

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060325\
 Data File : VX046485.D
 Acq On : 03 Jun 2025 20:02
 Operator : JC/MD
 Sample : Q2169-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 303-PPR-2

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046485.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.646	1234	1240	1246	rBV	255352	397300	1.07%	0.576%
2	8.714	1246	1251	1265	rVB	766713	1183184	3.19%	1.715%
3	10.189	1488	1493	1505	rBV	631383	851454	2.29%	1.234%
4	10.299	1505	1511	1518	rVV	2258203	2981898	8.04%	4.323%
5	10.640	1561	1567	1582	rVB	1348315	1752077	4.72%	2.540%
6	11.378	1683	1688	1695	rVV	899388	1474646	3.97%	2.138%
7	11.451	1695	1700	1711	rVB	452570	582376	1.57%	0.844%
8	11.609	1722	1726	1735	rVB2	463619	772568	2.08%	1.120%
9	11.750	1744	1749	1754	rBV	1949518	2297955	6.19%	3.331%
10	12.018	1788	1793	1799	rVB2	303611	447872	1.21%	0.649%
11	12.085	1799	1804	1815	rBV	884071	1090577	2.94%	1.581%
12	12.219	1821	1826	1828	rBV	1687781	2226150	6.00%	3.227%
13	12.317	1837	1842	1848	rVB4	278292	429284	1.16%	0.622%
14	12.603	1882	1889	1901	rVV	22955023	37108854	100.00%	53.793%
15	12.695	1901	1904	1913	rVB2	247988	449734	1.21%	0.652%
16	13.292	1997	2002	2007	rVB2	597283	809970	2.18%	1.174%
17	13.420	2018	2023	2032	rBV	1050643	1308560	3.53%	1.897%
18	13.774	2077	2081	2088	rVB	877472	1074655	2.90%	1.558%
19	14.194	2145	2150	2167	rBV	7517574	9909753	26.70%	14.365%
20	14.633	2214	2222	2226	rBV	848450	1116349	3.01%	1.618%
21	14.773	2239	2245	2250	rBV	538471	718932	1.94%	1.042%

