LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082801.D
Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

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-BF110715.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	3.550	126	128	134	rVB	38023	68539	1.05%	0.108%
2	5.036	254	258	260	rBV	2214852	3214995	49.17%	5.069%
3	5.459	292	295	297	rBV	5216659	6271160	95.90%	9.888%
4	6.487	381	385	387	rVB	4377218	6539079	100.00%	10.311%
5	6.613	393	396	399	rBV	5450318	5590173	85.49%	8.814%
6	6.842	414	416	419	rBV	1401614	1540947	23.57%	2.430%
7	7.002	428	430	433	rVB	4104524	3911478	59.82%	6.167%
8	7.413	462	466	468	rBV	3348748	4192966	64.12%	6.611%
9	7.516	472	475	478	rVV2	85983	125996	1.93%	0.199%
10	8.042	519	521	523	rBV	72560	69678	1.07%	0.110%
11	8.133	526	529	531	rBV	2448929	2181406	33.36%	3.440%
12	9.093	610	613	615	rBV	101532	105505	1.61%	0.166%
13	9.207	620	623	626	rVV	4198279	5265352	80.52%	8.302%
14	9.608	655	658	660	rBV	2178408	1936158	29.61%	3.053%
15	9.882	680	682	685	rBV	1757055	2417274	36.97%	3.811%
16	10.305	717	719	720	rBV	259319	219537	3.36%	0.346%
17	10.670	748	751	754	rBV	3793854	3923636	60.00%	6.187%
