

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
 Data File : VX033038.D
 Acq On : 24 Nov 2022 04:55
 Operator : JC/MD
 Sample : N5741-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-22

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033038.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	26	29	35	rBV	64956	64099	6.33%	0.536%
2	1.374	43	47	53	rVB	62473	66885	6.60%	0.559%
3	1.752	103	109	122	rVB	440979	586293	57.85%	4.900%
4	1.959	137	143	152	rVB2	53536	83060	8.20%	0.694%
5	2.215	180	185	196	rVB	26733	42006	4.14%	0.351%
6	2.343	199	206	212	rBV2	11941	23649	2.33%	0.198%
7	2.782	262	278	282	rBV3	36642	93980	9.27%	0.785%
8	2.831	282	286	288	rVV	37023	68968	6.81%	0.576%
9	2.867	288	292	305	rVV	98153	208732	20.60%	1.744%
10	3.008	305	315	323	rVV3	9228	39048	3.85%	0.326%
11	3.105	323	331	346	rVB2	80440	197149	19.45%	1.648%
12	3.739	427	435	444	rBV4	10584	34624	3.42%	0.289%
13	3.837	444	451	457	rVV2	10620	25900	2.56%	0.216%
14	3.904	457	462	470	rVB2	7024	16619	1.64%	0.139%
15	4.105	487	495	503	rVB2	5242	12005	1.18%	0.100%
16	4.306	518	528	541	rVV	174460	497028	49.04%	4.154%
17	4.422	541	547	562	rVB5	7271	21567	2.13%	0.180%
18	5.196	666	674	686	rVB5	5722	18766	1.85%	0.157%
19	5.385	694	705	712	rBV2	101328	299109	29.51%	2.500%
20	5.477	712	720	726	rVV	141411	439670	43.39%	3.675%
21	5.550	726	732	759	rVB	241050	712114	70.27%	5.951%
22	5.842	771	780	789	rBV6	5852	17564	1.73%	0.147%
23	5.958	789	799	805	rVV	104672	275024	27.14%	2.299%
24	6.038	805	812	825	rVV	227338	609789	60.17%	5.096%
25	6.202	825	839	845	rVV4	14124	61757	6.09%	0.516%
26	6.251	845	847	857	rVV3	11589	29941	2.95%	0.250%
27	6.361	857	865	874	rVB6	9868	30853	3.04%	0.258%
28	6.763	920	931	941	rBV	368791	874990	86.34%	7.313%
29	6.848	943	945	957	rVB4	6744	13949	1.38%	0.117%
30	7.178	990	999	1005	rVB3	7738	17227	1.70%	0.144%
31	7.379	1021	1032	1041	rBV3	38488	101490	10.01%	0.848%
32	7.854	1104	1110	1112	rBV3	9223	17286	1.71%	0.144%
33	7.879	1112	1114	1122	rVV2	12009	21164	2.09%	0.177%
34	7.988	1122	1132	1138	rVB	5709	13244	1.31%	0.111%
35	8.104	1144	1151	1153	rBV	12265	20789	2.05%	0.174%
36	8.141	1153	1157	1164	rVB	26619	49407	4.88%	0.413%

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Integrator: RTE

Smoothing : ON

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37	8.433	1200	1205	1211	rBV2	5662	11169	1.10%	0.093%
38	8.507	1211	1217	1225	rVB	24369	43504	4.29%	0.364%
39	8.647	1225	1240	1248	rBV	463595	725306	71.57%	6.062%
40	8.720	1248	1252	1258	rVB	11458	17061	1.68%	0.143%
41	8.958	1281	1291	1299	rVB2	42031	73125	7.22%	0.611%
42	9.049	1299	1306	1313	rBV	39547	64208	6.34%	0.537%
43	9.159	1319	1324	1334	rVB	11249	18627	1.84%	0.156%
44	9.458	1364	1373	1377	rBV3	10238	20499	2.02%	0.171%
45	9.945	1445	1453	1461	rBV4	4820	10346	1.02%	0.086%
46	10.055	1465	1471	1478	rBV	752201	1013414	100.00%	8.470%
47	10.195	1489	1494	1500	rVV	290291	373486	36.85%	3.121%
48	10.305	1500	1512	1518	rVB	14916	32345	3.19%	0.270%
49	10.963	1614	1620	1626	rBV	133414	166611	16.44%	1.392%
50	11.079	1634	1639	1646	rBV	493800	606919	59.89%	5.072%
51	11.305	1671	1676	1683	rVB	118580	146089	14.42%	1.221%
52	11.616	1721	1727	1734	rVB	29918	39676	3.92%	0.332%
53	11.756	1746	1750	1759	rVB	12455	16585	1.64%	0.139%
54	11.866	1762	1768	1770	rBV	13887	18280	1.80%	0.153%
55	11.890	1770	1772	1778	rVB	16538	17883	1.76%	0.149%
56	12.024	1788	1794	1802	rBV	774411	978347	96.54%	8.177%
57	12.244	1824	1830	1837	rBV	490445	590762	58.29%	4.937%
58	12.317	1837	1842	1852	rVB2	14370	26335	2.60%	0.220%
59	12.402	1852	1856	1861	rBV2	19101	26741	2.64%	0.223%
60	12.463	1861	1866	1873	rVB	42948	53266	5.26%	0.445%
61	12.616	1884	1891	1893	rBV	9329	13780	1.36%	0.115%
62	12.646	1893	1896	1900	rVV	41490	50787	5.01%	0.424%
63	12.701	1900	1905	1912	rVB	181878	232321	22.92%	1.942%
64	12.847	1924	1929	1934	rVB3	18420	26751	2.64%	0.224%
65	12.920	1934	1941	1945	rVV	89390	114642	11.31%	0.958%
66	12.963	1945	1948	1954	rVV	77184	89235	8.81%	0.746%
67	13.030	1954	1959	1964	rVB3	7635	10915	1.08%	0.091%
68	13.134	1972	1976	1979	rBV2	9672	12948	1.28%	0.108%
69	13.170	1979	1982	1985	rVV	24283	26495	2.61%	0.221%
70	13.292	1998	2002	2006	rVB	84268	100294	9.90%	0.838%
71	13.341	2006	2010	2013	rBV3	8053	12638	1.25%	0.106%
72	13.420	2019	2023	2030	rVB	49187	63697	6.29%	0.532%
73	13.500	2030	2036	2040	rBV4	5966	10460	1.03%	0.087%
74	13.542	2040	2043	2046	rVV	18999	26741	2.64%	0.223%
75	13.579	2046	2049	2056	rVV3	28200	57713	5.69%	0.482%
76	13.664	2060	2063	2069	rVB2	19082	30183	2.98%	0.252%

