LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011216\
Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

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-BF123115.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	4.361	196	199	202	rVB2	59567	90058	1.14%	0.136%
2	5.013	253	256	266	rVB	1145255	1280031	16.20%	1.930%
3	5.447	292	294	296	rBV	4466737	3930353	49.75%	5.926%
4	5.847	327	329	331	rBV	149404	141666	1.79%	0.214%
5	6.476	382	384	387	rBV	2189325	2395901	30.33%	3.612%
6	6.613	393	396	398	rBV	6970679	6356911	80.46%	9.585%
7	6.842	414	416	418	rBV	2106724	1731166	21.91%	2.610%
8	7.002	427	430	432	rBV	5977305	6034414	76.38%	9.098%
9	7.185	443	446	448	rBV2	84713	94810	1.20%	0.143%
10	7.413	463	466	468	rVB	4331391	5337720	67.56%	8.048%
11	7.493	471	473	474	rBV	70292	86095	1.09%	0.130%
12	7.539	474	477	479	rBV	98933	108170	1.37%	0.163%
13	7.619	479	484	486	rVB3	61991	107634	1.36%	0.162%
14	7.688	489	490	492	rBV	68605	92213	1.17%	0.139%
15	7.779	495	498	500	rBV	116571	131650	1.67%	0.198%
16	7.813	500	501	503	rVB	172042	148329	1.88%	0.224%
17	7.870	503	506	508	rBV	79122	126349	1.60%	0.191%
18	8.065	521	523	526	rBV2	96826	91462	1.16%	0.138%
19	8.122	526	528	530	rBV	1565421	2207769	27.94%	3.329%
20	8.156	530	531	532	rVB	123506	87643	1.11%	0.132%
21	8.328	543	546	548	rBV3	107253	170961	2.16%	0.258%
22	8.373	548	550	552	rVB	140968	146249	1.85%	0.221%
23	8.510	561	562	564	rVB	140137	101960	1.29%	0.154%
24	8.602	564	570	572	rBV2	317271	490342	6.21%	0.739%
25	8.636	572	573	576	rVV2	76519	137860	1.74%	0.208%
26	8.693	576	578	579	rVV	238185	233764	2.96%	0.352%
27	8.750	579	583	585	rVV4	75183	161724	2.05%	0.244%
28	8.796	585	587	588	rVV	190016	192157	2.43%	0.290%
29	8.853	588	592	595	rVV5	84993	221535	2.80%	0.334%
30	8.933	595	599	601	rVV4	89166	163784	2.07%	0.247%
31	8.968	601	602	605	rVB2	72178	122277	1.55%	0.184%
32	9.048	605	609	610	rBV3	132721	294739	3.73%	0.444%
33	9.070	610	611	613	rVV2	168181	213801	2.71%	0.322%
34	9.105	613	614	618	rVV3	179694	255465	3.23%	0.385%

LSC Area Percent Report

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Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.208	620	623	625	rVV	8524888	7900598	100.00%	11.912%
36	9.253	625	627	629	rVV2	99956	108575	1.37%	0.164%
37	9.311	629	632	633	rVV2	80048	161491	2.04%	0.243%
38	9.356	633	636	638	rVV3	135608	307991	3.90%	0.464%
39	9.413	638	641	643	rVV3	111755	199577	2.53%	0.301%
40	9.471	644	646	647	rVV2	181083	190590	2.41%	0.287%
41	9.551	650	653	654	rVV3	118184	298235	3.77%	0.450%
42	9.573	654	655	657	rVV	180841	209852	2.66%	0.316%
43	9.619	657	659	661	rVV2	93151	194428	2.46%	0.293%
44	9.676	661	664	665	rVV	435357	691059	8.75%	1.042%
45	9.745	667	670	672	rVB3	136180	198572	2.51%	0.299%
46	9.882	679	682	684	rBV	2791958	2638696	33.40%	3.978%
47	9.916	684	685	687	rVB	321447	239827	3.04%	0.362%
48	10.042	694	696	698	rVB	101015	118873	1.50%	0.179%
49	10.111	698	702	704	rVB3	90966	245893	3.11%	0.371%
50	10.202	707	710	711	rVV3	66488	105444	1.33%	0.159%
51	10.282	714	717	718	rVV2	145217	197030	2.49%	0.297%
52	10.305	718	719	721	rVV2	80245	93044	1.18%	0.140%
53	10.373	724	725	728	rBV3	116782	173607	2.20%	0.262%
54	10.419	728	729	731	rVB	272188	231594	2.93%	0.349%
55	10.511	731	737	739	rBV2	324056	623569	7.89%	0.940%
56	10.591	741	744	748	rVV4	128415	289009	3.66%	0.436%
57	10.671	748	751	753	rVV	4539864	4754558	60.18%	7.169%
58	10.716	753	755	757	rVB3	84618	111075	1.41%	0.167%
59	10.876	766	769	770	rBV2	57748	106544	1.35%	0.161%
60	10.968	775	777	779	rVV3	108884	184042	2.33%	0.277%
61	11.025	779	782	784	rVB4	75124	181513	2.30%	0.274%
62	11.368	810	812	814	rBV	2370021	2144626	27.15%	3.234%
63	11.482	820	822	825	rBV2	73139	118949	1.51%	0.179%
64	11.574	828	830	837	rVB7	67855	179620	2.27%	0.271%
65	11.974	863	865	867	rVB	50691	84479	1.07%	0.127%
66	12.957	948	951	953	rBV	6659461	6647656	84.14%	10.023%
67	13.997	1040	1042	1045	rBV	1532247	1546244	19.57%	2.331%
68	15.425	1164	1167	1170	rBV	1125591	1360091	17.22%	2.051%

