

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040924\
 Data File : VX040946.D
 Acq On : 09 Apr 2024 11:15
 Operator : JC/MD
 Sample : P1995-05
 Misc : 1.97g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MOO-23-00113

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\82X040124W.M
 Title : SW846 8260

Signal : TIC: VX040946.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.410	210	217	250	rBV	283983	858965	3.77%	1.504%
2	8.647	1235	1240	1245	rBV	145736	232050	1.02%	0.406%
3	8.726	1245	1253	1265	rVB	8742389	13885398	60.87%	24.308%
4	10.195	1487	1494	1504	rBV	4713824	6392128	28.02%	11.190%
5	10.311	1505	1513	1518	rVV	14387083	22810470	100.00%	39.932%
6	10.646	1561	1568	1577	rBV	4389787	5785843	25.36%	10.129%
7	11.085	1634	1640	1650	rVB2	202939	374349	1.64%	0.655%
8	11.378	1684	1688	1694	rBV	134764	237245	1.04%	0.415%
9	11.476	1698	1704	1710	rVB2	329742	467659	2.05%	0.819%
10	11.750	1746	1749	1759	rVB	231468	345754	1.52%	0.605%
11	12.024	1789	1794	1799	rBV2	219172	321673	1.41%	0.563%
12	12.317	1837	1842	1848	rVB3	176392	337161	1.48%	0.590%
13	12.421	1848	1859	1863	rVV	278175	392888	1.72%	0.688%
14	13.292	1999	2002	2007	rVB3	225638	289254	1.27%	0.506%
15	13.420	2019	2023	2032	rVB2	188952	335524	1.47%	0.587%
16	13.853	2088	2094	2099	rVB4	131989	253098	1.11%	0.443%
17	13.926	2099	2106	2111	rBV4	123892	268994	1.18%	0.471%
18	14.225	2149	2155	2162	rVB2	302148	502643	2.20%	0.880%
19	14.481	2192	2197	2205	rBV4	203923	368236	1.61%	0.645%
20	14.615	2215	2219	2225	rBV2	336107	558669	2.45%	0.978%
21	14.670	2225	2228	2233	rVB2	162041	229548	1.01%	0.402%
22	15.182	2307	2312	2315	rBV	211754	325895	1.43%	0.571%
23	15.560	2368	2374	2379	rBV	1106662	1550390	6.80%	2.714%

