

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020624\
 Data File : VY017271.D
 Acq On : 06 Feb 2024 17:47
 Operator : SY/MD
 Sample : P1358-05
 Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RT5149

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\82Y020124S.M
 Title : SW846 8260

Signal : TIC: VY017271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	59	65	68	rBV3	4307	7534	1.57%	0.282%
2	4.716	465	475	487	rBV3	10408	32018	6.69%	1.198%
3	5.759	636	646	656	rBV4	3380	10686	2.23%	0.400%
4	6.990	837	848	858	rBV2	3147	10410	2.18%	0.389%
5	7.722	958	968	973	rBV	60415	141892	29.65%	5.307%
6	7.795	973	980	992	rVB	97551	222582	46.52%	8.325%
7	8.142	1024	1037	1047	rBV	58069	129396	27.04%	4.840%
8	8.691	1115	1127	1141	rBV	161509	321540	67.20%	12.027%
9	10.185	1364	1372	1380	rBV	260510	450225	94.09%	16.840%
10	10.581	1432	1437	1443	rBV2	8304	14269	2.98%	0.534%
11	10.947	1494	1497	1506	rVB8	2680	5152	1.08%	0.193%
12	11.496	1580	1587	1597	rVB	235924	380738	79.57%	14.241%
13	12.142	1682	1693	1694	rBV5	21199	54079	11.30%	2.023%
14	12.343	1723	1726	1730	rVB	7799	8618	1.80%	0.322%
15	12.489	1744	1750	1756	rBV	168267	277660	58.03%	10.385%
16	13.428	1898	1904	1920	rVB	231980	478511	100.00%	17.898%
17	13.654	1931	1941	1943	rBV9	17688	51884	10.84%	1.941%
18	15.507	2238	2245	2256	rBV4	23941	76371	15.96%	2.857%

