LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100615\
Data File : BF082094.D
Acq On : 6 Oct 2015 20:12
Operator : UM/IZ
Sample : G3906-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

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-BF092815.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	5.074	253	257	267	rVB	822550	1311498	50.65%	5.546%
2	5.486	290	293	295	rBV	2215076	2464090	95.17%	10.420%
3	6.514	380	383	386	rBV	1802774	2249804	86.89%	9.514%
4	6.652	392	395	397	rBV	2626757	2589215	100.00%	10.949%
5	6.880	413	415	418	rBV	552833	479393	18.51%	2.027%
6	7.040	426	429	431	rBV	2191596	2043160	78.91%	8.640%
7	7.452	462	465	467	rBV	1486103	1481984	57.24%	6.267%
8	8.172	525	528	530	rBV	589648	606577	23.43%	2.565%
9	9.246	619	622	625	rBV	2759395	2559681	98.86%	10.824%
10	9.646	654	657	659	rBV	300803	375111	14.49%	1.586%
11	9.921	679	681	684	rBV	580399	684371	26.43%	2.894%
12	10.355	715	719	720	rBV	31944	42332	1.63%	0.179%
13	10.721	748	751	753	rBV	1576040	1732821	66.92%	7.327%
14	10.823	758	760	765	rVB	61164	77132	2.98%	0.326%
15	11.269	797	799	800	rBV	45374	38353	1.48%	0.162%
16	11.304	800	802	805	rVB	21907	29068	1.12%	0.123%
17	11.418	809	812	814	rBV	506332	674818	26.06%	2.854%
18	11.932	854	857	861	rBV3	24965	48712	1.88%	0.206%
19	12.629	916	918	920	rBV	51525	76437	2.95%	0.323%
20	12.858	935	938	941	rBV	59176	96161	3.71%	0.407%
21	13.007	948	951	953	rBV	1793644	2365439	91.36%	10.003%
