

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
 Data File : VX028828.D
 Acq On : 19 May 2022 16:19
 Operator : JC/MD
 Sample : N2943-18 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-23

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: VX028828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	52	rBV	130766	137095	2.02%	0.299%
2	1.745	103	108	122	rBV	551535	768415	11.33%	1.677%
3	1.953	137	142	154	rVB2	362874	582145	8.58%	1.270%
4	2.069	156	161	168	rVV	78207	112898	1.66%	0.246%
5	2.166	172	177	180	rVV	44380	68096	1.00%	0.149%
6	2.215	180	185	194	rVB	163368	244422	3.60%	0.533%
7	2.782	258	278	280	rBV4	60680	178168	2.63%	0.389%
8	2.825	280	285	289	rVV	169920	370730	5.47%	0.809%
9	2.867	289	292	302	rVV2	146391	330939	4.88%	0.722%
10	3.105	319	331	343	rBV	132188	308295	4.54%	0.673%
11	3.318	357	366	378	rBV	30187	73865	1.09%	0.161%
12	3.446	378	387	400	rBV	78813	178983	2.64%	0.391%
13	3.733	428	434	443	rVB2	62604	148601	2.19%	0.324%
14	3.843	443	452	457	rBV2	39223	99377	1.46%	0.217%
15	4.105	485	495	504	rVB3	44217	117119	1.73%	0.256%
16	4.306	518	528	540	rVB	332307	947949	13.97%	2.069%
17	5.196	651	674	687	rVB3	62130	205793	3.03%	0.449%
18	5.391	692	706	712	rBV2	180825	529418	7.80%	1.155%
19	5.477	712	720	726	rVV2	186263	555889	8.19%	1.213%
20	5.556	726	733	743	rVB	259965	709591	10.46%	1.549%
21	5.836	764	779	790	rBV5	29035	94603	1.39%	0.206%
22	5.958	790	799	806	rBV	183387	487160	7.18%	1.063%
23	6.037	806	812	823	rVB	109472	283433	4.18%	0.619%
24	6.165	824	833	836	rBV2	26527	69874	1.03%	0.152%
25	6.257	844	848	857	rVB3	33463	83345	1.23%	0.182%
26	6.360	857	865	875	rVB2	31717	90711	1.34%	0.198%
27	6.763	922	931	942	rBV	453280	1140294	16.81%	2.489%
28	7.177	991	999	1008	rVB2	31438	75110	1.11%	0.164%
29	7.379	1020	1032	1044	rBV3	154012	391719	5.77%	0.855%
30	8.147	1153	1158	1162	rVB	44964	72916	1.07%	0.159%
31	8.506	1210	1217	1227	rVB	56948	99161	1.46%	0.216%
32	8.653	1234	1241	1247	rVV	934143	1489852	21.96%	3.251%
33	8.720	1247	1252	1259	rVB	330360	495066	7.30%	1.080%
34	8.958	1287	1291	1299	rVB2	47390	80939	1.19%	0.177%
35	10.055	1465	1471	1477	rBV	1045724	1357583	20.01%	2.963%
36	10.195	1489	1494	1505	rVV	2333381	2902314	42.78%	6.334%

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37	10.305	1505	1512	1527	rVB	5085998	6783699	100.00%	14.805%
38	10.640	1562	1567	1577	rVB	1691525	2239914	33.02%	4.888%
39	10.963	1613	1620	1627	rVB	212139	259500	3.83%	0.566%
40	11.085	1634	1640	1652	rBV	1027569	1339394	19.74%	2.923%
41	11.305	1671	1676	1683	rBV	530205	638583	9.41%	1.394%
42	11.378	1683	1688	1691	rBV	1318105	2032982	29.97%	4.437%
43	11.451	1696	1700	1708	rVB	676316	809752	11.94%	1.767%
44	11.616	1721	1727	1736	rBV	1025524	1262279	18.61%	2.755%
45	11.756	1744	1750	1756	rVB	3691770	4506968	66.44%	9.836%
46	12.024	1789	1794	1799	rVV	1408372	1692210	24.95%	3.693%
47	12.085	1800	1804	1810	rVB	1070295	1366854	20.15%	2.983%
48	12.244	1825	1830	1838	rBV2	1133583	1519176	22.39%	3.315%
49	12.317	1838	1842	1851	rVB4	211488	319520	4.71%	0.697%
50	12.408	1852	1857	1862	rBV2	51436	72487	1.07%	0.158%
51	12.463	1862	1866	1872	rVB	83338	98943	1.46%	0.216%
52	12.530	1872	1877	1879	rBV	174690	214315	3.16%	0.468%
53	12.555	1879	1881	1886	rVB	152710	172210	2.54%	0.376%
54	12.615	1886	1891	1894	rBV	314722	373896	5.51%	0.816%
55	12.646	1894	1896	1900	rVV	91174	97767	1.44%	0.213%
56	12.701	1900	1905	1913	rVB2	283982	373589	5.51%	0.815%
57	12.847	1925	1929	1935	rVB	91409	115354	1.70%	0.252%
58	12.920	1935	1941	1945	rBV	186118	232278	3.42%	0.507%
59	12.963	1945	1948	1954	rVB	276528	318173	4.69%	0.694%
60	13.170	1978	1982	1986	rVB	215318	250788	3.70%	0.547%
61	13.292	1997	2002	2007	rVB2	514806	658574	9.71%	1.437%
62	13.426	2019	2024	2032	rVB	113786	149033	2.20%	0.325%
63	13.664	2060	2063	2069	rVB2	49686	76478	1.13%	0.167%
64	13.774	2074	2081	2091	rBV	958344	1236024	18.22%	2.698%
65	14.225	2149	2155	2164	rVB4	35553	71515	1.05%	0.156%
66	14.639	2218	2223	2234	rVB	308931	386786	5.70%	0.844%
67	14.780	2241	2246	2256	rBV	204642	269696	3.98%	0.589%

