

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080521\
 Data File : VX023576.D
 Acq On : 05 Aug 2021 16:37
 Operator : JC/MD
 Sample : M3298-06 200X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1940

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\82X072221W.M
 Title : SW846 8260

Signal : TIC: VX023576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.794	273	280	287	rVB	8249	14406	1.82%	0.310%
2	5.397	695	707	722	rBV	91338	261833	33.16%	5.641%
3	5.562	722	734	747	rBV	154259	429153	54.35%	9.245%
4	5.970	790	801	814	rBV	101514	270475	34.25%	5.827%
5	6.769	922	932	944	rBV	243149	571683	72.40%	12.316%
6	8.653	1234	1241	1253	rBV	512878	789615	100.00%	17.011%
7	10.055	1465	1471	1481	rBV	492602	673416	85.28%	14.508%
8	11.085	1634	1640	1651	rVB	381124	484491	61.36%	10.438%
9	12.024	1789	1794	1802	rVB	437574	525820	66.59%	11.328%
10	14.182	2139	2148	2151	rBV8	5822	14233	1.80%	0.307%
11	14.335	2167	2173	2174	rBV6	4154	8058	1.02%	0.174%
12	14.615	2216	2219	2222	rBV4	9713	13722	1.74%	0.296%
13	14.755	2239	2242	2245	rBV3	13983	17564	2.22%	0.378%
14	14.792	2246	2248	2253	rVB5	10446	13296	1.68%	0.286%
15	14.847	2253	2257	2261	rBV5	12253	23482	2.97%	0.506%
16	14.963	2273	2276	2283	rVB7	21417	32543	4.12%	0.701%
17	15.097	2296	2298	2306	rVB8	13072	25965	3.29%	0.559%
18	15.176	2308	2311	2314	rVV5	9489	16483	2.09%	0.355%
19	15.213	2314	2317	2321	rVB2	22593	26602	3.37%	0.573%
20	15.249	2321	2323	2327	rBV5	9307	12000	1.52%	0.259%
21	15.420	2347	2351	2356	rBV	74099	103406	13.10%	2.228%
22	15.682	2392	2394	2398	rVV3	24115	27113	3.43%	0.584%
23	15.743	2400	2404	2410	rVB2	74880	125875	15.94%	2.712%
24	15.865	2421	2424	2430	rVB5	29544	47521	6.02%	1.024%
25	16.097	2458	2462	2466	rBV4	26841	45639	5.78%	0.983%
26	16.712	2558	2563	2569	rBV2	37587	67429	8.54%	1.453%

