

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070011.D
 Acq On : 11 Dec 2021 16:27
 Operator : JC/MD
 Sample : M4873-06
 Misc : 6.93g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A2-7-6.5

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070011.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.233	81	91	132	rVB4	113694	411792	5.24%	0.683%
2	2.443	161	169	186	rVB2	92139	167038	2.12%	0.277%
3	2.998	369	376	386	rVB3	112795	179263	2.28%	0.297%
4	3.397	514	525	543	rVB3	39984	92185	1.17%	0.153%
5	5.302	1211	1235	1262	rBV2	46568	168657	2.14%	0.280%
6	5.484	1271	1303	1325	rBV2	301961	1260704	16.03%	2.091%
7	5.615	1327	1352	1390	rVB2	1661806	5939621	75.51%	9.853%
8	6.079	1506	1525	1550	rVB4	34820	108459	1.38%	0.180%
9	7.023	1859	1877	1895	rBV5	25941	80376	1.02%	0.133%
10	7.125	1897	1915	1916	rBV4	57734	96696	1.23%	0.160%
11	8.018	2225	2248	2258	rBV	884336	2169802	27.59%	3.600%
12	8.080	2259	2271	2290	rVV	1594055	3698734	47.02%	6.136%
13	8.163	2292	2302	2321	rVB3	78585	194031	2.47%	0.322%
14	8.284	2330	2347	2362	rBV5	68761	155529	1.98%	0.258%
15	8.437	2383	2404	2433	rBV3	1237519	3281633	41.72%	5.444%
16	8.576	2437	2456	2459	rBV6	190082	378910	4.82%	0.629%
17	8.820	2532	2547	2575	rVB5	62227	174492	2.22%	0.289%
18	8.965	2580	2601	2645	rVB	2637030	5562938	70.72%	9.229%
19	9.453	2754	2783	2795	rBV6	99262	263182	3.35%	0.437%
20	9.877	2926	2941	2962	rVB2	104489	218681	2.78%	0.363%
21	10.011	2980	2991	3005	rVB2	132666	264735	3.37%	0.439%
22	10.215	3045	3067	3074	rBV2	79789	171184	2.18%	0.284%
23	10.368	3110	3124	3134	rBV2	78453	137563	1.75%	0.228%
24	10.440	3134	3151	3170	rBV	4106246	7778596	98.89%	12.904%
25	10.564	3187	3197	3208	rBV5	49893	99395	1.26%	0.165%
26	10.623	3212	3219	3234	rVB5	62706	114568	1.46%	0.190%
27	11.626	3582	3593	3614	rBV4	47851	93270	1.19%	0.155%
28	11.746	3620	3638	3661	rBV	4264790	7631951	97.03%	12.661%
29	11.846	3664	3675	3697	rVV	280815	509315	6.48%	0.845%
30	11.953	3698	3715	3740	rVV3	268106	581453	7.39%	0.965%
31	12.280	3819	3837	3852	rVB3	57603	133821	1.70%	0.222%
32	12.733	3990	4006	4031	rVB	3543347	6097762	77.52%	10.116%
33	12.921	4065	4076	4087	rVB	124872	194854	2.48%	0.323%
34	12.983	4089	4099	4107	rBV	166970	283652	3.61%	0.471%
35	13.055	4119	4126	4143	rVB3	180279	328761	4.18%	0.545%
36	13.224	4173	4189	4205	rBV	175557	341588	4.34%	0.567%

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37	13.369	4231	4243	4257	rVB	352203	570187	7.25%	0.946%
38	13.675	4342	4357	4392	rVB	4301955	7865827	100.00%	13.049%
39	13.841	4409	4419	4423	rBV4	65726	99592	1.27%	0.165%
40	13.876	4424	4432	4441	rVV3	147502	238527	3.03%	0.396%
41	13.994	4466	4476	4489	rBV2	148988	227964	2.90%	0.378%
42	14.217	4548	4559	4570	rBV	185740	303014	3.85%	0.503%
43	14.326	4592	4600	4613	rVB3	104069	173231	2.20%	0.287%
44	14.812	4772	4781	4786	rBV4	80749	123443	1.57%	0.205%
45	14.847	4788	4794	4808	rVB4	190320	286309	3.64%	0.475%
46	14.927	4809	4824	4835	rBV4	176035	431816	5.49%	0.716%
47	15.469	5017	5026	5030	rBV4	58305	83717	1.06%	0.139%
48	15.507	5033	5040	5053	rVB	126548	217147	2.76%	0.360%
49	15.702	5108	5113	5136	rVB4	89324	153289	1.95%	0.254%
50	16.620	5445	5455	5469	rVB	72553	140176	1.78%	0.233%

