

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051322\
 Data File : VY008759.D
 Acq On : 13 May 2022 19:09
 Operator : KP/MD
 Sample : N2802-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SHALLOW-WC-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\82Y051222S.M
 Title : SW846 8260

Signal : TIC: VY008759.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	43	54	56	rBV5	2718	7880	6.69%	1.100%
2	2.180	56	59	63	rVV5	1145	1879	1.59%	0.262%
3	2.235	63	68	71	rBV6	1856	3014	2.56%	0.421%
4	2.503	108	112	114	rBV4	1864	2418	2.05%	0.337%
5	2.534	115	117	122	rVB4	2245	2455	2.08%	0.343%
6	2.662	135	138	144	rVB5	2510	3679	3.12%	0.513%
7	2.827	161	165	168	rBV5	818	1470	1.25%	0.205%
8	2.875	170	173	174	rVV3	1134	1215	1.03%	0.170%
9	3.009	193	195	198	rVV4	2121	1656	1.41%	0.231%
10	3.046	200	201	211	rVB3	4230	8480	7.19%	1.183%
11	3.948	342	349	353	rBV3	946	1962	1.66%	0.274%
12	4.198	382	390	400	rBV4	1123	3435	2.91%	0.479%
13	4.704	463	473	475	rBV6	2670	5231	4.44%	0.730%
14	6.984	840	847	849	rBV3	2551	5237	4.44%	0.731%
15	7.716	957	967	973	rBV2	18215	44145	37.45%	6.160%
16	7.789	973	979	991	rVB	31200	70898	60.15%	9.894%
17	8.130	1024	1035	1045	rVB4	24134	67931	57.64%	9.480%
18	8.691	1118	1127	1136	rBV2	44747	88942	75.46%	12.412%
19	9.746	1295	1300	1306	rVB5	879	1710	1.45%	0.239%
20	10.179	1364	1371	1379	rBV	69426	117862	100.00%	16.447%
21	10.575	1429	1436	1444	rBV3	7089	13187	11.19%	1.840%
22	10.947	1492	1497	1505	rBV3	3280	6005	5.09%	0.838%
23	11.319	1552	1558	1563	rVB3	3884	6818	5.78%	0.951%
24	11.490	1576	1586	1598	rVB	58443	97020	82.32%	13.539%
25	12.483	1742	1749	1758	rVB2	43433	72623	61.62%	10.134%
26	13.422	1894	1903	1910	rBV	46690	74700	63.38%	10.424%
27	13.965	1986	1992	1996	rVB5	1136	1852	1.57%	0.258%
28	15.318	2209	2214	2219	rVV4	1852	2898	2.46%	0.404%

