LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

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_F\METHODS\8270-BF060716.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	1.667	3	7	9	rVB	3928240	6094542	100.00%	19.215%
2	1.747	13	14	24	rVB	322016	636009	10.44%	2.005%
3	1.884	24	26	40	rVB	2030564	3205885	52.60%	10.108%
4	2.067	40	42	81	rVB3	71504	512240	8.40%	1.615%
5	5.004	296	299	305	rVB	114311	163216	2.68%	0.515%
6	5.427	333	336	338	rBV	2017568	2454229	40.27%	7.738%
7	6.456	423	426	429	rBV	1674076	2272252	37.28%	7.164%
8	6.593	435	438	440	rBV	2410404	2255468	37.01%	7.111%
9	6.822	456	458	461	rBV	686225	630448	10.34%	1.988%
10	6.982	469	472	474	rBV	2190731	1864460	30.59%	5.878%
11	7.393	505	508	510	rBV	1525777	1651123	27.09%	5.206%
12	8.113	568	571	573	rBV	900765	849823	13.94%	2.679%
13	9.188	663	665	668	rBV	1860911	2426564	39.82%	7.651%
14	9.588	698	700	702	rBV	372257	297175	4.88%	0.937%
15	9.873	722	725	727	rBV	613316	770628	12.64%	2.430%
16	10.651	791	793	796	rBV2	1013605	1216884	19.97%	3.837%
17	11.348	852	854	858	rBV	704521	671061	11.01%	2.116%
18	12.559	958	960	962	rBV	86767	71768	1.18%	0.226%
19	12.788	976	980	982	rBV	73225	90016	1.48%	0.284%
20	12.937	991	993	996	rBV	1669966	1740716	28.56%	5.488%
21	13.851	1070	1073	1082	rBV2	82157	128860	2.11%	0.406%
22	13.988	1082	1085	1087	rBV	637702	788987	12.95%	2.488%
23	14.491	1125	1129	1133	rBV3	38545	88885	1.46%	0.280%
24	14.628	1138	1141	1143	rVV	161873	158925	2.61%	0.501%
25	15.005	1171	1174	1178	rBV	28656	73249	1.20%	0.231%
26	15.405	1206	1209	1212	rBV	401042	506715	8.31%	1.598%
27	16.103	1267	1270	1278	rVB5	32541	97572	1.60%	0.308%

Sum of corrected areas: 31717700

LSC Report - Integrated Chromatogram

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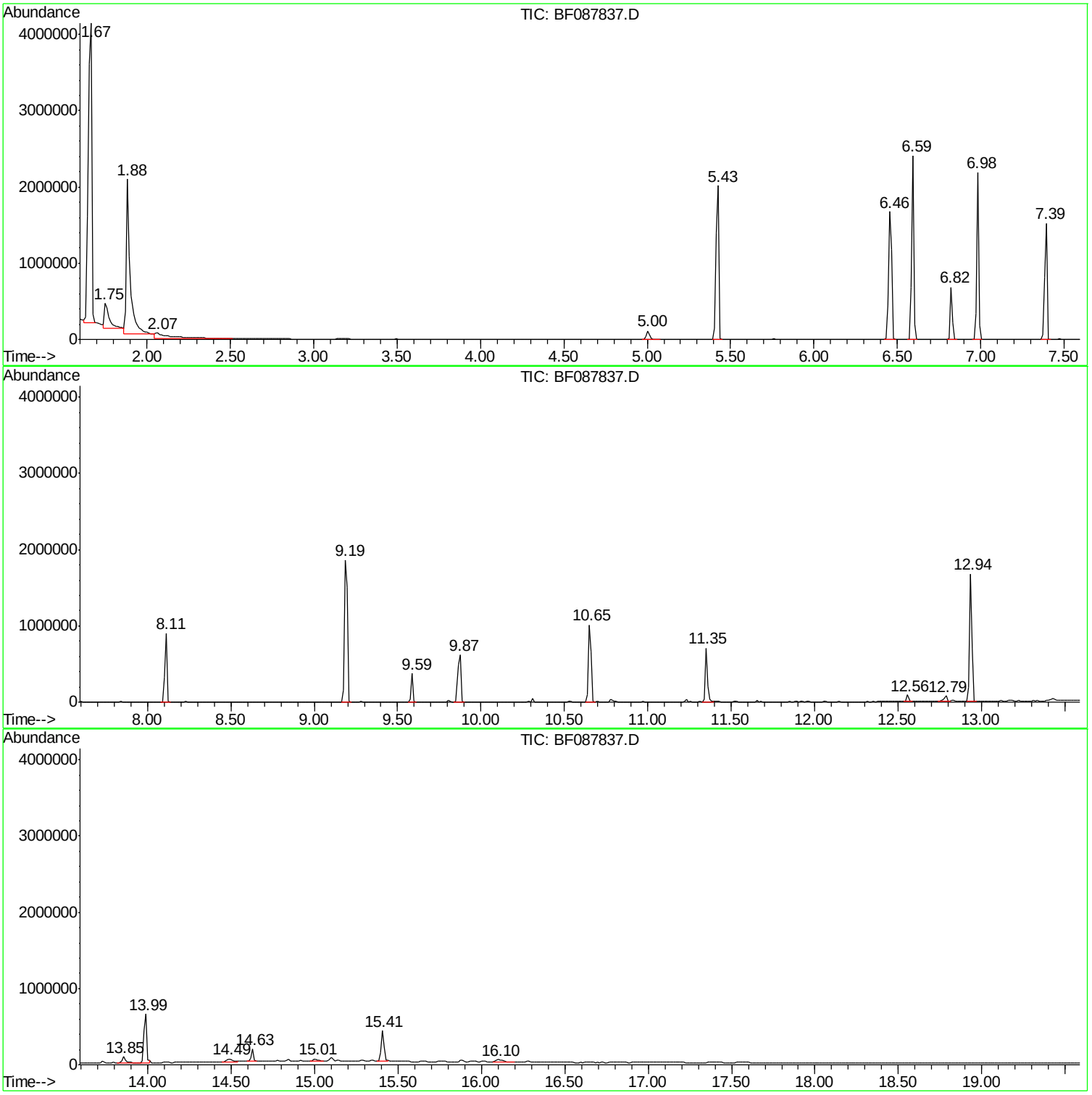
Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

