LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080615\
Data File : BF080908.D
Acq On : 7 Aug 2015 2:10
Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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-BF080615.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	4.281	190	192	195	rBV	20227	29529	1.40%	0.207%
2	4.956	249	251	254	rBV	360154	378100	17.98%	2.651%
3	5.379	286	288	291	rVB	306481	382112	18.17%	2.680%
4	5.801	322	325	327	rBV2	29013	35076	1.67%	0.246%
5	5.962	337	339	341	rBV	54960	51527	2.45%	0.361%
6	6.213	360	361	362	rBV	30320	25823	1.23%	0.181%
7	6.339	371	372	374	rVB	25656	25176	1.20%	0.177%
8	6.430	378	380	382	rVB	338897	284684	13.54%	1.996%
9	6.510	384	387	390	rVB	48416	63502	3.02%	0.445%
10	6.567	390	392	394	rBV	849819	727221	34.58%	5.100%
11	6.807	410	413	414	rBV	470604	390395	18.56%	2.738%
12	6.830	414	415	418	rVB	53557	51596	2.45%	0.362%
13	6.967	424	427	428	rVB	1165272	1224166	58.21%	8.584%
14	7.024	430	432	434	rVB	41900	35973	1.71%	0.252%
15	7.082	434	437	439	rBV	42273	43954	2.09%	0.308%
16	7.127	439	441	443	rBV	41193	36918	1.76%	0.259%
17	7.219	445	449	452	rBV4	37462	69069	3.28%	0.484%
18	7.287	452	455	456	rVB3	19792	27745	1.32%	0.195%
19	7.367	459	462	465	rBV	847984	1121000	53.31%	7.861%
20	7.493	471	473	475	rVB	38387	32637	1.55%	0.229%
21	7.802	498	500	501	rBV	35120	38558	1.83%	0.270%
22	7.962	512	514	516	rVB3	21869	24908	1.18%	0.175%
23	8.007	516	518	519	rBV	22017	27884	1.33%	0.196%
