

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060424\
 Data File : VY018472.D
 Acq On : 04 Jun 2024 18:35
 Operator : SY/MD
 Sample : P2686-03
 Misc : 4.58g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WCS-TPQ-VOC

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\82Y060324S.M

Title : SW846 8260

Signal : TIC: VY018472.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.119	43	49	52	rBV4	3075	6860	4.83%	1.033%
2	2.369	88	90	94	rVB5	1891	1669	1.17%	0.251%
3	2.643	129	135	139	rBV8	1807	3064	2.16%	0.462%
4	2.924	178	181	183	rBV5	1562	1682	1.18%	0.253%
5	3.058	201	203	210	rVB3	2856	5606	3.95%	0.844%
6	3.192	223	225	228	rBV3	1405	1824	1.28%	0.275%
7	3.838	329	331	337	rBV5	1220	2294	1.61%	0.346%
8	4.094	368	373	376	rBV3	813	1776	1.25%	0.268%
9	4.686	464	470	471	rBV4	2336	4031	2.84%	0.607%
10	6.960	839	843	844	rBV4	1914	2897	2.04%	0.436%
11	6.972	844	845	856	rVB6	3143	5180	3.65%	0.780%
12	7.710	955	966	971	rBV3	20350	50187	35.33%	7.560%
13	7.777	971	977	988	rVB2	22665	53151	37.41%	8.007%
14	8.130	1024	1035	1043	rBV2	23597	54459	38.33%	8.204%
15	8.374	1070	1075	1078	rBV5	1145	1433	1.01%	0.216%
16	8.679	1119	1125	1135	rVB	37377	81395	57.29%	12.261%
17	10.173	1362	1370	1378	rBV	84713	142070	100.00%	21.401%
18	11.483	1579	1585	1597	rVB	54772	92042	64.79%	13.865%
19	12.233	1705	1708	1712	rBV5	917	1869	1.32%	0.282%
20	12.477	1741	1748	1756	rBV	48410	81764	57.55%	12.317%
21	13.422	1895	1903	1910	rBV2	39036	64447	45.36%	9.708%
22	15.312	2209	2213	2217	rVB5	1307	2009	1.41%	0.303%
23	15.848	2296	2301	2307	rBV5	1044	2135	1.50%	0.322%