18	10.808	761	763	768	rVB	84216	163450	2.50%	0.258%
19	11.253	800	802	803	rBV	151824	135831	2.08%	0.214%
20	11.368	809	812	814	rVV	2843830	2485611	38.01%	3.919%
21	11.608	830	833	837	rBV4	35668	78323	1.20%	0.123%
22	11.676	837	839	842	rVB	106267	94921	1.45%	0.150%
23	11.905	857	859	864	rVV3	283207	415573	6.36%	0.655%
24	12.088	871	875	877	rBV	62689	99936	1.53%	0.158%
25	12.236	885	888	889	rBV	78962	96973	1.48%	0.153%
26	12.476	903	909	910	rVB4	51621	91355	1.40%	0.144%
27	12.579	916	918	920	rBV	54361	70369	1.08%	0.111%
28	12.625	920	922	924	rVV	99961	98152	1.50%	0.155%
29	12.694	926	928	931	rVV2	192393	236671	3.62%	0.373%
30	12.785	935	936	940	rVB2	301485	369966	5.66%	0.583%
31	12.956	948	951	953	rBV	4754632	4260497	65.15%	6.718%
32	13.196	968	972	974	rBV2	47372	67948	1.04%	0.107%
33	13.391	986	989	990	rBV	68361	66893	1.02%	0.105%
34	13.425	990	992	996	rVV5	33283	73566	1.13%	0.116%

LSC Area Percent Report

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Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

