

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
 Data File : VX041274.D
 Acq On : 29 Apr 2024 14:16
 Operator : JC/MD
 Sample : P2183-01
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1229

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\82X042224W.M
 Title : SW846 8260

Signal : TIC: VX041274.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.422	210	219	298	rBV	3329064	14218981	79.70%	25.954%
2	5.385	688	705	713	rBV2	84310	260887	1.46%	0.476%
3	5.543	724	731	753	rVB	159114	583467	3.27%	1.065%
4	5.805	761	774	787	rBV2	144887	423267	2.37%	0.773%
5	5.952	789	798	808	rBV	88880	243113	1.36%	0.444%
6	6.757	920	930	955	rBV	227902	557781	3.13%	1.018%
7	7.372	1018	1031	1042	rBV2	99497	254066	1.42%	0.464%
8	8.646	1235	1240	1245	rBV	448890	681724	3.82%	1.244%
9	8.720	1245	1252	1270	rVB	11227089	17840062	100.00%	32.564%
10	10.055	1466	1471	1478	rBV	491757	658766	3.69%	1.202%
11	10.195	1487	1494	1500	rBV	1090346	1424478	7.98%	2.600%
12	10.299	1502	1511	1518	rBV	3960777	5384063	30.18%	9.828%
13	10.640	1561	1567	1582	rVB	1314900	1745000	9.78%	3.185%
14	11.085	1634	1640	1645	rBV	435979	590265	3.31%	1.077%
15	11.305	1671	1676	1683	rBV	173201	228214	1.28%	0.417%
16	11.378	1683	1688	1695	rVV	520606	874376	4.90%	1.596%
17	11.451	1695	1700	1710	rVB	286574	395552	2.22%	0.722%
