LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081372.D
Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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	4.387	243	245	246	rBV	4851	7025	1.23%	0.092%
2	4.421	246	248	256	rVB	256310	323930	56.59%	4.238%
3	4.936	291	293	302	rBB	470372	481612	84.14%	6.301%
4	6.056	389	391	393	rBV	601972	517863	90.47%	6.775%
5	6.159	398	400	402	rBV	378110	488625	85.37%	6.392%
6	6.387	418	420	422	rBV	468433	404233	70.62%	5.288%
7	6.536	431	433	436	rBV	308921	332676	58.12%	4.352%
8	6.959	468	470	472	rBV	407244	324454	56.68%	4.245%
9	7.679	530	533	535	rBV	614112	526736	92.03%	6.891%
10	8.639	615	617	620	rBV2	3133	6406	1.12%	0.084%
11	8.753	625	627	630	rVB	485251	421927	73.71%	5.520%
12	9.050	651	653	655	rBV2	7750	10549	1.84%	0.138%
13	9.130	658	660	661	rVB	7401	7234	1.26%	0.095%
14	9.165	661	663	665	rBV	98984	106025	18.52%	1.387%
15	9.279	671	673	676	rBV3	4305	6901	1.21%	0.090%
16	9.325	676	677	679	rVB	8802	7270	1.27%	0.095%
17	9.416	683	685	687	rBV	608920	519782	90.81%	6.800%
18	9.736	712	713	716	rVB2	5470	7194	1.26%	0.094%
19	9.816	719	720	722	rBV2	6421	7031	1.23%	0.092%
20	9.953	731	732	734	rBV2	4703	6212	1.09%	0.081%
21	10.068	741	742	744	rBV2	29370	34086	5.96%	0.446%
22	10.102	744	745	747	rVB	11668	9488	1.66%	0.124%
23	10.193	751	753	756	rBV	296417	286753	50.10%	3.751%
24	10.262	756	759	761	rBV4	3369	7254	1.27%	0.095%
25	10.296	761	762	764	rBV2	4604	8161	1.43%	0.107%
26	10.365	765	768	770	rVV	30503	38357	6.70%	0.502%
27	10.399	770	771	773	rVV2	11777	12110	2.12%	0.158%
28	10.468	775	777	778	rVV	45200	41152	7.19%	0.538%
29	10.536	781	783	785	rBV2	8116	11689	2.04%	0.153%
30	10.628	789	791	794	rBV4	9752	17845	3.12%	0.233%
31	10.788	804	805	807	rBV2	9396	12550	2.19%	0.164%
32	10.822	807	808	811	rVB2	119133	122088	21.33%	1.597%
33	10.879	811	813	817	rBV	590229	572383	100.00%	7.488%
34	10.982	821	822	826	rVB2	32462	46248	8.08%	0.605%

LSC Area Percent Report

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Data File : BF081372.D
Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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

35	11.165	836	838	840	rBV2	17610	26412	4.61%	0.346%
36	11.233	841	844	848	rVB	99295	127582	22.29%	1.669%
37	11.302	848	850	853	rBV3	50367	59616	10.42%	0.780%
38	11.371	854	856	861	rBV4	22759	70890	12.39%	0.927%
39	11.451	861	863	865	rBV3	12899	25414	4.44%	0.332%
40	11.508	865	868	869	rVV2	38663	62935	11.00%	0.823%
41	11.542	869	871	874	rVB3	21511	36400	6.36%	0.476%
42	11.668	881	882	886	rBV4	29301	64160	11.21%	0.839%
43	11.771	890	891	893	rVB2	25538	26673	4.66%	0.349%
44	11.896	900	902	904	rBV	22135	40257	7.03%	0.527%
45	11.999	909	911	914	rBV3	26028	57078	9.97%	0.747%
46	12.079	916	918	919	rBV	124532	112893	19.72%	1.477%
47	12.136	919	923	927	rVV2	28329	82035	14.33%	1.073%
48	12.296	935	937	939	rVB	128158	136774	23.90%	1.789%
49	12.342	939	941	942	rBV2	19381	19694	3.44%	0.258%
50	12.468	950	952	953	rBV	265972	332081	58.02%	4.344%
51	13.485	1039	1041	1043	rBV	254735	383730	67.04%	5.020%
52	14.800	1154	1156	1159	rVB	219787	245514	42.89%	3.212%

Sum of corrected areas: 7643987

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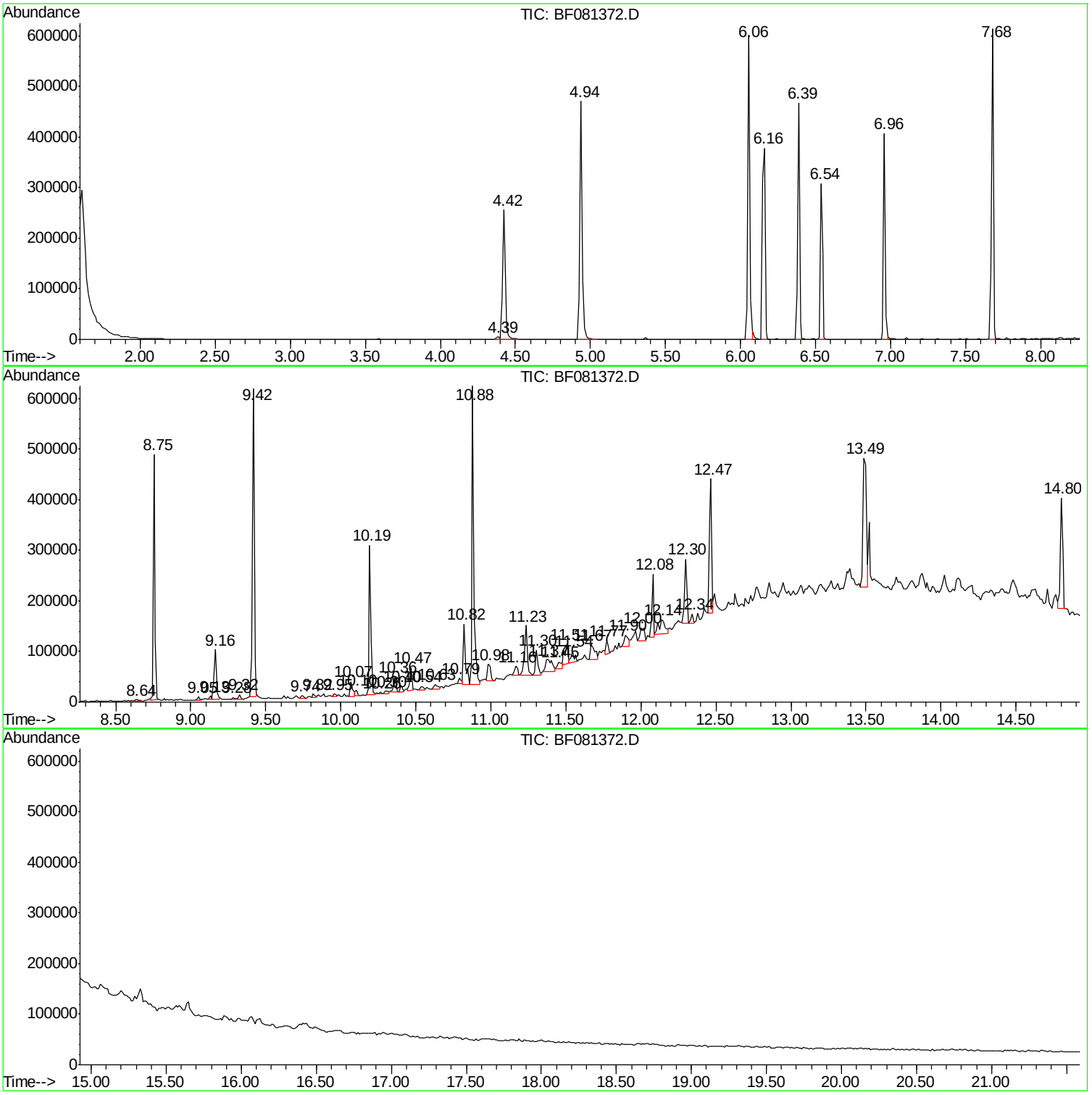
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
6TPB(4.5-5)