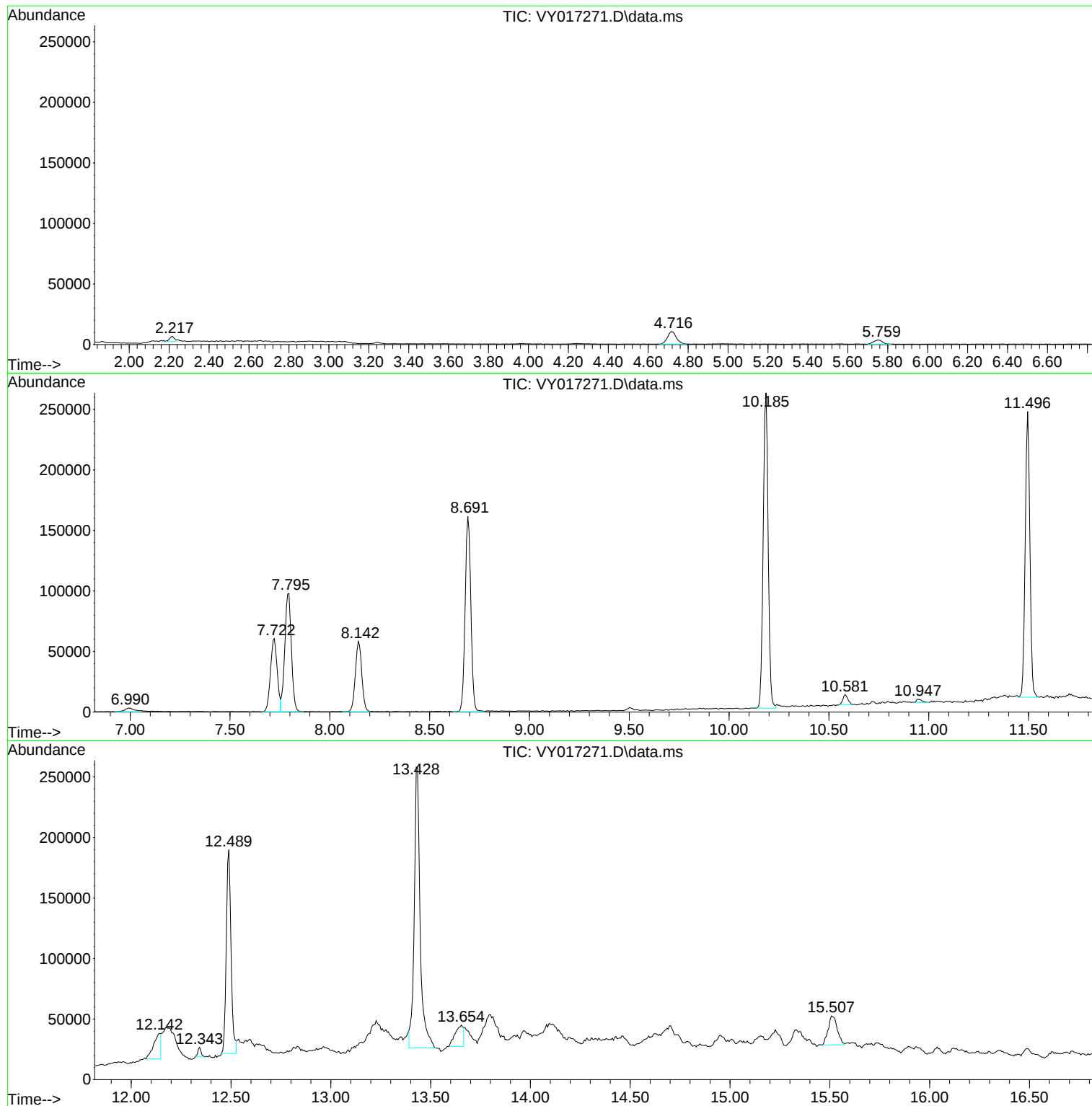
Sum of corrected areas: 2673565

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020624\
Data File : VY017271.D
Acq On : 06 Feb 2024 17:47
Operator : SY/MD
Sample : P1358-05
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT5149

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020624\
Data File : VY017271.D
Acq On : 06 Feb 2024 17:47
Operator : SY/MD
Sample : P1358-05
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT5149