18	11.615	1722	1727	1734	rVB	274452	391650	2.20%	0.715%
19	11.750	1745	1749	1758	rVB	1049048	1346932	7.55%	2.459%
20	12.024	1789	1794	1799	rVB	561561	728603	4.08%	1.330%
21	12.085	1799	1804	1809	rBV	305844	382814	2.15%	0.699%
22	12.243	1825	1830	1832	rBV	228334	292381	1.64%	0.534%
23	12.268	1832	1834	1838	rVV	170675	191526	1.07%	0.350%
24	12.317	1838	1842	1849	rVB3	230396	364118	2.04%	0.665%
25	12.530	1872	1877	1879	rBV	142840	179882	1.01%	0.328%
26	12.615	1886	1891	1894	rVV	155221	185257	1.04%	0.338%
27	12.701	1899	1905	1913	rBV3	109973	229154	1.28%	0.418%
28	12.963	1944	1948	1950	rVV	174784	201438	1.13%	0.368%
29	13.170	1974	1982	1986	rBV3	148830	237149	1.33%	0.433%
30	13.292	1998	2002	2007	rVB2	340260	453190	2.54%	0.827%
31	13.420	2019	2023	2032	rVB	185591	314086	1.76%	0.573%
32	13.774	2077	2081	2088	rVB	173672	264556	1.48%	0.483%
33	13.847	2088	2093	2099	rVB3	122354	206258	1.16%	0.376%
34	14.225	2149	2155	2161	rVB2	220102	374469	2.10%	0.684%
35	14.438	2183	2190	2193	rBV	197588	255237	1.43%	0.466%
36	14.481	2193	2197	2205	rVB2	141946	205937	1.15%	0.376%

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Instrument :
MSVOA_X
ClientSampleId :
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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\82X042224W.M
Title : SW846 8260

37	14.633	2215	2222	2226	rBV2	259044	504496	2.83%	0.921%