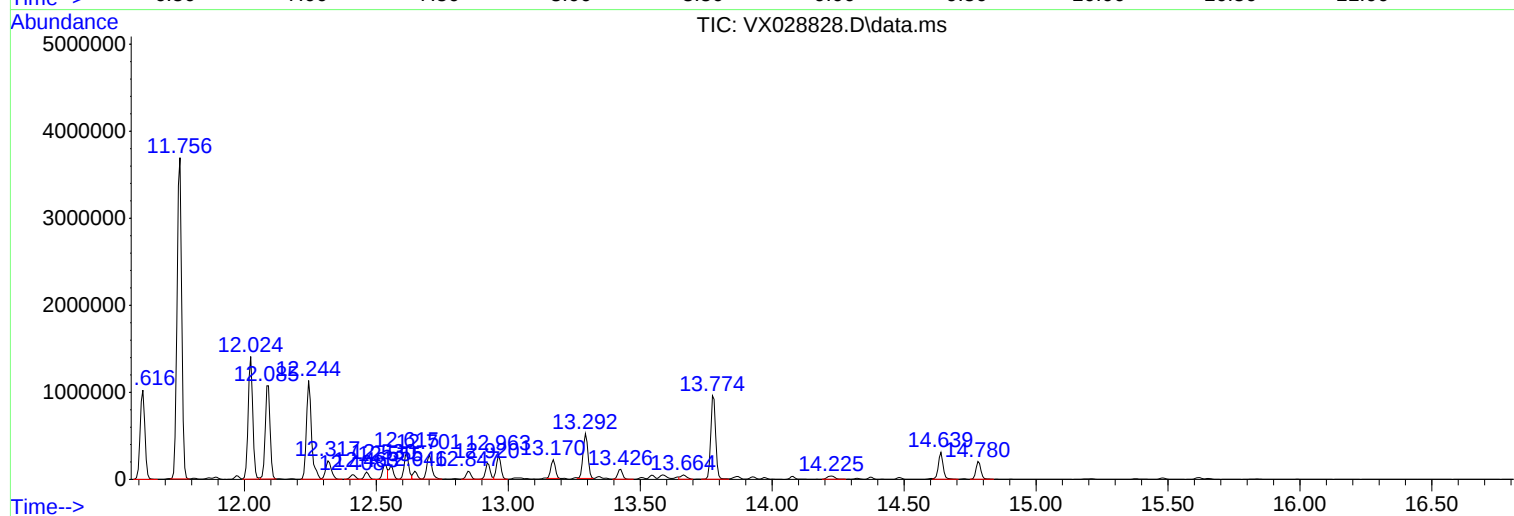
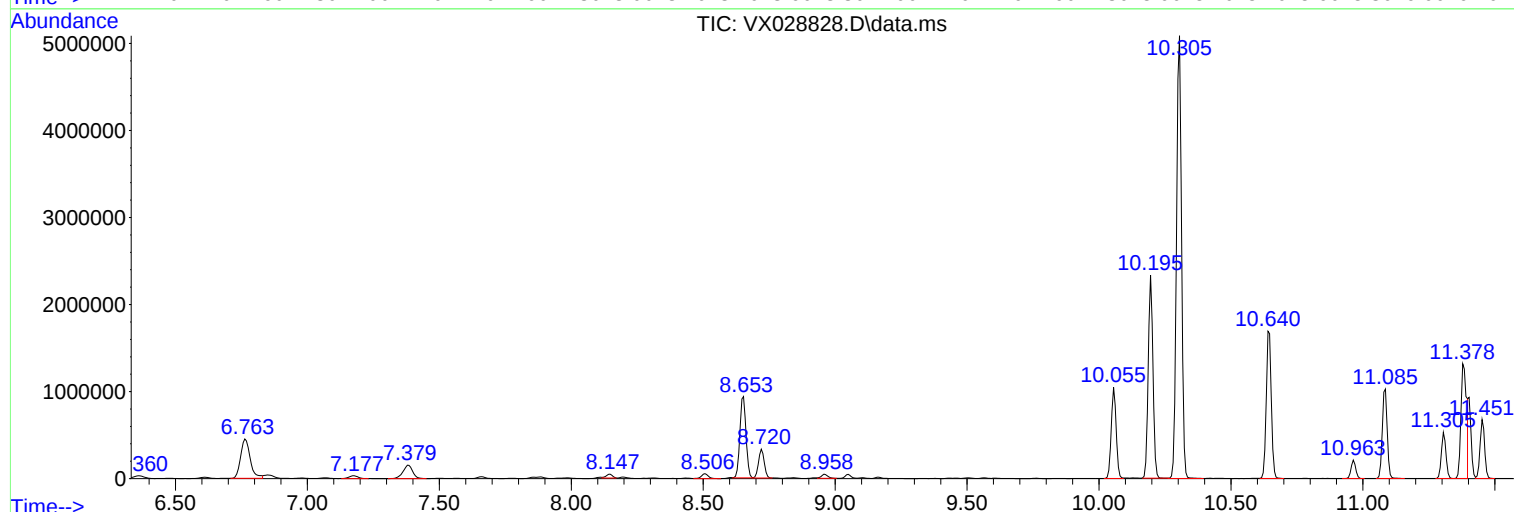
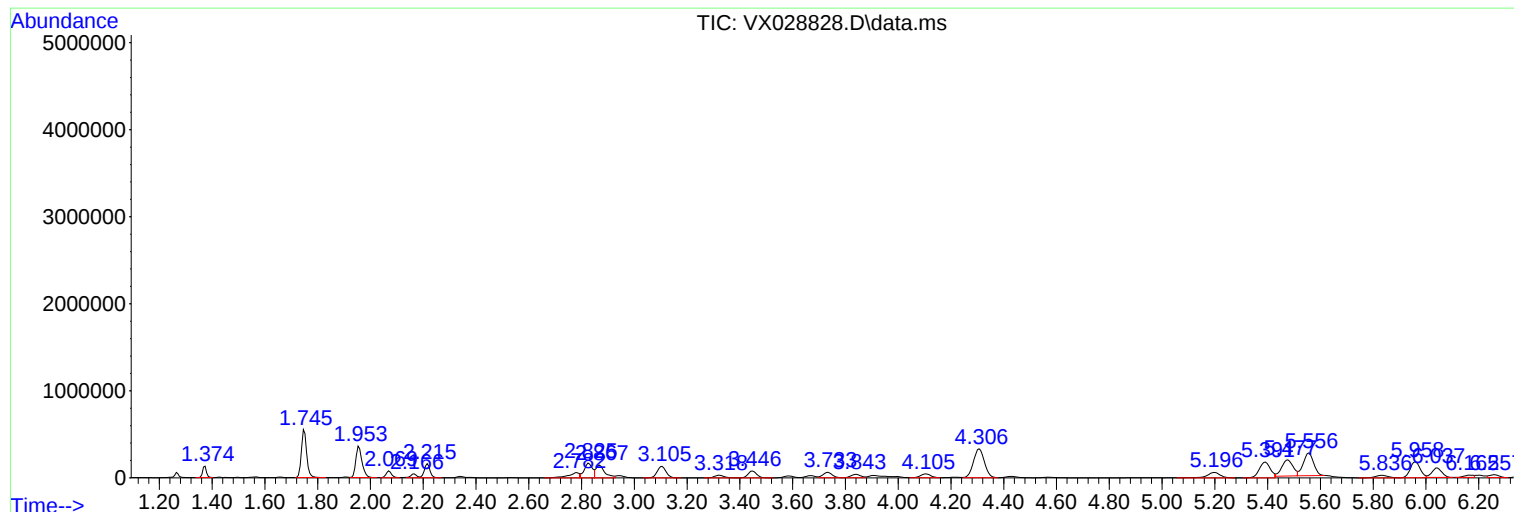
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
MSVOA_X
ClientSampleId :
MW-23