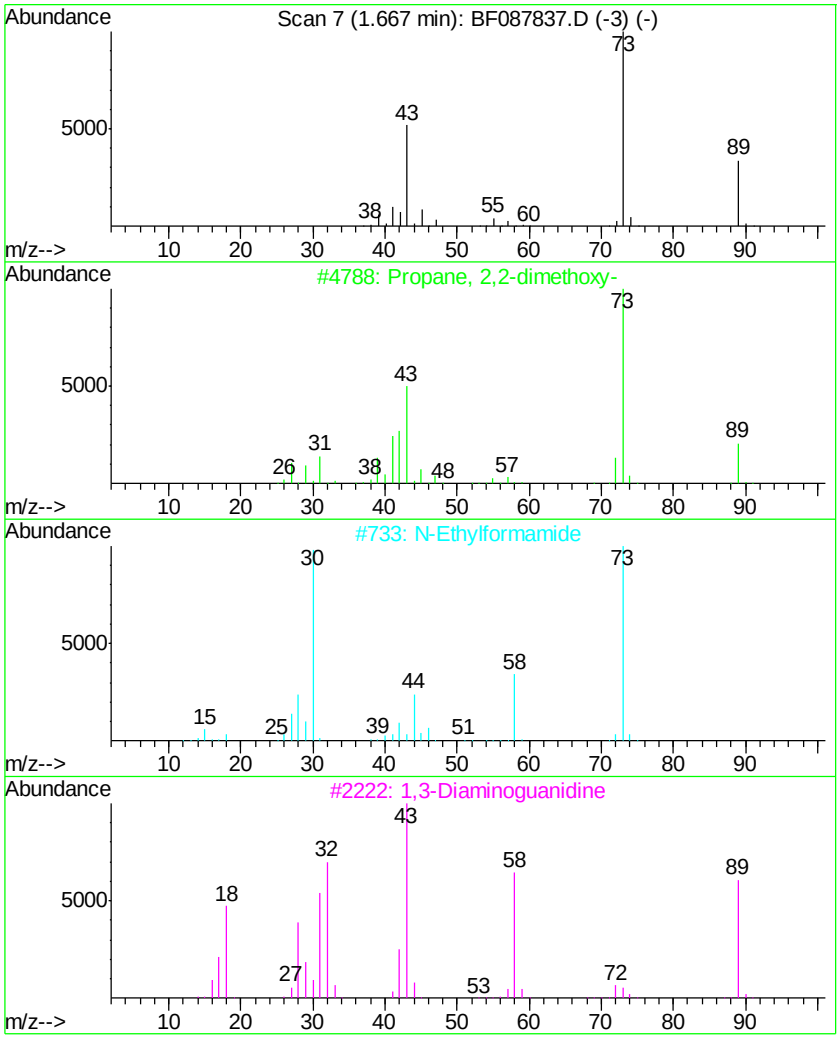
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

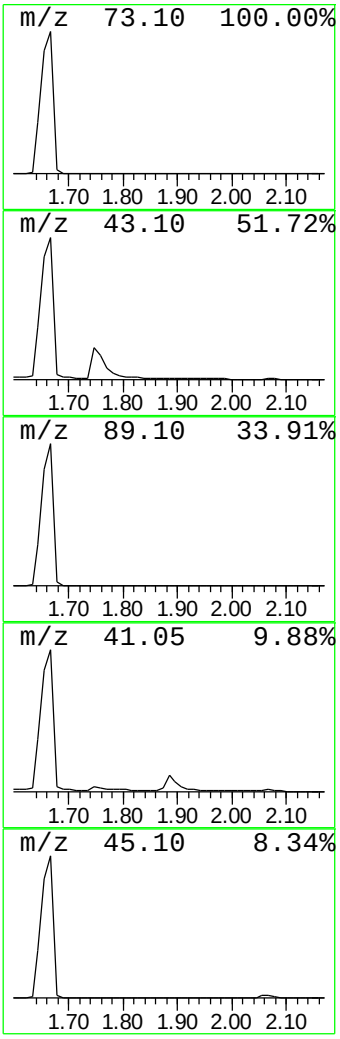
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	193.34 ng	6094540	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

