

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
 Data File : VX029022.D
 Acq On : 27 May 2022 14:27
 Operator : JC/MD
 Sample : N2968-04 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-25

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: VX029022.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	27	29	41	rVV	60698	63343	3.12%	0.263%
2	1.374	41	47	53	rVV	112226	126126	6.22%	0.524%
3	1.752	103	109	117	rVB	153643	217295	10.71%	0.903%
4	1.904	130	134	138	rBV	19127	26402	1.30%	0.110%
5	1.953	138	142	154	rVV3	84215	157565	7.77%	0.655%
6	2.069	156	161	170	rVV	83659	121336	5.98%	0.504%
7	2.166	172	177	181	rVV	50948	82237	4.06%	0.342%
8	2.215	181	185	196	rVB	105474	162460	8.01%	0.675%
9	2.751	261	273	282	rBV	36940	96596	4.76%	0.401%
10	2.867	287	292	299	rVV	65812	142680	7.04%	0.593%
11	2.946	300	305	315	rVB	20190	48166	2.38%	0.200%
12	3.111	319	332	341	rBV2	28734	73846	3.64%	0.307%
13	3.727	428	433	444	rVB2	13863	34766	1.71%	0.144%
14	3.843	444	452	457	rBV	10389	24770	1.22%	0.103%
15	3.910	457	463	468	rBV	9637	23994	1.18%	0.100%
16	4.105	485	495	505	rVB2	10993	30462	1.50%	0.127%
17	4.306	516	528	540	rBV3	57020	168852	8.33%	0.702%
18	5.202	665	675	683	rBV2	11915	37649	1.86%	0.156%
19	5.391	693	706	715	rBV	228637	670016	33.04%	2.784%
20	5.476	715	720	725	rVV3	38524	112543	5.55%	0.468%
21	5.556	725	733	759	rVB	363994	1048696	51.71%	4.358%
22	5.958	789	799	806	rBV	227928	604216	29.79%	2.511%
23	6.043	806	813	827	rVV	208029	563954	27.81%	2.343%
24	6.208	828	840	857	rVB5	13484	67029	3.31%	0.279%
25	6.763	922	931	945	rBV	589453	1399429	69.01%	5.815%
26	7.385	1023	1033	1043	rBV4	12573	32482	1.60%	0.135%
27	8.506	1209	1217	1226	rVB3	12414	21680	1.07%	0.090%
28	8.653	1234	1241	1247	rBV	1203130	1889798	93.19%	7.853%
29	8.720	1247	1252	1262	rVB	983431	1484909	73.22%	6.170%
30	8.958	1283	1291	1297	rBV	32647	52732	2.60%	0.219%
31	9.049	1297	1306	1313	rVB	33627	49970	2.46%	0.208%
32	10.055	1465	1471	1483	rBV	1321843	1735987	85.60%	7.214%
33	10.195	1488	1494	1501	rVV	1095019	1402868	69.17%	5.829%
34	10.305	1505	1512	1526	rVB	1524745	2028001	100.00%	8.427%
35	10.640	1562	1567	1580	rVB	804683	1081515	53.33%	4.494%
36	10.963	1613	1620	1625	rBV	47497	59670	2.94%	0.248%

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37	11.079	1634	1639	1652	rBV	1037433	1384974	68.29%	5.755%
38	11.305	1670	1676	1682	rBV	102992	130330	6.43%	0.542%
39	11.378	1682	1688	1690	rBV	226052	290866	14.34%	1.209%
40	11.451	1696	1700	1708	rVB	147839	182867	9.02%	0.760%
41	11.616	1720	1727	1738	rBV	274106	342119	16.87%	1.422%
42	11.756	1744	1750	1757	rVB	862894	1086666	53.58%	4.515%
43	12.024	1788	1794	1800	rBV	1448902	1764850	87.02%	7.334%
44	12.091	1800	1805	1810	rVB	280174	351093	17.31%	1.459%
45	12.244	1824	1830	1838	rBV	428920	531368	26.20%	2.208%
46	12.317	1838	1842	1851	rVB3	41354	68293	3.37%	0.284%
47	12.414	1852	1858	1862	rBV2	29992	40685	2.01%	0.169%
48	12.463	1862	1866	1871	rVB	18688	23657	1.17%	0.098%
49	12.530	1871	1877	1880	rBV	47123	68490	3.38%	0.285%
50	12.554	1880	1881	1886	rVV	37710	31456	1.55%	0.131%
51	12.615	1886	1891	1894	rVV	87553	103830	5.12%	0.431%
52	12.646	1894	1896	1900	rVV	28757	29138	1.44%	0.121%
53	12.701	1900	1905	1914	rVB2	89373	121887	6.01%	0.506%
54	12.847	1924	1929	1934	rVB2	23902	30165	1.49%	0.125%
55	12.920	1934	1941	1945	rBV	58001	74150	3.66%	0.308%
56	12.963	1945	1948	1953	rVB	73789	87904	4.33%	0.365%
57	13.140	1972	1977	1980	rBV	89173	132708	6.54%	0.551%
58	13.170	1980	1982	1988	rVB	89728	96223	4.74%	0.400%
59	13.292	1997	2002	2007	rVB2	195151	251823	12.42%	1.046%
60	13.426	2019	2024	2030	rVB	40066	52700	2.60%	0.219%
61	13.542	2040	2043	2047	rBV	16676	21180	1.04%	0.088%
62	13.591	2047	2051	2056	rVV4	20107	32848	1.62%	0.136%
63	13.664	2060	2063	2070	rVB4	17318	28806	1.42%	0.120%
64	13.774	2076	2081	2091	rBV	362605	472245	23.29%	1.962%
65	13.871	2091	2097	2102	rVB	25937	36976	1.82%	0.154%
66	14.103	2132	2135	2141	rVB2	16917	24087	1.19%	0.100%
67	14.213	2146	2153	2159	rBV3	18261	37998	1.87%	0.158%
68	14.322	2166	2171	2175	rBV3	17184	28564	1.41%	0.119%
69	14.371	2175	2179	2189	rVB3	13355	27310	1.35%	0.113%
70	14.639	2219	2223	2233	rVB	32777	44706	2.20%	0.186%
71	14.780	2241	2246	2257	rVB	65638	88407	4.36%	0.367%