22	13.898	1027	1029	1035	rBV	83332	160916	6.21%	0.680%
23	14.047	1040	1042	1049	rVV	388157	643945	24.87%	2.723%
24	15.087	1130	1133	1136	rBV2	30284	74375	2.87%	0.315%
25	15.441	1162	1164	1167	rBV	27147	42980	1.66%	0.182%
26	15.510	1167	1170	1174	rVV	309818	513093	19.82%	2.170%
27	16.184	1226	1229	1233	rVB	31261	73637	2.84%	0.311%
28	16.595	1263	1265	1273	rVB2	28448	74429	2.87%	0.315%
29	17.156	1312	1314	1319	rVB5	18044	38728	1.50%	0.164%

Sum of corrected areas: 23648260

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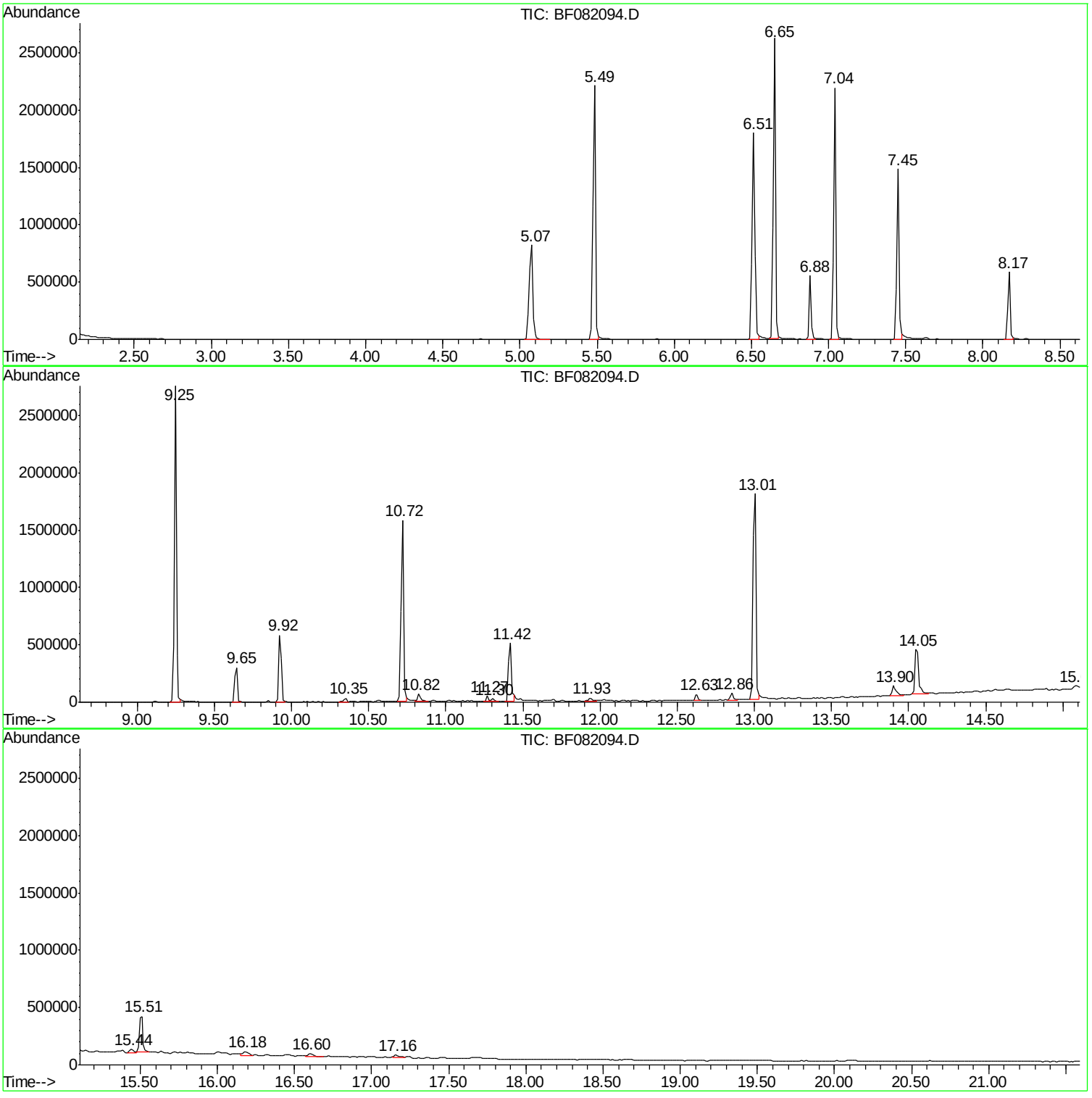
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100615\
Data File : BF082094.D
Acq On : 6 Oct 2015 20:12
Operator : UM/IZ
Sample : G3906-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

