LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

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-BF050916.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	1.633	3	4	13	rVB	609310	988007	21.21%	2.362%
2	1.747	13	14	18	rBV	2218315	3154840	67.74%	7.542%
3	4.787	277	280	295	rVB	364116	749482	16.09%	1.792%
4	5.233	317	319	322	rBV	3996260	4224178	90.70%	10.098%
5	5.633	352	354	359	rVB	62929	76593	1.64%	0.183%
6	6.307	410	413	415	rBV	3435722	4657445	100.00%	11.133%
7	6.410	419	422	424	rBV	4457497	4550978	97.71%	10.879%
8	6.627	439	441	444	rBV	744081	887366	19.05%	2.121%
9	6.787	453	455	458	rBV	3396937	3139401	67.41%	7.505%
10	7.073	478	480	484	rBV	172034	245859	5.28%	0.588%
11	7.210	489	492	494	rBV	2999624	3230721	69.37%	7.723%
12	7.919	552	554	556	rBV	1251527	1081570	23.22%	2.585%
13	9.005	646	649	651	rBV	3427264	3789554	81.37%	9.059%
14	9.130	658	660	662	rBV	61449	59094	1.27%	0.141%
15	9.405	681	684	686	rBV	364908	456876	9.81%	1.092%
16	9.610	700	702	704	rBV	101000	103627	2.22%	0.248%