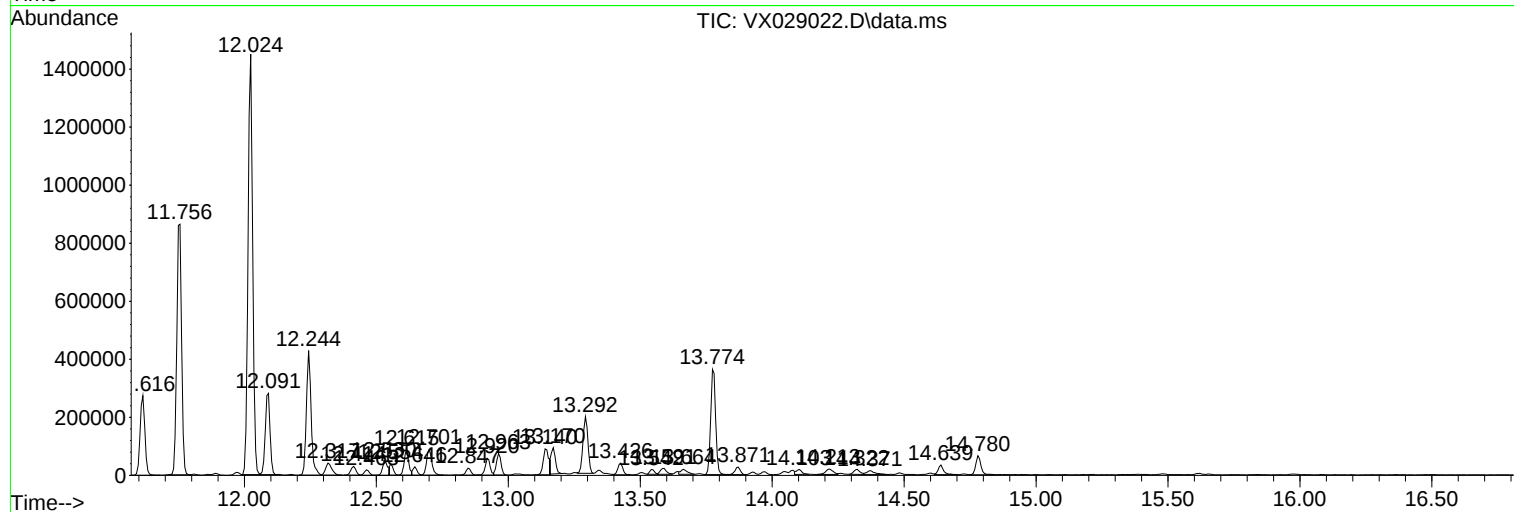
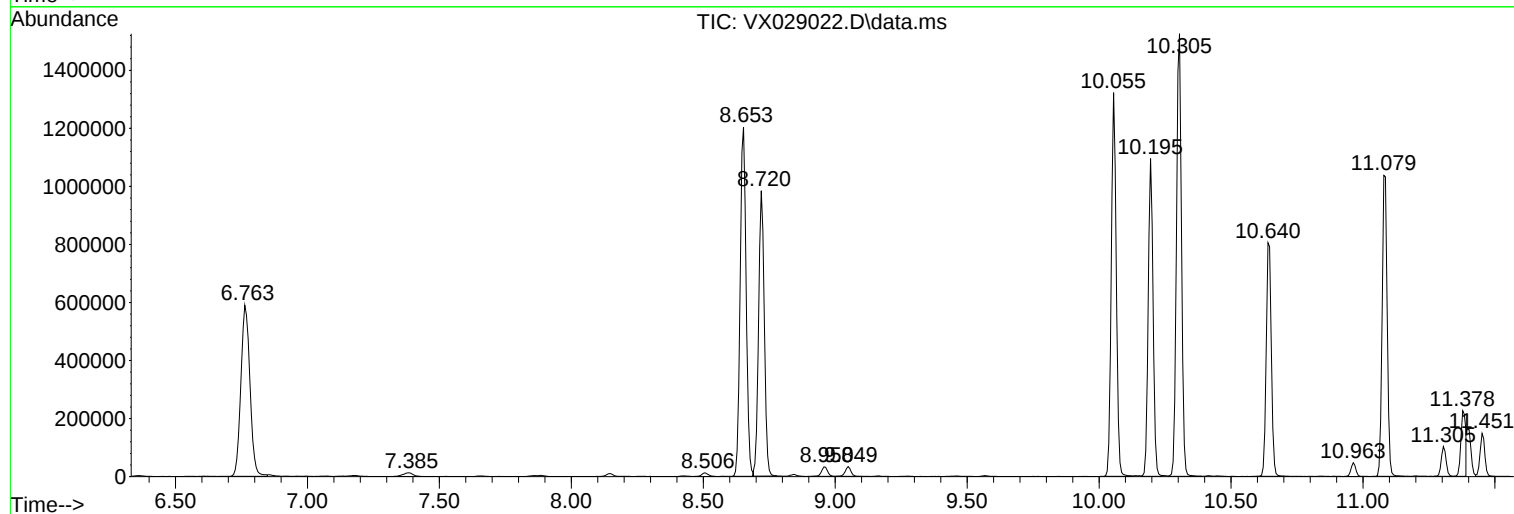
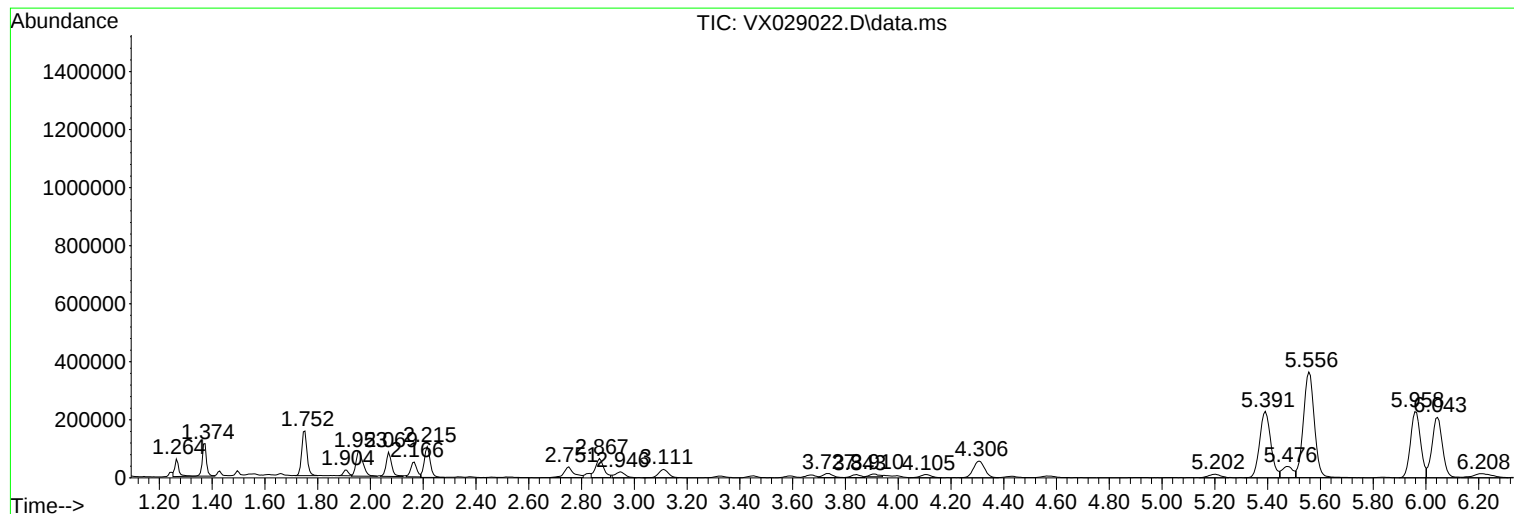
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Instrument :
MSVOA_X
ClientSampleId :
MW-25