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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Data File : BF081372.D
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Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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

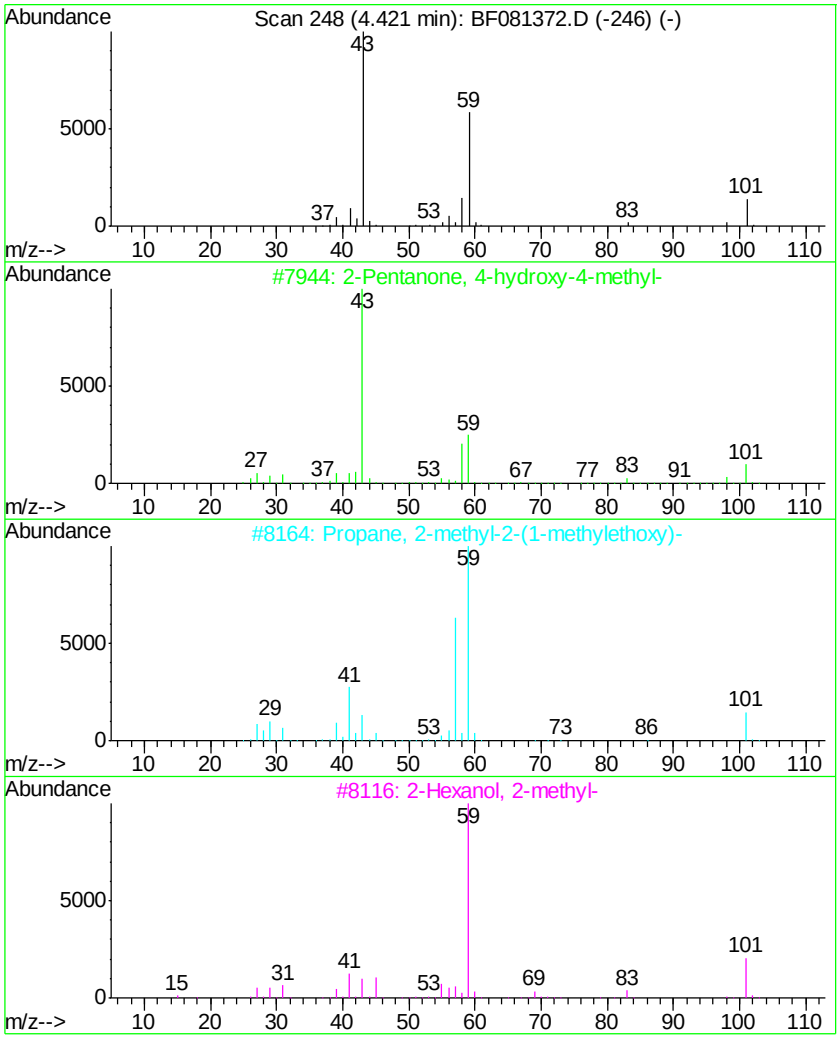
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

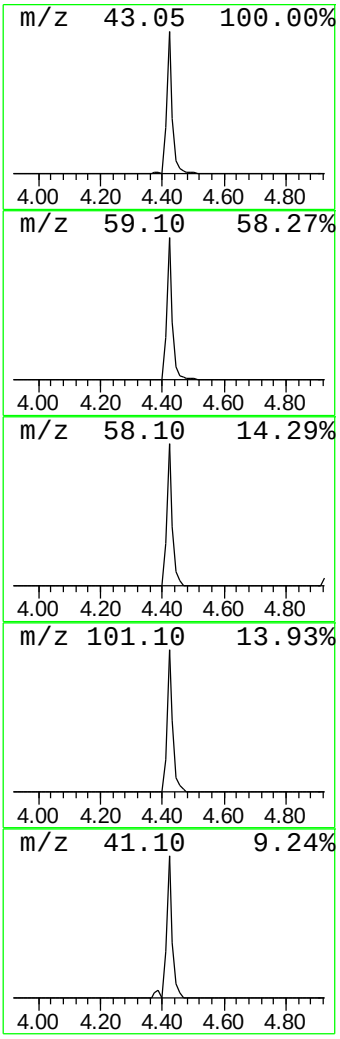
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	16.03 ng	323930	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





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Data File : BF081372.D
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Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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