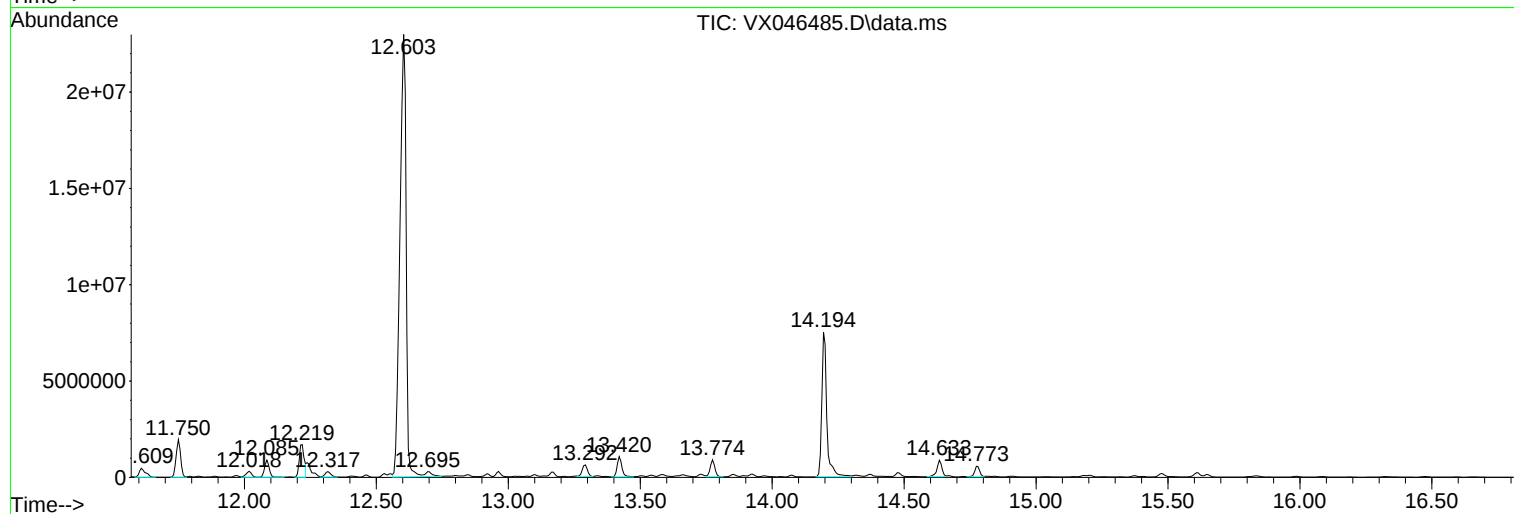
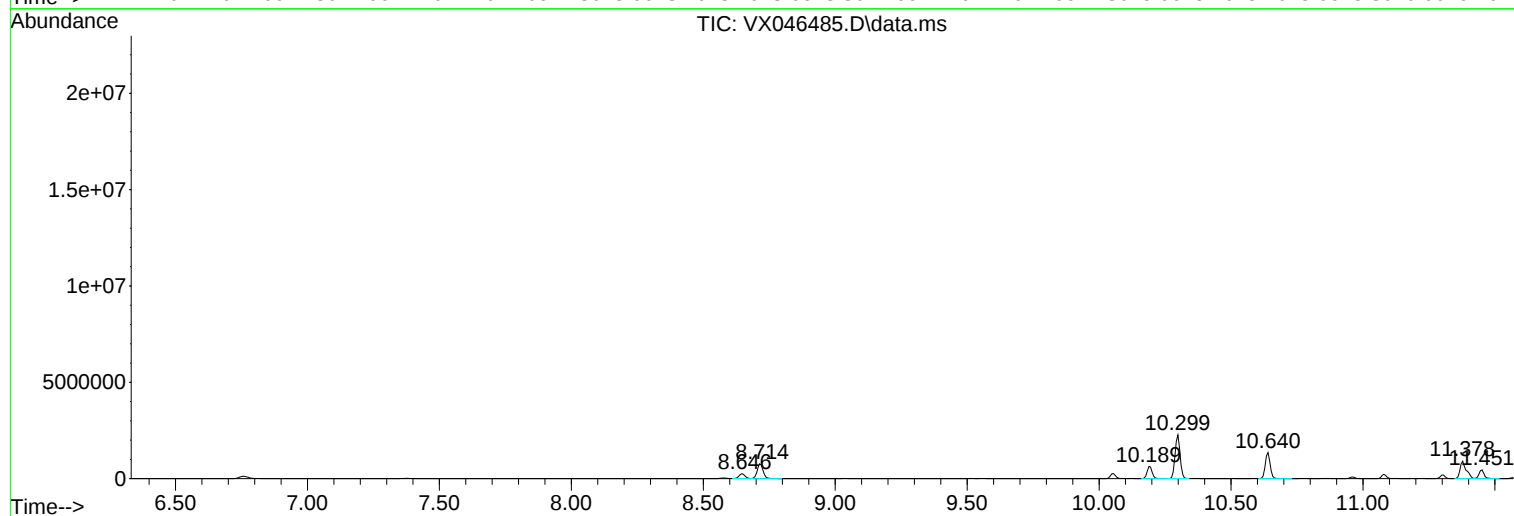
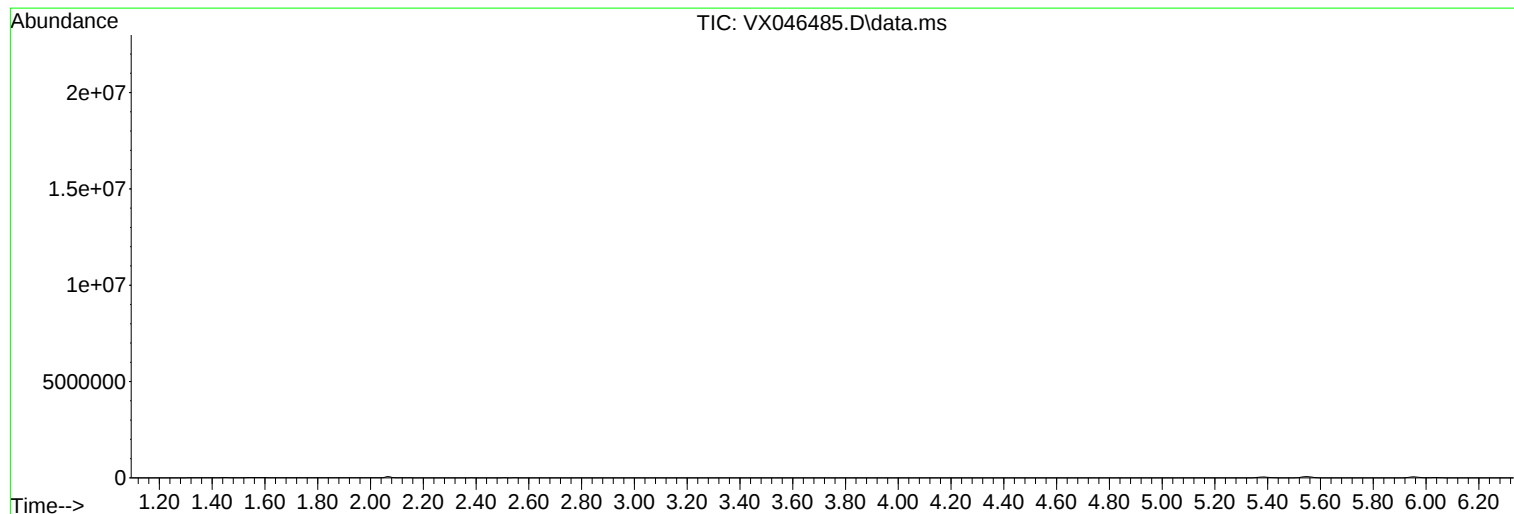
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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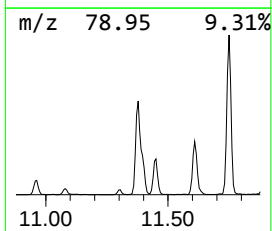
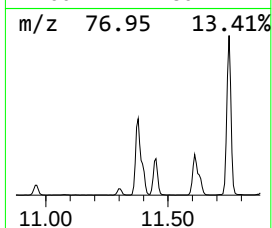
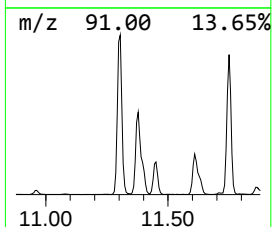
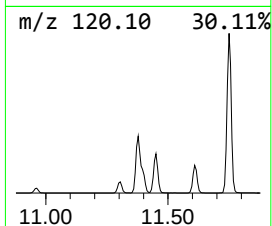
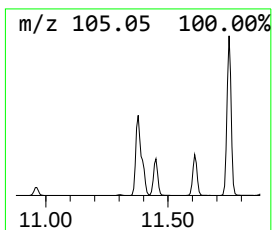
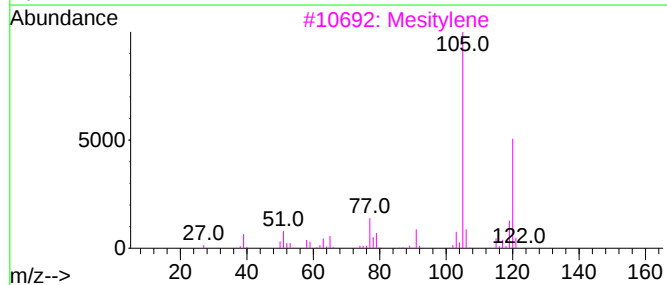
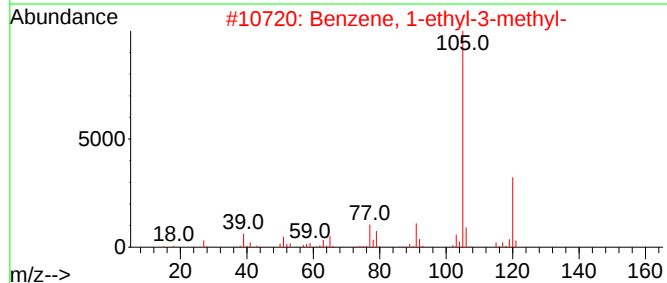
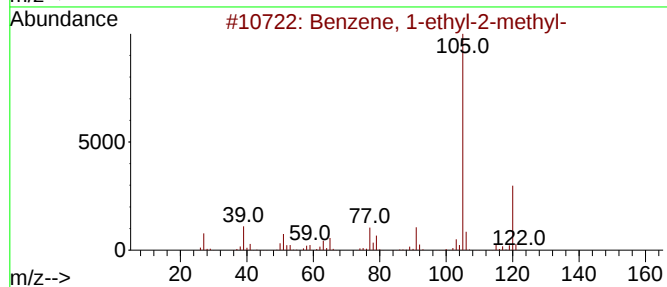
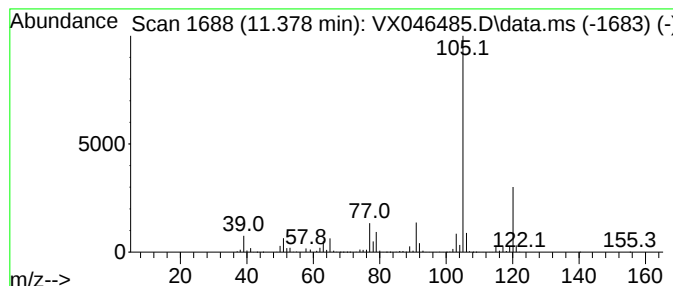
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	164.63 ug/l	1474650	1,4-Dichlorobenzene-d4	12.018

