

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
 Data File : VX028860.D
 Acq On : 20 May 2022 18:53
 Operator : JC/MD
 Sample : N2943-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP051822

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028860.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	21	29	41	rBV2	758696	799766	1.25%	0.206%
2	1.368	43	46	52	rVV	1524138	1574960	2.46%	0.405%
3	1.752	103	109	127	rVB	6232973	8792593	13.75%	2.262%
4	1.953	137	142	156	rVB	3714530	5416277	8.47%	1.394%
5	2.069	156	161	168	rVV	850855	1190138	1.86%	0.306%
6	2.166	168	177	181	rVV	514962	784081	1.23%	0.202%
7	2.215	181	185	194	rVB	1089717	1560428	2.44%	0.402%
8	2.782	258	278	281	rBV3	675374	2141478	3.35%	0.551%
9	2.825	281	285	289	rVV	1929928	4019995	6.29%	1.034%
10	2.867	289	292	319	rVV2	1553114	3461275	5.41%	0.891%
11	3.105	319	331	350	rVB	1541252	3506346	5.48%	0.902%
12	3.446	377	387	401	rBV	951528	2094170	3.27%	0.539%
13	3.672	416	424	429	rBV	263971	643499	1.01%	0.166%
14	3.733	429	434	443	rVB	397012	915615	1.43%	0.236%
15	3.837	443	451	457	rBV	266655	681176	1.07%	0.175%
16	4.306	518	528	541	rVB	3667231	10515527	16.44%	2.706%
17	5.477	710	720	730	rBV	2116929	6703123	10.48%	1.725%
18	5.623	740	744	766	rVB3	274501	932502	1.46%	0.240%
19	5.830	766	778	791	rBV4	321798	1052944	1.65%	0.271%
20	6.044	805	813	823	rVB	1180599	3014725	4.71%	0.776%
21	6.166	823	833	836	rBV2	308386	850799	1.33%	0.219%
22	6.361	857	865	876	rVB	320208	897151	1.40%	0.231%
23	6.763	924	931	938	rBV	440079	1084841	1.70%	0.279%
24	7.385	1019	1033	1044	rBV2	1717645	4337589	6.78%	1.116%
25	8.147	1153	1158	1163	rVB	447469	755558	1.18%	0.194%
26	8.507	1210	1217	1227	rVB	596754	1031939	1.61%	0.266%
27	8.653	1236	1241	1246	rVB	911131	1455089	2.28%	0.374%
28	8.720	1246	1252	1258	rBV	3610278	5418539	8.47%	1.394%
29	8.958	1287	1291	1300	rVB	554099	942045	1.47%	0.242%
30	9.049	1300	1306	1311	rBV	543457	803848	1.26%	0.207%
31	10.055	1461	1471	1476	rBV	930265	1372276	2.15%	0.353%
32	10.201	1489	1495	1500	rBV	21148556	28908220	45.20%	7.439%
33	10.317	1506	1514	1519	rBV	39647479	63955832	100.00%	16.457%
34	10.646	1562	1568	1577	rVB	16821467	22232520	34.76%	5.721%
35	10.963	1613	1620	1627	rBV	2448098	2968981	4.64%	0.764%
36	11.085	1635	1640	1645	rVB	937877	1203528	1.88%	0.310%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	11.305	1668	1676	1683	rVB	5973763	7212012	11.28%	1.856%
38	11.384	1683	1689	1691	rBV	14002043	19656037	30.73%	5.058%
39	11.457	1696	1701	1707	rVB	6825988	8529769	13.34%	2.195%
40	11.616	1721	1727	1736	rBV	11261663	13974652	21.85%	3.596%
41	11.762	1745	1751	1756	rVB	31307119	42826649	66.96%	11.020%
42	12.024	1789	1794	1798	rVV2	1391155	1831633	2.86%	0.471%
43	12.091	1798	1805	1810	rVB	12375221	15220433	23.80%	3.916%
44	12.244	1825	1830	1838	rBV2	12421519	17299265	27.05%	4.451%
45	12.317	1838	1842	1850	rVB4	2484559	3803398	5.95%	0.979%
46	12.408	1852	1857	1862	rBV2	681308	956595	1.50%	0.246%
47	12.463	1862	1866	1872	rVB	1004877	1177352	1.84%	0.303%
48	12.530	1872	1877	1880	rBV	2044928	3014394	4.71%	0.776%
49	12.555	1880	1881	1886	rVB	1809647	1583188	2.48%	0.407%
50	12.616	1886	1891	1894	rBV	3660232	4432746	6.93%	1.141%
51	12.646	1894	1896	1900	rVB	1093454	1153617	1.80%	0.297%
52	12.701	1900	1905	1913	rBV2	3313008	4365988	6.83%	1.123%
53	12.847	1925	1929	1934	rVB	1078950	1352145	2.11%	0.348%
54	12.920	1934	1941	1945	rBV	2131017	2760380	4.32%	0.710%
55	12.963	1945	1948	1954	rVB	3175970	3710929	5.80%	0.955%
56	13.170	1978	1982	1987	rVB	2663432	3030410	4.74%	0.780%
57	13.292	1998	2002	2007	rVB2	5748828	7454006	11.65%	1.918%
58	13.426	2019	2024	2032	rVB	1137020	1500725	2.35%	0.386%
59	13.585	2047	2050	2056	rVB2	425725	667884	1.04%	0.172%
60	13.664	2061	2063	2069	rVB2	487767	660883	1.03%	0.170%
61	13.780	2075	2082	2088	rBV	9926696	12578588	19.67%	3.237%
62	14.225	2149	2155	2164	rBV3	385439	768513	1.20%	0.198%
63	14.640	2218	2223	2233	rVB	3999633	5011595	7.84%	1.290%
64	14.780	2241	2246	2255	rBV	2731790	3369716	5.27%	0.867%
65	15.615	2373	2383	2386	rBV	467327	701360	1.10%	0.180%