Sum of corrected areas: 66323913

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Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
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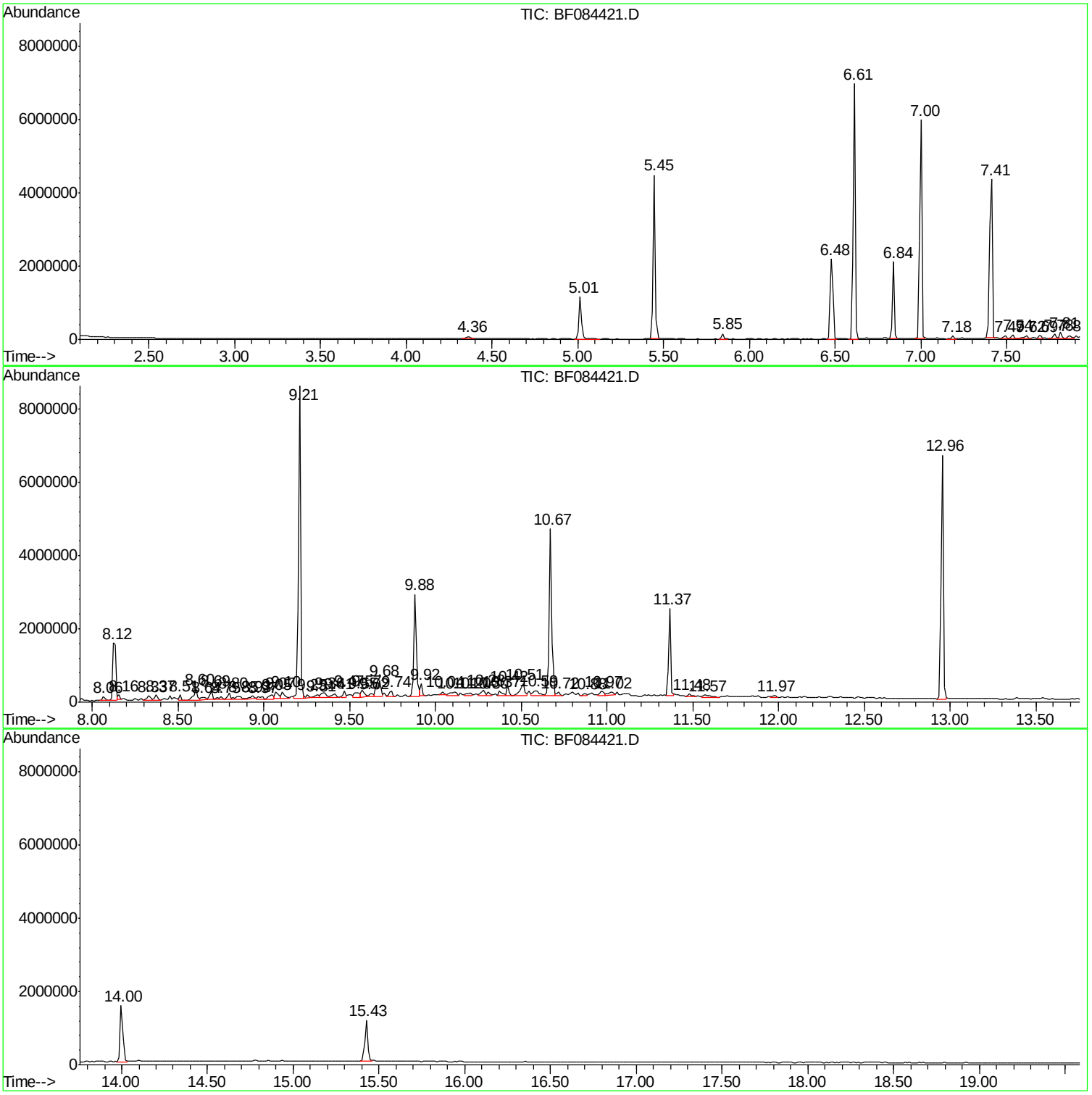
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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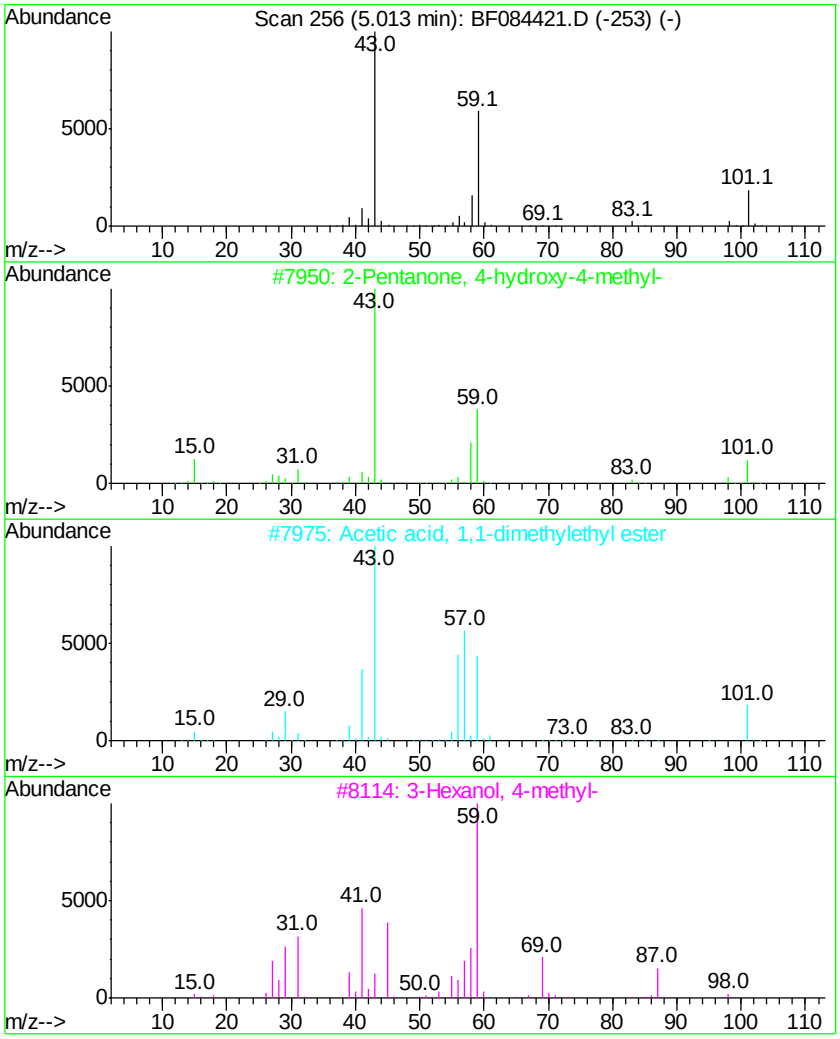
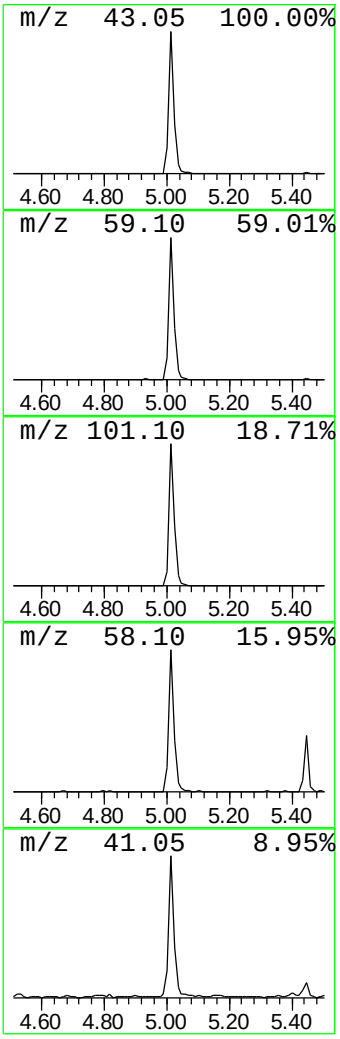
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	14.79 ng	1280030	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

