LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031424\
Data File : BG060643.D
Acq On : 14 Mar 2024 17:55
Operator : MA/JU
Sample : P1747-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-01

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: BG060643.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.807	404	412	427	rBV	840914	1394459	19.43%	4.489%
2	7.429	681	688	699	rVB	524911	920712	12.83%	2.964%
3	8.322	832	840	847	rBV	341418	586206	8.17%	1.887%
4	9.521	1035	1044	1054	rBV	1270493	2239680	31.21%	7.210%
5	11.166	1314	1324	1336	rBV	496366	893648	12.45%	2.877%
6	12.411	1527	1536	1545	rBV	121785	213427	2.97%	0.687%
7	13.575	1726	1734	1741	rBV	3671433	5647904	78.70%	18.181%
8	14.950	1961	1968	1977	rVB	801712	1255460	17.49%	4.041%
9	15.126	1993	1998	2008	rBV	137849	214347	2.99%	0.690%
10	15.655	2080	2088	2095	rBV	391624	554852	7.73%	1.786%
11	16.154	2167	2173	2181	rBV	560632	858322	11.96%	2.763%
12	16.430	2212	2220	2227	rBV	2508290	3911560	54.51%	12.591%
13	17.693	2428	2435	2444	rBV	988205	1489926	20.76%	4.796%
14	17.852	2457	2462	2469	rBV3	136262	207687	2.89%	0.669%
15	18.510	2569	2574	2586	rBV	100477	163388	2.28%	0.526%
16	19.773	2785	2789	2795	rBV3	57317	85987	1.20%	0.277%
17	20.273	2867	2874	2880	rBV	5440632	7176501	100.00%	23.101%
18	21.565	3088	3094	3099	rBV5	56902	103184	1.44%	0.332%
19	22.012	3163	3170	3181	rBV	834641	1453325	20.25%	4.678%
20	23.070	3344	3350	3359	rBV2	95228	176927	2.47%	0.570%
21	25.561	3763	3774	3790	rVB2	474590	1517648	21.15%	4.885%