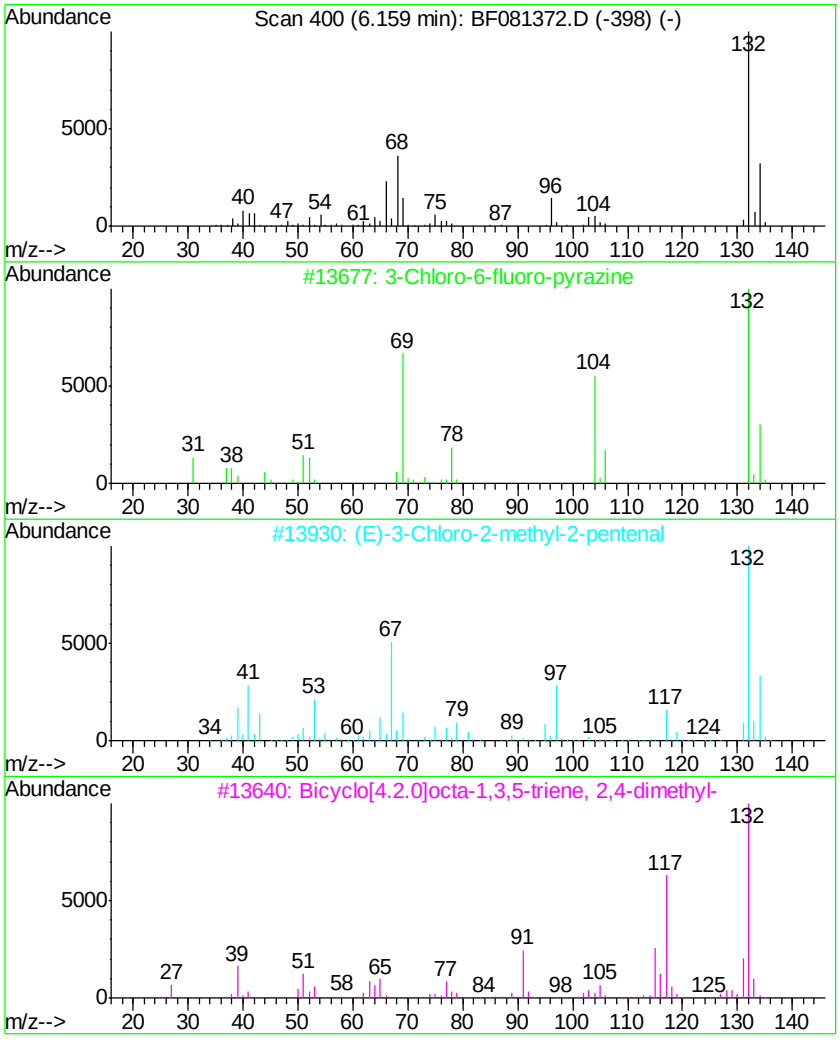
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

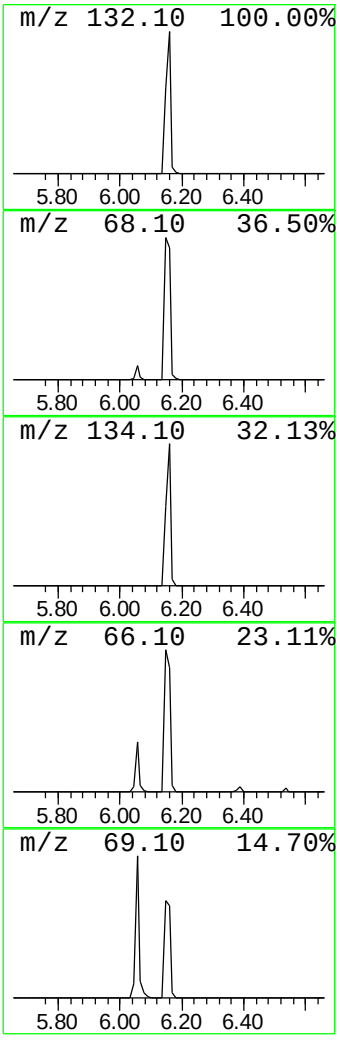
****

Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	24.18 ng	488625	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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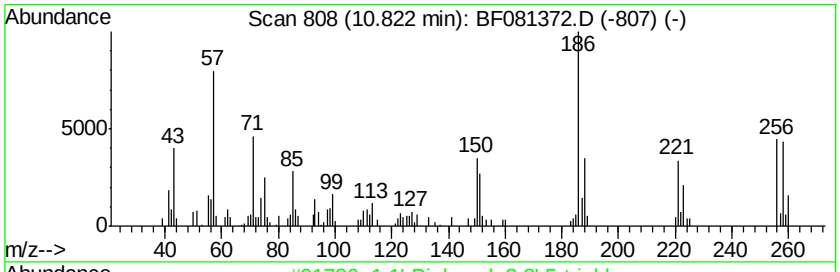
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

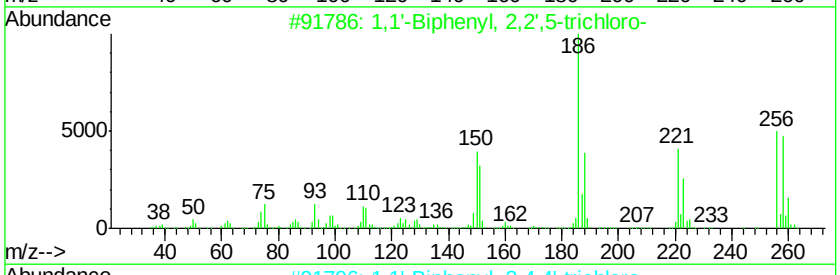
****

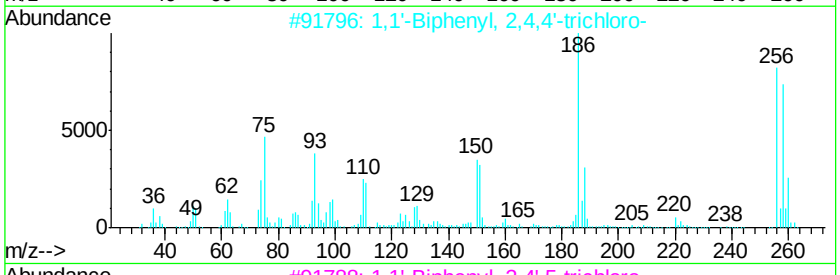
Peak Number 4 1,1'-Biphenyl, 2,2',5-trich... Concentration Rank 5

