

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
 Data File : VY014649.D
 Acq On : 14 Jul 2023 15:51
 Operator : SY/MD
 Sample : 03580-02
 Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SAMPLE-1

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_Y\methods\82Y071323S.M
 Title : SW846 8260

Signal : TIC: VY014649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.150	42	54	57	rBV9	6903	26005	88.74%	10.406%
2	2.393	92	94	97	rVB2	993	611	2.09%	0.245%
3	2.668	135	139	145	rVB4	1864	3752	12.80%	1.501%
4	2.729	148	149	154	rVB4	692	722	2.46%	0.289%
5	2.954	182	186	189	rVB4	644	928	3.17%	0.371%
6	2.991	189	192	195	rBV5	557	785	2.68%	0.314%
7	3.101	209	210	214	rBV2	734	752	2.57%	0.301%
8	3.332	245	248	250	rVB4	621	564	1.92%	0.226%
9	3.363	250	253	256	rVB5	740	681	2.32%	0.273%
10	3.570	285	287	290	rVB2	613	564	1.92%	0.226%
11	3.777	319	321	323	rVB3	615	535	1.83%	0.214%
12	3.820	323	328	331	rBV4	804	1453	4.96%	0.581%
13	3.857	331	334	335	rVB3	410	421	1.44%	0.168%
14	4.003	354	358	360	rBV3	440	681	2.32%	0.273%
15	4.100	371	374	376	rBV4	643	729	2.49%	0.292%
16	4.222	392	394	400	rBV4	554	689	2.35%	0.276%
17	4.369	414	418	420	rBV3	503	725	2.47%	0.290%
18	4.399	420	423	425	rVV2	585	509	1.74%	0.204%
19	4.442	428	430	435	rVB4	541	729	2.49%	0.292%
20	4.600	454	456	458	rBV2	607	725	2.47%	0.290%
21	4.698	466	472	473	rBV4	1218	1867	6.37%	0.747%
22	4.948	511	513	516	rVB4	421	473	1.61%	0.189%
23	5.021	523	525	527	rBV3	392	421	1.44%	0.168%
24	5.161	546	548	550	rVB3	743	630	2.15%	0.252%
25	5.186	550	552	553	rBV2	825	705	2.41%	0.282%
26	5.381	583	584	587	rBV3	539	487	1.66%	0.195%
27	5.515	603	606	610	rBV5	362	619	2.11%	0.248%
28	5.570	610	615	617	rVB3	502	885	3.02%	0.354%
29	5.606	617	621	622	rBV3	543	536	1.83%	0.214%
30	5.679	628	633	636	rBV4	473	829	2.83%	0.332%
31	5.716	636	639	640	rBV3	443	468	1.60%	0.187%
32	5.771	646	648	651	rVB4	526	503	1.72%	0.201%
33	5.826	653	657	658	rBV3	488	529	1.81%	0.212%
34	5.850	658	661	665	rVB5	399	610	2.08%	0.244%
35	5.917	668	672	673	rBV2	426	463	1.58%	0.185%
36	5.978	680	682	685	rVB3	586	505	1.72%	0.202%

