

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092723\
 Data File : VX037926.D
 Acq On : 27 Sep 2023 16:03
 Operator : JC/MD
 Sample : 04614-02
 Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AUD-1055

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\82X091523W.M
 Title : SW846 8260

Signal : TIC: VX037926.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	693	706	719	rBV	126976	391931	2.61%	0.993%
2	5.544	721	731	750	rVB	246538	716559	4.78%	1.815%
3	5.952	788	798	804	rBV	147626	390135	2.60%	0.988%
4	6.032	804	811	823	rVB	261330	696352	4.64%	1.764%
5	6.757	921	930	950	rBV	373779	905388	6.04%	2.293%
6	8.647	1234	1240	1246	rBV	802204	1219191	8.13%	3.088%
7	8.720	1246	1252	1266	rVB	773701	1242157	8.28%	3.146%
8	10.055	1466	1471	1481	rBV	788353	1089289	7.26%	2.759%
9	10.299	1502	1511	1518	rBV	1234792	1661741	11.08%	4.208%
10	10.640	1562	1567	1578	rVB	650073	915255	6.10%	2.318%
11	11.085	1634	1640	1650	rBV	648147	896311	5.98%	2.270%
12	11.378	1683	1688	1695	rBV	121838	218507	1.46%	0.553%
13	11.451	1695	1700	1709	rVB	590473	794292	5.30%	2.012%
14	11.756	1745	1750	1755	rVB	928816	1183702	7.89%	2.998%
15	11.963	1777	1784	1789	rBV	237426	323424	2.16%	0.819%
16	12.024	1789	1794	1800	rVV	1001721	1265225	8.44%	3.204%
17	12.085	1800	1804	1809	rVB	357393	471182	3.14%	1.193%
18	12.244	1825	1830	1838	rBV2	124003	206338	1.38%	0.523%
19	12.317	1838	1842	1848	rBV2	123756	180386	1.20%	0.457%
20	12.415	1848	1858	1863	rBV	1097101	1369933	9.14%	3.469%
21	12.963	1944	1948	1956	rBV2	278096	384568	2.56%	0.974%
22	13.286	1991	2001	2007	rBV3	154312	254796	1.70%	0.645%
23	13.420	2017	2023	2032	rVB	992427	1247076	8.32%	3.158%
24	13.774	2074	2081	2089	rBV	11788139	14993923	100.00%	37.973%
25	13.865	2092	2096	2103	rVB	156845	225254	1.50%	0.570%
26	14.634	2218	2222	2232	rVB	2643963	3230005	21.54%	8.180%
27	14.780	2240	2246	2253	rVB	1491011	1834107	12.23%	4.645%
28	15.207	2307	2316	2319	rBV	136897	201952	1.35%	0.511%
29	15.475	2354	2360	2373	rBV	238642	395623	2.64%	1.002%
30	15.609	2377	2382	2386	rVV	240852	395001	2.63%	1.000%
31	15.646	2386	2388	2397	rVB	135605	186269	1.24%	0.472%

