LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
Data File : BG021144.D
Acq On : 28 Feb 2016 10:03
Operator : UM/SJ
Sample : H1558-17
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-19

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:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.084	37	42	62	rVV	1209815	1665622	100.00%	25.342%
2	3.231	62	67	76	rVB	15553	29574	1.78%	0.450%
3	5.258	405	412	421	rVB	51575	79253	4.76%	1.206%
4	5.722	484	491	498	rVB	229933	365559	21.95%	5.562%
5	7.315	754	762	771	rBV	254439	433592	26.03%	6.597%
6	7.697	820	827	834	rBB	241857	405159	24.32%	6.164%
7	8.167	900	907	915	rBB	34777	56327	3.38%	0.857%
8	8.490	955	962	969	rBB	156377	265723	15.95%	4.043%
9	9.330	1097	1105	1113	rBB	158074	272075	16.33%	4.140%
10	10.975	1378	1385	1392	rBB	53401	91673	5.50%	1.395%
11	13.402	1791	1798	1804	rBV	386307	581550	34.91%	8.848%
12	14.218	1931	1937	1944	rBB	52291	75522	4.53%	1.149%
13	14.771	2025	2031	2039	rVB2	87562	133735	8.03%	2.035%
14	15.593	2167	2171	2176	rVB	16805	20652	1.24%	0.314%
15	16.251	2272	2283	2290	rBV	337565	508159	30.51%	7.732%
16	16.451	2312	2317	2320	rBV	16622	22008	1.32%	0.335%
17	17.503	2490	2496	2503	rBV2	112987	165049	9.91%	2.511%
18	18.372	2640	2644	2650	rBV2	35252	47903	2.88%	0.729%
19	20.094	2931	2937	2943	rBV	694455	880415	52.86%	13.395%
20	20.764	3044	3051	3056	rBV	19333	24743	1.49%	0.376%
21	21.386	3153	3157	3164	rBV	35035	53711	3.22%	0.817%
22	21.768	3215	3222	3230	rVB	112684	183615	11.02%	2.794%
23	23.255	3469	3475	3485	rBV2	14677	30861	1.85%	0.470%
24	23.478	3507	3513	3521	rVB4	9741	19120	1.15%	0.291%
25	25.047	3770	3780	3790	rBV2	59579	160888	9.66%	2.448%

Sum of corrected areas: 6572488

LSC Report - Integrated Chromatogram

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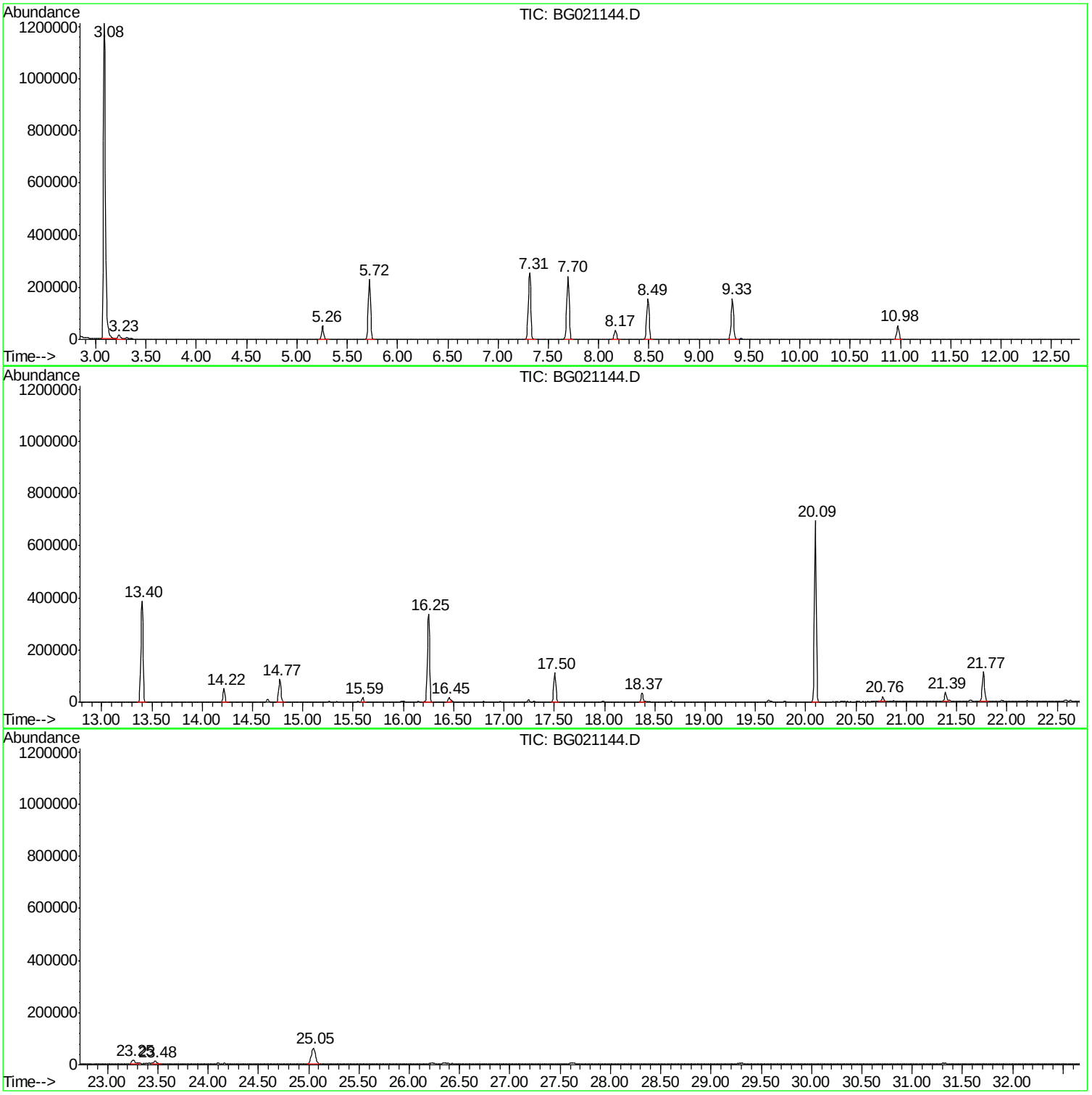
ClientSampleId : S-19