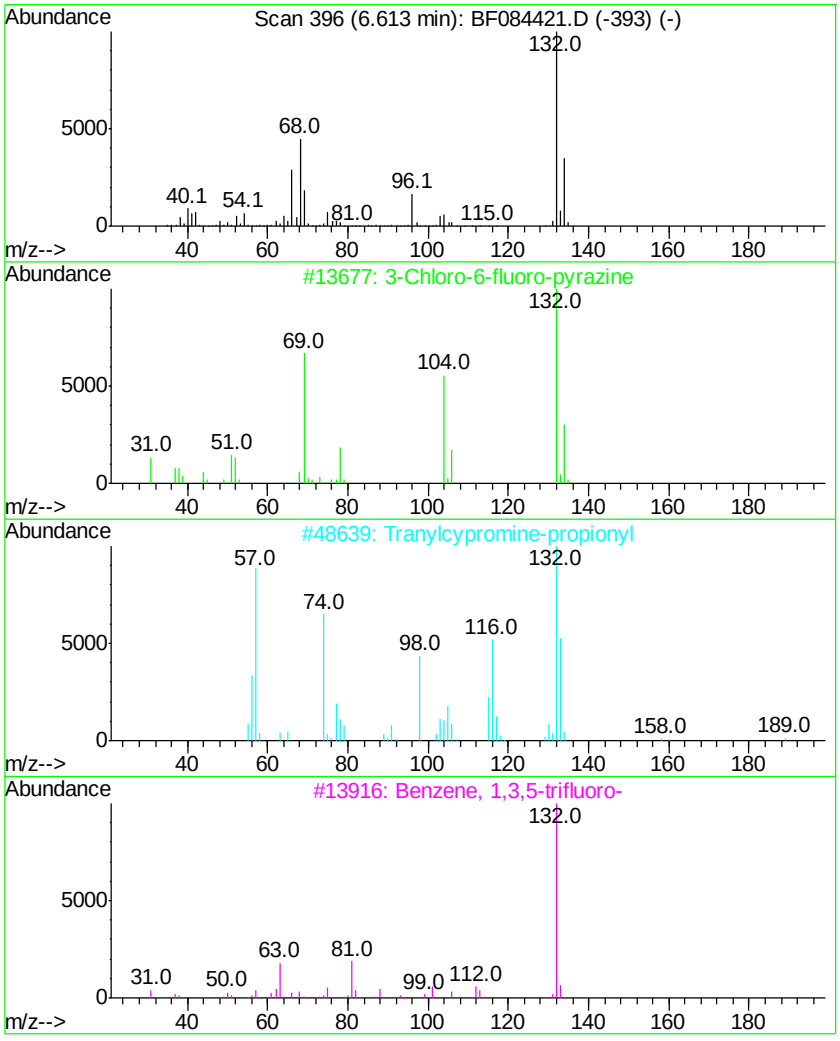
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

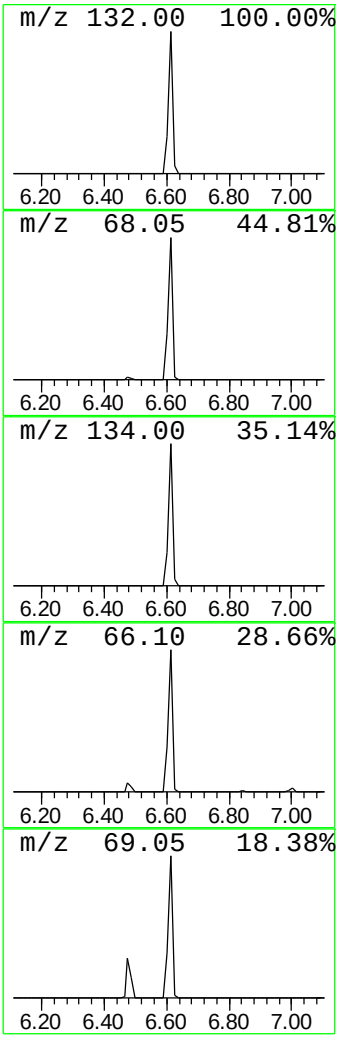
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	73.44 ng	6356910	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : H1078-11
Misc :
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Instrument : BNA_F
ClientSampleId : MW35

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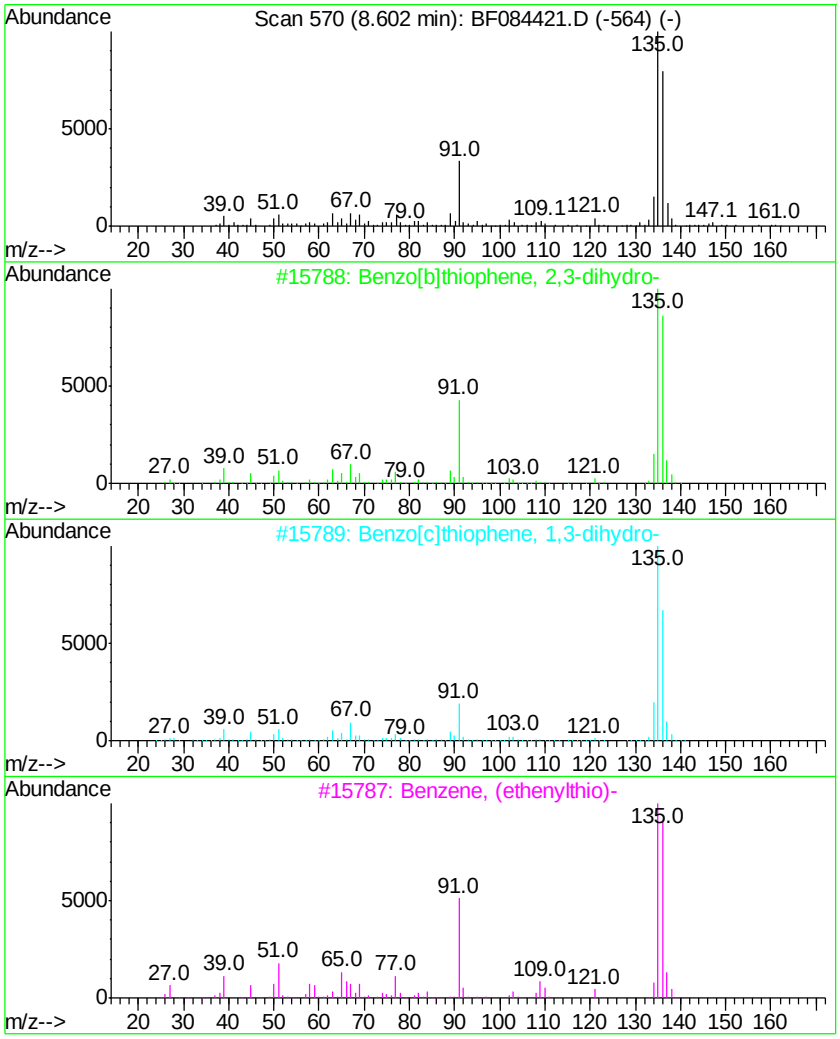
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

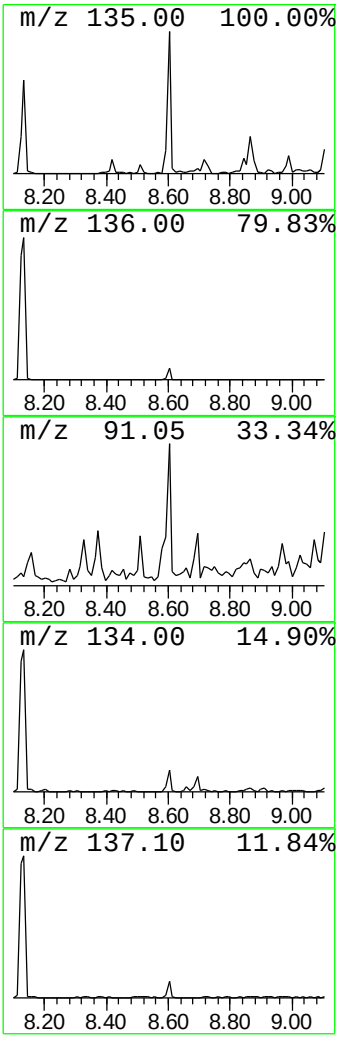
****

Peak Number 4 Benzo[b]thiophene, 2,3-dihy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.60	4.44 ng	490342	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	91
2	Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	90
3	Benzene, (ethenylthio)-	136	C8H8S	001822-73-7	87
4	4-Hydroxy-2-methylbenzaldehyde	136	C8H8O2	041438-18-0	72
5	Pyrazine, 2,6-diethyl-	136	C8H12N2	013067-27-1	72





