

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
 Data File : BF095586.D
 Acq On : 1 Jun 2017 4:53
 Operator : SJ/MA
 Sample : I3355-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW-3

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-BF050217.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	4.801	500	504	516	rBV2	24556	62100	2.34%	0.354%
2	5.472	615	618	653	rBV	378648	1067175	40.26%	6.077%
3	7.119	895	898	909	rBV	211341	490338	18.50%	2.792%
4	7.213	909	914	931	rVB	1340412	2240306	84.51%	12.758%
5	7.554	968	972	984	rBV	388069	511715	19.30%	2.914%
6	7.789	1007	1012	1032	rBV	1516177	2006458	75.69%	11.426%
7	8.466	1122	1127	1146	rBV	967140	1372680	51.78%	7.817%
8	9.583	1313	1317	1330	rBV	402610	568512	21.45%	3.237%
9	10.666	1498	1501	1507	rVB	31470	45622	1.72%	0.260%
10	10.889	1534	1539	1545	rVB5	12252	28496	1.07%	0.162%
11	11.360	1613	1619	1639	rVB	2032173	2650962	100.00%	15.096%
12	11.519	1639	1646	1652	rBV9	19626	57880	2.18%	0.330%
13	11.819	1690	1697	1701	rBV4	20438	42920	1.62%	0.244%
14	12.054	1733	1737	1743	rBV	79762	107361	4.05%	0.611%
15	12.413	1793	1798	1805	rBV2	506422	686269	25.89%	3.908%
16	13.254	1937	1941	1948	rVB5	21329	39322	1.48%	0.224%
17	13.401	1959	1966	1970	rBV5	18234	29896	1.13%	0.170%
18	13.707	2013	2018	2033	rBV	1005084	1431253	53.99%	8.151%
19	14.024	2066	2072	2075	rBV4	23749	32792	1.24%	0.187%
20	14.812	2201	2206	2215	rBV	444319	576055	21.73%	3.280%
21	15.018	2237	2241	2246	rBV6	15281	28982	1.09%	0.165%
22	15.801	2370	2374	2381	rVB	96959	126384	4.77%	0.720%
23	16.895	2555	2560	2566	rBV2	54156	82262	3.10%	0.468%
24	17.006	2575	2579	2584	rVB	74996	86407	3.26%	0.492%
25	17.159	2600	2605	2609	rBV2	1835977	2141360	80.78%	12.194%
26	17.936	2733	2737	2740	rBV	57797	62354	2.35%	0.355%
