LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

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-BF060517.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	4.593	506	511	529	rBV	60769	181759	8.35%	1.022%
2	5.269	621	626	656	rBV	1222969	2019236	92.81%	11.355%
3	6.934	903	909	920	rBV	1202841	1989431	91.44%	11.187%
4	7.028	920	925	940	rVB	1579512	2175729	100.00%	12.235%
5	7.369	979	983	994	rBV	282333	364529	16.75%	2.050%
6	7.604	1018	1023	1039	rBV	1136830	1546027	71.06%	8.694%
7	8.286	1133	1139	1163	rBV	834297	1235351	56.78%	6.947%
8	9.398	1323	1328	1343	rBV	418058	499237	22.95%	2.807%
9	11.180	1623	1631	1643	rBV	1527451	2055628	94.48%	11.559%
10	11.869	1744	1748	1755	rBV	208671	258429	11.88%	1.453%
11	12.221	1802	1808	1813	rBV2	429299	526400	24.19%	2.960%
12	13.080	1948	1954	1960	rBV	24742	29821	1.37%	0.168%
13	13.521	2023	2029	2037	rBV	820597	1143353	52.55%	6.429%
14	13.851	2081	2085	2092	rBV2	26370	34526	1.59%	0.194%
15	14.615	2210	2215	2220	rVB	357207	434076	19.95%	2.441%
16	15.639	2385	2389	2394	rVB2	92909	113386	5.21%	0.638%
17	16.439	2522	2525	2529	rVB	28220	35283	1.62%	0.198%
18	16.521	2536	2539	2543	rBV	27395	26141	1.20%	0.147%
19	16.739	2571	2576	2584	rBV2	51468	68837	3.16%	0.387%
20	16.851	2592	2595	2599	rVB	33759	38118	1.75%	0.214%
21	16.992	2611	2619	2623	rBV	1224865	1410225	64.82%	7.930%
22	17.398	2684	2688	2692	rVB2	24820	28467	1.31%	0.160%
23	17.780	2748	2753	2757	rBV3	24459	28531	1.31%	0.160%
24	17.839	2760	2763	2767	rVB	25768	29795	1.37%	0.168%
25	18.245	2827	2832	2840	rBV2	130508	229738	10.56%	1.292%
26	18.327	2842	2846	2852	rBV	359452	430304	19.78%	2.420%
27	18.662	2899	2903	2908	rBV	37661	46273	2.13%	0.260%
28	19.050	2965	2969	2976	rBV	99228	126621	5.82%	0.712%
29	19.415	3028	3031	3035	rBV2	28143	31781	1.46%	0.179%
