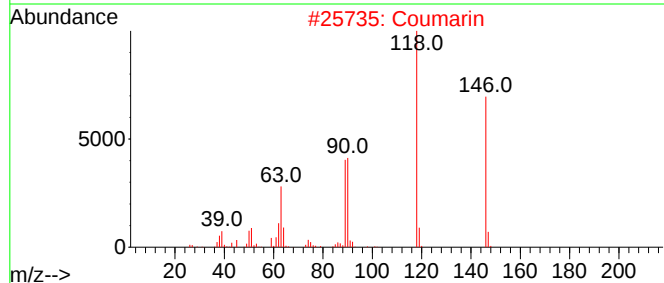
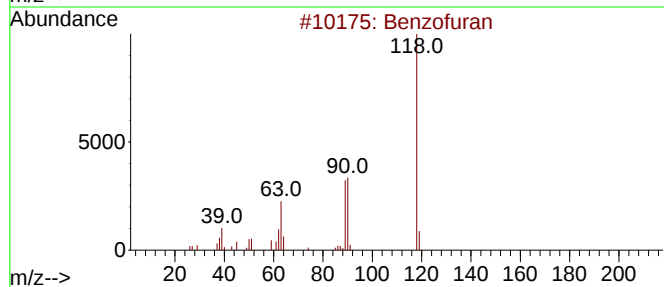
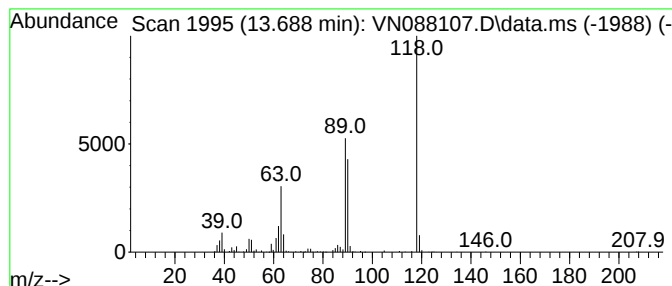
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Peak Number 2 Benzofuran Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	15.92 ug/l	630866	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran	118	C8H6O	000271-89-6	94
2			Coumarin	146	C9H6O2	000091-64-5	86
3			3-Hydroxyphenylacetylene	118	C8H6O	010401-11-3	81
4			4-Methylphthalic anhydride	162	C9H6O3	019438-61-0	72
5			1,2-Benzenedicarboxylic acid, 4-...	180	C9H8O4	004316-23-8	50



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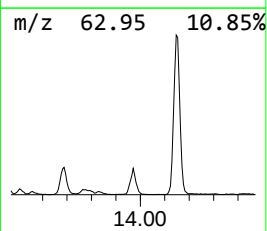
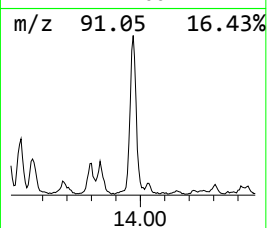
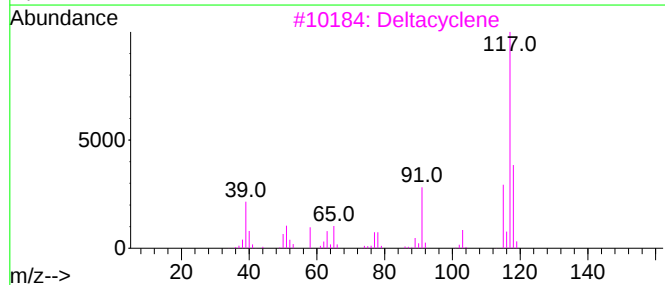
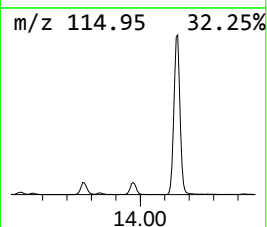
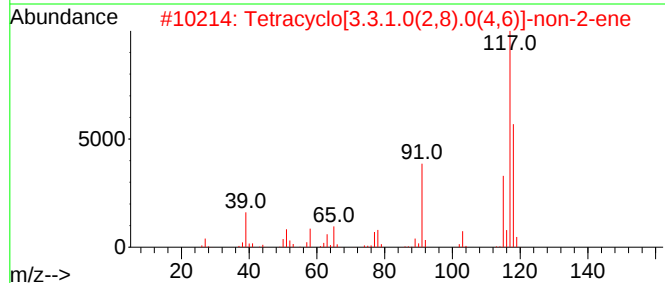
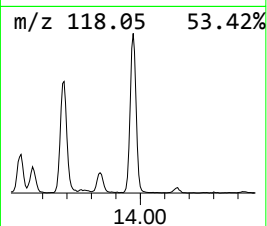
