LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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-BF072315.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	3.207	95	98	103	rBV3	7126	17093	1.26%	0.157%
2	3.881	155	157	160	rBV	11947	17550	1.29%	0.161%
3	5.104	262	264	269	rBV	74522	75626	5.56%	0.694%
4	5.516	298	300	303	rVB	469713	590720	43.44%	5.422%
5	5.881	330	332	334	rVB	16460	19290	1.42%	0.177%
6	5.950	334	338	339	rBV2	17524	27063	1.99%	0.248%
7	6.099	349	351	353	rBV	35660	45453	3.34%	0.417%
8	6.179	356	358	364	rVB2	19469	32629	2.40%	0.299%
9	6.350	371	373	376	rVB2	27284	39860	2.93%	0.366%
10	6.476	383	384	386	rBV2	32119	27900	2.05%	0.256%
11	6.556	389	391	393	rVB	424739	390175	28.69%	3.581%
12	6.636	396	398	402	rBV	57374	54328	4.00%	0.499%
13	6.704	402	404	406	rBV	1295718	1065715	78.37%	9.781%
14	6.944	423	425	427	rBV	404115	363040	26.70%	3.332%
15	7.104	436	439	441	rVB	1057585	947875	69.71%	8.699%
16	7.150	441	443	446	rVB	29655	31526	2.32%	0.289%
17	7.219	446	449	451	rBV	29285	30875	2.27%	0.283%
18	7.264	451	453	455	rBV	29857	27459	2.02%	0.252%
19	7.344	458	460	463	rVB2	33343	34968	2.57%	0.321%
20	7.424	463	467	468	rVB2	10786	25338	1.86%	0.233%