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77	13.774	2075	2081	2090	rVB	86945	114187	11.27%	0.954%
78	13.859	2090	2095	2100	rBV3	11014	19894	1.96%	0.166%
79	13.926	2100	2106	2110	rBV2	14155	18939	1.87%	0.158%
80	14.073	2126	2130	2134	rBV	10148	12302	1.21%	0.103%
81	14.213	2148	2153	2164	rBV	16024	26933	2.66%	0.225%
82	14.317	2166	2170	2175	rVV	8631	11893	1.17%	0.099%
83	14.371	2175	2179	2184	rVB	11807	14778	1.46%	0.124%
84	14.780	2241	2246	2255	rBV	54339	70462	6.95%	0.589%

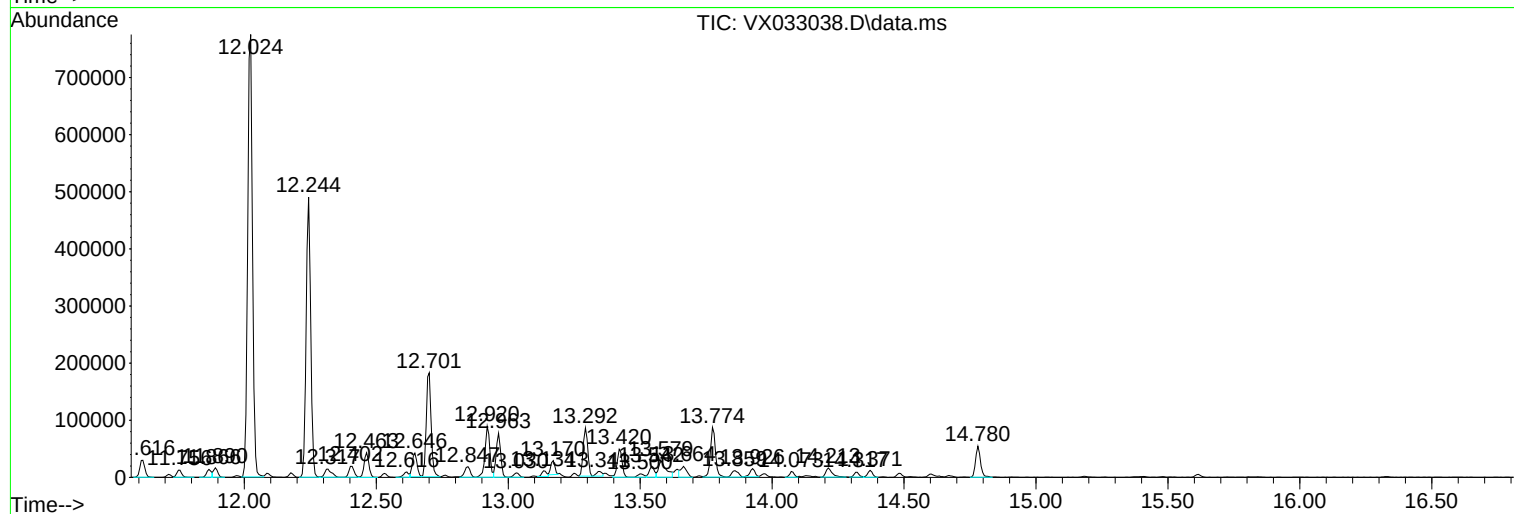
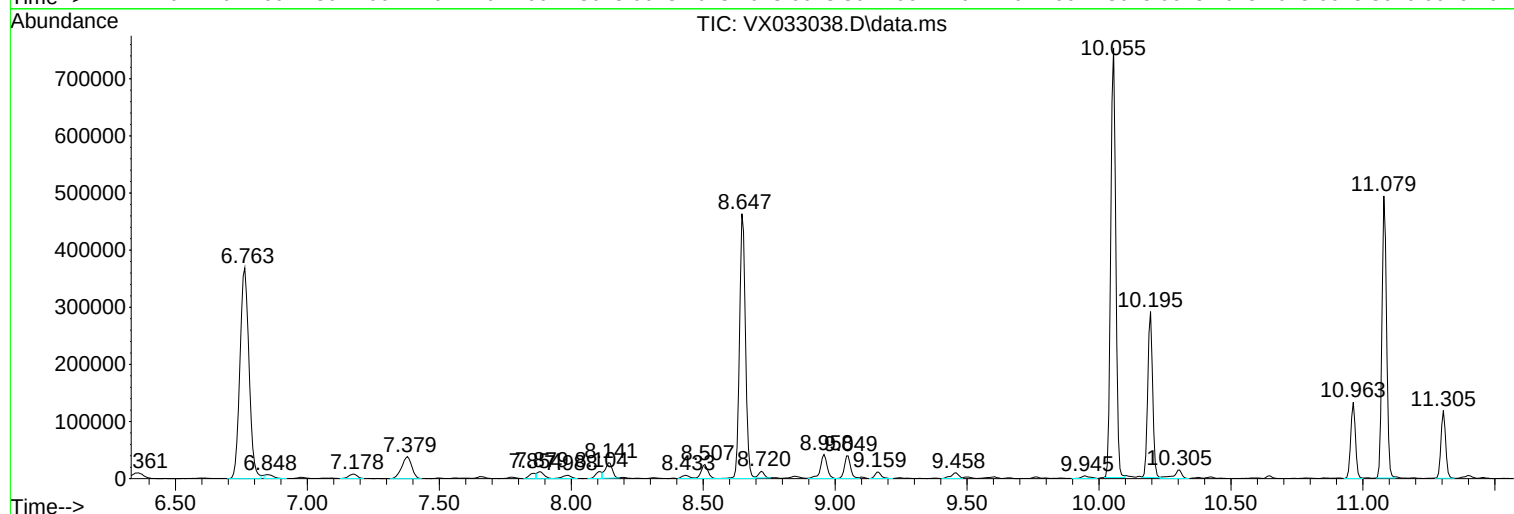
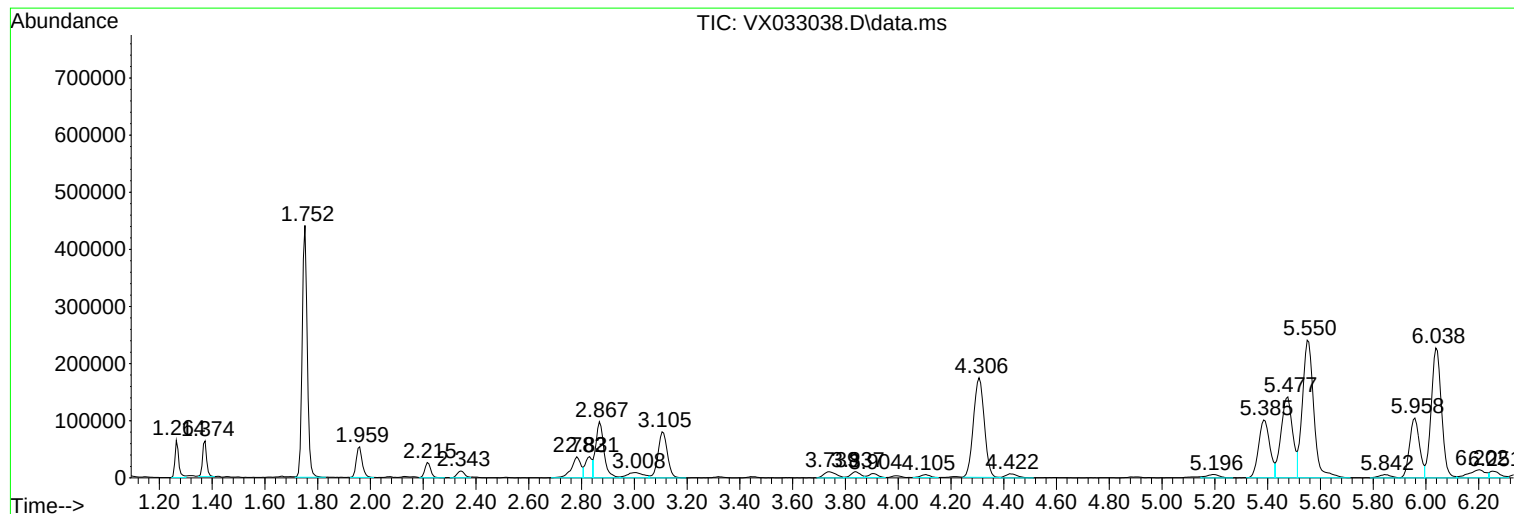
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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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ALS Vial : 33 Sample Multiplier: 1