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
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

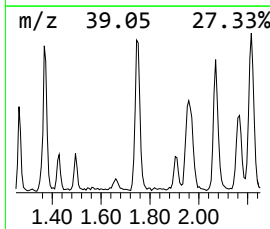
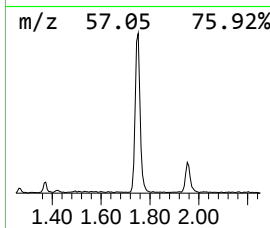
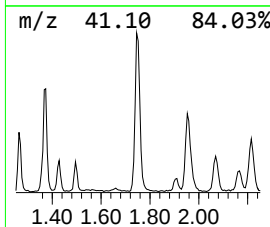
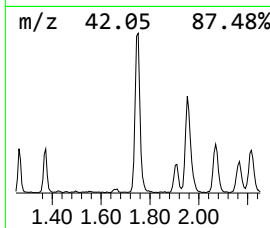
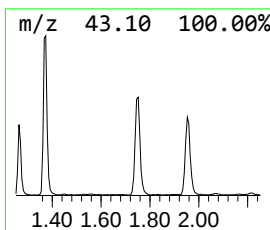
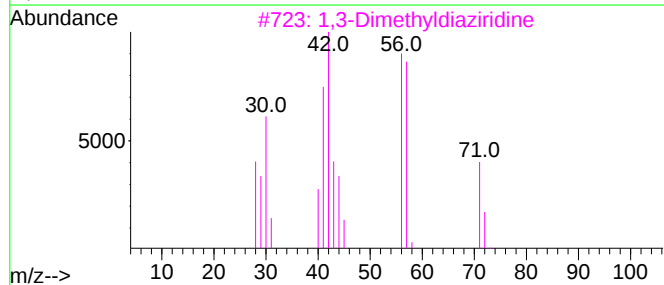
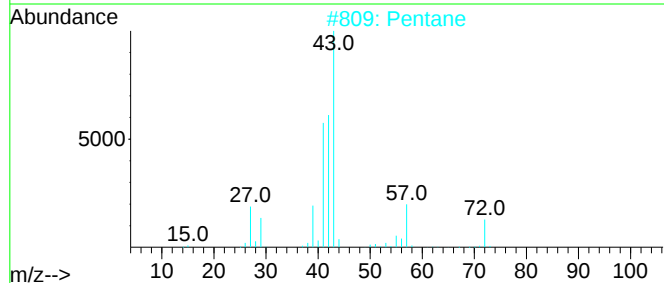
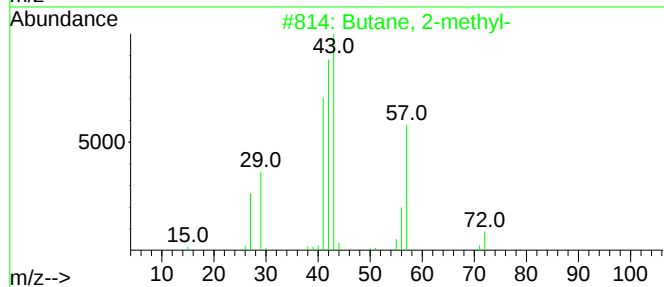
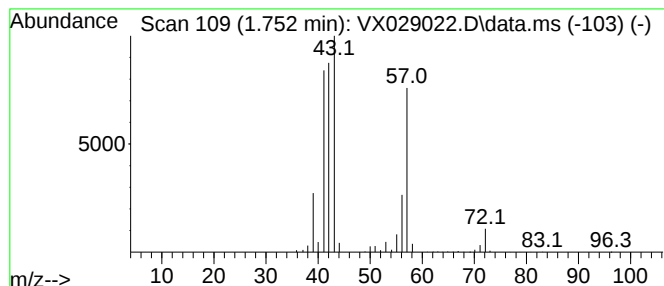
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	10.36 ug/l	217295	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			Pentane	72	C5H12	000109-66-0	43
3			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36
4			Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10



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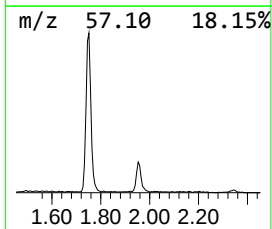
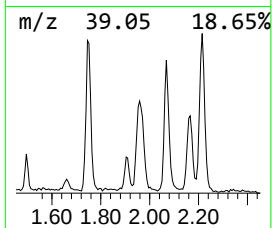
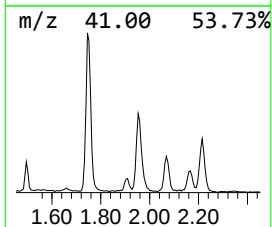
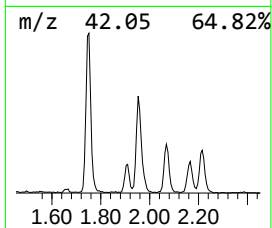
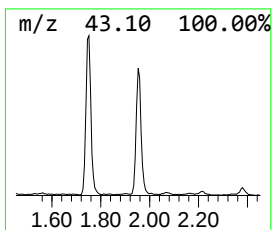
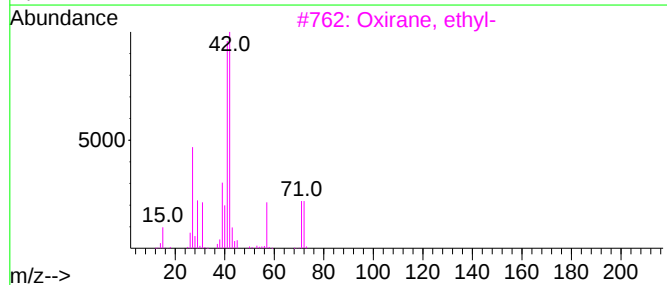
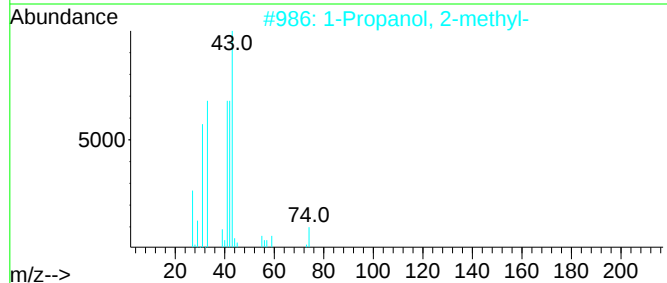
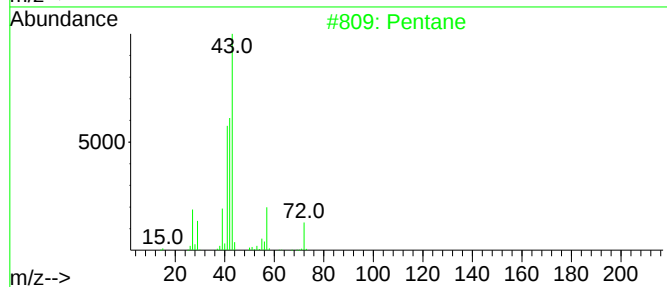
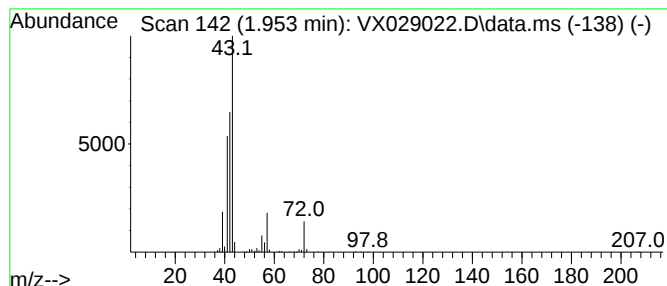
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	7.51 ug/l	157565	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	50
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	38
4			Butane, 2-methyl-	72	C5H12	000078-78-4	38
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	37