24	8.030	519	520	523	rVV	25453	40145	1.91%	0.282%
25	8.087	523	525	527	rVB	419283	470288	22.36%	3.298%
26	8.373	545	550	554	rVB5	16718	59402	2.82%	0.417%
27	8.476	556	559	562	rBV2	26283	55074	2.62%	0.386%
28	8.682	573	577	578	rVB3	25567	45604	2.17%	0.320%
29	8.773	582	585	587	rBV2	20930	29362	1.40%	0.206%
30	8.865	589	593	598	rBV7	12490	40374	1.92%	0.283%
31	8.945	598	600	604	rVB5	11960	27239	1.30%	0.191%
32	9.013	604	606	609	rBV3	9790	25929	1.23%	0.182%
33	9.070	609	611	615	rBV2	57736	98127	4.67%	0.688%
34	9.173	617	620	622	rVB	2208482	2022677	96.19%	14.184%

LSC Area Percent Report

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Data File : BF080908.D
Acq On : 7 Aug 2015 2:10
Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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-BF080615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.402	638	640	643	rBV4	16744	42083	2.00%	0.295%
36	9.562	653	654	656	rBV	99170	76623	3.64%	0.537%
37	9.722	664	668	670	rBV3	18846	54866	2.61%	0.385%
38	9.768	670	672	676	rVB5	19831	46253	2.20%	0.324%
39	9.848	676	679	681	rBV	551160	621894	29.57%	4.361%
40	9.928	683	686	689	rBV3	18765	36206	1.72%	0.254%
41	10.019	691	694	695	rBV2	21984	36321	1.73%	0.255%
42	10.088	698	700	702	rBV2	12462	21689	1.03%	0.152%
43	10.145	702	705	707	rVB3	31062	40357	1.92%	0.283%
44	10.202	708	710	711	rBV	22746	21859	1.04%	0.153%
45	10.259	713	715	720	rVB5	33877	58073	2.76%	0.407%
46	10.556	738	741	745	rBV2	21250	69346	3.30%	0.486%
