LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

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-BF013017.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	4.247	187	189	205	rBV	70624	176861	12.22%	0.945%
2	4.922	245	248	260	rBV	281664	381500	26.35%	2.039%
3	5.379	286	288	296	rBV	457415	705768	48.75%	3.772%
4	6.030	341	345	347	rBV	25784	28476	1.97%	0.152%
5	6.373	373	375	378	rVB	22398	23406	1.62%	0.125%
6	6.430	378	380	389	rBV	686066	942804	65.13%	5.039%
7	6.556	389	391	394	rVV	793333	792696	54.76%	4.236%
8	6.602	394	395	399	rVB3	42895	41324	2.85%	0.221%
9	6.785	408	411	413	rBV	1137971	1127797	77.90%	6.027%
10	6.842	413	416	419	rVB	19898	28635	1.98%	0.153%
11	6.933	422	424	427	rBV	537705	651349	44.99%	3.481%
12	7.356	459	461	467	rBV	486085	502940	34.74%	2.688%
13	7.848	502	504	510	rBV	22375	56851	3.93%	0.304%
14	8.076	521	524	526	rBV	1432859	1440760	99.52%	7.700%
15	8.133	527	529	537	rVB5	20448	50278	3.47%	0.269%
16	8.499	558	561	565	rVB3	9541	20194	1.39%	0.108%
17	8.888	593	595	599	rBV	18495	29511	2.04%	0.158%
18	9.002	603	605	609	rBV	17964	30231	2.09%	0.162%
19	9.150	615	618	620	rBV	760795	860460	59.44%	4.599%
