

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062822\
 Data File : VN073227.D
 Acq On : 29 Jun 2022 03:31
 Operator : JC\MD
 Sample : N3376-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 220615003-01-VOA

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073227.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.293	404	409	421	rVB4	15678	38788	1.12%	0.223%
2	5.281	560	577	607	rBV	873450	3194945	91.99%	18.391%
3	7.234	895	909	937	rBV	1178995	3472962	100.00%	19.991%
4	7.610	962	973	997	rBV	296567	788009	22.69%	4.536%
5	7.951	1020	1031	1036	rBV	224523	550639	15.86%	3.170%
6	8.016	1036	1042	1057	rVB	429408	991261	28.54%	5.706%
7	8.369	1092	1102	1111	rBV	241172	567591	16.34%	3.267%
8	8.463	1112	1118	1129	rVB2	47730	112904	3.25%	0.650%
9	8.904	1183	1193	1207	rBV	590880	1250634	36.01%	7.199%
10	10.186	1404	1411	1417	rBV5	27553	61308	1.77%	0.353%
11	10.375	1435	1443	1451	rBV	798802	1513066	43.57%	8.709%
12	11.680	1655	1665	1676	rBV	888096	1572607	45.28%	9.052%
13	12.669	1826	1833	1841	rVB	742545	1219896	35.13%	7.022%
14	13.016	1882	1892	1899	rBV2	20312	42737	1.23%	0.246%
15	13.610	1986	1993	2001	rBV	954234	1601275	46.11%	9.217%
16	14.139	2078	2083	2090	rVB2	38283	65176	1.88%	0.375%
17	14.469	2131	2139	2148	rBV2	85522	169250	4.87%	0.974%
18	15.086	2235	2244	2249	rBV5	52678	114525	3.30%	0.659%
19	15.580	2323	2328	2334	rBV3	24545	45125	1.30%	0.260%

