LSC Area Percent Report

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085362.D
Acq On : 11 Mar 2016 5:05
Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

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-BF030316.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	5.144	248	250	257	rBV	207735	316997	6.78%	0.827%
2	5.544	282	285	288	rBV	3552773	3954492	84.53%	10.319%
3	6.573	371	375	377	rBV	3004464	4613958	98.62%	12.040%
4	6.710	384	387	389	rBV	4164096	4678397	100.00%	12.208%
5	6.939	405	407	409	rVB	1133633	937655	20.04%	2.447%
6	7.099	418	421	423	rBV	3560156	3572891	76.37%	9.324%
7	7.499	453	456	459	rBV	2385866	2747092	58.72%	7.169%
8	8.219	517	519	522	rBV	1154086	1106183	23.64%	2.887%
9	9.305	611	614	616	rBV	3491378	4374602	93.51%	11.416%
10	9.693	646	648	650	rBV	819663	769502	16.45%	2.008%
11	9.910	665	667	669	rBV	126151	108448	2.32%	0.283%
12	9.979	671	673	675	rVB	1331350	1187530	25.38%	3.099%
13	10.402	707	710	712	rBV	126473	175070	3.74%	0.457%
14	10.630	727	730	733	rBV	51580	98600	2.11%	0.257%
15	10.768	739	742	744	rBV	2354349	2384792	50.97%	6.223%
16	10.882	750	752	759	rBV	164218	209159	4.47%	0.546%
17	11.328	789	791	792	rBV	75928	64478	1.38%	0.168%
18	11.465	800	803	805	rBV	1088440	1109127	23.71%	2.894%
19	11.979	846	848	851	rBV2	68982	103842	2.22%	0.271%
20	12.676	906	909	911	rBV	45722	60006	1.28%	0.157%
21	12.768	915	917	921	rBV	44588	52702	1.13%	0.138%
22	13.054	939	942	944	rBV	2259502	3197868	68.35%	8.345%
23	13.934	1017	1019	1029	rBV	195322	324745	6.94%	0.847%
24	14.094	1029	1033	1036	rBV	734509	885996	18.94%	2.312%
25	14.574	1073	1075	1082	rBV	55940	113887	2.43%	0.297%
26	15.134	1121	1124	1128	rBV	24121	54368	1.16%	0.142%
27	15.214	1128	1131	1132	rBV	40042	51125	1.09%	0.133%
28	15.557	1158	1161	1164	rBV	595476	751018	16.05%	1.960%
29	16.025	1199	1202	1204	rBV	47083	74028	1.58%	0.193%
30	16.082	1204	1207	1210	rVV2	20674	47132	1.01%	0.123%
31	17.603	1336	1340	1345	rBV4	36772	108140	2.31%	0.282%
32	18.631	1426	1430	1438	rBV6	23231	87322	1.87%	0.228%

LSC Area Percent Report

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085362.D
Acq On : 11 Mar 2016 5:05
Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

