LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : C0AH1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN029633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.517	61	73	108	rBV3	238613	2044519	2.07%	1.079%
2	3.740	108	111	123	rVB	245879	387926	0.39%	0.205%
3	7.046	667	673	682	rBV	217911	365767	0.37%	0.193%
4	7.222	696	703	717	rBV	841681	1356746	1.37%	0.716%
5	7.411	727	735	742	rBV	786559	1273403	1.29%	0.672%
6	7.881	807	815	823	rBV	808331	1264583	1.28%	0.667%
7	8.587	928	935	946	rBV	582459	939937	0.95%	0.496%
8	8.993	996	1004	1008	rBV	143501	261982	0.27%	0.138%
9	9.046	1008	1013	1025	rVB	900305	1494404	1.51%	0.788%
10	9.763	1128	1135	1148	rBV	619368	1057724	1.07%	0.558%
11	10.299	1217	1226	1237	rBV	975658	1637184	1.66%	0.864%
12	10.681	1283	1291	1306	rVB	944729	1680700	1.70%	0.887%
13	10.828	1306	1316	1331	rBV	590659	1502475	1.52%	0.793%
14	11.334	1394	1402	1415	rBV	3246975	5695509	5.77%	3.004%
15	12.081	1523	1529	1537	rBV	81034	151348	0.15%	0.080%
16	13.369	1742	1748	1753	rBV	112329	160369	0.16%	0.085%
17	13.945	1839	1846	1852	rBV	1672892	2368483	2.40%	1.249%
18	14.216	1886	1892	1902	rVB2	1859347	2765484	2.80%	1.459%
19	14.522	1938	1944	1950	rBV	1199700	1750783	1.77%	0.924%
20	14.587	1950	1955	1974	rBV	382132	847045	0.86%	0.447%
21	14.728	1974	1979	1984	rBV	108380	175983	0.18%	0.093%
22	14.840	1993	1998	2012	rVB6	64640	135110	0.14%	0.071%
23	15.098	2035	2042	2069	rBV	3384156	7025683	7.11%	3.706%
24	15.287	2071	2074	2089	rVB2	148330	346966	0.35%	0.183%
25	15.516	2108	2113	2120	rVB	2332717	3424133	3.47%	1.806%
26	15.640	2128	2134	2140	rBV	752535	1016534	1.03%	0.536%
27	15.740	2146	2151	2156	rBV	166002	243422	0.25%	0.128%
28	15.857	2167	2171	2175	rBV	96336	123416	0.12%	0.065%
29	16.022	2194	2199	2206	rBV	182190	253092	0.26%	0.134%
30	16.245	2226	2237	2255	rBV	3329175	6879823	6.97%	3.629%
31	17.081	2374	2379	2384	rVB	886141	1081996	1.10%	0.571%
32	17.139	2384	2389	2394	rBV	1699488	2086602	2.11%	1.101%
33	17.192	2394	2398	2406	rVB	750573	986411	1.00%	0.520%
34	17.275	2406	2412	2417	rBV	1382716	1922592	1.95%	1.014%
35	17.375	2423	2429	2435	rBV	2584844	3632200	3.68%	1.916%
36	17.592	2460	2466	2478	rBV	10289082	13775485	13.95%	7.267%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Title : SVOA CALIBRATION

37	17.875	2509	2514	2520	rBV	1146177	1544069	1.56%	0.815%
38	17.957	2525	2528	2535	rVB2	135872	181494	0.18%	0.096%
39	18.186	2562	2567	2572	rBV	183633	260570	0.26%	0.137%
40	18.516	2616	2623	2640	rBV	813222	2321925	2.35%	1.225%
41	19.045	2694	2713	2716	rBV	27034781	98769966	100.00%	52.102%
42	19.086	2716	2720	2737	rVB	437211	881612	0.89%	0.465%
43	19.286	2750	2754	2763	rVB2	143429	223765	0.23%	0.118%
44	19.469	2781	2785	2794	rBV3	87730	128836	0.13%	0.068%
45	19.675	2814	2820	2828	rBV	3048536	4057307	4.11%	2.140%
46	20.175	2900	2905	2909	rBV	520304	624861	0.63%	0.330%
47	21.474	3120	3126	3134	rBV	1408947	1918884	1.94%	1.012%
48	21.922	3199	3202	3208	rVB	192361	249010	0.25%	0.131%
49	23.692	3496	3503	3514	rBV2	2073300	4100494	4.15%	2.163%
50	23.845	3522	3529	3544	rVB2	1058589	2190568	2.22%	1.156%

Sum of corrected areas: 189569180

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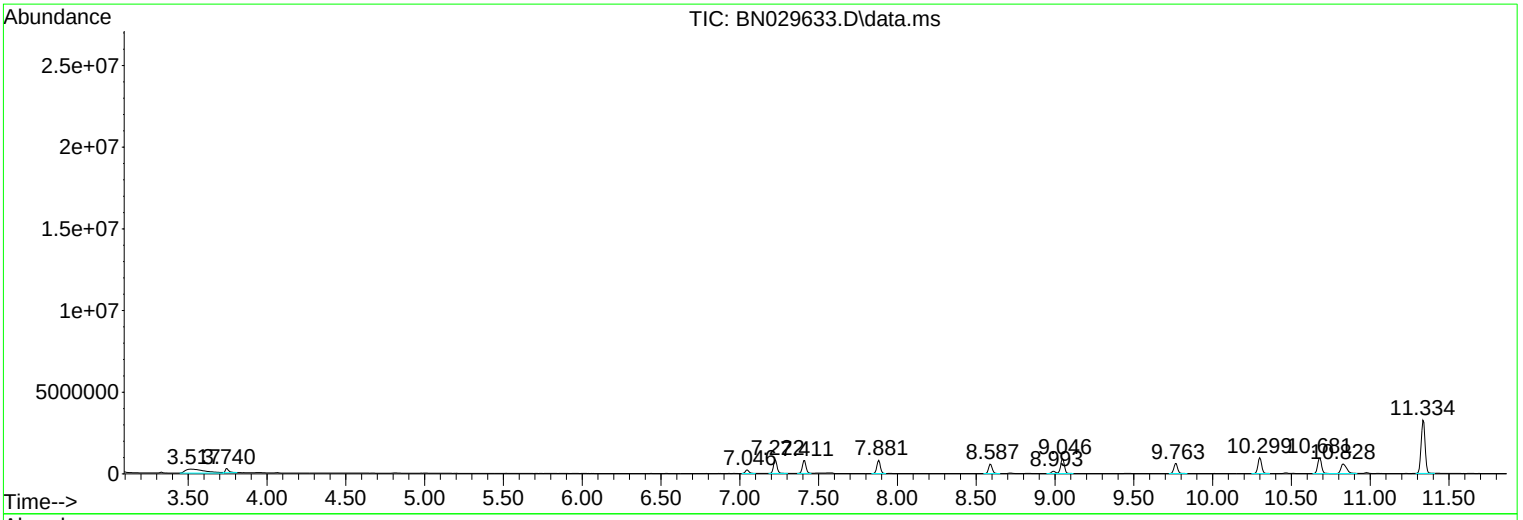
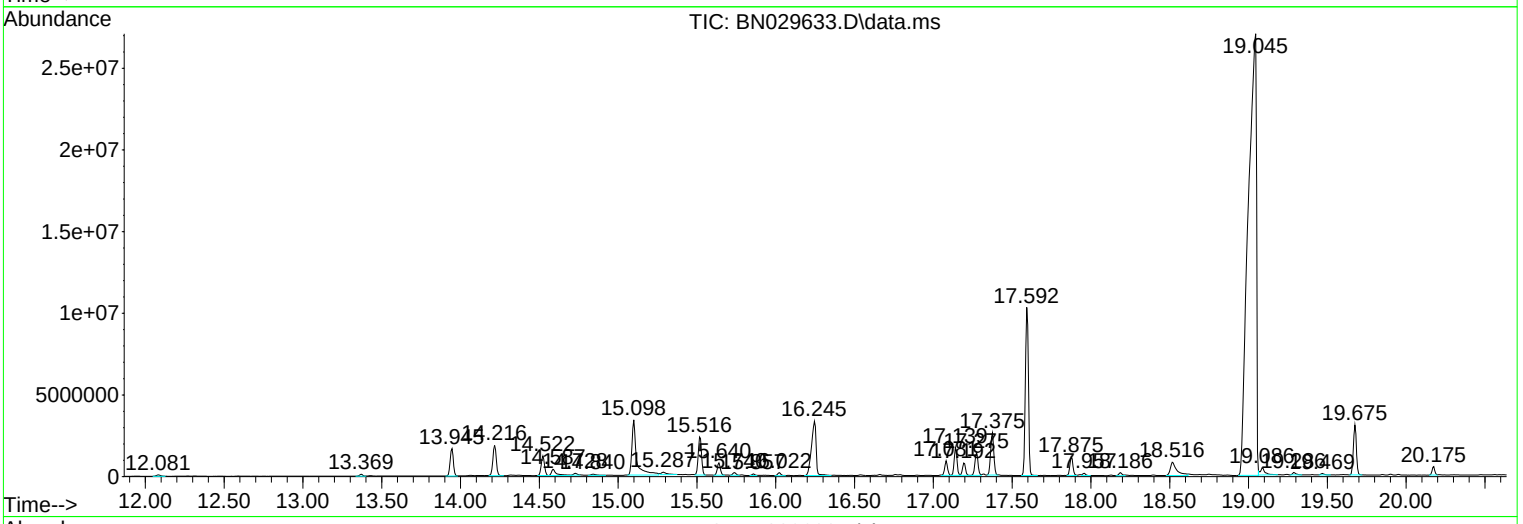
ALS Vial : 25 Sample Multiplier: 1

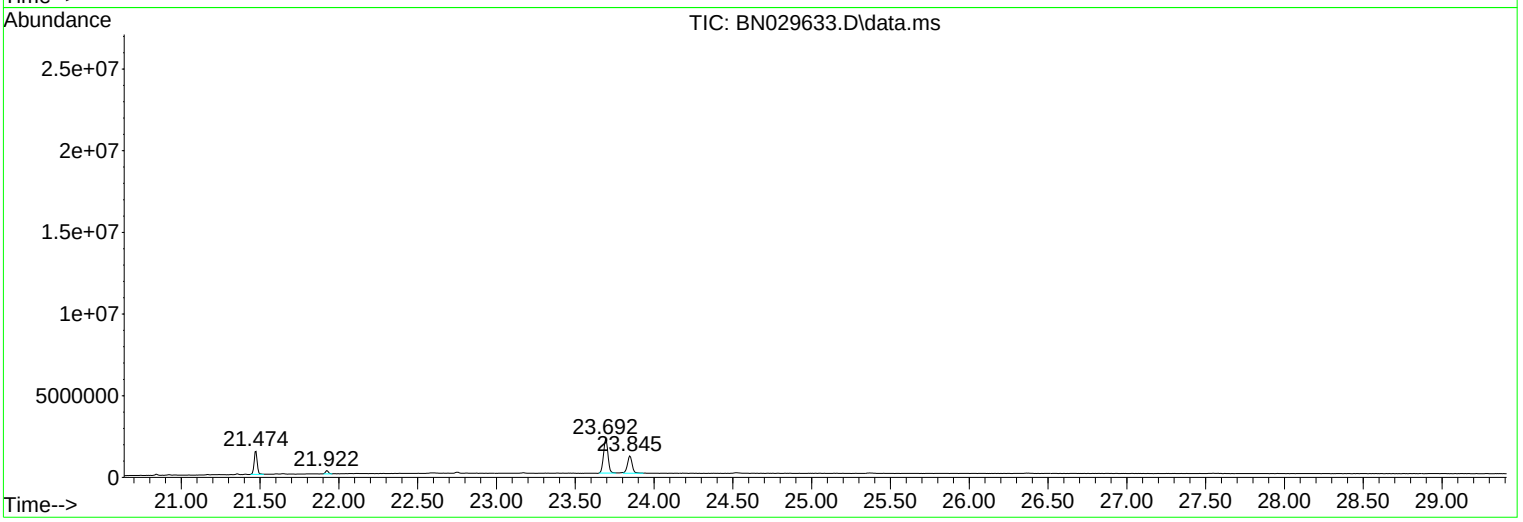
Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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