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-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.494	996	998	1000	rVV	263573	234682	3.59%	0.370%
36	13.539	1000	1002	1007	rVB5	40206	100562	1.54%	0.159%
37	13.745	1016	1020	1024	rBV4	40311	107244	1.64%	0.169%
38	13.871	1026	1031	1037	rBV	454293	884505	13.53%	1.395%
39	13.997	1040	1042	1045	rBV	1772367	2294384	35.09%	3.618%
40	14.191	1054	1059	1061	rBV	55810	111205	1.70%	0.175%
41	14.499	1083	1086	1095	rBV2	171936	358865	5.49%	0.566%
42	14.774	1108	1110	1115	rBV2	73911	126137	1.93%	0.199%
43	15.117	1138	1140	1142	rBV	145808	215260	3.29%	0.339%
44	15.437	1164	1168	1170	rBV	1064131	1699719	25.99%	2.680%
45	15.677	1187	1189	1192	rVB	62609	78897	1.21%	0.124%
46	15.905	1206	1209	1211	rBV	62373	98005	1.50%	0.155%
47	15.962	1211	1214	1217	rBV2	54221	131472	2.01%	0.207%
48	17.243	1322	1326	1331	rVB2	65456	142906	2.19%	0.225%
49	17.414	1337	1341	1345	rBV5	61898	198178	3.03%	0.312%
50	17.928	1382	1386	1391	rVB5	28873	78373	1.20%	0.124%
51	19.346	1506	1510	1515	rVB6	24821	80593	1.23%	0.127%

Sum of corrected areas: 63420901

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Misc :
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Instrument : BNA_F
