

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
 Data File : VX027355.D
 Acq On : 09 Mar 2022 17:27
 Operator : JC/MD
 Sample : N1815-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PW-1

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\82X030822W.M
 Title : SW846 8260

Signal : TIC: VX027355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	103	108	124	rVB	679282	972190	1.11%	0.273%
2	1.953	137	142	155	rVB2	558716	938129	1.07%	0.264%
3	2.825	280	285	289	rVV	859794	1843874	2.11%	0.518%
4	2.867	289	292	306	rVB2	737311	1600418	1.83%	0.450%
5	3.099	320	330	349	rVB	748097	1707941	1.95%	0.480%
6	3.446	378	387	400	rBV	593274	1323089	1.51%	0.372%
7	4.306	518	528	540	rVB	1629181	4677688	5.34%	1.315%
8	5.196	645	674	689	rVB	273345	1063546	1.22%	0.299%
9	5.477	711	720	730	rBV3	1101556	3969144	4.53%	1.116%
10	5.623	739	744	763	rVB2	315471	1089928	1.25%	0.306%
11	5.830	766	778	791	rBV3	616716	1919538	2.19%	0.540%
12	6.202	822	839	842	rBV3	490326	1924670	2.20%	0.541%
13	6.257	843	848	857	rVV2	802713	2241392	2.56%	0.630%
14	6.361	857	865	877	rVB2	425591	1192296	1.36%	0.335%
15	6.617	893	907	918	rBV2	362425	915690	1.05%	0.257%
16	6.763	922	931	938	rVV	586539	1552239	1.77%	0.436%
17	7.385	1020	1033	1043	rBV	2143190	5193623	5.93%	1.460%
18	7.988	1122	1132	1143	rVB2	433504	1233358	1.41%	0.347%
19	8.147	1154	1158	1162	rVV	719964	1269034	1.45%	0.357%
20	8.506	1212	1217	1226	rVB	869673	1518117	1.73%	0.427%
21	8.604	1226	1233	1236	rBV4	637279	1266553	1.45%	0.356%
22	8.653	1236	1241	1248	rVB	1232988	2196761	2.51%	0.617%
23	9.458	1365	1373	1377	rBV2	739959	1245520	1.42%	0.350%
24	10.055	1468	1471	1476	rVB	1203455	1539419	1.76%	0.433%
25	10.213	1489	1497	1502	rVB2	45138951	87528005	100.00%	24.602%
26	10.311	1510	1513	1518	rVB2	562525	879018	1.00%	0.247%
27	10.780	1582	1590	1594	rBV2	594635	962081	1.10%	0.270%
28	10.963	1614	1620	1625	rBV	4244301	5209362	5.95%	1.464%
29	11.085	1634	1640	1643	rBV	1241486	1666980	1.90%	0.469%
30	11.305	1671	1676	1686	rBV	8251258	10496524	11.99%	2.950%
31	11.402	1686	1692	1695	rVV	1779585	2167837	2.48%	0.609%
32	11.457	1695	1701	1710	rVB	7071584	9463588	10.81%	2.660%
33	11.616	1722	1727	1735	rVB	2310033	3015029	3.44%	0.847%
34	11.756	1745	1750	1755	rVB	16438314	20517599	23.44%	5.767%
35	11.896	1770	1773	1777	rVB	710102	892426	1.02%	0.251%
36	12.024	1789	1794	1800	rVB2	1494537	2263549	2.59%	0.636%

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Integrator: RTE

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Sampling : 1

Min Area: 3 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.091	1800	1805	1810	rBV	18511646	24596764	28.10%	6.913%
38	12.250	1825	1831	1837	rBV	20405482	26088809	29.81%	7.333%
39	12.317	1837	1842	1849	rVB3	4404308	6930372	7.92%	1.948%
40	12.408	1852	1857	1862	rBV2	923380	1336460	1.53%	0.376%
41	12.463	1862	1866	1873	rVB	1914712	2382257	2.72%	0.670%
42	12.536	1873	1878	1880	rBV	2826685	3842167	4.39%	1.080%
43	12.555	1880	1881	1886	rVV	1516954	1499822	1.71%	0.422%
44	12.616	1886	1891	1894	rVV	7306450	8565122	9.79%	2.407%
45	12.646	1894	1896	1900	rVB	1217120	1292728	1.48%	0.363%
46	12.701	1900	1905	1913	rBV2	4316751	6481492	7.41%	1.822%
47	12.847	1925	1929	1934	rVB	1763243	2253435	2.57%	0.633%
48	12.926	1934	1942	1945	rBV	4223342	5459717	6.24%	1.535%
49	12.963	1945	1948	1954	rVB	4493786	5537250	6.33%	1.556%
50	13.170	1978	1982	1987	rVB	4151979	4607713	5.26%	1.295%
51	13.292	1998	2002	2008	rVV2	9416453	12833501	14.66%	3.607%
52	13.426	2020	2024	2030	rVB	2180378	2758963	3.15%	0.775%
53	13.548	2040	2044	2047	rBV	796989	1002204	1.15%	0.282%
54	13.585	2047	2050	2056	rVB3	923740	1518643	1.74%	0.427%
55	13.670	2061	2064	2070	rVB2	931739	1465580	1.67%	0.412%
56	13.780	2077	2082	2089	rVB	23421492	32973102	37.67%	9.268%
57	13.871	2089	2097	2101	rVV	1003767	1407285	1.61%	0.396%
58	14.079	2126	2131	2138	rBV	685821	981254	1.12%	0.276%
59	14.219	2149	2154	2159	rBV2	629300	1013188	1.16%	0.285%
60	14.640	2218	2223	2233	rVB	4583368	5864042	6.70%	1.648%
61	14.780	2241	2246	2255	rVB	2805990	3630843	4.15%	1.021%

