

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070921\
 Data File : VX023214.D
 Acq On : 09 Jul 2021 10:12
 Operator : JC/MD
 Sample : VX0709MBL01
 Misc : 5.0g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0709MBL01

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_X\Method\82X070221W.M
 Title : SW846 8260

Signal : TIC: VX023214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.574	562	572	583	rBV	6839	23087	2.10%	0.313%
2	5.391	693	706	718	rBV	134273	393212	35.76%	5.325%
3	5.550	721	732	749	rVB	225931	644306	58.59%	8.725%
4	5.958	787	799	816	rVB	146172	385793	35.08%	5.224%
5	6.763	921	931	945	rBV	347241	822975	74.83%	11.144%
6	7.129	984	991	1000	rBV3	9372	21568	1.96%	0.292%
7	8.135	1137	1156	1176	rBV2	145950	669611	60.89%	9.068%
8	8.647	1234	1240	1249	rBV	692041	1099736	100.00%	14.892%
9	10.055	1464	1471	1479	rBV	700860	939388	85.42%	12.721%
10	10.970	1613	1621	1631	rBV	441194	746121	67.85%	10.104%
11	11.085	1634	1640	1649	rBV	571305	754094	68.57%	10.212%
12	12.024	1789	1794	1802	rVB	665061	813060	73.93%	11.010%
13	13.036	1954	1960	1967	rVB3	6333	13483	1.23%	0.183%
14	13.378	2012	2016	2022	rVB3	7064	11691	1.06%	0.158%
15	13.554	2041	2045	2048	rBV4	7309	13072	1.19%	0.177%
16	13.591	2048	2051	2056	rVB2	9502	15081	1.37%	0.204%
17	13.804	2076	2086	2091	rVB7	8123	18434	1.68%	0.250%