38	15.560	2368	2374	2379	rBV	787982	1111780	6.23%	2.029%

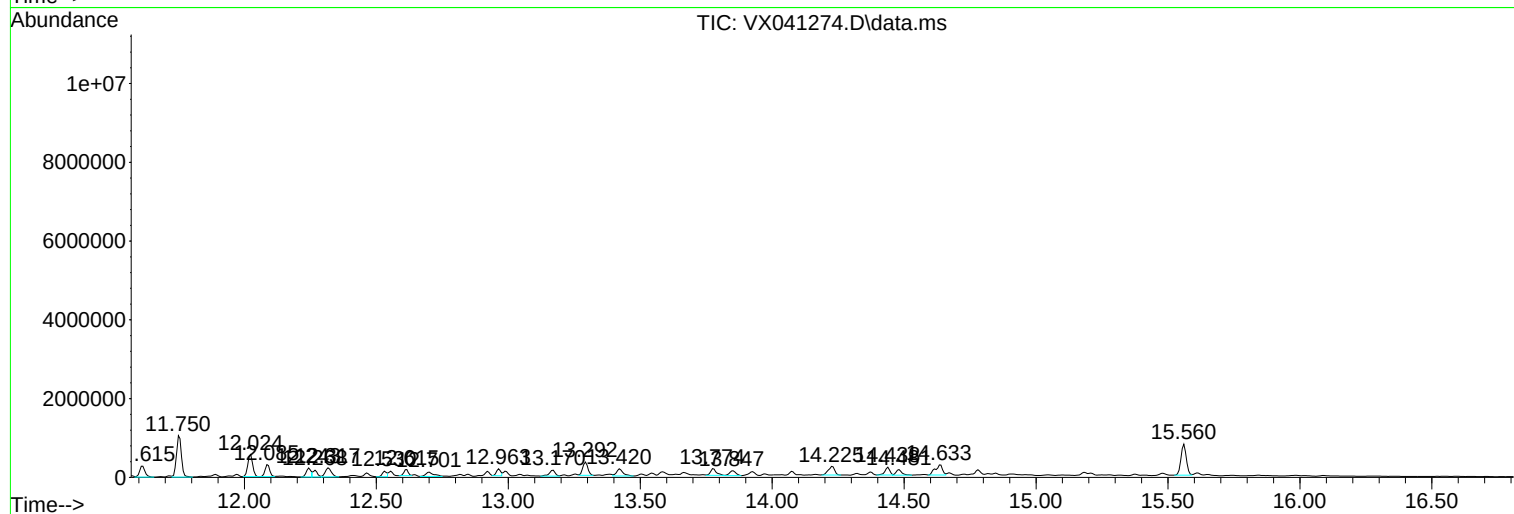
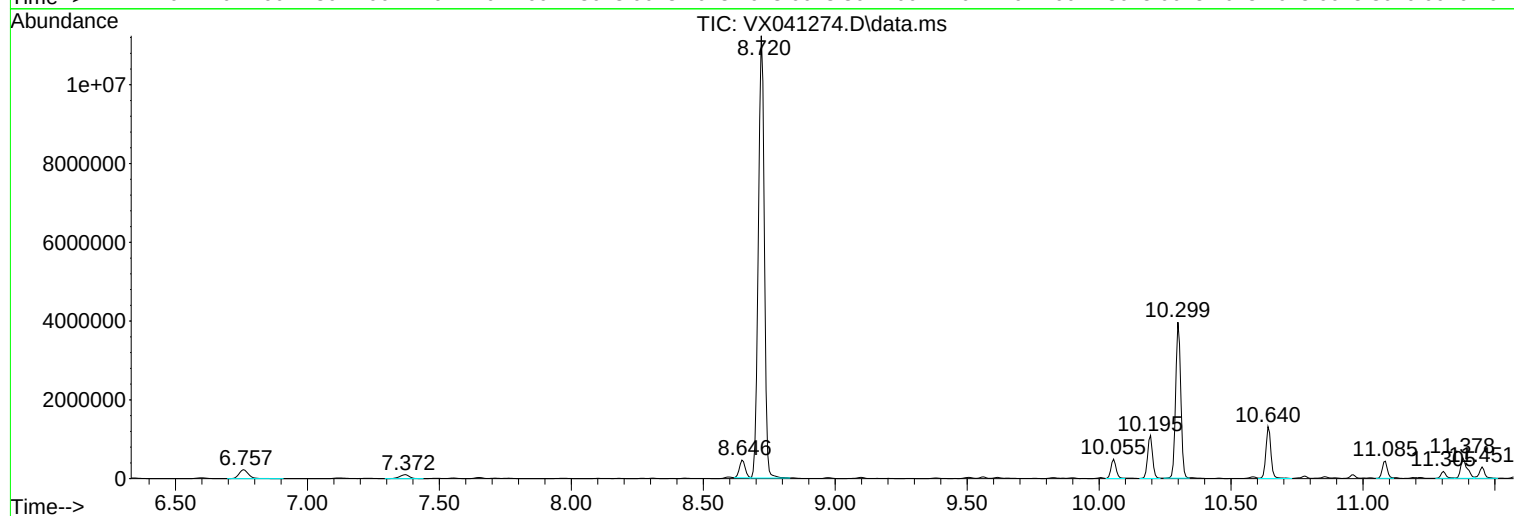
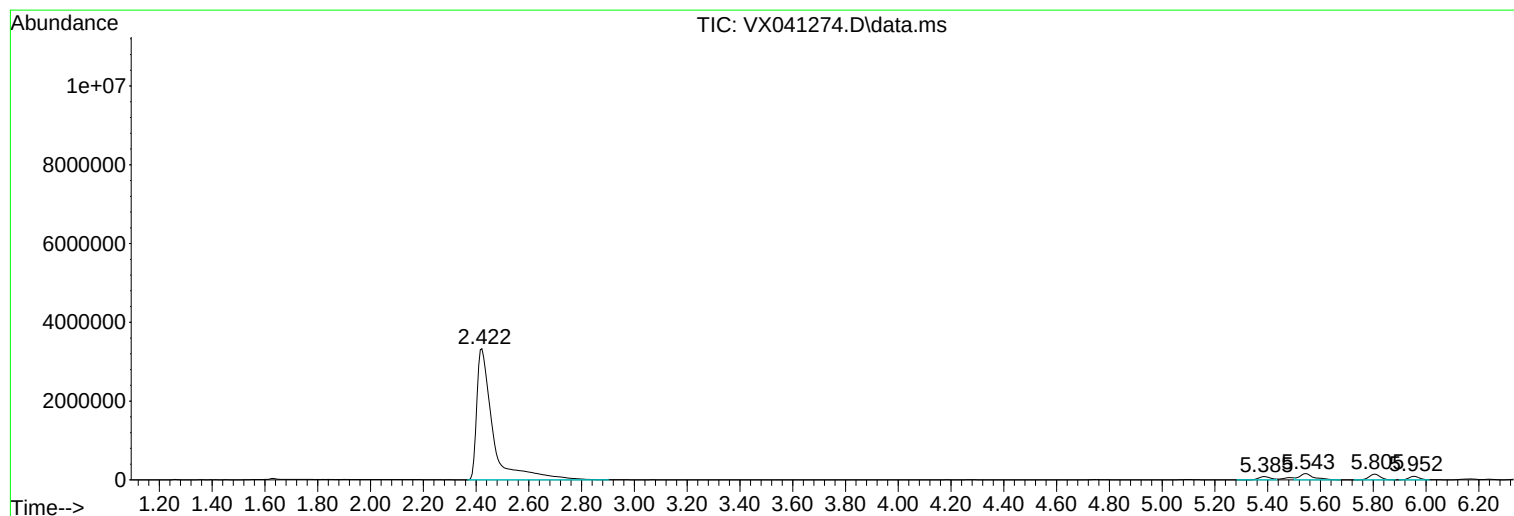
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
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Sample : P2183-01
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1229

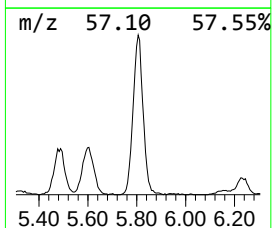
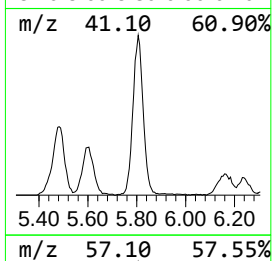
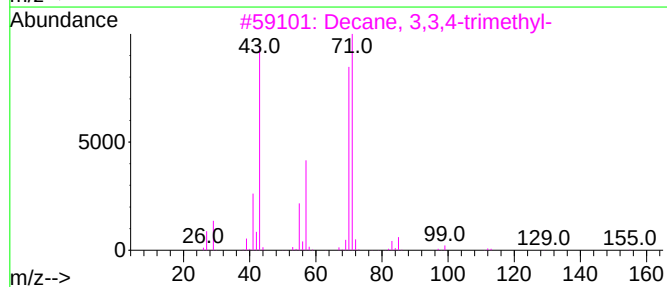
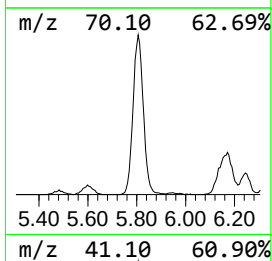
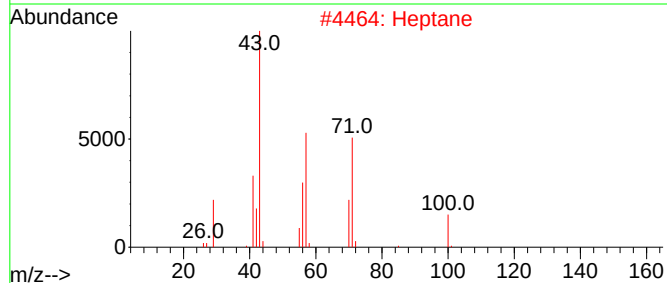
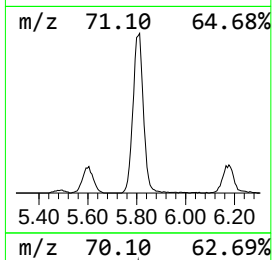
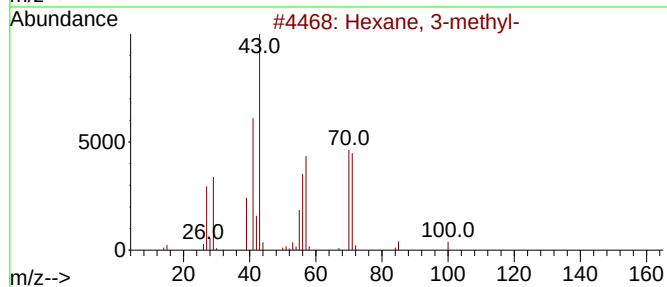
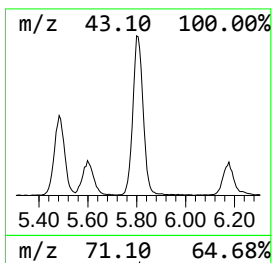
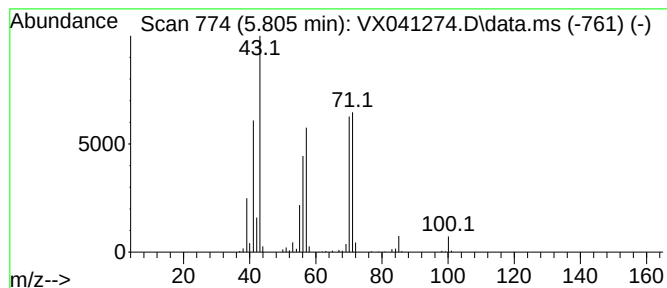
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.805	36.27 ug/l	423267	Pentafluorobenzene	5.543

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	80
3			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	50
5			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50



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Sample : P2183-01
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1229

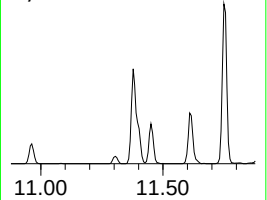
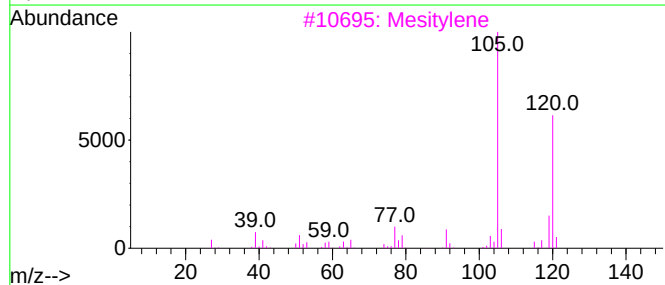
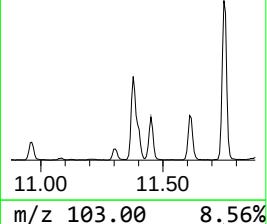
