

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042224\
 Data File : VX041195.D
 Acq On : 22 Apr 2024 17:20
 Operator : JC/MD
 Sample : P2218-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B-131-GW-01

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: VX041195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	68	84	85	rBV8	7377	27600	3.26%	0.458%
2	5.385	693	705	721	rBV2	97131	288280	34.03%	4.781%
3	5.544	721	731	753	rVV	174622	504074	59.51%	8.360%
4	5.952	787	798	814	rBV	96884	264225	31.19%	4.382%
5	6.757	920	930	950	rBV	253712	621898	73.42%	10.314%
6	8.647	1234	1240	1263	rBV	519660	847061	100.00%	14.048%
7	10.055	1465	1471	1491	rBV	538418	740678	87.44%	12.284%
8	11.079	1634	1639	1651	rBV	449294	599538	70.78%	9.943%
9	11.969	1780	1785	1788	rBV2	10926	13416	1.58%	0.222%
10	12.024	1788	1794	1802	rVV	563452	733035	86.54%	12.157%
11	12.317	1838	1842	1851	rVB4	16644	28224	3.33%	0.468%
12	12.530	1872	1877	1879	rBV	19746	25610	3.02%	0.425%
13	12.555	1879	1881	1886	rVB	20396	21449	2.53%	0.356%
14	12.616	1886	1891	1895	rBV	38566	50050	5.91%	0.830%
15	12.713	1901	1907	1916	rBV5	11549	24057	2.84%	0.399%
16	12.847	1924	1929	1934	rVB	19528	24554	2.90%	0.407%
17	12.920	1934	1941	1944	rBV	46144	57298	6.76%	0.950%
18	12.963	1944	1948	1954	rVB	77523	94601	11.17%	1.569%
19	13.024	1954	1958	1959	rBV	8808	9436	1.11%	0.156%
20	13.170	1975	1982	1986	rBV2	27865	38930	4.60%	0.646%
21	13.256	1992	1996	1998	rBV2	13160	18974	2.24%	0.315%
22	13.292	1998	2002	2012	rVV2	78199	124708	14.72%	2.068%
23	13.371	2012	2015	2020	rVB	12955	15619	1.84%	0.259%
24	13.426	2020	2024	2030	rVB3	7241	10619	1.25%	0.176%
25	13.579	2045	2049	2057	rVV	25046	49812	5.88%	0.826%
26	13.676	2060	2065	2070	rVB2	13354	18574	2.19%	0.308%
27	13.774	2076	2081	2091	rVB	73954	101893	12.03%	1.690%
28	13.926	2100	2106	2110	rBV3	6926	11514	1.36%	0.191%
29	14.079	2126	2131	2137	rBV	9527	11857	1.40%	0.197%
30	14.213	2149	2153	2159	rBV2	9390	14623	1.73%	0.243%
31	14.323	2166	2171	2175	rBV	8700	11563	1.37%	0.192%
32	14.633	2218	2222	2233	rVB	84221	116287	13.73%	1.929%
33	14.780	2239	2246	2256	rBV	113633	149167	17.61%	2.474%
34	15.213	2313	2317	2320	rVB	7326	9835	1.16%	0.163%
35	15.377	2336	2344	2347	rBV3	5815	10861	1.28%	0.180%
36	15.475	2354	2360	2372	rBV	29054	54688	6.46%	0.907%

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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	15.615	2374	2383	2386	rVV	47041	74992	8.85%	1.244%
38	15.652	2386	2389	2396	rVB	23280	34209	4.04%	0.567%
39	15.810	2410	2415	2418	rBV3	8440	15566	1.84%	0.258%
40	15.841	2418	2420	2426	rVB	9389	12517	1.48%	0.208%
41	16.328	2493	2500	2511	rBV	71562	131735	15.55%	2.185%
42	16.694	2555	2560	2566	rVB	8104	16063	1.90%	0.266%