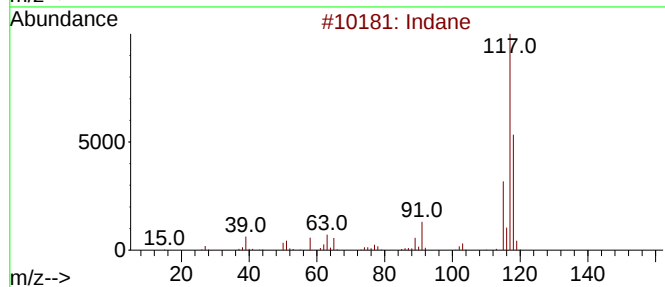
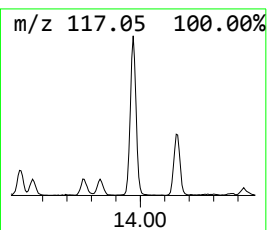
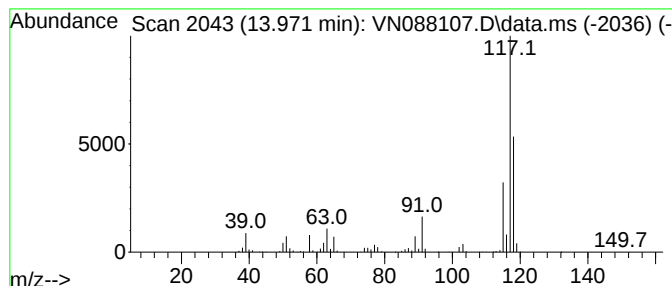
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Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.970	37.07 ug/l	1469330	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
3			Deltacyclene	118	C9H10	007785-10-6	59
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53



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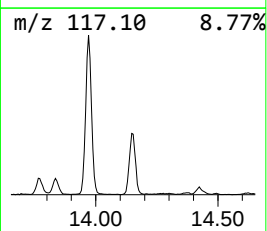
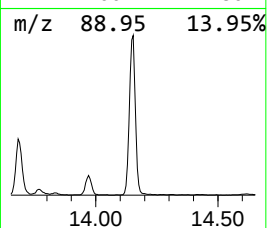
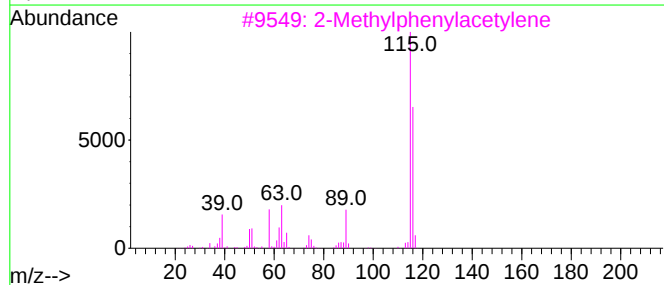
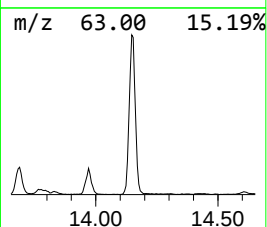
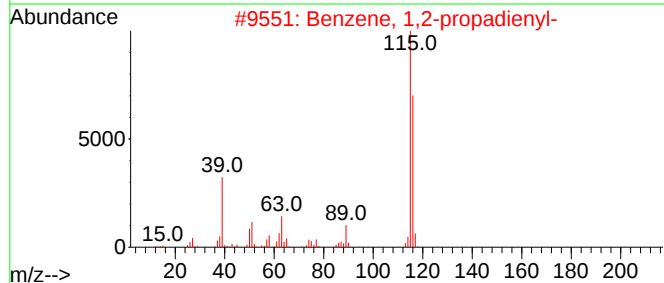
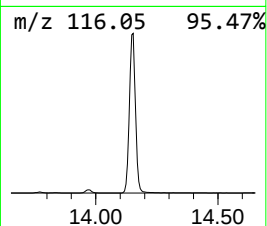
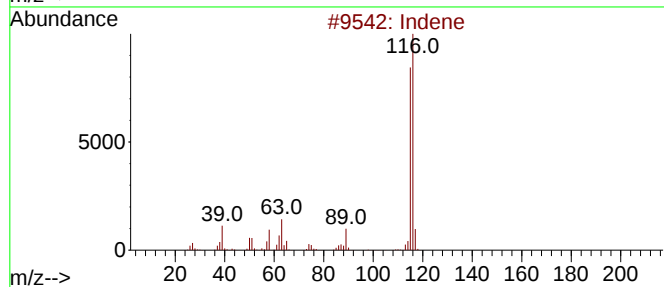
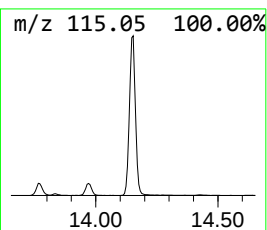
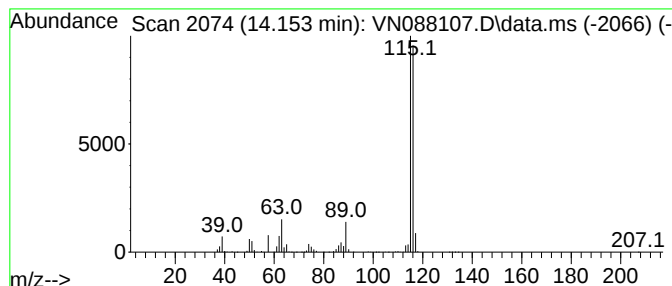