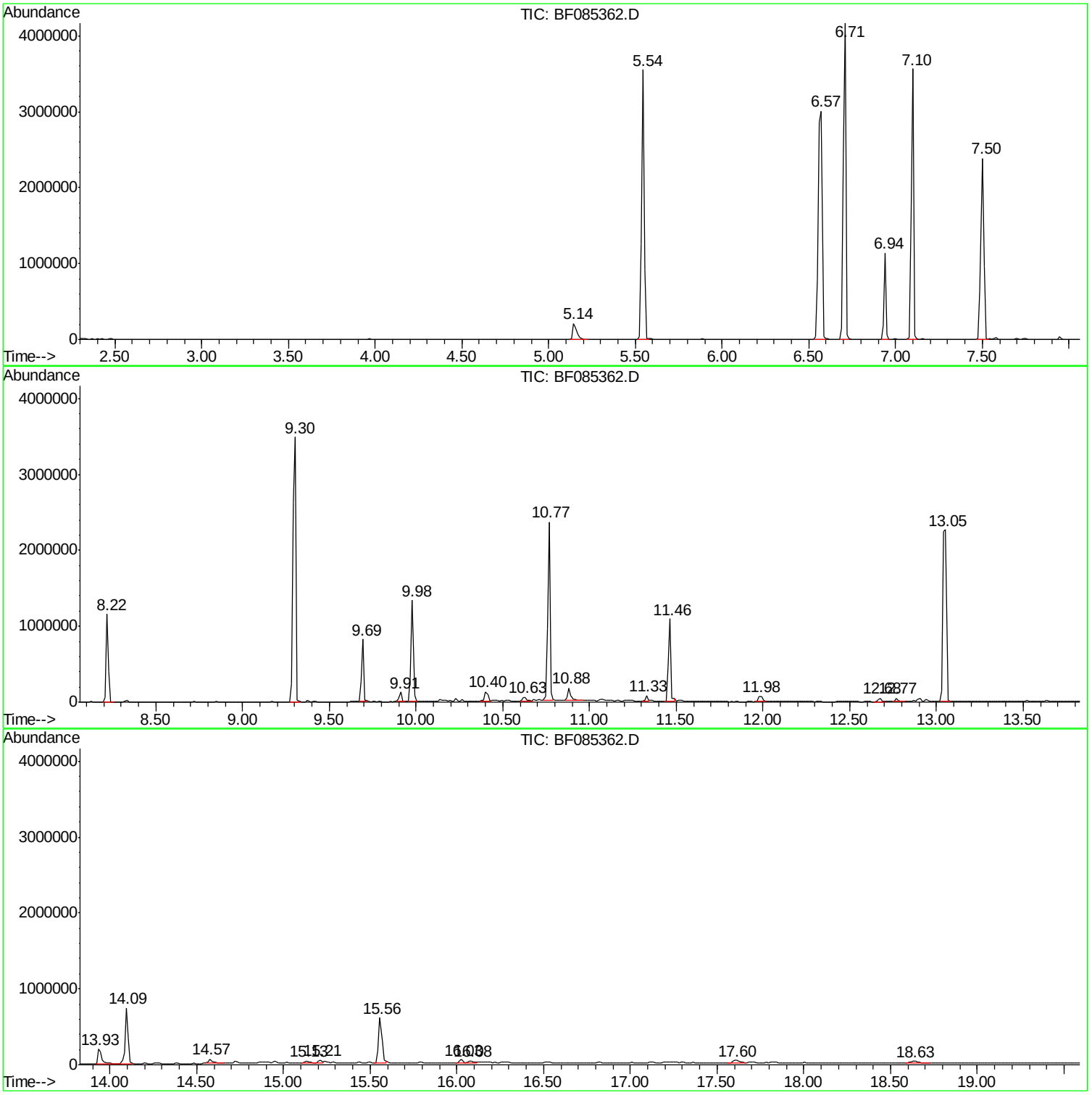
Sum of corrected areas: 38321152

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085362.D
Acq On : 11 Mar 2016 5:05
Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

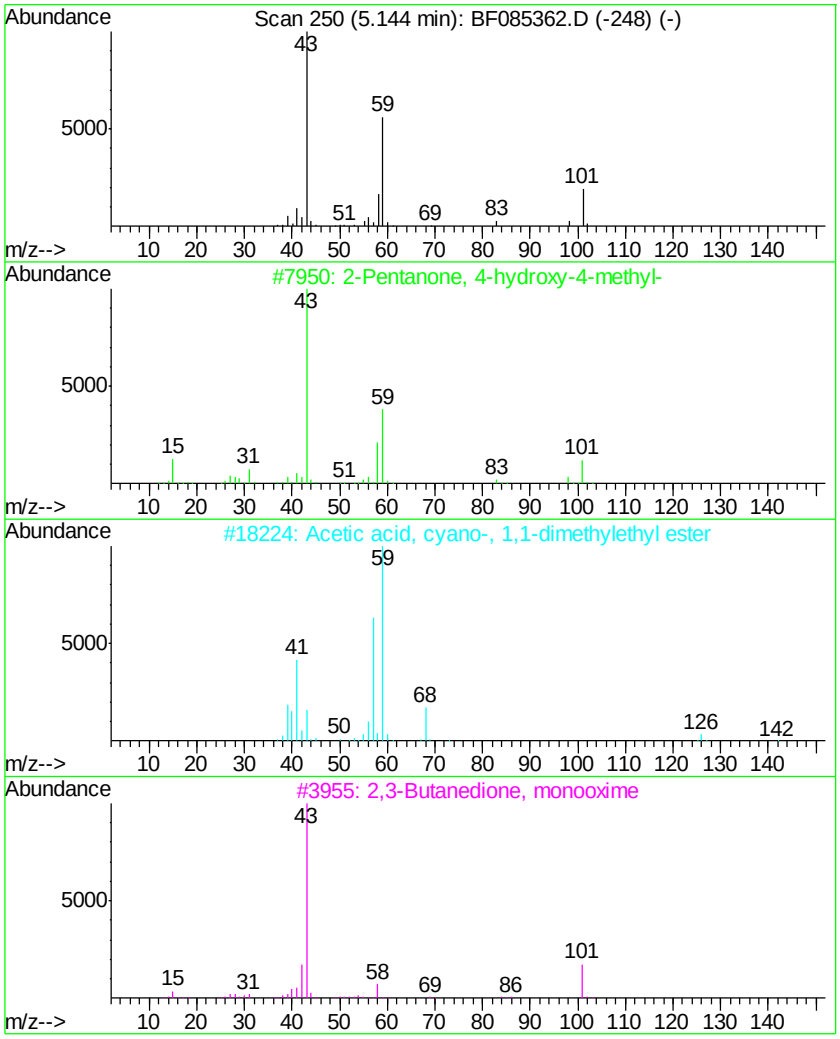
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

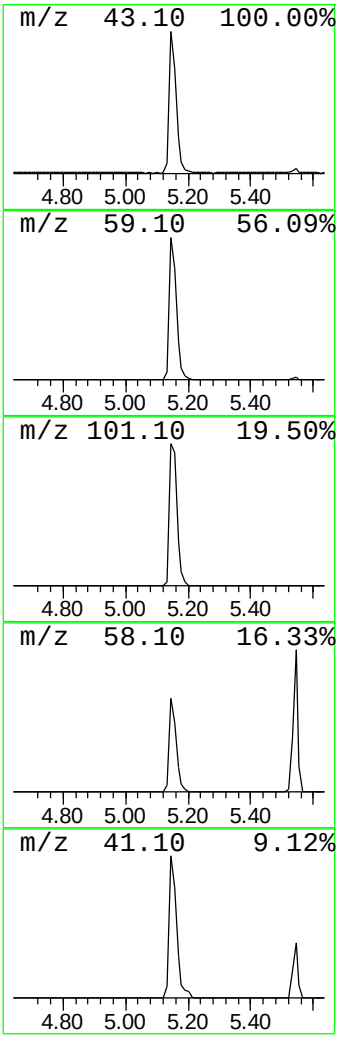
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.76 ng	316997	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane	58	C4H10	000106-97-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF085362.D
Acq On : 11 Mar 2016 5:05
Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