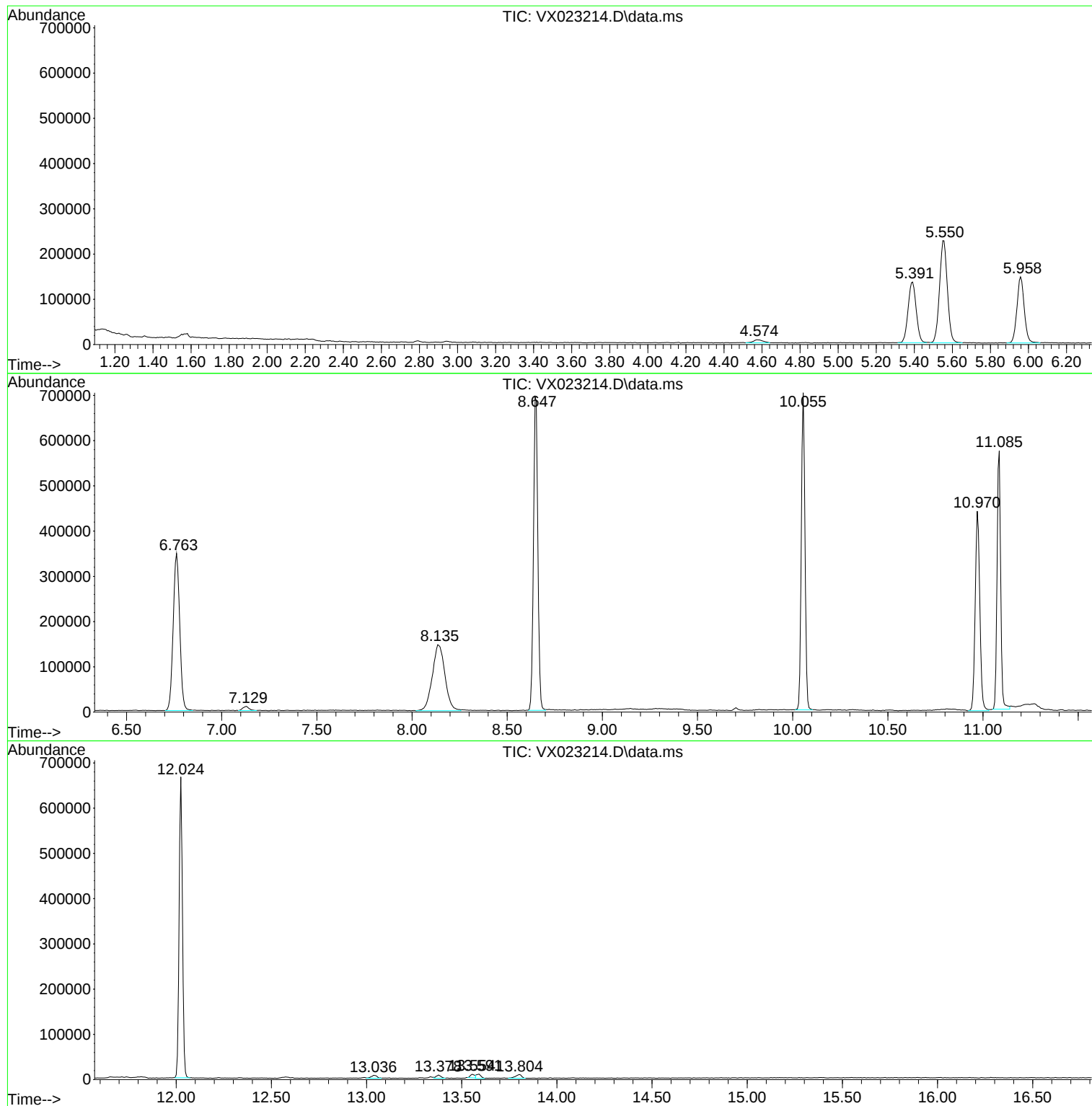
Sum of corrected areas: 7384712

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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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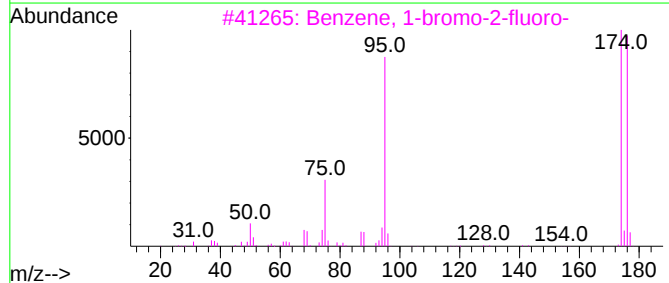
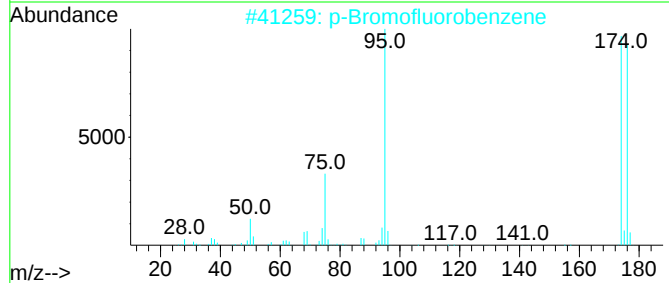
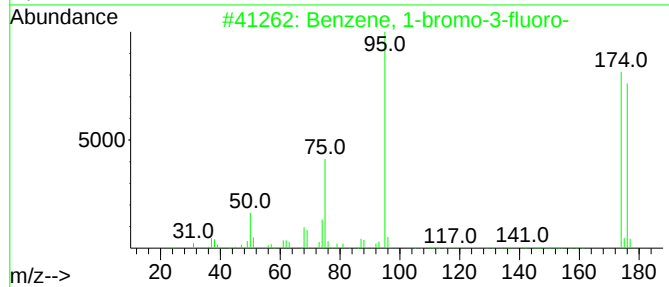
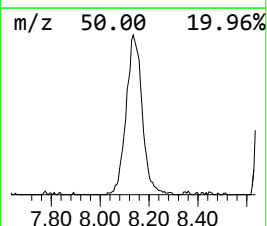
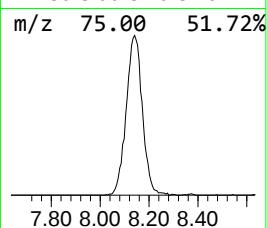
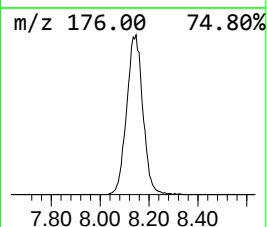
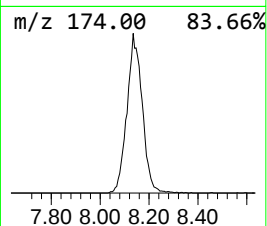
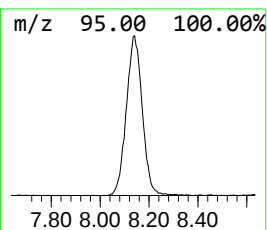
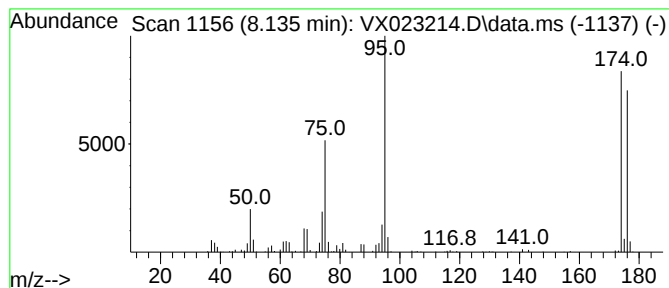
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, 1-bromo-3-fluoro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.135	40.68 ug/l	669611	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	95
2			p-Bromofluorobenzene	174	C6H4BrF	000460-00-4	94
3			Benzene, 1-bromo-2-fluoro-	174	C6H4BrF	001072-85-1	94
4			4(1H)-Pyrimidinone, 5-bromo-	174	C4H3BrN2O	019808-30-1	32
5			Benzene, 1-fluoro-4-(methylsulfo...	174	C7H7FO2S	000455-15-2	12