21	7.504	472	474	476	rVB	1017368	789775	58.08%	7.248%
22	7.630	482	485	487	rVB3	21694	32479	2.39%	0.298%
23	7.710	487	492	494	rVB4	7743	17022	1.25%	0.156%
24	7.904	505	509	510	rVB4	11370	23449	1.72%	0.215%
25	7.927	510	511	515	rVB2	18329	26538	1.95%	0.244%
26	8.007	517	518	520	rBV	15304	19082	1.40%	0.175%
27	8.133	528	529	531	rBV2	18575	23980	1.76%	0.220%
28	8.236	536	538	540	rBV	502323	414257	30.46%	3.802%
29	8.339	546	547	549	rBV2	13329	16290	1.20%	0.150%
30	8.510	560	562	564	rBV	30363	30868	2.27%	0.283%
31	8.602	568	570	572	rBV	138501	118888	8.74%	1.091%
32	8.819	585	589	591	rVB5	14728	23557	1.73%	0.216%
33	8.910	594	597	600	rBV2	15961	25808	1.90%	0.237%
34	9.013	600	606	610	rVV6	10508	32431	2.38%	0.298%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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-BF072315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.207	620	623	624	rBV2	43438	47985	3.53%	0.440%
36	9.310	630	632	634	rVB	1680849	1359831	100.00%	12.480%
37	9.482	645	647	650	rBV2	12381	21303	1.57%	0.196%
38	9.539	650	652	654	rVV3	10471	17210	1.27%	0.158%
39	9.573	654	655	659	rVB3	11586	23862	1.75%	0.219%
40	9.710	665	667	668	rBV	59265	73869	5.43%	0.678%