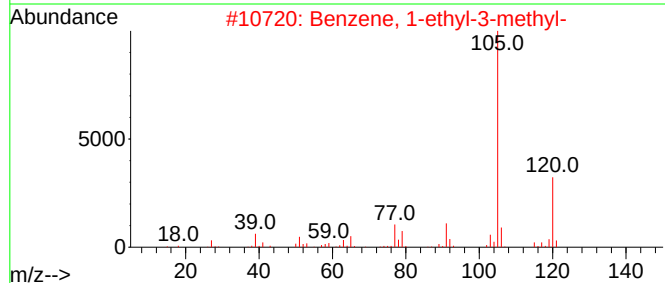
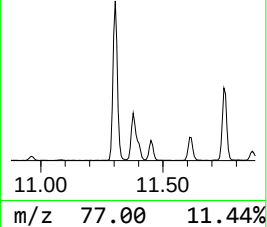
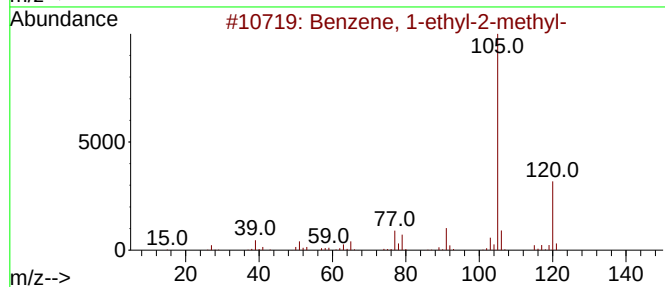
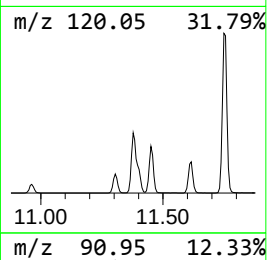
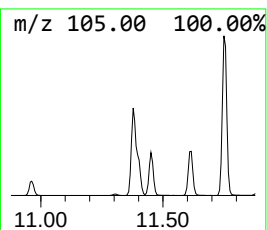
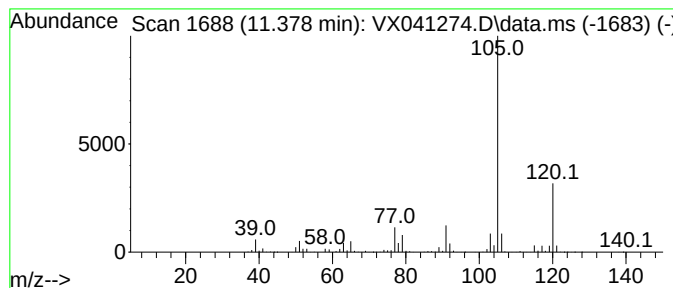
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	60.00 ug/l	874376	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	95
3			Mesitylene	120	C9H12	000108-67-8	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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Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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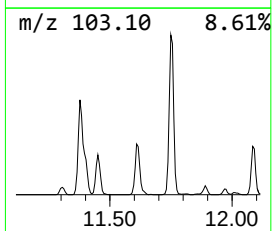
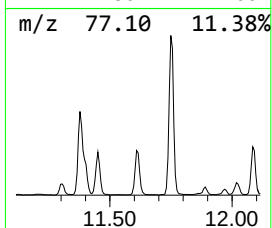
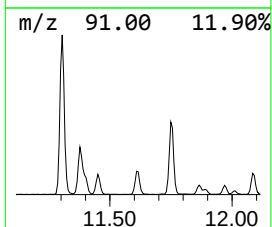
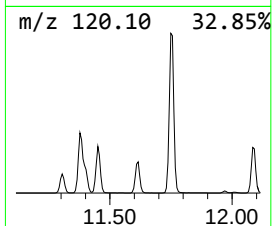
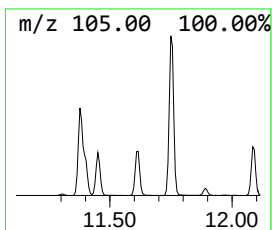
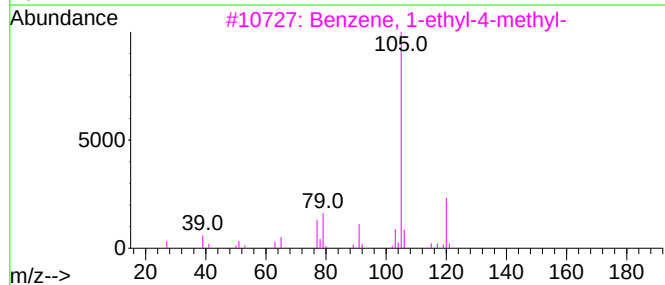
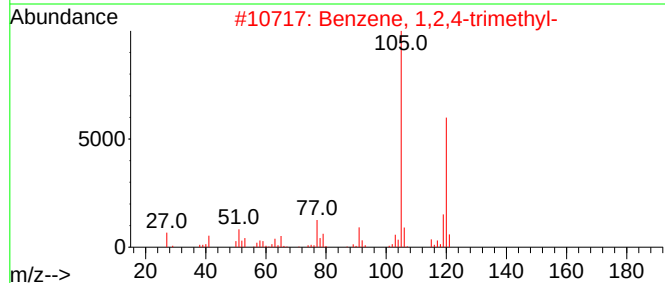
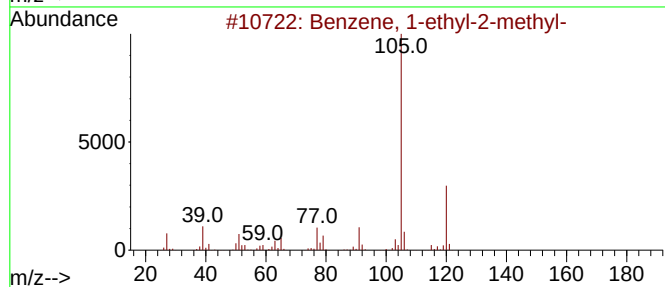
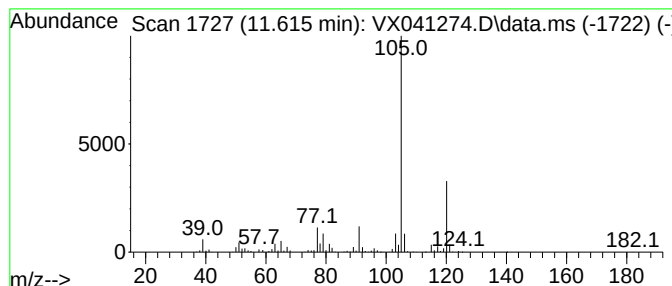
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	26.88 ug/l	391650	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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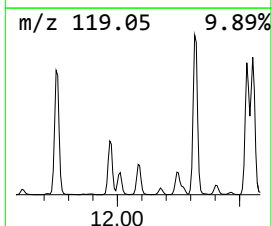
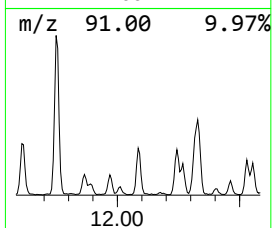
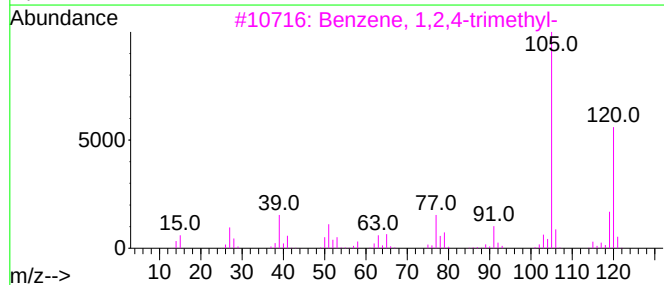
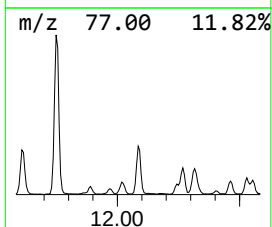
