

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
 Data File : VN074963.D
 Acq On : 21 Oct 2022 15:47
 Operator : JC\MD
 Sample : N5222-09
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-9

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_N\methods\82N102022W.M
 Title : SW846 8260

Signal : TIC: VN074963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.294	33	41	51	rBV	193951	467056	6.81%	1.359%
2	2.847	126	135	147	rVB6	146511	556732	8.11%	1.620%
3	7.947	991	1002	1010	rBV10	20337	74435	1.08%	0.217%
4	8.171	1029	1040	1045	rBV	896170	2132925	31.09%	6.205%
5	8.229	1045	1050	1062	rVV	1059051	2312275	33.70%	6.727%
6	8.582	1100	1110	1120	rBV	980826	2252974	32.84%	6.554%
7	8.782	1131	1144	1153	rVB3	298062	819948	11.95%	2.385%
8	9.106	1189	1199	1212	rBV	1427885	3064563	44.67%	8.915%
9	9.341	1232	1239	1242	rBV5	36072	70491	1.03%	0.205%
10	9.388	1243	1247	1256	rVB3	53741	104645	1.53%	0.304%
11	9.959	1342	1344	1350	rVV6	40706	83207	1.21%	0.242%
12	10.012	1350	1353	1361	rVB6	33339	70563	1.03%	0.205%
13	10.147	1372	1376	1383	rVB2	57739	105490	1.54%	0.307%
14	10.570	1439	1448	1468	rBV	3671635	6861048	100.00%	19.960%
15	10.735	1468	1476	1479	rBV5	41884	111810	1.63%	0.325%
16	10.835	1487	1493	1500	rVB6	37455	81210	1.18%	0.236%
17	10.982	1511	1518	1528	rVB4	69719	156643	2.28%	0.456%
18	11.106	1528	1539	1546	rBV3	159912	315478	4.60%	0.918%
19	11.864	1661	1668	1681	rVV	2178336	3934034	57.34%	11.445%
20	11.970	1681	1686	1696	rVB2	55054	126334	1.84%	0.368%
21	12.070	1696	1703	1709	rBV	77817	167981	2.45%	0.489%
22	12.847	1825	1835	1843	rBV	2596965	4463667	65.06%	12.985%
23	13.482	1938	1943	1951	rVV	75710	133847	1.95%	0.389%