30	19.768	3087	3091	3100	rBV3	60270	115518	5.31%	0.650%
31	19.997	3126	3130	3139	rVB	310474	376853	17.32%	2.119%
32	20.450	3203	3207	3210	rBV	41816	60443	2.78%	0.340%
33	20.486	3210	3213	3218	rVB4	28836	47676	2.19%	0.268%
34	21.027	3303	3305	3312	rVB7	19733	23313	1.07%	0.131%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.762	3427	3430	3434	rVB6	14981	22468	1.03%	0.126%

Sum of corrected areas: 17783303

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
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Acq On : 8 Jun 2017 15:00
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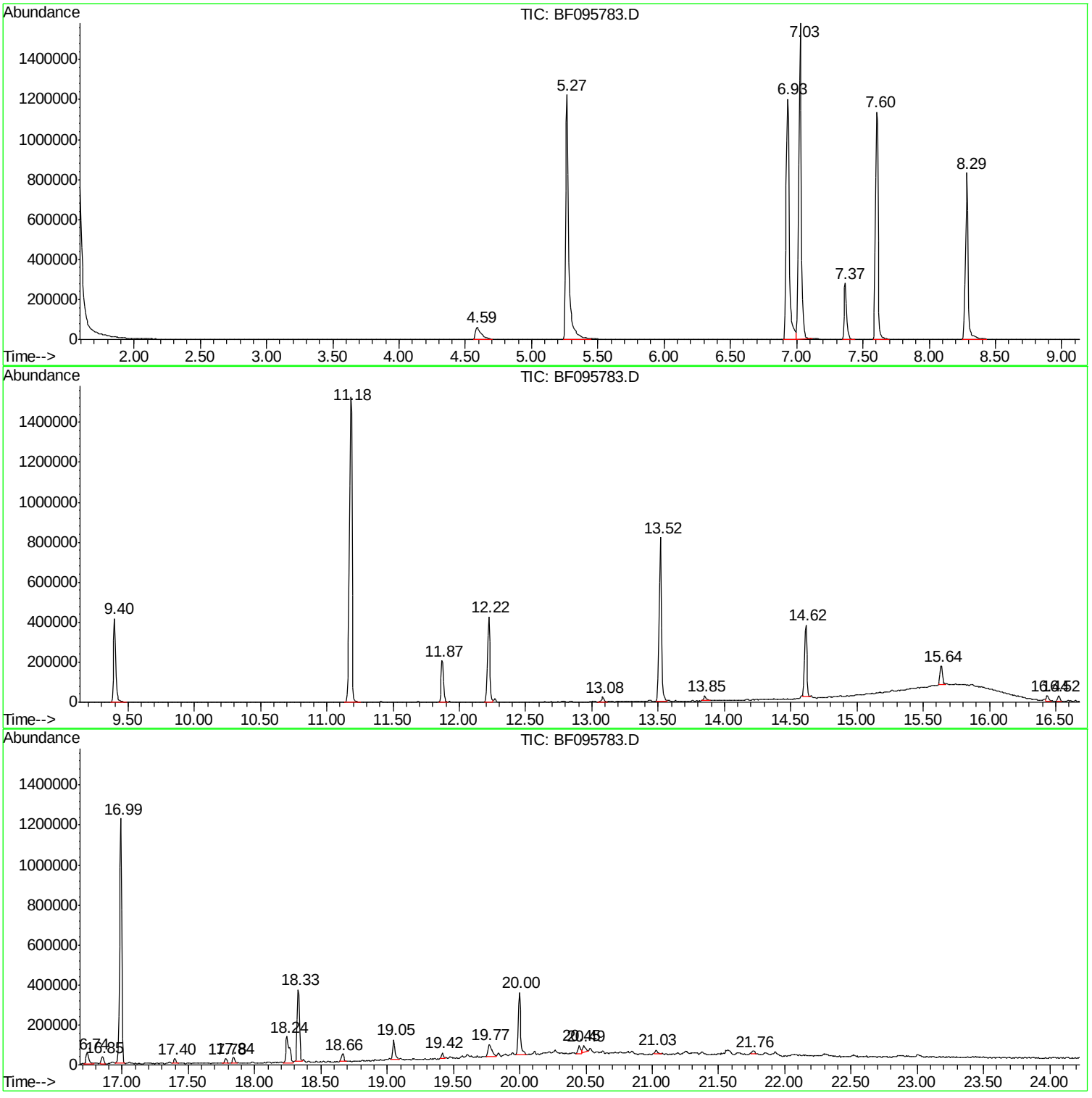
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
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Sample : I3469-13
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

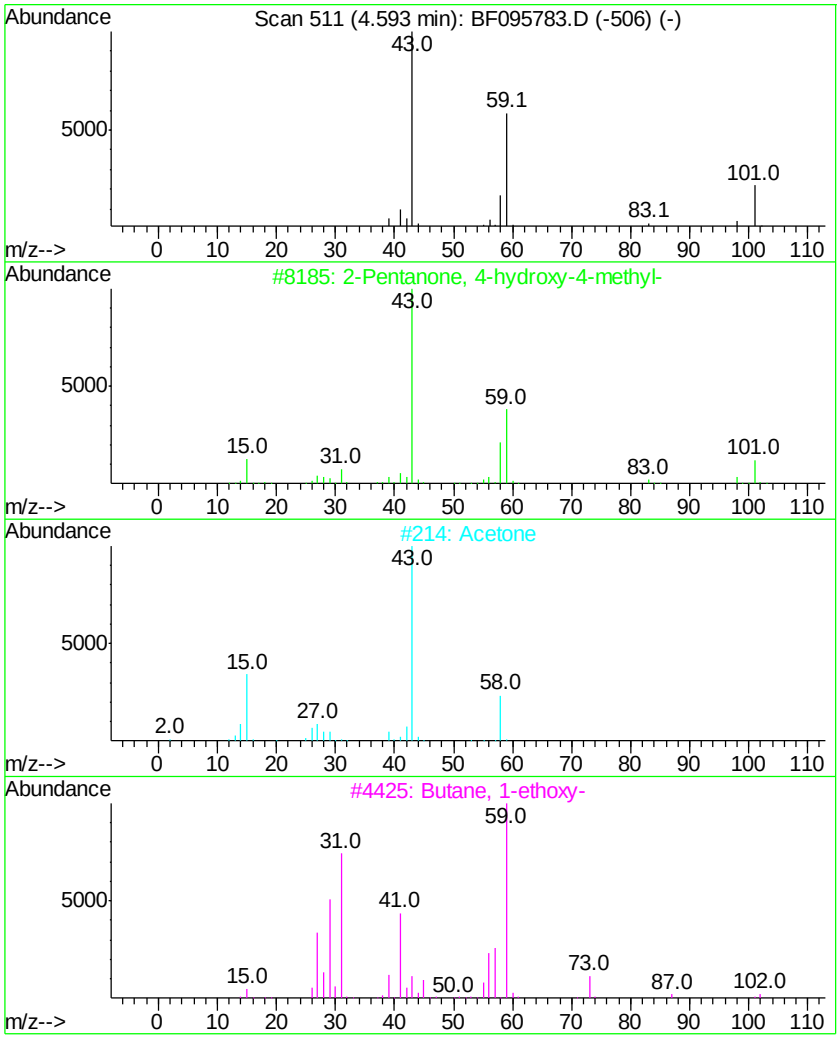
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