Instrument :
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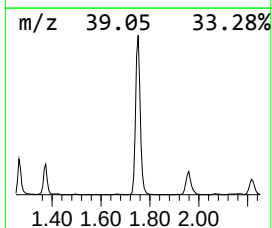
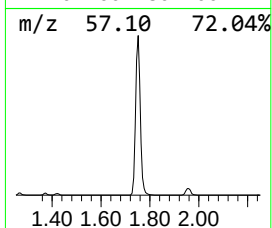
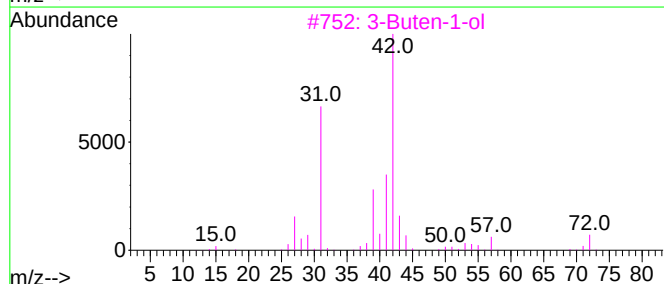
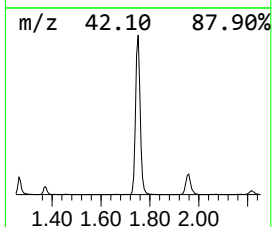
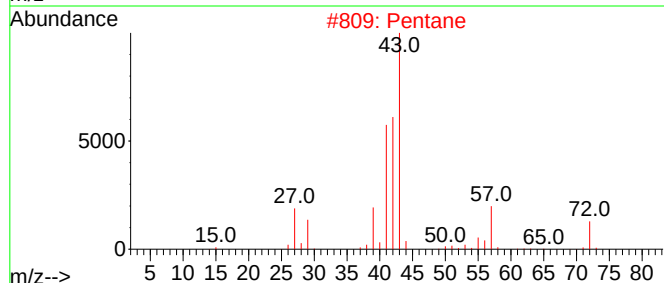
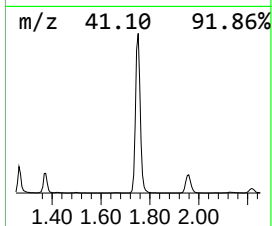
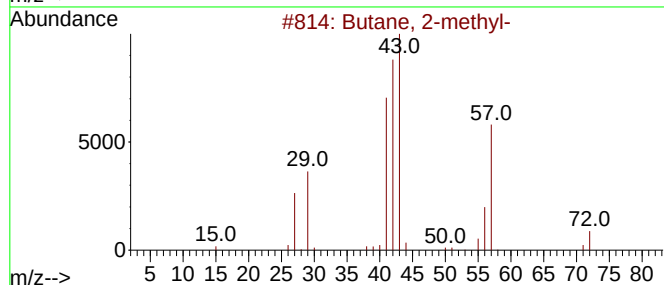
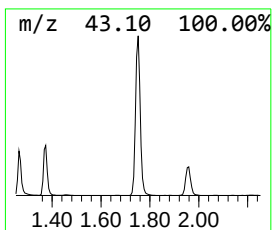
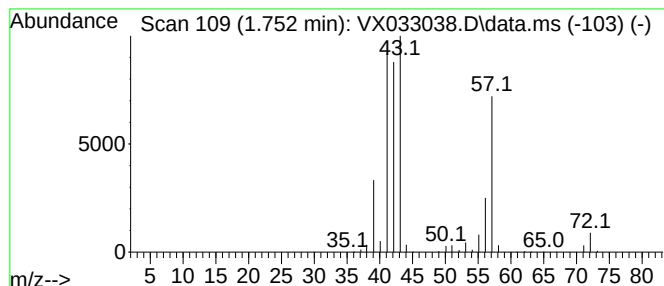
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	41.17 ug/l	586293	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	37
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Butene	56	C4H8	000106-98-9	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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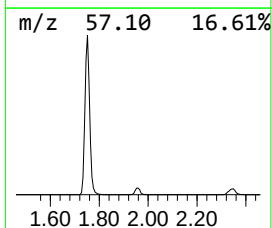
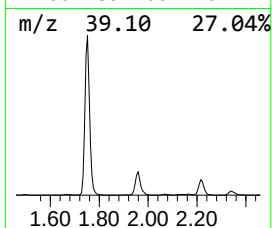
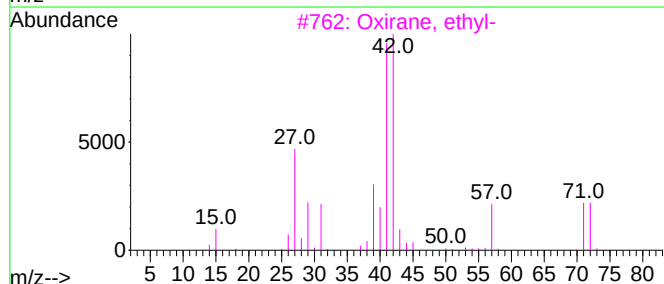
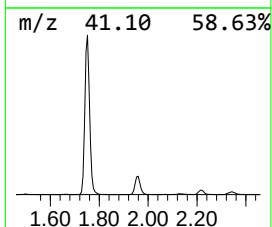
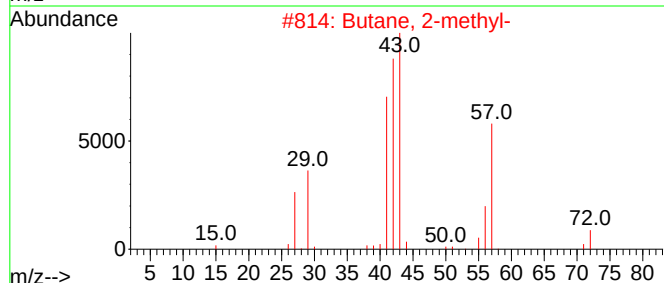
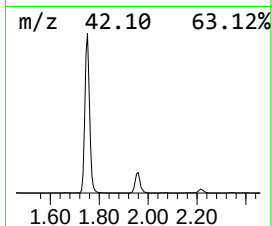
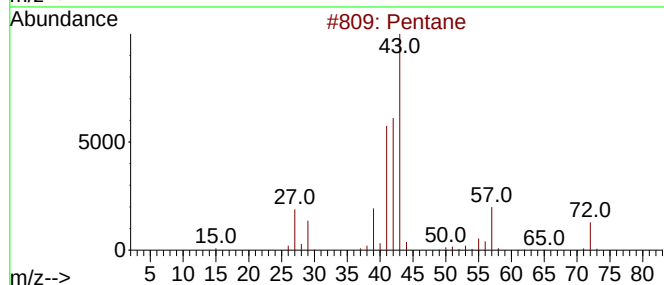
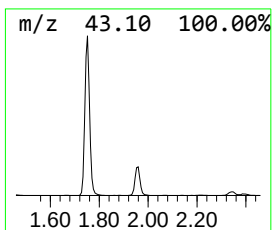
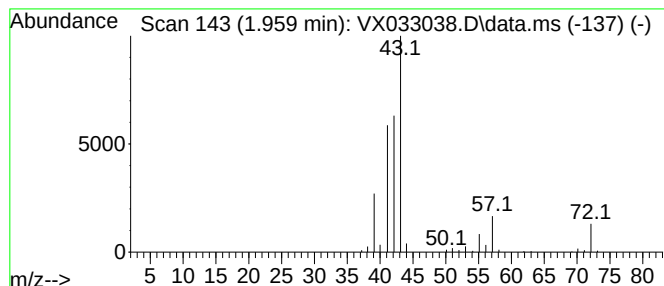
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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.
1.959	5.83 ug/l	83060	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	64
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	32
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	17