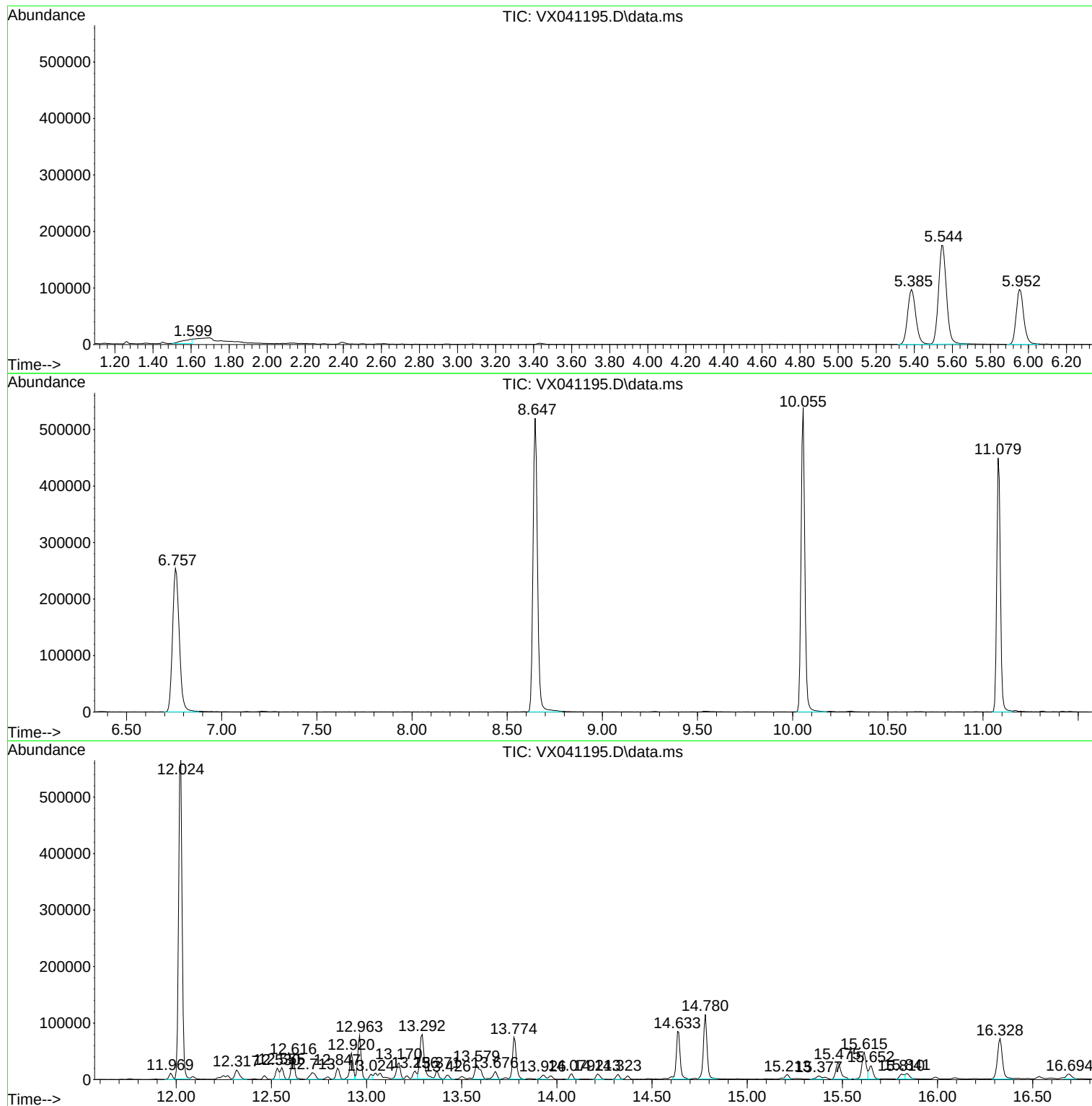
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



