

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
 Data File : VX027222.D
 Acq On : 28 Feb 2022 16:02
 Operator : JC/MD
 Sample : N1688-06 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 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\82X022322W.M
 Title : SW846 8260

Signal : TIC: VX027222.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	27	30	42	rVB	27983	27206	2.46%	0.251%
2	1.374	42	47	53	rBV	50720	47229	4.28%	0.436%
3	1.752	104	109	120	rVB	163892	224220	20.31%	2.068%
4	1.959	138	143	154	rVB2	83016	137314	12.44%	1.267%
5	2.075	156	162	169	rVV	13695	19117	1.73%	0.176%
6	2.166	172	177	181	rVV	8885	12761	1.16%	0.118%
7	2.221	181	186	195	rVV	41652	68208	6.18%	0.629%
8	2.343	199	206	217	rBB2	5923	12876	1.17%	0.119%
9	2.782	261	278	281	rBV2	24030	68501	6.21%	0.632%
10	2.831	281	286	289	rVV	59317	120200	10.89%	1.109%
11	2.873	289	293	305	rVB2	52795	119800	10.85%	1.105%
12	3.105	322	331	342	rVB	50406	116559	10.56%	1.075%
13	3.325	359	367	377	rVB2	11959	26921	2.44%	0.248%
14	3.453	381	388	396	rBV	6709	14832	1.34%	0.137%
15	3.587	402	410	416	rBV3	7347	18608	1.69%	0.172%
16	3.672	416	424	428	rVV3	4302	11475	1.04%	0.106%
17	3.739	428	435	443	rVV	24957	60520	5.48%	0.558%
18	3.843	443	452	458	rVV2	16717	42565	3.86%	0.393%
19	3.910	458	463	470	rVV3	8390	25326	2.29%	0.234%
20	4.105	486	495	505	rVB2	16691	44806	4.06%	0.413%
21	4.306	519	528	540	rVV	117168	331375	30.02%	3.057%
22	4.428	540	548	560	rVB2	8782	25804	2.34%	0.238%
23	5.202	662	675	695	rVB	29801	97488	8.83%	0.899%
24	5.391	695	706	713	rBV	56304	165435	14.99%	1.526%
25	5.477	713	720	727	rVV2	69356	214798	19.46%	1.982%
26	5.556	727	733	759	rVB	96376	307878	27.89%	2.840%
27	5.836	768	779	790	rBV5	8587	28114	2.55%	0.259%
28	5.958	790	799	807	rBV	57233	153436	13.90%	1.415%
29	6.044	807	813	823	rVB	31778	80991	7.34%	0.747%
30	6.172	824	834	837	rBV2	9977	28350	2.57%	0.262%
31	6.263	844	849	857	rVB3	12067	31225	2.83%	0.288%
32	6.361	857	865	875	rVB	12495	33338	3.02%	0.308%
33	6.763	922	931	942	rBV	148560	386013	34.97%	3.561%
34	6.854	943	946	959	rVB4	16459	38104	3.45%	0.352%
35	7.171	989	998	1008	rVB2	17018	40674	3.68%	0.375%
36	7.385	1021	1033	1047	rVB2	57646	143997	13.04%	1.328%

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37	7.659	1073	1078	1085	rVB3	7223	13743	1.24%	0.127%
38	8.147	1143	1158	1162	rBV	31400	65260	5.91%	0.602%
39	8.196	1162	1166	1176	rVB2	9281	17309	1.57%	0.160%
40	8.507	1208	1217	1225	rVB	21250	36264	3.28%	0.335%
41	8.653	1234	1241	1247	rVB	305228	484598	43.90%	4.470%
42	8.720	1247	1252	1258	rVB	34299	51104	4.63%	0.471%
43	8.964	1287	1292	1299	rVB3	13763	25223	2.28%	0.233%
44	9.049	1299	1306	1312	rBV	14018	23647	2.14%	0.218%
45	9.165	1320	1325	1335	rVB	9213	15479	1.40%	0.143%
46	10.055	1465	1471	1480	rBV	315074	422440	38.27%	3.897%
47	10.195	1489	1494	1504	rVB	429321	546925	49.54%	5.045%
48	10.305	1504	1512	1522	rBV	798651	1103939	100.00%	10.184%
49	10.640	1562	1567	1578	rVB	256029	337960	30.61%	3.118%
50	11.079	1634	1639	1650	rVB	244105	323424	29.30%	2.984%
51	11.378	1683	1688	1690	rBV	186859	249133	22.57%	2.298%
52	11.402	1690	1692	1696	rVV	172521	178455	16.17%	1.646%
53	11.451	1696	1700	1711	rVB	123369	151563	13.73%	1.398%
54	11.616	1721	1727	1737	rBV	225517	290643	26.33%	2.681%
55	11.750	1745	1749	1756	rVB	484881	605990	54.89%	5.590%
56	11.969	1781	1785	1789	rBV	10133	11246	1.02%	0.104%
57	12.024	1789	1794	1799	rVV	329235	413411	37.45%	3.814%
58	12.085	1799	1804	1810	rVB	240958	306749	27.79%	2.830%
59	12.244	1825	1830	1838	rBV	279051	365861	33.14%	3.375%
60	12.317	1838	1842	1848	rVB2	46254	61424	5.56%	0.567%
61	12.408	1852	1857	1862	rBV3	13476	18621	1.69%	0.172%
62	12.463	1862	1866	1871	rVB	22558	26062	2.36%	0.240%
63	12.530	1872	1877	1879	rBV	40619	50670	4.59%	0.467%
64	12.555	1879	1881	1886	rVV	37644	41225	3.73%	0.380%
65	12.616	1886	1891	1894	rVV	84582	103141	9.34%	0.951%
66	12.646	1894	1896	1900	rVB	23136	24055	2.18%	0.222%
67	12.701	1900	1905	1913	rBV2	74755	100128	9.07%	0.924%
68	12.847	1924	1929	1934	rVB2	24008	29777	2.70%	0.275%
69	12.920	1935	1941	1945	rBV	50927	64185	5.81%	0.592%
70	12.963	1945	1948	1955	rVB	79180	89329	8.09%	0.824%
71	13.042	1955	1961	1968	rBV6	4250	11263	1.02%	0.104%
72	13.170	1978	1982	1987	rVB	53017	61954	5.61%	0.572%
73	13.292	1997	2002	2007	rVB2	134755	174597	15.82%	1.611%
74	13.426	2019	2024	2030	rVB	31156	42014	3.81%	0.388%
75	13.542	2040	2043	2046	rBV2	12278	16119	1.46%	0.149%
76	13.585	2046	2050	2056	rVV2	15080	26208	2.37%	0.242%

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77	13.664	2060	2063	2069	rVB2	14595	21416	1.94%	0.198%
78	13.774	2076	2081	2090	rVB	235397	294767	26.70%	2.719%
79	14.079	2126	2131	2138	rBV	9839	12617	1.14%	0.116%
80	14.219	2149	2154	2164	rBV3	10921	21889	1.98%	0.202%
81	14.640	2218	2223	2233	rVB	72785	92503	8.38%	0.853%
82	14.780	2241	2246	2256	rBV	60003	75639	6.85%	0.698%
83	15.615	2378	2383	2387	rBV2	8916	14091	1.28%	0.130%

