LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097410.D
Acq On : 5 Aug 2017 21:15
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

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-BF072517.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	4.540	464	468	476	rBV	17227	29962	4.68%	0.627%
2	5.040	550	553	568	rBV	69524	150092	23.46%	3.143%
3	6.116	734	736	749	rBV	76990	142766	22.32%	2.989%
4	6.210	749	752	764	rVB	131002	171234	26.77%	3.585%
5	6.422	785	788	803	rVB	488351	491867	76.89%	10.299%
6	6.581	812	815	828	rBV	100076	102342	16.00%	2.143%
7	7.004	884	887	897	rBV	57763	78123	12.21%	1.636%
8	7.710	1003	1007	1016	rBV	709943	639711	100.00%	13.395%
9	8.786	1186	1190	1198	rBV	148303	134260	20.99%	2.811%
10	9.186	1256	1258	1263	rBV2	9311	11308	1.77%	0.237%
11	9.451	1299	1303	1313	rVB	589968	515429	80.57%	10.792%
12	10.127	1411	1418	1423	rBV	5105	7255	1.13%	0.152%
13	10.239	1434	1437	1444	rVB	49969	55753	8.72%	1.167%
14	10.374	1455	1460	1468	rBV2	12068	18277	2.86%	0.383%
15	10.816	1532	1535	1538	rBV	9174	8559	1.34%	0.179%
16	10.922	1550	1553	1562	rVB	523026	465668	72.79%	9.750%
17	11.245	1605	1608	1613	rVB2	11174	10171	1.59%	0.213%
18	11.645	1673	1676	1678	rBV2	9176	6761	1.06%	0.142%
19	12.039	1740	1743	1746	rVB2	16383	15081	2.36%	0.316%
20	12.127	1755	1758	1764	rBV	28348	30259	4.73%	0.634%
21	12.351	1793	1796	1800	rBV	35441	34508	5.39%	0.723%
22	12.404	1802	1805	1807	rBV3	7875	7715	1.21%	0.162%
23	12.498	1818	1821	1825	rBV	138916	129118	20.18%	2.704%
24	12.757	1863	1865	1867	rVB3	7691	6916	1.08%	0.145%
25	12.786	1867	1870	1874	rBV5	6338	8543	1.34%	0.179%
26	12.910	1888	1891	1893	rBV4	6524	9142	1.43%	0.191%
27	12.933	1893	1895	1900	rVB5	9761	13375	2.09%	0.280%
28	13.098	1921	1923	1927	rBV4	10732	17536	2.74%	0.367%
29	13.298	1955	1957	1958	rBV2	11779	7491	1.17%	0.157%
30	13.545	1995	1999	2003	rBV	519276	493206	77.10%	10.327%
31	13.615	2007	2011	2012	rBV3	13355	18421	2.88%	0.386%
32	13.892	2056	2058	2060	rBV3	21191	18133	2.83%	0.380%