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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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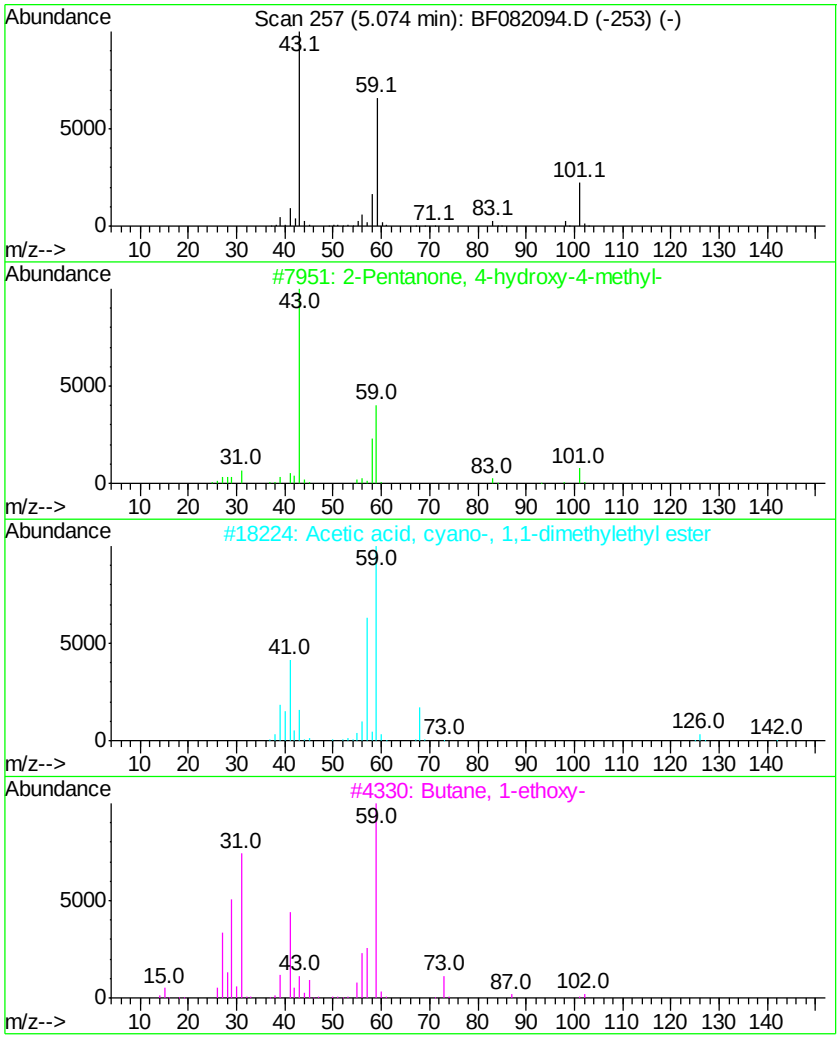
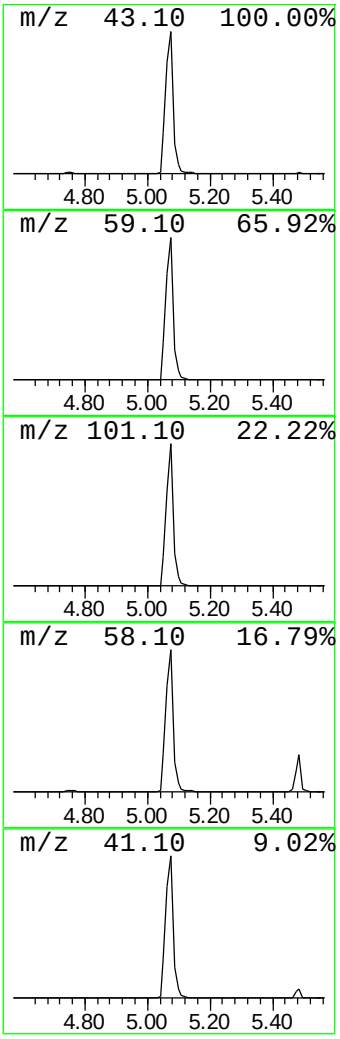
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	54.71 ng	1311500	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Acq On : 6 Oct 2015 20:12
Operator : UM/IZ
Sample : G3906-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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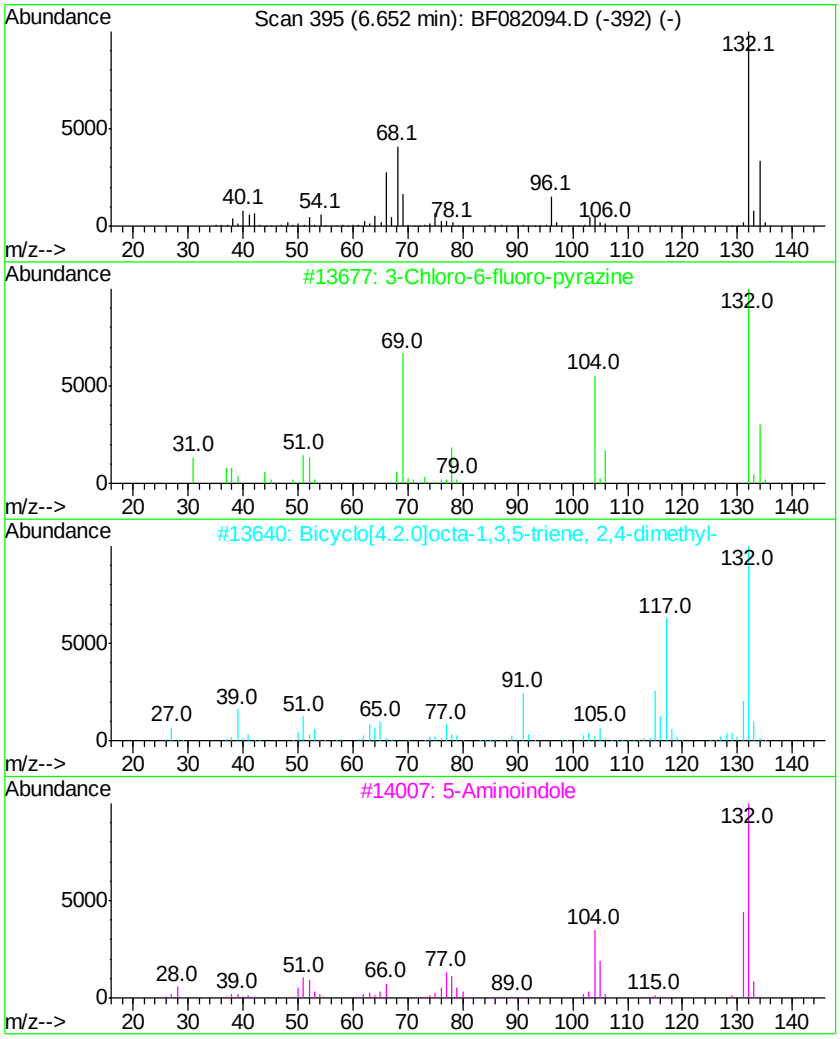
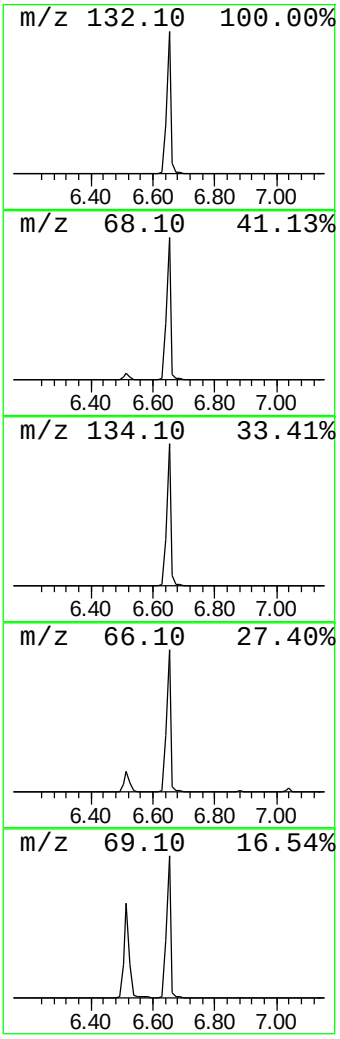
Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	108.02 ng	2589220	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	5-Aminoindole	132	C8H8N2	005192-03-0	9
