LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

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-BF032217.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	4.110	373	378	387	rBV	405829	576277	10.87%	1.118%
2	4.498	438	444	447	rBV	4192493	4661558	87.90%	9.046%
3	5.563	618	625	628	rBV	3750566	4937158	93.10%	9.581%
4	5.710	644	650	653	rBV	4326118	4891059	92.23%	9.491%
5	5.957	688	692	696	rBV	1083013	1023307	19.30%	1.986%
6	6.140	718	723	727	rBV	3585443	3831687	72.25%	7.435%
7	6.610	796	803	806	rBV	2675790	3233110	60.96%	6.274%
8	6.734	817	824	831	rBV2	34933	53412	1.01%	0.104%
9	7.463	943	948	952	rBV	1486508	1415123	26.68%	2.746%
10	8.645	1146	1149	1152	rBV	76106	72686	1.37%	0.141%
11	8.792	1164	1174	1177	rBV	4702804	5303324	100.00%	10.291%
12	8.875	1182	1188	1191	rBV3	41135	59855	1.13%	0.116%
13	8.945	1197	1200	1205	rVB	124132	129007	2.43%	0.250%
14	9.198	1241	1243	1246	rVB2	61426	57771	1.09%	0.112%
15	9.257	1249	1253	1255	rVV	207900	230857	4.35%	0.448%
16	9.281	1255	1257	1262	rVV	400328	333270	6.28%	0.647%
17	9.433	1279	1283	1287	rBV2	64909	69140	1.30%	0.134%
18	9.522	1291	1298	1301	rVV	193381	246197	4.64%	0.478%