17	9.668	704	707	710	rVV	1110619	986970	21.19%	2.359%
18	9.988	732	735	738	rVB3	60399	79878	1.72%	0.191%
19	10.113	744	746	747	rVV	194064	183129	3.93%	0.438%
20	10.148	747	749	753	rVB4	41615	78046	1.68%	0.187%
21	10.262	757	759	762	rBV3	40698	68992	1.48%	0.165%
22	10.331	762	765	768	rBV	56330	79166	1.70%	0.189%
23	10.456	774	776	779	rBV	2179293	2096483	45.01%	5.012%
24	10.582	785	787	791	rVB	180995	192170	4.13%	0.459%
25	11.028	824	826	827	rBV	104164	82730	1.78%	0.198%
26	11.142	834	836	839	rBV	848092	808308	17.36%	1.932%
27	11.348	851	854	857	rBV	40585	60676	1.30%	0.145%
28	11.691	882	884	893	rBV	139961	278042	5.97%	0.665%
29	12.479	951	953	958	rVB3	30579	59595	1.28%	0.142%
30	12.571	958	961	964	rBV2	40865	61702	1.32%	0.147%
31	12.731	972	975	978	rBV	3105974	2852564	61.25%	6.819%
32	12.971	993	996	999	rBV	27811	54055	1.16%	0.129%
33	13.211	1016	1017	1020	rVB2	64624	69238	1.49%	0.166%
34	13.645	1052	1055	1062	rBV2	174431	353094	7.58%	0.844%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