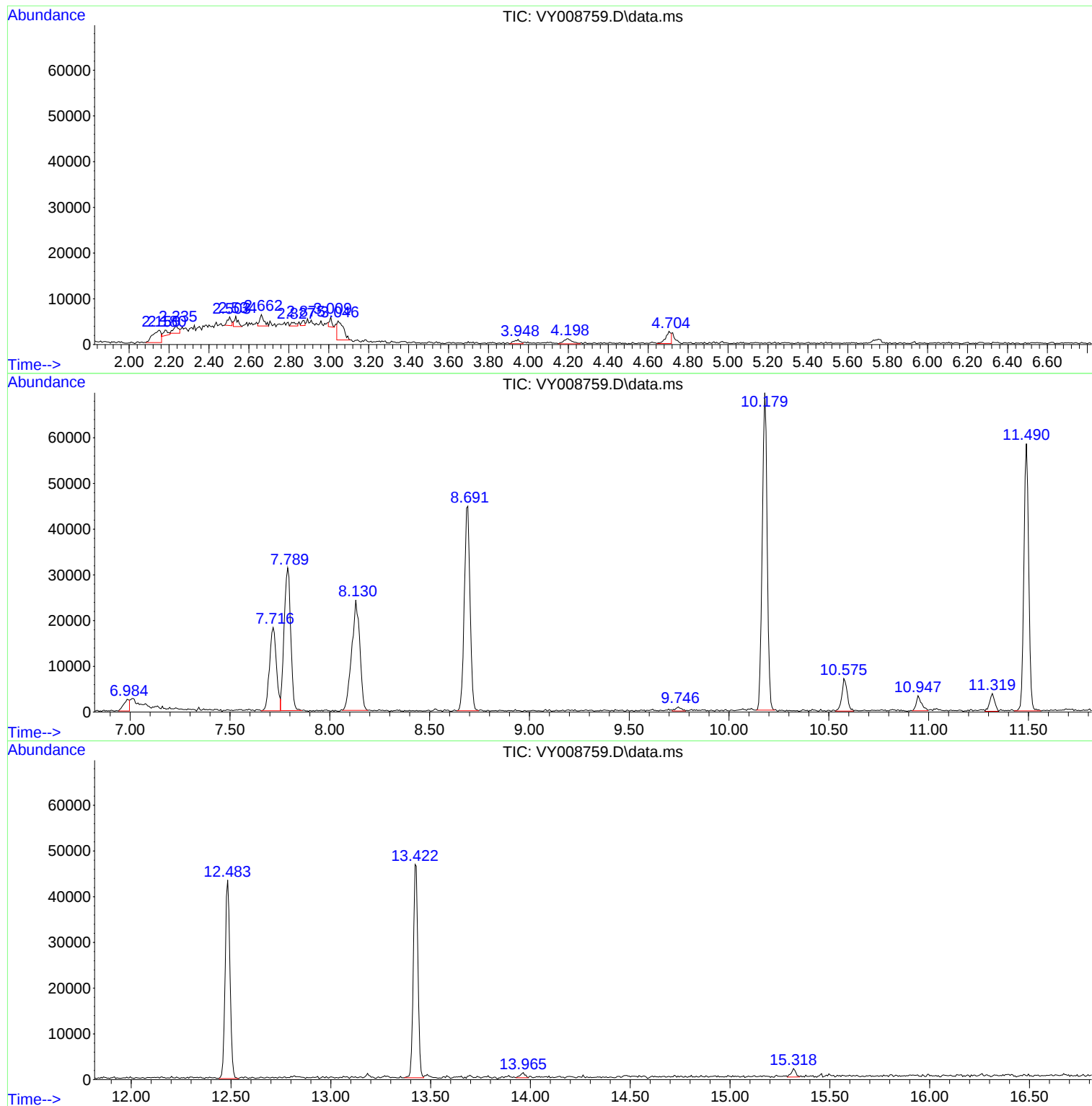
Sum of corrected areas: 716602

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Instrument :
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ClientSampleId :
SHALLOW-WC-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051222S.M
Quant Title : SW846 8260