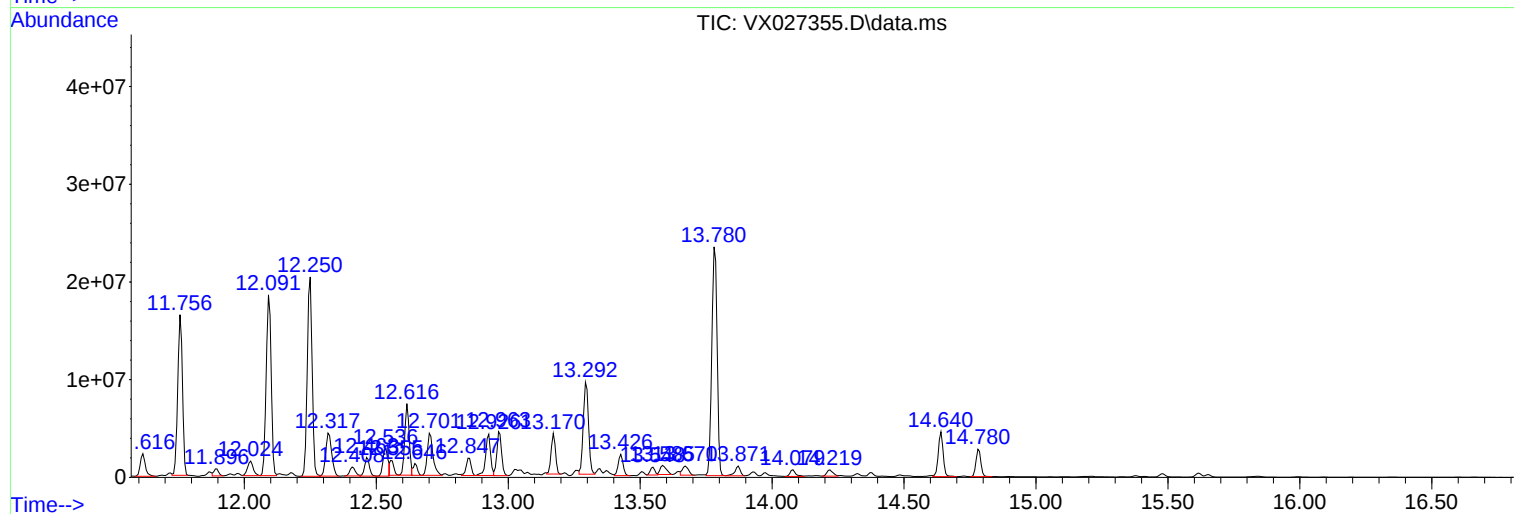
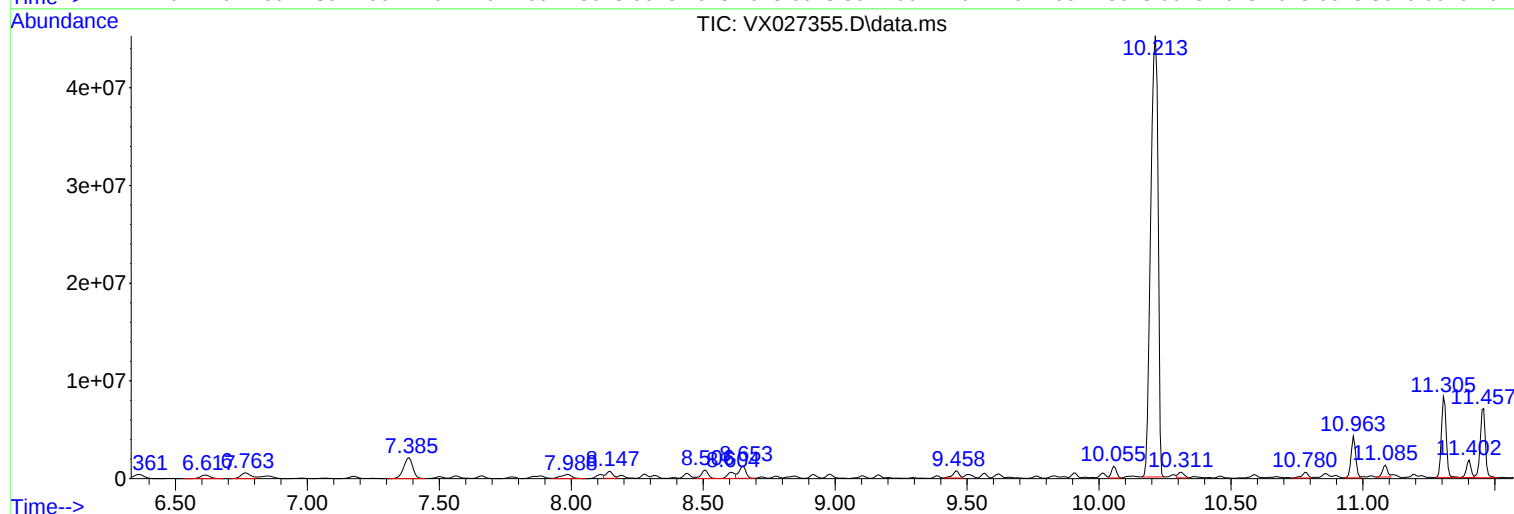
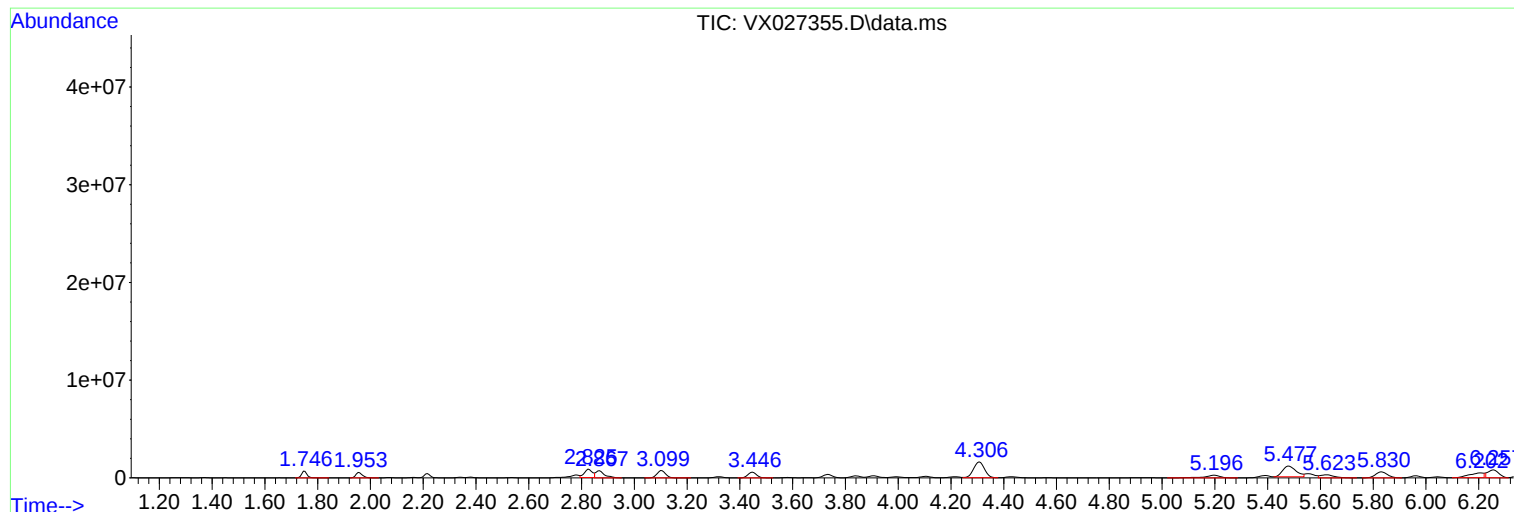
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ClientSampleId :
PW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

