LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022607.D
Acq On : 26 Jun 2016 12:45
Operator : UM/SJ
Sample : H3761-02
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-5F-9-11

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-BG062516.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	3.055	32	37	58	rBV	7444125	11991411	100.00%	19.108%
2	5.240	403	409	415	rBV	143230	227557	1.90%	0.363%
3	5.705	480	488	498	rBV	2241213	3584285	29.89%	5.711%
4	7.309	753	761	771	rVB	2378582	4189167	34.93%	6.675%
5	7.691	819	826	835	rVB	2210713	3846175	32.07%	6.129%
6	8.161	899	906	913	rBV	445522	772765	6.44%	1.231%
7	8.490	954	962	970	rBV	1586943	2784192	23.22%	4.437%
8	9.330	1095	1105	1113	rBV	1450658	2599049	21.67%	4.142%
9	10.987	1379	1387	1394	rBV	607799	1094903	9.13%	1.745%
10	13.419	1793	1801	1810	rBV	3462838	5360194	44.70%	8.541%
11	14.236	1930	1940	1946	rBV	487463	730768	6.09%	1.164%
12	14.794	2029	2035	2043	rBV2	986487	1625463	13.56%	2.590%
13	16.281	2277	2288	2298	rBV	3783890	5943200	49.56%	9.470%
14	17.550	2497	2504	2510	rBV2	1491655	2302072	19.20%	3.668%
15	18.425	2648	2653	2660	rBV2	339298	513545	4.28%	0.818%
16	19.688	2864	2868	2874	rBV5	172167	229270	1.91%	0.365%
17	19.959	2910	2914	2920	rVB	91699	127846	1.07%	0.204%
18	20.152	2940	2947	2954	rBV	6484930	8910388	74.31%	14.198%
19	21.463	3166	3170	3182	rVB5	274353	517126	4.31%	0.824%
20	21.845	3229	3235	3243	rBV	1642207	2769778	23.10%	4.414%
21	25.205	3798	3807	3818	rVB2	864017	2636820	21.99%	4.202%