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-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.771	1063	1066	1069	rBV	935737	870962	18.70%	2.082%
36	13.954	1080	1082	1087	rBV	34923	68339	1.47%	0.163%
37	14.228	1103	1106	1107	rBV	106634	168868	3.63%	0.404%
38	14.845	1158	1160	1162	rBV	59987	70421	1.51%	0.168%
39	15.131	1183	1185	1187	rBV	487394	615316	13.21%	1.471%
40	15.165	1187	1188	1191	rVB	42891	58283	1.25%	0.139%
41	15.542	1218	1221	1223	rBV	54496	77975	1.67%	0.186%
42	17.417	1382	1385	1387	rBV3	36224	62356	1.34%	0.149%

Sum of corrected areas: 41832949

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
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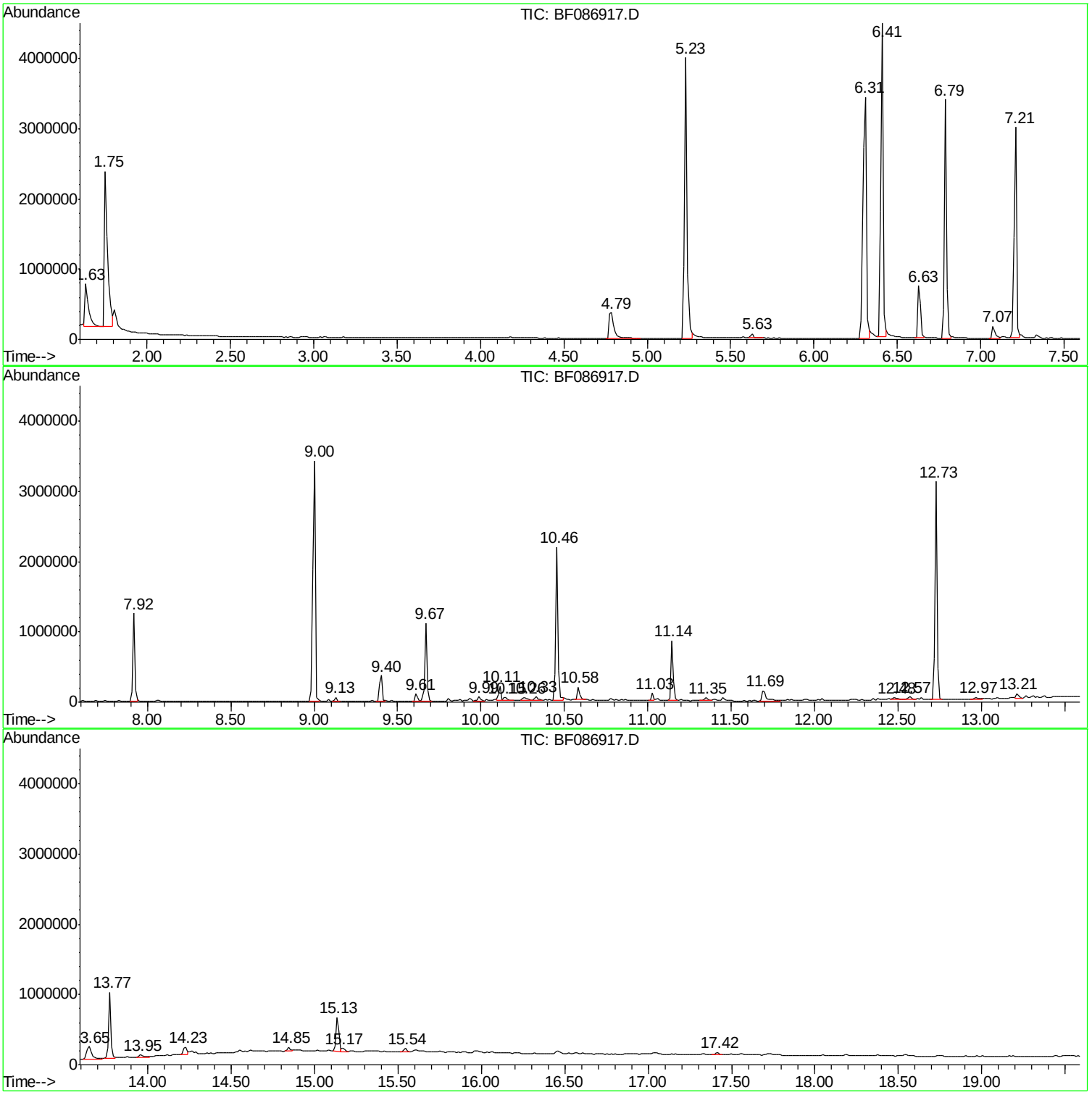
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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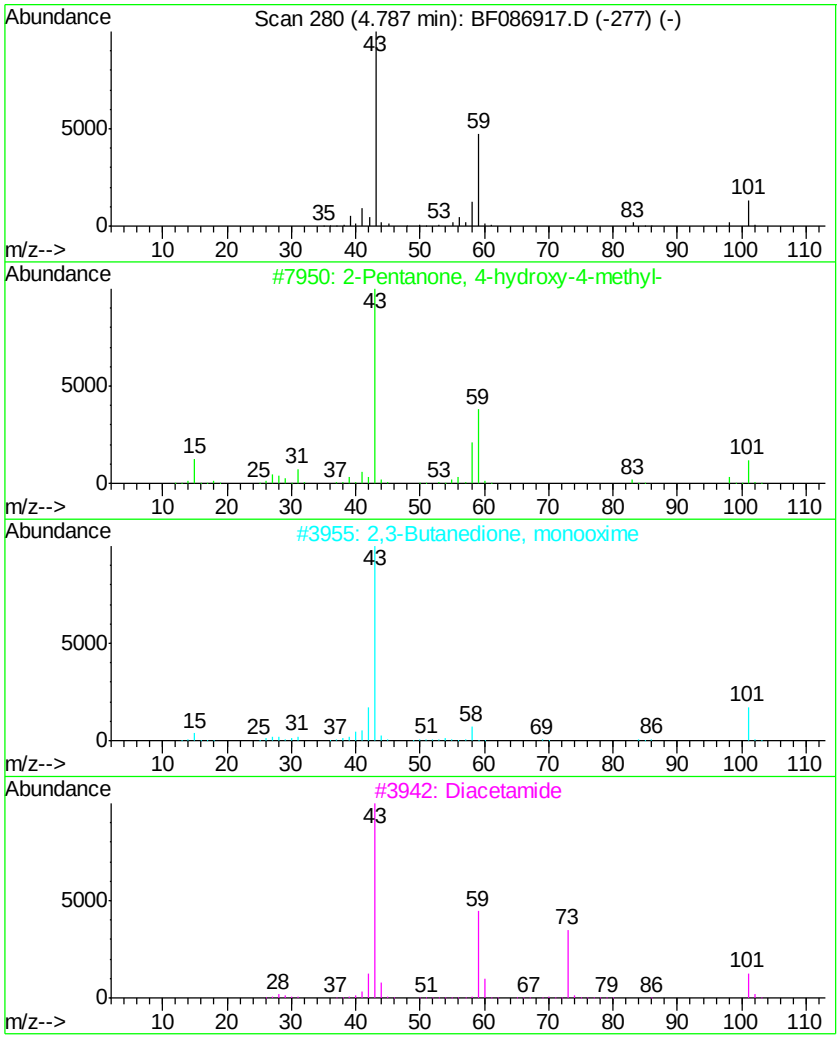
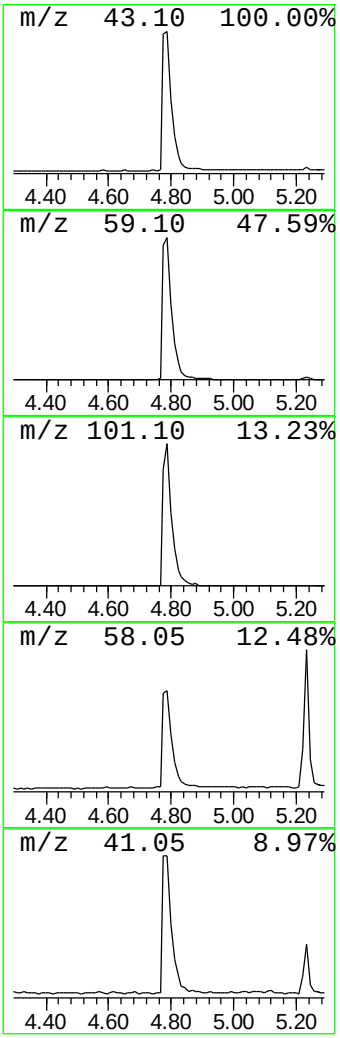
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	16.89 ng	749482	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9