24	13.617	1955	1966	1972	rBV5	64459	154913	2.26%	0.451%
25	13.794	1988	1996	2002	rBV	2643181	4492184	65.47%	13.068%
26	14.000	2024	2031	2038	rBV5	33400	83414	1.22%	0.243%
27	14.270	2071	2077	2084	rBV3	82205	149936	2.19%	0.436%
28	14.523	2113	2120	2127	rBV9	28403	73858	1.08%	0.215%
29	14.776	2158	2163	2170	rVB3	55437	96391	1.40%	0.280%
30	14.941	2184	2191	2197	rBV4	60190	116554	1.70%	0.339%
31	15.123	2216	2222	2229	rVB7	53991	102993	1.50%	0.300%
32	15.311	2247	2254	2261	rBV4	66506	147058	2.14%	0.428%
33	15.447	2265	2277	2284	rVB3	91289	257593	3.75%	0.749%
34	15.641	2303	2310	2317	rVB2	119309	232507	3.39%	0.676%

Sum of corrected areas: 34374757

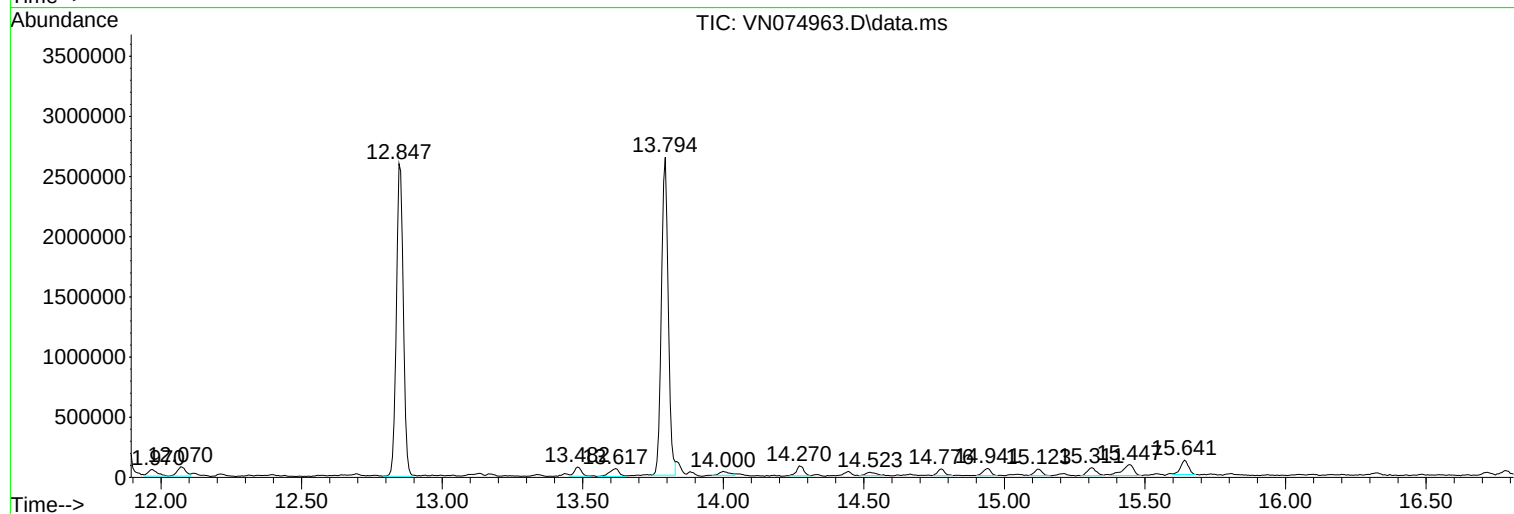
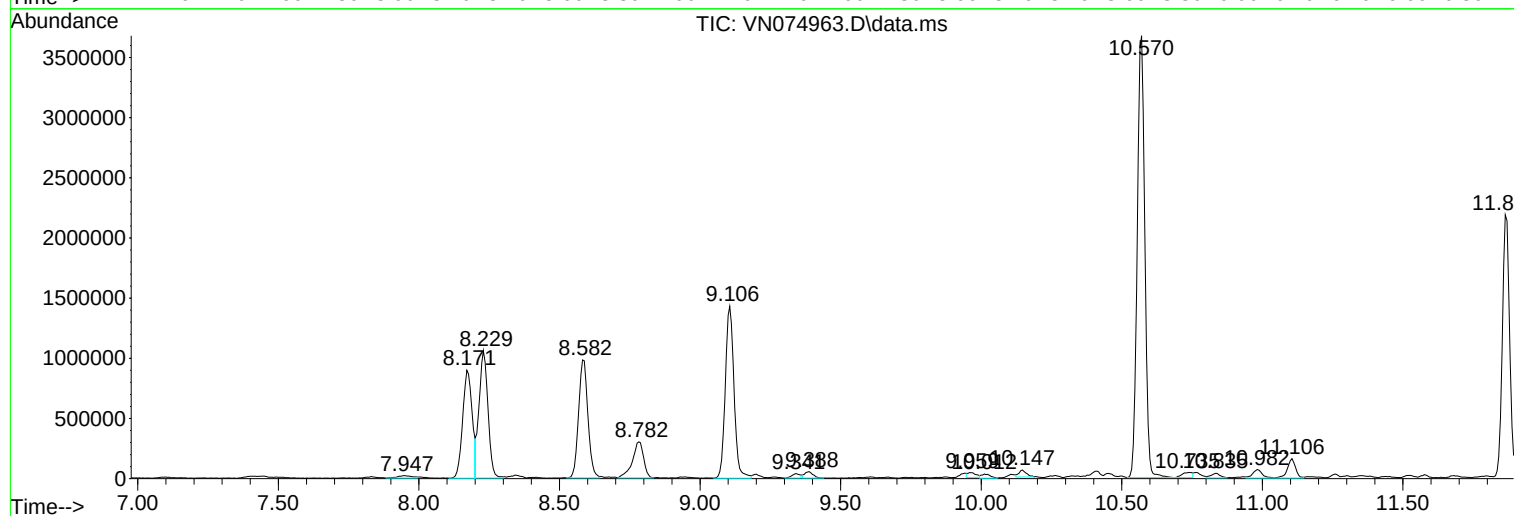
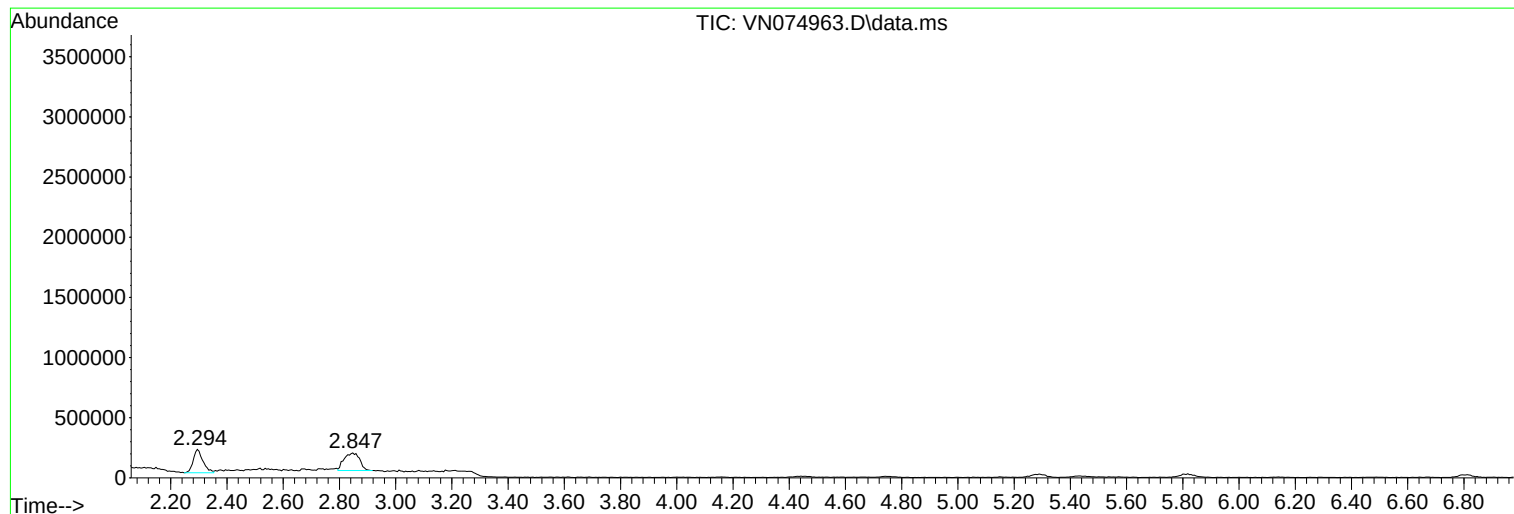
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