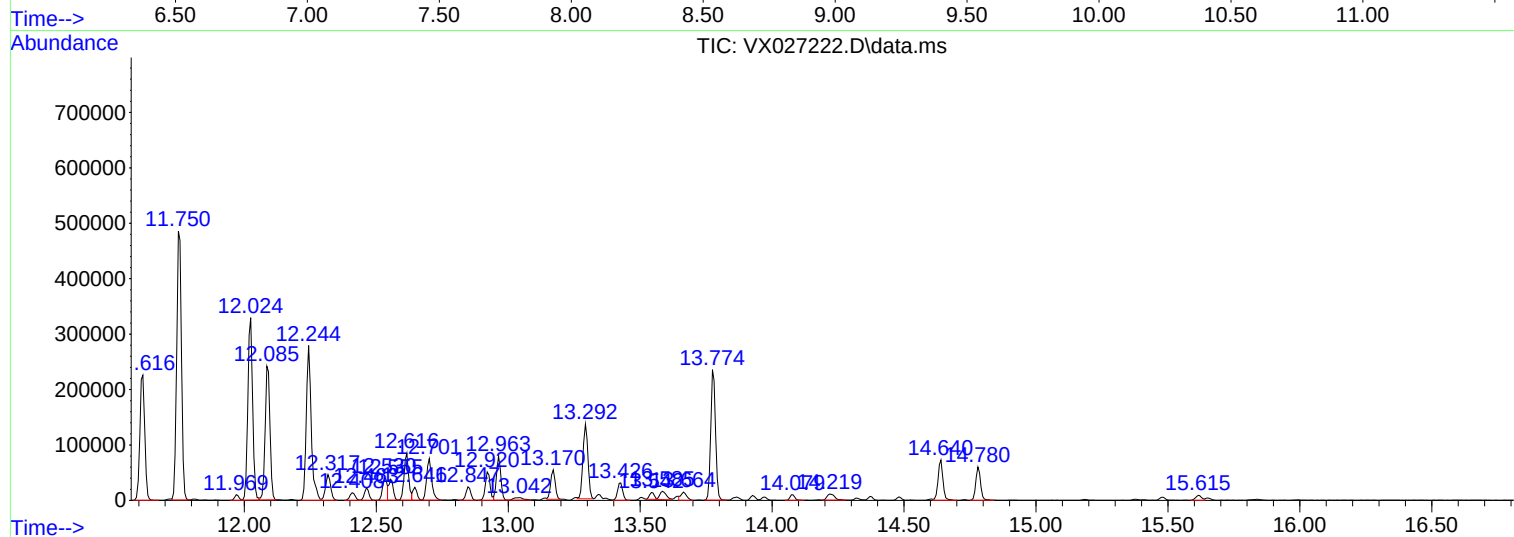
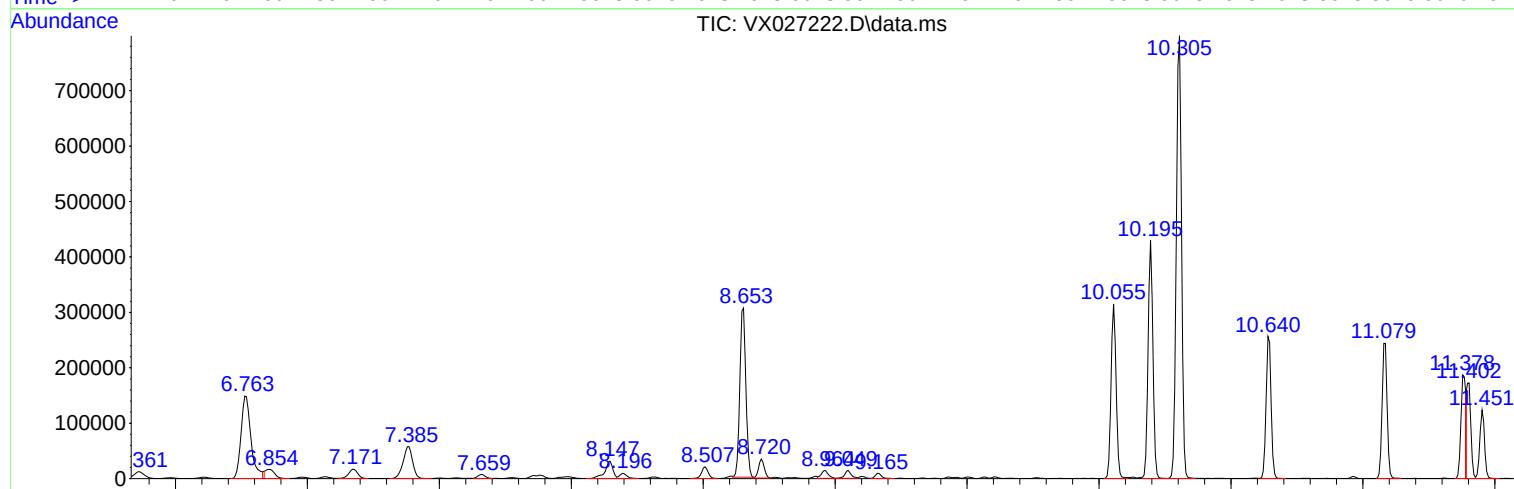
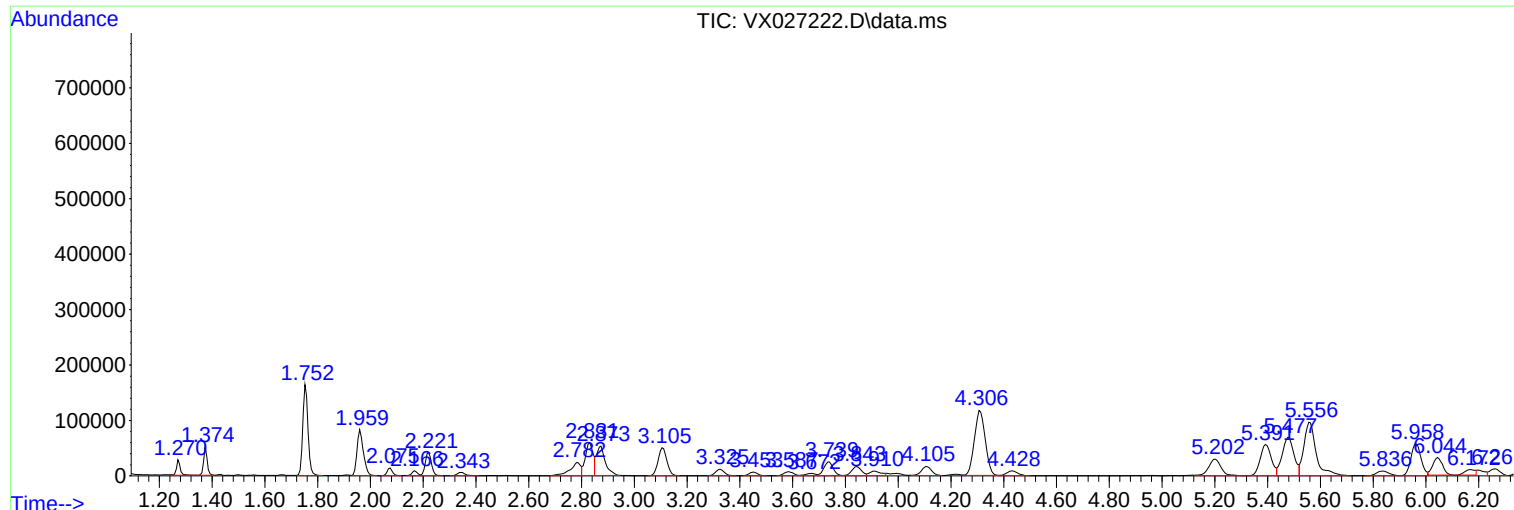
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