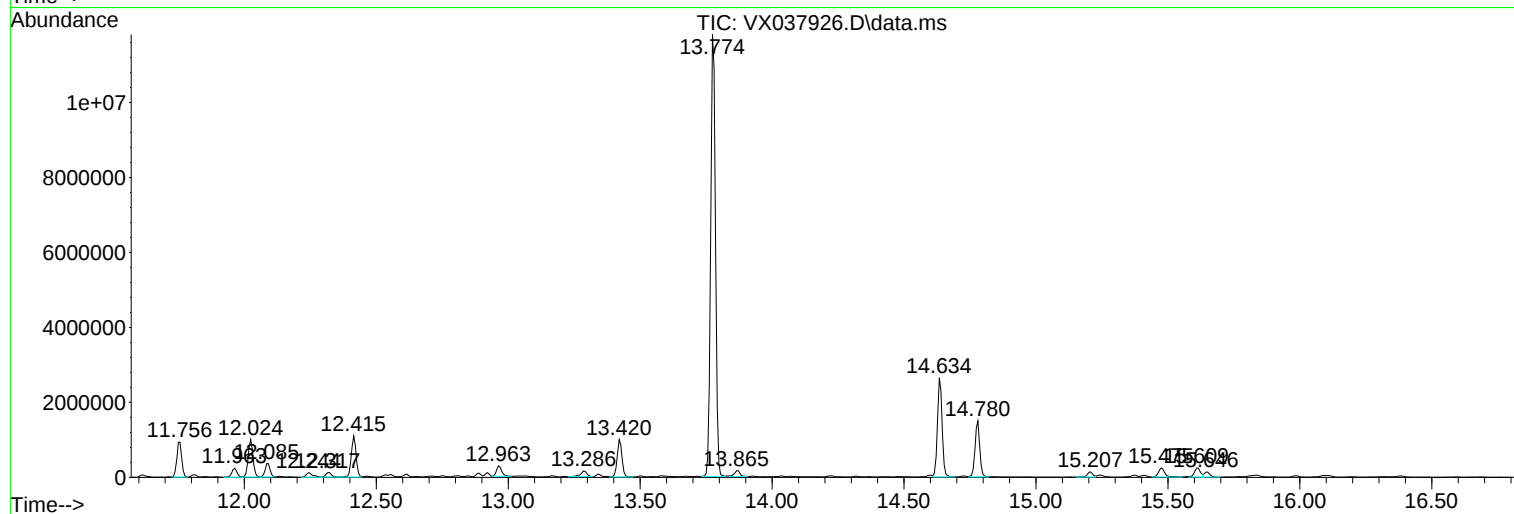
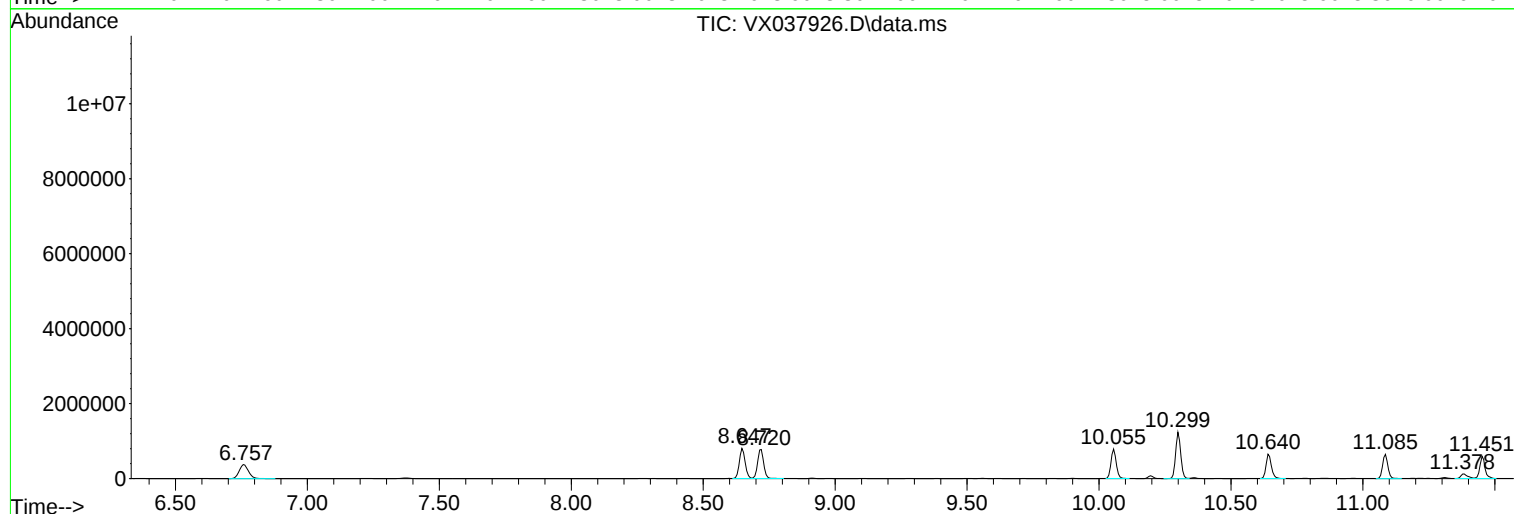
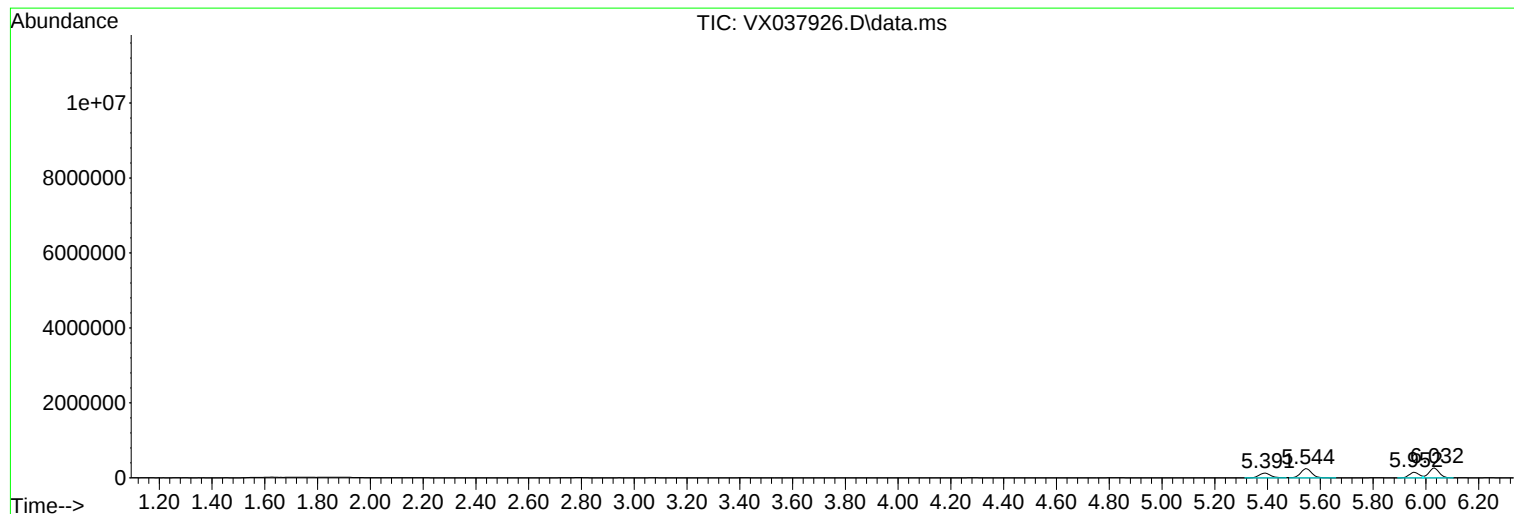
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ClientSampleId :
AUD-1055

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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



