LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

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-BF030316.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	5.156	248	251	257	rVB	230219	324954	6.46%	0.896%
2	5.556	284	286	289	rVB	1924967	1796930	35.73%	4.956%
3	6.573	373	375	378	rVB	1392896	1155133	22.97%	3.186%
4	6.722	385	388	391	rBV	2955281	3199066	63.61%	8.823%
5	6.962	407	409	411	rBV	914440	865235	17.20%	2.386%
6	7.019	412	414	416	rBV	224179	184823	3.68%	0.510%
7	7.122	420	423	425	rVB	3141900	3493938	69.47%	9.637%
8	7.522	455	458	460	rBV	2635685	2568003	51.06%	7.083%
9	8.242	519	521	524	rVB	1270550	1170783	23.28%	3.229%
10	8.345	529	530	534	rVV2	45028	58800	1.17%	0.162%
11	9.065	591	593	598	rBV3	18185	55109	1.10%	0.152%
12	9.145	598	600	603	rVB3	56610	81433	1.62%	0.225%
13	9.328	613	616	618	rBV	3987599	5029140	100.00%	13.871%
14	9.716	648	650	653	rVB	58389	95520	1.90%	0.263%
15	9.808	656	658	660	rBV	70934	61779	1.23%	0.170%
16	9.865	660	663	665	rBV3	87141	193822	3.85%	0.535%
17	9.922	667	668	672	rBV3	65894	137960	2.74%	0.381%
18	10.002	672	675	677	rBV	1454126	1354816	26.94%	3.737%
19	10.048	677	679	680	rVV2	51359	61296	1.22%	0.169%
20	10.196	688	692	693	rBV4	77704	176312	3.51%	0.486%
21	10.230	693	695	698	rVV4	168782	294252	5.85%	0.812%
22	10.288	698	700	702	rVV3	66307	107582	2.14%	0.297%
23	10.333	702	704	707	rVB3	103173	171017	3.40%	0.472%
24	10.402	707	710	711	rBV2	241788	269126	5.35%	0.742%
25	10.436	711	713	716	rVB4	212188	435779	8.67%	1.202%
26	10.493	716	718	720	rBV2	44509	54244	1.08%	0.150%
27	10.699	734	736	739	rBV3	26373	52507	1.04%	0.145%
28	10.791	741	744	746	rBV	2822834	2904834	57.76%	8.012%
29	10.905	752	754	757	rBV3	57698	85822	1.71%	0.237%
30	10.985	760	761	764	rVB3	44109	51744	1.03%	0.143%
31	11.076	766	769	771	rVB3	43489	72821	1.45%	0.201%
32	11.225	779	782	783	rBV2	48434	80076	1.59%	0.221%
33	11.293	785	788	789	rVV3	36496	56336	1.12%	0.155%
34	11.442	798	801	802	rBV2	31170	57553	1.14%	0.159%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.488	802	805	806	rBV	1284643	1324225	26.33%	3.652%
36	11.613	813	816	818	rBV4	46318	96881	1.93%	0.267%
37	11.659	818	820	821	rVV2	45966	61942	1.23%	0.171%
38	11.762	825	829	831	rBV3	51879	112700	2.24%	0.311%
39	11.888	839	840	843	rBV3	46827	69302	1.38%	0.191%
40	12.002	846	850	854	rBV5	106432	229645	4.57%	0.633%
41	12.299	873	876	878	rBV4	32714	53557	1.06%	0.148%
42	12.402	882	885	887	rVB3	40702	84152	1.67%	0.232%
43	12.436	887	888	891	rBV3	53441	85709	1.70%	0.236%
44	12.528	894	896	899	rVB4	33479	63912	1.27%	0.176%
45	12.574	899	900	905	rBV4	28140	59790	1.19%	0.165%
46	12.676	905	909	910	rBV3	49040	76347	1.52%	0.211%
47	12.734	913	914	917	rVB2	36642	51382	1.02%	0.142%
48	12.779	917	918	921	rBV3	57745	128110	2.55%	0.353%
49	12.825	921	922	925	rVB3	60083	94034	1.87%	0.259%
50	12.894	925	928	929	rBV2	48706	82838	1.65%	0.228%
51	13.065	941	943	946	rBV	2770283	3722814	74.02%	10.268%
52	13.122	946	948	954	rVB7	46325	124176	2.47%	0.342%
53	13.545	981	985	988	rVB3	32181	69488	1.38%	0.192%
54	13.774	1002	1005	1006	rBV2	30258	53327	1.06%	0.147%
55	13.911	1015	1017	1019	rBV3	26193	50810	1.01%	0.140%
56	13.957	1019	1021	1027	rVB2	51890	143827	2.86%	0.397%
57	14.117	1033	1035	1038	rBV	1095276	1055428	20.99%	2.911%
58	14.242	1045	1046	1051	rVB3	39538	72955	1.45%	0.201%
59	14.471	1064	1066	1070	rVV5	47426	95811	1.91%	0.264%
60	14.528	1070	1071	1075	rVB3	52357	85352	1.70%	0.235%
61	14.620	1075	1079	1082	rBV5	48896	129056	2.57%	0.356%
62	14.700	1084	1086	1089	rVB2	31680	51823	1.03%	0.143%
63	14.791	1092	1094	1095	rVV2	48109	60395	1.20%	0.167%
64	14.837	1095	1098	1100	rVV3	38869	72005	1.43%	0.199%
65	14.940	1104	1107	1110	rVB4	63526	142154	2.83%	0.392%
66	15.008	1110	1113	1117	rBV5	38002	107555	2.14%	0.297%
67	15.580	1160	1163	1166	rBV	512095	724922	14.41%	1.999%
68	18.083	1379	1382	1385	rVB2	29396	61392	1.22%	0.169%