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Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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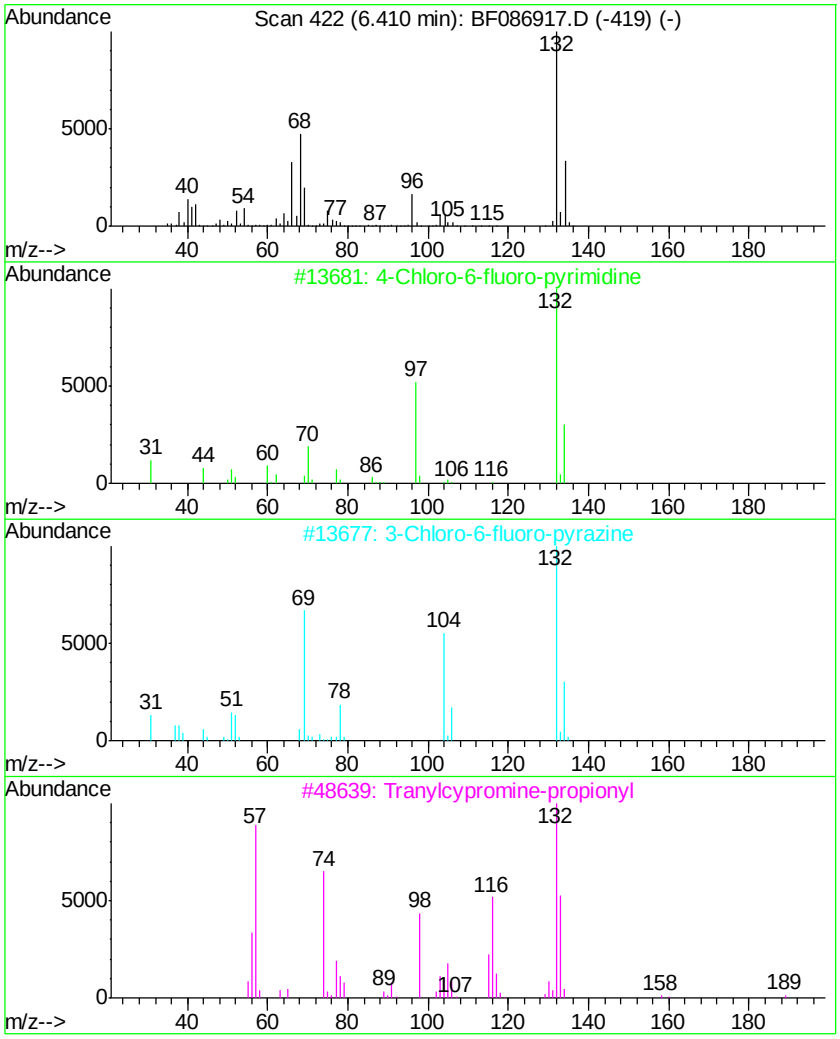
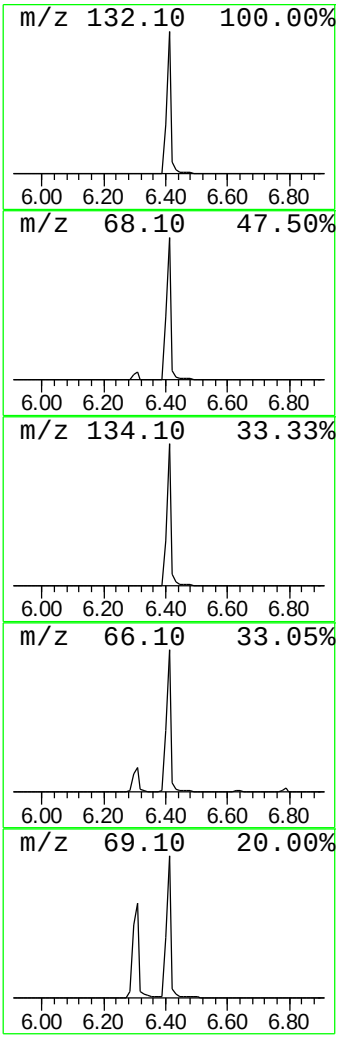
Peak Number 4 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	102.57 ng	4550980	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
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Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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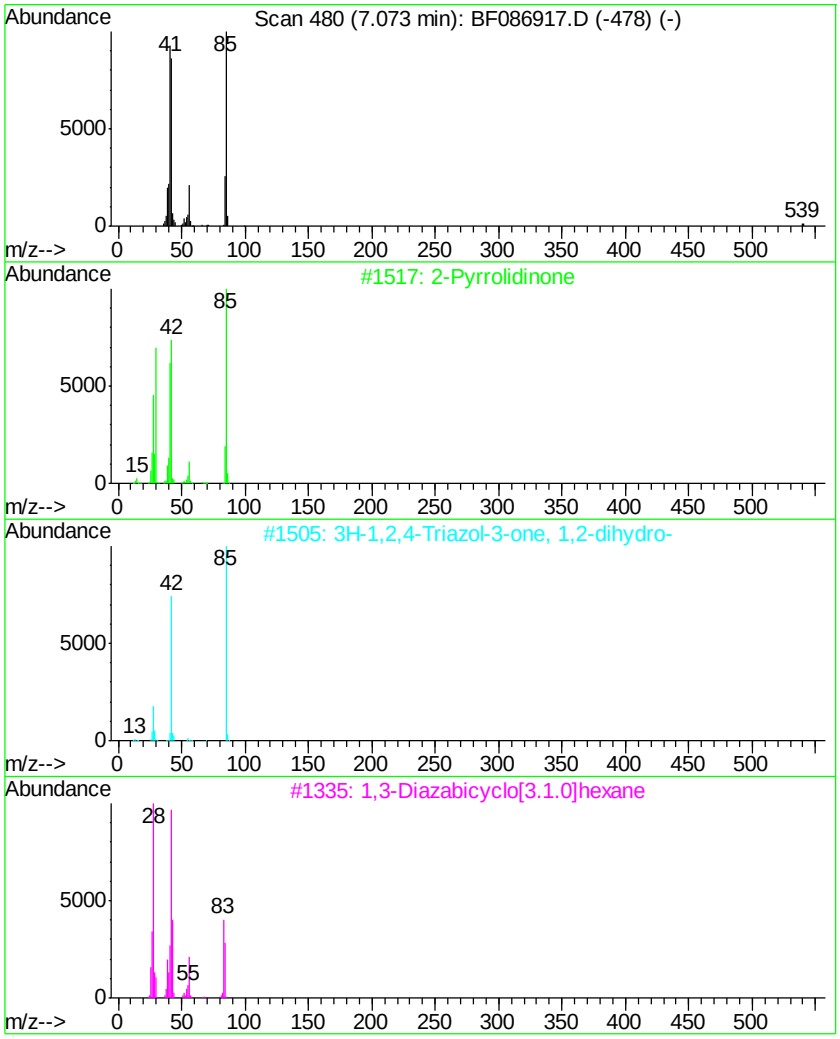
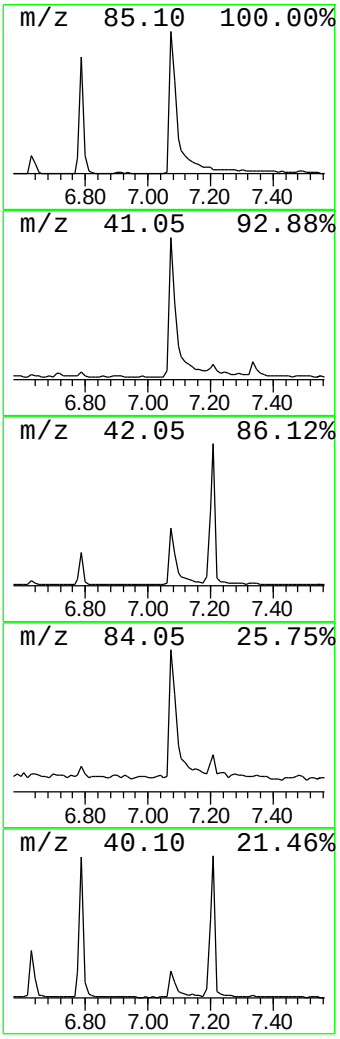
Peak Number 6 2-Pyrrolidinone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	5.54 ng	245859	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone	85	C4H7NO	000616-45-5	91
2	3H-1,2,4-Triazol-3-one, 1,2-dihy...	85	C2H3N3O	000930-33-6	53
3	1,3-Diazabicyclo[3.1.0]hexane	84	C4H8N2	017038-28-7	43
4	2-Butyl-1,2-oxaborolane	126	C7H15BO	005357-13-1	39
5	1-Bromo-7-(tetrahydro-2-pyranylo...	278	C12H23BrO2	010160-25-5	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