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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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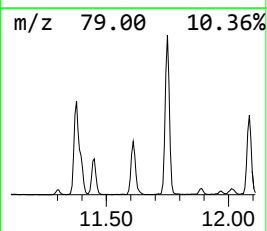
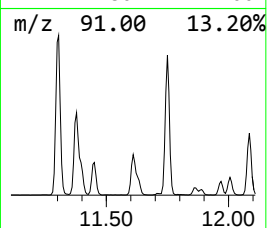
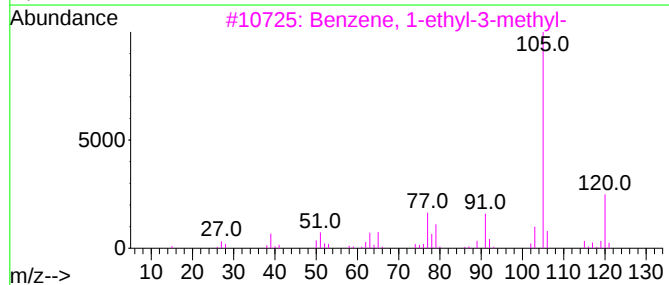
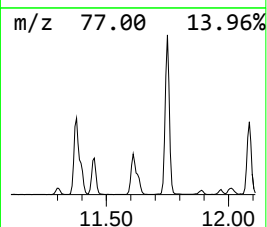
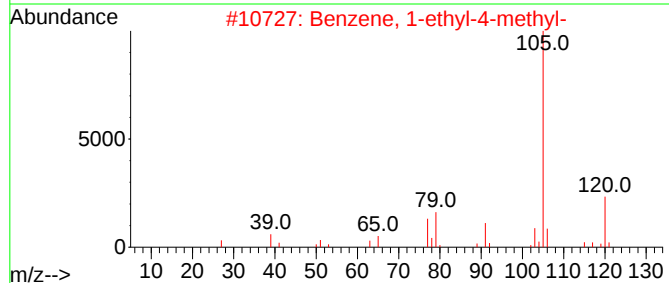
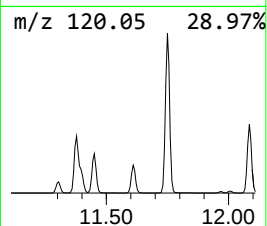
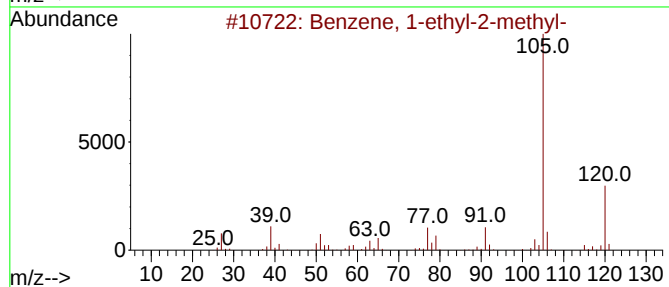
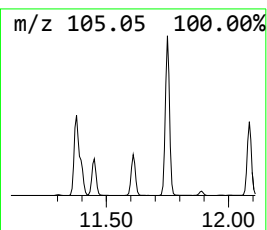
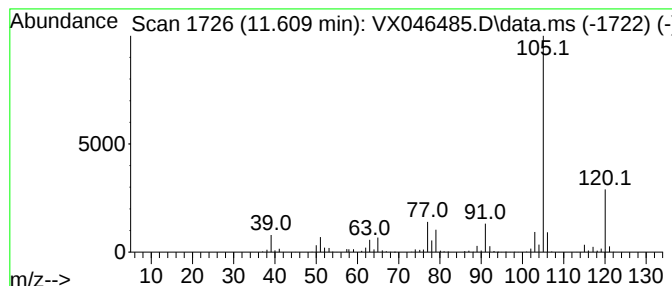
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.609	86.25 ug/l	772568	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
303-PPR-2