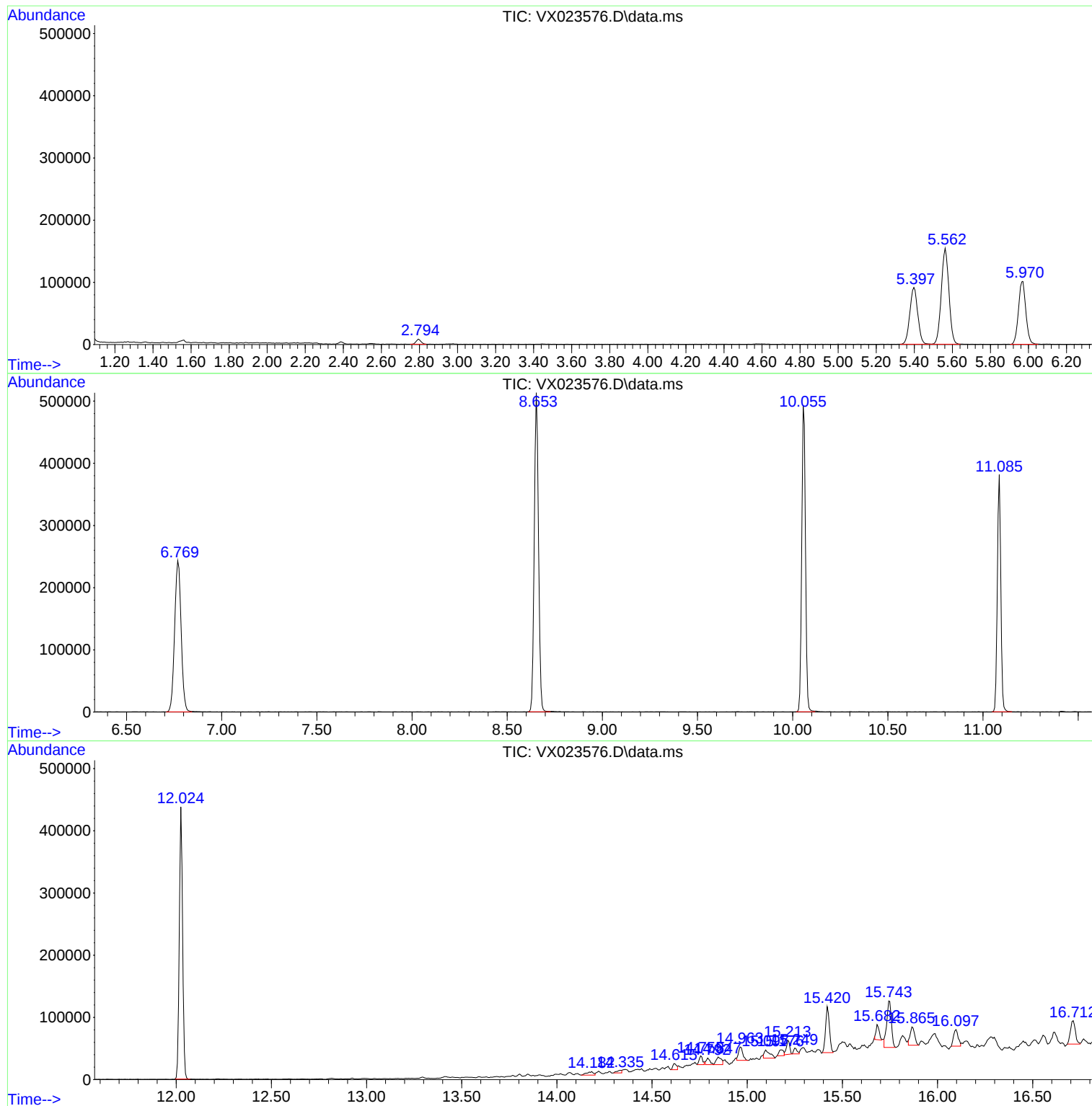
Sum of corrected areas: 4641823

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080521\
Data File : VX023576.D
Acq On : 05 Aug 2021 16:37
Operator : JC/MD
Sample : M3298-06 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1940

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080521\
Data File : VX023576.D
Acq On : 05 Aug 2021 16:37
Operator : JC/MD
Sample : M3298-06 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
1940