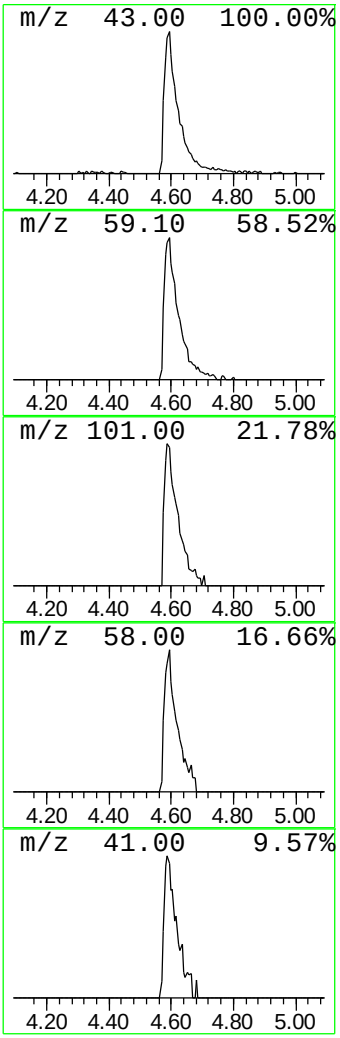
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	9.97 ng	181759	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetone	58	C3H6O	000067-64-1	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

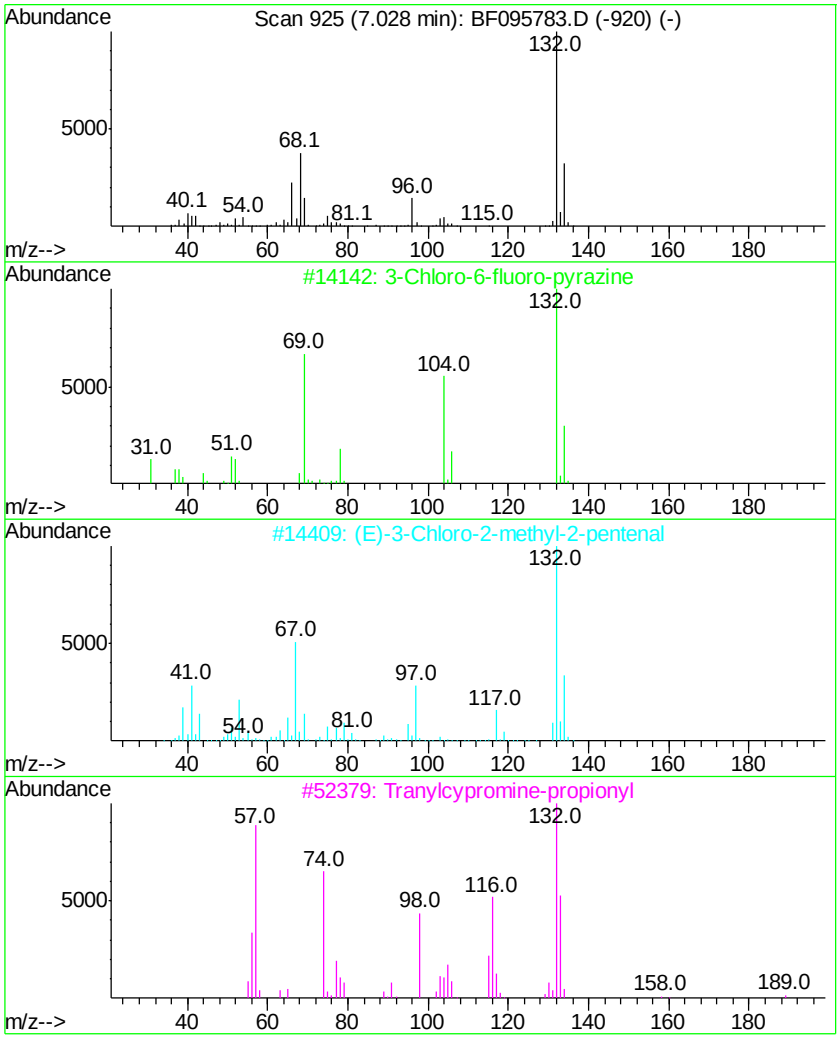
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

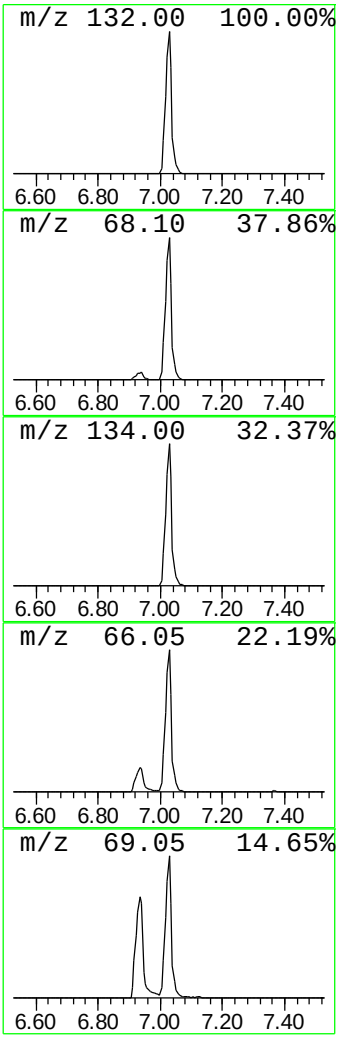
****

Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	119.37 ng	2175730	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
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Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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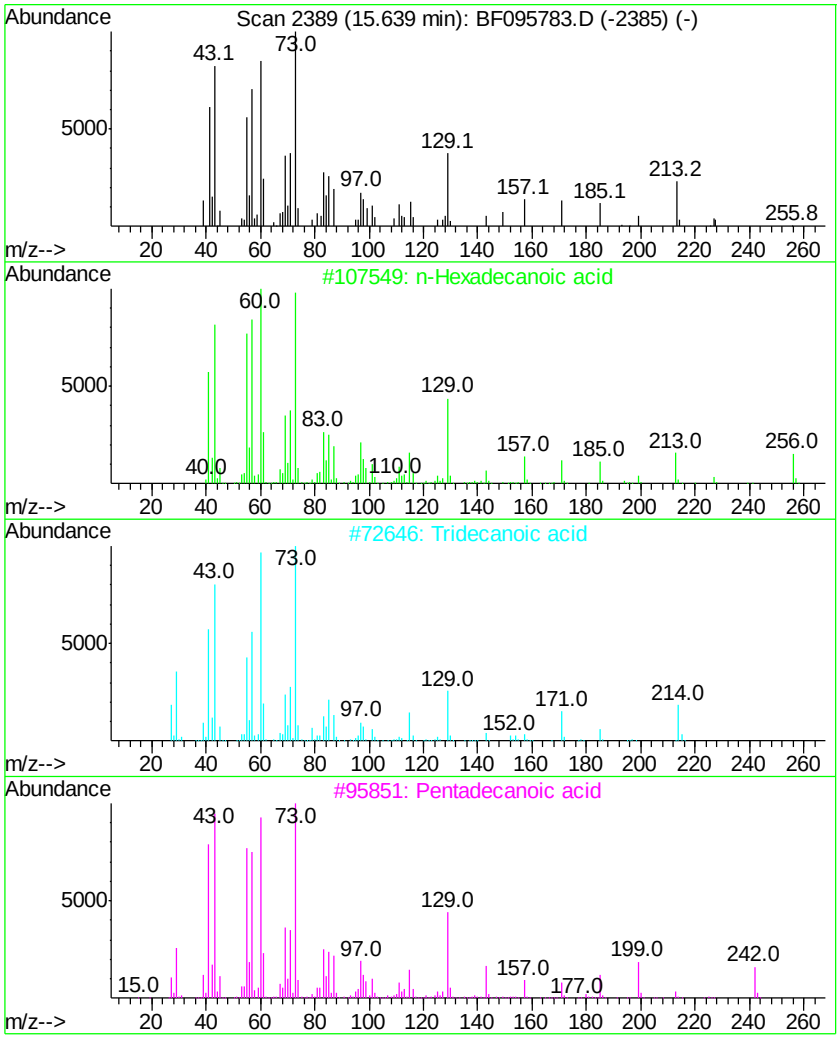
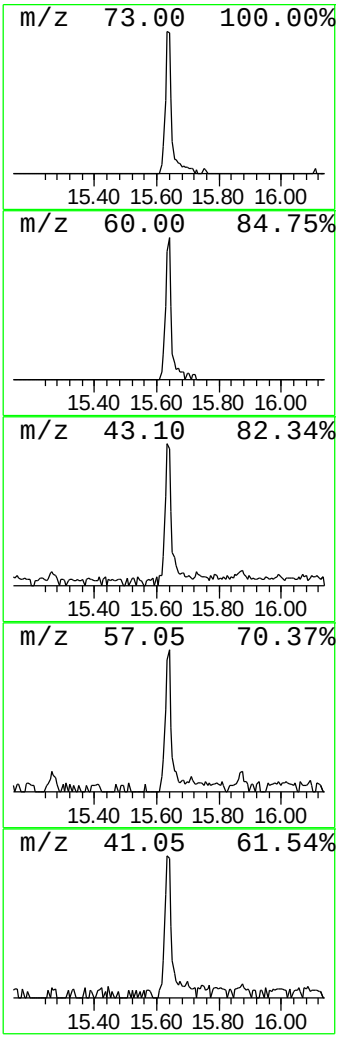
Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	5.22 ng	113386	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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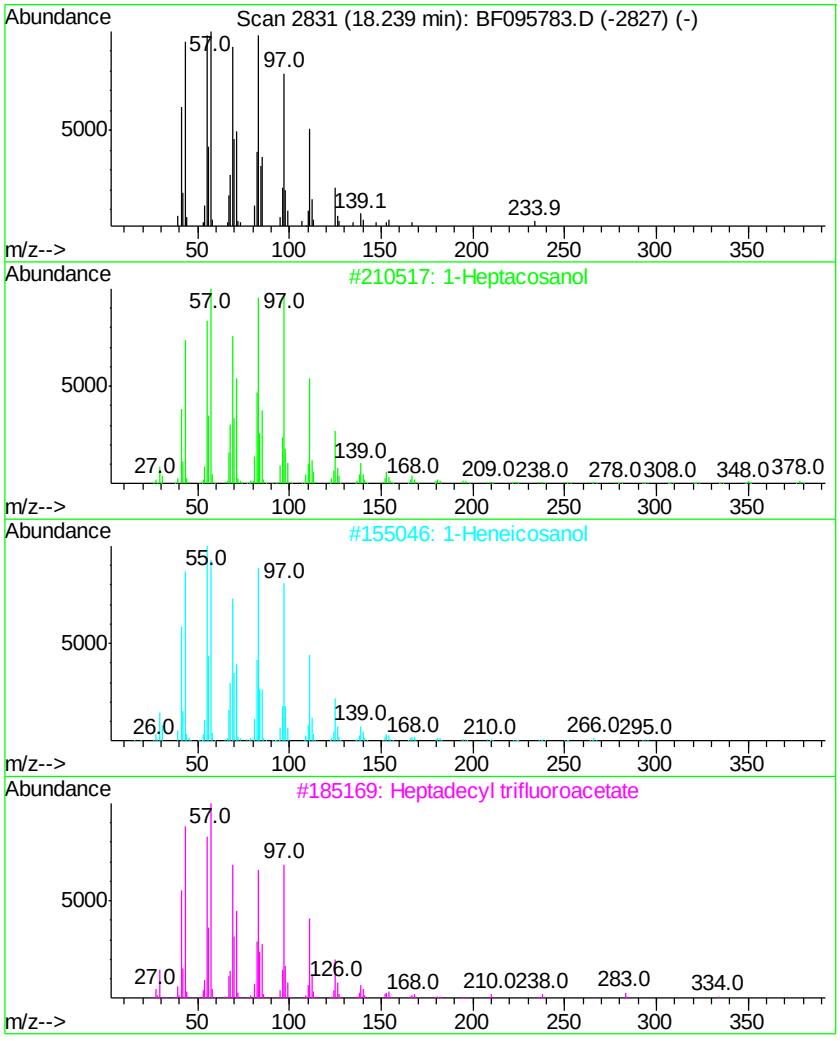