Library Search Compound Report

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Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
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Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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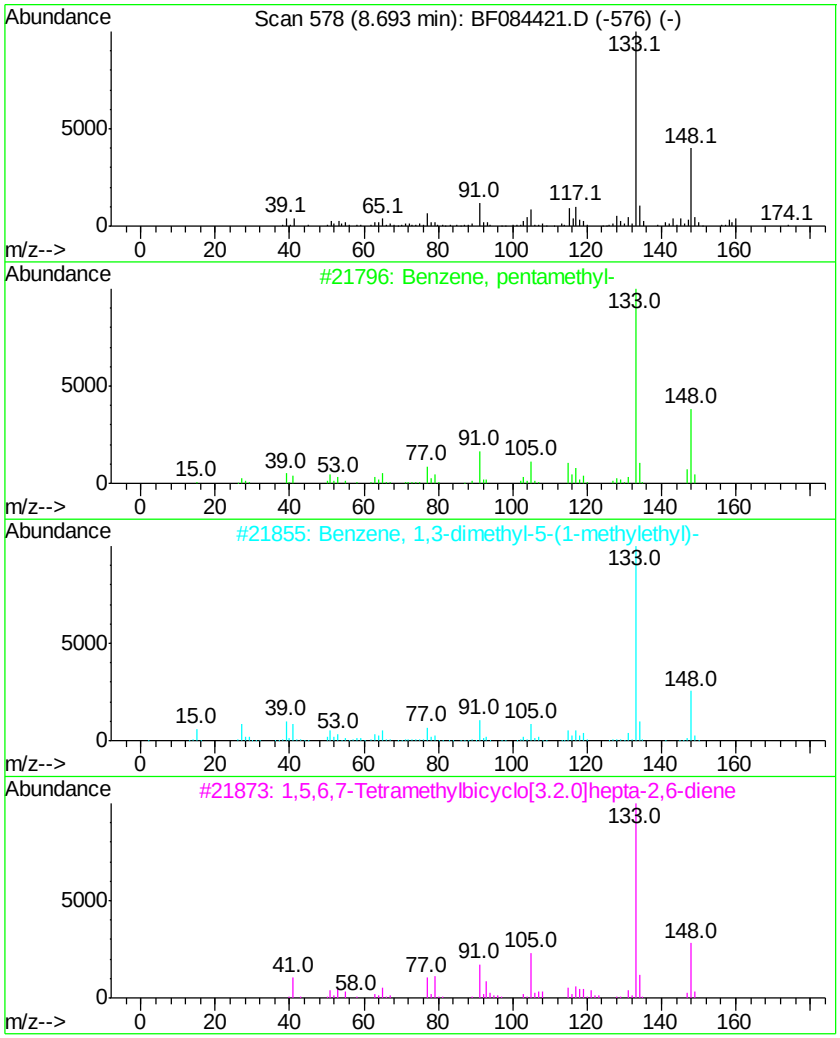
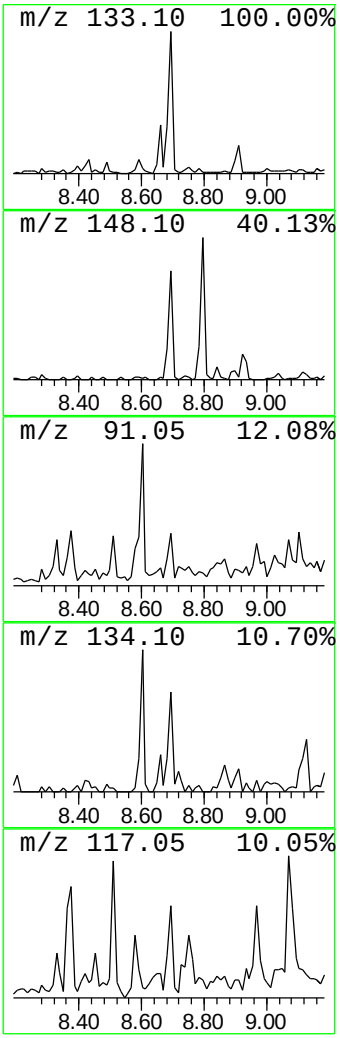
****

Peak Number 5 Benzene, pentamethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.12 ng	233764	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, pentamethyl-	148	C11H16	000700-12-9	91
2	Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	87
3	1,5,6,7-Tetramethylbicyclo[3.2.0...	148	C11H16	134329-46-7	81
4	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	80
5	Benzene, 2,4-dimethyl-1-(1-methy...	148	C11H16	004706-89-2	80





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Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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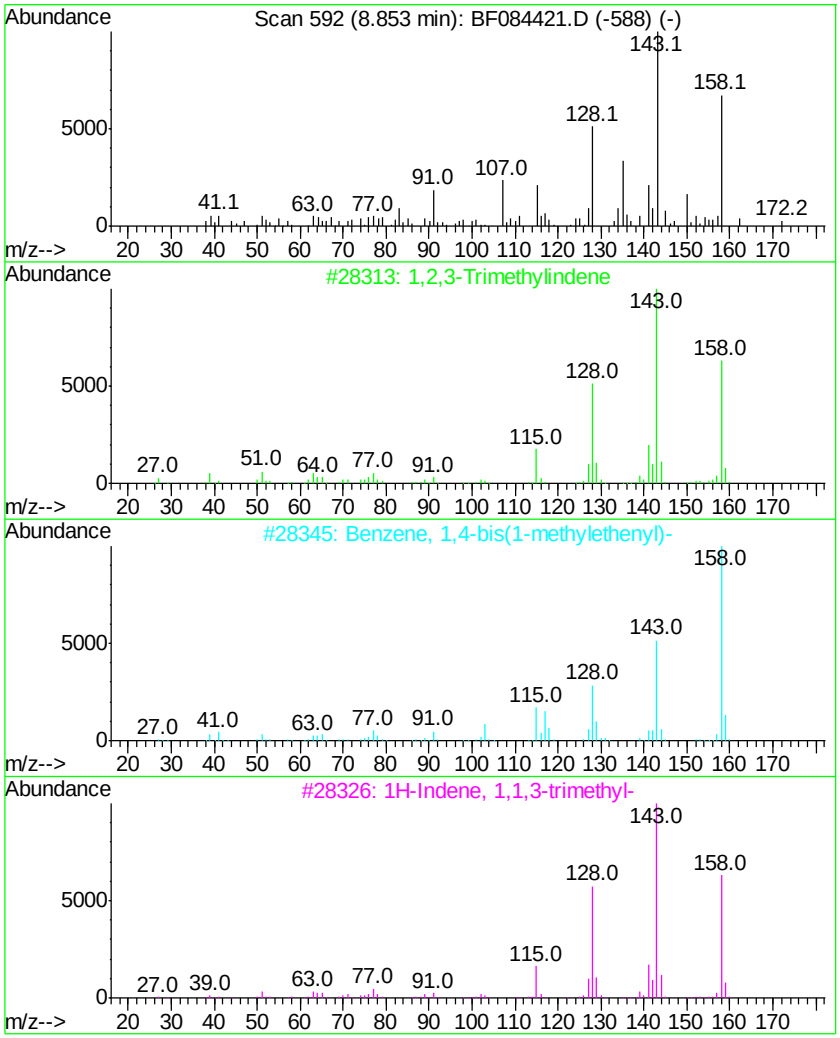
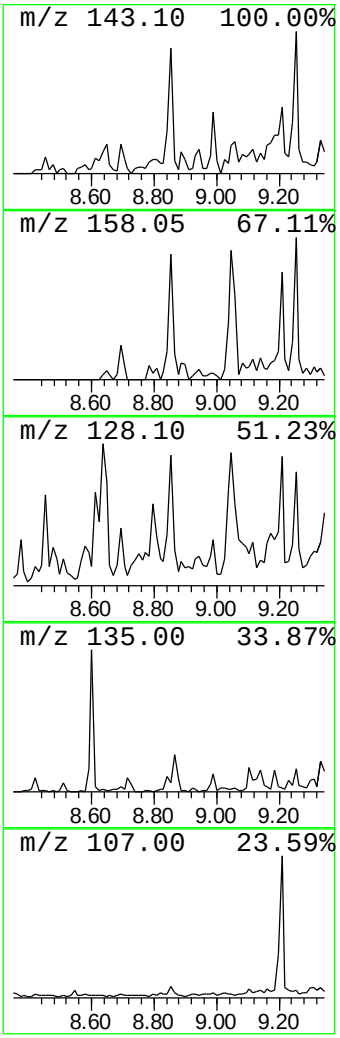
Peak Number 6 1,2,3-Trimethylindene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	2.01 ng	221535	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Trimethylindene	158	C12H14	004773-83-5	94
2	Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	58
3	1H-Indene, 1,1,3-trimethyl-	158	C12H14	002177-45-9	53
4	(1-Methylpenta-1,3-dienyl)benzene	158	C12H14	116669-49-9	53
5	Benzene, 1,3,5-trimethyl-2-(1,2-...	158	C12H14	029555-07-5	47