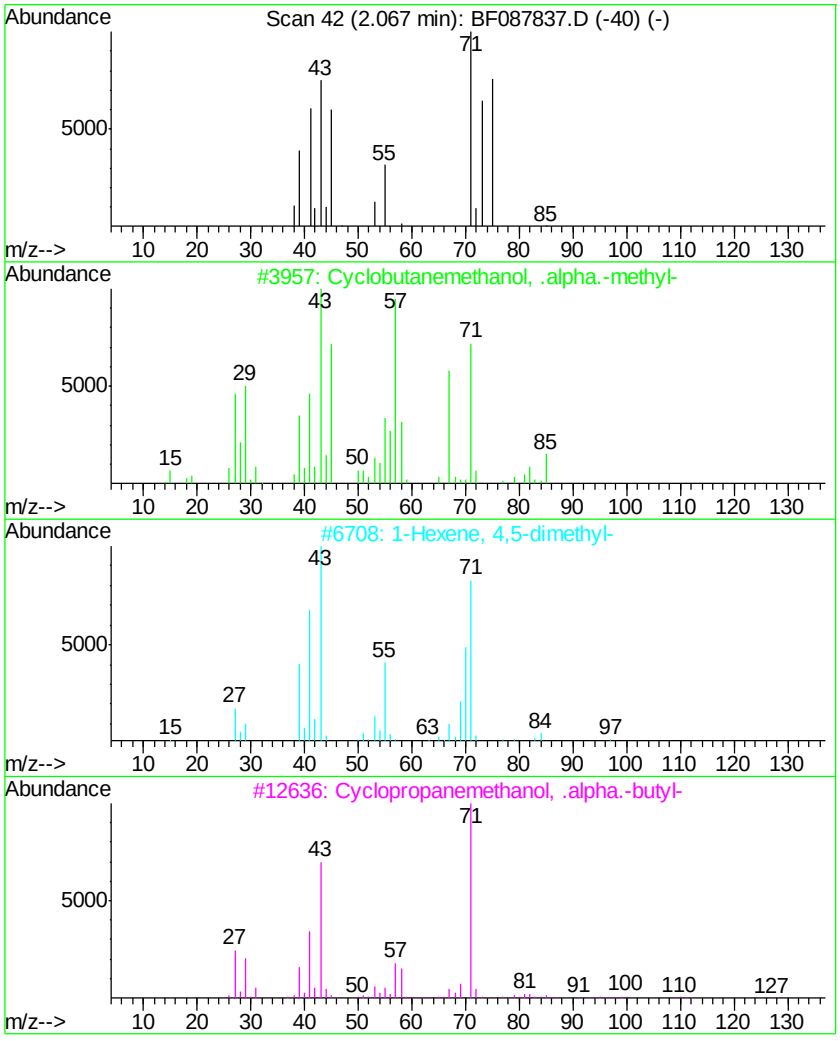
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

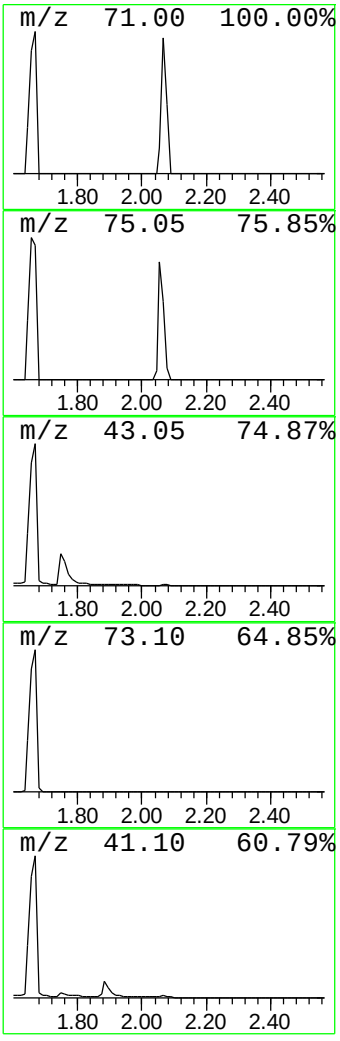
****

Peak Number 4 unknown2.07 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	16.25 ng	512240	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanemethanol, .alpha.-met...	100	C6H12O	007515-29-9	43
2	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	23
3	Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	17
4	Hexaborane	76	B6H10	023777-80-2	9
5	Oxirane, propyl-	86	C5H10O	001003-14-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