20	9.551	650	653	655	rBV	88852	103768	7.17%	0.555%
21	9.688	663	665	666	rBV	25577	26821	1.85%	0.143%
22	9.756	670	671	673	rVV2	12934	22306	1.54%	0.119%
23	9.825	674	677	679	rVV	1572119	1447669	100.00%	7.737%
24	9.859	679	680	685	rVB5	38551	46289	3.20%	0.247%
25	10.373	723	725	728	rVB	15545	20869	1.44%	0.112%
26	10.476	732	734	736	rVB	17105	24672	1.70%	0.132%
27	10.614	744	746	751	rBV	246523	291681	20.15%	1.559%
28	10.739	754	757	760	rVB	63830	93358	6.45%	0.499%
29	10.819	762	764	766	rVB	64460	53371	3.69%	0.285%
30	10.911	769	772	774	rBV	287406	323755	22.36%	1.730%
31	11.196	793	797	801	rBV3	43286	108539	7.50%	0.580%
32	11.254	801	802	804	rBV2	36269	46911	3.24%	0.251%
33	11.311	804	807	808	rBV	1229485	1190788	82.26%	6.364%
34	11.551	825	828	831	rBV2	57201	120577	8.33%	0.644%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.522	911	913	915	rBV	314400	307187	21.22%	1.642%
36	12.751	931	933	935	rVB	228706	235447	16.26%	1.258%
37	12.888	943	945	948	rVB	603171	538139	37.17%	2.876%
38	12.968	948	952	955	rBV	221189	471468	32.57%	2.520%
39	13.082	960	962	966	rVB	273000	428137	29.57%	2.288%
