

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092023\
 Data File : VX037836.D
 Acq On : 20 Sep 2023 16:39
 Operator : JC/MD
 Sample : 04511-02 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50095

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\82X091523W.M
 Title : SW846 8260

Signal : TIC: VX037836.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	26	30	34	rBV	15239	17199	1.27%	0.150%
2	1.374	41	47	52	rBV	89474	101515	7.51%	0.883%
3	1.453	57	60	65	rVB	55669	60516	4.48%	0.526%
4	1.557	70	77	83	rVB3	12031	25021	1.85%	0.218%
5	1.752	104	109	118	rVB	39253	53961	3.99%	0.469%
6	1.959	138	143	153	rVV3	20295	42137	3.12%	0.367%
7	2.057	153	159	173	rVV	328169	572549	42.36%	4.980%
8	2.166	173	177	181	rVV2	11994	23102	1.71%	0.201%
9	2.215	181	185	195	rVB	32051	56260	4.16%	0.489%
10	2.380	207	212	222	rVB	18383	32052	2.37%	0.279%
11	2.867	287	292	299	rVB2	7090	14223	1.05%	0.124%
12	3.117	323	333	345	rBV	20323	50779	3.76%	0.442%
13	4.721	586	596	610	rBV	33776	97700	7.23%	0.850%
14	5.391	693	706	723	rBV	147326	445325	32.95%	3.874%
15	5.556	723	733	752	rVB	257878	736918	54.52%	6.410%
16	5.958	789	799	806	rBV	160029	422281	31.24%	3.673%
17	6.044	806	813	826	rVB	219790	586320	43.38%	5.100%
18	6.763	920	931	944	rBV	402817	958313	70.90%	8.336%
19	8.653	1234	1241	1247	rBV	834388	1339232	99.08%	11.649%
20	8.720	1247	1252	1261	rVB	897223	1334255	98.71%	11.606%
21	9.616	1390	1399	1413	rBV5	14265	51519	3.81%	0.448%
22	10.006	1457	1463	1466	rBV2	17404	40433	2.99%	0.352%
23	10.055	1466	1471	1483	rVB	912797	1234721	91.35%	10.740%
24	10.195	1489	1494	1503	rVB	74366	99769	7.38%	0.868%
25	10.299	1505	1511	1521	rVB	214015	295361	21.85%	2.569%