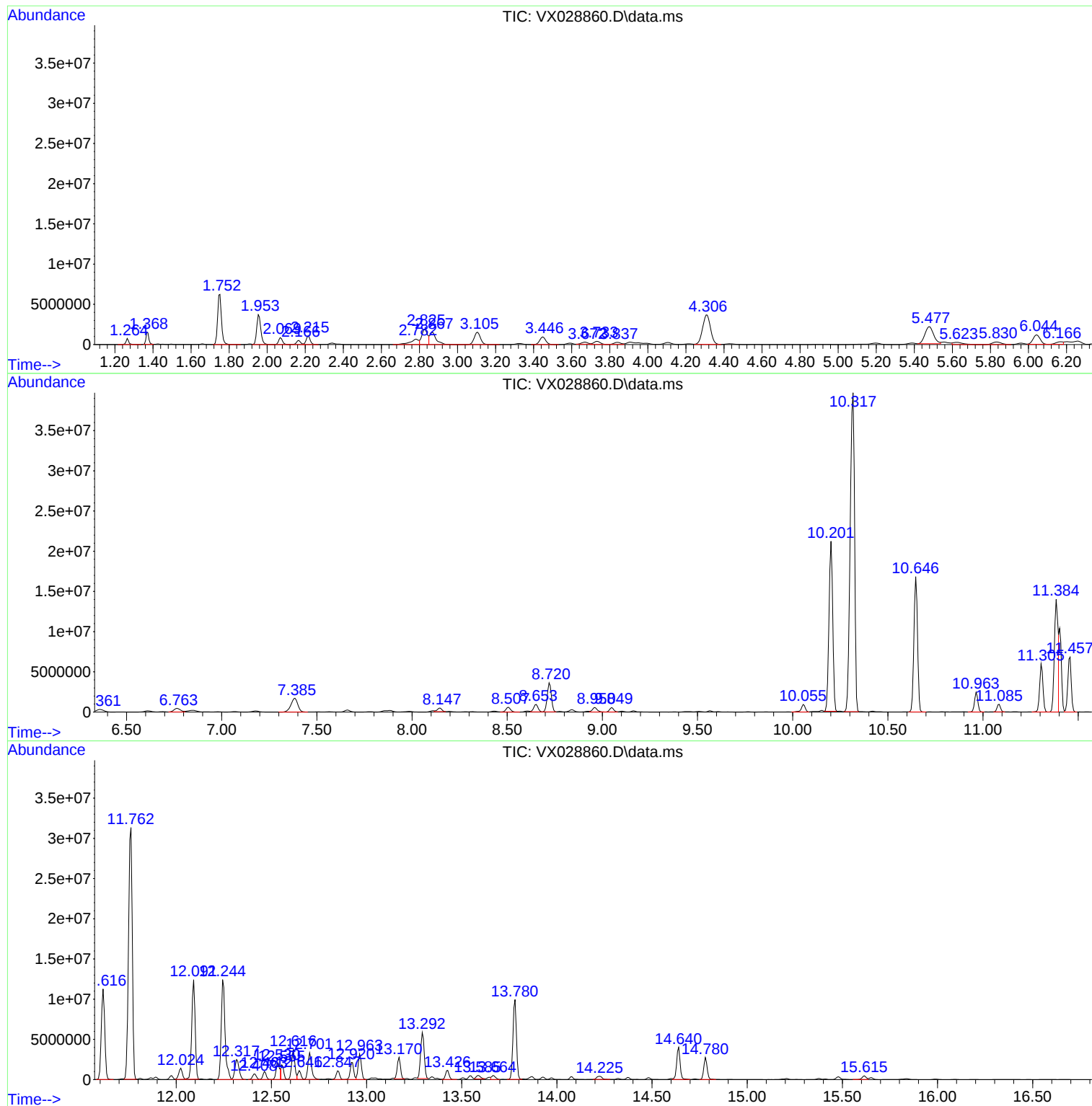
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ClientSampleId :
DUP051822

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
DUP051822

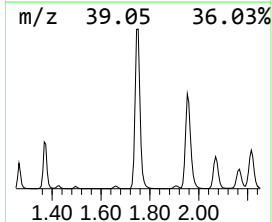
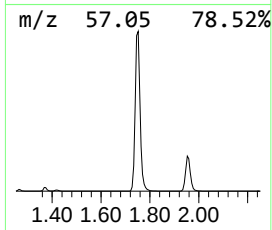
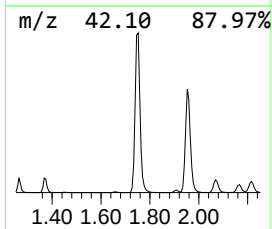
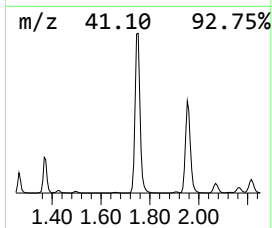
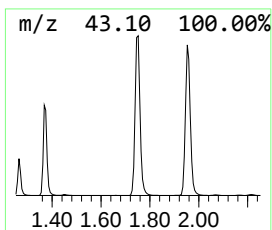
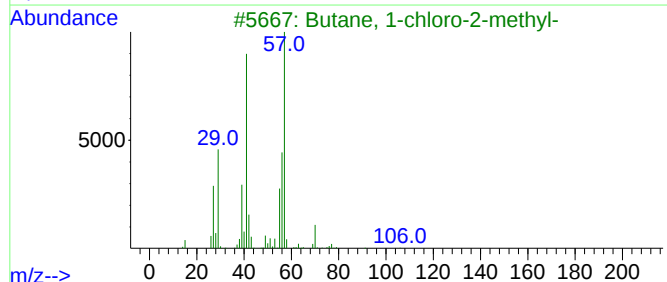
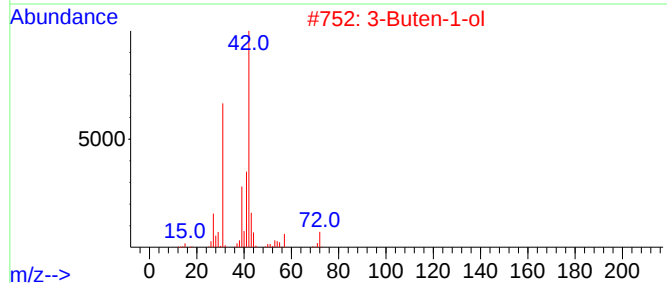
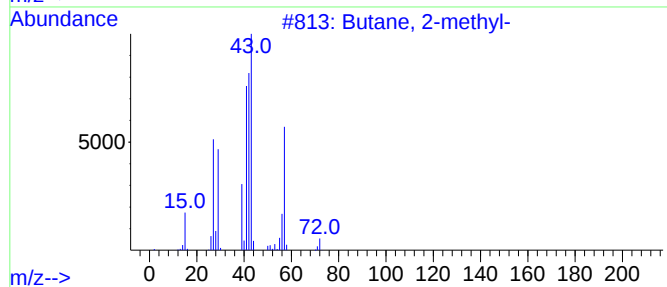
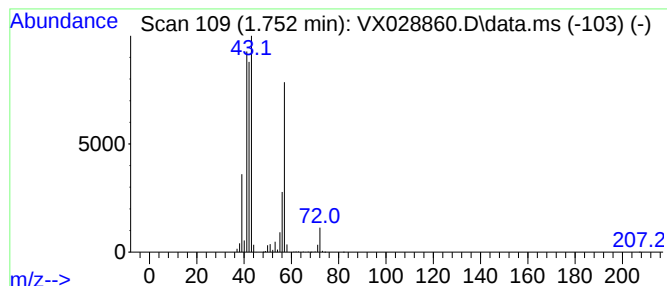
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	471.45 ug/l	8792590	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4			Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
5			Pentane	72	C5H12	000109-66-0	33



