

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060723\
 Data File : VN078099.D
 Acq On : 07 Jun 2023 13:28
 Operator : JC\MD
 Sample : 03066-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 606

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\82N060623W.M
 Title : SW846 8260

Signal : TIC: VN078099.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.430	69	81	82	rBV5	13738	32357	1.54%	0.285%
2	2.818	141	147	153	rVB2	20123	36437	1.74%	0.321%
3	7.500	935	943	952	rBV2	10860	25324	1.21%	0.223%
4	8.177	1048	1058	1062	rBV	294687	706959	33.72%	6.232%
5	8.230	1062	1067	1082	rVB	500156	1143710	54.55%	10.082%
6	8.588	1114	1128	1139	rBV2	299157	684502	32.65%	6.034%
7	9.106	1207	1216	1232	rBV	753195	1536434	73.29%	13.544%
8	10.571	1456	1465	1473	rBV	1111988	2096461	100.00%	18.481%
9	10.630	1473	1475	1483	rVB6	12769	25084	1.20%	0.221%
10	11.871	1677	1686	1699	rBV	962534	1787280	85.25%	15.756%
11	12.853	1845	1853	1862	rBV	683486	1185608	56.55%	10.452%
12	13.265	1914	1923	1930	rBV	270944	440154	21.00%	3.880%
13	13.506	1956	1964	1971	rBV3	44765	92772	4.43%	0.818%
14	13.612	1977	1982	1985	rBV4	17595	31355	1.50%	0.276%
15	13.800	2006	2014	2021	rBV	661971	1195389	57.02%	10.538%
16	13.865	2021	2025	2032	rVB6	30168	63775	3.04%	0.562%
17	14.000	2043	2048	2057	rVB8	11613	30560	1.46%	0.269%
18	14.676	2151	2163	2171	rBV7	20312	61544	2.94%	0.543%
19	14.935	2201	2207	2213	rBV6	26369	45799	2.18%	0.404%
20	15.053	2219	2227	2233	rBV4	26177	59654	2.85%	0.526%
21	15.217	2249	2255	2261	rVV3	13549	23761	1.13%	0.209%
22	15.323	2267	2273	2279	rBV8	17148	38812	1.85%	0.342%

