LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081514.D
Acq On : 6 Sep 2015 17:22
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

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-BF090115.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	4.399	243	246	263	rVB	508811	1004646	56.92%	6.826%
2	4.913	288	291	293	rBV	1413756	1765153	100.00%	11.993%
3	6.033	386	389	391	rBV	1616272	1679194	95.13%	11.409%
4	6.124	395	397	400	rBV	1582001	1576579	89.32%	10.712%
5	6.353	415	417	420	rVB	327037	324494	18.38%	2.205%
6	6.513	428	431	433	rBV	1259347	1077063	61.02%	7.318%
7	6.936	465	468	470	rBV	1040466	1024031	58.01%	6.957%
8	7.645	528	530	533	rBV	455626	397639	22.53%	2.702%
9	8.730	622	625	627	rBV	1786245	1528322	86.58%	10.384%
10	9.130	658	660	663	rBV	256751	251691	14.26%	1.710%
11	9.382	680	682	685	rVB2	301311	358902	20.33%	2.438%
12	10.171	748	751	754	rBV	929977	850109	48.16%	5.776%
13	10.319	762	764	768	rVB	26804	29606	1.68%	0.201%
14	10.765	801	803	804	rBV	26397	22207	1.26%	0.151%
15	10.856	808	811	814	rBV	252866	370436	20.99%	2.517%
16	11.428	859	861	862	rBV	63767	59928	3.40%	0.407%
17	11.451	862	863	867	rVB2	16648	27621	1.56%	0.188%
18	12.045	913	915	918	rVB	130158	111517	6.32%	0.758%
19	12.262	932	934	936	rBV	81751	111138	6.30%	0.755%
20	12.342	938	941	942	rBV	23740	38478	2.18%	0.261%
21	12.434	947	949	952	rBV	983362	1106407	62.68%	7.517%
22	12.605	960	964	966	rVB	14162	22929	1.30%	0.156%