Sum of corrected areas: 31065150

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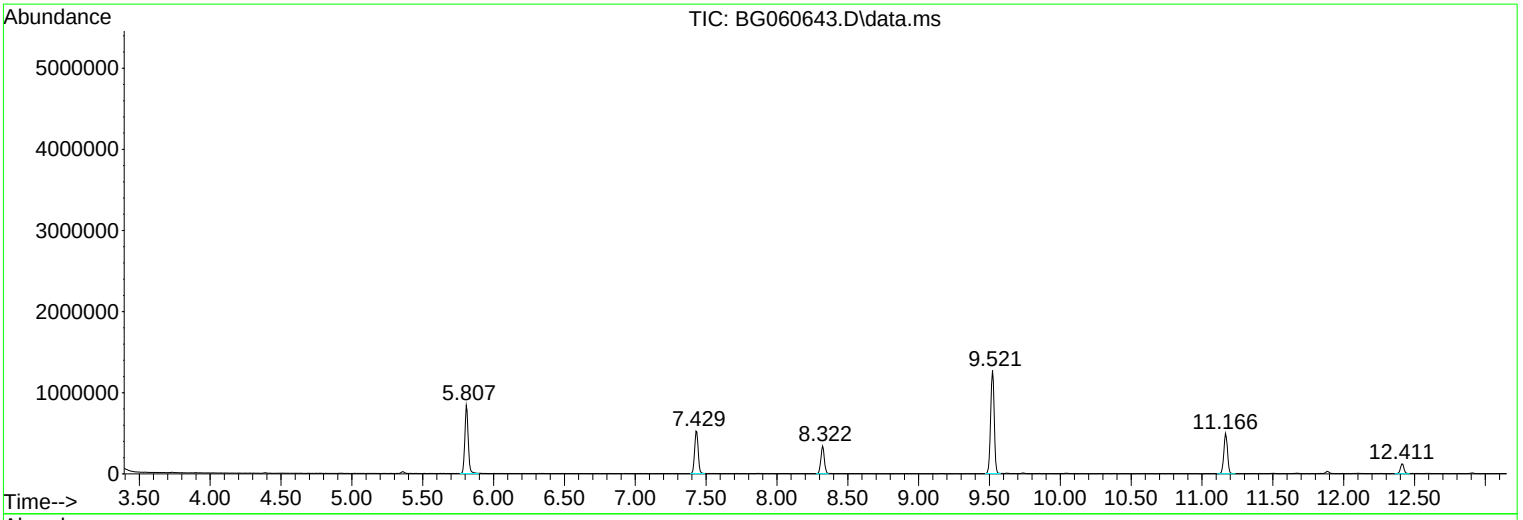
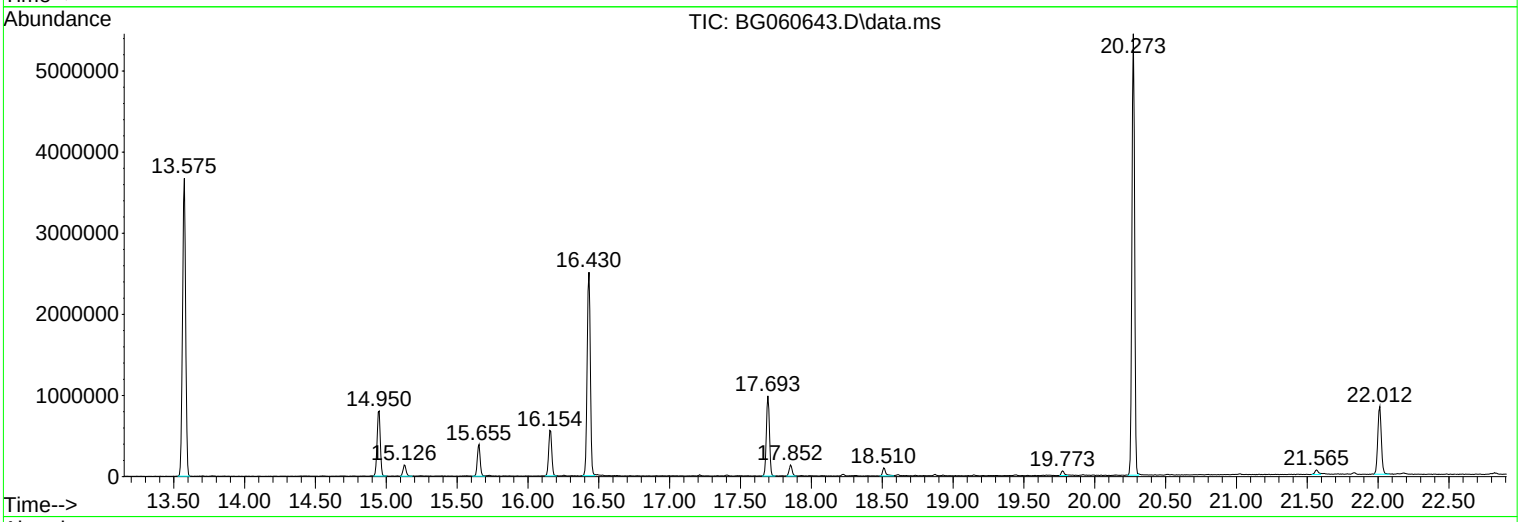
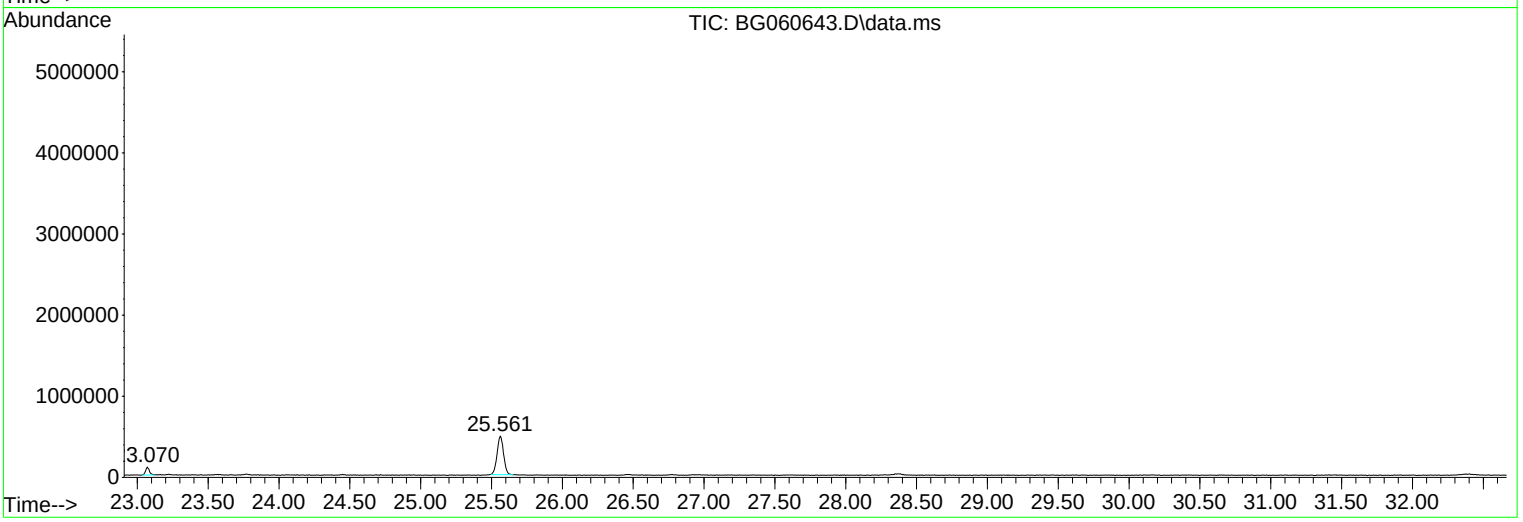
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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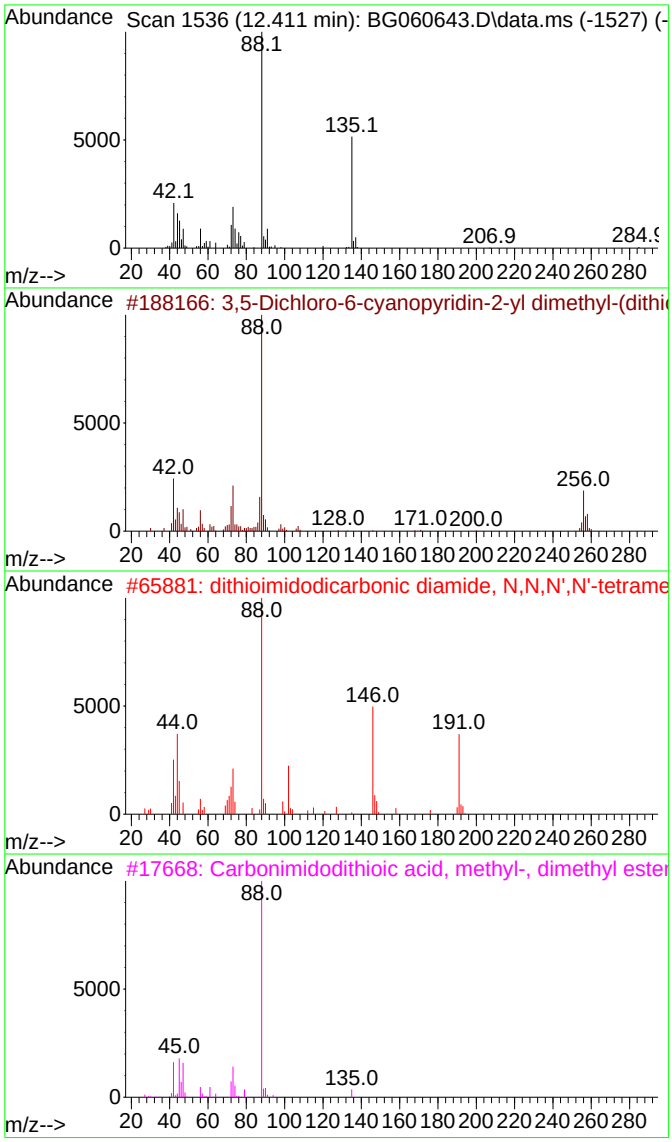
TIC Integration Parameters: LSCINT.P