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



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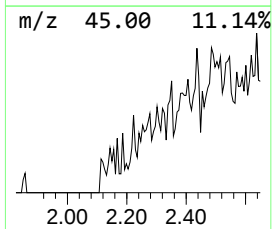
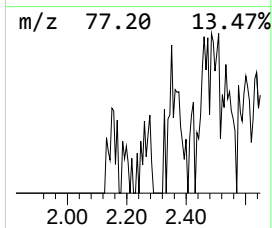
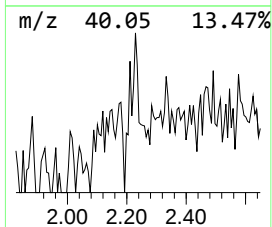
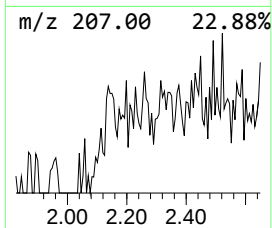
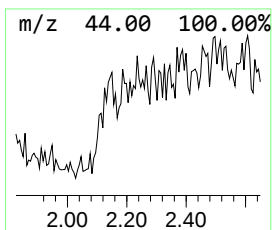
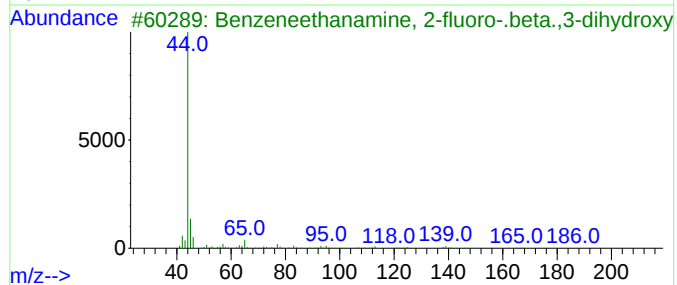
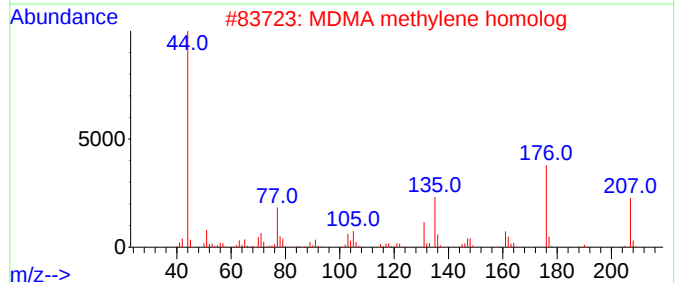
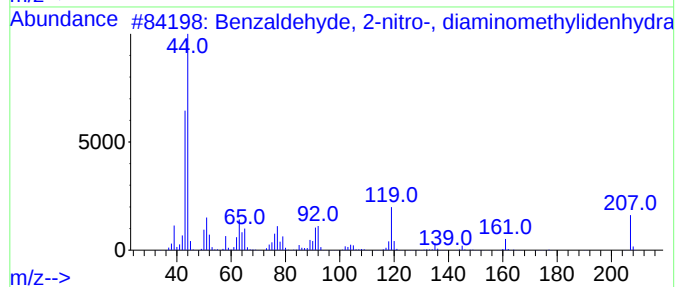
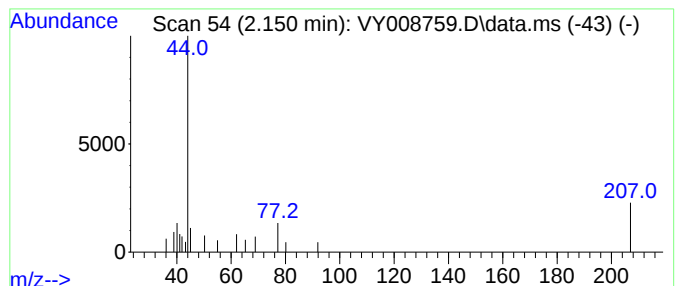
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051222S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.150 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.150	5.56 ug/l	7880	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2-nitro-, diaminom...	207	C8H9N5O2	102632-31-5	38
2			MDMA methylene homolog	207	C12H17NO2	1010386-32-2	9
3			Benzeneethanamine, 2-fluoro-.bet...	185	C9H12FN02	103439-04-9	9
4			Cathinone	149	C9H11NO	071031-15-7	9
5			2-Octanamine	129	C8H19N	000693-16-3	4