27	18.406	2813	2817	2824	rVB4	40349	61794	2.33%	0.352%
28	18.506	2830	2834	2842	rBV	447436	544037	20.52%	3.098%
29	20.183	3114	3119	3129	rBV	289345	378537	14.28%	2.156%

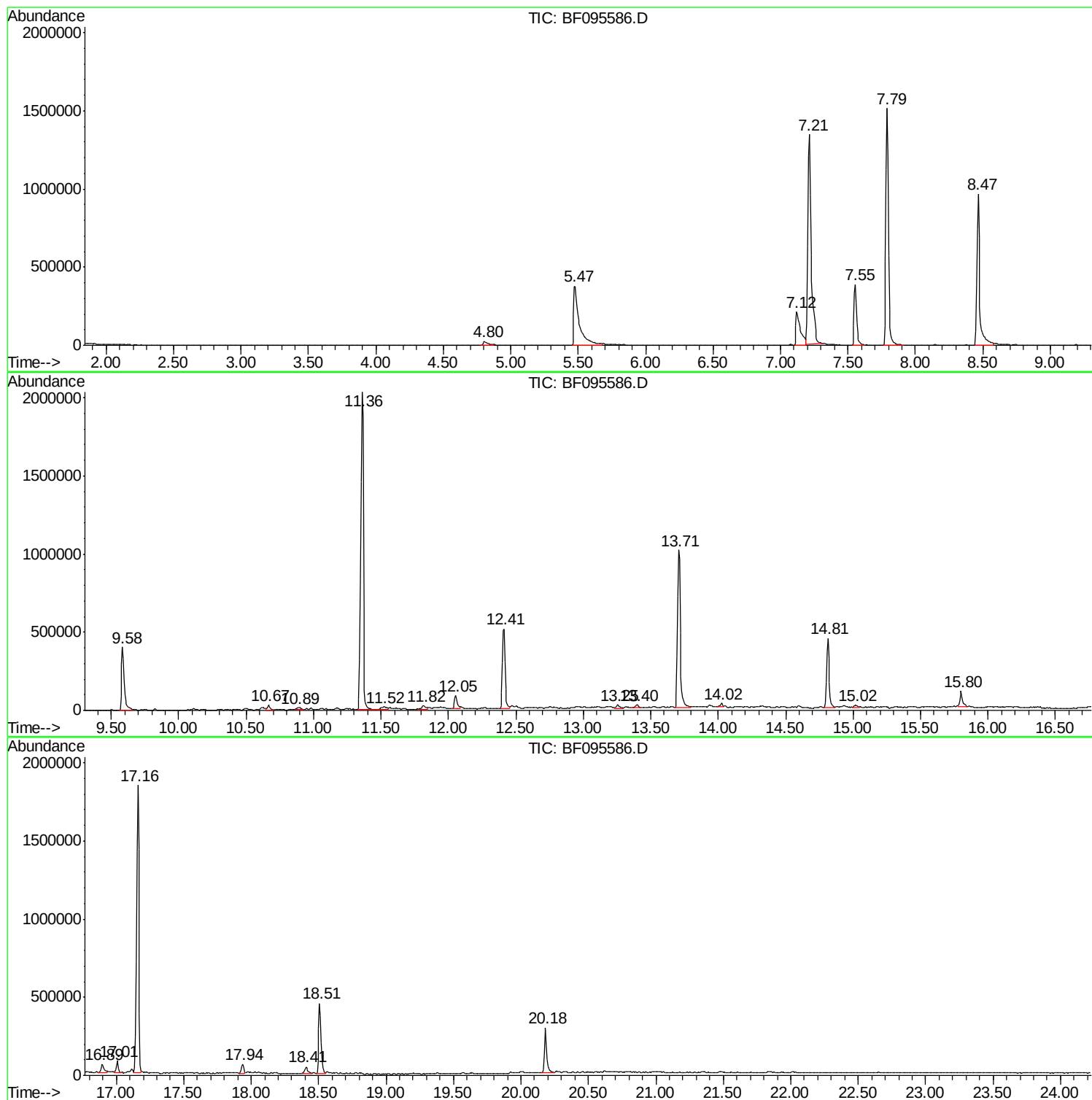
Sum of corrected areas: 17560229

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-3

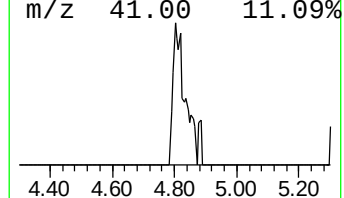
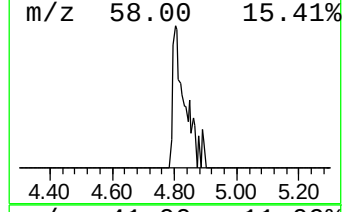
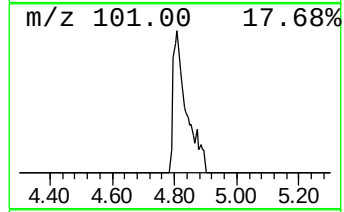
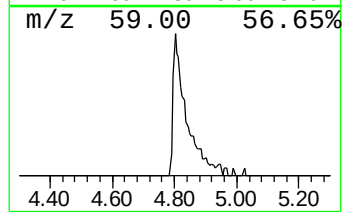
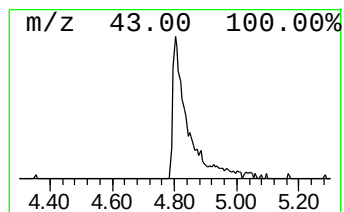
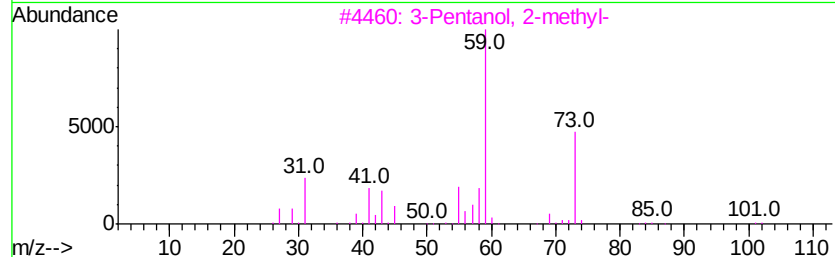
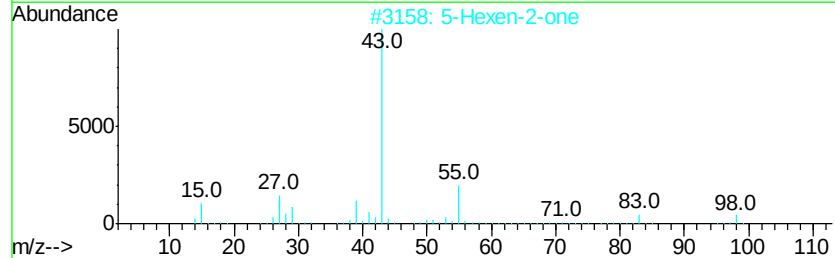
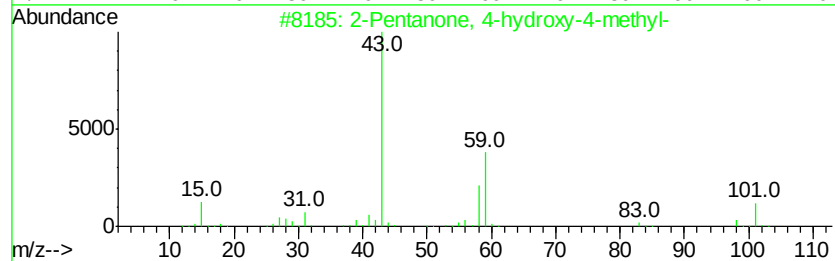
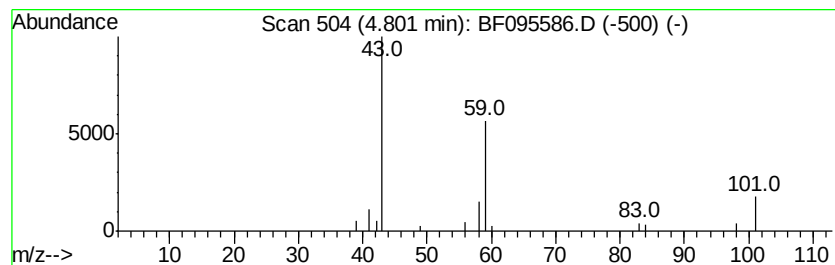
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	2.43 ng	62100	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
4		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