47	10.625	745	747	750	rVB2	663138	720247	34.25%	5.051%
48	10.751	757	758	762	rVB	27484	43244	2.06%	0.303%
49	11.128	790	791	793	rVB	44232	41430	1.97%	0.291%
50	11.196	795	797	803	rVB2	31724	58110	2.76%	0.407%
51	11.322	806	808	812	rVB	726185	616956	29.34%	4.326%
52	11.493	821	823	826	rVB	30507	31337	1.49%	0.220%
53	11.631	832	835	839	rBV2	24104	77086	3.67%	0.541%
54	11.711	841	842	844	rVB	41027	41504	1.97%	0.291%
55	11.859	853	855	857	rBV2	70770	84035	4.00%	0.589%
56	12.248	885	889	893	rBV6	10233	25993	1.24%	0.182%
57	12.739	930	932	934	rVB	22026	22216	1.06%	0.156%
58	12.911	944	947	949	rBV	2113953	2102863	100.00%	14.746%
59	13.448	992	994	996	rBV	18592	30392	1.45%	0.213%
60	13.871	1027	1031	1032	rBV3	13105	31667	1.51%	0.222%
61	13.951	1036	1038	1040	rBV	689876	627997	29.86%	4.404%
62	15.357	1158	1161	1164	rBV	450426	538052	25.59%	3.773%

Sum of corrected areas: 14260473

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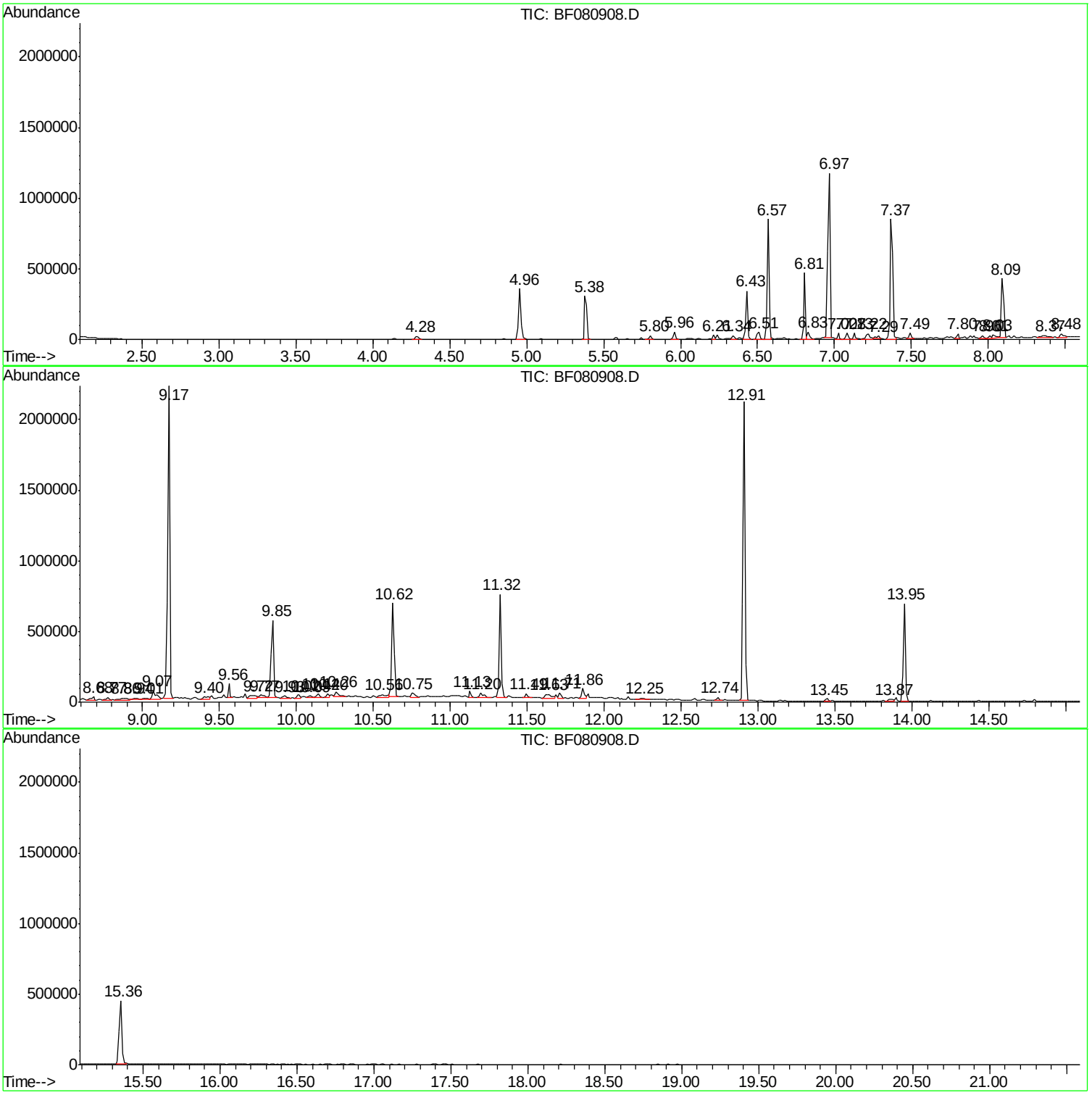
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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Data File : BF080908.D
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Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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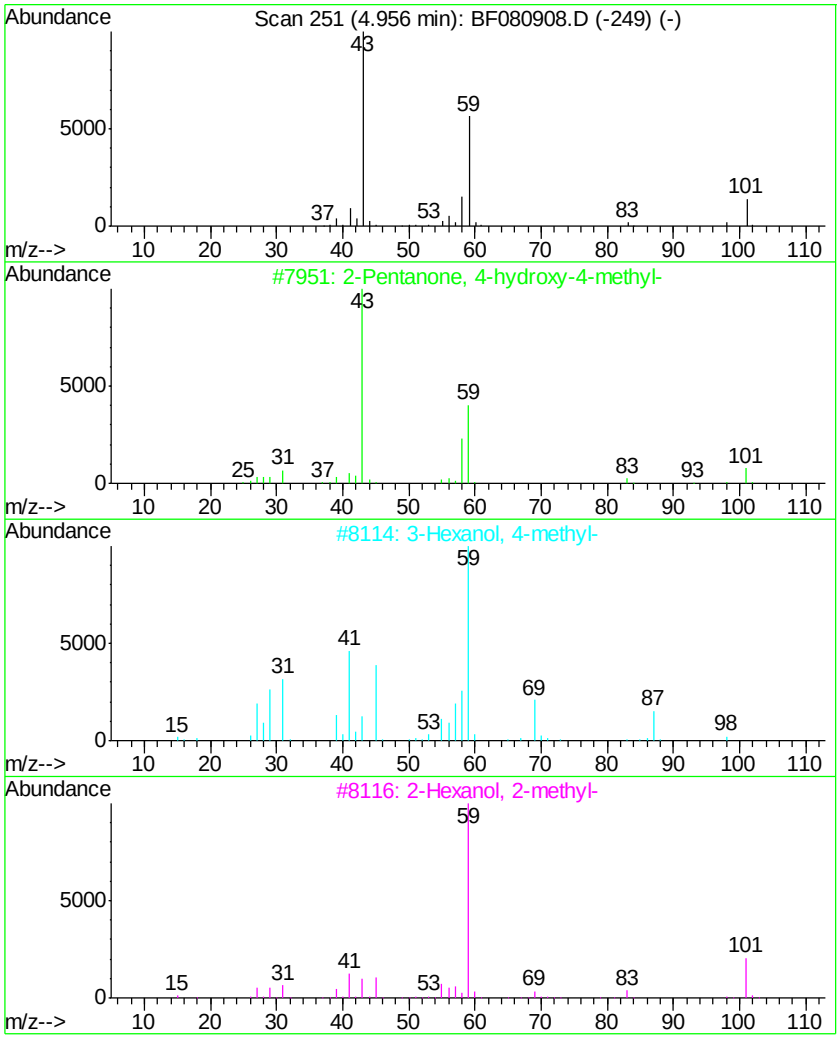
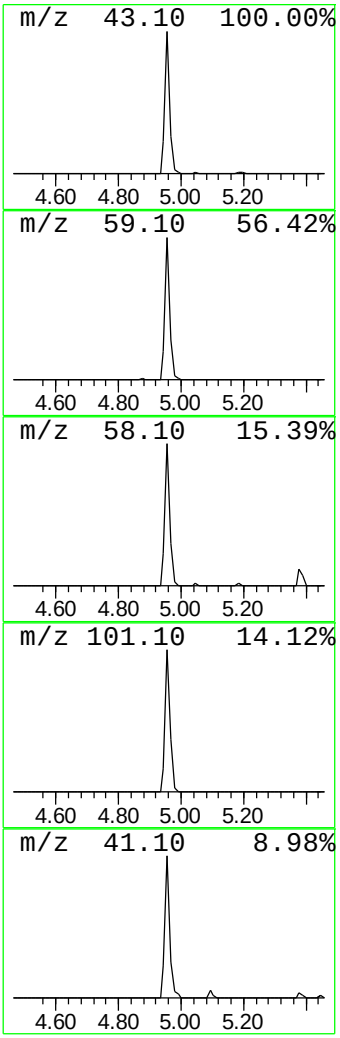
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	19.37 ng	378100	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