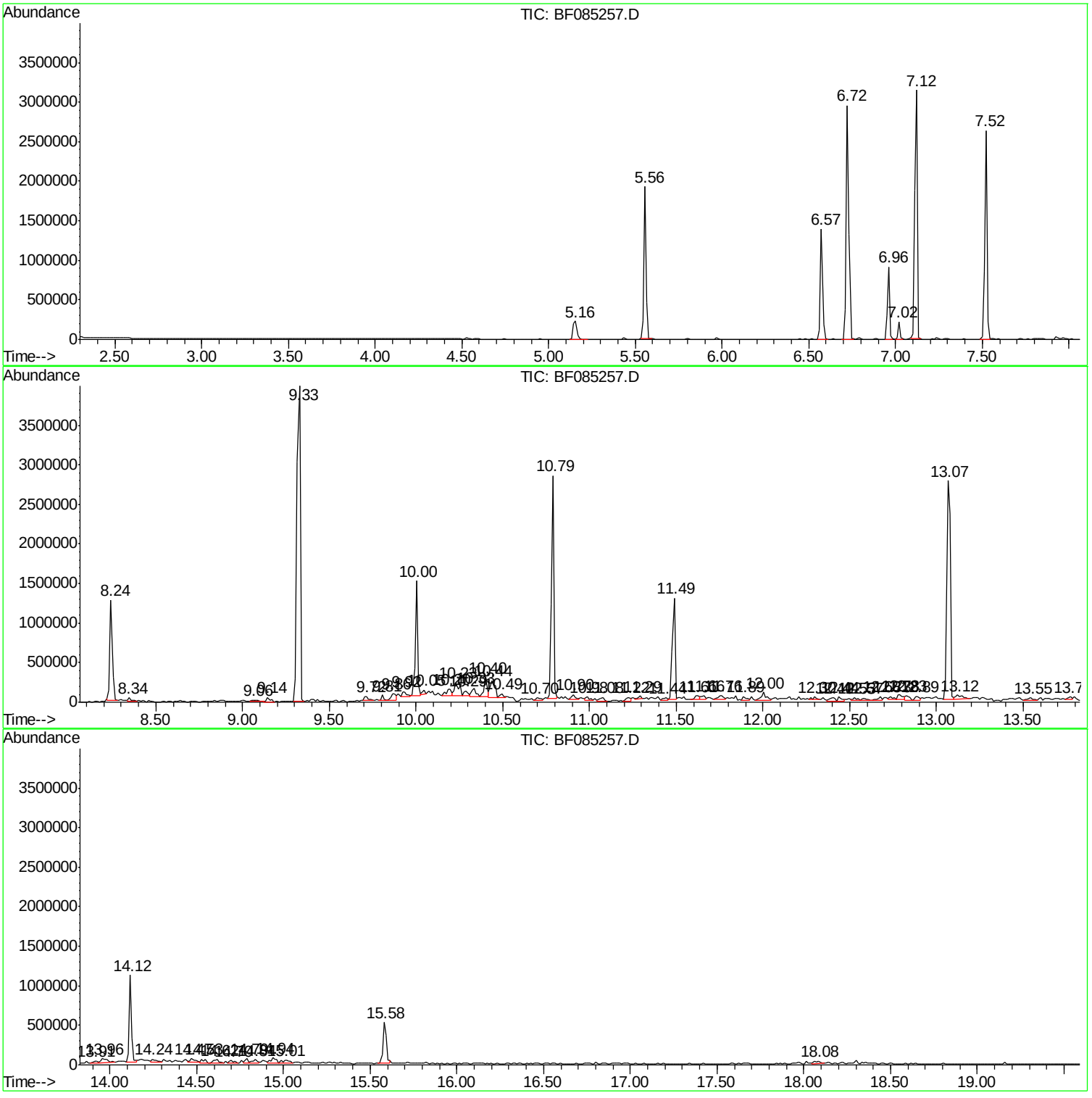
Sum of corrected areas: 36256361

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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 : BF085257.D
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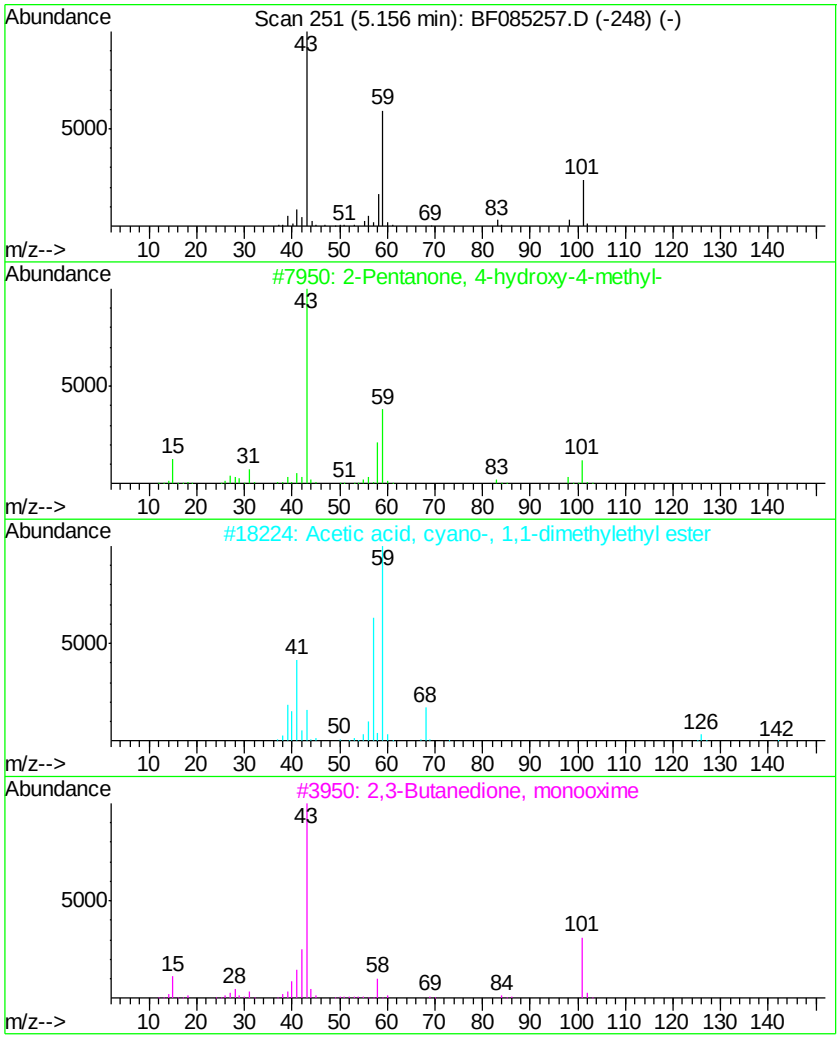
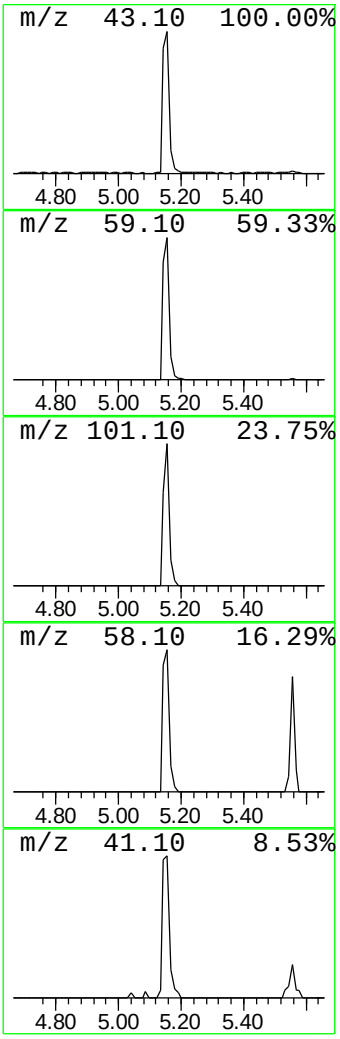
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	7.51 ng	324954	