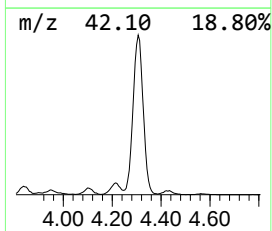
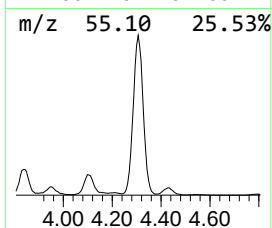
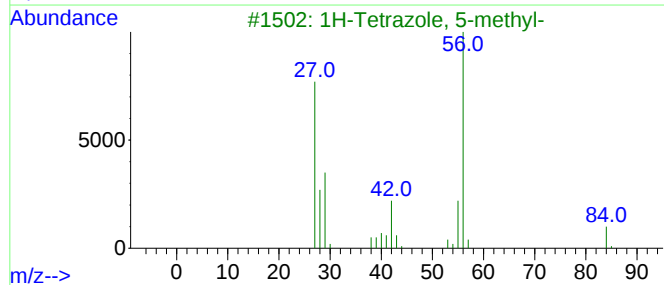
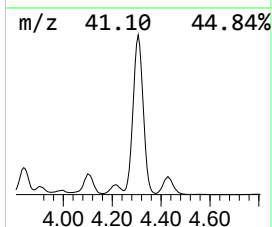
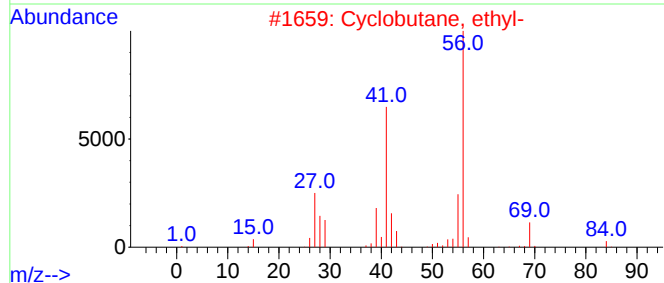
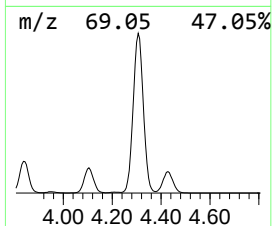
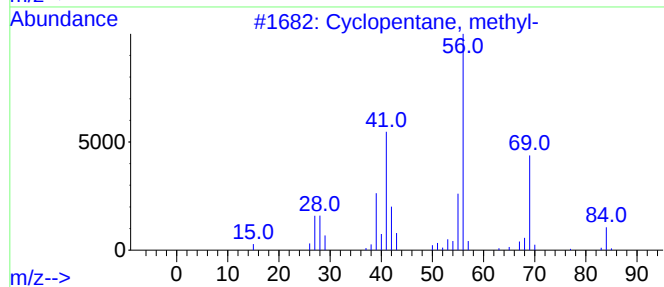
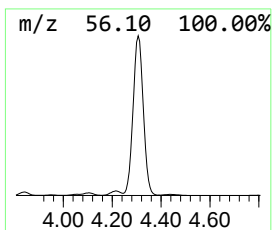
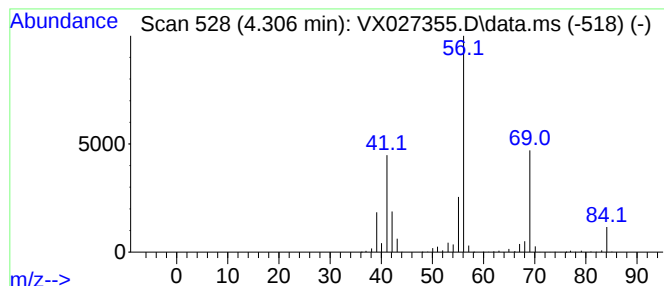
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	214.59 ug/l	4677690	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46
5			1-Octene, 7-methyl-	126	C9H18	013151-06-9	43



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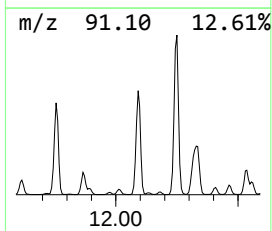
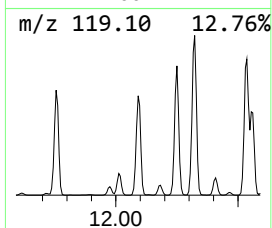
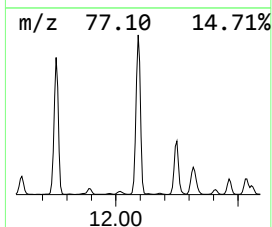
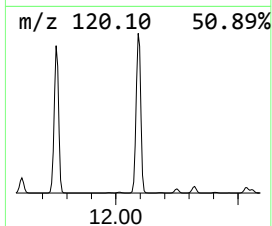
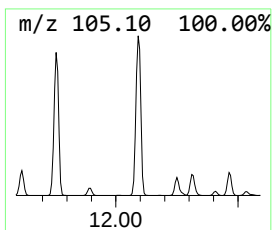
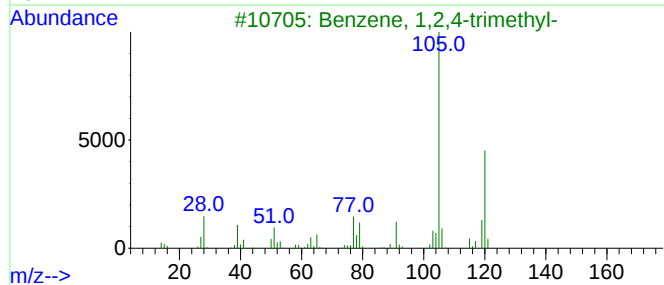
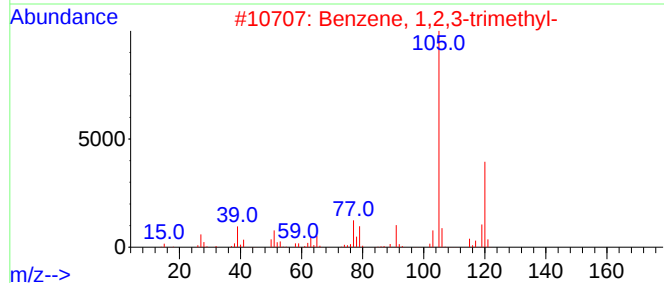
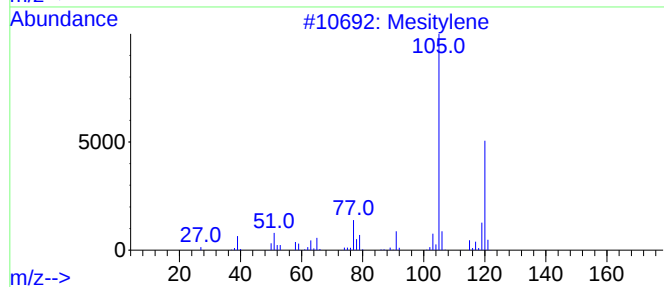
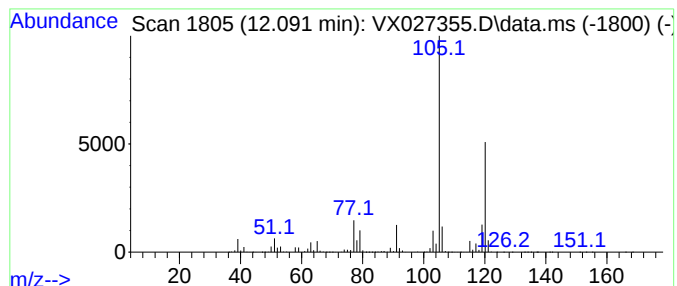
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	543.32 ug/l	24596800	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	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