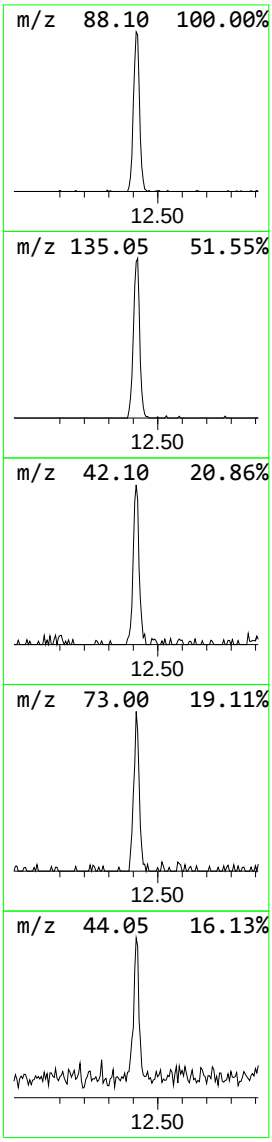
****

Peak Number 1 3,5-Dichloro-6-cyanopyridin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.411	4.78 ng	213427	Naphthalene-d8	11.166

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dichloro-6-cyanopyridin-2-yl...	291	C9H7Cl2N3S2	1000305-58-3	59
2	dithioimidodicarbonic diamide, N...	191	C6H13N3S2	1000400-23-8	53
3	Carbonimidodithioic acid, methyl...	135	C4H9NS2	018805-25-9	53
4	Bis(dimethylthiocarbamyl) sulfide	208	C6H12N2S3	000097-74-5	50
5	Methyl(methyl-4-deoxy-2-O-methyl...	218	C9H14O6	052545-23-0	43