5		3-Octanol	130	C8H18O	000589-98-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-3

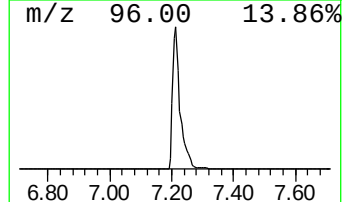
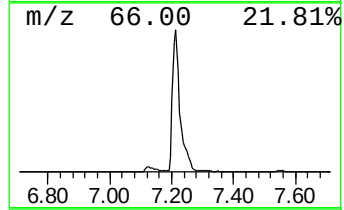
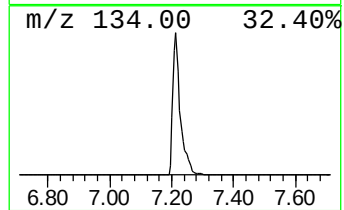
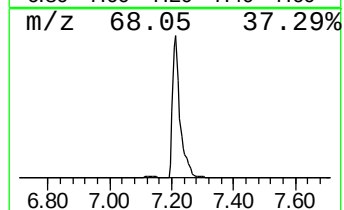
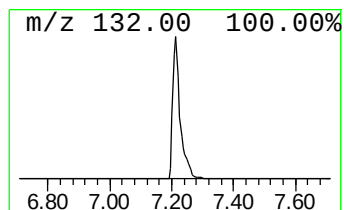
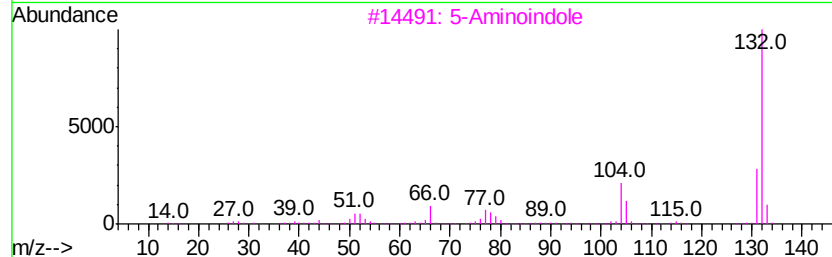
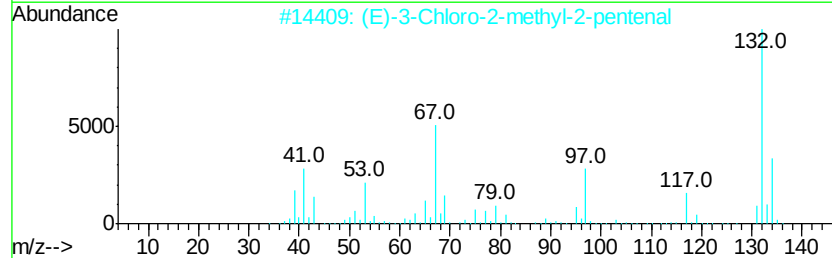
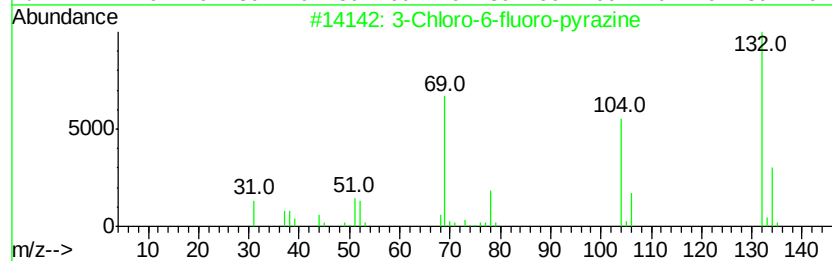
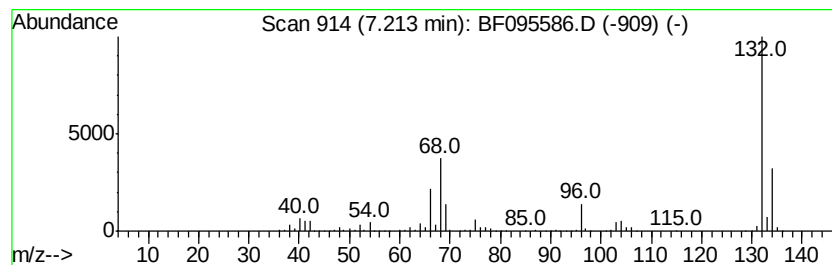
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	87.56 ng	2240310	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

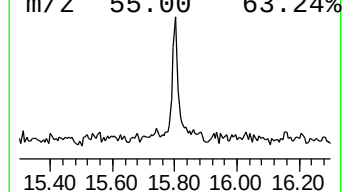
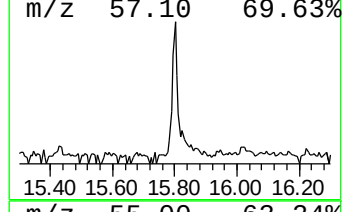
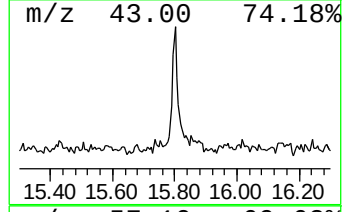
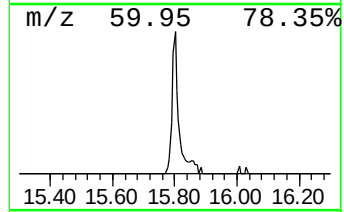
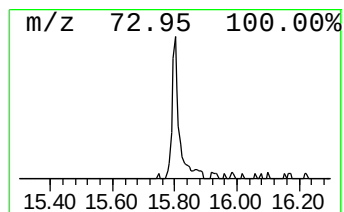
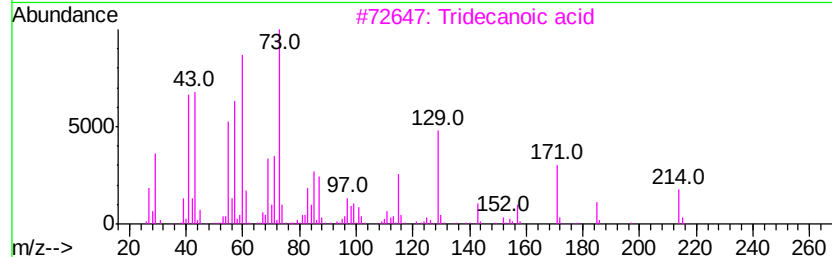
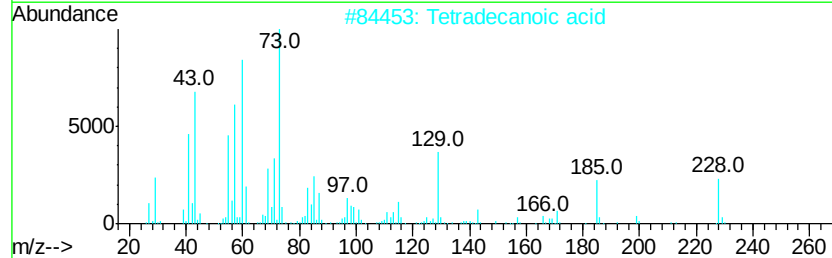