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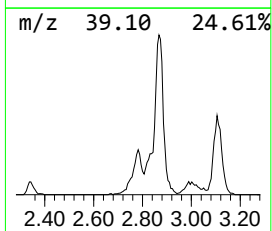
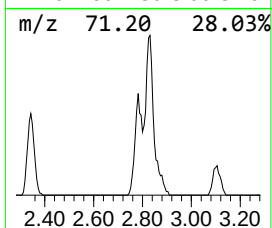
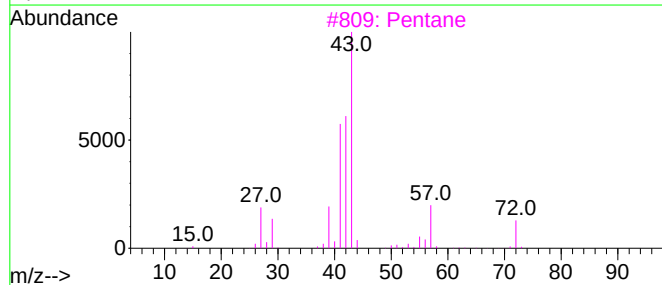
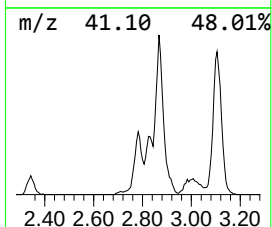
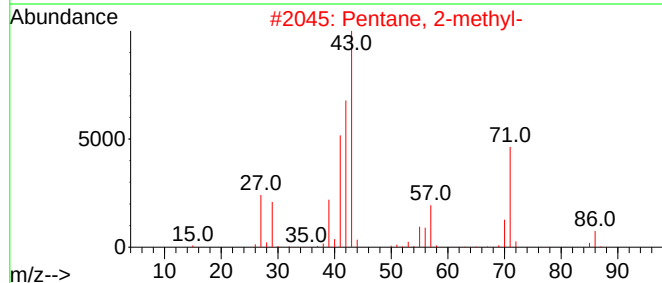
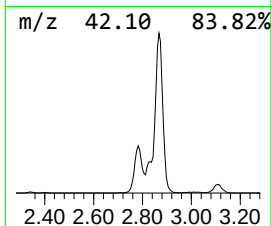
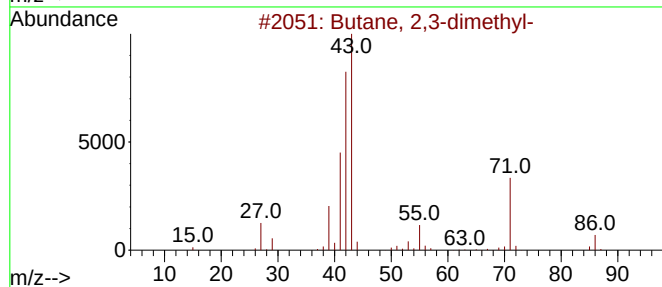
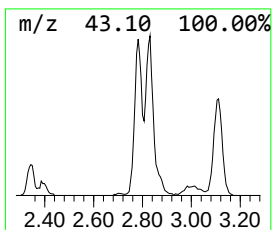
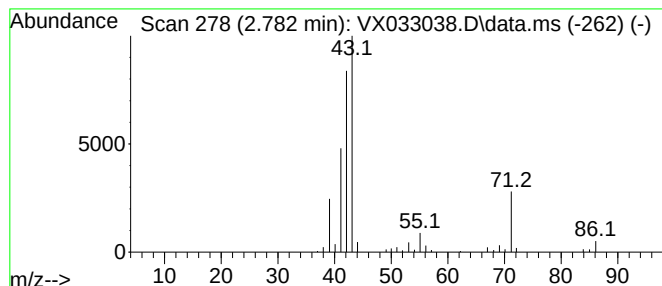
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	6.60 ug/l	93980	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3			Pentane	72	C5H12	000109-66-0	38
4			1-Pentene	70	C5H10	000109-67-1	28
5			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	12