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Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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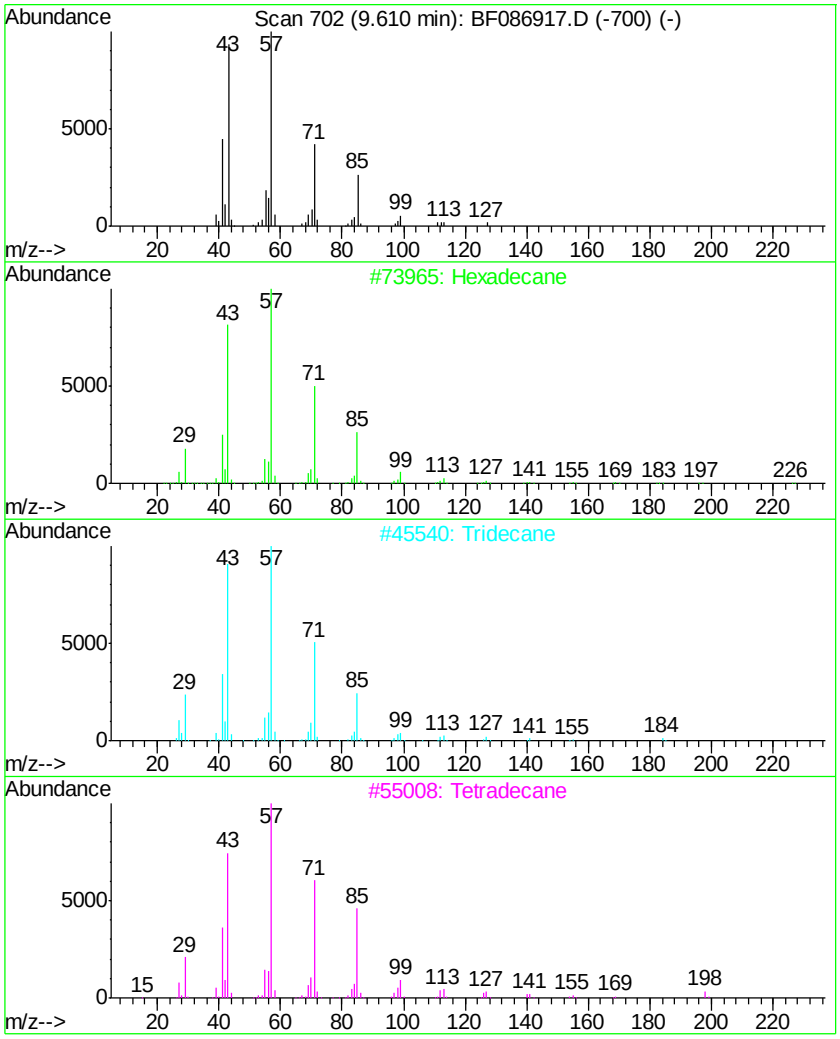
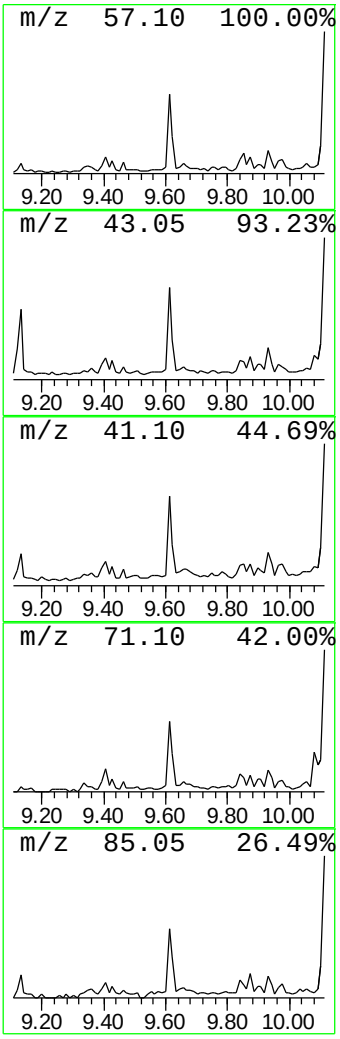
Peak Number 7 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.61	2.10 ng	103627	Acenaphthene-d10	9.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Tridecane	184	C13H28	000629-50-5	86
3	Tetradecane	198	C14H30	000629-59-4	83
4	Dotriacontane	451	C32H66	000544-85-4	83
5	Pentadecane	212	C15H32	000629-62-9	78





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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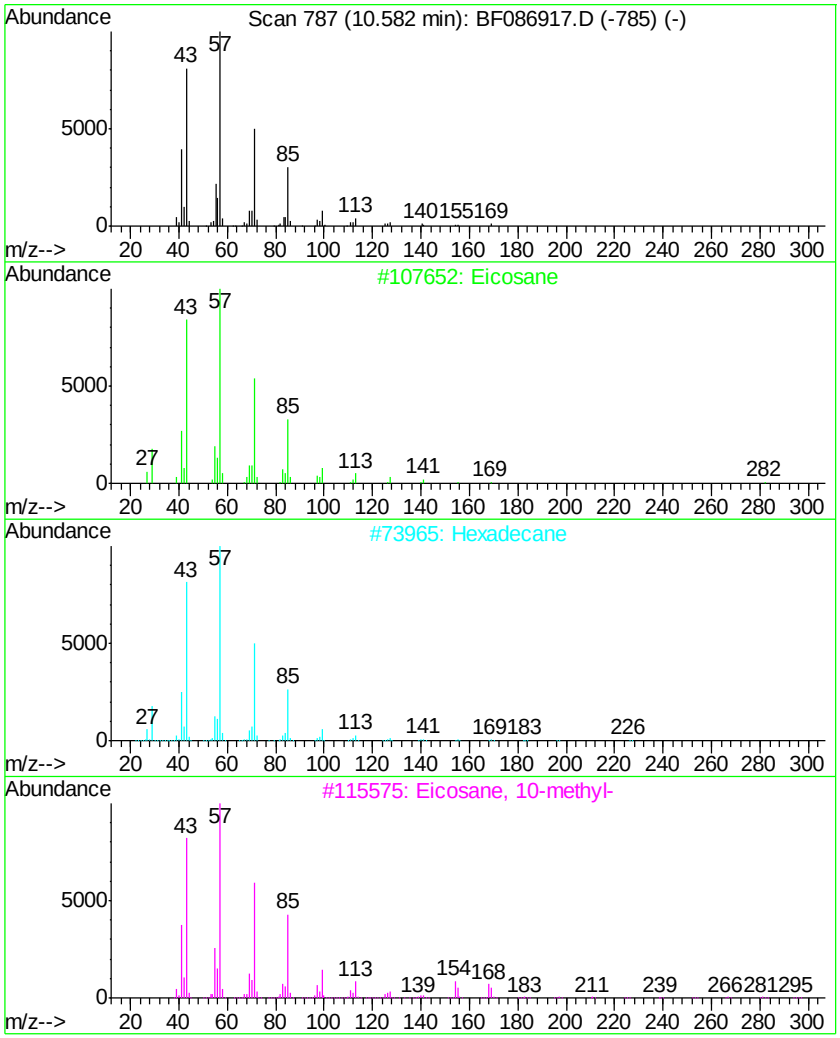
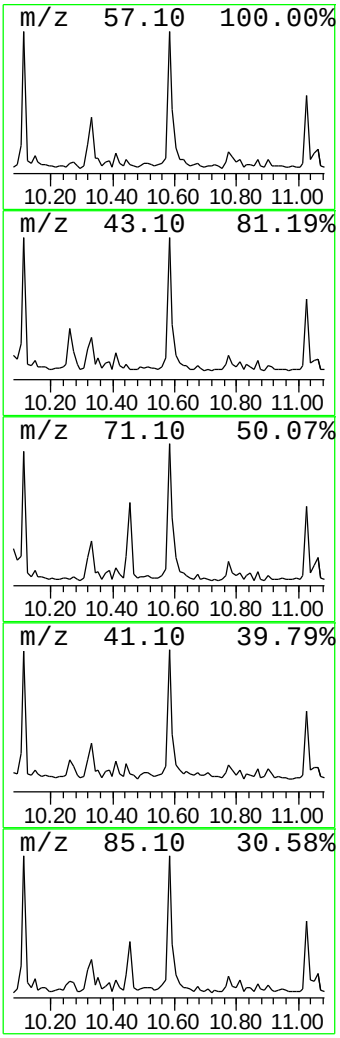
Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	4.75 ng	192170	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Octadecane	254	C18H38	000593-45-3	72
5	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