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\BF100615\
Data File : BF082094.D
Acq On : 6 Oct 2015 20:12
Operator : UM/IZ
Sample : G3906-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
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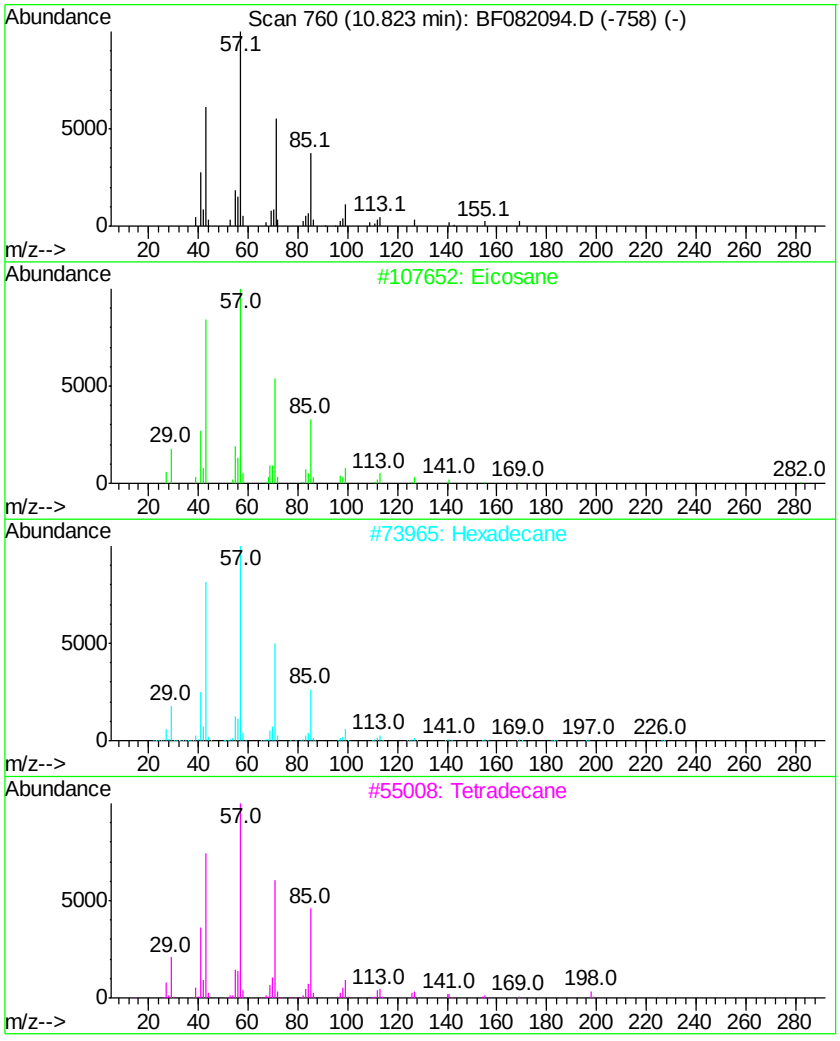
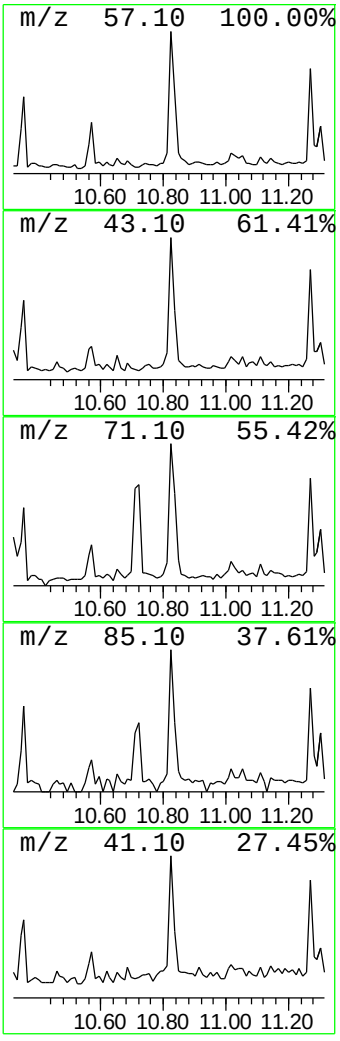
Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	2.29 ng	77132	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecane	198	C14H30	000629-59-4	86
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100615\
Data File : BF082094.D