19	9.598	1305	1311	1317	rVV2	3042570	3919920	73.91%	7.607%
20	9.669	1320	1323	1331	rVB3	166755	224989	4.24%	0.437%
21	9.786	1338	1343	1347	rBV	400697	418671	7.89%	0.812%
22	9.828	1347	1350	1353	rVB2	115273	137083	2.58%	0.266%
23	10.192	1407	1412	1416	rBV	130756	124200	2.34%	0.241%
24	10.469	1453	1459	1461	rBV	49350	74619	1.41%	0.145%
25	10.580	1472	1478	1482	rBV	2449806	2797637	52.75%	5.429%
26	10.780	1508	1512	1514	rBV	138558	154059	2.90%	0.299%
27	10.798	1514	1515	1520	rVB	76573	53883	1.02%	0.105%
28	11.198	1577	1583	1590	rVB3	104303	127927	2.41%	0.248%
29	11.333	1602	1606	1609	rBV	103118	97068	1.83%	0.188%
30	11.433	1618	1623	1625	rBV	1151575	1216615	22.94%	2.361%
31	11.457	1625	1627	1631	rVB	128056	111040	2.09%	0.215%
32	11.863	1689	1696	1701	rVB3	47946	77809	1.47%	0.151%
33	12.186	1747	1751	1754	rBV3	48279	59186	1.12%	0.115%
34	12.439	1788	1794	1797	rBV2	90824	112175	2.12%	0.218%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.921	1872	1876	1879	rBV	221224	209427	3.95%	0.406%
36	13.198	1918	1923	1927	rBV	194640	213308	4.02%	0.414%
37	13.410	1953	1959	1963	rBV	2931137	3522770	66.43%	6.836%
38	13.739	2012	2015	2022	rVB3	36869	56398	1.06%	0.109%