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Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
MSVOA_X
ClientSampleId :
MW-23

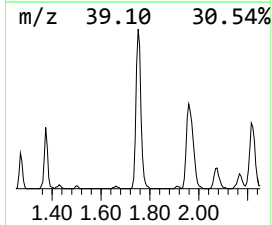
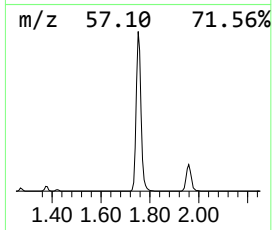
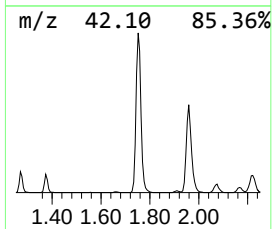
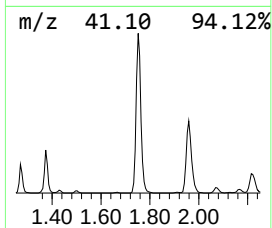
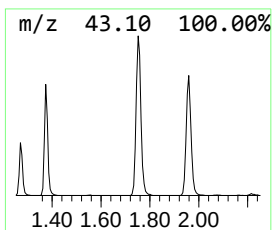
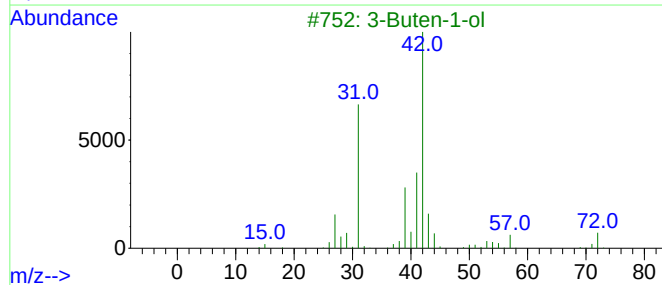
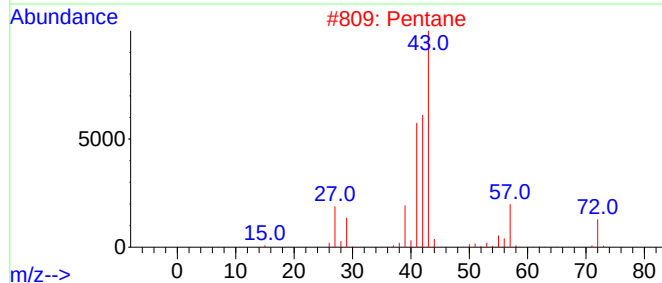
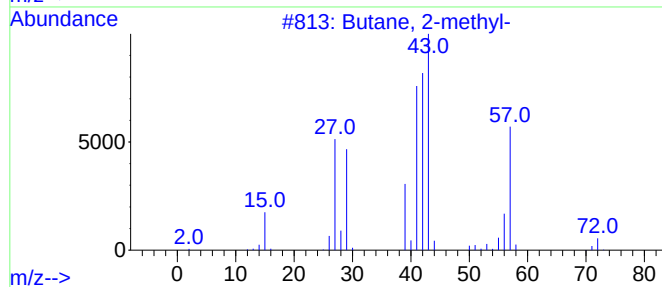
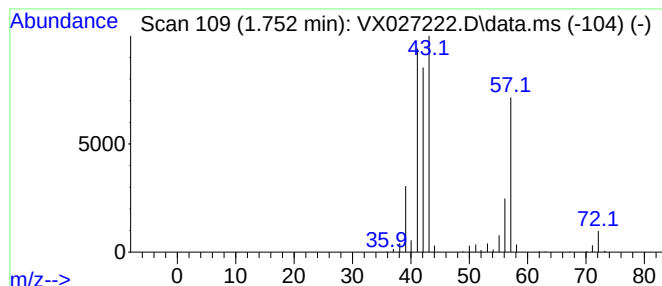
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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	36.41 ug/l	224220	Pentafluorobenzene	5.562

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	33
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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

Instrument :
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ClientSampleId :
MW-23