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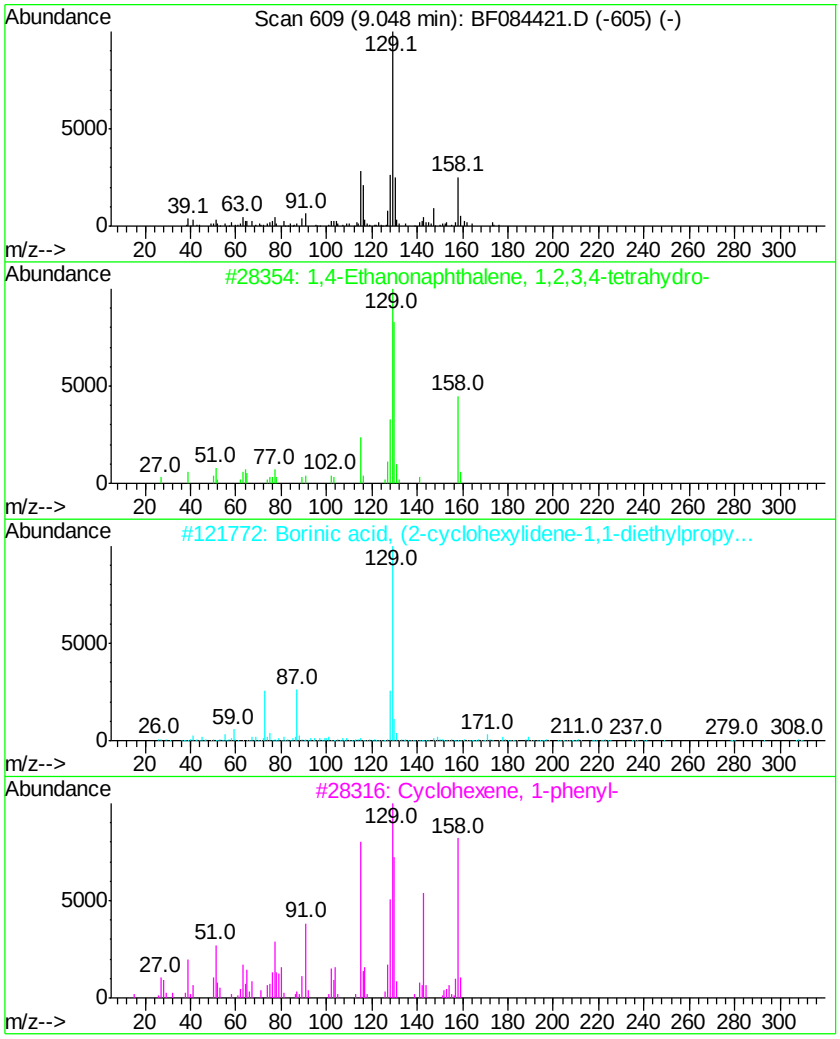
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

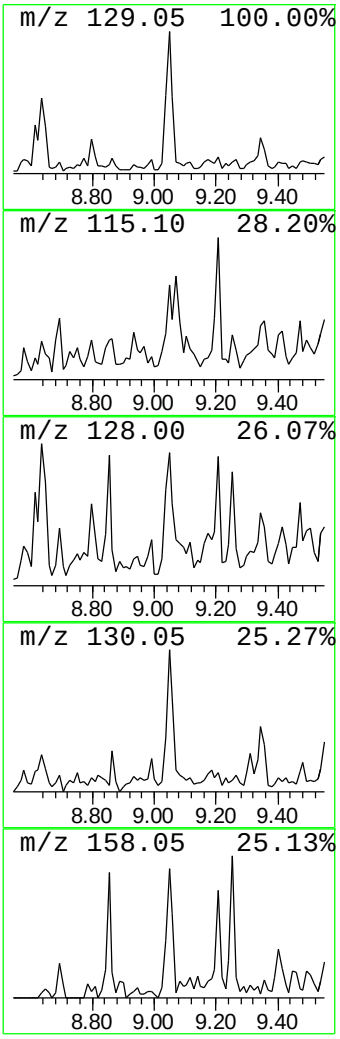
****

Peak Number 7 unknown9.05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	2.23 ng	294739	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Ethanonaphthalene, 1,2,3,4-t...	158	C12H14	004175-52-4	42
2	Borinic acid, (2-cyclohexylidene...	308	C18H37BOSi	074810-48-3	37
3	Cyclohexene, 1-phenyl-	158	C12H14	000771-98-2	32
4	Isoquinoline	129	C9H7N	000119-65-3	32
5	5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011216\
Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