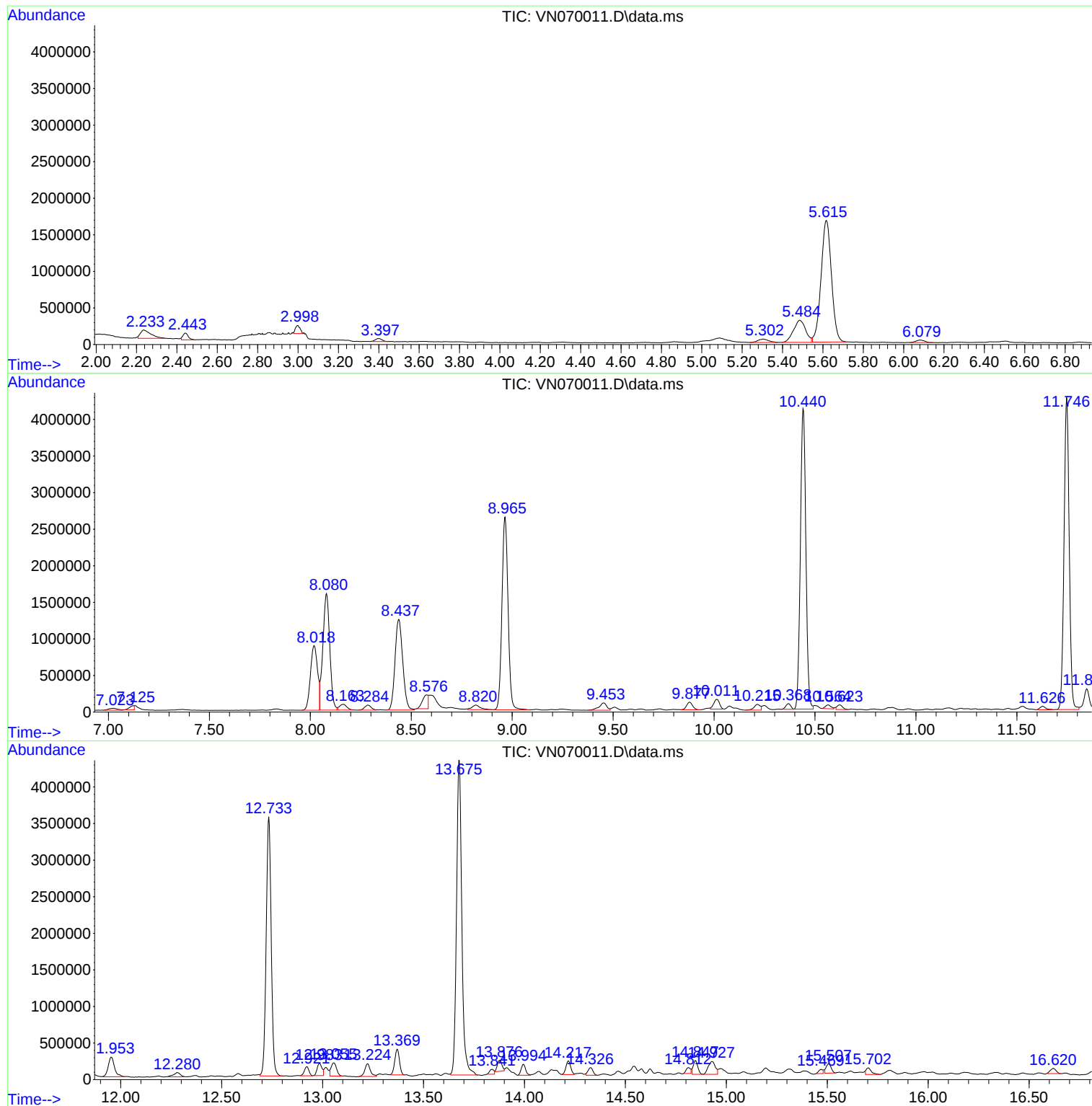
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Quant Title : SW846 8260