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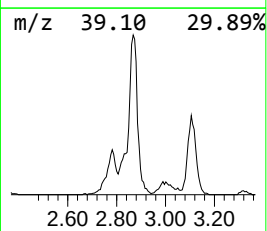
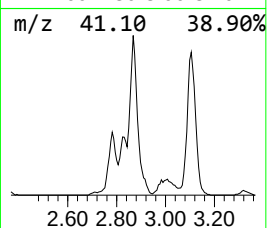
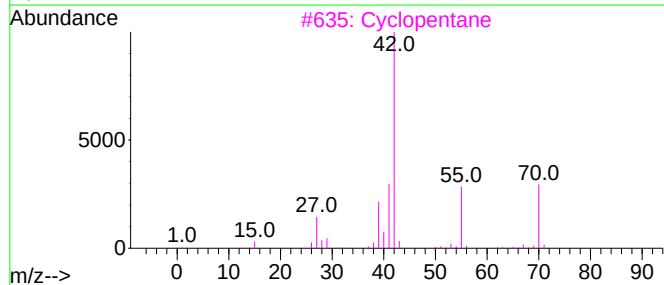
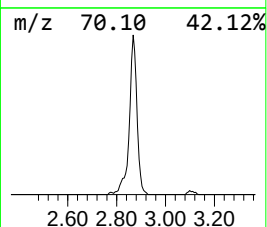
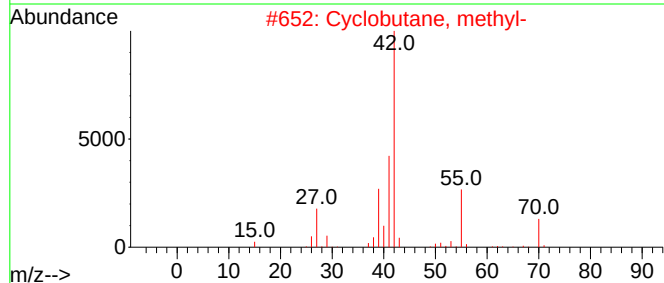
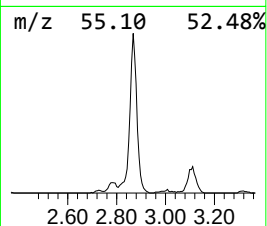
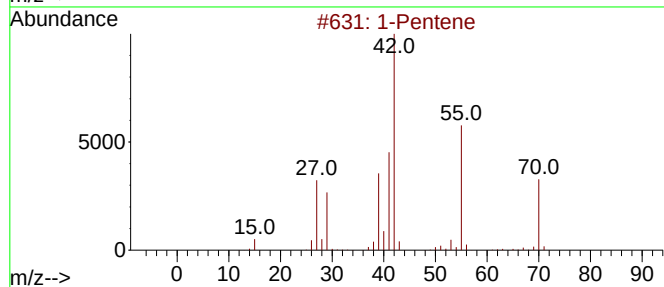
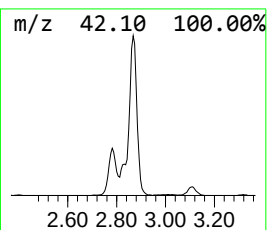
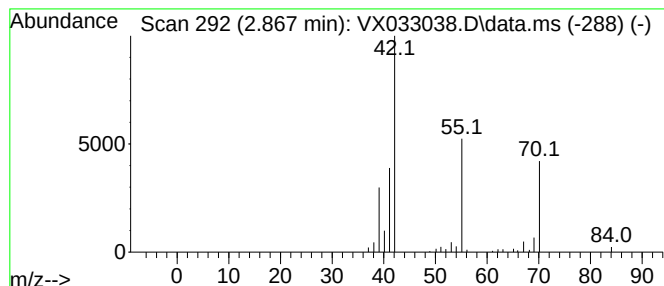
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Quant Title : SW846 8260

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

Peak Number 4 1-Pentene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	14.66 ug/l	208732	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	86
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
3			Cyclopentane	70	C5H10	000287-92-3	86
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
5			2-Pentene, (E)-	70	C5H10	000646-04-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033038.D
Acq On : 24 Nov 2022 04:55
Operator : JC/MD
Sample : N5741-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