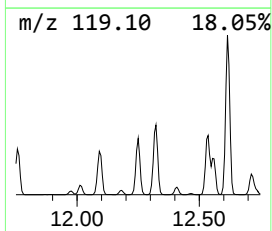
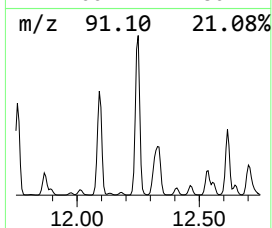
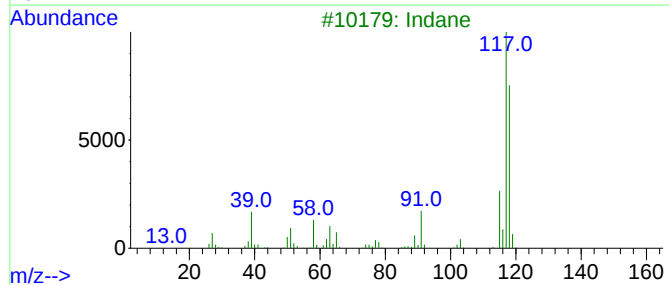
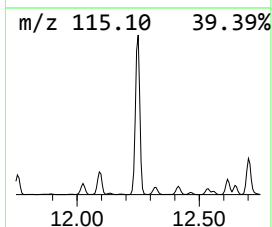
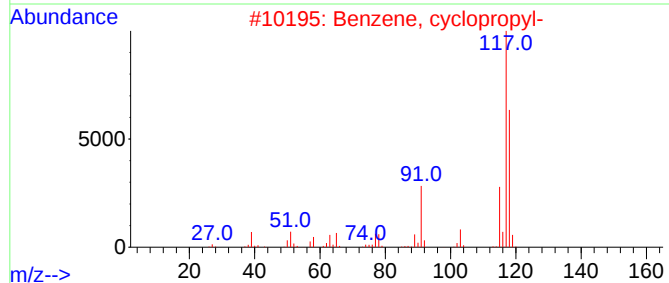
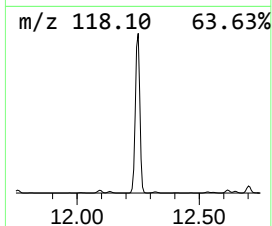
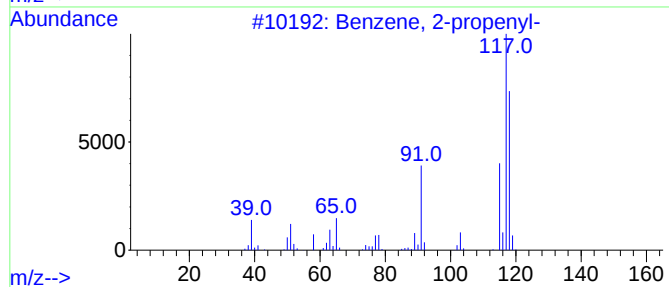
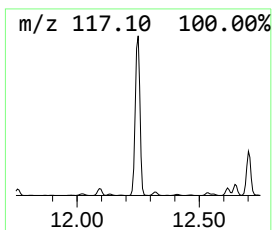
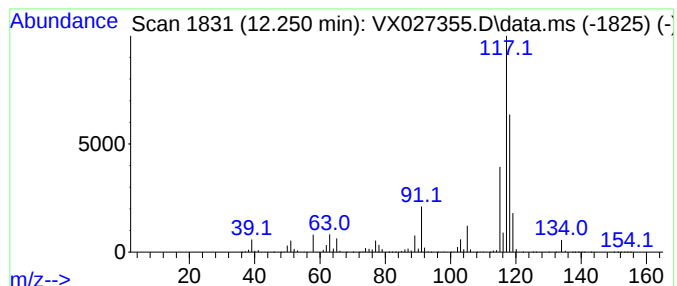
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	576.28 ug/l	26088800	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3			Indane	118	C9H10	000496-11-7	70
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	62
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50