40	13.162	966	969	970	rBV	163293	286414	19.78%	1.531%
41	13.185	970	971	973	rVB	297786	217522	15.03%	1.162%
42	13.288	978	980	982	rBV	289032	362120	25.01%	1.935%
43	13.368	984	987	988	rBV	1054878	1170670	80.87%	6.256%
44	13.642	1009	1011	1012	rBV	180290	174805	12.07%	0.934%
45	13.951	1035	1038	1043	rVB2	904373	1198271	82.77%	6.404%
46	14.134	1052	1054	1059	rVB	630324	672852	46.48%	3.596%
47	14.294	1066	1068	1069	rBV	189413	199949	13.81%	1.069%
48	15.368	1160	1162	1164	rVB	555524	635552	43.90%	3.397%

Sum of corrected areas: 18711748

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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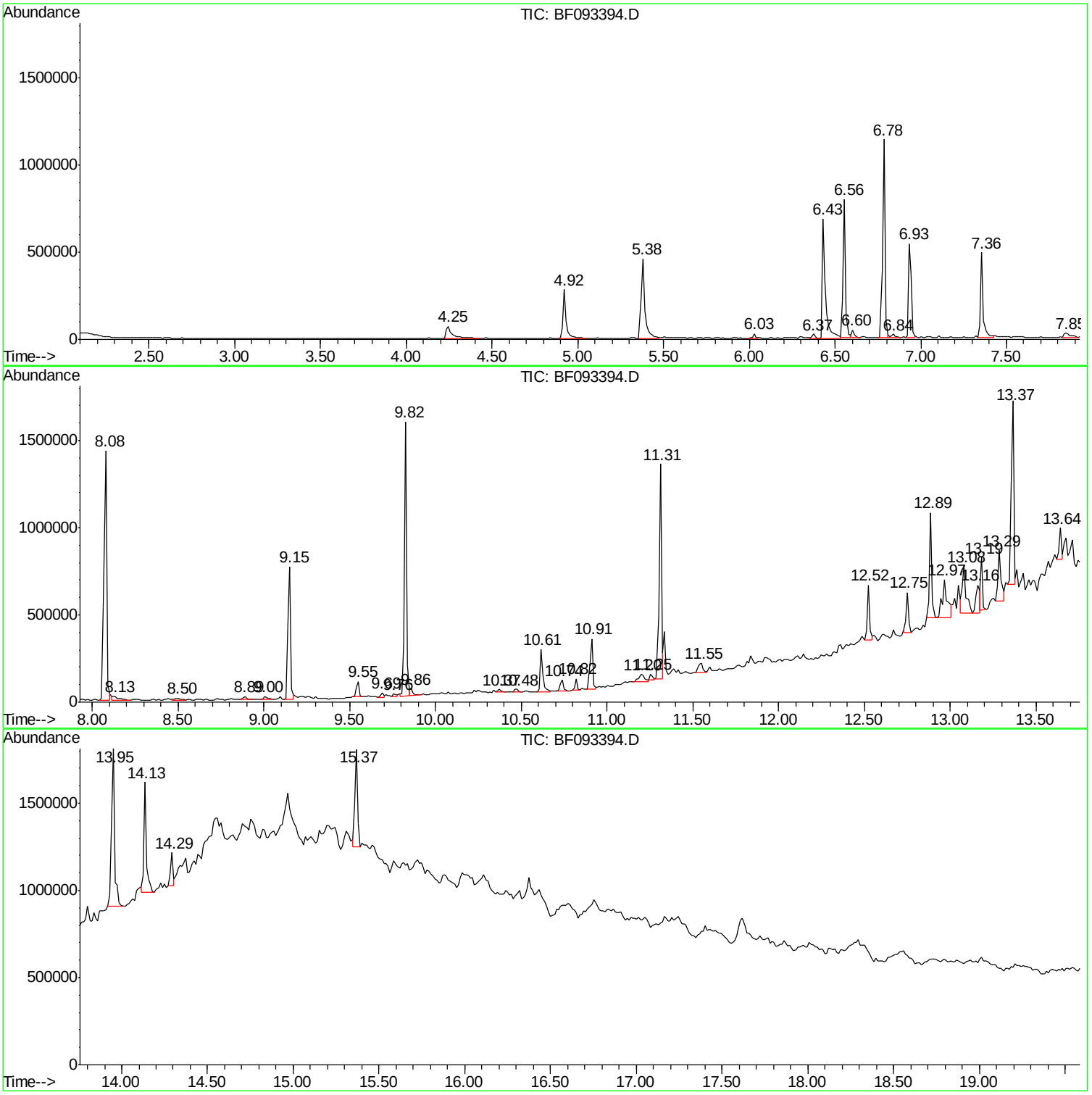
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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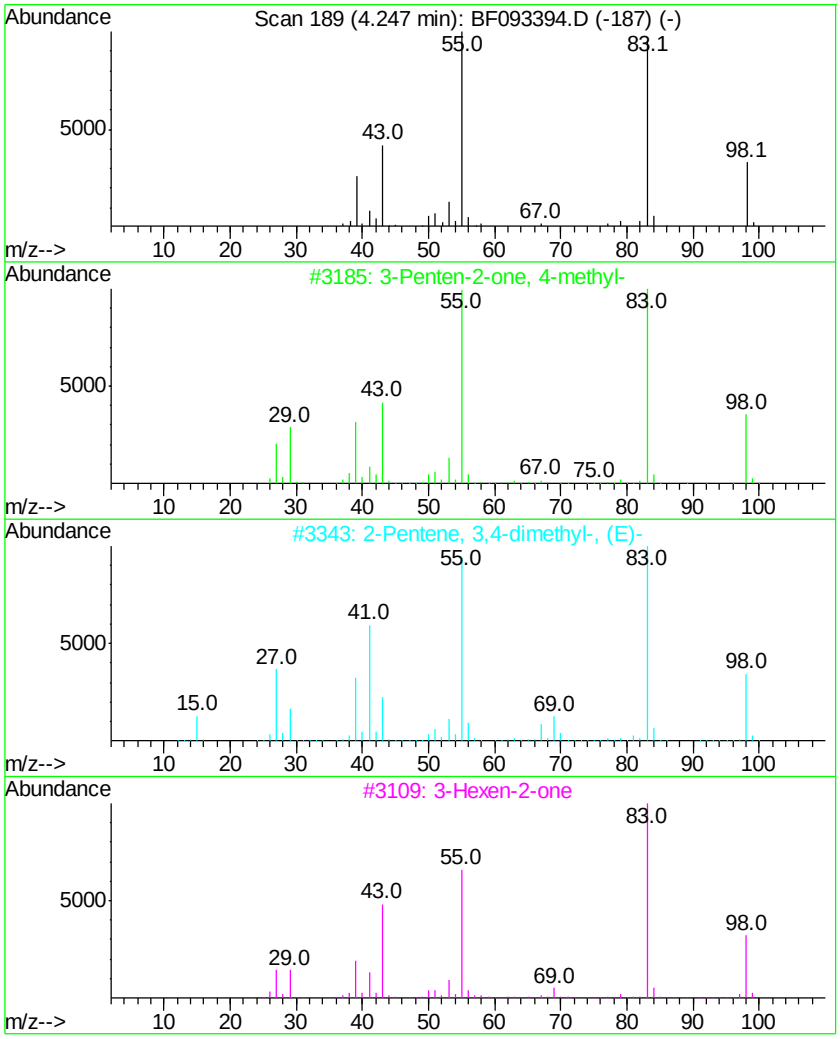
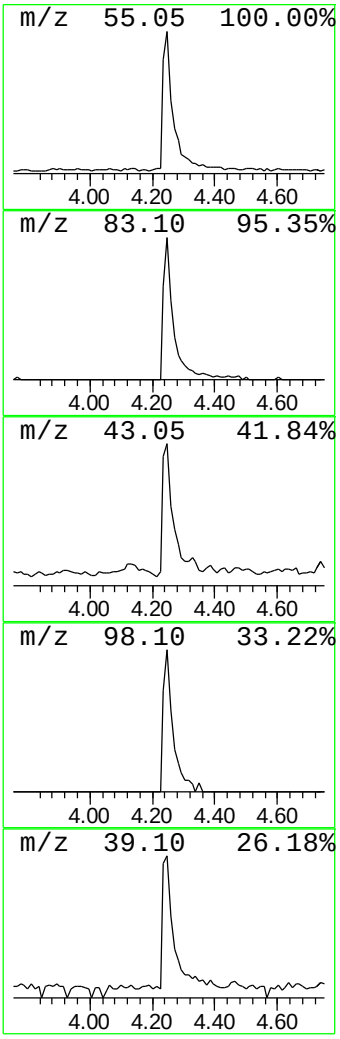
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	3.14 ng	176861	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	87
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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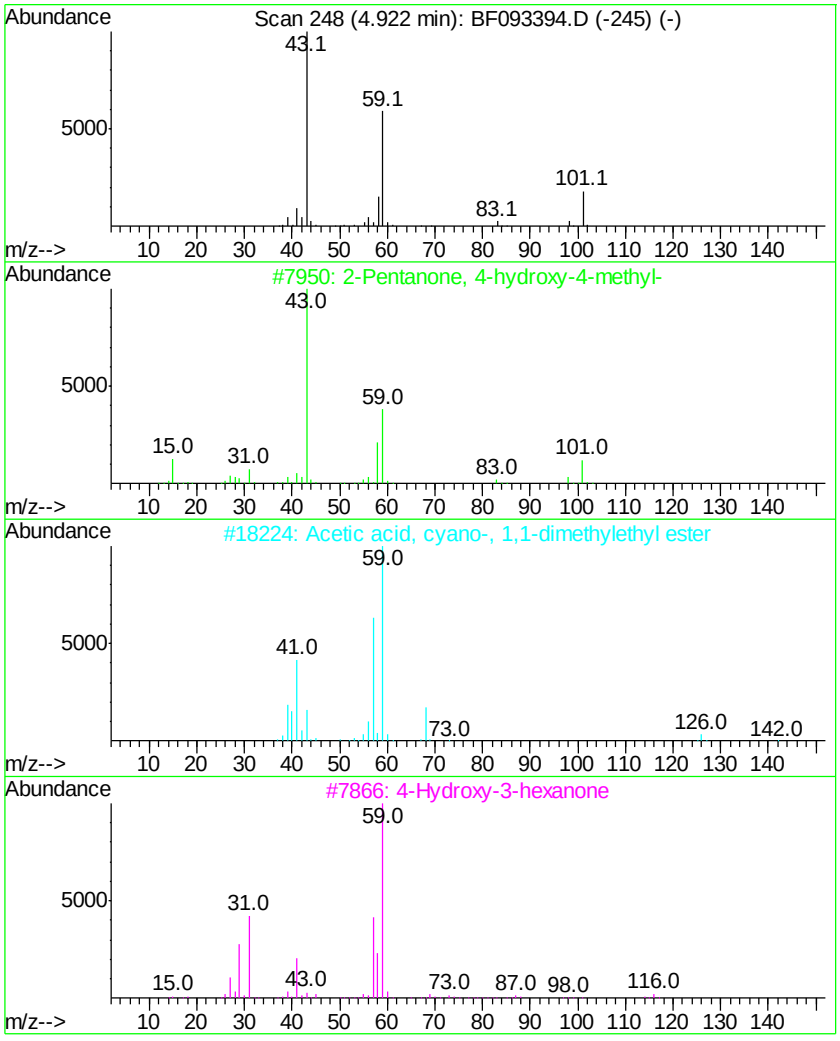