Sum of corrected areas: 62755974

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Misc :
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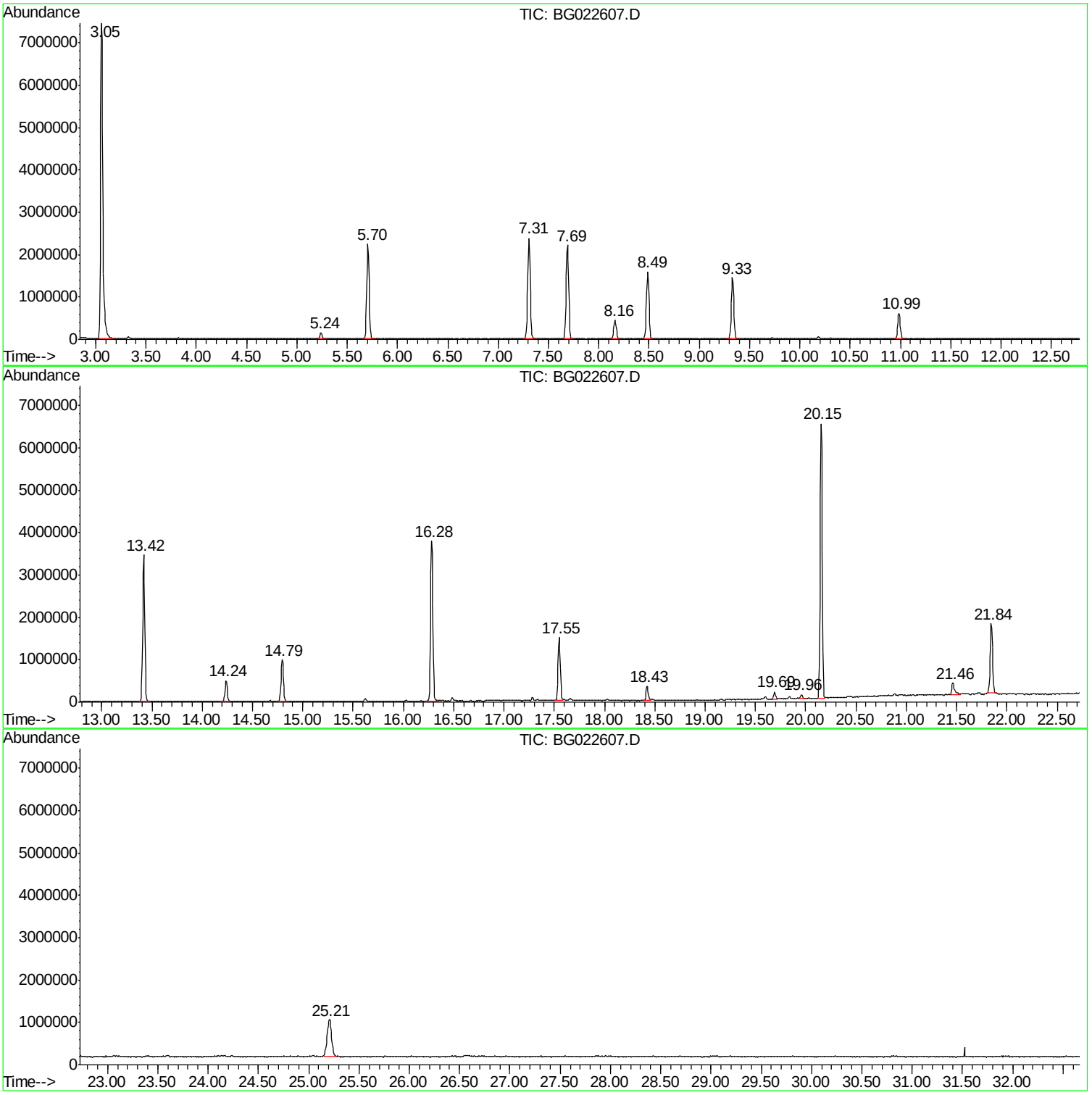
Instrument :
BNA_G
ClientSampleId :
LOCATION-5F-9-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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