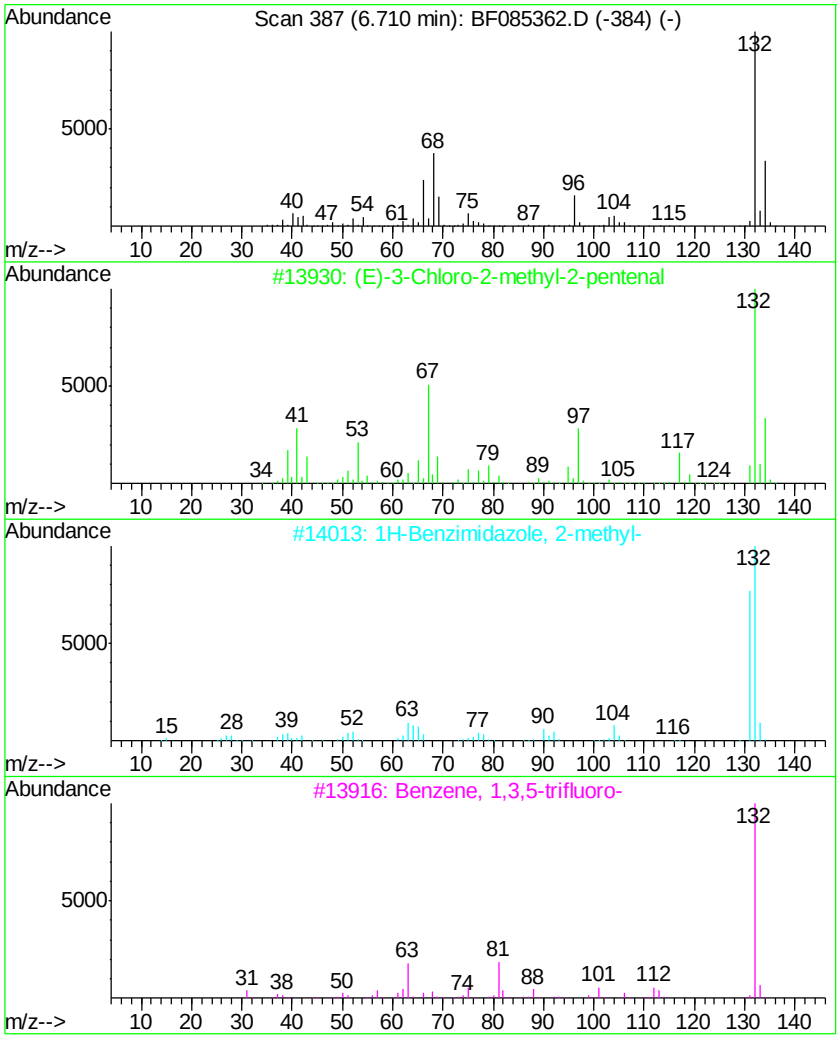
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