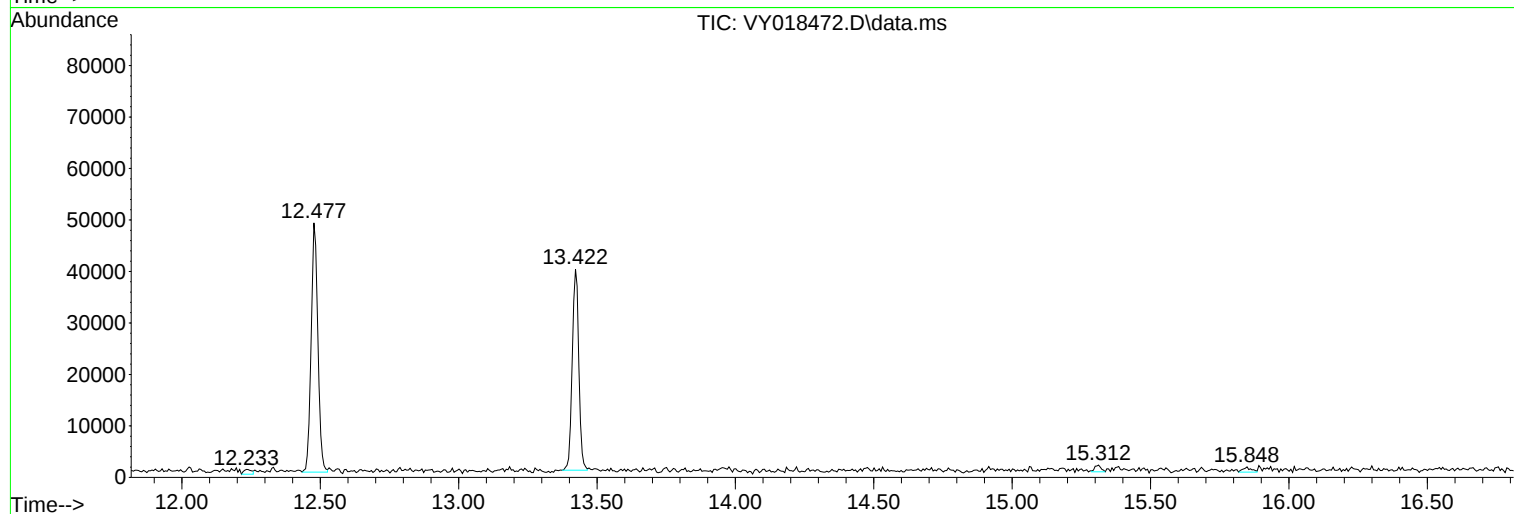
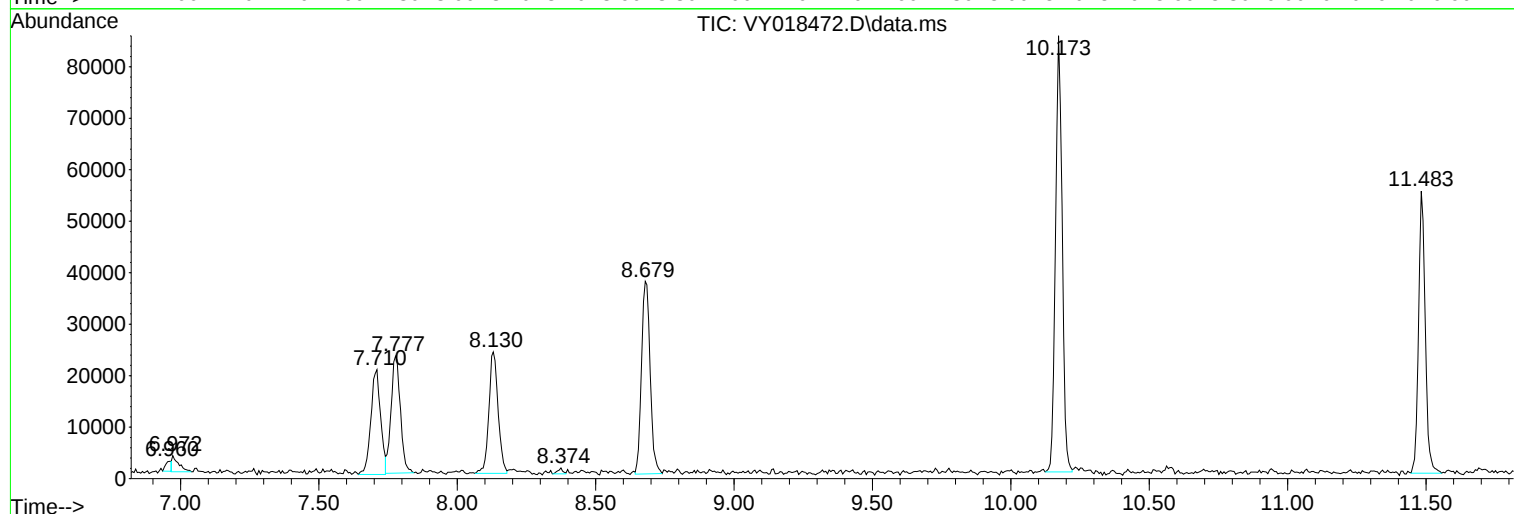