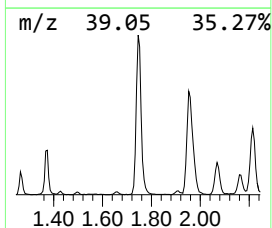
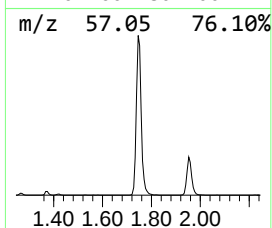
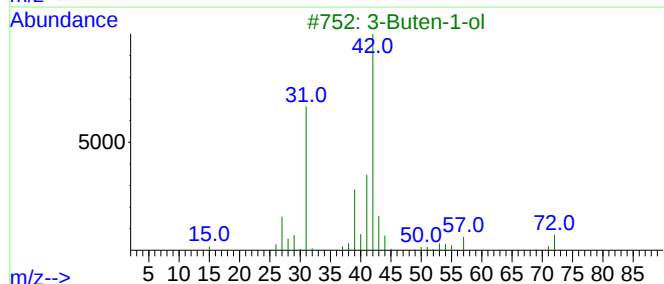
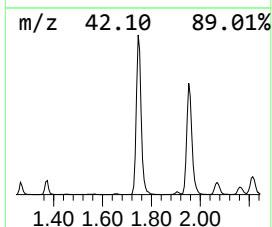
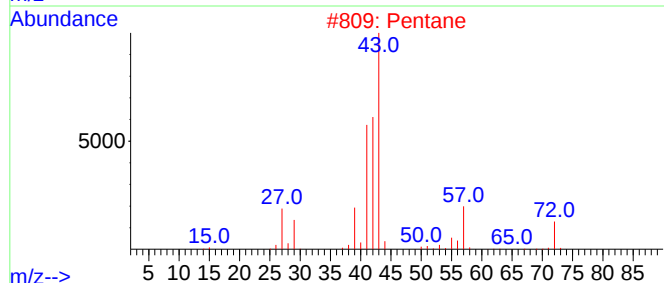
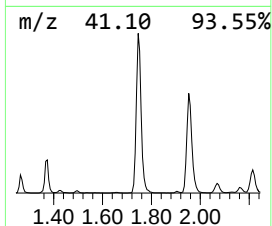
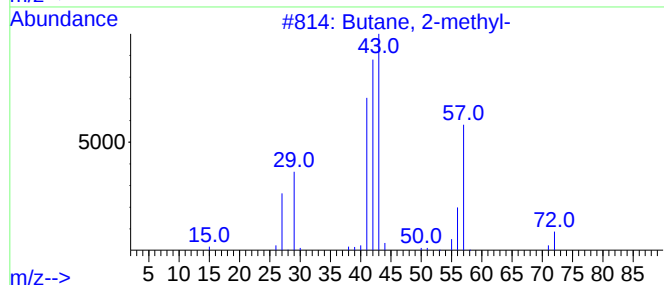
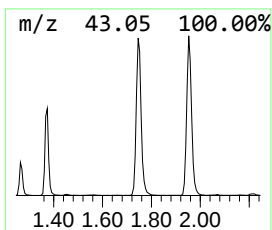
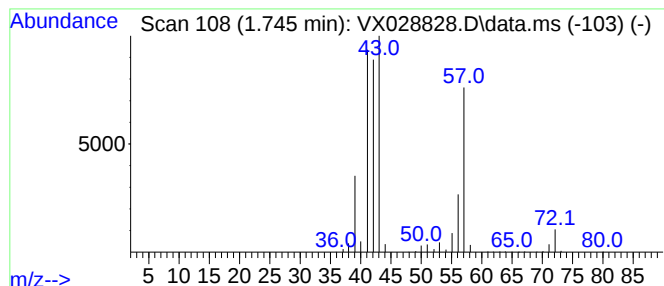
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	54.14 ug/l	768415	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	28
3			3-Buten-1-ol	72	C4H8O	000627-27-0	25
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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ClientSampleId :
MW-23

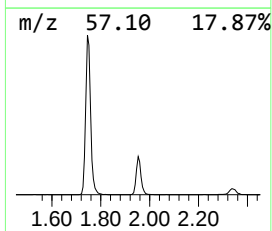
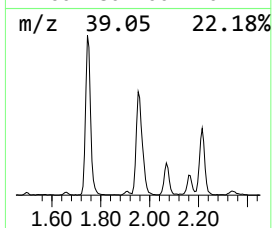
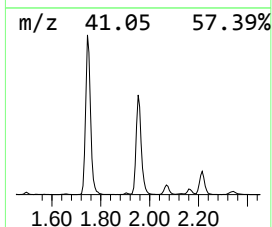
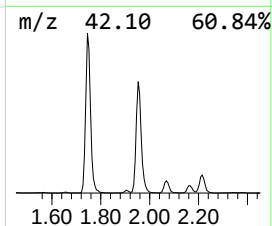
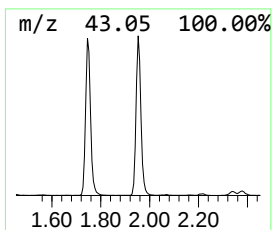
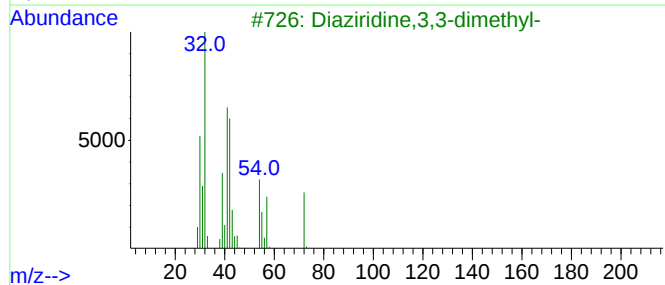
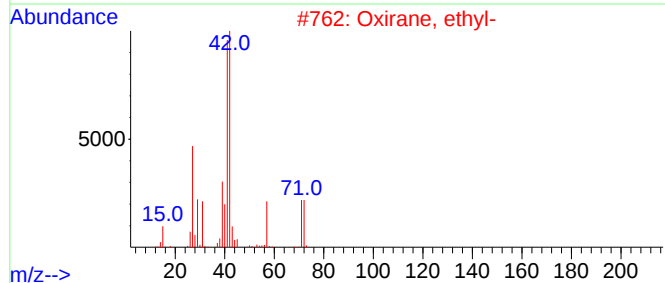
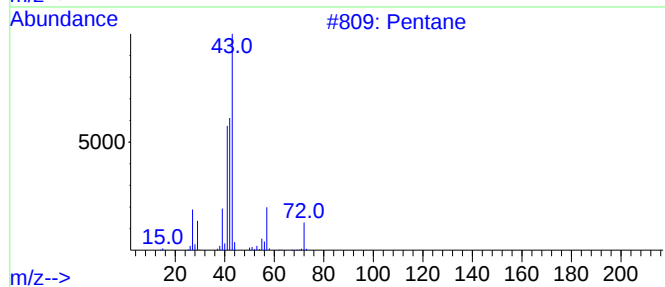
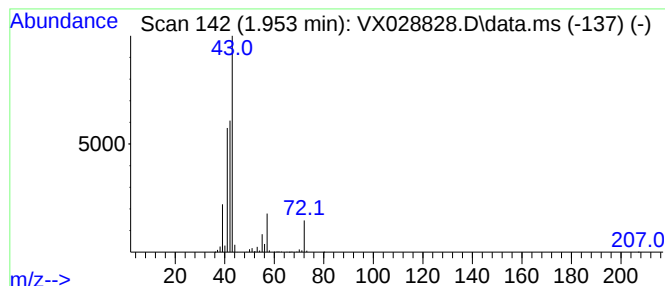
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	41.02 ug/l	582145	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	43
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	25



