LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031424\
Data File : BG060644.D
Acq On : 14 Mar 2024 18:36
Operator : MA/JU
Sample : P1747-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-01-DUP

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.809	405	412	424	rBV	864795	1408358	17.83%	4.170%
2	7.430	681	688	697	rBV	550000	953413	12.07%	2.823%
3	8.323	832	840	848	rVB	372103	635271	8.04%	1.881%
4	9.522	1036	1044	1052	rBV	1369162	2422800	30.67%	7.174%
5	11.167	1316	1324	1335	rBV	540511	972862	12.31%	2.881%
6	12.413	1529	1536	1545	rBV	147147	241621	3.06%	0.715%
7	13.570	1726	1733	1741	rVB	3848965	6143470	77.76%	18.192%
8	14.945	1960	1967	1974	rBV	880878	1387889	17.57%	4.110%
9	15.127	1993	1998	2006	rBV	164879	232254	2.94%	0.688%
10	15.656	2081	2088	2095	rBV	430463	633270	8.02%	1.875%
11	16.155	2167	2173	2180	rBV	661798	982151	12.43%	2.908%
12	16.431	2213	2220	2228	rVB	2640951	3988985	50.49%	11.812%
13	17.695	2427	2435	2446	rVB	1117634	1675836	21.21%	4.962%
14	17.853	2455	2462	2472	rBV2	158194	242971	3.08%	0.719%
15	18.511	2569	2574	2586	rBV2	108464	178202	2.26%	0.528%
16	19.769	2784	2788	2794	rBV	85617	121272	1.54%	0.359%
17	20.274	2867	2874	2881	rBV	5924862	7900327	100.00%	23.394%
18	21.567	3089	3094	3100	rBV3	61109	102753	1.30%	0.304%
19	22.007	3162	3169	3186	rVB2	897679	1657278	20.98%	4.908%
20	23.071	3344	3350	3357	rBV2	101220	173731	2.20%	0.514%
21	25.562	3761	3774	3786	rBV	553867	1715458	21.71%	5.080%