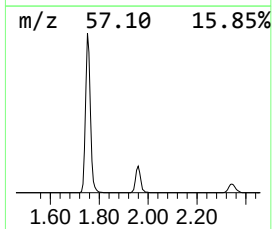
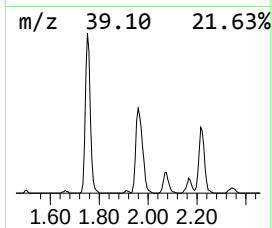
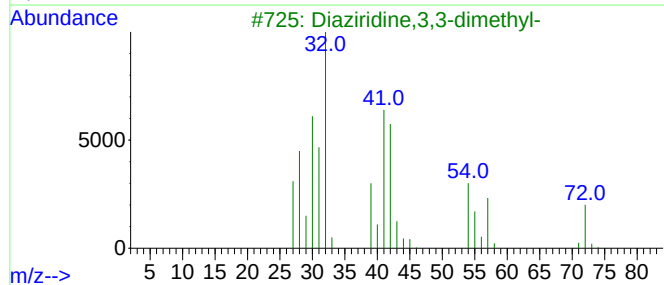
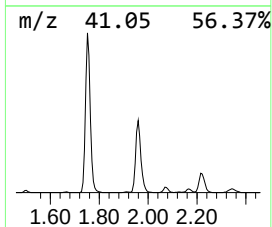
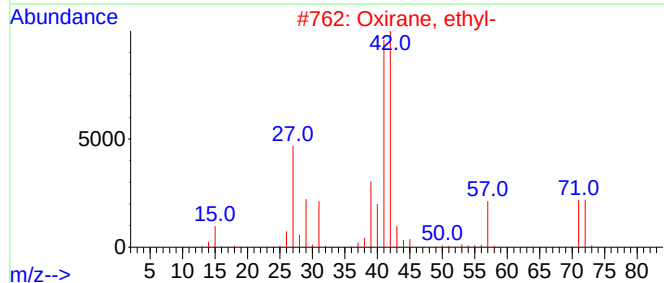
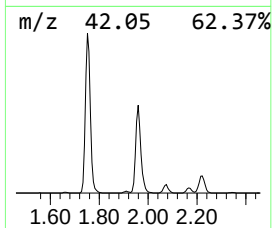
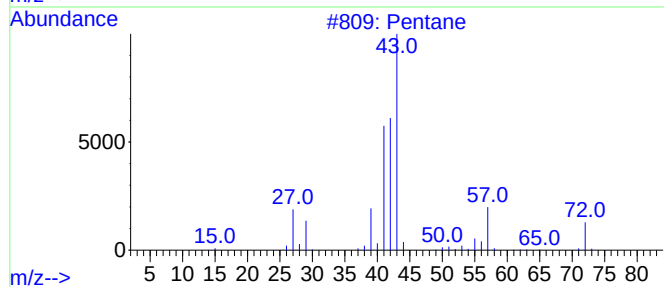
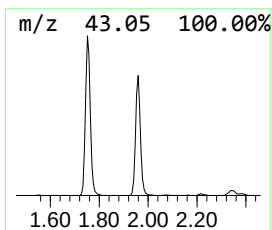
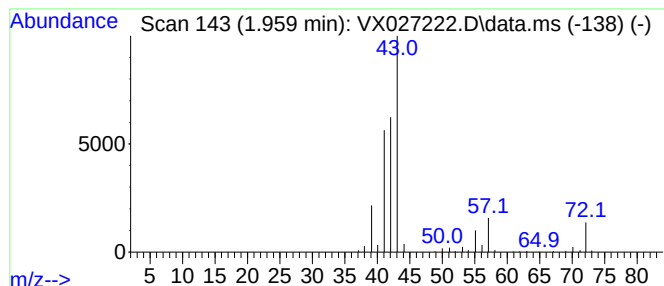
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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.
1.959	22.30 ug/l	137314	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	90
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	25
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12



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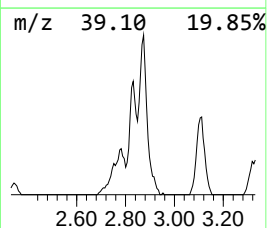
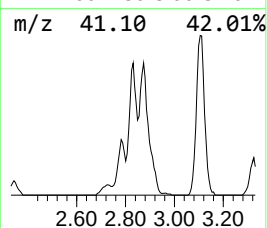
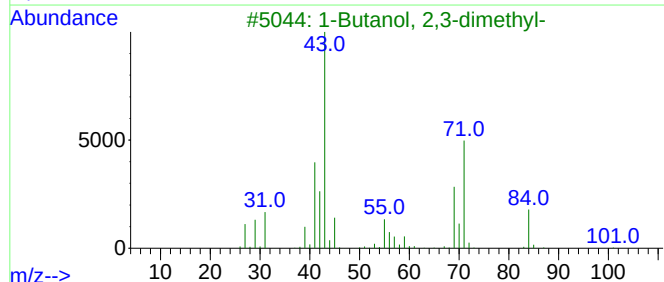
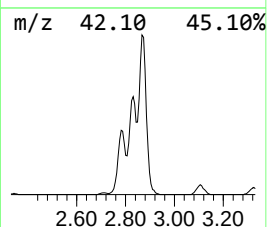
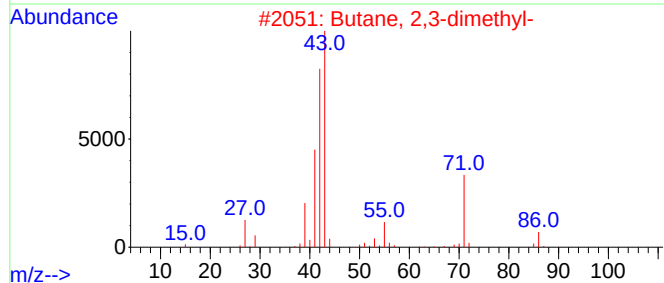
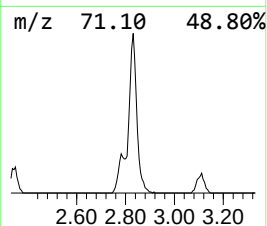
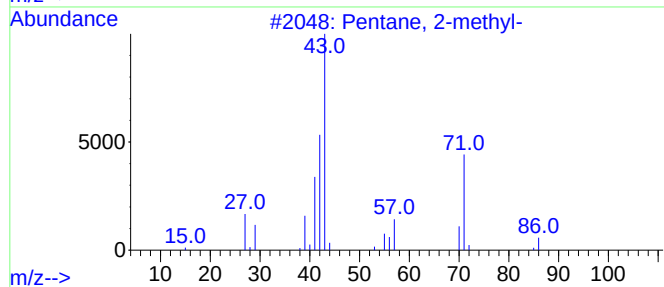
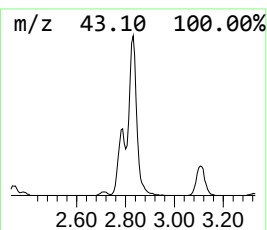
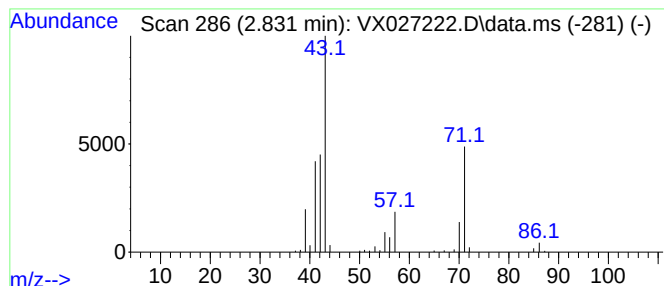
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.831	19.52 ug/l	120200	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	42
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
5			Pentane	72	C5H12	000109-66-0	38