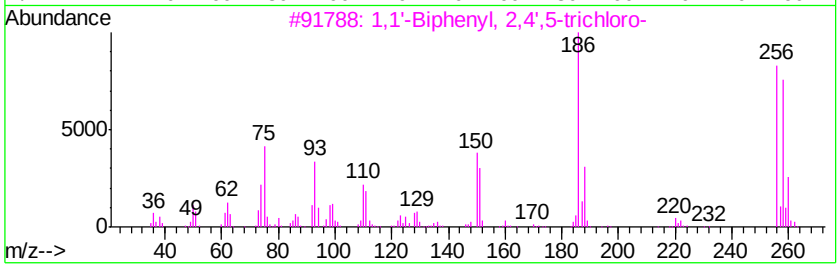
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	4.27 ng	122088	Phenanthrene-d10	10.88

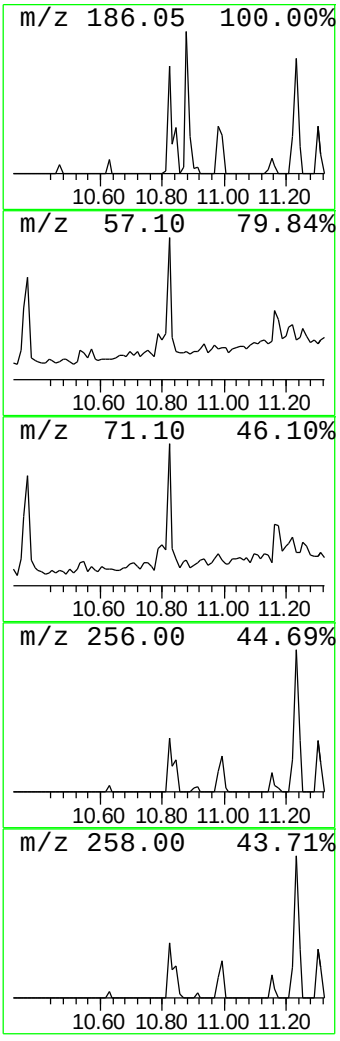
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2',5-trichloro-	256	C12H7Cl3	037680-65-2	99
2	1,1'-Biphenyl, 2,4,4'-trichloro-	256	C12H7Cl3	007012-37-5	87
3	1,1'-Biphenyl, 2,4',5-trichloro-	256	C12H7Cl3	016606-02-3	83
4	1,1'-Biphenyl, 2,2',6-trichloro-	256	C12H7Cl3	038444-73-4	83
5	4-Acetamido-1,2,5-trimethyl-4-ph...	260	C16H24N2O	201055-92-7	25











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Data File : BF081372.D
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Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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

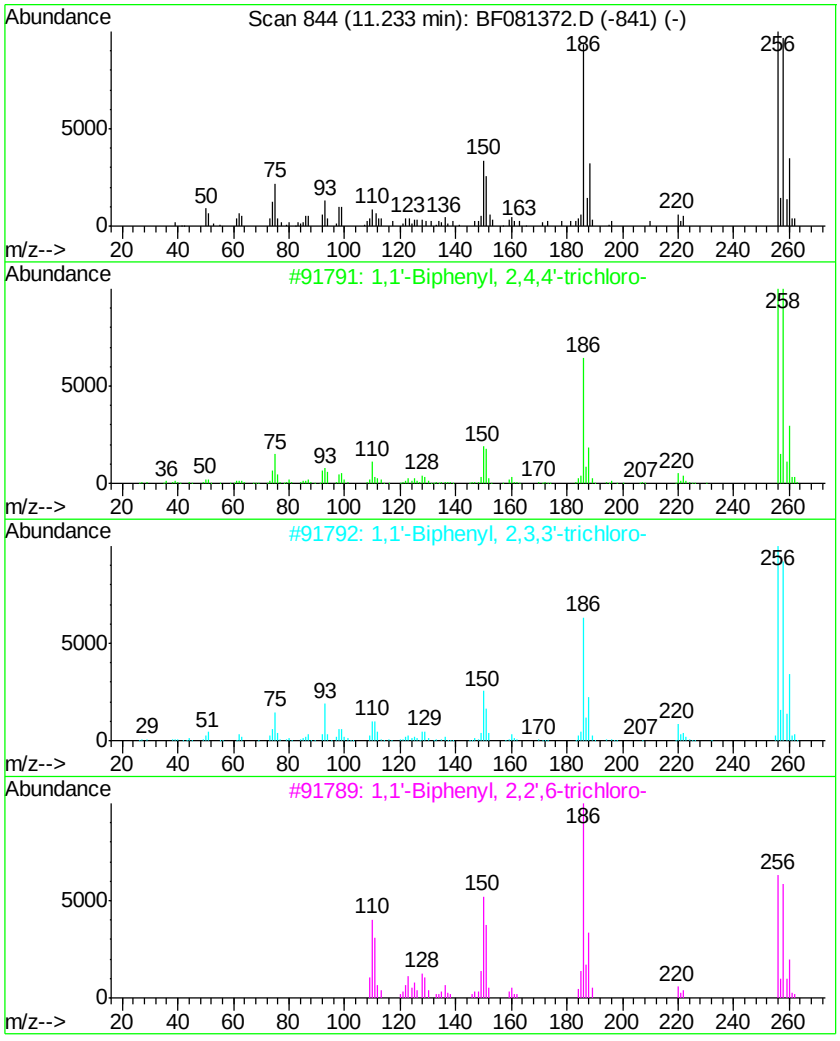
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

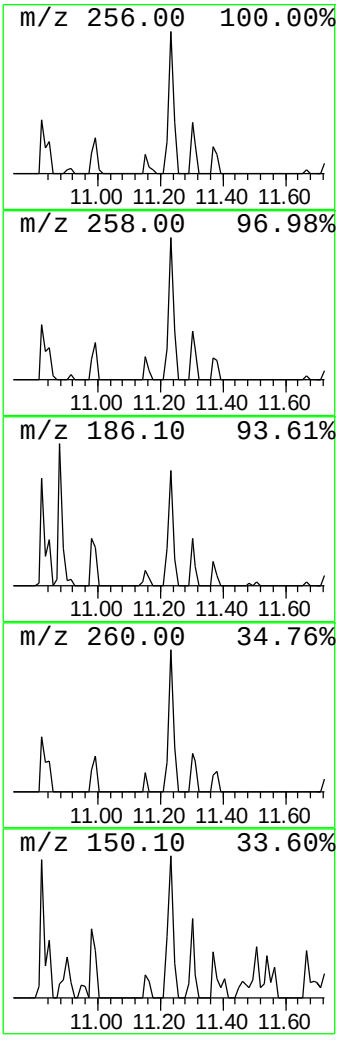
****

Peak Number 5 1,1'-Biphenyl, 2,4,4'-trich... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	4.46 ng	127582	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,4,4'-trichloro-	256	C12H7Cl3	007012-37-5	98
2	1,1'-Biphenyl, 2,3,3'-trichloro-	256	C12H7Cl3	038444-84-7	95
3	1,1'-Biphenyl, 2,2',6-trichloro-	256	C12H7Cl3	038444-73-4	95
4	1,1'-Biphenyl, 2,4,5-trichloro-	256	C12H7Cl3	015862-07-4	95
5	1,1'-Biphenyl, 2',3,4-trichloro-	256	C12H7Cl3	038444-86-9	95