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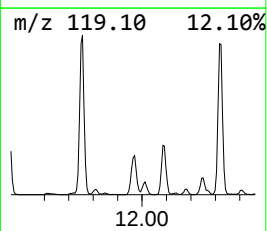
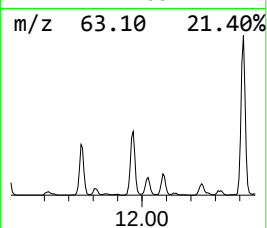
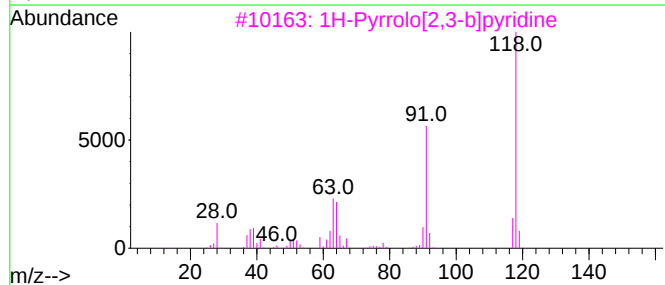
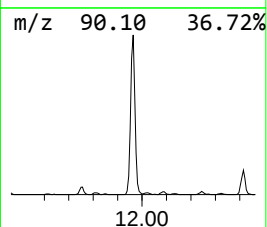
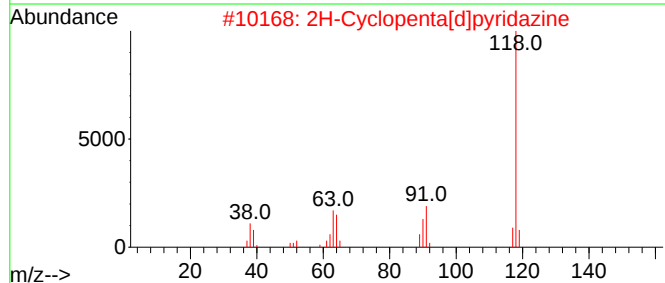
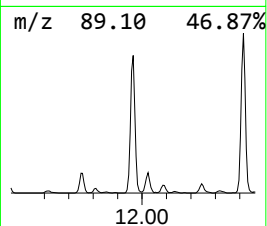
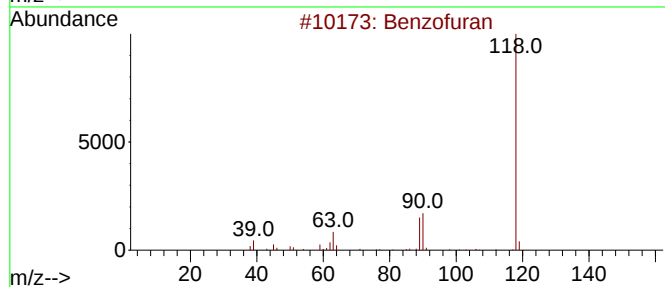
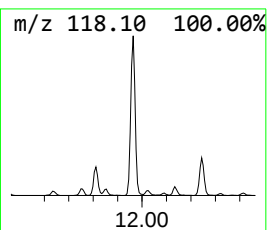
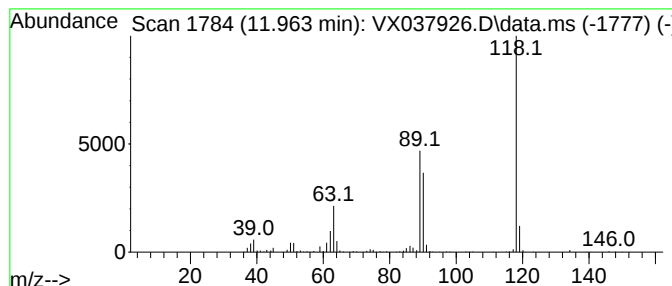
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzofuran Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	12.78 ug/l	323424	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran	118	C8H6O	000271-89-6	90
2			2H-Cyclopenta[d]pyridazine	118	C7H6N2	000270-64-4	64
3			1H-Pyrrolo[2,3-b]pyridine	118	C7H6N2	000271-63-6	45
4			1H-Tetrazole, 5-phenyl-	146	C7H6N4	018039-42-4	45
5			3-Hydroxyphenylacetylene	118	C8H6O	010401-11-3	42



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Instrument :
MSVOA_X
ClientSampleId :
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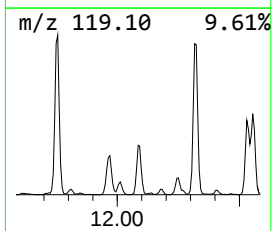
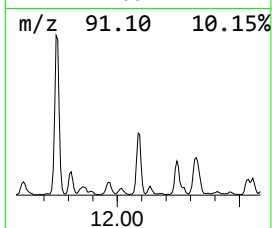
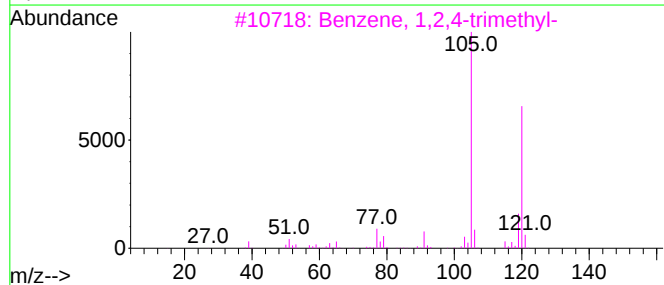
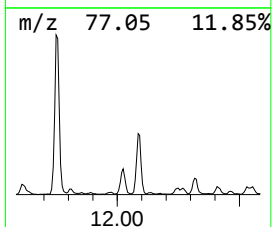
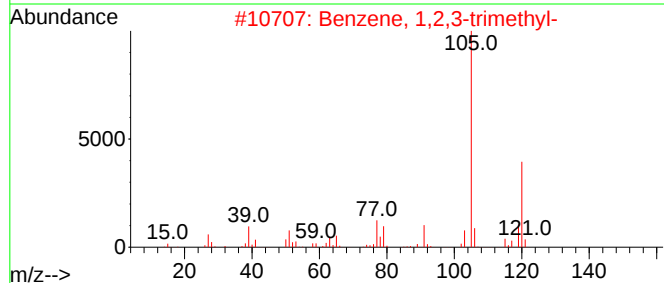
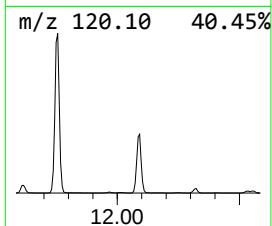
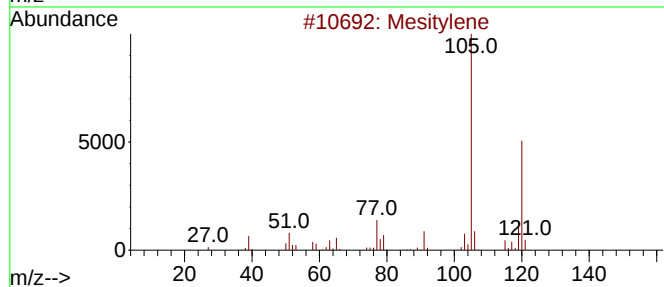
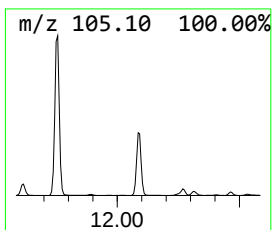
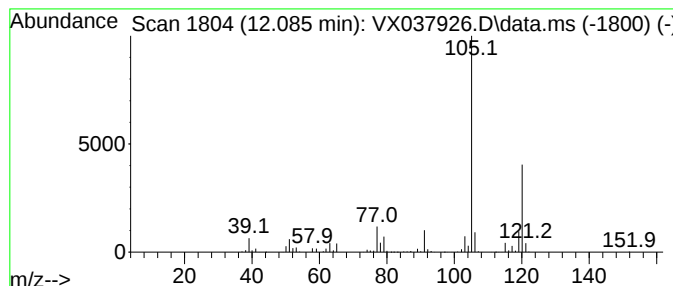
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	18.62 ug/l	471182	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