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Sample : P1747-01
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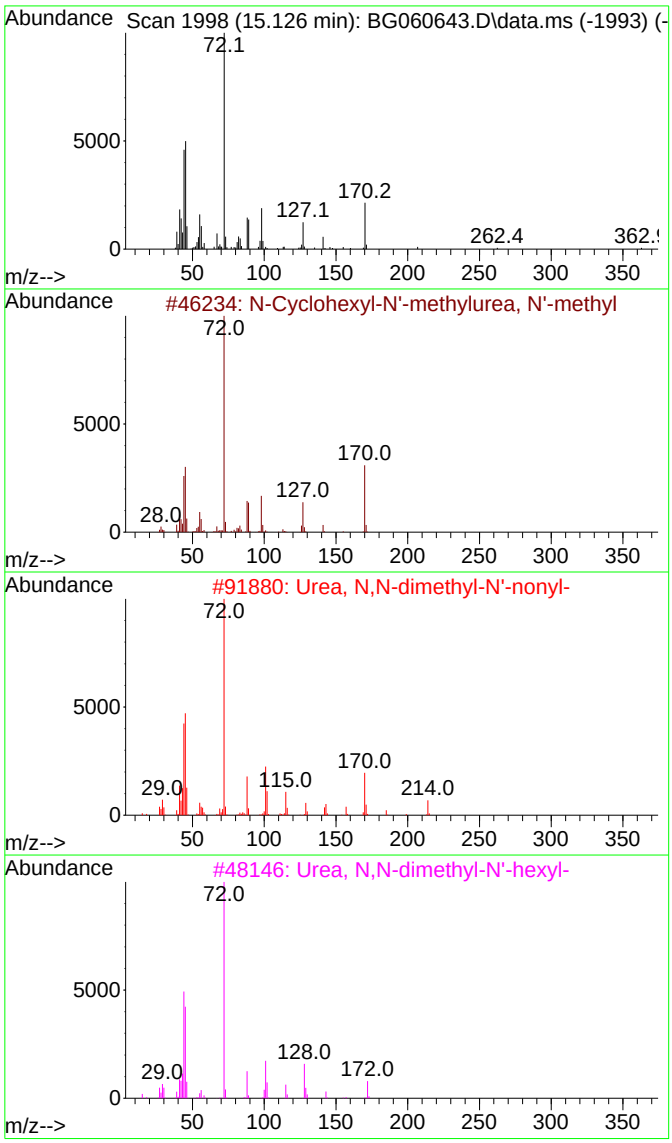
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

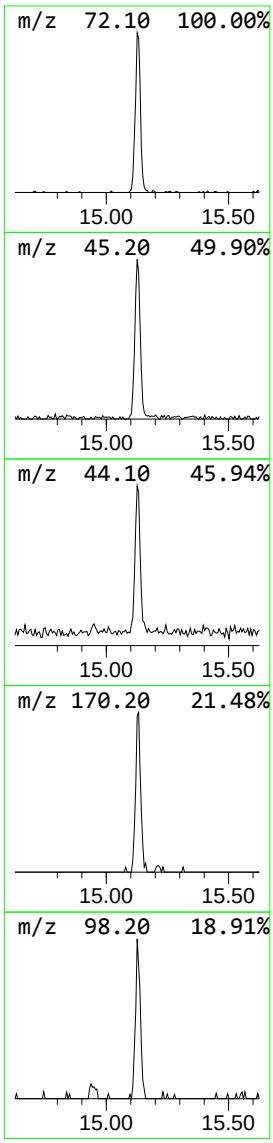
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.126	3.41 ng	214347	Acenaphthene-d10	14.950

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Cyclohexyl-N'-methylurea, N'-m...	170	C9H18N2O	031468-12-9	94
2	Urea, N,N-dimethyl-N'-nonyl-	214	C12H26N2O	1000419-88-7	72
3	Urea, N,N-dimethyl-N'-hexyl-	172	C9H20N2O	1000419-88-3	59
4	Urea, N,N-dimethyl-N'-octyl-	200	C11H24N2O	1000419-88-6	59
5	Urea, N,N-dimethyl-N'-pentyl-	158	C8H18N2O	1000419-88-1	59





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Sample : P1747-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-01