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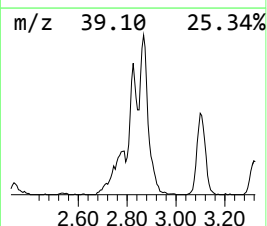
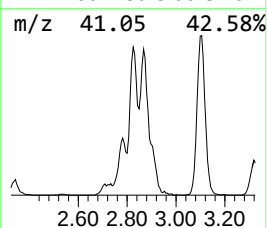
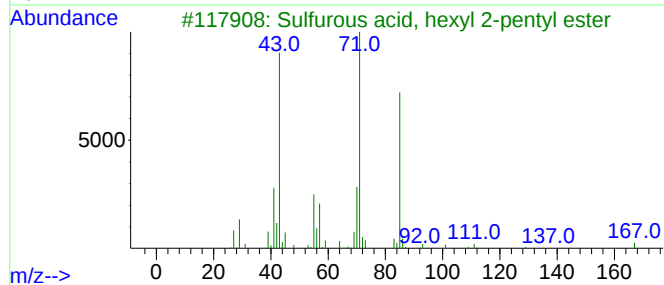
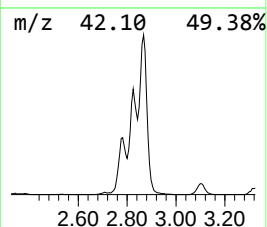
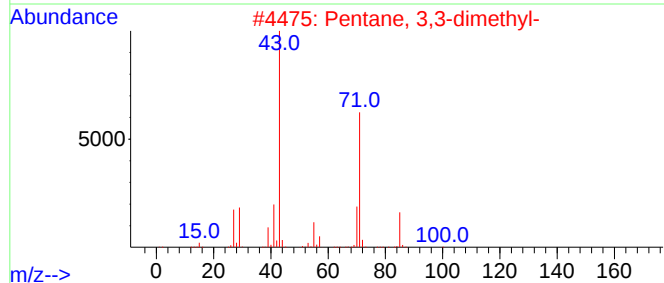
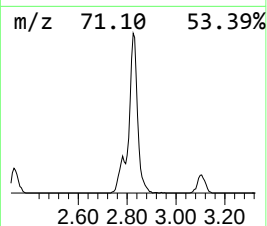
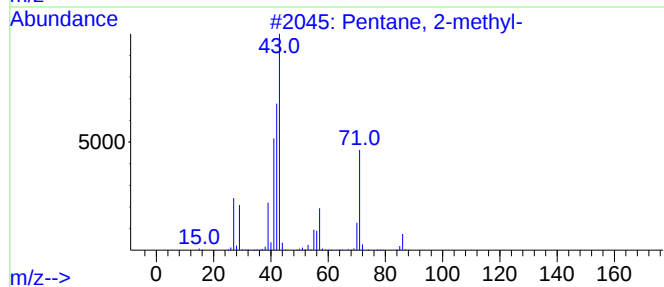
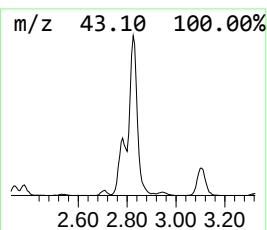
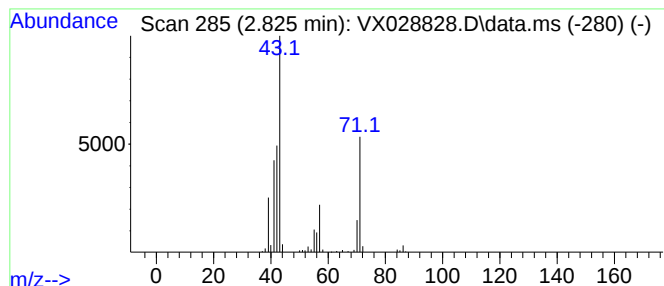
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	26.12 ug/l	370730	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	94
2			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	47
3			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	40
4			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	39
5			Pentane	72	C5H12	000109-66-0	38