39	14.374	2117	2123	2127	rBV	3404763	4050126	76.37%	7.859%
40	14.563	2151	2155	2166	rVB2	179747	243299	4.59%	0.472%
41	14.686	2170	2176	2179	rBV	834829	1025233	19.33%	1.989%
42	14.710	2179	2180	2185	rVB	84600	79663	1.50%	0.155%
43	15.351	2286	2289	2296	rVB2	92157	112788	2.13%	0.219%
44	15.904	2379	2383	2386	rBV	79332	127714	2.41%	0.248%
45	16.068	2408	2411	2415	rBV3	63298	89891	1.69%	0.174%
46	16.251	2440	2442	2446	rVB	43045	53065	1.00%	0.103%
47	16.321	2449	2454	2460	rVB	633453	814601	15.36%	1.581%
48	16.857	2541	2545	2549	rBV2	66512	102931	1.94%	0.200%

Sum of corrected areas: 51532893

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
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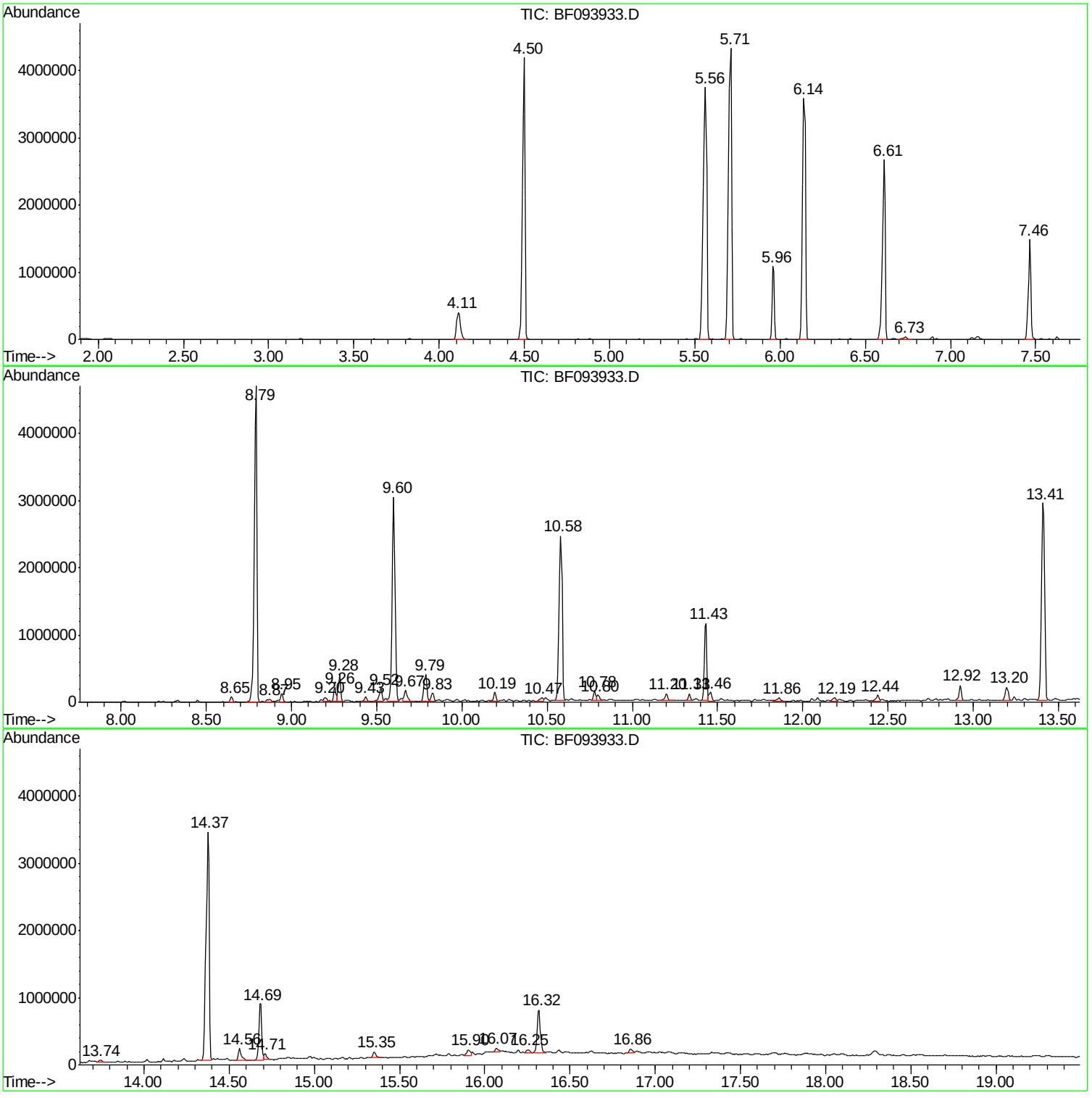
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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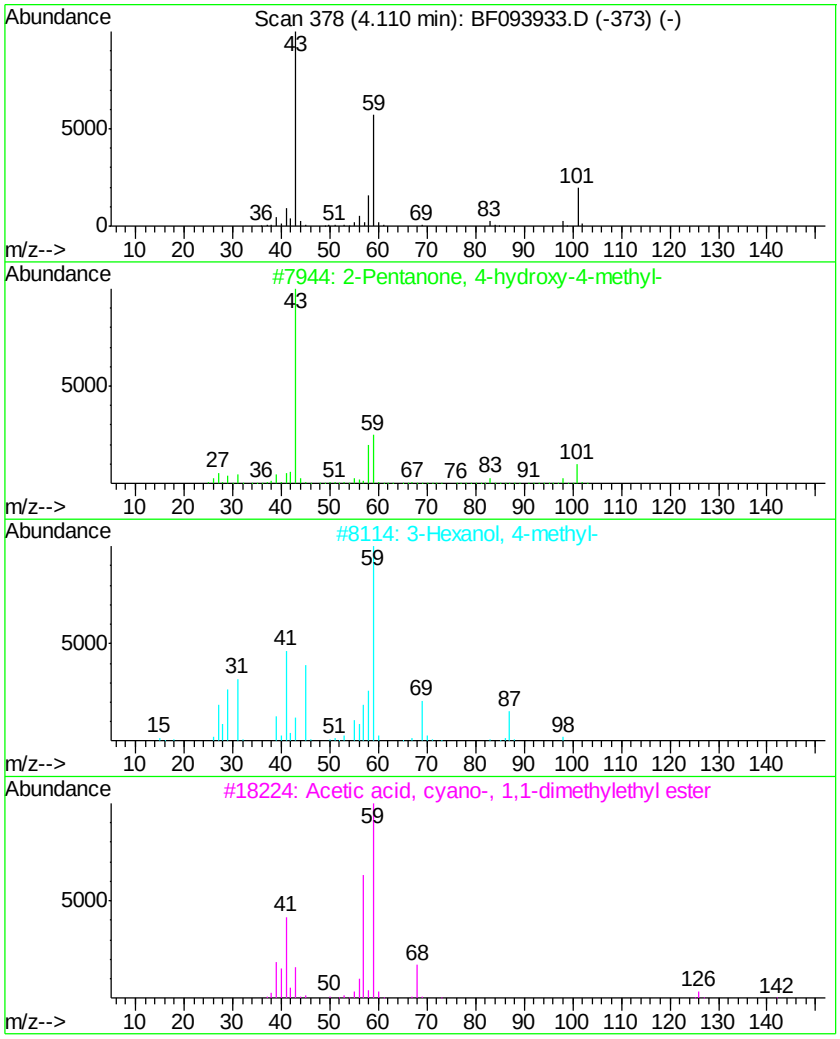
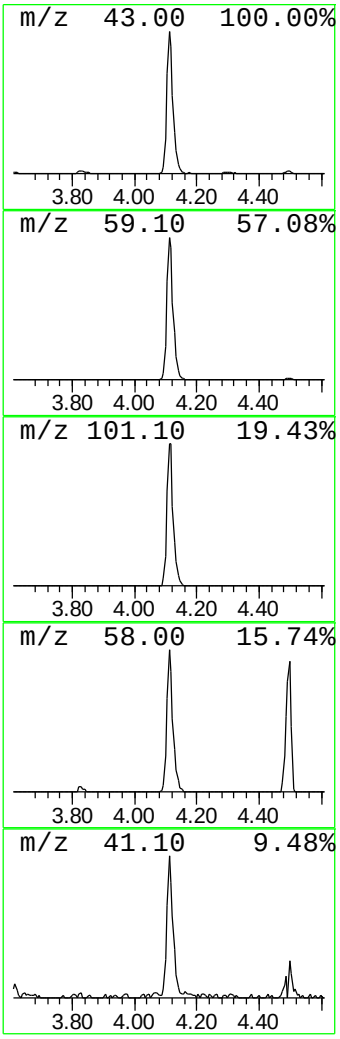
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	11.26 ng	576277	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