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ClientSampleId :
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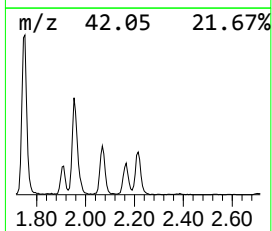
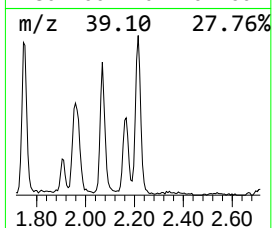
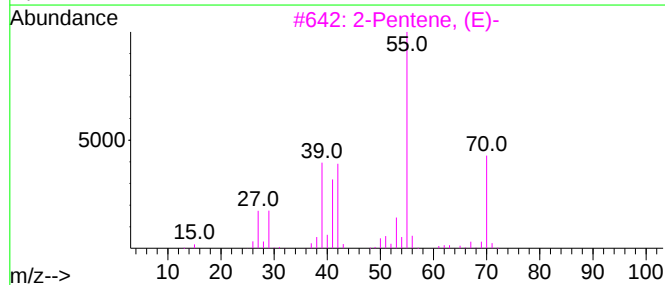
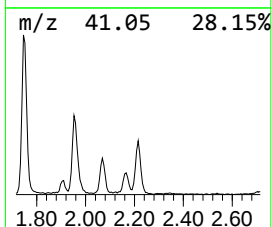
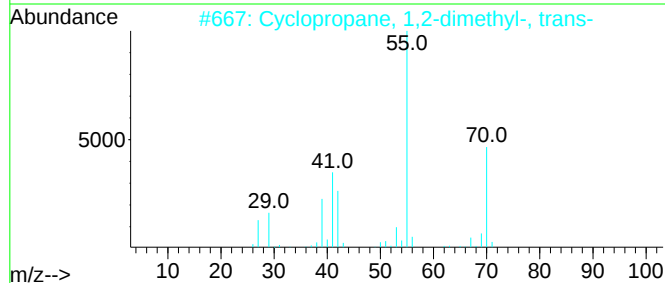
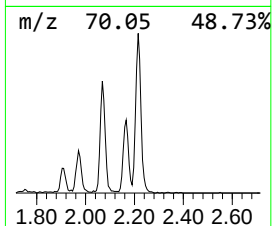
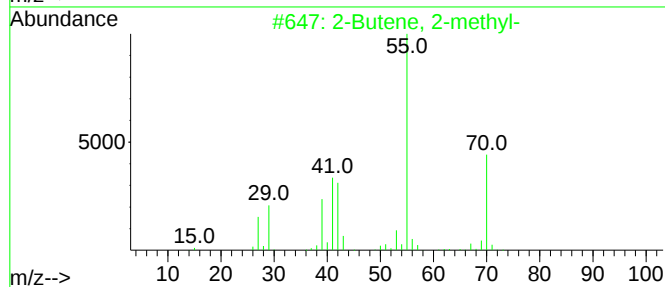
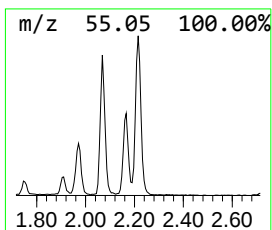
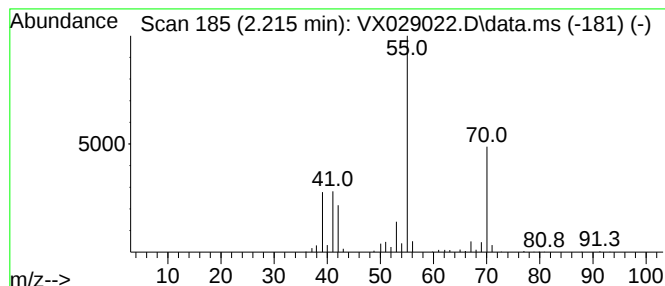
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Quant Title : SW846 8260

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

Peak Number 3 2-Butene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	7.75 ug/l	162460	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-			70	C5H10	000513-35-9	91
2	Cyclopropane, 1,2-dimethyl-, trans-			70	C5H10	002402-06-4	90
3	2-Pentene, (E)-			70	C5H10	000646-04-8	87
4	2-Methyl-1-butene			70	C5H10	000563-46-2	78
5	1-Butene, 3-methyl-			70	C5H10	000563-45-1	78