Sum of corrected areas: 33770172

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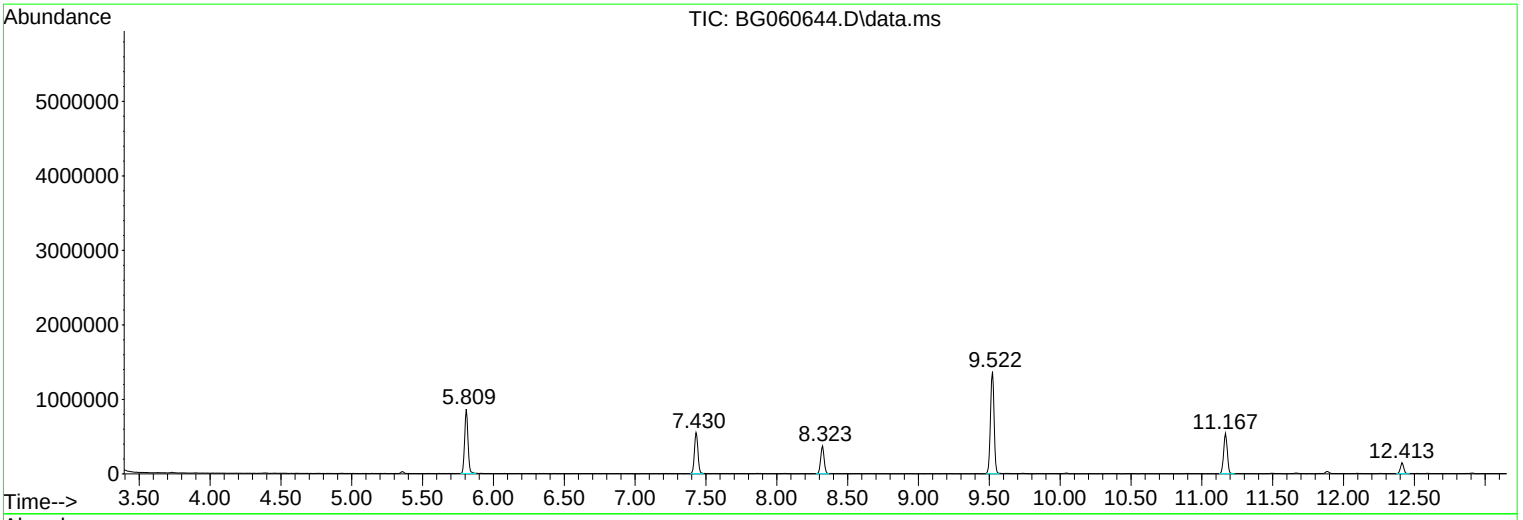
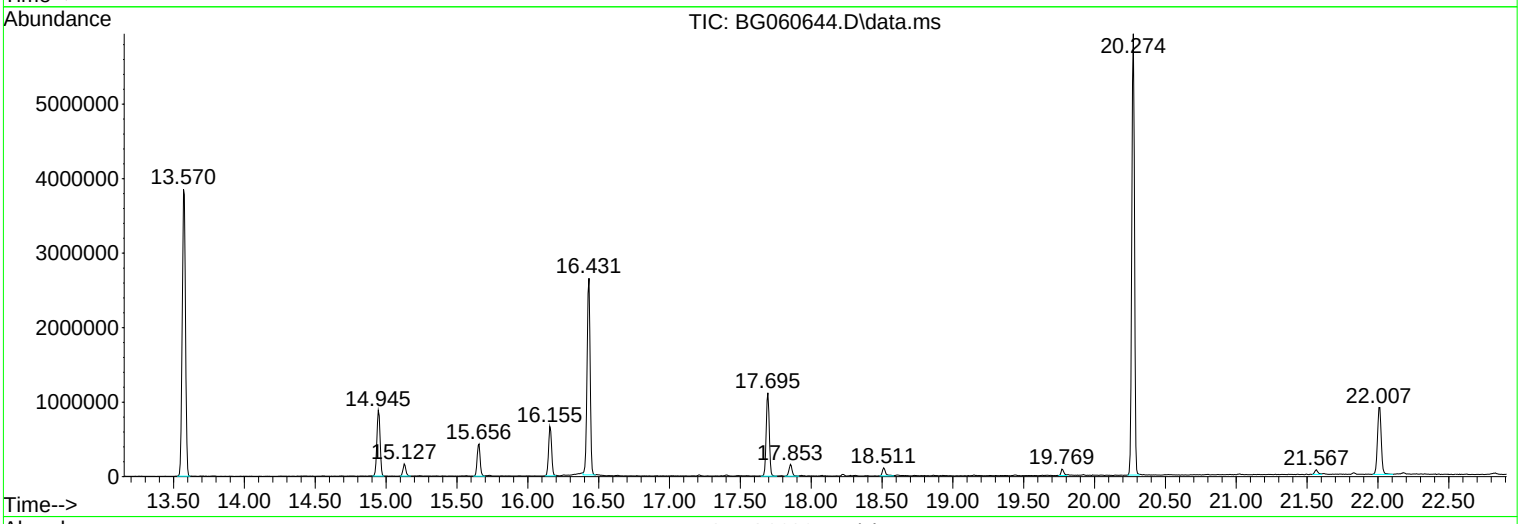
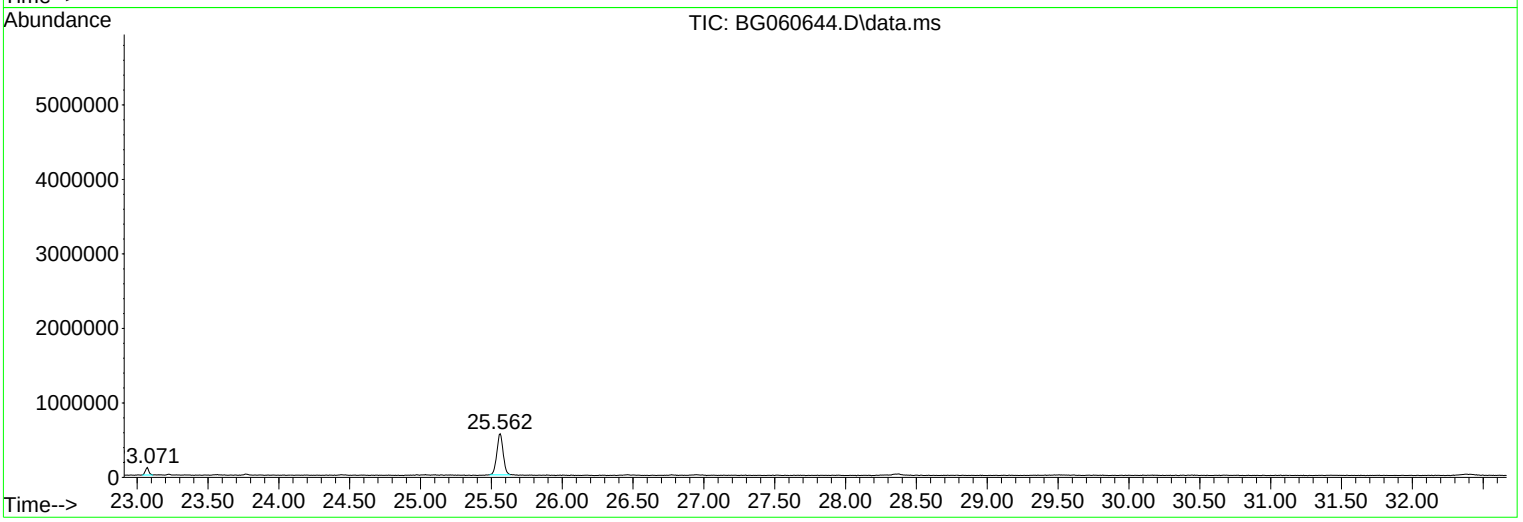
Instrument :
BNA_G
ClientSampleId :
MW-01-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BG060644.D
Acq On : 14 Mar 2024 18:36
Operator : MA/JU
Sample : P1747-02
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