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Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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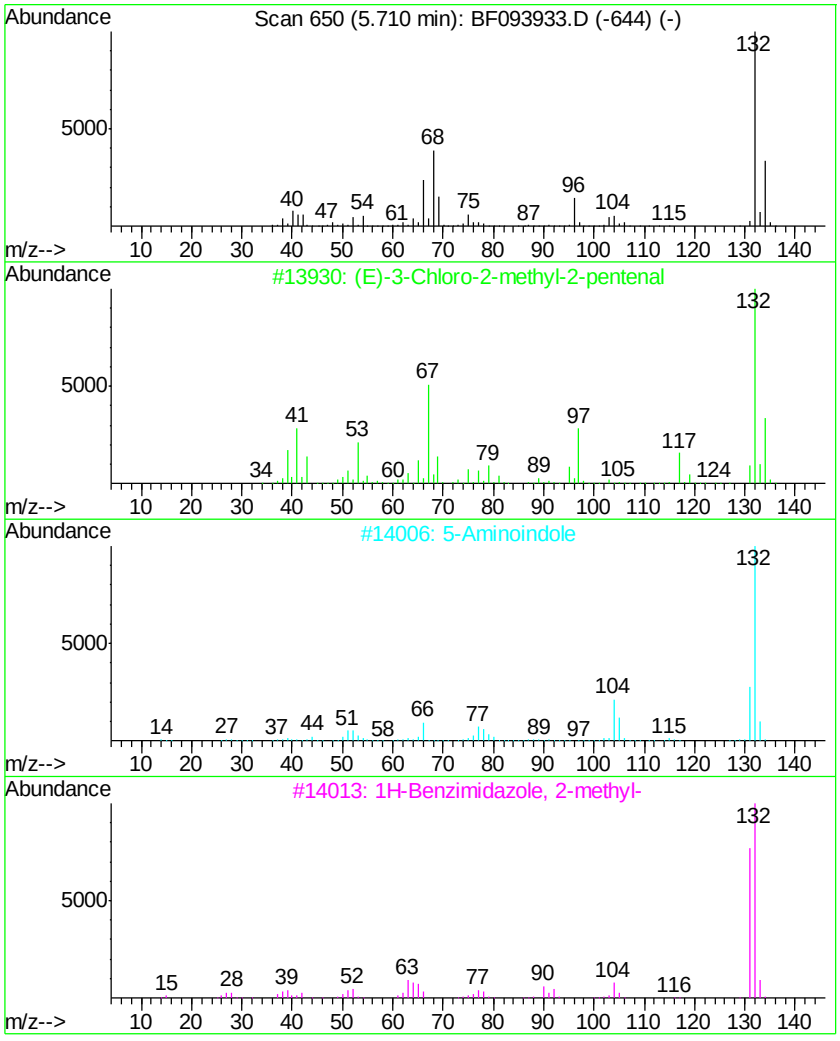
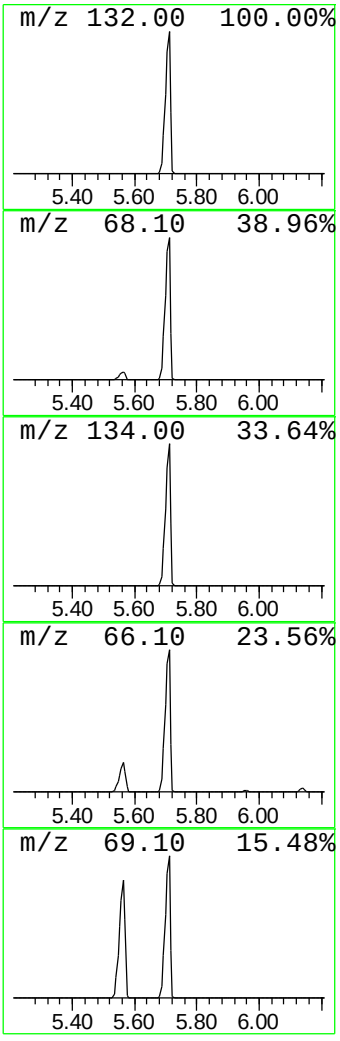
Peak Number 2 unknown5.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	95.59 ng	4891060	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
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Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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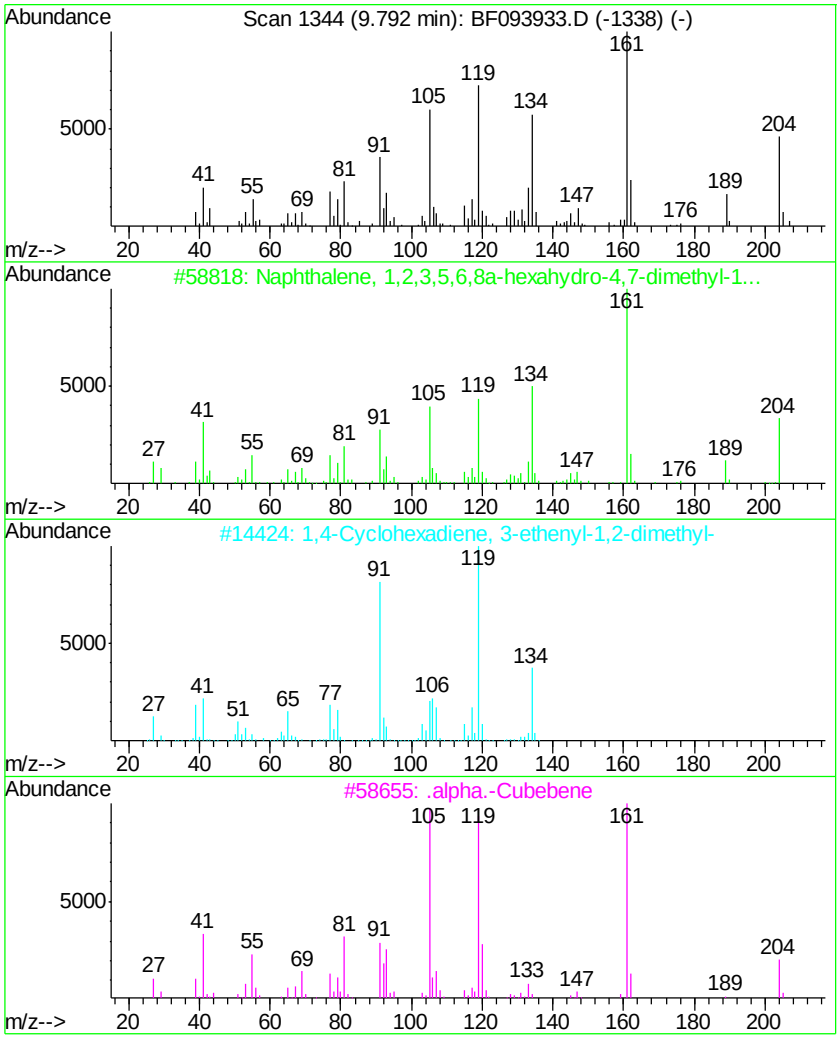
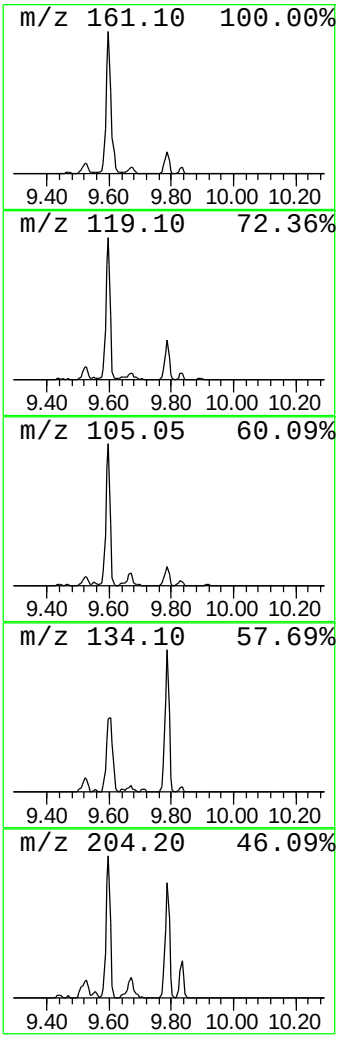
Peak Number 4 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	2.14 ng	418671	Acenaphthene-d10	9.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	97
2	1,4-Cyclohexadiene, 3-ethenyl-1,...	134	C10H14	062338-57-2	89
3	.alpha.-Cubebene	204	C15H24	017699-14-8	70
4	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	030021-74-0	60
5	Benzofuran, 2,3-dihydro-2-methyl-	134	C9H10O	001746-11-8	50





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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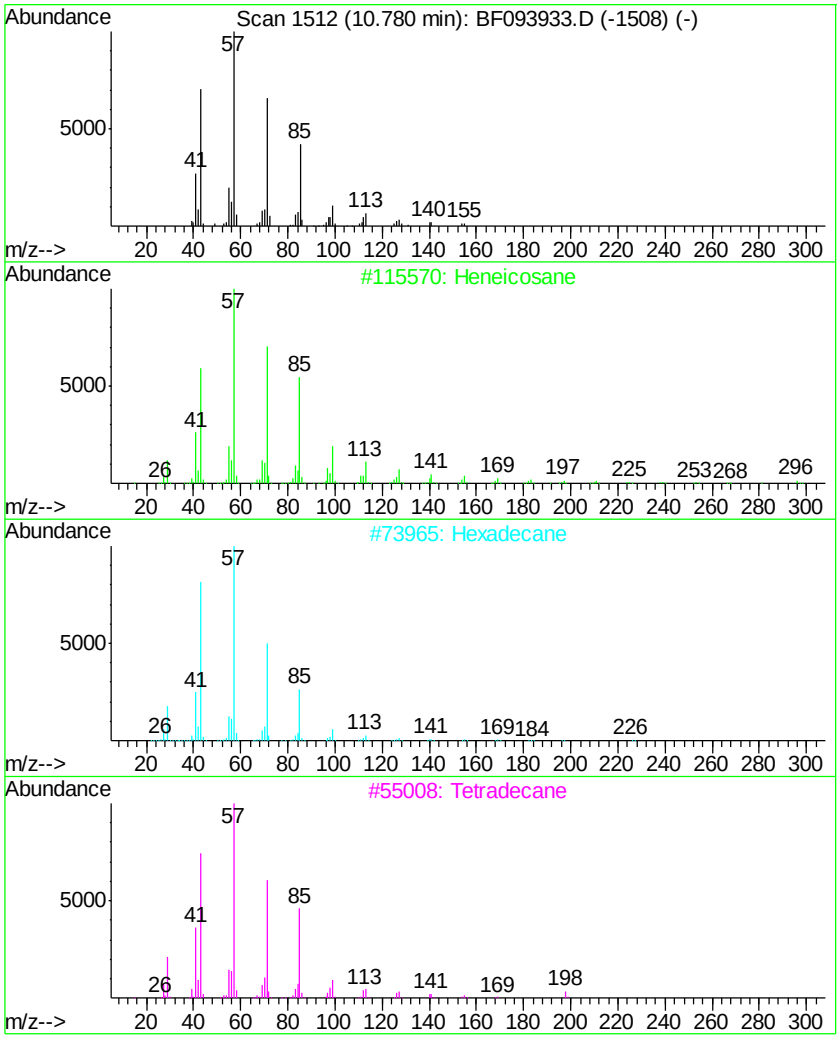
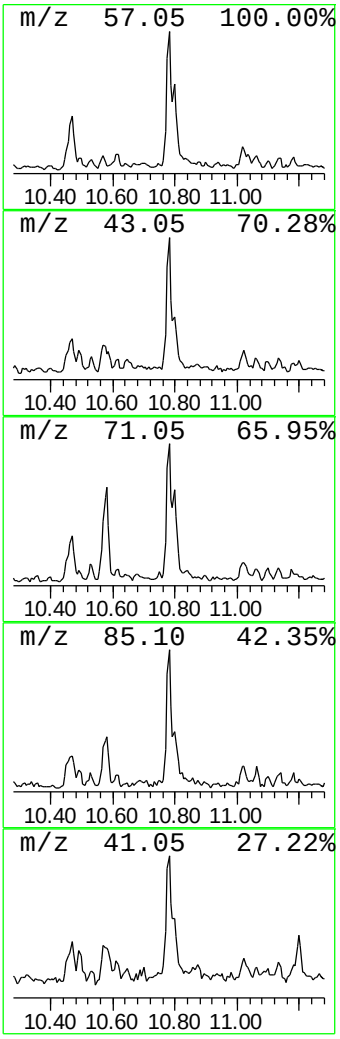
Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	2.53 ng	154059	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecane	198	C14H30	000629-59-4	87
4	Eicosane	282	C20H42	000112-95-8	86
5	Pentadecane	212	C15H32	000629-62-9	78





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
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Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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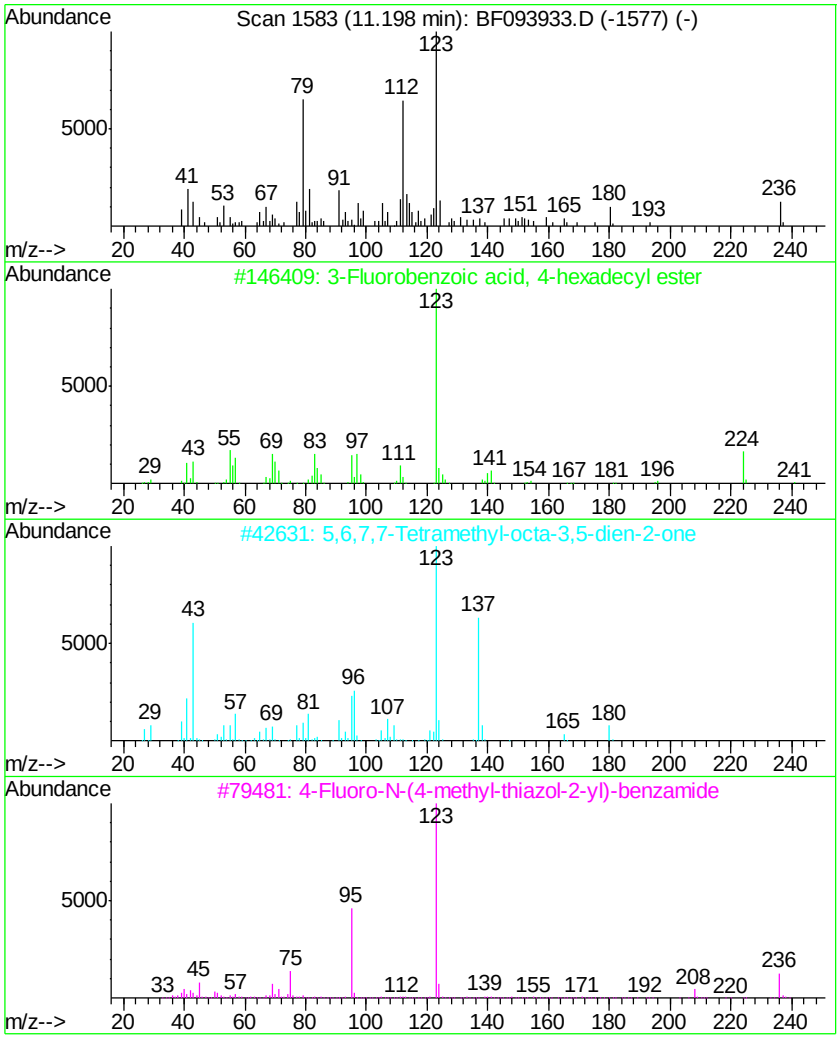
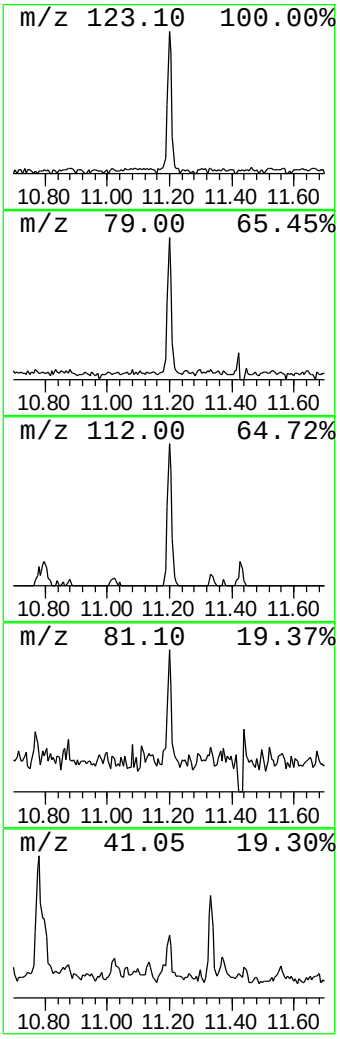
Peak Number 6 unknown11.20 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	2.10 ng	127927	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, 4-hexadecv...	364	C23H37FO2	1000283-01-7	35
2	5,6,7,7-Tetramethyl-octa-3,5-die...	180	C12H20O	1000190-70-9	35
3	4-Fluoro-N-(4-methyl-thiazol-2-y...	236	C11H9FN2OS	1000274-33-8	35
4	Phenol, 4-amino-3-methyl-	123	C7H9NO	002835-99-6	30
5	Phenol, 2-amino-4-methyl-	123	C7H9NO	000095-84-1	30





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Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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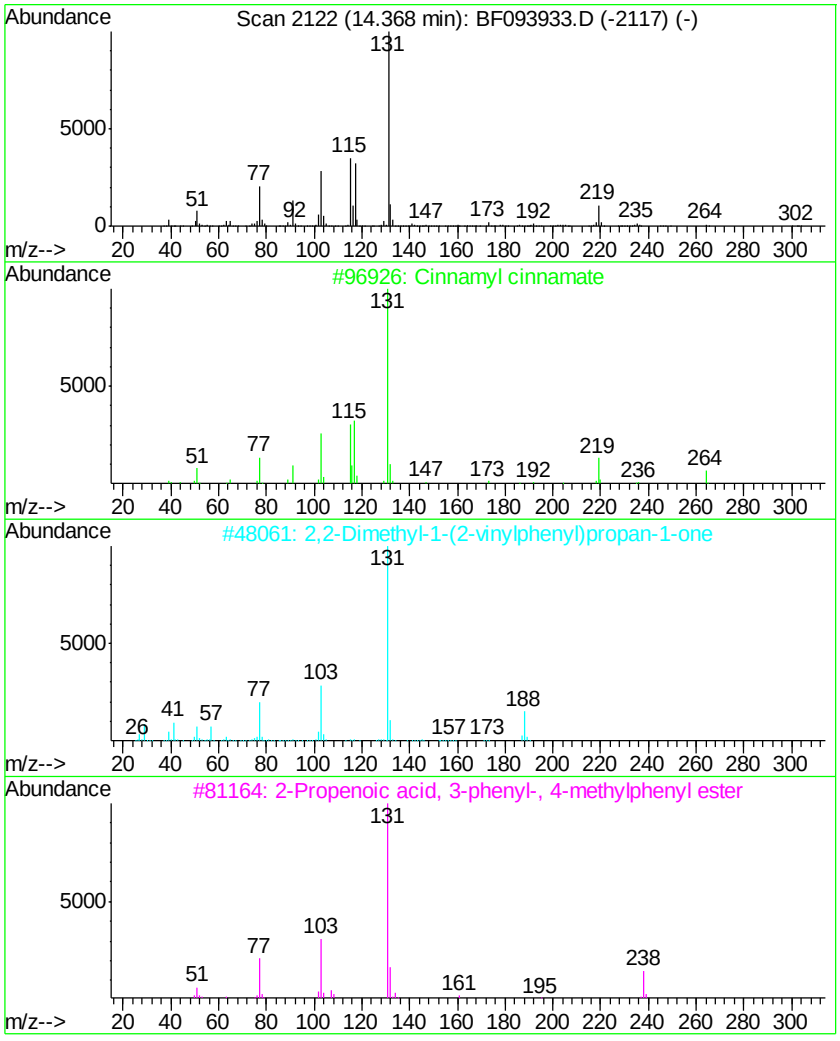