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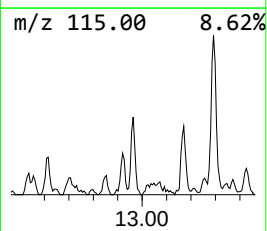
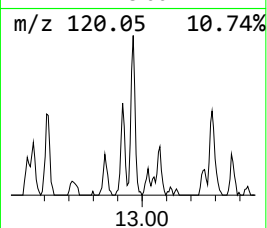
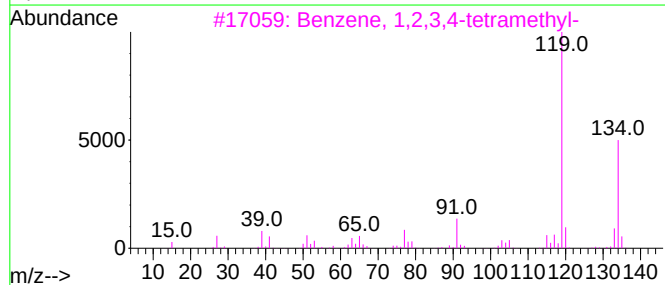
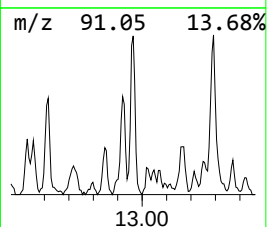
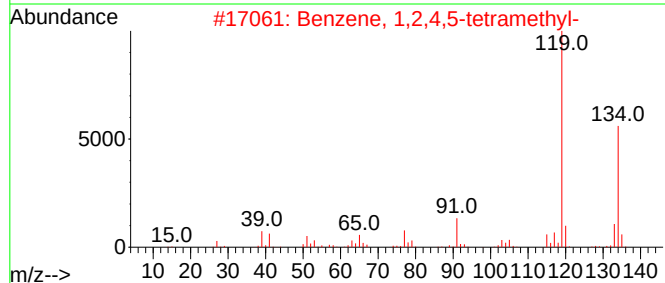
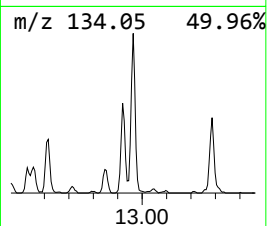
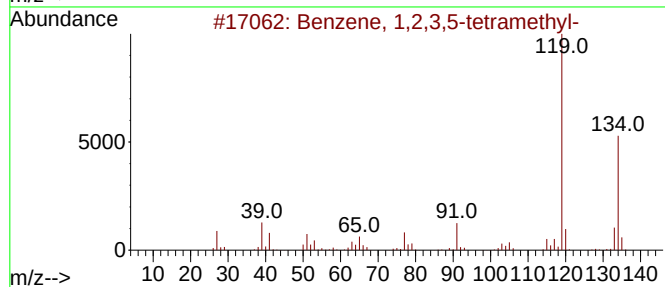
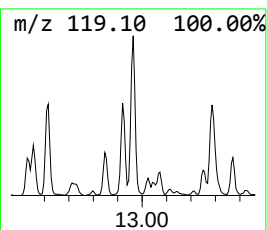
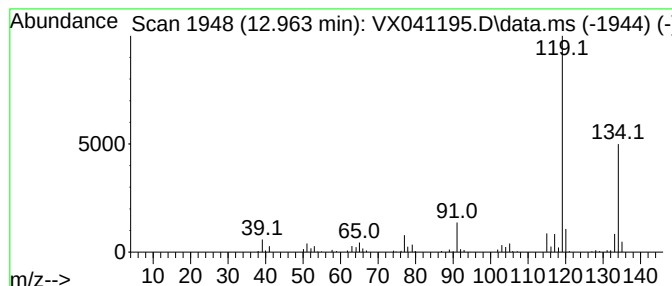
Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

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 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.963	6.45 ug/l	94601	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	o-Cymene	134	C10H14	000527-84-4	95



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Sample : P2218-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