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Data File : BN029633.D
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

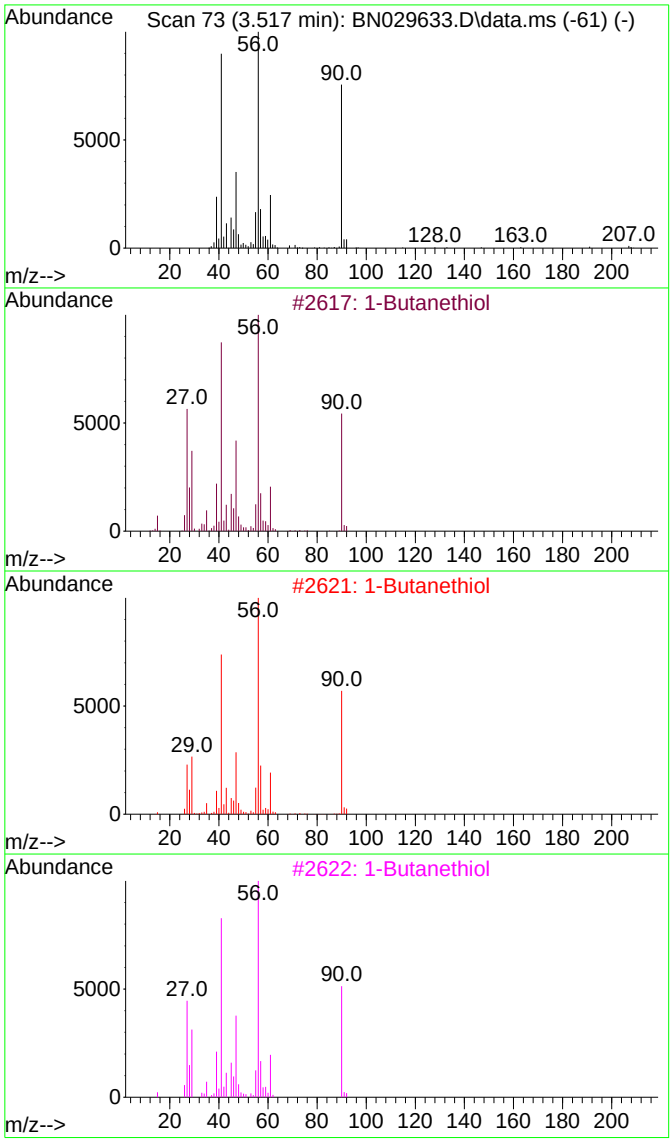
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

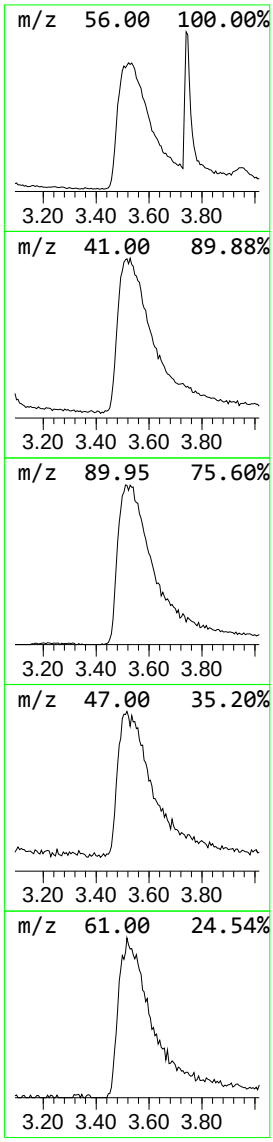
****

Peak Number 1 1-Butanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.517	32.34 ng/ul	2044520	1,4-Dichlorobenzene-d4	7.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanethiol	90	C4H10S	000109-79-5	91
2	1-Butanethiol	90	C4H10S	000109-79-5	91
3	1-Butanethiol	90	C4H10S	000109-79-5	91
4	1-Butanethiol	90	C4H10S	000109-79-5	83
5	1-Propanethiol, 2-methyl-	90	C4H10S	000513-44-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

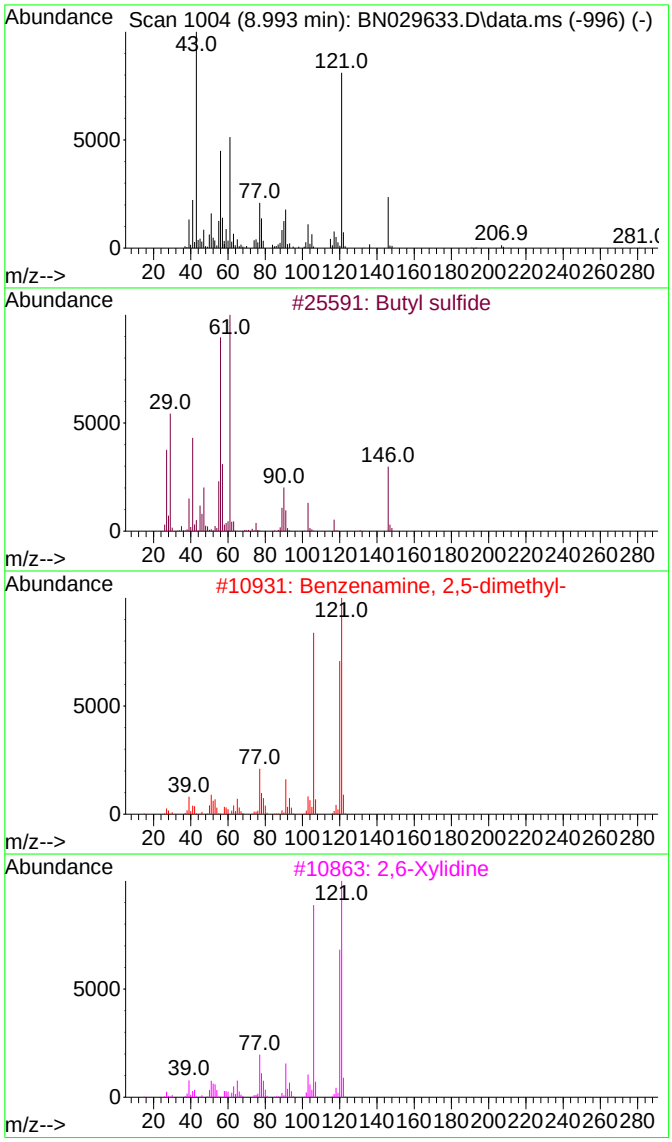
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

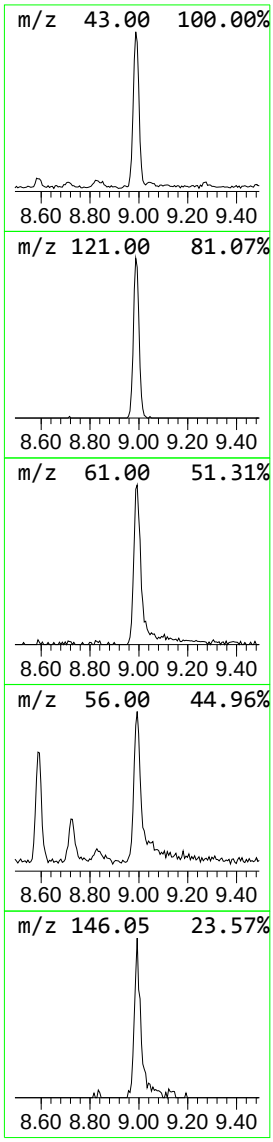
****

Peak Number 2 unknown-01 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.993	4.14 ng/ul	261982	1,4-Dichlorobenzene-d4	7.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl sulfide	146	C8H18S	000544-40-1	45
2	Benzenamine, 2,5-dimethyl-	121	C8H11N	000095-78-3	43
3	2,6-Xylidine	121	C8H11N	000087-62-7	38
4	Acetamide, 2-methoxy-2-phenyl-N-...	303	C17H18ClNO2	327991-45-7	38
5	Butyl sulfide	146	C8H18S	000544-40-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

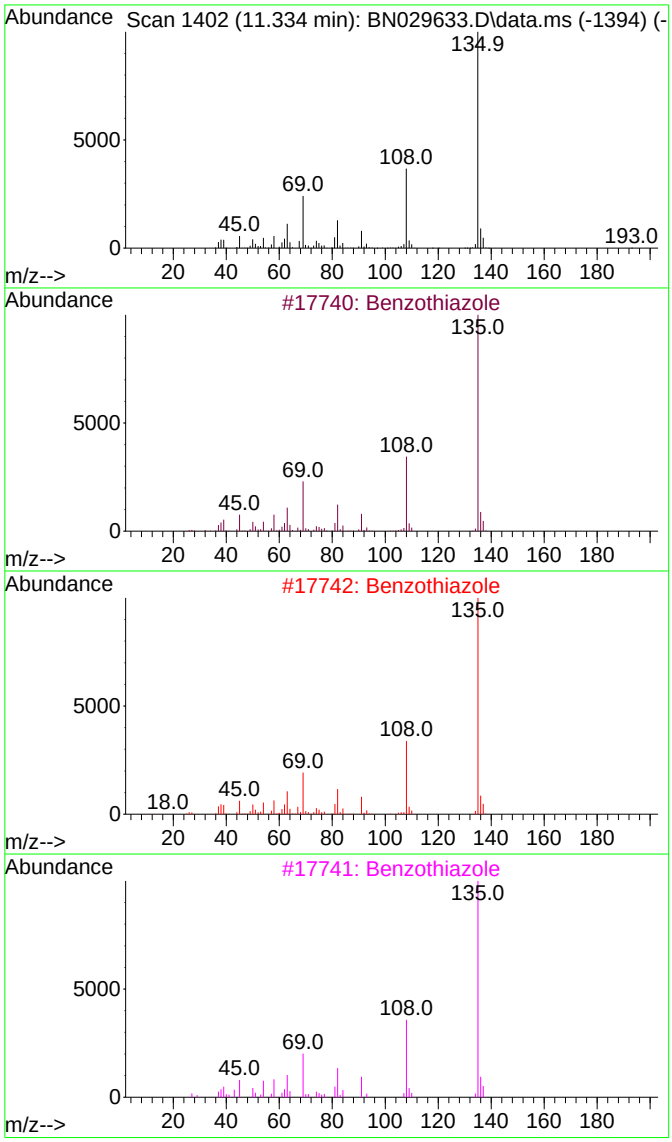
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

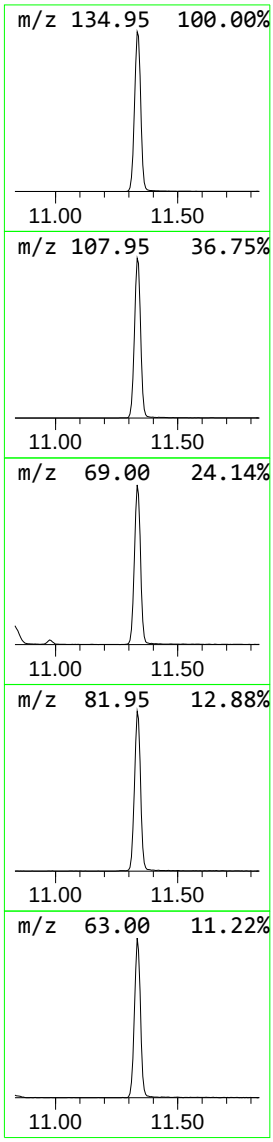
****

Peak Number 3 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.334	67.78 ng/ul	5695510	Naphthalene-d8	10.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	97
2	Benzothiazole	135	C7H5NS	000095-16-9	95
3	Benzothiazole	135	C7H5NS	000095-16-9	95
4	Benzothiazole	135	C7H5NS	000095-16-9	94
5	Benzothiazole	135	C7H5NS	000095-16-9	91