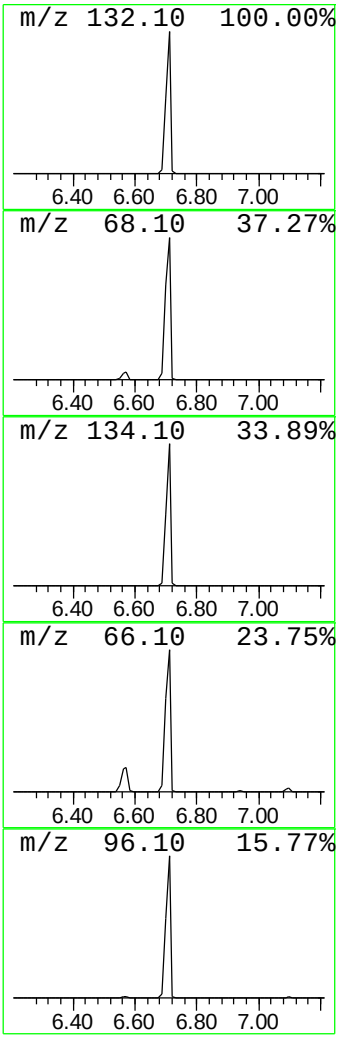
****

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	99.79 ng	4678400	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : H1731-06
Misc :
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Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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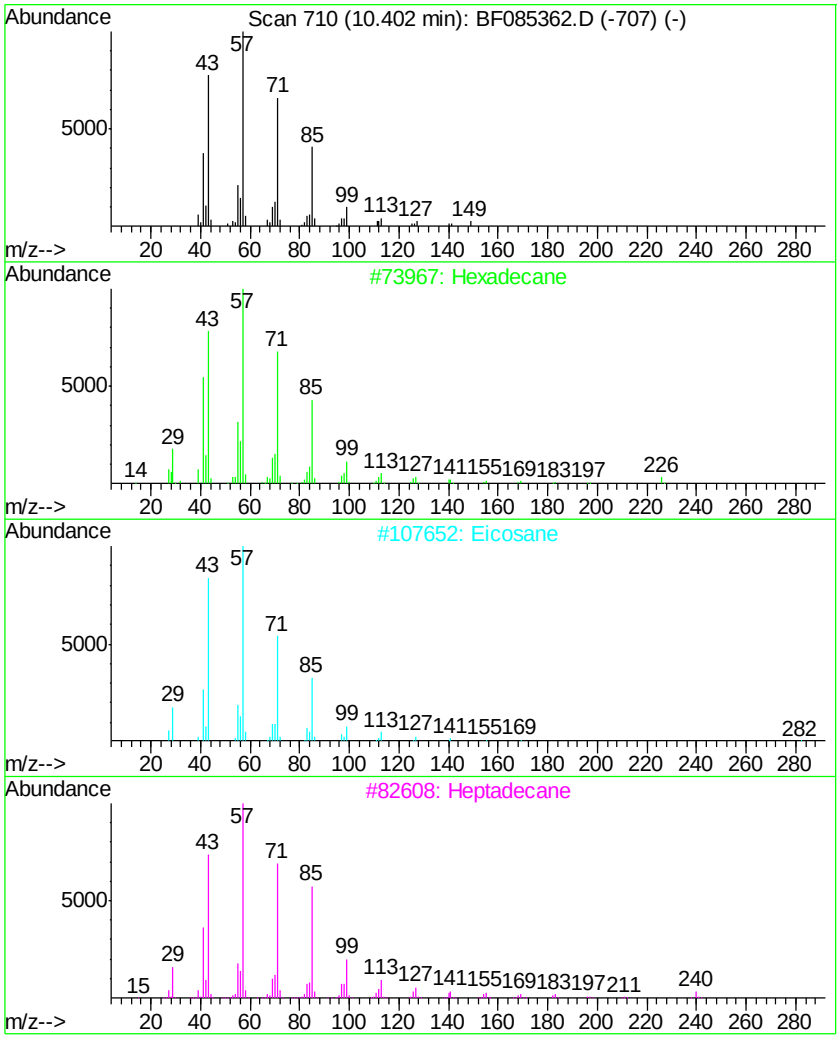
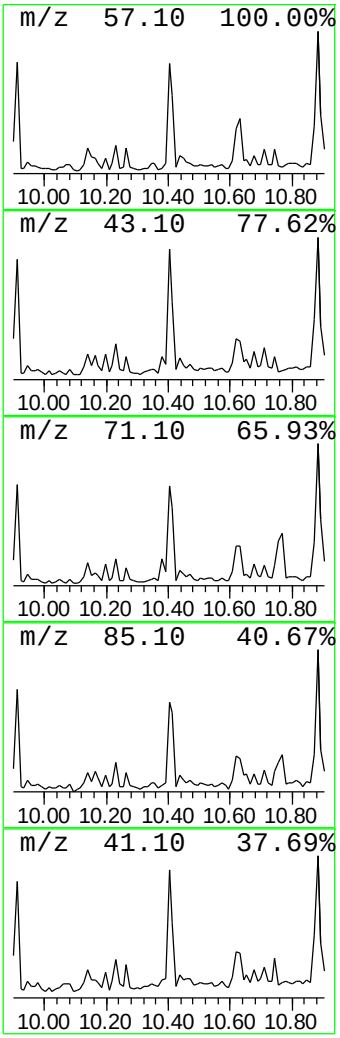
Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.95 ng	175070	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Tridecane	184	C13H28	000629-50-5	86
5	Pentadecane	212	C15H32	000629-62-9	86





Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085362.D
Acq On : 11 Mar 2016 5:05
Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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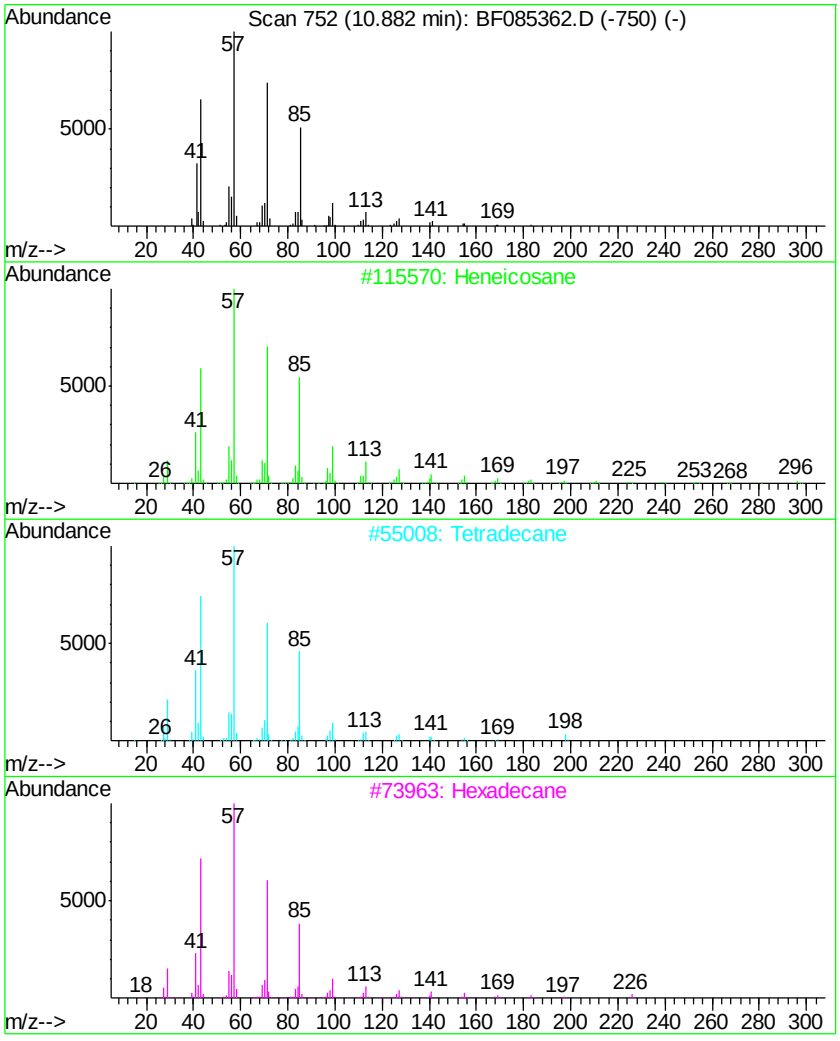
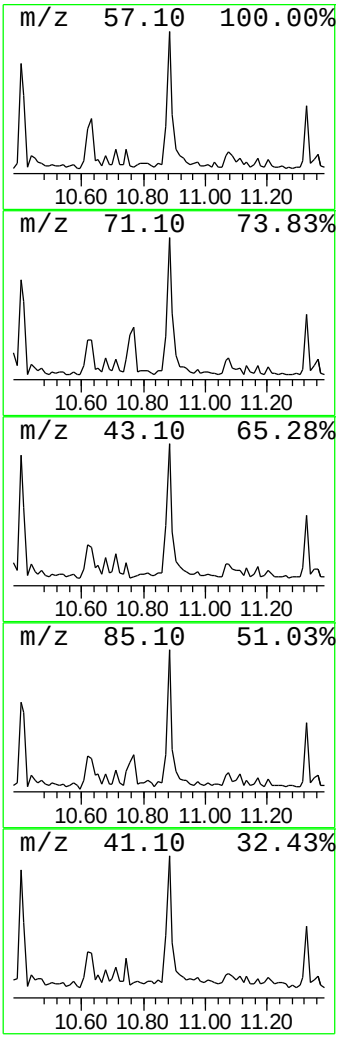
Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	3.77 ng	209159	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetradecane	198	C14H30	000629-59-4	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





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Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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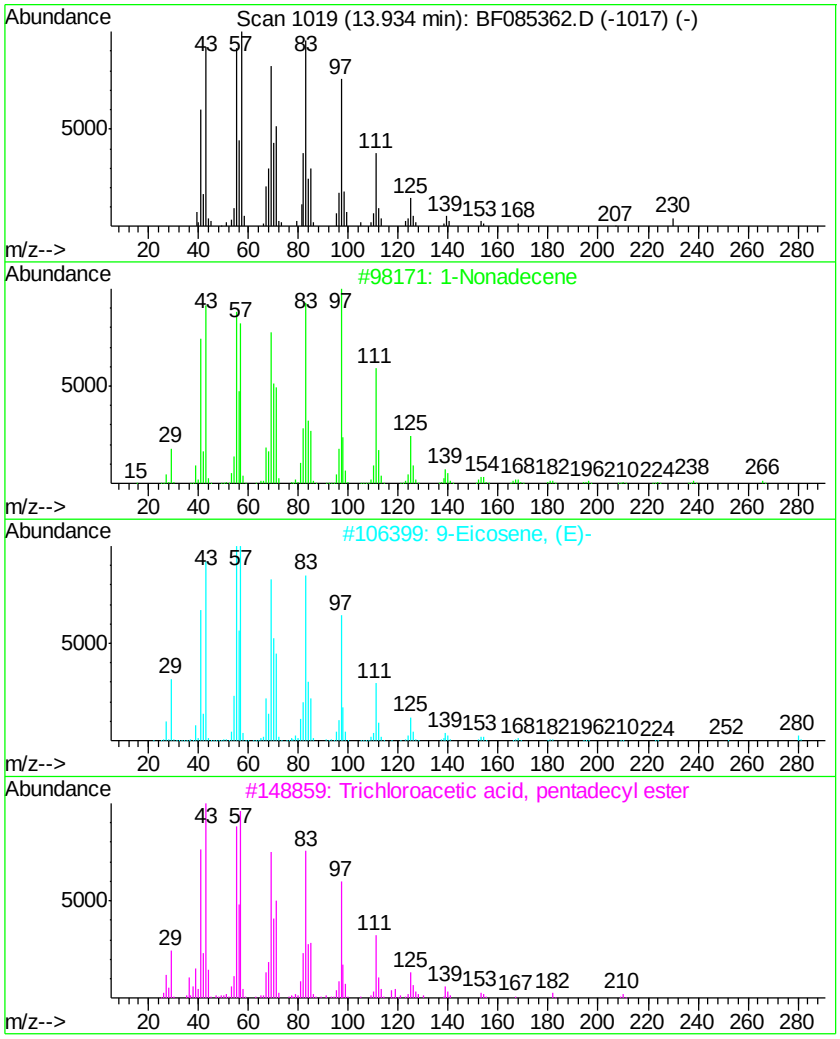
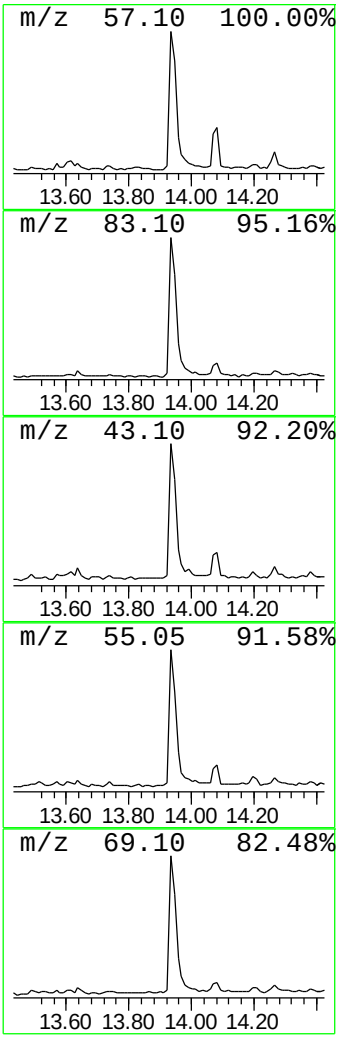
Peak Number 6 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	7.33 ng	324745	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