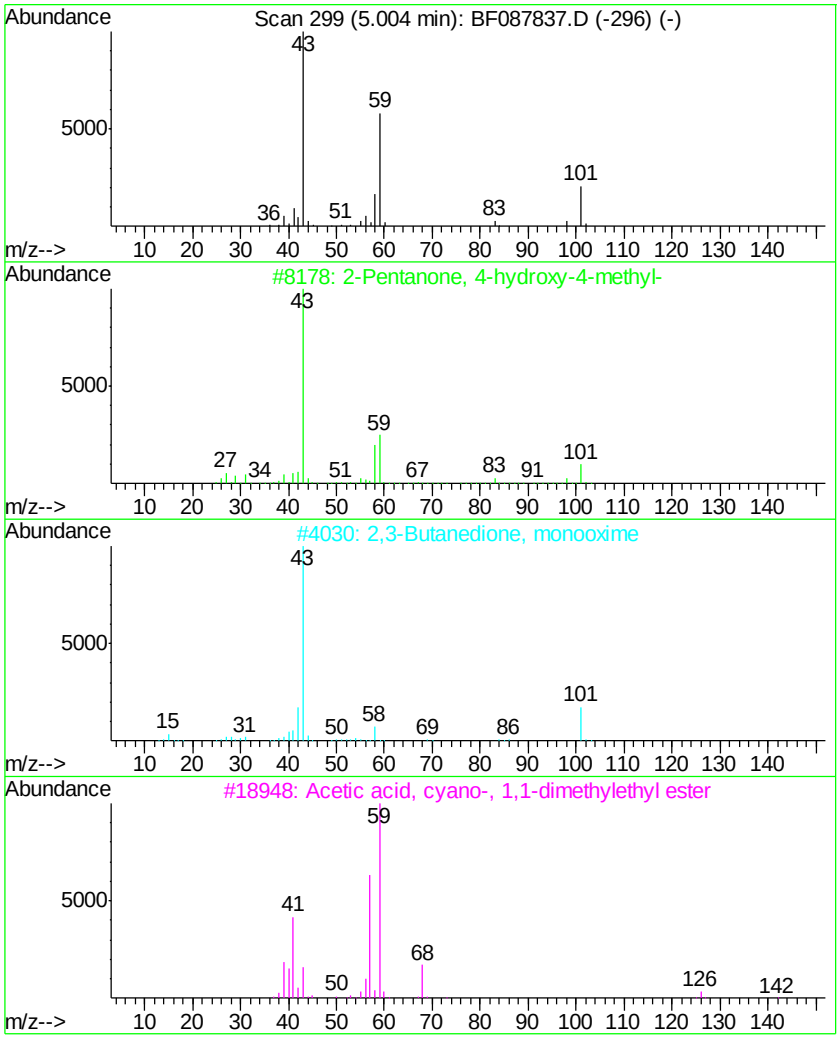
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

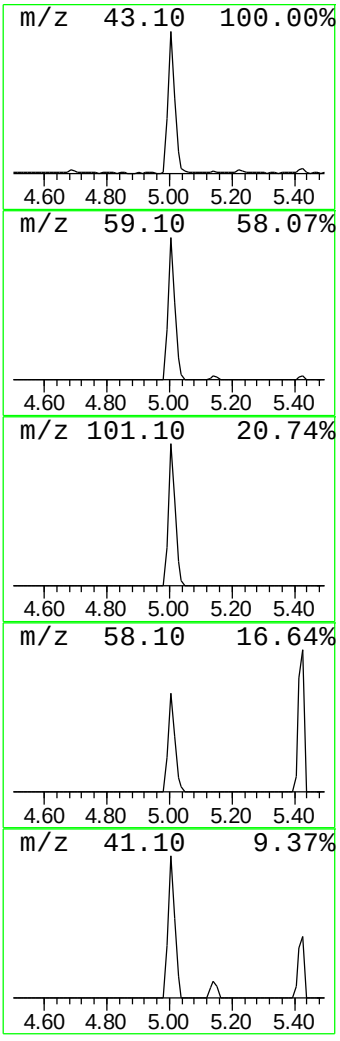
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	5.18 ng	163216	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

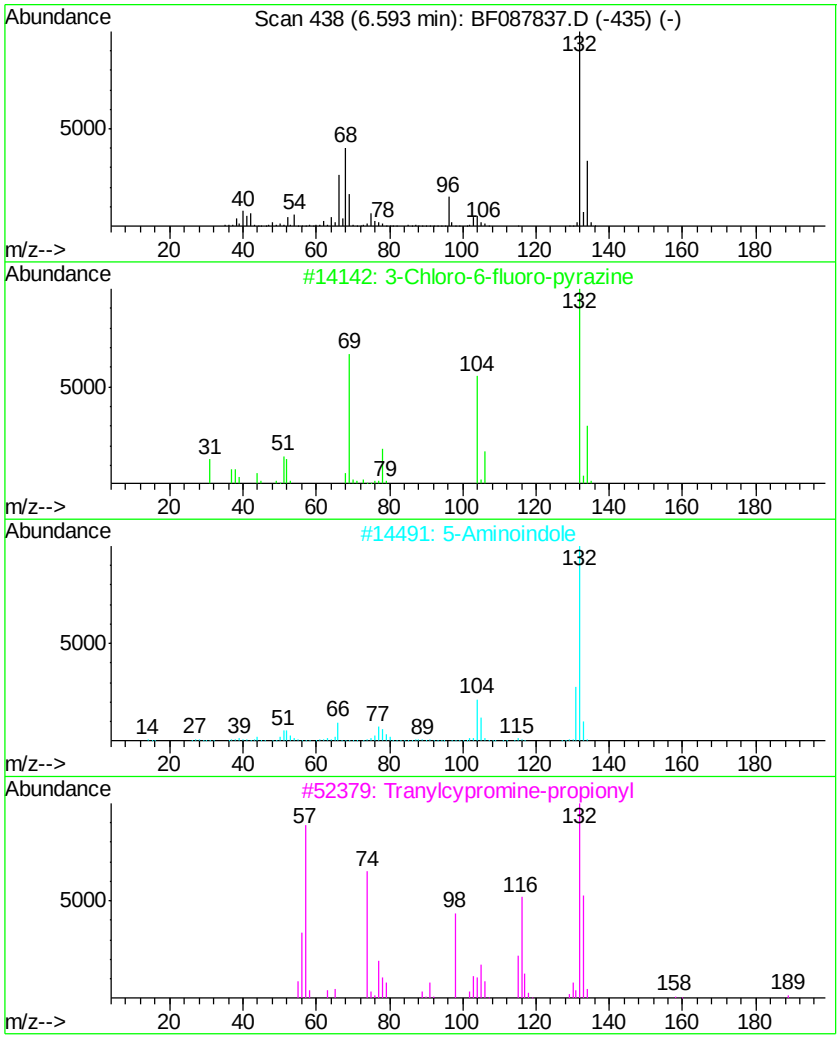
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