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Silane, dimethyl-	60	C2H8Si	001111-74-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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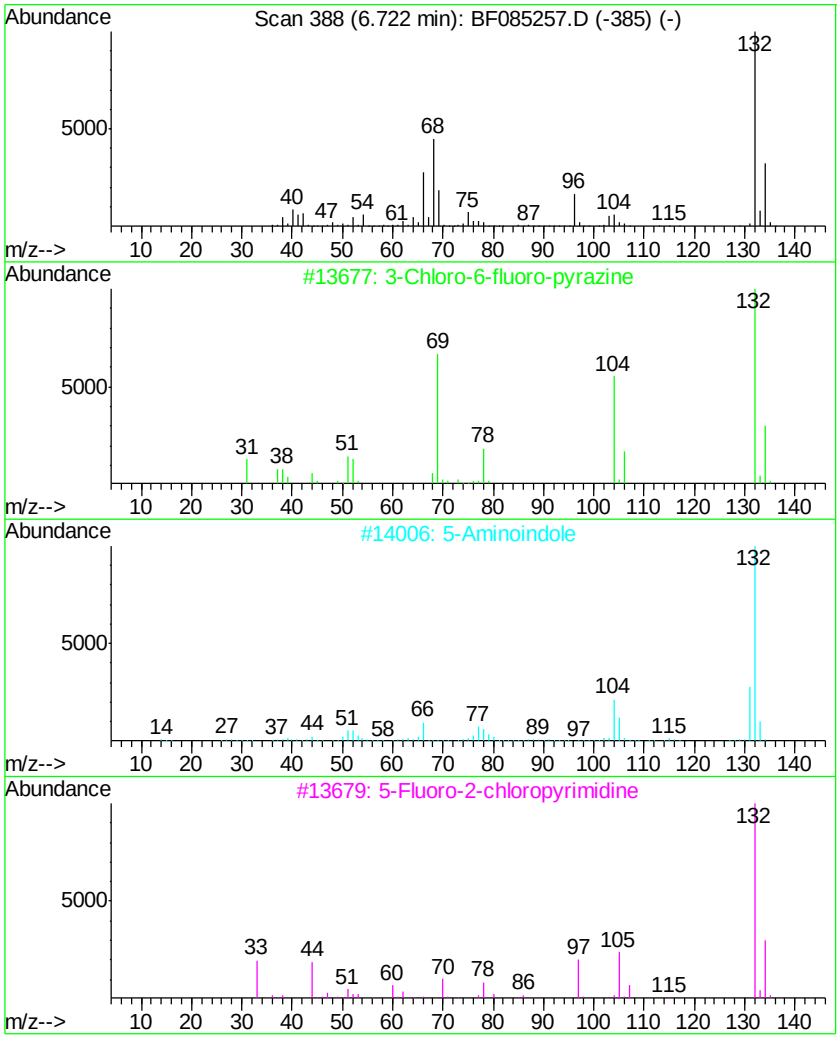
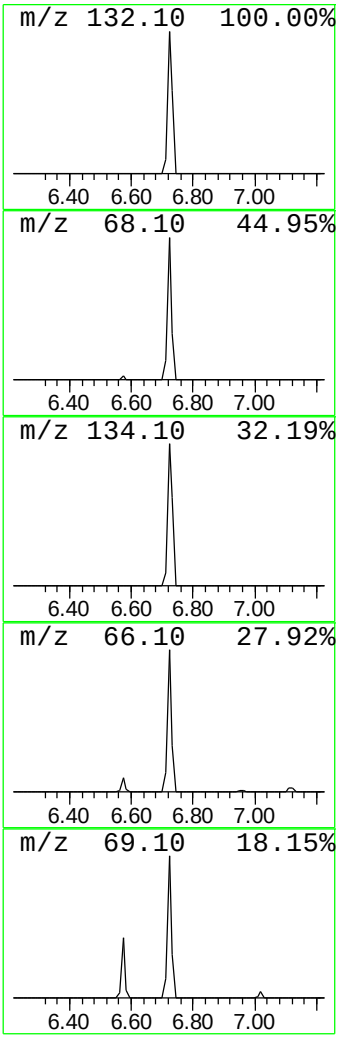
Peak Number 2 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	73.95 ng	3199070	1,4-Dichlorobenzene-d4	6.96