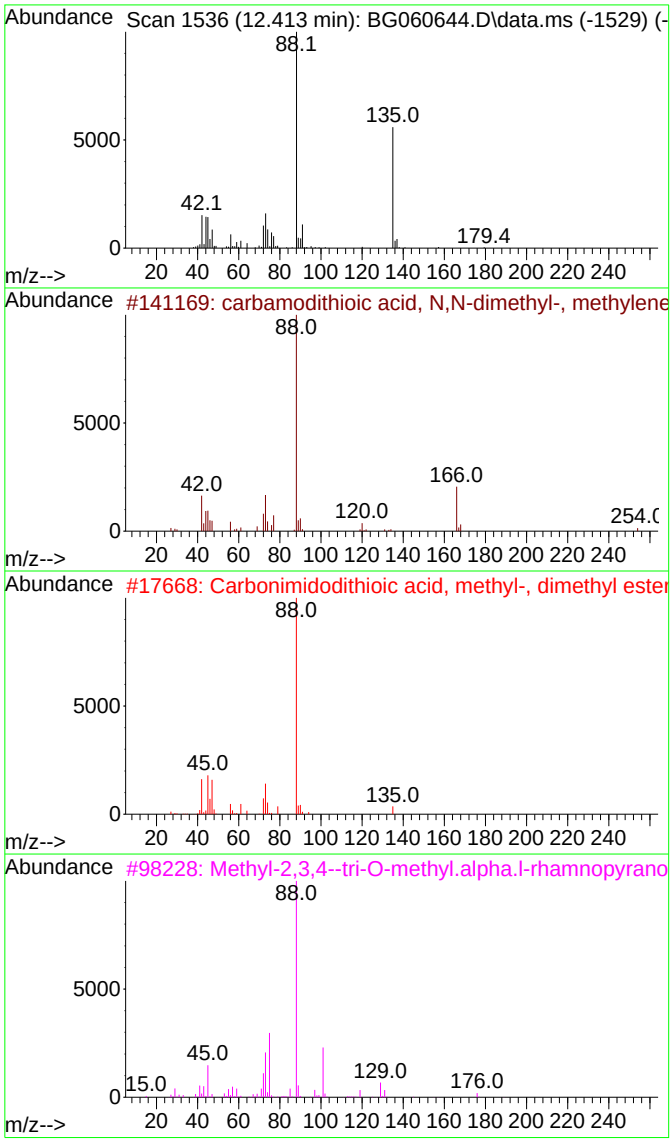
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

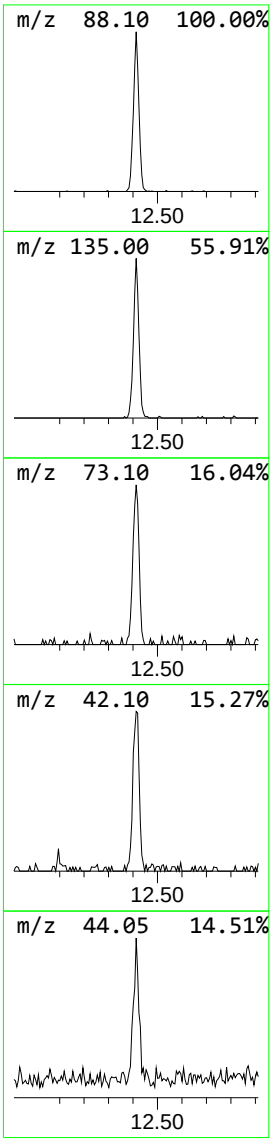
****

Peak Number 1 unknown12.413 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.413	4.97 ng	241621	Naphthalene-d8	11.167

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	carbamodithioic acid, N,N-dimeth...	254	C7H14N2S4	1000401-44-5	47
2	Carbonimidodithioic acid, methyl...	135	C4H9NS2	018805-25-9	40
3	Methyl-2,3,4--tri-O-methyl.alpha...	220	C10H20O5	003253-23-4	38
4	Dithiocarbamic acid, N,N-dimethy...	164	C5H12N2S2	002801-22-1	37
5	Methyl 4-O-acetyl-2,3-di-O-methy...	248	C11H20O6	072945-56-3	32