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP051822

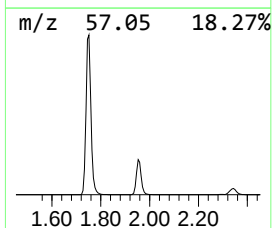
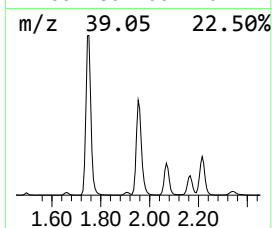
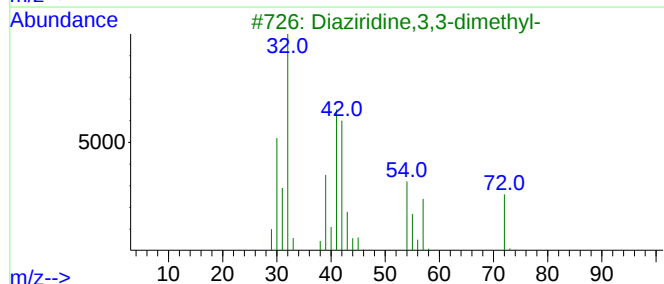
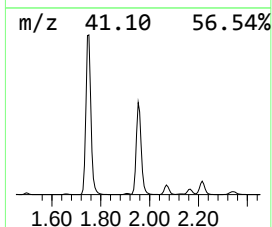
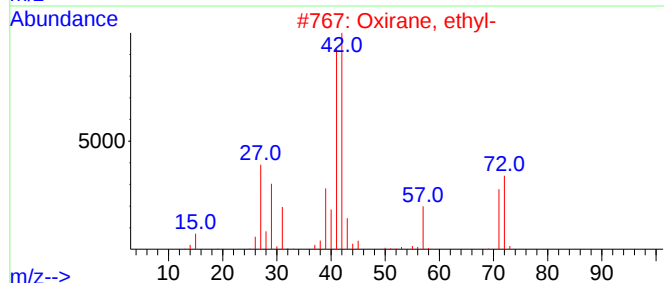
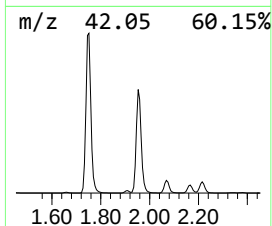
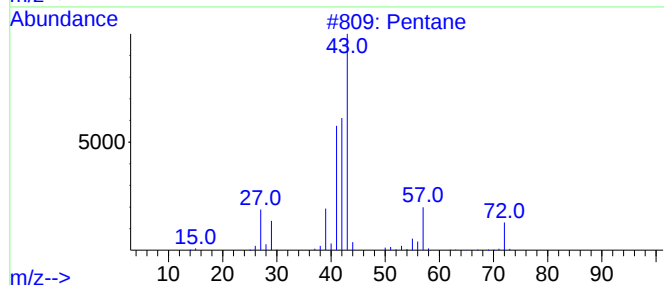
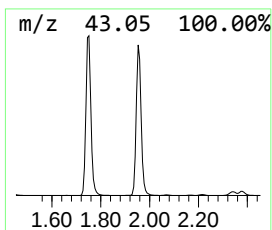
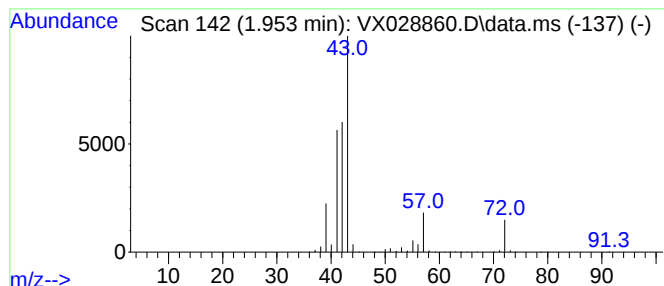
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	290.42 ug/l	5416280	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4			Butane, 2-methyl-	72	C5H12	000078-78-4	38
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	25