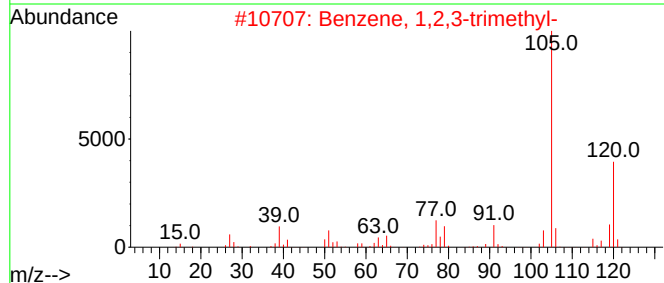
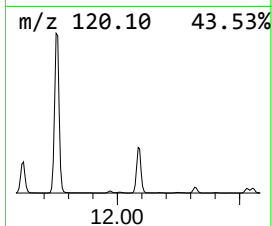
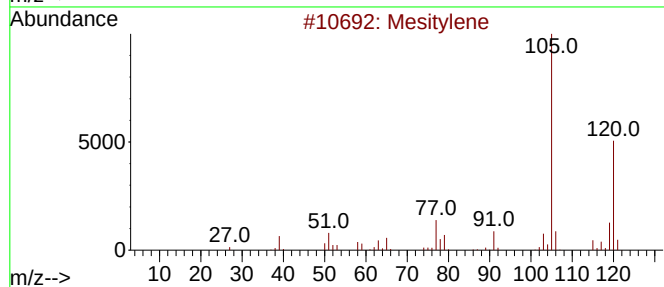
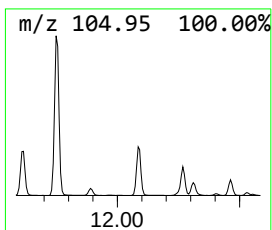
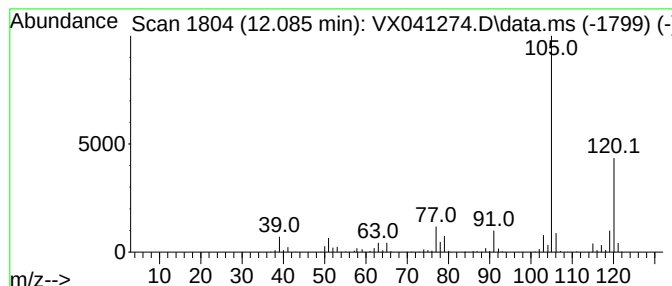
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	26.27 ug/l	382814	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	93
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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Instrument :
MSVOA_X
ClientSampleId :
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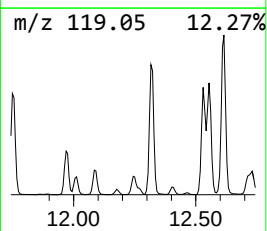
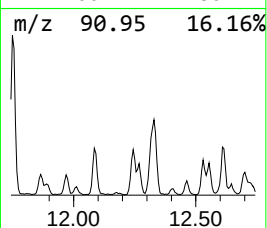
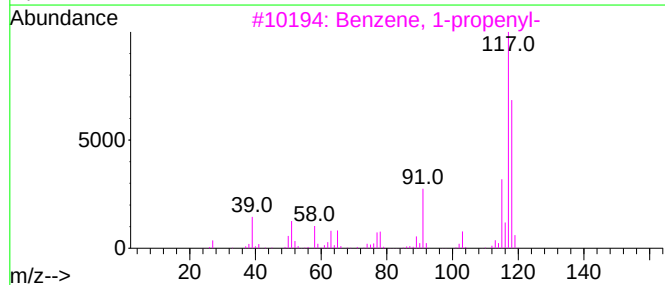
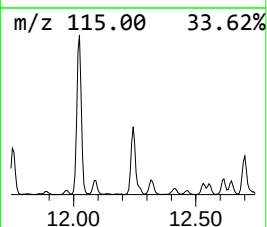
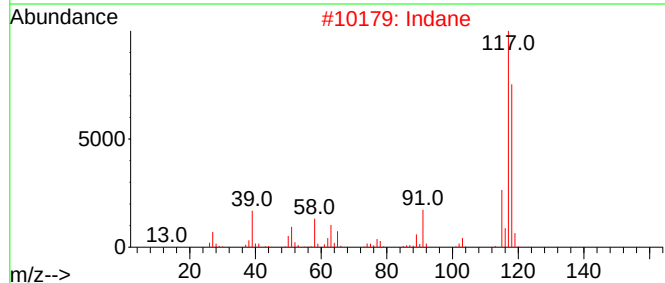
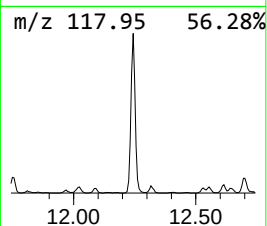
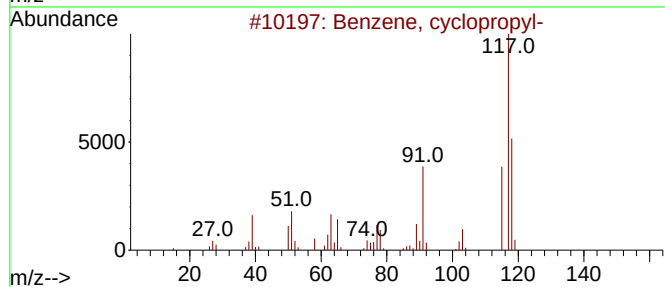
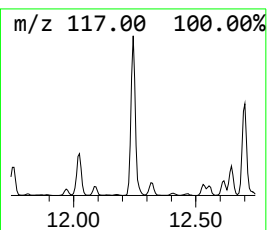
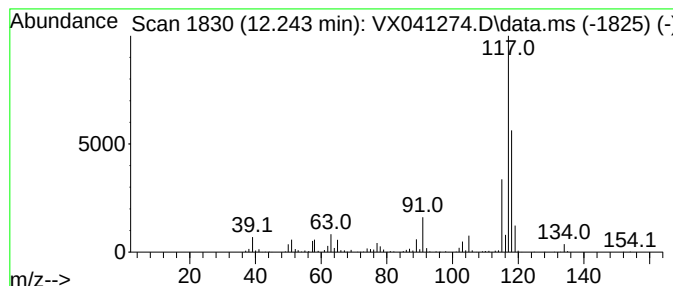
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	20.06 ug/l	292381	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041274.D
Acq On : 29 Apr 2024 14:16
Operator : JC/MD
Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1229

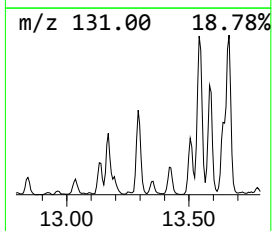
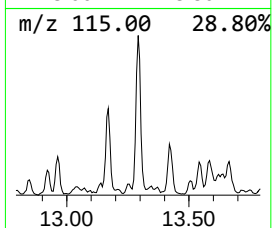
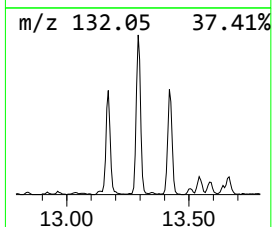
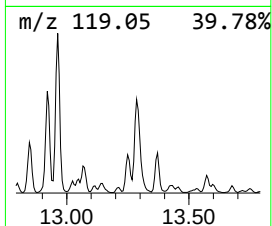