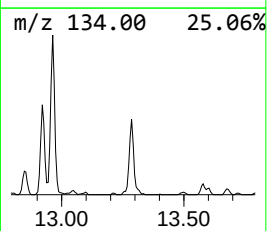
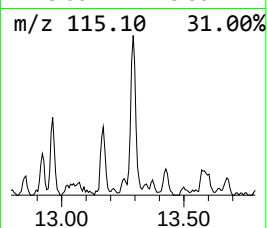
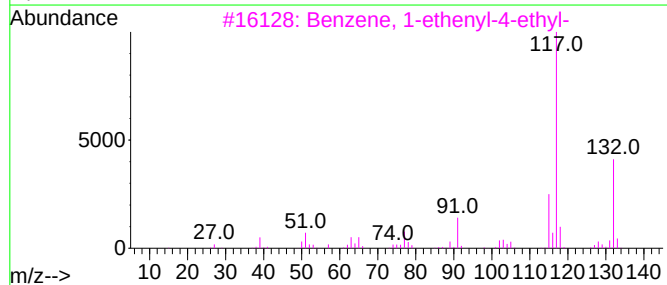
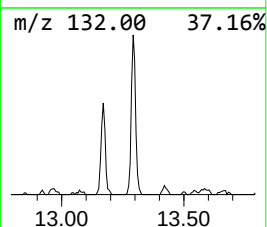
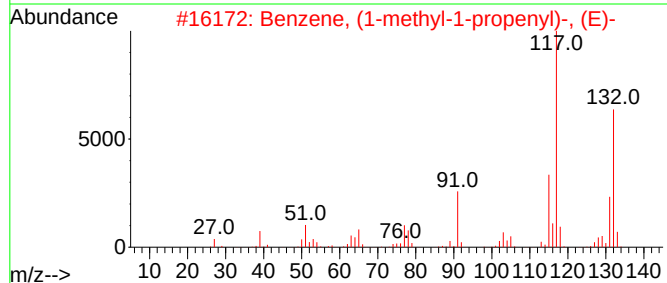
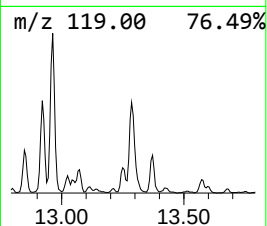
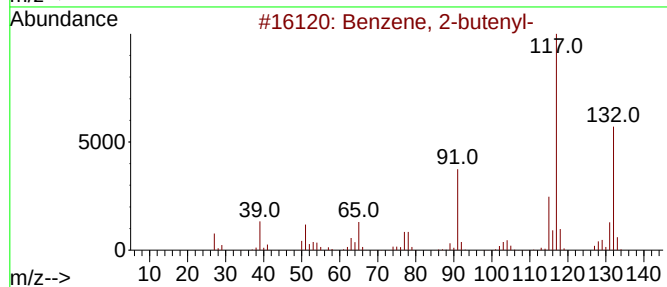
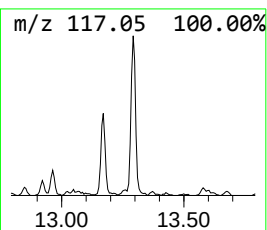
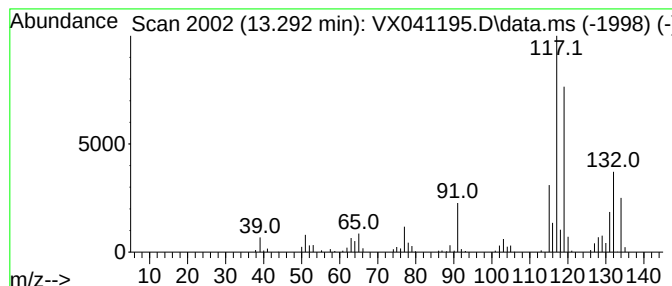
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 2-butenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	8.51 ug/l	124708	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	53
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	53
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	50
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	49
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	49



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Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

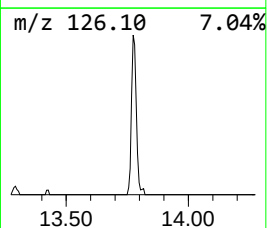
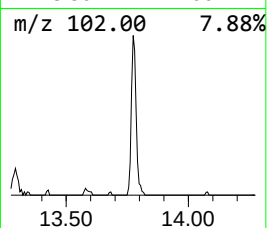
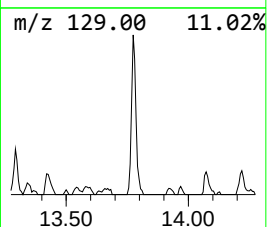
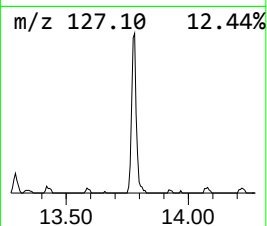
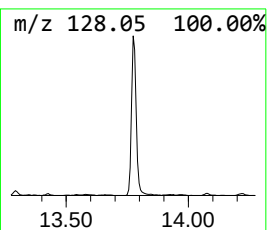
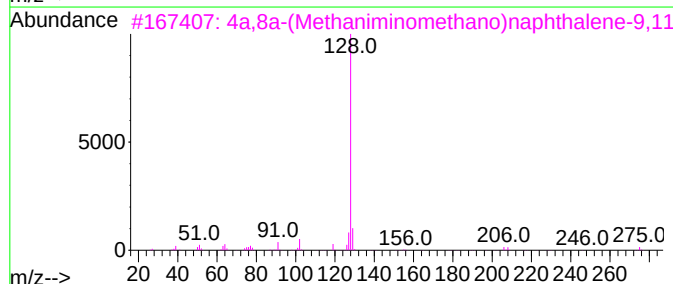
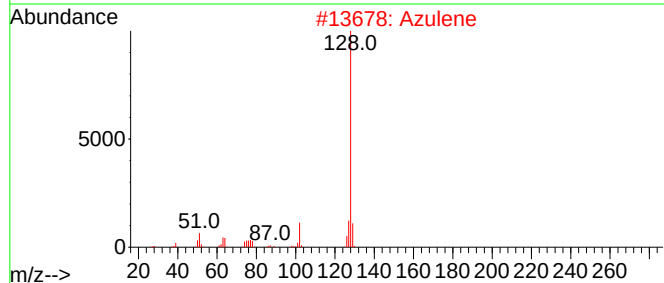
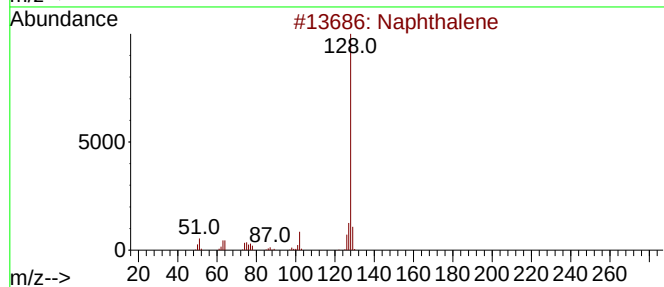
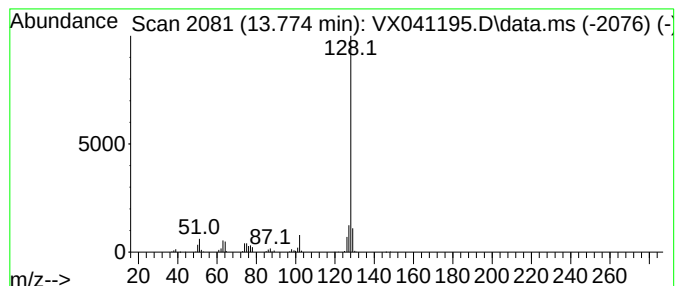
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 3 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	6.95 ug/l	101893	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	93
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50