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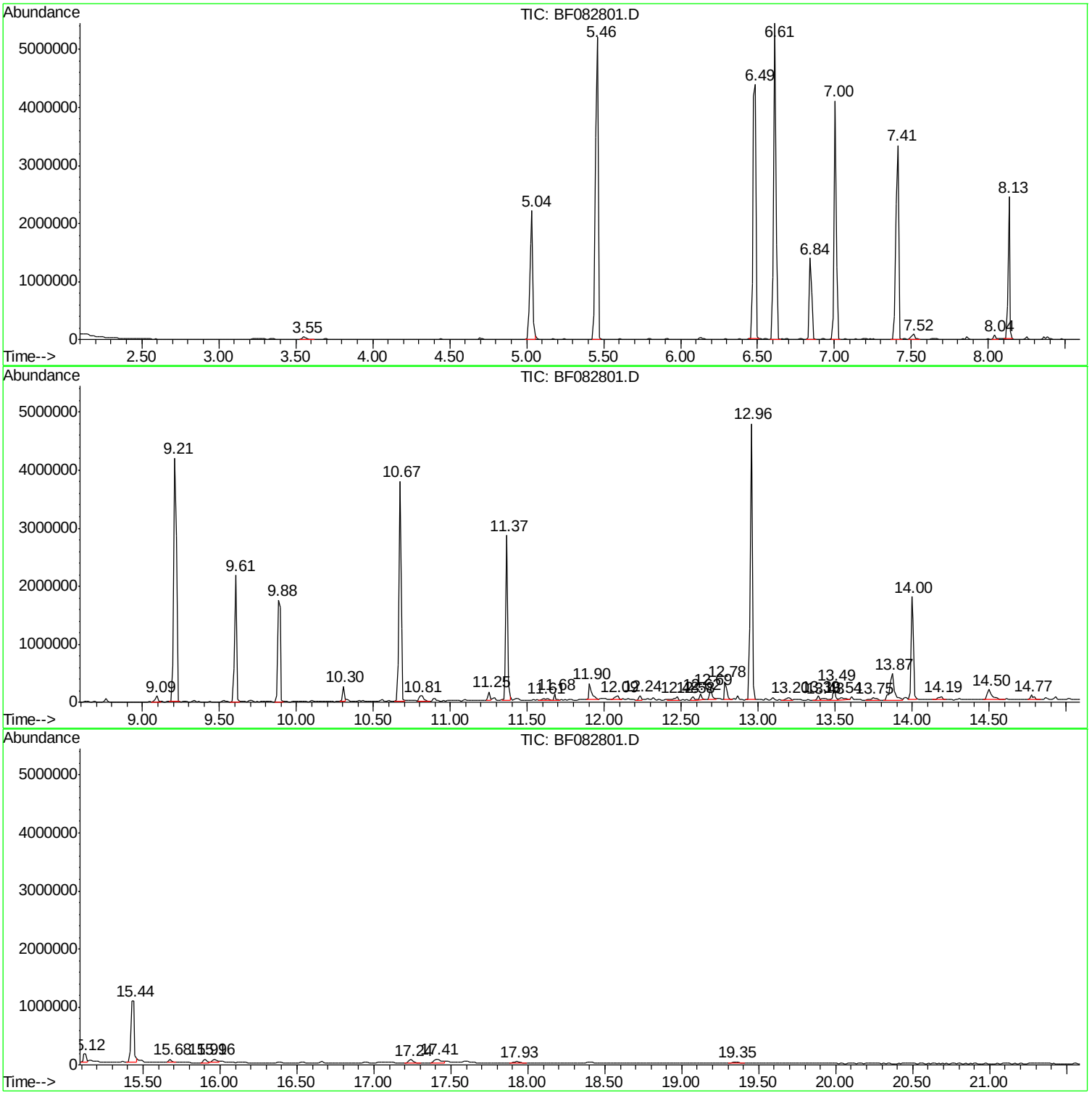
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082801.D
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Operator : UM/IZ
Sample : G4246-05
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Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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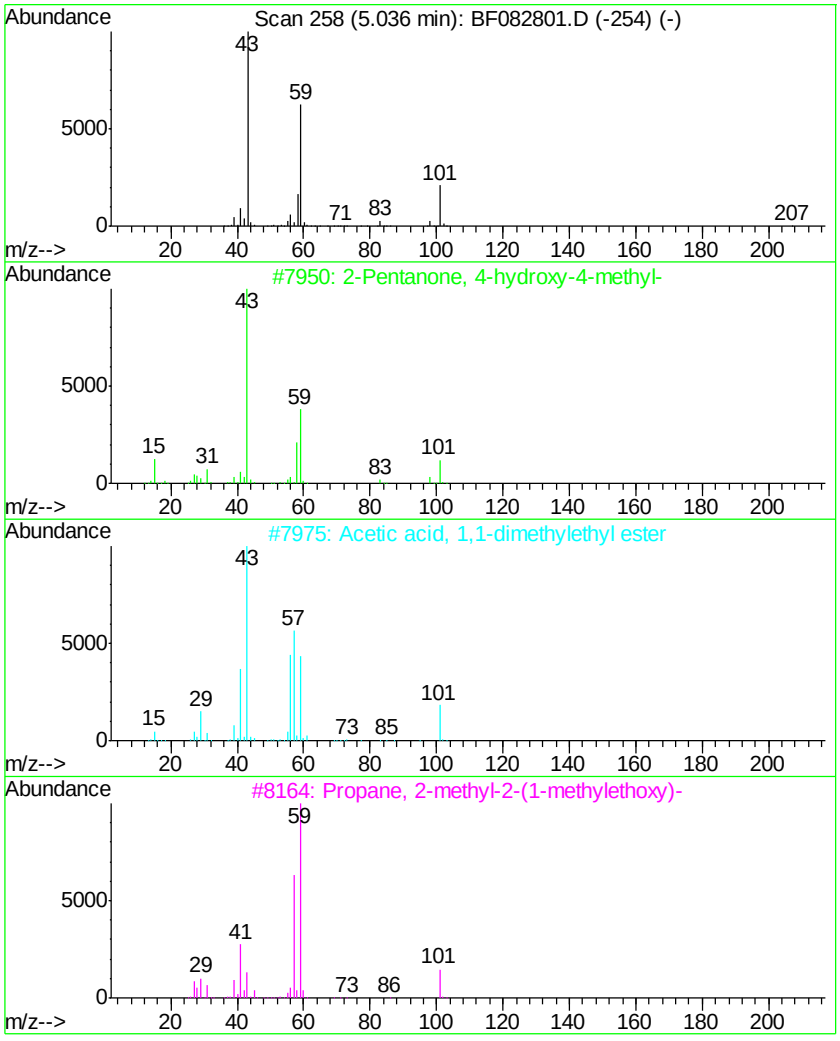
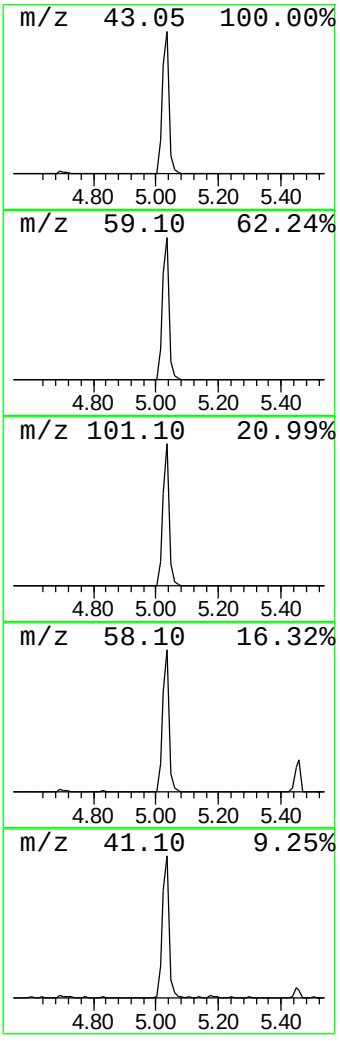
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	41.73 ng	3215000	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
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Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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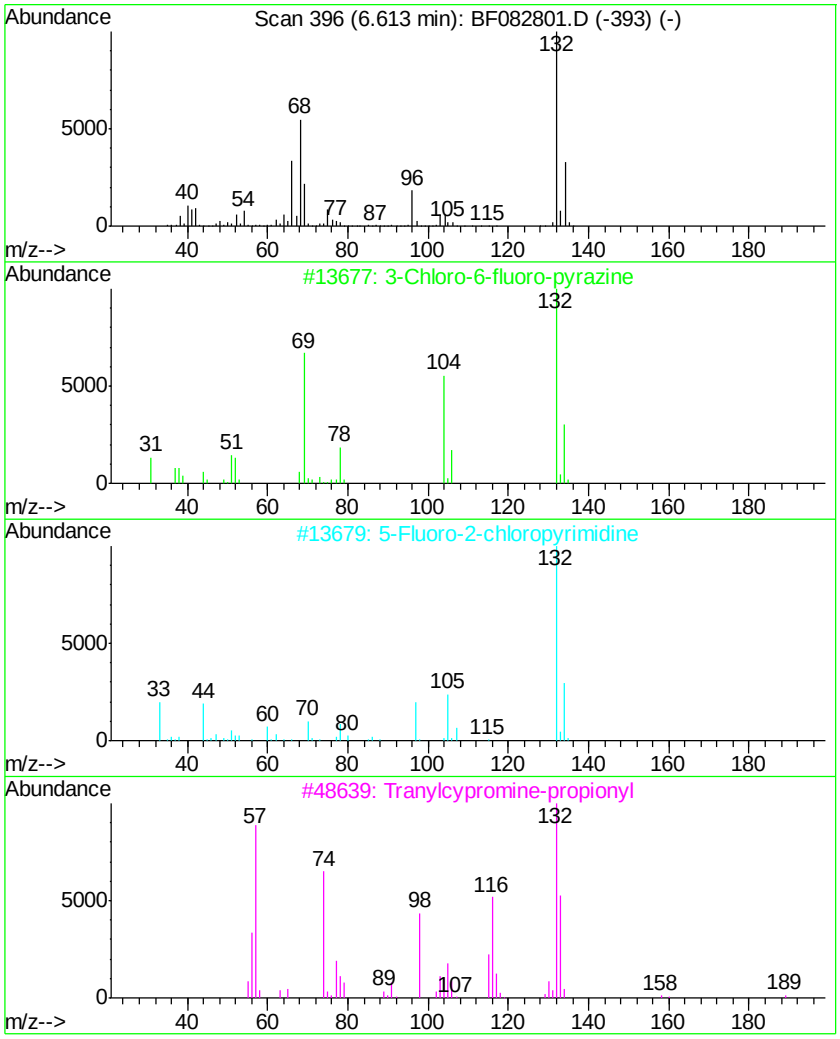
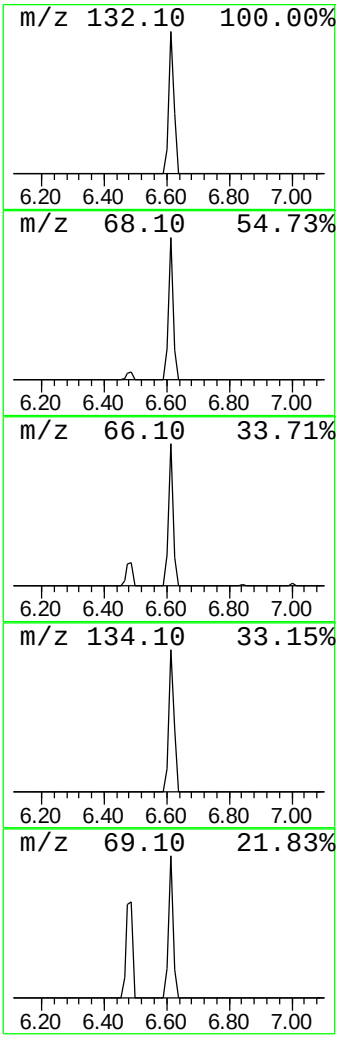
Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	72.56 ng	5590170	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082801.D
Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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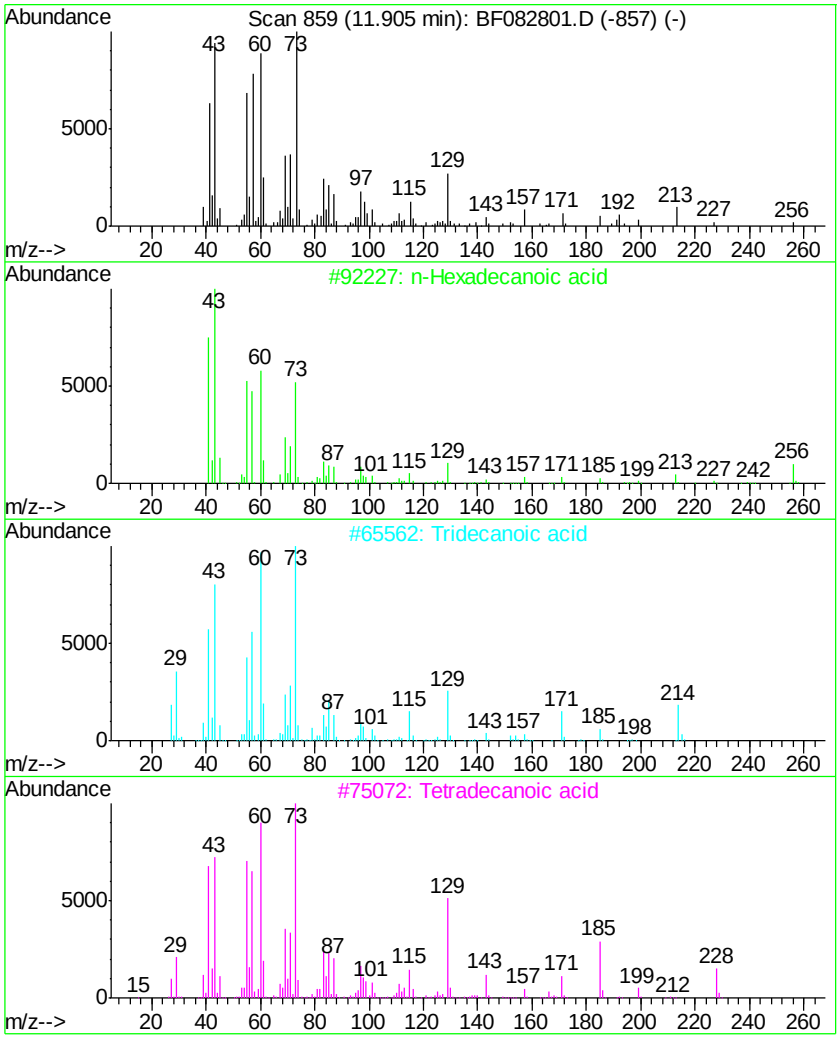