41	9.745	668	670	671	rVB2	14380	17442	1.28%	0.160%
42	9.996	689	692	694	rBV	392493	411797	30.28%	3.779%
43	10.065	696	698	701	rBV3	14342	29798	2.19%	0.273%
44	10.156	704	706	711	rVB6	16693	38580	2.84%	0.354%
45	10.236	711	713	716	rBV4	9446	22089	1.62%	0.203%
46	10.350	721	723	725	rBV	11789	19684	1.45%	0.181%
47	10.408	727	728	730	rVB	21253	17201	1.26%	0.158%
48	10.453	730	732	735	rBV3	12170	21677	1.59%	0.199%
49	10.705	750	754	756	rBV3	12357	31831	2.34%	0.292%
50	10.773	758	760	763	rVV2	859784	839825	61.76%	7.708%
51	10.865	763	768	770	rVV5	13429	20192	1.48%	0.185%
52	10.899	770	771	775	rVB4	16050	20837	1.53%	0.191%
53	10.956	775	776	778	rBV2	12854	16546	1.22%	0.152%
54	11.185	794	796	801	rVB5	7926	16876	1.24%	0.155%
55	11.482	820	822	824	rBV	395135	403119	29.64%	3.700%
56	11.539	824	827	830	rVB5	11827	26972	1.98%	0.248%
57	11.631	833	835	838	rBV	111217	105213	7.74%	0.966%
58	11.711	838	842	844	rVB4	9434	21786	1.60%	0.200%
59	11.848	851	854	859	rVB6	6757	23340	1.72%	0.214%
60	12.008	865	868	870	rBV2	29158	45857	3.37%	0.421%
61	12.179	882	883	886	rVB2	13908	16242	1.19%	0.149%
62	12.796	935	937	940	rVB3	16878	17331	1.27%	0.159%
63	13.082	960	962	964	rBV	1351618	1147424	84.38%	10.531%