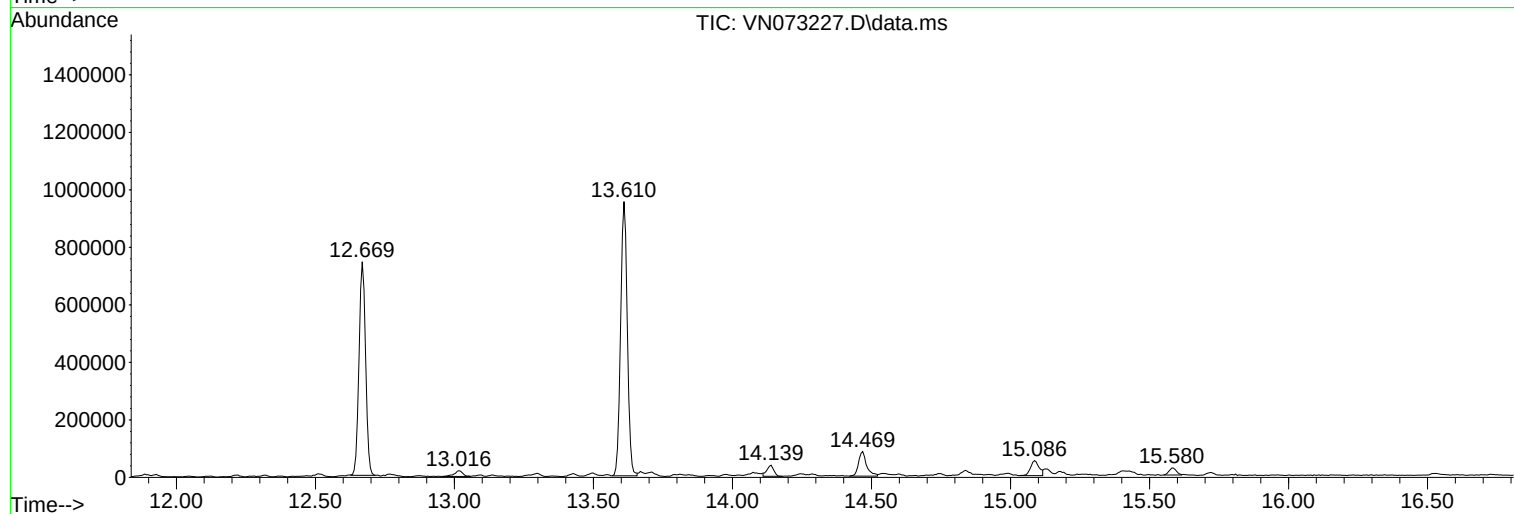
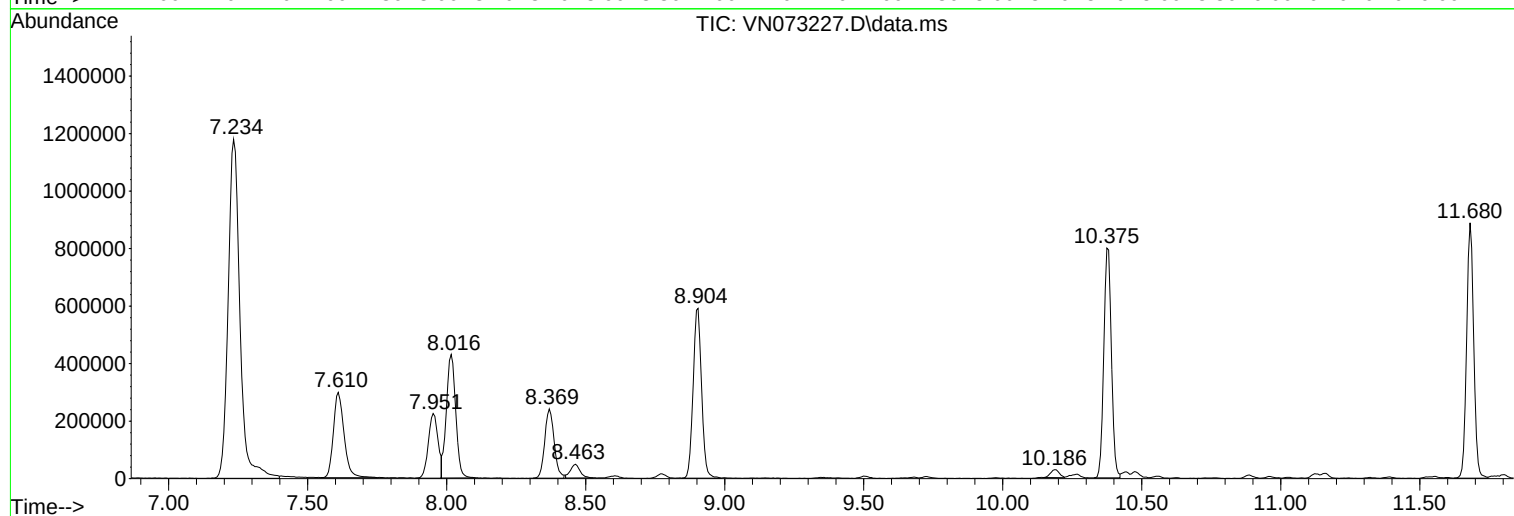
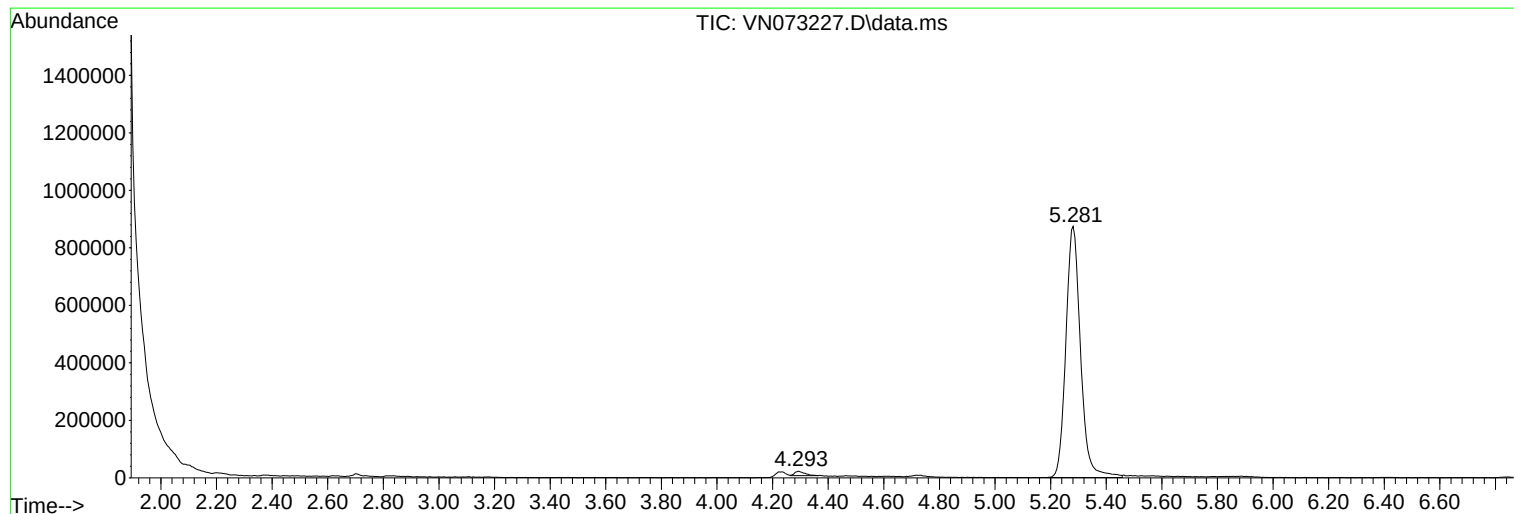
Sum of corrected areas: 17372698