23	13.359	1028	1030	1036	rBV2	70028	116752	6.61%	0.793%
24	13.462	1036	1039	1040	rBV2	287427	361732	20.49%	2.458%
25	13.577	1045	1049	1052	rVV2	7442	18623	1.06%	0.127%
26	13.679	1055	1058	1063	rBV2	11124	23032	1.30%	0.156%
27	13.988	1081	1085	1089	rVB4	8557	19646	1.11%	0.133%
28	14.445	1123	1125	1129	rBV	53147	95357	5.40%	0.648%
29	14.674	1143	1145	1147	rBV	31712	32681	1.85%	0.222%
30	14.720	1147	1149	1151	rVB	44529	39124	2.22%	0.266%
31	14.765	1151	1153	1158	rBV	182060	210789	11.94%	1.432%
32	15.234	1189	1194	1197	rBV3	5282	19003	1.08%	0.129%
33	15.840	1244	1247	1252	rVB2	13996	22526	1.28%	0.153%
34	16.160	1272	1275	1279	rBV	11165	21200	1.20%	0.144%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081514.D
Acq On : 6 Sep 2015 17:22
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

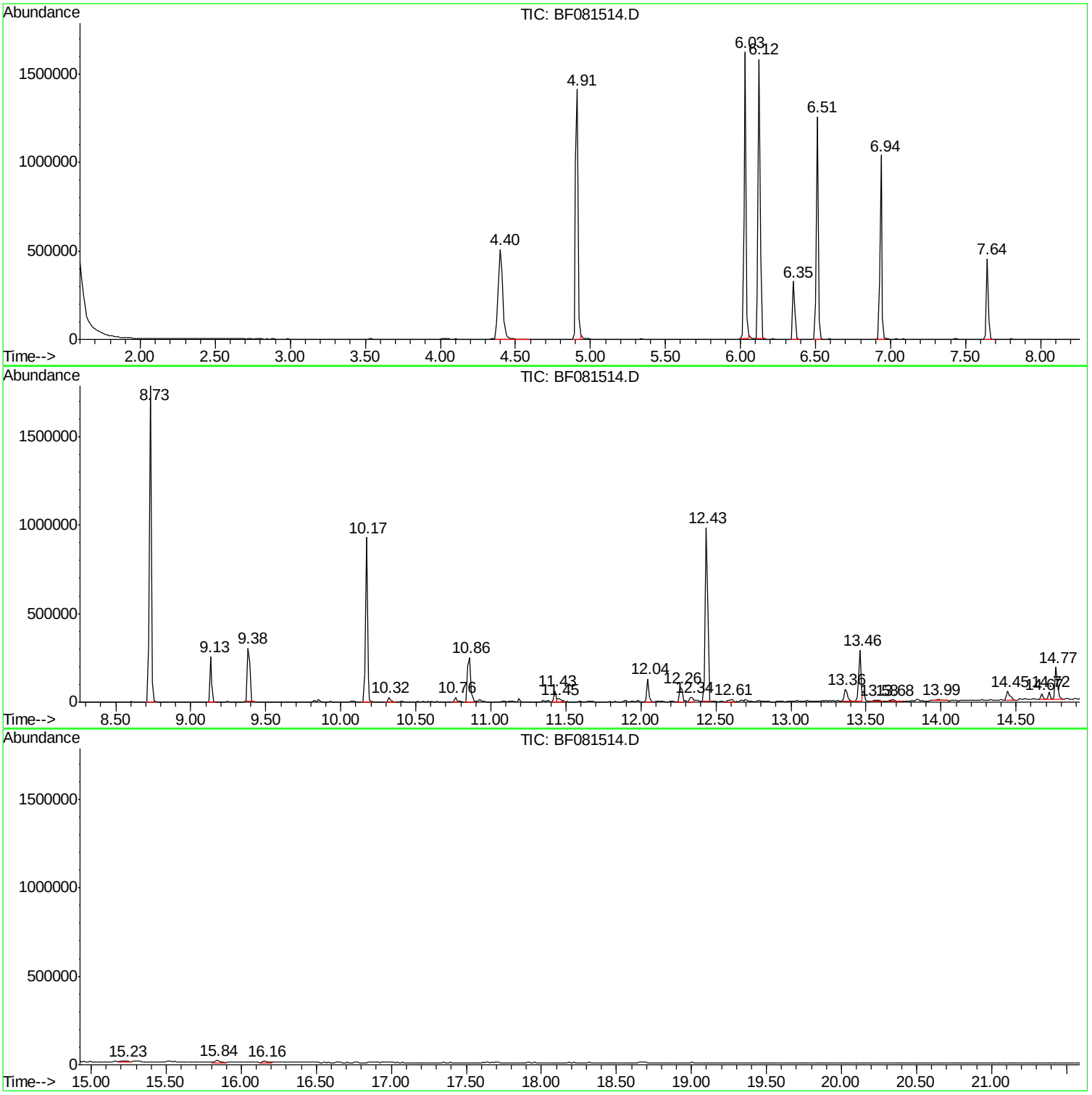
Sum of corrected areas: 14718555

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081514.D
Acq On : 6 Sep 2015 17:22
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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Acq On : 6 Sep 2015 17:22
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

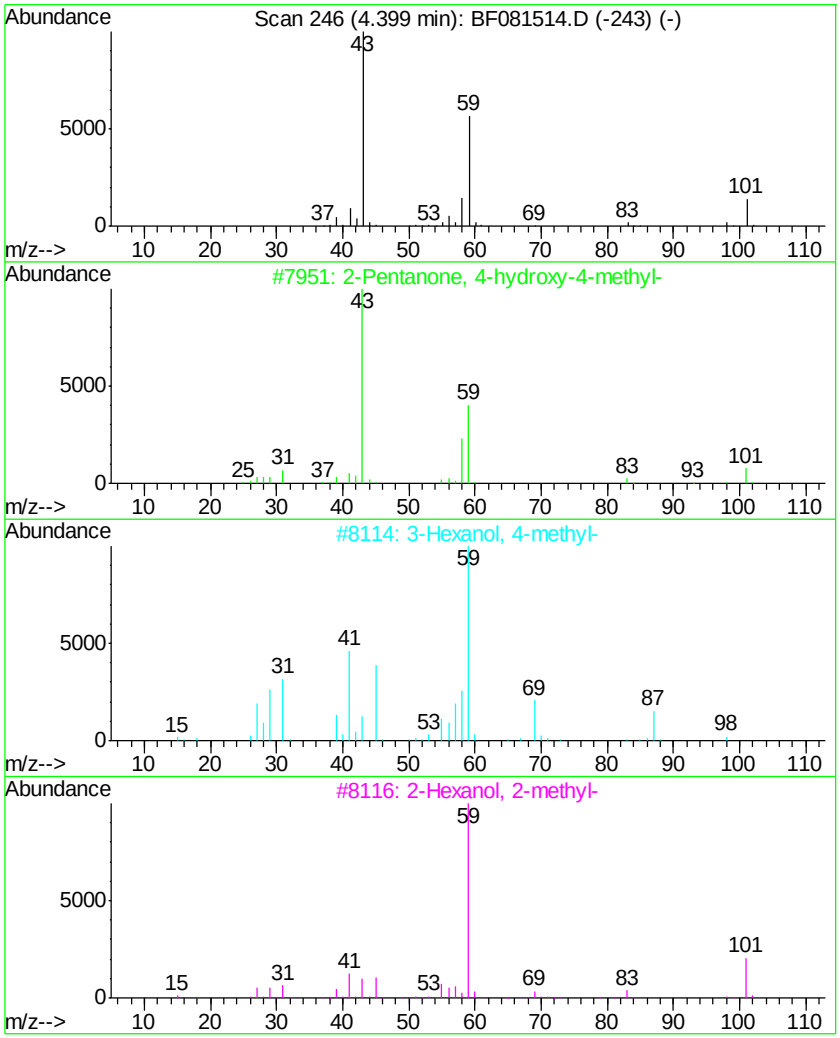
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

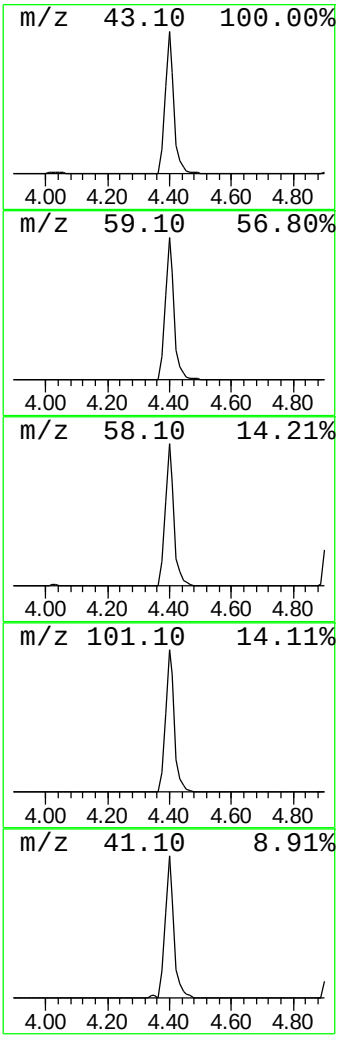
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	61.92 ng	1004650	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081514.D
Acq On : 6 Sep 2015 17:22