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Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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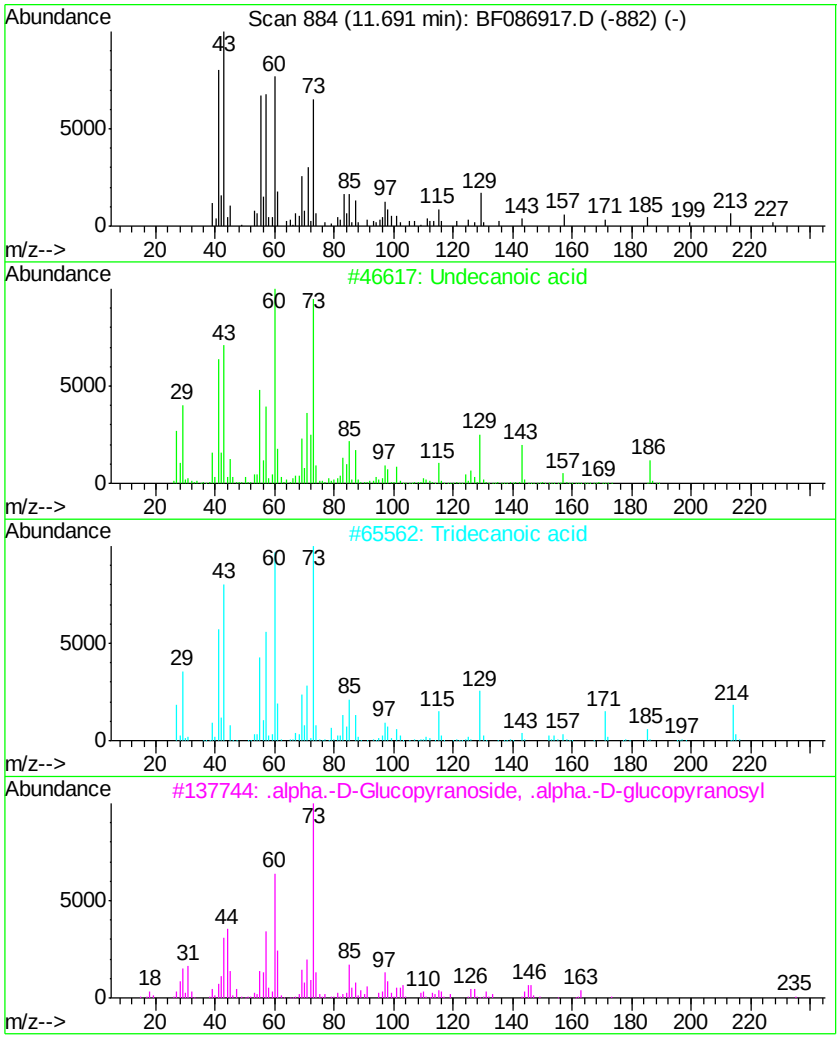
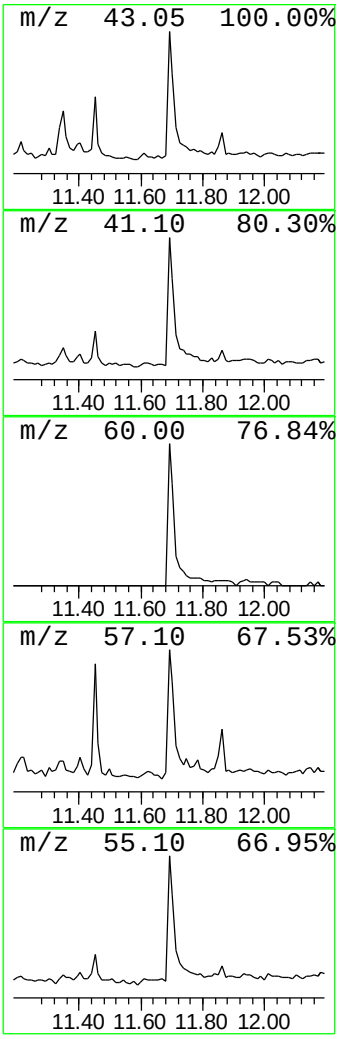
Peak Number 11 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	6.88 ng	278042	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	59
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





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Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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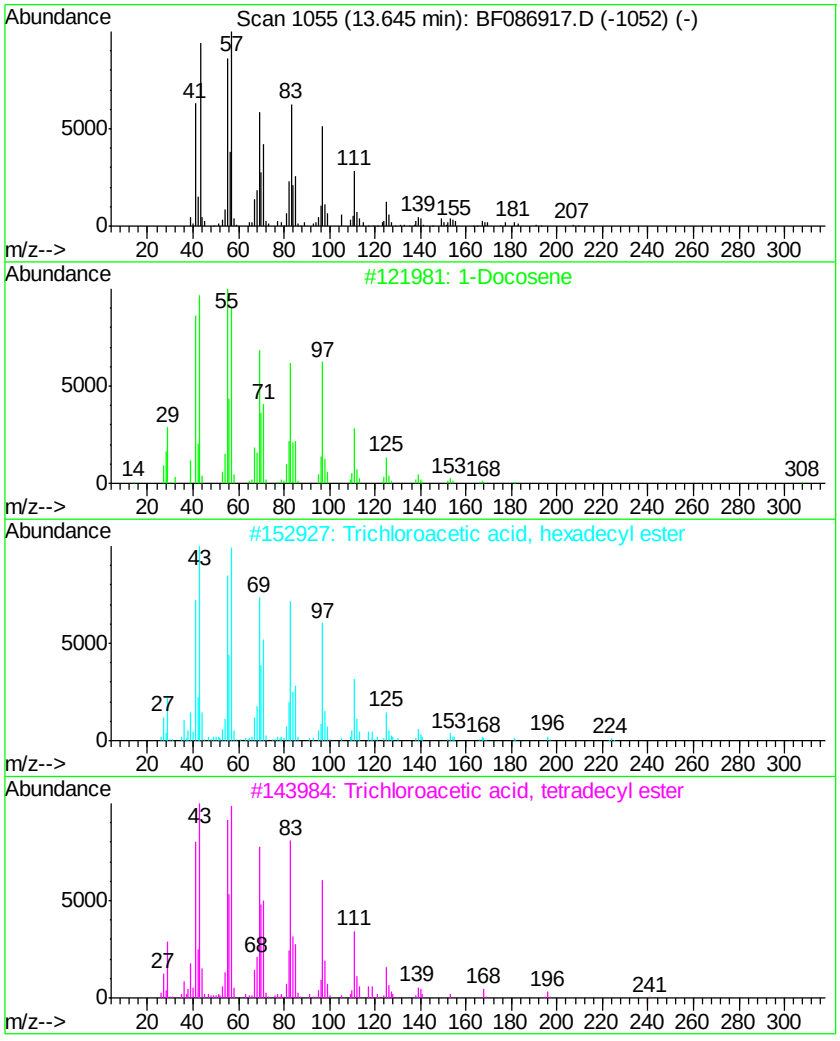
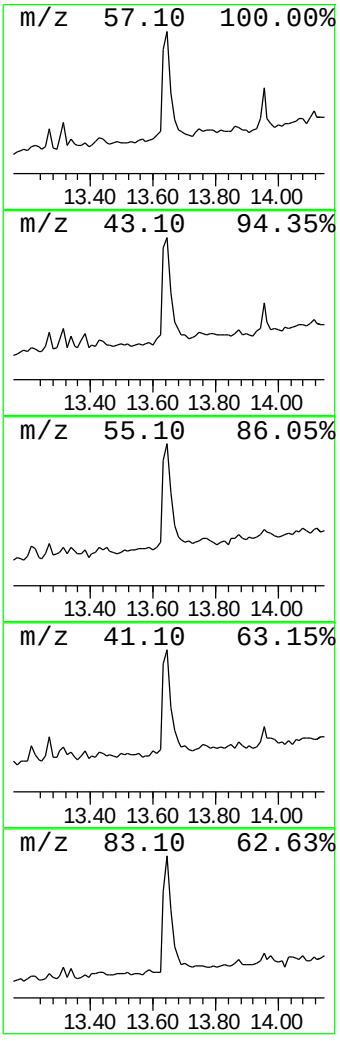
Peak Number 12 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	8.11 ng	353094	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





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Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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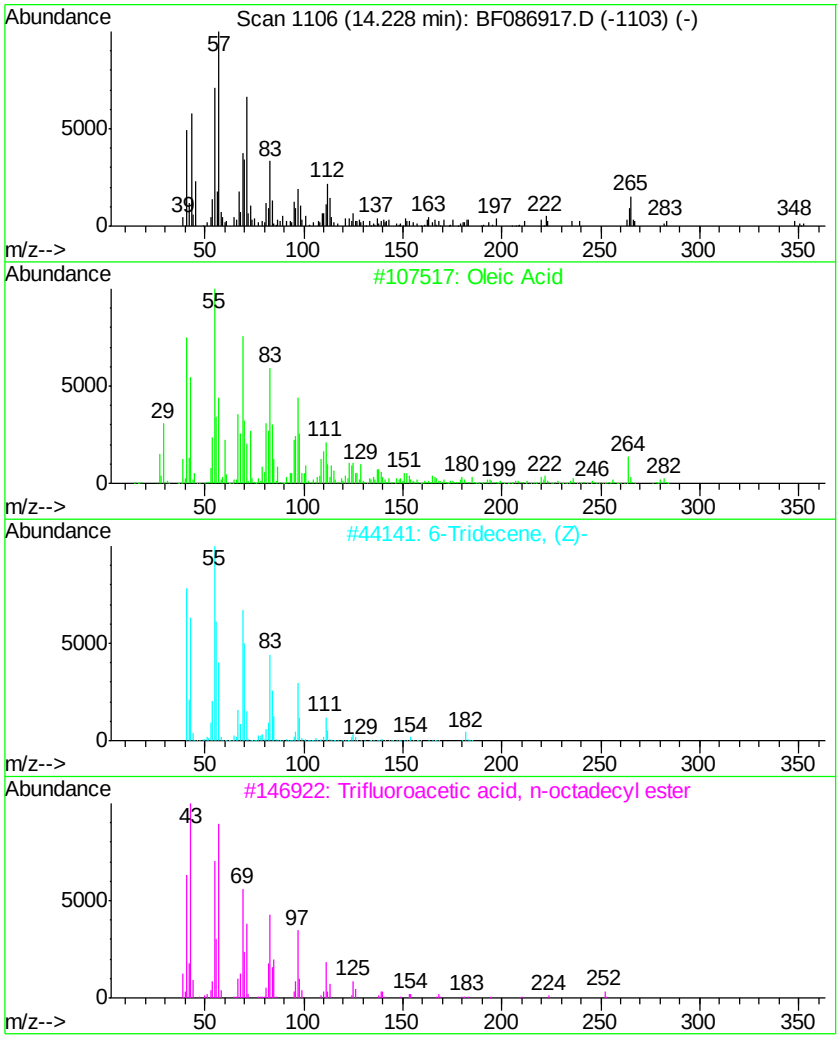