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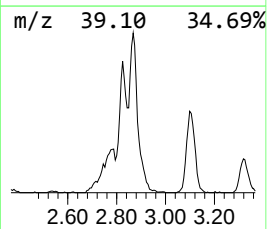
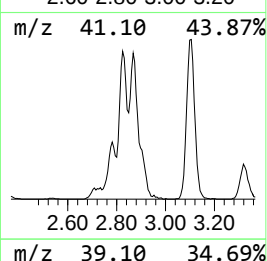
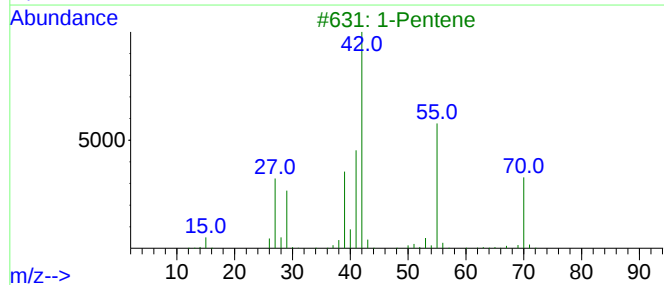
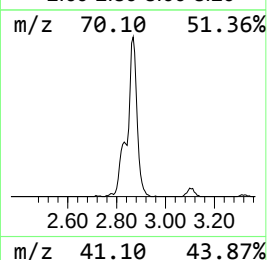
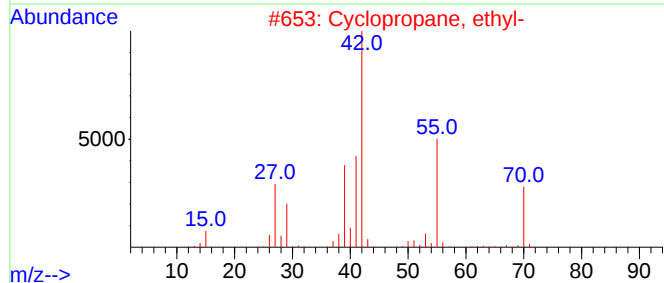
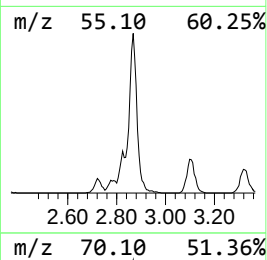
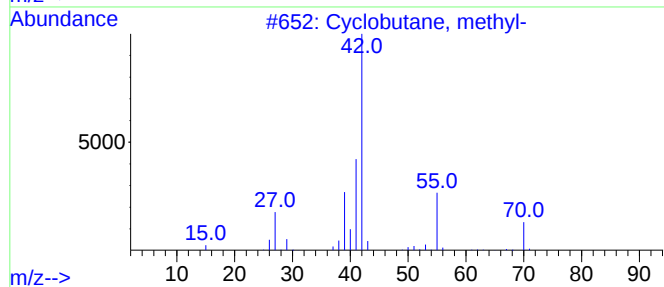
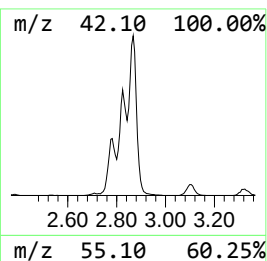
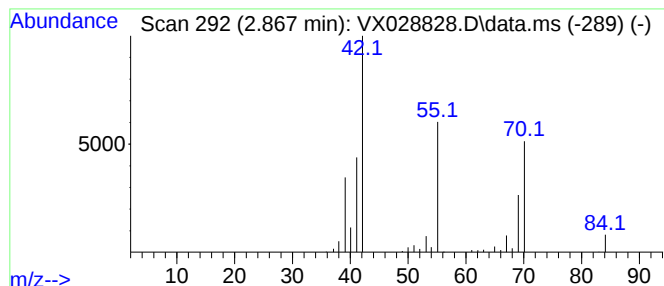
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
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Peak Number 4 Cyclobutane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	23.32 ug/l	330939	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	83
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	80
3			1-Pentene	70	C5H10	000109-67-1	80
4			2-Pentene	70	C5H10	000109-68-2	43
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

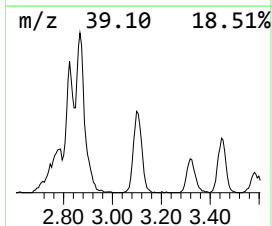
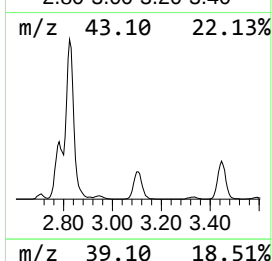
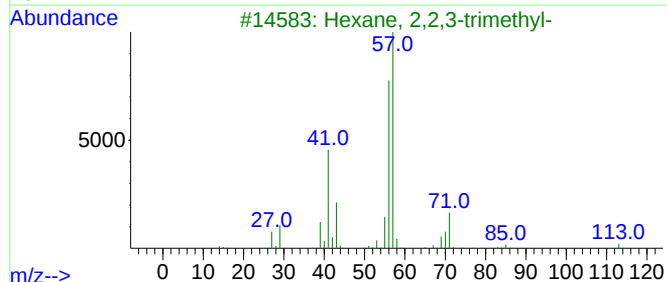
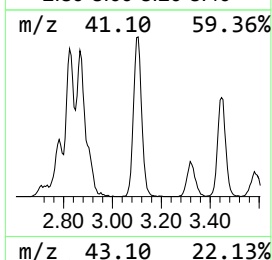
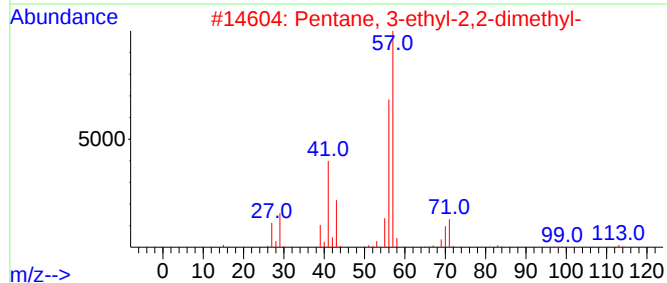
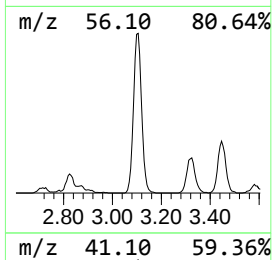
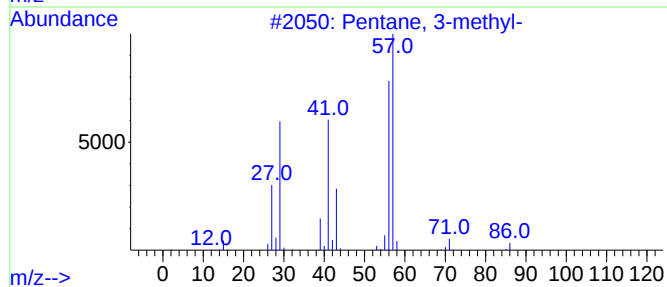
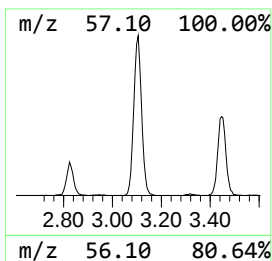
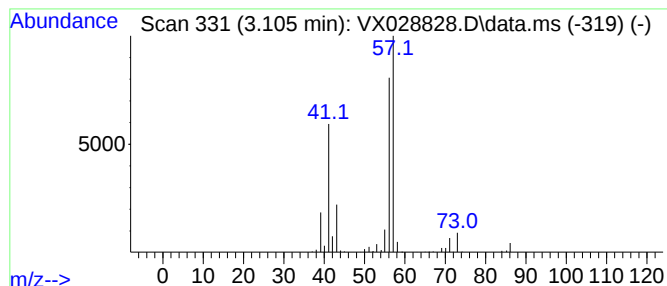
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	21.72 ug/l	308295	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	72
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