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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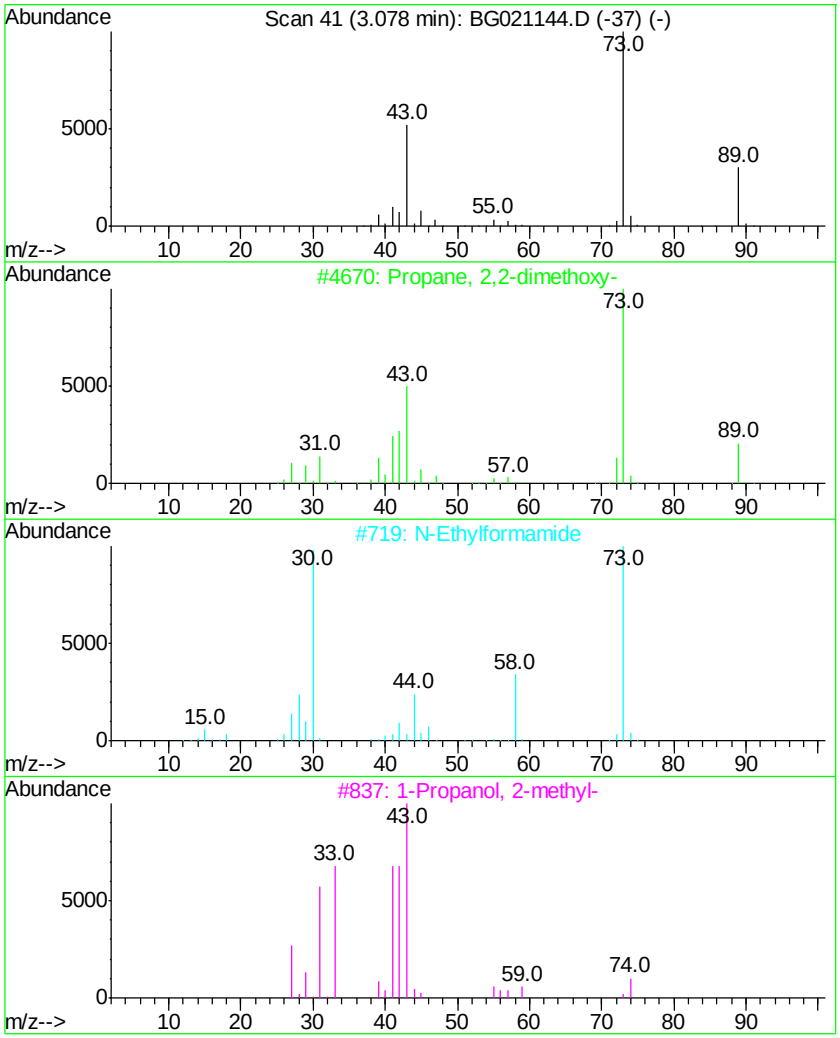
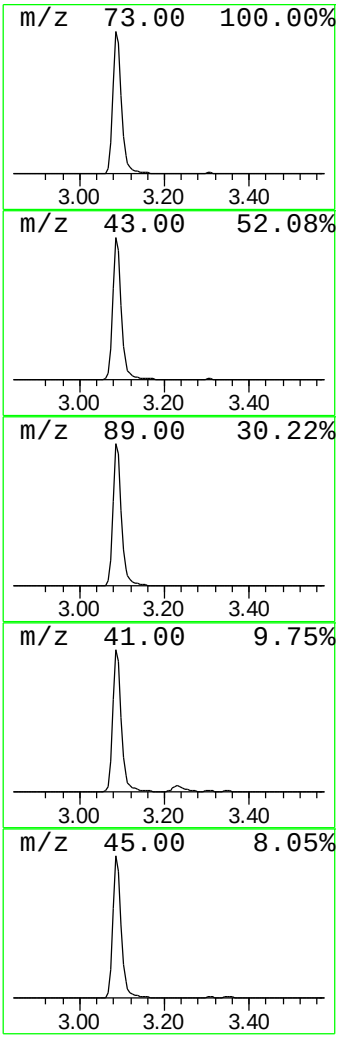
Peak Number 1 unknown3.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.08	591.41 ng	1665620	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : S-19

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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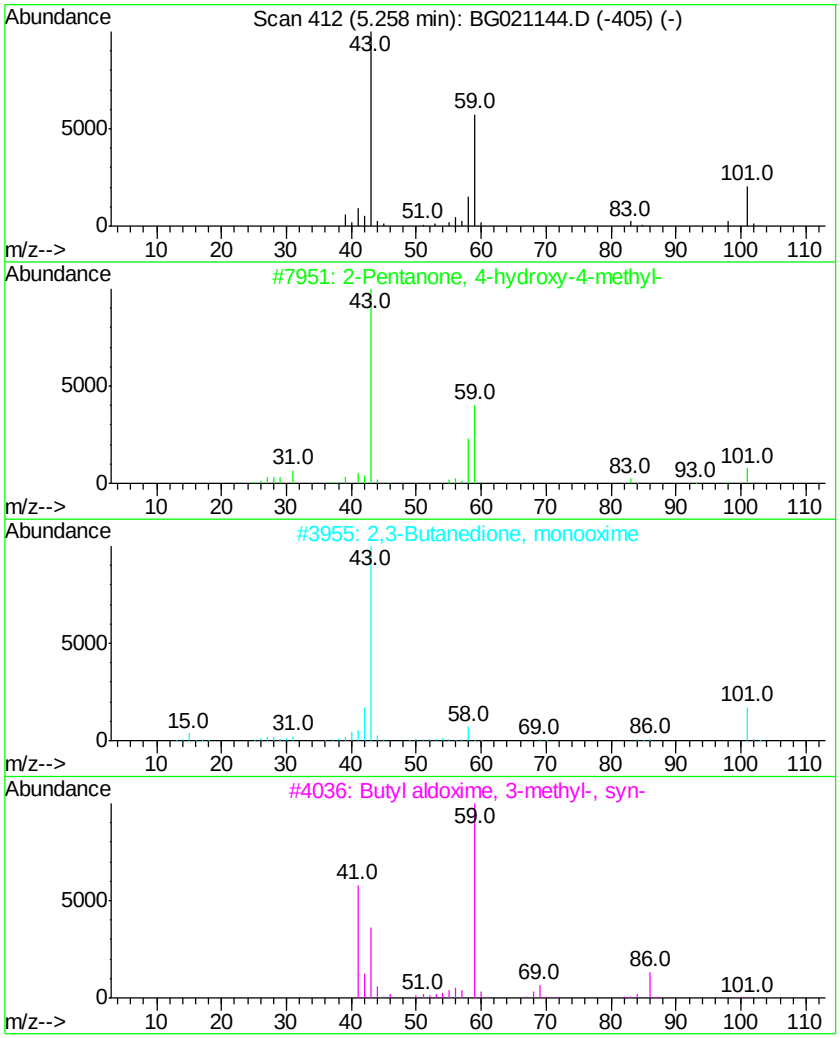
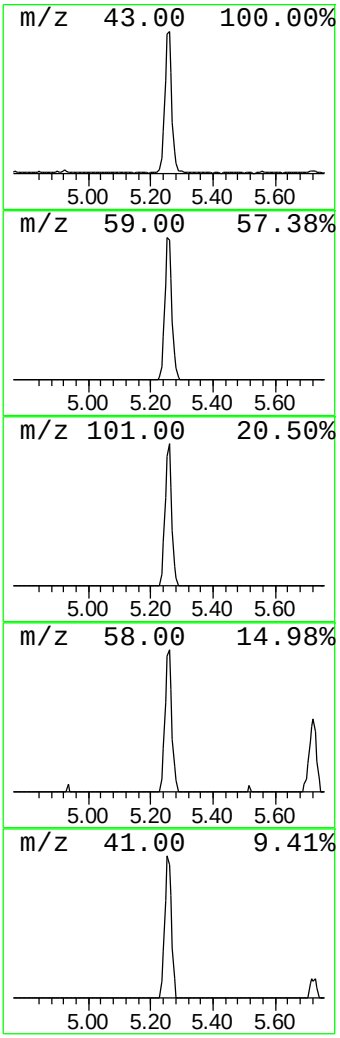
Peak Number 3 unknown5.26 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	28.14 ng	79253	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	23
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument : BNA_G
ClientSampleId : S-19