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

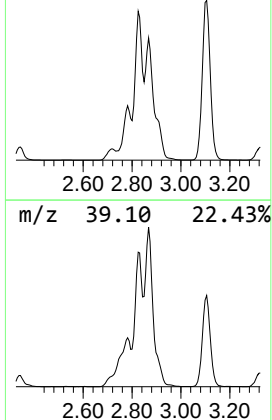
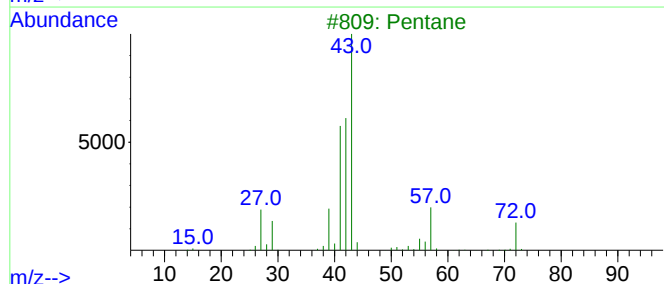
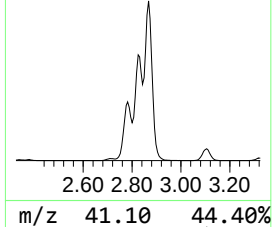
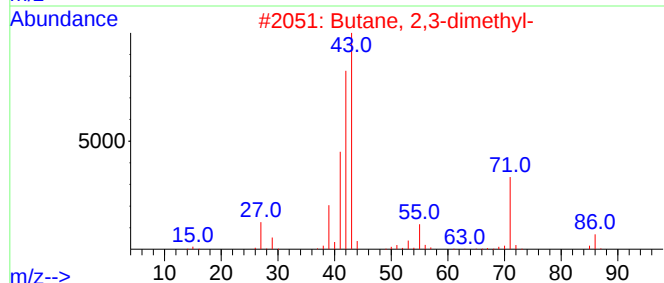
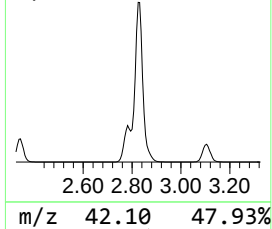
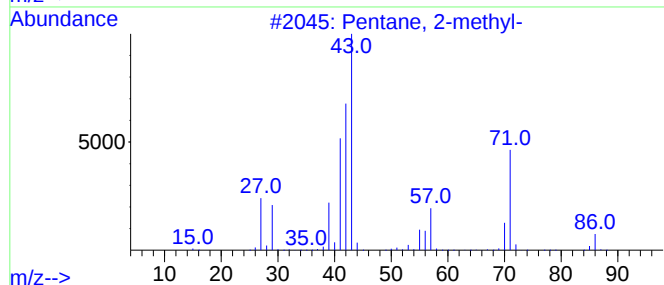
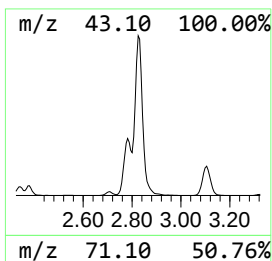
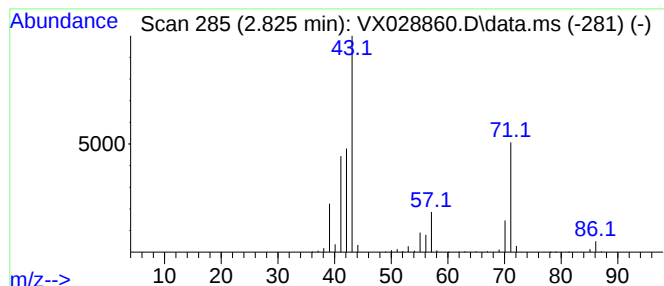
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	215.55 ug/l	4020000	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	94
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	49
3			Pentane	72	C5H12	000109-66-0	49
4			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	42
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

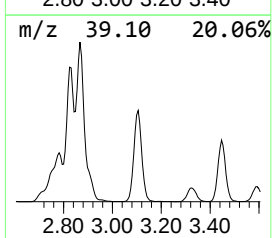
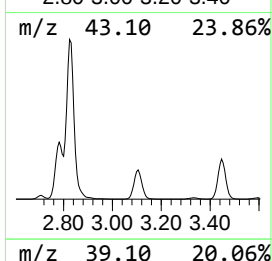
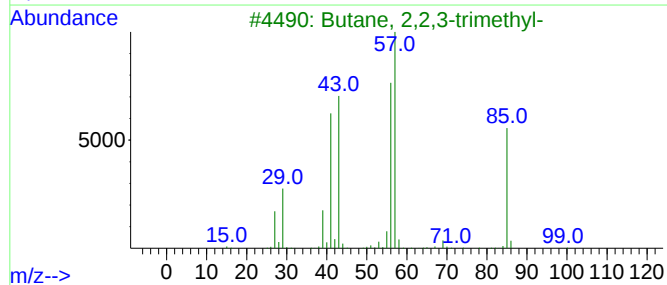
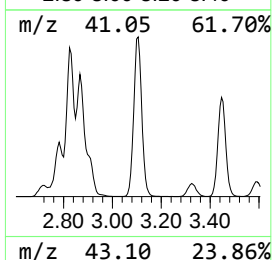
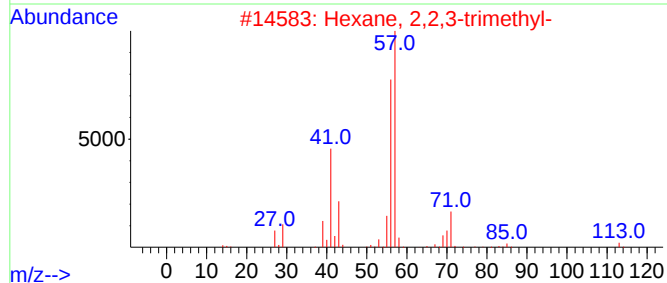
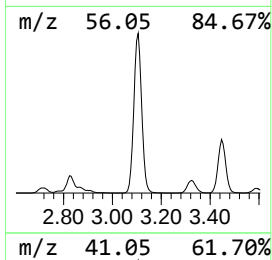
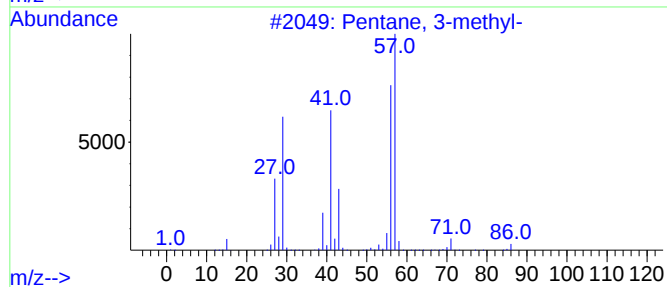
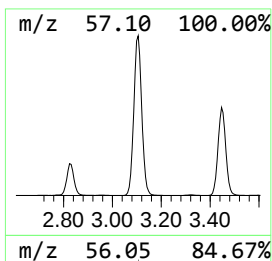
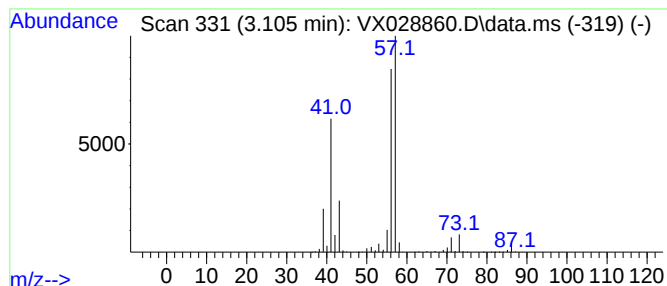
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	188.01 ug/l	3506350	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
5			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40