64	13.151	966	968	970	rVB	51338	45362	3.34%	0.416%
65	14.214	1059	1061	1064	rBV	316854	301932	22.20%	2.771%
66	15.825	1199	1202	1205	rBV	176809	213879	15.73%	1.963%

Sum of corrected areas: 10895799

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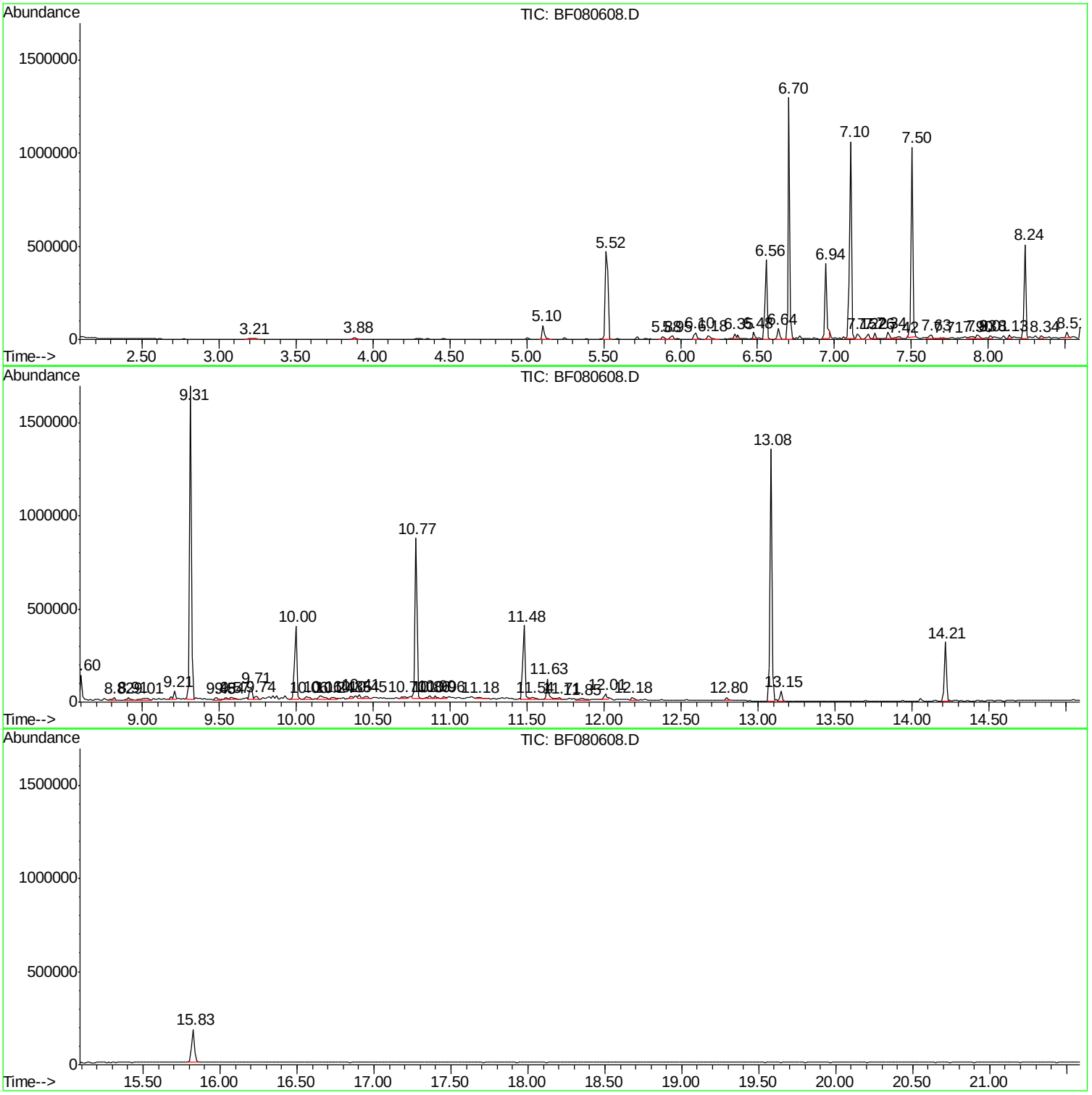
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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Operator : TP/UM
Sample : G3045-07
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

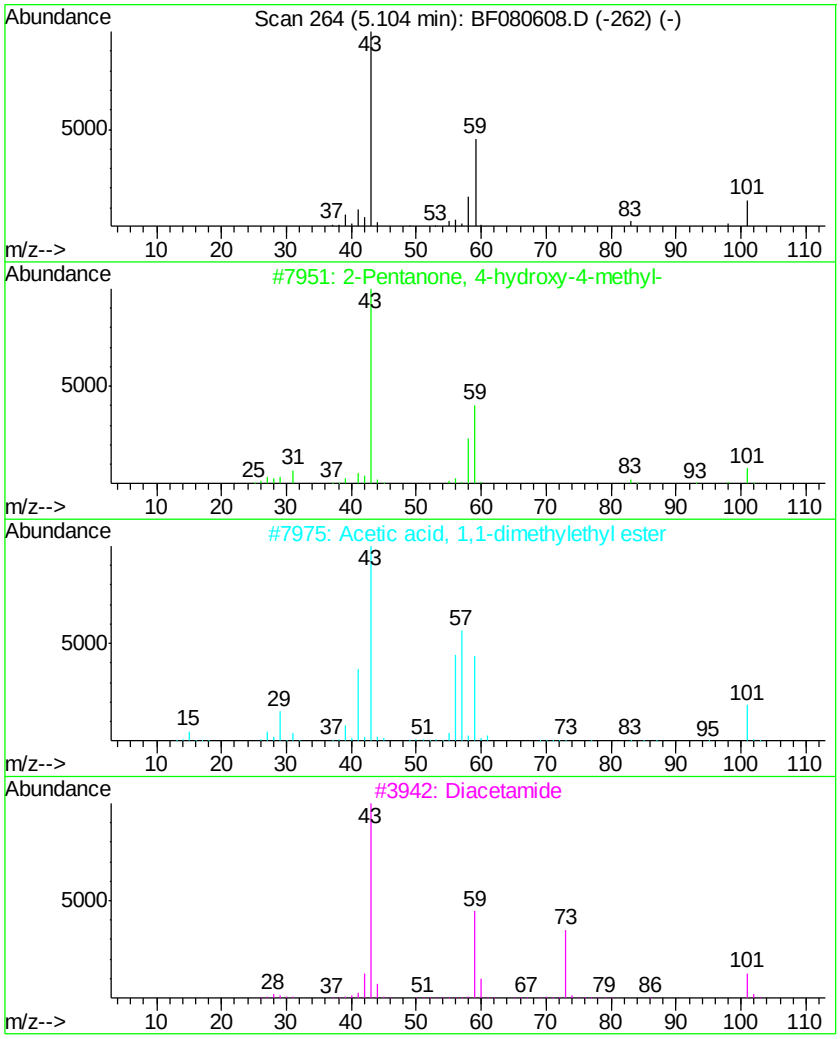
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

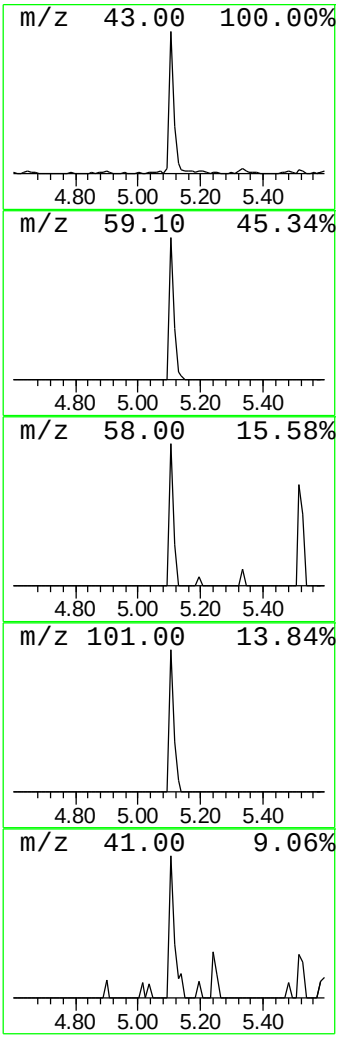
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	4.17 ng	75626	1,4-Dichlorobenzene-d4	6.94

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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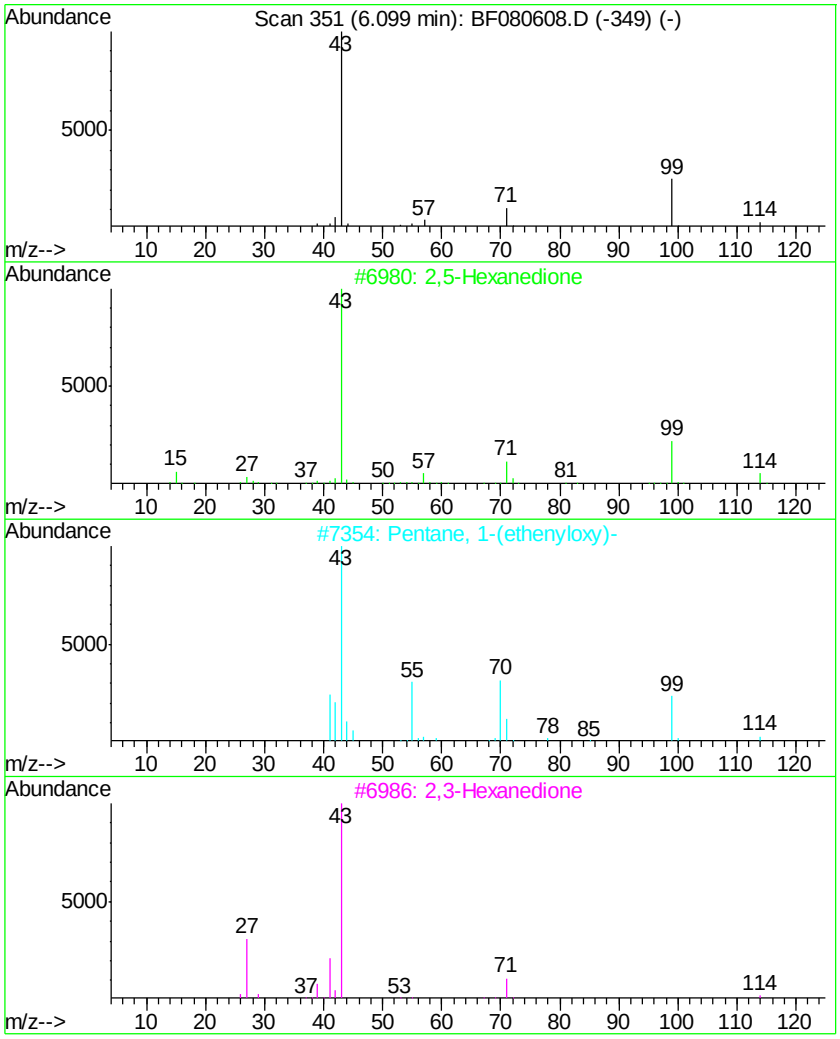
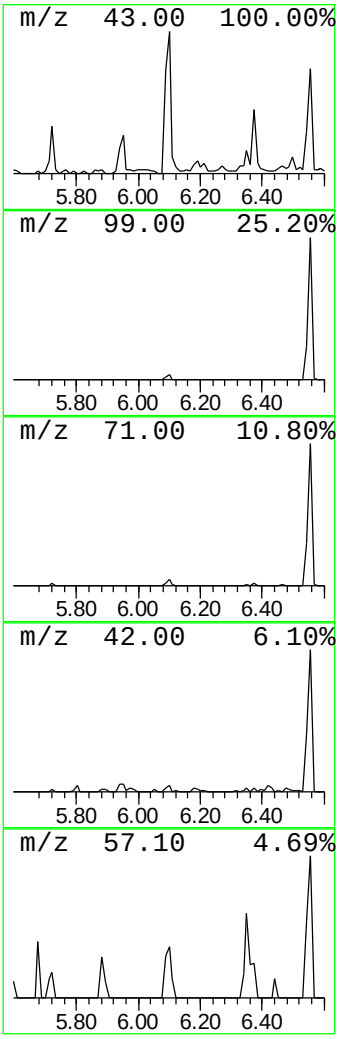
Peak Number 2 2,5-Hexanedione Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.10	2.50 ng	45453	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanedione	114	C6H10O2	000110-13-4	78
2	Pentane, 1-(ethenyloxy)-	114	C7H14O	005363-63-3	64
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	38