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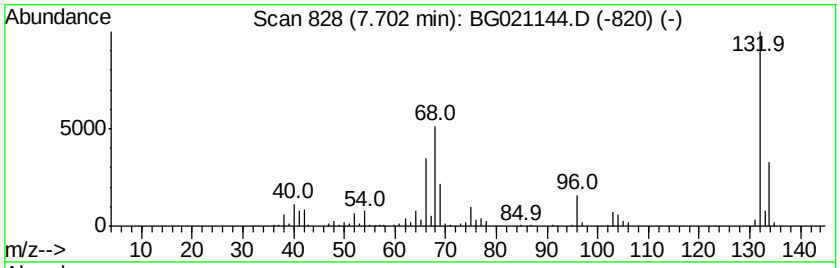
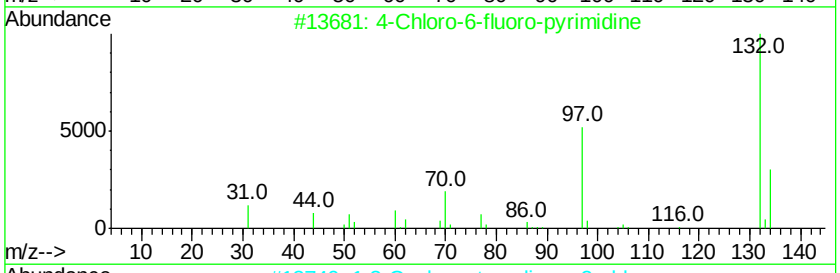
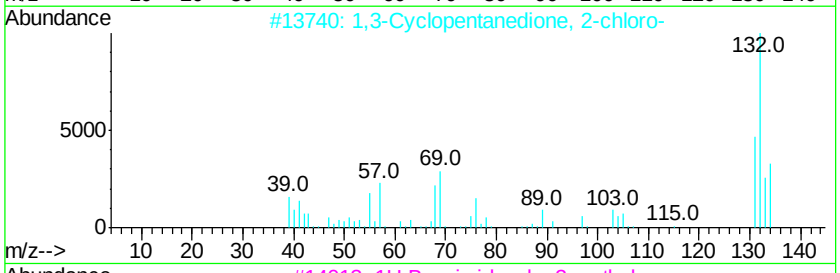
Peak Number 4 unknown7.70 Concentration Rank 2

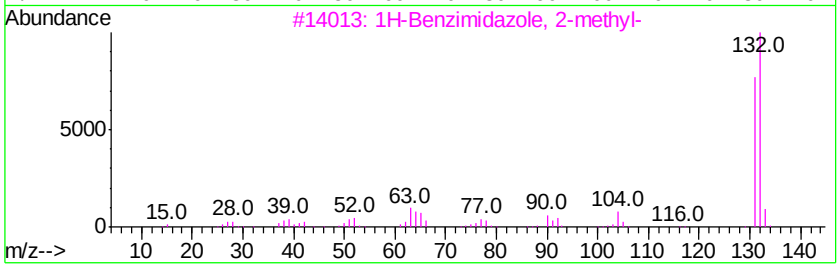
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	143.86 ng	405159	1,4-Dichlorobenzene-d4	8.16

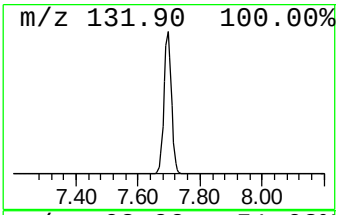
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16

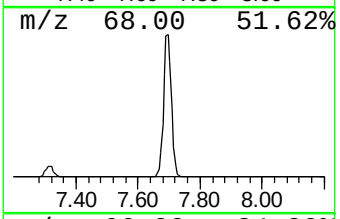


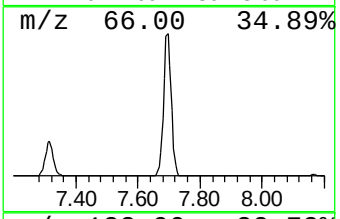


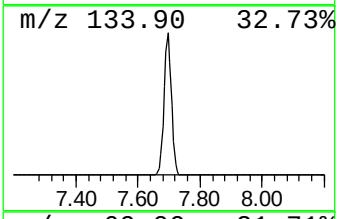


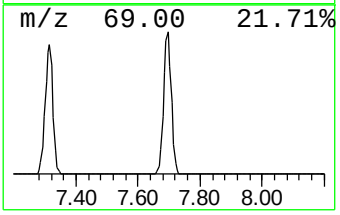












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Instrument : BNA_G
ClientSampleId : S-19