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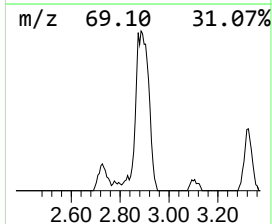
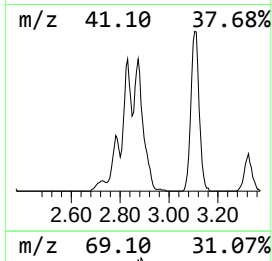
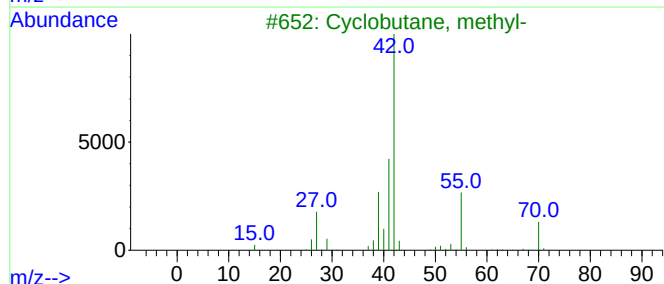
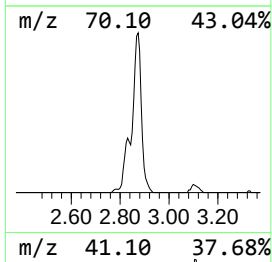
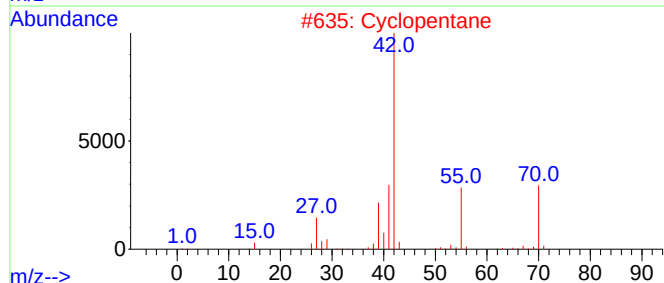
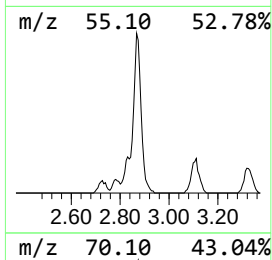
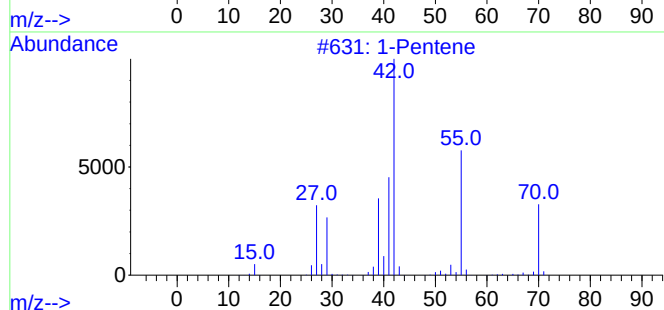
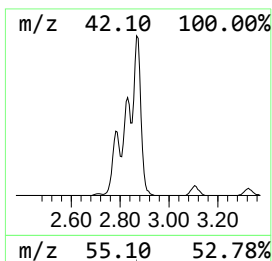
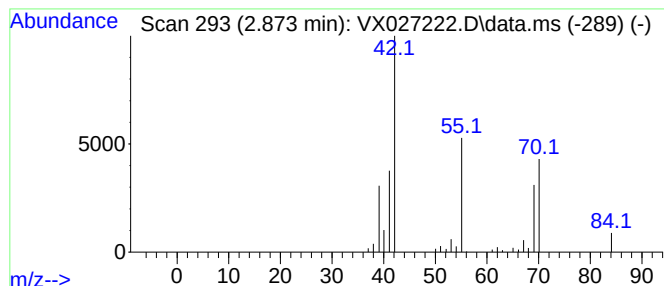
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Pentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.873	19.46 ug/l	119800	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene		70	C5H10	000109-67-1	80
2	Cyclopentane		70	C5H10	000287-92-3	80
3	Cyclobutane, methyl-		70	C5H10	000598-61-8	80
4	2-Pentene, (E)-		70	C5H10	000646-04-8	43
5	2-Pentene, (Z)-		70	C5H10	000627-20-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

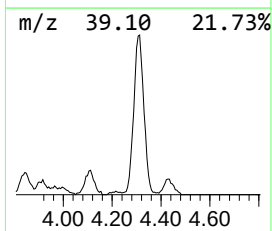
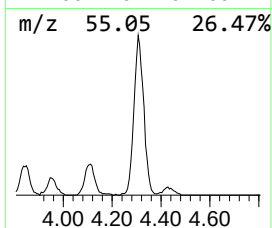
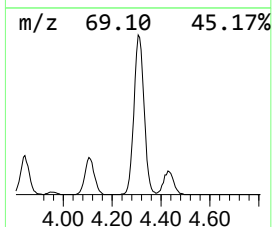
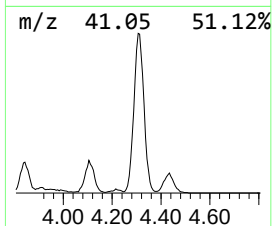
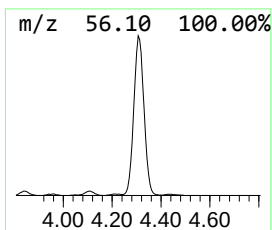
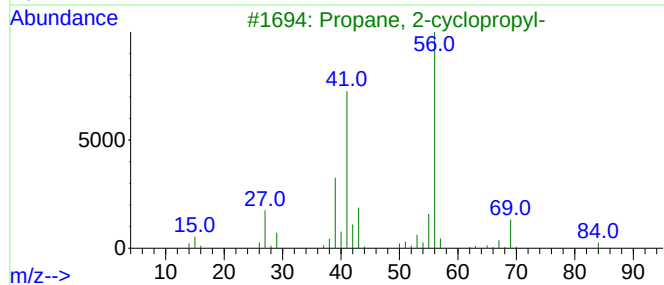
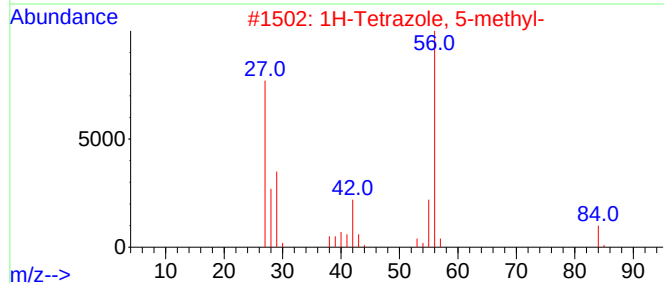
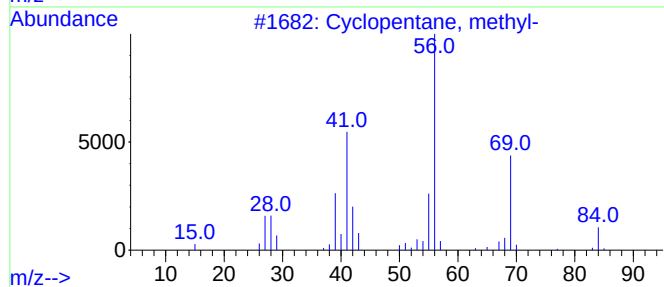
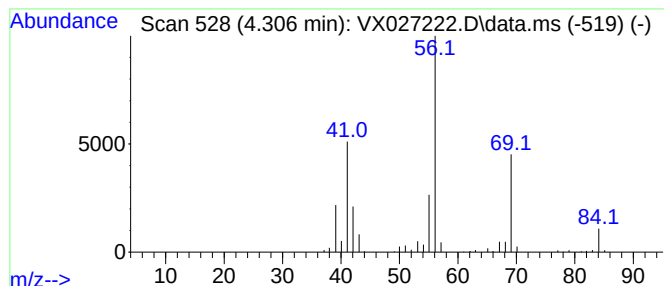
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Quant Title : SW846 8260