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

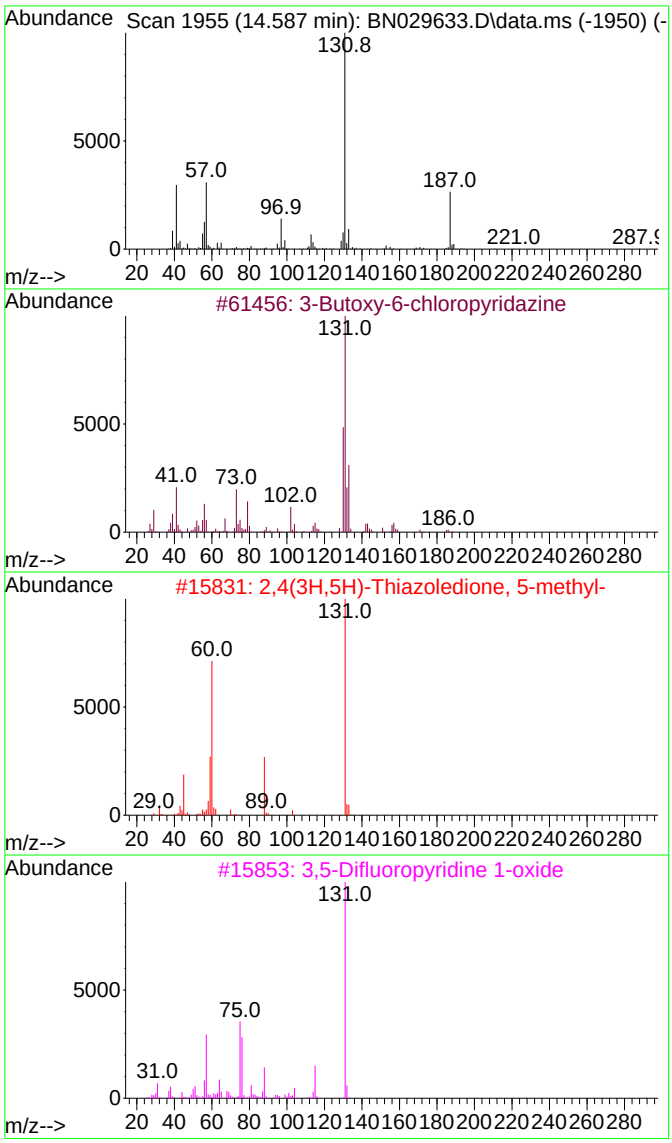
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

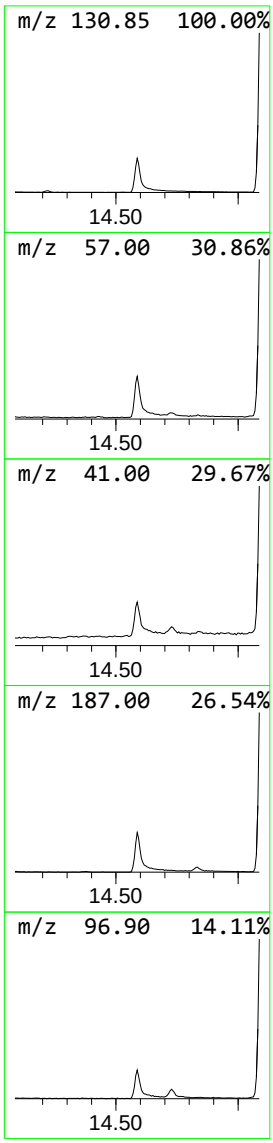
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown-02 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.587	9.68 ng/ul	847045	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Butoxy-6-chloropyridazine	186	C8H11ClN2O	017321-22-1	37
2	2,4(3H,5H)-Thiazoledione, 5-methyl-	131	C4H5NO2S	1000319-17-7	9
3	3,5-Difluoropyridine 1-oxide	131	C5H3F2NO	210169-07-6	9
4	5-(3-Hydroxy-4,4,10,13,14-pentam...	690	C39H74O4Si3	1000495-09-2	9
5	4-Chloro-5-methyl-1H-pyrazol-3-a...	215	C8H10ClN3O2	1000511-78-2	9





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Data File : BN029633.D
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Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

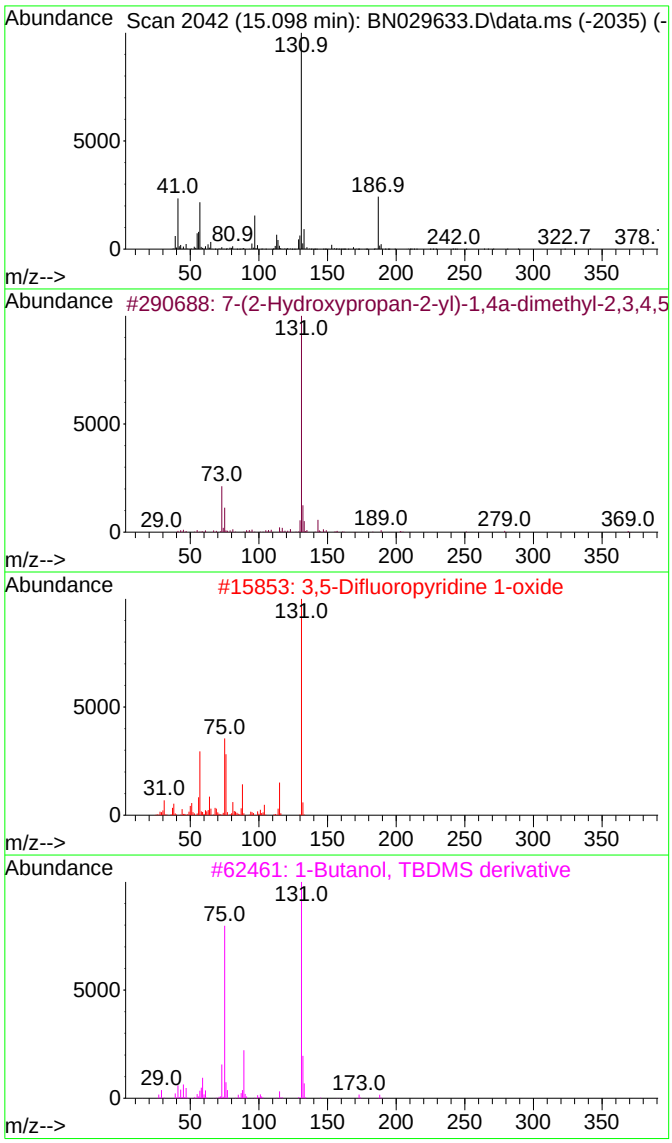
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

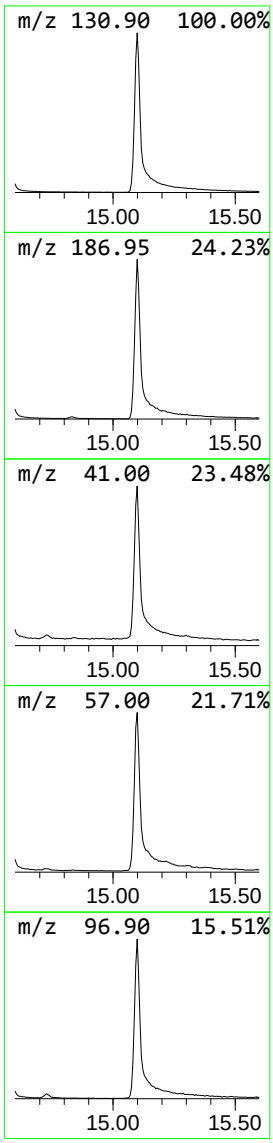
****

Peak Number 5 unknown-03 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	80.26 ng/ul	7025680	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-(2-Hydroxypropan-2-yl)-1,4a-di...	384	C21H44O2Si2	1010495-95-3	33
2	3,5-Difluoropyridine 1-oxide	131	C5H3F2NO	210169-07-6	9
3	1-Butanol, TBDMS derivative	188	C10H24OSi	1000333-04-7	9
4	2,2-Dimethyl-3-pentanol, TMS der...	188	C10H24OSi	1000364-14-3	9
5	2,4(3H,5H)-Thiazoledione, 5-methyl-	131	C4H5NO2S	1000319-17-7	7





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

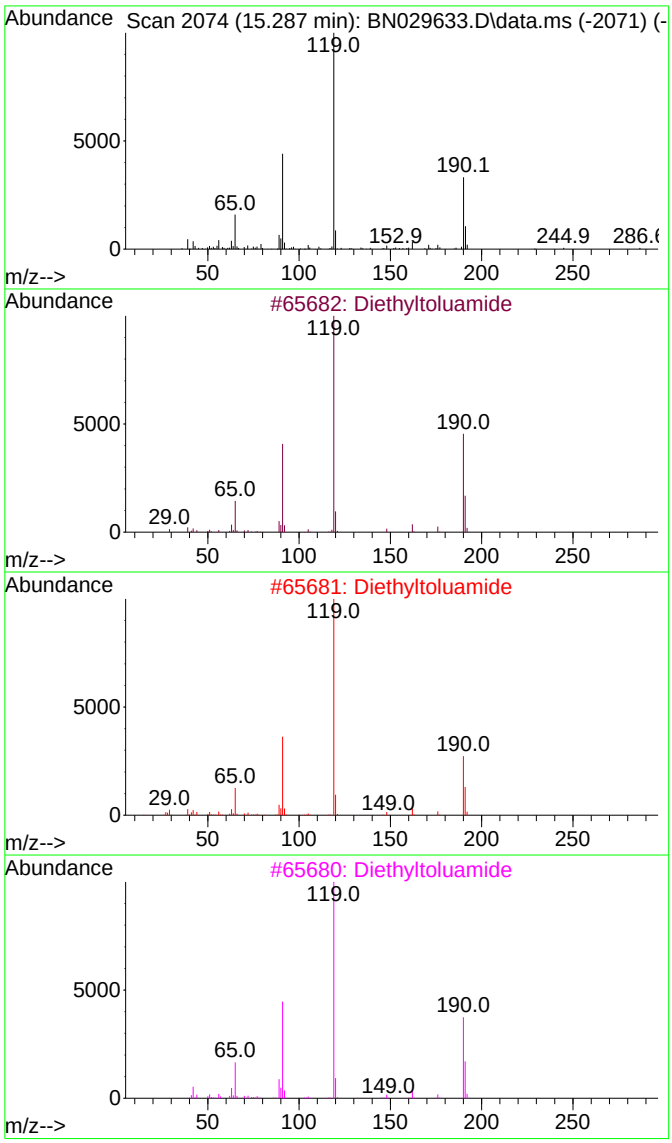
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

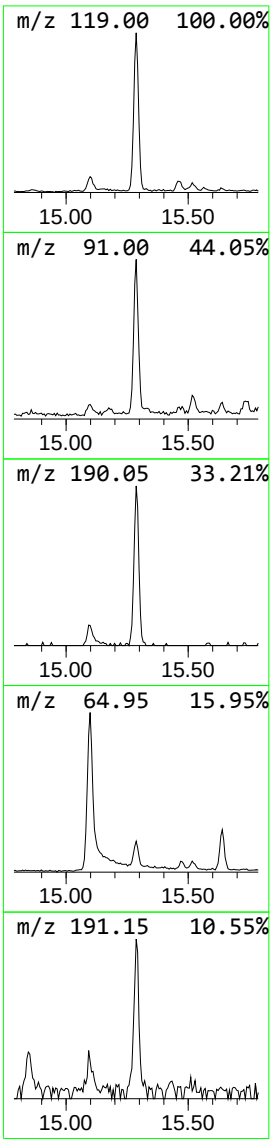
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Diethyltoluamide Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.287	3.96 ng/ul	346966	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	97
2	Diethyltoluamide	191	C12H17NO	000134-62-3	95
3	Diethyltoluamide	191	C12H17NO	000134-62-3	94
4	Diethyltoluamide	191	C12H17NO	000134-62-3	94
5	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	90





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Data File : BN029633.D
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Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