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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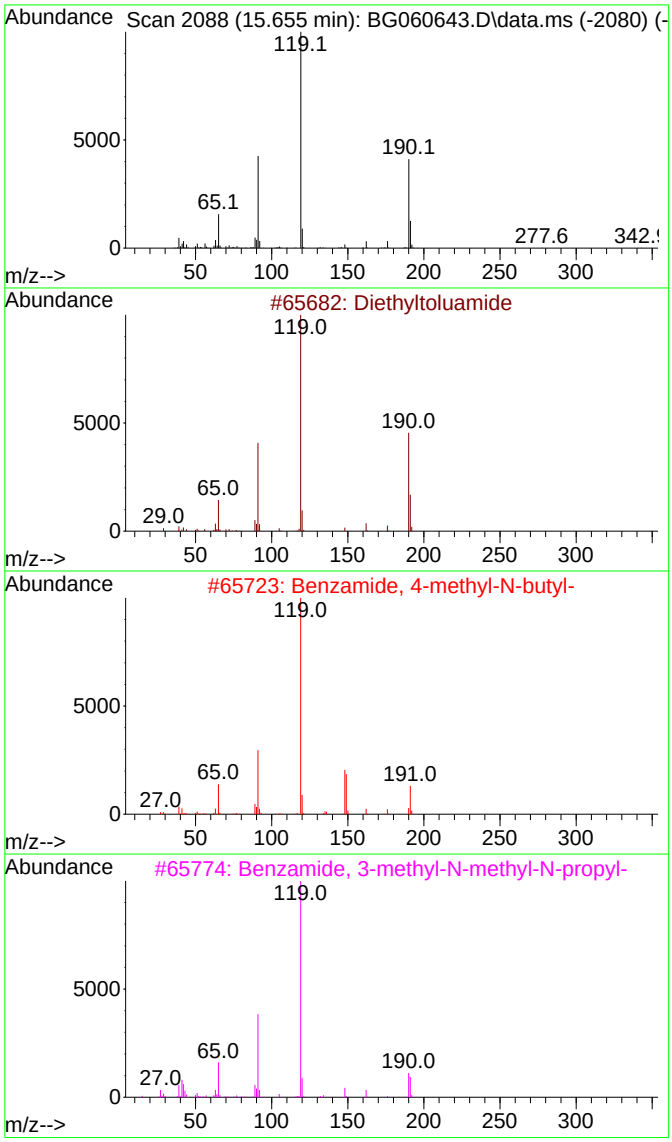
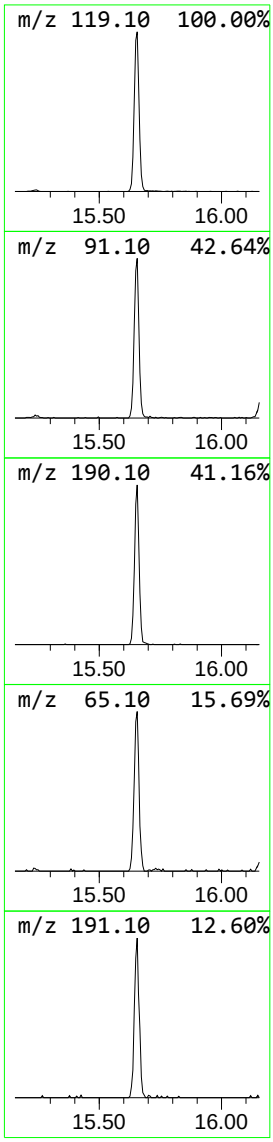
****

Peak Number 3 Diethyltoluamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.655	8.84 ng	554852	Acenaphthene-d10	14.950

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	76
3	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	76
4	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76
5	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	76





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Sample : P1747-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
MW-01

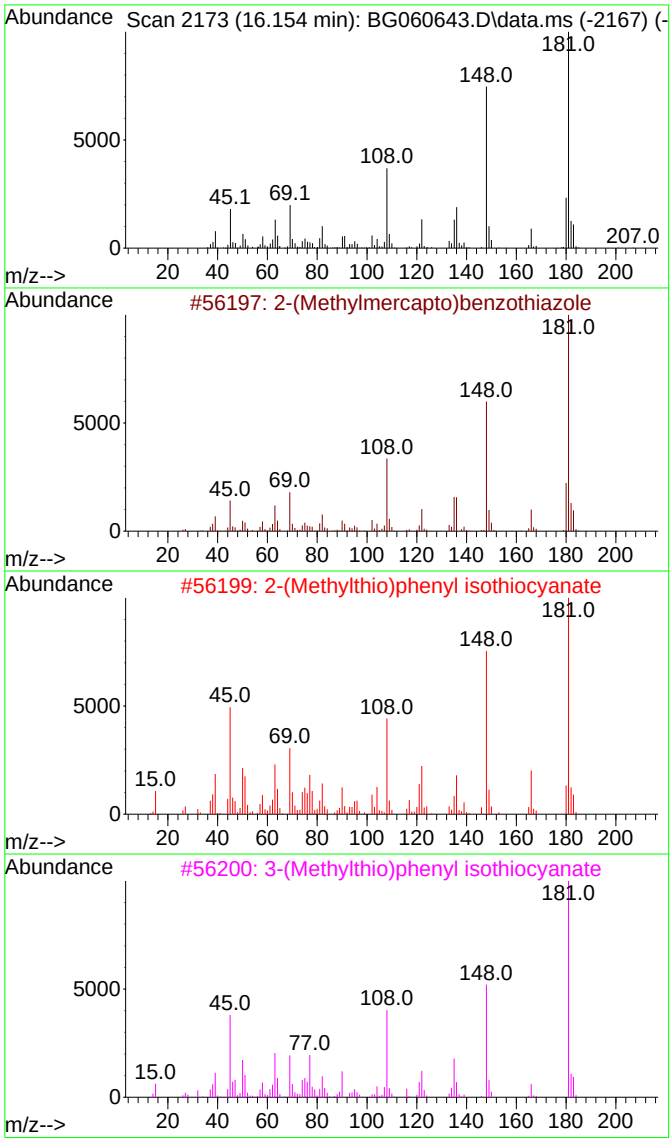
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