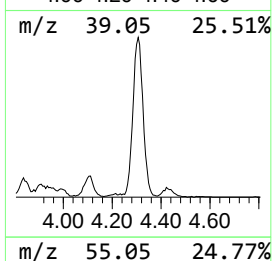
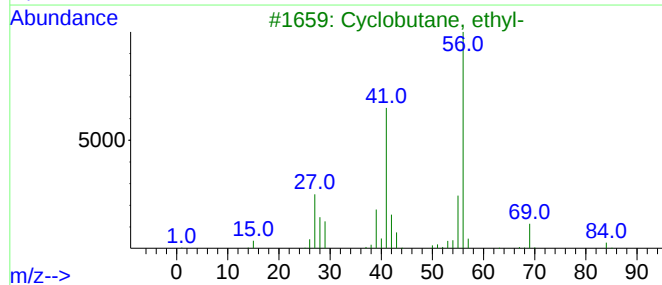
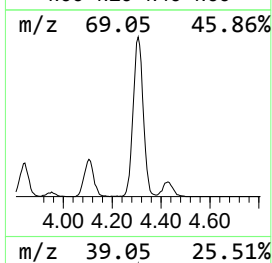
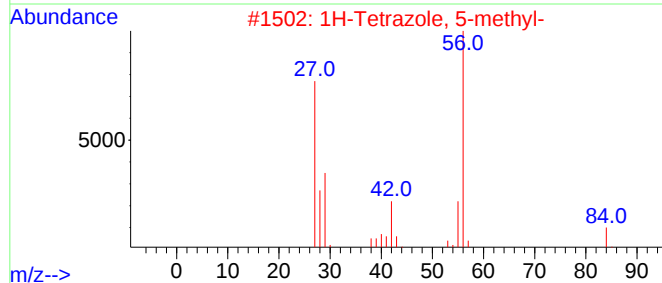
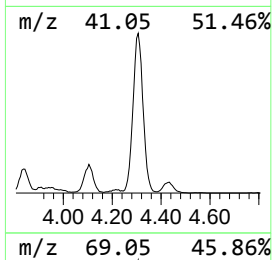
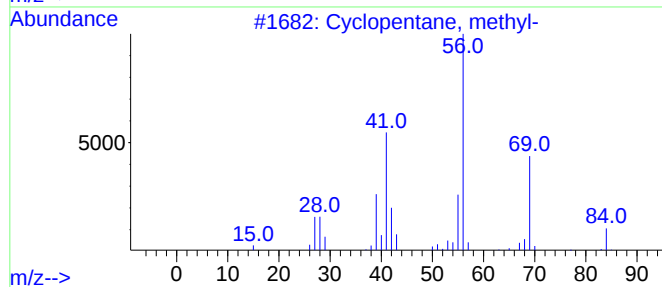
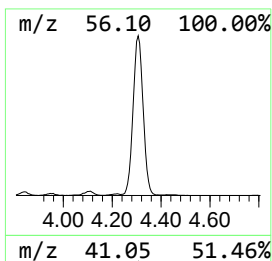
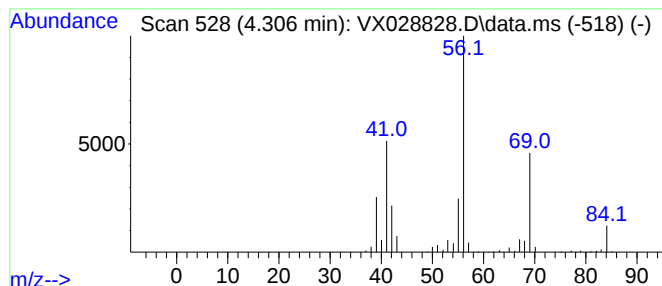
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	66.80 ug/l	947949	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			Cyclobutane	56	C4H8	000287-23-0	53
5			Cyclohexane	84	C6H12	000110-82-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

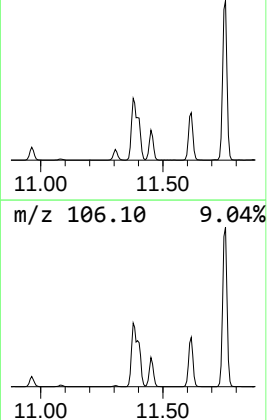
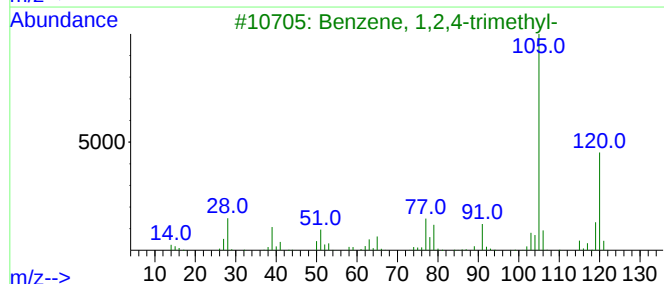
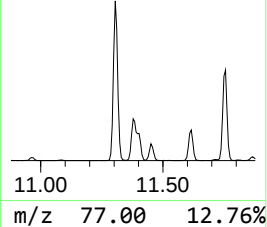
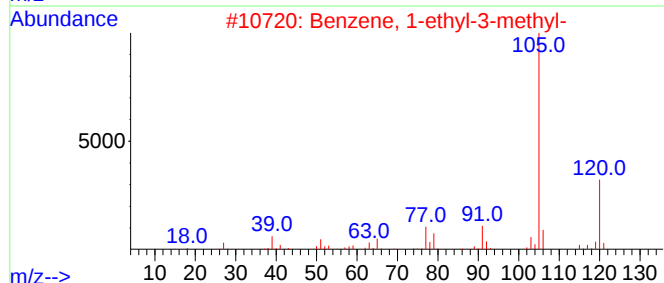
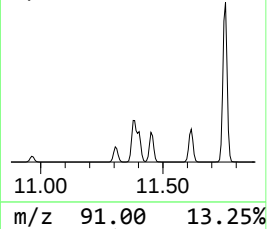
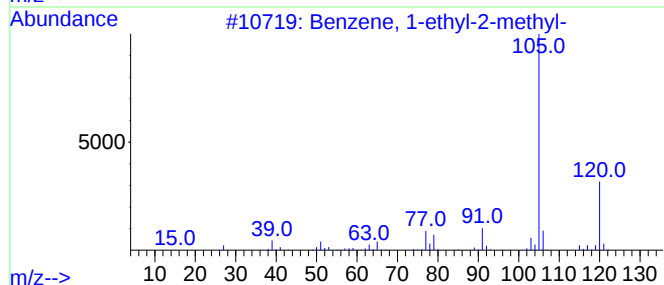
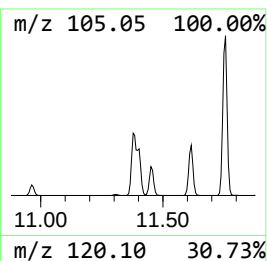
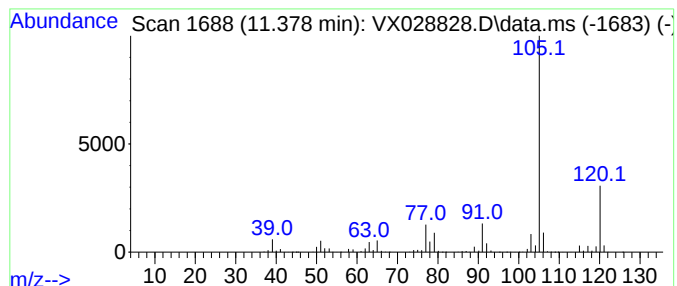
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	60.07 ug/l	2032980	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