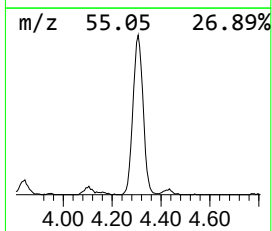
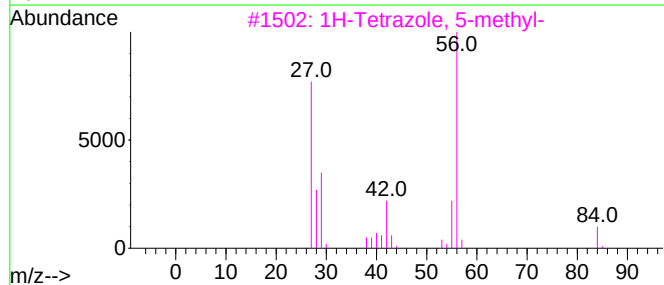
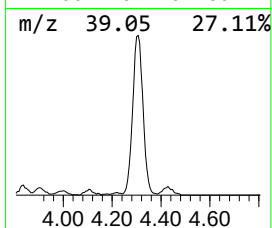
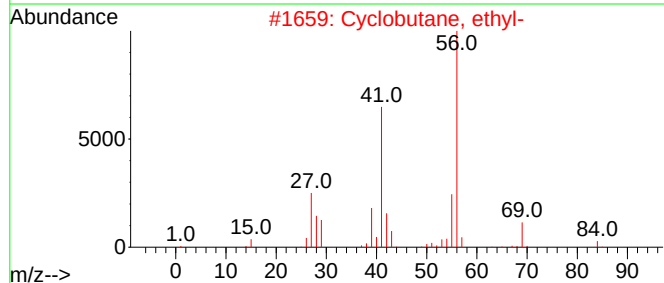
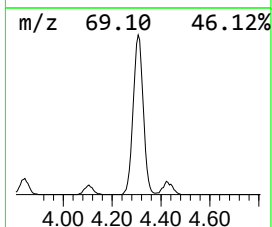
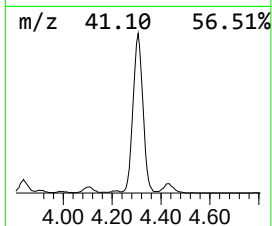
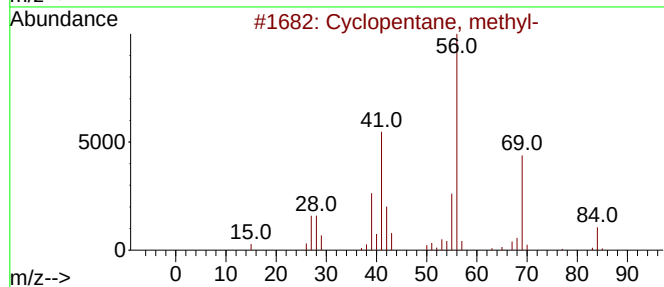
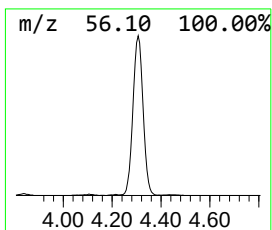
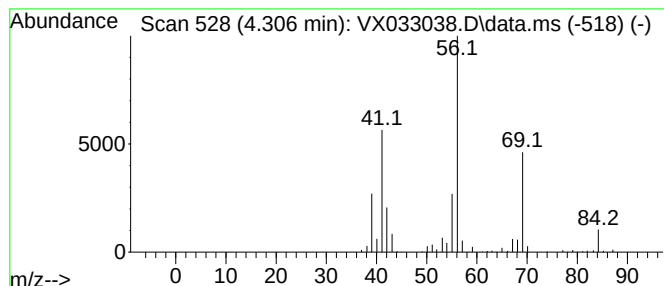
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	34.90 ug/l	497028	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	64
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4			Cyclobutane	56	C4H8	000287-23-0	50
5			Cyclohexane	84	C6H12	000110-82-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033038.D
Acq On : 24 Nov 2022 04:55
Operator : JC/MD
Sample : N5741-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

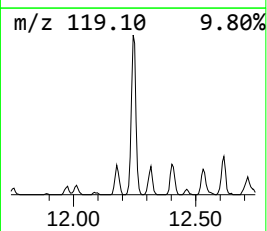
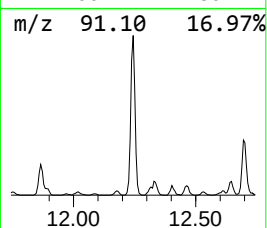
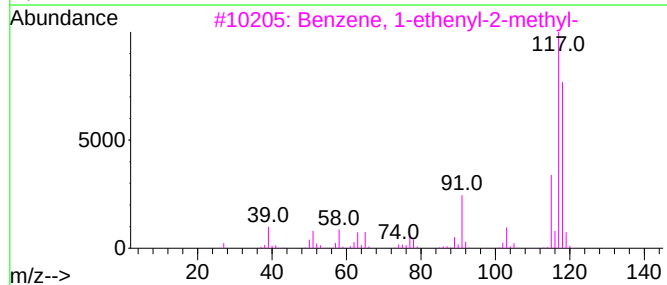
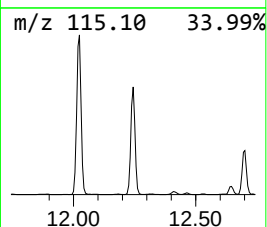
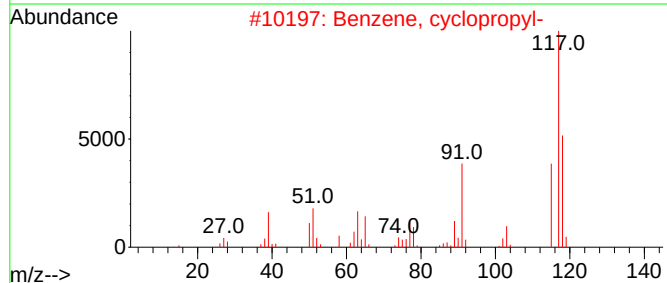
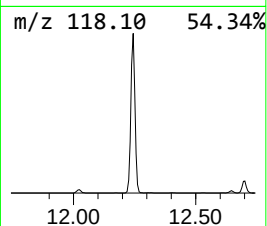
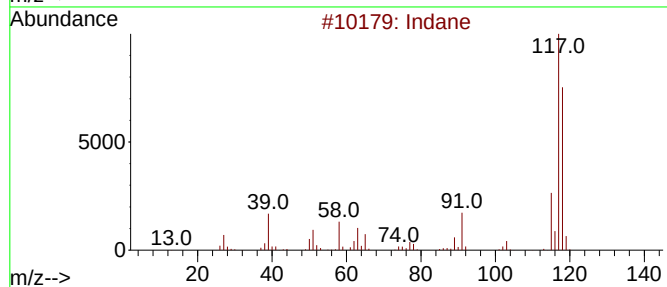
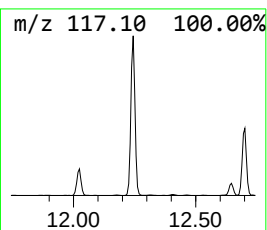
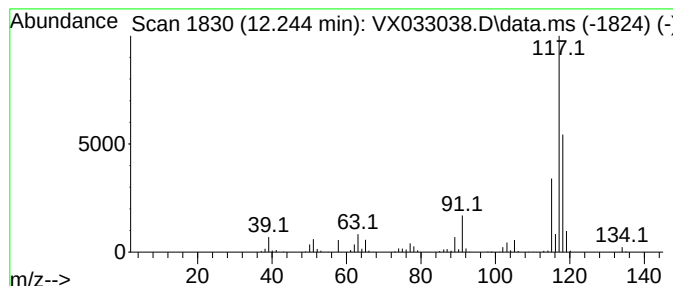
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	30.19 ug/l	590762	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, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Deltacyclene	118	C9H10	007785-10-6	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033038.D
Acq On : 24 Nov 2022 04:55
Operator : JC/MD
Sample : N5741-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