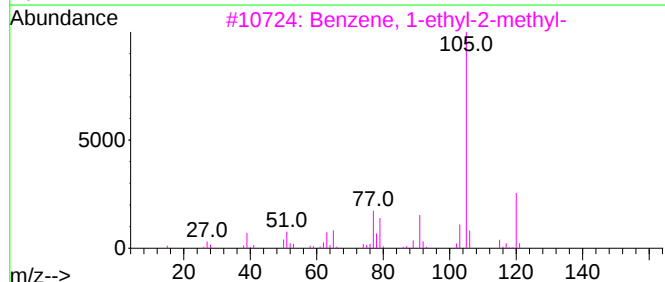
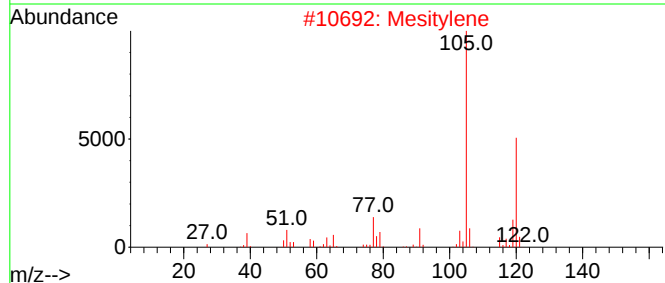
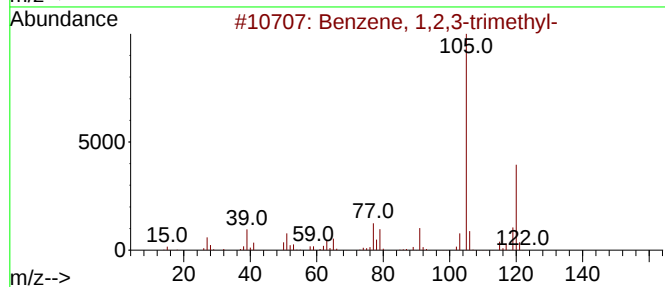
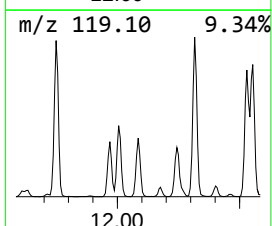
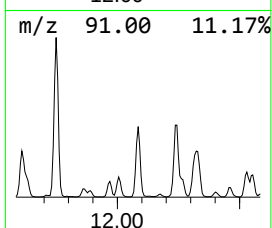
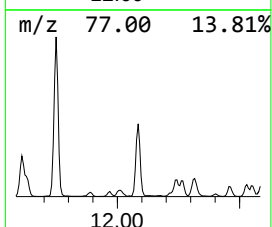
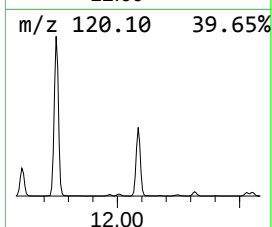
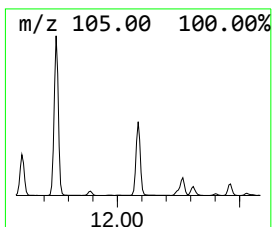
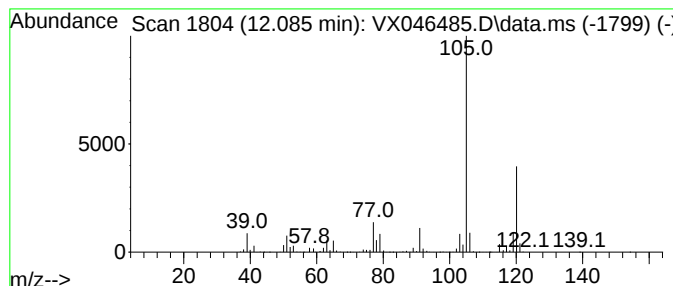
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	121.75 ug/l	1090580	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	95
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

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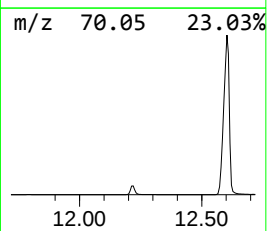
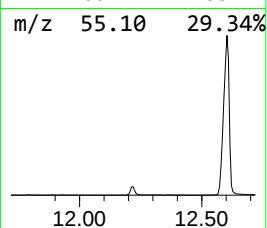
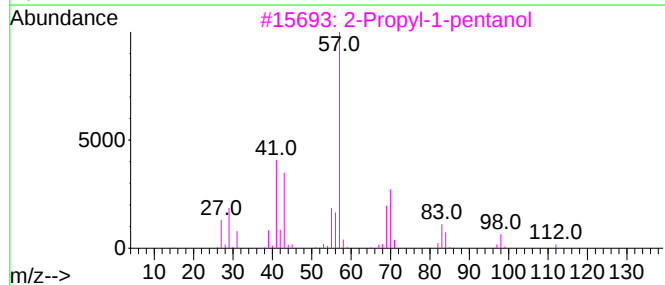
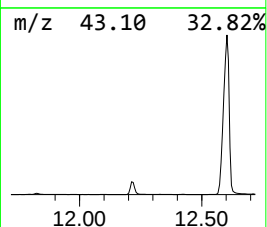
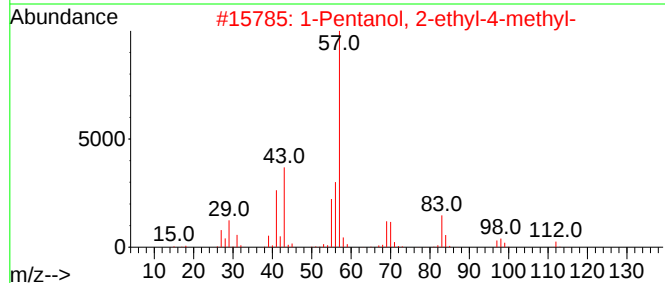
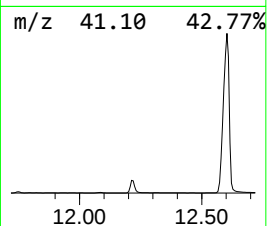
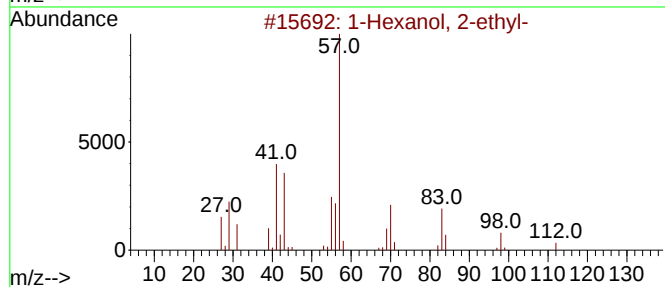
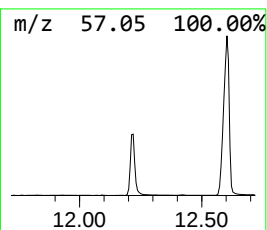
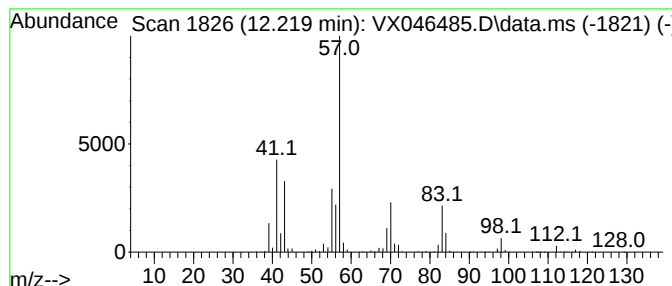
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	248.53 ug/l	2226150	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4		3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47
5		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	45