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Peak Number 4 Benzene, 1,2-propadienyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.153	164.02 ug/l	6501220	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
3			2-Methylphenylacetylene	116	C9H8	000766-47-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91



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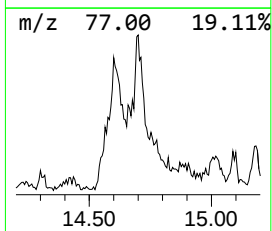
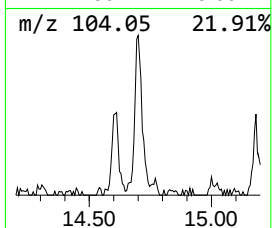
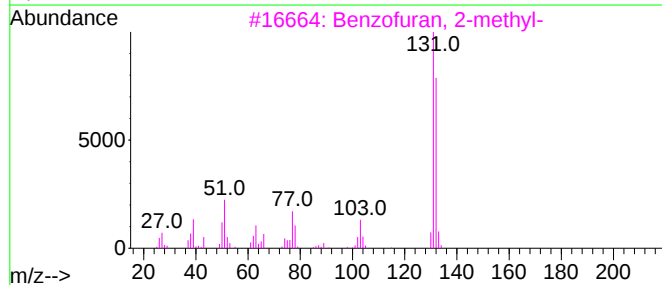
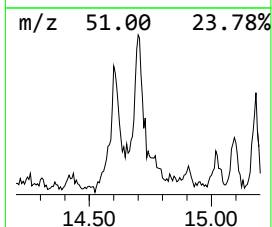
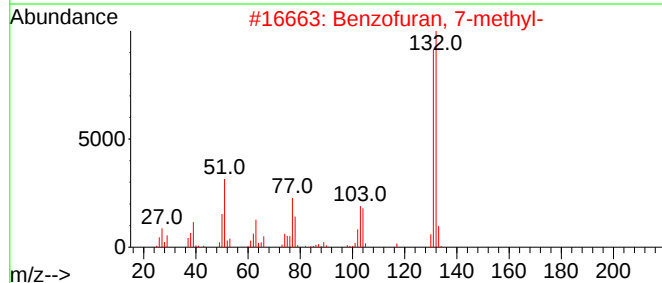
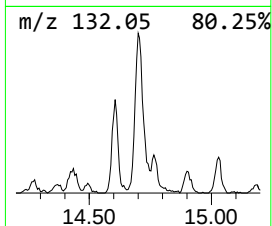
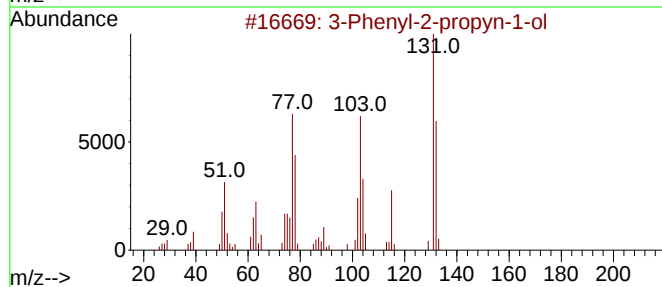
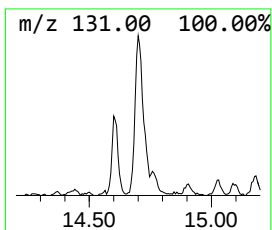
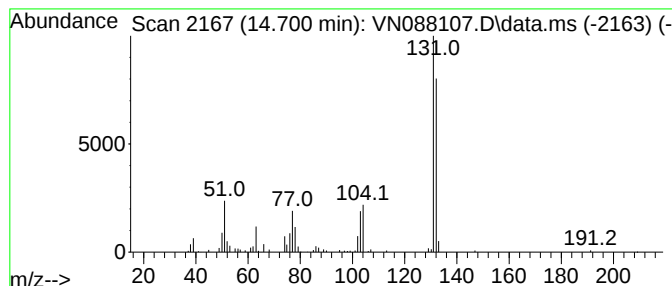
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Phenyl-2-propyn-1-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.700	7.43 ug/l	294621	1,4-Dichlorobenzene-d4	13.771