33	14.057	2084	2086	2092	rVB6	25000	29062	4.54%	0.609%
34	14.780	2207	2209	2214	rBV4	37446	44733	6.99%	0.937%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097410.D
Acq On : 5 Aug 2017 21:15
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.886	2223	2227	2232	rVB	240271	254275	39.75%	5.324%
36	15.086	2259	2261	2269	rVB7	43678	70969	11.09%	1.486%
37	15.274	2291	2293	2295	rBV2	35605	42701	6.68%	0.894%
38	15.674	2358	2361	2366	rBV6	38435	77206	12.07%	1.617%
39	15.874	2393	2395	2397	rBV3	33070	37926	5.93%	0.794%
40	16.421	2486	2488	2494	rBV5	28923	52449	8.20%	1.098%
41	18.062	2765	2767	2771	rBV5	30119	43863	6.86%	0.918%
42	18.256	2798	2800	2802	rBV3	26572	34328	5.37%	0.719%
43	18.445	2830	2832	2837	rBV6	24675	50131	7.84%	1.050%
44	18.568	2851	2853	2860	rBV7	29621	69661	10.89%	1.459%
45	19.209	2960	2962	2967	rBV5	24707	50410	7.88%	1.056%
46	19.292	2974	2976	2982	rBV7	25028	35677	5.58%	0.747%
47	19.339	2982	2984	2986	rBV2	30718	33492	5.24%	0.701%

Sum of corrected areas: 4775865