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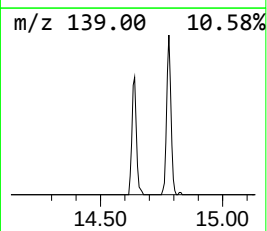
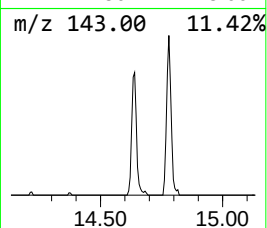
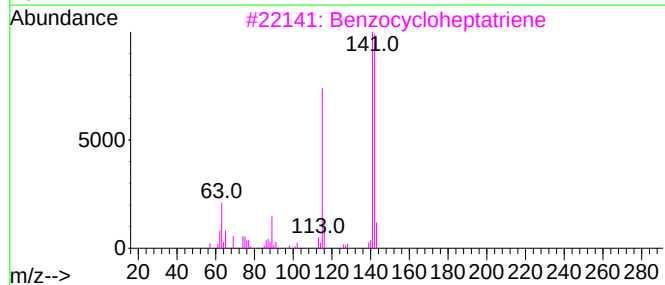
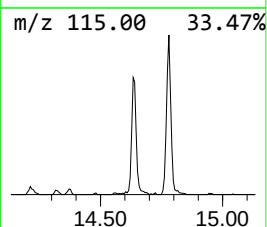
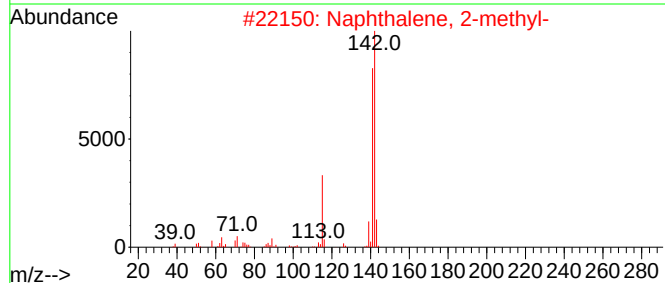
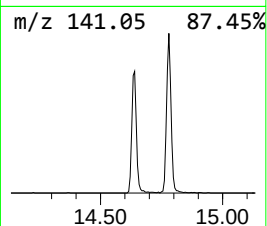
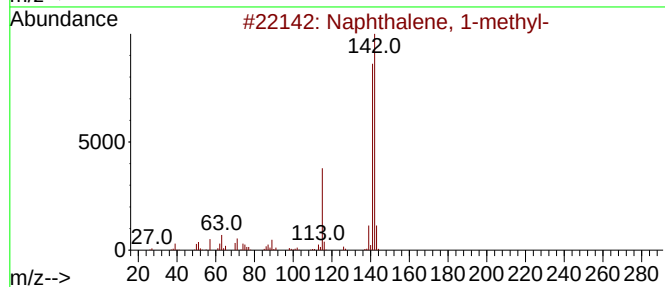
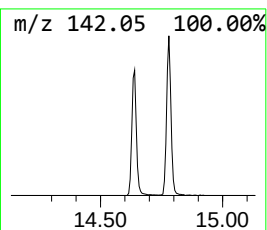
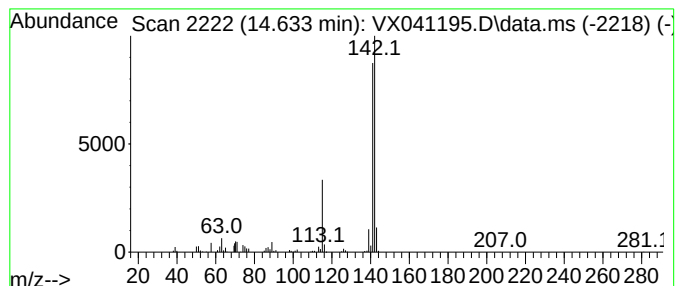
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	7.93 ug/l	116287	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59