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DUP051822

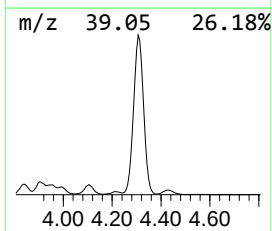
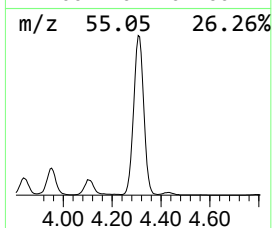
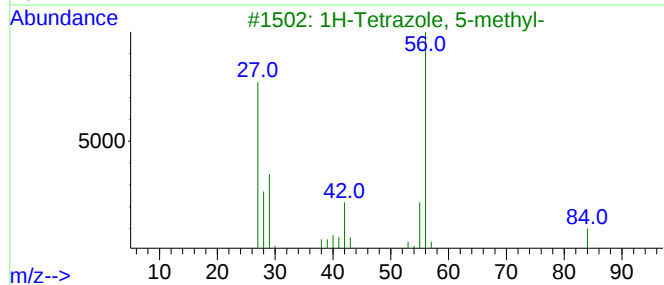
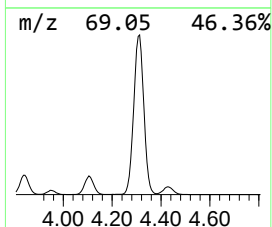
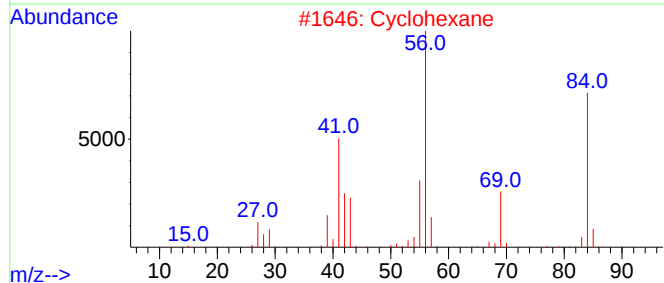
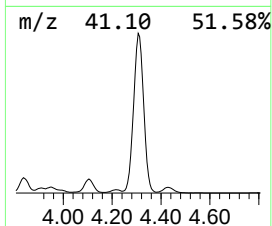
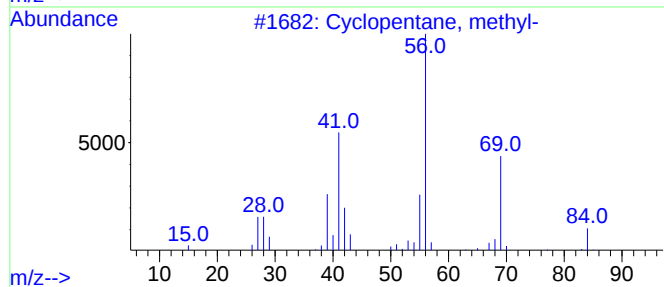
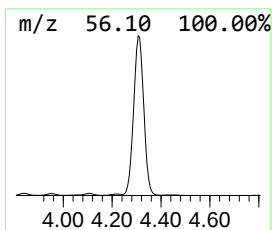
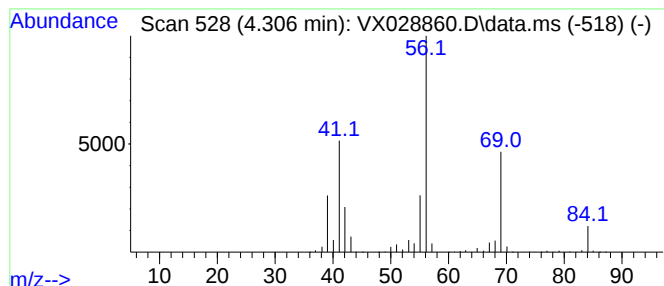
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	563.83 ug/l	10515500	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclohexane	84	C6H12	000110-82-7	78
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5		Cyclobutane	56	C4H8	000287-23-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028860.D
Acq On : 20 May 2022 18:53
Operator : JC/MD
Sample : N2943-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