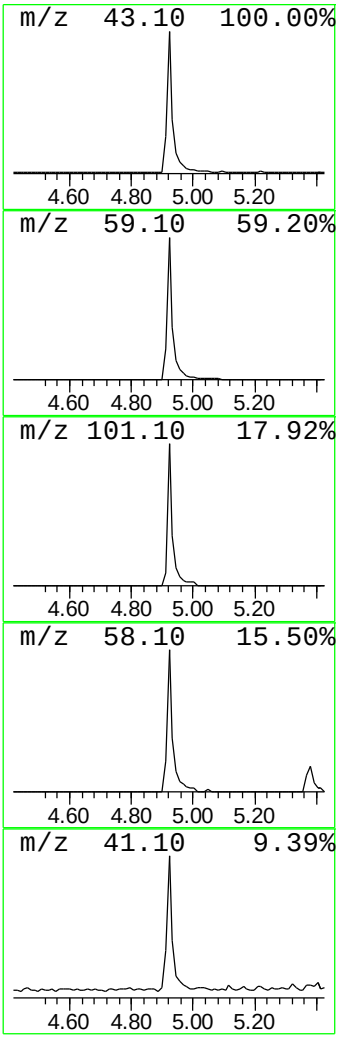
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.77 ng	381500	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

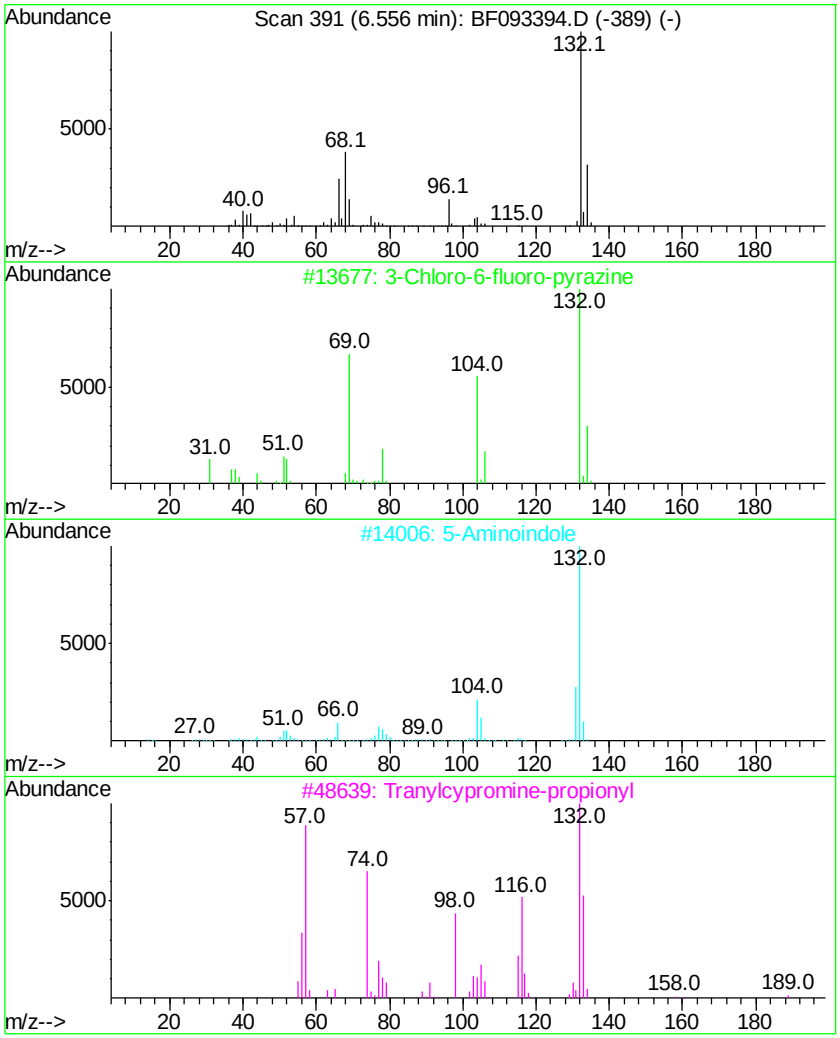
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

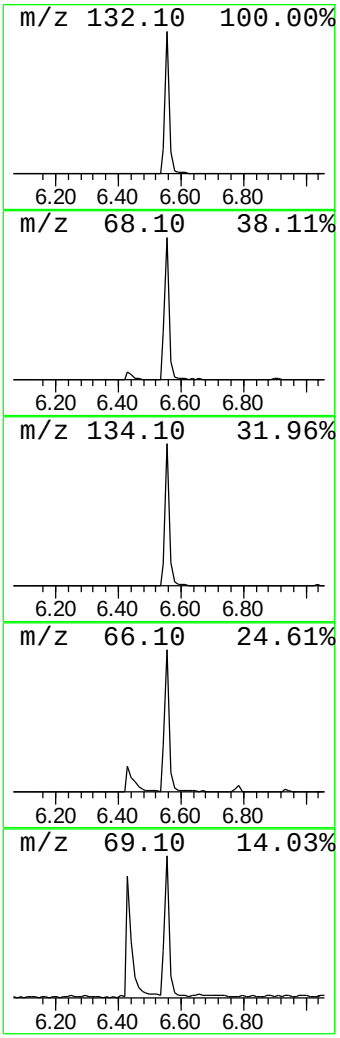
****

Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	14.06 ng	792696	1,4-Dichlorobenzene-d4	6.78

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	Amphetaminil	250	C17H18N2	017590-01-1	10
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Acq On : 4 Mar 2017 9:22
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Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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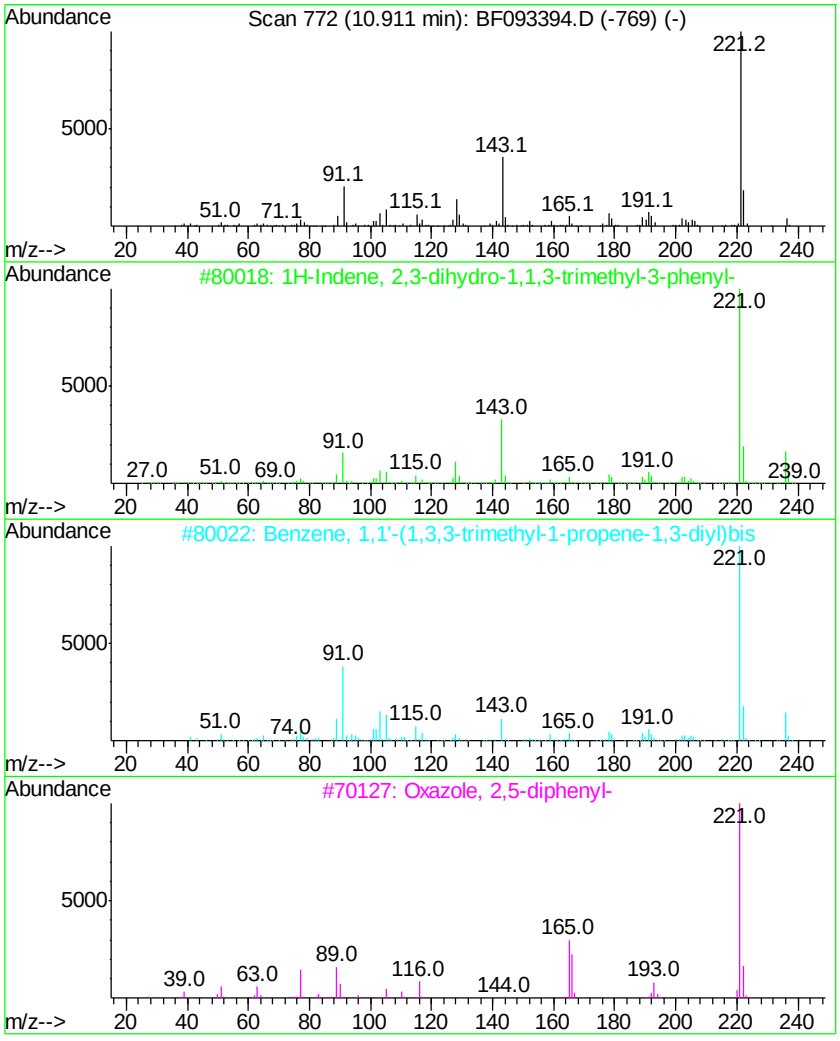
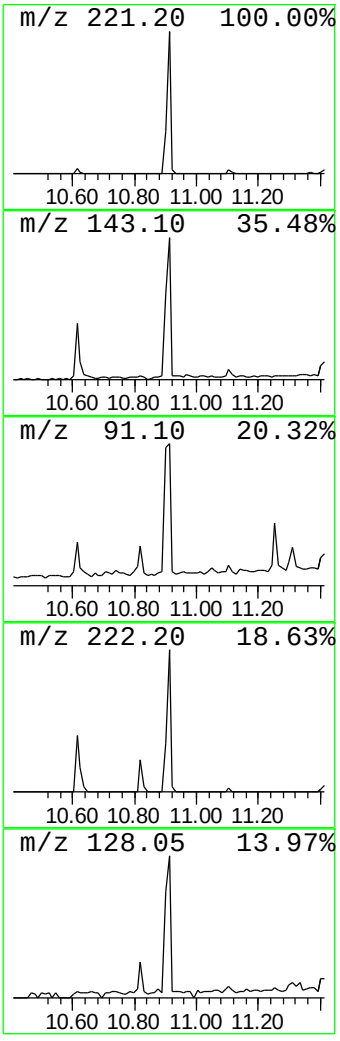
Peak Number 5 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	5.44 ng	323755	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	86
2	Benzene, 1,1'-(1,3,3-trimethyl-1...	236	C18H20	006258-73-7	64
3	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	50