26	10.640	1562	1567	1577	rVB	111558	152369	11.27%	1.325%
27	11.079	1634	1639	1649	rBV	776258	989916	73.24%	8.611%
28	11.311	1671	1677	1683	rVV2	12929	19017	1.41%	0.165%
29	11.378	1683	1688	1697	rVV	25389	48442	3.58%	0.421%
30	11.451	1697	1700	1711	rVB2	15758	21252	1.57%	0.185%
31	11.616	1722	1727	1732	rBV	11503	15692	1.16%	0.136%
32	11.756	1746	1750	1759	rVB	48396	65468	4.84%	0.569%
33	12.024	1781	1794	1801	rBV	1075012	1351643	100.00%	11.757%
34	12.085	1801	1804	1812	rVB	18247	25915	1.92%	0.225%
35	12.244	1824	1830	1839	rBV3	13468	21872	1.62%	0.190%
36	13.292	1998	2002	2007	rVB2	10064	13847	1.02%	0.120%

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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\82X091523W.M
Title : SW846 8260

37	13.780	2076	2082	2089	rBV	15023	21034	1.56%	0.183%
38	14.640	2214	2223	2233	rBV5	5775	13881	1.03%	0.121%
39	15.487	2357	2362	2367	rBV2	11240	14801	1.10%	0.129%
40	16.371	2501	2507	2515	rVB2	17396	29964	2.22%	0.261%

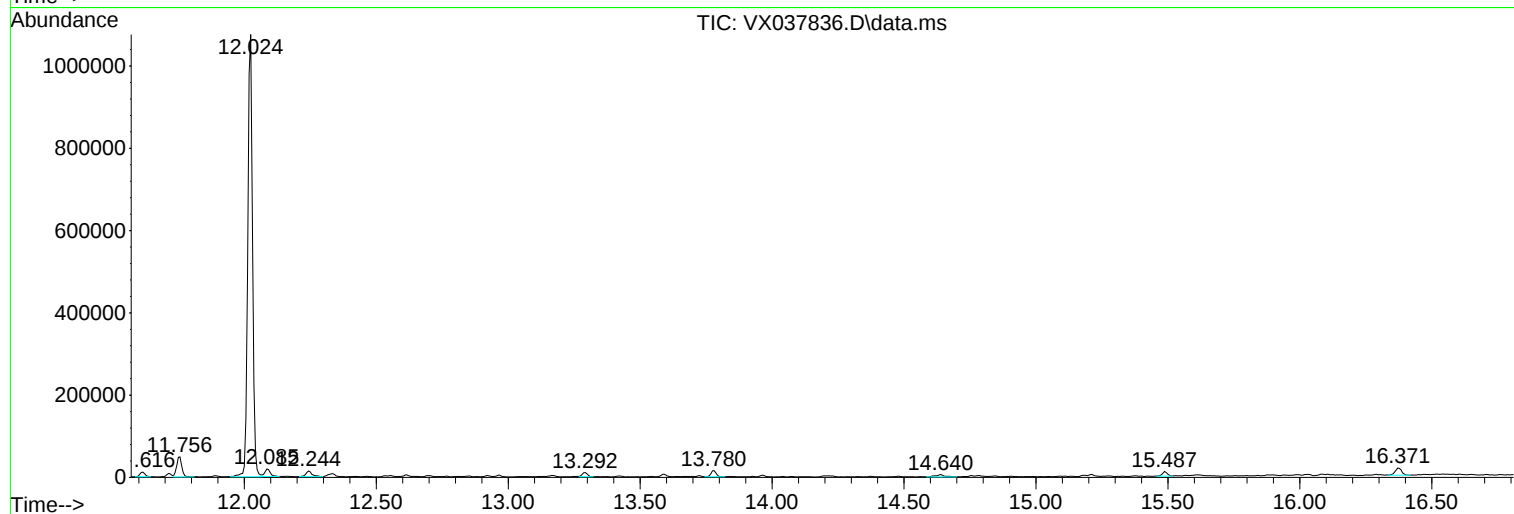
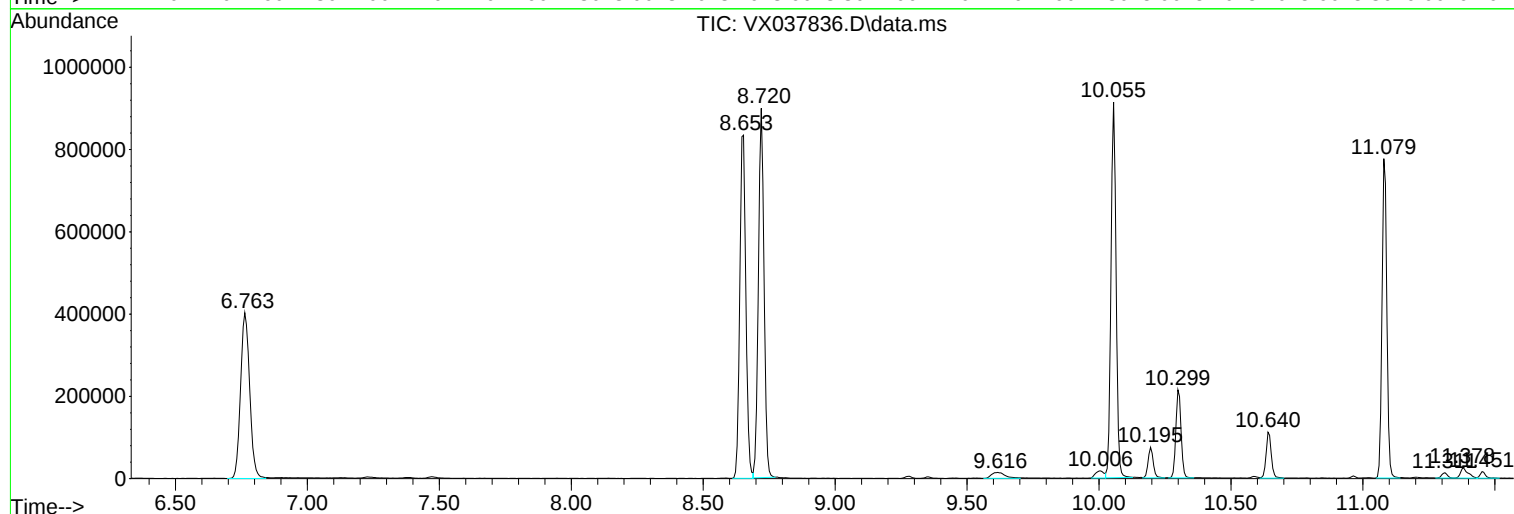
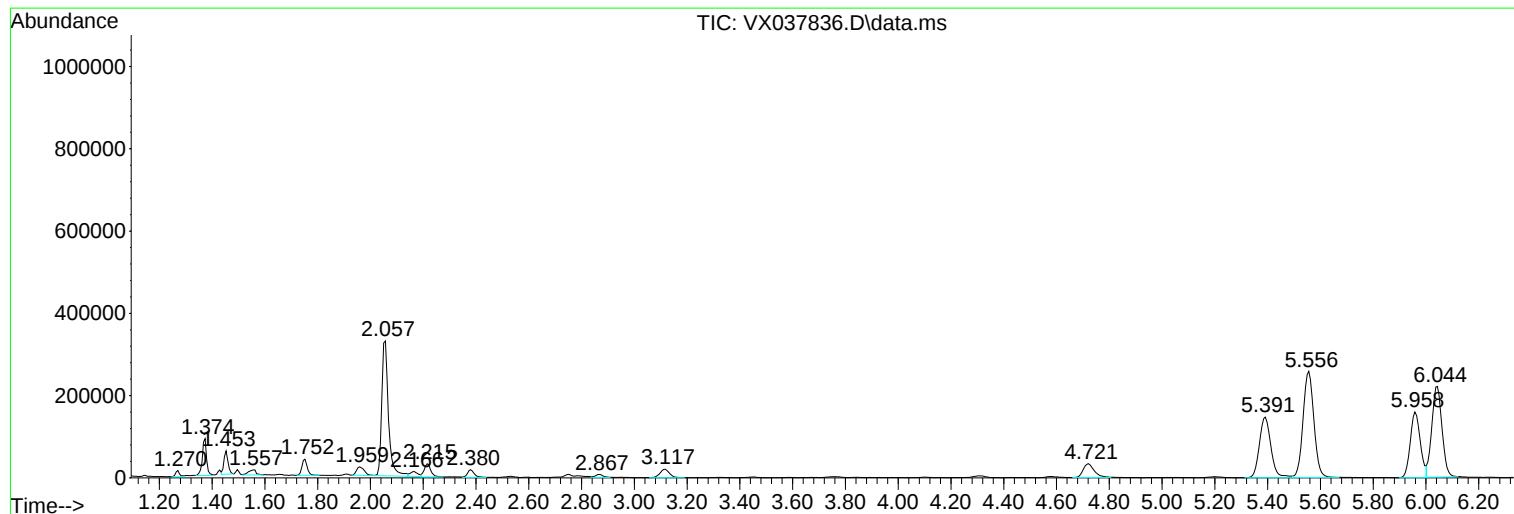
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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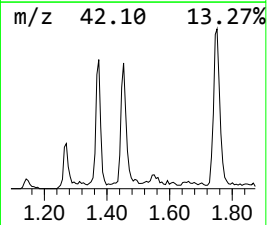
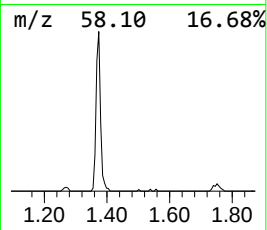
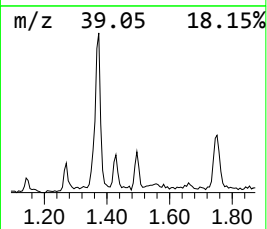
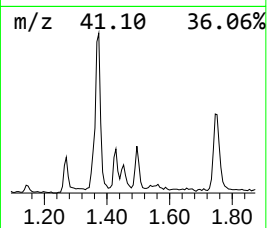
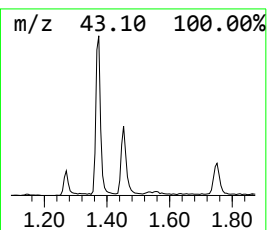
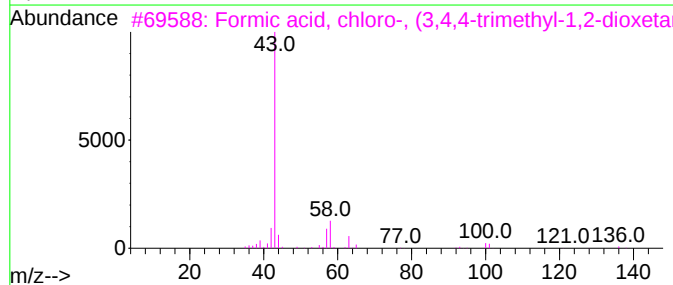
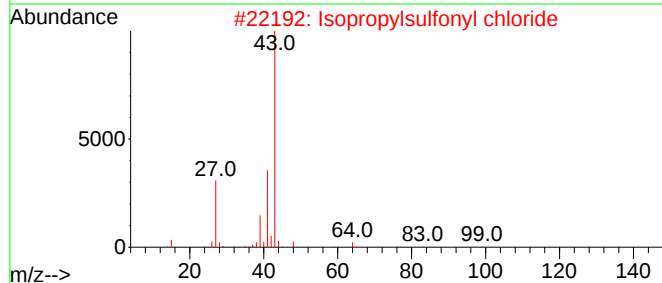
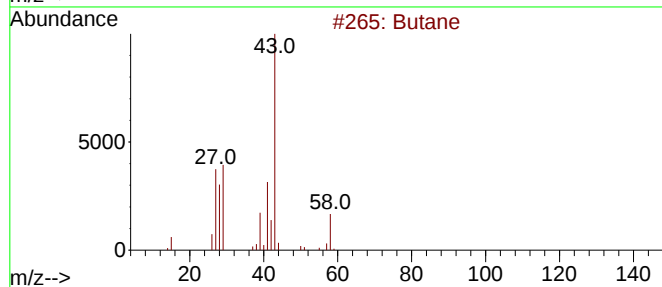
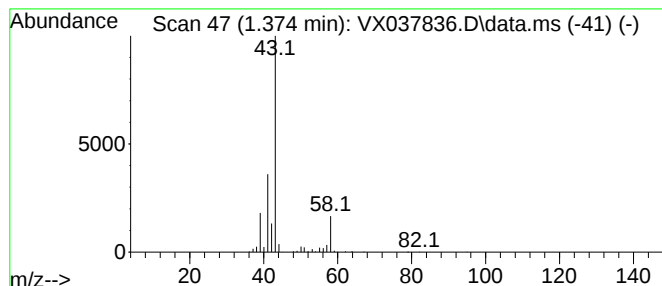
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	6.89 ug/l	101515	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