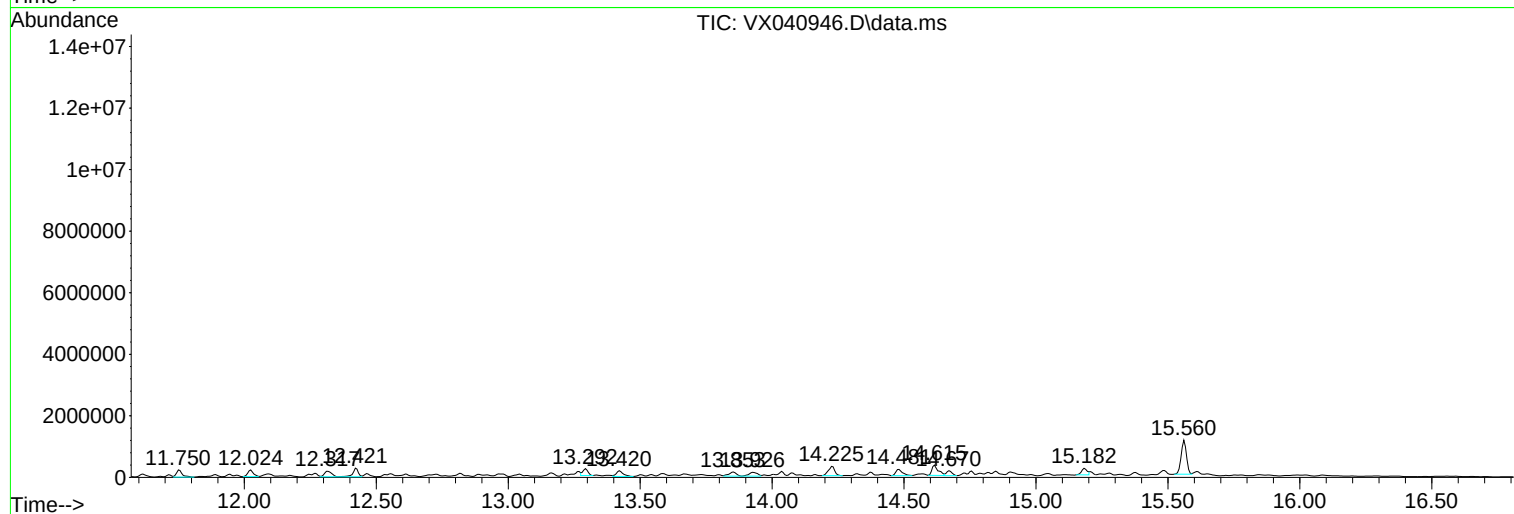
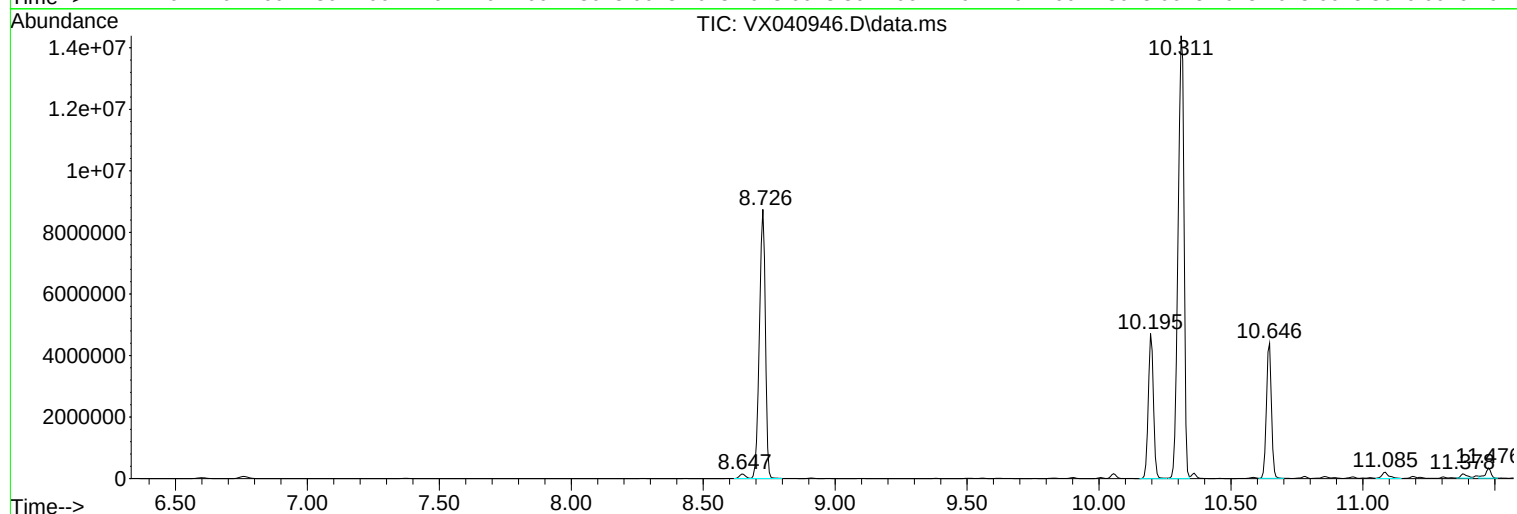
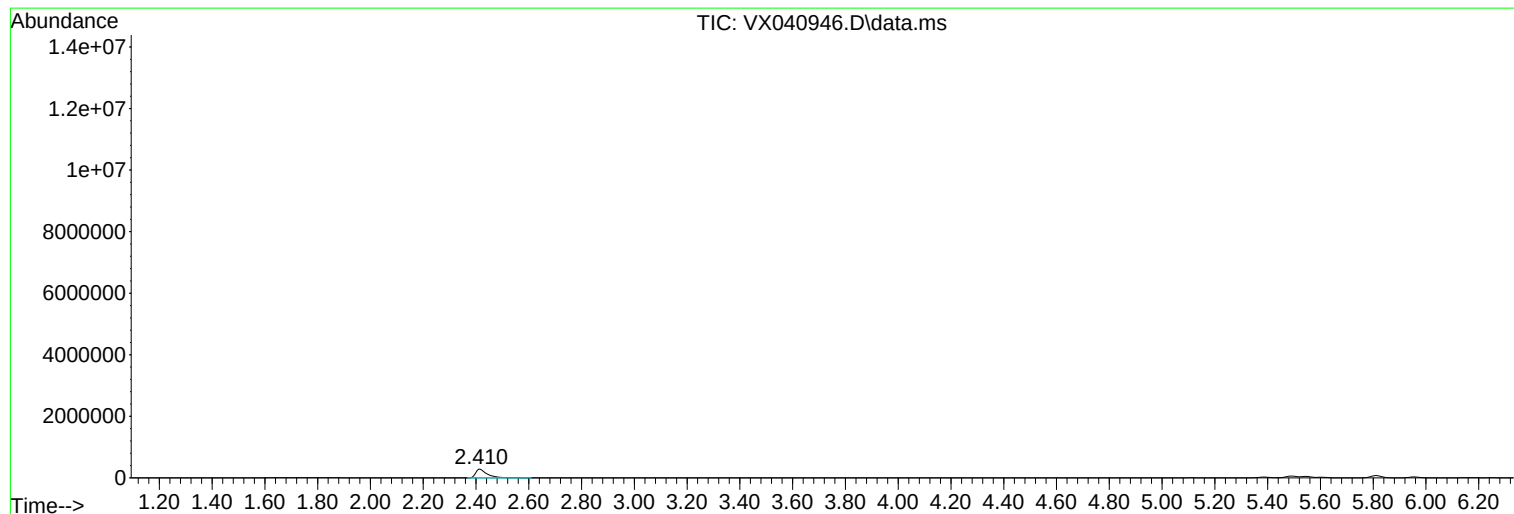
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Instrument :
MSVOA_X
ClientSampleId :
MOO-23-00113

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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