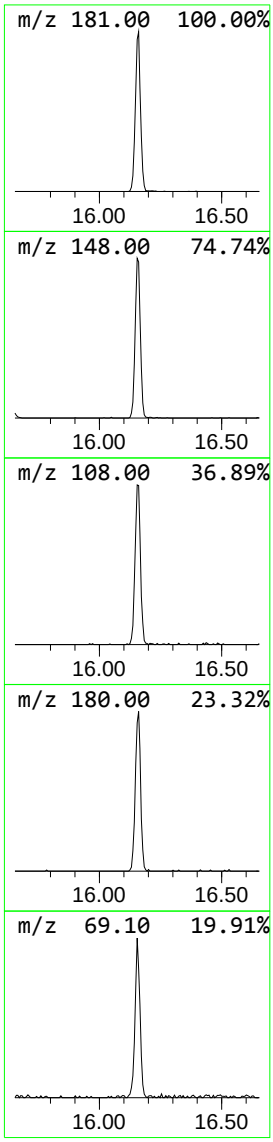
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.154	13.67 ng	858322	Acenaphthene-d10	14.950

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	99
2	2-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-75-6	80
3	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	68
4	2(3H)-Benzothiazolethione, 3-met...	181	C8H7NS2	002254-94-6	58
5	4-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	015863-41-9	50





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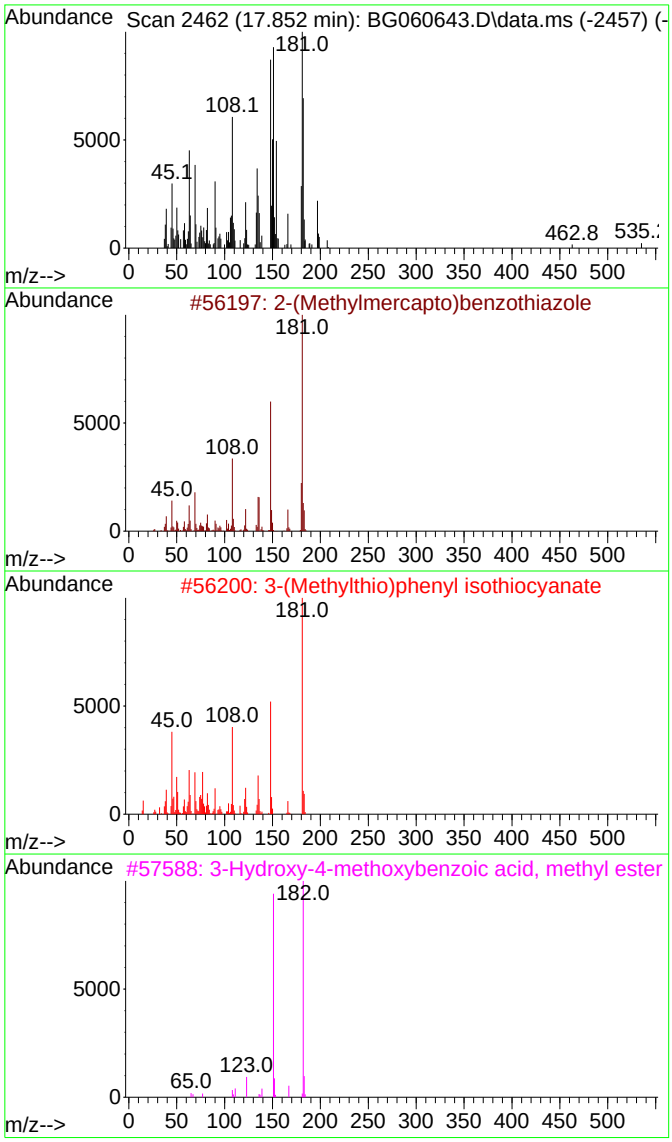
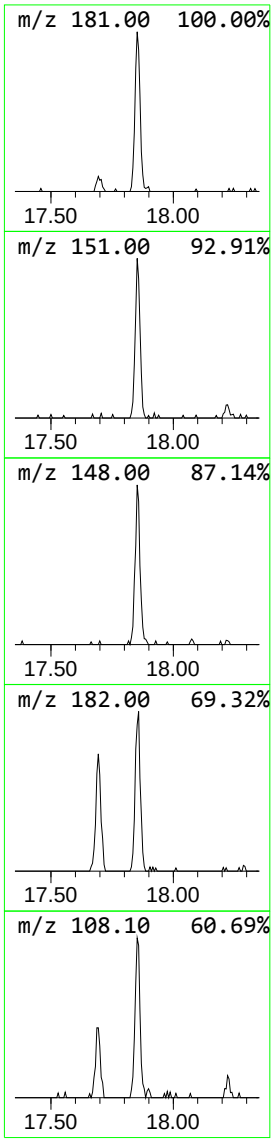
Peak Number 5 unknown17.582 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.852	2.79 ng	207687	Phenanthrene-d10	17.694