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Sample : P1747-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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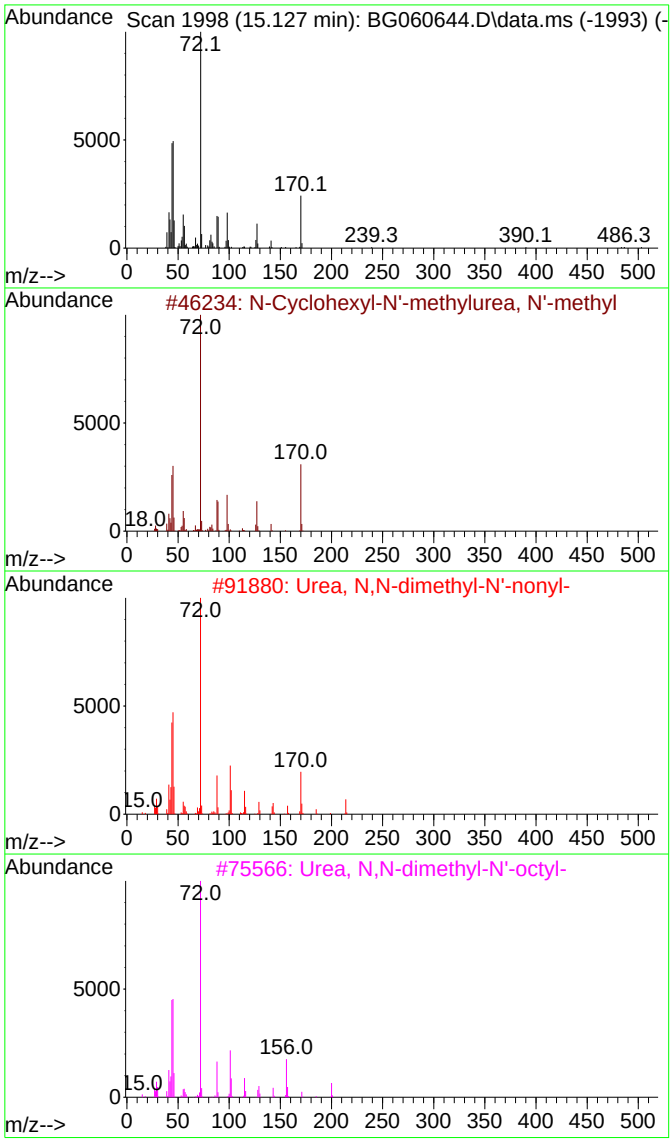
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

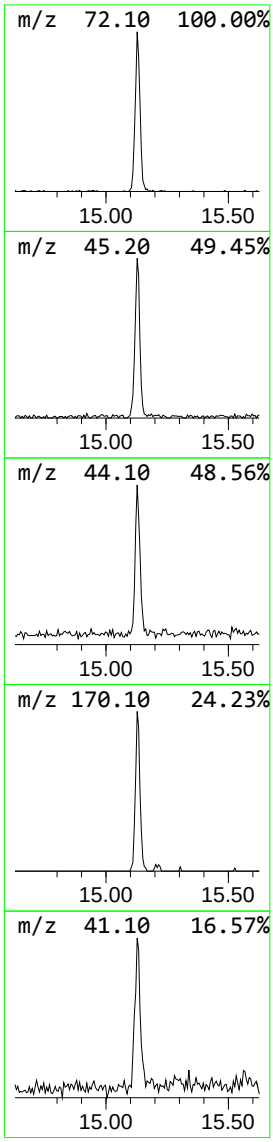
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 N-Cyclohexyl-N'-methylurea,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	3.35 ng	232254	Acenaphthene-d10	14.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Cyclohexyl-N'-methylurea, N'-m...	170	C9H18N2O	031468-12-9	91
2	Urea, N,N-dimethyl-N'-nonyl-	214	C12H26N2O	1000419-88-7	72
3	Urea, N,N-dimethyl-N'-octyl-	200	C11H24N2O	1000419-88-6	59
4	Urea, N,N-dimethyl-N'-pentyl-	158	C8H18N2O	1000419-88-1	59
5	Urea, N,N-dimethyl-N'-hexyl-	172	C9H20N2O	1000419-88-3	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031424\
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Sample : P1747-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-01-DUP