4	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	33
5	2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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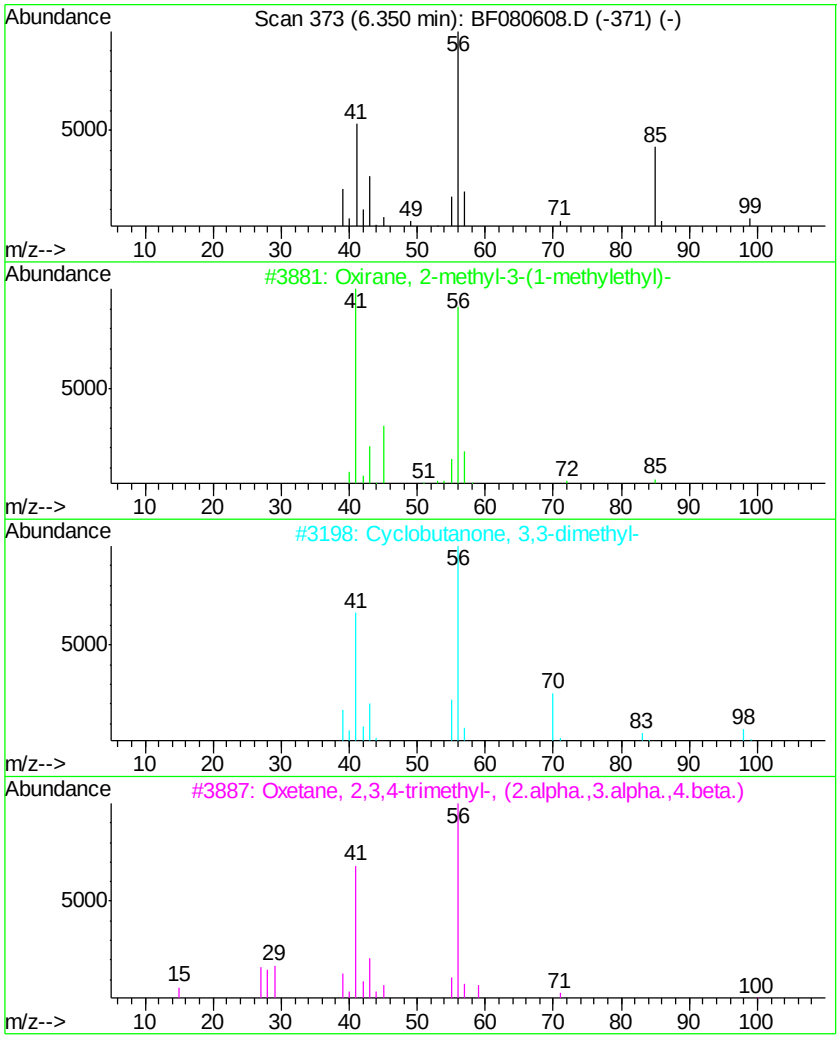
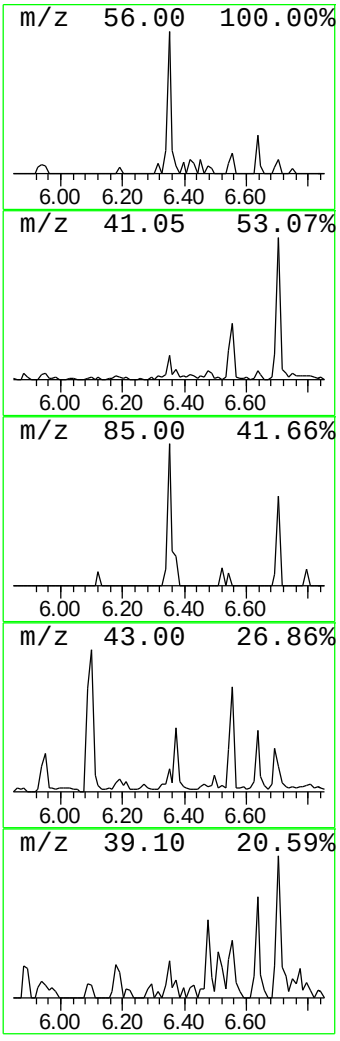
Peak Number 3 Oxirane, 2-methyl-3-(1-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	2.20 ng	39860	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	50
2	Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	33
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	33
4	Methacrylamide	85	C4H7NO	000079-39-0	9
5	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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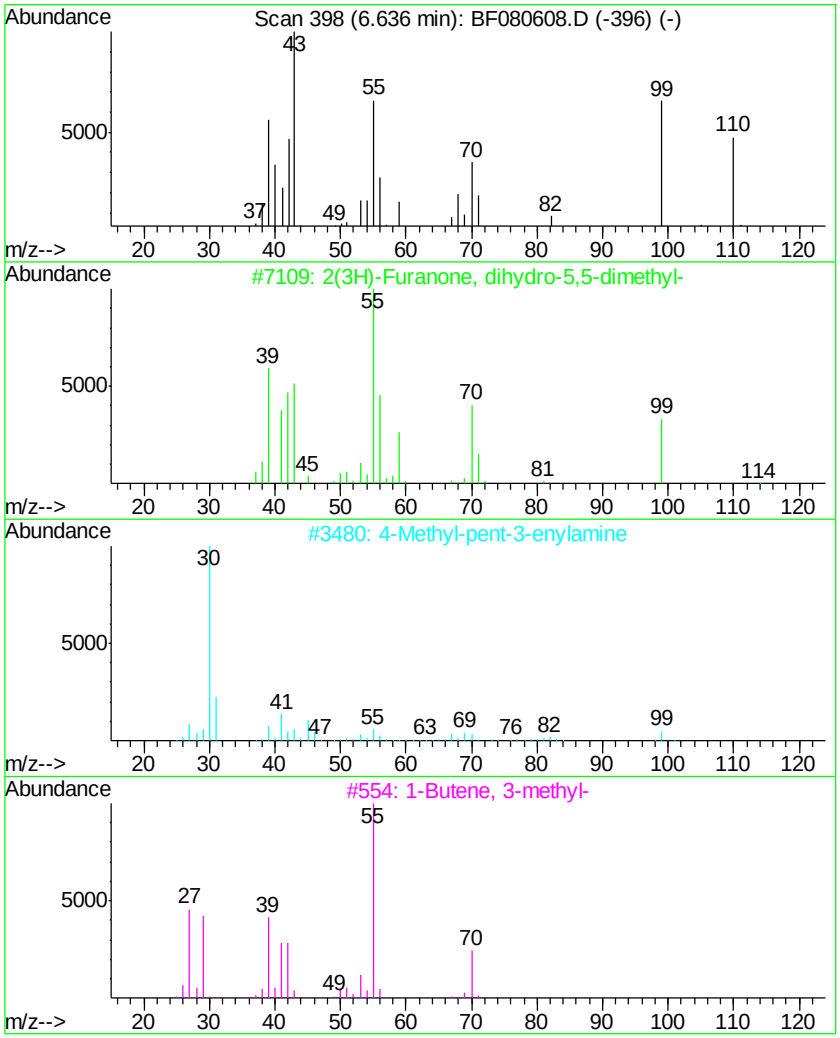
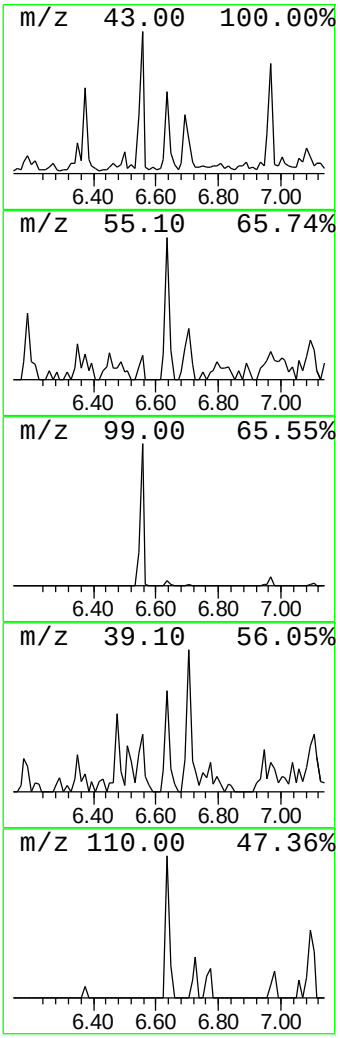
Peak Number 4 unknown6.64 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	2.99 ng	54328	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5,5-dime...	114	C6H10O2	003123-97-5	47
2	4-Methyl-pent-3-enylamine	99	C6H13N	013296-28-1	37
3	1-Butene, 3-methyl-	70	C5H10	000563-45-1	35
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	27
5	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