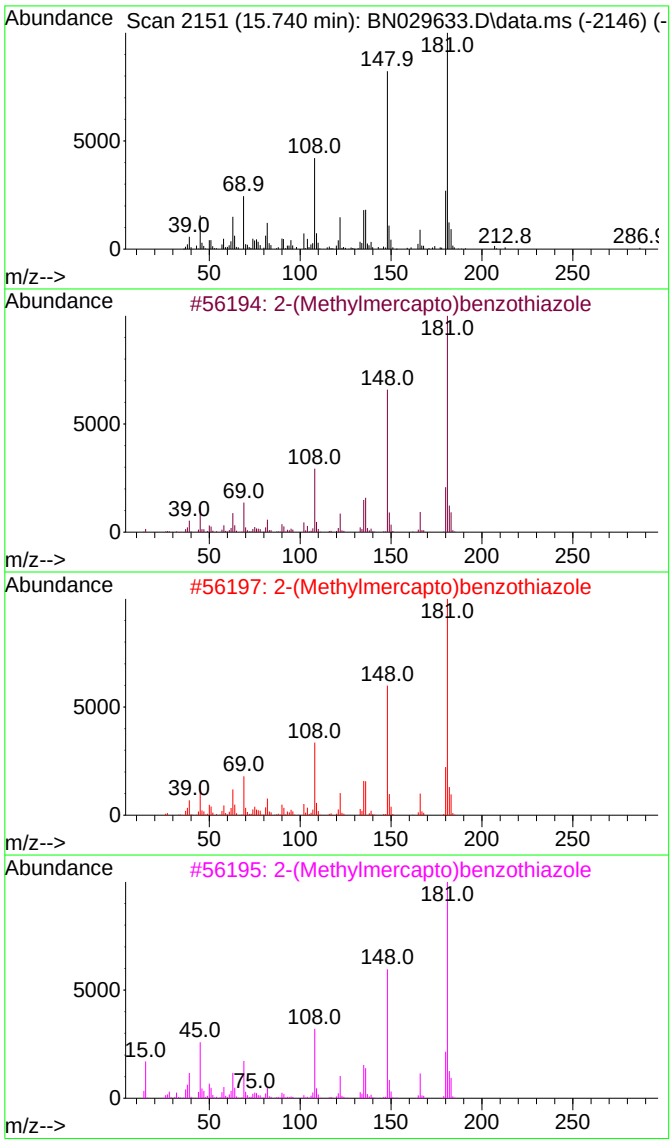
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

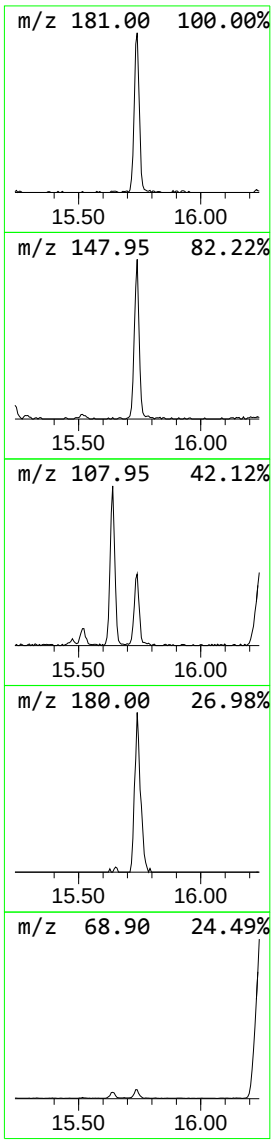
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-(Methylmercapto)benzothia... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.740	2.78 ng/ul	243422	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	98
2	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	96
3	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	94
4	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	90
5	2(3H)-Benzothiazolethione, 3-met...	181	C8H7NS2	002254-94-6	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

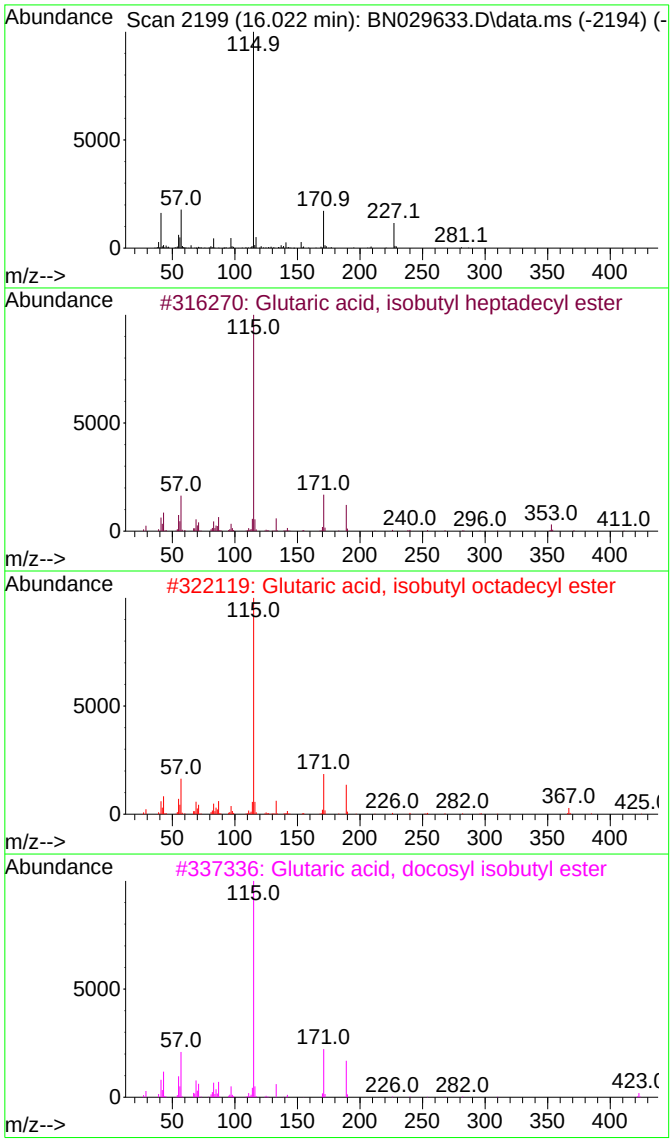
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

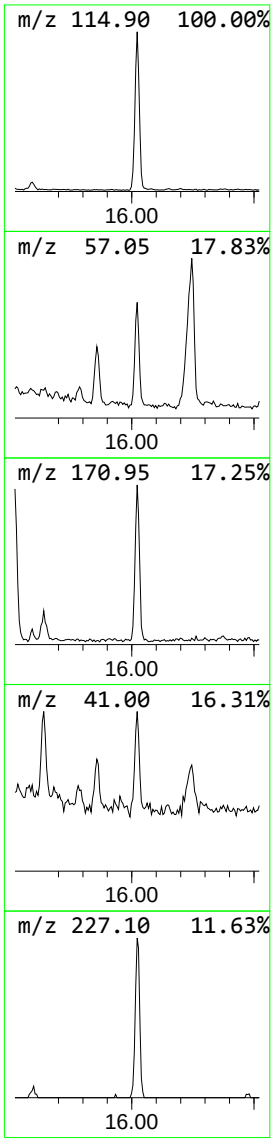
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Glutaric acid, isobutyl hep... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.022	2.63 ng/ul	253092	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutaric acid, isobutyl heptadec...	426	C26H50O4	1000358-26-5	64
2	Glutaric acid, isobutyl octadecy...	440	C27H52O4	1000358-26-6	64
3	Glutaric acid, docosyl isobutyl ...	496	C31H60O4	1000359-69-8	45
4	Glutaric acid, isobutyl 3-methyl...	258	C14H26O4	1000359-71-9	45
5	Glutaric acid, isobutyl hexadecy...	412	C25H48O4	1000358-26-4	39





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Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

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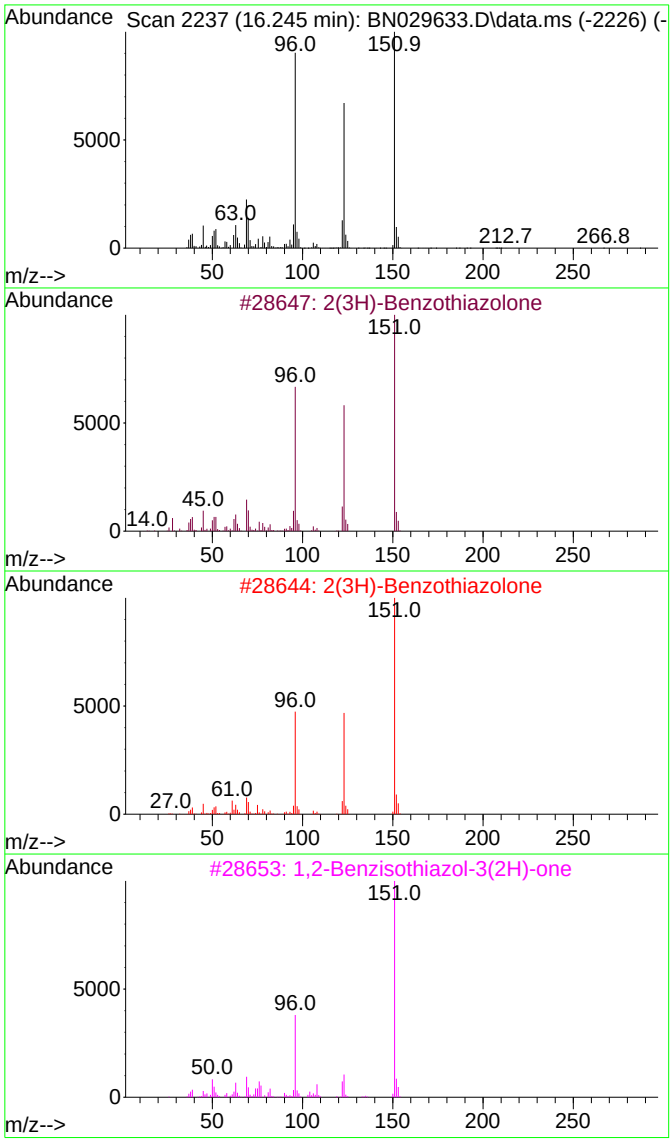
Quant Title : SVOA CALIBRATION

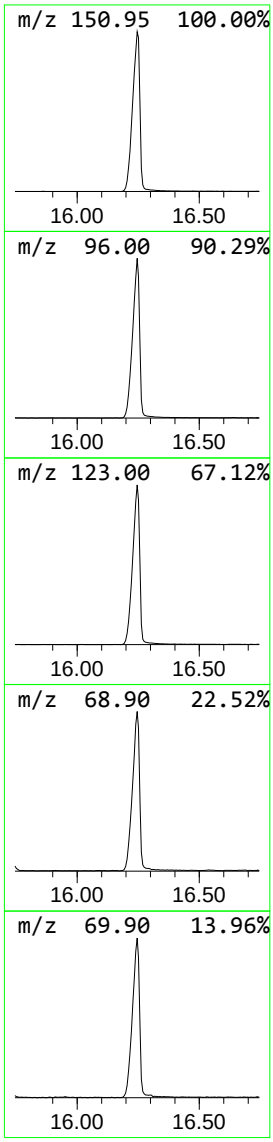
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2(3H)-Benzothiazolone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	71.57 ng/ul	6879820	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	95
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
4	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	49
5	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	43