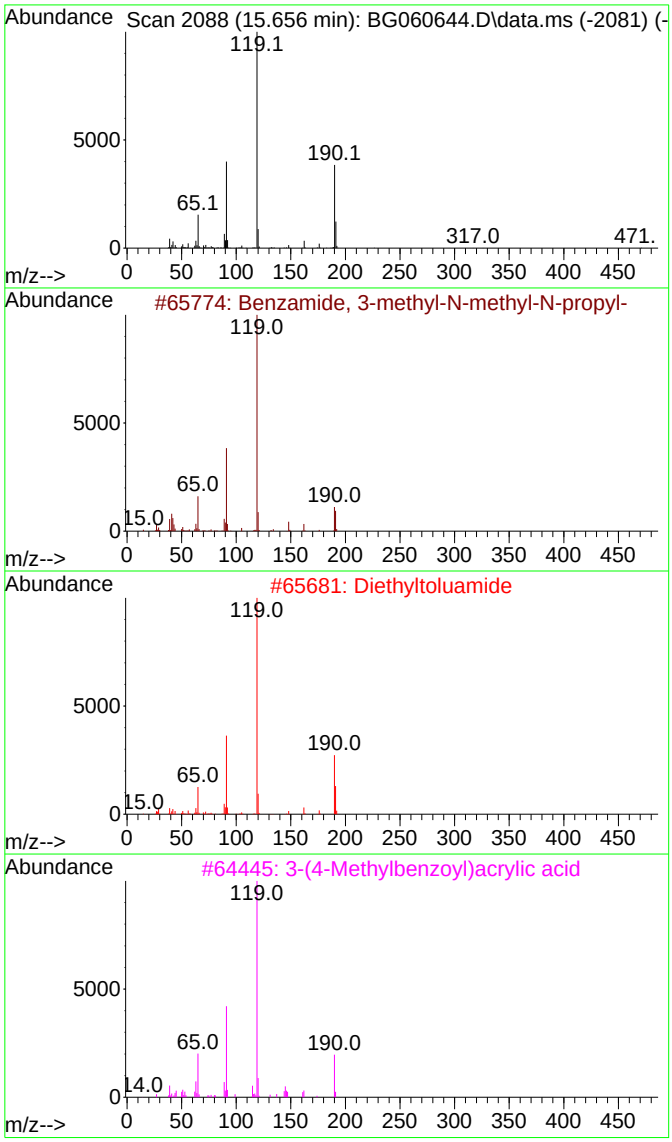
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

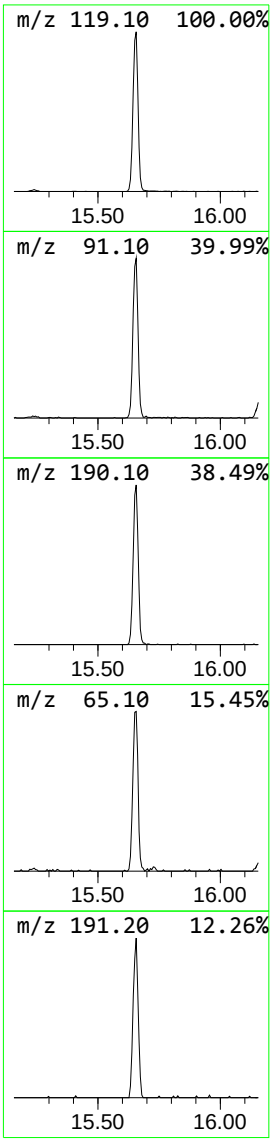
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzamide, 3-methyl-N-methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	9.13 ng	633270	Acenaphthene-d10	14.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	93
2	Diethyltoluamide	191	C12H17NO	000134-62-3	91
3	3-(4-Methylbenzoyl)acrylic acid	190	C11H10O3	020972-36-5	78
4	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	64
5	Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	64





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Sample : P1747-02
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-01-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

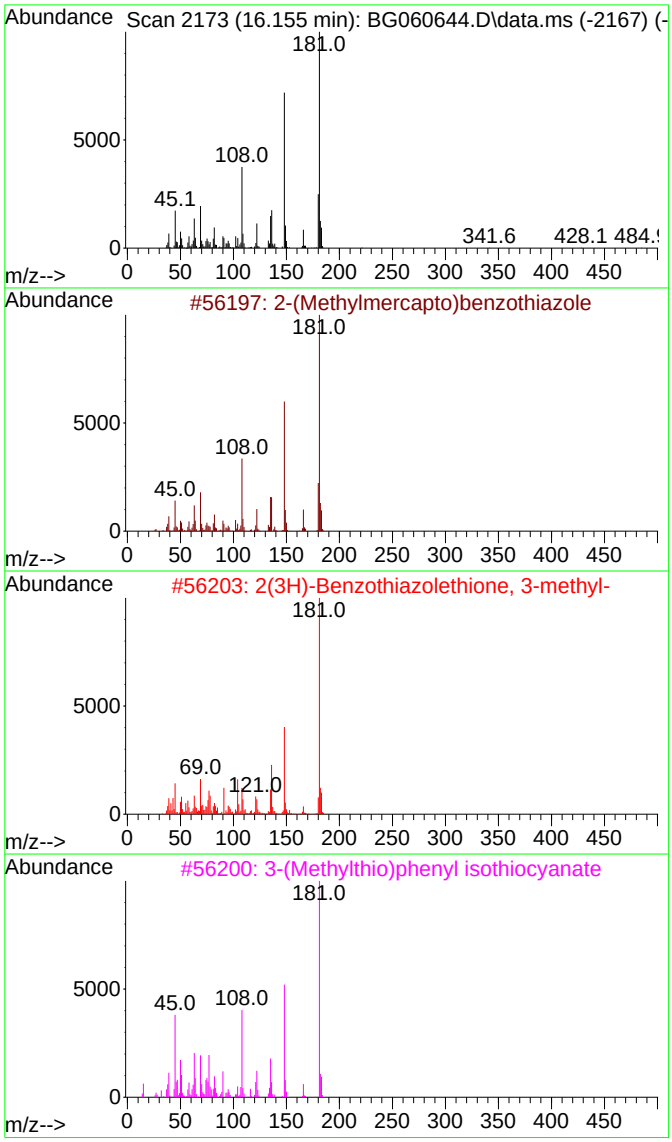
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