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Operator : TP/UM
Sample : G3045-07
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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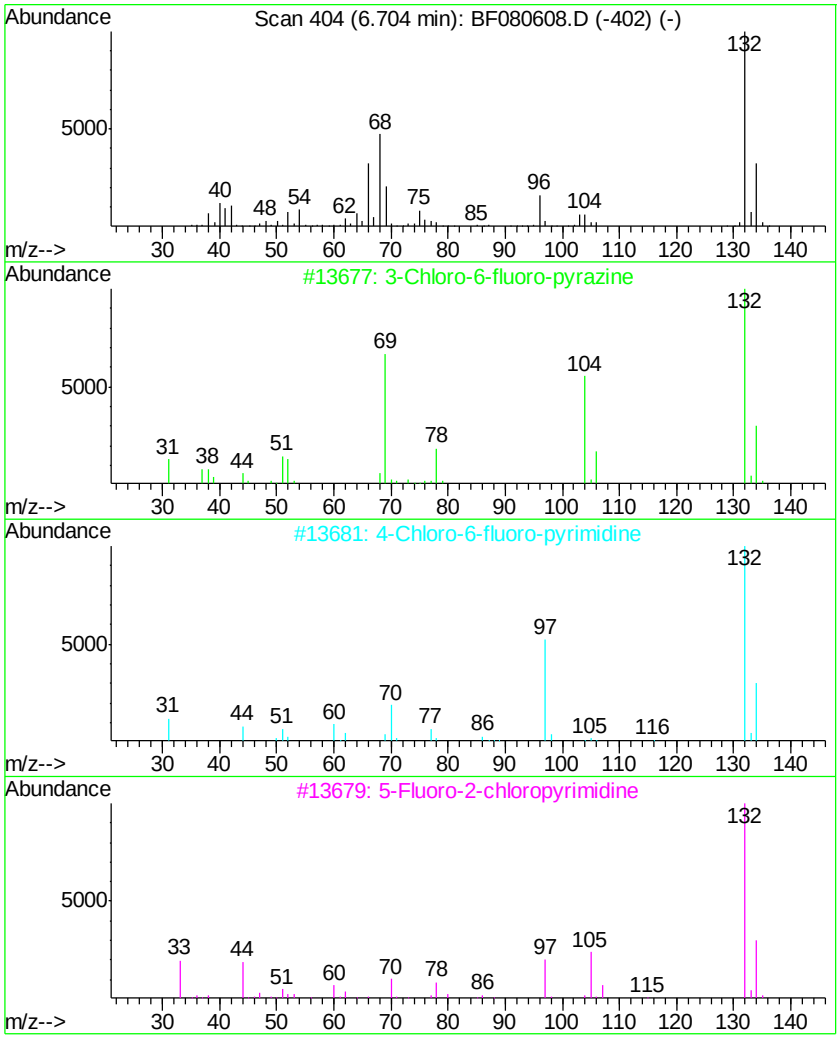
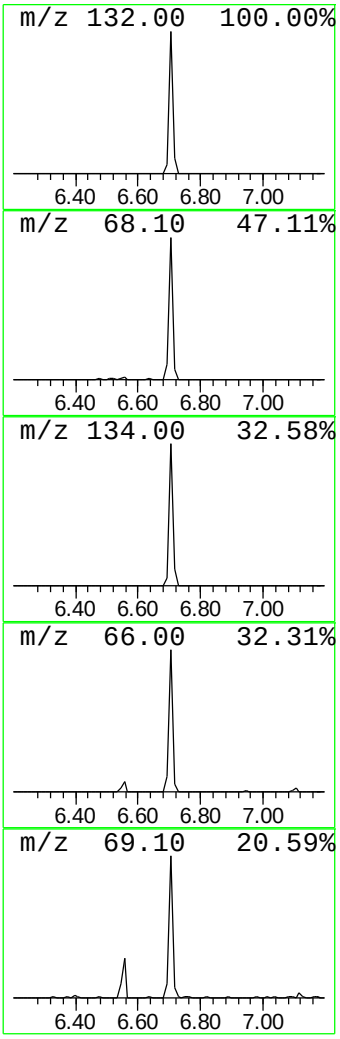
Peak Number 5 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	58.71 ng	1065720	1,4-Dichlorobenzene-d4	6.94

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Sample : G3045-07
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Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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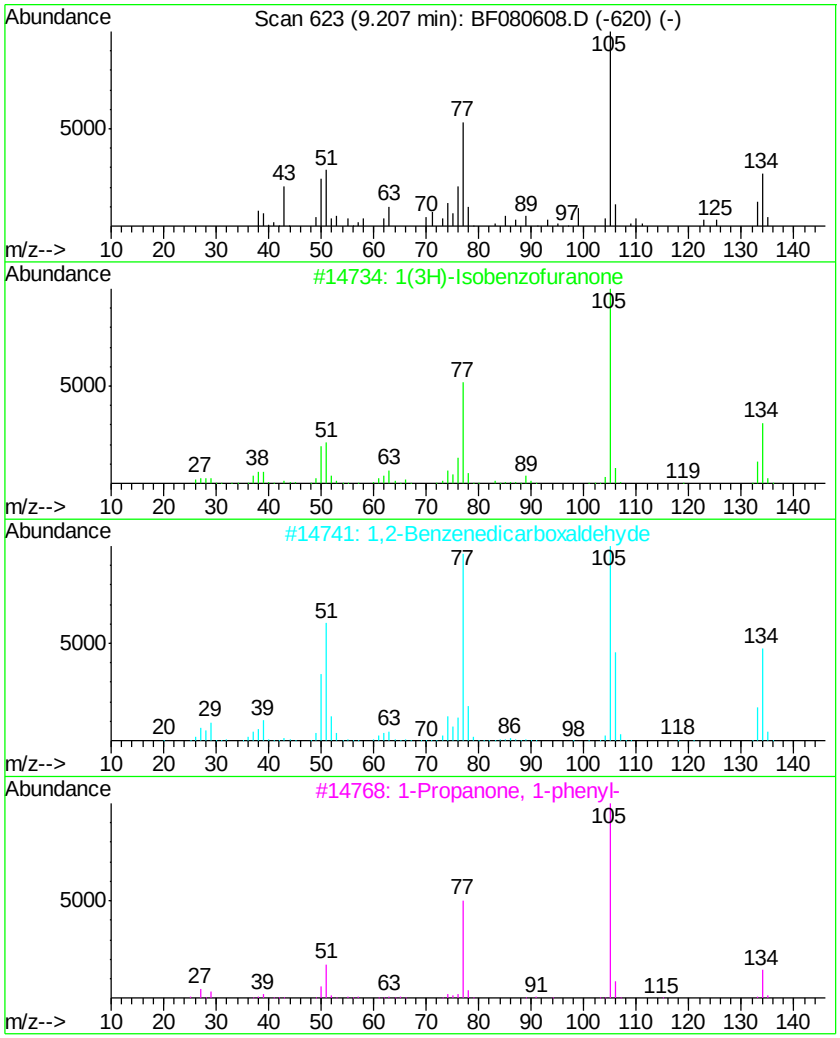
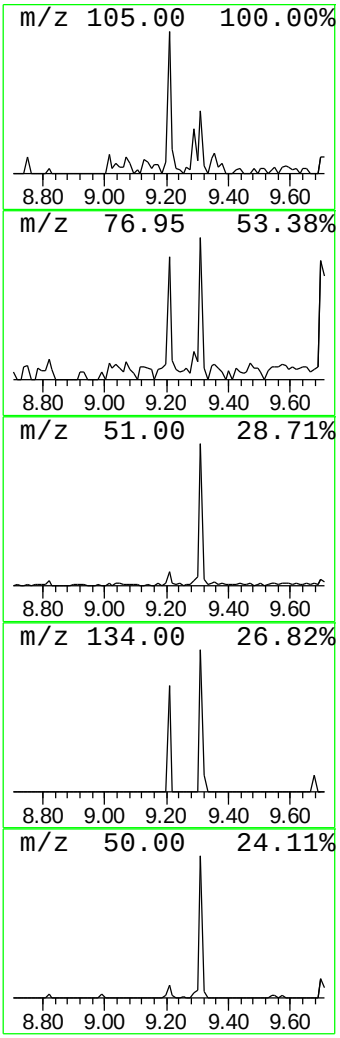
Peak Number 8 1(3H)-Isobenzofuranone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	2.33 ng	47985	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(3H)-Isobenzofuranone	134	C8H6O2	000087-41-2	87
2	1,2-Benzenedicarboxaldehyde	134	C8H6O2	000643-79-8	53
3	1-Propanone, 1-phenyl-	134	C9H10O	000093-55-0	53
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	50
5	Ethanone, 2,2-dibromo-1-phenyl-	276	C8H6Br2O	013665-04-8	47