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

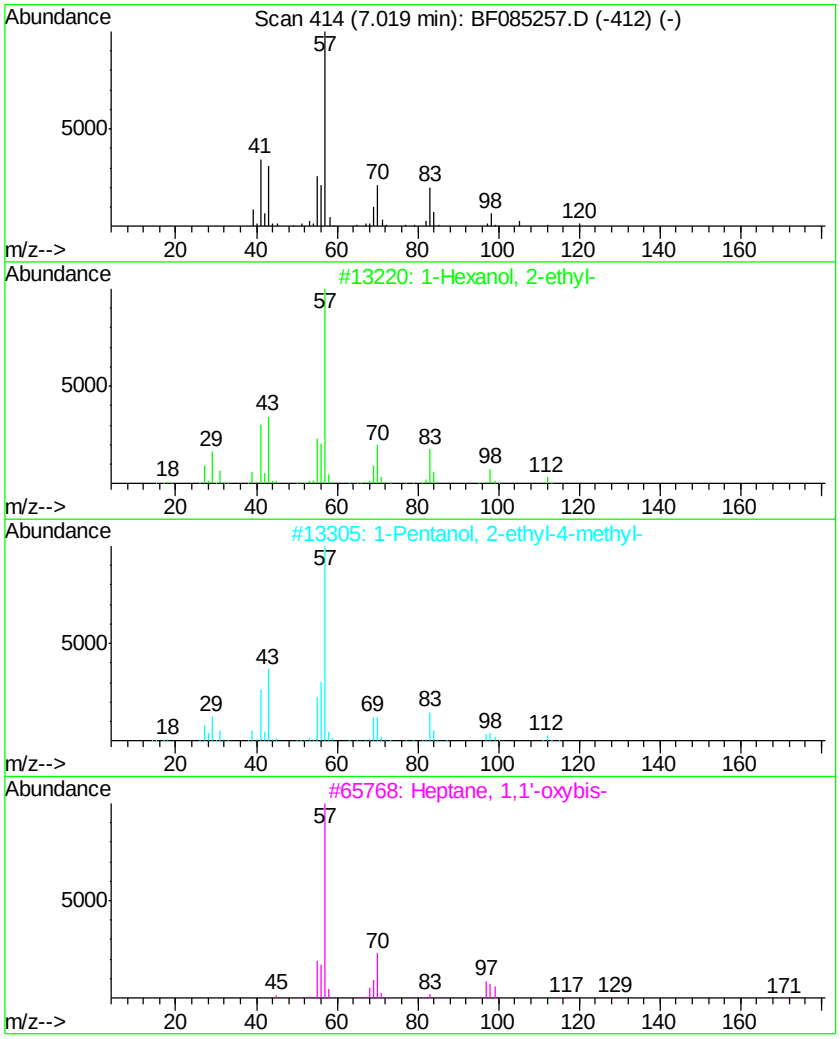
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

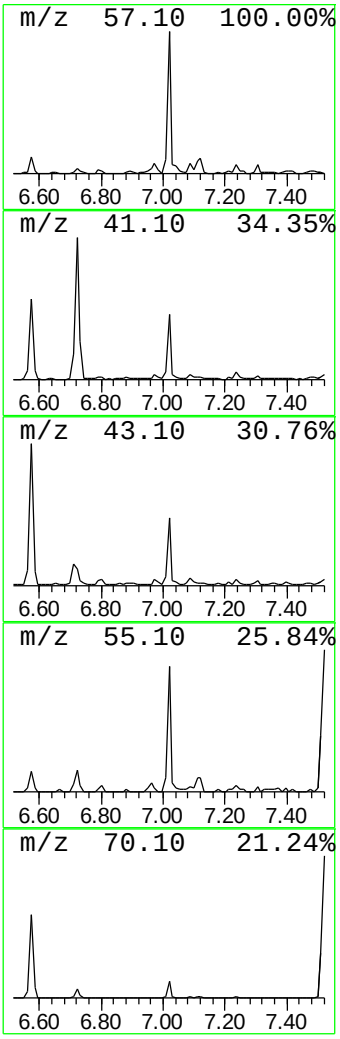
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	4.27 ng	184823	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	45





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

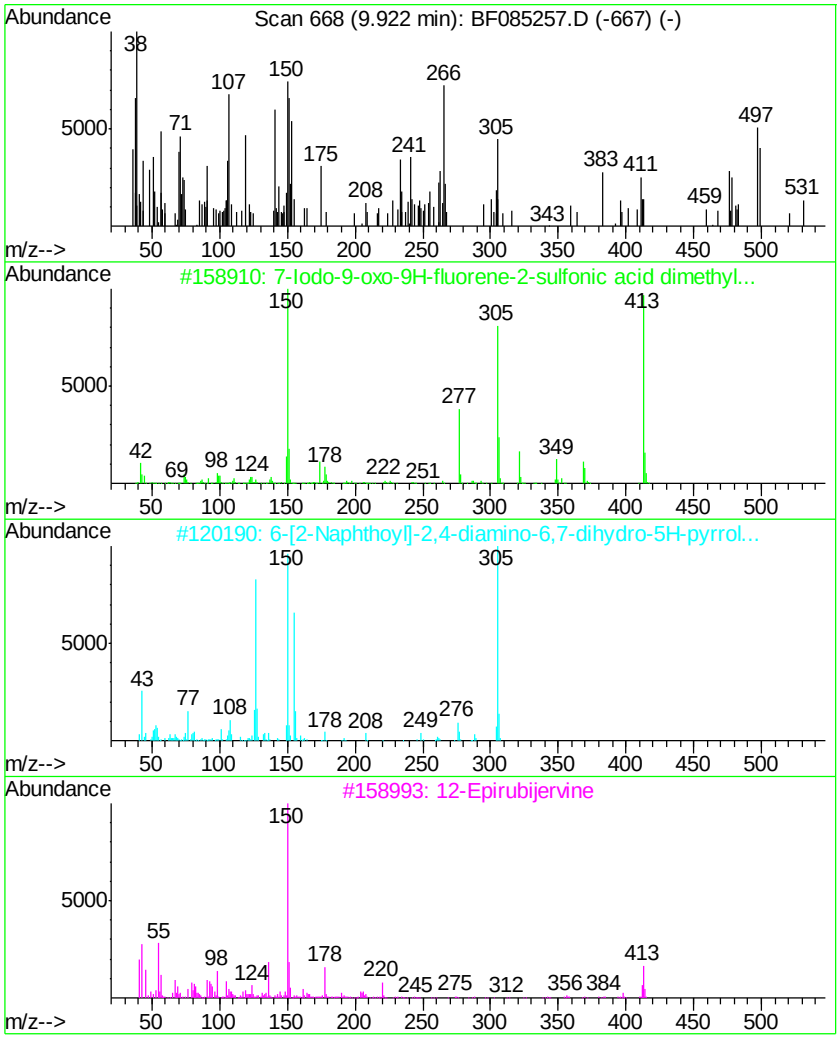
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