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Acq On : 7 Aug 2015 2:10
Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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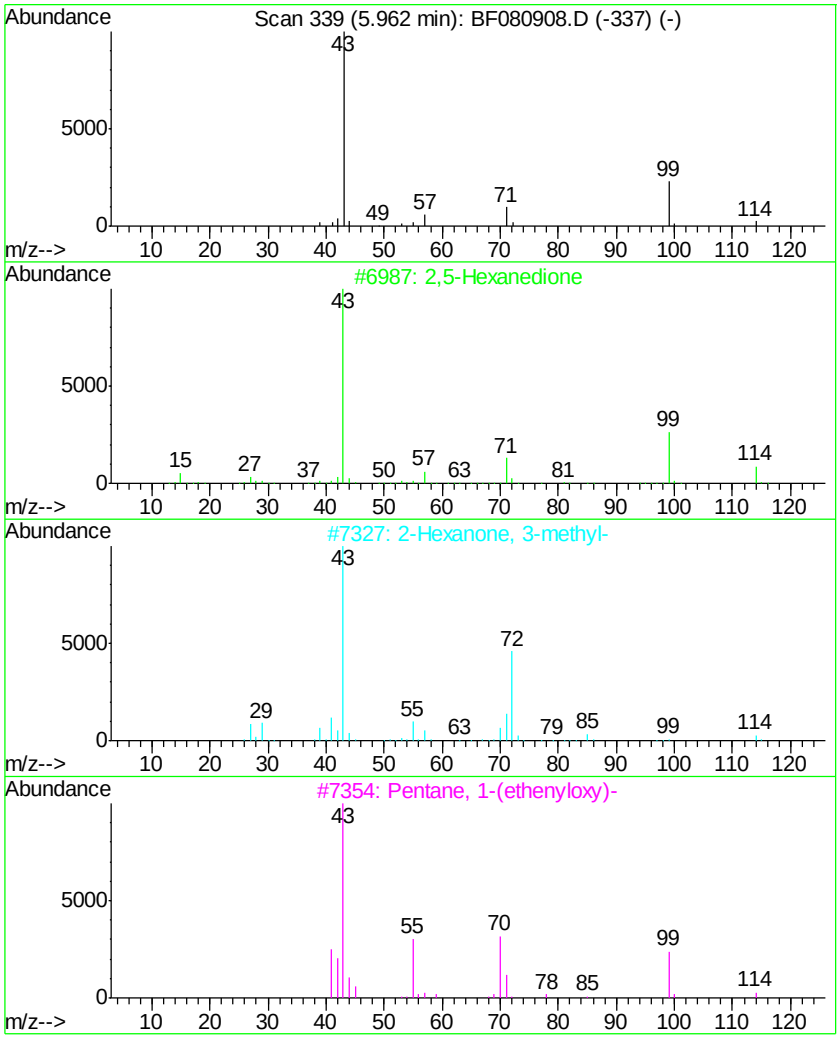
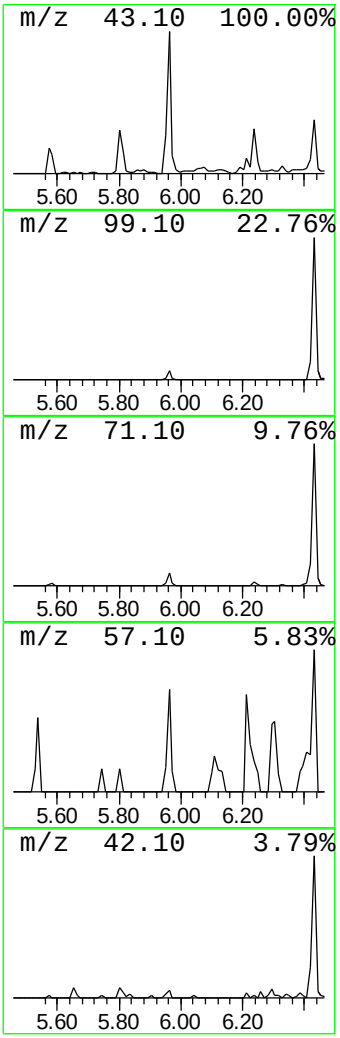
Peak Number 2 2,5-Hexanedione Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	2.64 ng	51527	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanedione	114	C6H10O2	000110-13-4	53
2	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	47
3	Pentane, 1-(ethenyloxy)-	114	C7H14O	005363-63-3	39
4	2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	9
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080615\
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Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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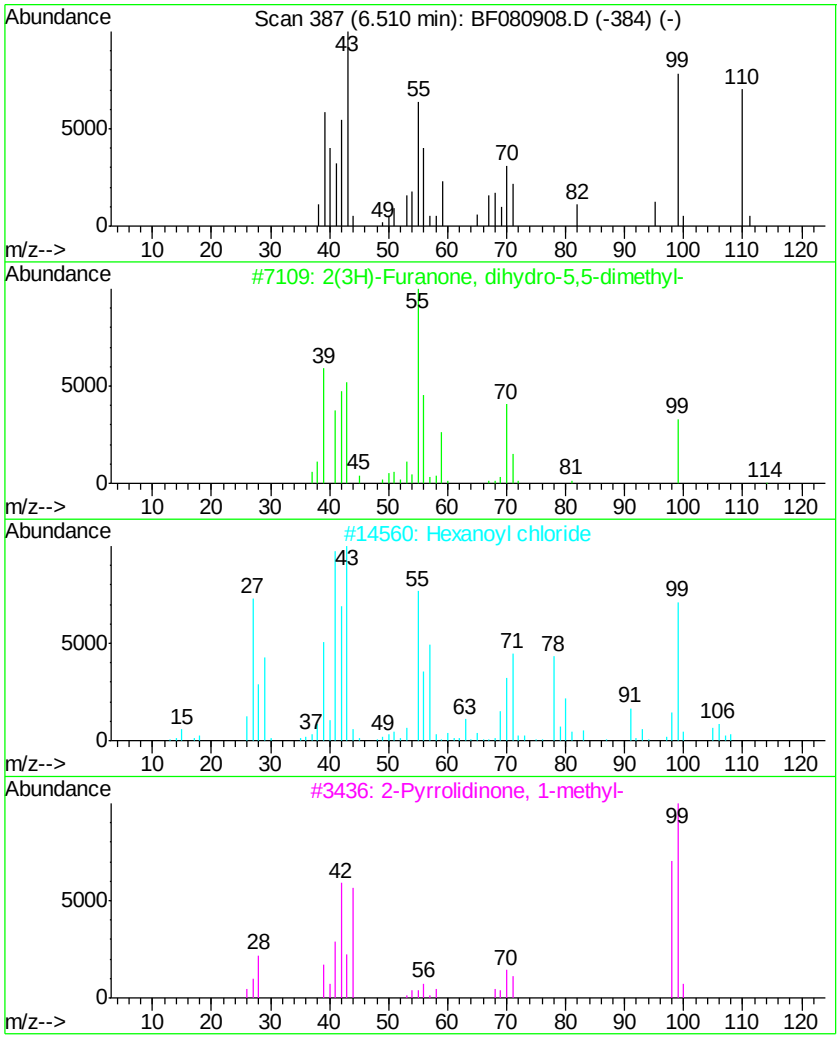
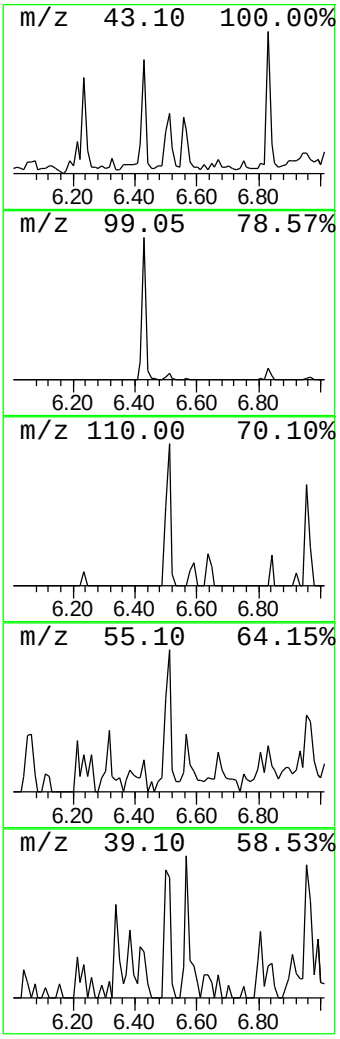
Peak Number 3 2(3H)-Furanone, dihydro-5,5... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	3.25 ng	63502	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5,5-dime...	114	C6H10O2	003123-97-5	64
2	Hexanoyl chloride	134	C6H11ClO	000142-61-0	53
3	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	43
4	Cyclopropane, isothiocyanato-	99	C4H5NS	056601-42-4	38
5	1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	35





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Data File : BF080908.D