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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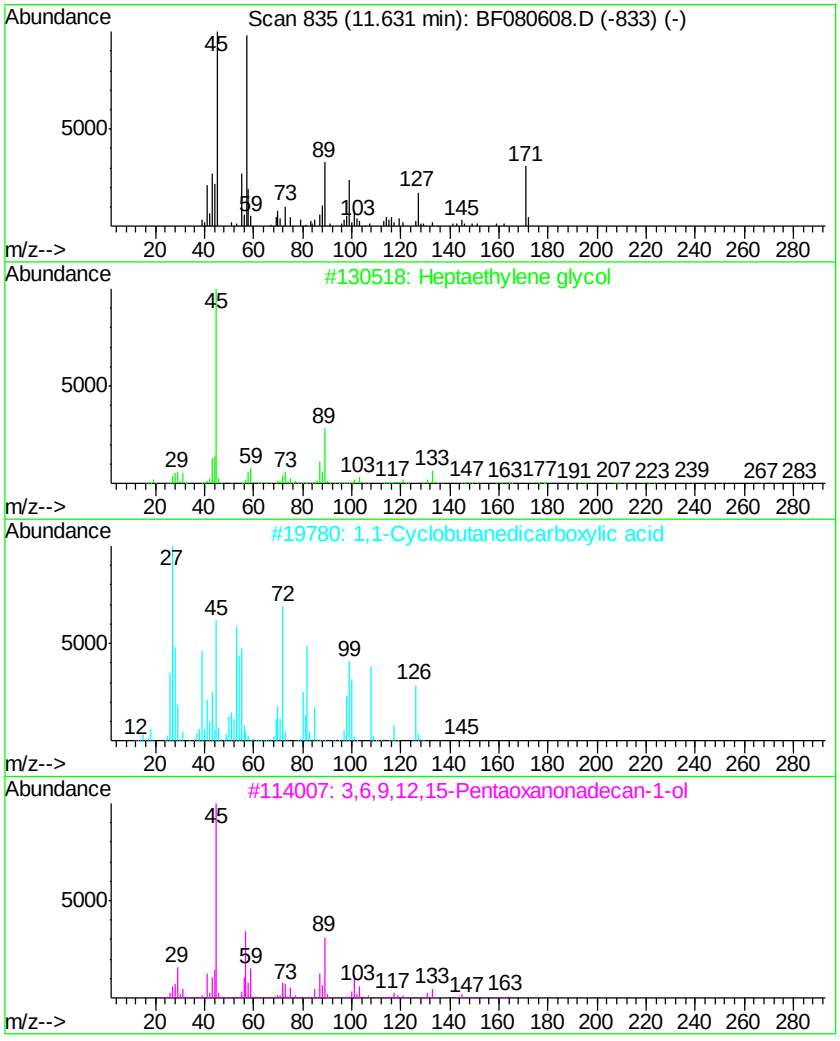
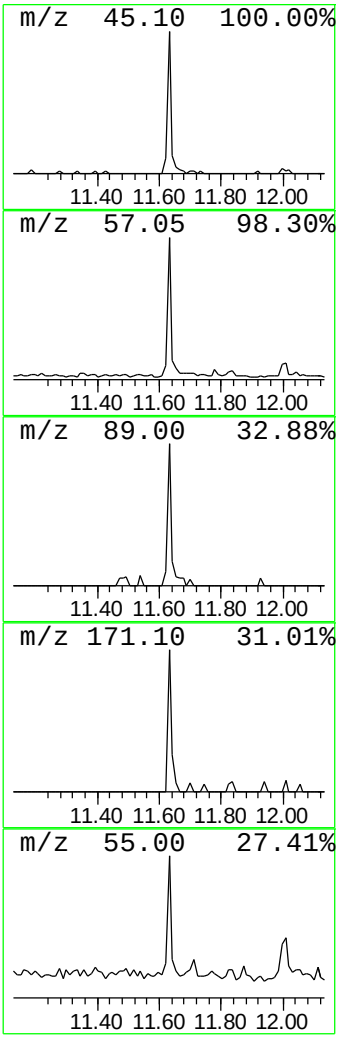
Peak Number 9 unknown11.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	5.22 ng	105213	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	38
2	1,1-Cyclobutanedicarboxylic acid	144	C6H8O4	005445-51-2	38
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	38
4	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	38
5	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
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Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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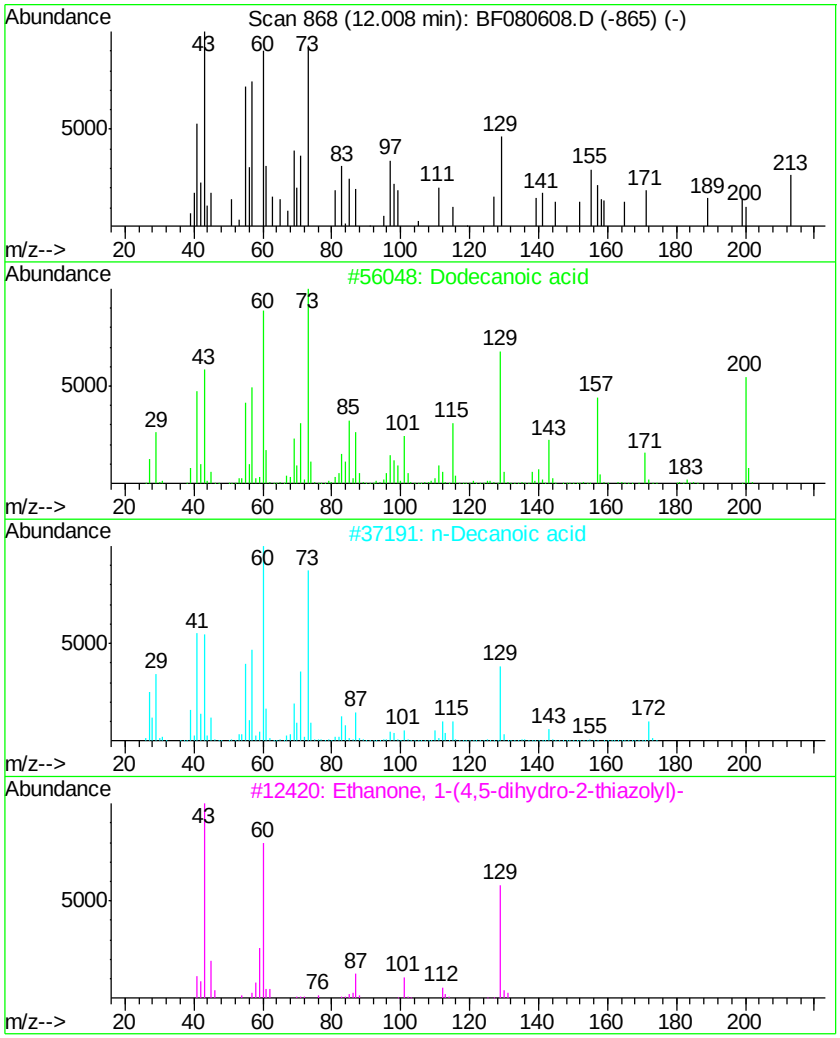
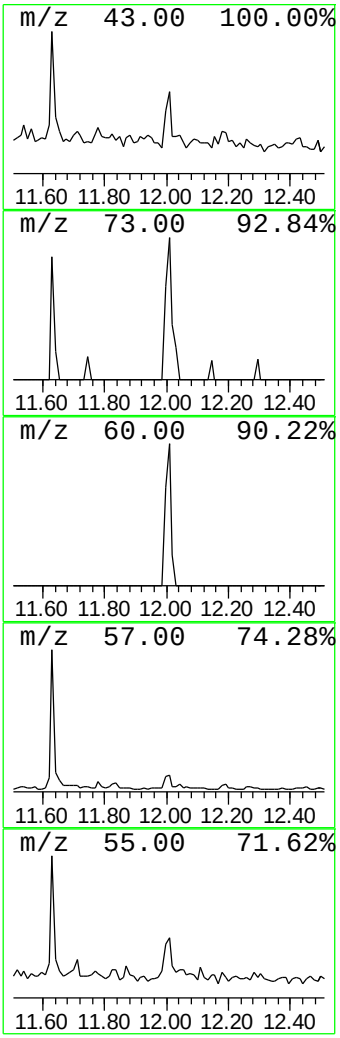
Peak Number 10 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.28 ng	45857	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	62
2	n-Decanoic acid	172	C10H20O2	000334-48-5	38
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
4	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	25
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	16





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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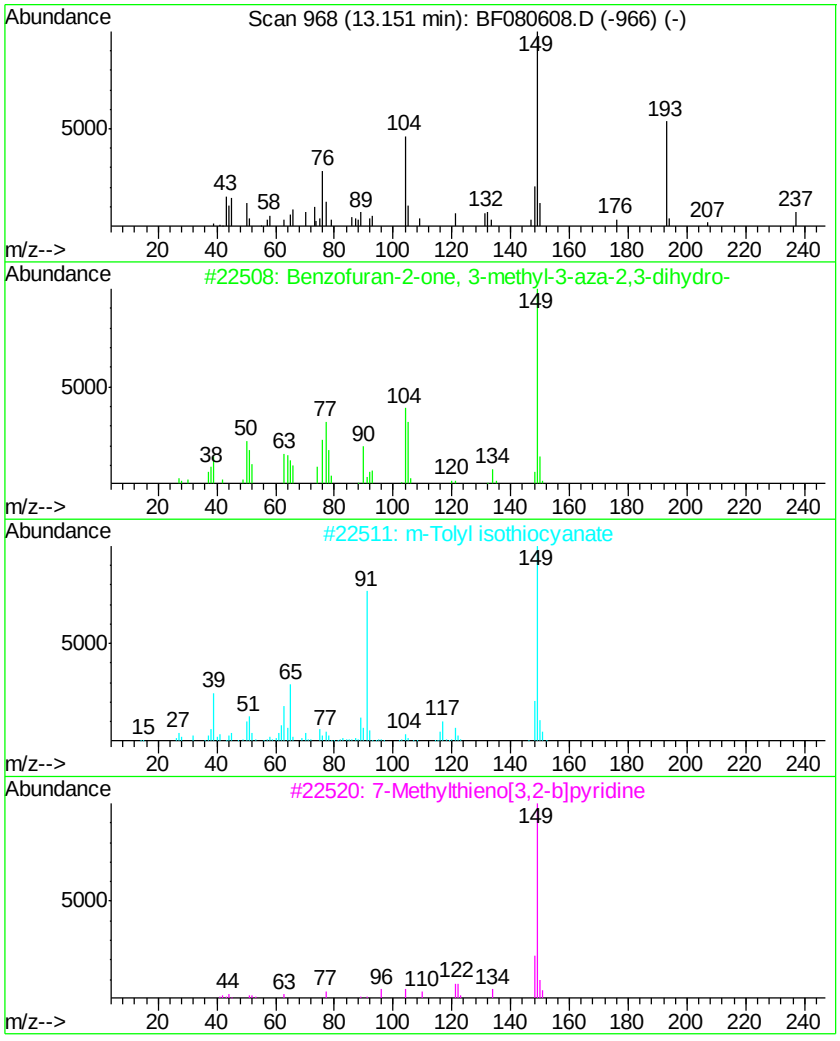