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

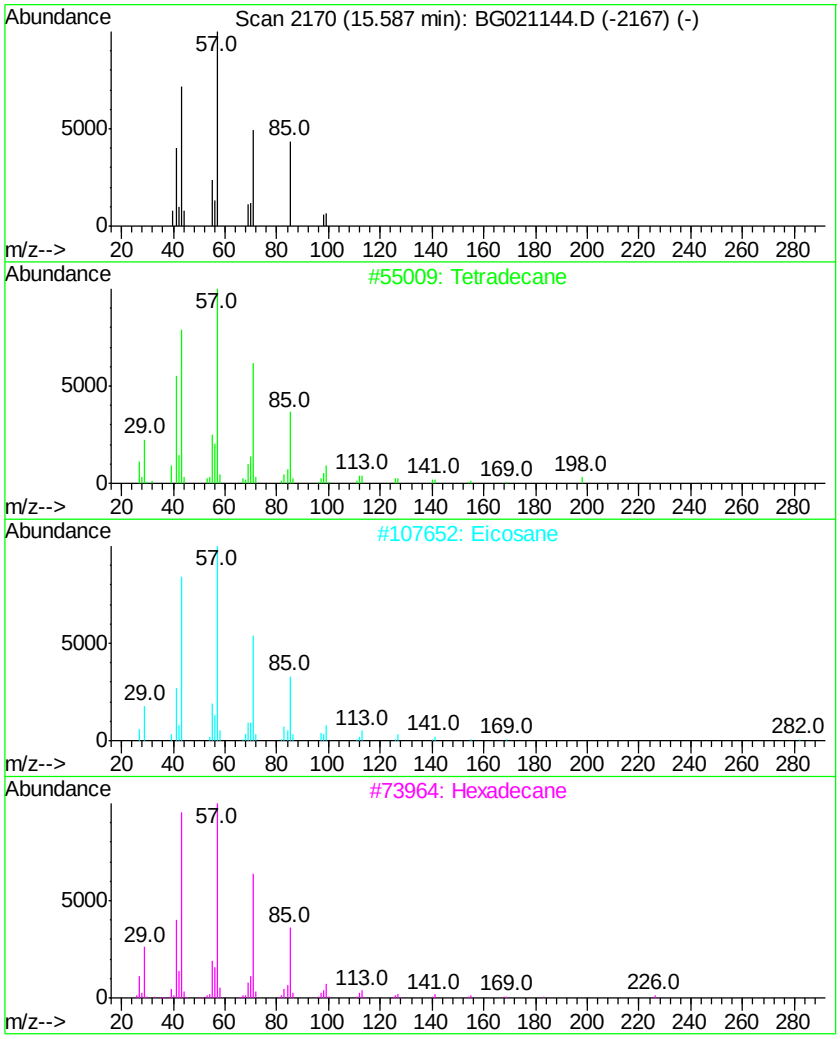
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

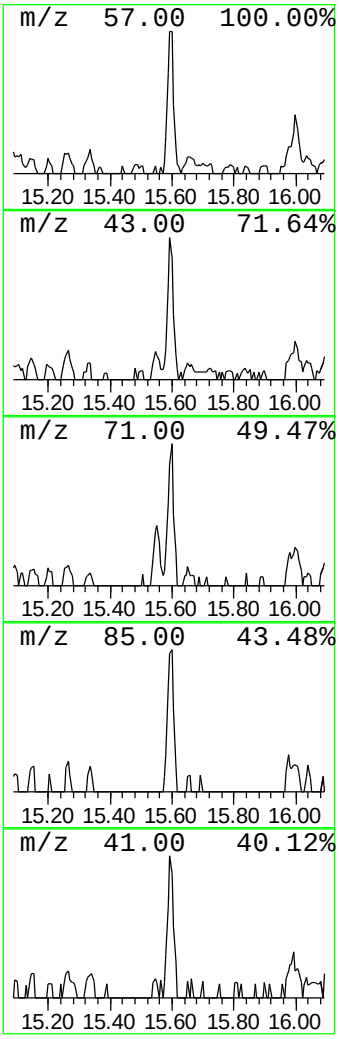
****

Peak Number 6 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	3.09 ng	20652	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Hexadecane	226	C16H34	000544-76-3	86
4	Tridecane	184	C13H28	000629-50-5	78
5	Pentadecane	212	C15H32	000629-62-9	78