4	4(1H)-Quinolinone, 2-phenyl-	221	C15H11NO	014802-18-7	40
5	4-Quinolinol, 2-phenyl-	221	C15H11NO	001144-20-3	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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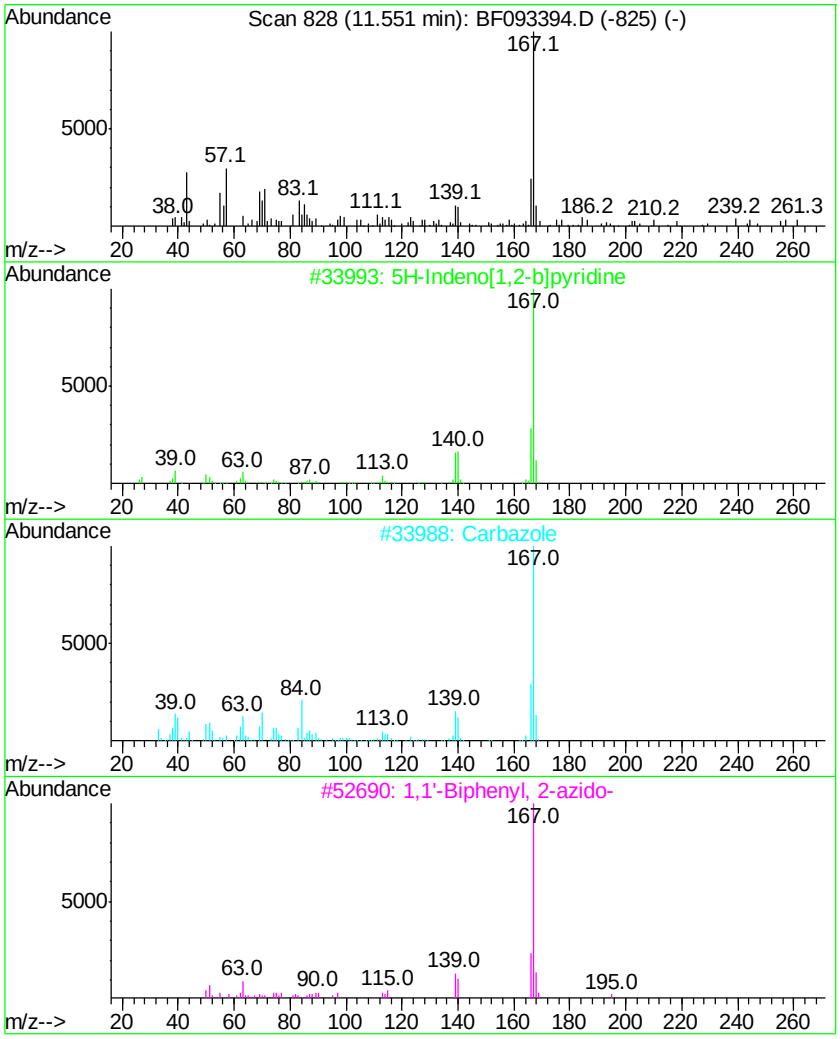
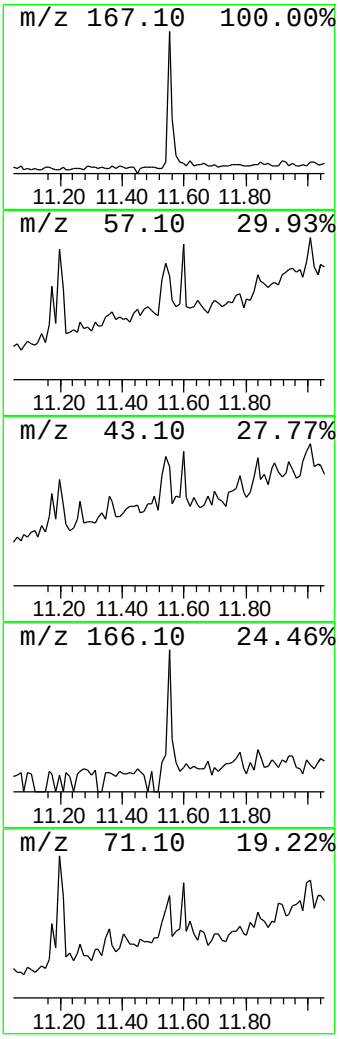
****

Peak Number 6 5H-Indeno[1,2-b]pyridine Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.03 ng	120577	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	76
2	Carbazole	167	C12H9N	000086-74-8	76
3	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	64
4	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	59
5	D-Galactitol, 2-(acetylmethylami...	363	C16H29NO8	074410-42-7	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
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Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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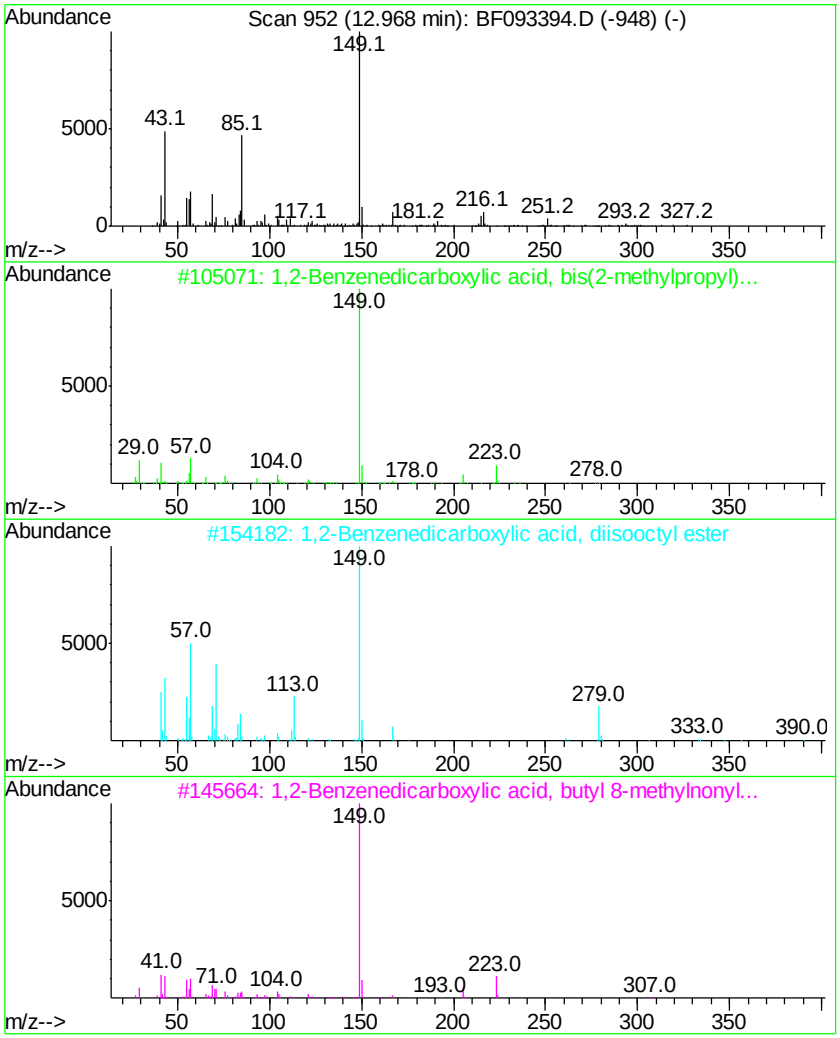
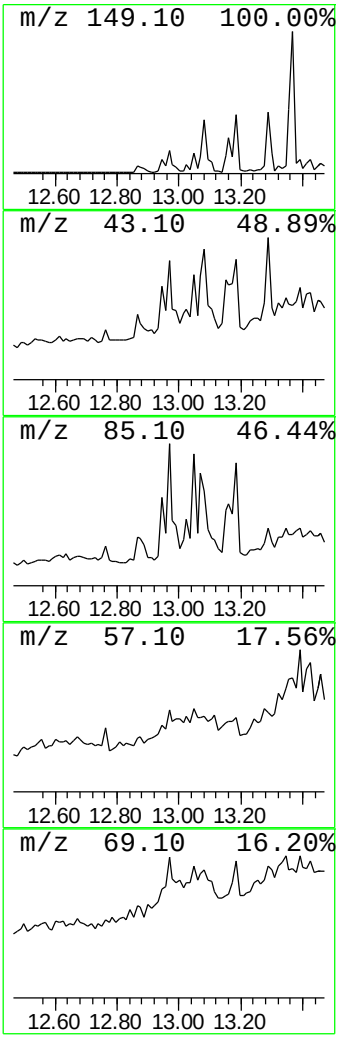
Peak Number 7 unknown12.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	7.87 ng	471468	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	47