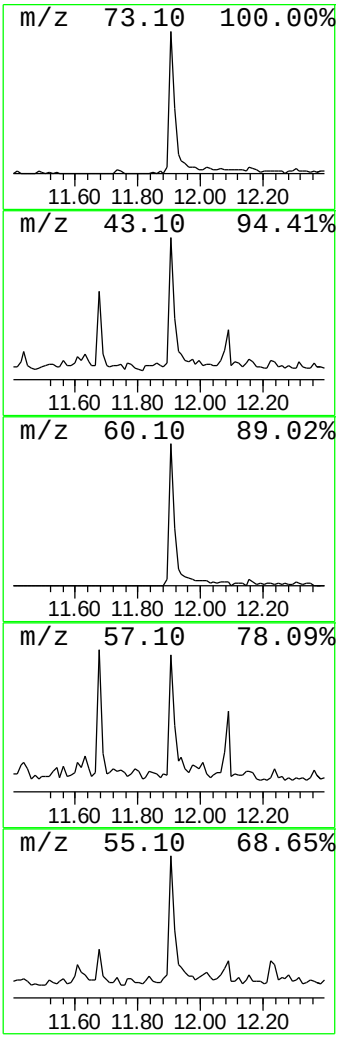
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.34 ng	415573	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Data File : BF082801.D
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Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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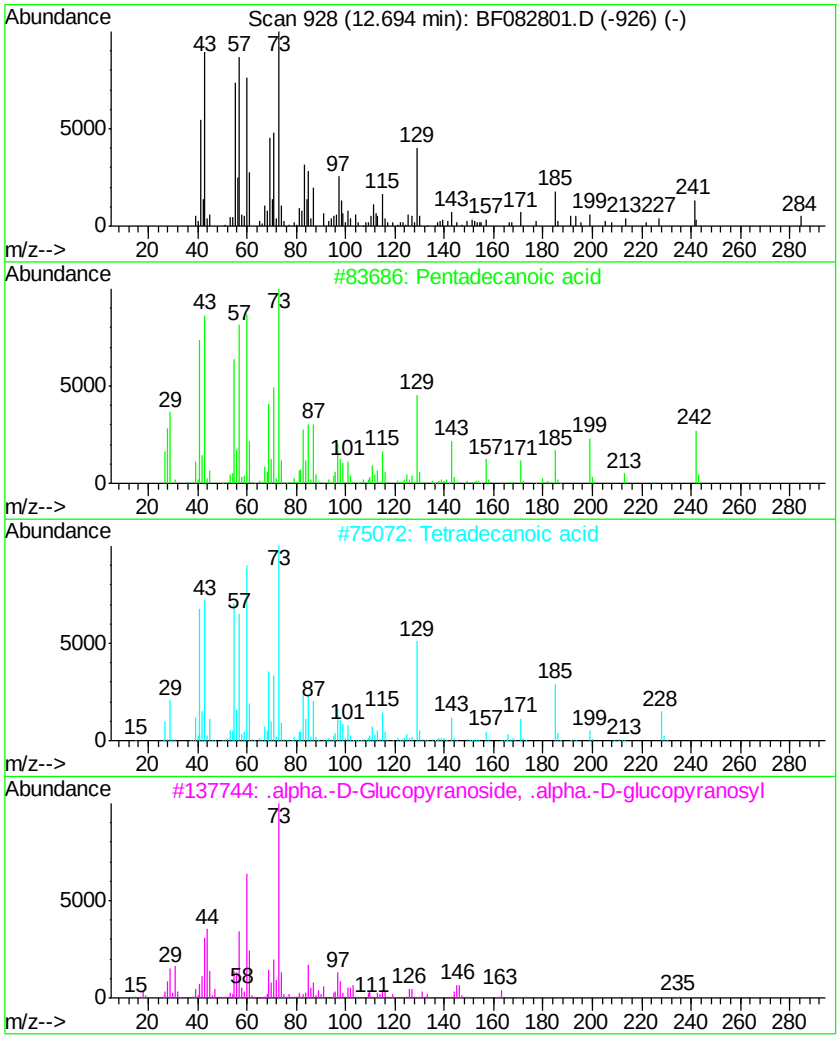
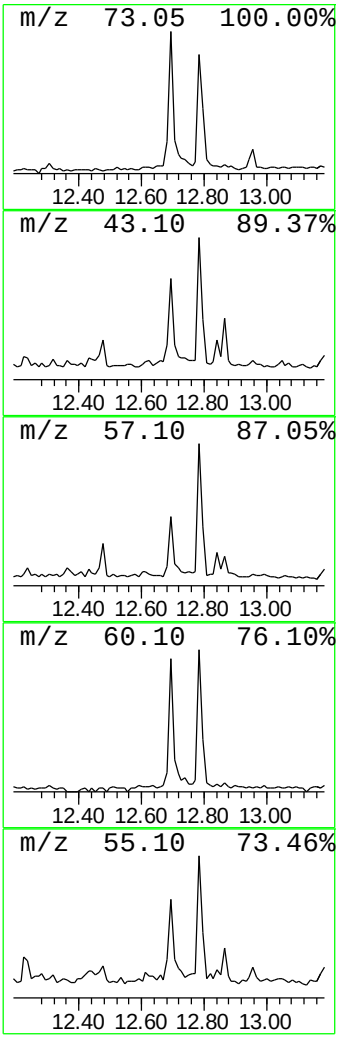
Peak Number 5 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.06 ng	236671	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	18
5	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	11





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Data File : BF082801.D
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Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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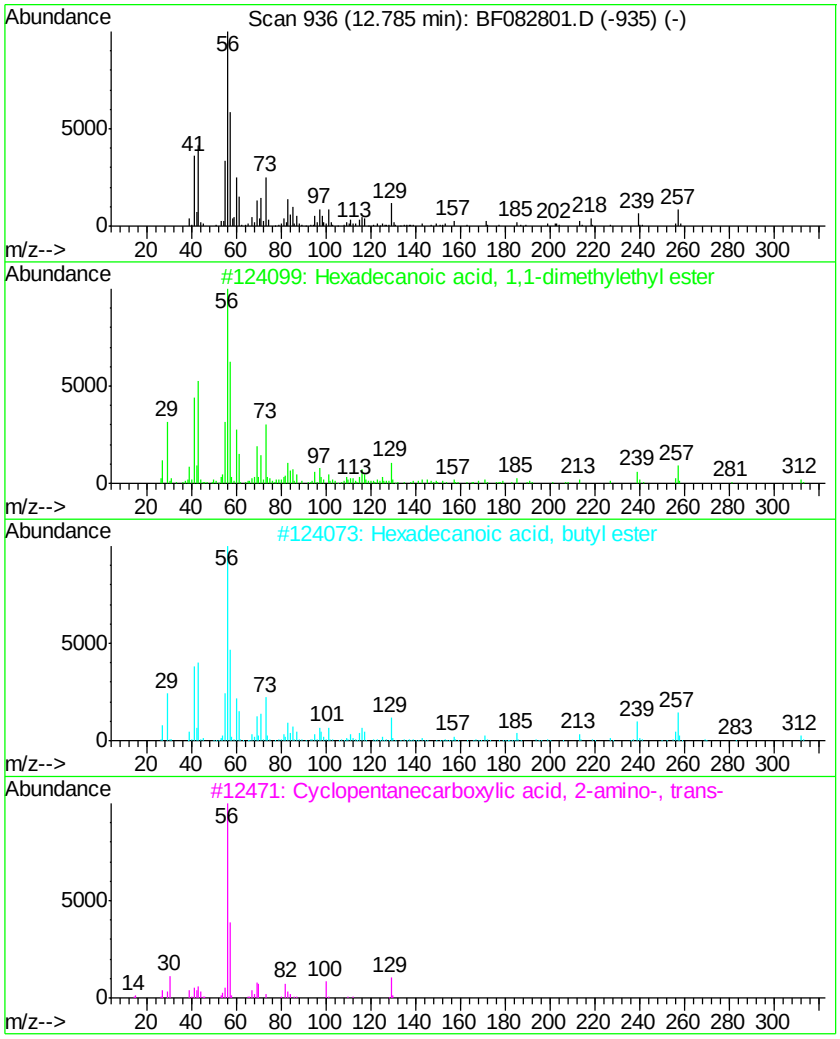
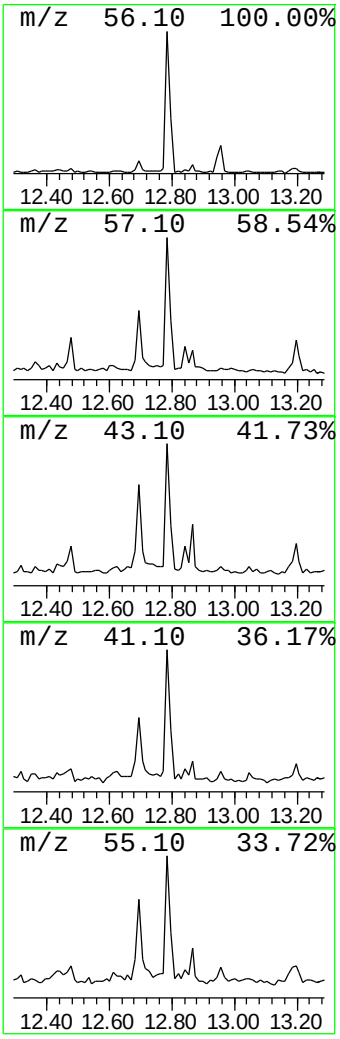
Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	3.22 ng	369966	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38