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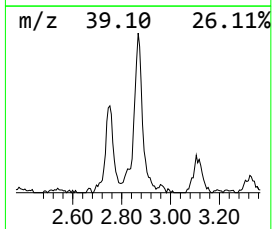
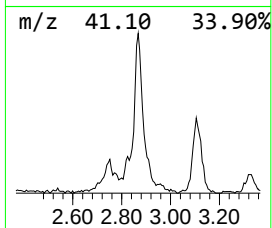
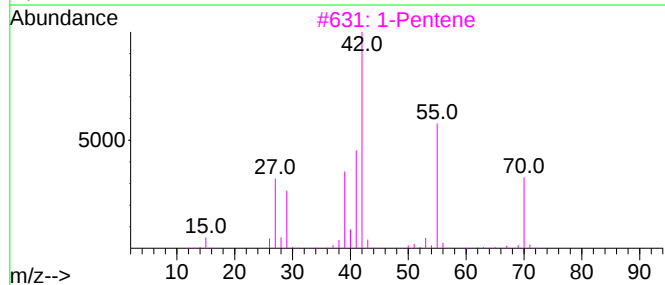
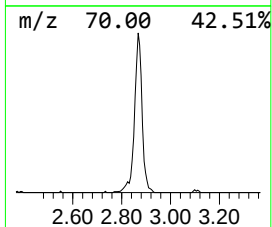
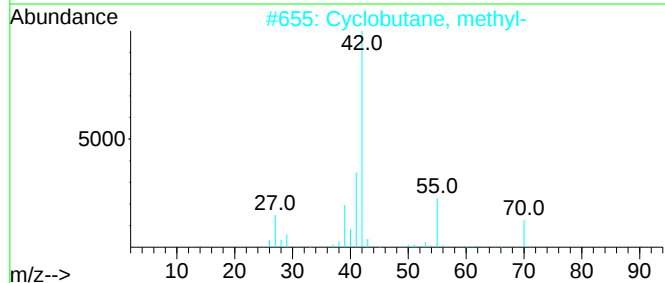
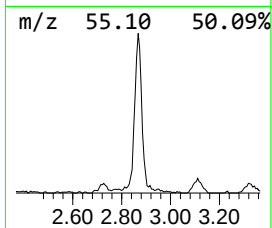
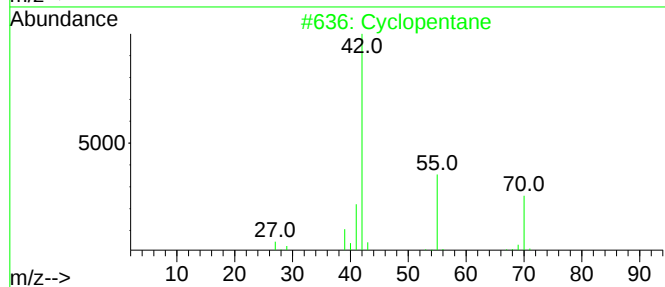
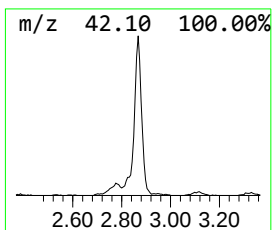
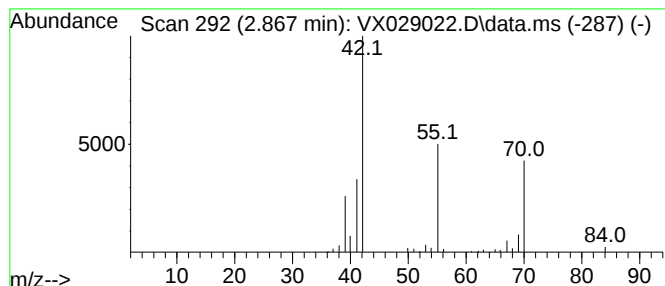
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	6.80 ug/l	142680	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	86
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3			1-Pentene	70	C5H10	000109-67-1	72
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	38
5			2-Pentene	70	C5H10	000109-68-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

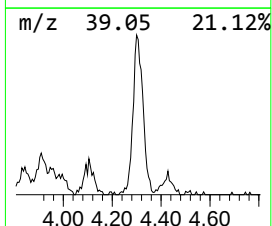
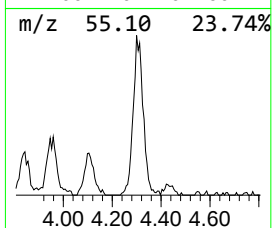
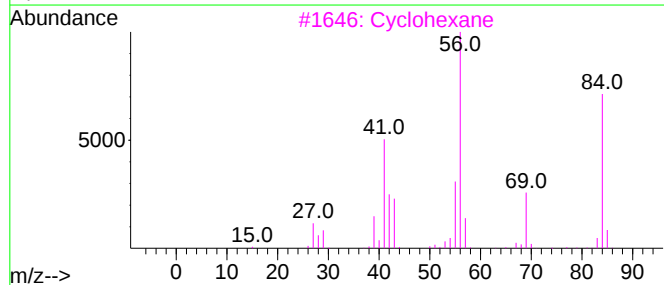
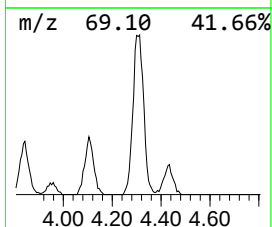
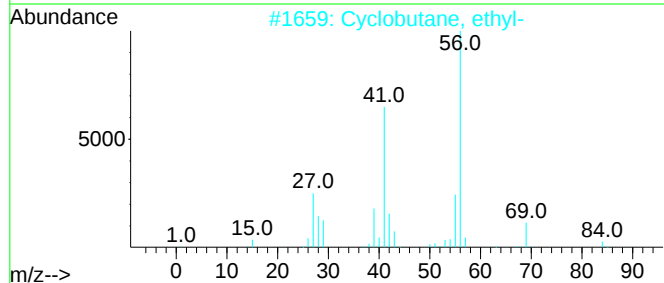
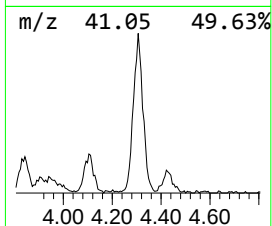
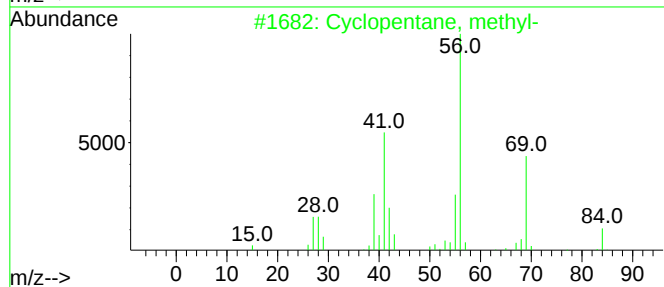
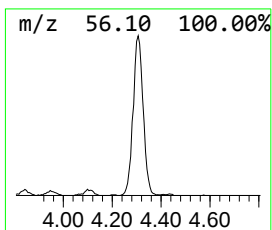
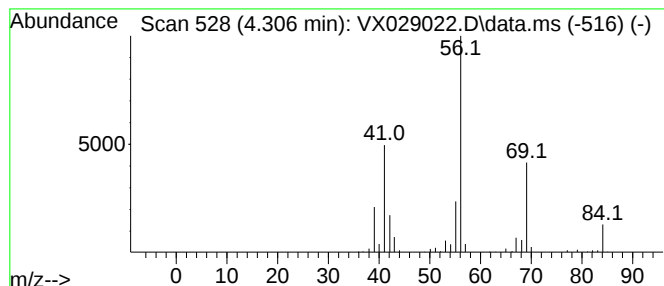
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	8.05 ug/l	168852	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	78
3			Cyclohexane	84	C6H12	000110-82-7	78
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