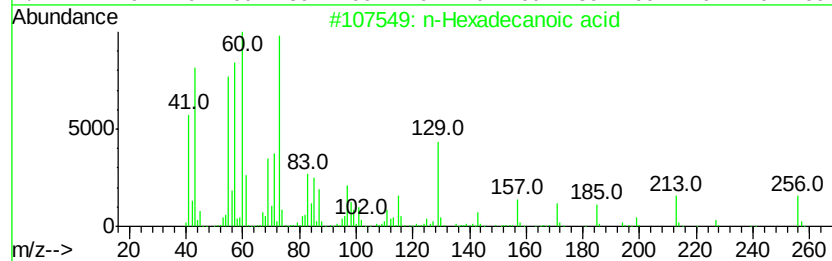
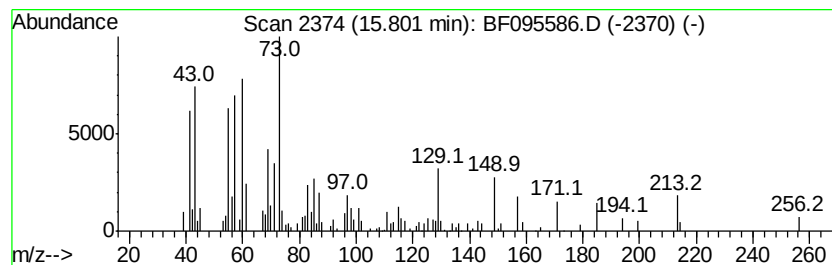
Instrument :
BNA_F
ClientSampleId :
RW-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.80	4.39 ng	126384	Phenanthrene-d10	14.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

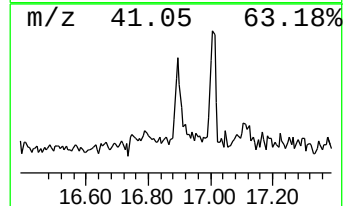
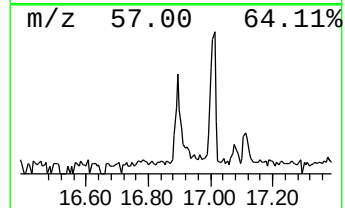
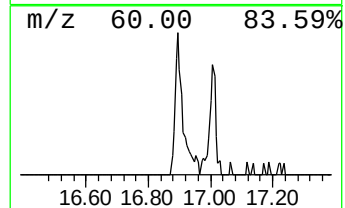
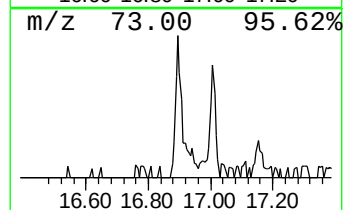
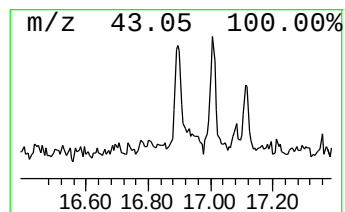
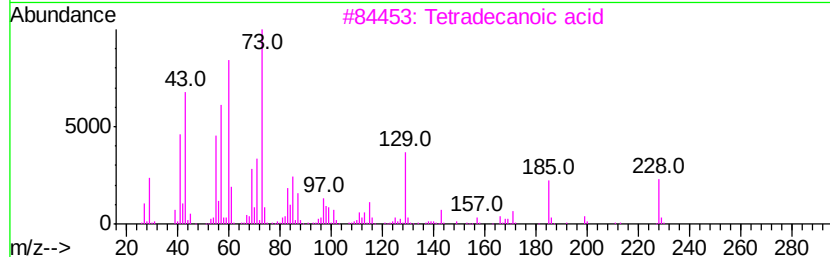
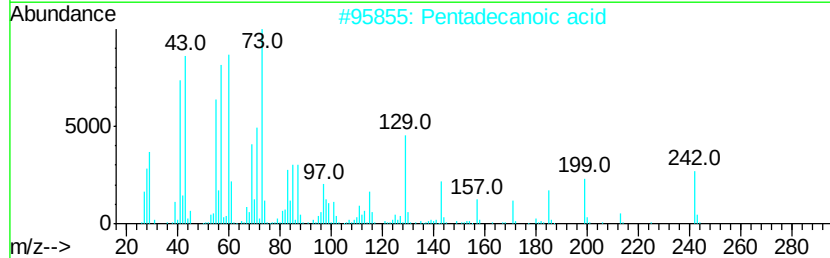
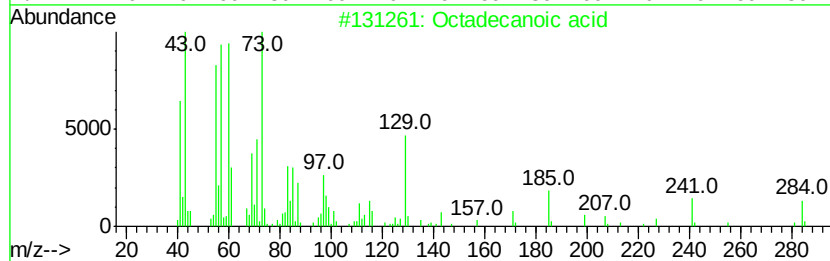
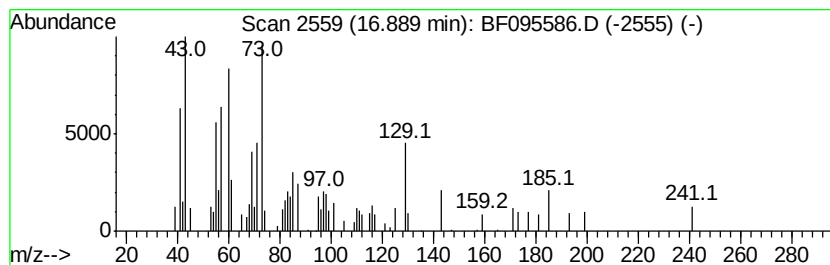
Instrument :
BNA_F
ClientSampleId :
RW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.89	3.02 ng	82262	Chrysene-d12	18.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-3

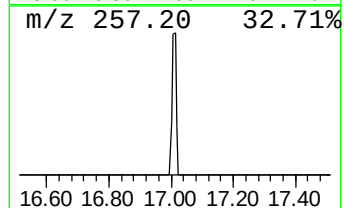
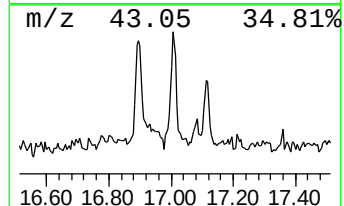