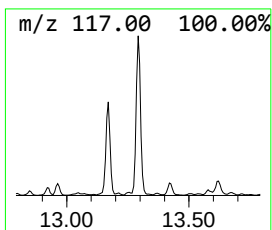
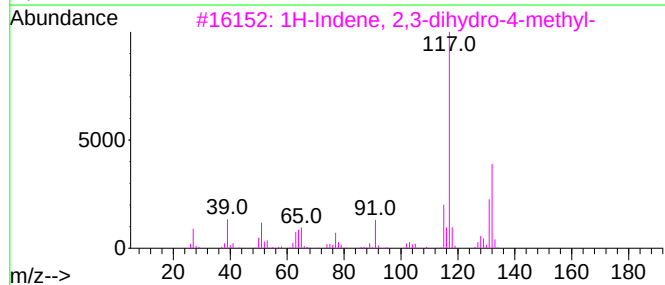
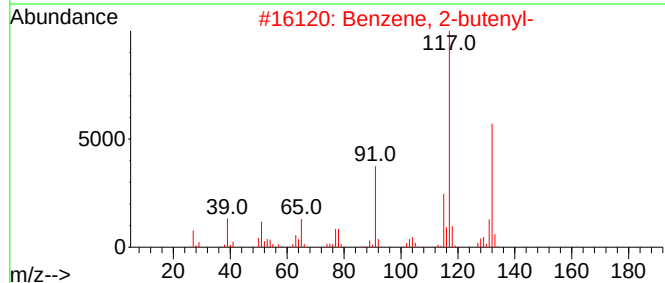
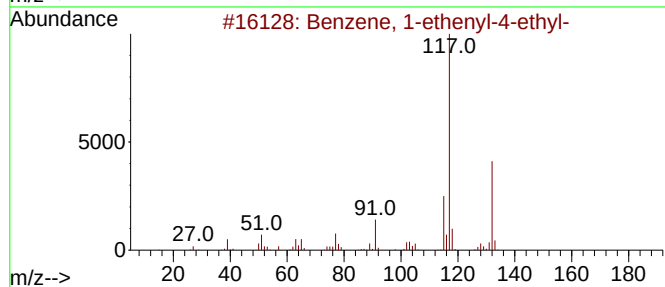
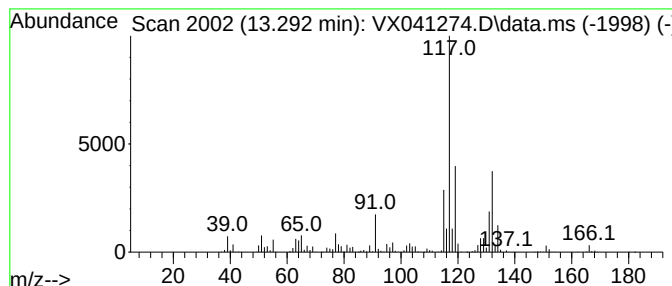
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	31.10 ug/l	453190	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
5			Indan, 1-methyl-	132	C10H12	000767-58-8	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041274.D
Acq On : 29 Apr 2024 14:16
Operator : JC/MD
Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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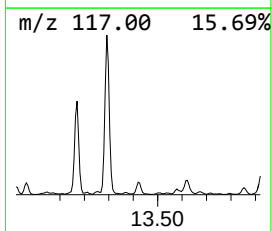
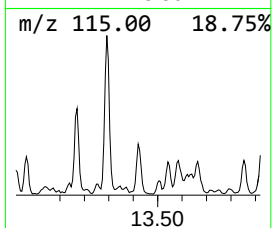
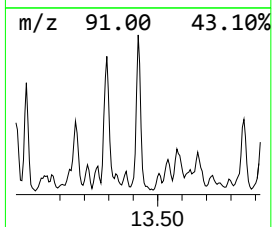
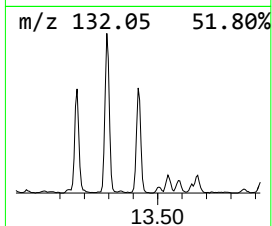
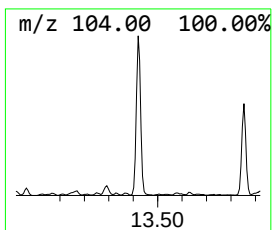
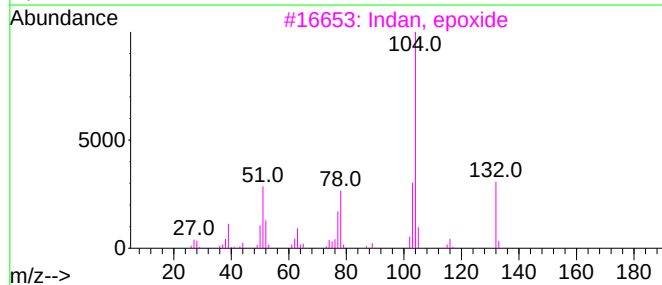
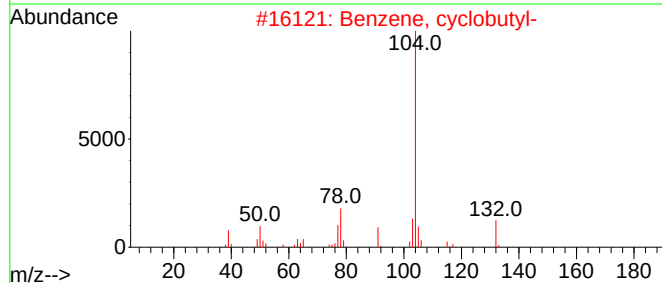
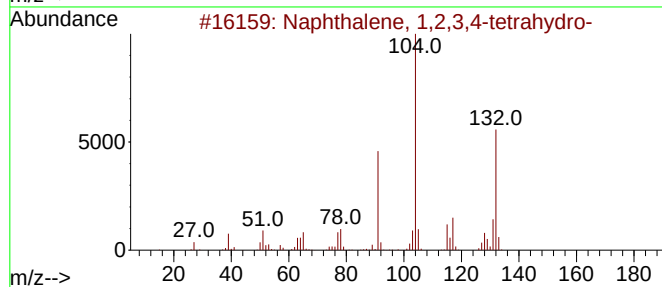
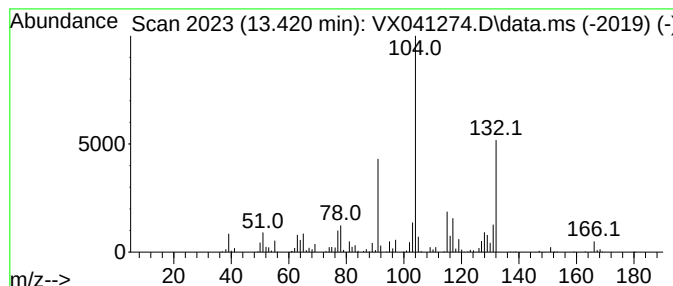
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	21.55 ug/l	314086	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	96
2			Benzene, cyclobutyl-	132	C10H12	004392-30-7	53
3			Indan, epoxide	132	C9H8O	000768-22-9	52
4			Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	50
5			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041274.D
Acq On : 29 Apr 2024 14:16