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097410.D
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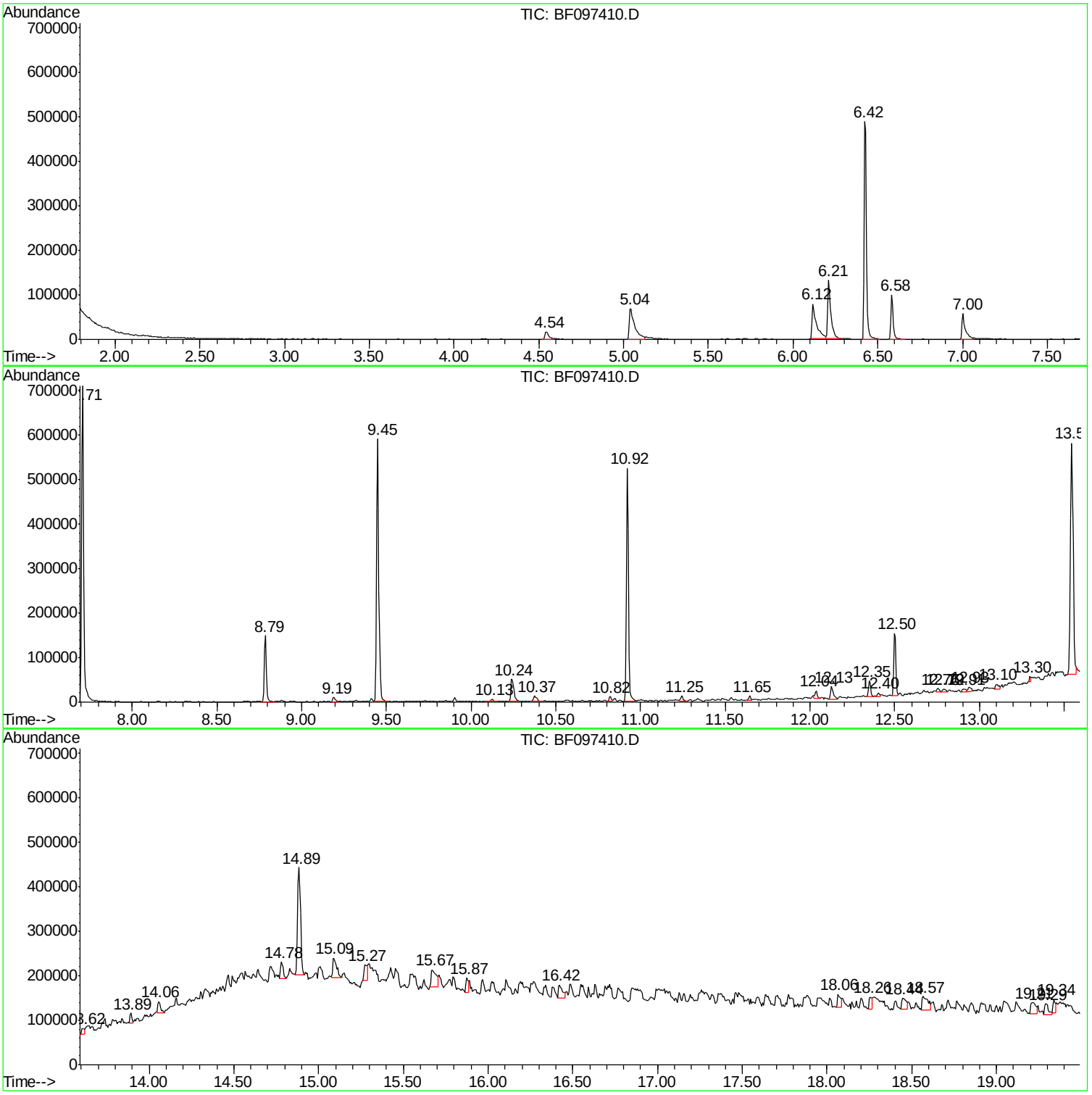
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097410.D
Acq On : 5 Aug 2017 21:15
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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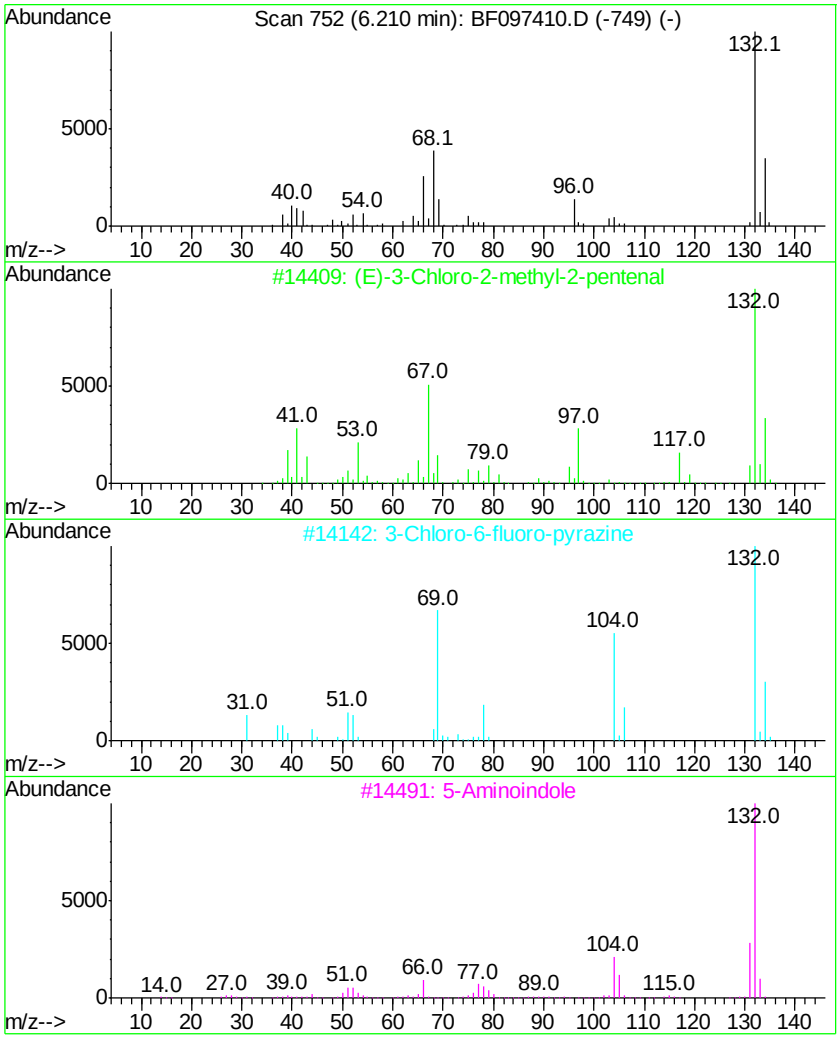
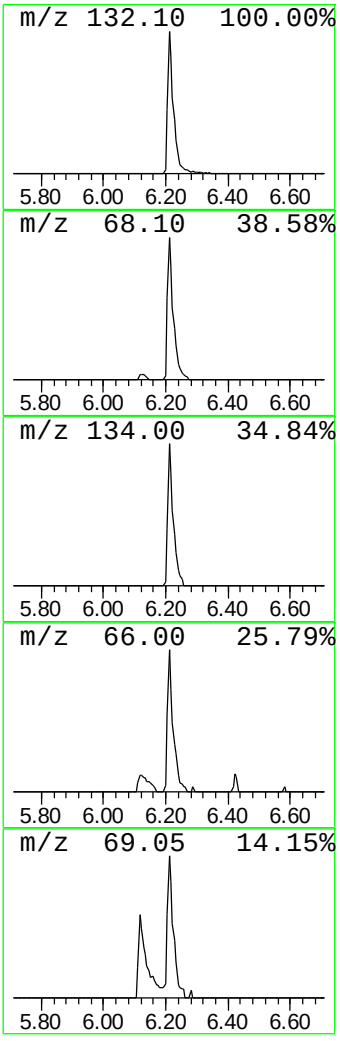
Peak Number 1 unknown6.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	6.96 ng	171234	1,4-Dichlorobenzene-d4	6.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097410.D
Acq On : 5 Aug 2017 21:15
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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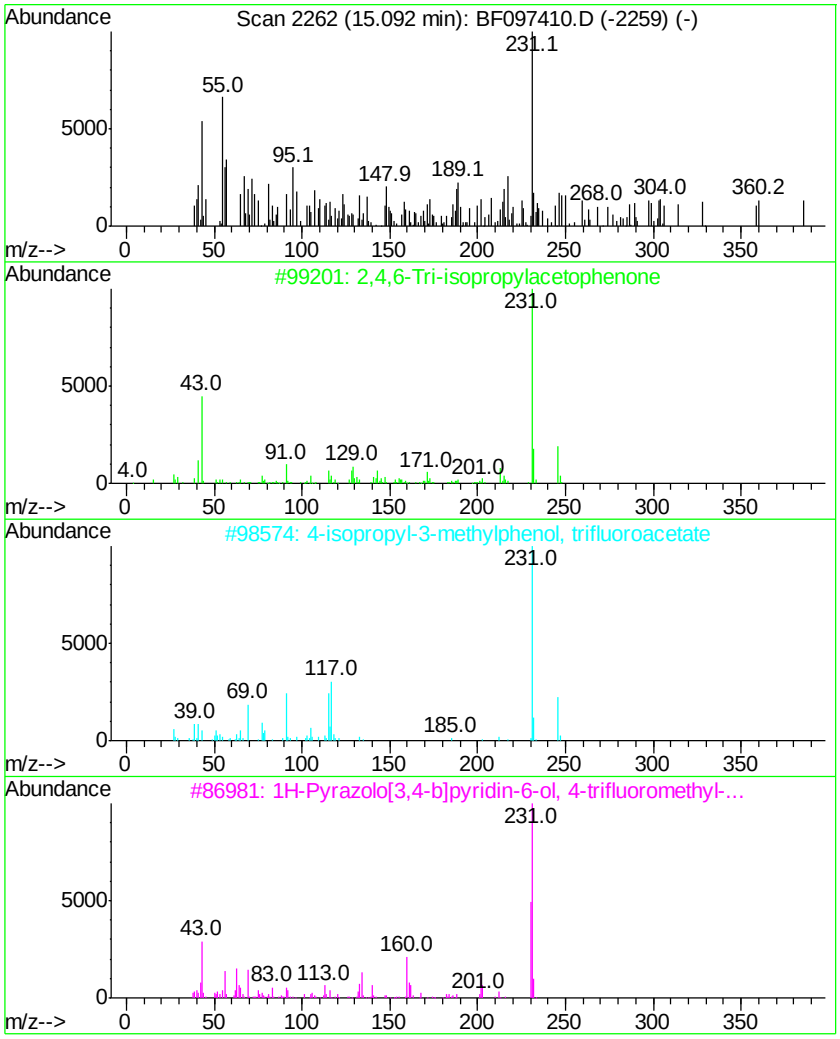
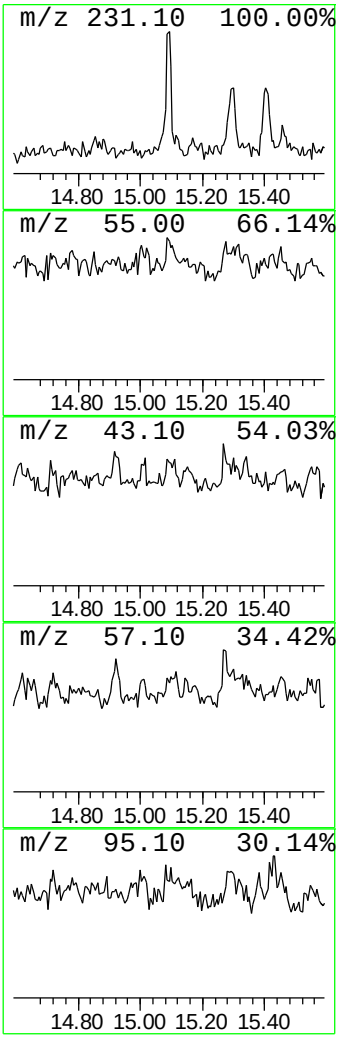
Peak Number 4 unknown15.09 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	5.58 ng	70969	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Tri-isopropylacetophenone	246	C17H26O	002234-14-2	38