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37	6.021	686	689	694	rBV4	611	991	3.38%	0.397%
38	6.118	702	705	709	rBV6	369	532	1.82%	0.213%
39	6.234	721	724	729	rBV6	569	861	2.94%	0.345%
40	6.271	729	730	733	rBV2	598	512	1.75%	0.205%
41	6.344	739	742	745	rBV4	417	577	1.97%	0.231%
42	6.442	754	758	761	rBV5	335	454	1.55%	0.182%
43	6.533	770	773	776	rVB4	498	614	2.10%	0.246%
44	6.655	789	793	796	rVB4	612	713	2.43%	0.285%
45	6.759	808	810	815	rVB4	401	527	1.80%	0.211%
46	6.813	815	819	820	rBV4	449	552	1.88%	0.221%
47	6.966	834	844	853	rVV2	2765	9643	32.91%	3.859%
48	7.106	865	867	870	rBV4	471	520	1.77%	0.208%
49	7.143	870	873	876	rBV5	527	624	2.13%	0.250%
50	7.356	905	908	909	rBV3	571	561	1.91%	0.224%
51	7.405	912	916	917	rBV4	543	511	1.74%	0.204%
52	7.472	924	927	930	rBV4	268	430	1.47%	0.172%
53	7.533	934	937	939	rBV4	662	552	1.88%	0.221%
54	7.649	954	956	959	rVB3	468	446	1.52%	0.178%
55	7.716	961	967	973	rVV4	2814	6159	21.02%	2.465%
56	7.783	973	978	987	rVV3	6444	14866	50.73%	5.949%
57	7.990	1011	1012	1015	rVB2	494	421	1.44%	0.168%
58	8.057	1020	1023	1026	rVB4	527	616	2.10%	0.247%
59	8.094	1026	1029	1030	rBV2	624	528	1.80%	0.211%
60	8.142	1030	1037	1044	rVV2	4267	10358	35.35%	4.145%
61	8.197	1044	1046	1049	rVB4	430	532	1.82%	0.213%
62	8.325	1064	1067	1069	rBV3	458	588	2.01%	0.235%
63	8.526	1098	1100	1102	rBV3	417	464	1.58%	0.186%
64	8.685	1119	1126	1135	rVV2	10444	22145	75.57%	8.862%
65	8.789	1139	1143	1146	rVV5	383	608	2.07%	0.243%
66	8.825	1148	1149	1153	rVB2	401	541	1.85%	0.216%
67	9.124	1196	1198	1201	rVB2	572	543	1.85%	0.217%
68	9.161	1201	1204	1206	rBV3	730	977	3.33%	0.391%
69	9.228	1212	1215	1218	rVB4	487	650	2.22%	0.260%
70	9.307	1224	1228	1230	rBV3	530	705	2.41%	0.282%
71	9.374	1237	1239	1244	rVB4	536	949	3.24%	0.380%
72	9.459	1251	1253	1257	rBV4	466	661	2.26%	0.265%
73	9.599	1274	1276	1279	rVB3	729	571	1.95%	0.228%
74	9.801	1307	1309	1312	rBV3	699	461	1.57%	0.184%
75	9.831	1312	1314	1317	rVB4	569	568	1.94%	0.227%
76	9.904	1321	1326	1328	rBV4	330	550	1.88%	0.220%

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77	10.002	1340	1342	1343	rVV2	544	500	1.71%	0.200%
78	10.045	1348	1349	1352	rVB3	644	486	1.66%	0.194%
79	10.118	1359	1361	1363	rVB3	732	533	1.82%	0.213%
80	10.179	1365	1371	1378	rVV	16096	29304	100.00%	11.727%
81	10.264	1383	1385	1392	rVB6	755	1231	4.20%	0.493%
82	10.392	1403	1406	1408	rVB3	539	593	2.02%	0.237%
83	10.477	1419	1420	1424	rBV4	656	756	2.58%	0.303%
84	10.581	1435	1437	1440	rVB4	629	547	1.87%	0.219%
85	10.929	1492	1494	1497	rBV3	1072	1542	5.26%	0.617%
86	11.002	1504	1506	1508	rBV3	488	555	1.89%	0.222%
87	11.154	1529	1531	1533	rBV2	646	602	2.05%	0.241%
88	11.215	1539	1541	1543	rVB2	582	461	1.57%	0.184%
89	11.270	1547	1550	1551	rBV3	865	883	3.01%	0.353%
90	11.306	1554	1556	1559	rVV3	719	882	3.01%	0.353%
91	11.343	1559	1562	1564	rVB4	574	788	2.69%	0.315%
92	11.489	1581	1586	1594	rBV	14831	25340	86.47%	10.140%
93	11.648	1610	1612	1613	rBV	714	619	2.11%	0.248%
94	11.831	1641	1642	1644	rBV2	716	507	1.73%	0.203%
95	11.886	1648	1651	1656	rBV5	946	1681	5.74%	0.673%
96	12.020	1670	1673	1676	rBV5	1154	1588	5.42%	0.635%
97	12.343	1723	1726	1728	rBV4	1092	1125	3.84%	0.450%
98	12.483	1743	1749	1755	rVB2	11662	19924	67.99%	7.973%
99	13.422	1899	1903	1913	rVB2	12685	20221	69.00%	8.092%
100	13.782	1960	1962	1965	rBV4	1545	2056	7.02%	0.823%