2	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	47
3	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	47
4	2-t-Butyl-5-[hydroxy-(2,4,6-trim...	306	C18H26O4	092572-63-9	43
5	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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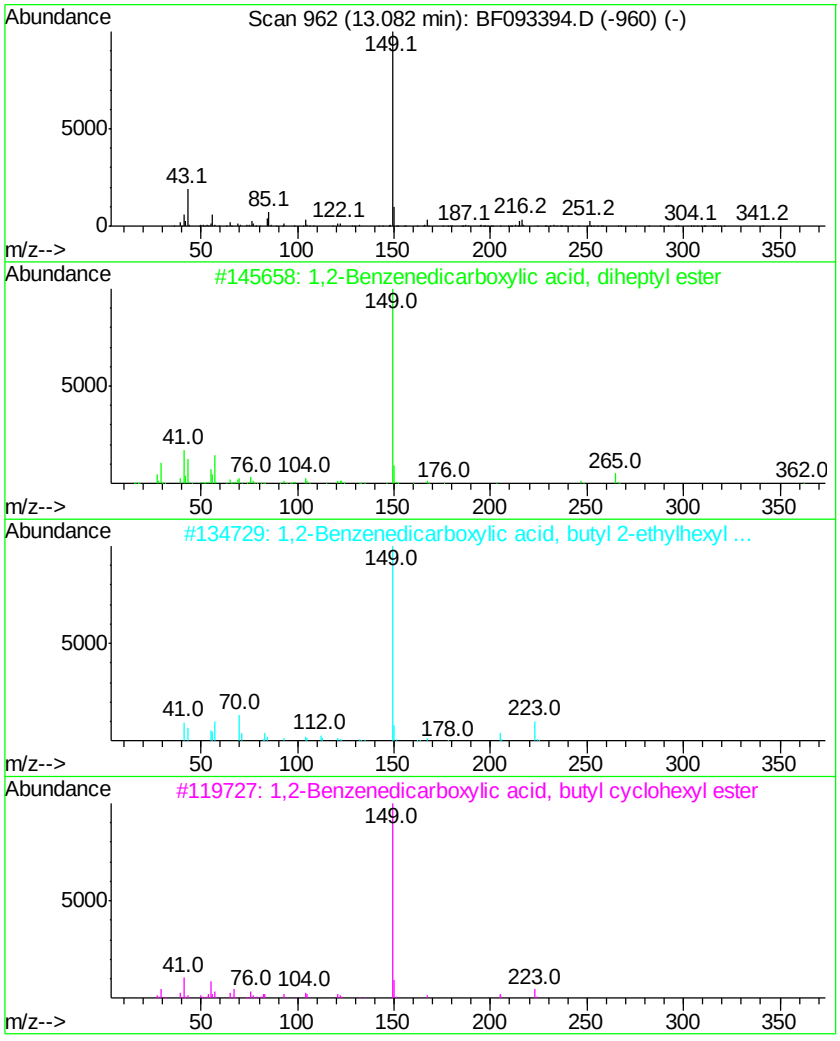
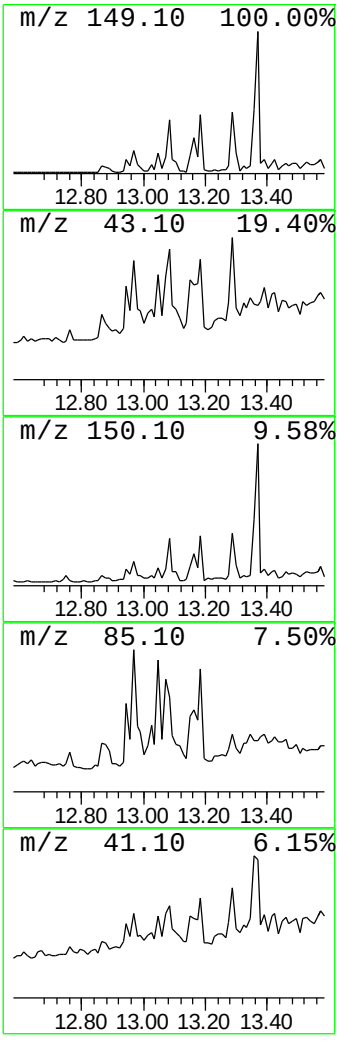
Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.08	7.15 ng	428137	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	64
2	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	64
3	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	64
4	1,2-Benzenedicarboxylic acid, di...	334	C20H30O4	000084-75-3	64
5	1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	56





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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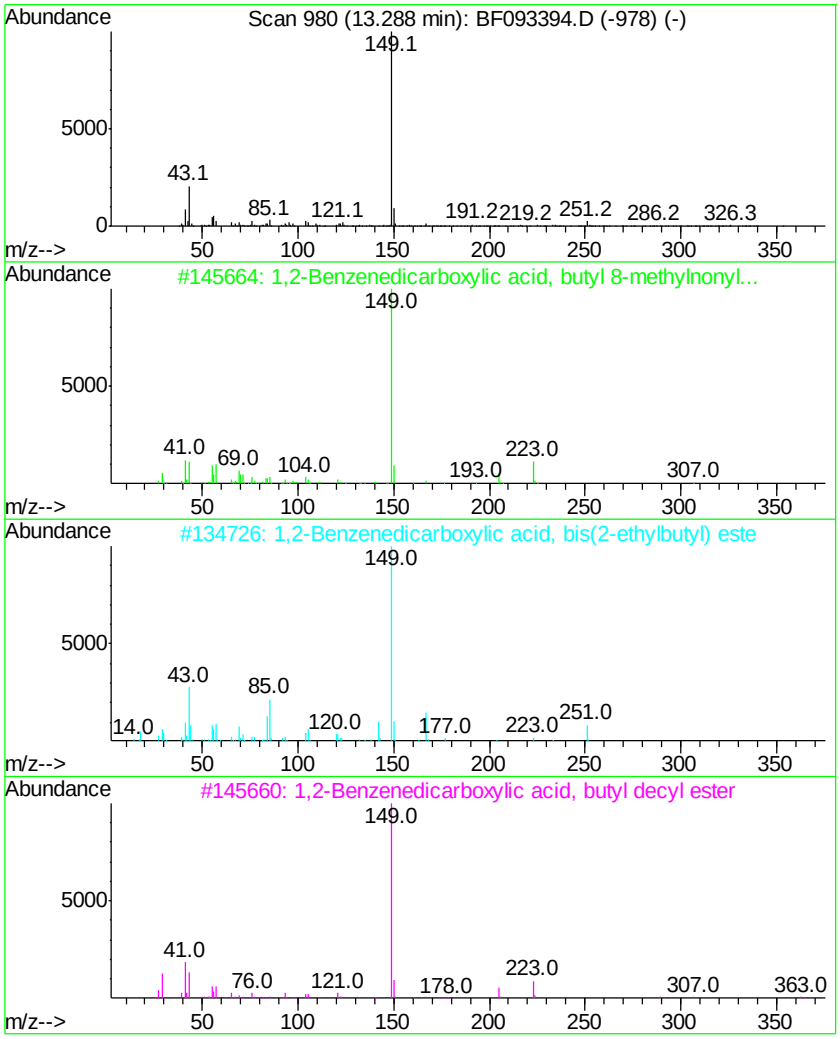
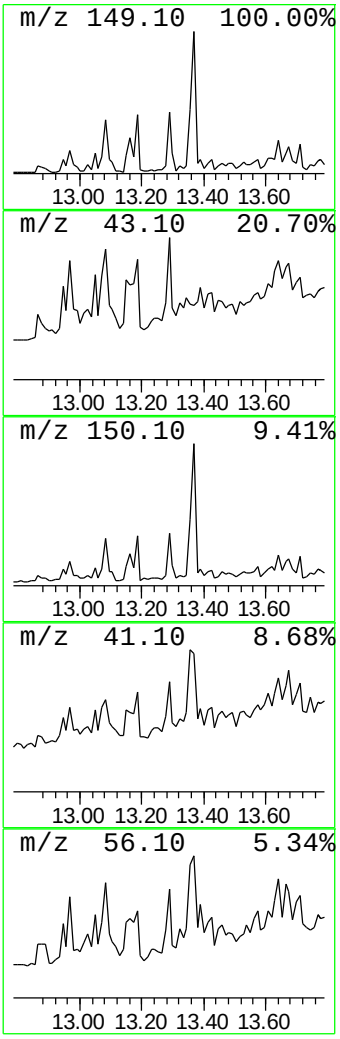
Peak Number 11 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	6.04 ng	362120	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	64
2	1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	007299-89-0	56