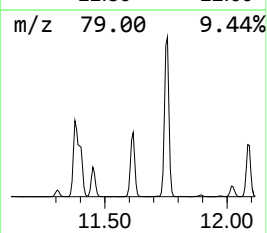
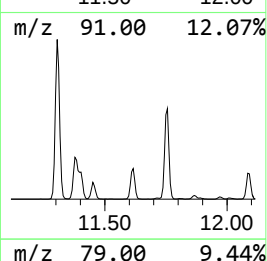
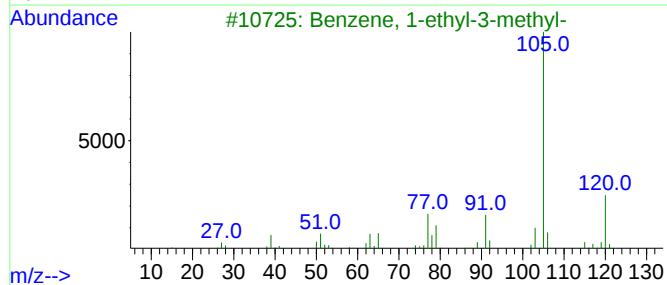
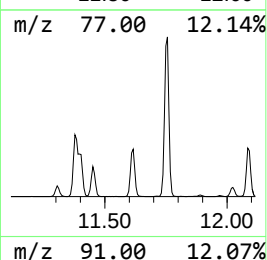
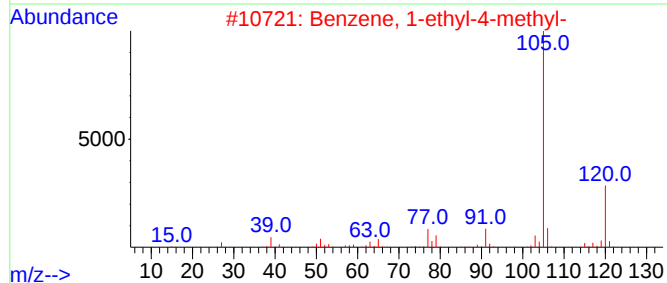
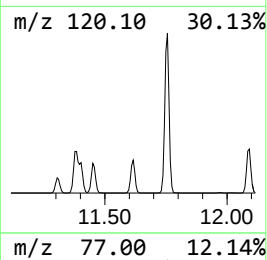
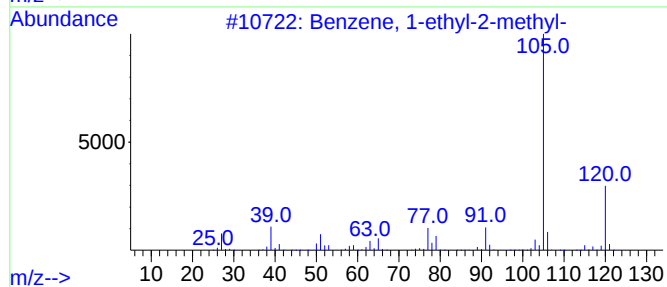
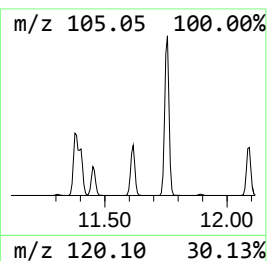
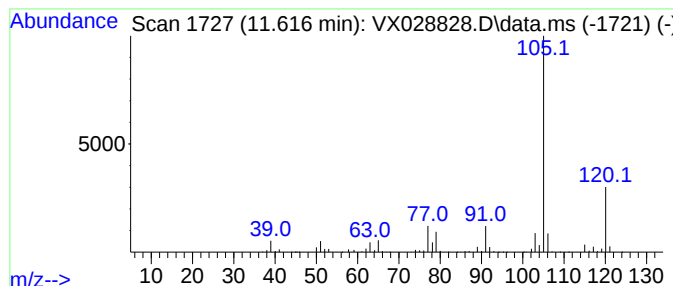
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	37.30 ug/l	1262280	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

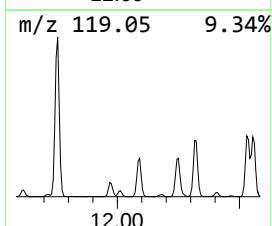
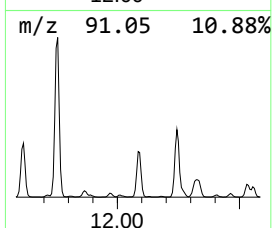
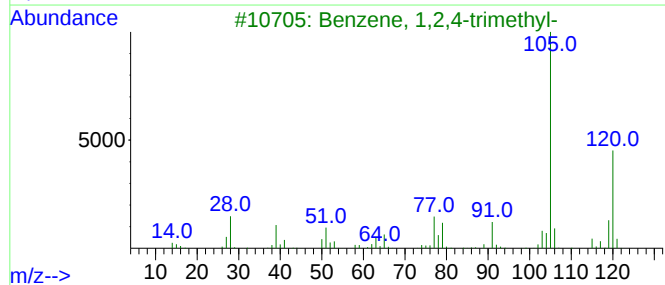
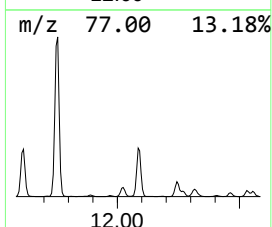
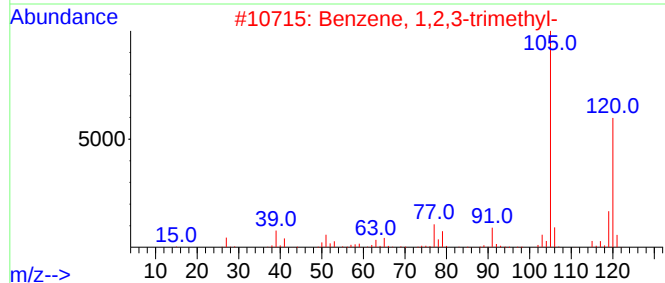
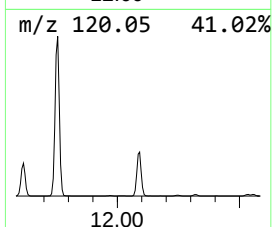
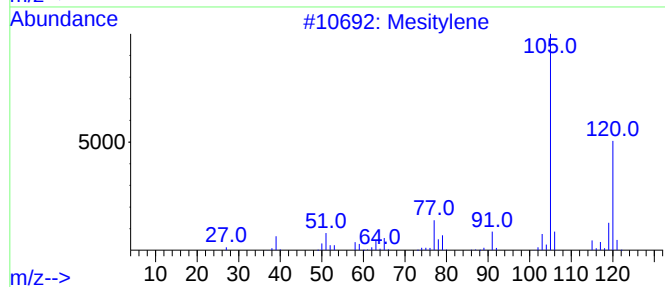
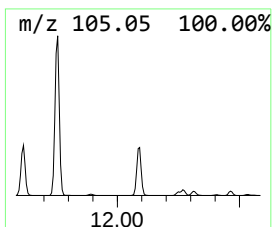
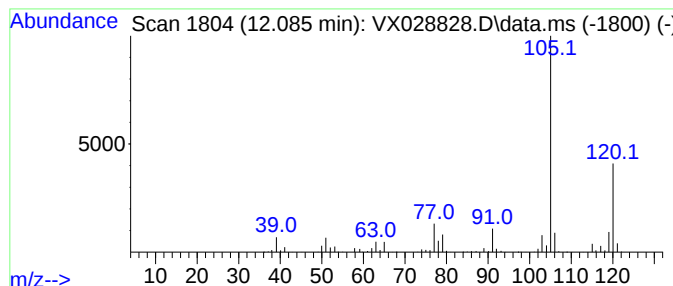
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	40.39 ug/l	1366850	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-2-methyl-	120	C9H12	000611-14-3	93
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