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Data File : BG022607.D
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Sample : H3761-02
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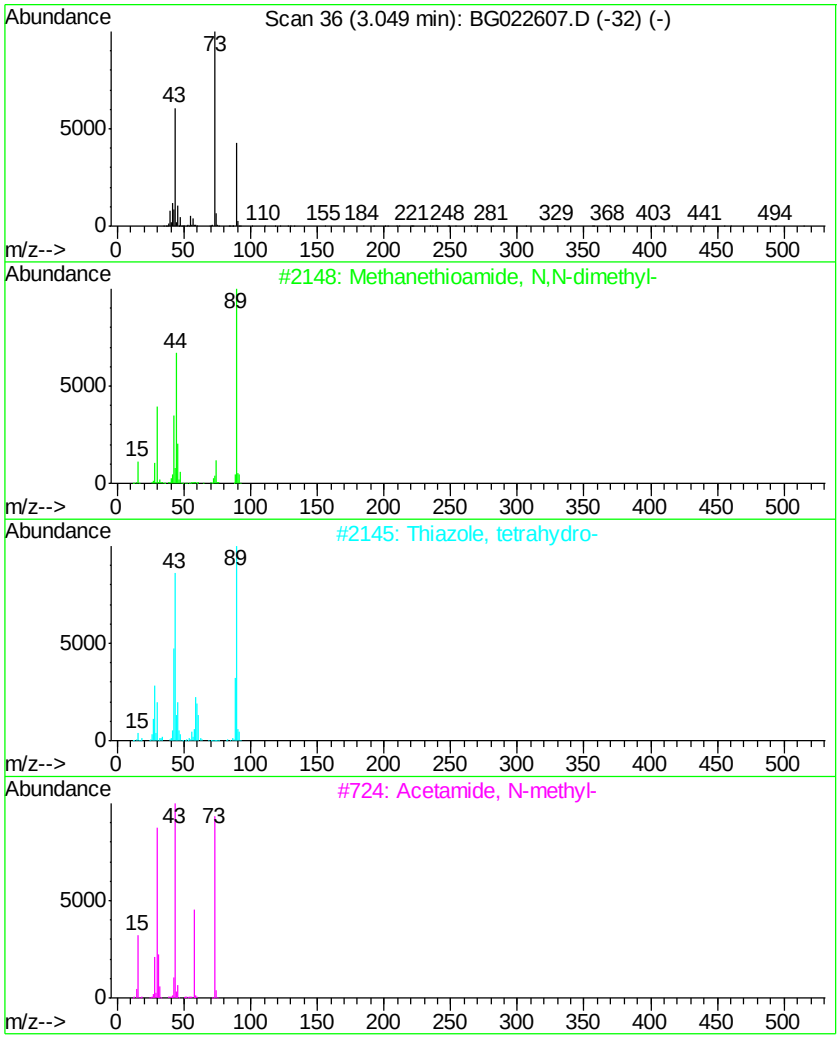
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