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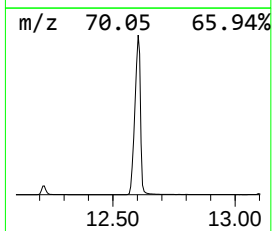
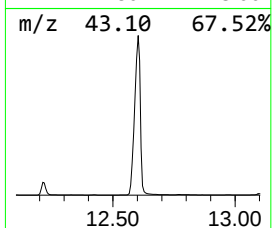
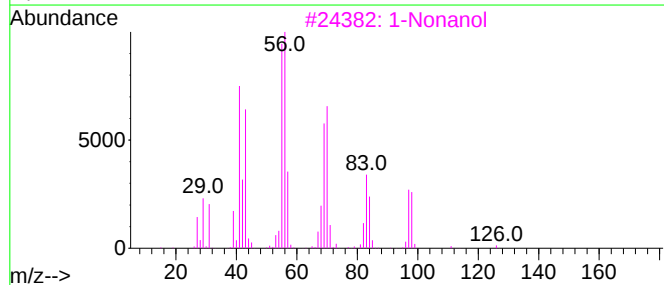
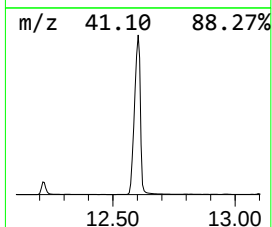
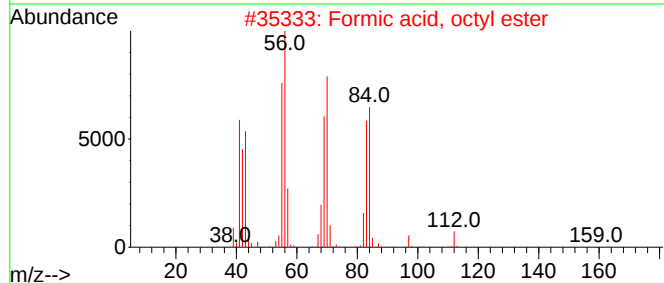
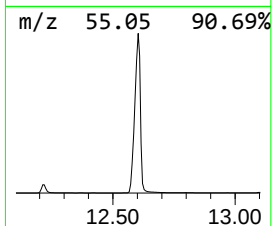
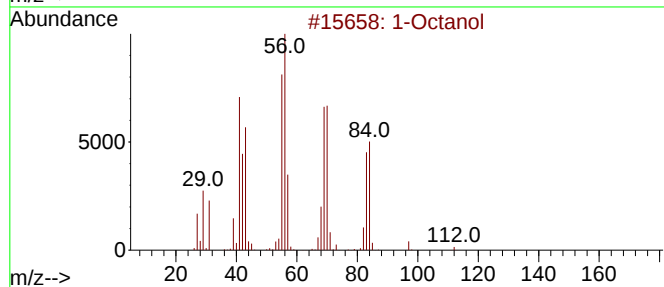
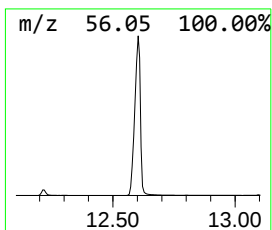
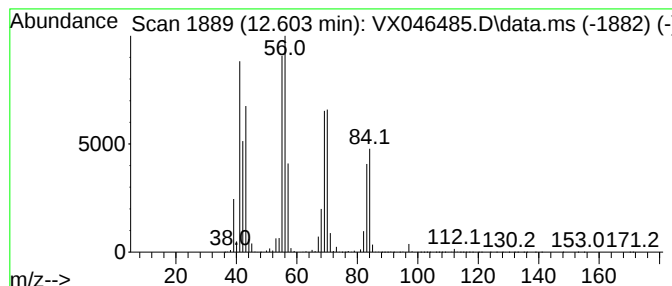
Instrument :
MSVOA_X
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.603	4142.80 ug/l	37108900	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3	1-Nonanol	144	C9H20O	000143-08-8	72
4	Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	53
5	1-Hexanol, 3-methyl-	116	C7H16O	013231-81-7	50



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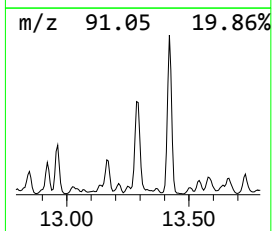
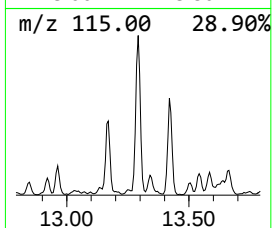
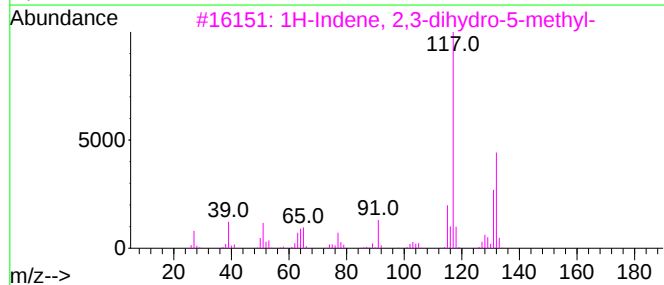
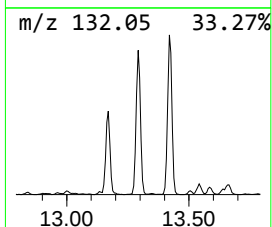
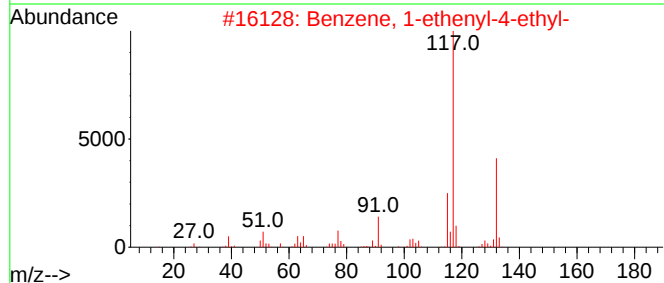
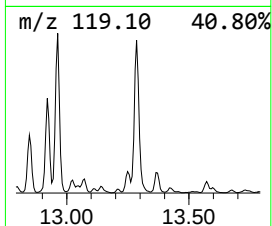
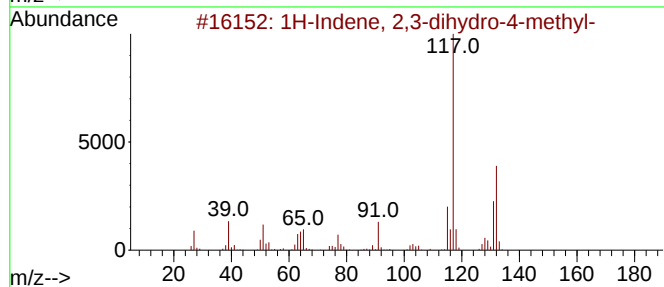
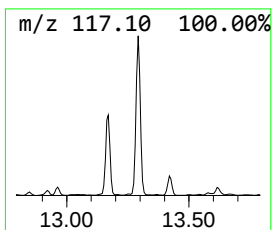
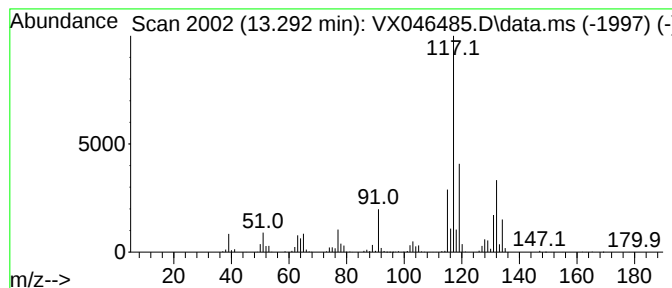
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	90.42 ug/l	809970	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	92	
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	92	
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	92	
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	87	
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060325\
Data File : VX046485.D
Acq On : 03 Jun 2025 20:02
Operator : JC/MD
Sample : Q2169-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
303-PPR-2