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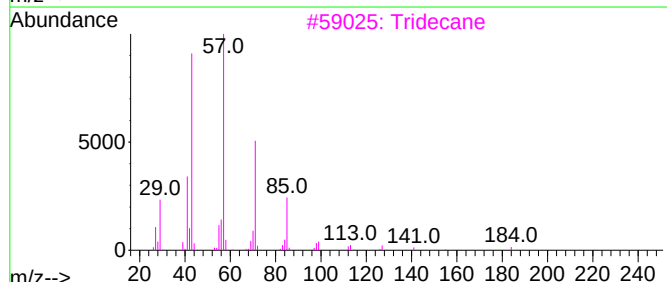
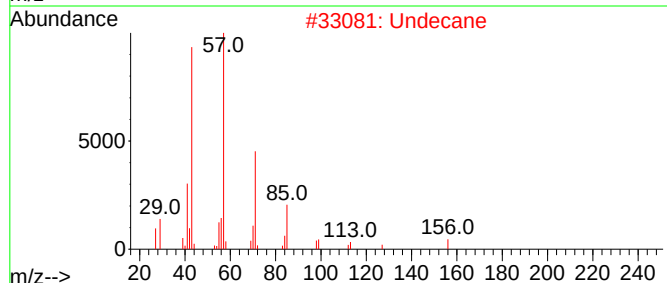
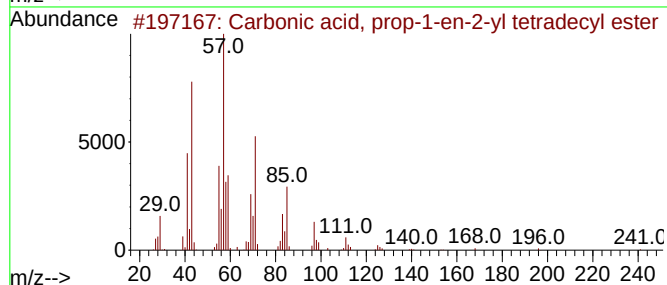
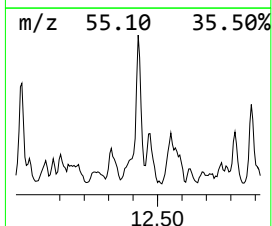
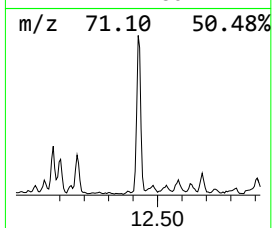
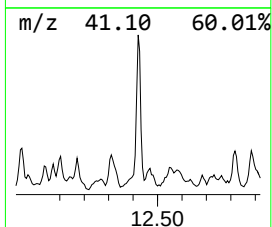
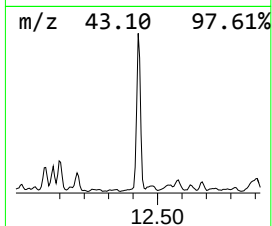
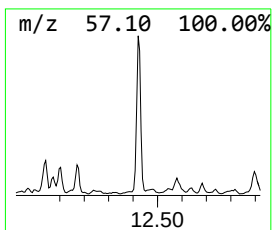
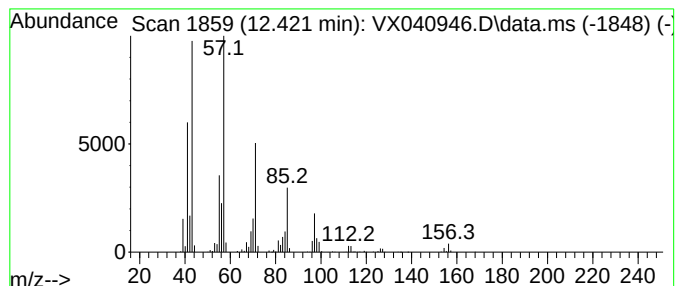
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 1 Carbonic acid, prop-1-en-2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	61.07 ug/l	392888	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
2			Undecane	156	C11H24	001120-21-4	76
3			Tridecane	184	C13H28	000629-50-5	72
4			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	64
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	64



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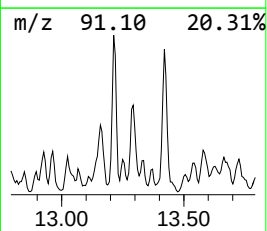
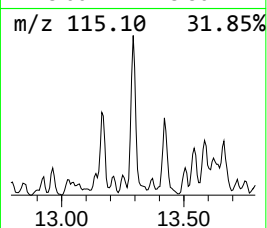
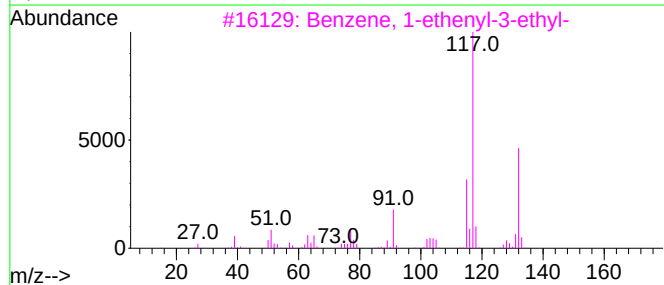
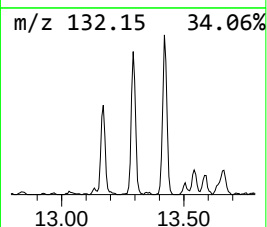
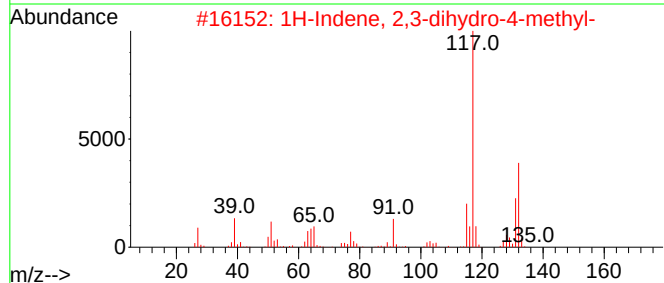
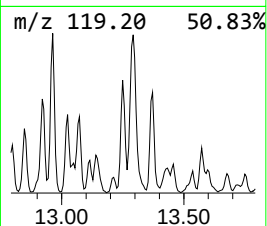
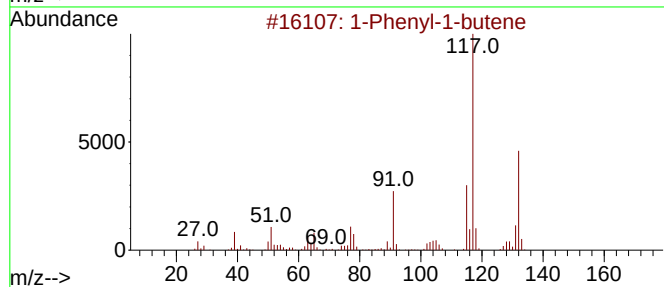
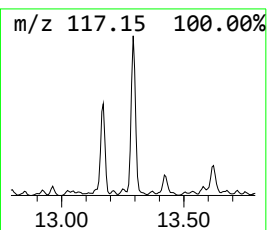
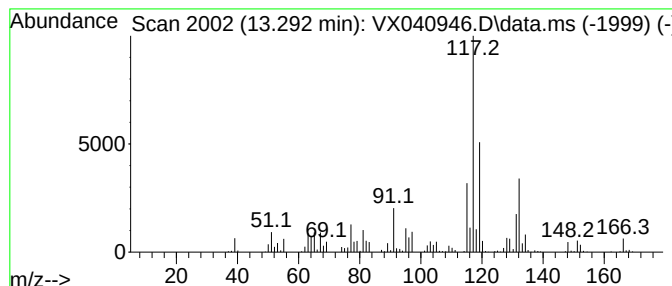
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Quant Title : SW846 8260