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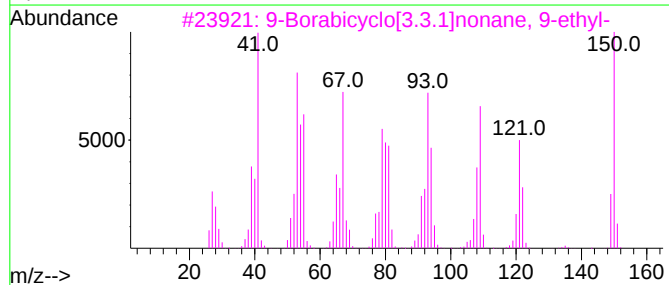
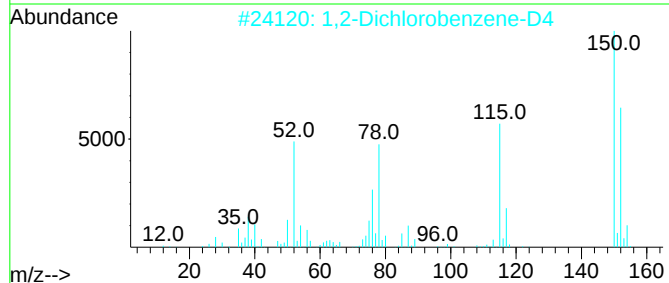
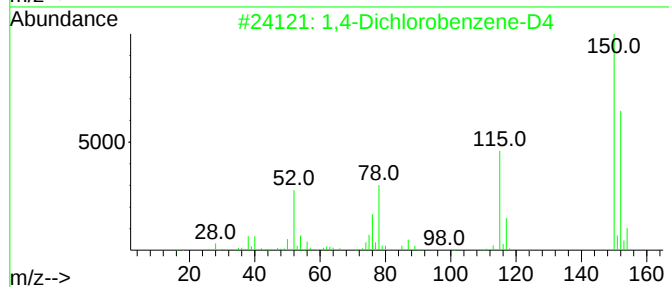
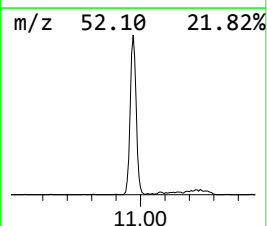
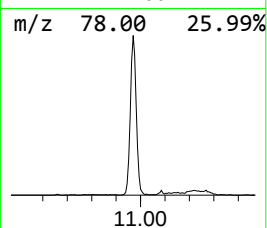
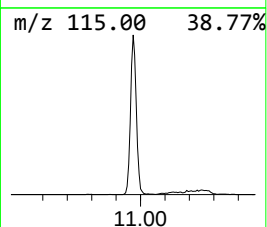
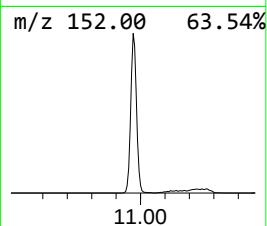
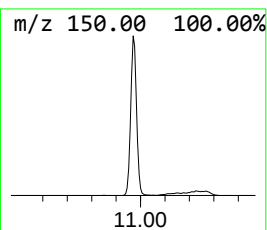
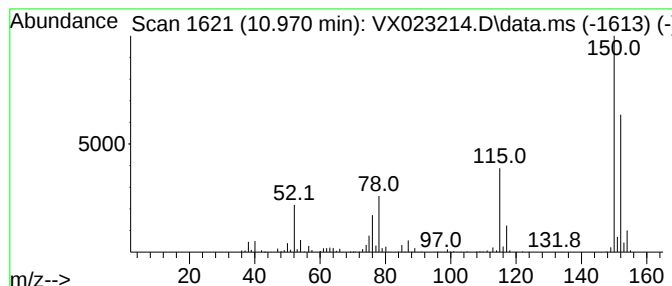
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Peak Number 2 1,4-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.970	39.71 ug/l	746121	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
2			1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
3			9-Borabicyclo[3.3.1]nonane, 9-ethyl-	150	C10H19B	052102-17-7	38
4			3-Amino-1,2,4-dithiazole-5-thione	150	C2H2N2S3	006846-35-1	10
5			6-Benzothiazolamine	150	C7H6N2S	000533-30-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-brom...	8.135	40.7	ug/l	669611	2	6.763	822975	50.0
1,4-Dichloroben...	10.970	39.7	ug/l	746121	3	10.055	939388	50.0