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

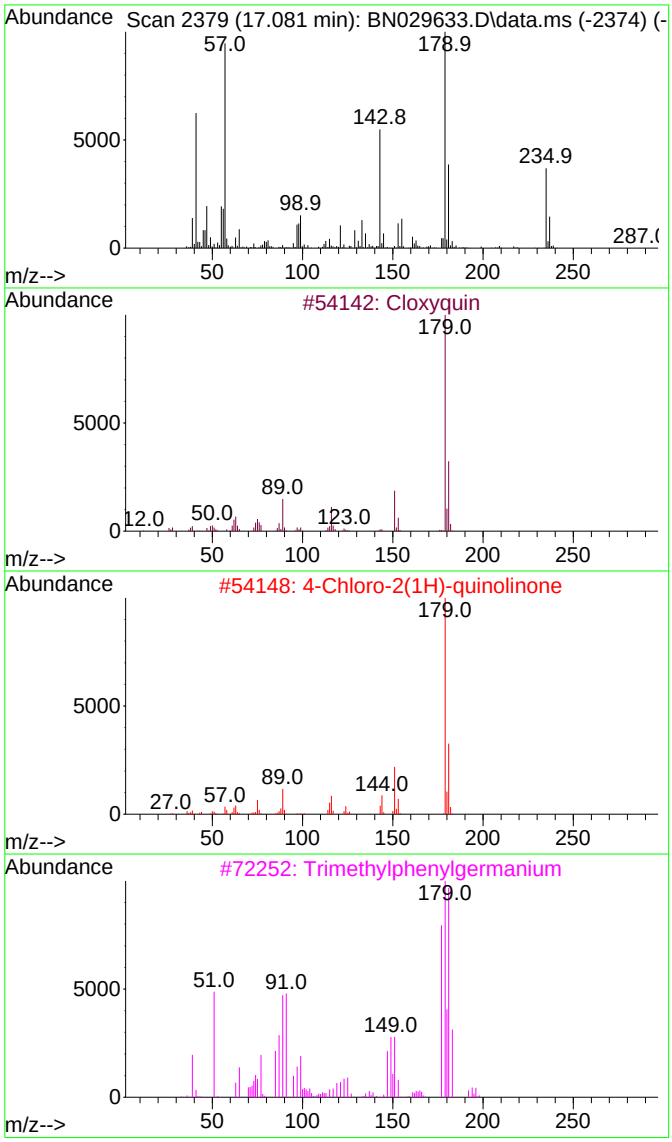
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

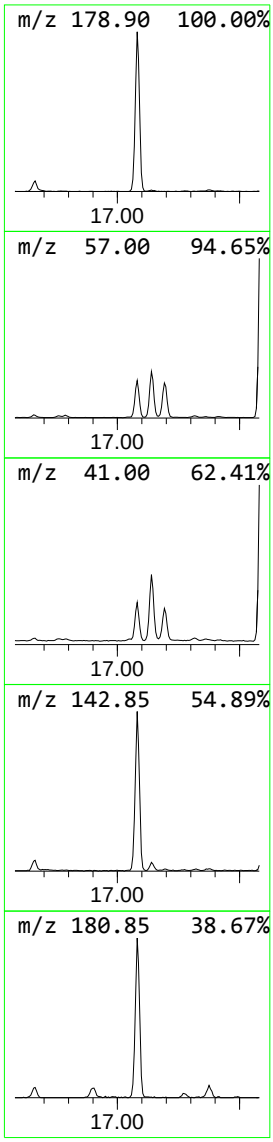
****

Peak Number 10 unknown-04 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.081	11.26 ng/ul	1082000	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cloxyquin	179	C9H6ClNO	000130-16-5	32
2	4-Chloro-2(1H)-quinolinone	179	C9H6ClNO	020146-59-2	32
3	Trimethylphenylgermanium	196	C9H14Ge	001626-00-2	17
4	1,4-Bis(trimethylsilyl)-1,3-buta...	194	C10H18Si2	004526-07-2	10
5	Phenanthridine	179	C13H9N	000229-87-8	9





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

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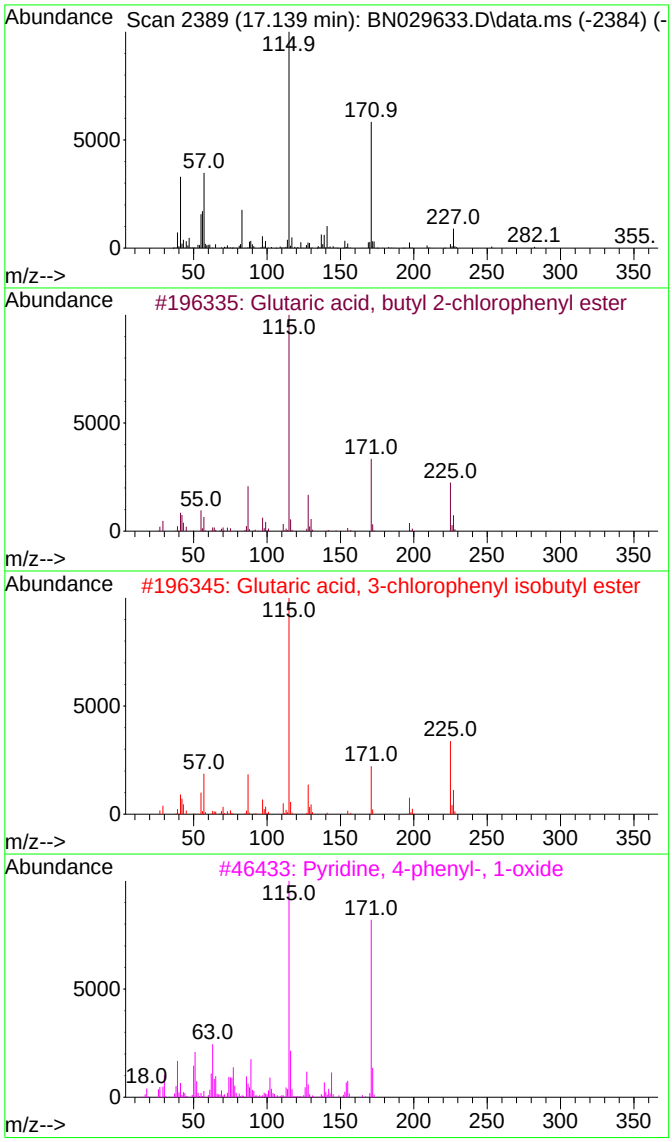
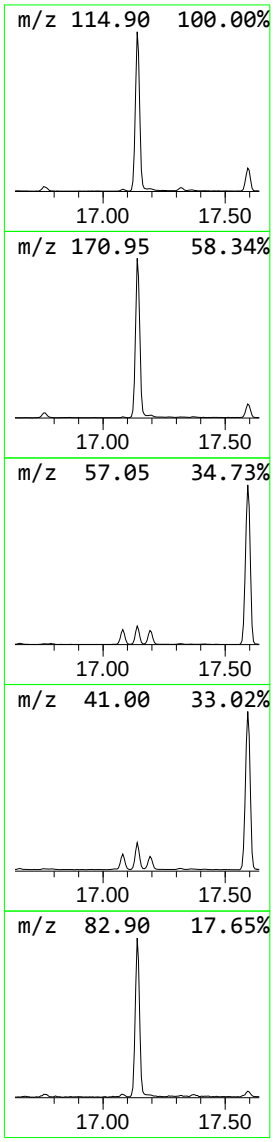
Peak Number 11 unknown-05 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	21.71 ng/ul	2086600	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutaric acid, butyl 2-chlorophe...	298	C15H19ClO4	1000358-59-9	40
2	Glutaric acid, 3-chlorophenyl is...	298	C15H19ClO4	1000358-81-0	38
3	Pyridine, 4-phenyl-, 1-oxide	171	C11H9NO	001131-61-9	38
4	Glutaric acid, butyl docosyl ester	496	C31H60O4	1000359-69-9	38
5	Glutaric acid, 4-chlorophenyl pe...	312	C16H21ClO4	1000359-21-1	37





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Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

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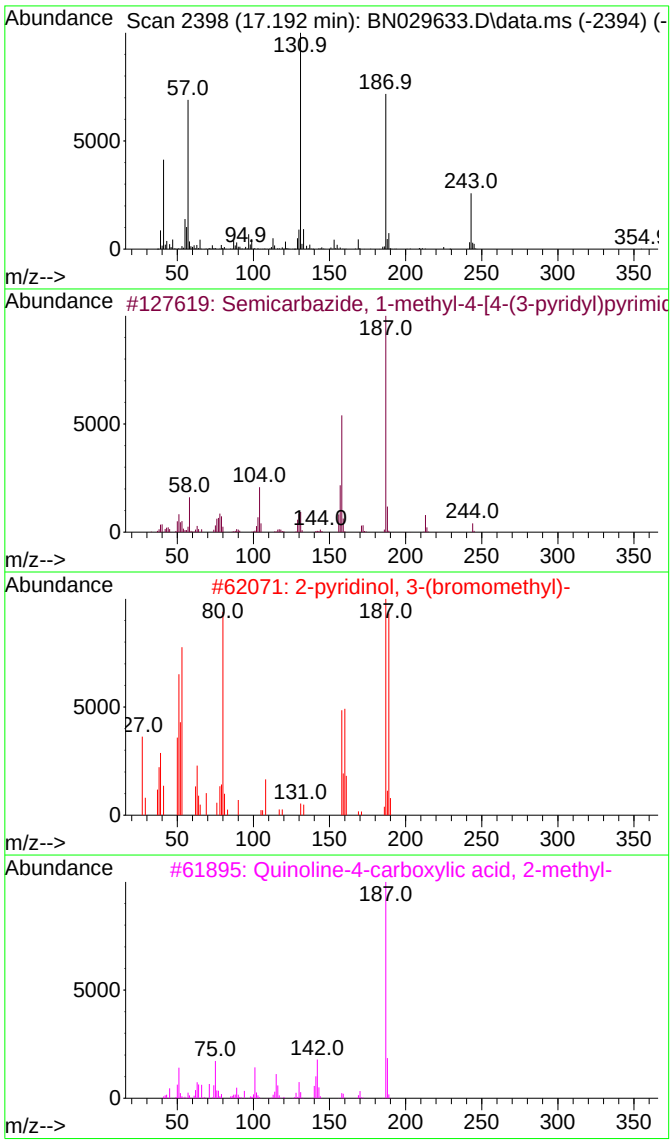
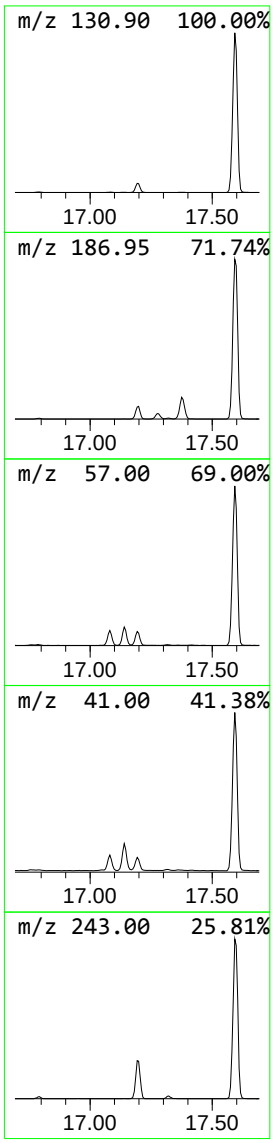
Peak Number 12 unknown-06 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.192	10.26 ng/ul	986411	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Semicarbazide, 1-methyl-4-[4-(3-...	244	C11H12N6O	1000270-46-2	14
2	2-pyridinol, 3-(bromomethyl)-	187	C6H6BrNO	1000400-15-7	9
3	Quinoline-4-carboxylic acid, 2-m...	187	C11H9NO2	000634-38-8	9
4	Benzene, 2-chloro-1-methoxy-4-ni...	187	C7H6ClNO3	004920-79-0	9
5	N-Benzylmaleimide	187	C11H9NO2	001631-26-1	9





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Acq On : 10 Feb 2024 05:33
Operator : MA/JU
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