2	4-isopropyl-3-methylphenol, trif...	246	C12H13F3O2	1000376-51-7	38
3	1H-Pyrazolo[3,4-b]pyridin-6-ol, ...	231	C9H8F3N3O	094835-66-2	38
4	Cyclopropanecarboxylic acid, 2,2...	354	C22H30N2O2	1000317-04-7	37
5	4-(O-Chlorobenzylidene)-2-ethylt...	266	C12H11ClN2OS	033449-97-7	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097410.D
Acq On : 5 Aug 2017 21:15
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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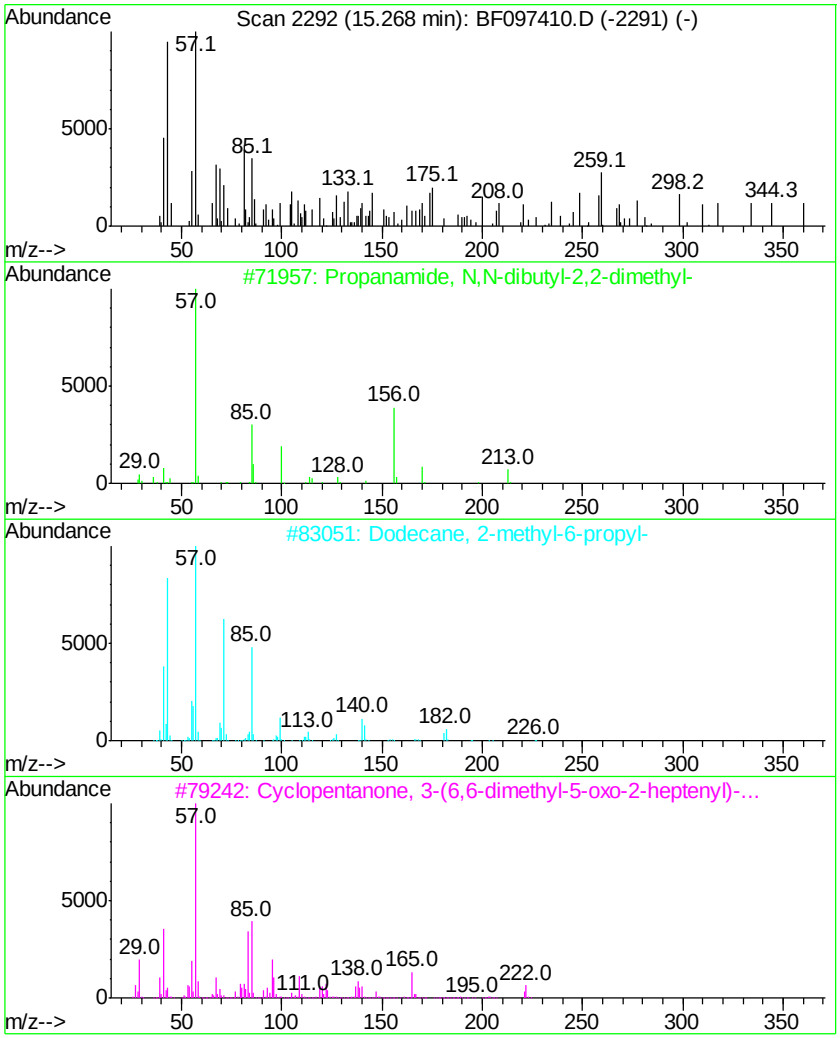
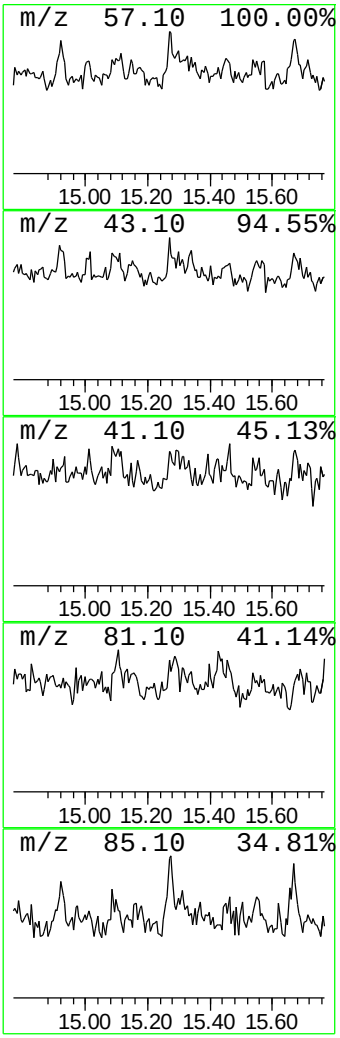
Peak Number 5 unknown15.27 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.36 ng	42701	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanamide, N,N-dibutyl-2,2-dim...	213	C13H27NO	1000308-12-4	14
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	14
3	Cyclopentanone, 3-(6,6-dimethyl-...	222	C14H22O2	083040-98-6	14
4	2-Hydroxy-1,1,10-trimethyl-6,9-e...	226	C13H22O3	108511-85-9	14