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91
2		Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	91
3		Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	87
4		Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	87
5		2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	86



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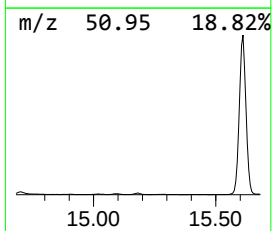
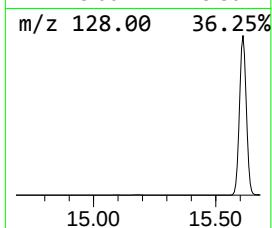
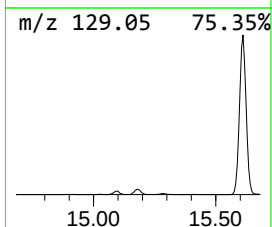
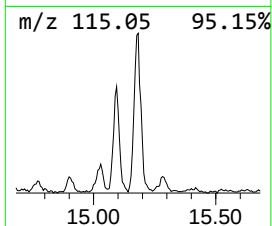
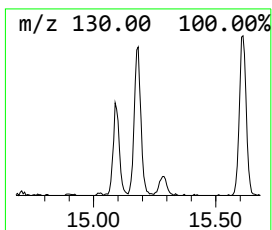
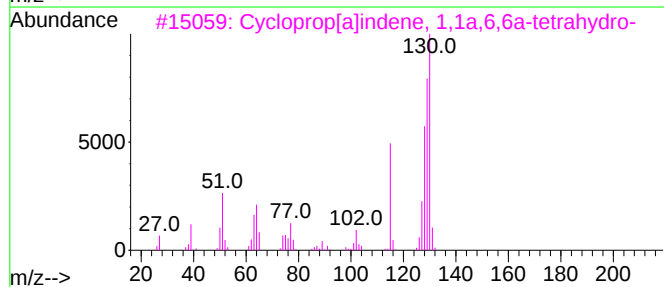
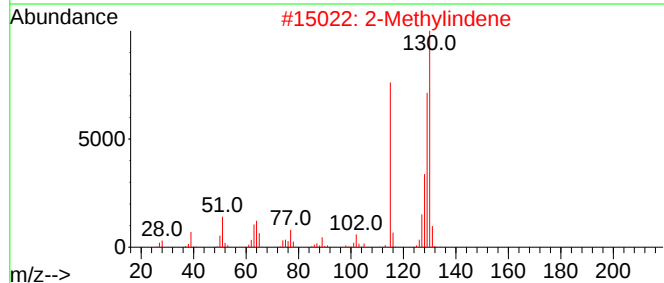
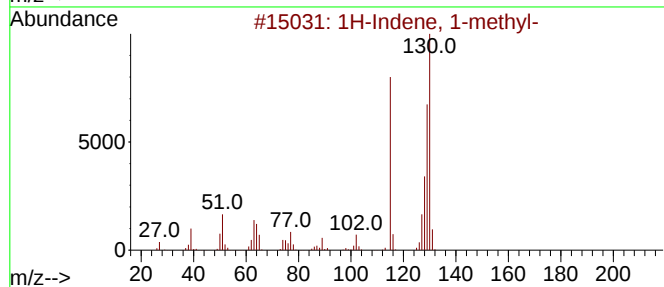
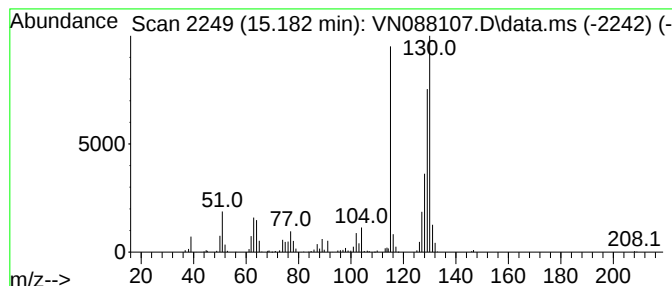
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	8.92 ug/l	353548	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2			2-Methylindene	130	C10H10	002177-47-1	96