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Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

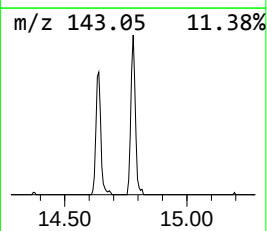
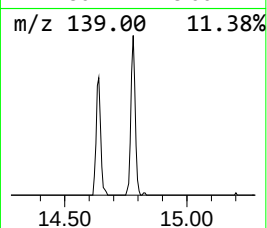
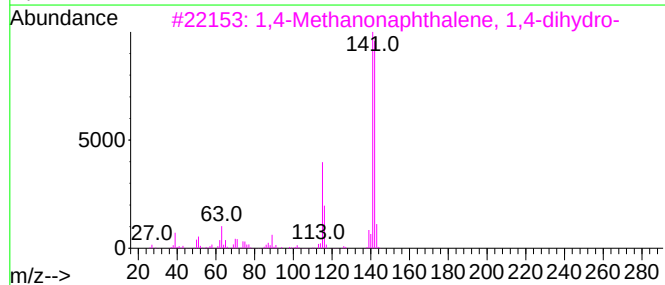
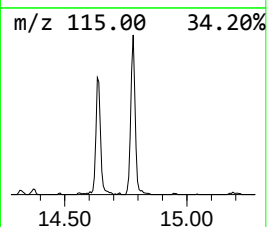
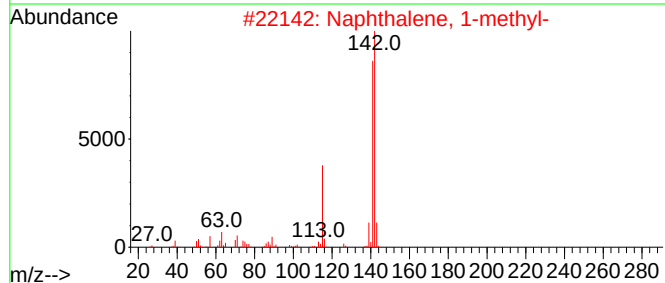
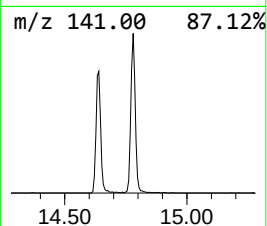
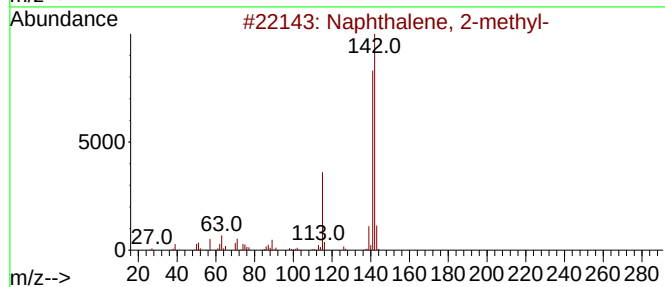
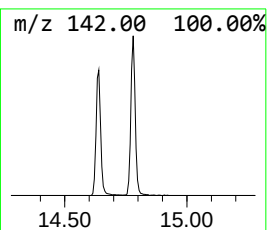
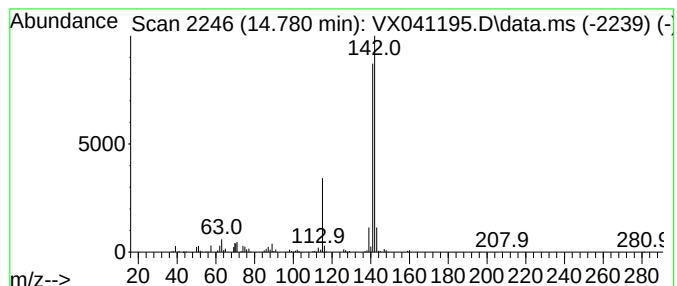
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 5 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	10.17 ug/l	149167	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042224\
Data File : VX041195.D
Acq On : 22 Apr 2024 17:20
Operator : JC/MD
Sample : P2218-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