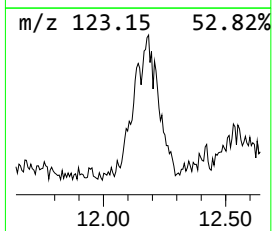
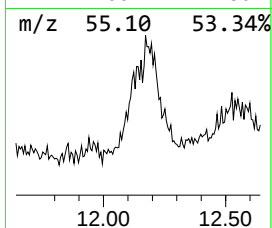
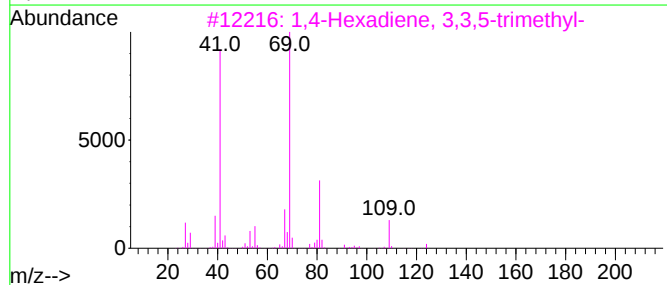
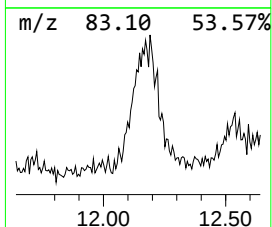
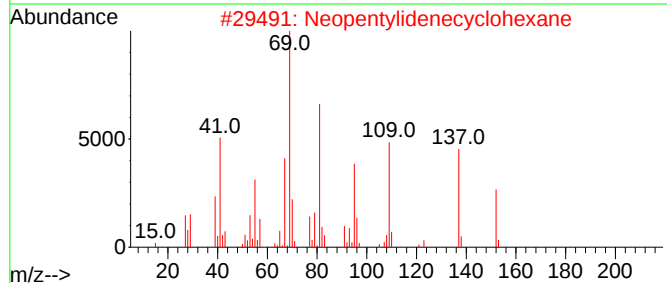
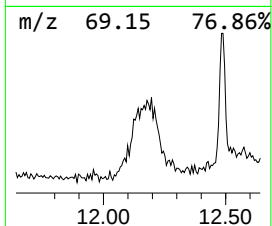
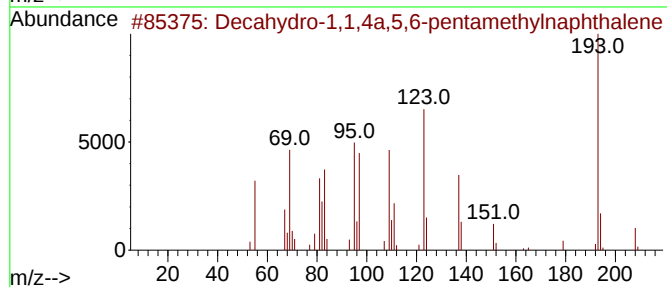
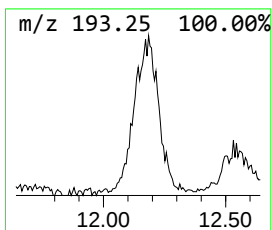
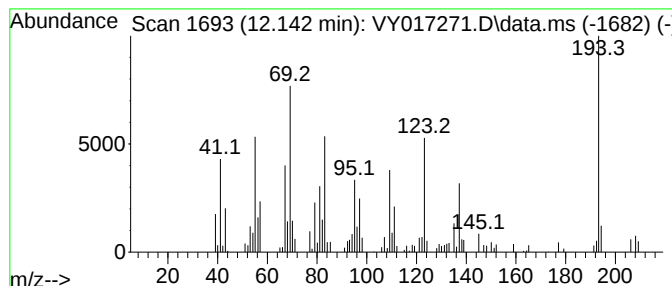
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 1 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.142	7.10 ug/l	54079	Chlorobenzene-d5	11.496

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	70
2		Neopentylidenecyclohexane	152	C11H20	039546-80-0	27
3		1,4-Hexadiene, 3,3,5-trimethyl-	124	C9H16	074753-00-7	18
4		2-Anthracenamine	193	C14H11N	000613-13-8	14
5		6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020624\
Data File : VY017271.D
Acq On : 06 Feb 2024 17:47
Operator : SY/MD
Sample : P1358-05
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT5149