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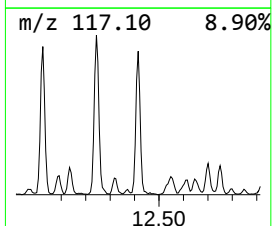
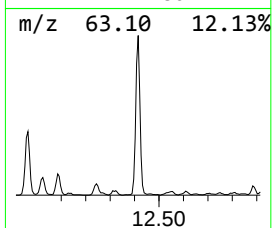
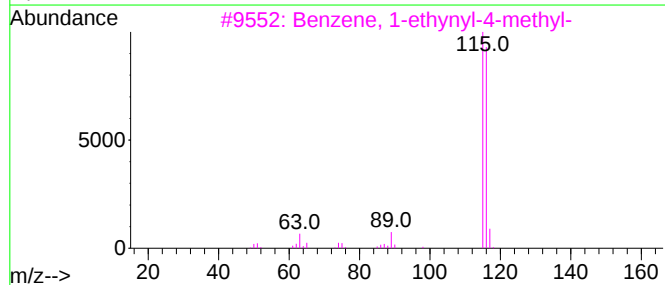
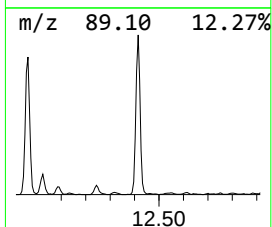
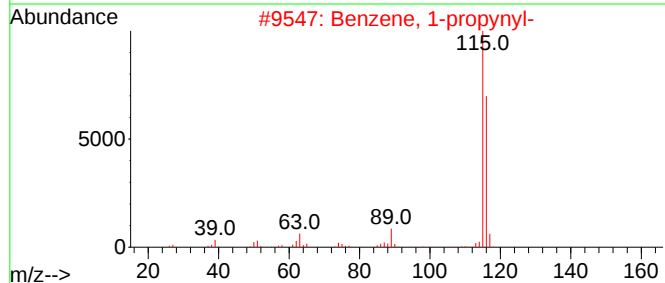
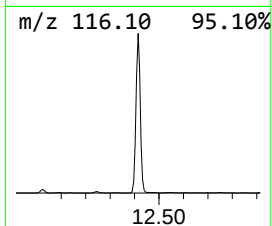
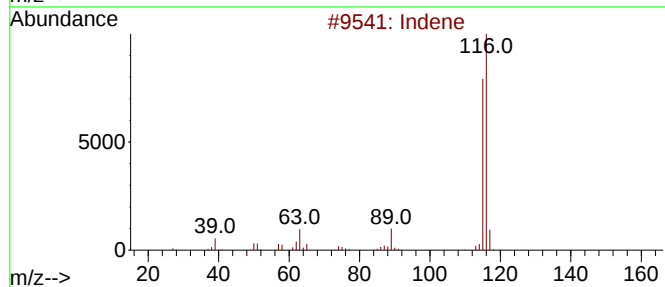
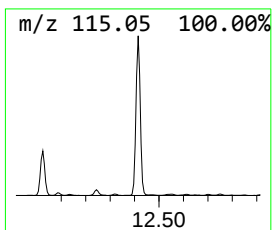
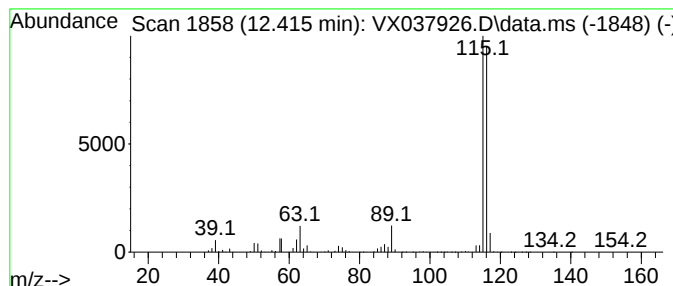
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	54.14 ug/l	1369930	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90



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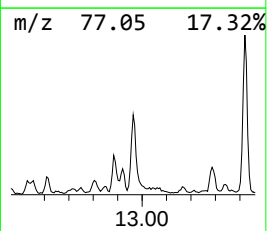
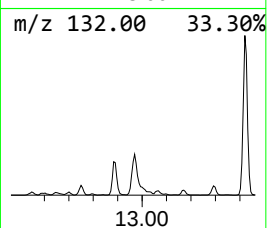
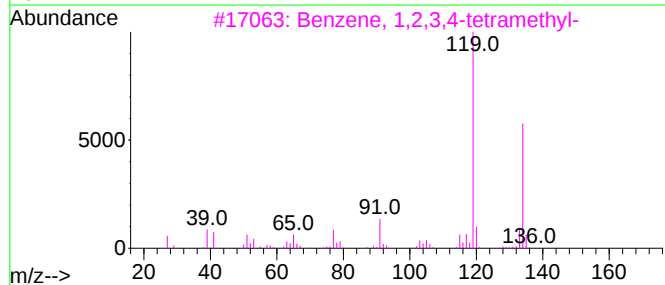
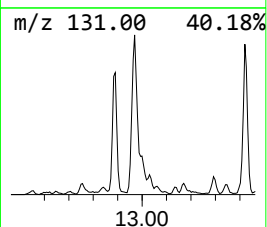
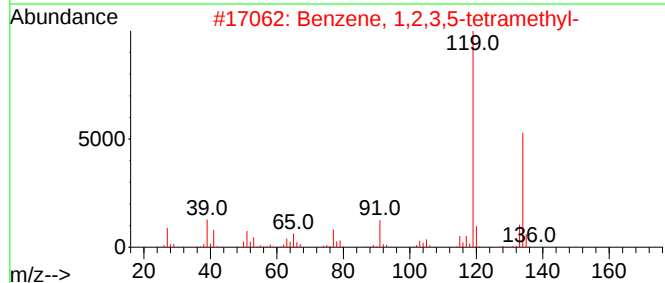
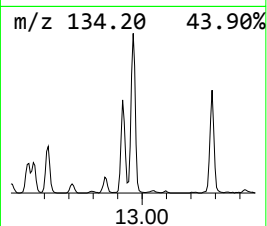
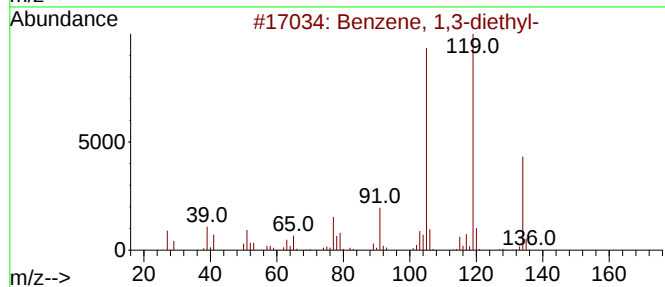
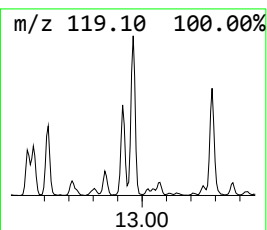
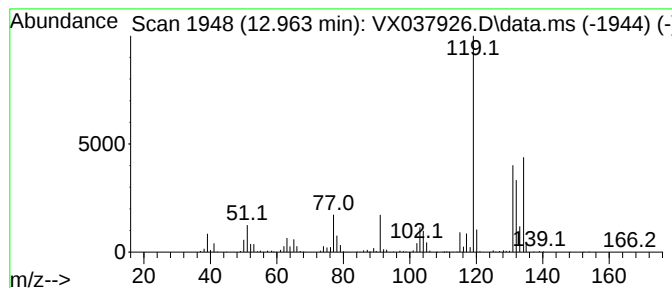
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,3-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	15.20 ug/l	384568	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	92
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	64