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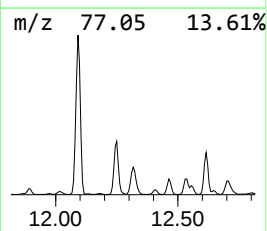
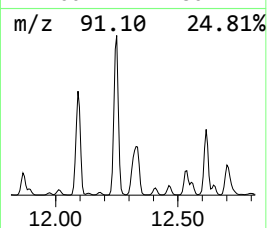
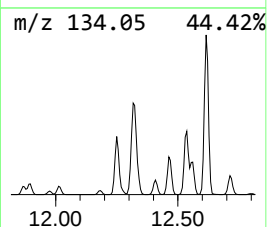
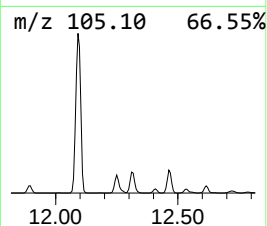
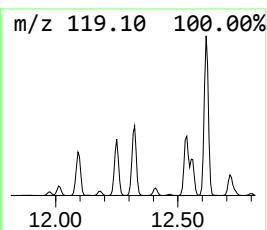
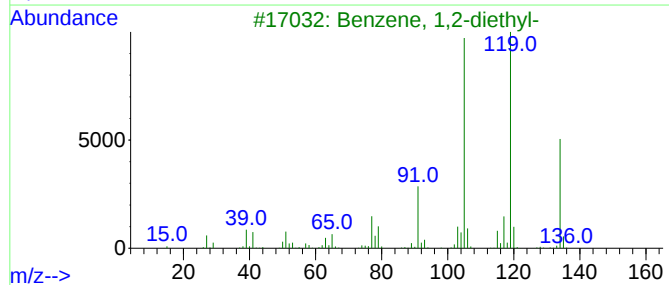
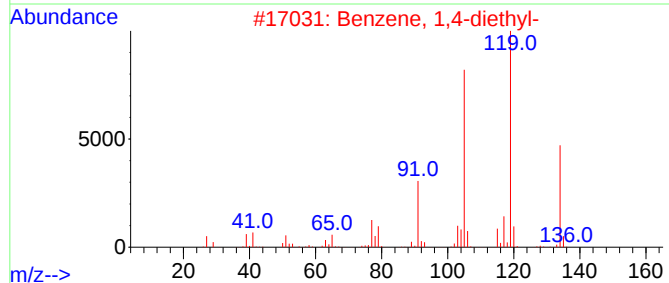
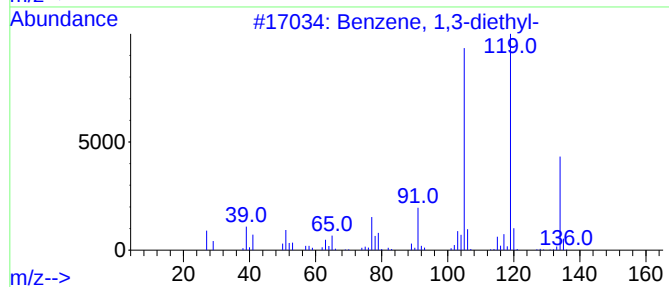
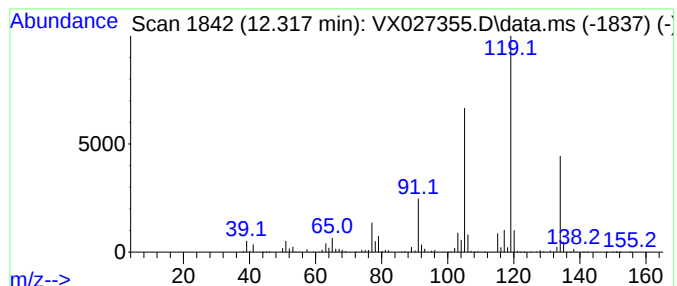
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,3-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	153.09 ug/l	6930370	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	96
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



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Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

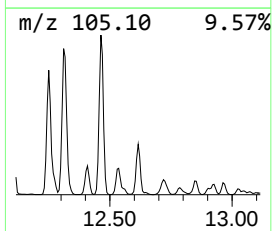
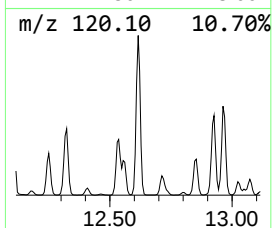
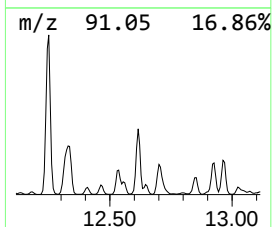
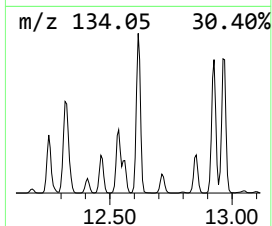
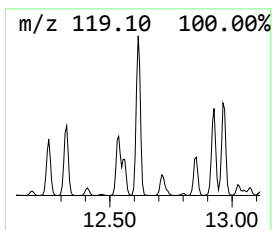
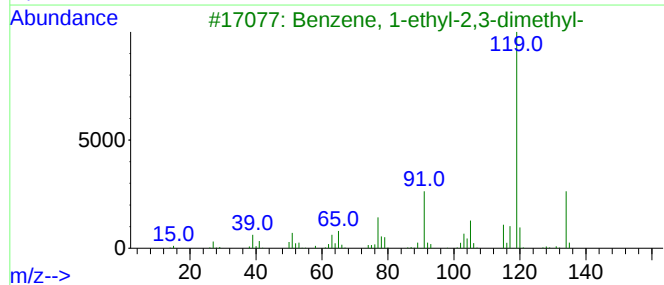
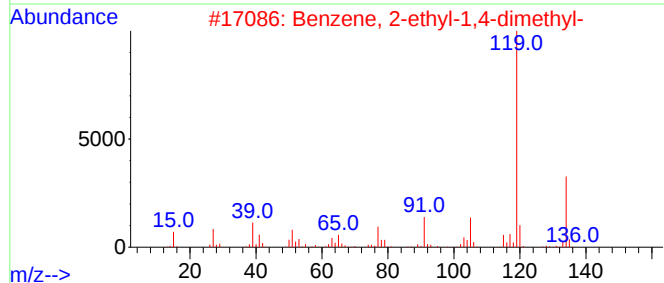
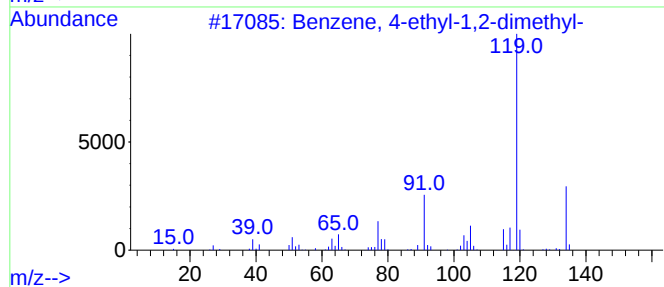
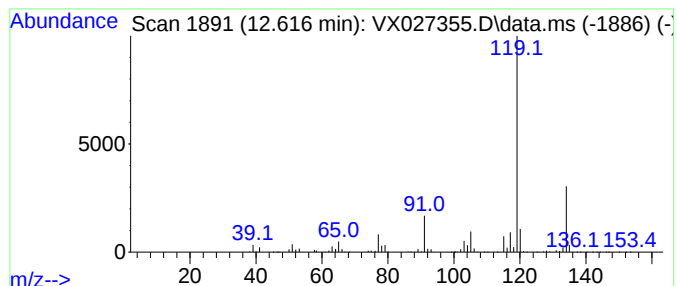
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	189.20 ug/l	8565120	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
Data File : VX027355.D
Acq On : 09 Mar 2022 17:27
Operator : JC/MD
Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