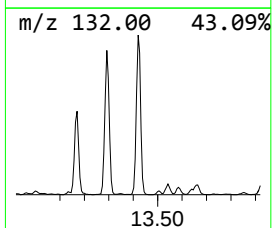
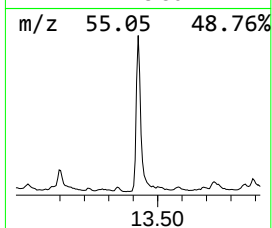
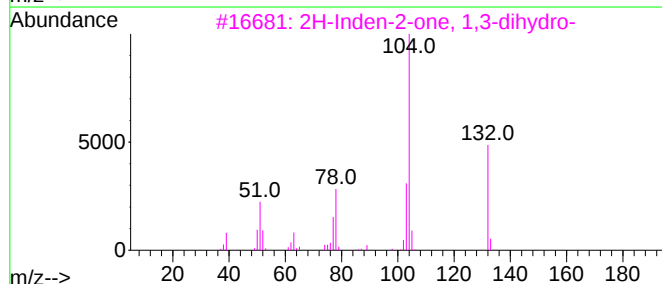
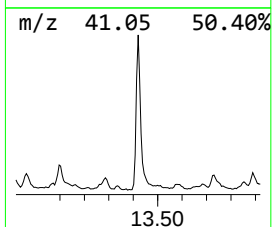
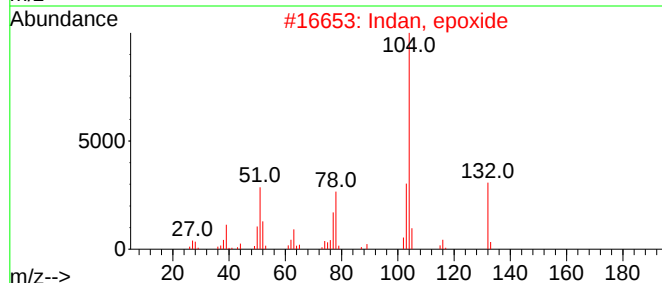
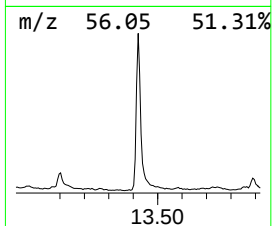
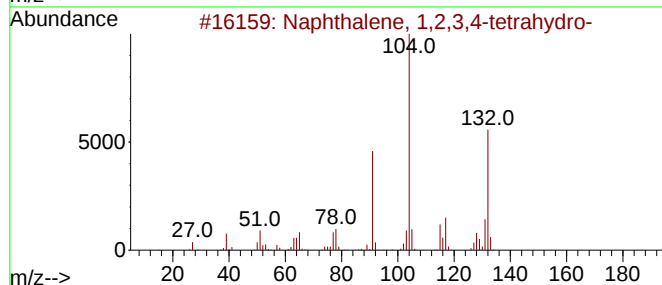
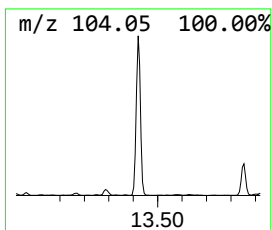
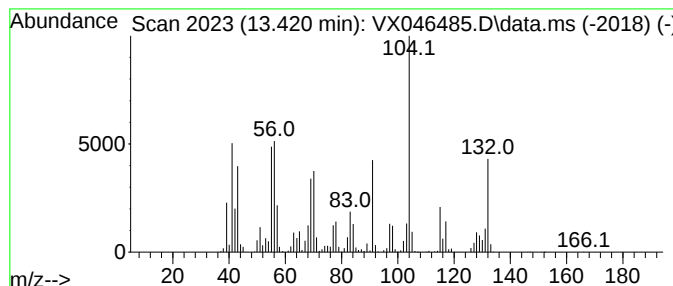
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	146.09 ug/l	1308560	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	91
2			Indan, epoxide	132	C9H8O	000768-22-9	45
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	45
4			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	30
5			Isopropylcyclobutane	98	C7H14	000872-56-0	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060325\
Data File : VX046485.D
Acq On : 03 Jun 2025 20:02
Operator : JC/MD
Sample : Q2169-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
303-PPR-2