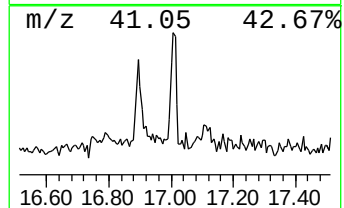
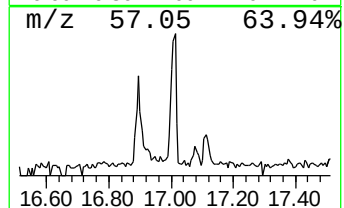
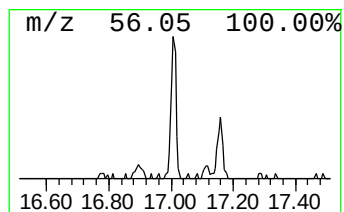
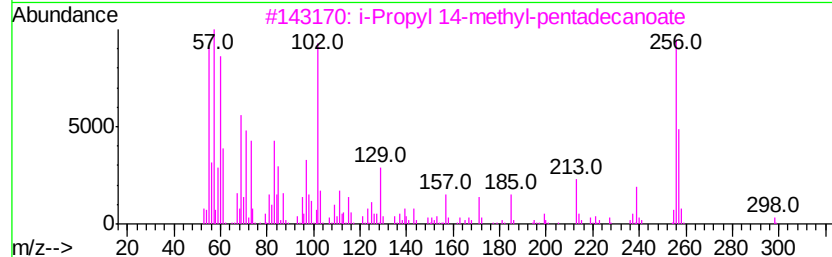
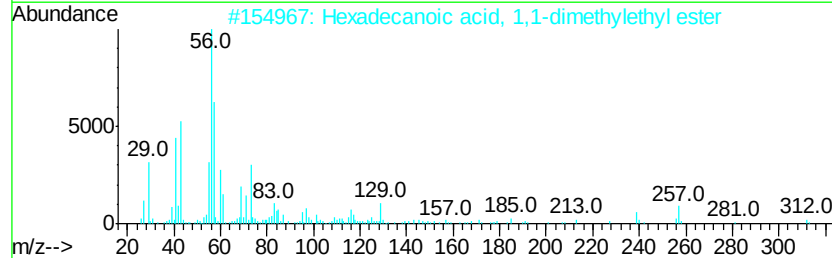
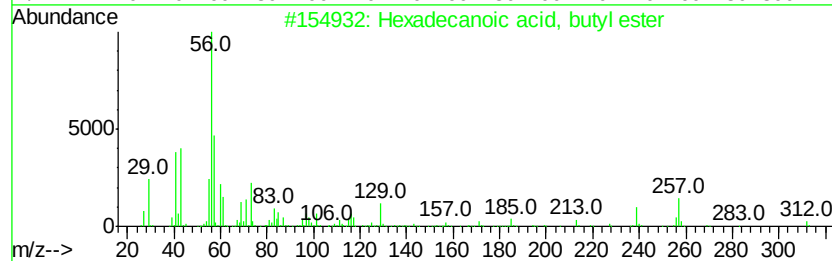
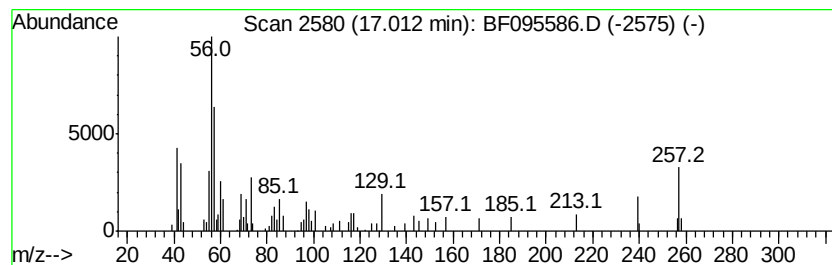
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.01	3.18 ng	86407	Chrysene-d12	18.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	25
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-3

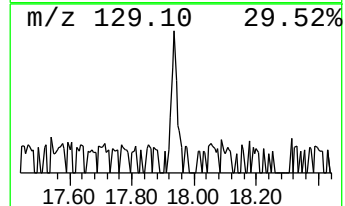
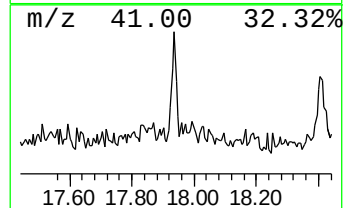
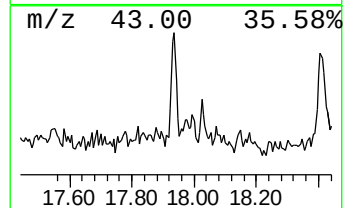
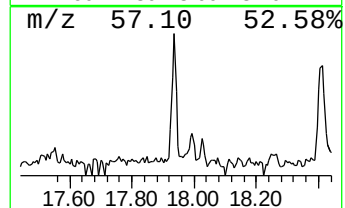
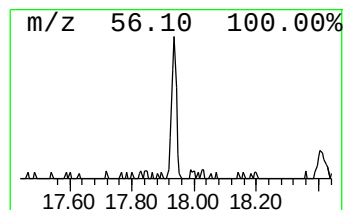
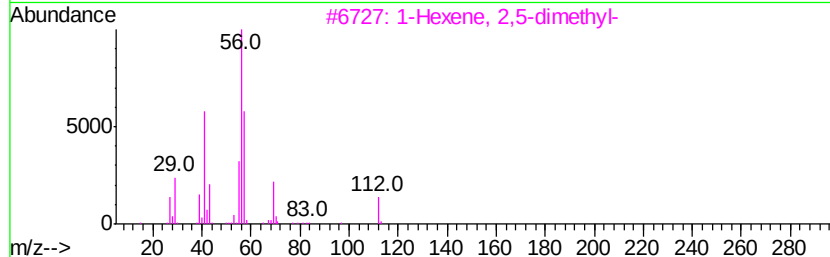
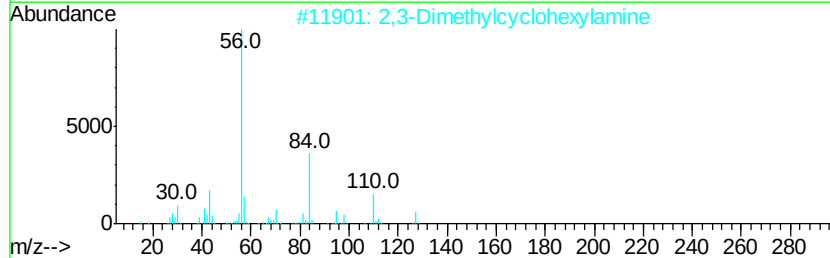
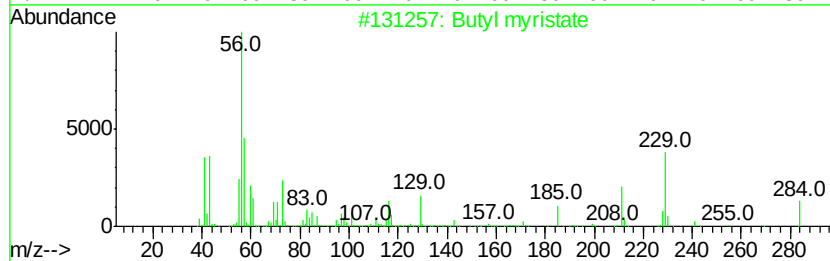
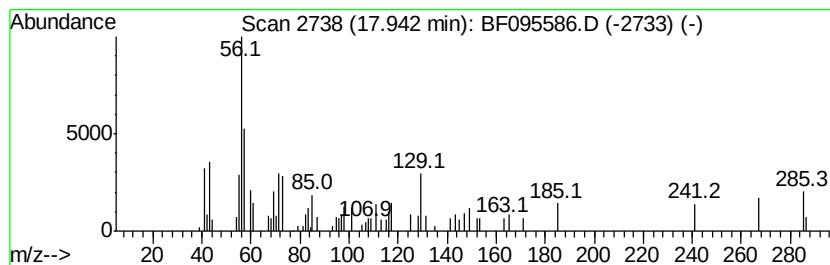