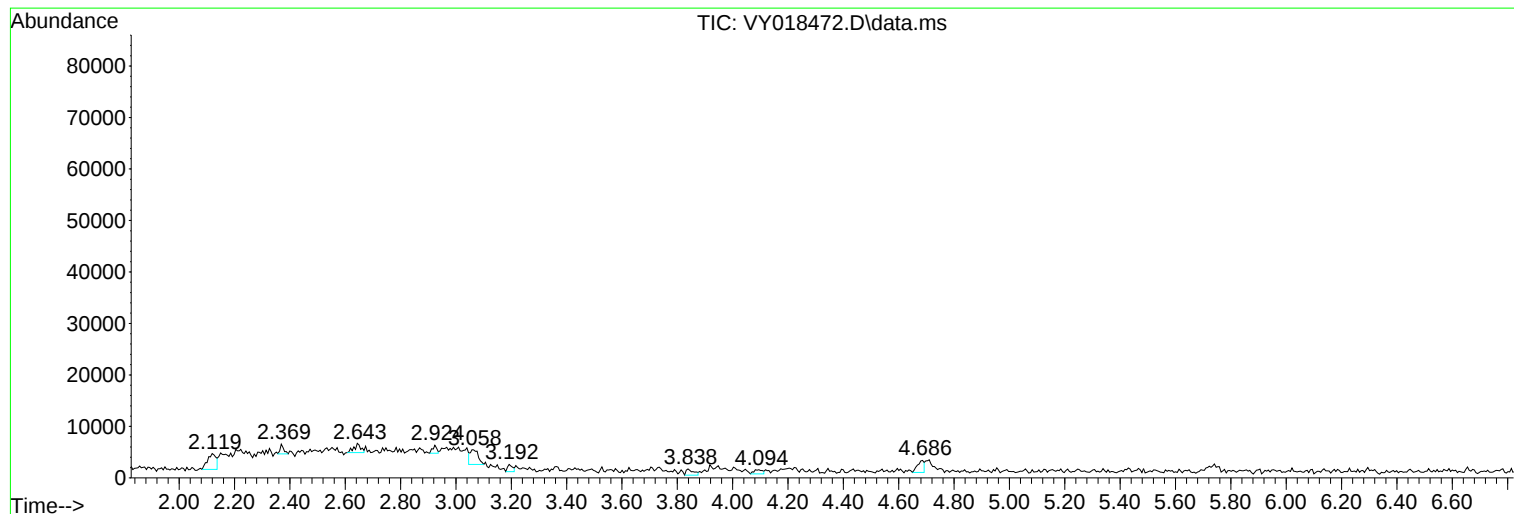
Sum of corrected areas: 663844