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

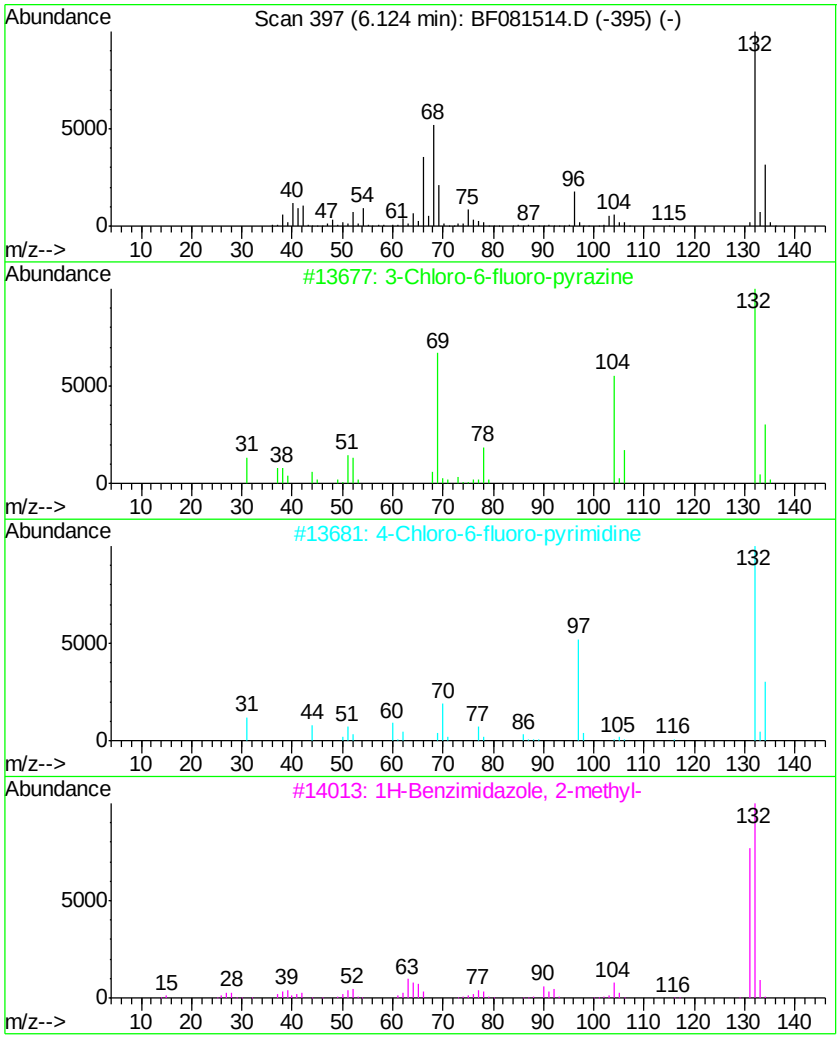
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

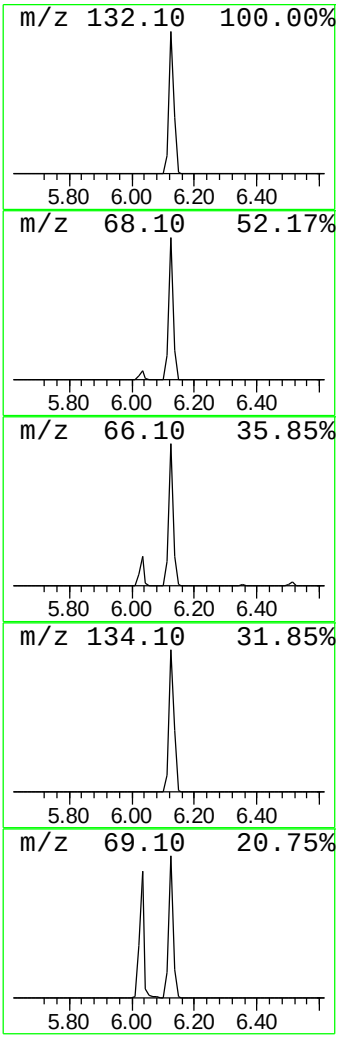
****

Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	97.17 ng	1576580	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081514.D
Acq On : 6 Sep 2015 17:22
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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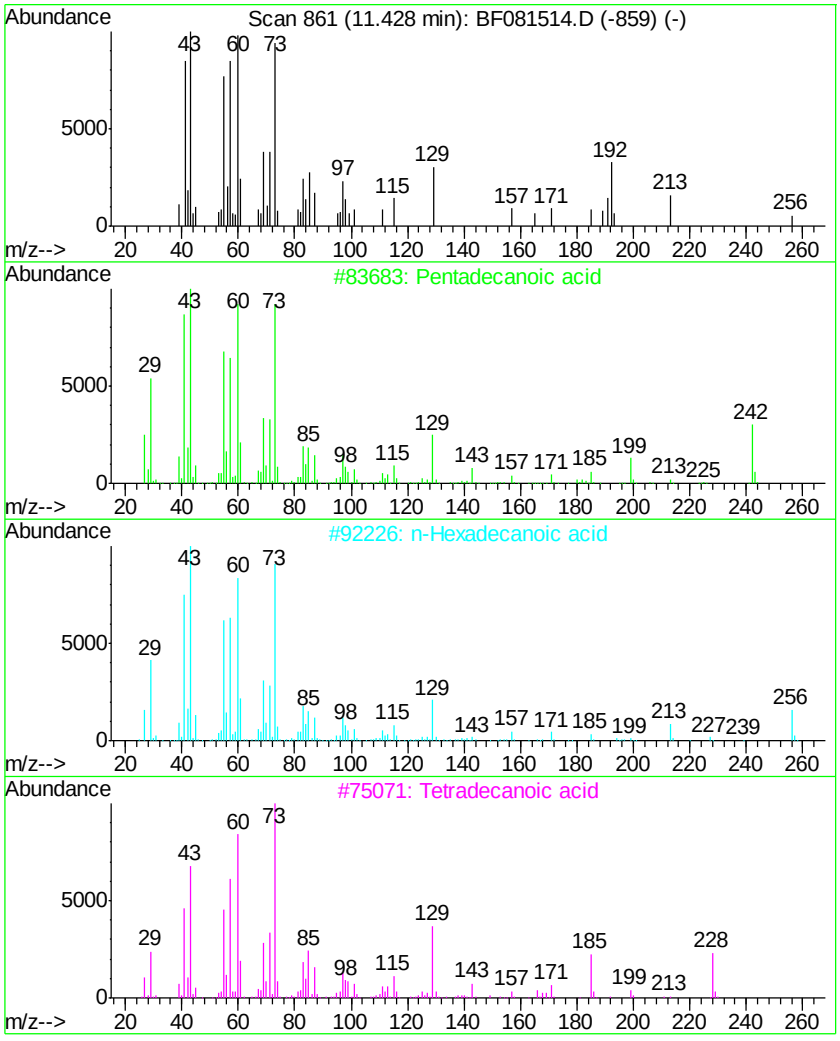
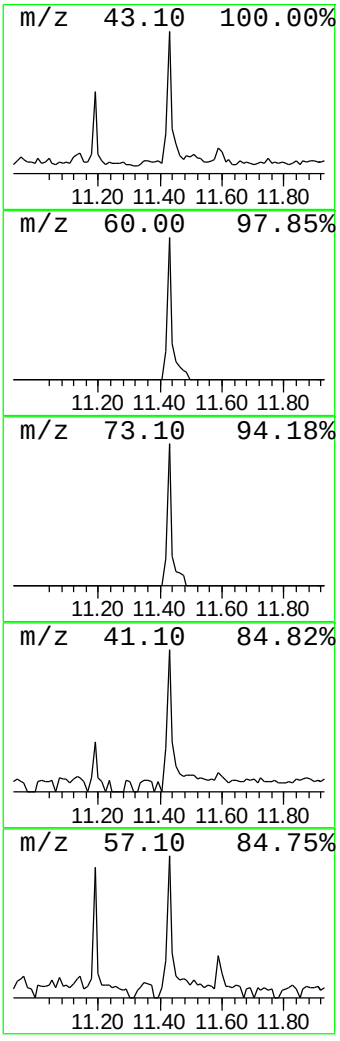
Peak Number 4 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	3.24 ng	59928	Phenanthrene-d10	10.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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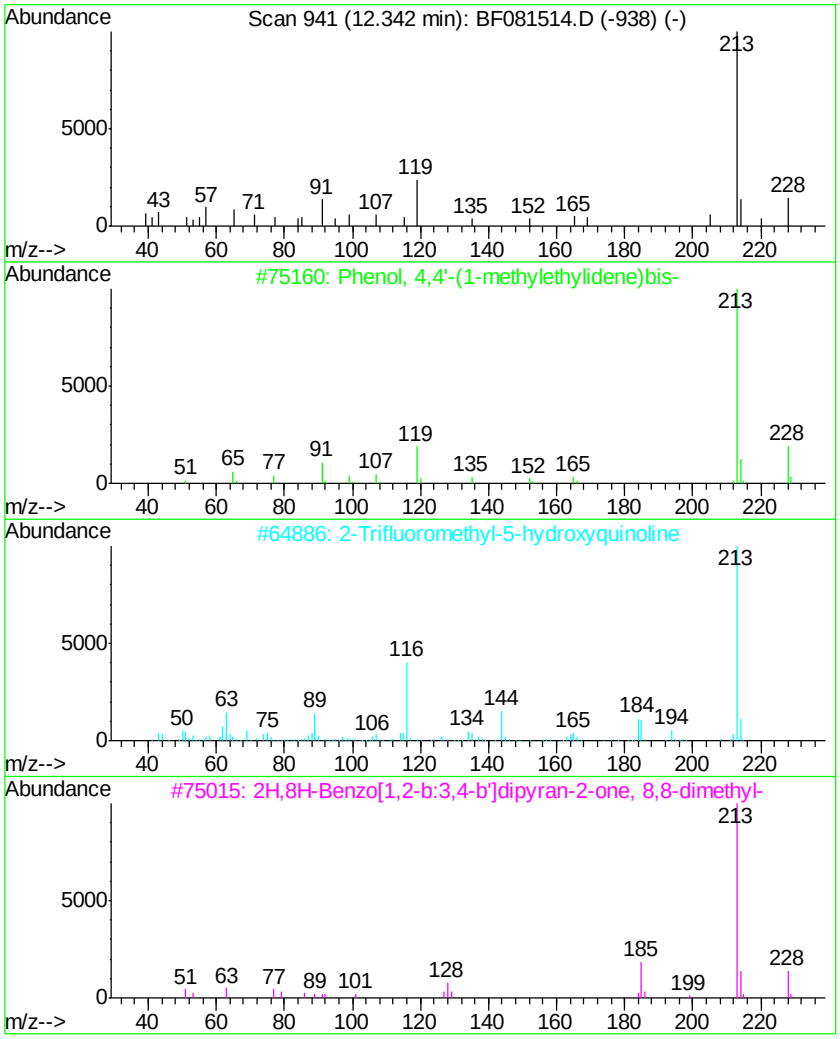