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062822\
Data File : VN073227.D
Acq On : 29 Jun 2022 03:31
Operator : JC\MD
Sample : N3376-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
220615003-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062822\
Data File : VN073227.D
Acq On : 29 Jun 2022 03:31
Operator : JC\MD
Sample : N3376-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
220615003-01-VOA

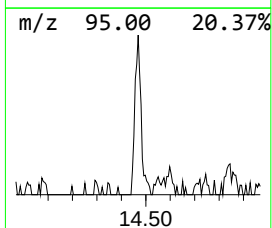
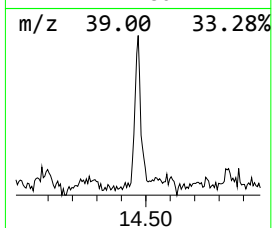
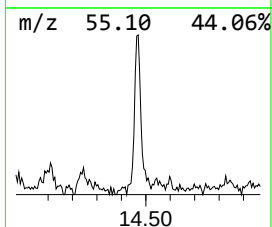
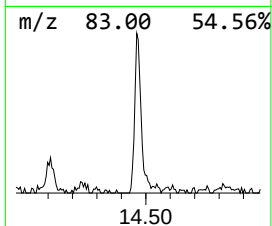
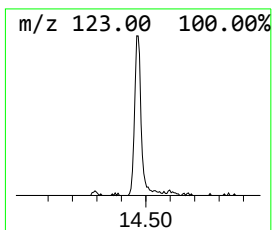
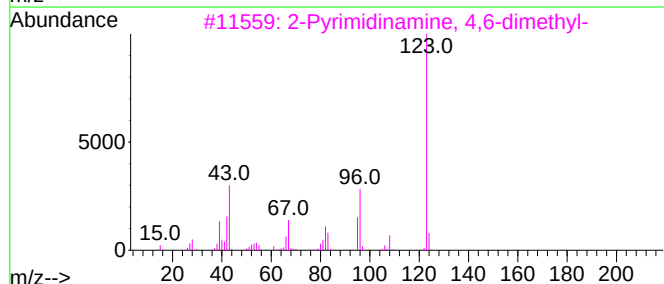
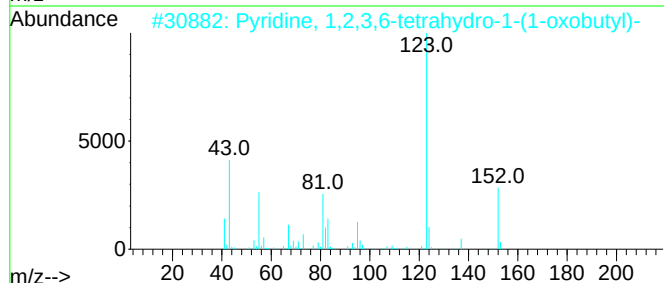
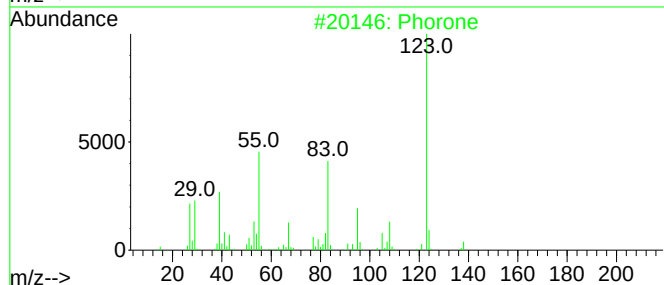
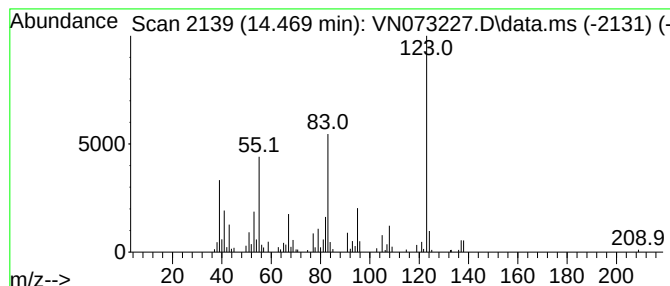
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Phorone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.469	5.28 ug/l	169250	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phorone	138	C9H14O	000504-20-1	97
2			Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	53
3			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	52
4			4-(3-Fluorobenzoyl)-3-phenyl-5-i...	283	C16H10FNO3	1000434-46-1	47
5			3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062822\
Data File : VN073227.D
Acq On : 29 Jun 2022 03:31
Operator : JC\MD
Sample : N3376-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
220615003-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
Phorone	14.469	5.3	ug/l	169250	4	13.610	1601280	50.0