3			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	96
4			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102725\
Data File : VN088107.D
Acq On : 27 Oct 2025 12:50
Operator : JC\MD
Sample : Q3454-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101625

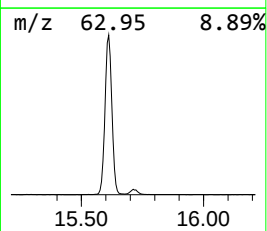
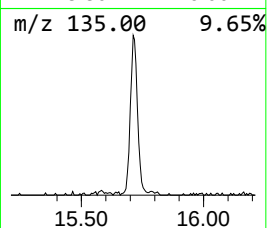
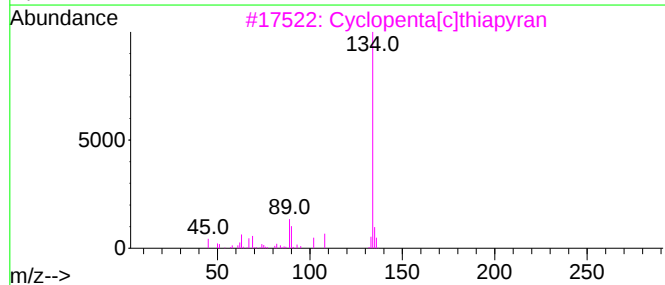
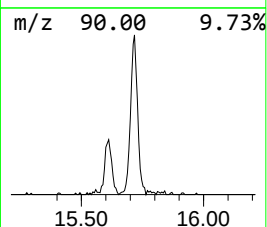
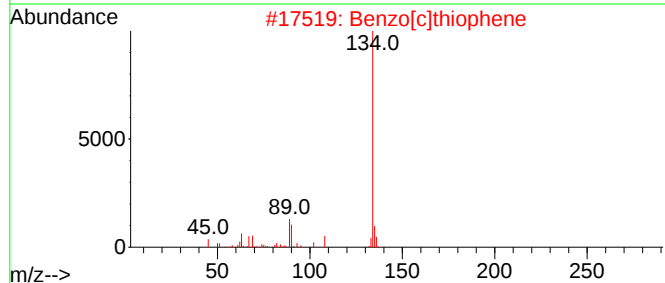
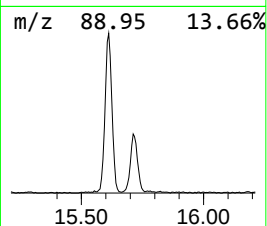
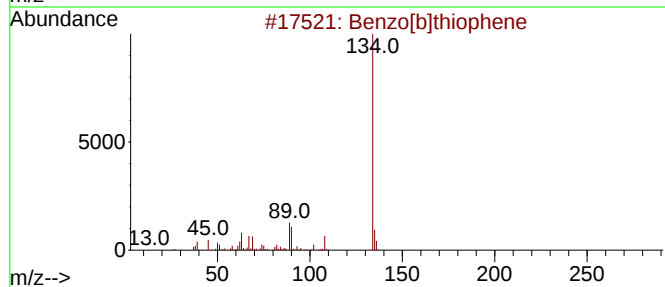
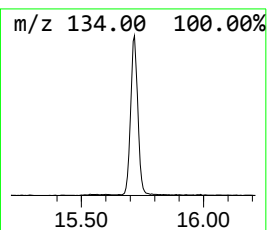
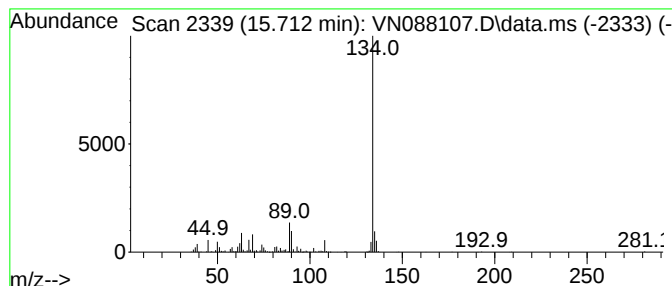
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[b]thiophene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.712	23.97 ug/l	950042	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			(5E)-(E)-5-Benzylidene-2-thioxot...	221	C10H7NOS2	1000497-38-8	83