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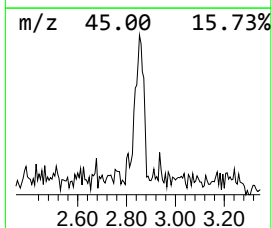
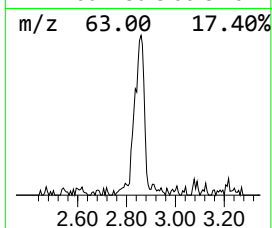
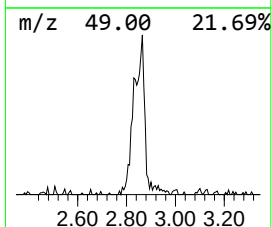
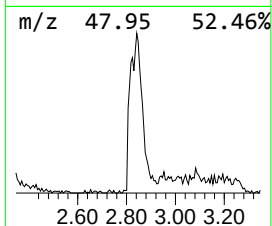
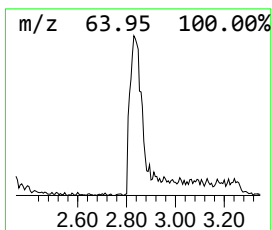
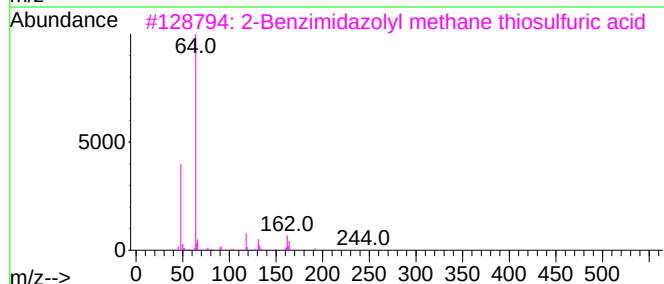
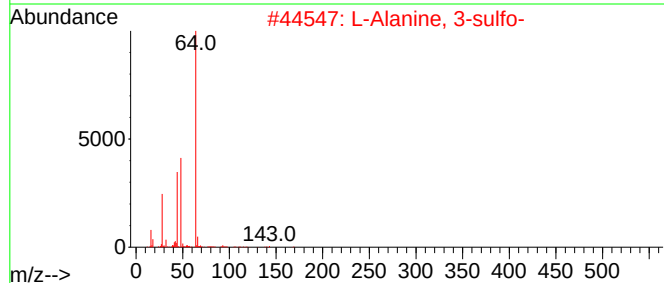
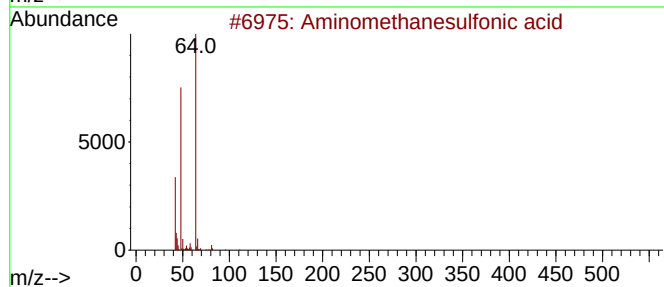
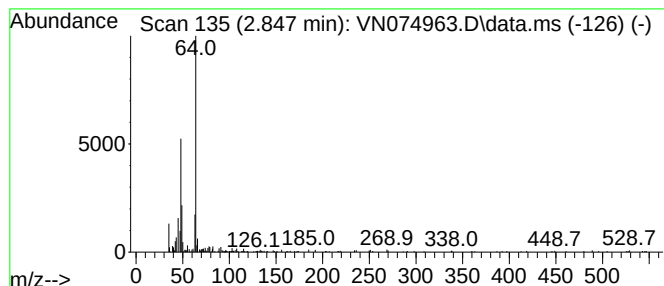
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Peak Number 2 unknown2.847 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.847	12.04 ug/l	556732	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	45
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	45
3			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	45
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	45