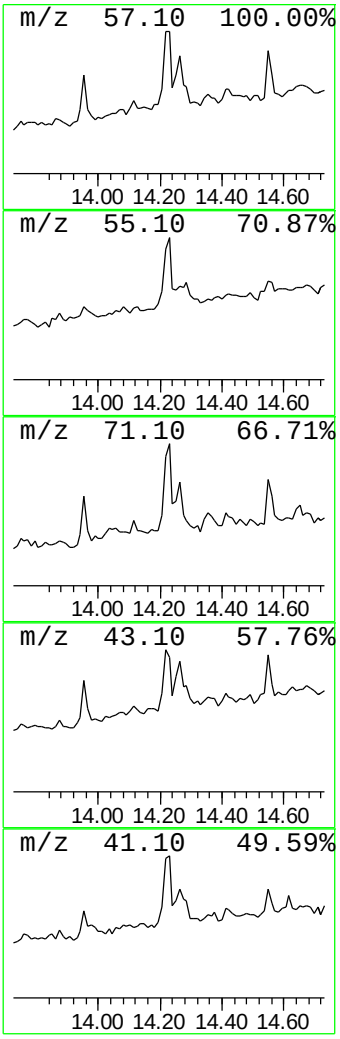
Peak Number 13 Oleic Acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	3.88 ng	168868	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	83
2	6-Tridecene, (Z)-	182	C13H26	006508-77-6	48
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	41
4	1-Nonadecene	266	C19H38	018435-45-5	38
5	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
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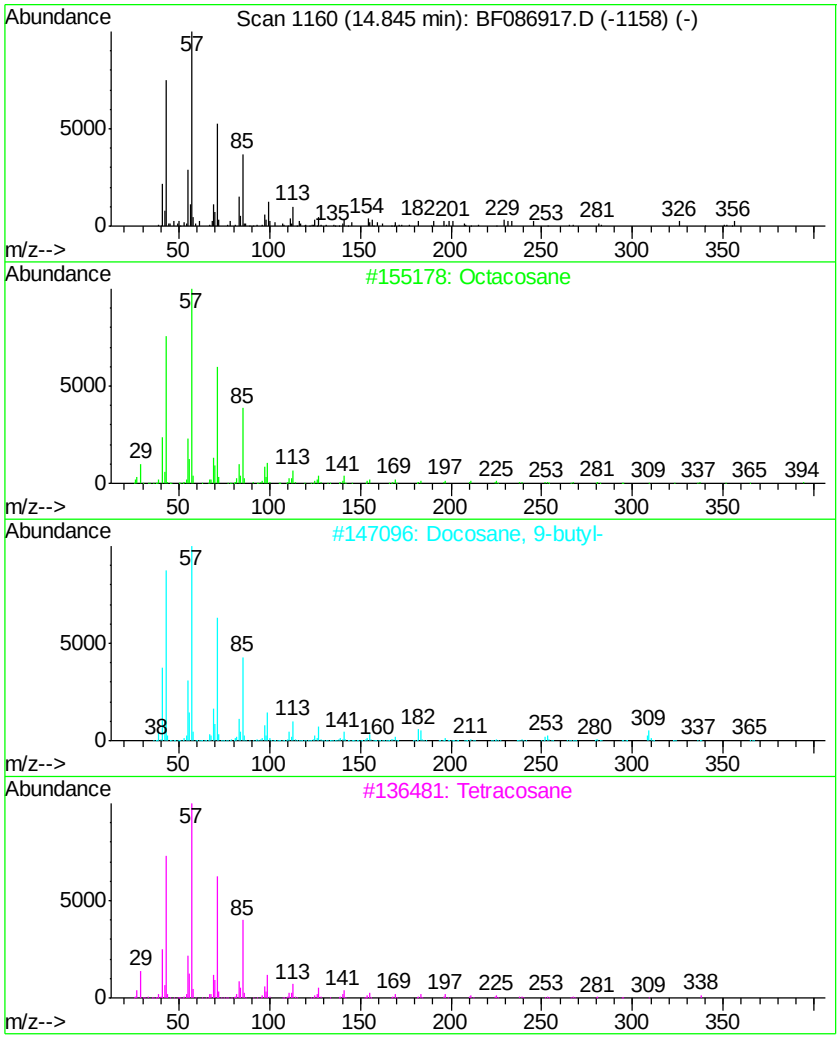
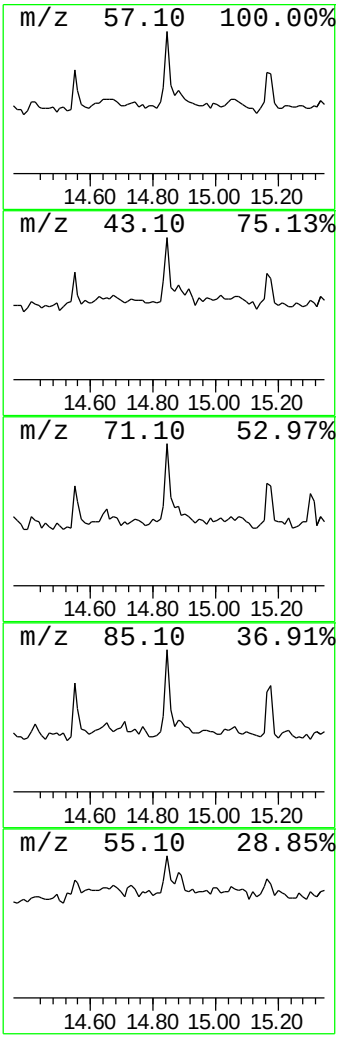
Peak Number 14 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.29 ng	70421	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Docosane, 9-butyl-	366	C26H54	055282-14-9	83
3	Tetracosane	338	C24H50	000646-31-1	83
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	83
5	Eicosane	282	C20H42	000112-95-8	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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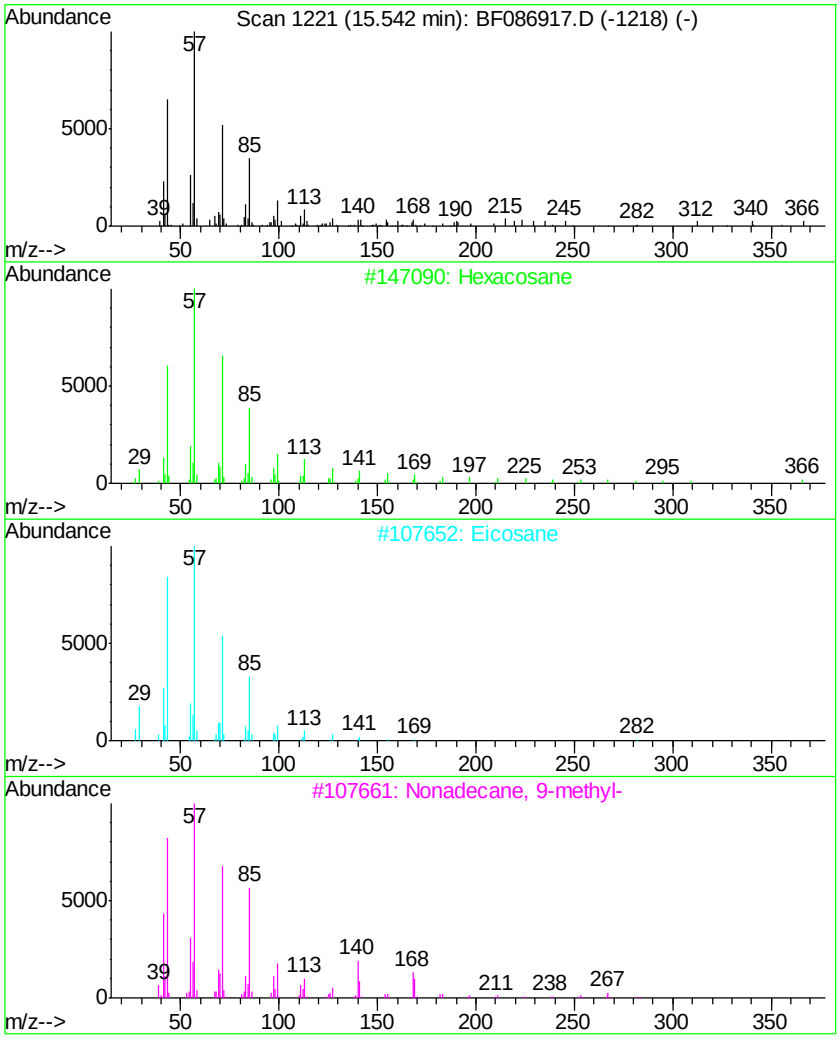
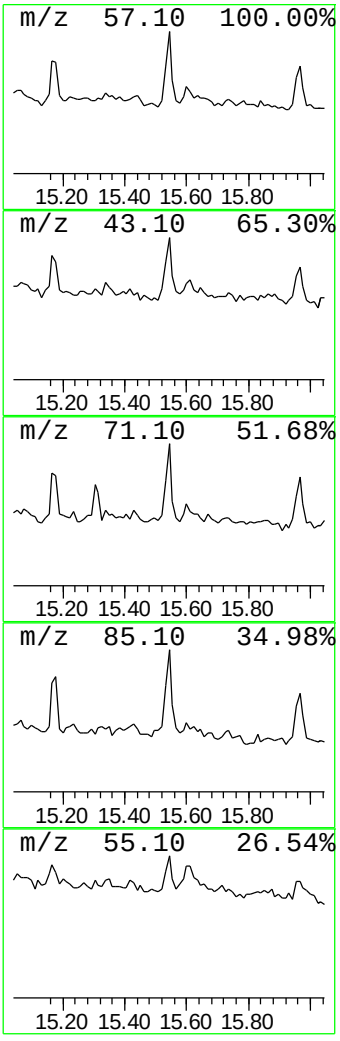
Peak Number 15 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	2.53 ng	77975	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	95
2	Eicosane	282	C20H42	000112-95-8	81
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	74
4	Hexadecane	226	C16H34	000544-76-3	72
5	Octacosane	394	C28H58	000630-02-4	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086917.D
Acq On : 12 May 2016 5:18
Operator : UM/SJ
Sample : H2916-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-9K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.79	16.9	ng	749482	1	6.63	887366	20.0
unknown6.41	6.41	102.6	ng	4550980	1	6.63	887366	20.0
2-Pyrrolidinone	7.07	5.5	ng	245859	1	6.63	887366	20.0
Hexadecane	9.61	2.1	ng	103627	3	9.67	986970	20.0
Eicosane	10.58	4.8	ng	192170	4	11.14	808308	20.0
Undecanoic acid	11.69	6.9	ng	278042	4	11.14	808308	20.0
1-Docosene	13.65	8.1	ng	353094	5	13.77	870962	20.0
Oleic Acid	14.23	3.9	ng	168868	5	13.77	870962	20.0
Octacosane	14.85	2.3	ng	70421	6	15.13	615316	20.0
Hexacosane	15.54	2.5	ng	77975	6	15.13	615316	20.0