5			Thiepino[3,2-e]isobenzofuran-1,3...	260	C14H12O3S	055044-57-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102725\
Data File : VN088107.D
Acq On : 27 Oct 2025 12:50
Operator : JC\MD
Sample : Q3454-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101625

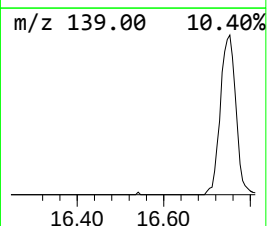
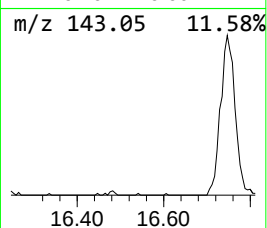
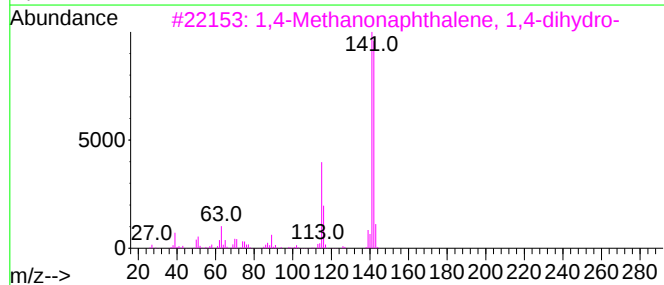
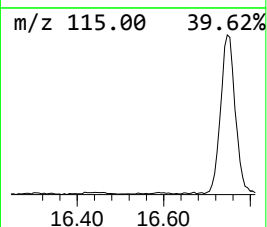
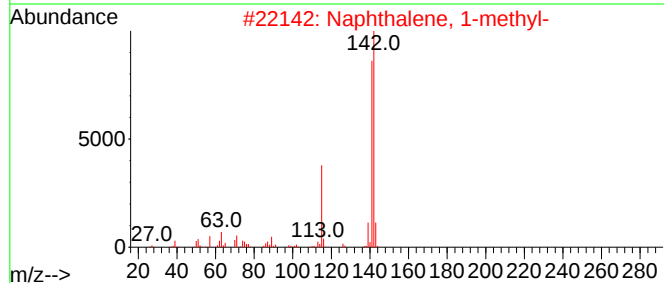
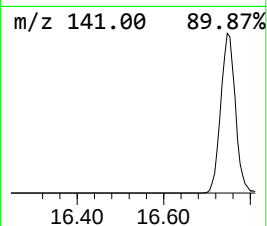
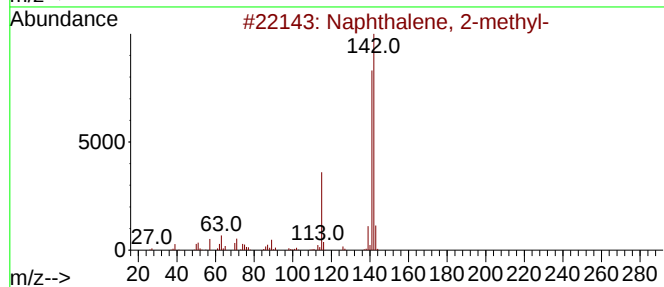
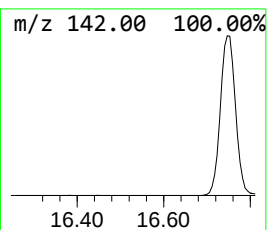
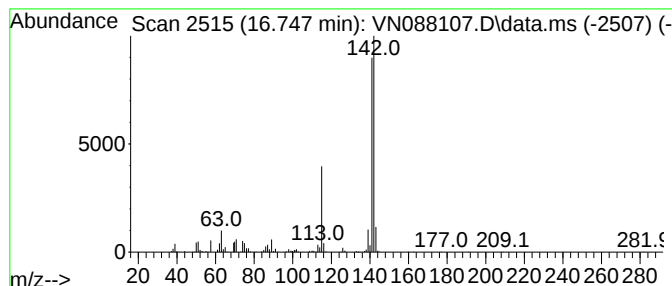
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.747	28.44 ug/l	1127270	1,4-Dichlorobenzene-d4	13.771

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	94
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	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102725\
Data File : VN088107.D
Acq On : 27 Oct 2025 12:50
Operator : JC\MD
Sample : Q3454-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
101625

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.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
Cyclopentanone,...	12.165	16.8	ug/l	542330	3	11.841	1615770	50.0
Benzofuran	13.688	15.9	ug/l	630866	4	13.771	1981800	50.0
Indane	13.970	37.1	ug/l	1469330	4	13.771	1981800	50.0
Benzene, 1,2-pr...	14.153	164.0	ug/l	6501220	4	13.771	1981800	50.0
3-Phenyl-2-prop...	14.700	7.4	ug/l	294621	4	13.771	1981800	50.0
1H-Indene, 1-me...	15.182	8.9	ug/l	353548	4	13.771	1981800	50.0
Benzo[b]thiophene	15.712	24.0	ug/l	950042	4	13.771	1981800	50.0
Naphthalene, 2-...	16.747	28.4	ug/l	1127270	4	13.771	1981800	50.0