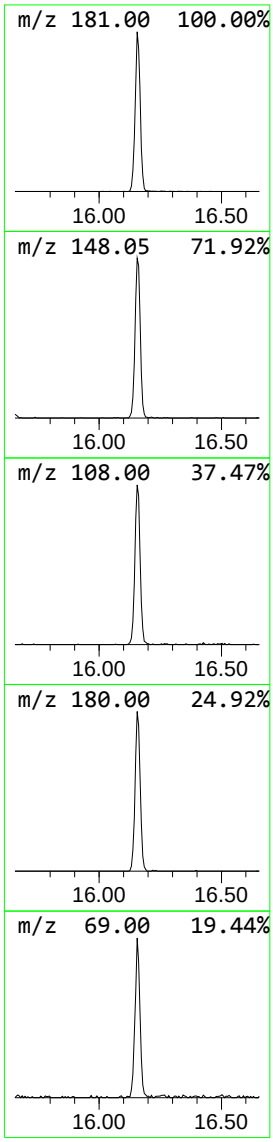
****

Peak Number 4 2-(Methylmercapto)benzothia... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.155	14.15 ng	982151	Acenaphthene-d10	14.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	99
2	2(3H)-Benzothiazolethione, 3-met...	181	C8H7NS2	002254-94-6	83
3	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	83
4	2-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-75-6	74
5	4-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	015863-41-9	60





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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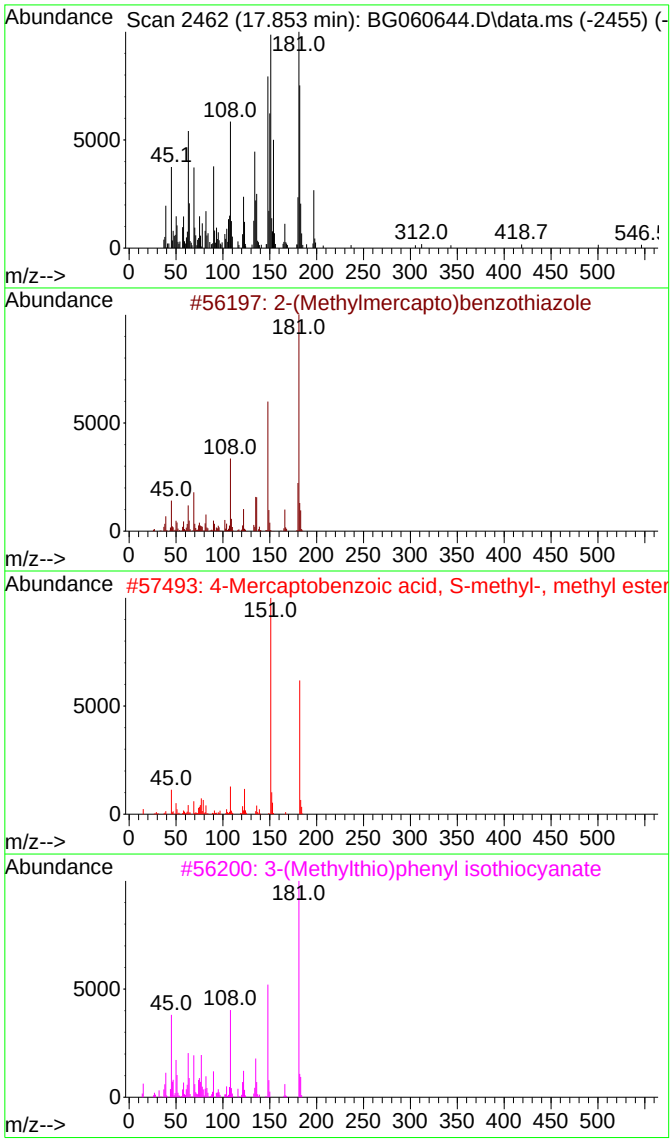
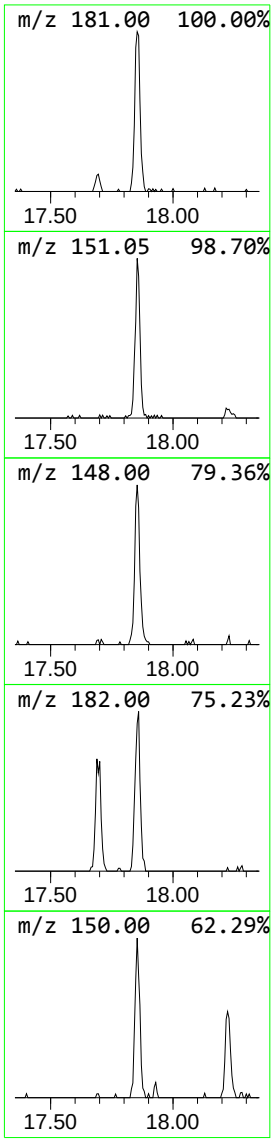
****