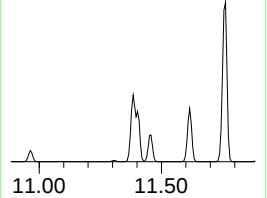
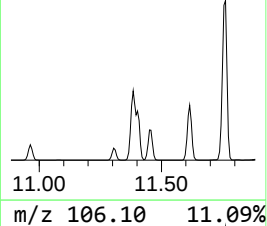
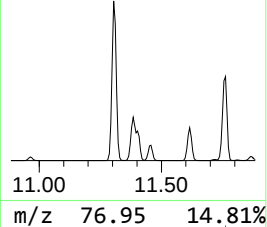
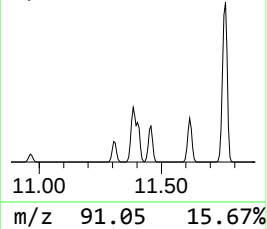
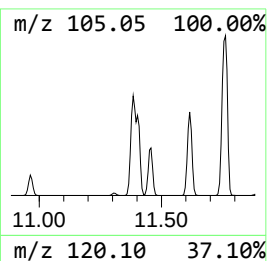
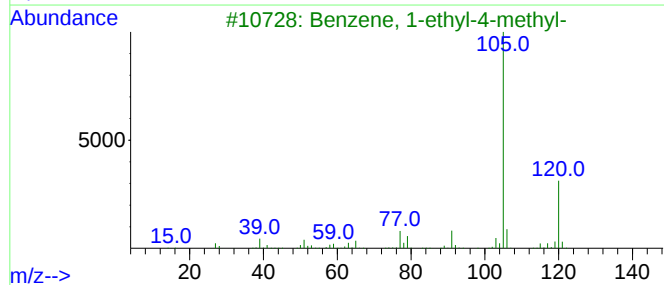
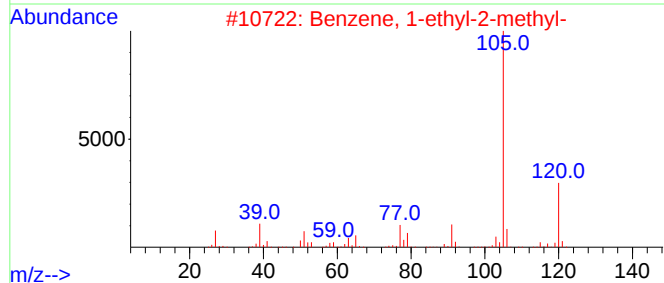
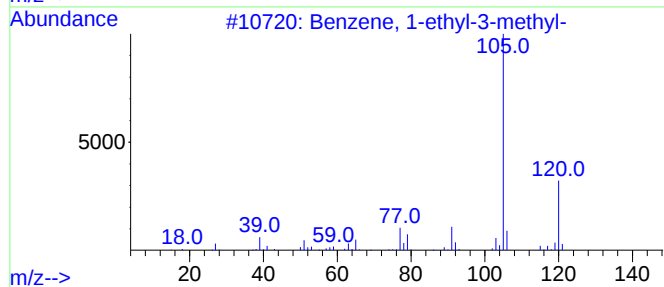
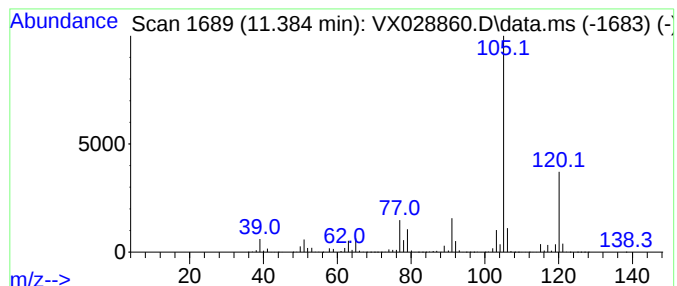
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	536.57 ug/l	19656000	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028860.D
Acq On : 20 May 2022 18:53
Operator : JC/MD
Sample : N2943-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

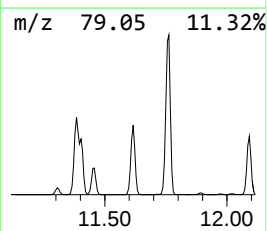
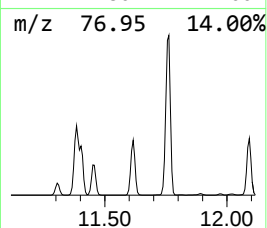
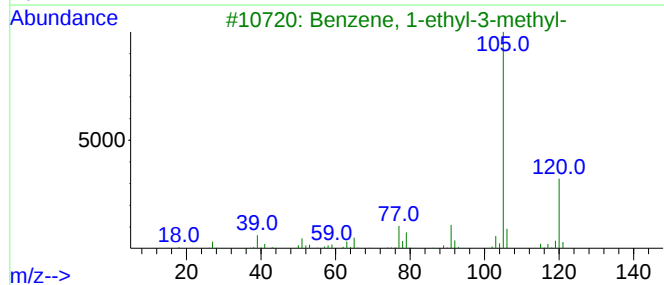
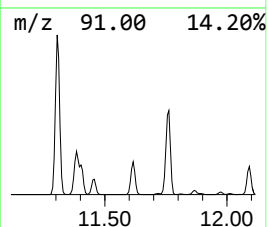
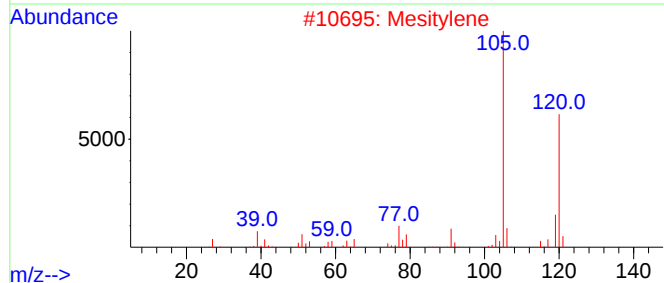
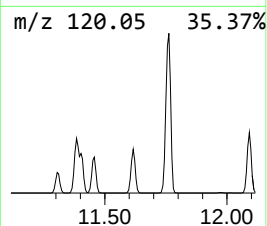
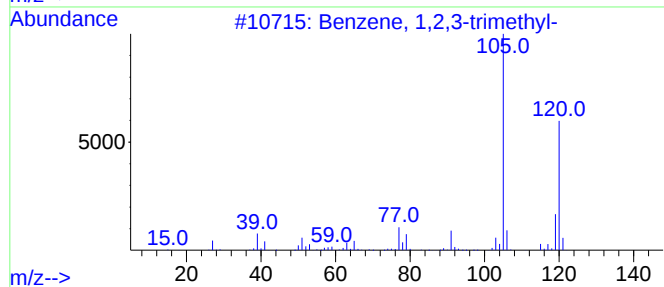
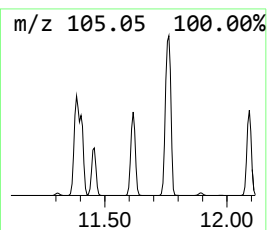
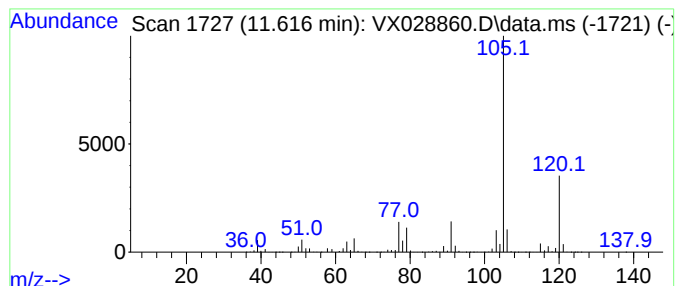
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	381.48 ug/l	13974700	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
2			Mesitylene	120	C9H12	000108-67-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028860.D
Acq On : 20 May 2022 18:53
Operator : JC/MD
Sample : N2943-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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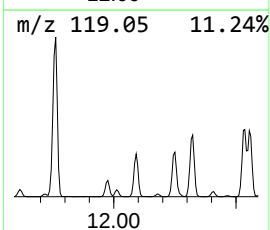
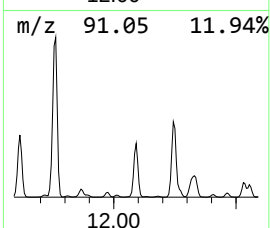
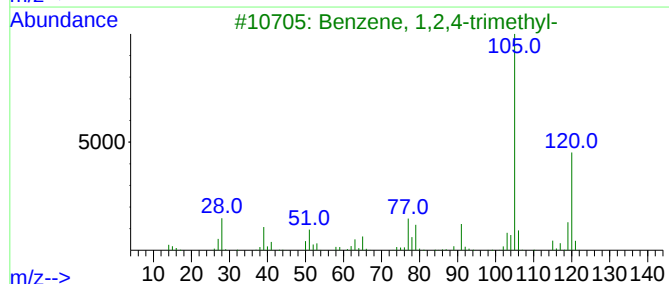
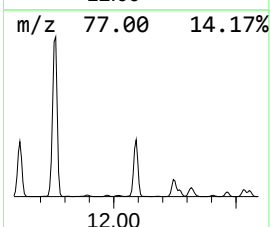
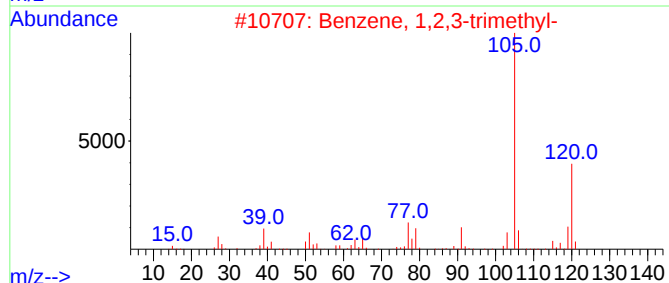
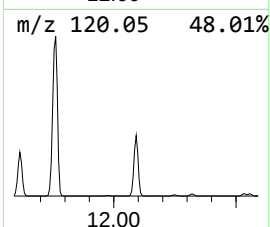
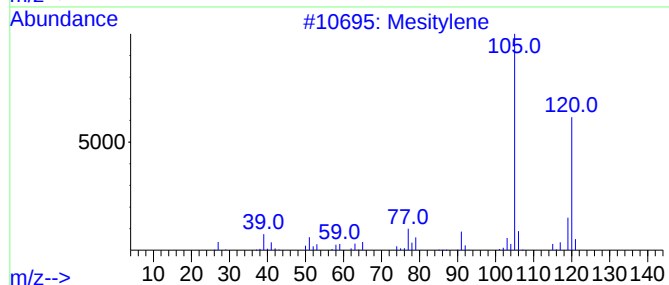
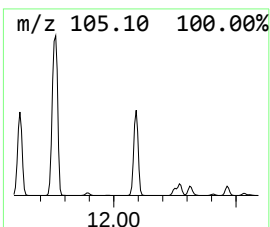
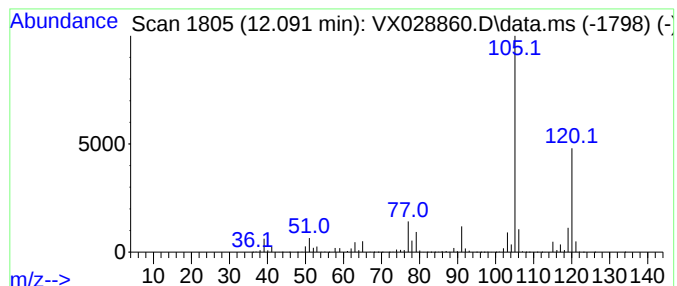
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	415.49 ug/l	15220400	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	94
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028860.D
Acq On : 20 May 2022 18:53
Operator : JC/MD
Sample : N2943-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