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Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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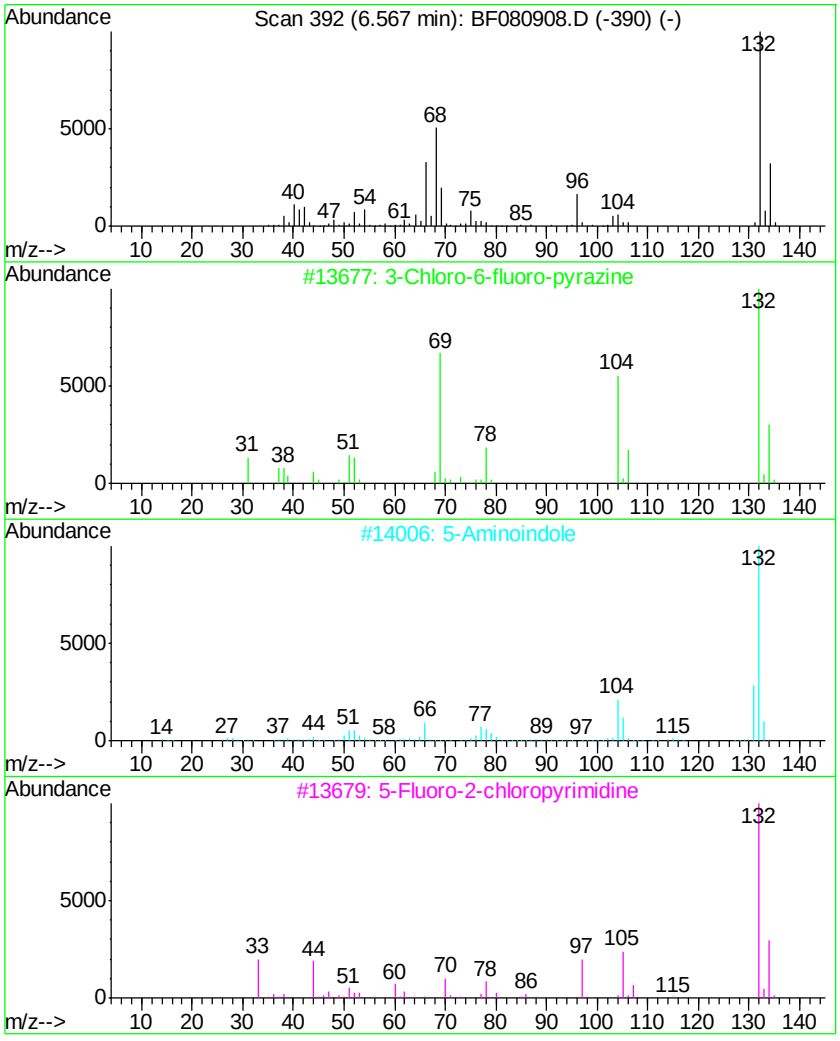
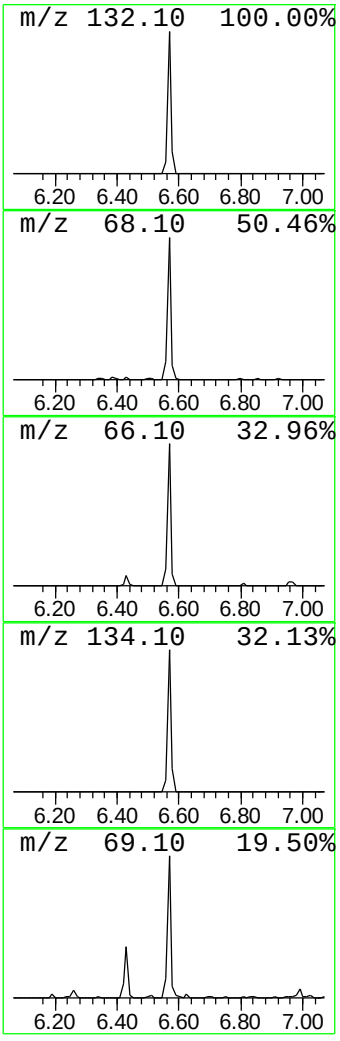
Peak Number 4 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	37.26 ng	727221	1,4-Dichlorobenzene-d4	6.81

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	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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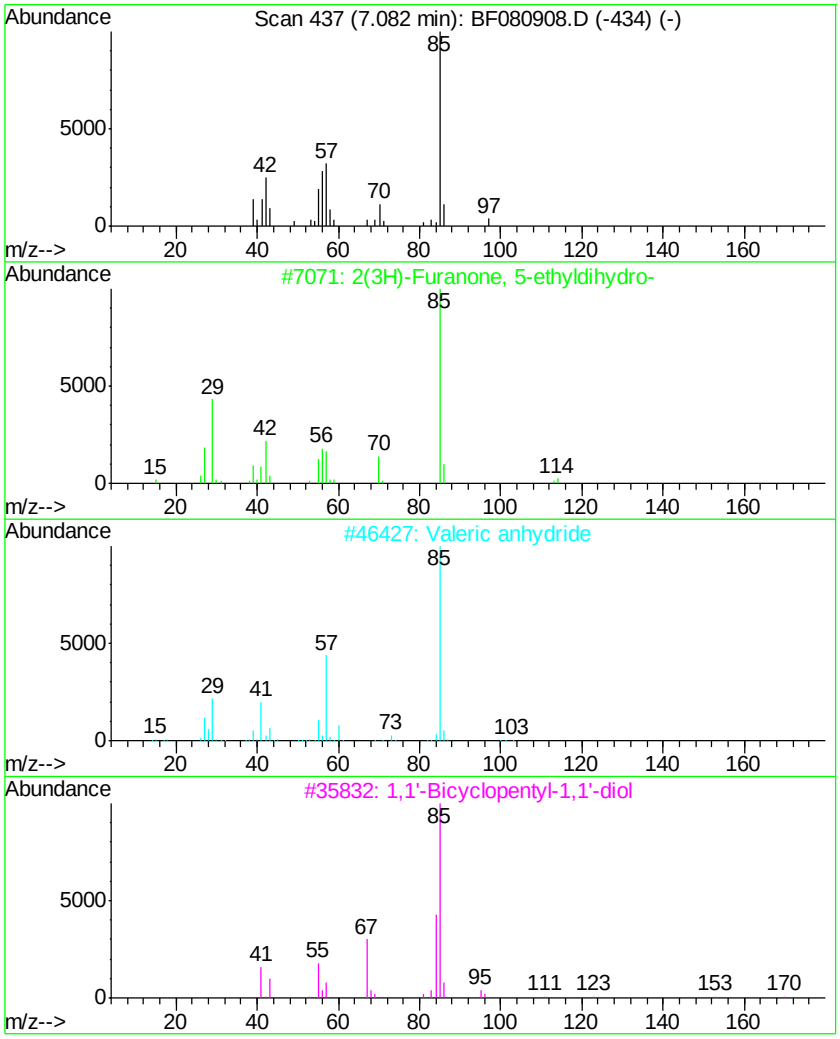
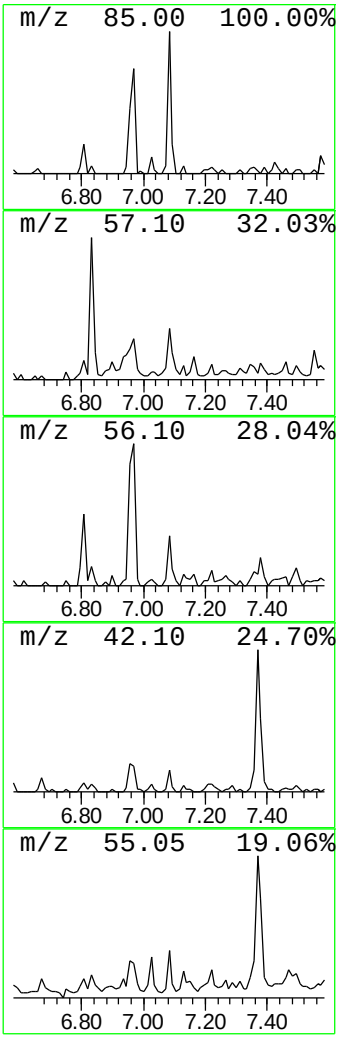
Peak Number 6 2(3H)-Furanone, 5-ethyldihy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	2.25 ng	43954	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, 5-ethyldihydro-	114	C6H10O2	000695-06-7	56
2	Valeric anhydride	186	C10H18O3	002082-59-9	9
3	1,1'-Bicyclopentyl-1,1'-diol	170	C10H18O2	005181-75-9	9
4	Oxirane, (2-methylpropyl)-	100	C6H12O	023850-78-4	9
5	3,3,6-Trimethyl-1,5-heptadien-4-ol	154	C10H18O	057590-19-9	9





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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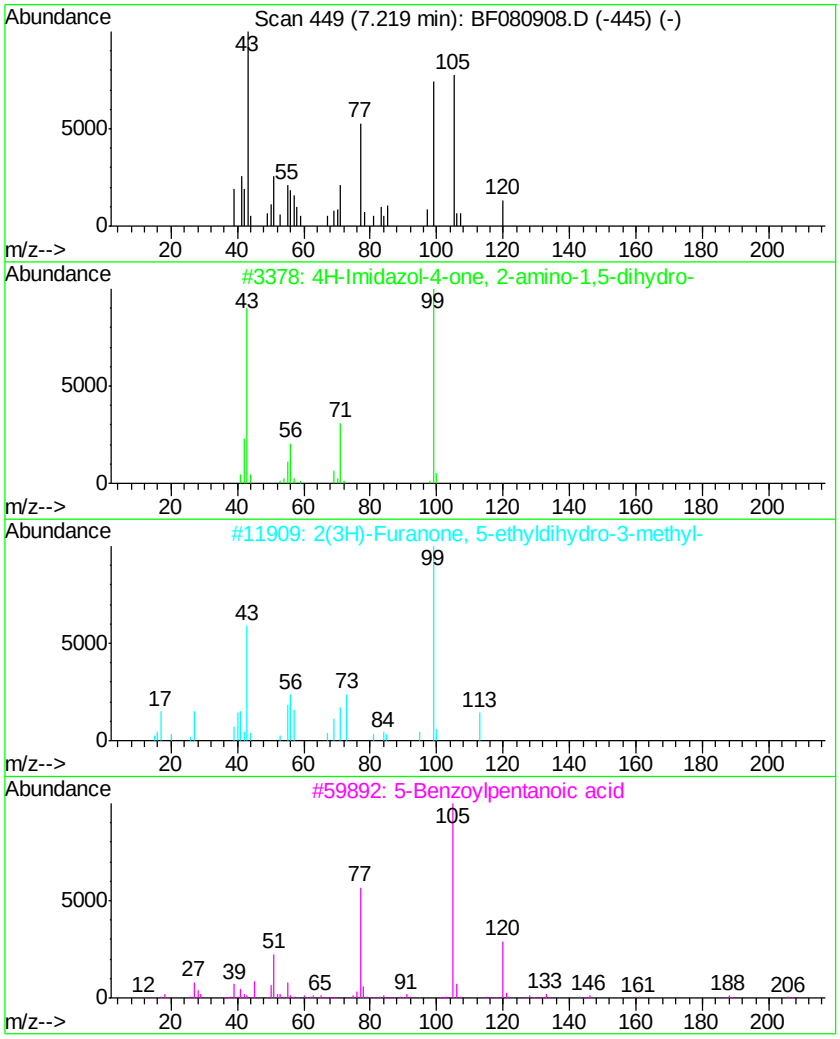
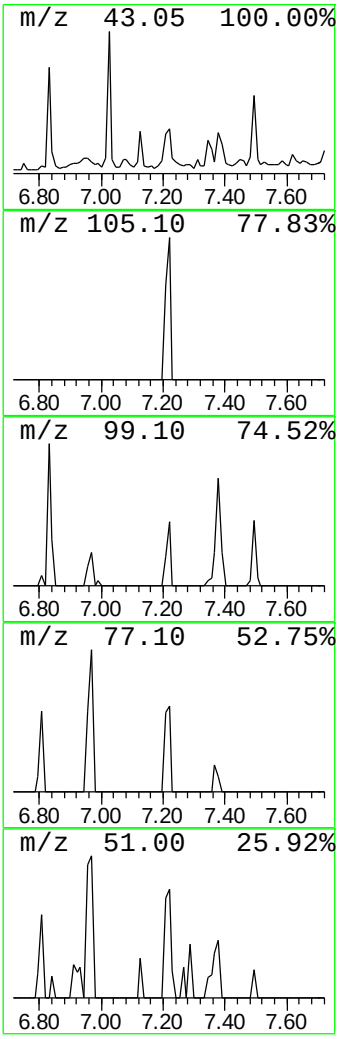
Peak Number 7 unknown7.22 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	3.54 ng	69069	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	38
2	2(3H)-Furanone, 5-ethyldihydro-3...	128	C7H12O2	002610-98-2	27