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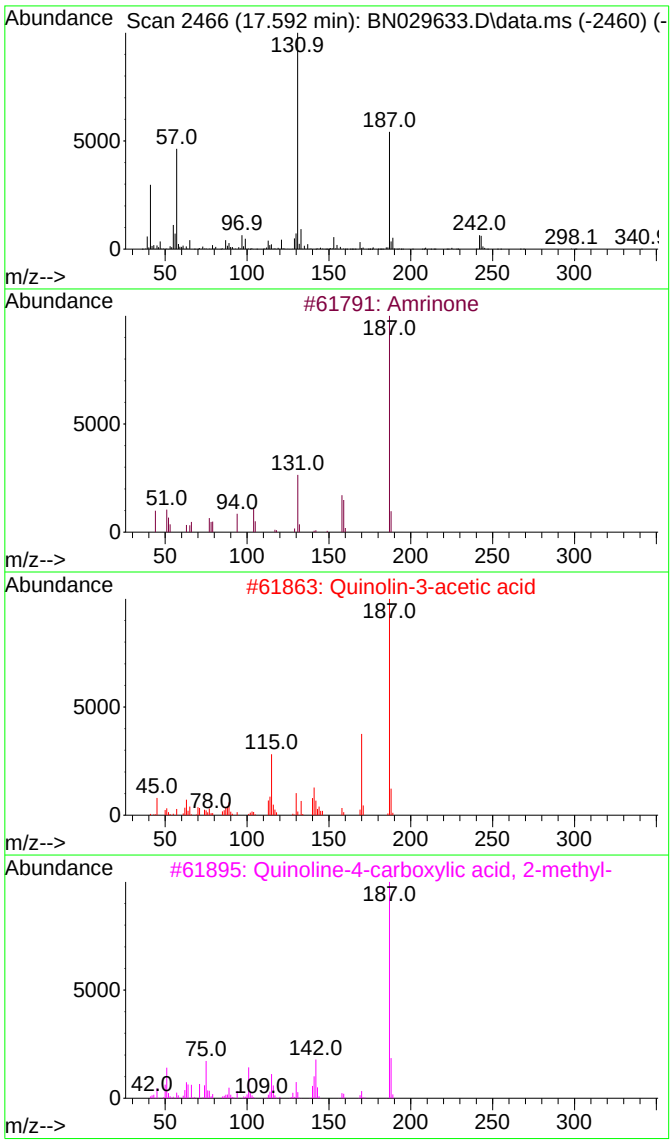
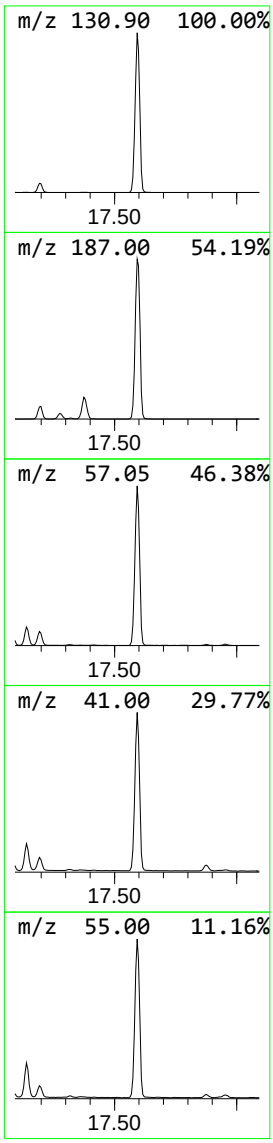
Peak Number 13 unknown-07 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.592	143.30 ng/ul	13775500	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amrinone	187	C10H9N3O	060719-84-8	9
2	Quinolin-3-acetic acid	187	C11H9NO2	021168-40-1	9
3	Quinoline-4-carboxylic acid, 2-m...	187	C11H9NO2	000634-38-8	9
4	Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	041195-90-8	9
5	6-Hydroxy-2-methylcyclohepta(b)p...	187	C11H9NO2	109338-95-6	9





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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Quant Title : SVOA CALIBRATION

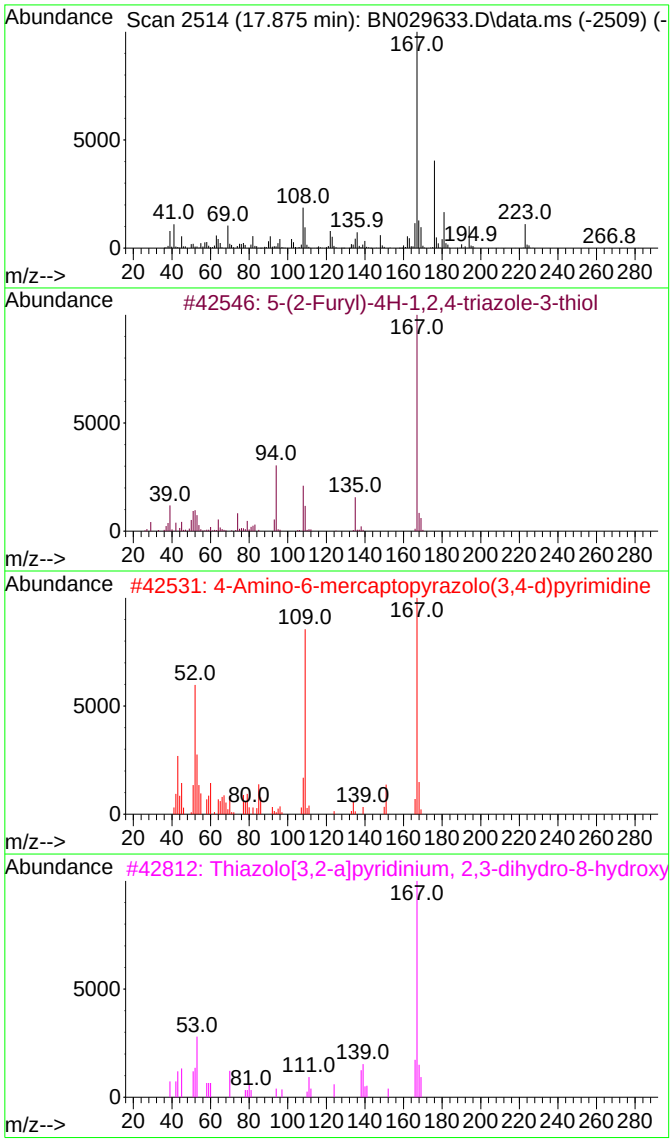
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

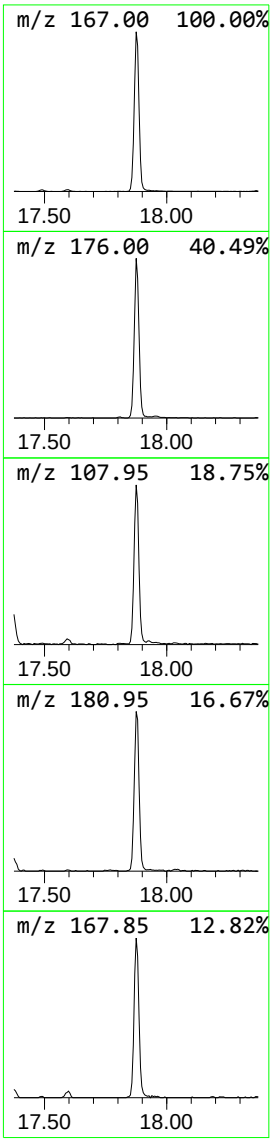
****

Peak Number 14 unknown-08 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.875	16.06 ng/ul	1544070	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(2-Furyl)-4H-1,2,4-triazole-3-...	167	C6H5N3OS	035771-65-4	47
2	4-Amino-6-mercaptopyrazolo(3,4-d...	167	C5H5N5S	023771-52-0	43
3	Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	43
4	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	38
5	Glutaric acid, 2-fluorophenyl di...	392	C24H21FO4	1000393-34-5	38





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

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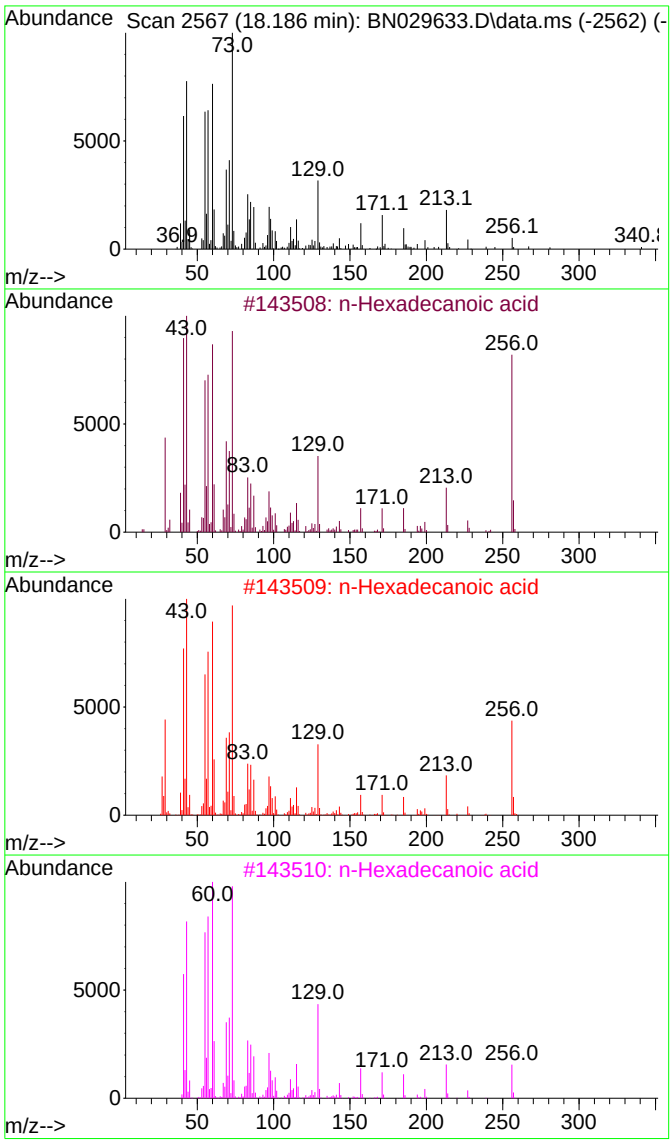
Quant Title : SVOA CALIBRATION

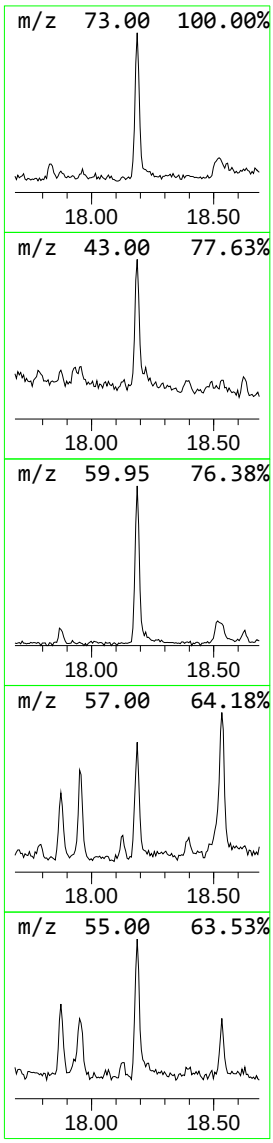
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 n-Hexadecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	2.71 ng/ul	260570	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81





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Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

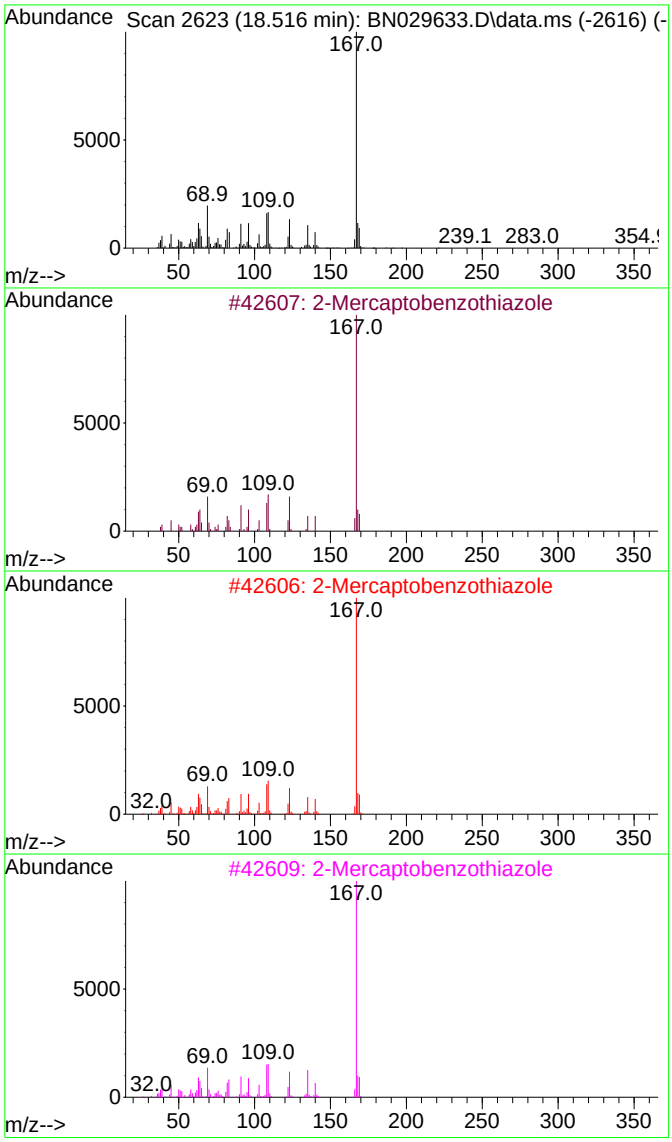
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