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

Peak Number 5 1H-Tetrazole, 5-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	53.82 ug/l	331375	Pentafluorobenzene	5.562

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	80
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

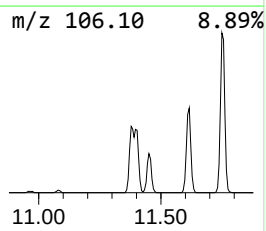
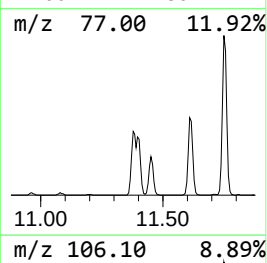
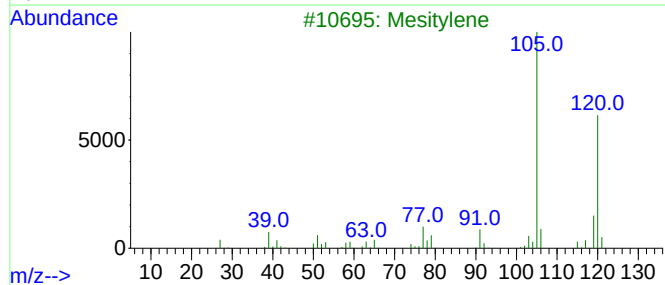
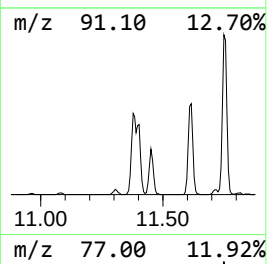
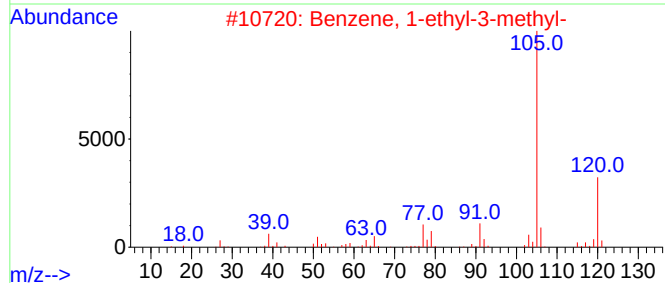
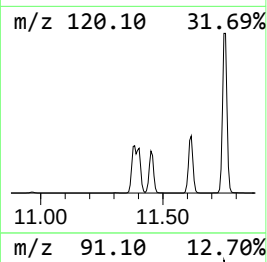
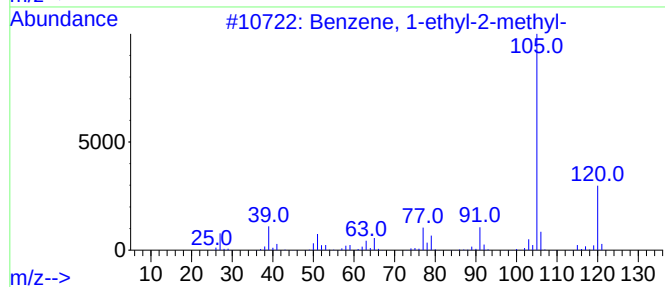
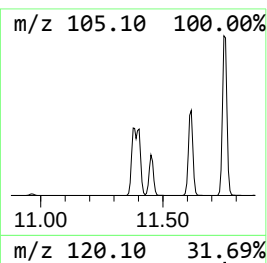
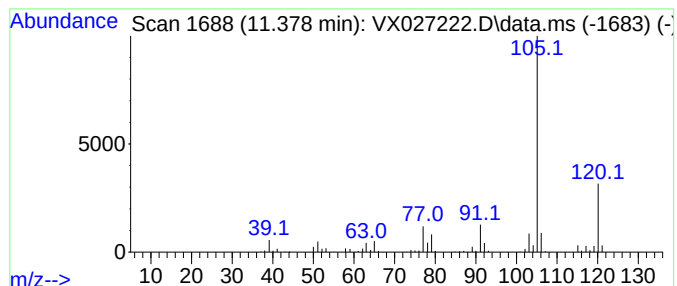
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	30.13 ug/l	249133	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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

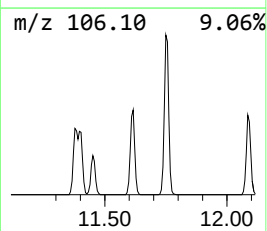
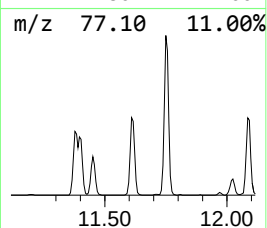
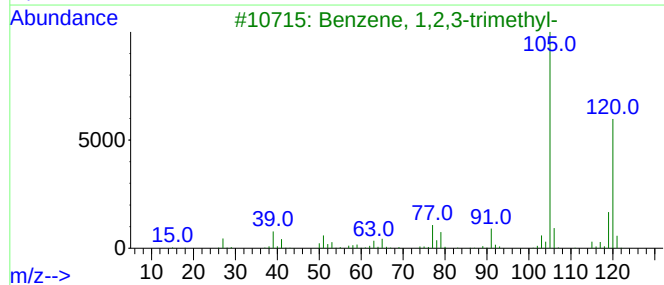
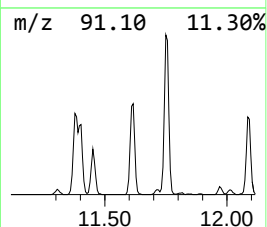
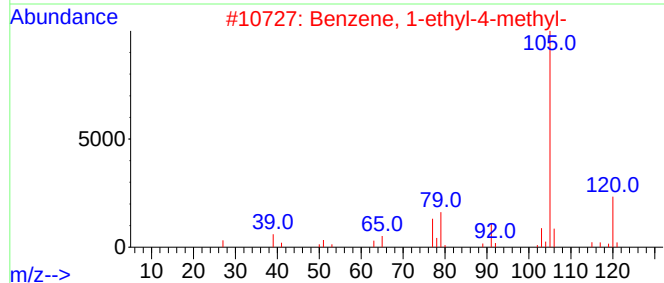
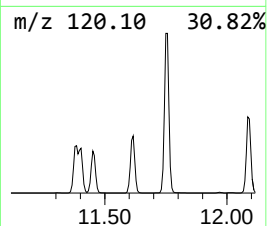
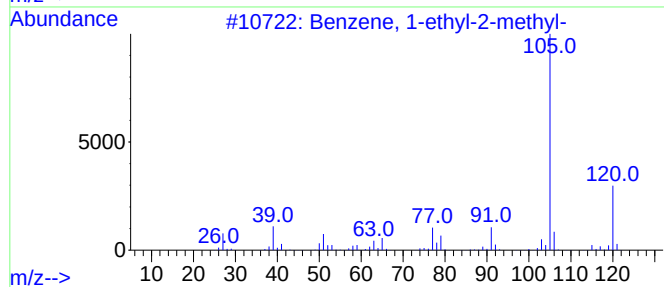
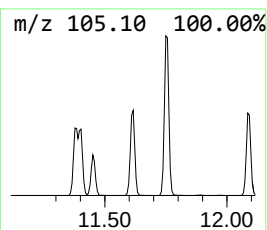
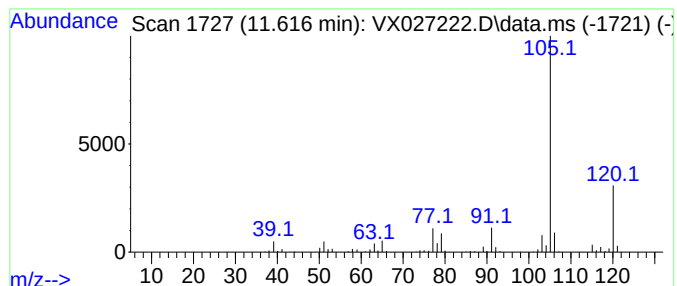
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	35.15 ug/l	290643	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-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Mesitylene	120	C9H12	000108-67-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