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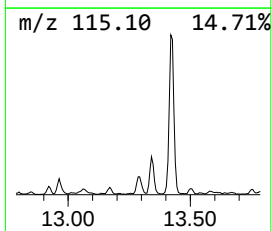
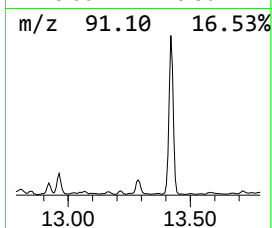
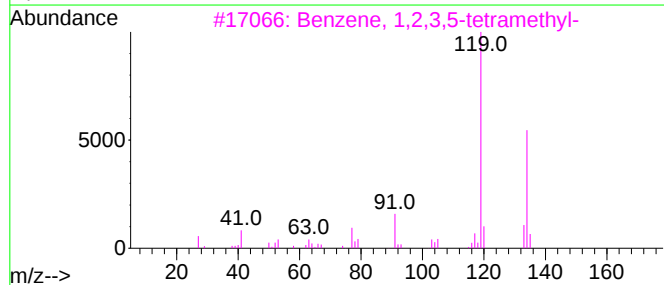
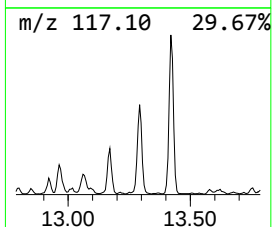
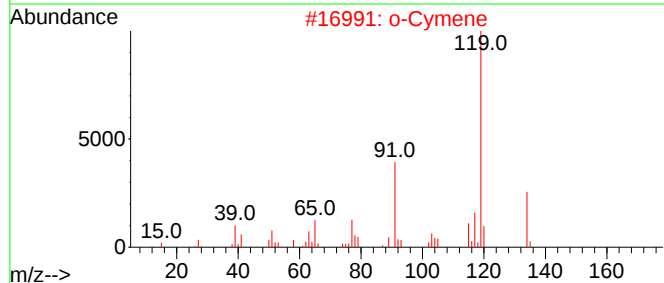
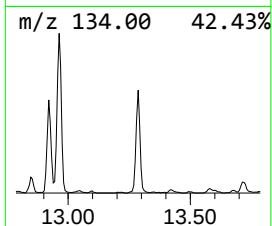
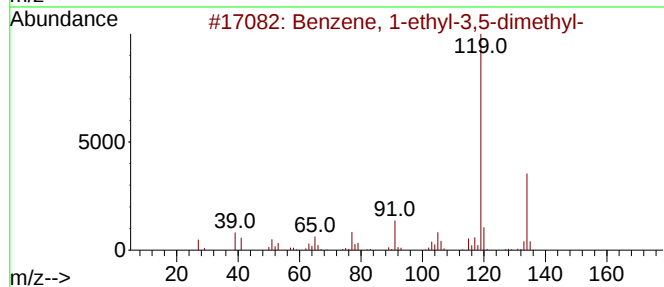
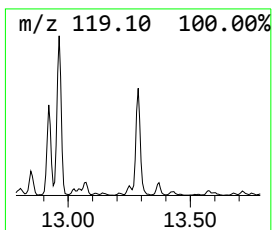
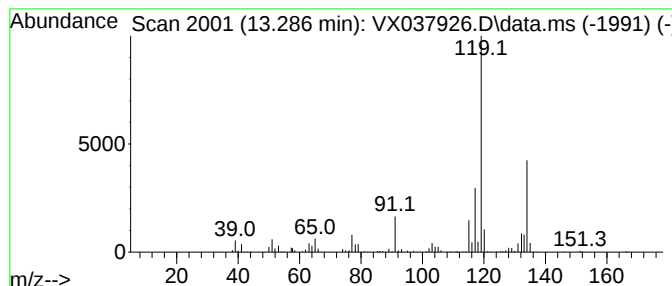
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	10.07 ug/l	254796	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87
2			o-Cymene	134	C10H14	000527-84-4	87
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	87
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87



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Operator : JC/MD
Sample : 04614-02
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1055