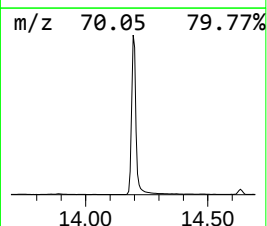
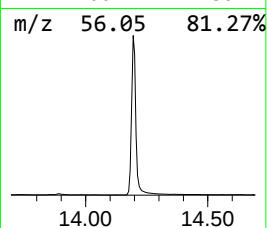
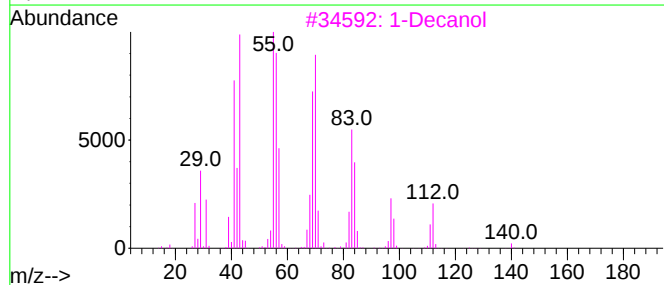
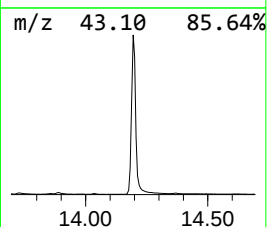
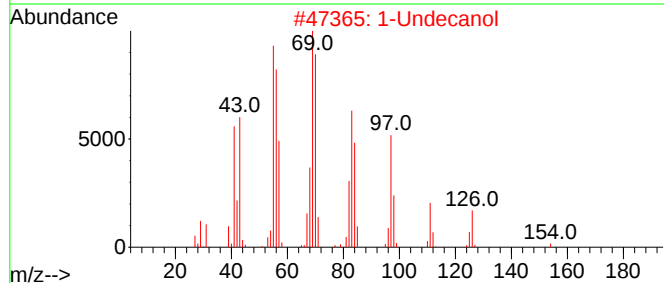
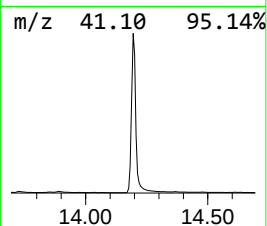
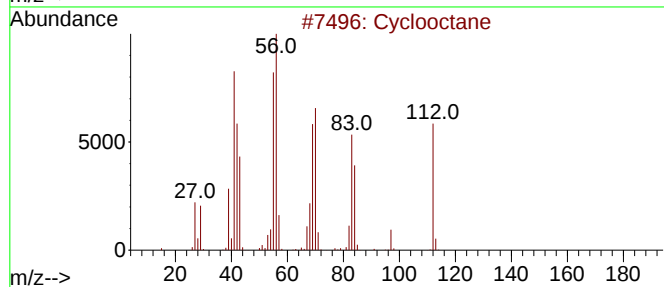
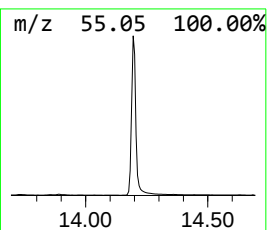
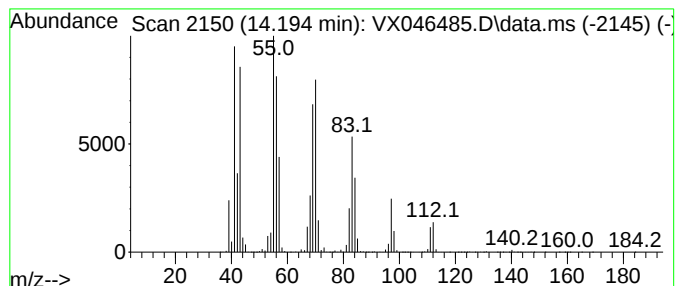
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Quant Title : SW846 8260

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

Peak Number 8 Cyclooctane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.194	1106.32 ug/l	9909750	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane	112	C8H16	000292-64-8	87
2			1-Undecanol	172	C11H24O	000112-42-5	86
3			1-Decanol	158	C10H22O	000112-30-1	86
4			Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	81
5			Cyclopropane, octyl-	154	C11H22	001472-09-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060325\
Data File : VX046485.D
Acq On : 03 Jun 2025 20:02
Operator : JC/MD
Sample : Q2169-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
303-PPR-2

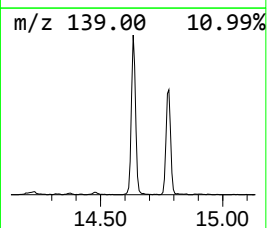
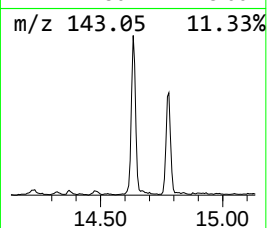
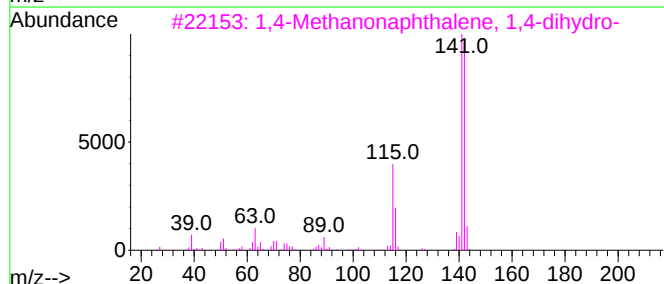
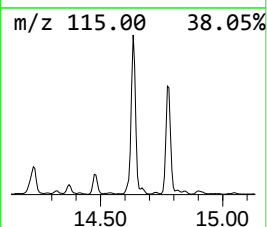
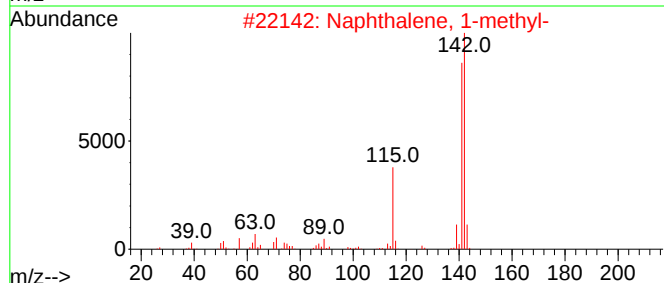
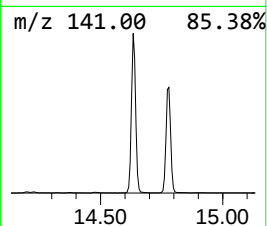
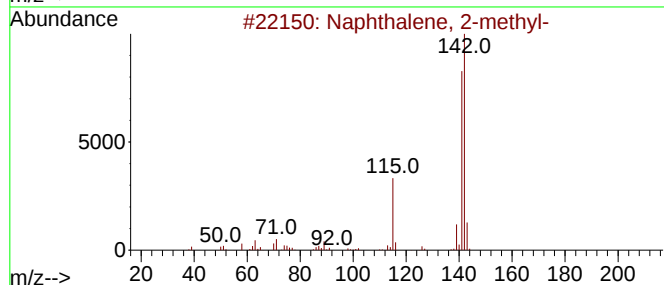
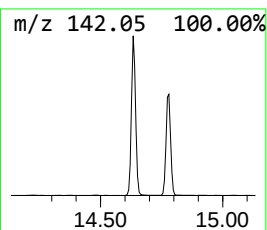
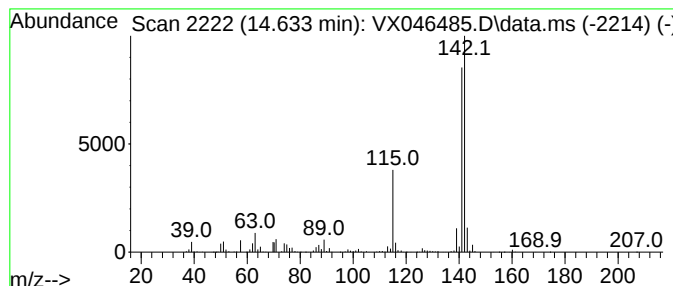
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	124.63 ug/l	1116350	1,4-Dichlorobenzene-d4	12.018