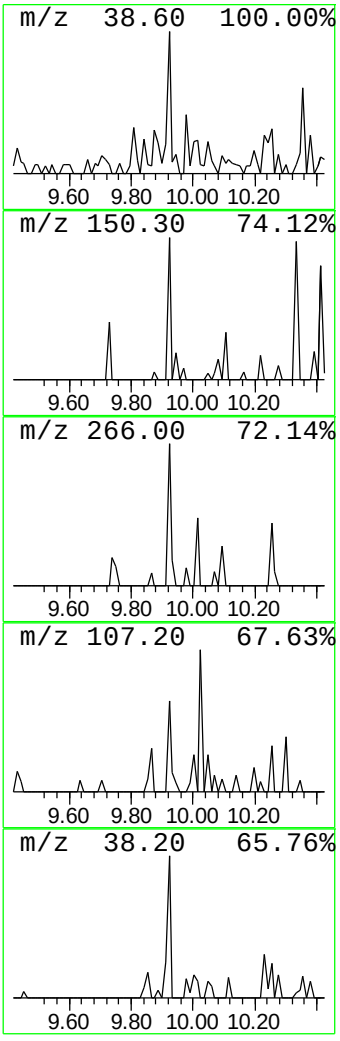
****

Peak Number 6 unknown9.92 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	2.04 ng	137960	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Iodo-9-oxo-9H-fluorene-2-sulfo...	413	C15H12INO3S	324052-46-2	22
2	6-[2-Naphthoyl]-2,4-diamino-6,7-...	305	C17H15N5O	1000251-30-4	12
3	12-Epirubijervine	413	C27H43NO2	000472-00-4	9
4	Dihydroisosolanidin-3-one oxime	412	C27H44N2O	1000255-37-1	9
5	6-[1-Naphthoyl]-2,4-diamino-6,7-...	305	C17H15N5O	329203-17-0	9





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Data File : BF085257.D
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Misc :
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Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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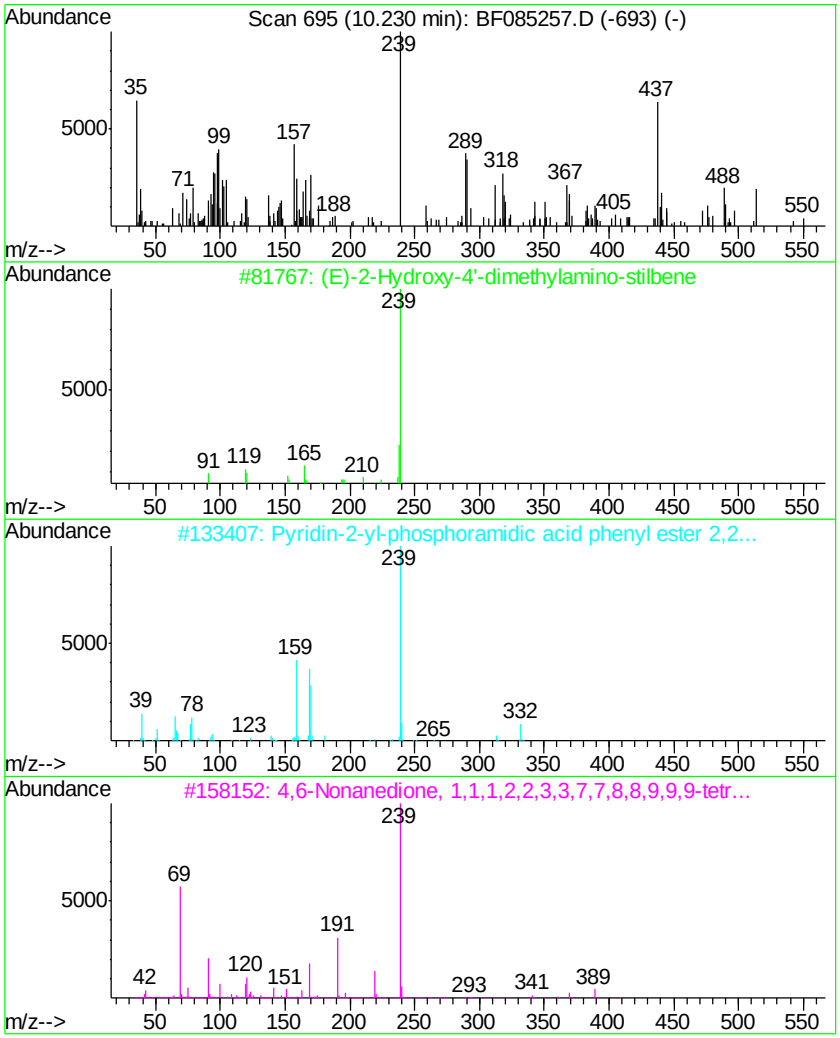
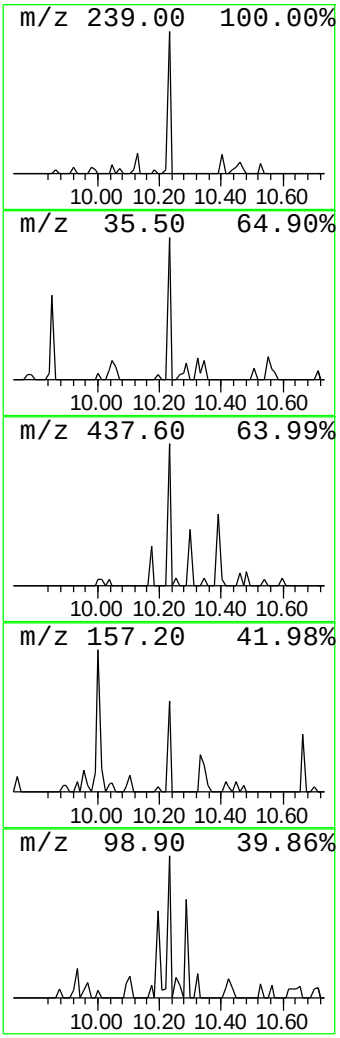
Peak Number 8 unknown10.23 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	4.34 ng	294252	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-2-Hydroxy-4'-dimethylamino-s...	239	C16H17NO	110983-42-1	22
2	Pyridin-2-yl-phosphoramidic acid...	332	C13H12F3N2O3P	292852-63-2	10
3	4,6-Nonanedione, 1,1,1,2,2,3,3,7...	408	C9H2F14O2	113116-18-0	10
4	Ethyl .alpha.-fluoro-4-nitro-cin...	239	C11H10FNO4	1000148-09-1	10
5	2-Ethylidenehydrazono-3-methyl-6...	239	C10H10ClN3S	1000148-09-0	10