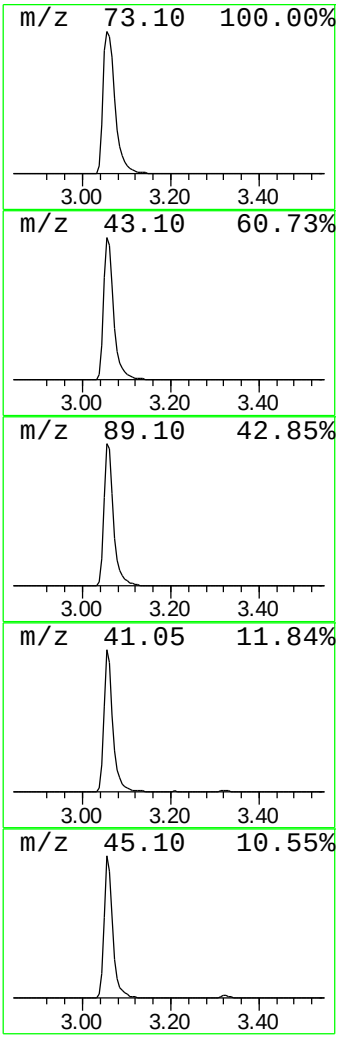
****

Peak Number 1 unknown3.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	310.35 ng	11991400	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	43
2	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	28
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022607.D
Acq On : 26 Jun 2016 12:45
Operator : UM/SJ
Sample : H3761-02
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-5F-9-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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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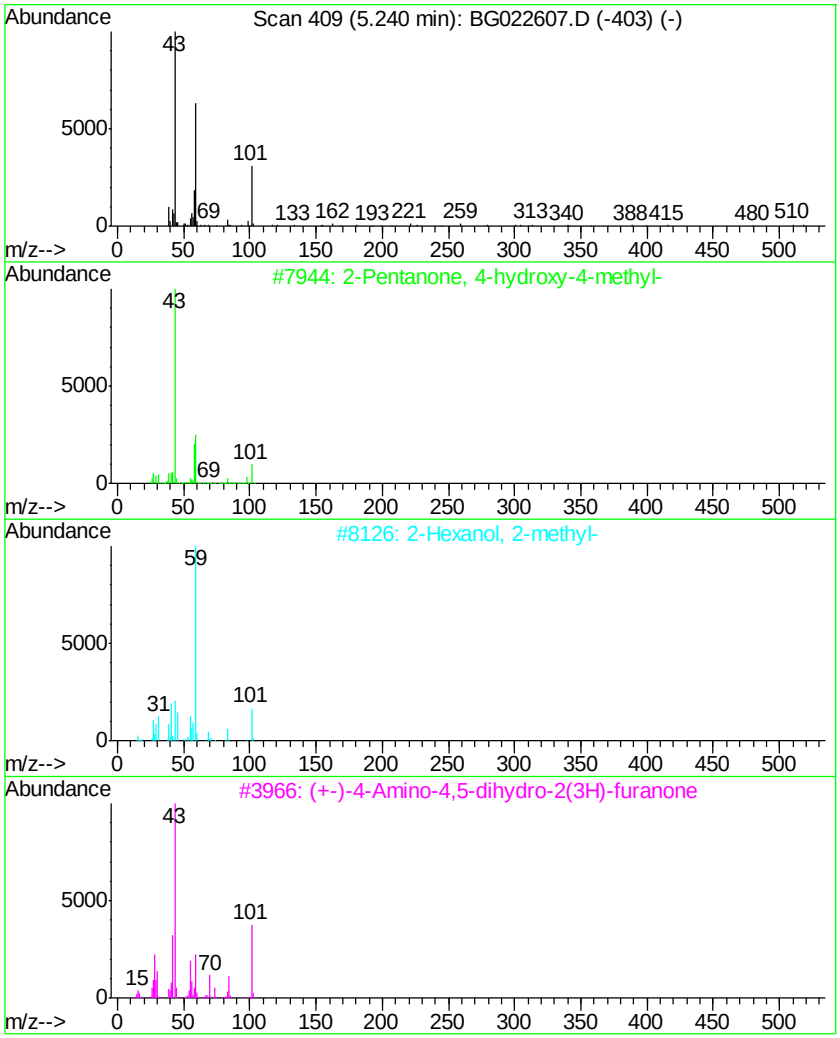
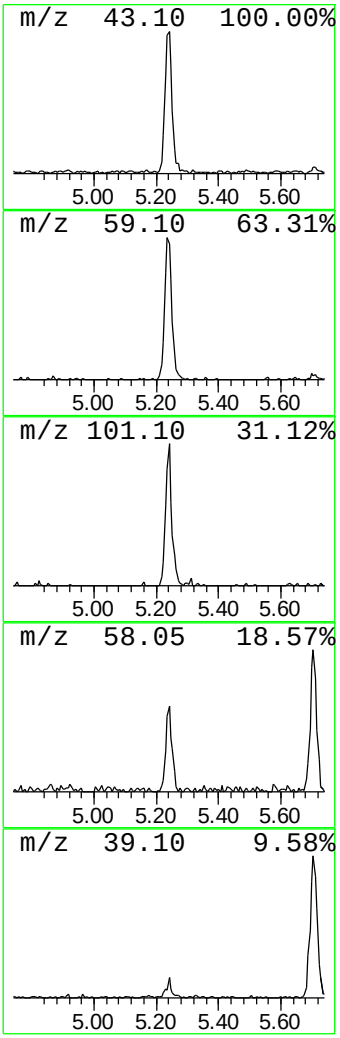
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	5.89 ng	227557	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	32
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	17