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.94 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	2.29 ng	62354	Chrysene-d12	18.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl myristate	284	C18H36O2	000110-36-1	45
2		2,3-Dimethylcyclohexylamine	127	C8H17N	042195-92-6	27
3		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27
5		Cyclohexanecarboxylic acid, 2-am...	143	C7H13NO2	005691-20-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

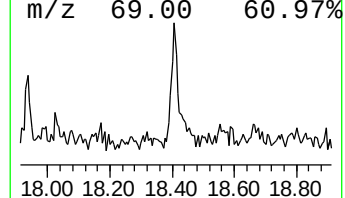
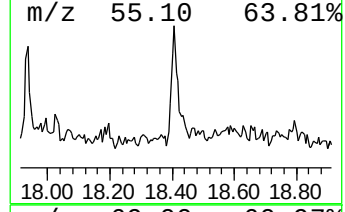
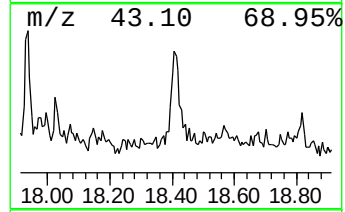
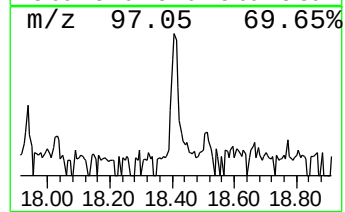
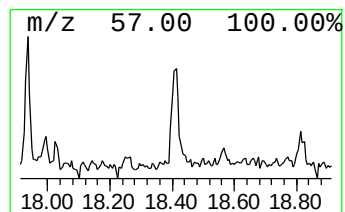
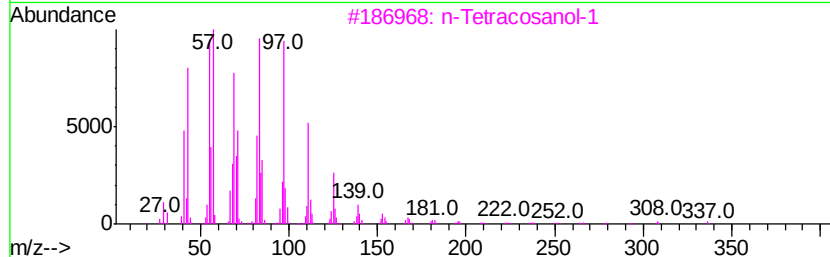
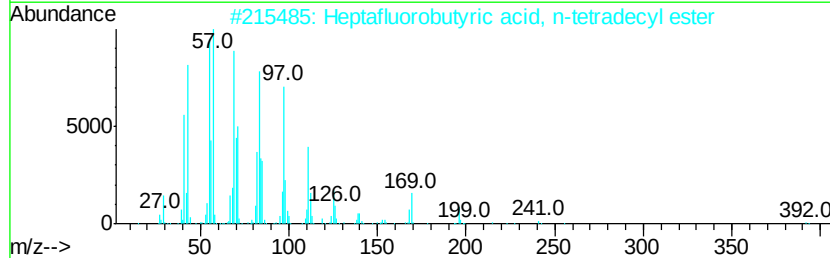
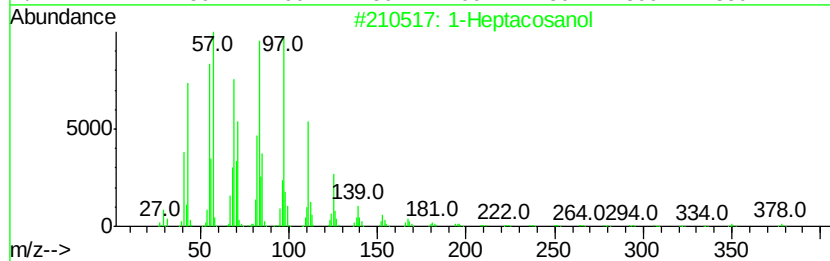
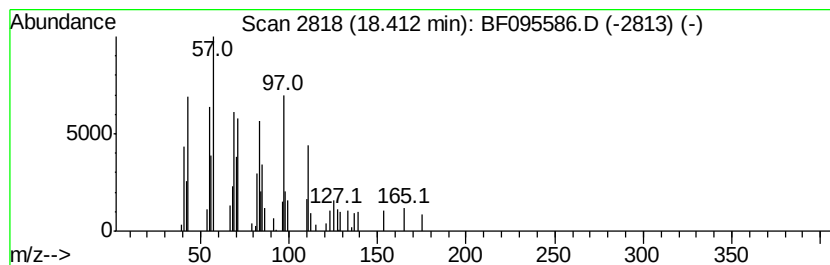
Instrument :
BNA_F
ClientSampleId :
RW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	2.27 ng	61794	Chrysene-d12	18.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	91
2	Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8	90
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	87
4	1-Heneicosanol	312 C21H44O	015594-90-8	83
5	Behenic alcohol	326 C22H46O	000661-19-8	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095586.D
Acq On : 1 Jun 2017 4:53
Operator : SJ/MA
Sample : I3355-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	2.4	ng	62100	1	7.55	511715	20.0
unknown7.21	7.21	87.6	ng	2240310	1	7.55	511715	20.0
n-Hexadecanoic acid	15.80	4.4	ng	126384	4	14.81	576055	20.0
Octadecanoic acid	16.89	3.0	ng	82262	5	18.51	544037	20.0
Hexadecanoic acid...	17.01	3.2	ng	86407	5	18.51	544037	20.0
unknown17.94	17.94	2.3	ng	62354	5	18.51	544037	20.0
1-Heptacosanol	18.41	2.3	ng	61794	5	18.51	544037	20.0