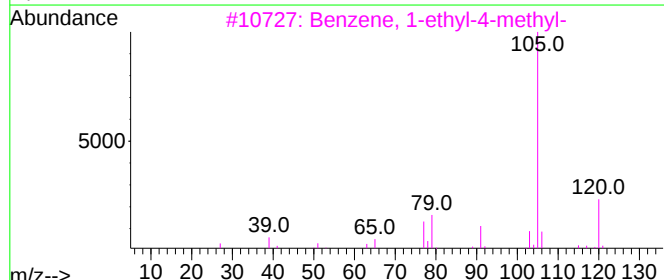
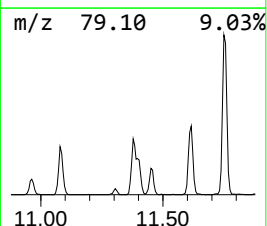
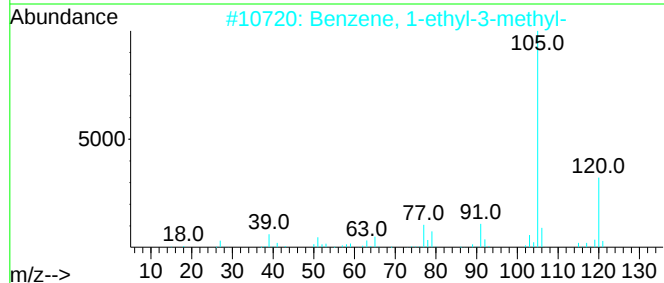
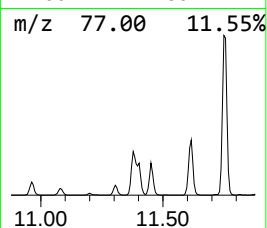
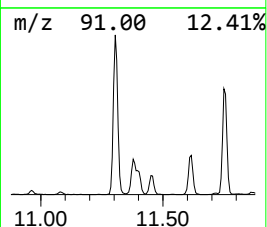
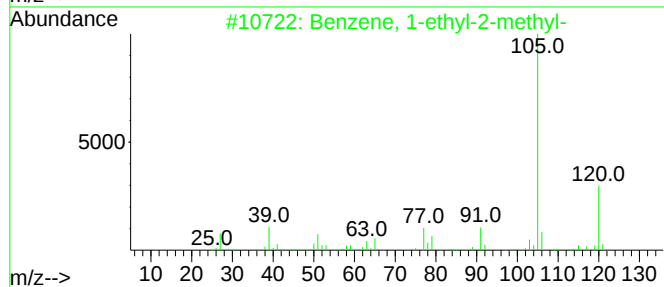
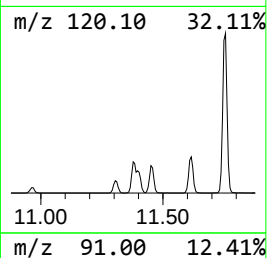
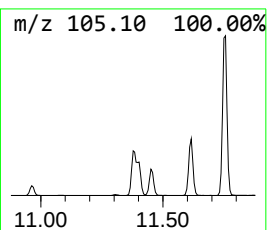
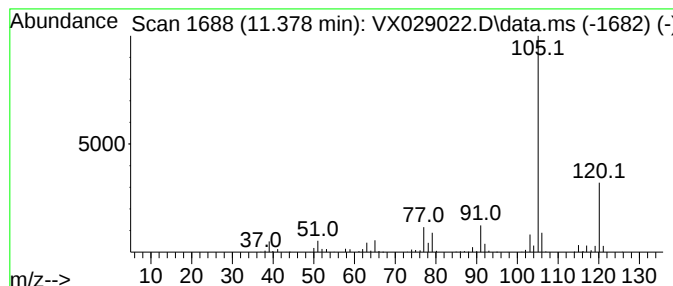
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	8.24 ug/l	290866	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	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	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

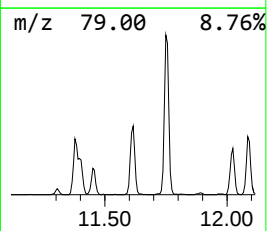
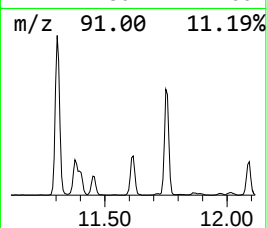
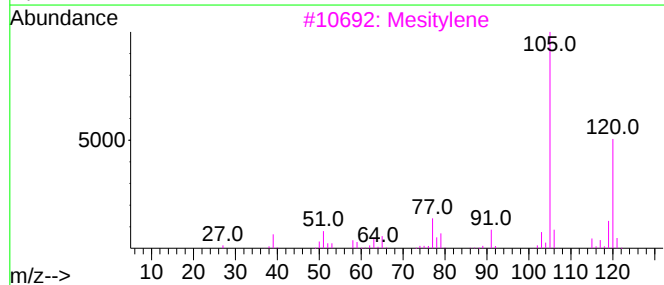
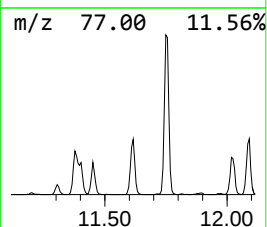
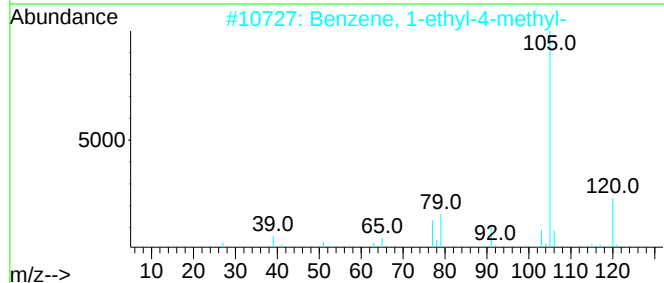
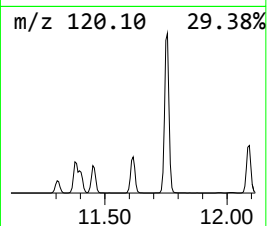
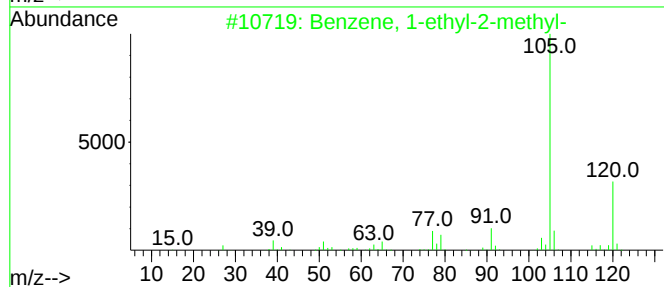
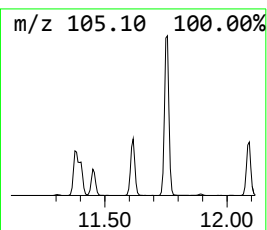
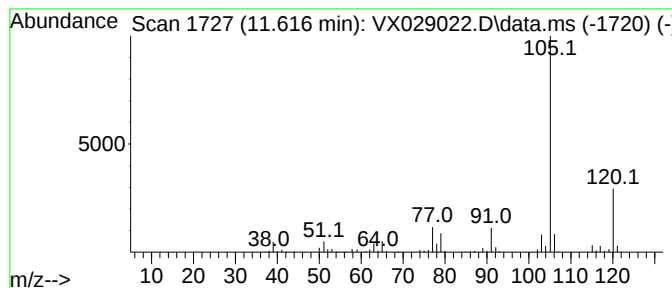
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	9.69 ug/l	342119	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	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