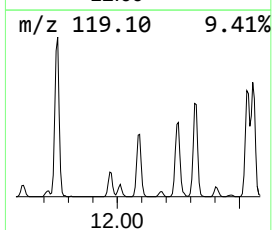
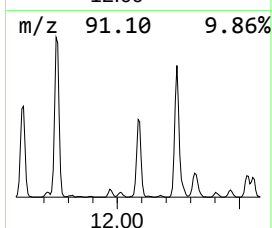
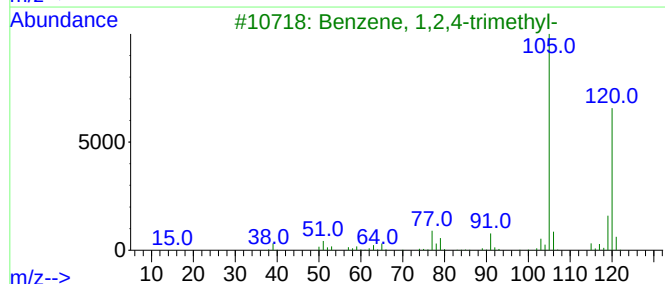
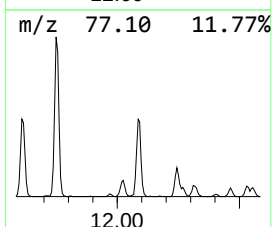
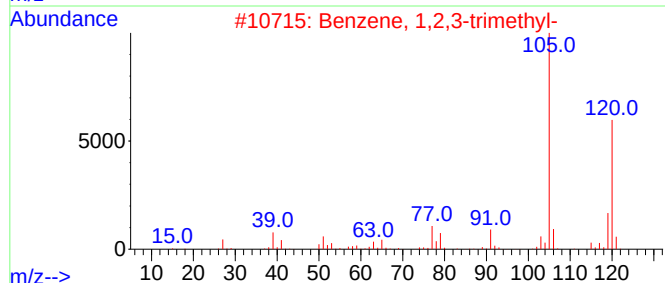
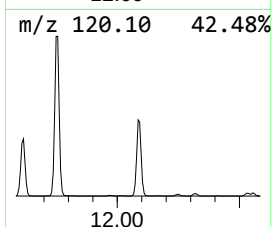
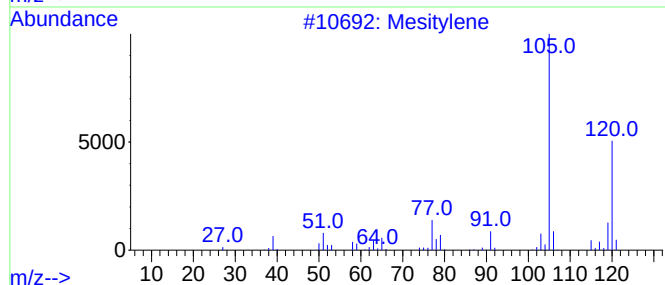
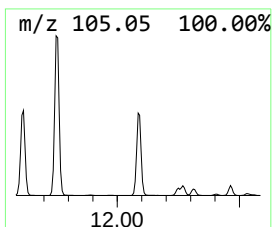
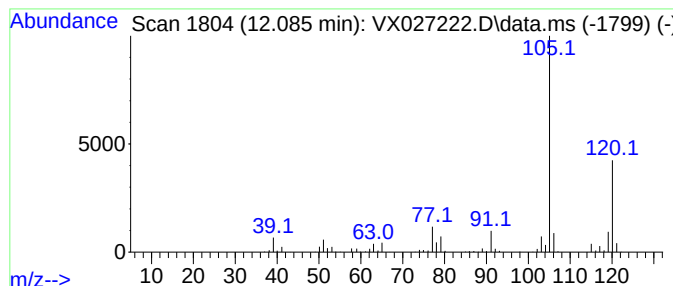
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	37.10 ug/l	306749	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