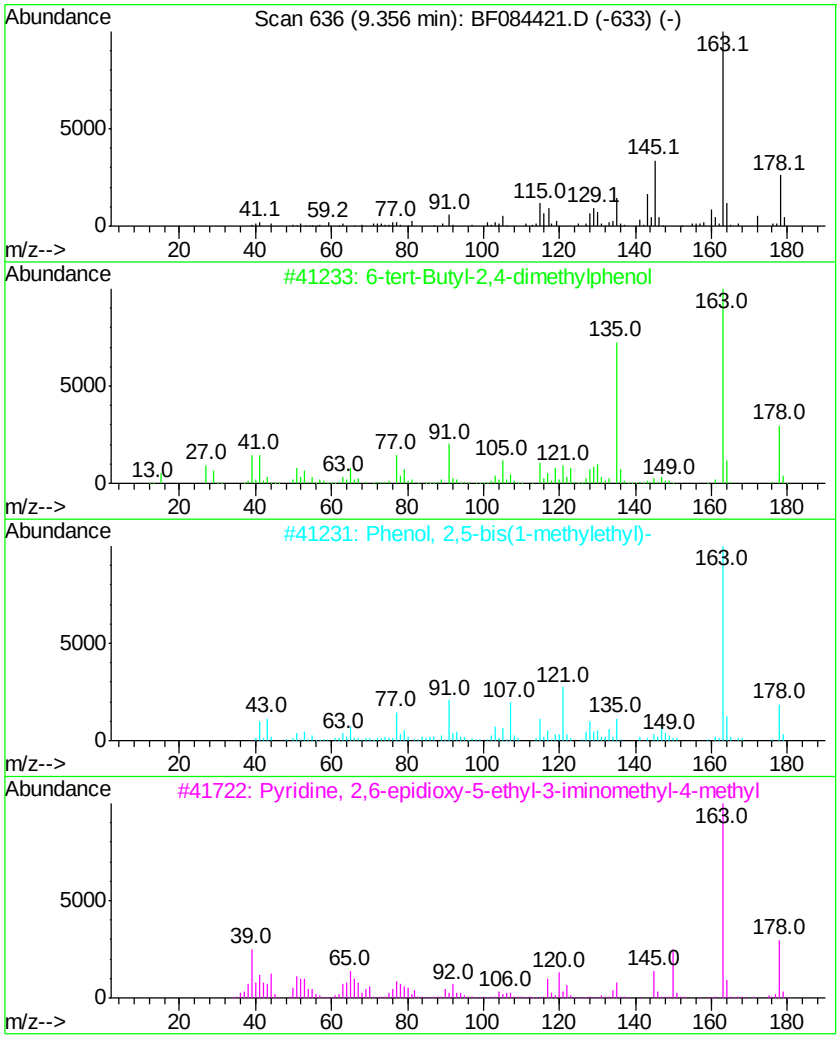
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

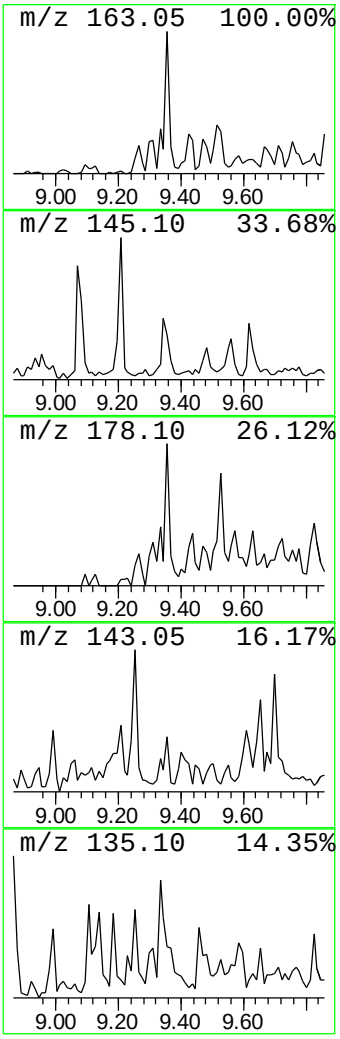
****

Peak Number 8 6-tert-Butyl-2,4-dimethylph... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	2.33 ng	307991	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
2	Phenol, 2,5-bis(1-methylethyl)-	178	C12H18O	035946-91-9	64
3	Pyridine, 2,6-epidioxy-5-ethyl-3...	178	C9H10N2O2	1000263-31-1	59
4	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	58
5	Propofol	178	C12H18O	002078-54-8	53





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Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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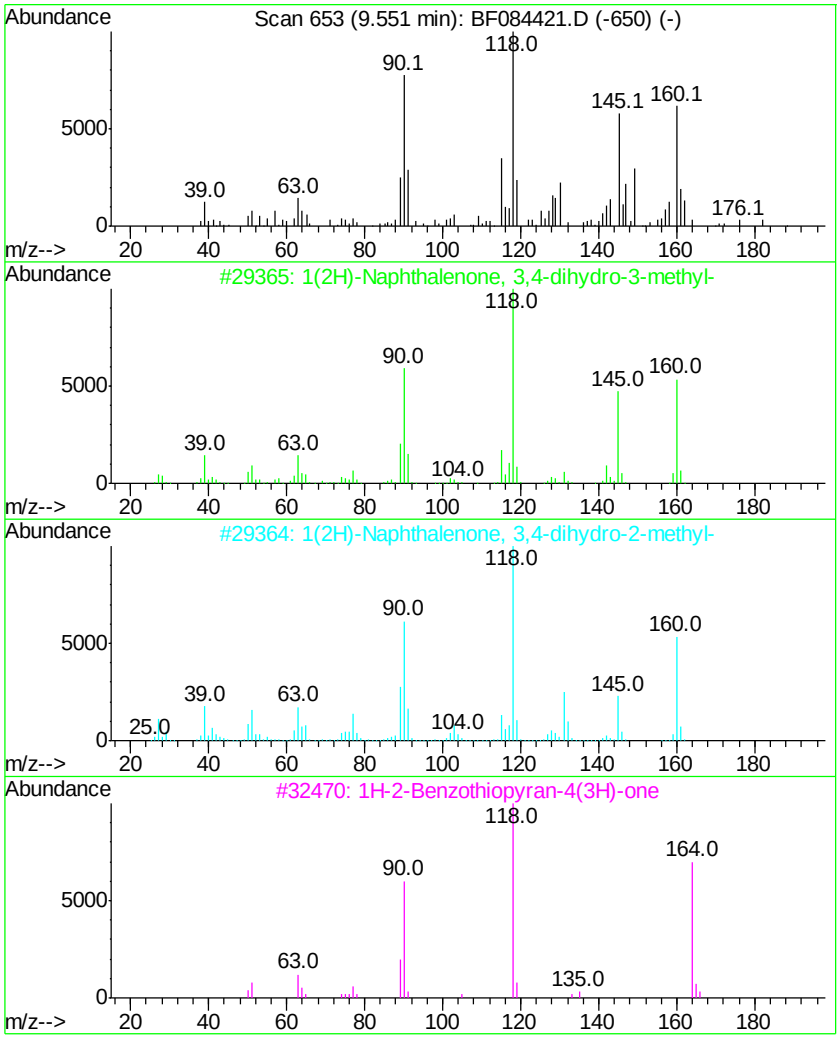
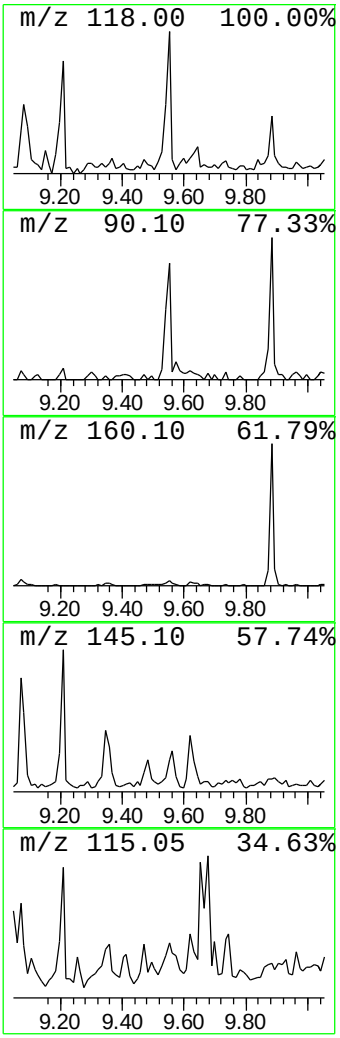
Peak Number 9 1(2H)-Naphthalenone, 3,4-di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	2.26 ng	298235	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	83
2	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	001590-08-5	72
3	1H-2-Benzothiopyran-4(3H)-one	164	C9H8OS	004426-76-0	53
4	1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	53
5	1,3,5-Norcaratriene	90	C7H6	004646-69-9	46