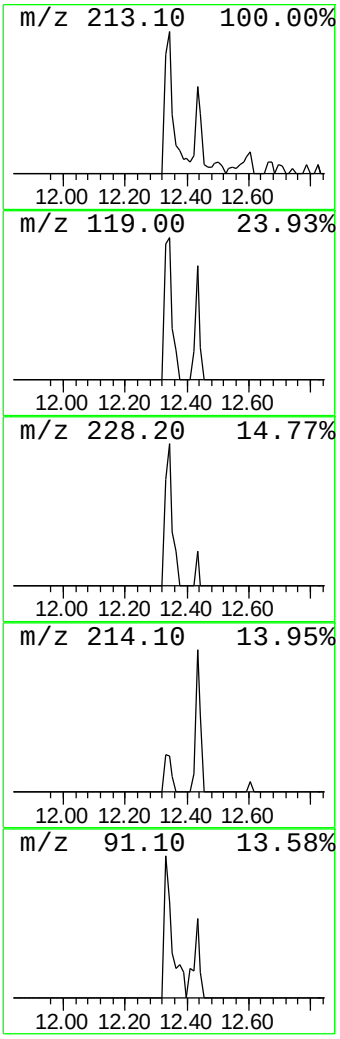
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	2.13 ng	38478	Chrysene-d12	13.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	81
2	2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	50
3	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	50
4	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	47
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47





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Sample : G3555-10
Misc :
ALS Vial : 89 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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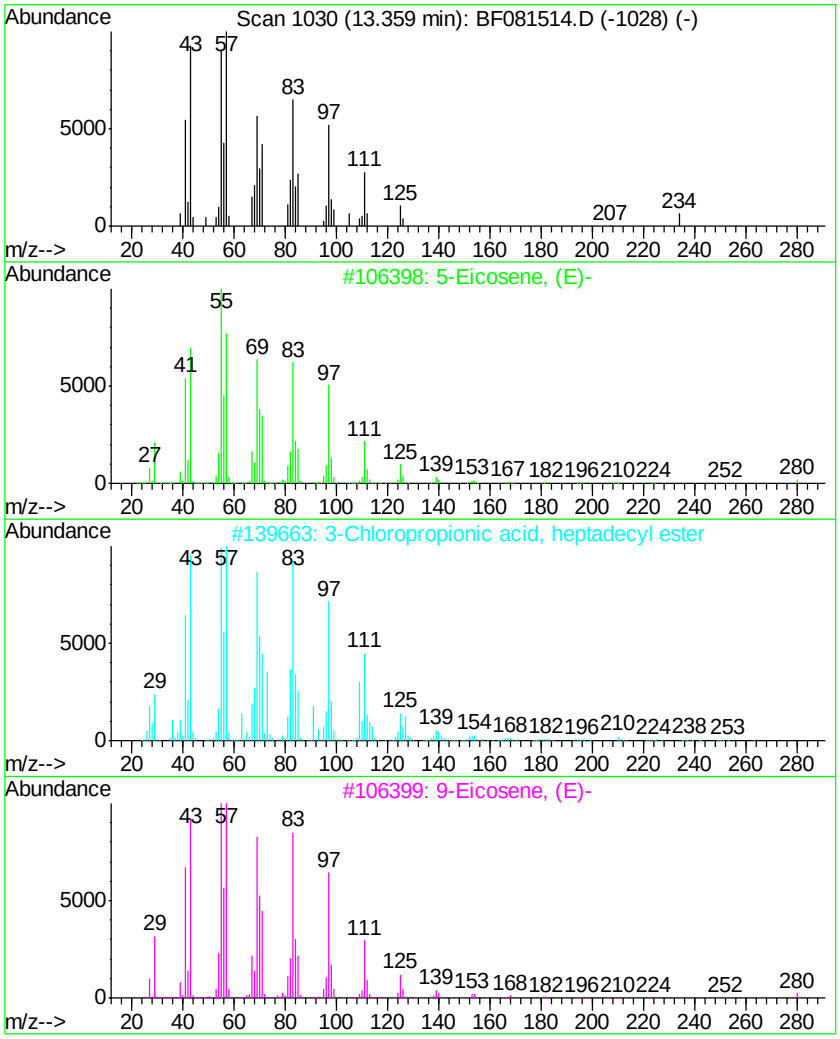