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Sample : H1731-06
Misc :
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Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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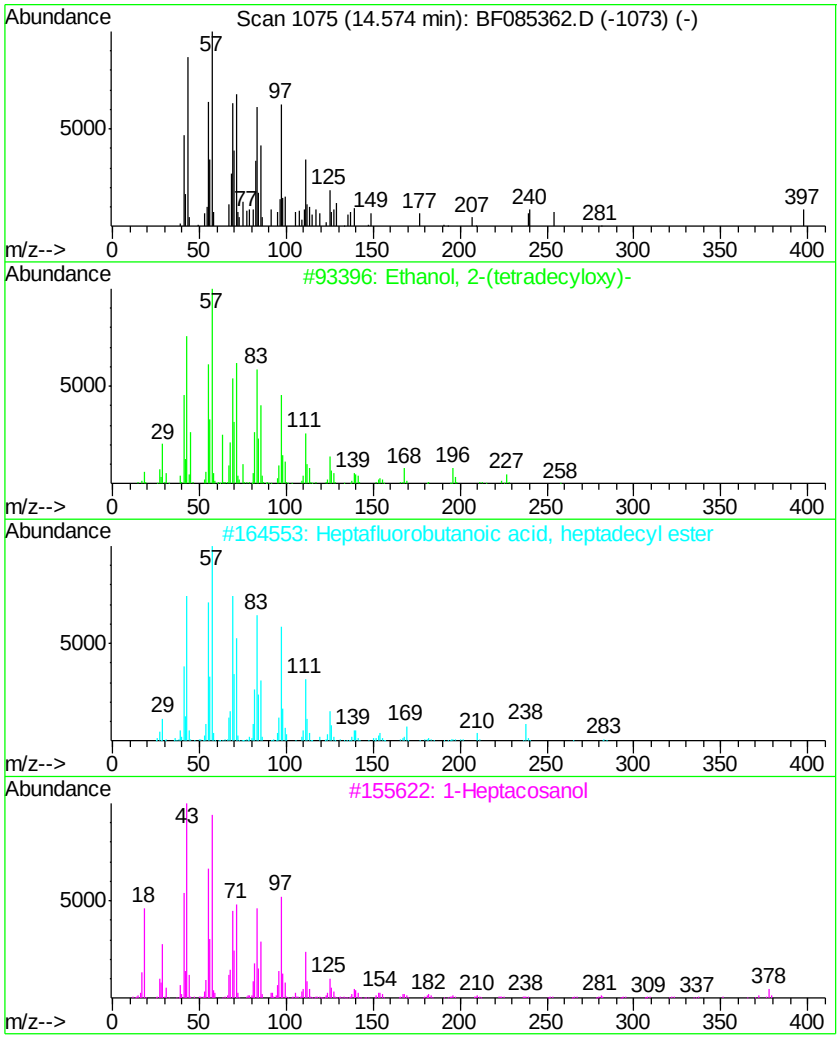
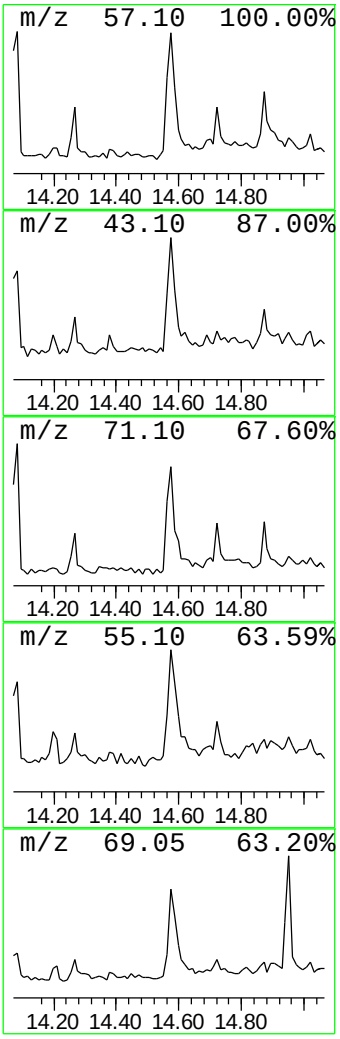
Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.57 ng	113887	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
3	1-Heptacosanol	396	C27H56O	002004-39-9	86
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	83
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	83