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Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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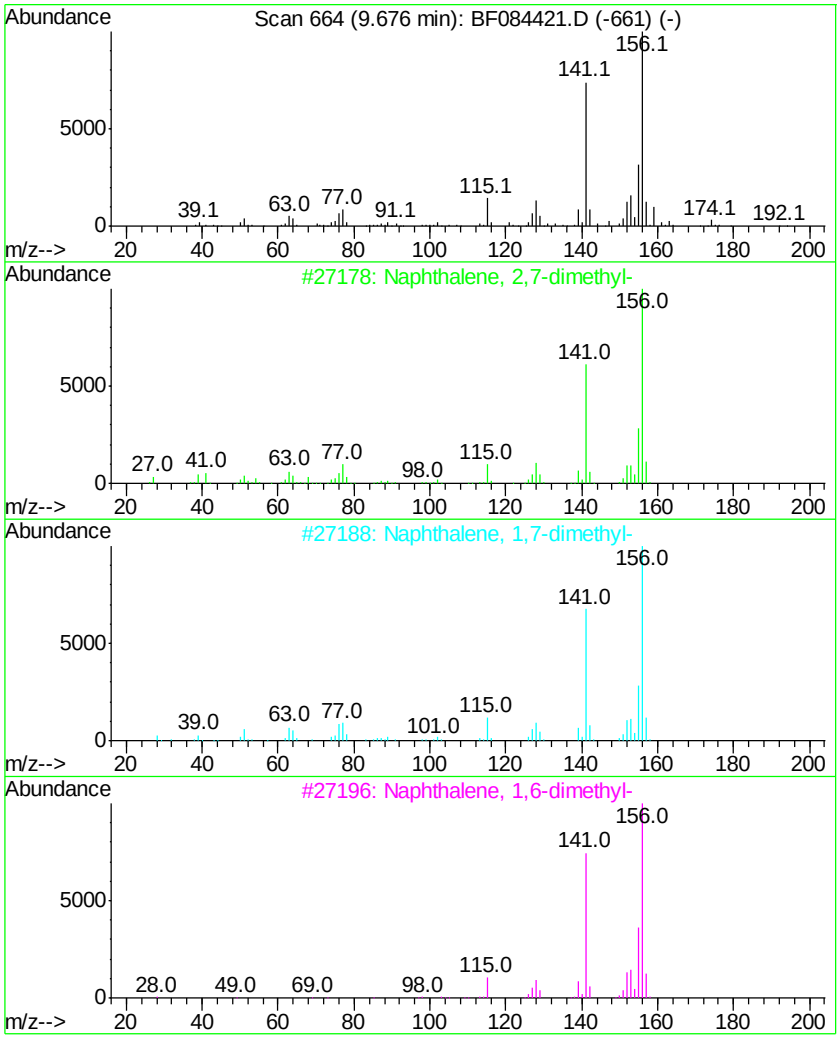
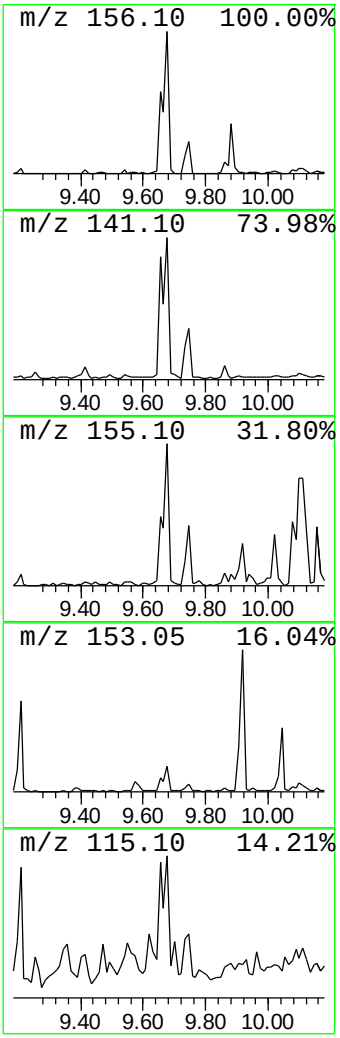
Peak Number 10 Naphthalene, 2,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	5.24 ng	691059	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011216\
Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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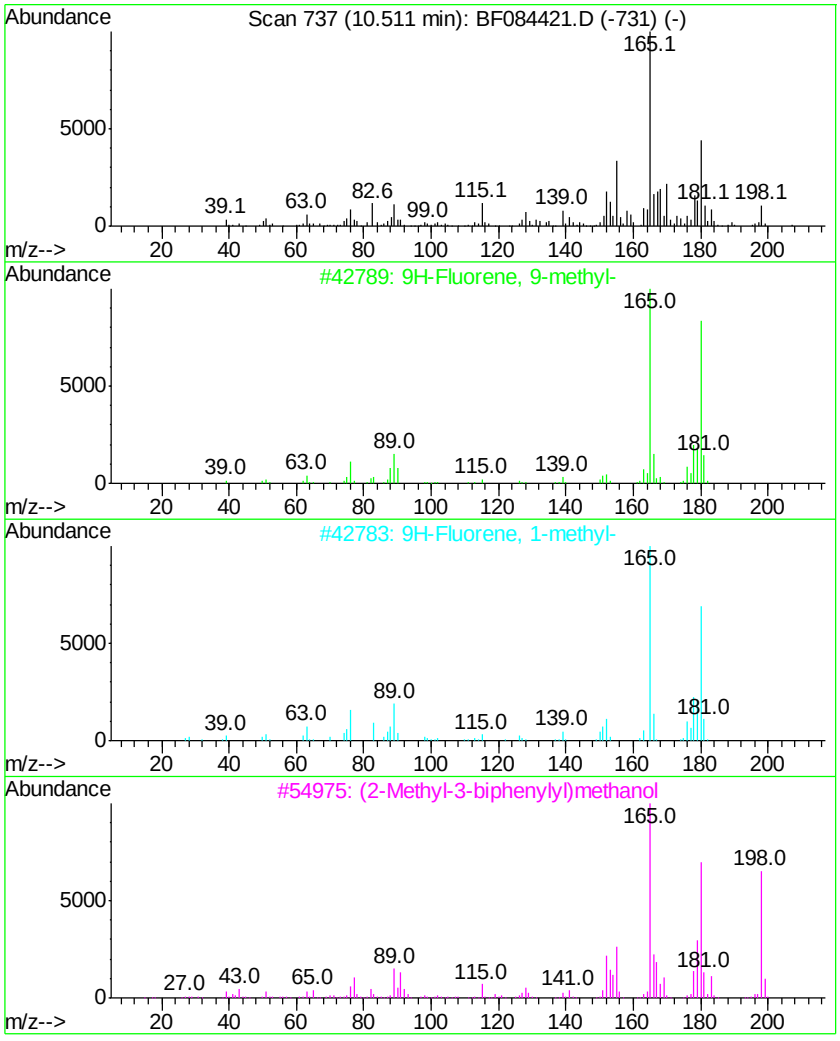
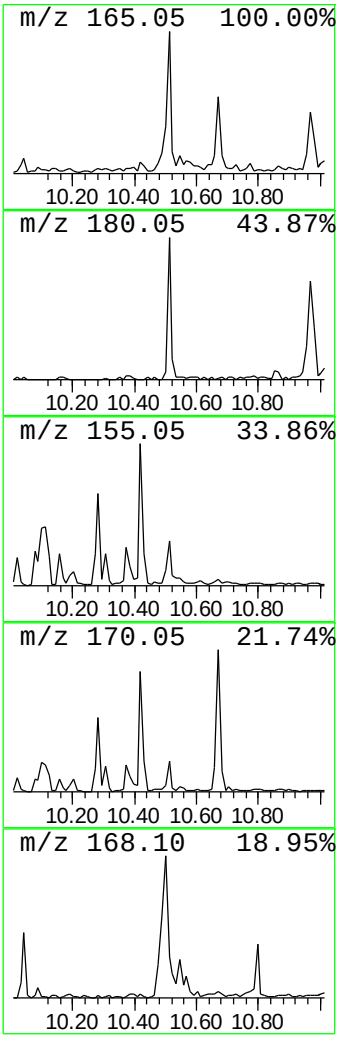
Peak Number 11 9H-Fluorene, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	4.73 ng	623569	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9-methyl-	180	C14H12	002523-37-7	78
2	9H-Fluorene, 1-methyl-	180	C14H12	001730-37-6	60
3	(2-Methyl-3-biphenylyl)methanol	198	C14H14O	076350-90-8	60
4	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	53
5	9H-Fluorene, 2-methyl-	180	C14H12	001430-97-3	53