Peak Number 5 unknown17.853 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.853	2.90 ng	242971	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	47
2	4-Mercaptobenzoic acid, S-methyl...	182	C9H10O2S	003795-79-7	25
3	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	18
4	Benzoic acid, 4-(methylamino)-	151	C8H9NO2	010541-83-0	15
5	2,6-Pyridinedimethanol, 4-(dimet...	182	C9H14N2O2	001882-25-3	14





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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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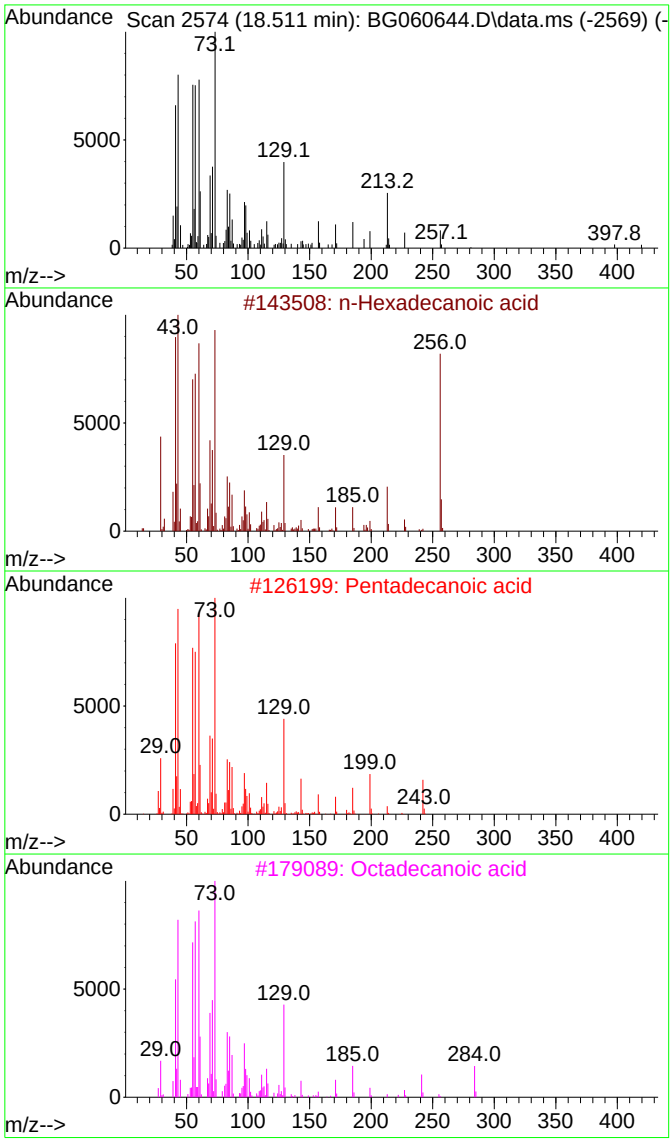
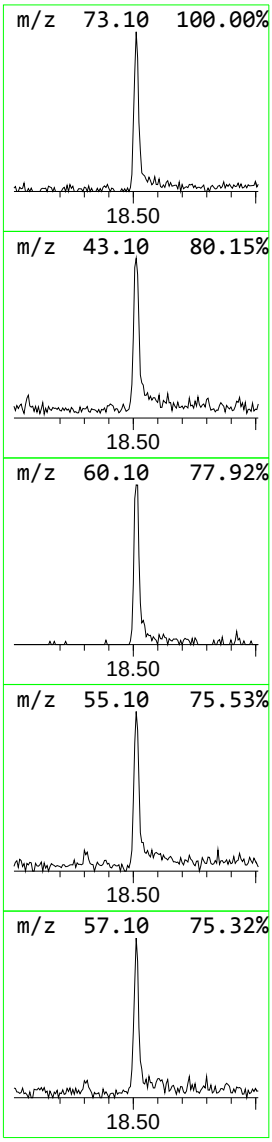
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	2.13 ng	178202	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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ClientSampleId :
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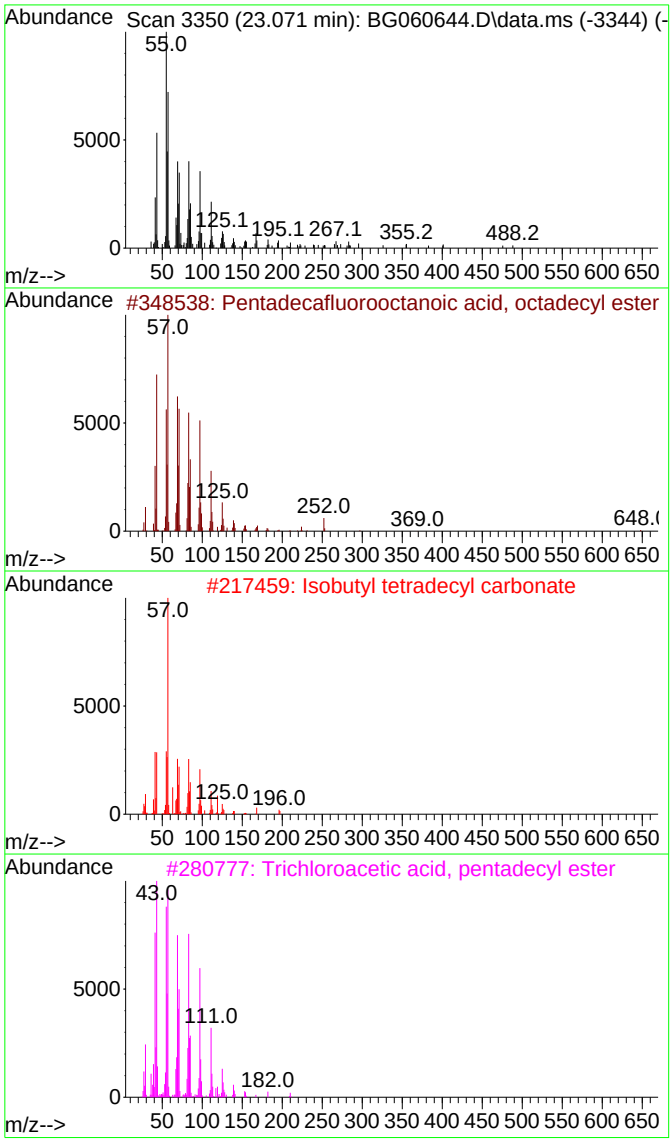
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