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Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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

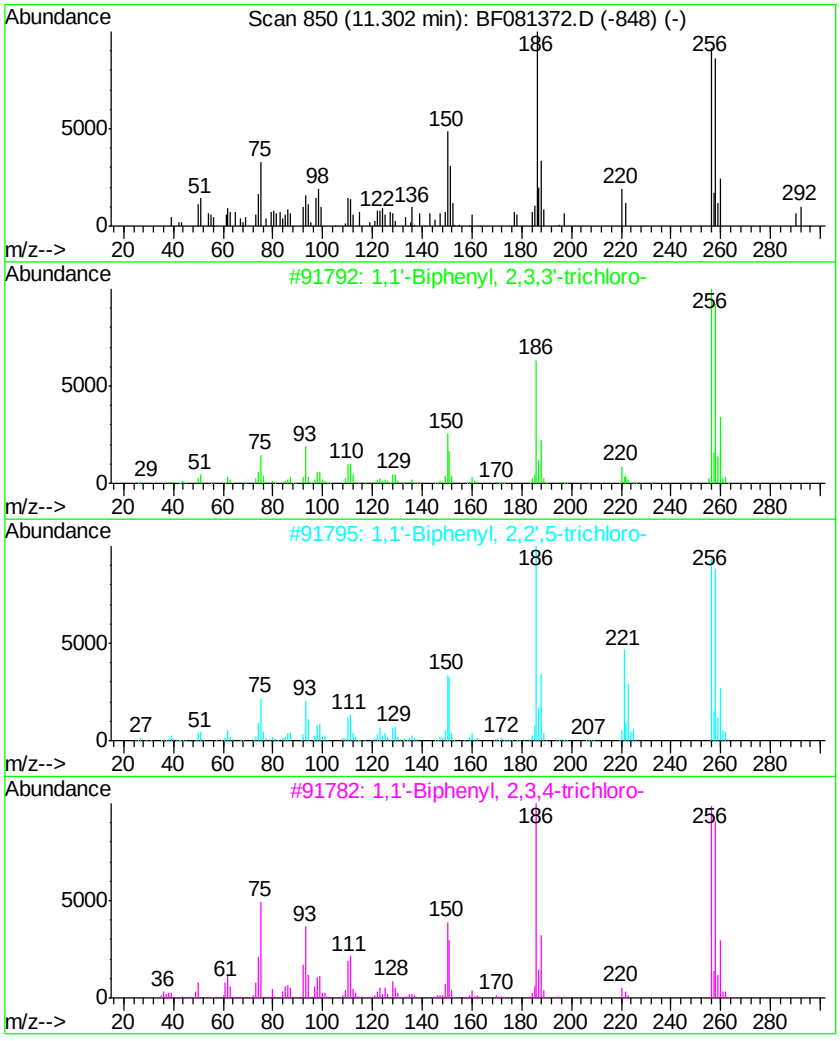
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

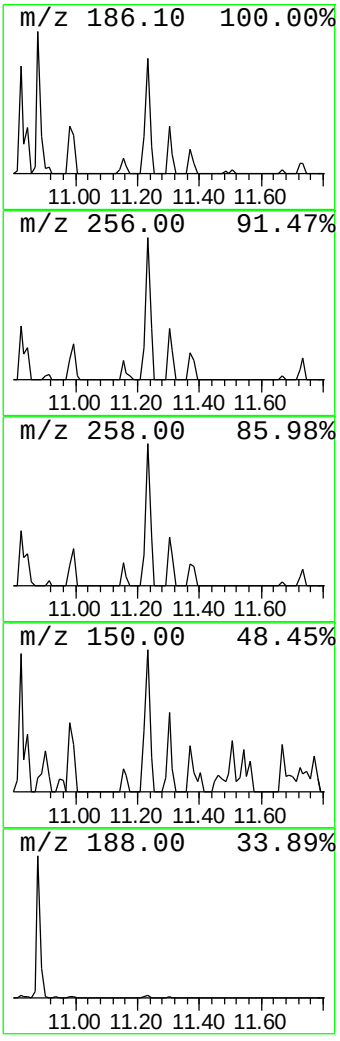
****

Peak Number 6 1,1'-Biphenyl, 2,3,3'-trich... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	2.08 ng	59616	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,3,3'-trichloro-	256	C12H7Cl3	038444-84-7	98
2	1,1'-Biphenyl, 2,2',5-trichloro-	256	C12H7Cl3	037680-65-2	98
3	1,1'-Biphenyl, 2,3,4-trichloro-	256	C12H7Cl3	055702-46-0	96
4	1,1'-Biphenyl, 2',3,4-trichloro-	256	C12H7Cl3	038444-86-9	96
5	1,1'-Biphenyl, 2,4,4'-trichloro-	256	C12H7Cl3	007012-37-5	95





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Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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