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Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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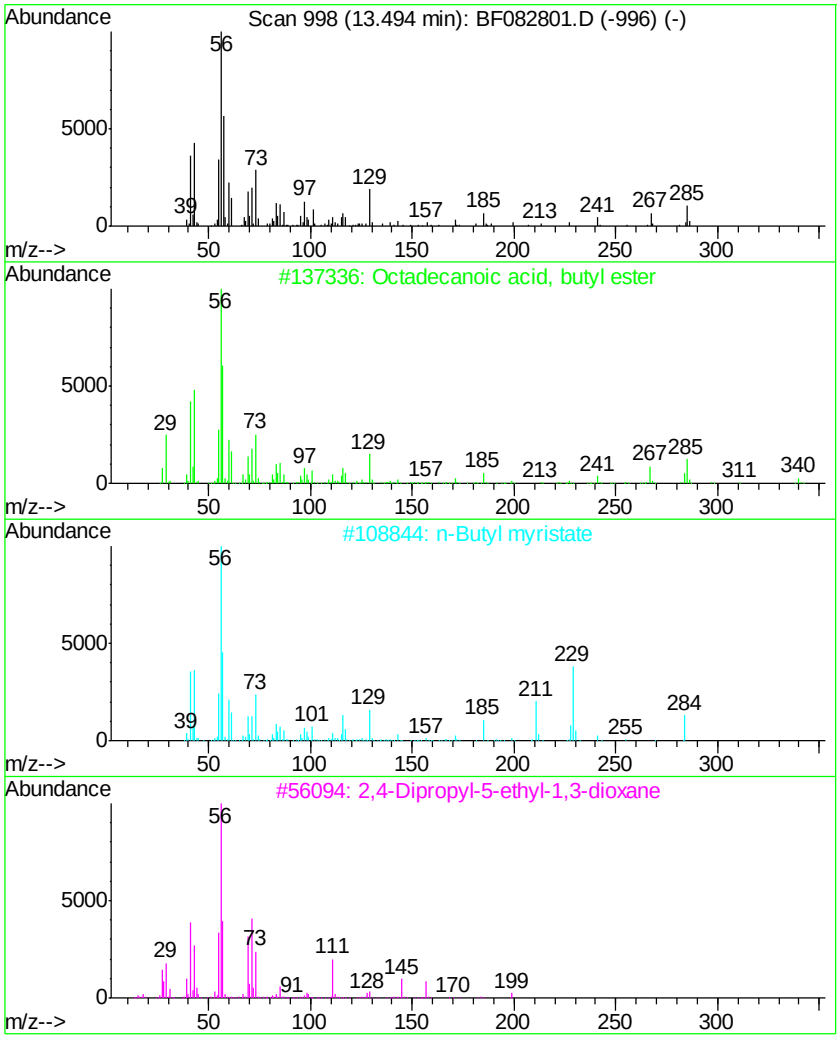
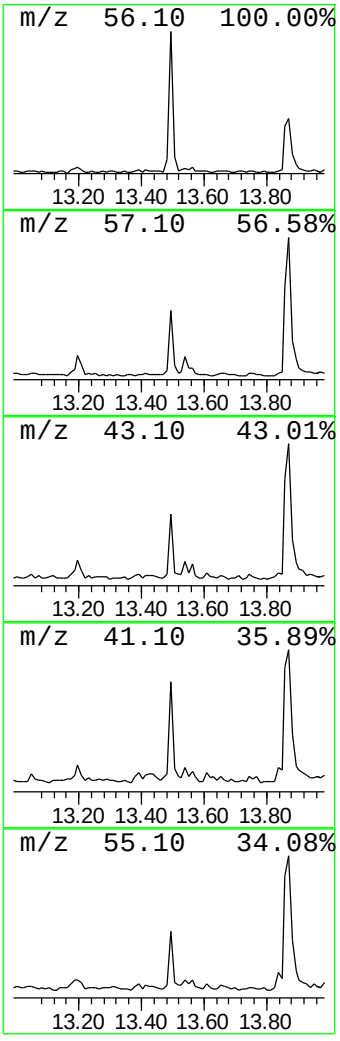
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.05 ng	234682	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	72
3	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47
4	Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	43
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38





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Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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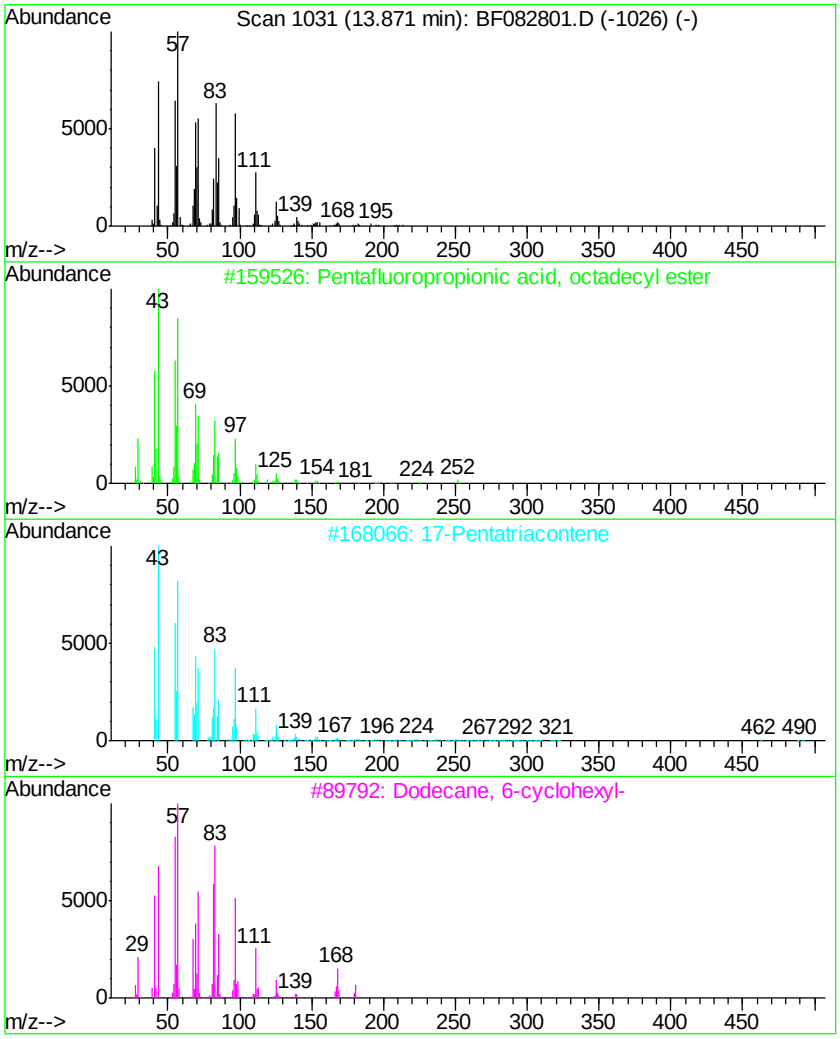
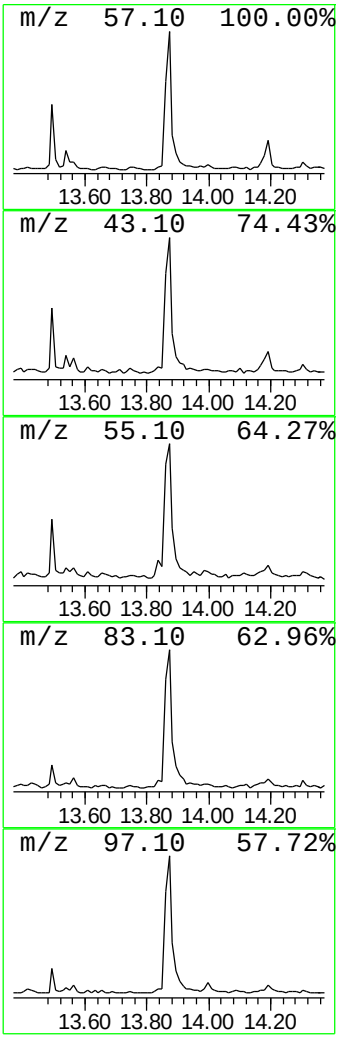
Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.71 ng	884505	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	90
3	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	86
4	1-Pentadecanol	228	C15H32O	000629-76-5	76
5	1-Nonadecene	266	C19H38	018435-45-5	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082801.D
Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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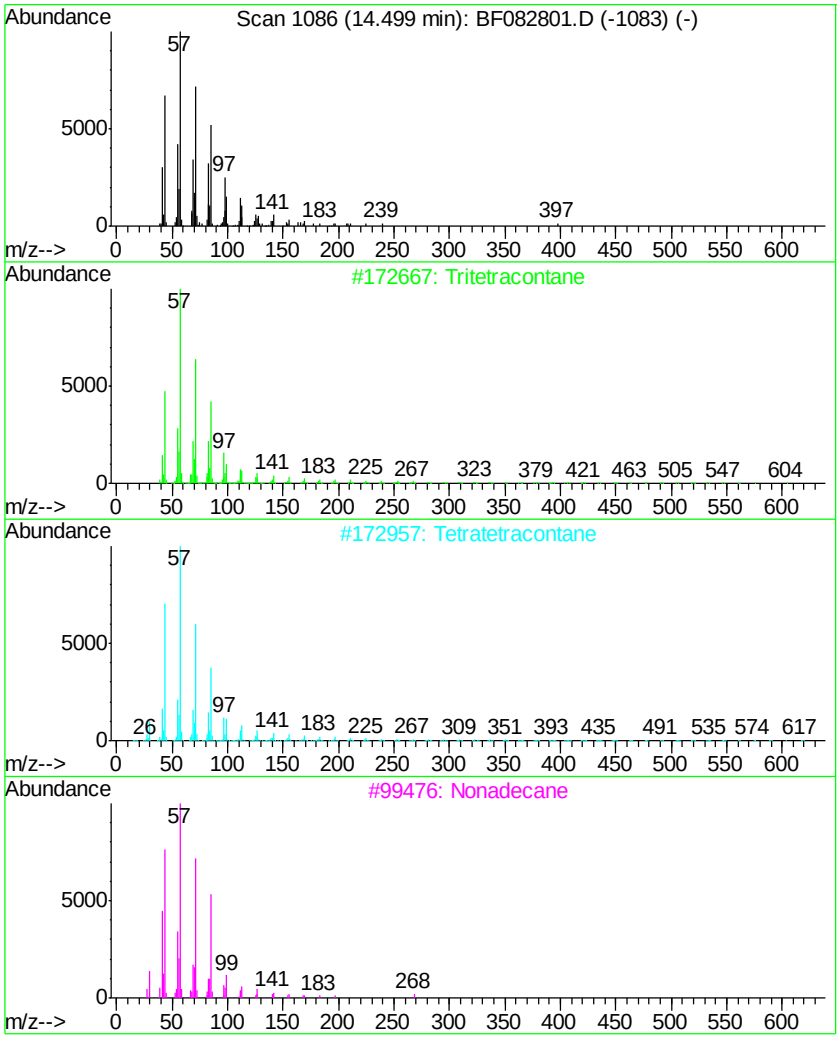
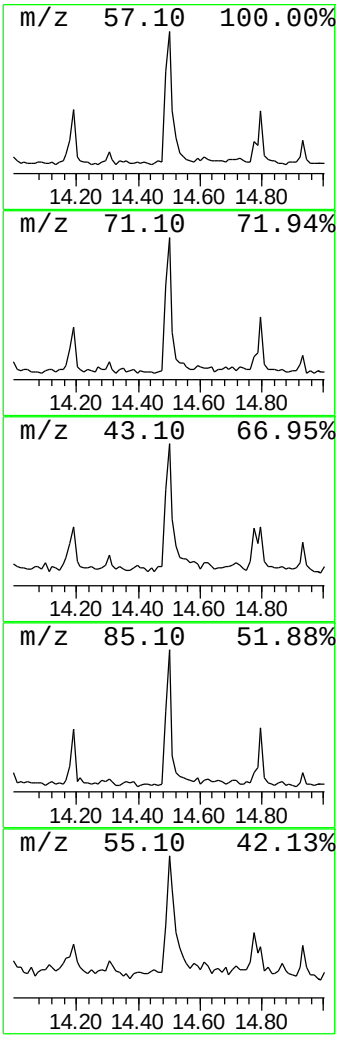
Peak Number 9 Tritetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	3.13 ng	358865	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	Nonadecane	268	C19H40	000629-92-5	68
4	Tetradecane	198	C14H30	000629-59-4	62
5	Octadecane	254	C18H38	000593-45-3	62





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Data File : BF082801.D
Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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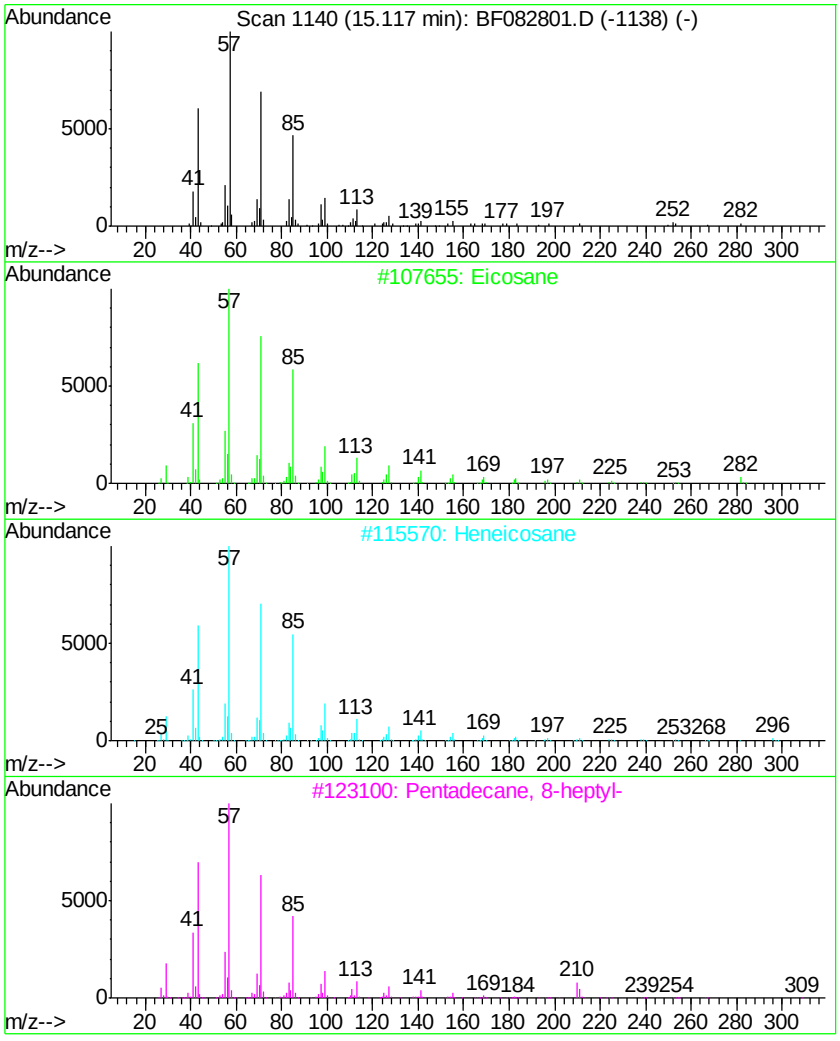
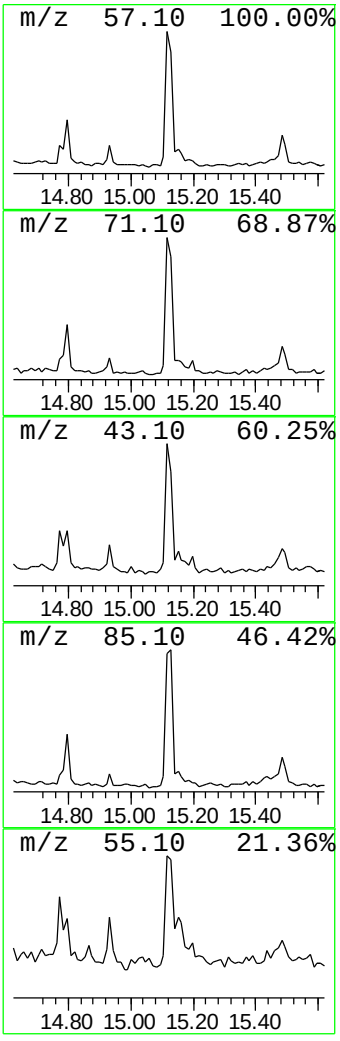
Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	2.53 ng	215260	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4	Nonacosane	408	C29H60	000630-03-5	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082801.D
Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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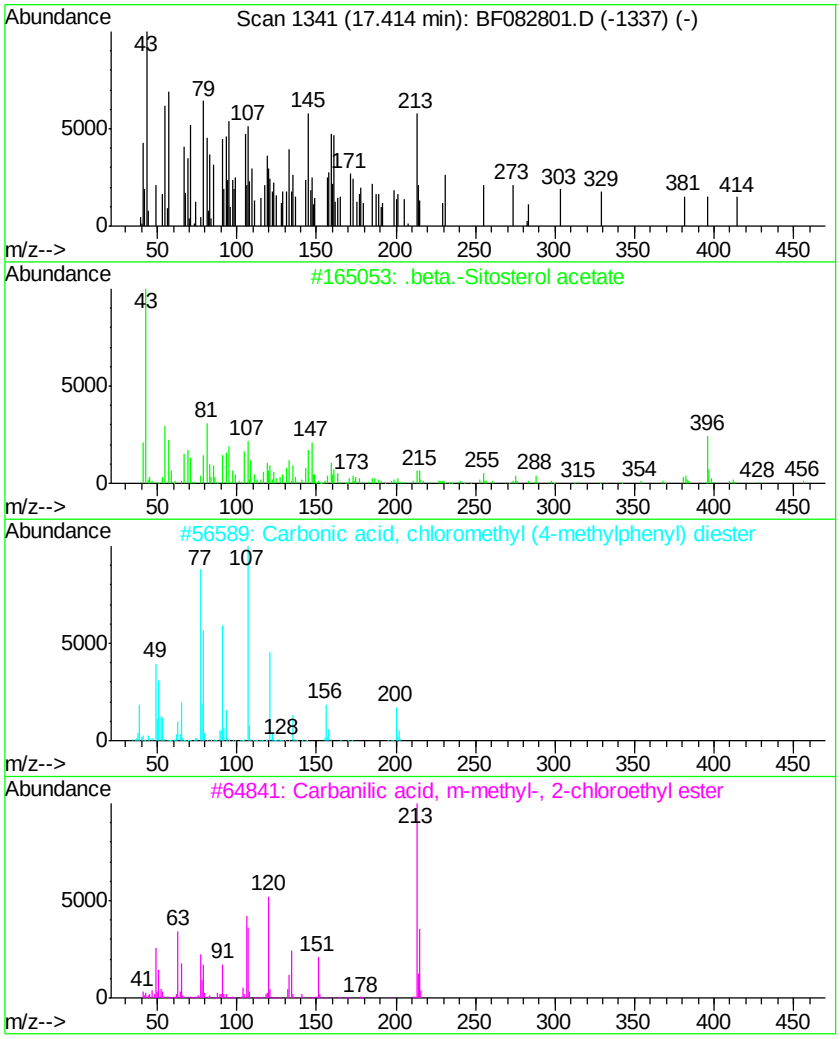
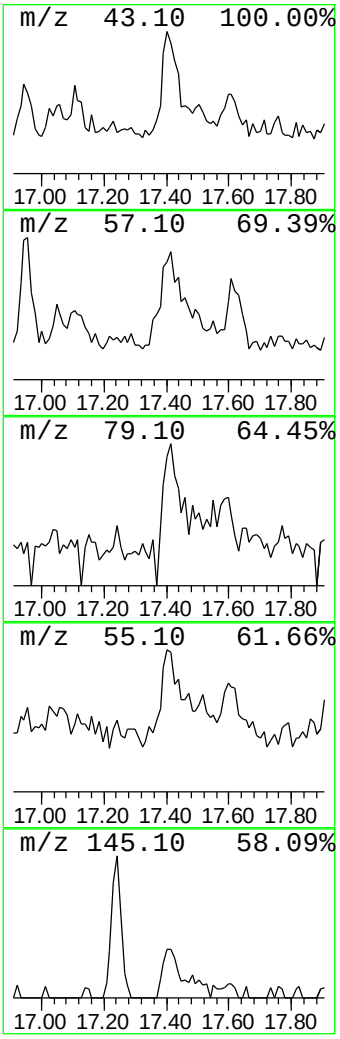