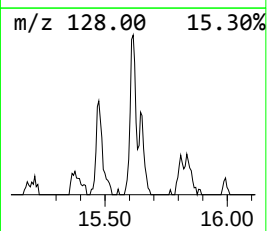
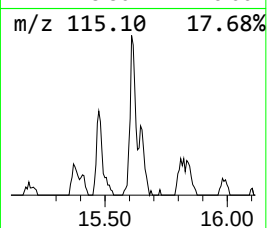
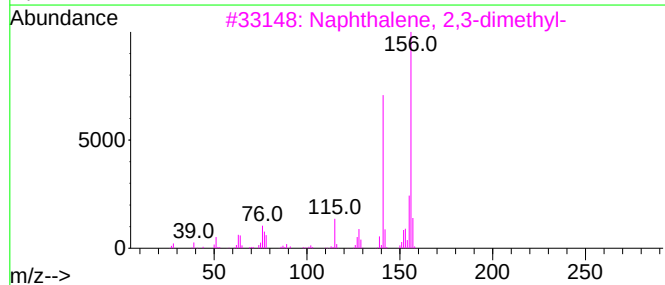
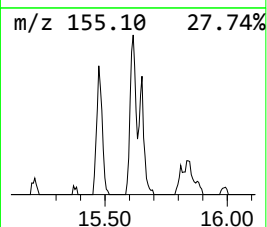
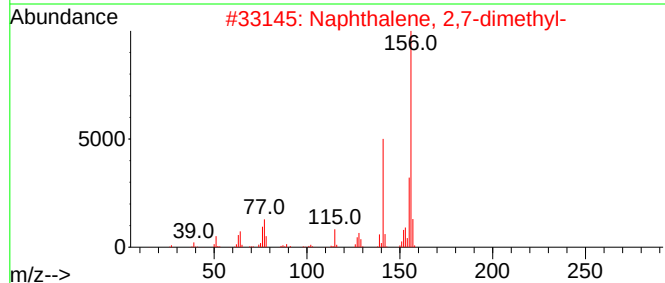
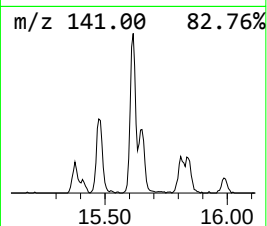
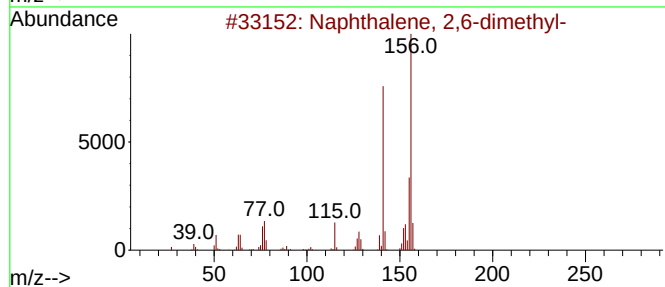
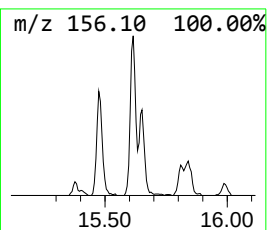
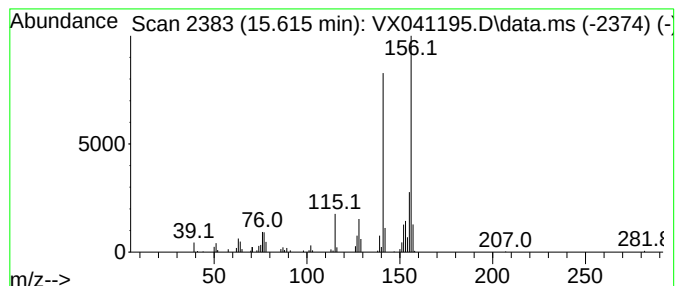
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	5.12 ug/l	74992	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042224\
Data File : VX041195.D
Acq On : 22 Apr 2024 17:20
Operator : JC/MD
Sample : P2218-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