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ClientSampleId :
WCS-TPQ-VOC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
Quant Title : SW846 8260

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



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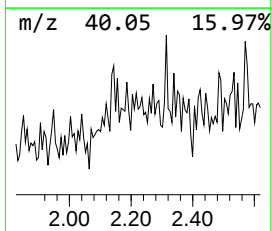
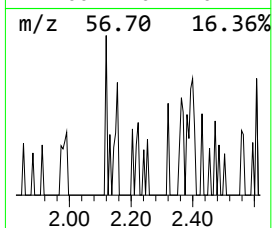
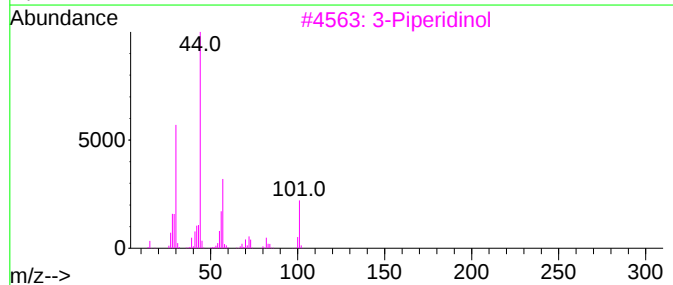
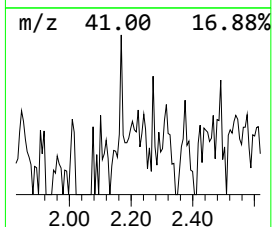
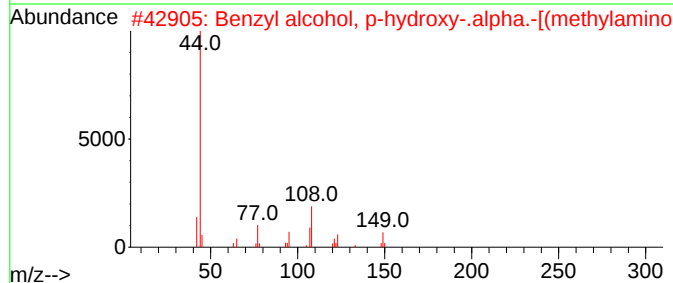
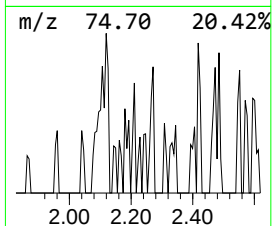
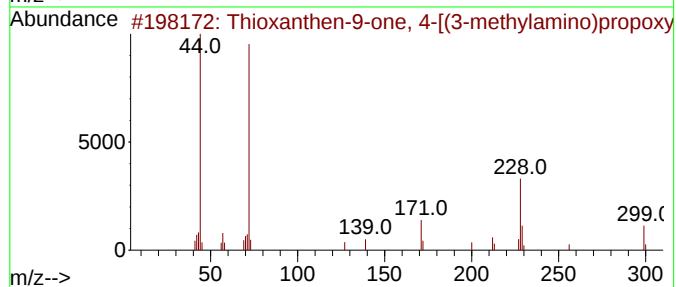
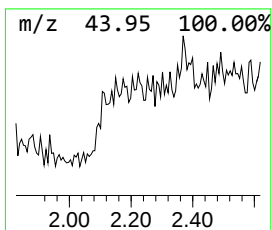
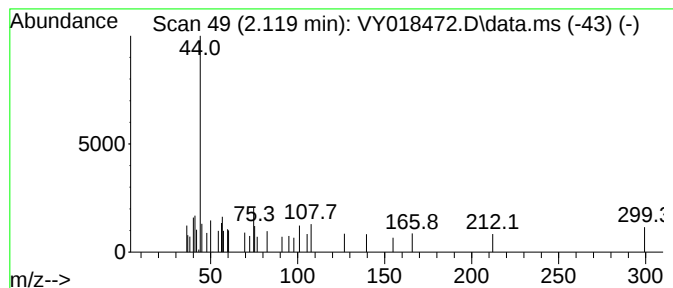
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.119 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.119	6.45 ug/l	6860	Pentafluorobenzene	7.777

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thioxanthen-9-one, 4-[(3-methyla...	299	C17H17NO2S	118793-90-1	43
2			Benzyl alcohol, p-hydroxy-.alpha...	167	C9H13NO2	000094-07-5	23
3			3-Piperidinol	101	C5H11NO	006859-99-0	9
4			3-Methyl-3,5--(cyanoethyl)tetrah...	236	C12H16N2OS	1000140-32-3	9
5			4-Fluorohistamine	129	C5H8FN3	049872-60-8	9