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	50
2	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	30
3	3-Hydroxy-4-methoxybenzoic acid,...	182	C9H10O4	006702-50-7	18
4	3-Mercaptobenzoic acid, S-methyl...	182	C9H10O2S	090721-40-7	15
5	Benzoic acid, 4-(methylamino)-	151	C8H9NO2	010541-83-0	15





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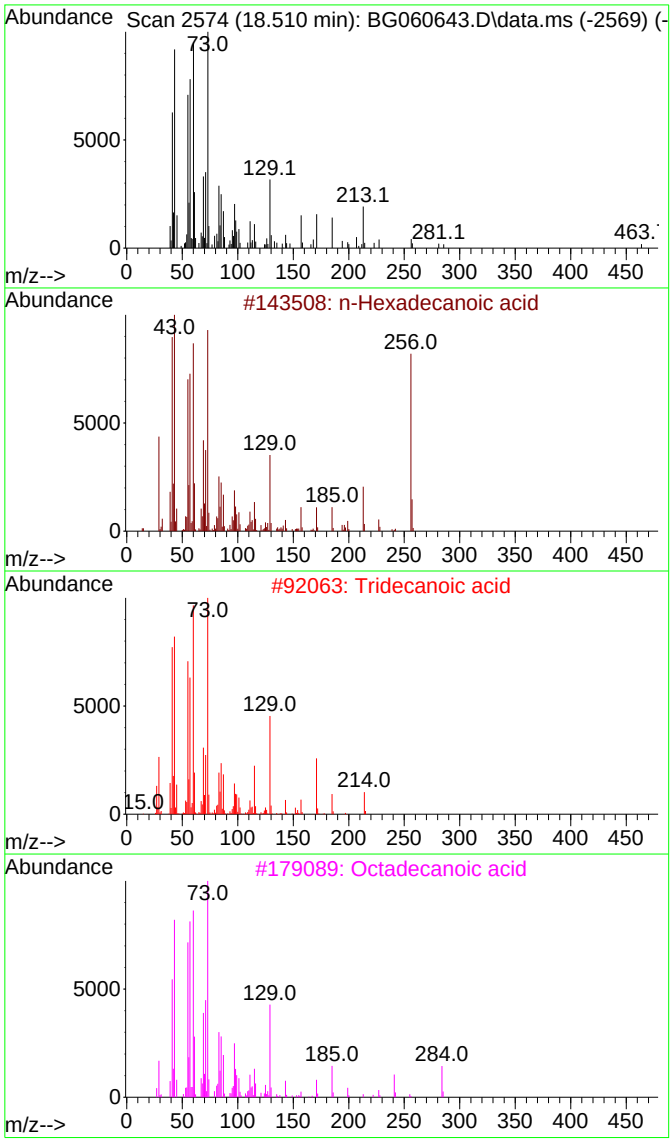
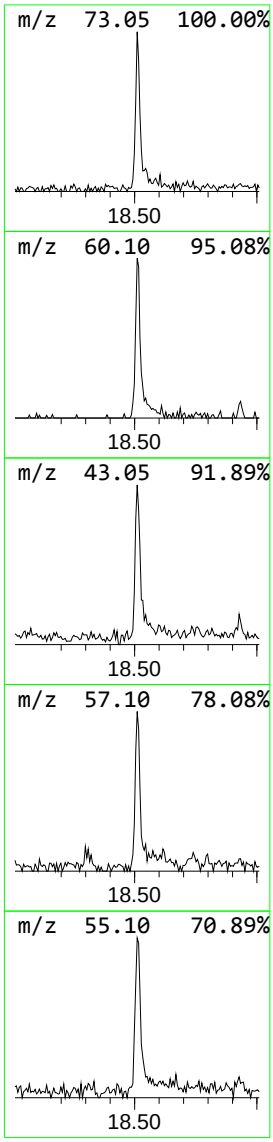
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.510	2.19 ng	163388	Phenanthrene-d10	17.694