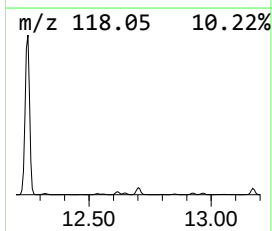
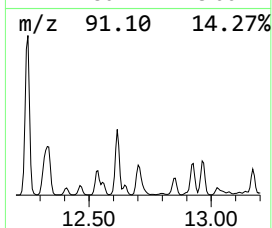
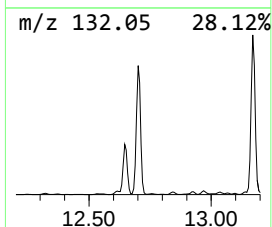
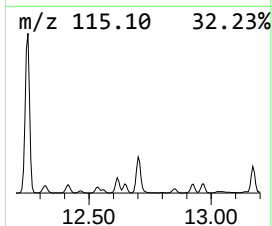
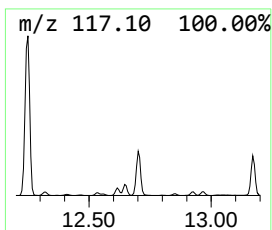
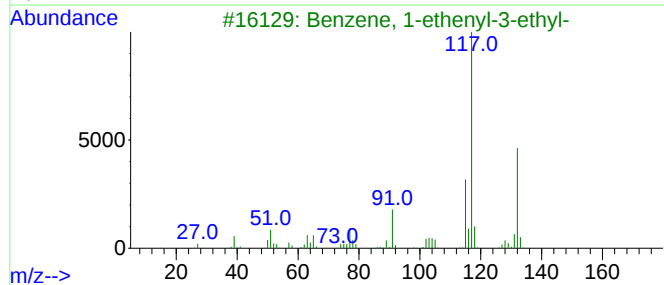
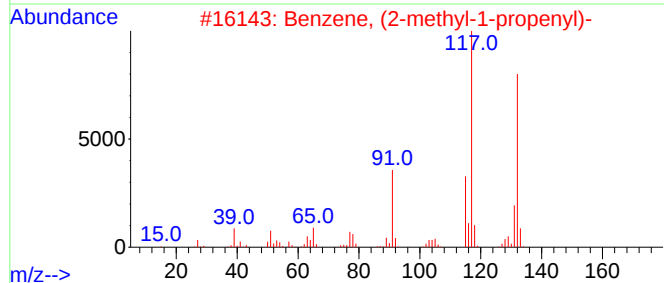
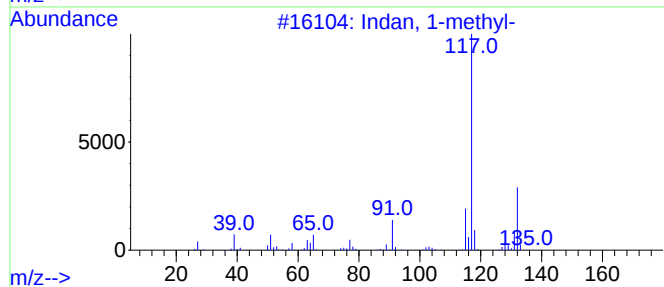
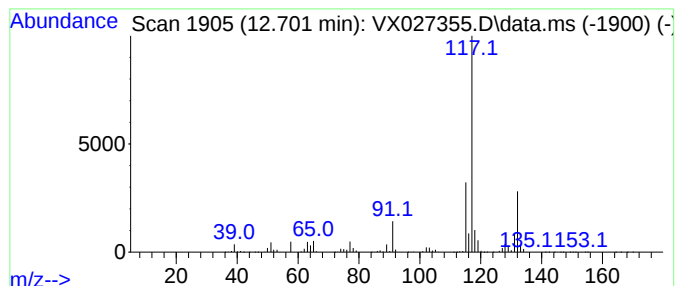
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Quant Title : SW846 8260

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

Peak Number 6 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	143.17 ug/l	6481490	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
Data File : VX027355.D
Acq On : 09 Mar 2022 17:27
Operator : JC/MD
Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

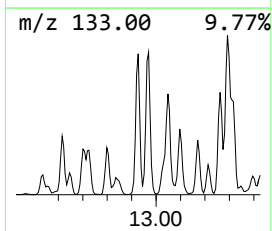
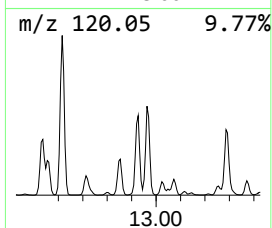
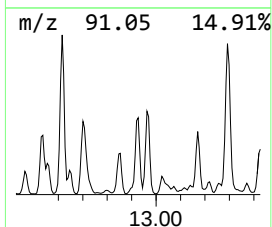
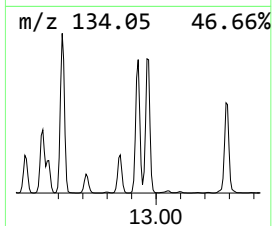
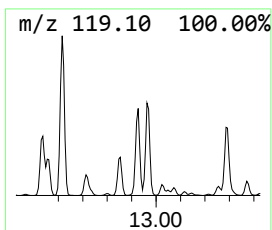
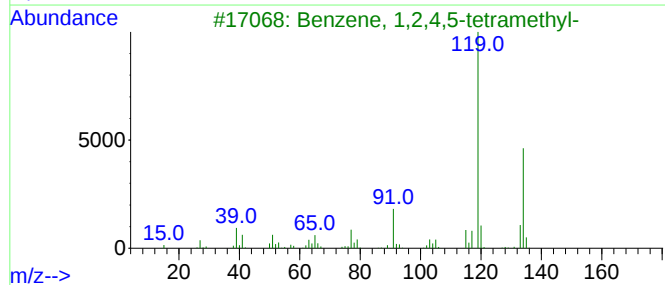
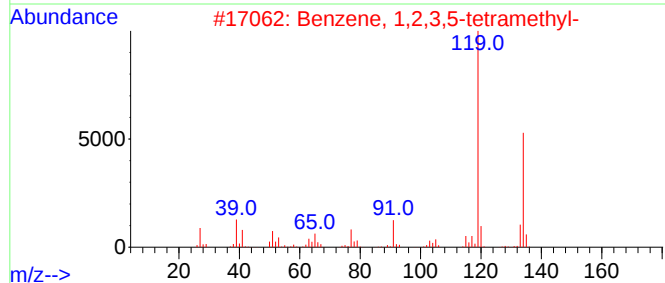
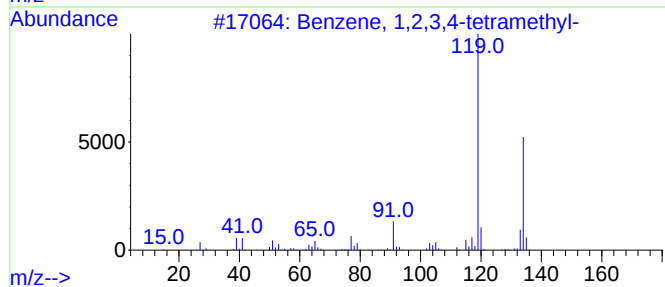
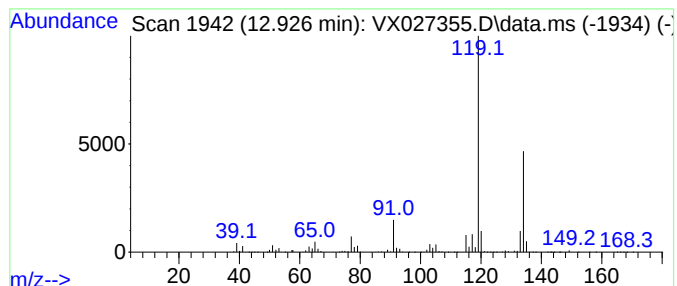
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.926	120.60 ug/l	5459720	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
Data File : VX027355.D
Acq On : 09 Mar 2022 17:27
Operator : JC/MD
Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