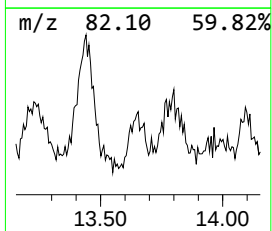
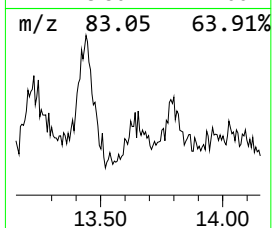
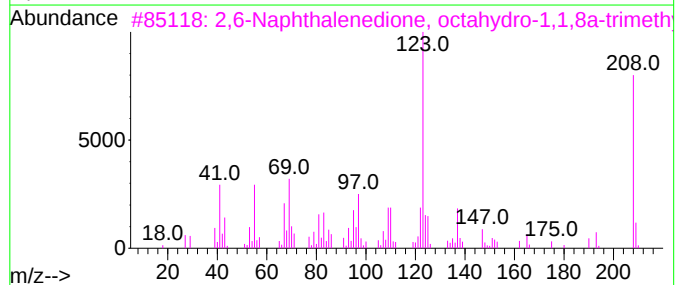
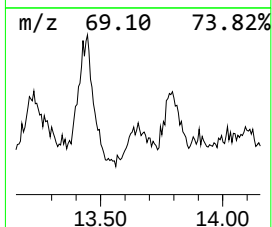
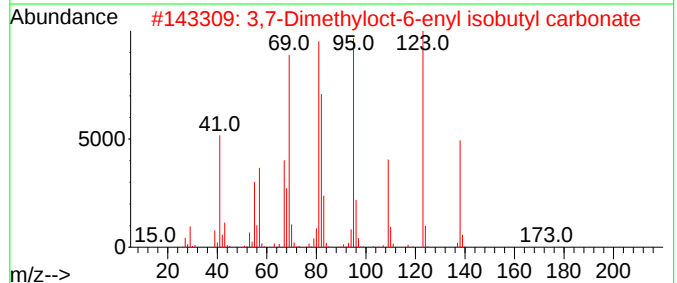
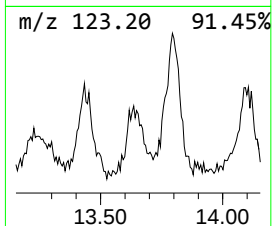
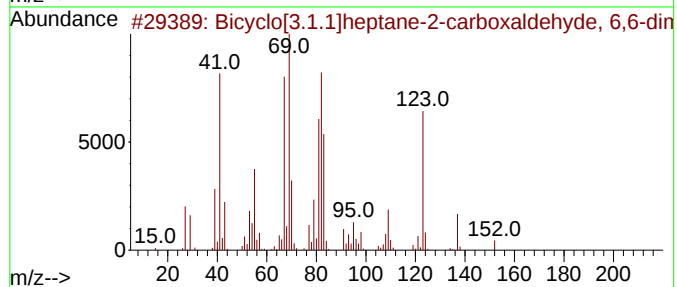
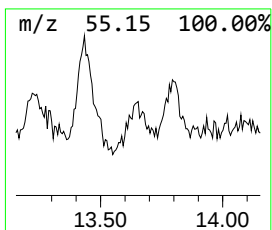
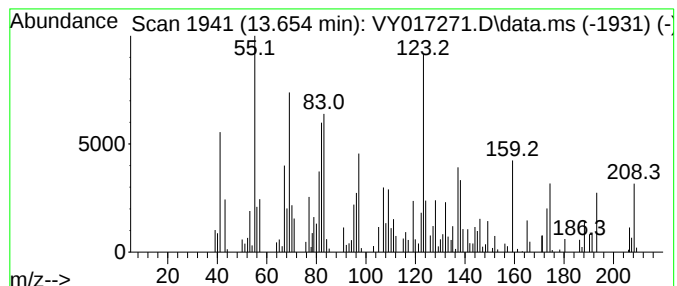
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.654 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.654	5.42 ug/l	51884	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	38
2			3,7-Dimethyloct-6-enyl isobutyl ...	256	C15H28O3	1000372-79-6	35
3			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	30
4			Heptanedioic acid, 3-methyl-, di...	202	C10H18O4	014226-72-3	14
5			5,6,7,7-Tetramethyl-octa-3,5-die...	180	C12H20O	1000190-70-9	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020624\
Data File : VY017271.D
Acq On : 06 Feb 2024 17:47
Operator : SY/MD
Sample : P1358-05
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT5149