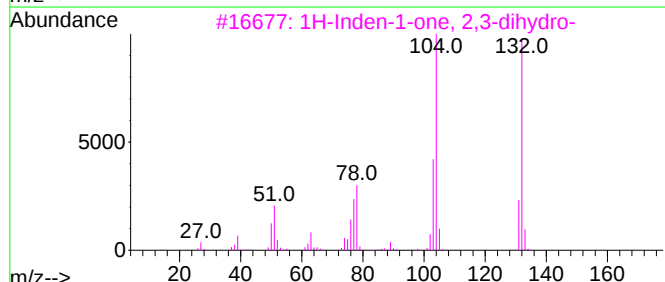
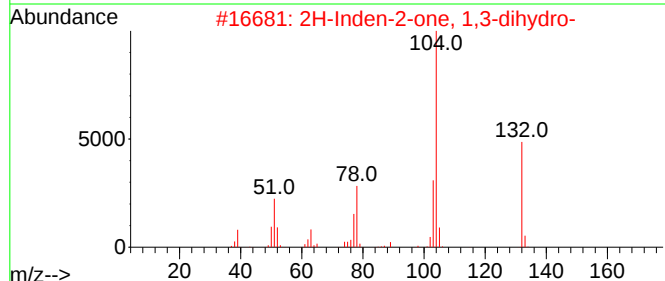
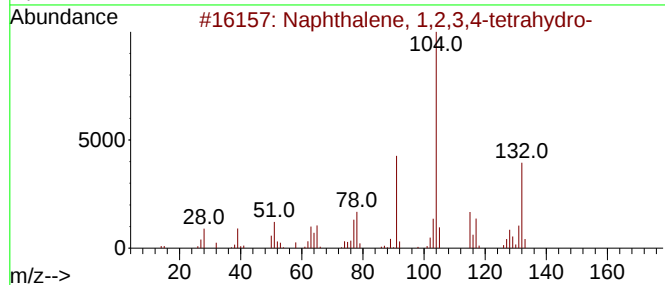
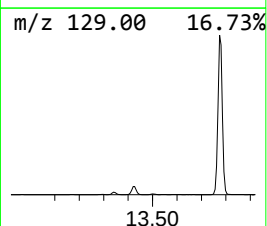
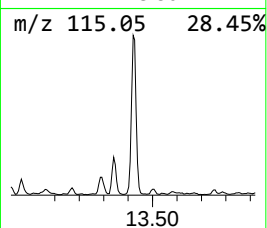
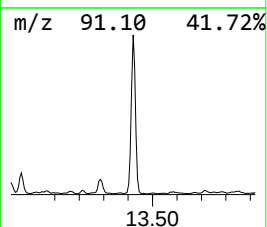
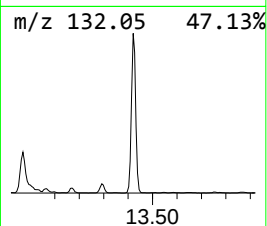
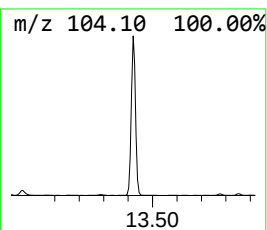
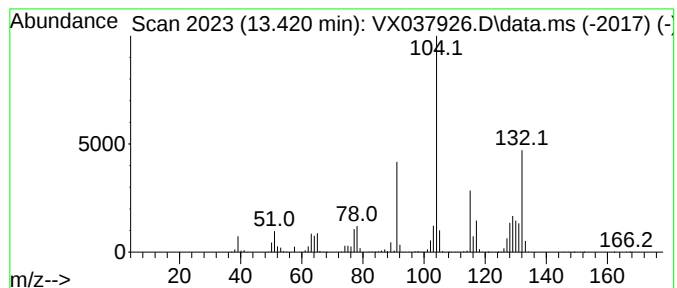
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	49.28 ug/l	1247080	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
3			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	50
4			Benzene, cyclobutyl-	132	C10H12	004392-30-7	50
5			Indan, epoxide	132	C9H8O	000768-22-9	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092723\
Data File : VX037926.D
Acq On : 27 Sep 2023 16:03
Operator : JC/MD
Sample : 04614-02
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1055

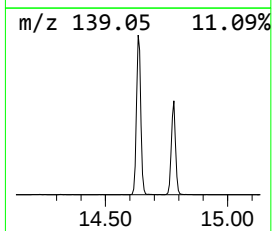
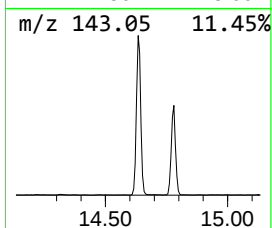
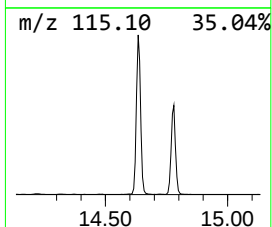
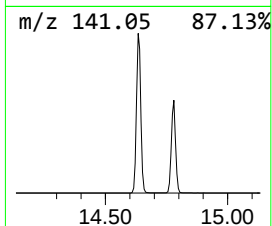
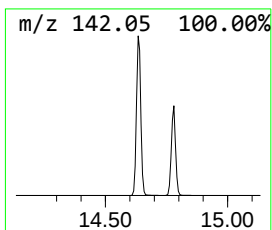
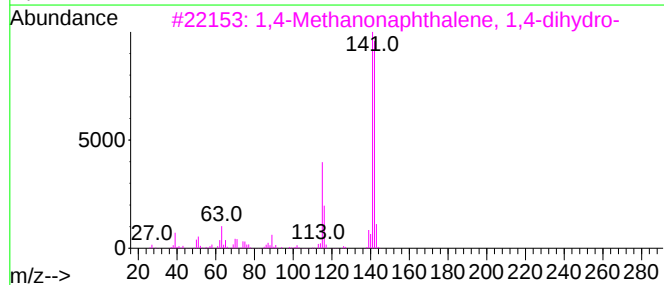
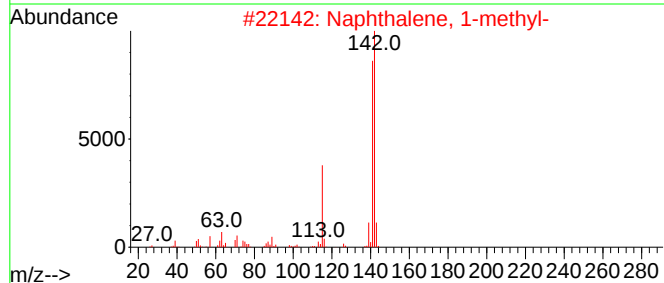
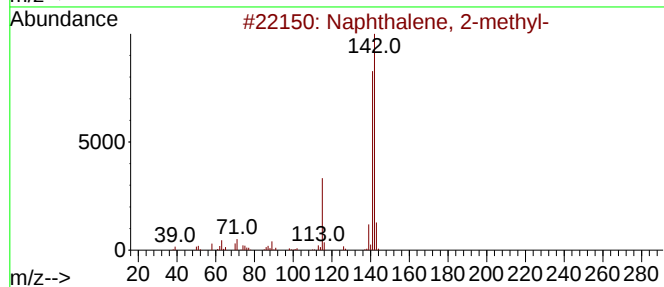
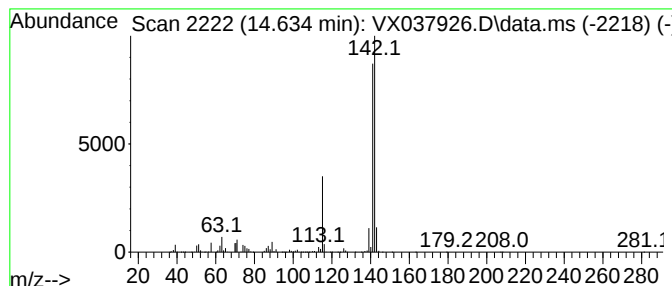
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	127.65 ug/l	3230010	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			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	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092723\
Data File : VX037926.D
Acq On : 27 Sep 2023 16:03
Operator : JC/MD
Sample : 04614-02
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1055