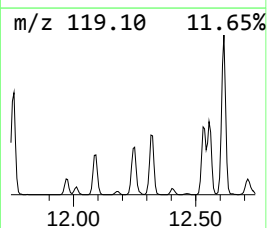
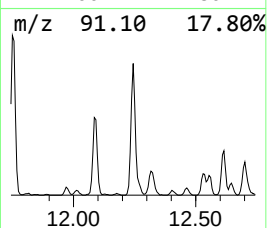
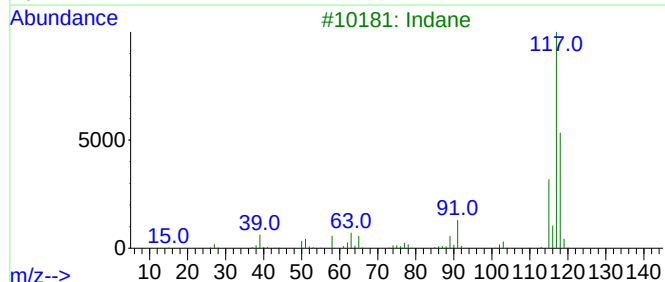
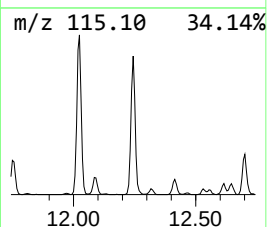
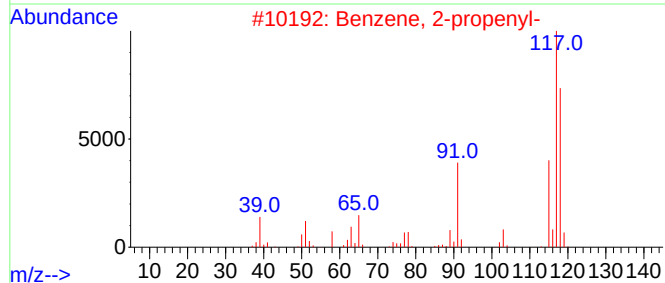
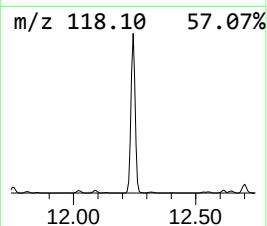
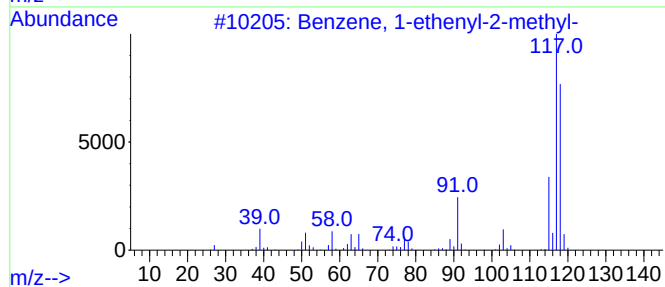
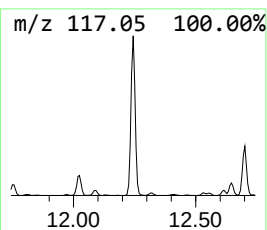
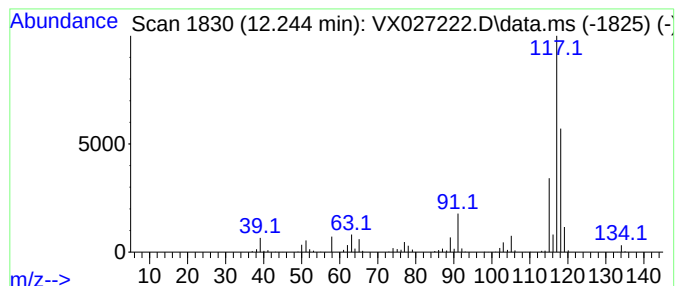
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-ethenyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	44.25 ug/l	365861	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
3			Indane	118	C9H10	000496-11-7	81
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
5			Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

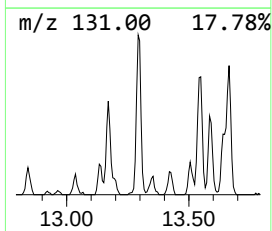
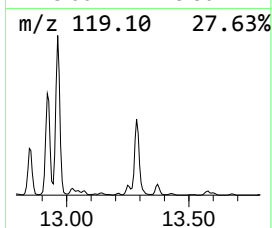
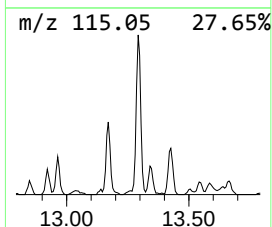
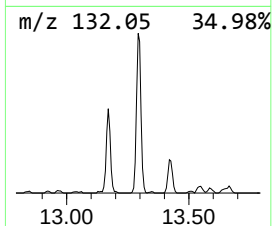
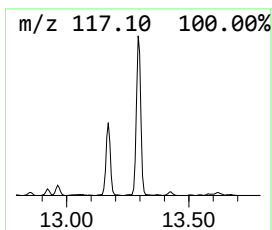
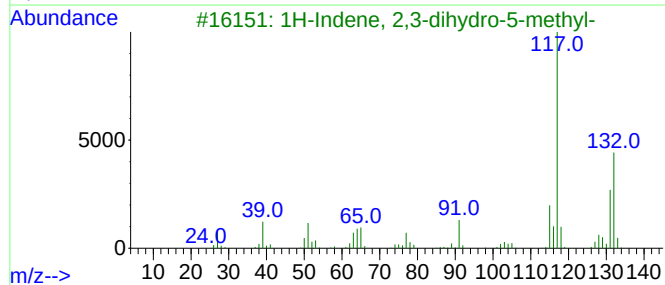
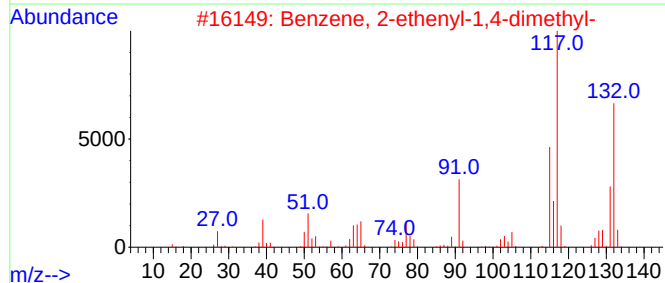
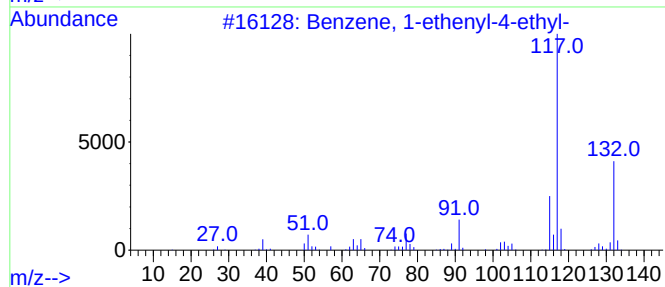
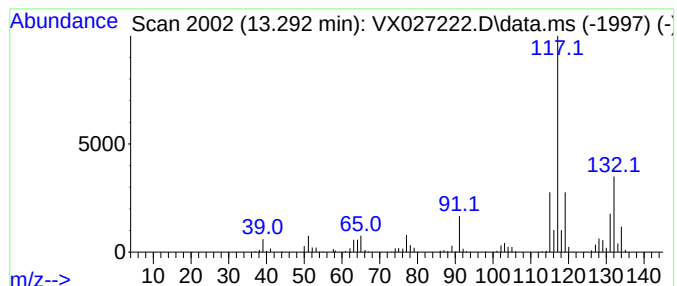
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	21.12 ug/l	174597	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			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027222.D
Acq On : 28 Feb 2022 16:02
Operator : JC/MD
Sample : N1688-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.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
Butane, 2-methyl-	1.752	36.4	ug/l	224220	1	5.562	307878	50.0
Pentane	1.959	22.3	ug/l	137314	1	5.562	307878	50.0
Pentane, 2-methyl-	2.831	19.5	ug/l	120200	1	5.562	307878	50.0
1-Pentene	2.873	19.5	ug/l	119800	1	5.562	307878	50.0
1H-Tetrazole, 5...	4.306	53.8	ug/l	331375	1	5.562	307878	50.0
Benzene, 1-ethy...	11.378	30.1	ug/l	249133	4	12.024	413411	50.0
Benzene, 1-ethy...	11.616	35.1	ug/l	290643	4	12.024	413411	50.0
Benzene, 1,2,3-...	12.085	37.1	ug/l	306749	4	12.024	413411	50.0
Benzene, 1-ethe...	12.244	44.3	ug/l	365861	4	12.024	413411	50.0
Benzene, 1-ethe...	13.292	21.1	ug/l	174597	4	12.024	413411	50.0