3	5-Benzoylpentanoic acid	206	C12H14O3	097547-93-8	27
4	3,5-Diamino-1,2,4-triazole	99	C2H5N5	000503-88-8	27
5	Benzoic acid, 3,3,5-trimethyl-6-...	336	C21H20O4	1000277-63-9	27





Library Search Compound Report

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ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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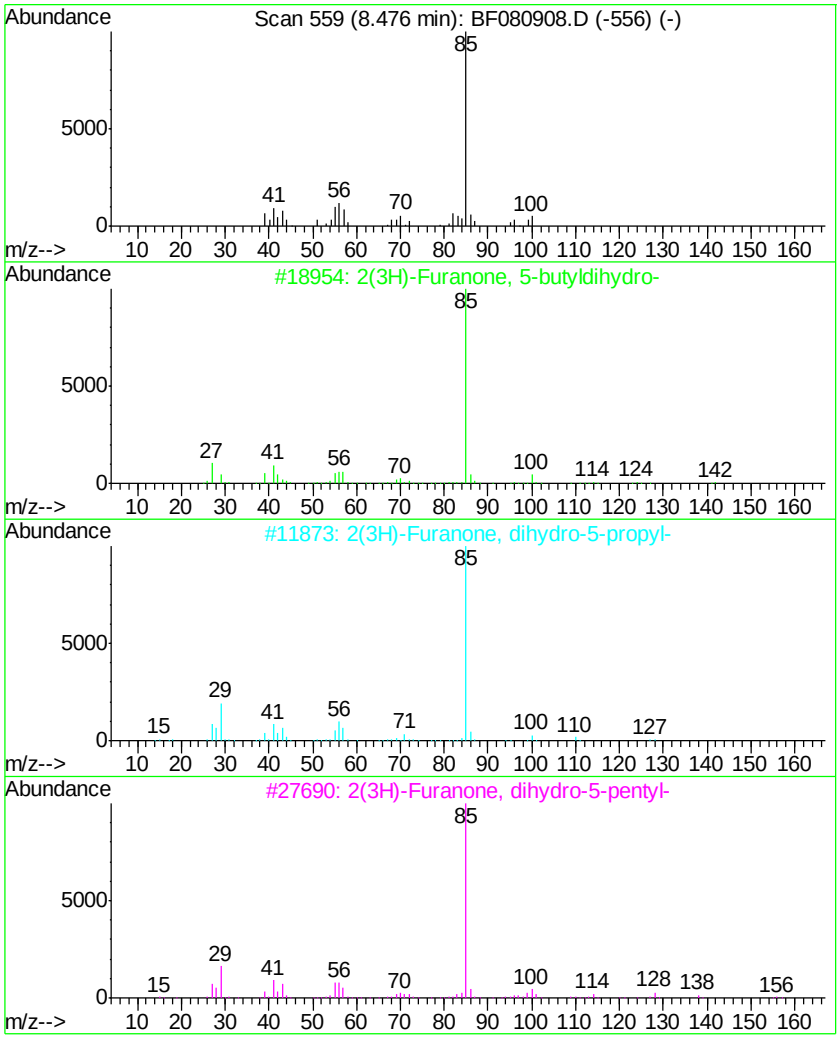
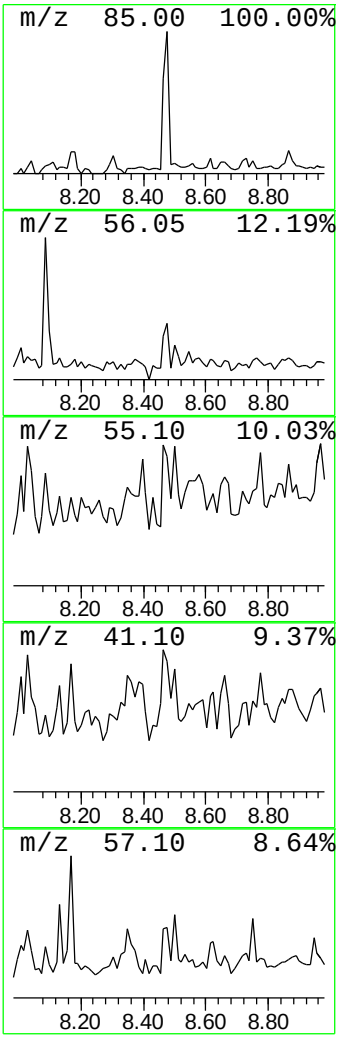
Peak Number 9 2(3H)-Furanone, 5-butyldihy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	2.34 ng	55074	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, 5-butyldihydro-	142	C8H14O2	000104-50-7	64
2	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	64
3	2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	64
4	2-Pyrrolidinone	85	C4H7NO	000616-45-5	59
5	Valeric anhydride	186	C10H18O3	002082-59-9	45





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Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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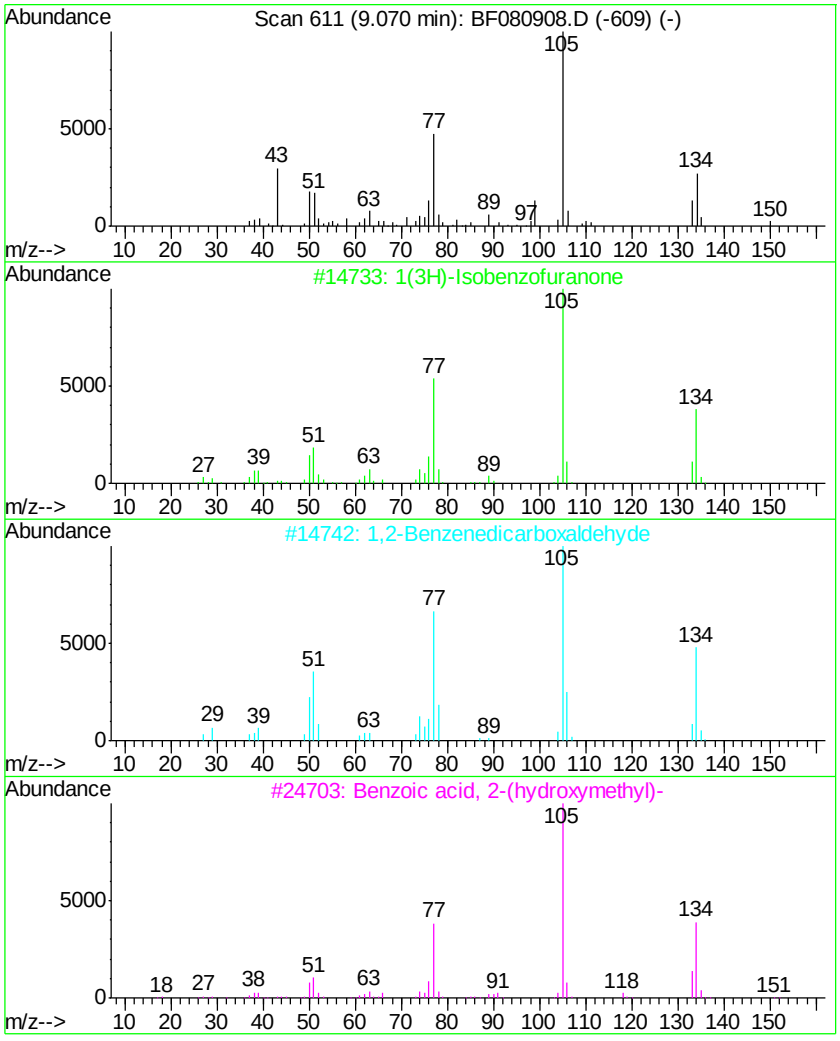
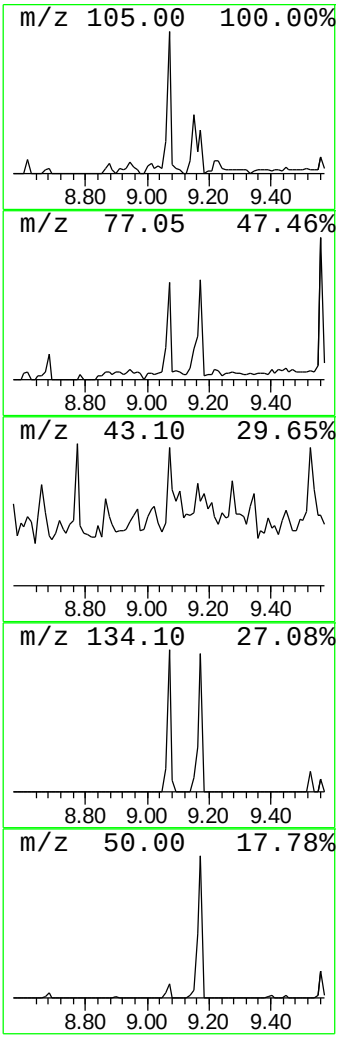
Peak Number 10 1(3H)-Isobenzofuranone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	3.16 ng	98127	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(3H)-Isobenzofuranone	134	C8H6O2	000087-41-2	93
2	1,2-Benzenedicarboxaldehyde	134	C8H6O2	000643-79-8	72
3	Benzoic acid, 2-(hydroxymethyl)-	152	C8H8O3	000612-20-4	53