Operator : JC/MD
Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1229

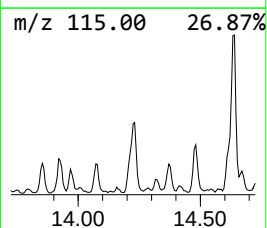
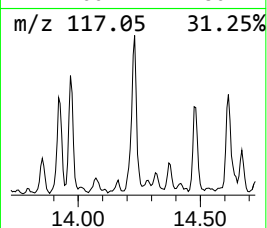
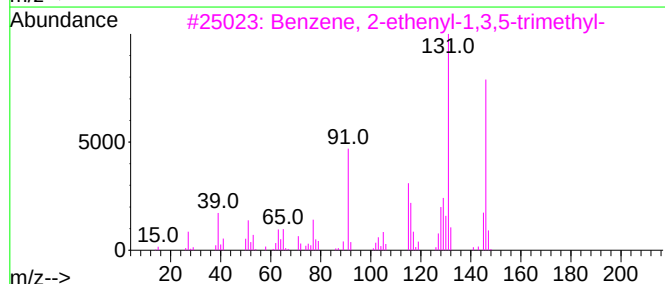
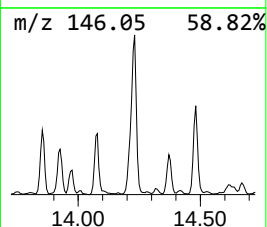
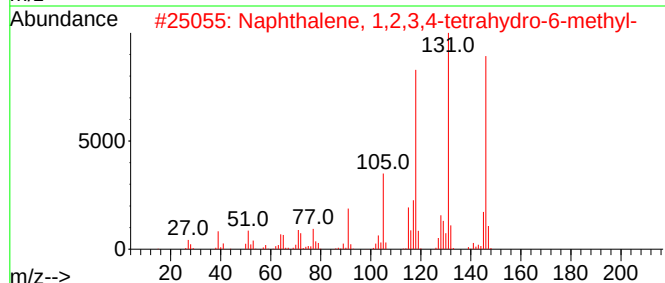
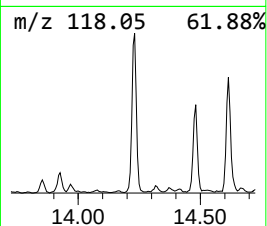
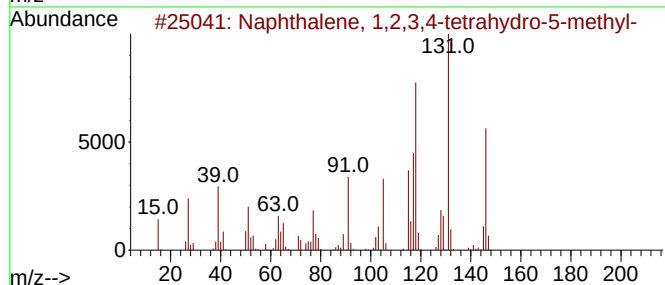
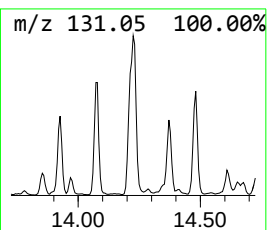
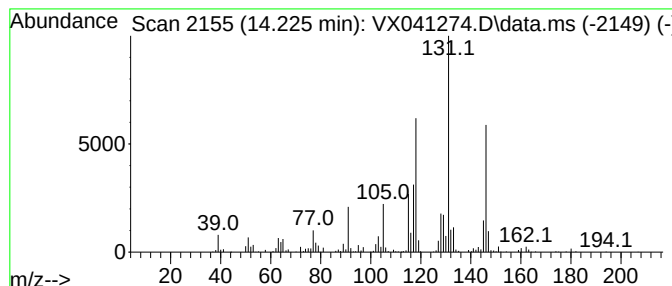
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	25.70 ug/l	374469	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	86
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	86
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041274.D
Acq On : 29 Apr 2024 14:16
Operator : JC/MD
Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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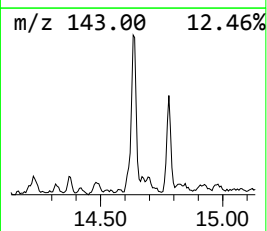
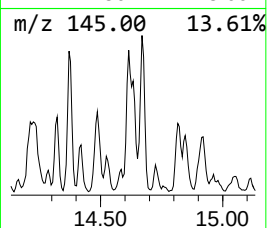
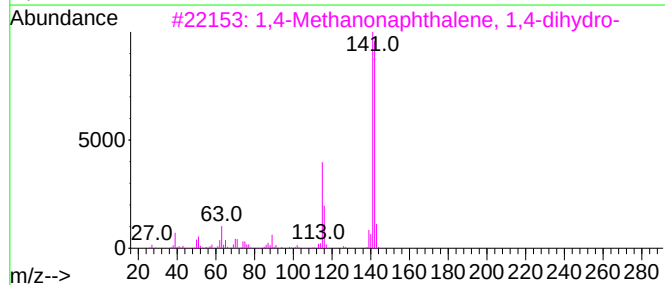
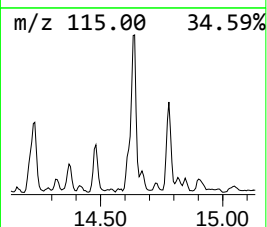
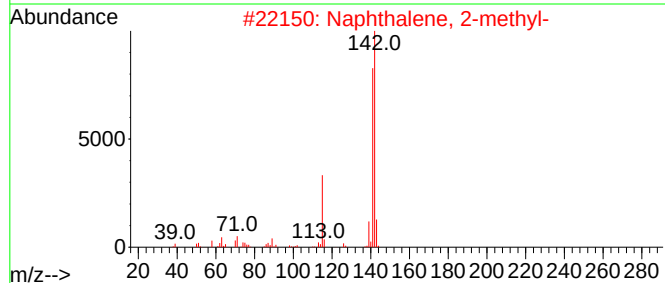
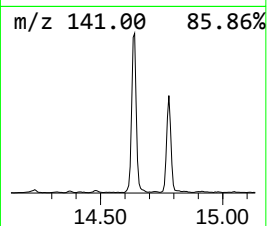
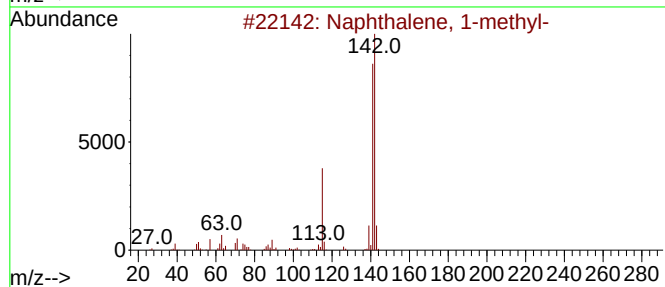
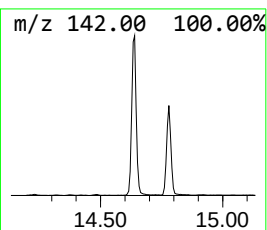
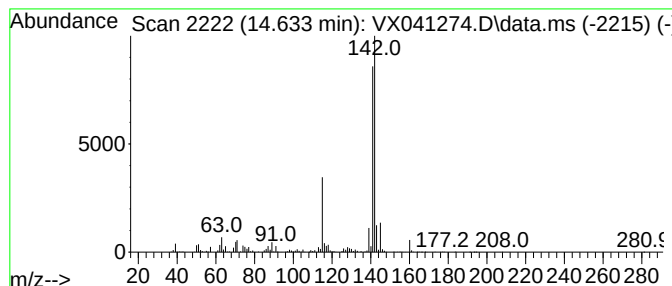
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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.