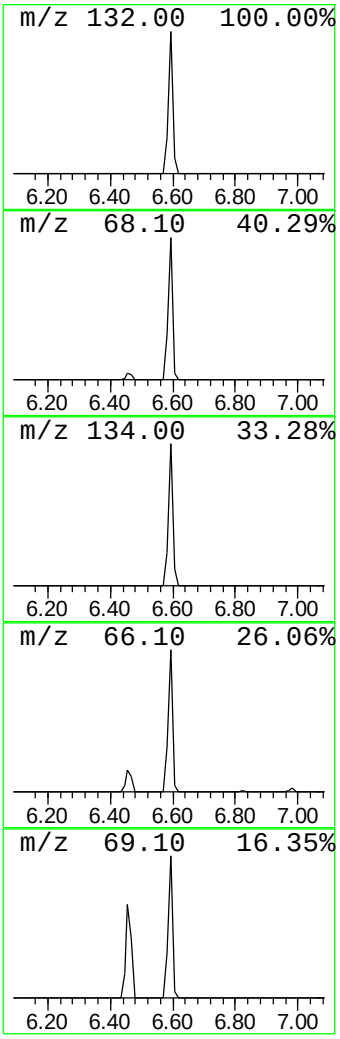
****

Peak Number 6 unknown6.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	71.55 ng	2255470	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

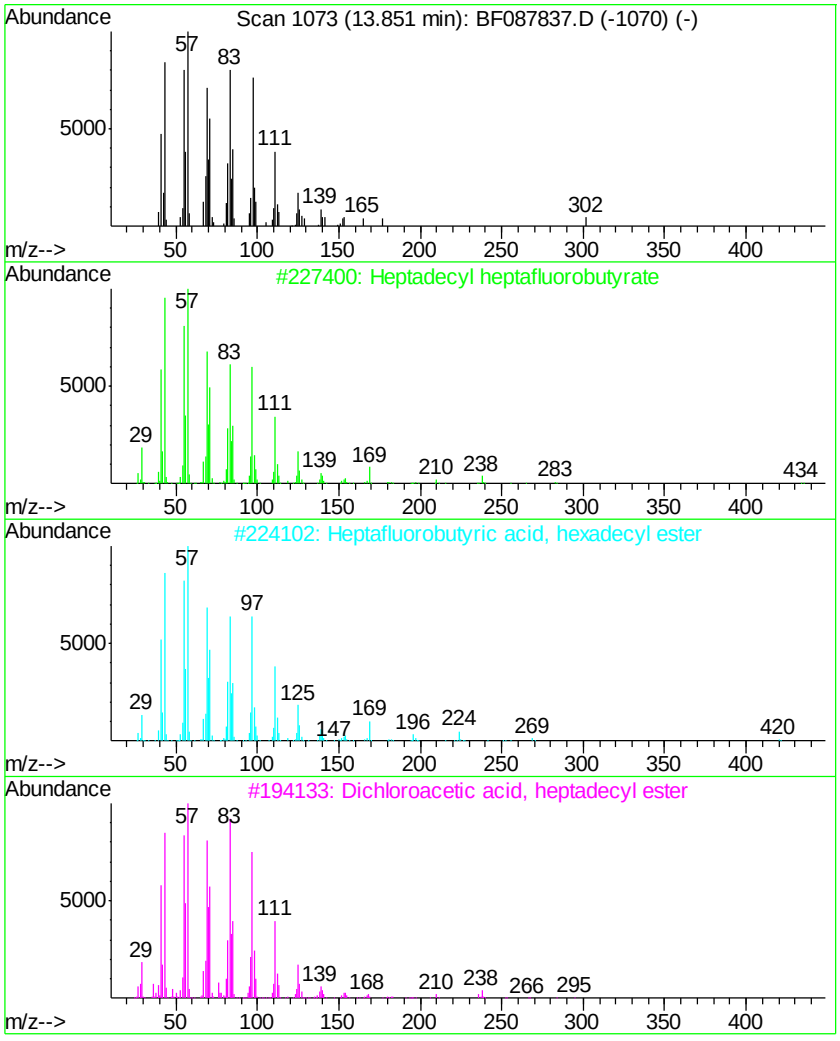
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