4			Isobutane	58	C4H10	000075-28-5	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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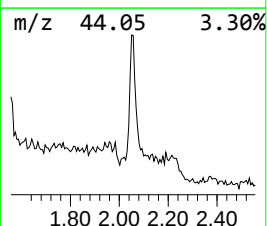
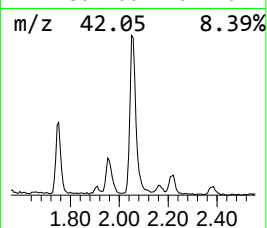
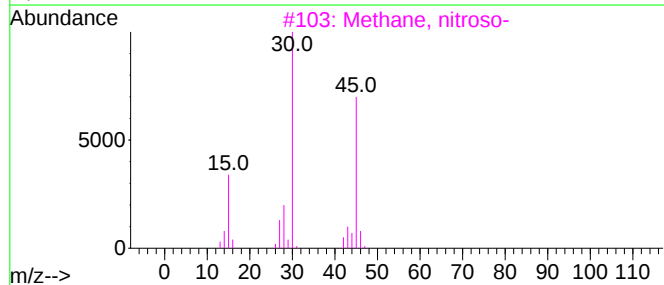
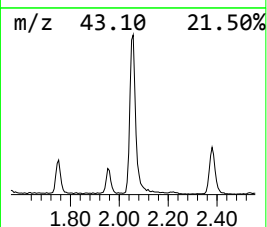
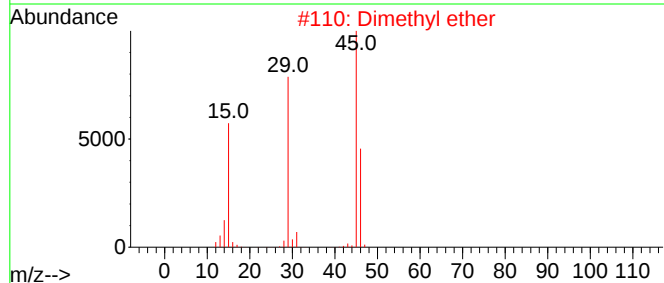
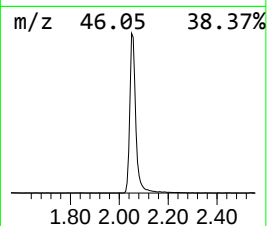
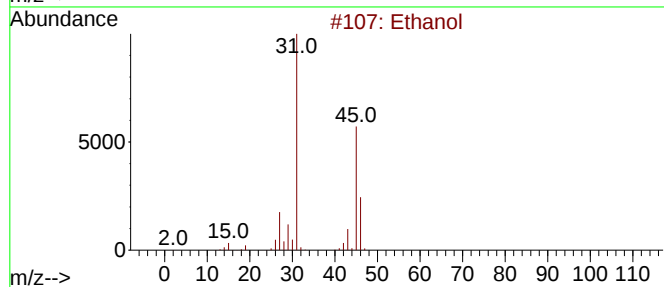
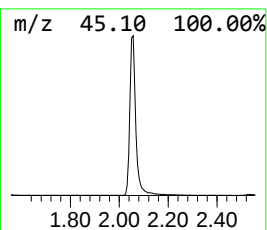
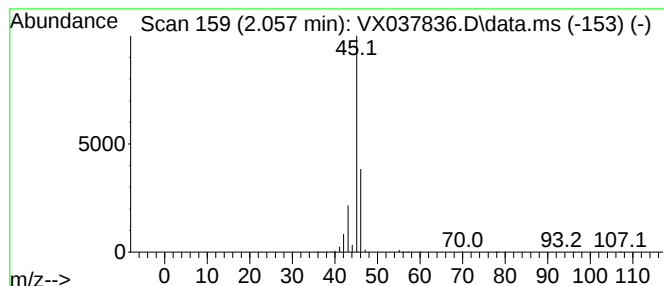
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	38.85 ug/l	572549	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	L-Lactic acid			90	C3H6O3	000079-33-4	2



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.374	6.9	ug/l	101515	1	5.556	736918	50.0
Ethanol	2.057	38.9	ug/l	572549	1	5.556	736918	50.0