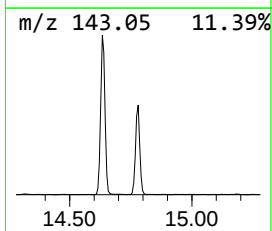
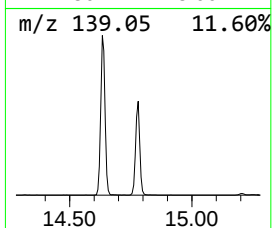
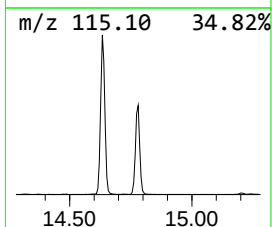
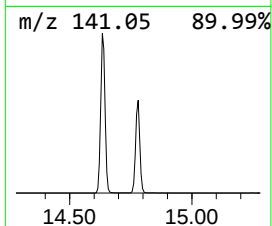
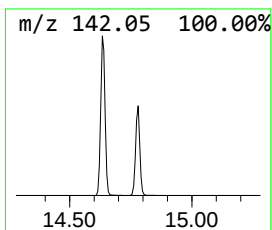
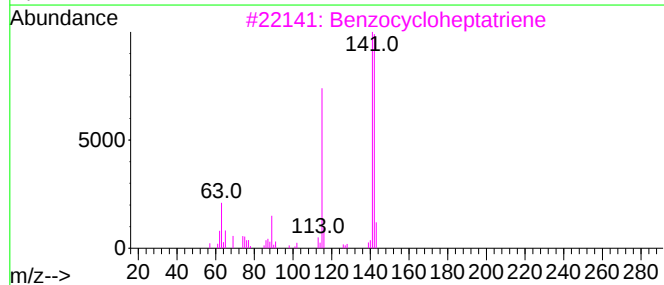
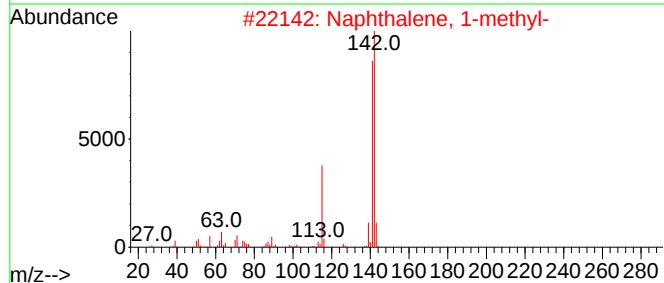
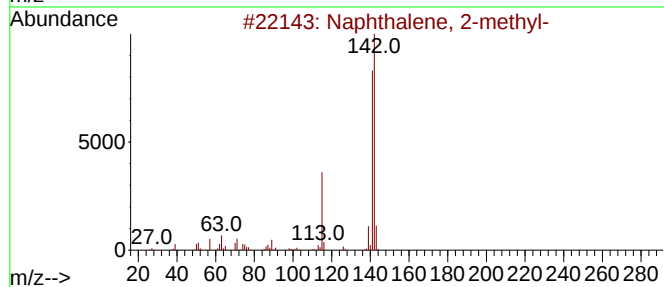
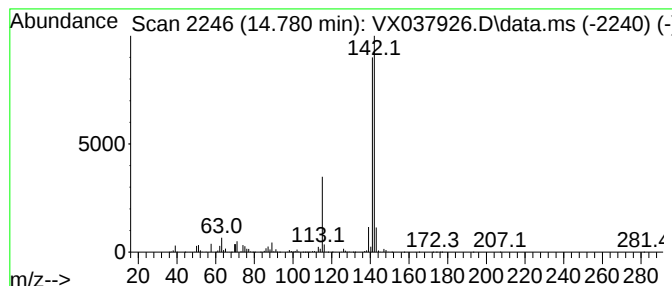
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	72.48 ug/l	1834110	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092723\
Data File : VX037926.D
Acq On : 27 Sep 2023 16:03
Operator : JC/MD
Sample : 04614-02
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1055

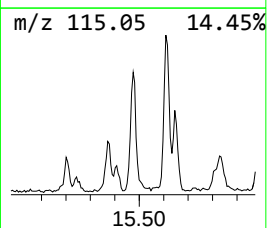
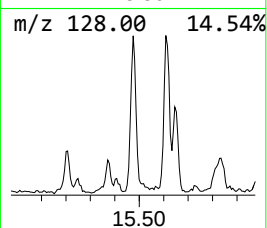
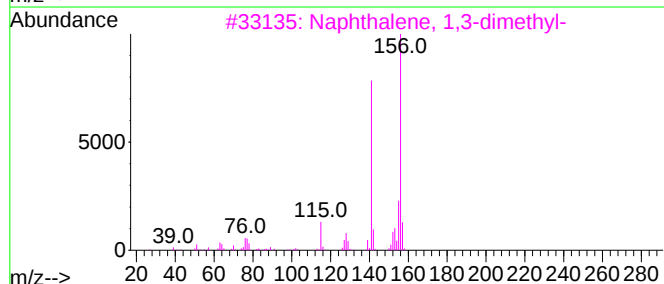
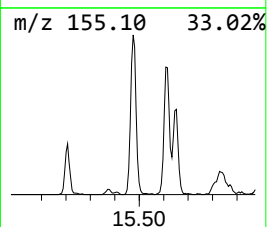
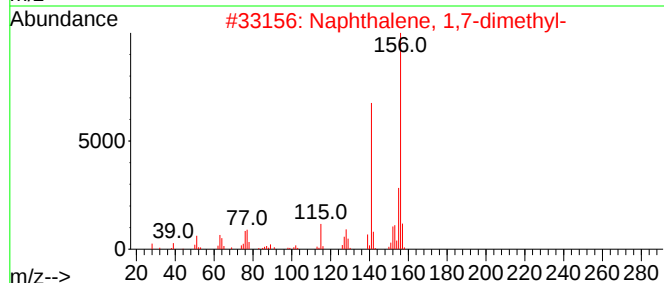
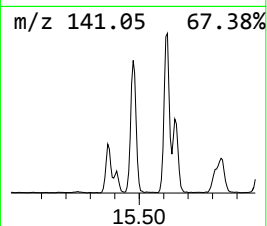
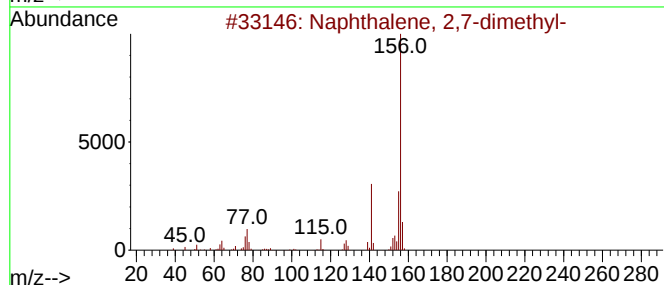
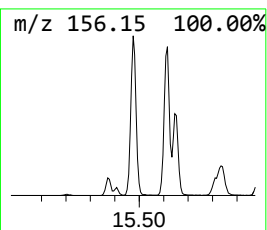
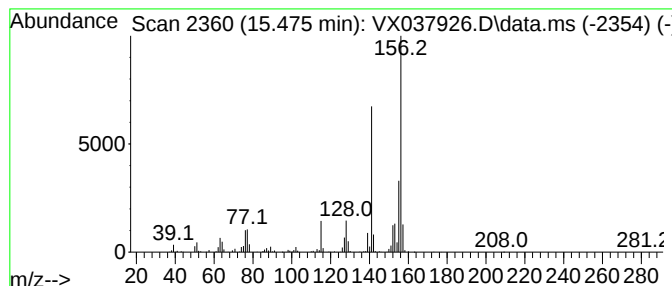
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	15.63 ug/l	395623	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092723\
Data File : VX037926.D
Acq On : 27 Sep 2023 16:03
Operator : JC/MD
Sample : 04614-02
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1055