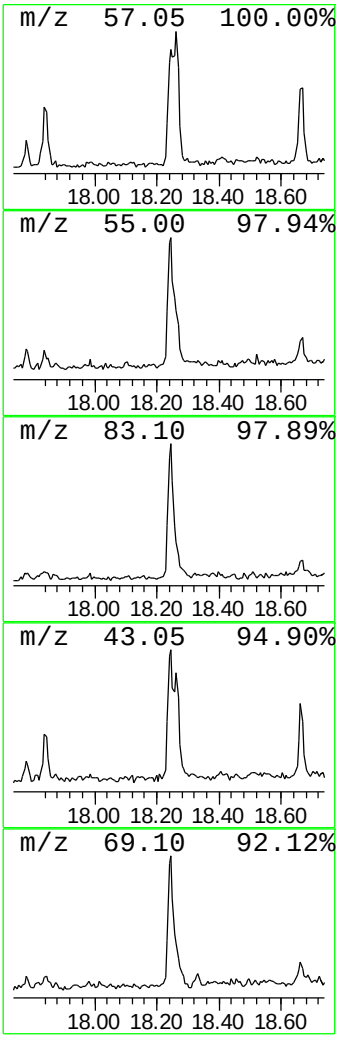
Peak Number 6 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	10.68 ng	229738	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	1-Nonadecene	266	C19H38	018435-45-5	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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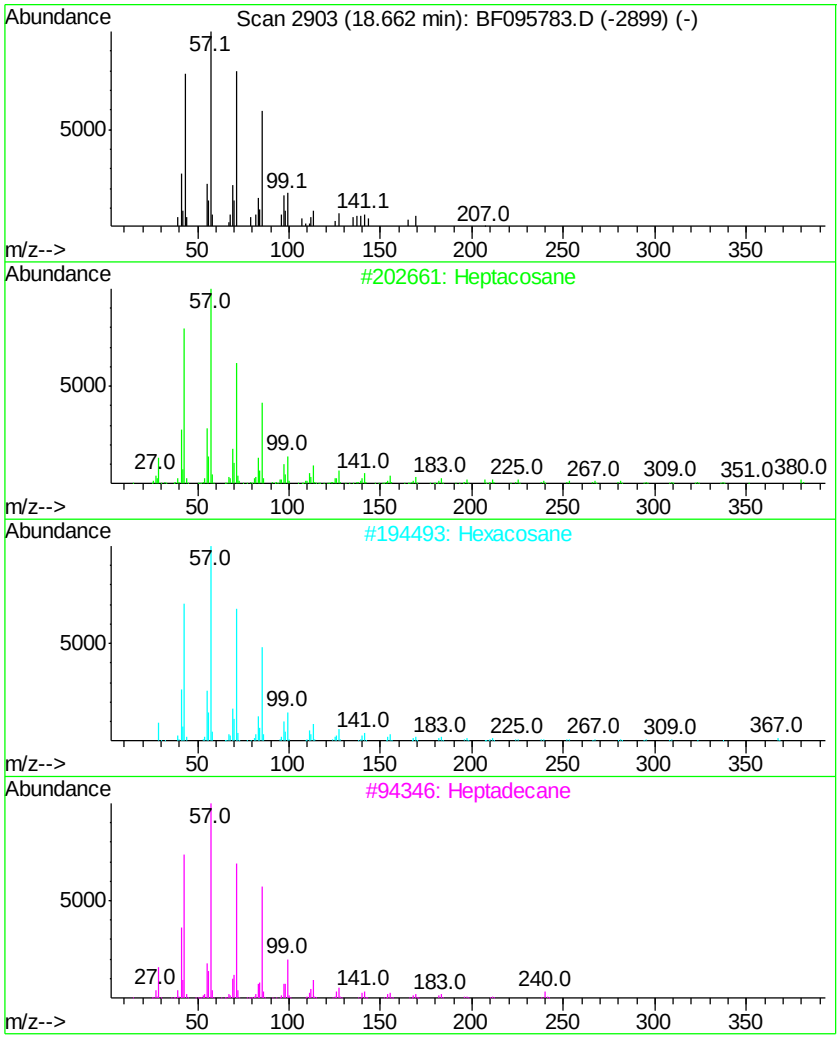
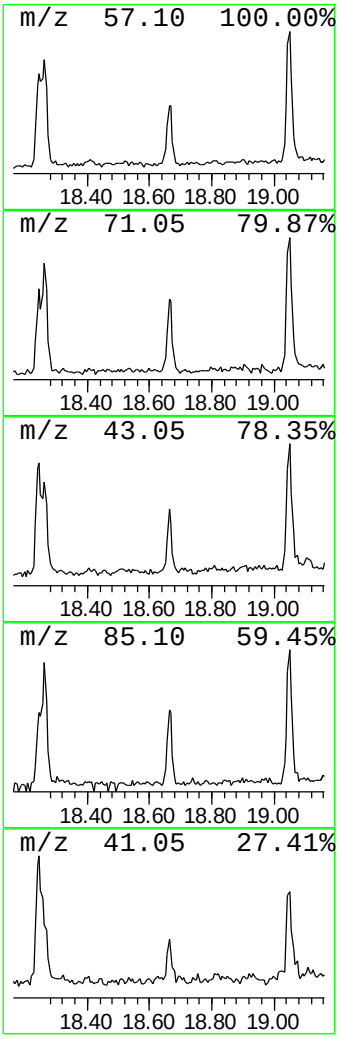
Peak Number 7 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.66	2.15 ng	46273	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Heneicosane	296	C21H44	000629-94-7	86
5	2-methyloctacosane	408	C29H60	1000376-72-8	83





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Sample : I3469-13
Misc :