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

Peak Number 2 1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	44.96 ug/l	289254	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	96
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90



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ALS Vial : 7 Sample Multiplier: 1

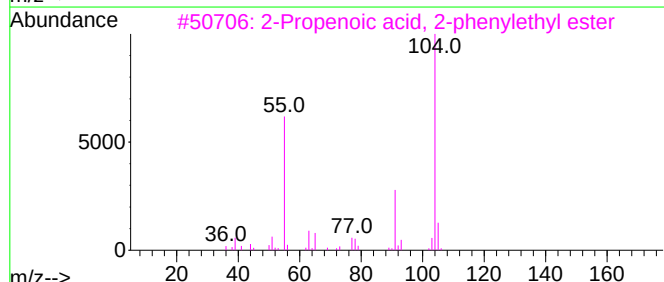
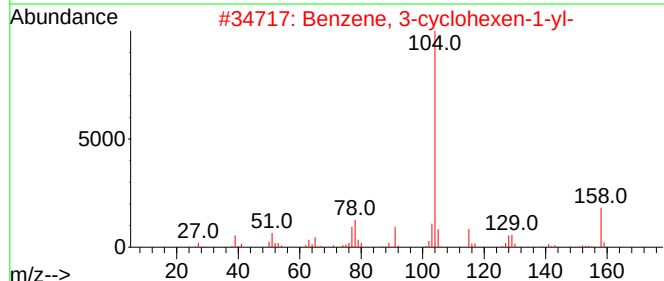
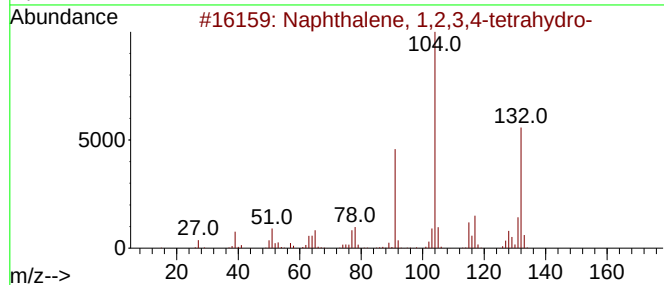
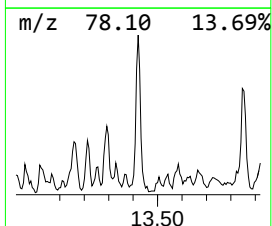
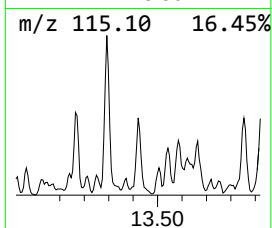
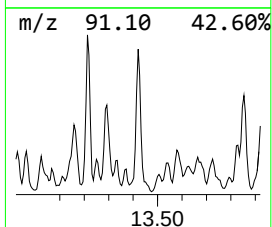
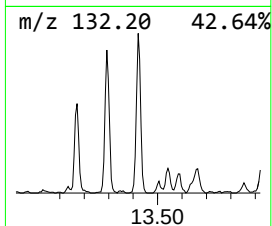
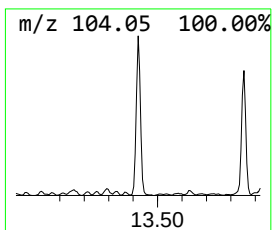
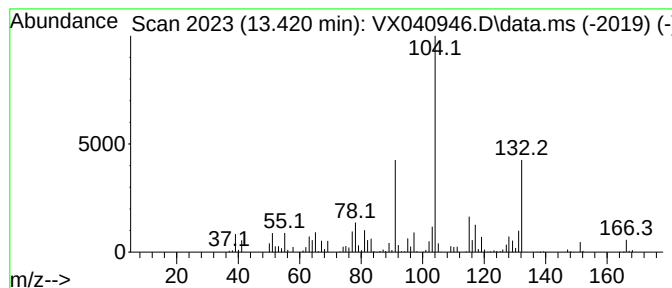
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.420	52.15 ug/l	335524	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	91
2	Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	43
3	2-Propenoic acid, 2-phenylethyl ...	176	C11H12O2	003530-36-7	38
4	Benzenepropanoic acid, methyl ester	164	C10H12O2	000103-25-3	38
5	3(2H)-Furanone, dihydro-2,2-dime...	190	C12H14O2	063678-00-2	38