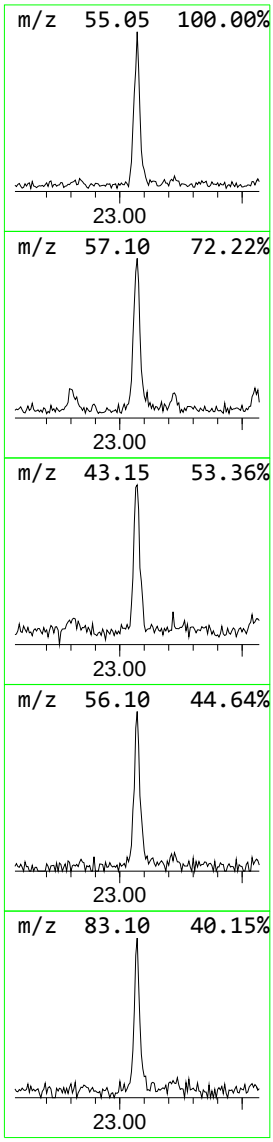
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.071	2.10 ng	173731	Chrysene-d12	22.007

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	87
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
4	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	74
5	Cyclooctacosane	392	C28H56	000297-24-5	72





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown12.413	12.413	5.0	ng	241621	2	11.167	972862	20.0
N-Cyclohexyl-N'...	15.127	3.4	ng	232254	3	14.945	1387890	20.0
Benzamide, 3-me...	15.656	9.1	ng	633270	3	14.945	1387890	20.0
2-(Methylmercap...	16.155	14.2	ng	982151	3	14.945	1387890	20.0
unknown17.853	17.853	2.9	ng	242971	4	17.695	1675840	20.0
n-Hexadecanoic ...	18.511	2.1	ng	178202	4	17.695	1675840	20.0
Pentadecafluoro...	23.071	2.1	ng	173731	5	22.007	1657280	20.0