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Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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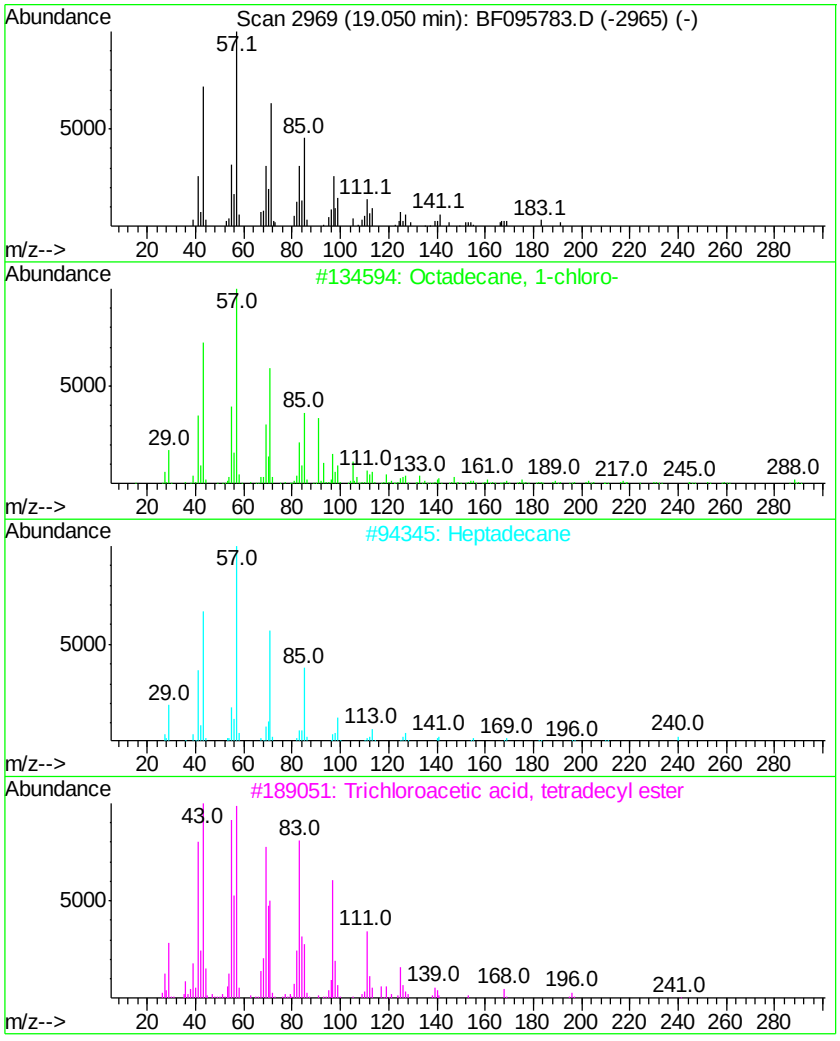
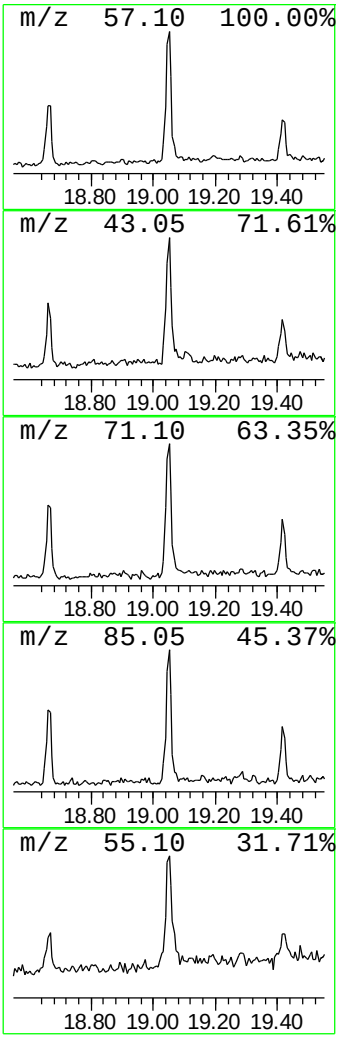
Peak Number 8 Octadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.05	5.89 ng	126621	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
2	Heptadecane	240	C17H36	000629-78-7	52
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	49
4	17-Pentatriacontene	491	C35H70	006971-40-0	49
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	49





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Sample : I3469-13
Misc :
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Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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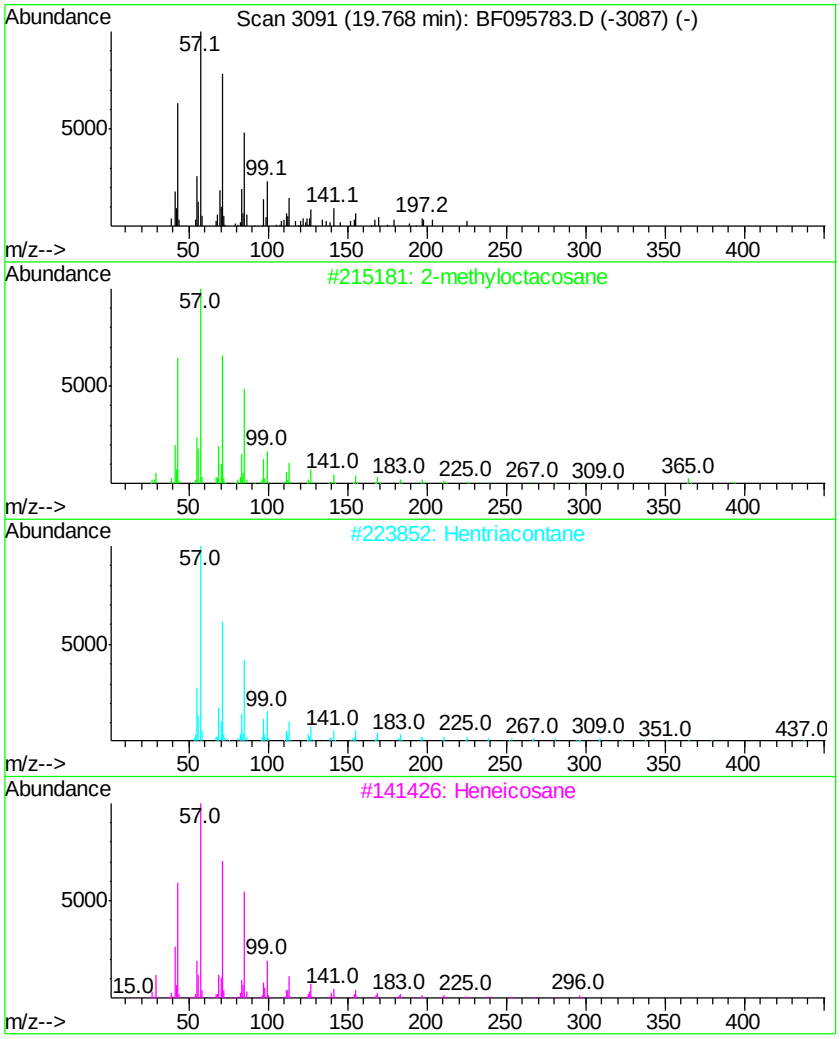
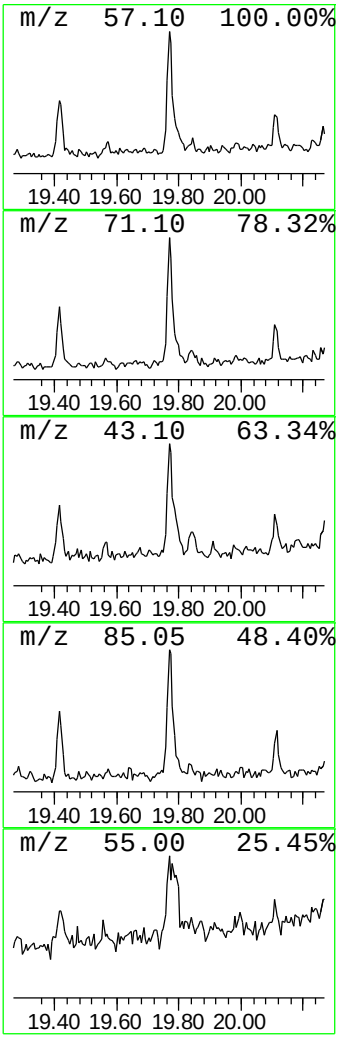