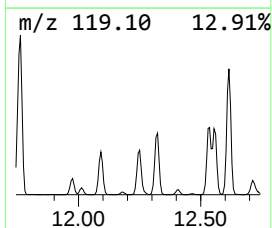
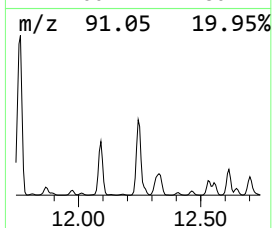
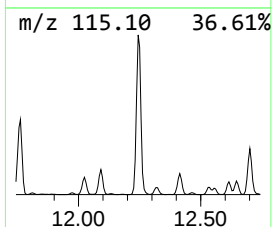
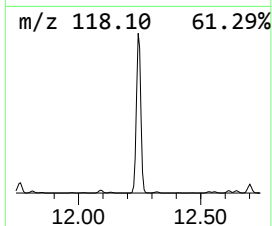
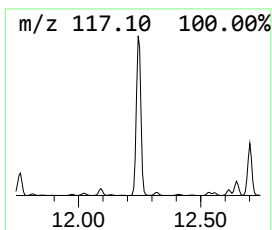
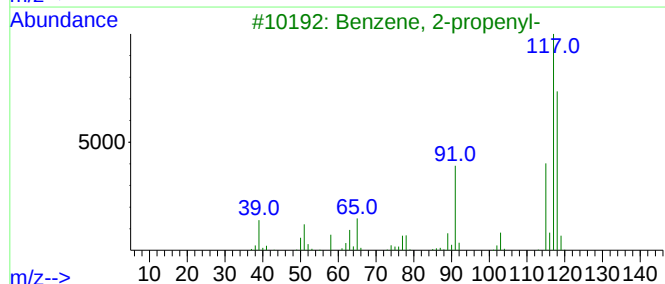
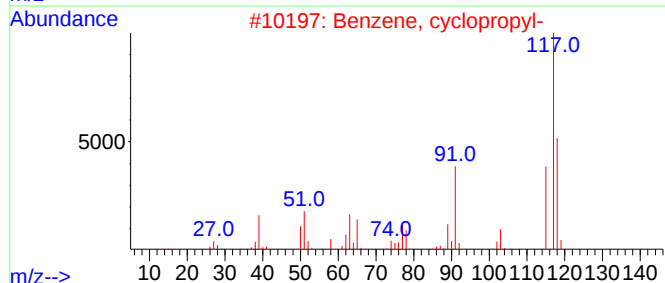
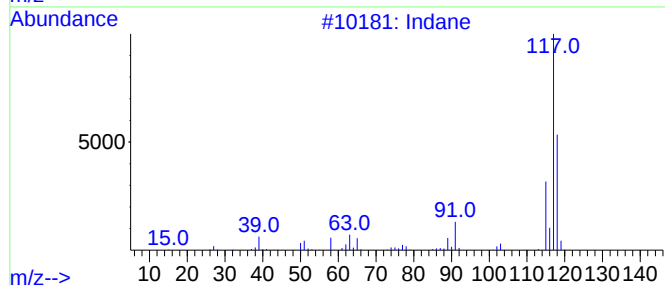
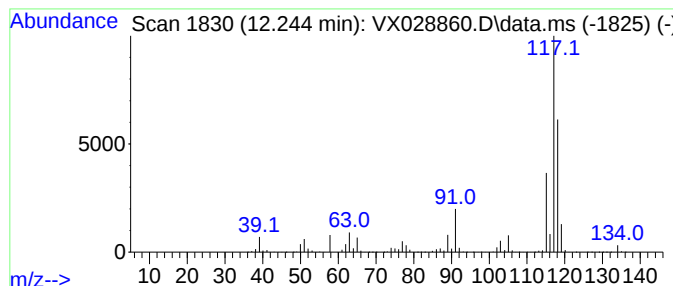
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	472.24 ug/l	17299300	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	68
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028860.D
Acq On : 20 May 2022 18:53
Operator : JC/MD
Sample : N2943-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