5			Sulfur dioxide	64	O2S	007446-09-5	45



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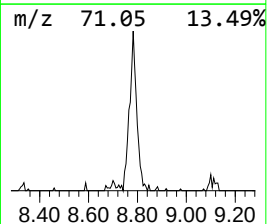
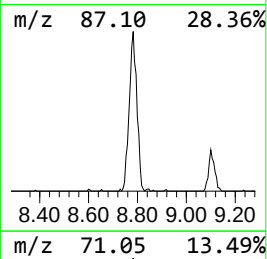
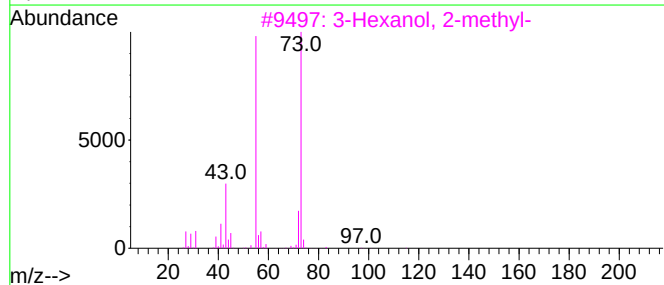
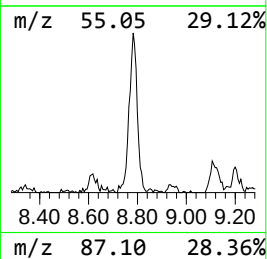
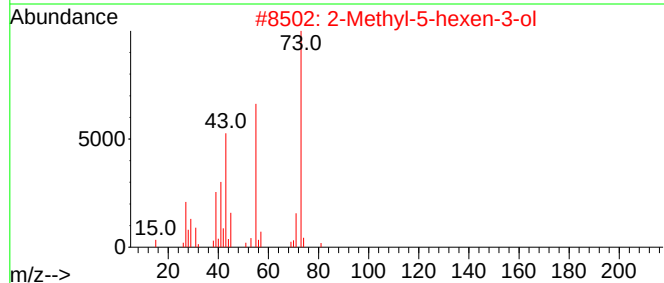
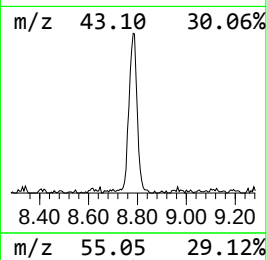
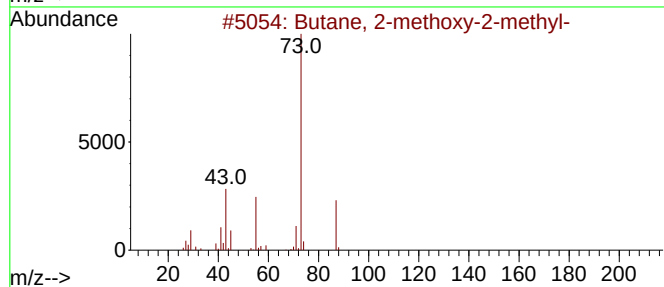
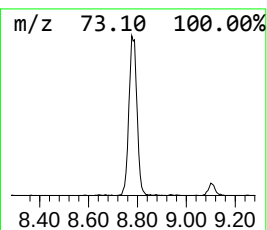
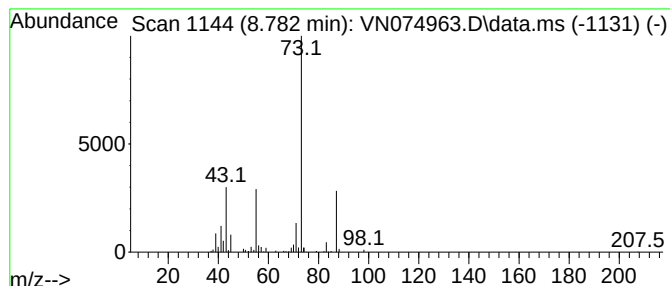
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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.782	13.38 ug/l	819948	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.294	10.1	ug/l	467056	1	8.229	2312280	50.0
unknown2.847	2.847	12.0	ug/l	556732	1	8.229	2312280	50.0
Butane, 2-metho...	8.782	13.4	ug/l	819948	2	9.106	3064560	50.0