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Sample : G3906-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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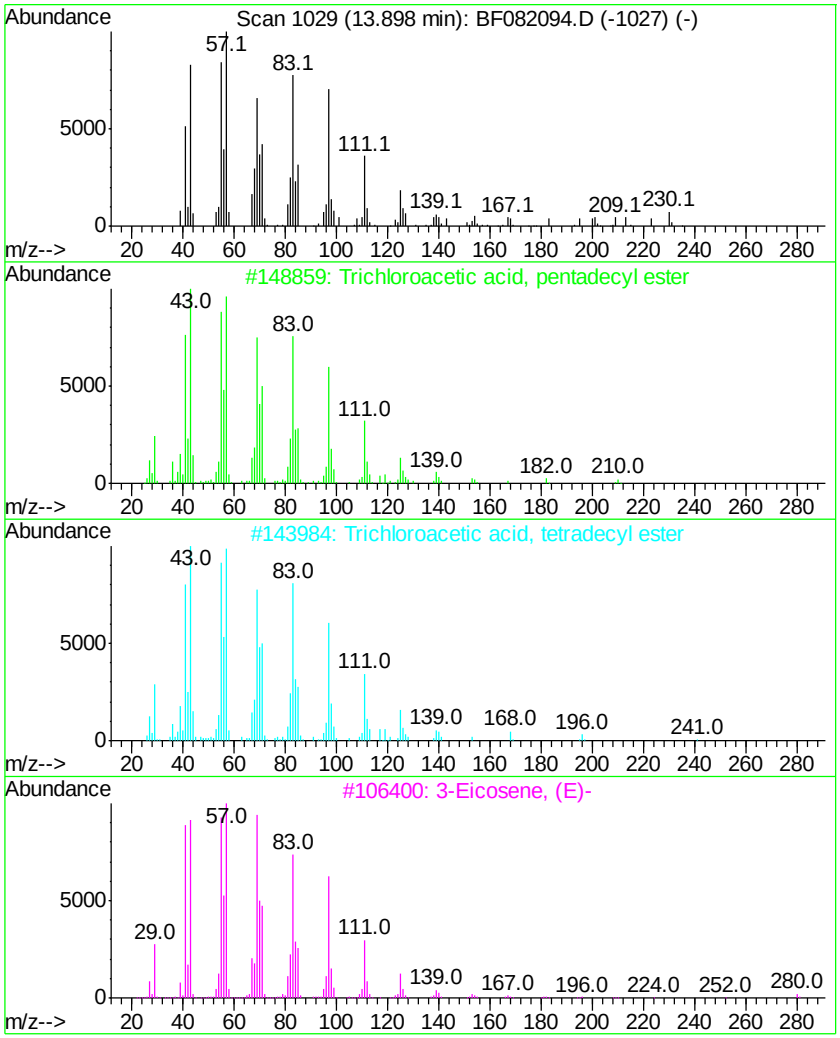
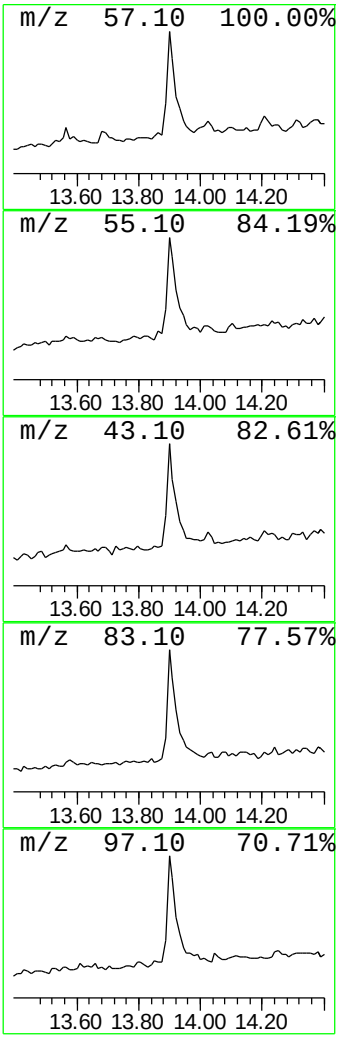
Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	5.00 ng	160916	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	1-Eicosanol	298	C20H42O	000629-96-9	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100615\
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Acq On : 6 Oct 2015 20:12
Operator : UM/IZ
Sample : G3906-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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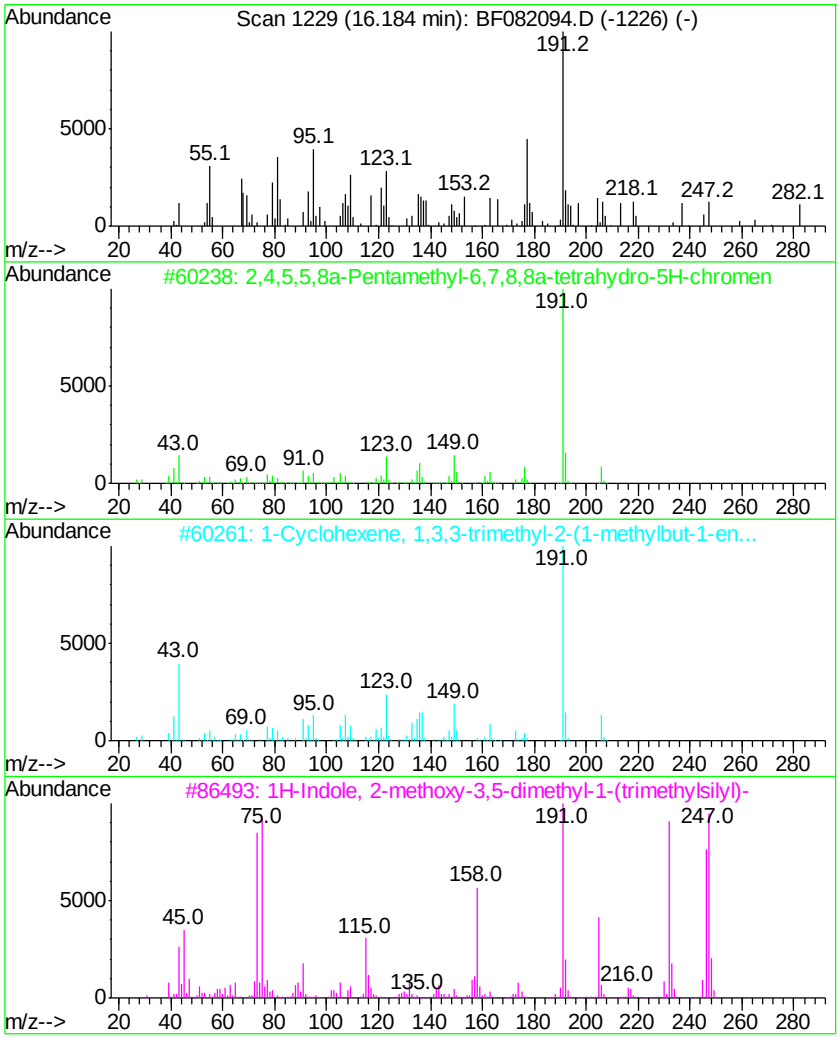
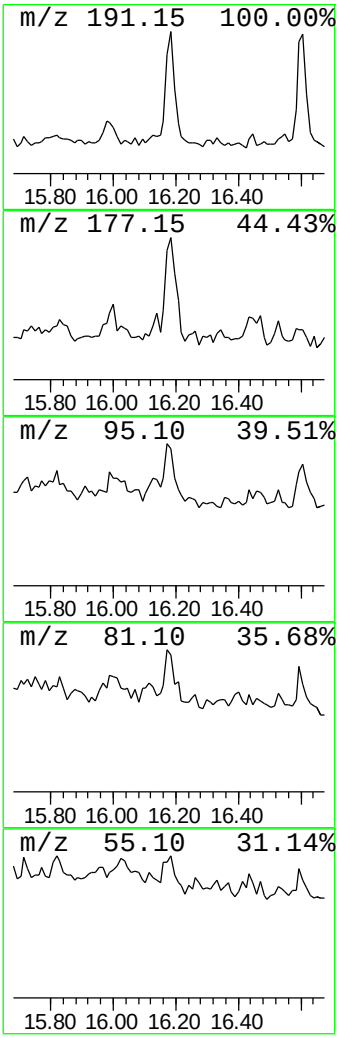