5	1-[3-Nitro-4-ethoxyphenyl]biguanide	266	C10H14N6O3	1000255-99-6	14





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Misc :
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Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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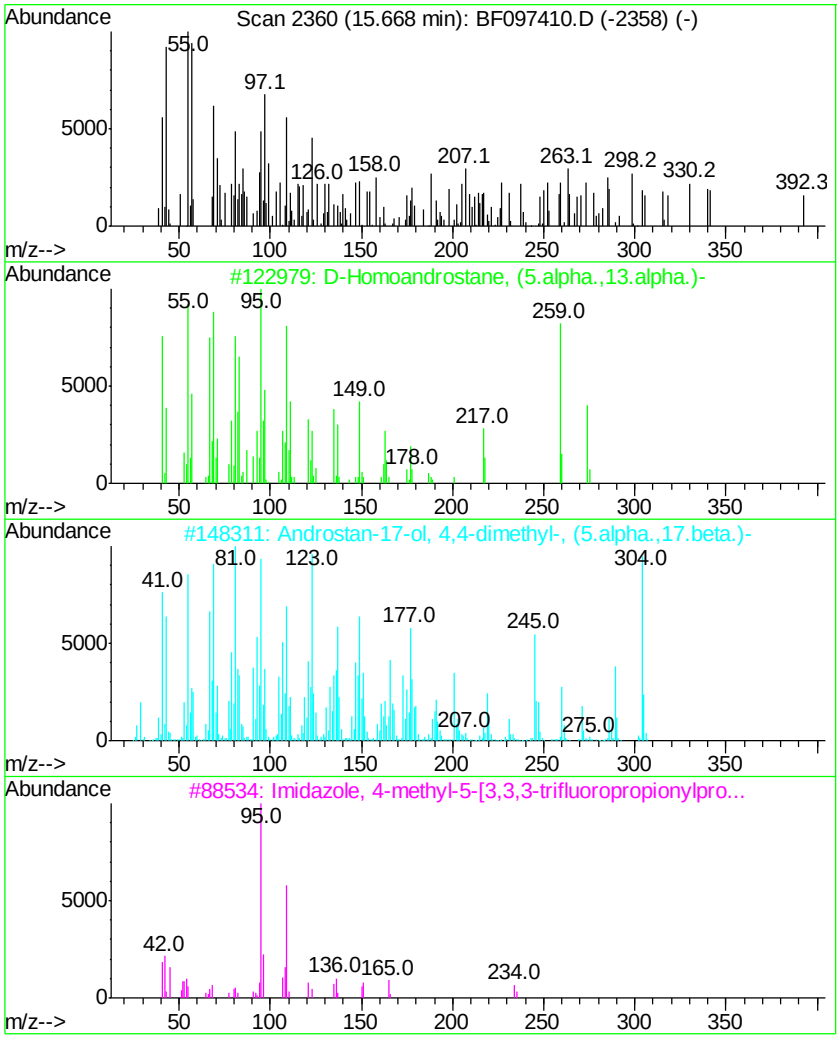
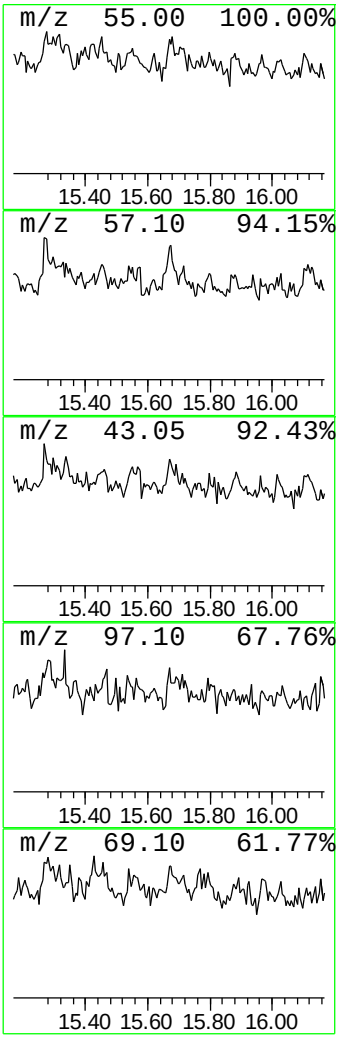
Peak Number 6 D-Homoandrostane, (5.alpha.... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	6.07 ng	77206	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Homoandrostane, (5.alpha.,13.a...	274	C20H34	054482-31-4	55
2	Androstan-17-ol, 4,4-dimethyl-, ...	304	C21H36O	006561-00-8	30
3	Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	27
4	Cyclopentene, 1-isopropyl-4,5-di...	138	C10H18	007712-74-5	25
5	7-Isopropyl-10-methyl-1-oxo-1,5-...	304	C14H24O3S2	1000189-33-1	25





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Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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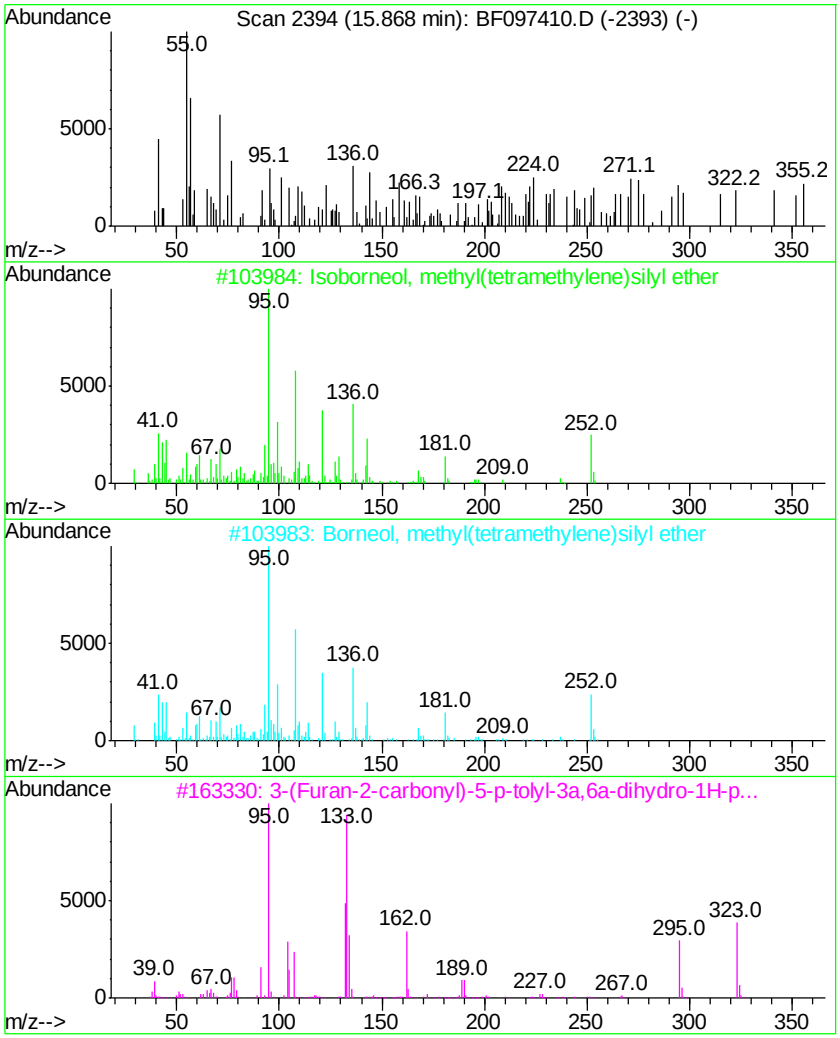