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Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

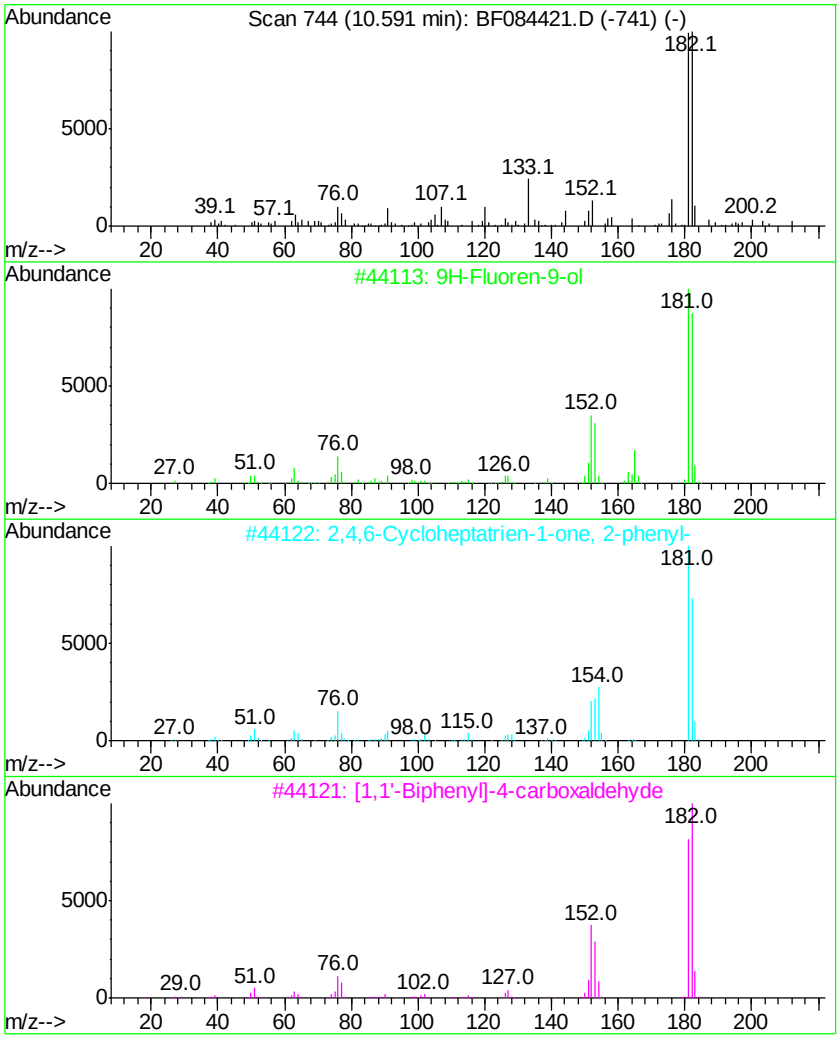
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

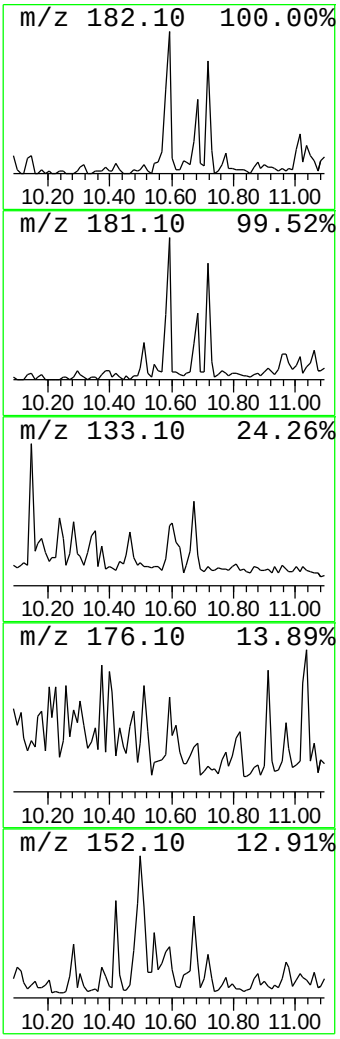
****

Peak Number 12 9H-Fluoren-9-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.19 ng	289009	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-ol	182	C13H10O	001689-64-1	59
2	2,4,6-Cycloheptatrien-1-one, 2-p...	182	C13H10O	014562-09-5	59
3	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	47
4	Pyridine, 4,4'-(1,2-ethenediyl)bis-	182	C12H10N2	001135-32-6	42
5	2-Hydroxyfluorene	182	C13H10O	002443-58-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011216\
Data File : BF084421.D
Acq On : 12 Jan 2016 20:24
Operator : SJ/UM
Sample : H1078-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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...	5.01	14.8	ng	1280030	1	6.84	1731170	20.0
unknown6.61	6.61	73.4	ng	6356910	1	6.84	1731170	20.0
Benzo[b]thiophene...	8.60	4.4	ng	490342	2	8.13	2207770	20.0
Benzene, pentamet...	8.69	2.1	ng	233764	2	8.13	2207770	20.0
1,2,3-Trimethylin...	8.85	2.0	ng	221535	2	8.13	2207770	20.0
unknown9.05	9.05	2.2	ng	294739	3	9.88	2638700	20.0
6-tert-Butyl-2,4-...	9.36	2.3	ng	307991	3	9.88	2638700	20.0
1(2H)-Naphthaleno...	9.55	2.3	ng	298235	3	9.88	2638700	20.0
Naphthalene, 2,7-...	9.68	5.2	ng	691059	3	9.88	2638700	20.0
9H-Fluorene, 9-me...	10.51	4.7	ng	623569	3	9.88	2638700	20.0
9H-Fluoren-9-ol	10.59	2.2	ng	289009	3	9.88	2638700	20.0