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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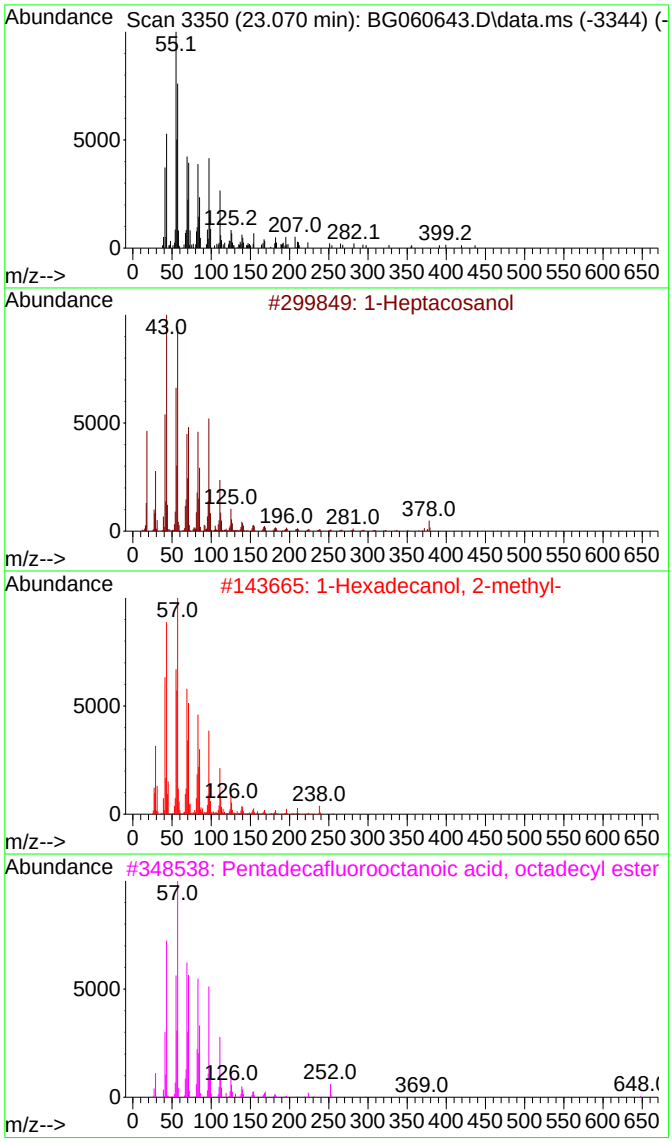
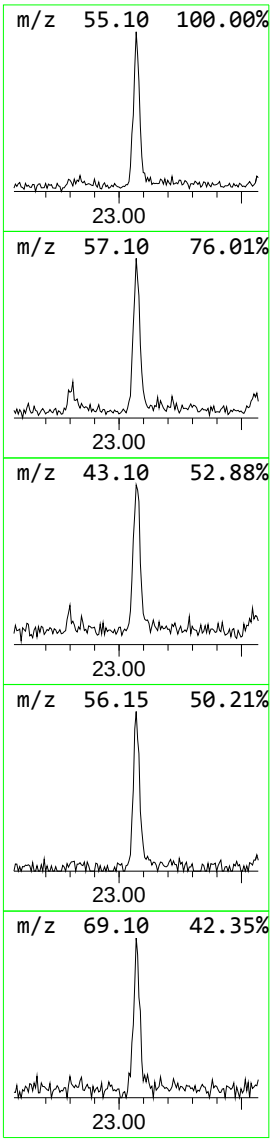
Peak Number 7 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.070	2.43 ng	176927	Chrysene-d12	22.012

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	83
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	74
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	74
4	Behenic alcohol	326	C22H46O	000661-19-8	72
5	17-Pentatriacontene	491	C35H70	006971-40-0	72





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3,5-Dichloro-6-...	12.411	4.8	ng	213427	2	11.166	893648	20.0
N-Cyclohexyl-N'...	15.126	3.4	ng	214347	3	14.950	1255460	20.0
Diethyltoluamide	15.655	8.8	ng	554852	3	14.950	1255460	20.0
2-(Methylmercap...	16.154	13.7	ng	858322	3	14.950	1255460	20.0
unknown17.582	17.852	2.8	ng	207687	4	17.694	1489930	20.0
n-Hexadecanoic ...	18.510	2.2	ng	163388	4	17.694	1489930	20.0
1-Heptacosanol	23.070	2.4	ng	176927	5	22.012	1453330	20.0