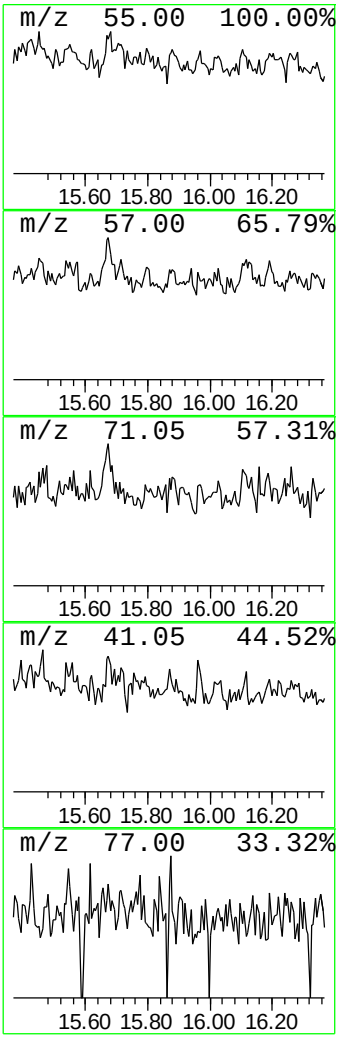
Peak Number 7 unknown15.87 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.98 ng	37926	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoborneol, methyl(tetramethylen...	252	C15H28OSi	1000278-62-1	30
2	Borneol, methyl(tetramethylene)s...	252	C15H28OSi	1000278-62-0	27
3	3-(Furan-2-carbonyl)-5-p-tolyl-3...	323	C17H13N3O4	1000296-77-7	16
4	1,5-Dihydropyrrol-2-one, 4-(fura...	357	C15H11N5O4S	1000303-76-0	14
5	Propanoic acid, 3,3,3-trifluoro-...	374	C16H14F4N2O4	1000362-44-3	14





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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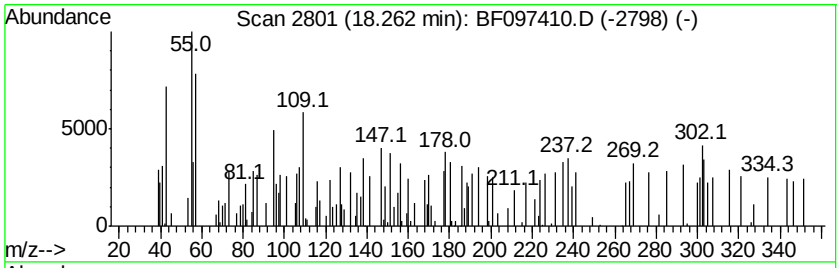
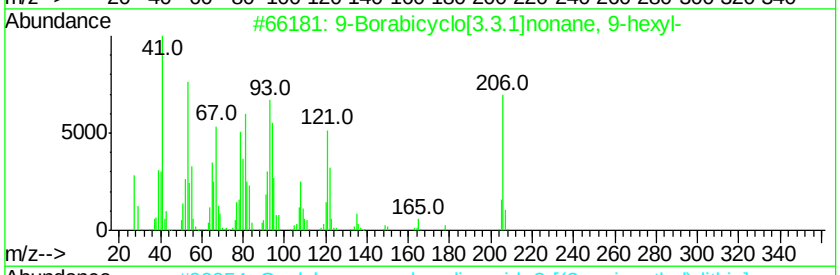
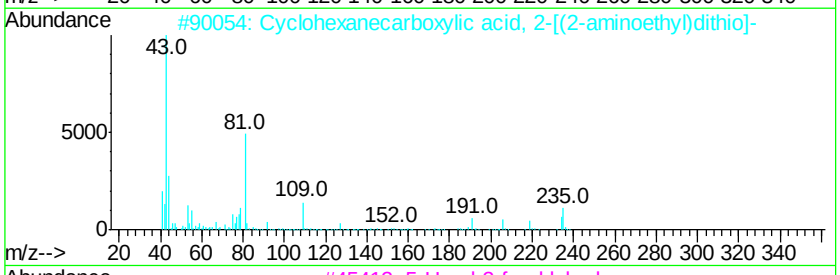
Peak Number 10 unknown18.26 Concentration Rank 14

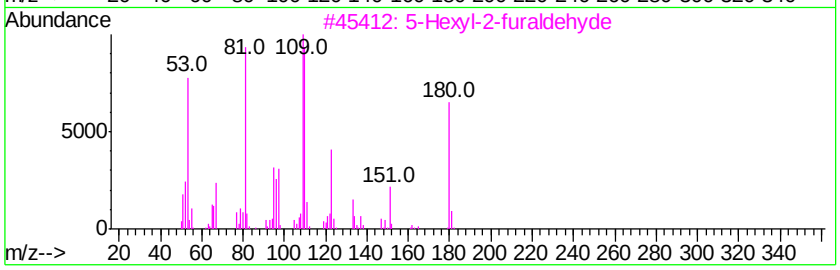
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.70 ng	34328	Perylene-d12	14.89