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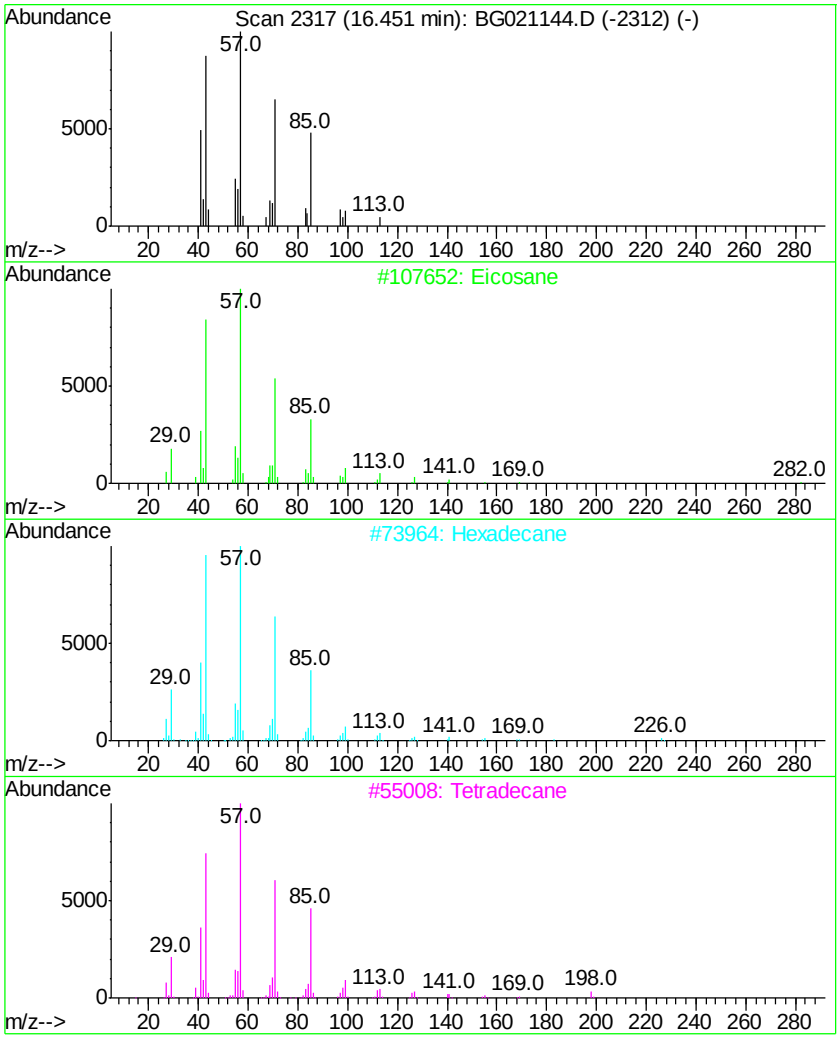
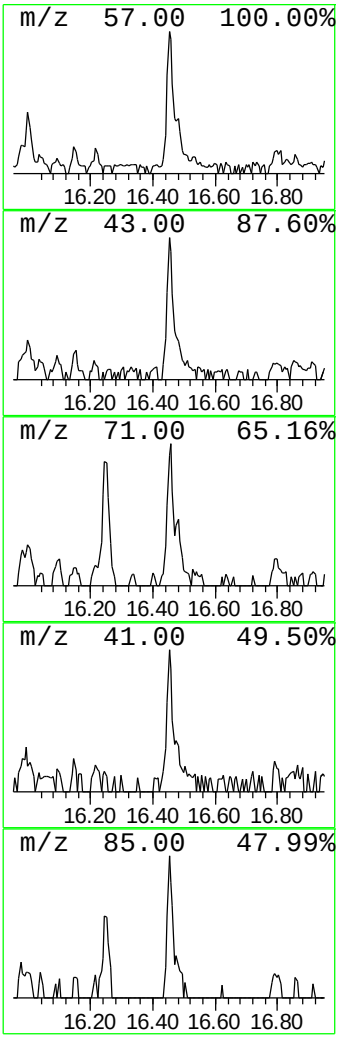
****

Peak Number 7 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	2.67 ng	22008	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetradecane	198	C14H30	000629-59-4	78
4	Pentadecane	212	C15H32	000629-62-9	59
5	Tridecane	184	C13H28	000629-50-5	59