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	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060325\
Data File : VX046485.D
Acq On : 03 Jun 2025 20:02
Operator : JC/MD
Sample : Q2169-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
303-PPR-2

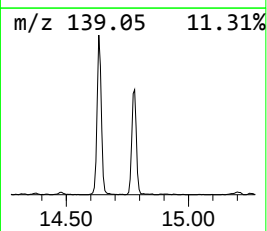
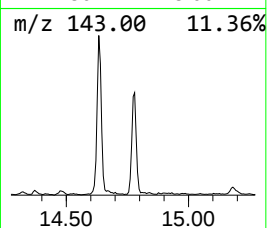
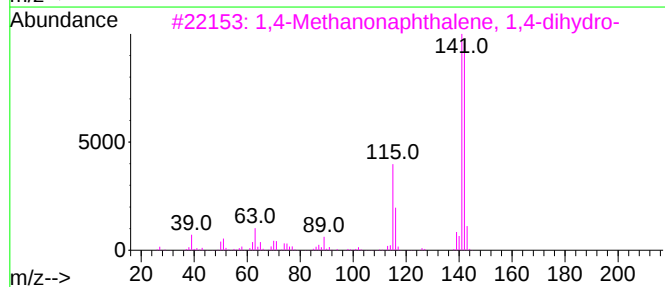
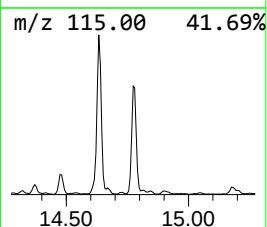
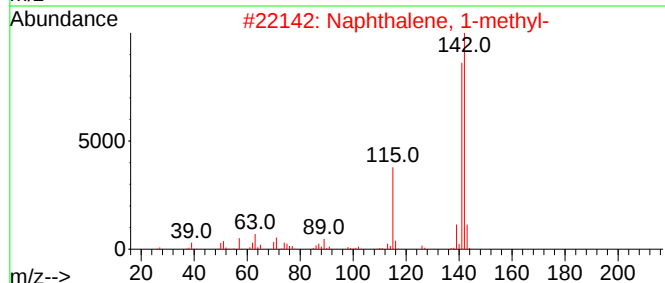
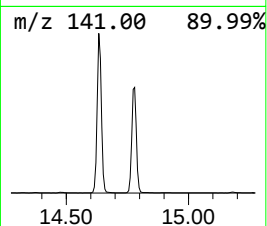
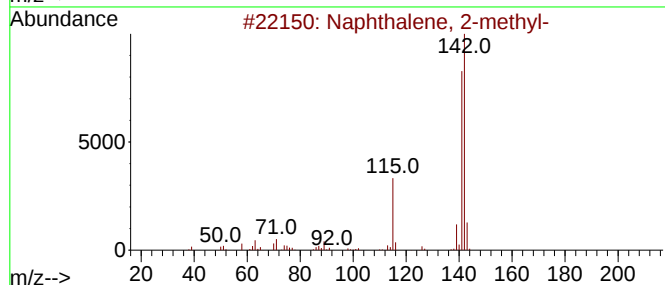
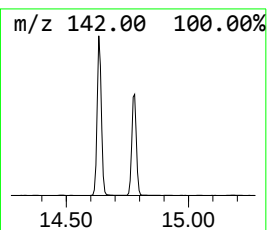
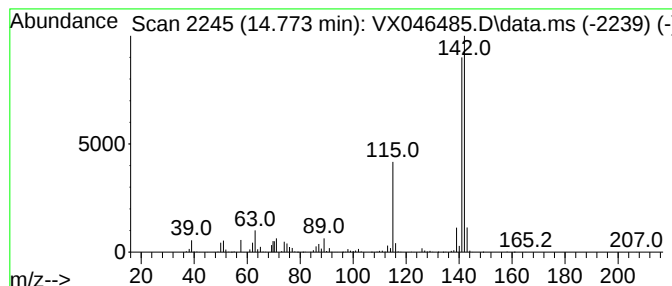
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.773	80.26 ug/l	718932	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060325\
Data File : VX046485.D
Acq On : 03 Jun 2025 20:02
Operator : JC/MD
Sample : Q2169-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
303-PPR-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.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
Benzene, 1-ethy...	11.378	164.6	ug/l	1474650	4	12.018	447872	50.0
Benzene, 1-ethy...	11.609	86.3	ug/l	772568	4	12.018	447872	50.0
Benzene, 1,2,3-...	12.085	121.8	ug/l	1090580	4	12.018	447872	50.0
1-Hexanol, 2-et...	12.219	248.5	ug/l	2226150	4	12.018	447872	50.0
1-Octanol	12.603	4142.8	ug/l	37108900	4	12.018	447872	50.0
1H-Indene, 2,3-...	13.292	90.4	ug/l	809970	4	12.018	447872	50.0
Naphthalene, 1,...	13.420	146.1	ug/l	1308560	4	12.018	447872	50.0
Cyclooctane	14.194	1106.3	ug/l	9909750	4	12.018	447872	50.0
Naphthalene, 2-...	14.633	124.6	ug/l	1116350	4	12.018	447872	50.0
Naphthalene, 1-...	14.773	80.3	ug/l	718932	4	12.018	447872	50.0