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Sample : H1713-01
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Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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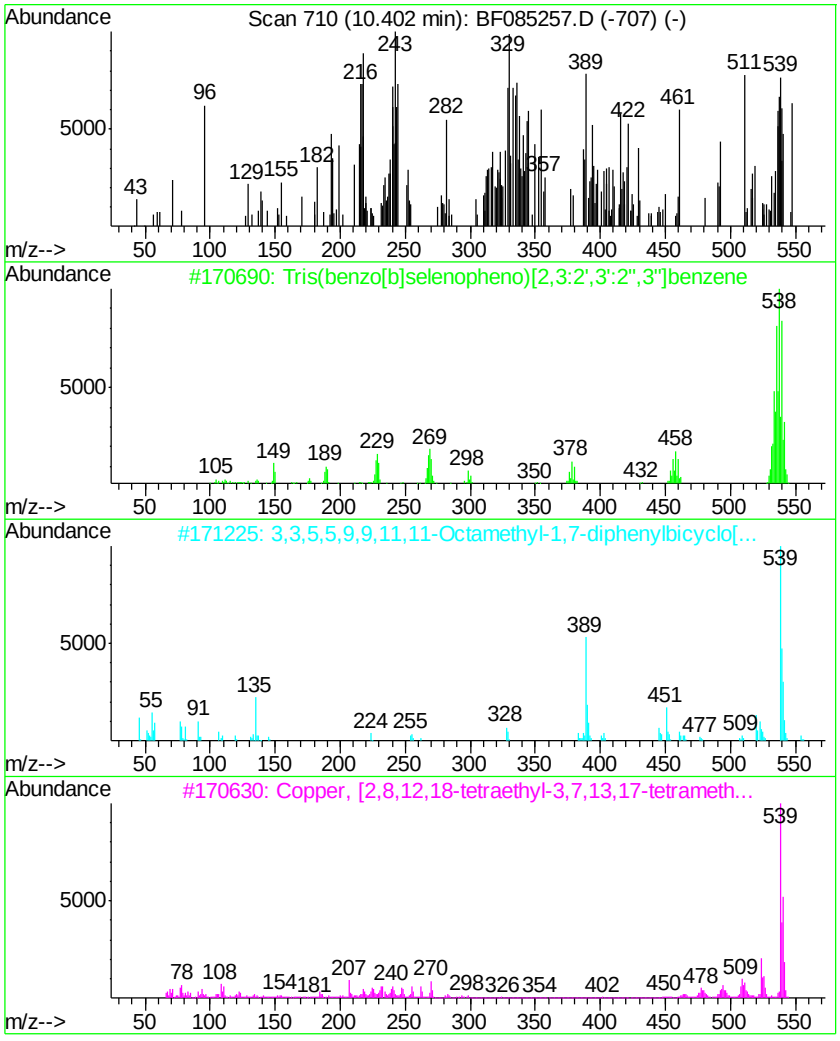
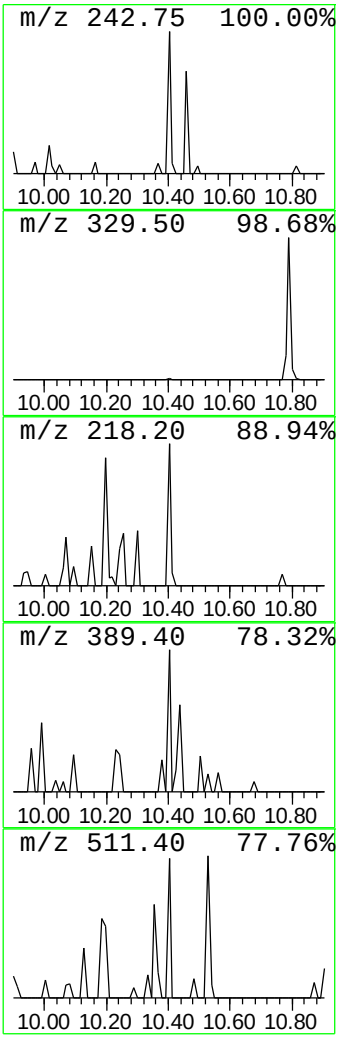
Peak Number 10 unknown10.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	3.97 ng	269126	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	42
2	3,3,5,5,9,9,11,11-Octamethyl-1,7...	554	C20H34O7Si6	049538-51-4	18
3	Copper, [2,8,12,18-tetraethyl-3,...	539	C32H36CuN4	014055-18-6	10
4	5-Germaspiro[4.4]nona-1,3,6,8-te...	538	C36H32Ge	150479-95-1	9
5	Bis(triphenylphosphoranylidene)a...	580	C36H30N4P2	038011-36-8	7