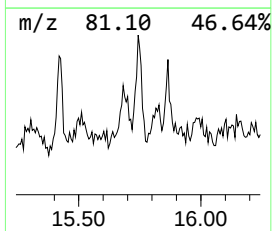
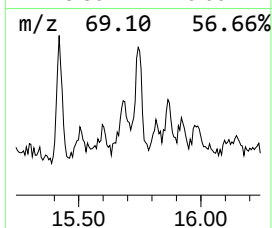
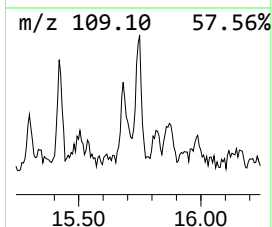
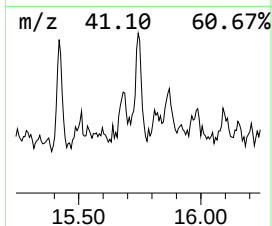
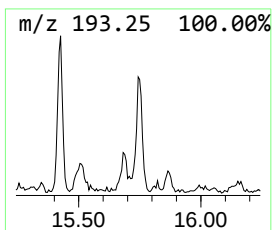
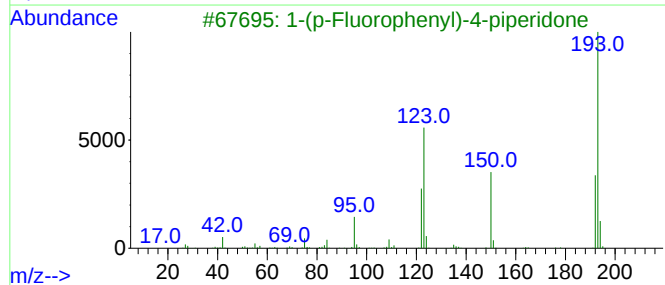
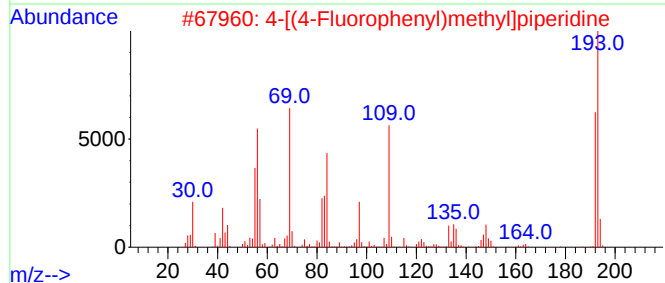
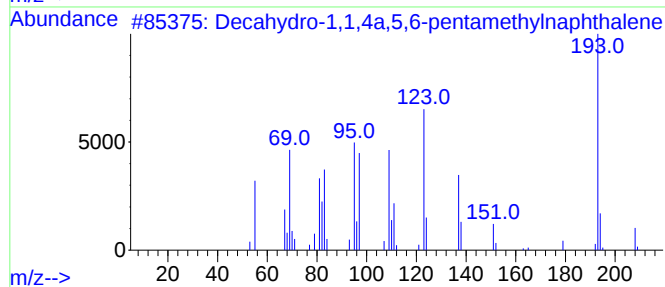
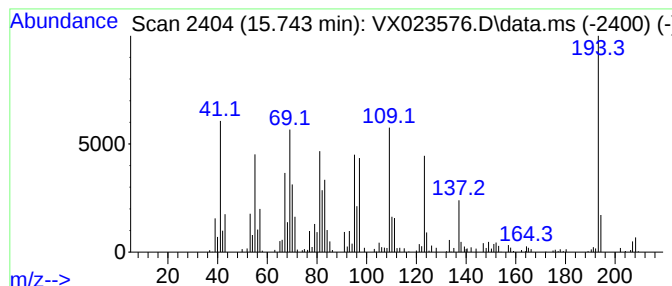
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072221W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown15.743 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	11.97 ug/l	125875	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2			4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	38
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	35
5			Neopentylidenecyclohexane	152	C11H20	039546-80-0	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080521\
Data File : VX023576.D
Acq On : 05 Aug 2021 16:37
Operator : JC/MD
Sample : M3298-06 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
1940