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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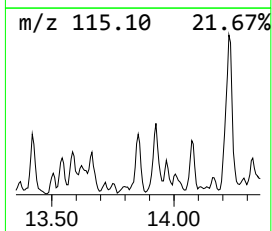
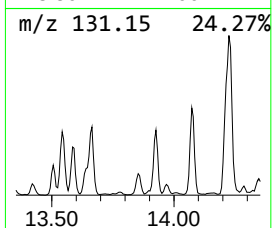
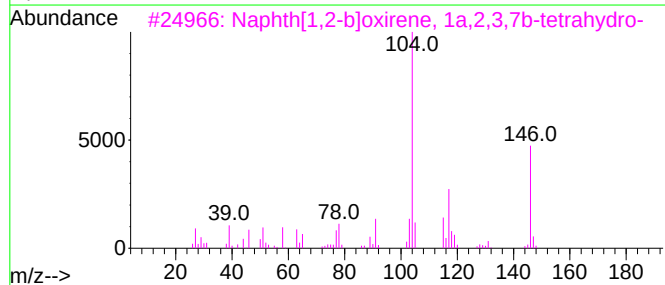
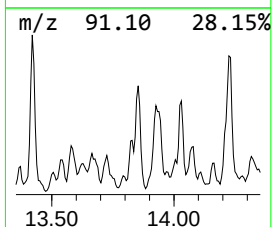
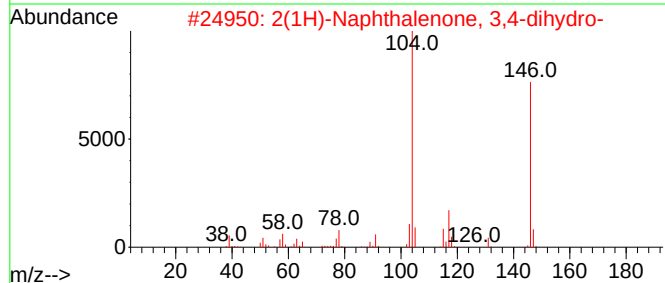
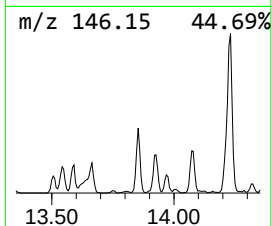
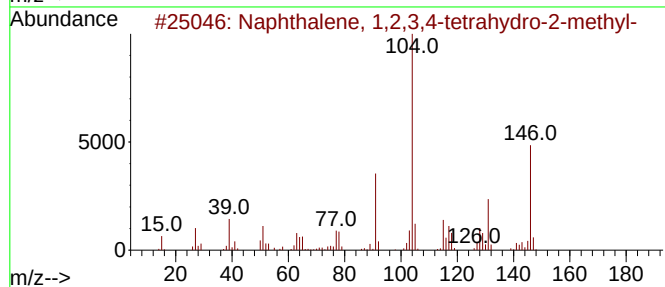
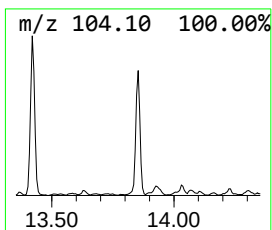
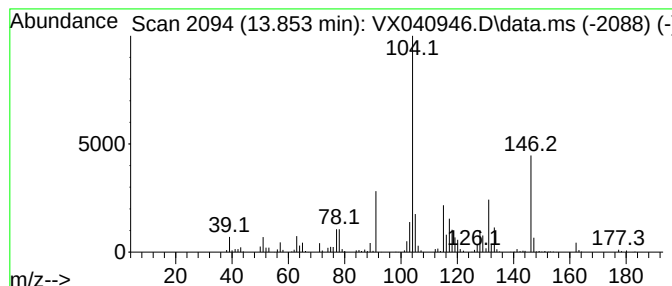
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Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.853	39.34 ug/l	253098	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	81
2			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	58
3			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
4			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	47
5			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38



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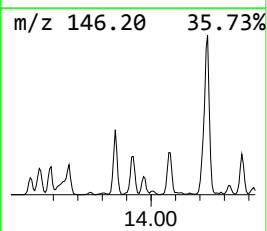
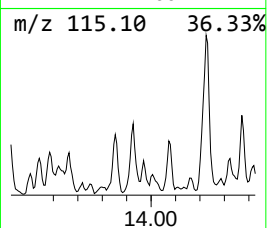
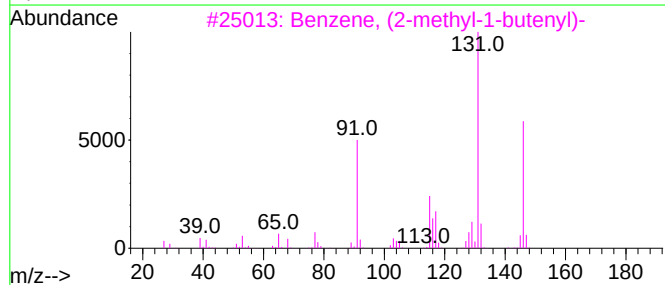
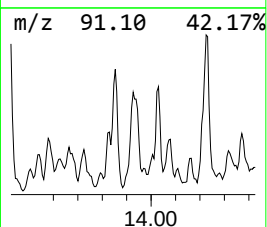
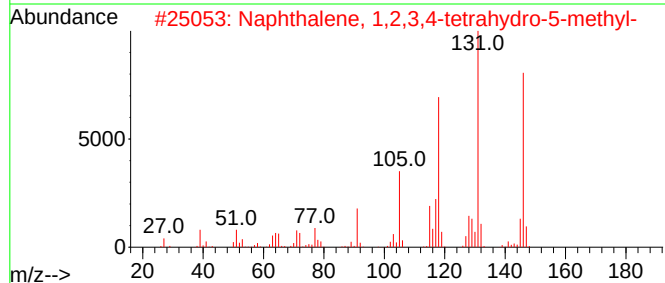
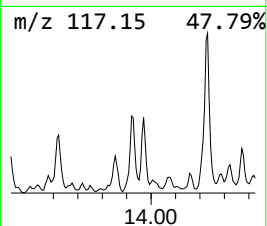
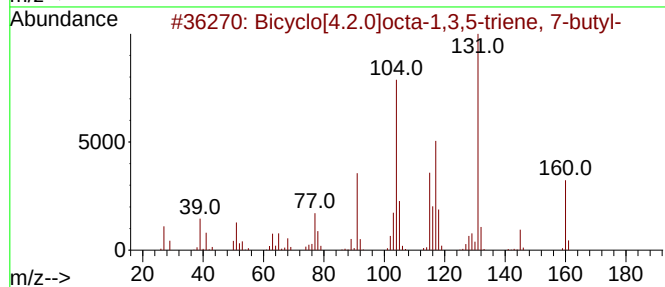
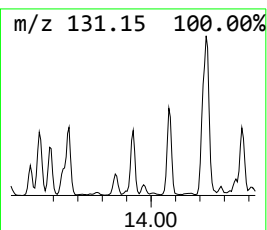
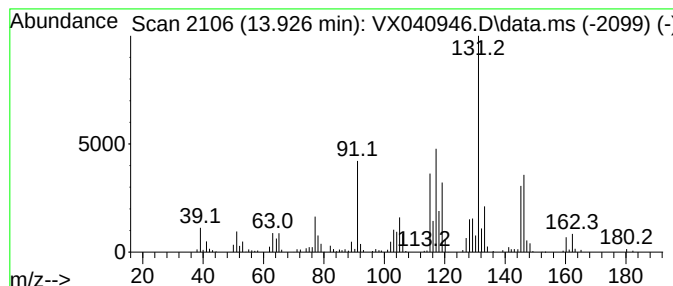
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 5 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	41.81 ug/l	268994	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.2.0]octa-1,3,5-triene,...	160	C12H16	078920-29-3	64
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	64
3			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	60
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	60
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	60