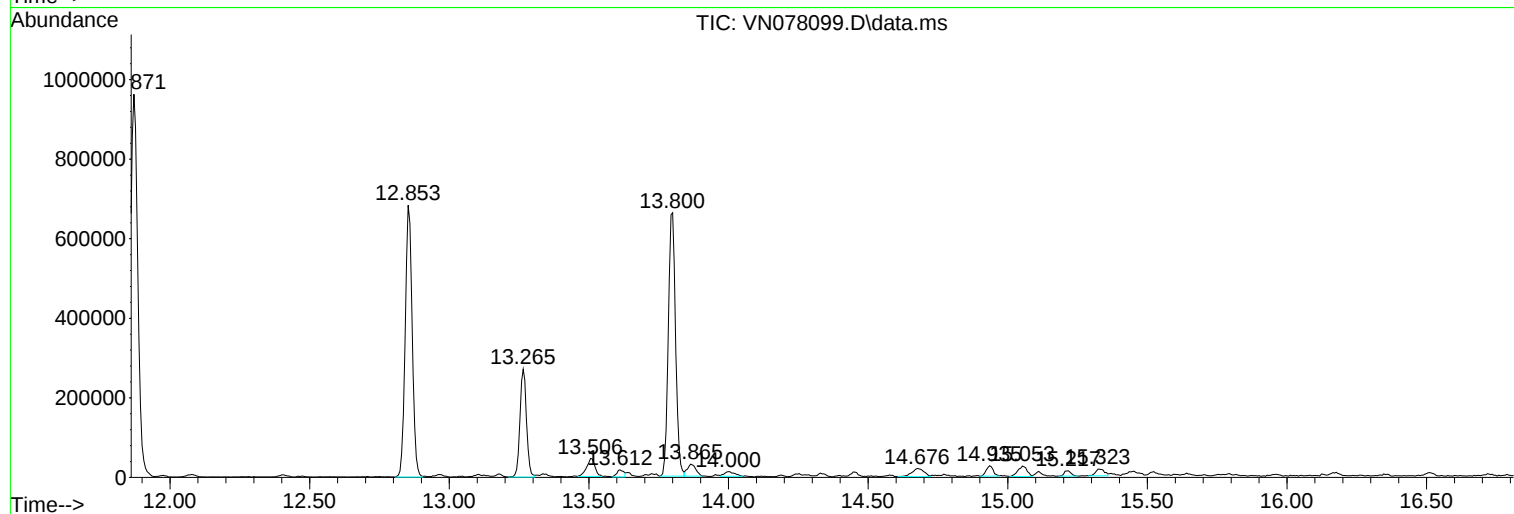
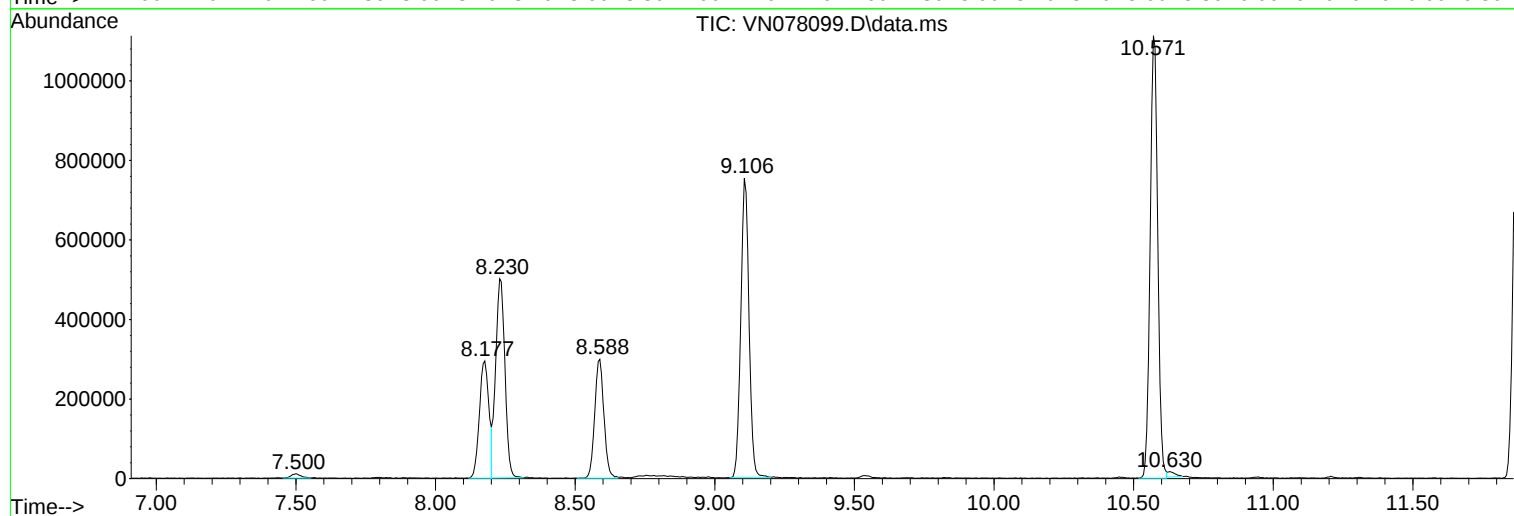
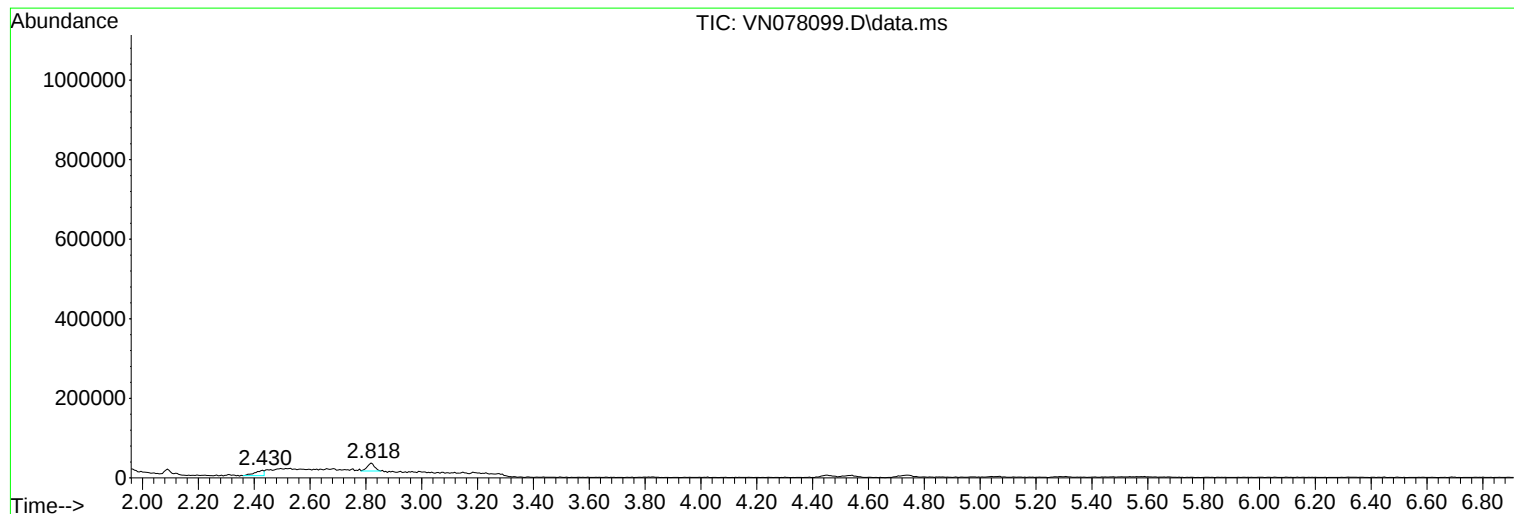
Sum of corrected areas: 11343731