Peak Number 7 2,4,5,5,8a-Pentamethyl-6,7,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.87 ng	73637	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	60
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	55
3	1H-Indole, 2-methoxy-3,5-dimethy...	247	C14H21NOSi	074367-60-5	41
4	3-(5-Fluoro-1,3-dioxo-1,3-dihydr...	237	C11H8FNO4	1000278-27-9	30
5	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	27





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Misc :
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Instrument : BNA_F
ClientSampleId : IM-MLA-DGA-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
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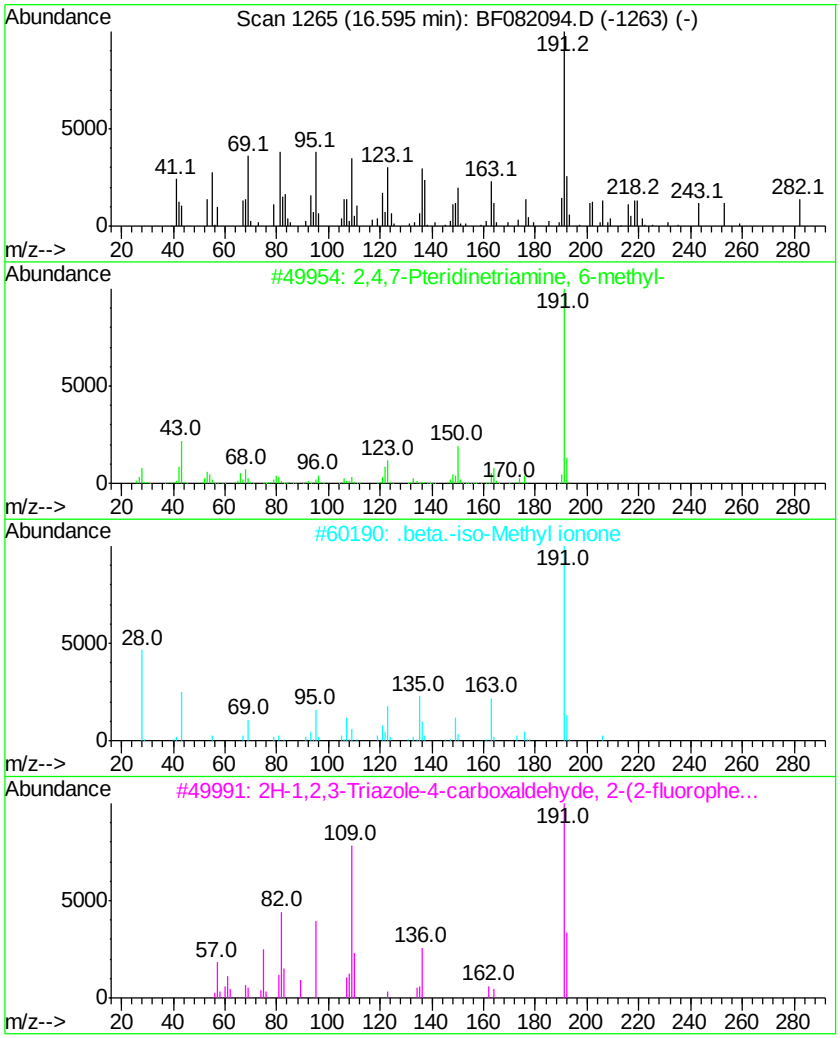