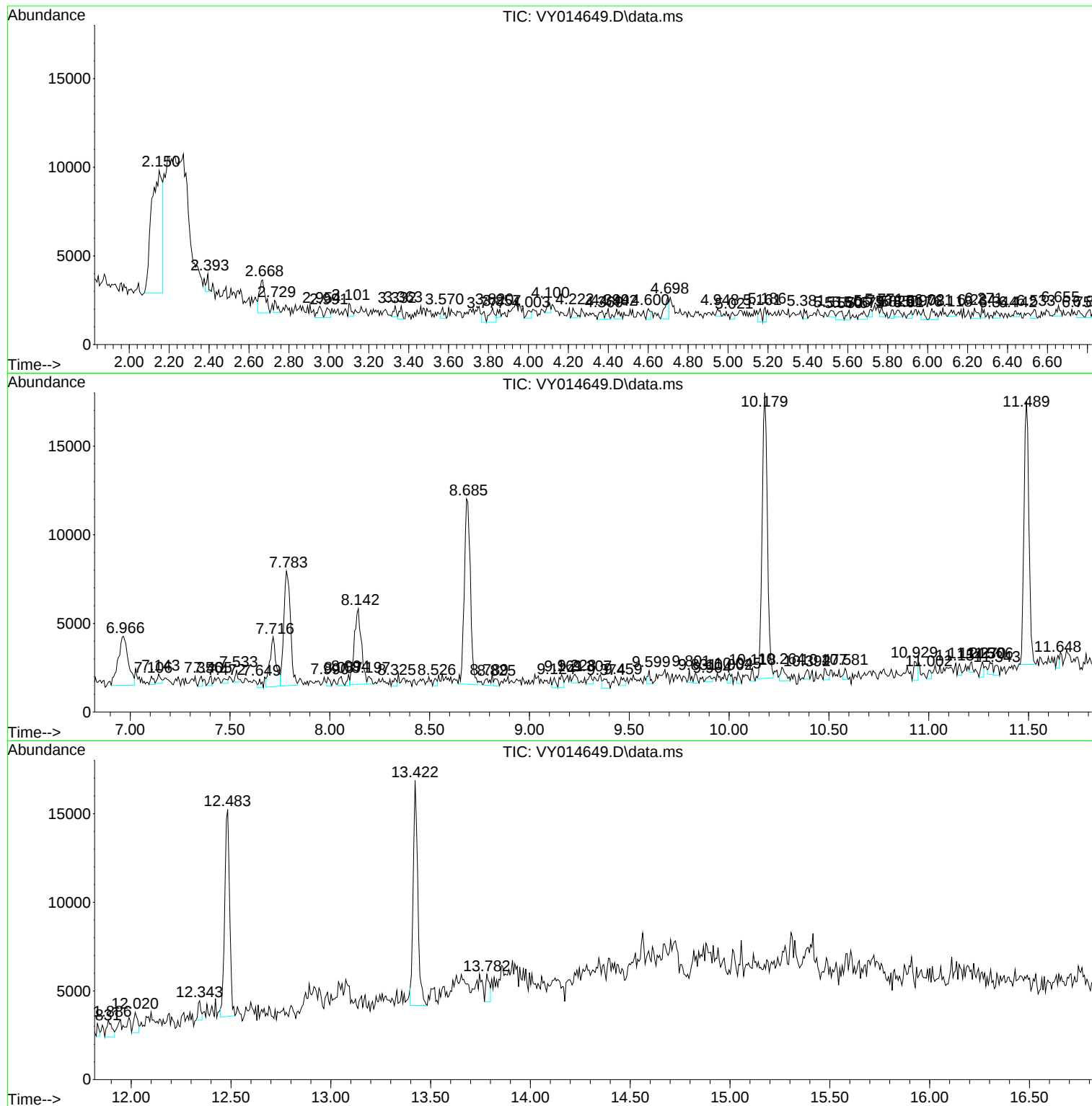
Sum of corrected areas: 249895

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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