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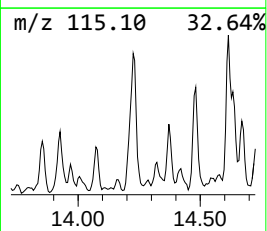
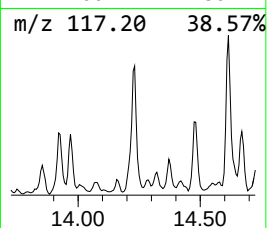
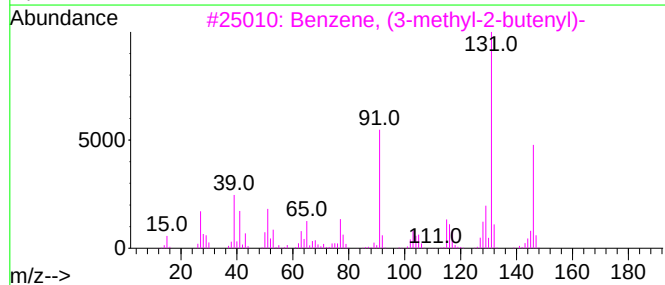
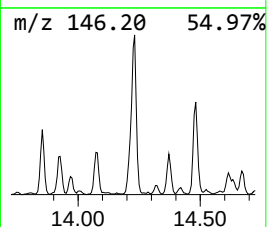
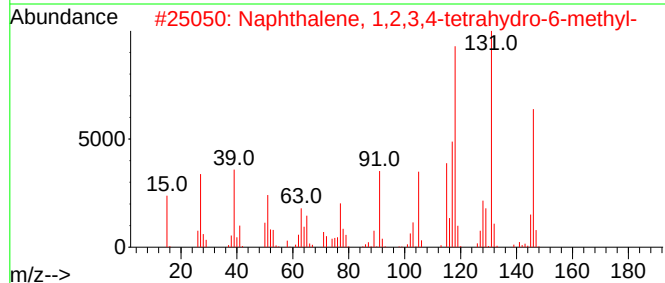
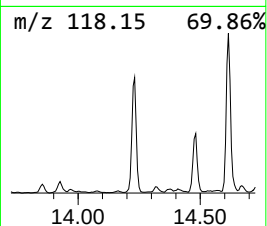
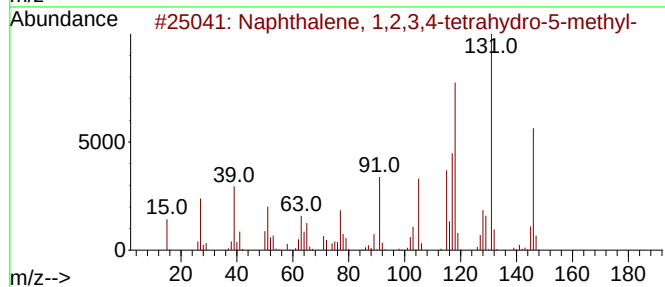
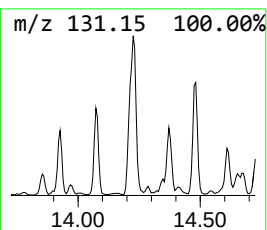
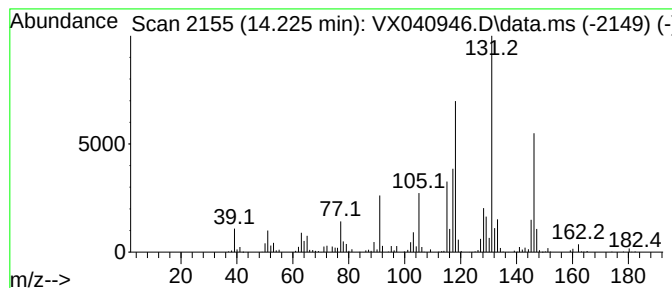
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	78.13 ug/l	502643	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	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040924\
Data File : VX040946.D
Acq On : 09 Apr 2024 11:15
Operator : JC/MD
Sample : P1995-05
Misc : 1.97g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-23-00113