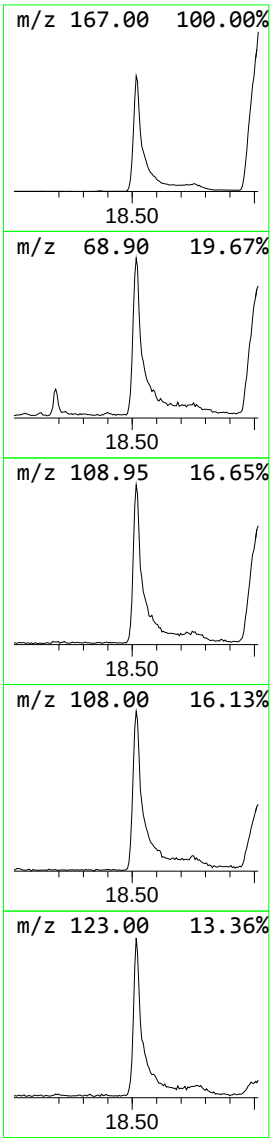
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 2-Mercaptobenzothiazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.516	24.15 ng/ul	2321930	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
3	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
4	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	90





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Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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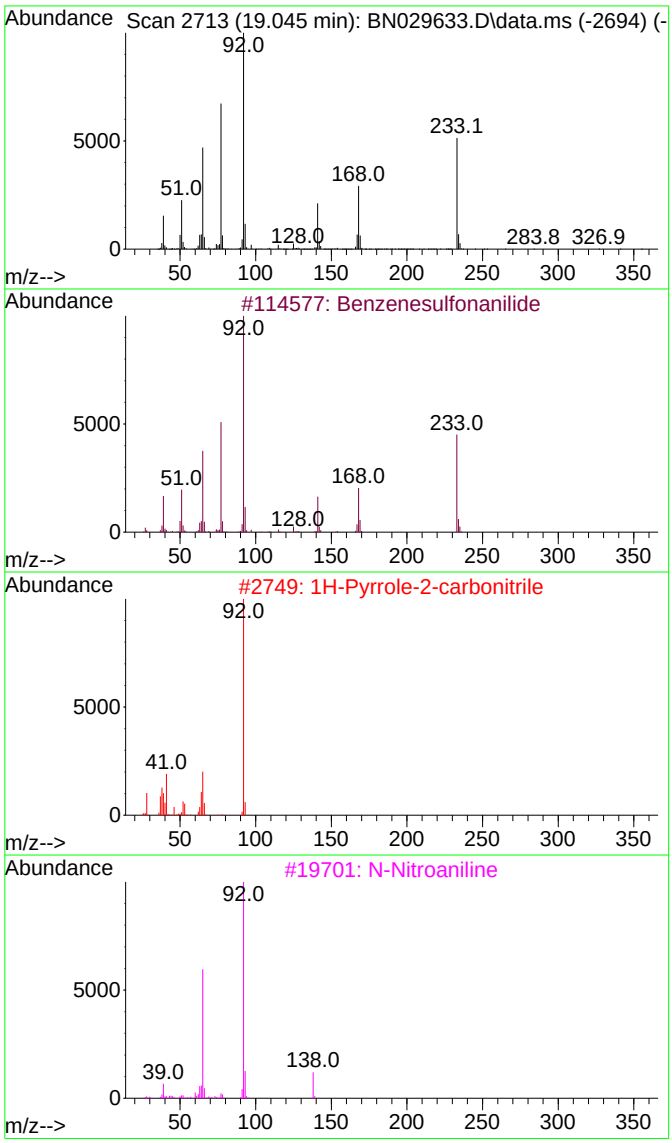
Quant Title : SVOA CALIBRATION

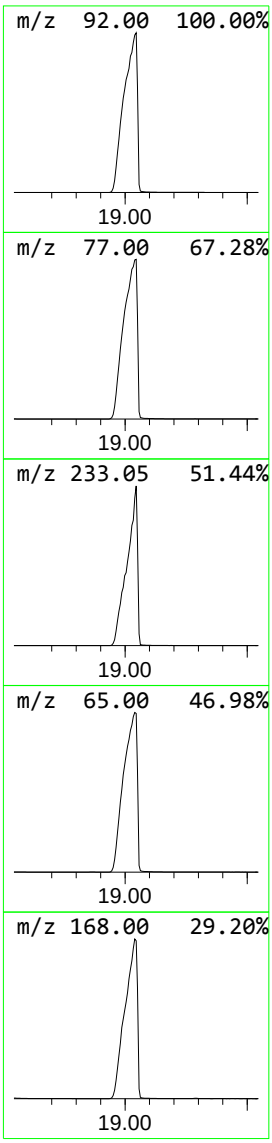
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Benzenesulfonanilide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.045	1027.47 ng/ul	98770000	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonanilide	233	C12H11NO2S	001678-25-7	99
2	1H-Pyrrole-2-carbonitrile	92	C5H4N2	009513-94-4	47
3	N-Nitroaniline	138	C6H6N2O2	000645-55-6	47
4	3-Picoline, 2-nitro-	138	C6H6N2O2	018368-73-5	47
5	Ethanone, 1-(2-chloro-10H-phenot...	381	C20H16ClN3OS	1000277-64-9	42





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

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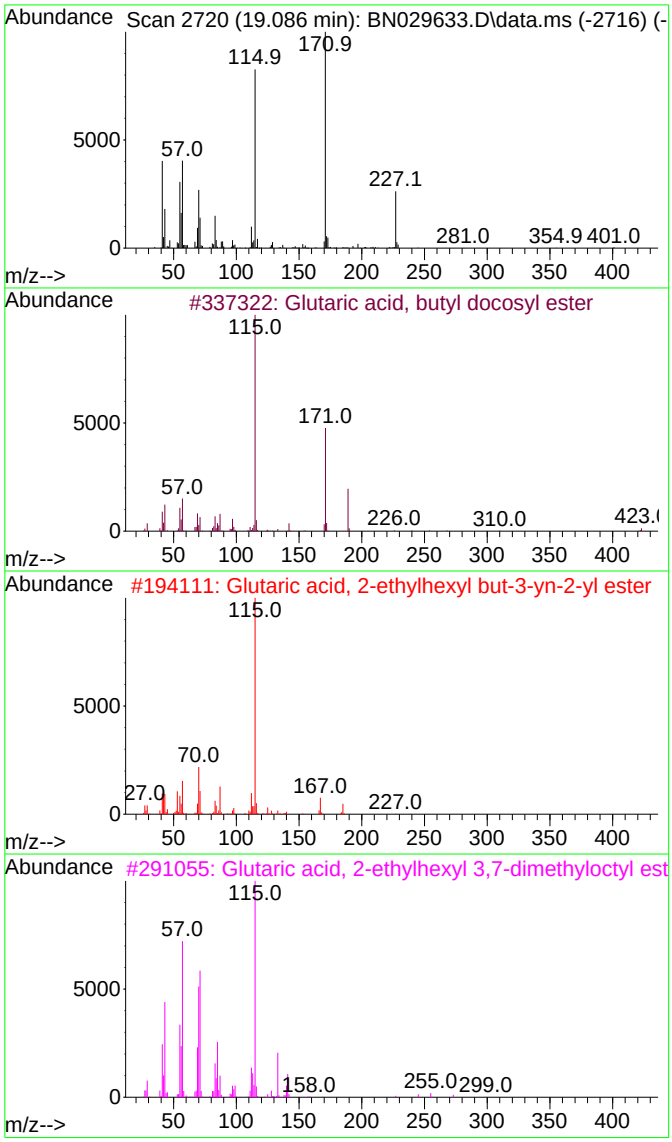
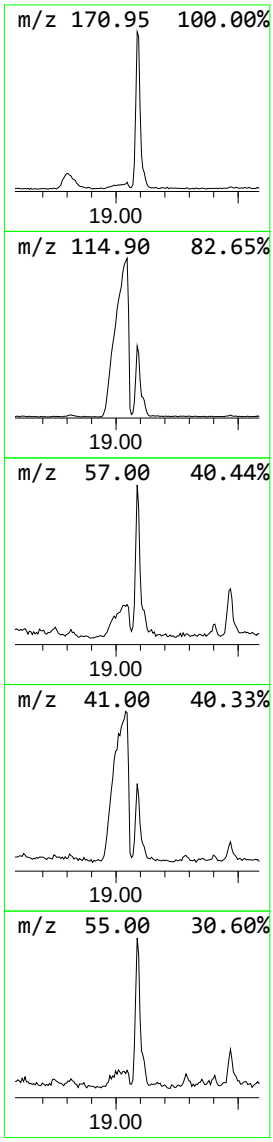
Peak Number 18 unknown-09 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.086	9.17 ng/ul	881612	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutaric acid, butyl docosyl ester	496	C31H60O4	1000359-69-9	43
2	Glutaric acid, 2-ethylhexyl but-...	296	C17H28O4	1000393-99-9	38
3	Glutaric acid, 2-ethylhexyl 3,7-...	384	C23H44O4	1000391-48-5	38
4	Ethylmalonic acid dibutyl ester	244	C13H24O4	001113-92-4	37
5	Glutaric acid, 2-nitro-4-chlorob...	427	C21H30ClNO6	1000377-05-4	35





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ALS Vial : 25 Sample Multiplier: 1

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ClientSampleId :
C0AH1

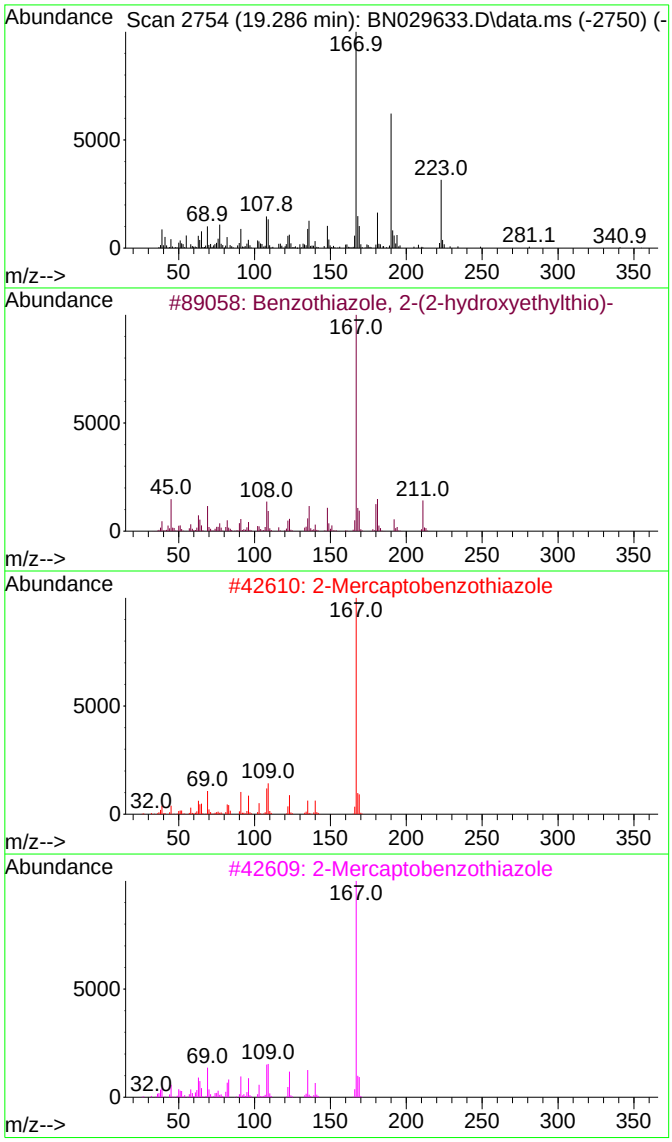
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