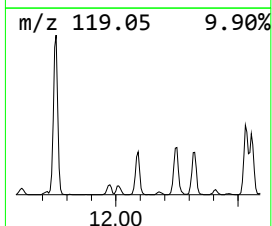
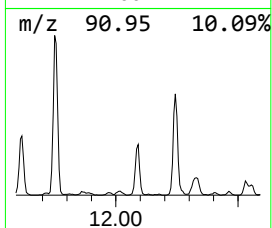
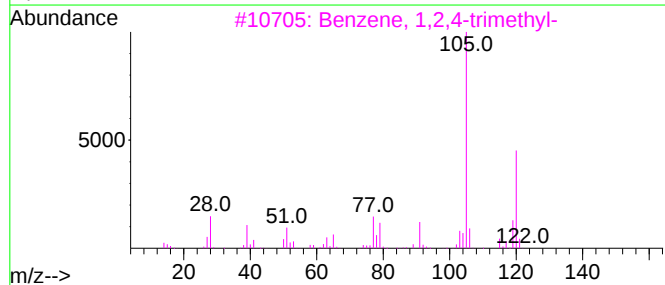
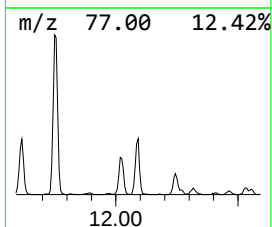
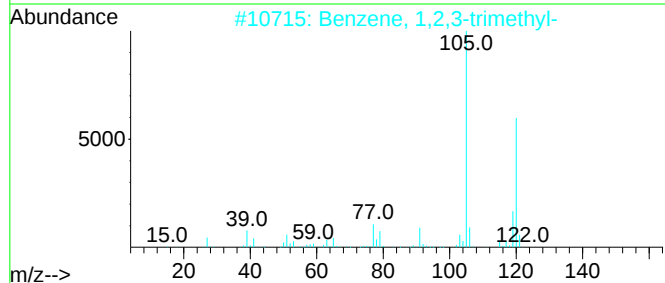
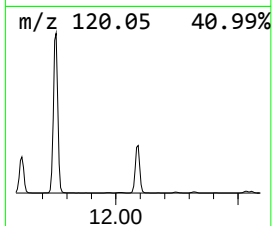
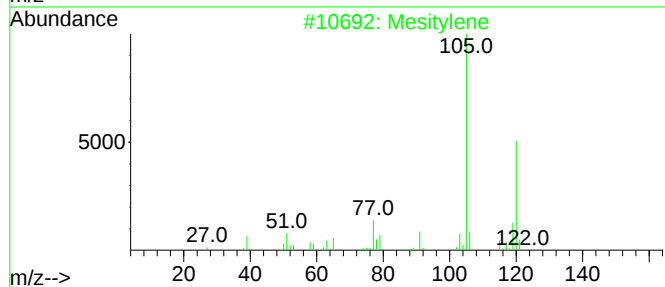
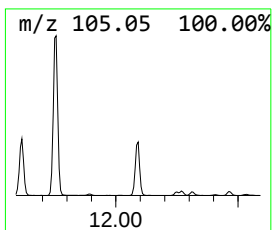
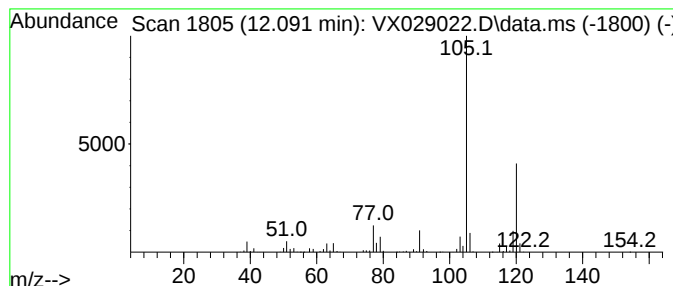
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	9.95 ug/l	351093	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	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