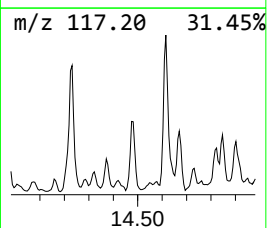
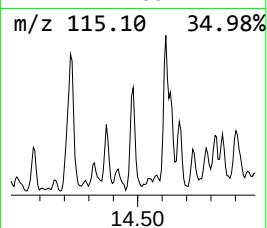
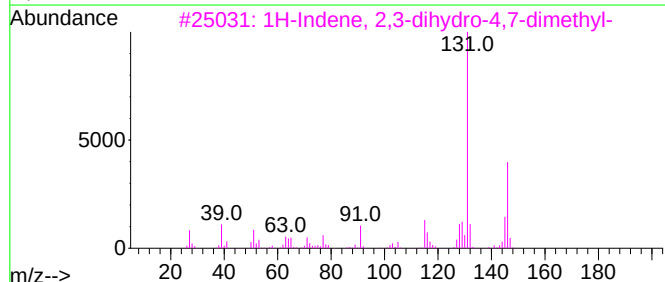
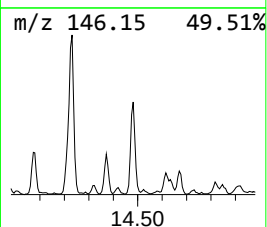
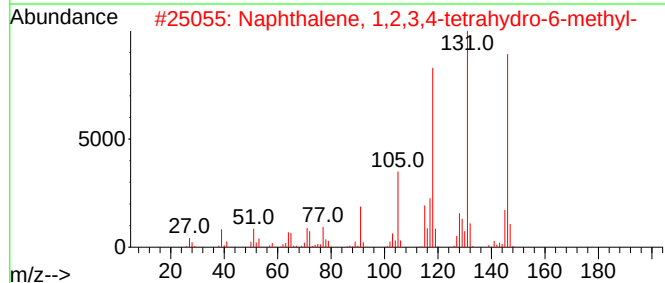
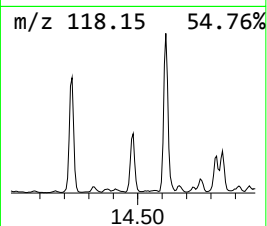
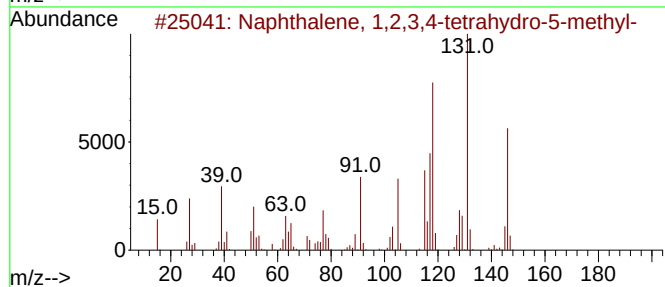
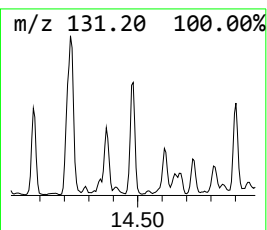
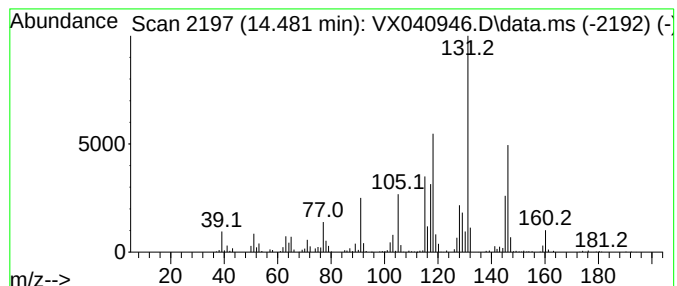
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Quant Title : SW846 8260

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.
14.481	57.24 ug/l	368236	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	90
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	81
3			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	64
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040924\
Data File : VX040946.D
Acq On : 09 Apr 2024 11:15
Operator : JC/MD
Sample : P1995-05
Misc : 1.97g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-23-00113

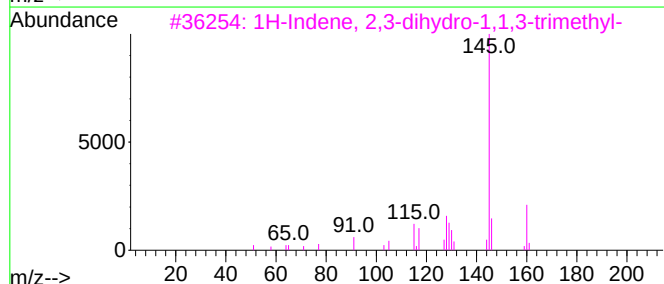
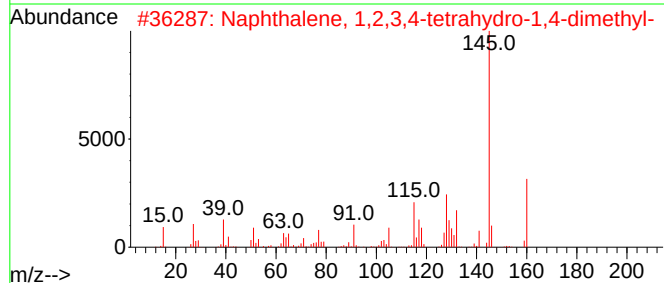
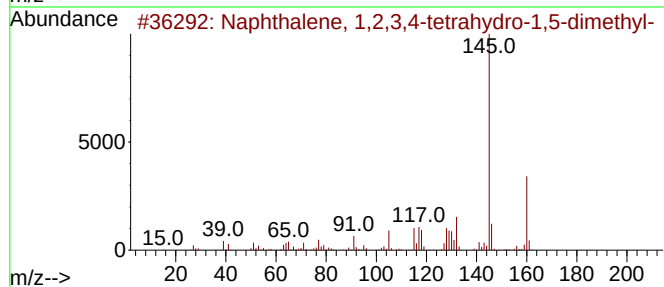
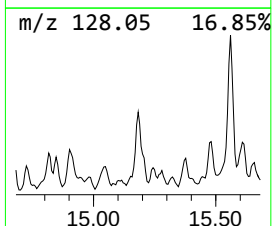
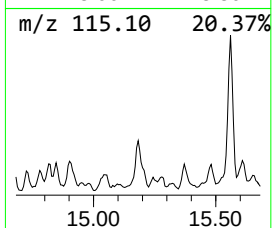
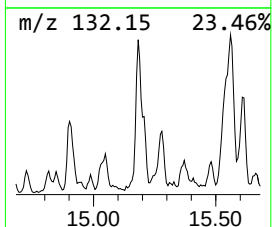
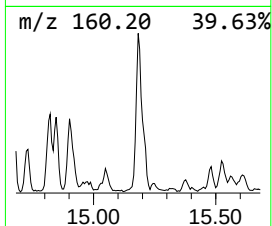
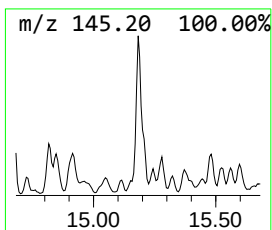
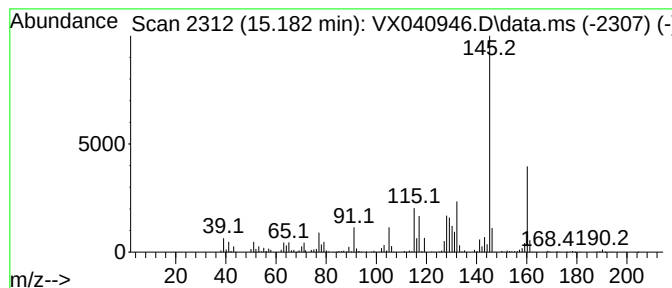
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	50.66 ug/l	325895	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
3			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	91
4			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	90
5			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	89