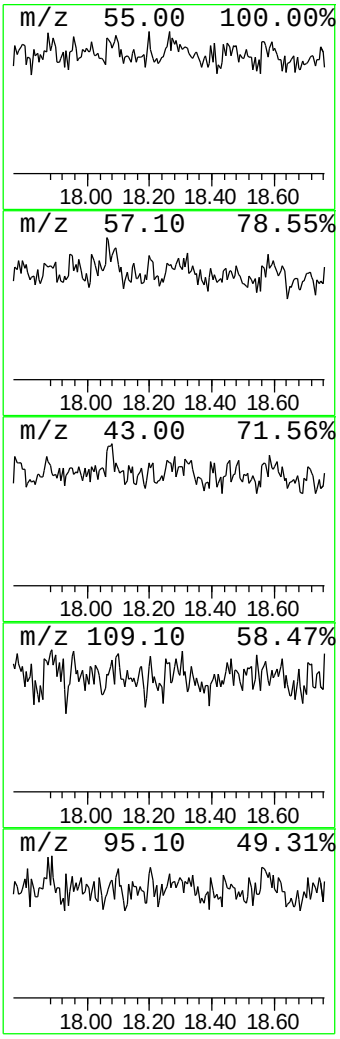
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Borabicyclo[3.3.1]nonane, 9-he...	206	C14H27B	042371-64-2	38
2	Cyclohexanecarboxylic acid, 2-[(...	235	C9H17NO2S2	025828-46-0	32
3	5-Hexyl-2-furaldehyde	180	C11H16O2	007011-80-5	27
4	4-Cyclopentene-1,3-diol, trans-	100	C5H8O2	000694-47-3	27
5	1,2-Oxazine, 3-ethoxycarbonyl-3-...	267	C10H12F3NO4	1000153-75-1	27











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080517\
Data File : BF097410.D
Acq On : 5 Aug 2017 21:15
Operator : SJ/JU
Sample : I4610-10 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-080317-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.21	6.21	7.0	ng	171234	1	6.43	491867	20.0
unknown15.09	15.09	5.6	ng	70969	6	14.89	254275	20.0
unknown15.27	15.27	3.4	ng	42701	6	14.89	254275	20.0
D-Homoandrostane,...	15.67	6.1	ng	77206	6	14.89	254275	20.0
unknown15.87	15.87	3.0	ng	37926	6	14.89	254275	20.0
unknown18.26	18.26	2.7	ng	34328	6	14.89	254275	20.0