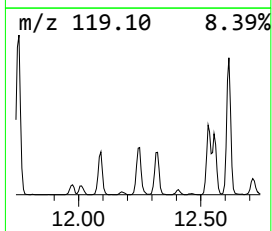
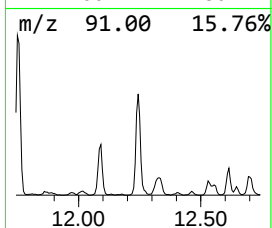
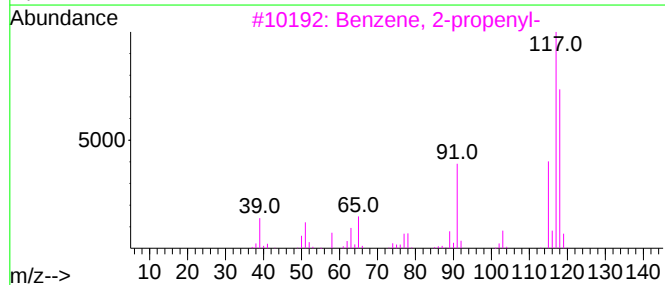
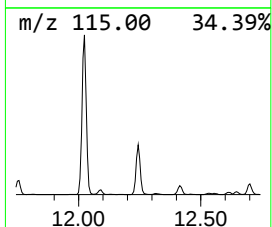
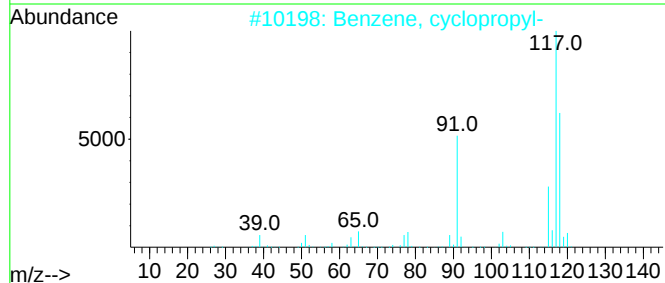
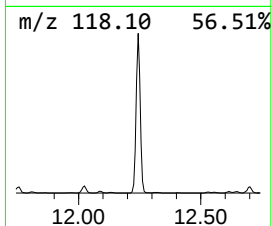
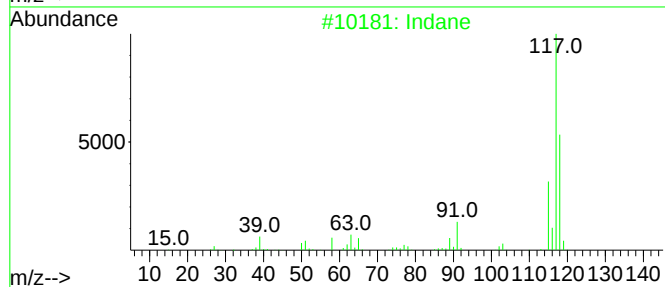
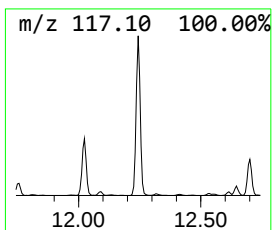
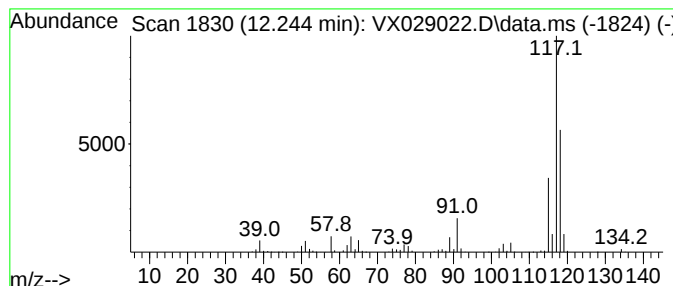
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	15.05 ug/l	531368	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	87
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

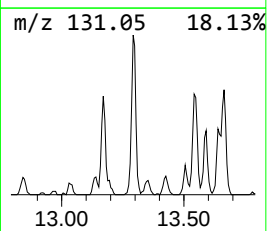
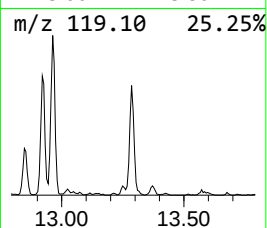
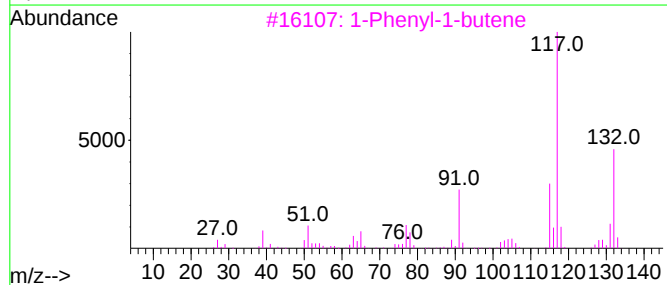
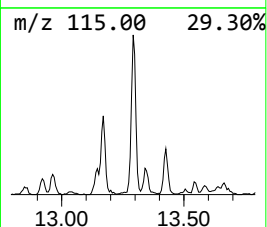
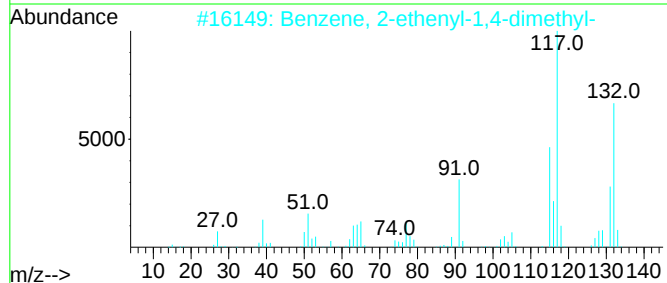
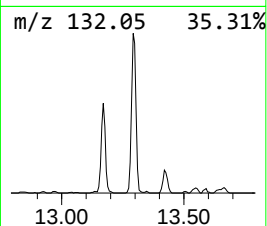
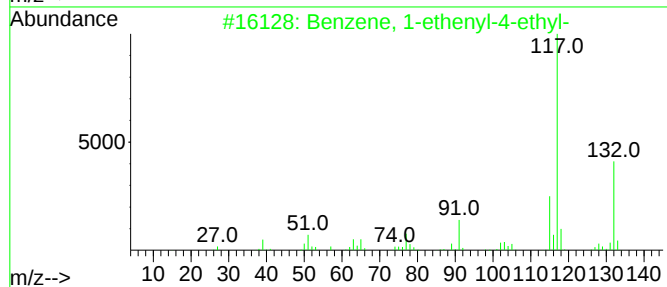
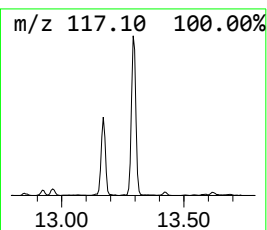
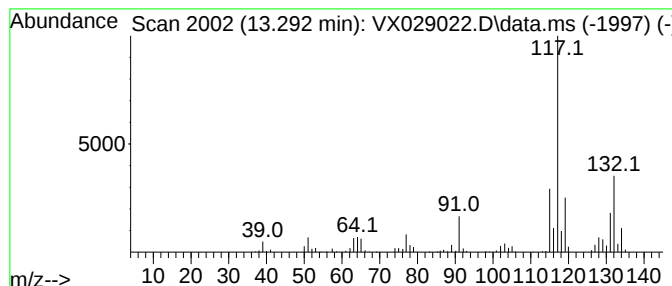
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	7.13 ug/l	251823	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029022.D
Acq On : 27 May 2022 14:27
Operator : JC/MD
Sample : N2968-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

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	7.5	ug/l	157565	1	5.556	1048700	50.0
2-Butene, 2-met...	2.215	7.8	ug/l	162460	1	5.556	1048700	50.0
Cyclopentane	2.867	6.8	ug/l	142680	1	5.556	1048700	50.0
Cyclopentane, m...	4.306	8.1	ug/l	168852	1	5.556	1048700	50.0
Benzene, 1-ethy...	11.378	8.2	ug/l	290866	4	12.024	1764850	50.0
Benzene, 1-ethy...	11.616	9.7	ug/l	342119	4	12.024	1764850	50.0
Benzene, 1,2,3-...	12.091	9.9	ug/l	351093	4	12.024	1764850	50.0
Indane	12.243	15.1	ug/l	531368	4	12.024	1764850	50.0
Benzene, 1-ethe...	13.292	7.1	ug/l	251823	4	12.024	1764850	50.0