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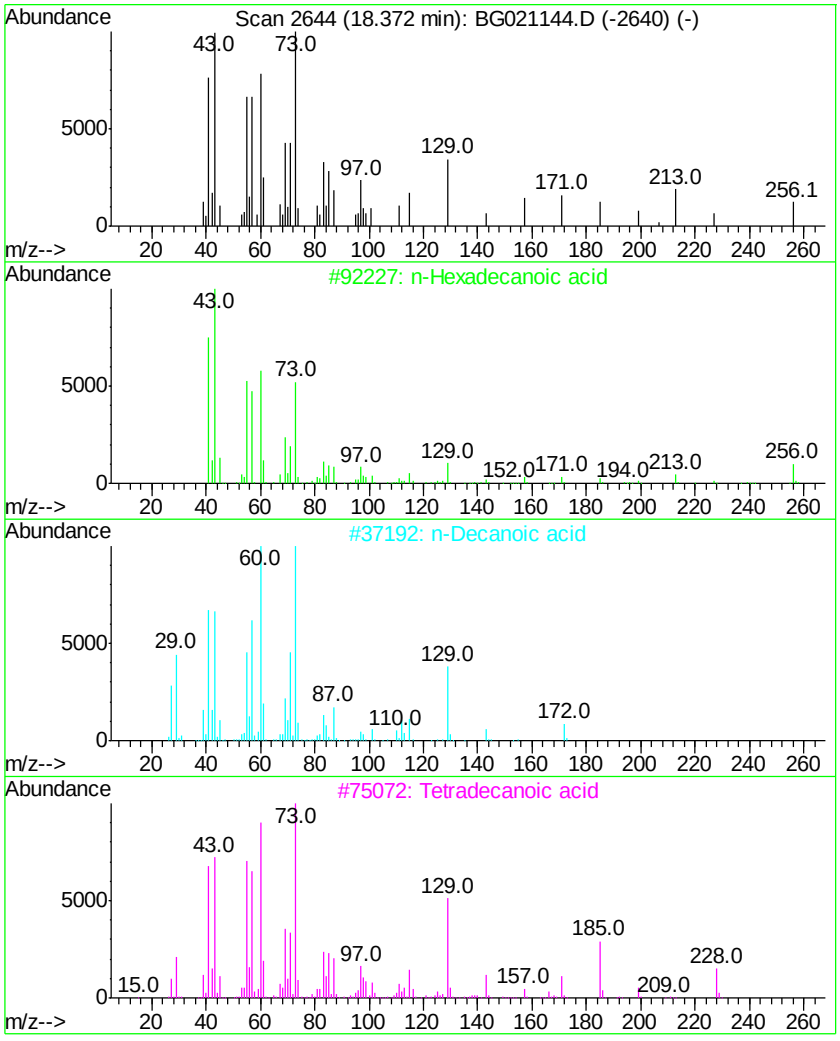
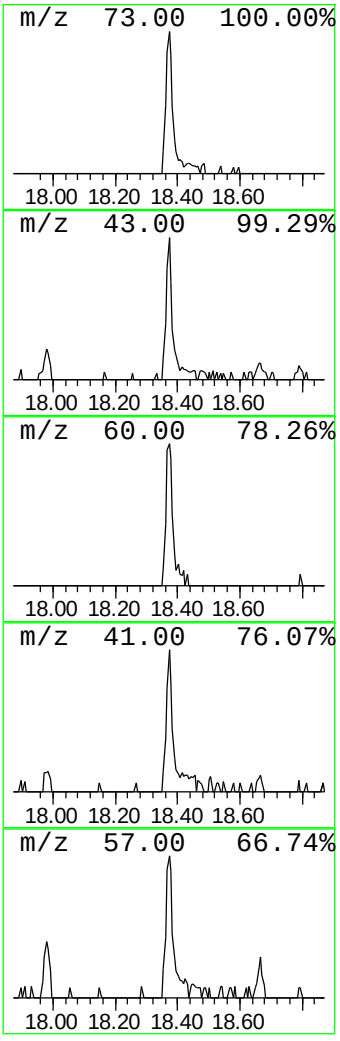
Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	5.80 ng	47903	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Lactose	342	C12H22O11	000063-42-3	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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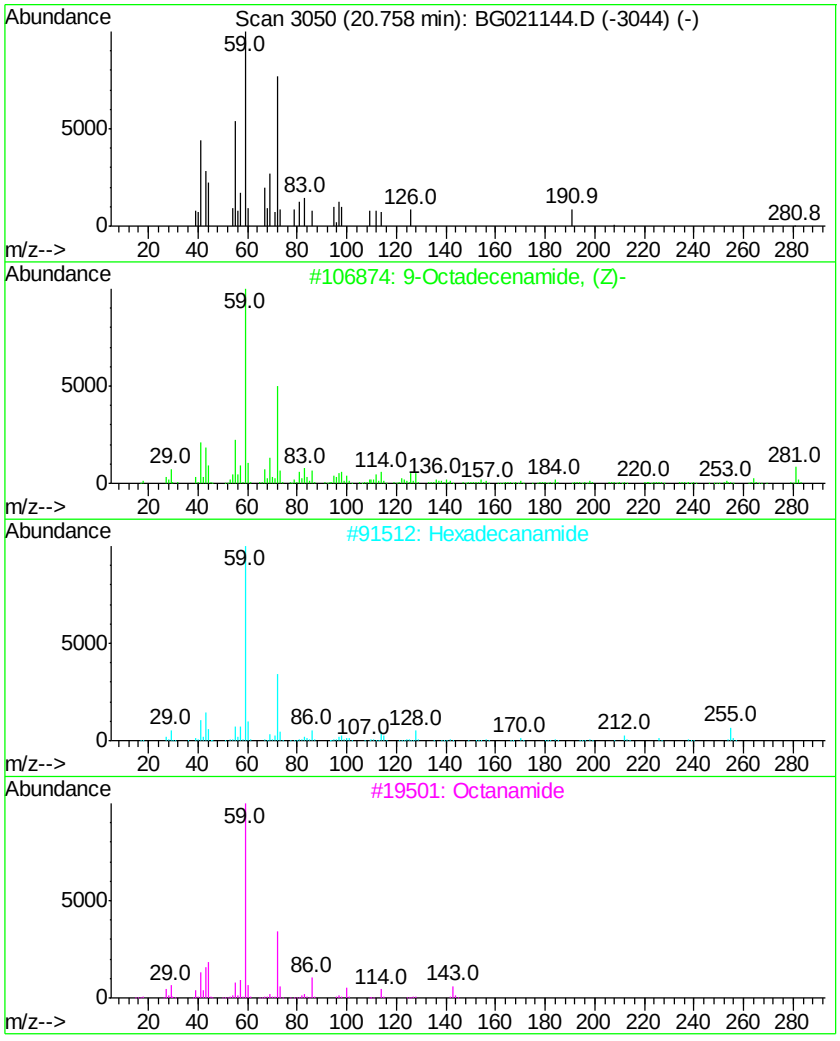
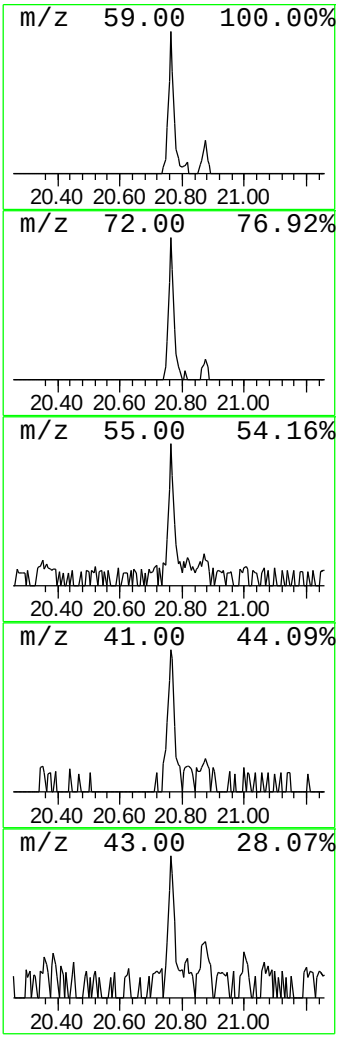
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	2.70 ng	24743	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2	Hexadecanamide	255	C16H33NO	000629-54-9	59
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Dodecanamide	199	C12H25NO	001120-16-7	50
5	Tetradecanamide	227	C14H29NO	000638-58-4	47