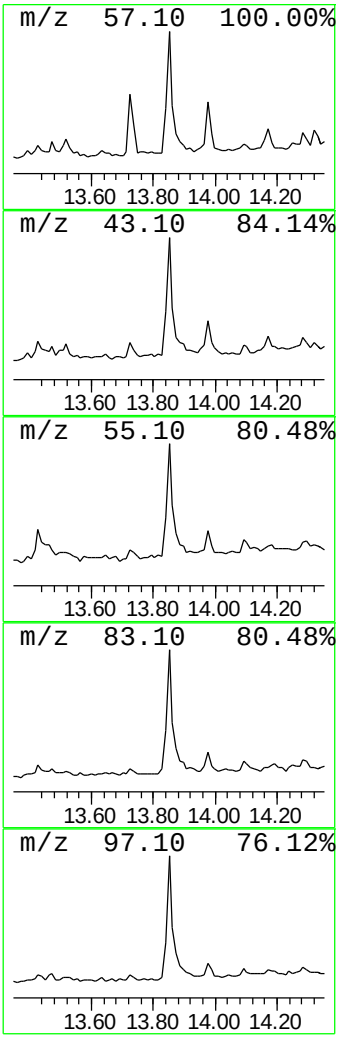
****

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.27 ng	128860	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Operator : UM/SJ
Sample : H3405-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

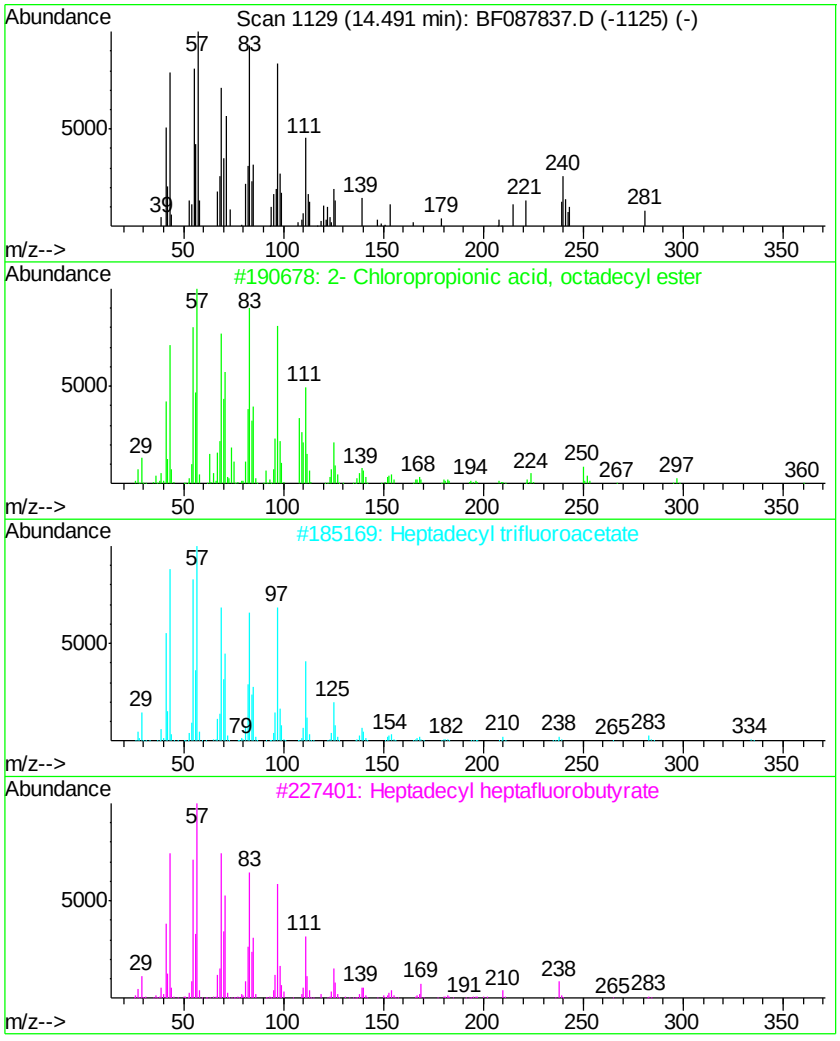
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

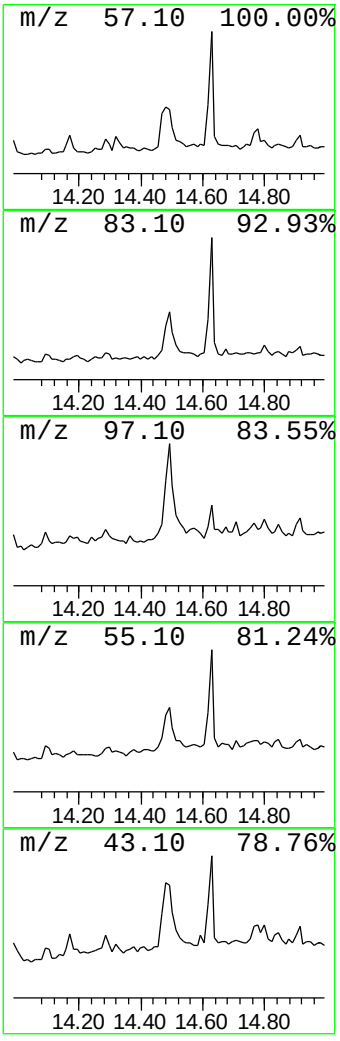
****

Peak Number 10 2- Chloropropionic acid, oc... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.25 ng	88885	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4	1-Heptacosanol	396	C27H56O	002004-39-9	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