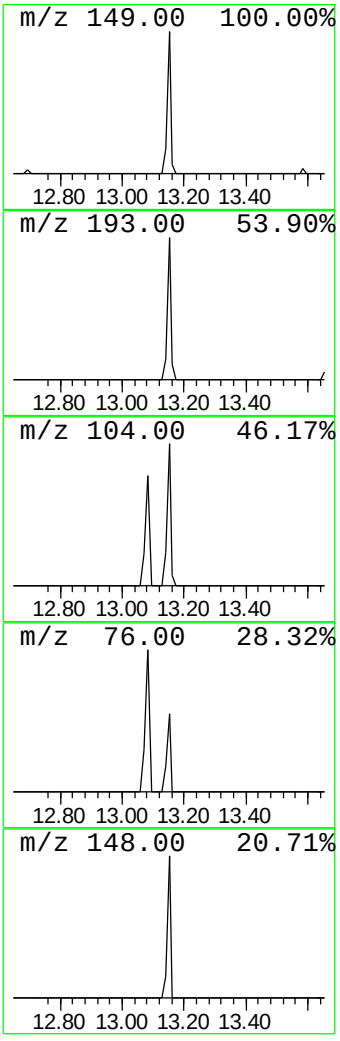
Peak Number 11 unknown13.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	3.00 ng	45362	Chrysene-d12	14.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran-2-one, 3-methyl-3-aza...	149	C8H7NO2	1000289-12-2	38
2	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	38
3	7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	35
4	2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	27
5	4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080608.D
Acq On : 23 Jul 2015 23:37
Operator : TP/UM
Sample : G3045-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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...	5.10	4.2	ng	75626	1	6.94	363040	20.0
2,5-Hexanedione	6.10	2.5	ng	45453	1	6.94	363040	20.0
Oxirane, 2-methyl...	6.35	2.2	ng	39860	1	6.94	363040	20.0
unknown6.64	6.64	3.0	ng	54328	1	6.94	363040	20.0
unknown6.70	6.70	58.7	ng	1065720	1	6.94	363040	20.0
1(3H)-Isobenzofur...	9.21	2.3	ng	47985	3	10.00	411797	20.0
unknown11.63	11.63	5.2	ng	105213	4	11.48	403119	20.0
Dodecanoic acid	12.01	2.3	ng	45857	4	11.48	403119	20.0
unknown13.15	13.15	3.0	ng	45362	5	14.21	301932	20.0