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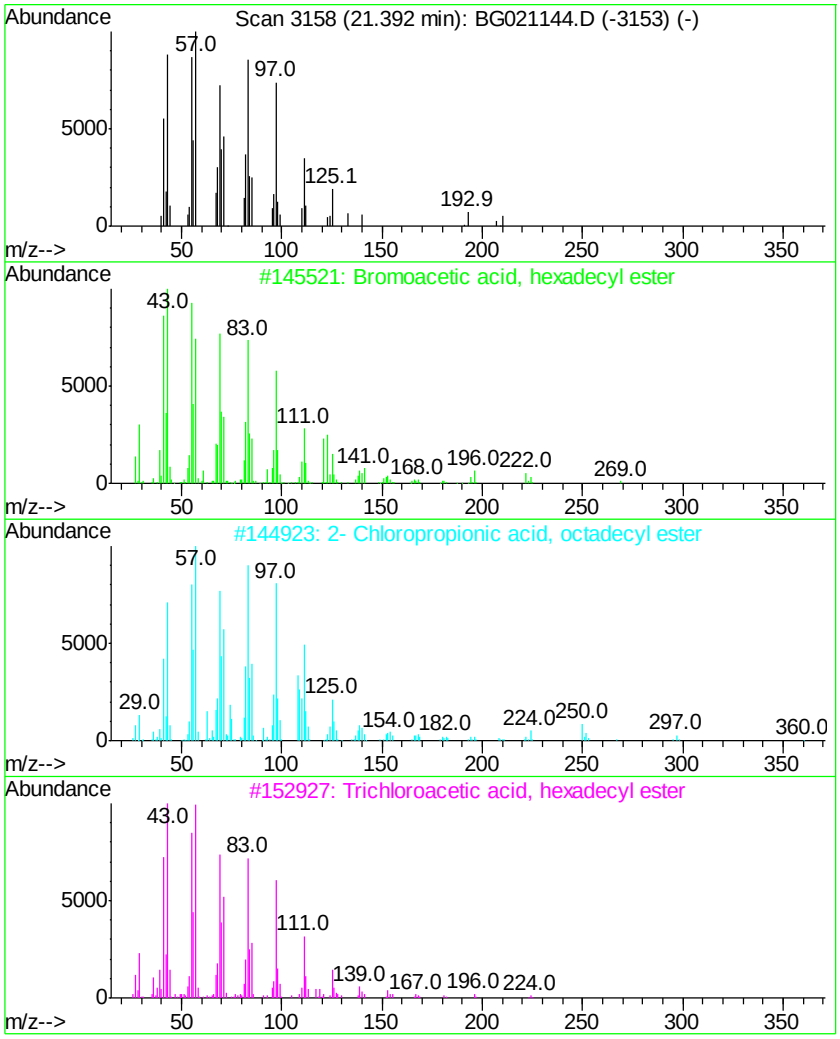
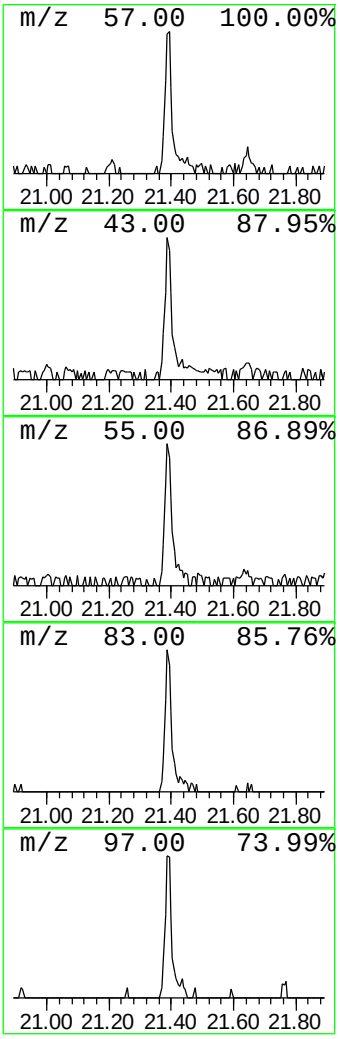
Peak Number 10 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	5.85 ng	53711	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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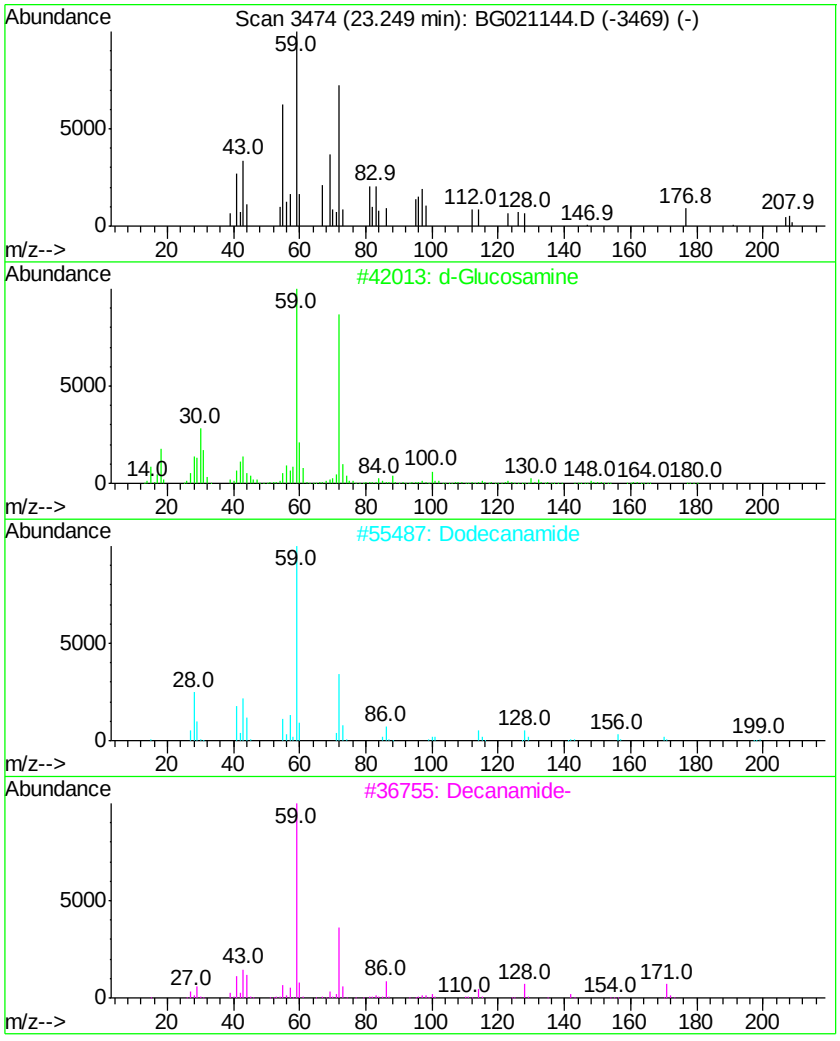
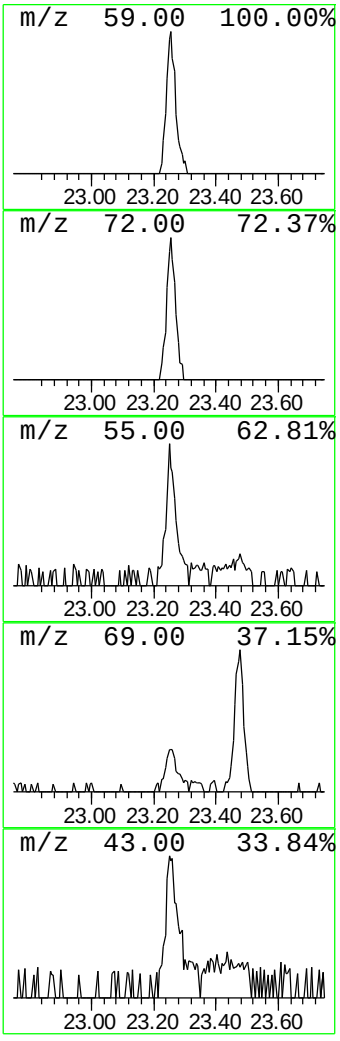
Peak Number 11 d-Glucosamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.25	3.36 ng	30861	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	d-Glucosamine	179	C6H13NO5	000090-77-7	53
2	Dodecanamide	199	C12H25NO	001120-16-7	47
3	Decanamide-	171	C10H21NO	002319-29-1	38
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	37
5	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	35





Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
Data File : BG021144.D
Acq On : 28 Feb 2016 10:03
Operator : UM/SJ
Sample : H1558-17
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-19

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

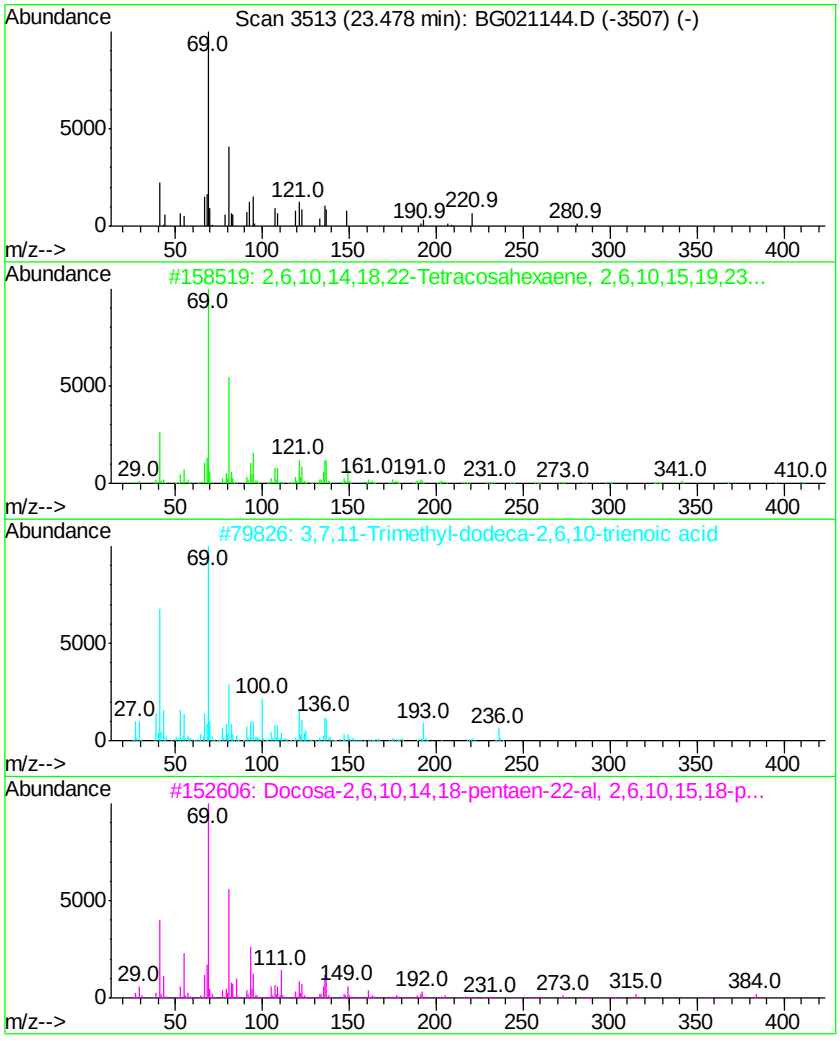
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

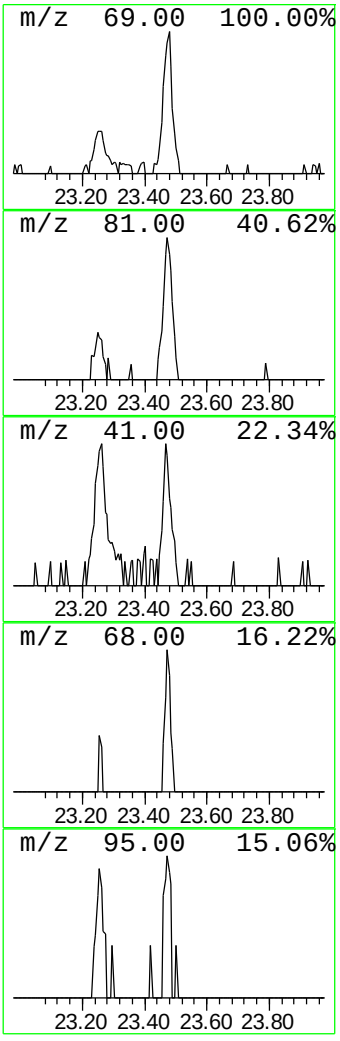
****

Peak Number 12 2,6,10,14,18,22-Tetracosahe... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.48	2.38 ng	19120	Perylene-d12	25.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
2	3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	78
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5	Squalene	410	C30H50	007683-64-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022716\
Data File : BG021144.D
Acq On : 28 Feb 2016 10:03
Operator : UM/SJ
Sample : H1558-17
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-19

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.08	3.08	591.4	ng	1665620	1	8.16	56327	20.0
unknown5.26	5.26	28.1	ng	79253	1	8.16	56327	20.0
unknown7.70	7.70	143.9	ng	405159	1	8.16	56327	20.0
Tetradecane	15.59	3.1	ng	20652	3	14.77	133735	20.0
Eicosane	16.45	2.7	ng	22008	4	17.50	165049	20.0
n-Hexadecanoic acid	18.37	5.8	ng	47903	4	17.50	165049	20.0
9-Octadecenamide,...	20.76	2.7	ng	24743	5	21.77	183615	20.0
Bromoacetic acid,...	21.39	5.8	ng	53711	5	21.77	183615	20.0
d-Glucosamine	23.25	3.4	ng	30861	5	21.77	183615	20.0
2,6,10,14,18,22-T...	23.48	2.4	ng	19120	6	25.05	160888	20.0