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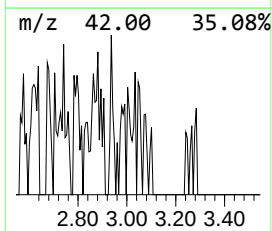
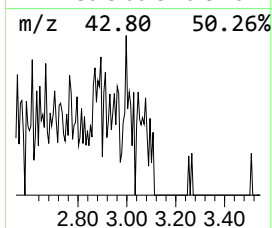
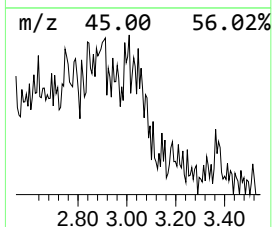
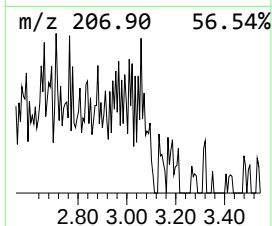
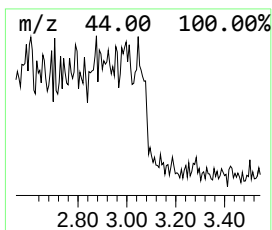
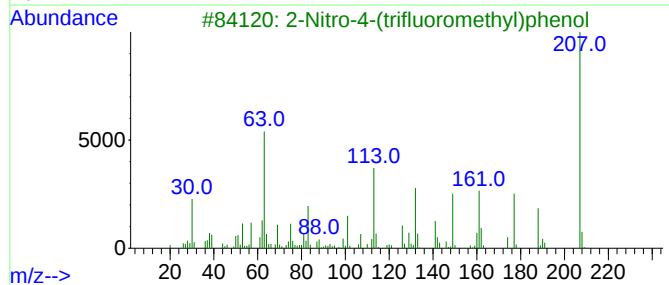
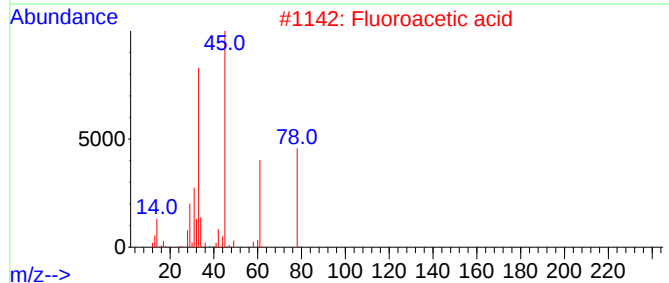
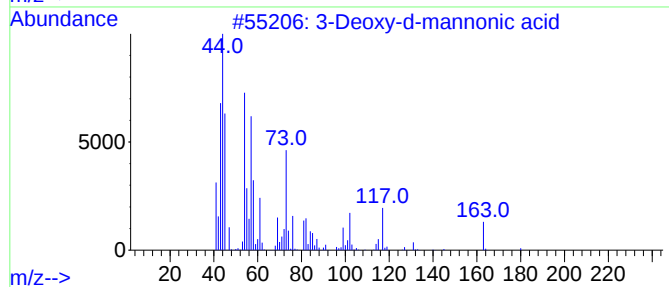
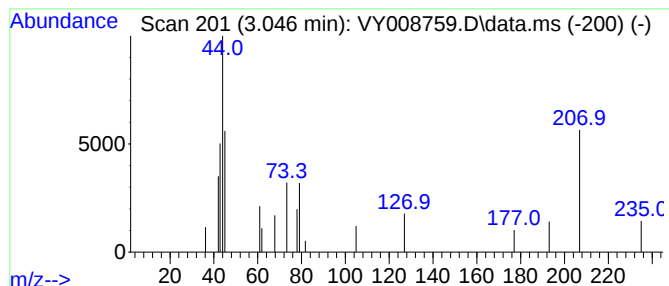
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Peak Number 2 unknown3.046 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	5.98 ug/l	8480	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Deoxy-d-mannonic acid	180	C6H12O6	001518-59-8	25
2			Fluoroacetic acid	78	C2H3FO2	000144-49-0	9
3			2-Nitro-4-(trifluoromethyl)phenol	207	C7H4F3NO3	000400-99-7	9
4			3,6-Dinitro-1H-indole	207	C8H5N3O4	004771-15-7	9
5			2,3-Dihydroxy-6-nitroquinoxaline	207	C8H5N3O4	002379-56-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.150	2.150	5.6	ug/l	7880	1	7.789	70898	50.0
unknown3.046	3.046	6.0	ug/l	8480	1	7.789	70898	50.0