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Data File : BF085362.D
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Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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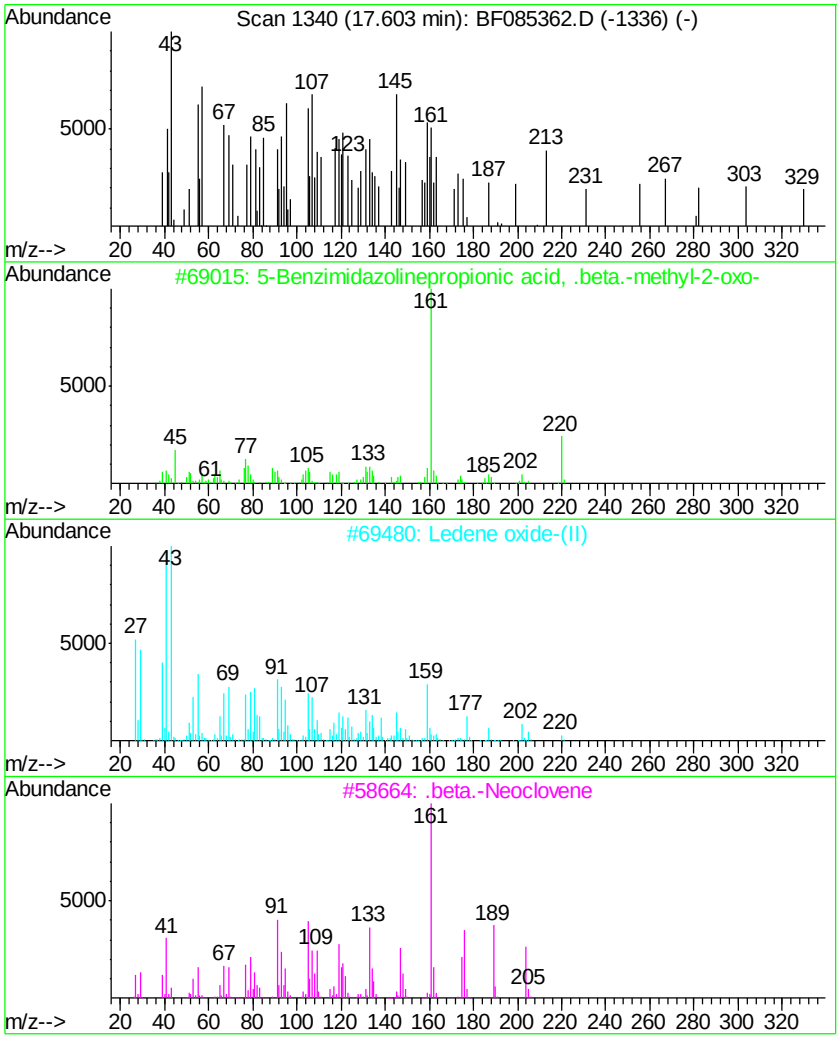
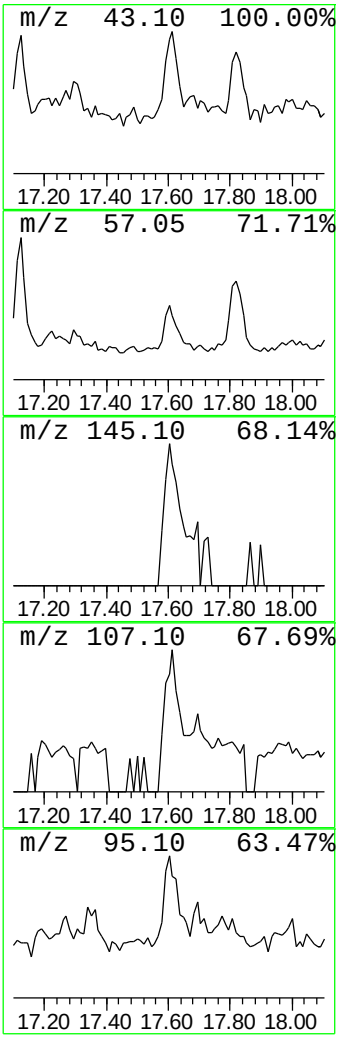
Peak Number 8 unknown17.60 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	2.88 ng	108140	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Benzimidazolinepropionic acid,...	220	C11H12N2O3	021190-17-0	35
2	Ledene oxide-(II)	220	C15H24O	1000159-36-7	35
3	.beta.-Neoclovene	204	C15H24	056684-96-9	22
4	2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	22
5	Lactic acid, pentamethylbenzyl e...	250	C15H22O3	019405-32-4	17