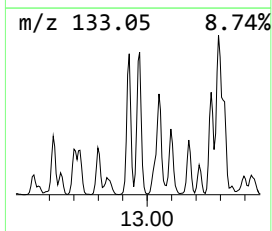
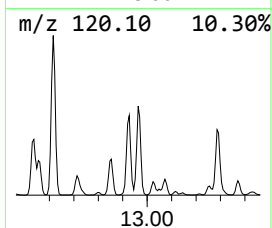
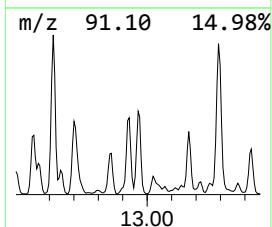
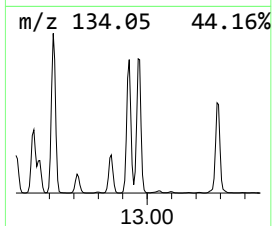
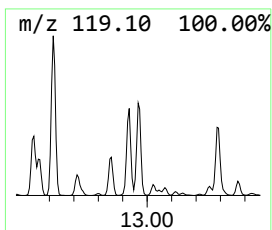
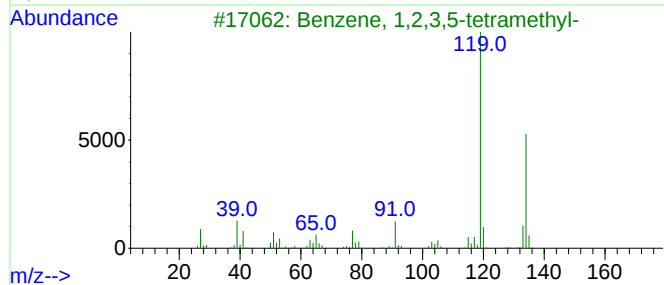
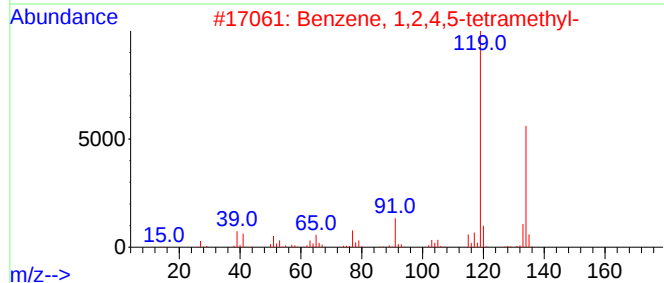
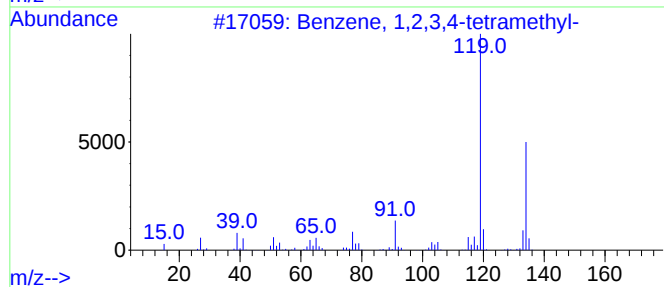
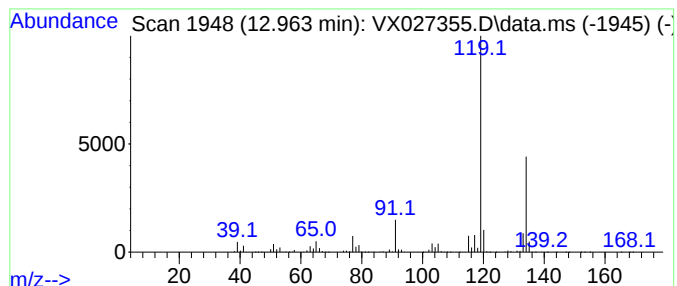
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	122.31 ug/l	5537250	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4			o-Cymene	134	C10H14	000527-84-4	96
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
Data File : VX027355.D
Acq On : 09 Mar 2022 17:27
Operator : JC/MD
Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

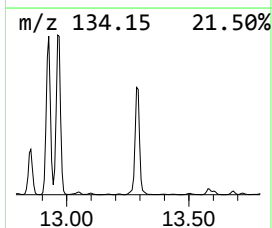
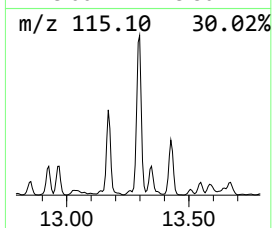
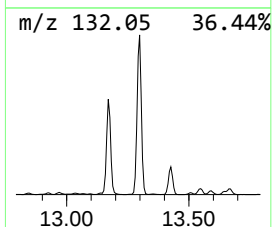
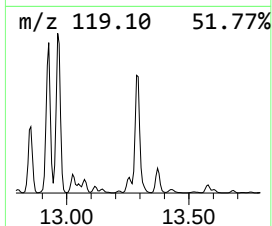
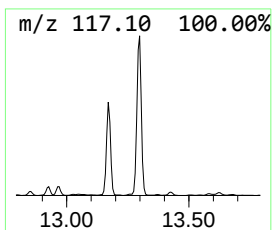
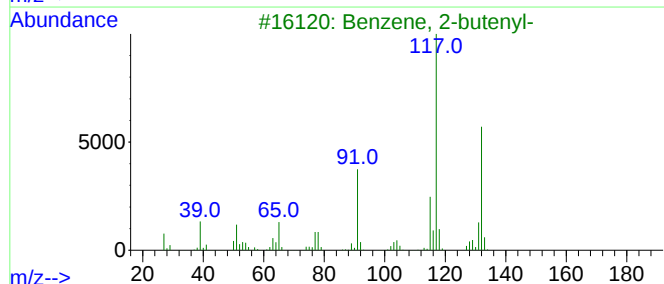
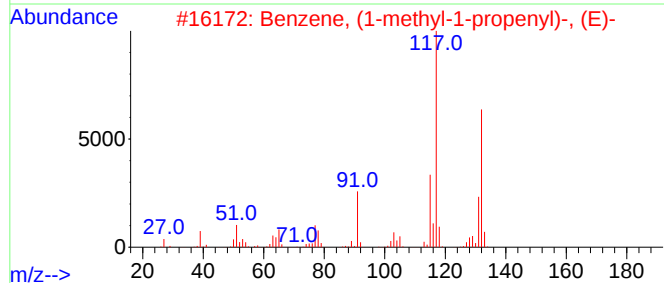
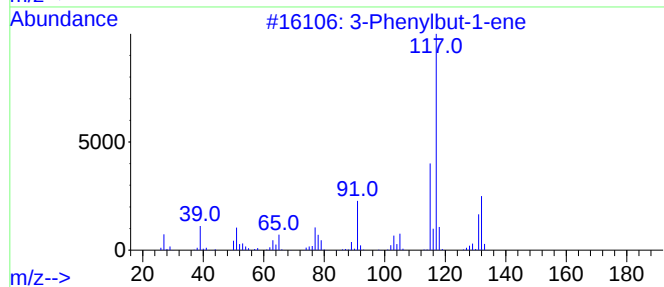
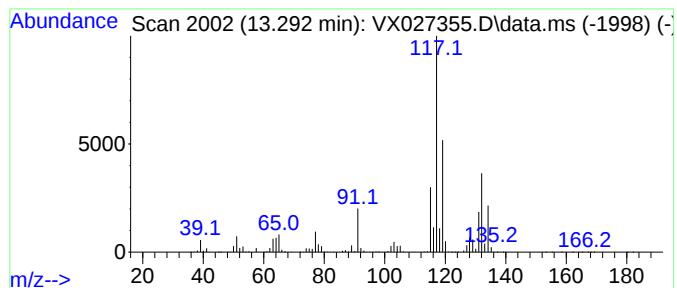
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Quant Title : SW846 8260