4	2-Phenyl-oxetane	134	C9H10O	1000145-26-5	53
5	1-Propanone, 1-phenyl-	134	C9H10O	000093-55-0	50





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Acq On : 7 Aug 2015 2:10
Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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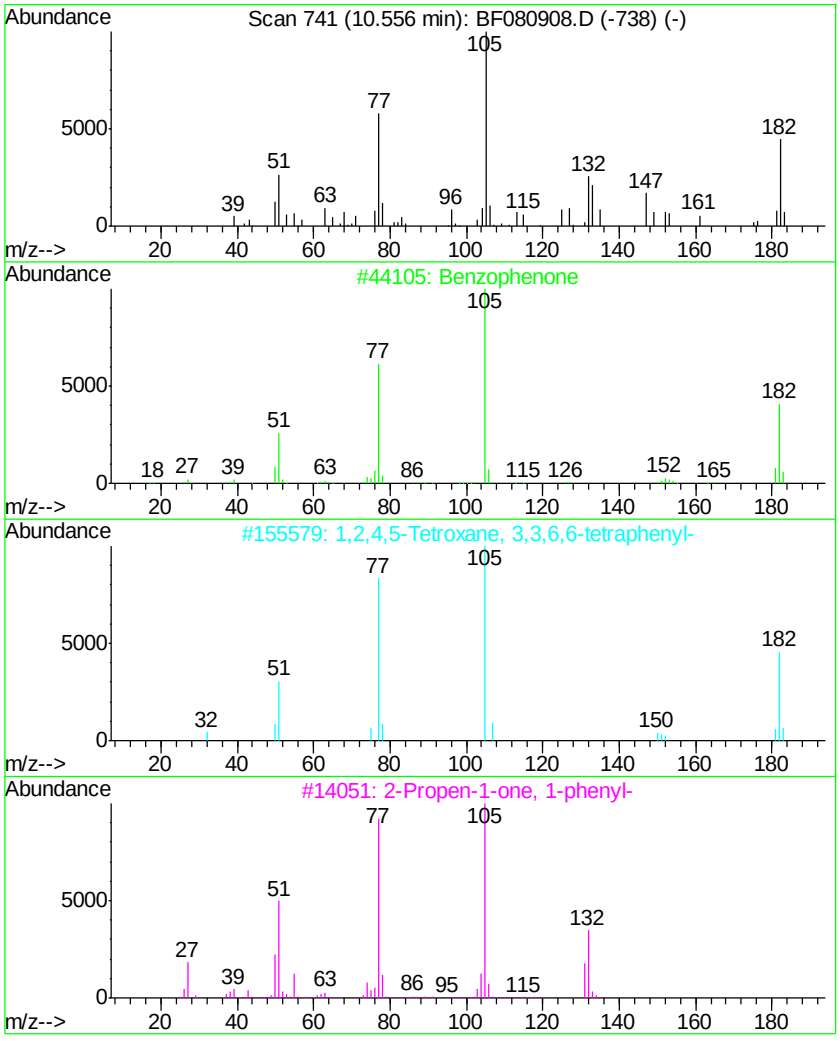
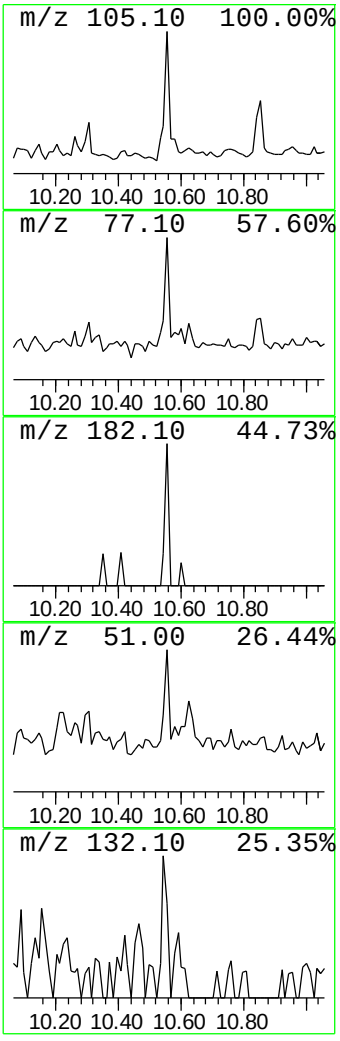
Peak Number 11 Benzophenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.23 ng	69346	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	62
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	50
3	2-Propen-1-one, 1-phenyl-	132	C9H8O	000768-03-6	49
4	Azobenzene	182	C12H10N2	000103-33-3	38
5	Azobenzene, (E)-	182	C12H10N2	017082-12-1	38





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Acq On : 7 Aug 2015 2:10
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Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.M
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TIC Library : C:\DATABASE\NIST02.L
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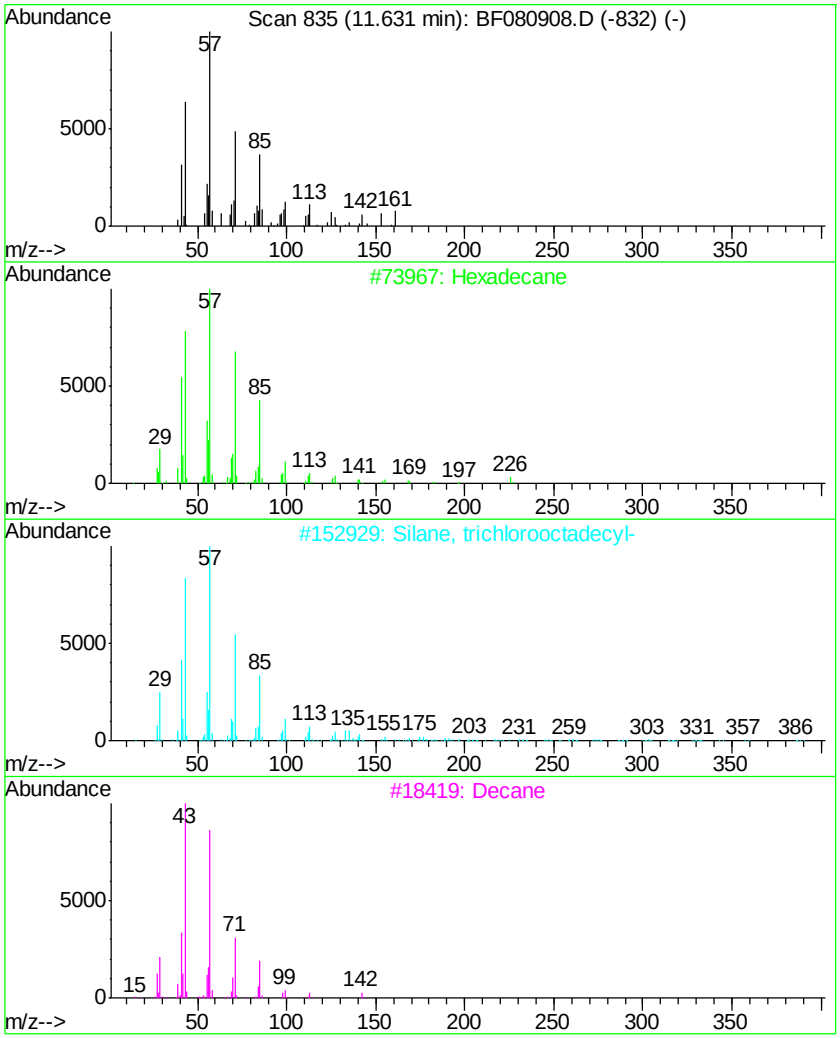
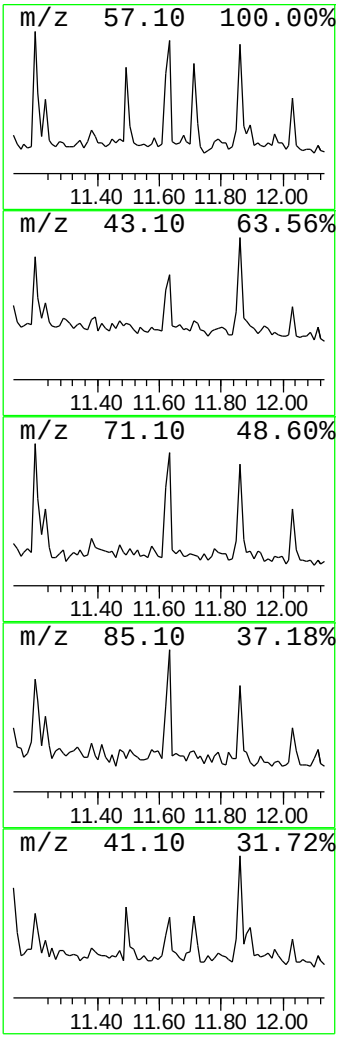
Peak Number 12 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	2.50 ng	77086	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	72
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72
3	Decane	142	C10H22	000124-18-5	72
4	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
5	Octacosane	394	C28H58	000630-02-4	64