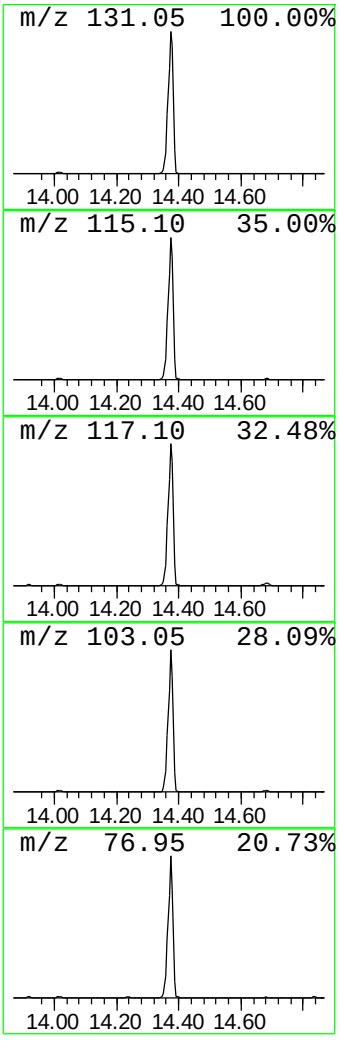
Peak Number 7 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	79.01 ng	4050130	Chrysene-d12	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3	2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	50
4	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	50
5	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	50





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Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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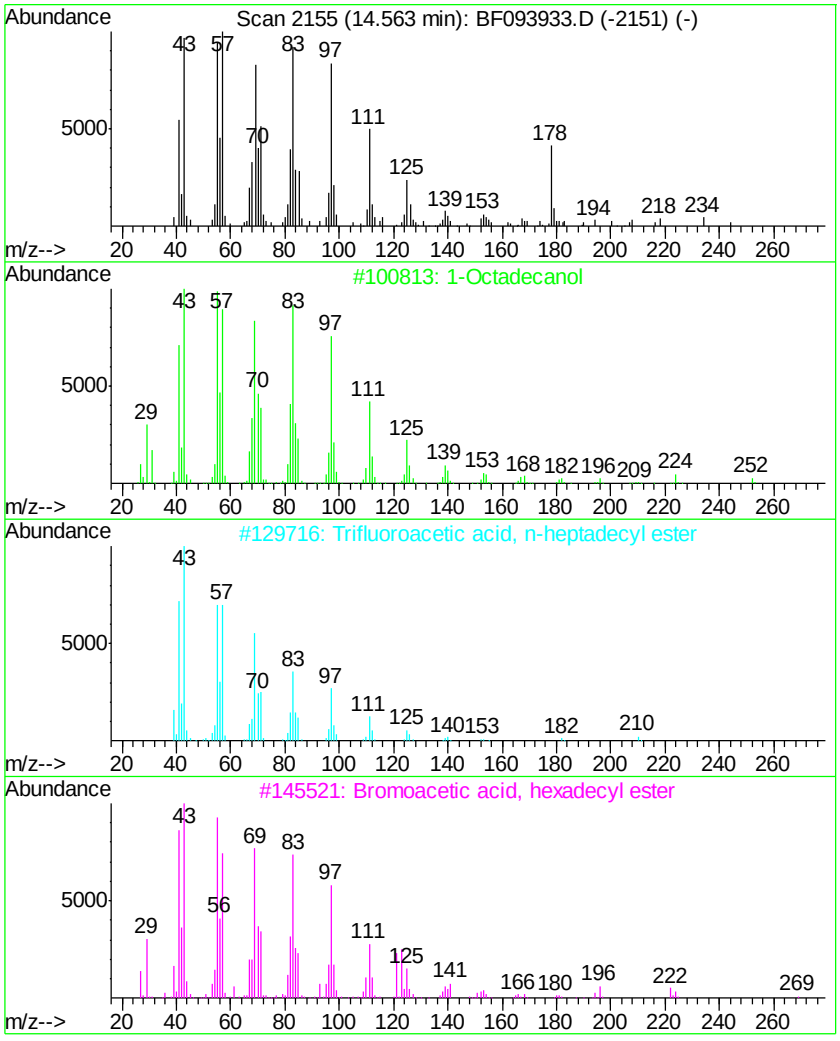
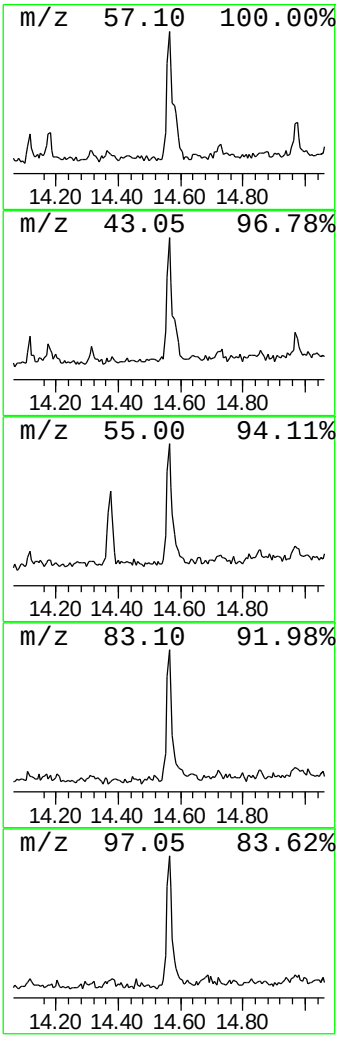
Peak Number 8 1-Octadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	4.75 ng	243299	Chrysene-d12	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	87
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	87
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
4	1-Nonadecene	266	C19H38	018435-45-5	87
5	1-Heptadecanol	256	C17H36O	001454-85-9	87





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093933.D
Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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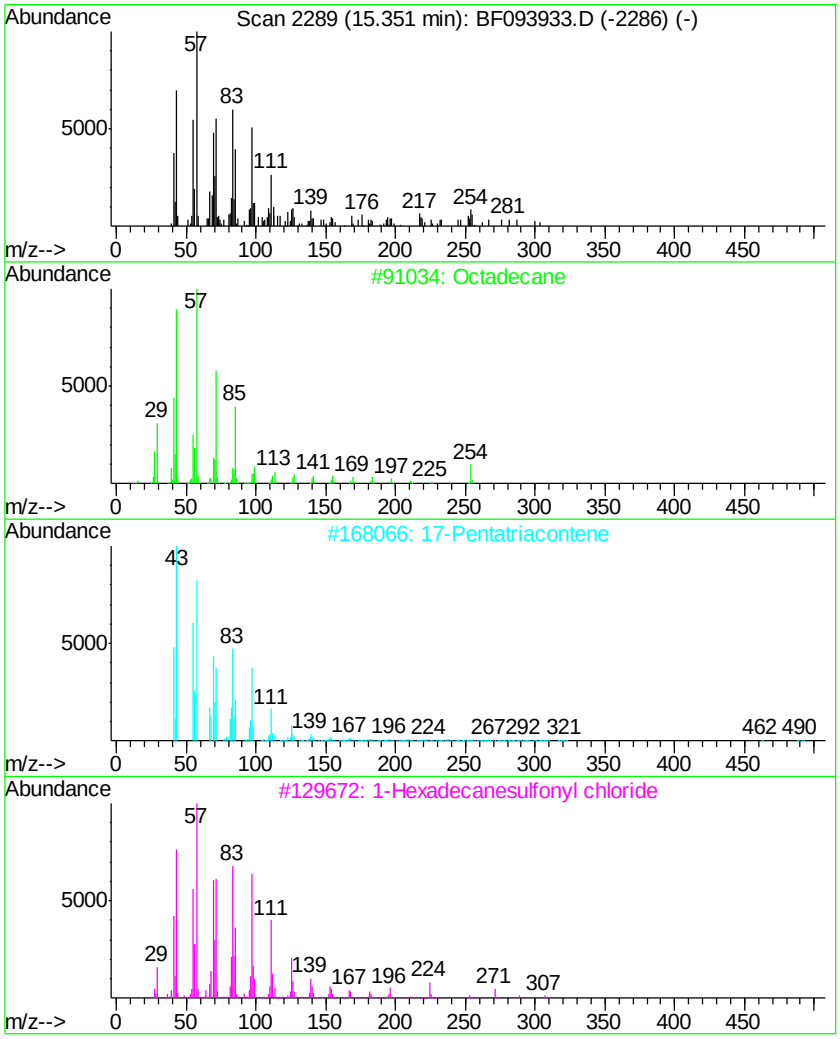