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060723\
Data File : VN078099.D
Acq On : 07 Jun 2023 13:28
Operator : JC\MD
Sample : 03066-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
606

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060723\
Data File : VN078099.D
Acq On : 07 Jun 2023 13:28
Operator : JC\MD
Sample : 03066-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
606

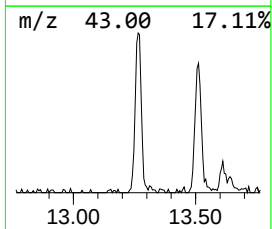
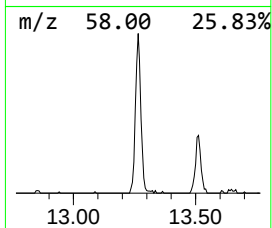
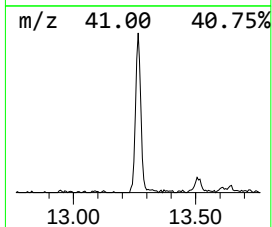
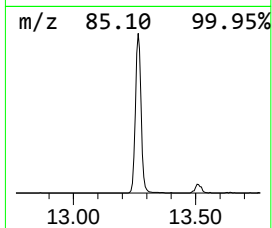
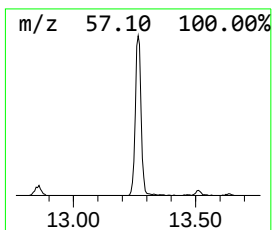
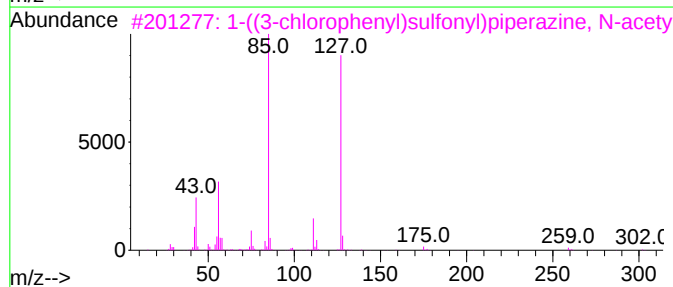
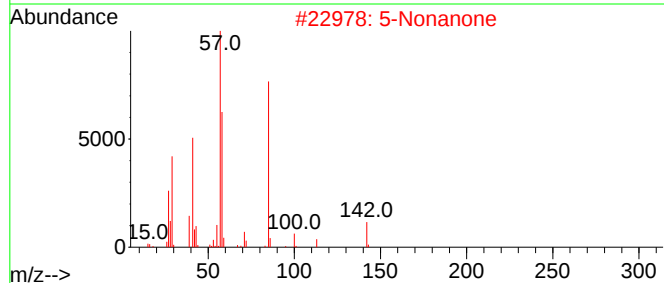
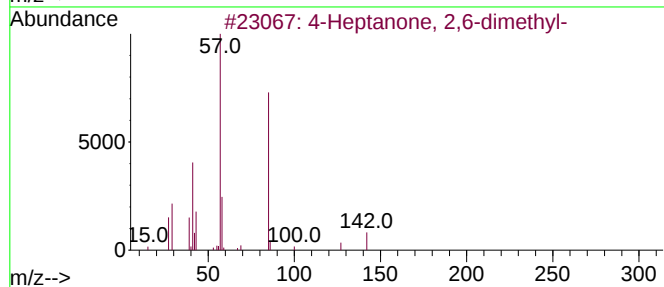
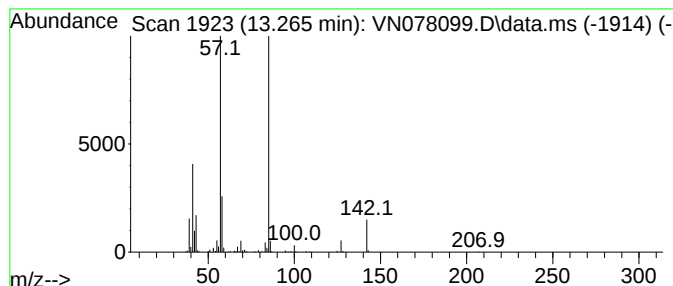
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	18.41 ug/l	440154	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			5-Nonanone	142	C9H18O	000502-56-7	59
3			1-((3-chlorophenyl)sulfonyl)pipe...	302	C12H15ClN2O3S	1000500-95-3	53
4			2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	53
5			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060723\
Data File : VN078099.D
Acq On : 07 Jun 2023 13:28
Operator : JC\MD
Sample : 03066-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
606

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
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
4-Heptanone, 2,...	13.265	18.4	ug/l	440154	4	13.794	1195390	50.0