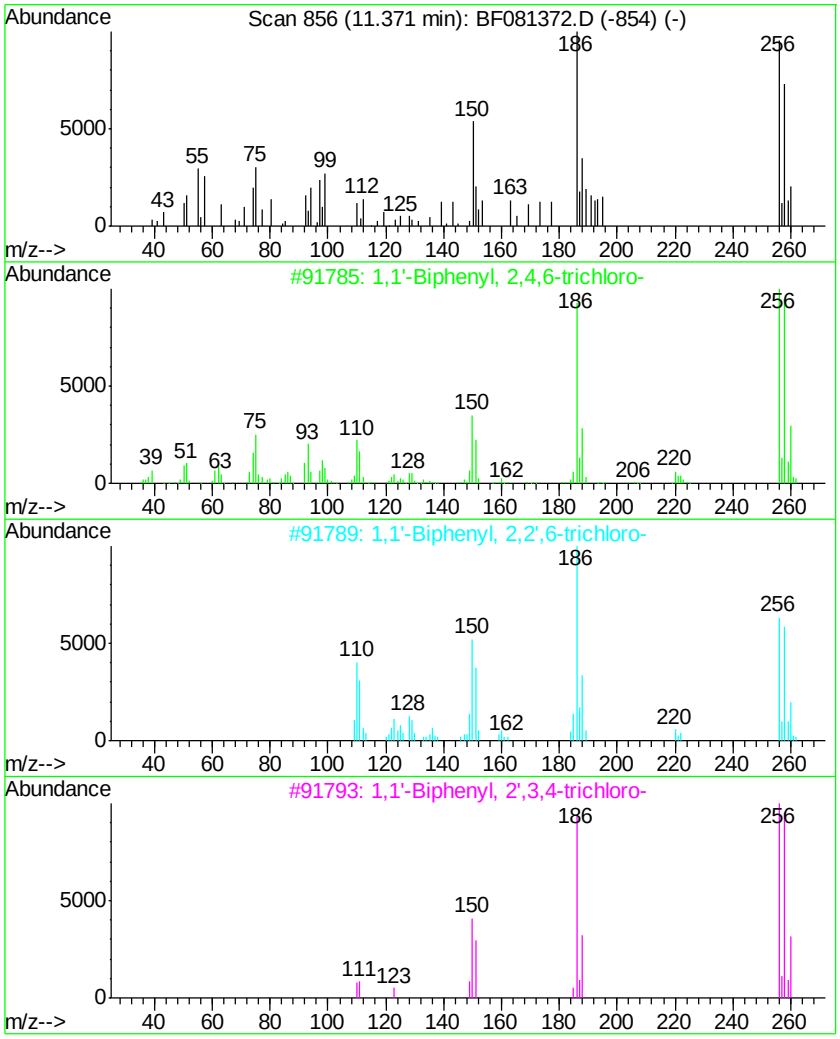
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

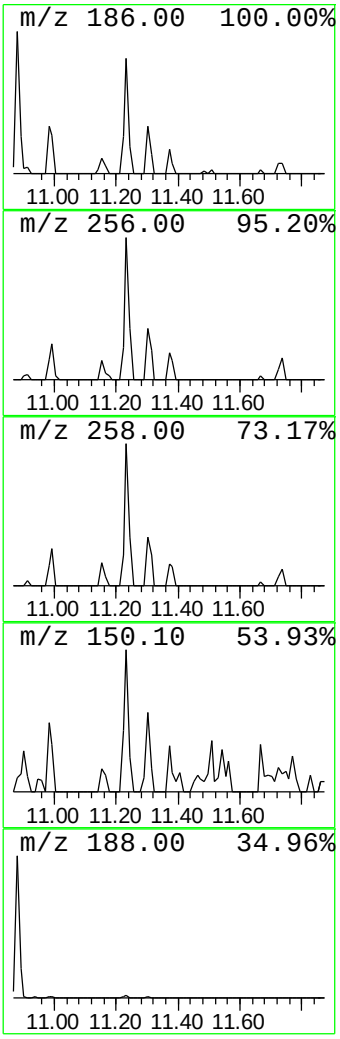
****

Peak Number 7 1,1'-Biphenyl, 2,4,6-trichl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	2.48 ng	70890	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,4,6-trichloro-	256	C12H7Cl3	035693-92-6	90
2	1,1'-Biphenyl, 2,2',6-trichloro-	256	C12H7Cl3	038444-73-4	76
3	1,1'-Biphenyl, 2',3,4-trichloro-	256	C12H7Cl3	038444-86-9	72
4	1,1'-Biphenyl, 2,3,6-trichloro-	256	C12H7Cl3	055702-45-9	60
5	1,1'-Biphenyl, 2,4',5-trichloro-	256	C12H7Cl3	016606-02-3	58