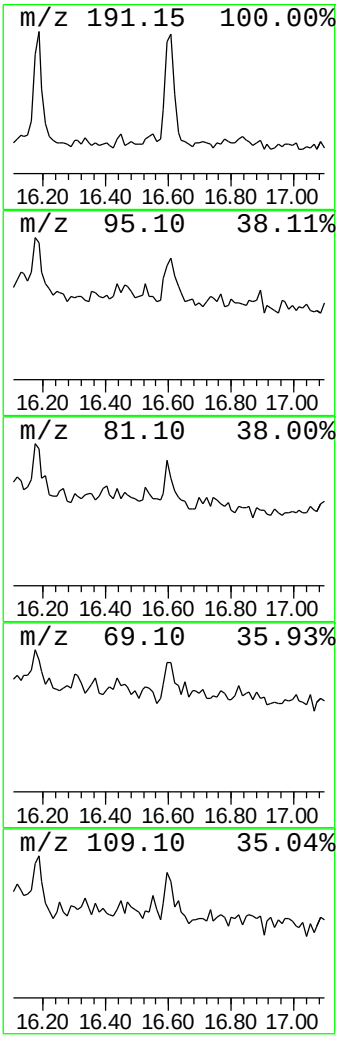
Peak Number 8 unknown16.60 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	2.90 ng	74429	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	38
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	37
3	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	37
4	2-(2-Hydroxyethylimino)-3,6-dime...	222	C11H14N2OS	068720-70-7	35
5	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.07	54.7	ng	1311500	1	6.88	479393	20.0
unknown6.65	6.65	108.0	ng	2589220	1	6.88	479393	20.0
Eicosane	10.82	2.3	ng	77132	4	11.42	674818	20.0
Trichloroacetic a...	13.90	5.0	ng	160916	5	14.06	643945	20.0
2,4,5,5,8a-Pentam...	16.18	2.9	ng	73637	6	15.51	513093	20.0
unknown16.60	16.60	2.9	ng	74429	6	15.51	513093	20.0