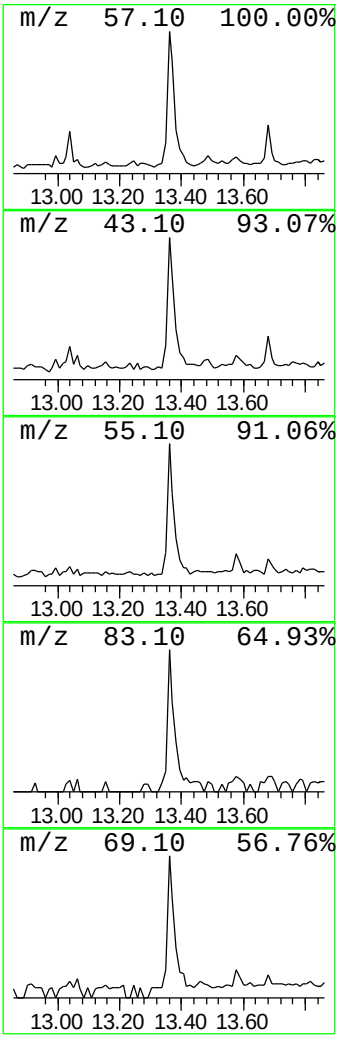
Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	6.46 ng	116752	Chrysene-d12	13.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
4	Cyclohexadecane	224	C16H32	000295-65-8	81
5	1-Tetracosanol	354	C24H50O	000506-51-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081514.D
Acq On : 6 Sep 2015 17:22
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Sample : G3555-10
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.40	61.9	ng	1004650	1	6.35	324494	20.0
unknown6.12	6.12	97.2	ng	1576580	1	6.35	324494	20.0
Pentadecanoic acid	11.43	3.2	ng	59928	4	10.86	370436	20.0
Phenol, 4,4'-(1-m...	12.34	2.1	ng	38478	5	13.46	361732	20.0
5-Eicosene, (E)-	13.36	6.5	ng	116752	5	13.46	361732	20.0