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081372.D
Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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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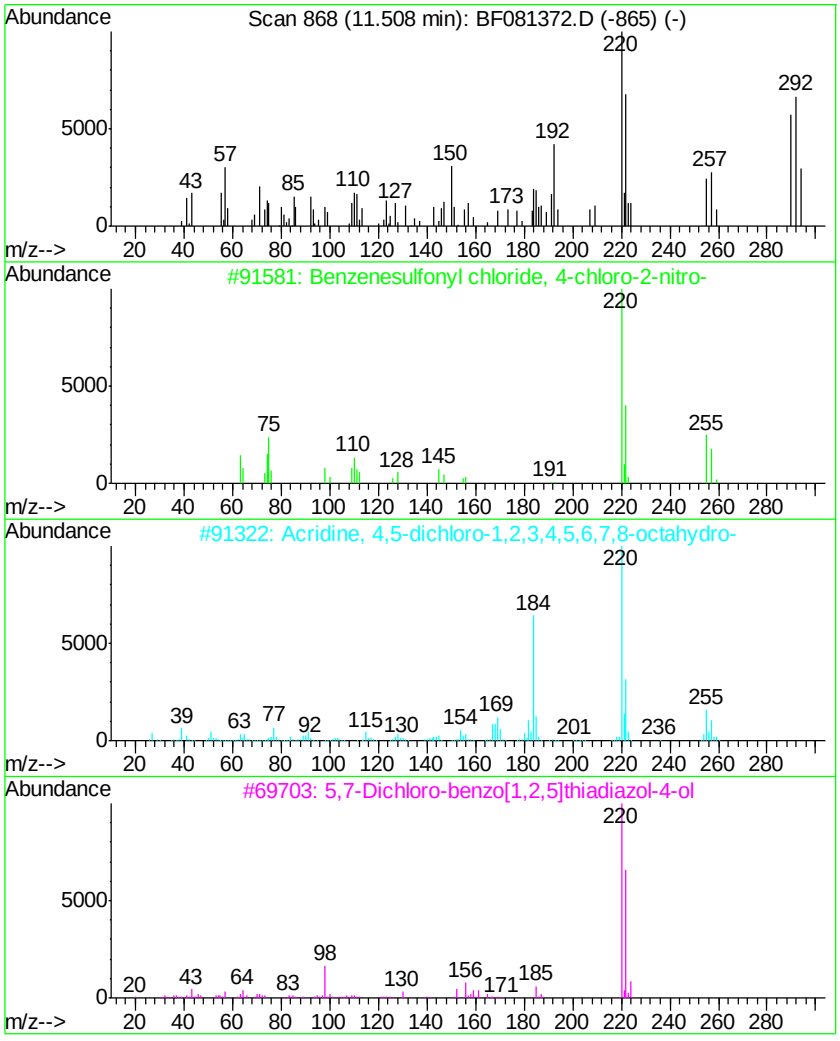
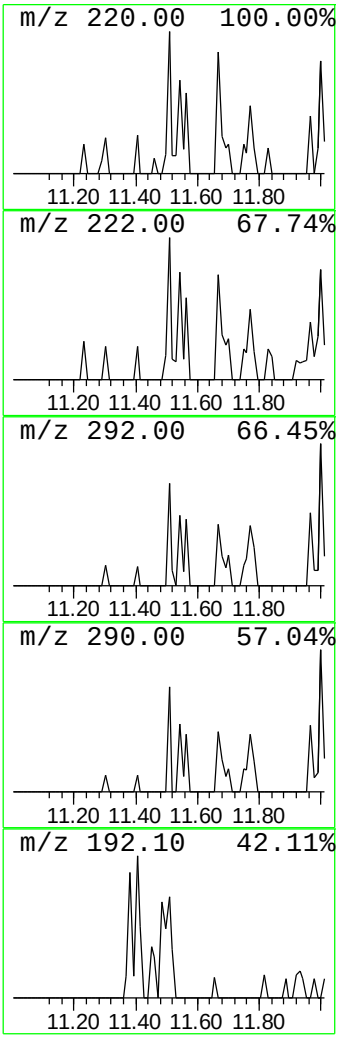
Peak Number 8 unknown11.51 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.51	2.20 ng	62935	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonyl chloride, 4-chlo...	255	C6H3Cl2NO4S	004533-96-4	38
2	Acridine, 4,5-dichloro-1,2,3,4,5...	255	C13H15Cl2N	022766-55-8	35
3	5,7-Dichloro-benzo[1,2,5]thiadia...	220	C6H2Cl2N2OS	016407-74-2	27
4	4-Chloro-3-(2-chloroethyl)-2-met...	255	C12H11Cl2NO	092696-18-9	27
5	2-Thiophenecarboxaldehyde, (2-th...	220	C10H8N2S2	024523-46-4	25





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Data File : BF081372.D
Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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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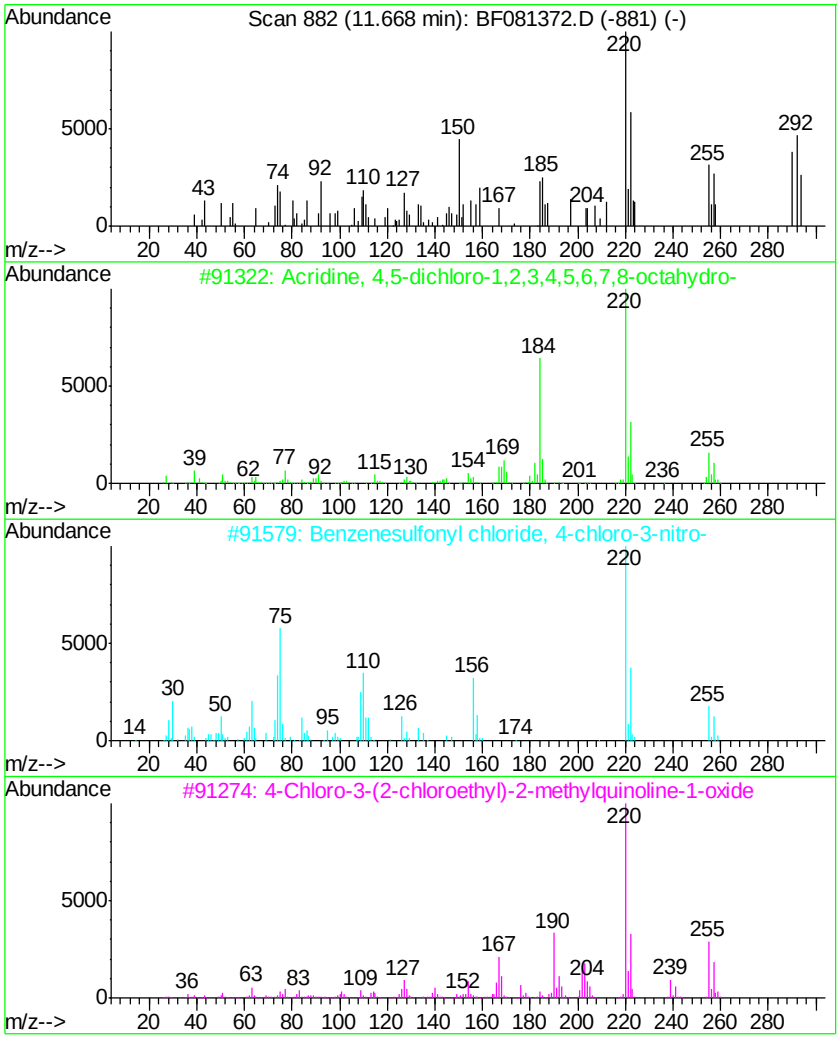
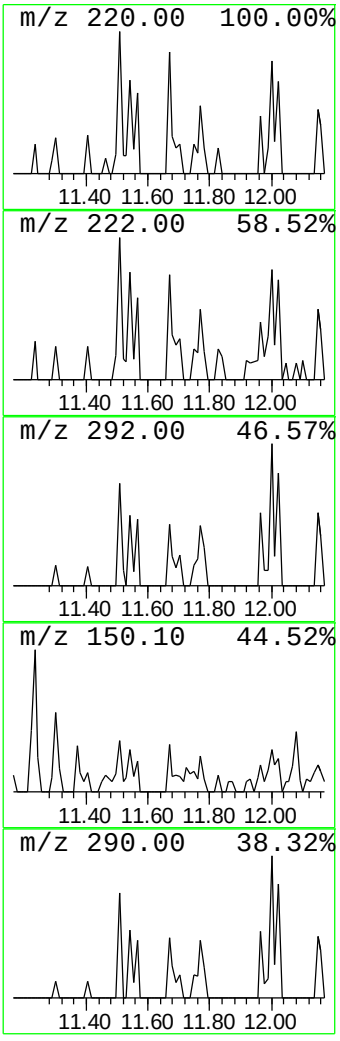
Peak Number 9 unknown11.67 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.24 ng	64160	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridine, 4,5-dichloro-1,2,3,4,5...	255	C13H15Cl2N	022766-55-8	38
2	Benzenesulfonyl chloride, 4-chlo...	255	C6H3Cl2NO4S	000097-08-5	35
3	4-Chloro-3-(2-chloroethyl)-2-met...	255	C12H11Cl2NO	092696-18-9	27
4	Phosphinous chloride, diphenyl-	220	C12H10ClP	001079-66-9	22
5	Benzenesulfonyl chloride, 4-chlo...	255	C6H3Cl2NO4S	004533-96-4	15