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Data File : BF080908.D
Acq On : 7 Aug 2015 2:10
Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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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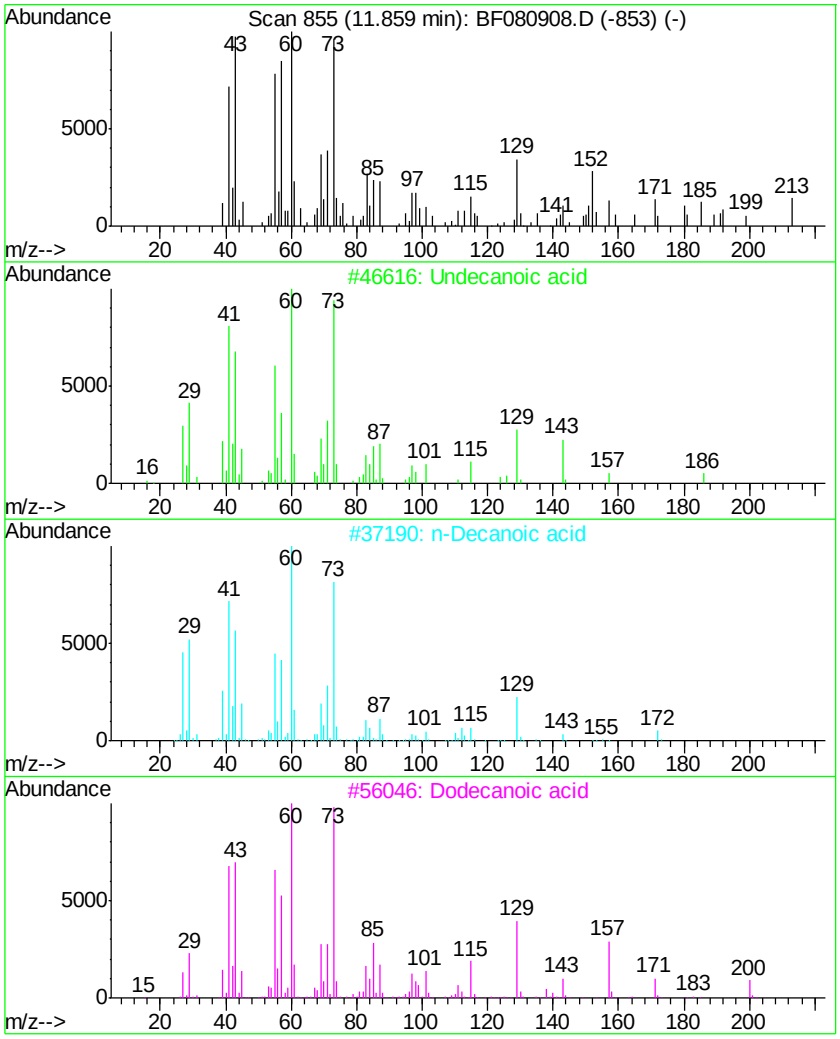
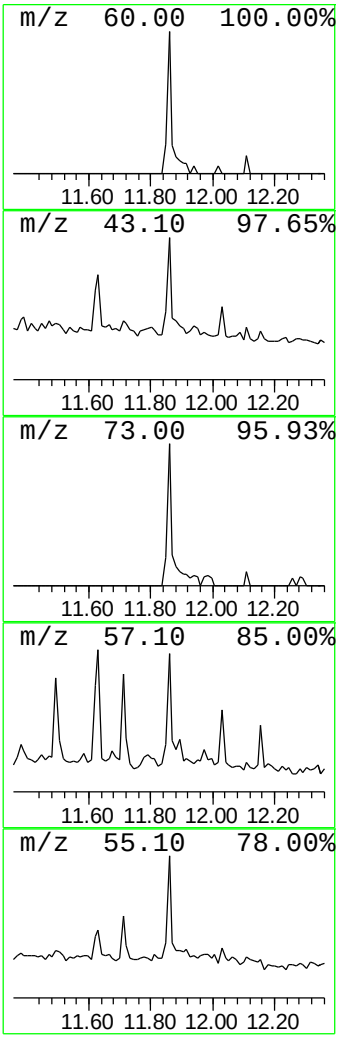
Peak Number 13 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.72 ng	84035	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	68
3	Dodecanoic acid	200	C12H24O2	000143-07-7	58
4	Amyl Nitrite	117	C5H11NO2	000110-46-3	38
5	Decane	142	C10H22	000124-18-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080615\
Data File : BF080908.D
Acq On : 7 Aug 2015 2:10
Operator : TP/UM
Sample : G3196-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.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...	4.96	19.4	ng	378100	1	6.81	390395	20.0
2,5-Hexanedione	5.96	2.6	ng	51527	1	6.81	390395	20.0
2(3H)-Furanone, d...	6.51	3.3	ng	63502	1	6.81	390395	20.0
unknown6.57	6.57	37.3	ng	727221	1	6.81	390395	20.0
2(3H)-Furanone, 5...	7.08	2.3	ng	43954	1	6.81	390395	20.0
unknown7.22	7.22	3.5	ng	69069	1	6.81	390395	20.0
2(3H)-Furanone, 5...	8.48	2.3	ng	55074	2	8.09	470288	20.0
1(3H)-Isobenzofur...	9.07	3.2	ng	98127	3	9.85	621894	20.0
Benzophenone	10.56	2.2	ng	69346	3	9.85	621894	20.0
Hexadecane	11.63	2.5	ng	77086	4	11.32	616956	20.0
Undecanoic acid	11.86	2.7	ng	84035	4	11.32	616956	20.0