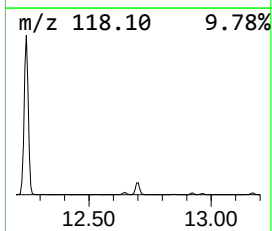
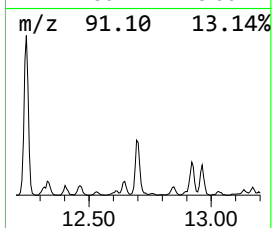
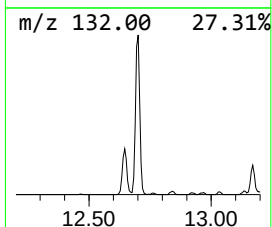
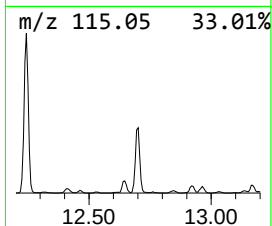
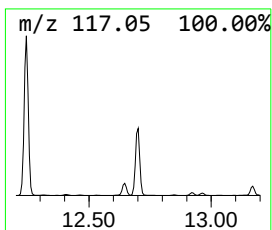
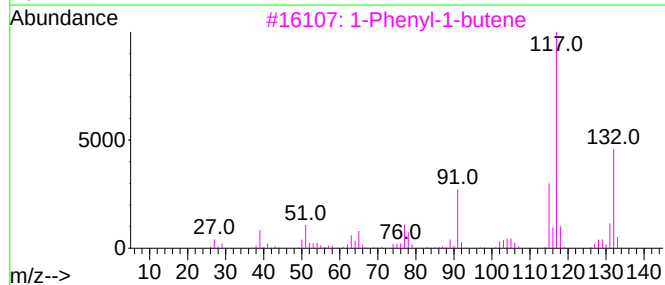
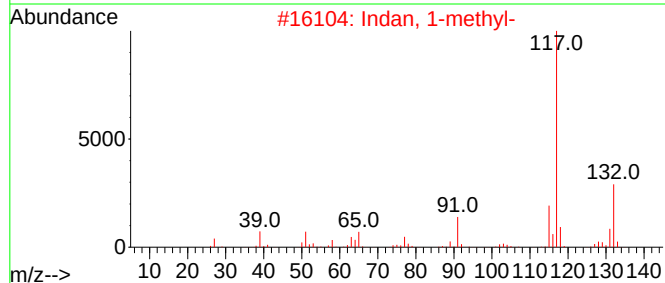
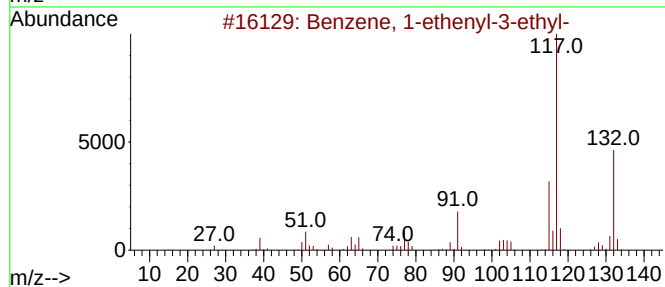
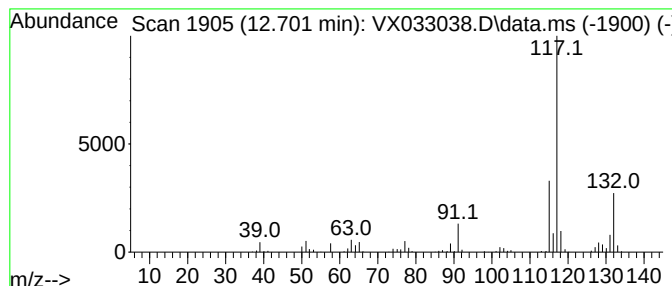
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	11.87 ug/l	232321	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033038.D
Acq On : 24 Nov 2022 04:55
Operator : JC/MD
Sample : N5741-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

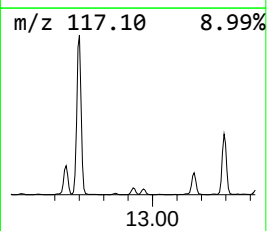
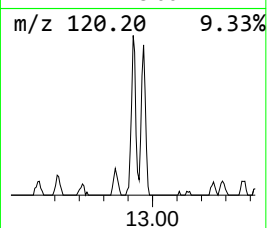
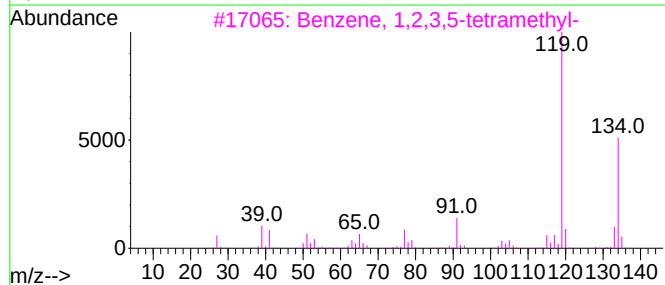
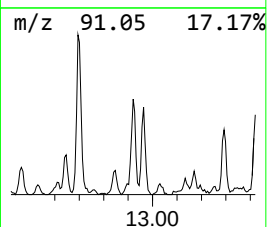
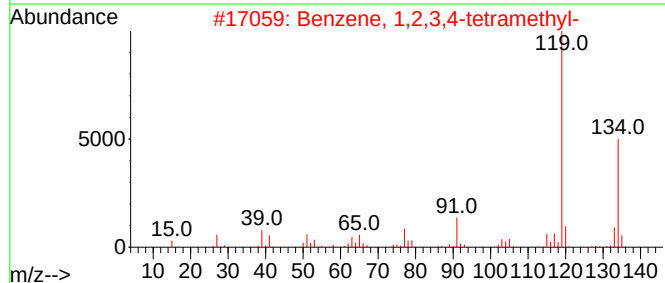
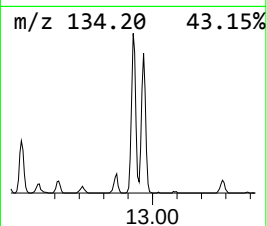
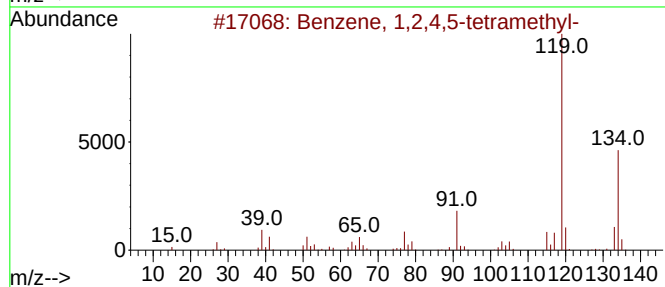
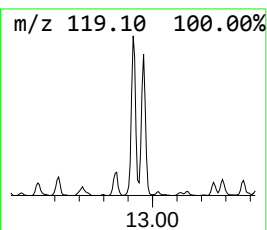
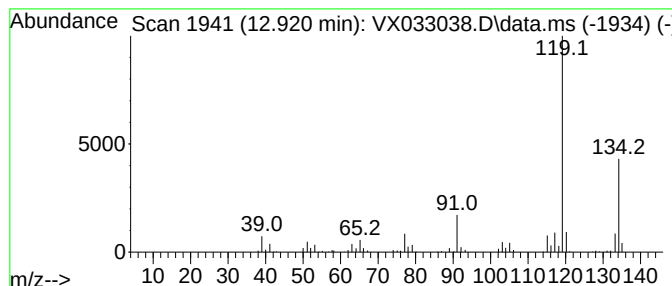
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	5.86 ug/l	114642	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033038.D
Acq On : 24 Nov 2022 04:55
Operator : JC/MD
Sample : N5741-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