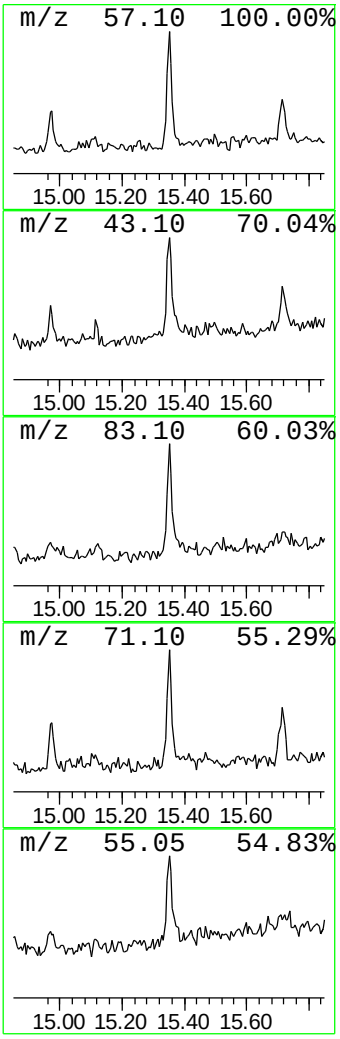
Peak Number 9 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	2.20 ng	112788	Chrysene-d12	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	89
2	17-Pentatriacontene	491	C35H70	006971-40-0	64
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	64
4	1-Octadecene	252	C18H36	000112-88-9	64
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	58





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Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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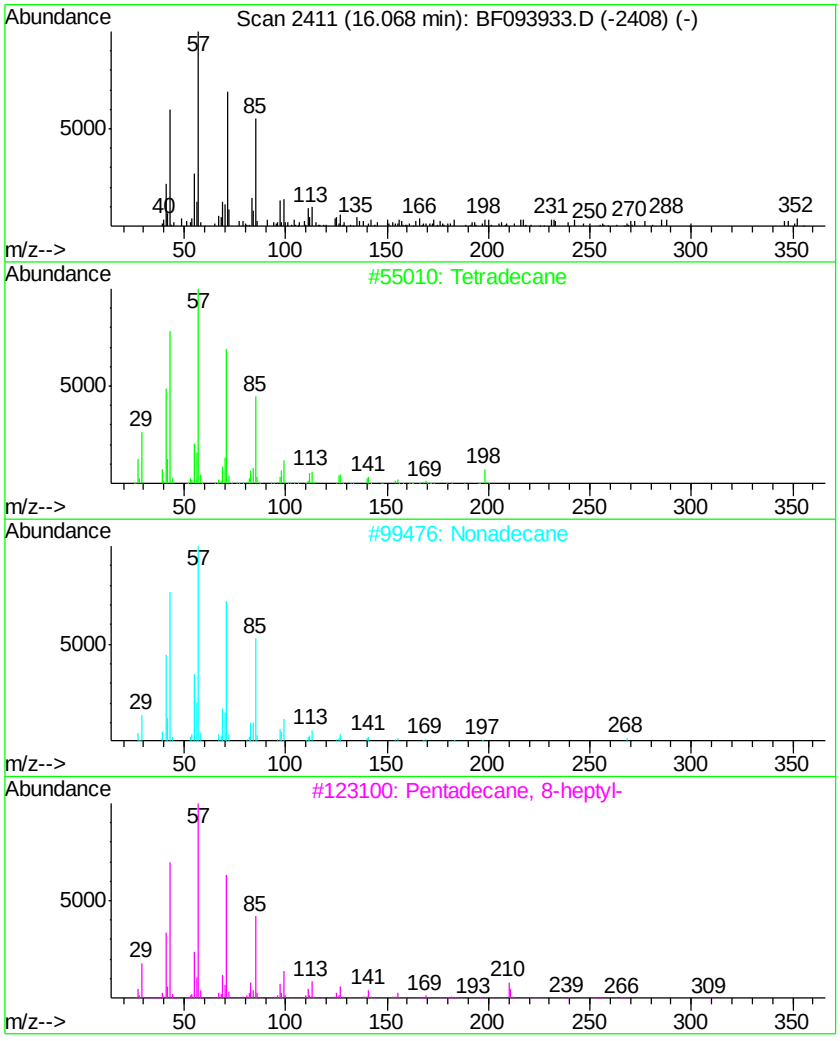
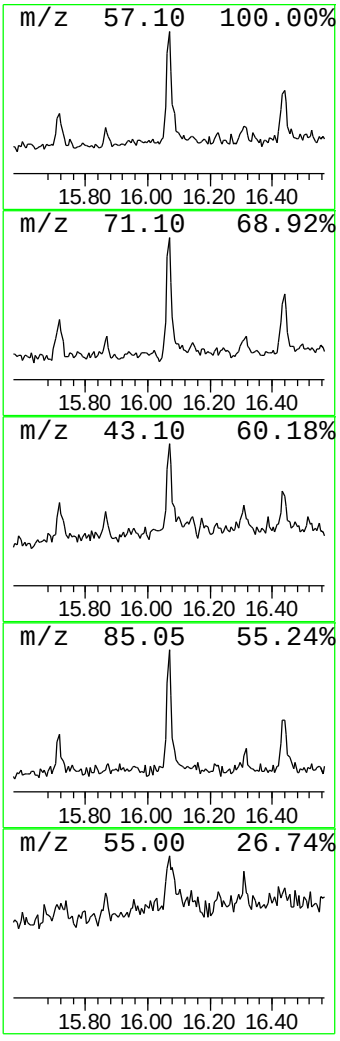
Peak Number 10 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.21 ng	89891	Perylene-d12	16.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Nonadecane	268	C19H40	000629-92-5	89
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Nonacosane	408	C29H60	000630-03-5	80





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Data File : BF093933.D
Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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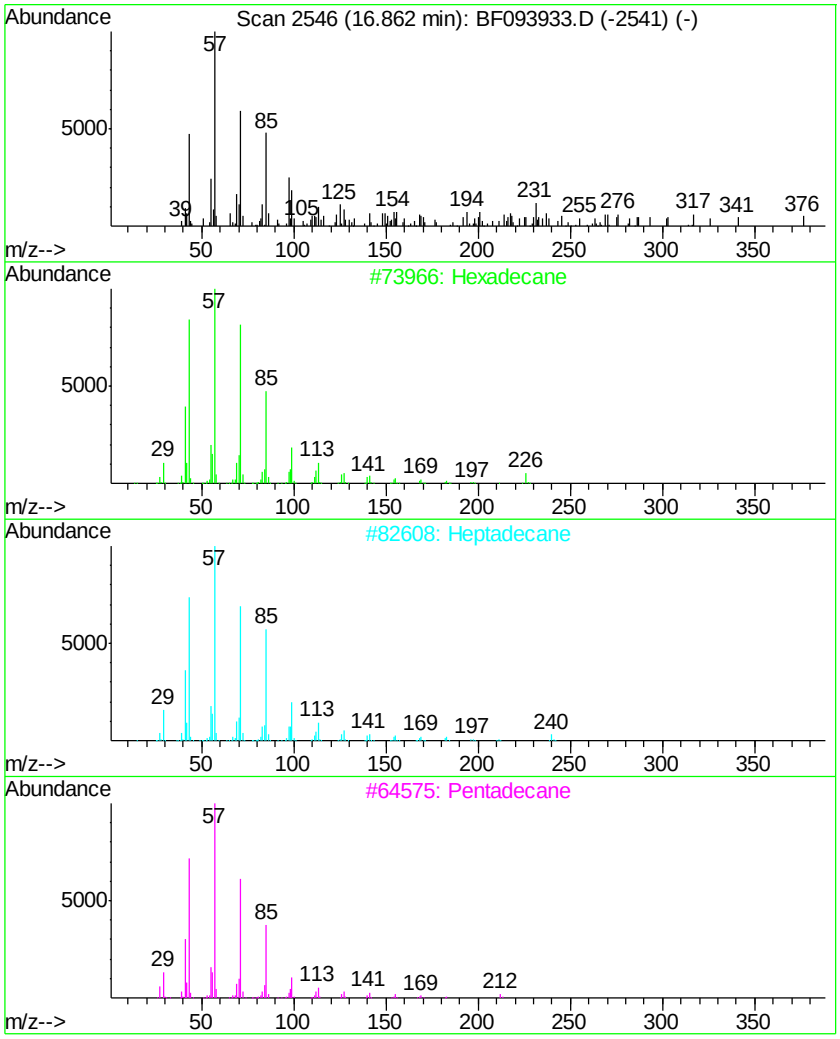