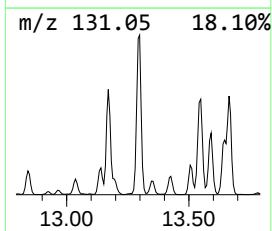
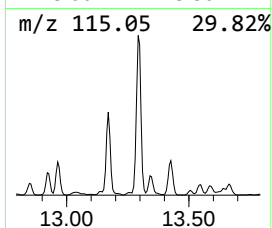
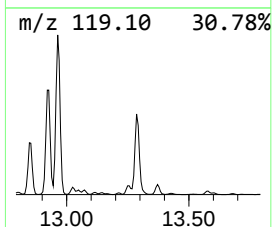
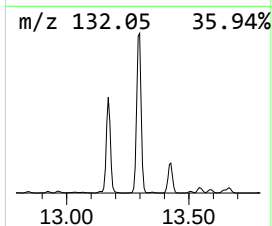
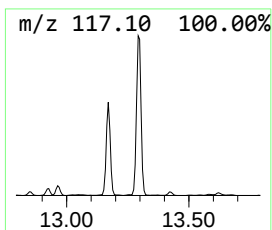
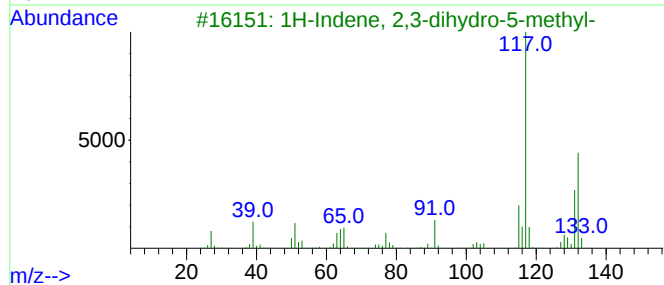
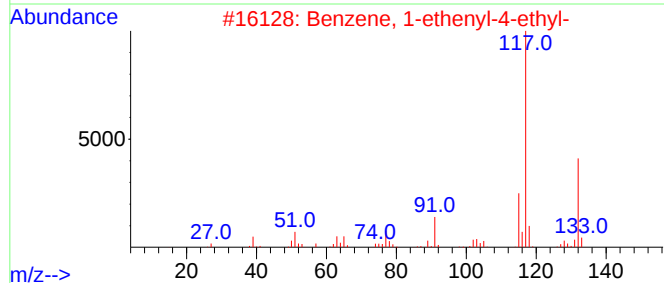
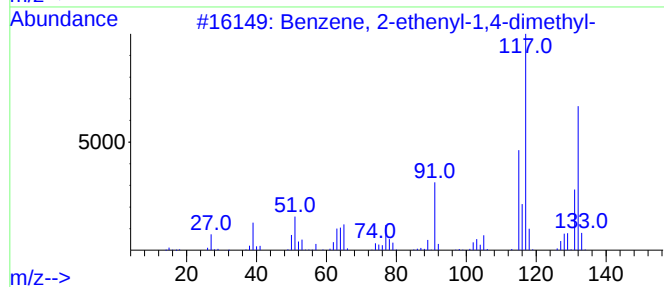
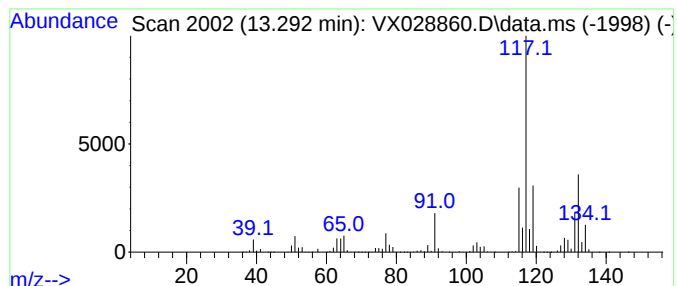
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	203.48 ug/l	7454010	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028860.D
Acq On : 20 May 2022 18:53
Operator : JC/MD
Sample : N2943-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP051822

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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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Pentane	1.953	290.4	ug/l	5416280	1	5.556	932502	50.0
Pentane, 2-methyl-	2.825	215.6	ug/l	4020000	1	5.556	932502	50.0
Pentane, 3-methyl-	3.105	188.0	ug/l	3506350	1	5.556	932502	50.0
Cyclopentane, m...	4.306	563.8	ug/l	10515500	1	5.556	932502	50.0
Benzene, 1-ethy...	11.384	536.6	ug/l	19656000	4	12.024	1831630	50.0
Benzene, 1,2,3-...	11.616	381.5	ug/l	13974700	4	12.024	1831630	50.0
Benzene, 1-ethy...	12.091	415.5	ug/l	15220400	4	12.024	1831630	50.0
Indane	12.244	472.2	ug/l	17299300	4	12.024	1831630	50.0
Benzene, 2-ethe...	13.292	203.5	ug/l	7454010	4	12.024	1831630	50.0