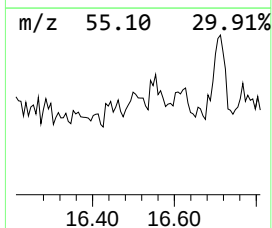
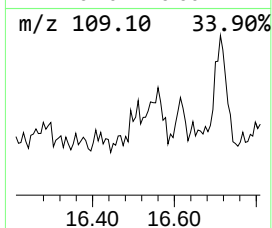
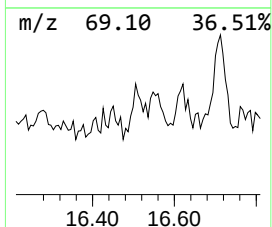
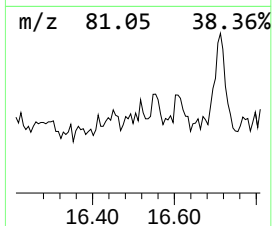
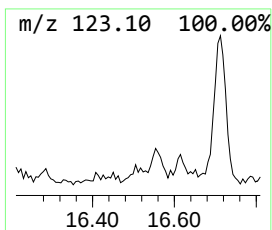
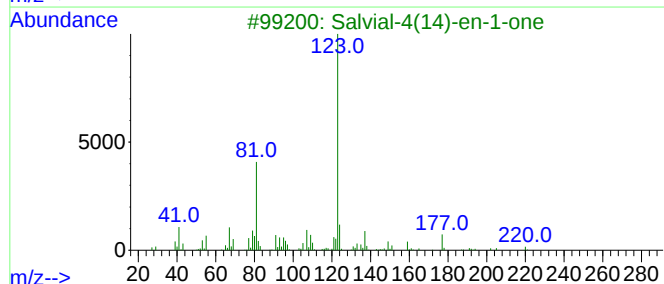
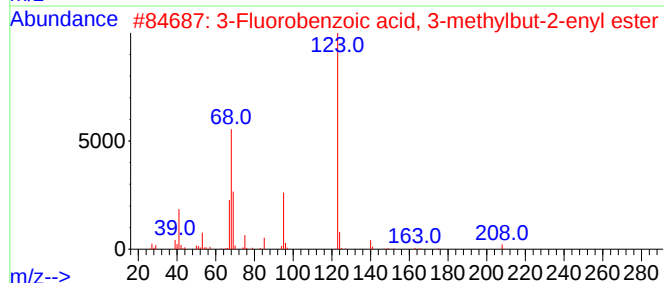
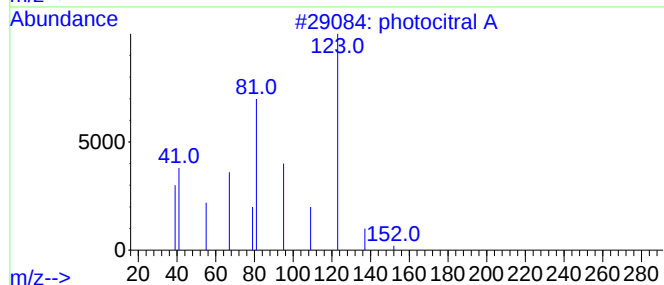
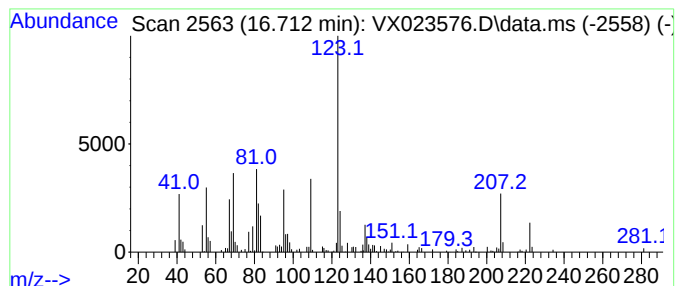
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072221W.M
Quant Title : SW846 8260

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

Peak Number 3 photocitral A Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.712	6.41 ug/l	67429	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			photocitral A	152	C10H16O	055253-28-6	50
2			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	47
3			Salvial-4(14)-en-1-one	220	C15H24O	073809-82-2	43
4			Hydrazine, N-(bicyclo[4.1.0]hept...	259	C14H17N3O2	1000259-41-4	43
5			Benzamide, 4-fluoro-N-(2-ethylhe...	251	C15H22FNO	1000407-32-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080521\
Data File : VX023576.D
Acq On : 05 Aug 2021 16:37
Operator : JC/MD
Sample : M3298-06 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1940

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072221W.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
unknown15.743	15.743	12.0	ug/l	125875	4	12.024	525820	50.0
photocitral A	16.712	6.4	ug/l	67429	4	12.024	525820	50.0