14.633	34.62 ug/l	504496	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	90
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041274.D
Acq On : 29 Apr 2024 14:16
Operator : JC/MD
Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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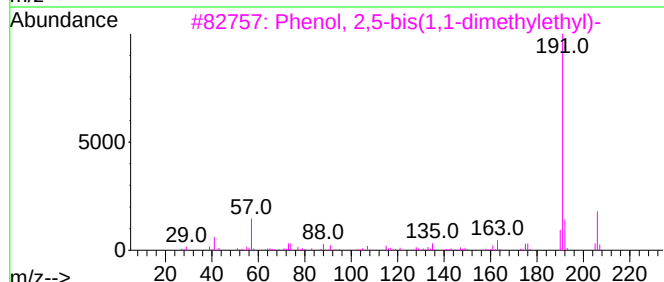
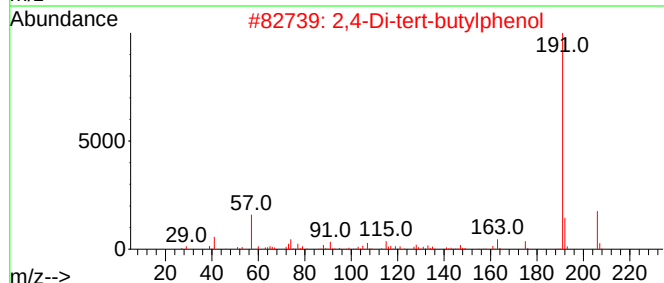
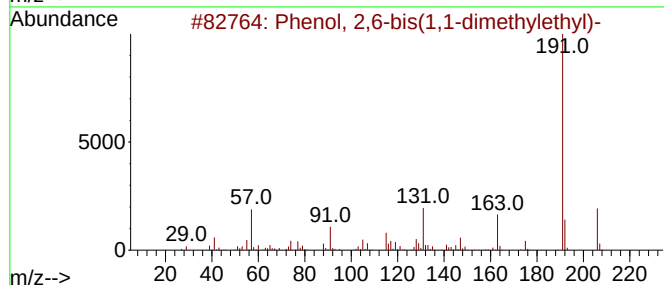
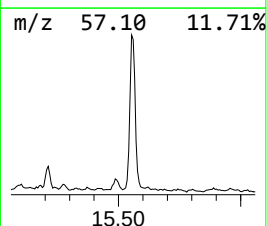
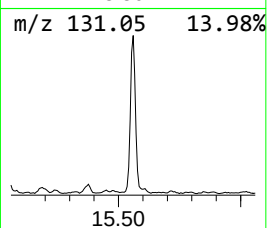
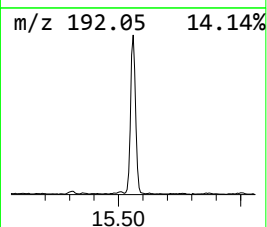
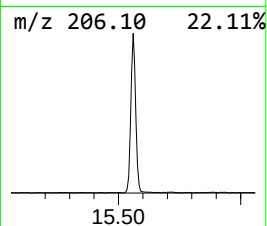
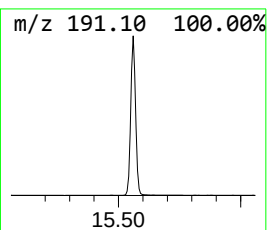
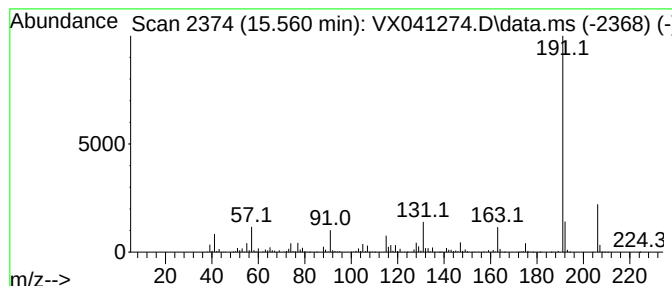
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Quant Title : SW846 8260

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

Peak Number 10 Phenol, 2,6-bis(1,1-dimethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	76.30 ug/l	1111780	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
3			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
4			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	72
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041274.D
Acq On : 29 Apr 2024 14:16
Operator : JC/MD
Sample : P2183-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.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-ethy...	11.378	60.0	ug/l	874376	4	12.024	728603	50.0
Benzene, 1-ethy...	11.615	26.9	ug/l	391650	4	12.024	728603	50.0
Benzene, 1-ethy...	12.085	26.3	ug/l	382814	4	12.024	728603	50.0
Benzene, cyclop...	12.243	20.1	ug/l	292381	4	12.024	728603	50.0
Benzene, 1-ethe...	13.292	31.1	ug/l	453190	4	12.024	728603	50.0
Naphthalene, 1,...	13.420	21.6	ug/l	314086	4	12.024	728603	50.0
Naphthalene, 1,...	14.225	25.7	ug/l	374469	4	12.024	728603	50.0
Naphthalene, 1-...	14.633	34.6	ug/l	504496	4	12.024	728603	50.0
Phenol, 2,6-bis...	15.560	76.3	ug/l	1111780	4	12.024	728603	50.0