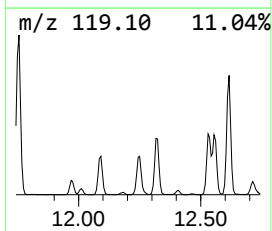
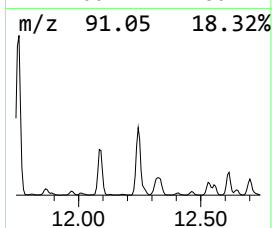
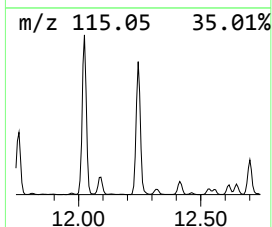
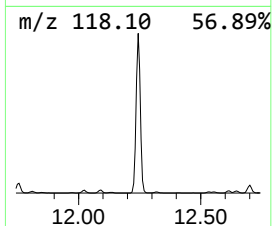
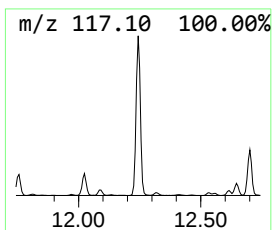
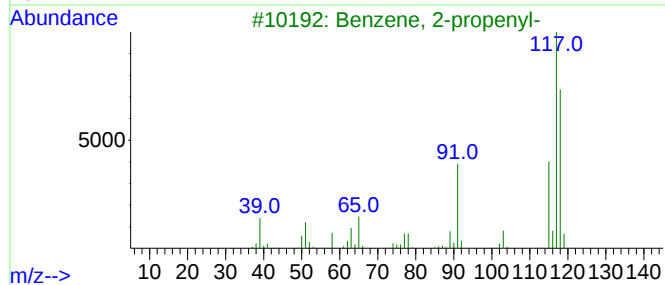
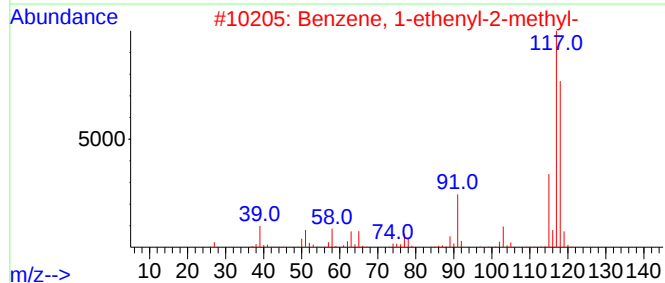
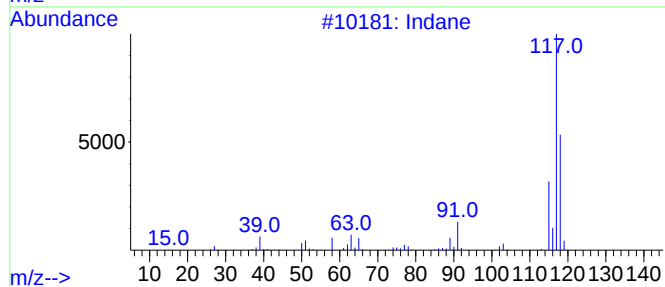
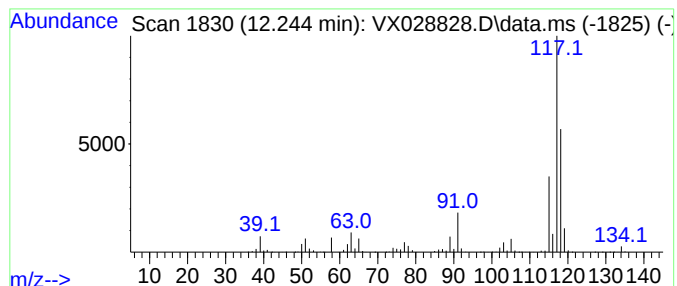
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	44.89 ug/l	1519180	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	89
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051922\
Data File : VX028828.D
Acq On : 19 May 2022 16:19
Operator : JC/MD
Sample : N2943-18 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

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	41.0	ug/l	582145	1	5.556	709591	50.0
Pentane, 2-methyl-	2.825	26.1	ug/l	370730	1	5.556	709591	50.0
Cyclobutane, me...	2.867	23.3	ug/l	330939	1	5.556	709591	50.0
Pentane, 3-methyl-	3.105	21.7	ug/l	308295	1	5.556	709591	50.0
Cyclopentane, m...	4.306	66.8	ug/l	947949	1	5.556	709591	50.0
Benzene, 1-ethy...	11.378	60.1	ug/l	2032980	4	12.024	1692210	50.0
Benzene, 1-ethy...	11.616	37.3	ug/l	1262280	4	12.024	1692210	50.0
Benzene, 1,2,3-...	12.085	40.4	ug/l	1366850	4	12.024	1692210	50.0
Indane	12.244	44.9	ug/l	1519180	4	12.024	1692210	50.0