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022607.D
Acq On : 26 Jun 2016 12:45
Operator : UM/SJ
Sample : H3761-02
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LOCATION-5F-9-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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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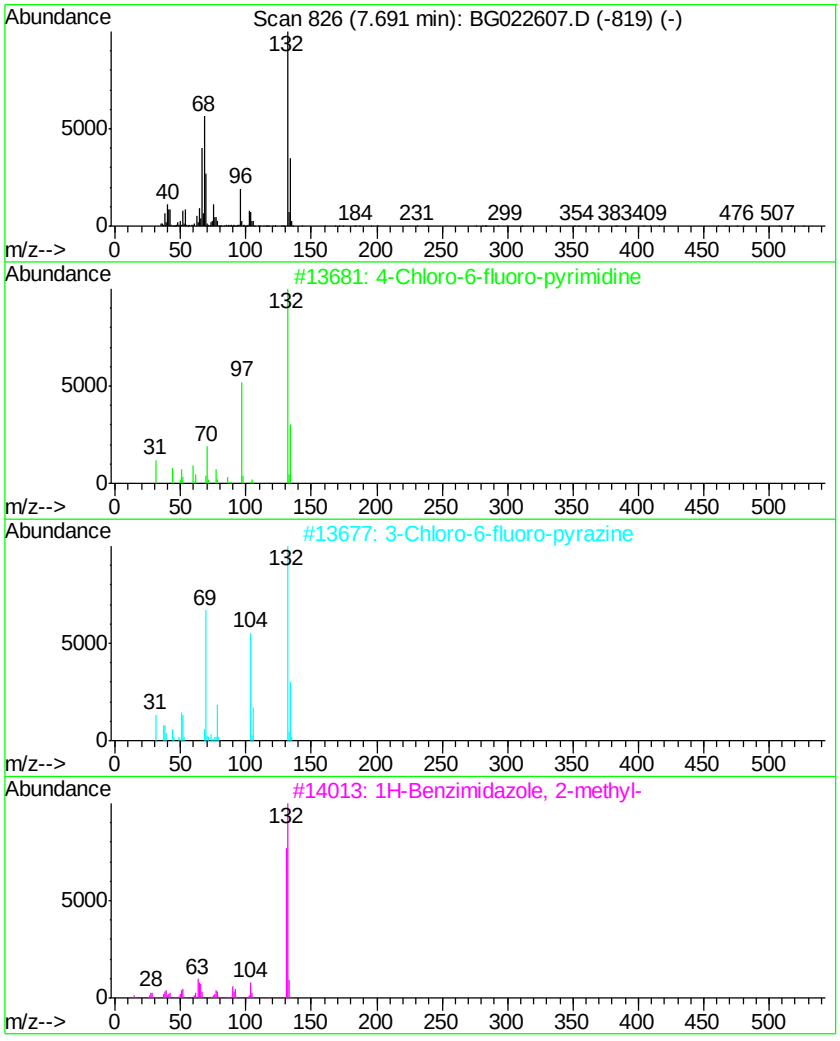
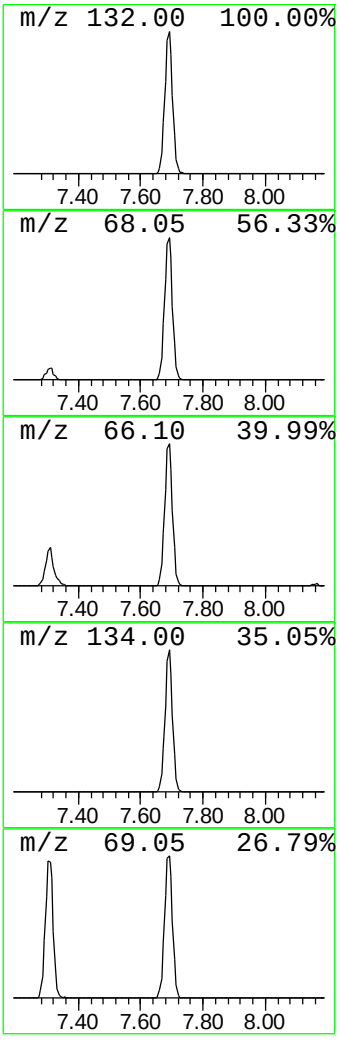
Peak Number 3 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	99.54 ng	3846180	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	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022607.D
Acq On : 26 Jun 2016 12:45
Operator : UM/SJ
Sample : H3761-02
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-5F-9-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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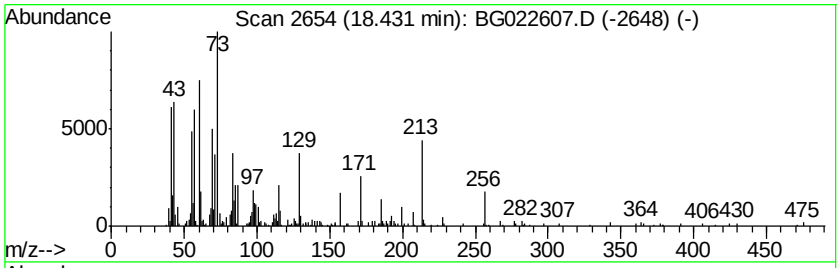
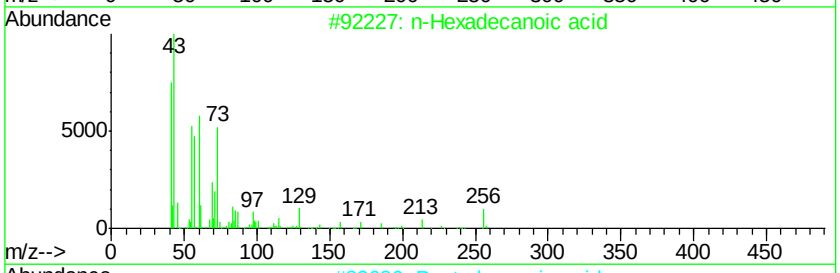
****