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081372.D
Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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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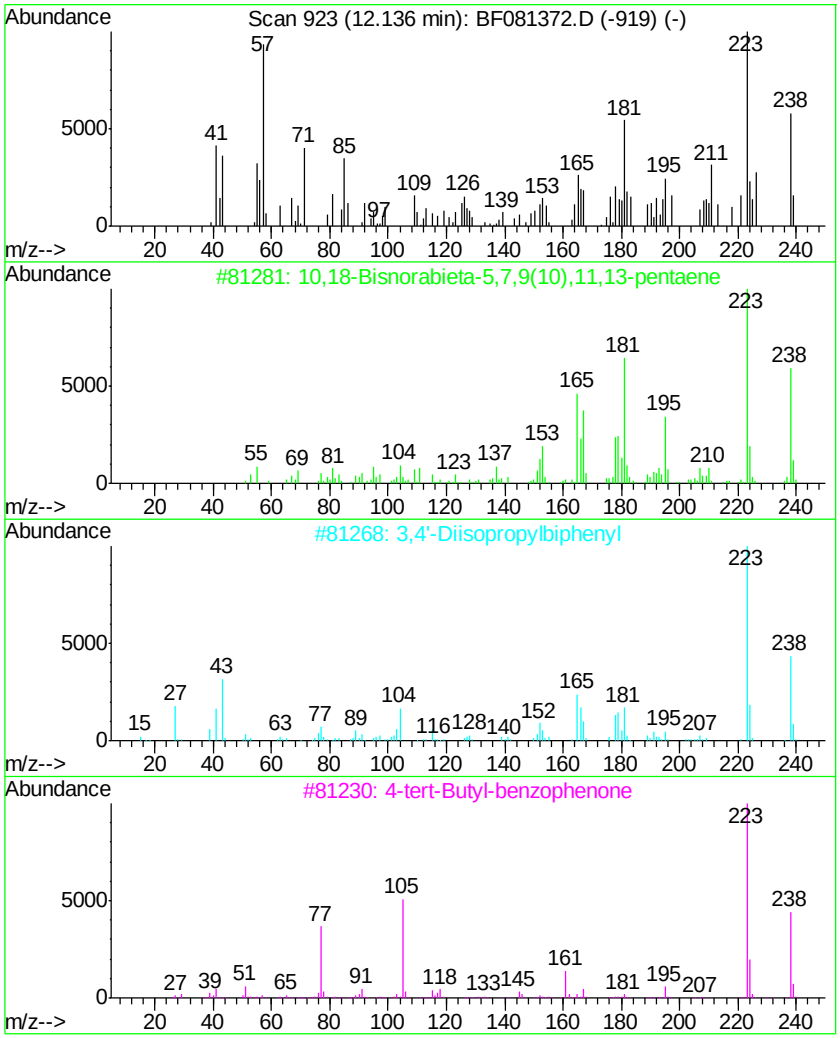
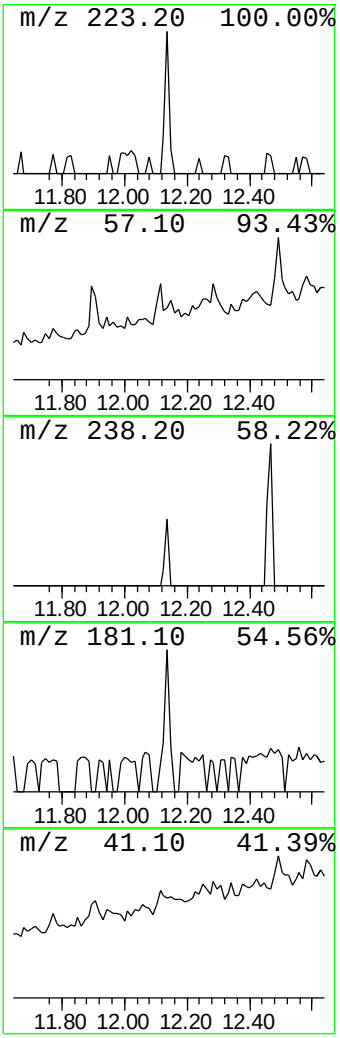
Peak Number 10 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	2.87 ng	82035	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	76
2	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	55
3	4-tert-Butyl-benzophenone	238	C17H18O	022679-54-5	46
4	Anthracene, 9,10-dimethoxy-	238	C16H14O2	002395-97-3	43
5	1,4,7-Trimethyl-2-azafluorenone	223	C15H13NO	064322-98-1	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081372.D
Acq On : 3 Sep 2015 3:27
Operator : UM/IZ
Sample : G3490-03 5X
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6TPB(4.5-5)

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...	4.42	16.0	ng	323930	1	6.39	404233	20.0
unknown6.16	6.16	24.2	ng	488625	1	6.39	404233	20.0
1,1'-Biphenyl, 2,...	10.82	4.3	ng	122088	4	10.88	572383	20.0
1,1'-Biphenyl, 2,...	11.23	4.5	ng	127582	4	10.88	572383	20.0
1,1'-Biphenyl, 2,...	11.30	2.1	ng	59616	4	10.88	572383	20.0
1,1'-Biphenyl, 2,...	11.37	2.5	ng	70890	4	10.88	572383	20.0
unknown11.51	11.51	2.2	ng	62935	4	10.88	572383	20.0
unknown11.67	11.67	2.2	ng	64160	4	10.88	572383	20.0
10,18-Bisnorabiet...	12.14	2.9	ng	82035	4	10.88	572383	20.0