3	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	50
4	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	50
5	1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	50





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Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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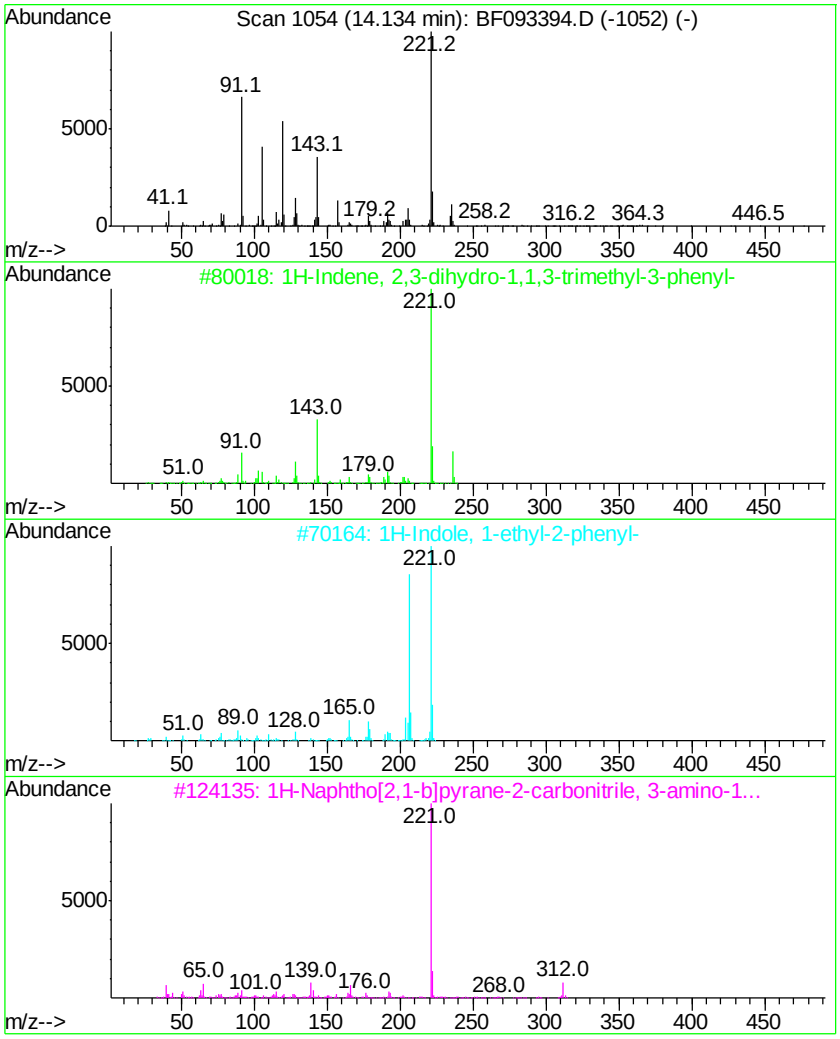
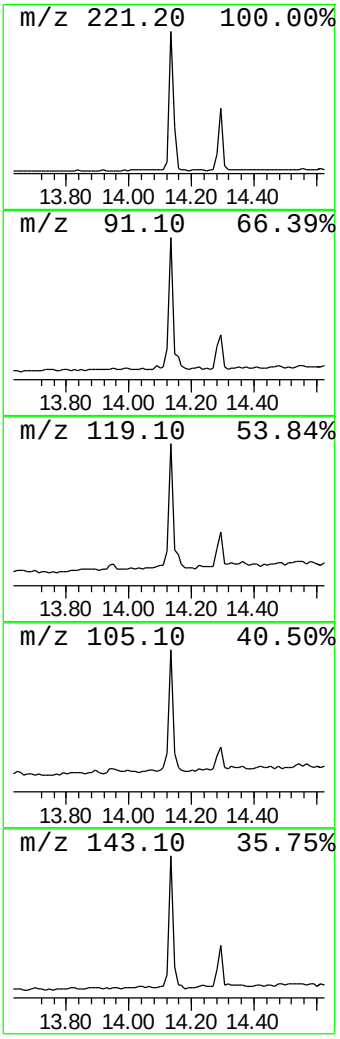
Peak Number 13 unknown14.13 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	11.23 ng	672852	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	49
2	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	45
3	1H-Naphtho[2,1-b]pyrane-2-carbon...	312	C21H16N2O	130715-41-2	38
4	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38
5	N-Methyl-m-hemipimide	221	C11H11NO4	092288-92-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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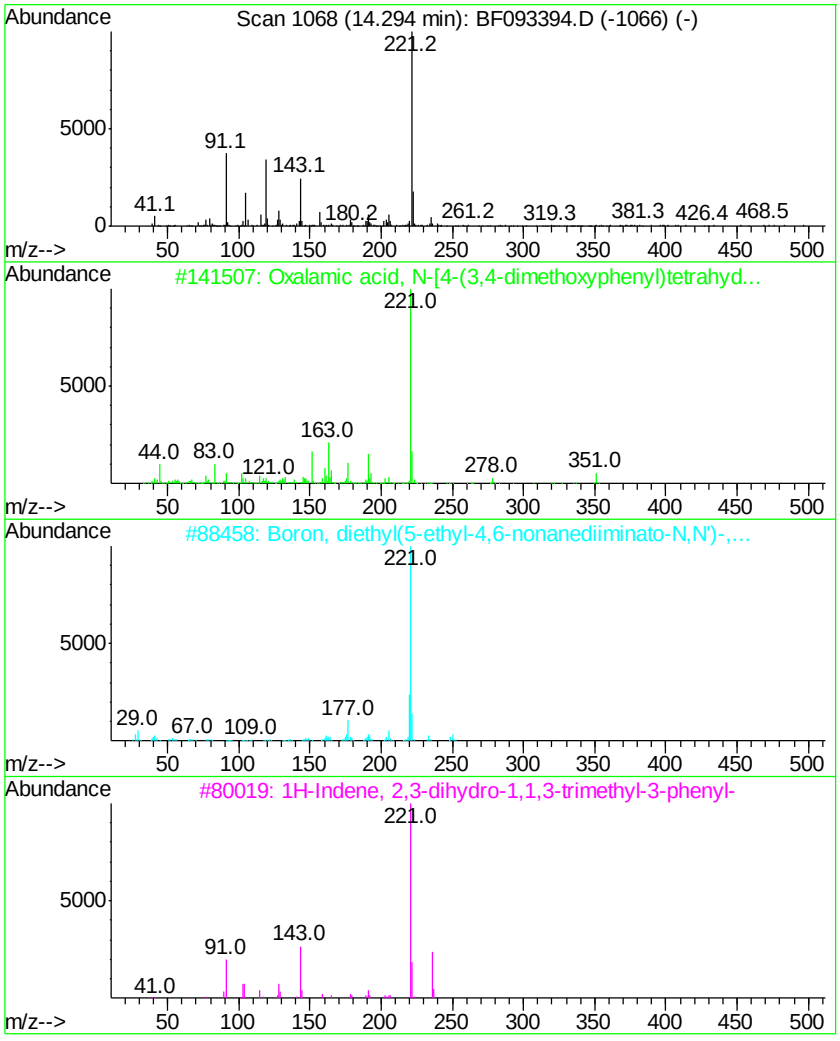
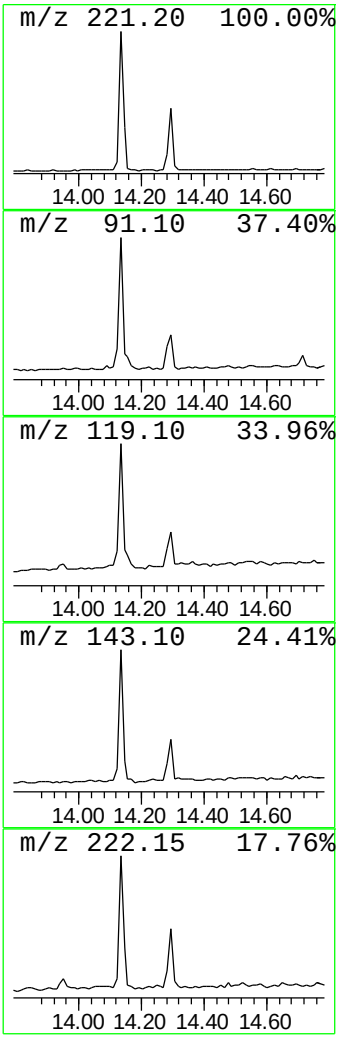
Peak Number 14 unknown14.29 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	3.34 ng	199949	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalamic acid, N-[4-(3,4-dimetho...	351	C18H25NO6	1000295-43-8	47