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040924\
Data File : VX040946.D
Acq On : 09 Apr 2024 11:15
Operator : JC/MD
Sample : P1995-05
Misc : 1.97g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-23-00113

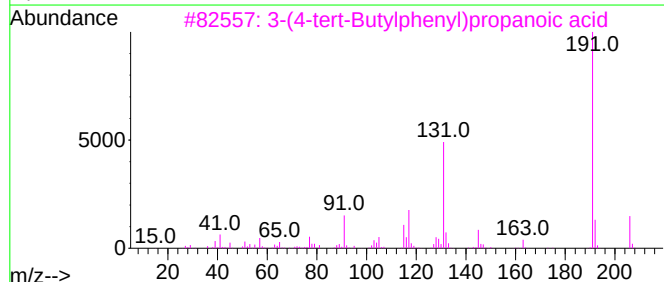
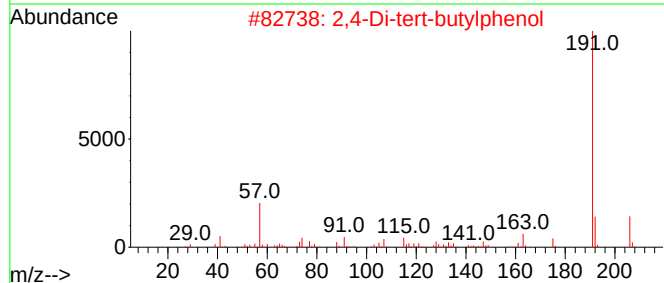
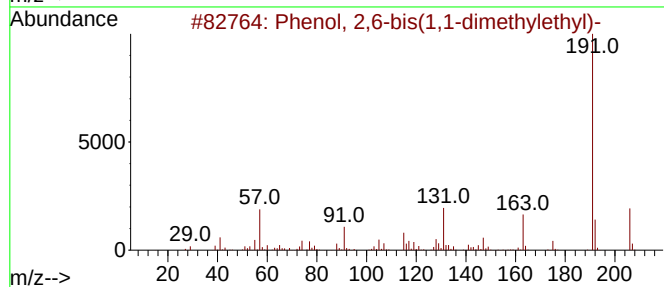
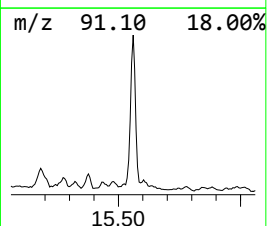
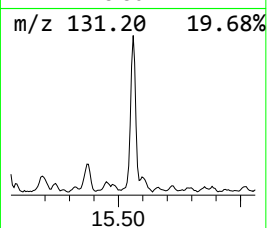
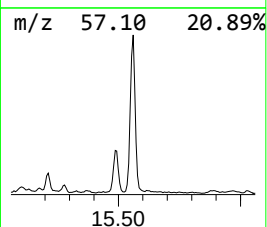
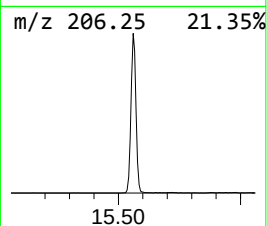
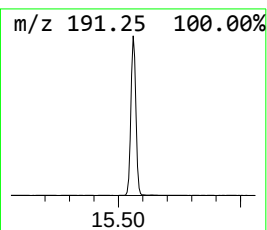
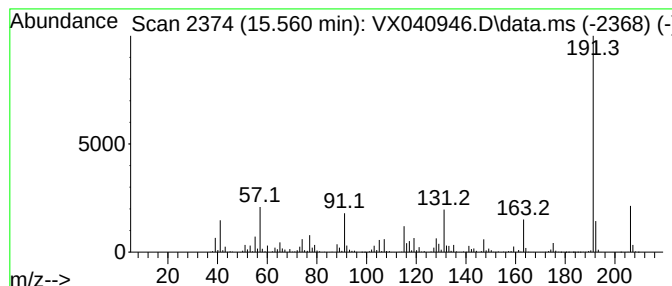
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	240.99 ug/l	1550390	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	98
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	90
3			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	83
4			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	81
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040924\
Data File : VX040946.D
Acq On : 09 Apr 2024 11:15
Operator : JC/MD
Sample : P1995-05
Misc : 1.97g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-23-00113

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Carbonic acid, ...	12.421	61.1	ug/l	392888	4	12.024	321673	50.0
1-Phenyl-1-butene	13.292	45.0	ug/l	289254	4	12.024	321673	50.0
Naphthalene, 1,...	13.420	52.1	ug/l	335524	4	12.024	321673	50.0
Naphthalene, 1,...	13.853	39.3	ug/l	253098	4	12.024	321673	50.0
Bicyclo[4.2.0]o...	13.926	41.8	ug/l	268994	4	12.024	321673	50.0
Naphthalene, 1,...	14.225	78.1	ug/l	502643	4	12.024	321673	50.0
Naphthalene, 1,...	14.481	57.2	ug/l	368236	4	12.024	321673	50.0
Naphthalene, 1,...	15.182	50.7	ug/l	325895	4	12.024	321673	50.0
Phenol, 2,6-bis...	15.560	241.0	ug/l	1550390	4	12.024	321673	50.0