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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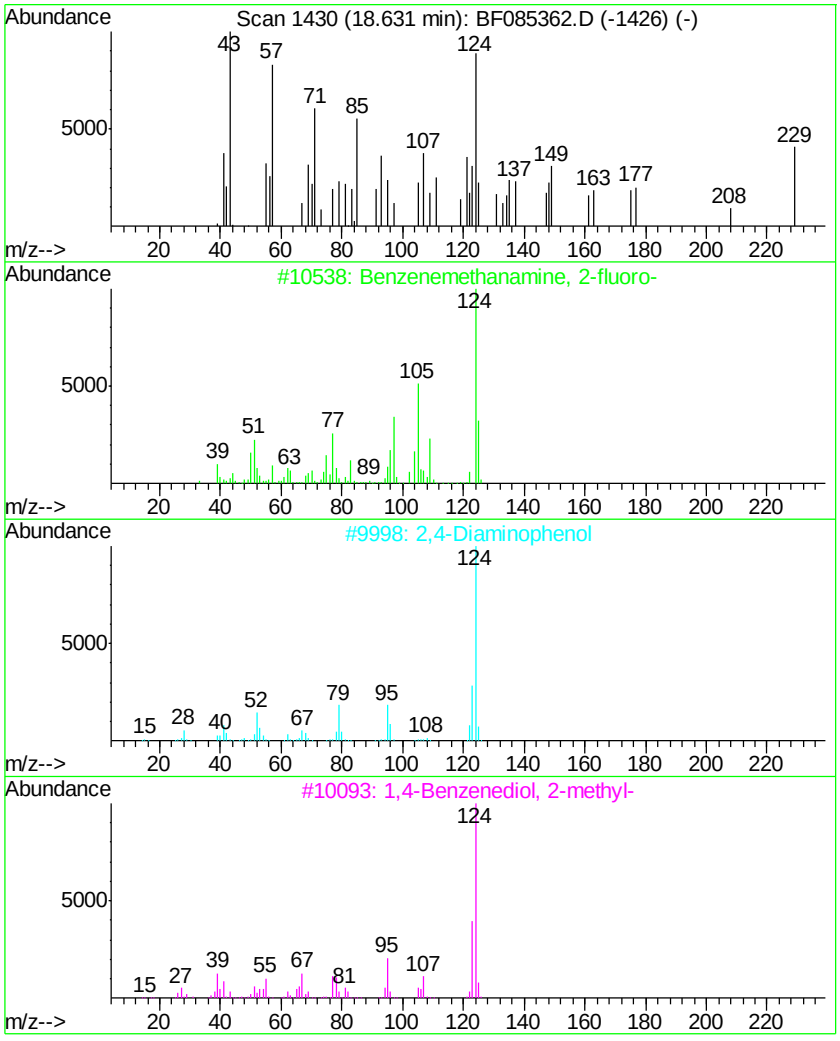
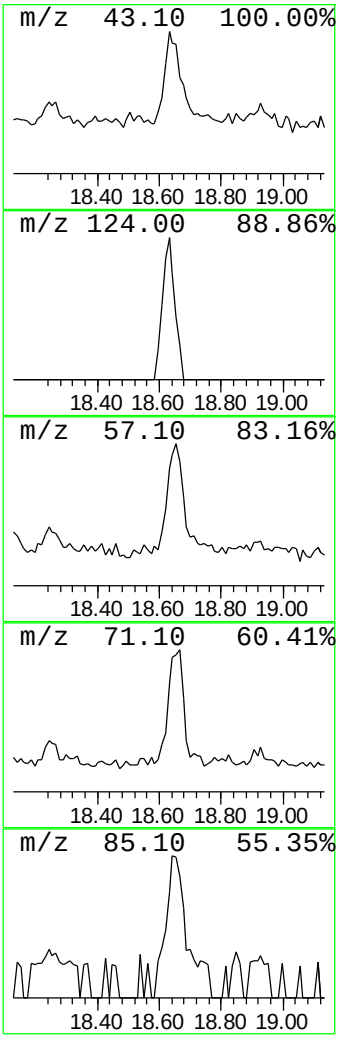
Peak Number 9 unknown18.63 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.63	2.33 ng	87322	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanamine, 2-fluoro-	125	C7H8FN	000089-99-6	25
2	2,4-Diaminophenol	124	C6H8N2O	000095-86-3	18
3	1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	14
4	4,5-Pyrimidinediamine, 6-methyl-	124	C5H8N4	022715-28-2	14
5	Homatropine	275	C16H21NO3	000087-00-3	14





Tentatively Identified Compound (LSC) summary

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085362.D
Acq On : 11 Mar 2016 5:05
Operator : UM/SJ
Sample : H1731-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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
2-Pentanone, 4-hy...	5.14	6.8	ng	316997	1	6.94	937655	20.0
unknown6.71	6.71	99.8	ng	4678400	1	6.94	937655	20.0
Hexadecane	10.40	3.0	ng	175070	3	9.98	1187530	20.0
Heneicosane	10.88	3.8	ng	209159	4	11.46	1109130	20.0
1-Nonadecene	13.93	7.3	ng	324745	5	14.09	885996	20.0
Ethanol, 2-(tetra...	14.57	2.6	ng	113887	5	14.09	885996	20.0
unknown17.60	17.60	2.9	ng	108140	6	15.56	751018	20.0
unknown18.63	18.63	2.3	ng	87322	6	15.56	751018	20.0