2	Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	47
3	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	45
4	Benzene, 1,1'-(1,3,3-trimethyl-1...	236	C18H20	006258-73-7	33
5	4-Toluenesulfonic acid, (1,3-dip...	406	C23H22N2O3S	1000286-65-2	33





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
Data File : BF093394.D
Acq On : 4 Mar 2017 9:22
Operator : SJ/MA
Sample : I2057-16 5X
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
3-Penten-2-one, 4...	4.25	3.1	ng	176861	1	6.78	1127800	20.0
2-Pentanone, 4-hy...	4.92	6.8	ng	381500	1	6.78	1127800	20.0
unknown6.56	6.56	14.1	ng	792696	1	6.78	1127800	20.0
1H-Indene, 2,3-di...	10.91	5.4	ng	323755	4	11.31	1190790	20.0
5H-Indeno[1,2-b]p...	11.55	2.0	ng	120577	4	11.31	1190790	20.0
unknown12.97	12.97	7.9	ng	471468	5	13.95	1198270	20.0
1,2-Benzenedicarb...	13.08	7.2	ng	428137	5	13.95	1198270	20.0
1,2-Benzenedicarb...	13.29	6.0	ng	362120	5	13.95	1198270	20.0
unknown14.13	14.13	11.2	ng	672852	5	13.95	1198270	20.0
unknown14.29	14.29	3.3	ng	199949	5	13.95	1198270	20.0