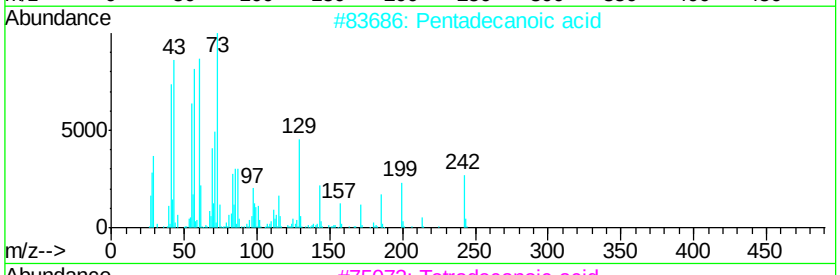
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

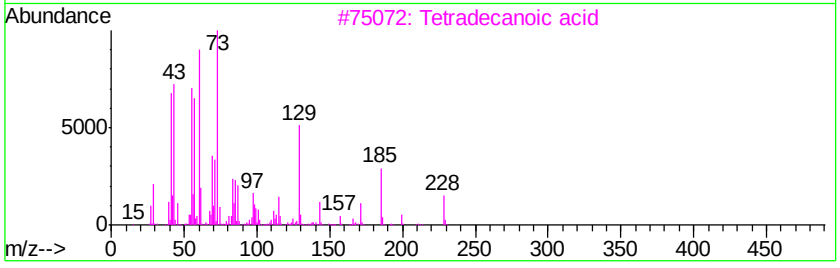
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	4.46 ng	513545	Phenanthrene-d10	17.55

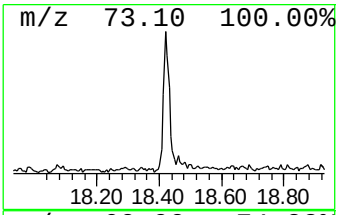
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	80