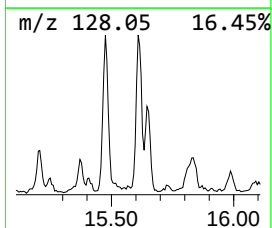
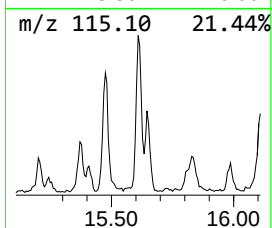
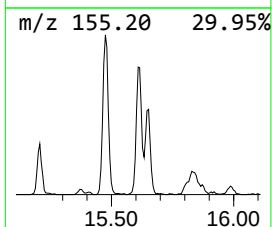
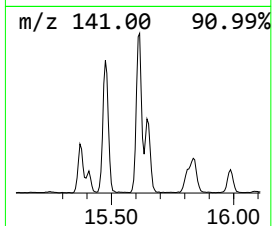
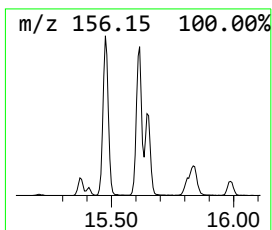
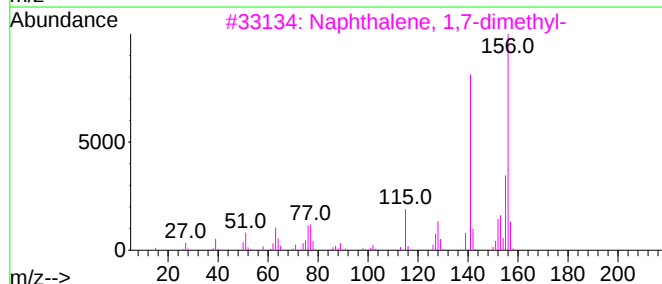
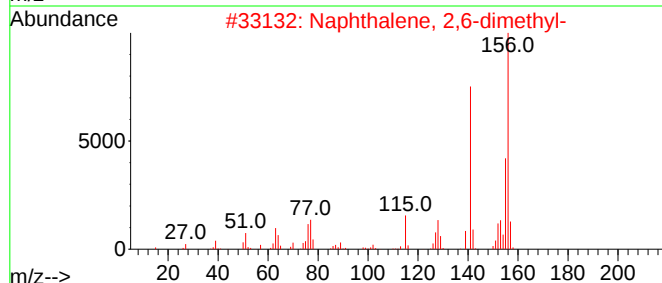
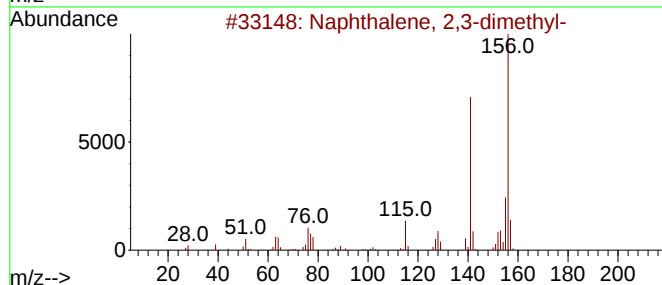
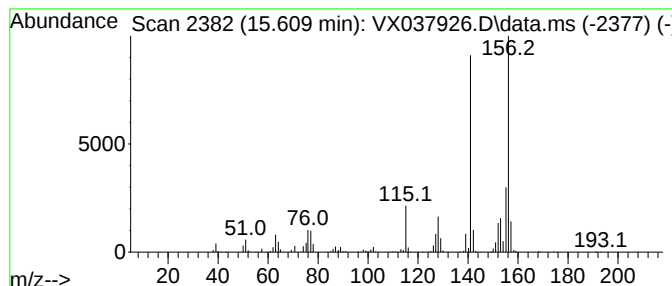
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Quant Title : SW846 8260

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.
15.609	15.61 ug/l	395001	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, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092723\
Data File : VX037926.D
Acq On : 27 Sep 2023 16:03
Operator : JC/MD
Sample : 04614-02
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1055

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.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, 1,2,3-...	12.085	18.6	ug/l	471182	4	12.024	1265230	50.0
Indene	12.415	54.1	ug/l	1369930	4	12.024	1265230	50.0
Benzene, 1,3-di...	12.963	15.2	ug/l	384568	4	12.024	1265230	50.0
Benzene, 1-ethy...	13.286	10.1	ug/l	254796	4	12.024	1265230	50.0
Naphthalene, 1,...	13.420	49.3	ug/l	1247080	4	12.024	1265230	50.0
Naphthalene, 2-...	14.634	127.7	ug/l	3230010	4	12.024	1265230	50.0
Naphthalene, 1-...	14.780	72.5	ug/l	1834110	4	12.024	1265230	50.0
Naphthalene, 2,...	15.475	15.6	ug/l	395623	4	12.024	1265230	50.0
Naphthalene, 2,...	15.609	15.6	ug/l	395001	4	12.024	1265230	50.0