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Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

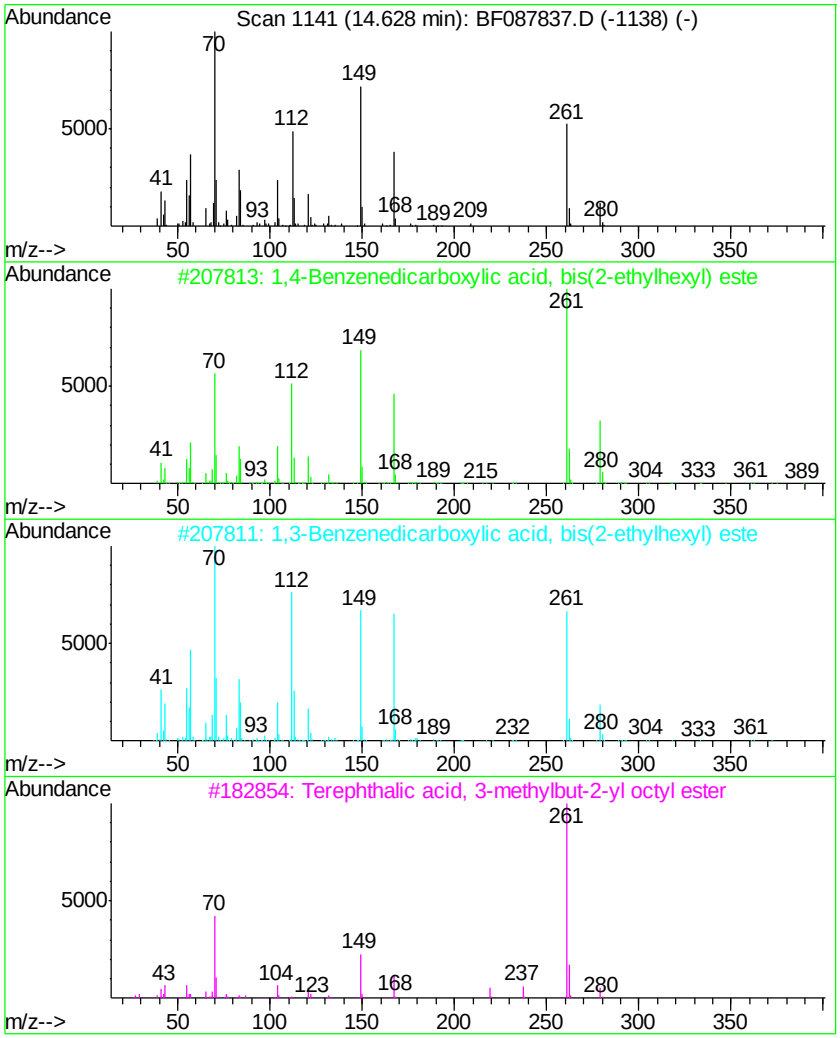
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

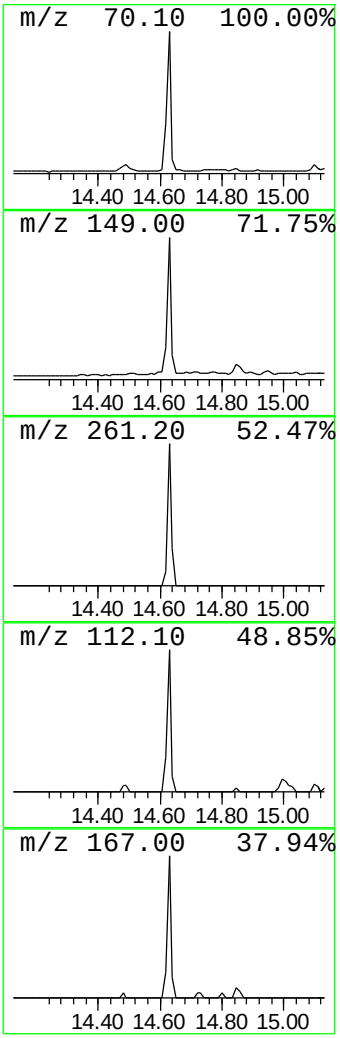
****

Peak Number 11 1,4-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	4.03 ng	158925	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	74
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
4	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	46
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	38