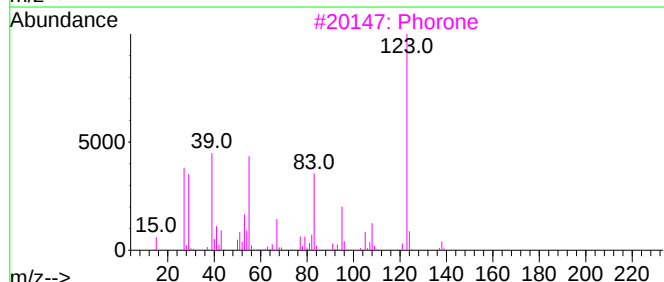
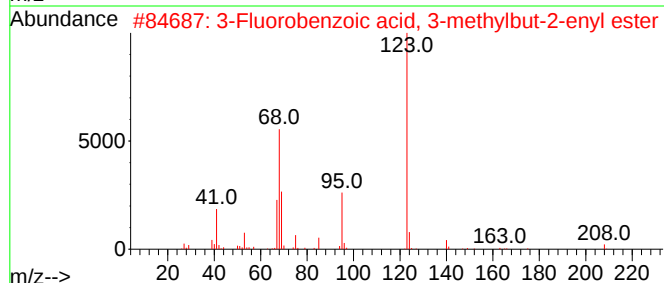
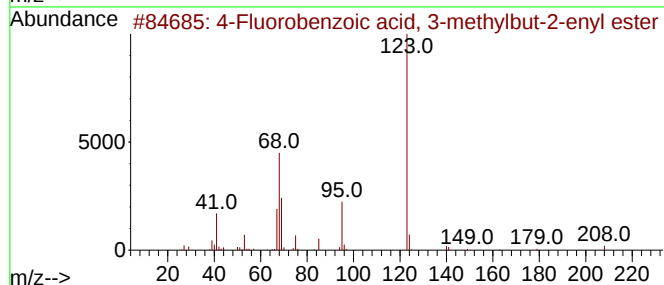
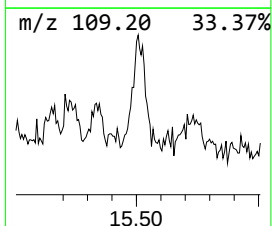
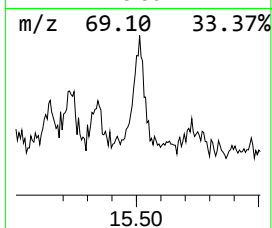
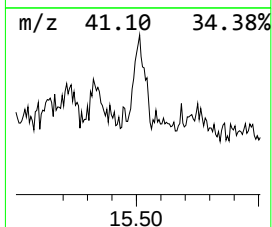
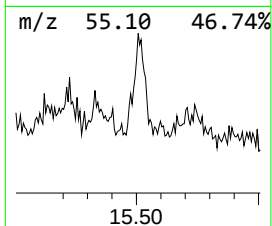
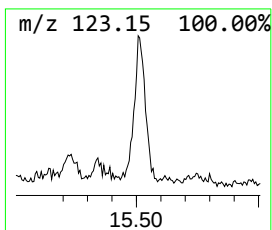
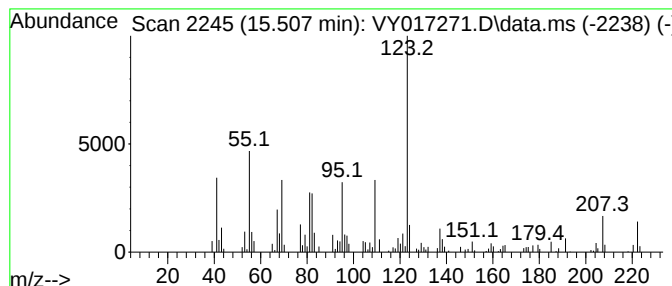
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.M
Quant Title : SW846 8260

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

Peak Number 3 4-Fluorobenzoic acid, 3-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.507	7.98 ug/l	76371	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13F02	1000299-15-1	52
2			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13F02	154559-38-3	52
3			Phorone	138	C9H14O	000504-20-1	50
4			1,3-Benzenediol, 4,5-dimethyl-	138	C8H10O2	000527-55-9	49
5			Benzamide, 4-fluoro-N-allyl-N-et...	207	C12H14FNO	1000446-42-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020624\
Data File : VY017271.D
Acq On : 06 Feb 2024 17:47
Operator : SY/MD
Sample : P1358-05
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT5149

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020124S.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
Decahydro-1,1,4...	12.142	7.1	ug/l	54079	3	11.496	380738	50.0
unknown13.654	13.654	5.4	ug/l	51884	4	13.434	478511	50.0
4-Fluorobenzoic...	15.507	8.0	ug/l	76371	4	13.434	478511	50.0