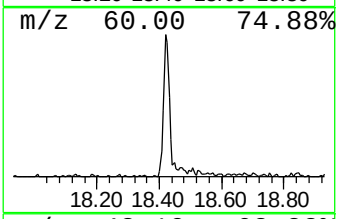


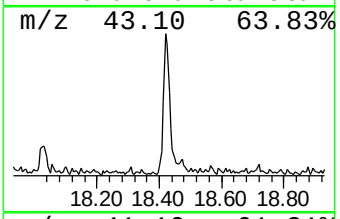


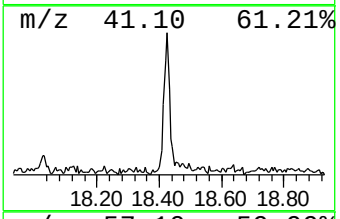


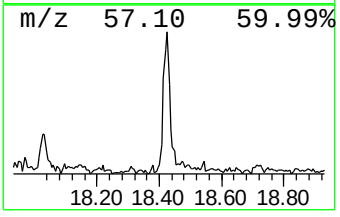












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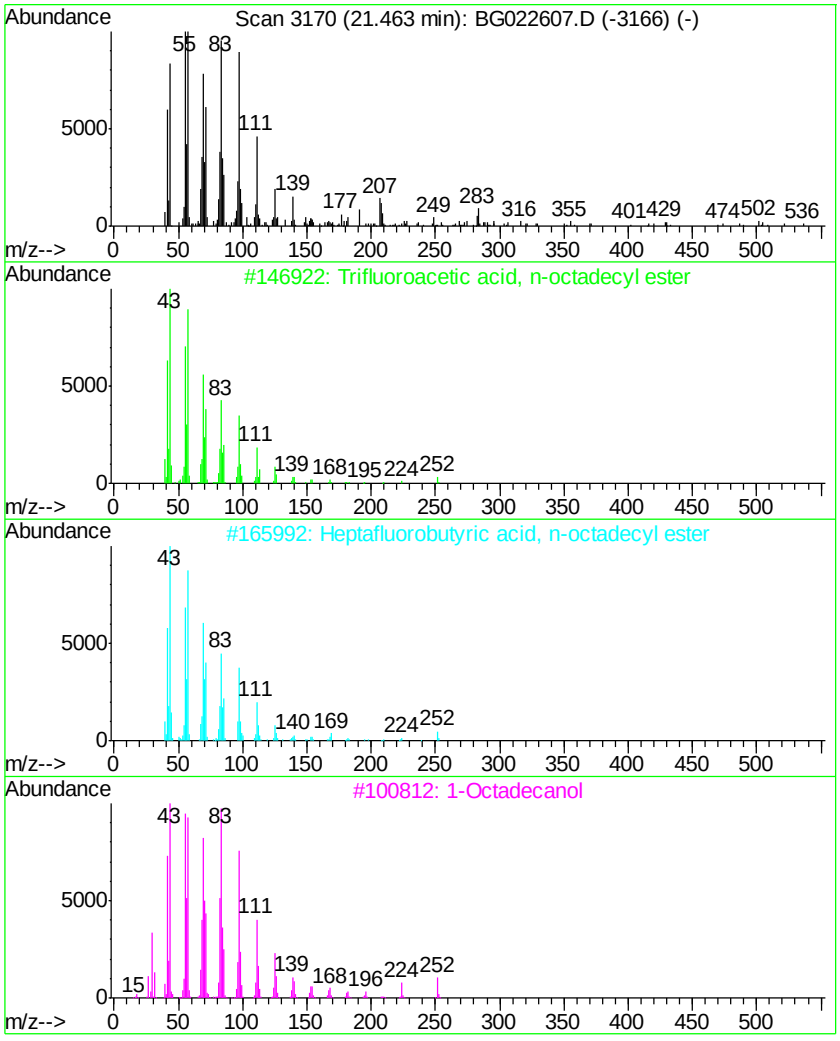
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

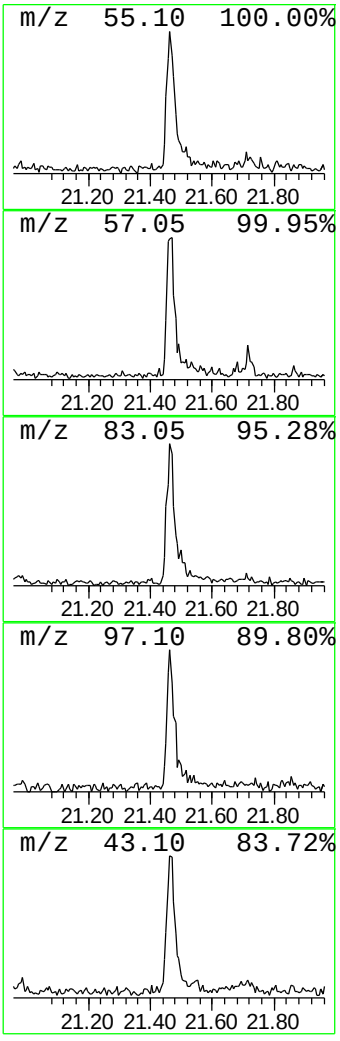
****

Peak Number 6 Trifluoroacetic acid, n-oct... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	3.73 ng	517126	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	86
3	1-Octadecanol	270	C18H38O	000112-92-5	86
4	1-Nonadecanol	284	C19H40O	001454-84-8	83
5	Isotridecanol-	200	C13H28O	027458-92-0	72





Tentatively Identified Compound (LSC) summary

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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
unknown3.05	3.05	310.4	ng	11991400	1	8.16	772765	20.0
2-Pentanone, 4-hy...	5.24	5.9	ng	227557	1	8.16	772765	20.0
unknown7.69	7.69	99.5	ng	3846180	1	8.16	772765	20.0
n-Hexadecanoic acid	18.43	4.5	ng	513545	4	17.55	2302070	20.0
Trifluoroacetic a...	21.46	3.7	ng	517126	5	21.84	2769780	20.0