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



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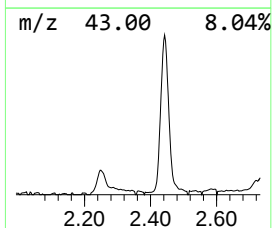
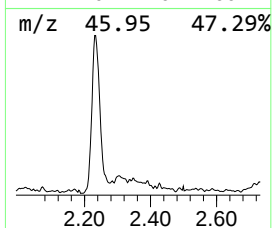
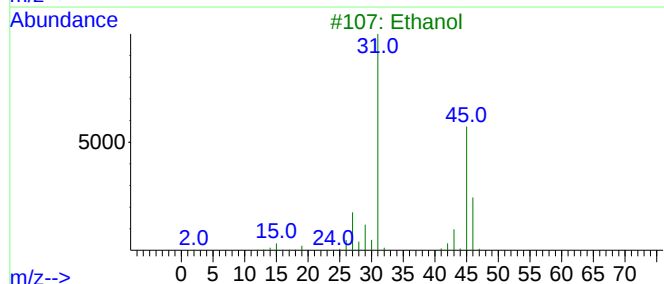
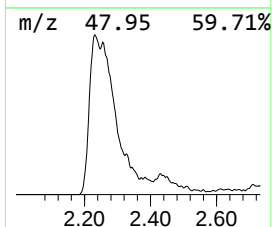
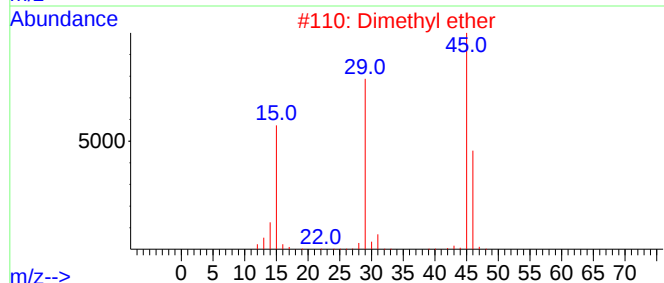
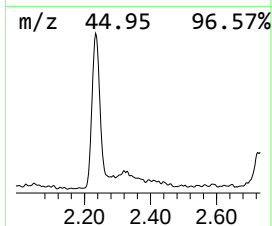
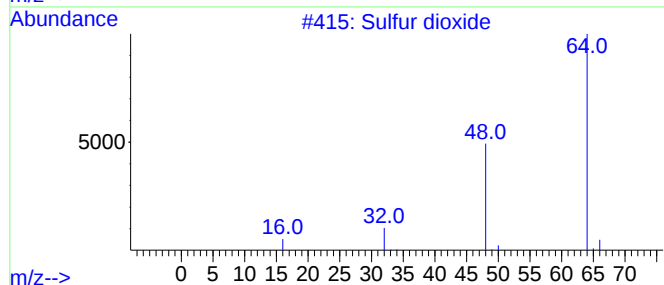
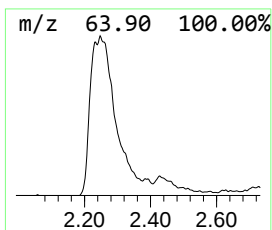
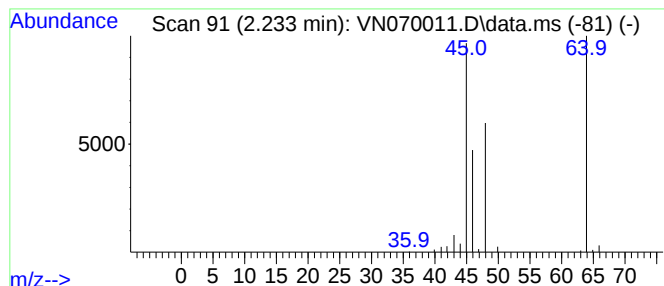
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.233	5.57 ug/l	411792	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	58
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Ethanol	46	C2H6O	000064-17-5	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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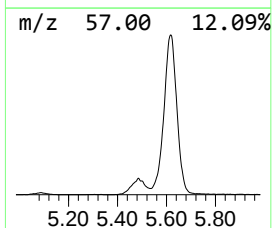
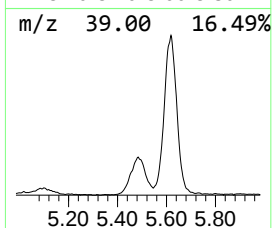