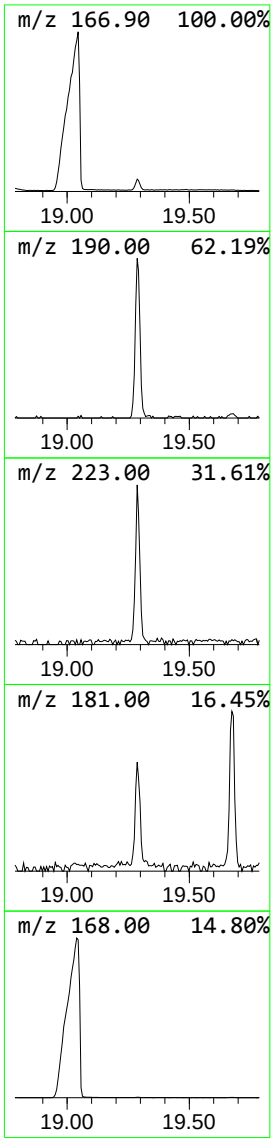
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Benzothiazole, 2-(2-hydroxy... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	2.33 ng/ul	223765	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole, 2-(2-hydroxyethyl...	211	C9H9NOS2	004665-63-8	58
2	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	50
3	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	43
4	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	43
5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	38





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Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

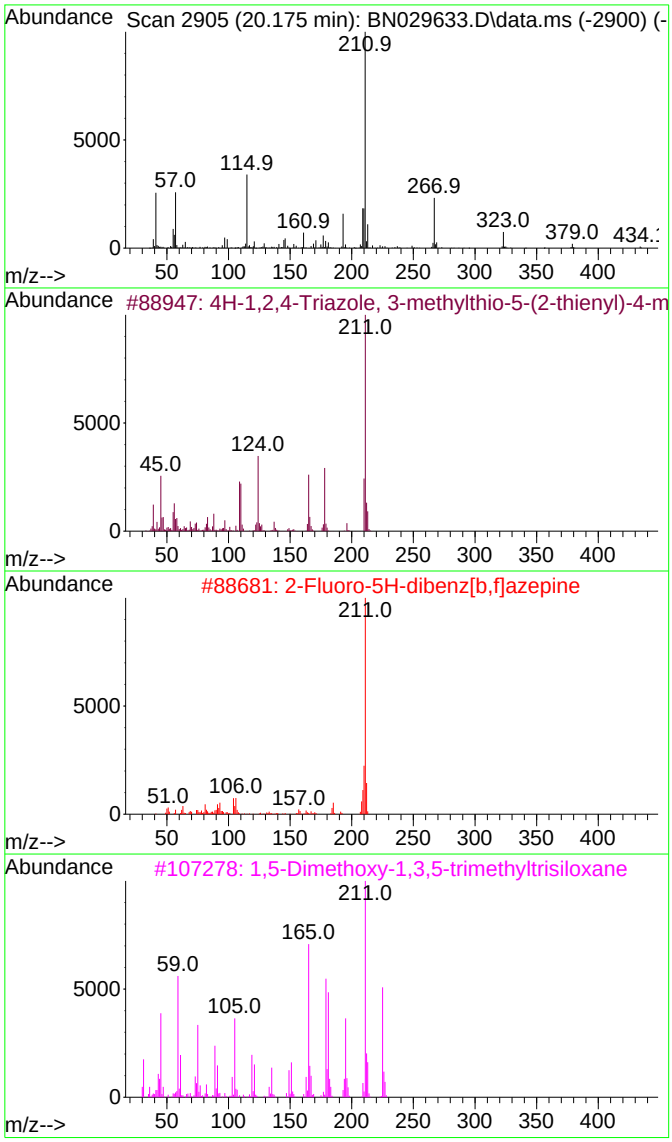
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

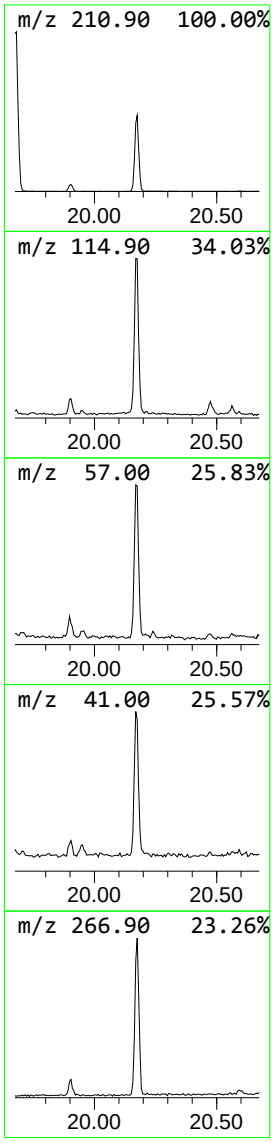
****

Peak Number 20 unknown-10 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.175	6.51 ng/ul	624861	Chrysene-d12	21.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,2,4-Triazole, 3-methylthio-...	211	C8H9N3S2	116850-51-2	37
2	2-Fluoro-5H-dibenz[b,f]azepine	211	C14H10FN	024986-53-6	25
3	1,5-Dimethoxy-1,3,5-trimethyltri...	226	C5H18O4Si3	1000245-86-1	17
4	Aspon	378	C12H28O5P2S2	003244-90-4	10
5	4-Amino-4'-hydroxystilbene	211	C14H13NO	000836-44-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

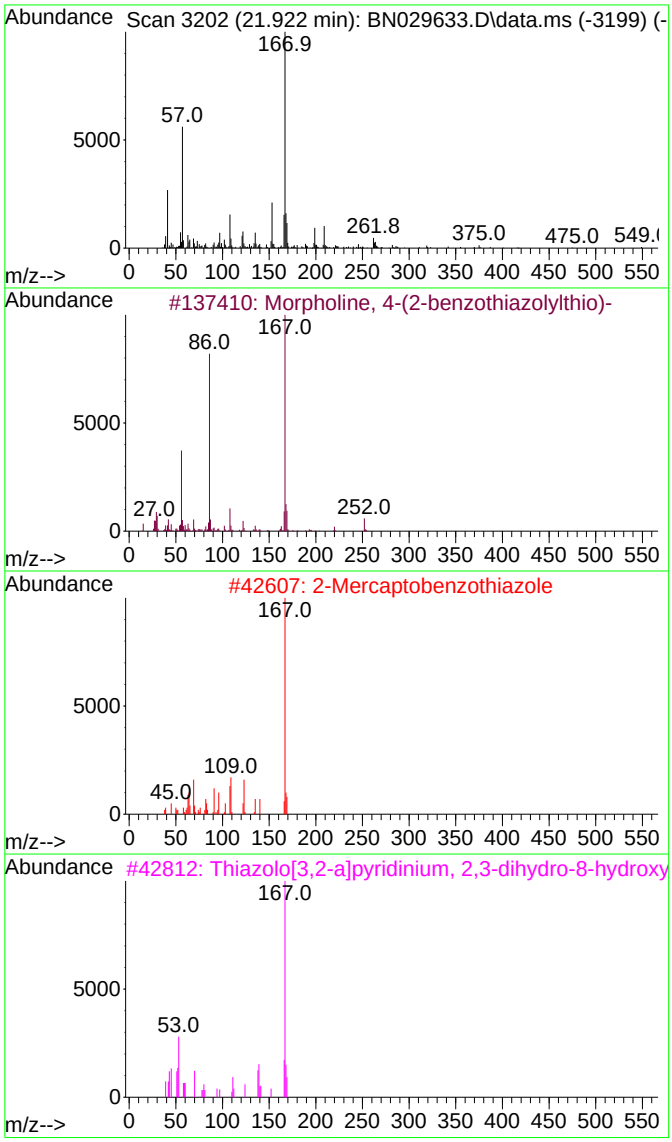
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

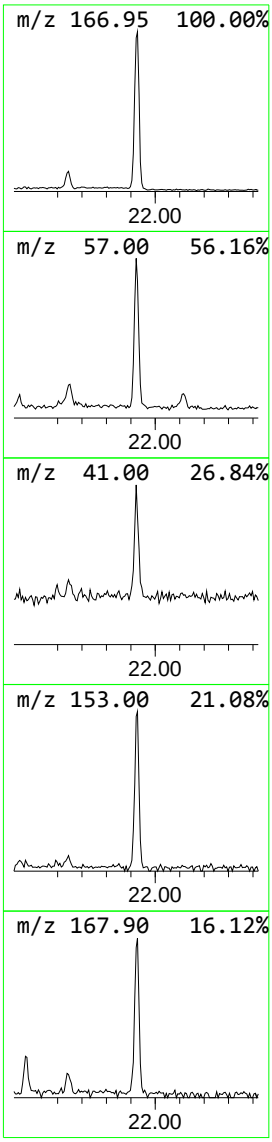
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 21 Morpholine, 4-(2-benzothiaz... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.922	2.60 ng/ul	249010	Chrysene-d12	21.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-(2-benzothiazolylt...	252	C11H12N2OS2	000102-77-2	53
2	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	50
3	Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	50
4	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	50
5	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020924\
Data File : BN029633.D
Acq On : 10 Feb 2024 05:33
Operator : MA/JU
Sample : P1398-17
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0AH1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Butanethiol	3.517	32.3	ng/ul	2044520	1	7.881	1264580	20.0
unknown-01	8.993	4.1	ng/ul	261982	1	7.881	1264580	20.0
Benzothiazole	11.334	67.8	ng/ul	5695510	2	10.681	1680700	20.0
unknown-02	14.587	9.7	ng/ul	847045	3	14.522	1750780	20.0
unknown-03	15.098	80.3	ng/ul	7025680	3	14.522	1750780	20.0
Diethyltoluamide	15.287	4.0	ng/ul	346966	3	14.522	1750780	20.0
2-(Methylmercap...	15.740	2.8	ng/ul	243422	3	14.522	1750780	20.0
Glutaric acid, ...	16.022	2.6	ng/ul	253092	4	17.275	1922590	20.0
2(3H)-Benzothia...	16.245	71.6	ng/ul	6879820	4	17.275	1922590	20.0
unknown-04	17.081	11.3	ng/ul	1082000	4	17.275	1922590	20.0
unknown-05	17.139	21.7	ng/ul	2086600	4	17.275	1922590	20.0
unknown-06	17.192	10.3	ng/ul	986411	4	17.275	1922590	20.0
unknown-07	17.592	143.3	ng/ul	13775500	4	17.275	1922590	20.0
unknown-08	17.875	16.1	ng/ul	1544070	4	17.275	1922590	20.0
n-Hexadecanoic ...	18.186	2.7	ng/ul	260570	4	17.275	1922590	20.0
2-Mercaptobenzo...	18.516	24.1	ng/ul	2321930	4	17.275	1922590	20.0
Benzenesulfonan...	19.045	1027.5	ng/ul	98770000	4	17.275	1922590	20.0
unknown-09	19.086	9.2	ng/ul	881612	4	17.275	1922590	20.0
Benzothiazole, ...	19.286	2.3	ng/ul	223765	4	17.275	1922590	20.0
unknown-10	20.175	6.5	ng/ul	624861	5	21.474	1918880	20.0
Morpholine, 4-(...	21.922	2.6	ng/ul	249010	5	21.474	1918880	20.0