Peak Number 9 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	6.13 ng	115518	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	2-methyltetracosane	352	C25H52	1000376-72-6	90
5	Pentacosane	352	C25H52	000629-99-2	87





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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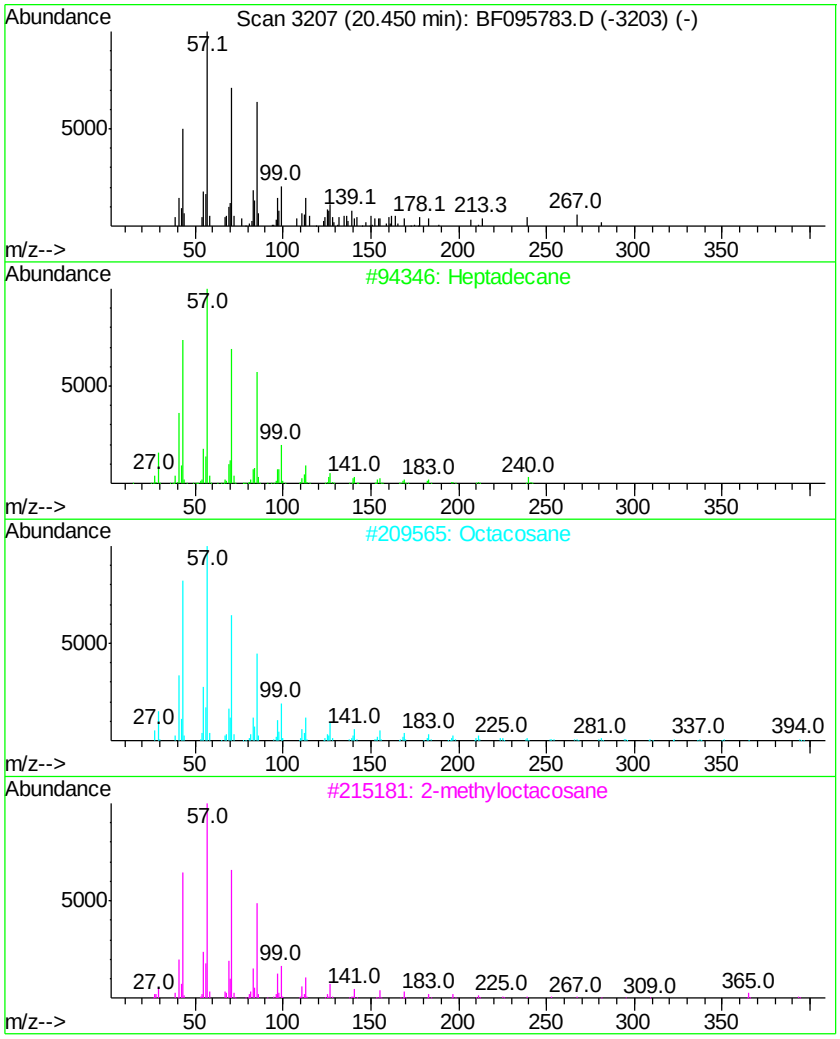
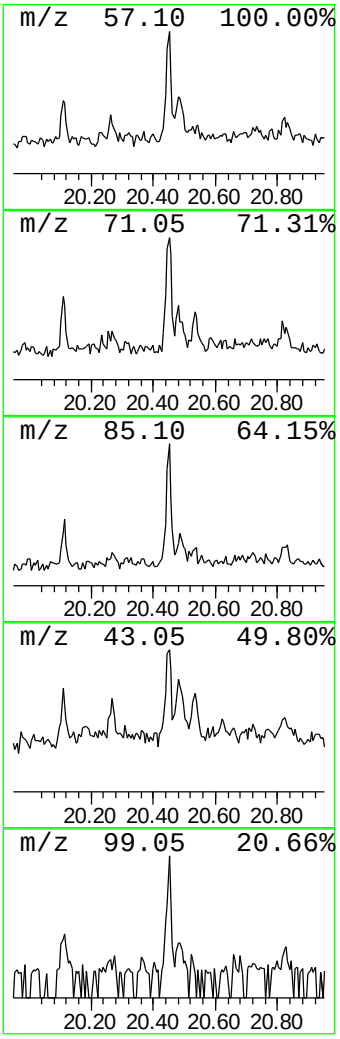
Peak Number 10 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.45	3.21 ng	60443	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octacosane	394	C28H58	000630-02-4	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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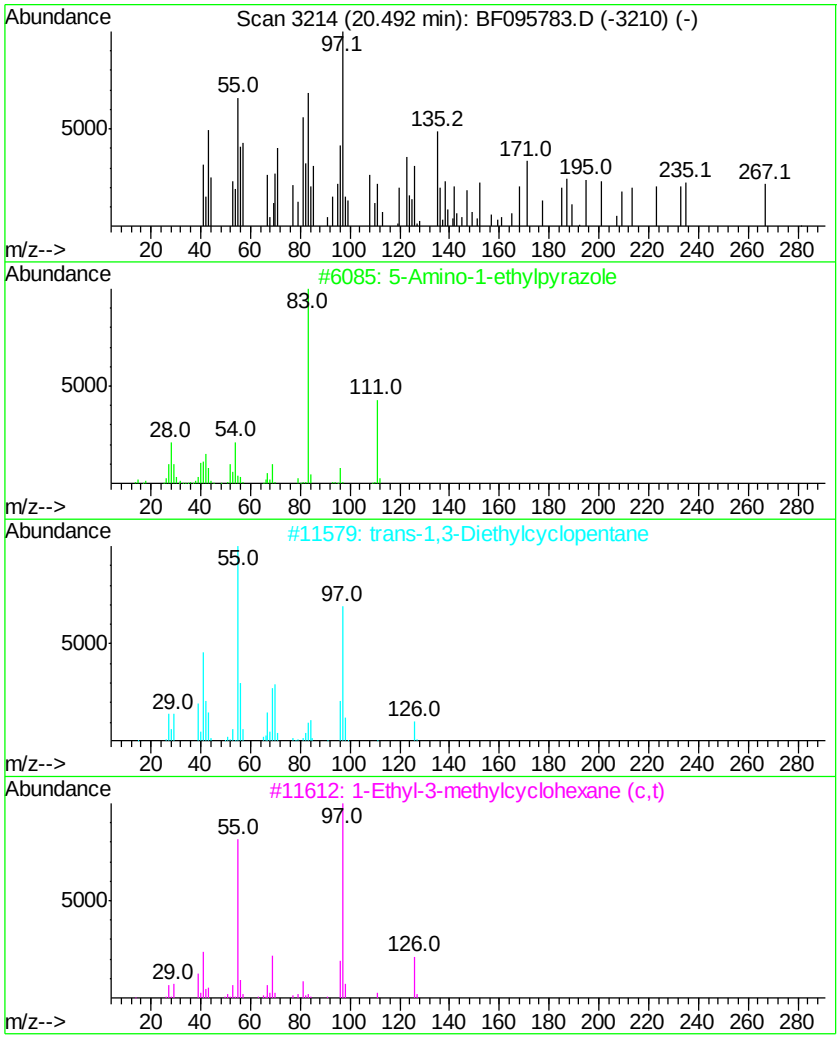
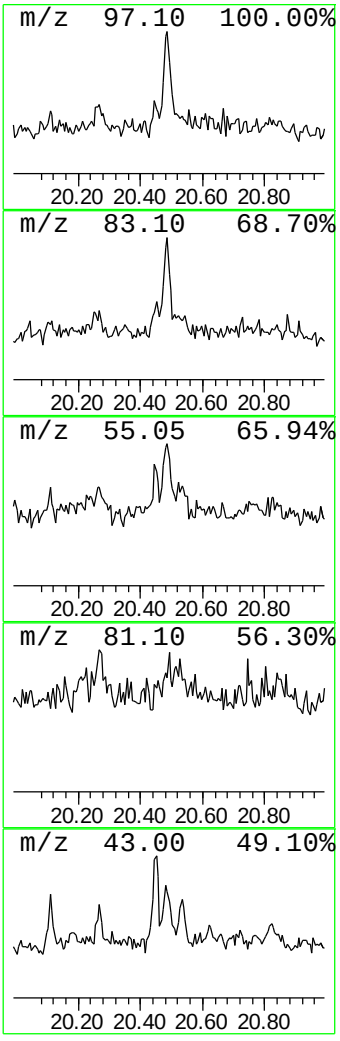
Peak Number 11 unknown20.49 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.49	2.53 ng	47676	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	30
2	trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	30
3	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	27
4	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	27
5	Cycloheptanecarboxylic acid	142	C8H14O2	001460-16-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095783.D
Acq On : 8 Jun 2017 15:00
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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
2-Pentanone, 4-hy...	4.59	10.0	ng	181759	1	7.37	364529	20.0
unknown7.03	7.03	119.4	ng	2175730	1	7.37	364529	20.0
n-Hexadecanoic acid	15.64	5.2	ng	113386	4	14.62	434076	20.0
1-Heptacosanol	18.24	10.7	ng	229738	5	18.33	430304	20.0
Heptacosane	18.66	2.1	ng	46273	5	18.33	430304	20.0
Octadecane, 1-chl...	19.05	5.9	ng	126621	5	18.33	430304	20.0
2-methyloctacosane	19.77	6.1	ng	115518	6	20.00	376853	20.0
Heptadecane	20.45	3.2	ng	60443	6	20.00	376853	20.0
unknown20.49	20.49	2.5	ng	47676	6	20.00	376853	20.0