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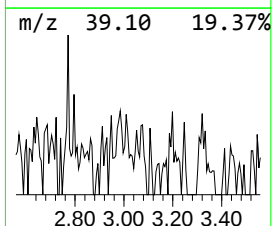
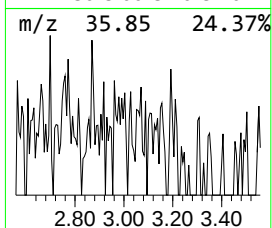
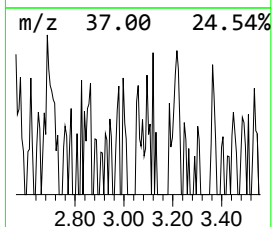
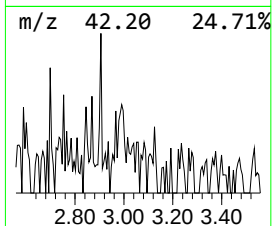
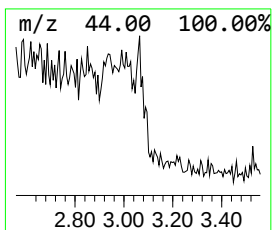
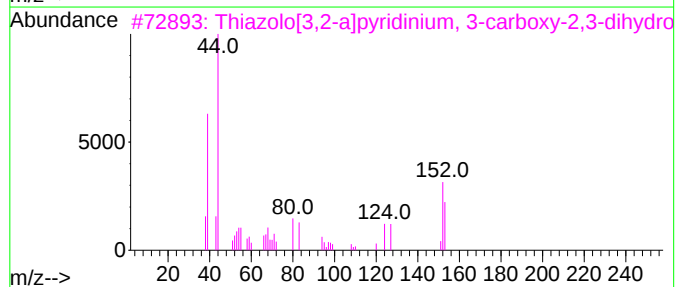
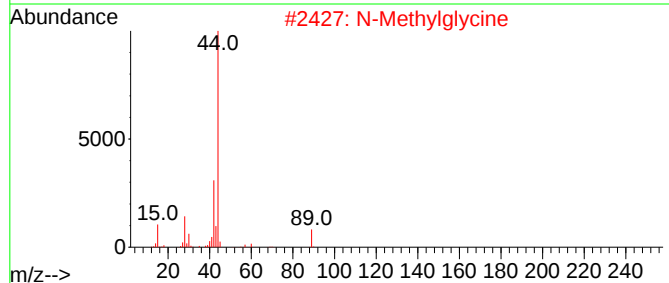
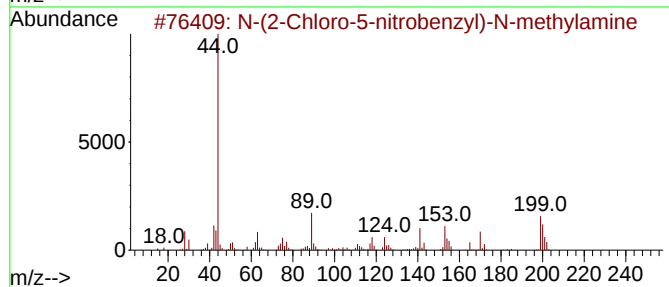
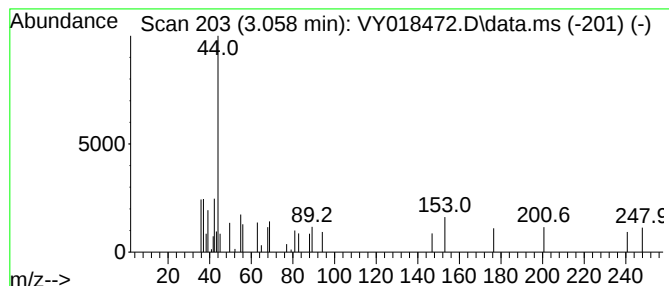
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.058 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.058	5.27 ug/l	5606	Pentafluorobenzene	7.777

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(2-Chloro-5-nitrobenzyl)-N-met...	200	C8H9ClN2O2	872107-89-6	25
2			N-Methylglycine	89	C3H7NO2	000107-97-1	9
3			Thiazolo[3,2-a]pyridinium, 3-car...	197	C8H7NO3S	023003-39-6	9
4			Methanesulfonamide, N,N-dimethyl-	123	C3H9NO2S	000918-05-8	9
5			5-Bromo-N,N-dimethyl-2H-1,2,4-tr...	218	C5H7BrN4O	1000387-99-1	9



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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
unknown2.119	2.119	6.5	ug/l	6860	1	7.777	53151	50.0
unknown3.058	3.058	5.3	ug/l	5606	1	7.777	53151	50.0