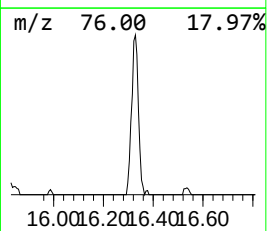
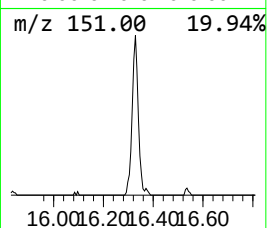
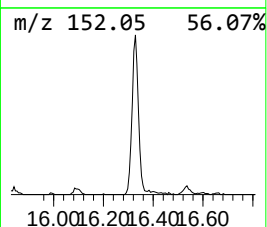
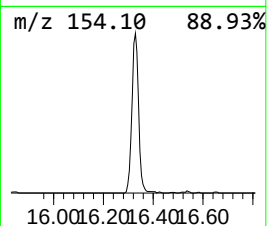
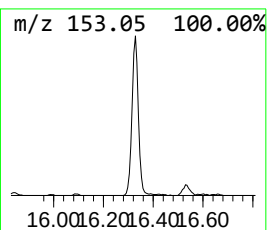
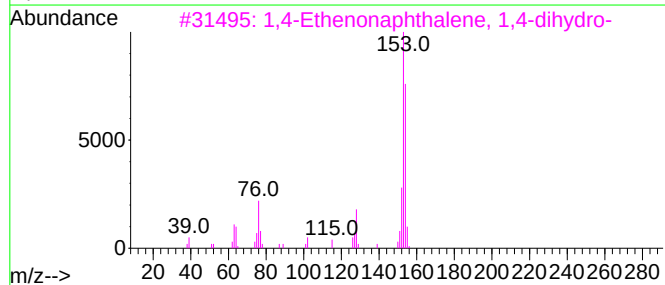
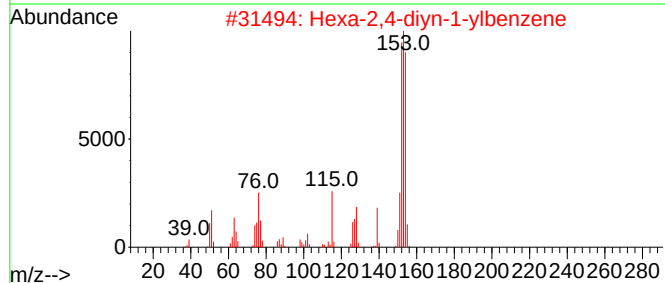
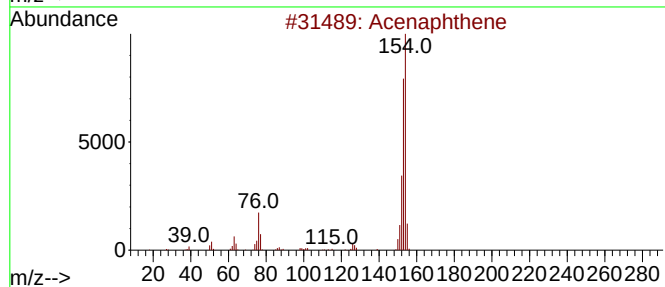
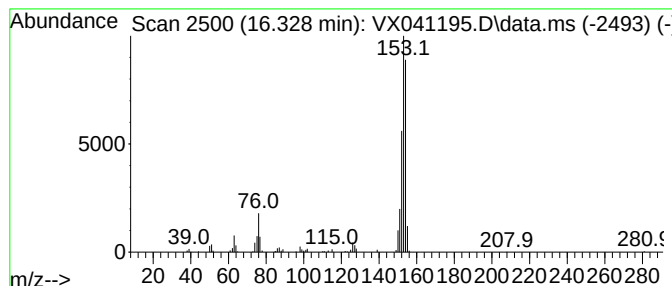
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Quant Title : SW846 8260

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

Peak Number 7 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	8.99 ug/l	131735	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	53
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042224\
Data File : VX041195.D
Acq On : 22 Apr 2024 17:20
Operator : JC/MD
Sample : P2218-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-131-GW-01

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
Benzene, 1,2,3,...	12.963	6.5	ug/l	94601	4	12.024	733035	50.0
Benzene, 2-bute...	13.292	8.5	ug/l	124708	4	12.024	733035	50.0
Azulene	13.774	7.0	ug/l	101893	4	12.024	733035	50.0
Benzocyclohepta...	14.634	7.9	ug/l	116287	4	12.024	733035	50.0
1,4-Methanonaph...	14.780	10.2	ug/l	149167	4	12.024	733035	50.0
Naphthalene, 2,...	15.615	5.1	ug/l	74992	4	12.024	733035	50.0
Hexa-2,4-diyne-1...	16.328	9.0	ug/l	131735	4	12.024	733035	50.0