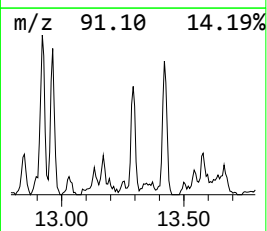
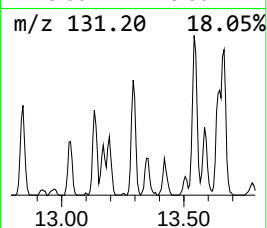
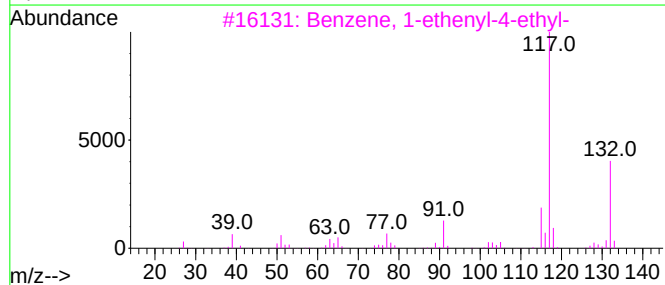
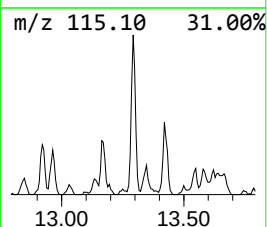
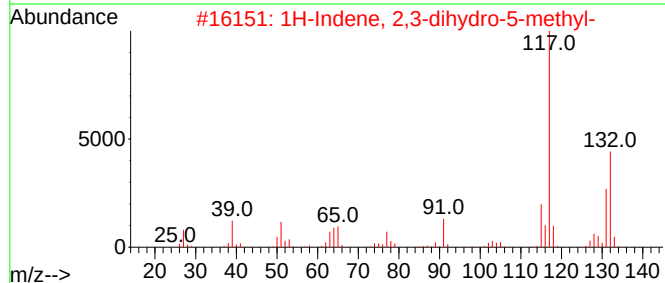
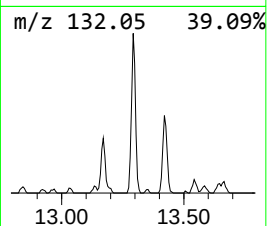
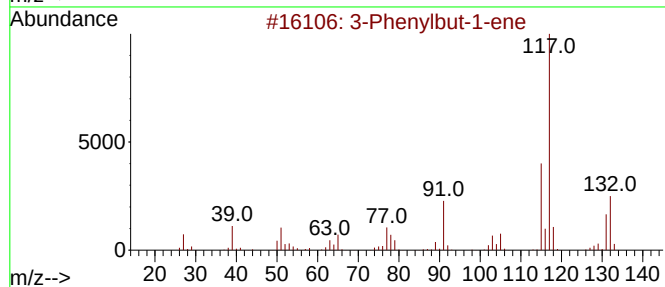
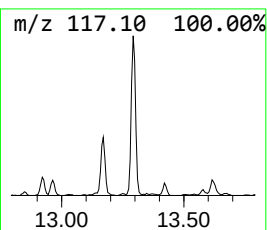
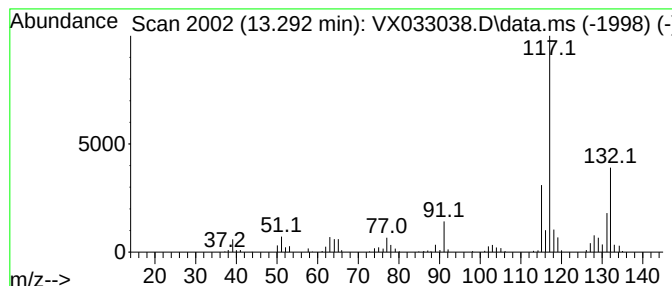
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.13 ug/l	100294	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
3		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5		Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033038.D
Acq On : 24 Nov 2022 04:55
Operator : JC/MD
Sample : N5741-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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	1.959	5.8	ug/l	83060	1	5.556	712114	50.0
Butane, 2,3-dim...	2.782	6.6	ug/l	93980	1	5.556	712114	50.0
1-Pentene	2.867	14.7	ug/l	208732	1	5.556	712114	50.0
Cyclopentane, m...	4.306	34.9	ug/l	497028	1	5.556	712114	50.0
Indane	12.244	30.2	ug/l	590762	4	12.024	978347	50.0
Benzene, 1-ethe...	12.701	11.9	ug/l	232321	4	12.024	978347	50.0
Benzene, 1,2,4,...	12.920	5.9	ug/l	114642	4	12.024	978347	50.0
3-Phenylbut-1-ene	13.292	5.1	ug/l	100294	4	12.024	978347	50.0