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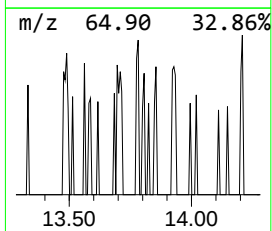
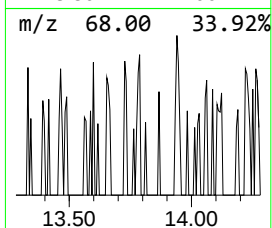
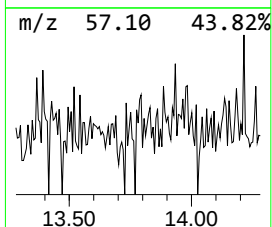
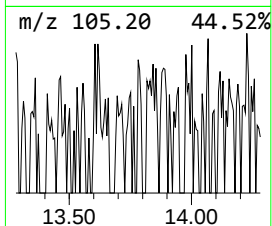
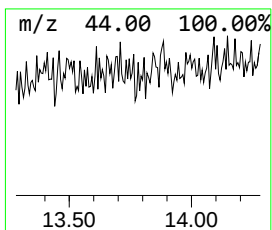
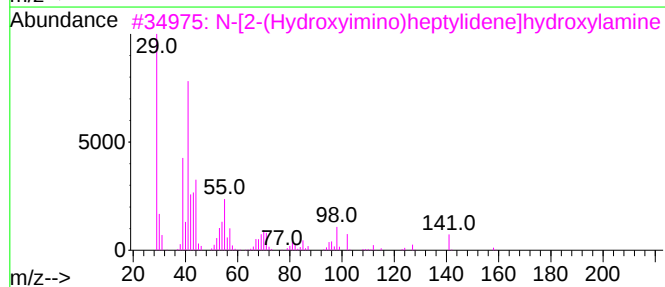
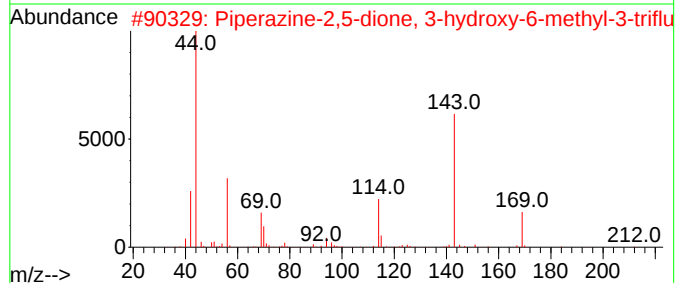
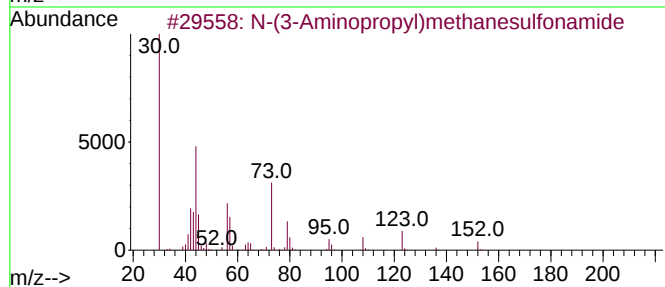
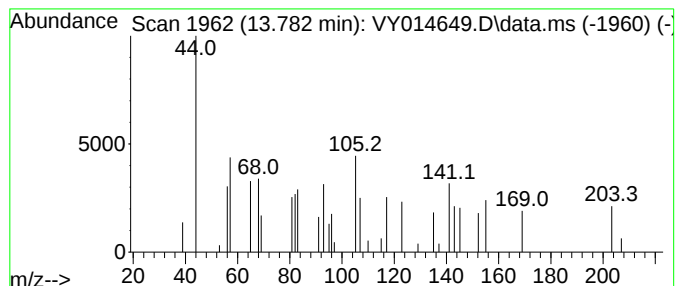
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.782 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.782	5.08 ug/l	2056	1,4-Dichlorobenzene-d4		13.428	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	N-(3-Aminopropyl)methanesulfonamide		152	C4H12N2O2S	1000443-88-2	22
2	Piperazine-2,5-dione, 3-hydroxy-...		212	C6H7F3N2O3	1000303-24-2	12
3	N-[2-(Hydroxyimino)heptylidene]h...		158	C7H14N2O2	098428-44-5	10
4	Acetamide, 2-chloro-		93	C2H4ClNO	000079-07-2	9
5	1,3-Oxazin-2-one, tetrahydro-3-m...		155	C8H13NO2	1000139-25-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown13.782	13.782	5.1	ug/l	2056	4	13.428	20221	50.0