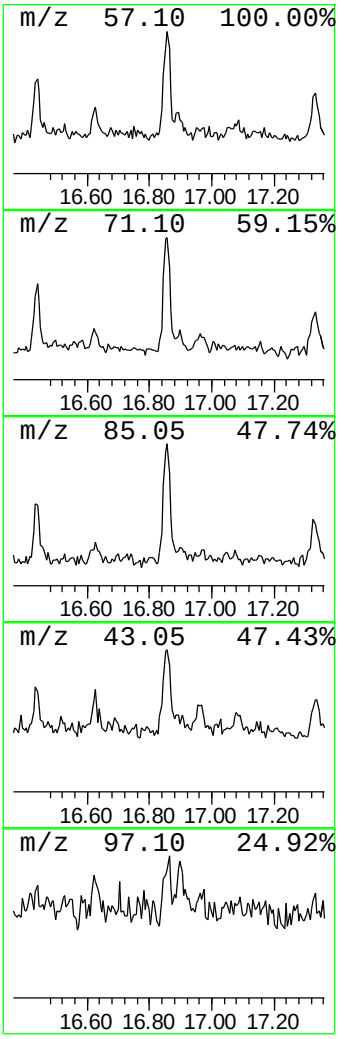
Peak Number 11 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	2.53 ng	102931	Perylene-d12	16.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Heptadecane	240	C17H36	000629-78-7	83
3	Pentadecane	212	C15H32	000629-62-9	64
4	Tetradecane, 2-methyl-	212	C15H32	001560-95-8	58
5	Tetratriacontane	479	C34H70	014167-59-0	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
Data File : BF093933.D
Acq On : 25 Mar 2017 3:31
Operator : SJ/MA
Sample : I2379-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	4.11	11.3	ng	576277	1	5.96	1023310	20.0
unknown5.71	5.71	95.6	ng	4891060	1	5.96	1023310	20.0
Naphthalene, 1,2,...	9.79	2.1	ng	418671	3	9.61	3919920	20.0
Heneicosane	10.78	2.5	ng	154059	4	11.43	1216620	20.0
unknown11.20	11.20	2.1	ng	127927	4	11.43	1216620	20.0
Cinnamyl cinnamate	14.37	79.0	ng	4050130	5	14.69	1025230	20.0
1-Octadecanol	14.56	4.8	ng	243299	5	14.69	1025230	20.0
Octadecane	15.35	2.2	ng	112788	5	14.69	1025230	20.0
Tetradecane	16.07	2.2	ng	89891	6	16.32	814601	20.0
Hexadecane	16.86	2.5	ng	102931	6	16.32	814601	20.0