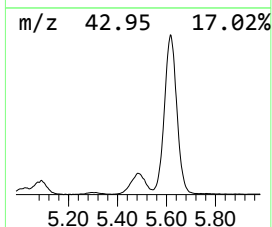
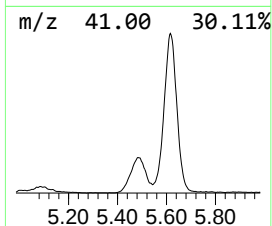
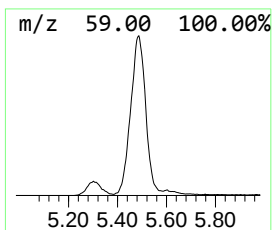
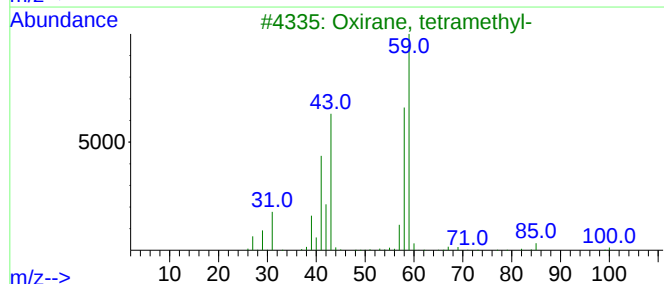
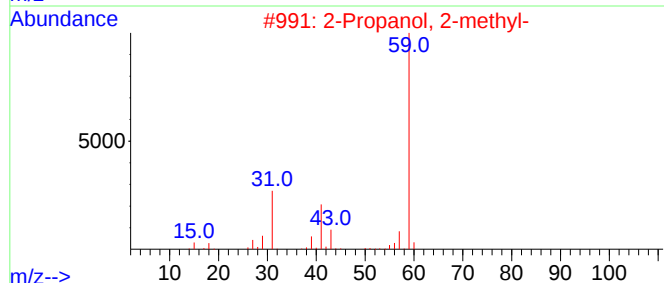
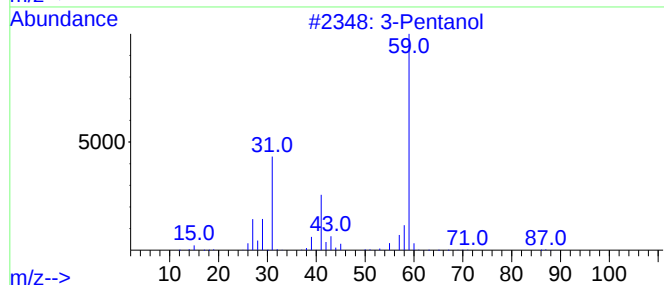
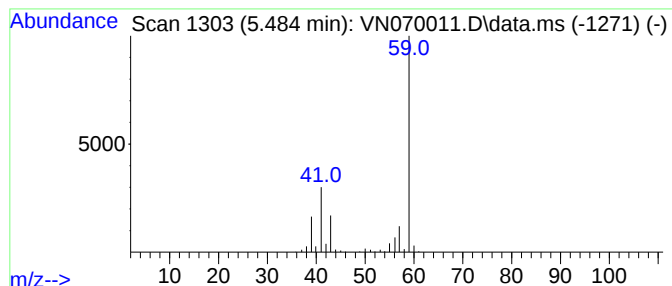
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown5.484 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.484	17.04 ug/l	1260700	Pentafluorobenzene	8.080

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Pentanol	88	C5H12O	000584-02-1	40
2		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9
3		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	9
4		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5		Acetaldoxime	59	C2H5NO	000107-29-9	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.233	5.6	ug/l	411792	1	8.080	3698730	50.0
unknown5.484	5.484	17.0	ug/l	1260700	1	8.080	3698730	50.0