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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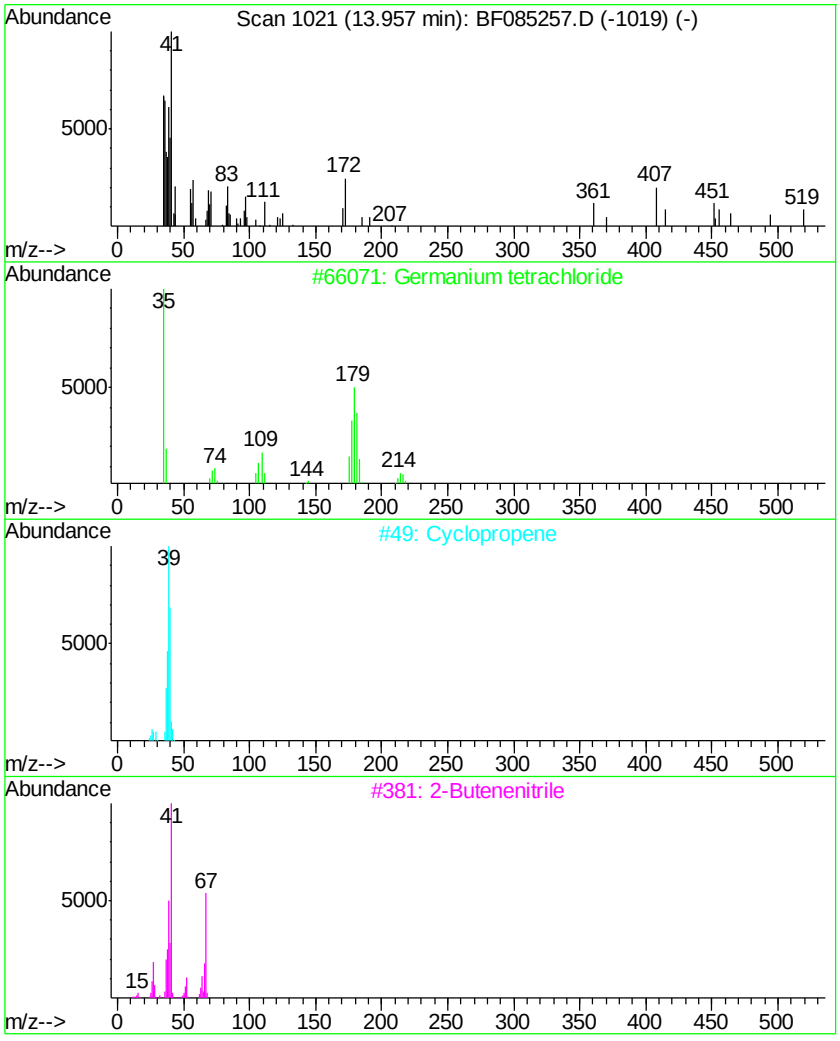
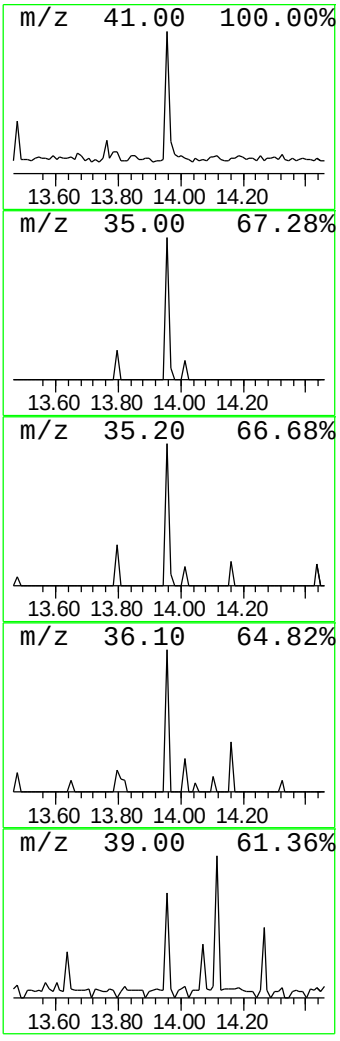
Peak Number 13 unknown13.96 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	2.73 ng	143827	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Germanium tetrachloride	214	Cl4Ge	010038-98-9	36
2	Cyclopropene	40	C3H4	002781-85-3	10
3	2-Butenenitrile	67	C4H5N	004786-20-3	9
4	2-Furanmethanol, 5-nitro-	143	C5H5NO4	002493-04-1	9
5	Methane, chlorotrinitro-	185	CClN3O6	001943-16-4	9





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Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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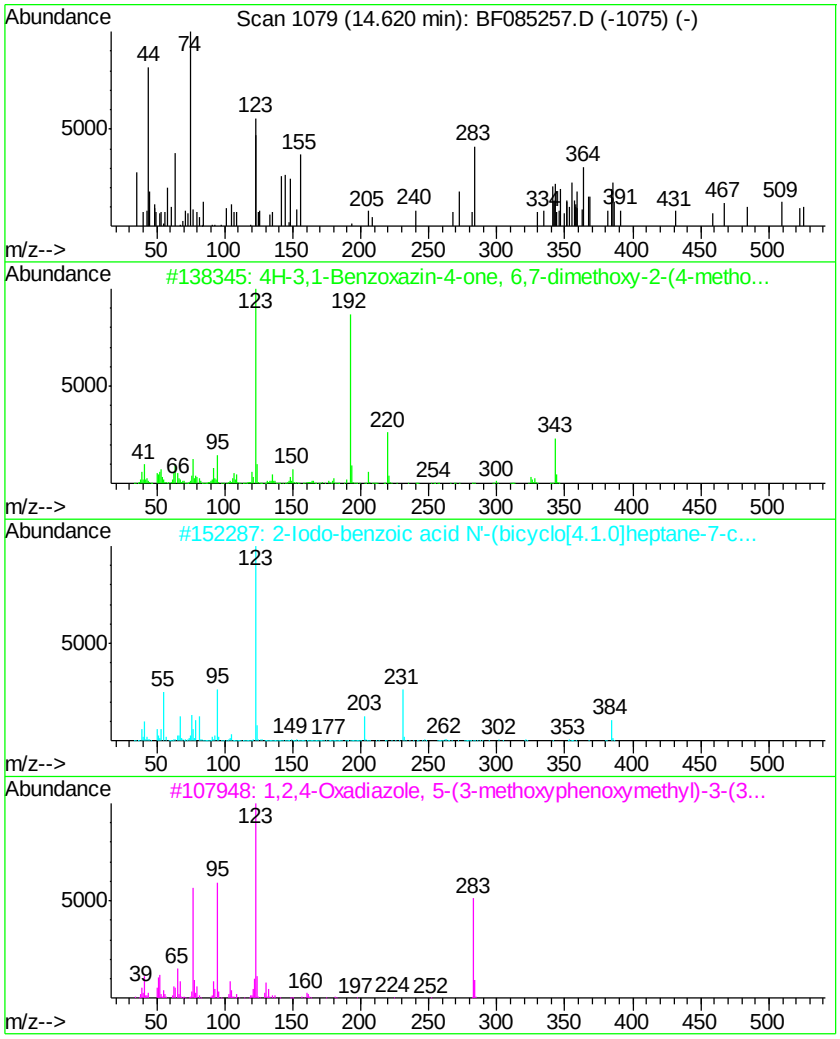
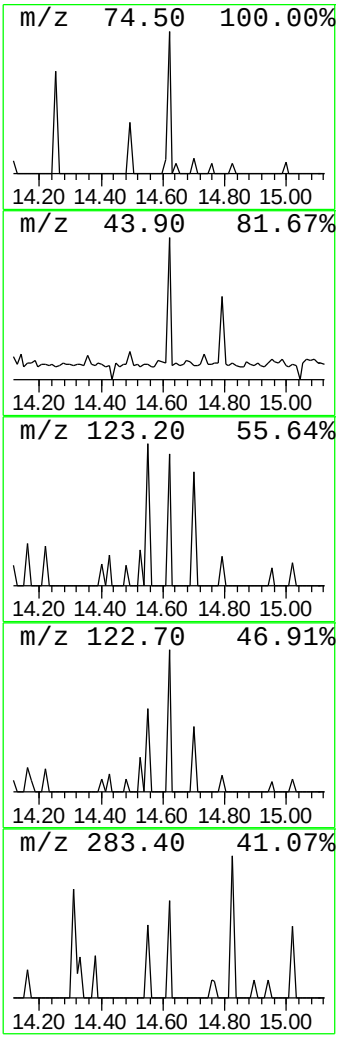
Peak Number 14 unknown14.62 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.45 ng	129056	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-3,1-Benzoxazin-4-one, 6,7-dim...	343	C18H17NO6	1000273-67-9	22
2	2-Iodo-benzoic acid N'-(bicyclo[...	384	C15H17IN2O2	1000278-50-1	4
3	1,2,4-Oxadiazole, 5-(3-methoxyph...	283	C15H13N3O3	1000264-11-5	4
4	2-Fluoro-1-(4-fluorophenyl)ethyl...	203	C8H7F2NO3	1000222-78-1	2
5	Ethyl 2-(o-anisidino)-3,3,3-trif...	414	C19H18F4N2O4	1000225-39-6	1