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Instrument : BNA_F
ClientSampleId : SB-05-COMP-0.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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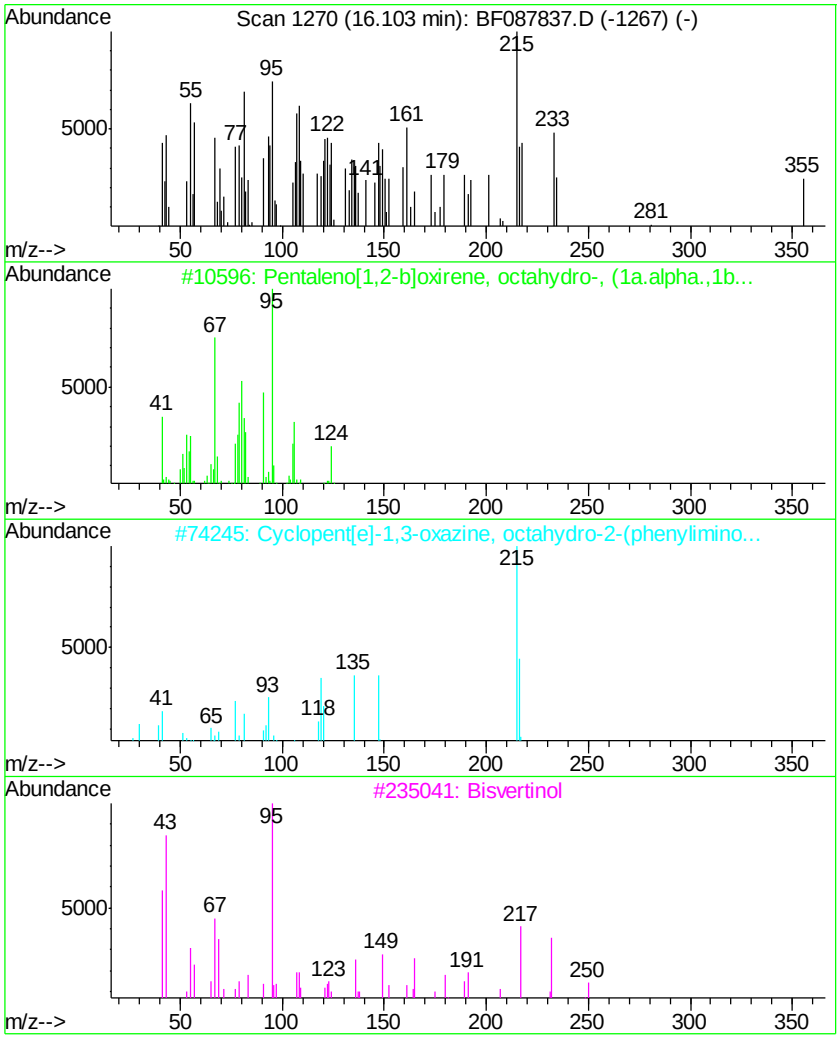
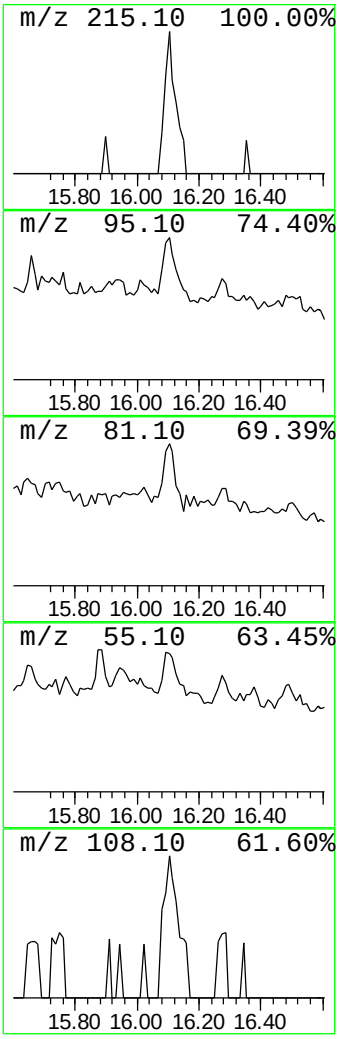
****

Peak Number 12 unknown16.10 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	3.85 ng	97572	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaleno[1,2-b]oxirene, octahyd...	124	C8H12O	055449-70-2	40
2	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	14
3	Bisvertinol	498	C28H34O8	103804-06-4	12
4	2-Amino-5,6-dichloro-1-methylben...	215	C8H7Cl2N3	030486-79-4	12
5	1,2-Dimethyl-4-oxocyclohex-2-ene...	152	C9H12O2	1000187-01-2	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087837.D
Acq On : 9 Jun 2016 6:44
Operator : UM/SJ
Sample : H3405-10
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	1.67	193.3	ng	6094540	1	6.82	630448	20.0
unknown2.07	2.07	16.3	ng	512240	1	6.82	630448	20.0
2-Pentanone, 4-hy...	5.00	5.2	ng	163216	1	6.82	630448	20.0
unknown6.59	6.59	71.5	ng	2255470	1	6.82	630448	20.0
Heptadecyl heptaf...	13.85	3.3	ng	128860	5	13.99	788987	20.0
2- Chloropropioni...	14.49	2.3	ng	88885	5	13.99	788987	20.0
1,4-Benzenedicarb...	14.63	4.0	ng	158925	5	13.99	788987	20.0
unknown16.10	16.10	3.9	ng	97572	6	15.41	506715	20.0