Peak Number 11 unknown17.41 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	2.33 ng	198178	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	22
2	Carbonic acid, chloromethyl (4-m...	200	C9H9ClO3	132905-79-4	18
3	Carbanilic acid, m-methyl-, 2-ch...	213	C10H12ClNO2	032508-30-8	12
4	5-O-Tolylcarbamoyl-3H-imidazole-...	273	C14H15N3O3	313251-31-9	11
5	2-Chloroethyl isopropyl sulfide	138	C5H11ClS	004303-41-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
Data File : BF082801.D
Acq On : 7 Nov 2015 10:36
Operator : UM/IZ
Sample : G4246-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	5.04	41.7	ng	3215000	1	6.84	1540950	20.0
unknown6.61	6.61	72.6	ng	5590170	1	6.84	1540950	20.0
n-Hexadecanoic acid	11.90	3.3	ng	415573	4	11.37	2485610	20.0
Pentadecanoic acid	12.69	2.1	ng	236671	5	14.00	2294380	20.0
Hexadecanoic acid...	12.79	3.2	ng	369966	5	14.00	2294380	20.0
Octadecanoic acid...	13.49	2.0	ng	234682	5	14.00	2294380	20.0
Pentafluoropropio...	13.87	7.7	ng	884505	5	14.00	2294380	20.0
Tritetracontane	14.50	3.1	ng	358865	5	14.00	2294380	20.0
Eicosane	15.12	2.5	ng	215260	6	15.44	1699720	20.0
unknown17.41	17.41	2.3	ng	198178	6	15.44	1699720	20.0