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

Peak Number 9 3-Phenylbut-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	283.48 ug/l	12833500	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
2		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
4		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	70
5		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
Data File : VX027355.D
Acq On : 09 Mar 2022 17:27
Operator : JC/MD
Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

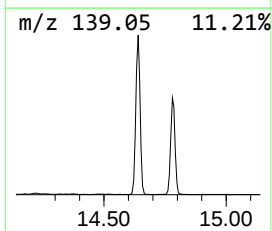
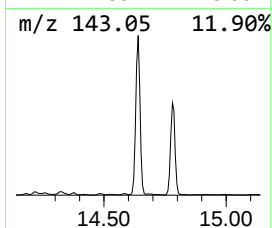
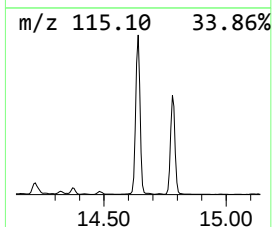
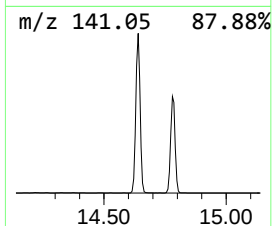
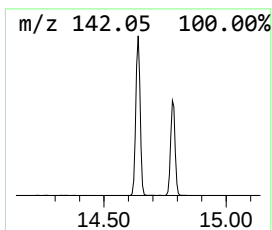
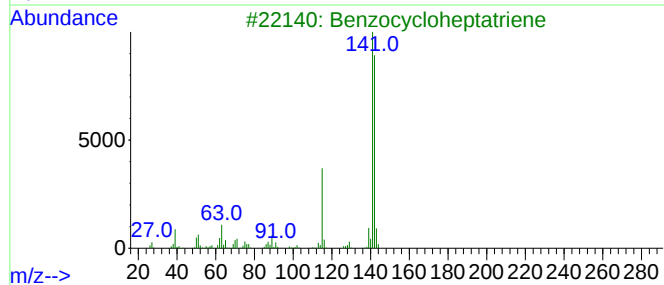
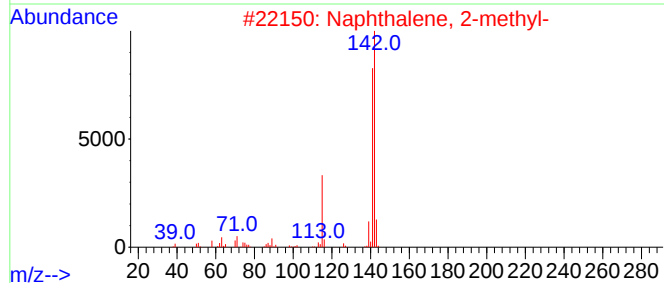
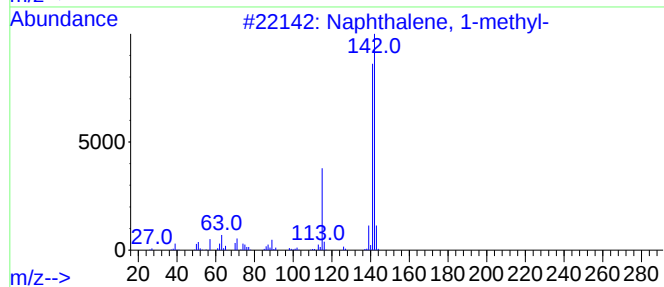
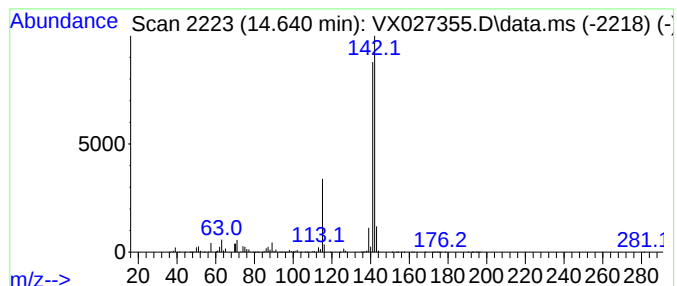
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	129.53 ug/l	5864040	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030922\
Data File : VX027355.D
Acq On : 09 Mar 2022 17:27
Operator : JC/MD
Sample : N1815-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.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-...	12.091	543.3	ug/l	24596800	4	12.024	2263550	50.0
Benzene, 2-prop...	12.250	576.3	ug/l	26088800	4	12.024	2263550	50.0
Benzene, 1,3-di...	12.317	153.1	ug/l	6930370	4	12.024	2263550	50.0
Benzene, 4-ethy...	12.616	189.2	ug/l	8565120	4	12.024	2263550	50.0
Indan, 1-methyl-	12.701	143.2	ug/l	6481490	4	12.024	2263550	50.0
Benzene, 1,2,3,...	12.926	120.6	ug/l	5459720	4	12.024	2263550	50.0
Benzene, 1,2,4,...	12.963	122.3	ug/l	5537250	4	12.024	2263550	50.0
3-Phenylbut-1-ene	13.292	283.5	ug/l	12833500	4	12.024	2263550	50.0
Benzocyclohepta...	14.640	129.5	ug/l	5864040	4	12.024	2263550	50.0