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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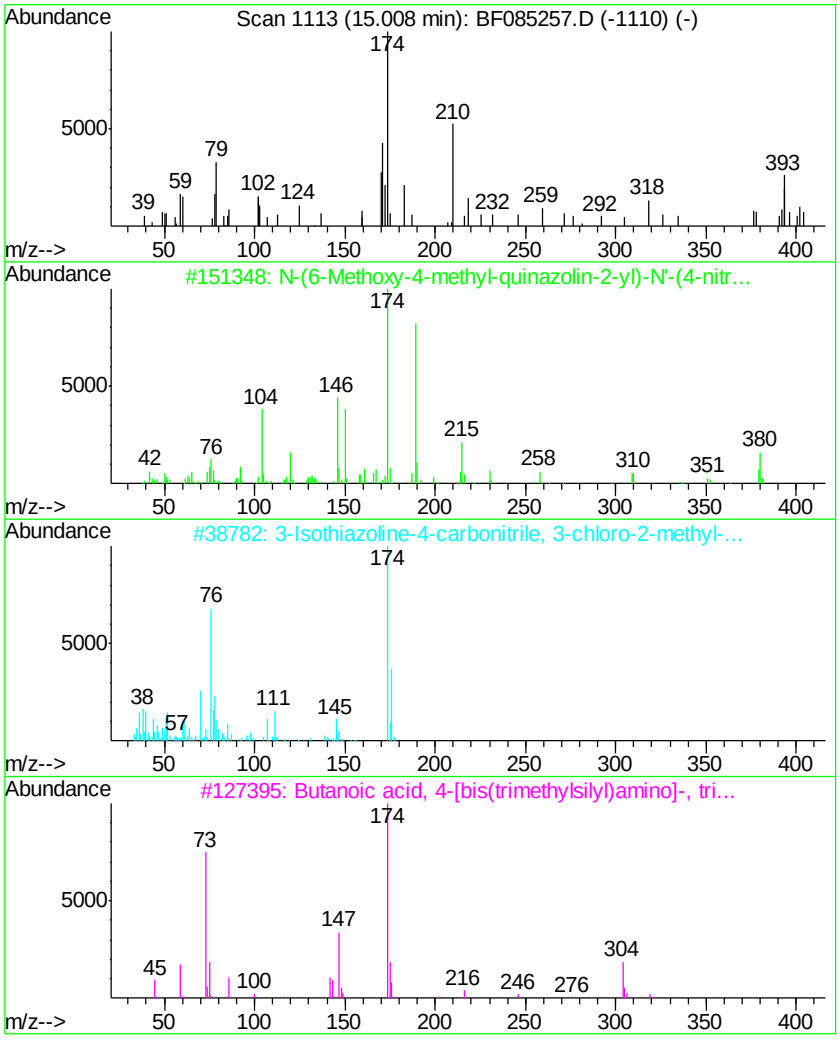
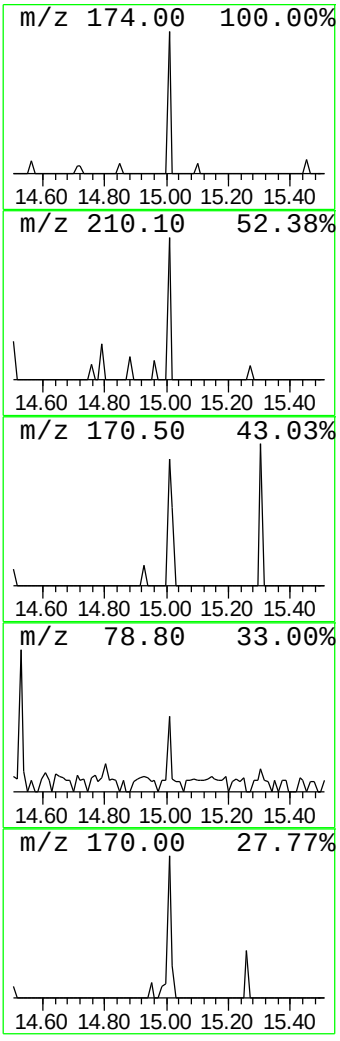
Peak Number 16 unknown15.01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	2.97 ng	107555	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(6-Methoxy-4-methyl-quinazolin...	380	C18H16N6O4	1000275-15-0	25
2	3-Isothiazoline-4-carbonitrile, ...	174	C5H3ClN2OS	1000267-49-1	10
3	Butanoic acid, 4-[bis(trimethyls...	319	C13H33NO2Si3	039508-23-1	10
4	2,2-Dimethyl-4-ethynyl-tetrahydr...	170	C9H14OS	015601-02-2	10
5	2,6-Dimethylpyrazino[2,3-c][2,7]...	210	C12H10N4	1000147-70-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085257.D
Acq On : 8 Mar 2016 15:55
Operator : UM/SJ
Sample : H1713-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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...	5.16	7.5	ng	324954	1	6.96	865235	20.0
unknown6.72	6.72	74.0	ng	3199070	1	6.96	865235	20.0
1-Hexanol, 2-ethyl-	7.02	4.3	ng	184823	1	6.96	865235	20.0
unknown9.92	9.92	2.0	ng	137960	3	10.00	1354820	20.0
unknown10.23	10.23	4.3	ng	294252	3	10.00	1354820	20.0
unknown10.40	10.40	4.0	ng	269126	3	10.00	1354820	20.0
unknown13.96	13.96	2.7	ng	143827	5	14.12	1055430	20.0
unknown14.62	14.62	2.5	ng	129056	5	14.12	1055430	20.0
unknown15.01	15.01	3.0	ng	107555	6	15.58	724922	20.0