

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
 Data File : BF095789.D
 Acq On : 8 Jun 2017 18:22
 Operator : SJ/MA
 Sample : I3559-15
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BACKFILL-01

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	4.569	503	507	526	rBV	83058	222330	12.87%	1.605%
2	5.263	621	625	655	rBV	719206	1291373	74.73%	9.325%
3	6.922	903	907	919	rBV	849257	1279364	74.03%	9.238%
4	7.022	919	924	938	rVB	1055646	1492351	86.36%	10.776%
5	7.363	978	982	998	rVB	257083	357988	20.72%	2.585%
6	7.604	1017	1023	1039	rBV	787412	1095898	63.42%	7.913%
7	8.280	1133	1138	1156	rBV	556469	814794	47.15%	5.883%
8	9.398	1323	1328	1341	rBV	353306	494940	28.64%	3.574%
9	11.180	1623	1631	1642	rBV	1181276	1728135	100.00%	12.478%
10	11.874	1744	1749	1760	rBV	129367	170296	9.85%	1.230%
11	12.221	1801	1808	1814	rBV2	409989	565765	32.74%	4.085%
12	13.080	1946	1954	1958	rBV	18865	25021	1.45%	0.181%
13	13.515	2023	2028	2044	rBV	665123	886656	51.31%	6.402%
14	13.851	2080	2085	2092	rBV2	17380	26096	1.51%	0.188%
15	14.615	2210	2215	2230	rVB	396723	565415	32.72%	4.083%
16	16.992	2613	2619	2623	rBV	1391455	1637683	94.77%	11.825%
17	18.244	2828	2832	2842	rBV2	55479	80718	4.67%	0.583%
18	18.327	2842	2846	2857	rVB	431896	526964	30.49%	3.805%
19	19.480	3038	3042	3046	rVB	80085	84796	4.91%	0.612%
20	19.997	3125	3130	3142	rBV	340232	447837	25.91%	3.234%
21	20.450	3199	3207	3211	rBV2	31638	54615	3.16%	0.394%

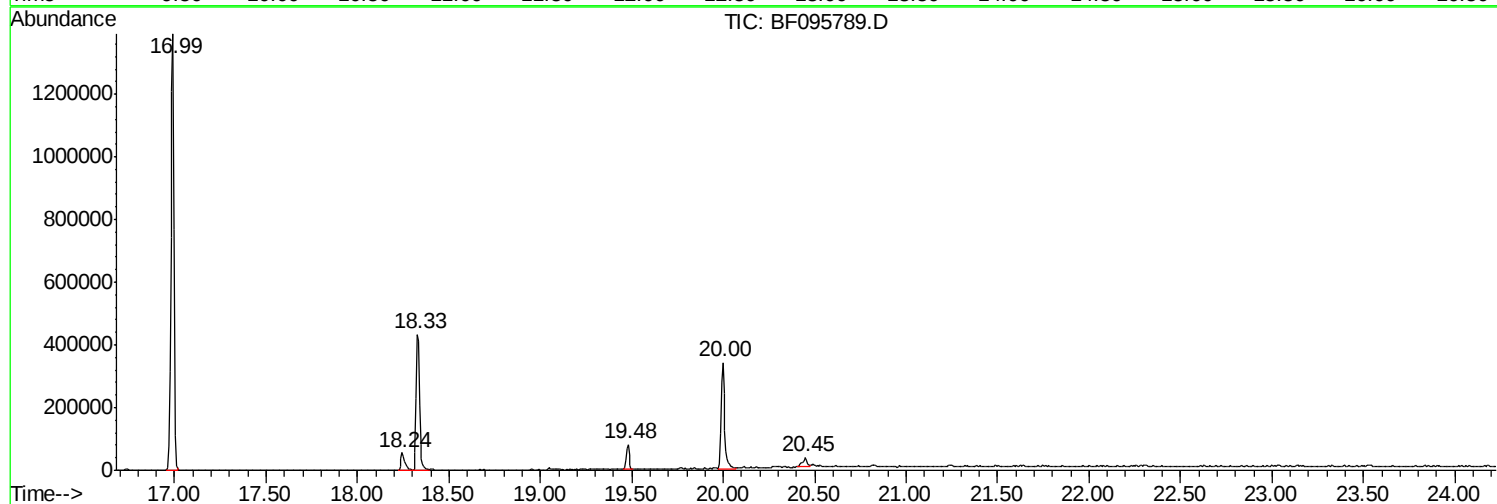
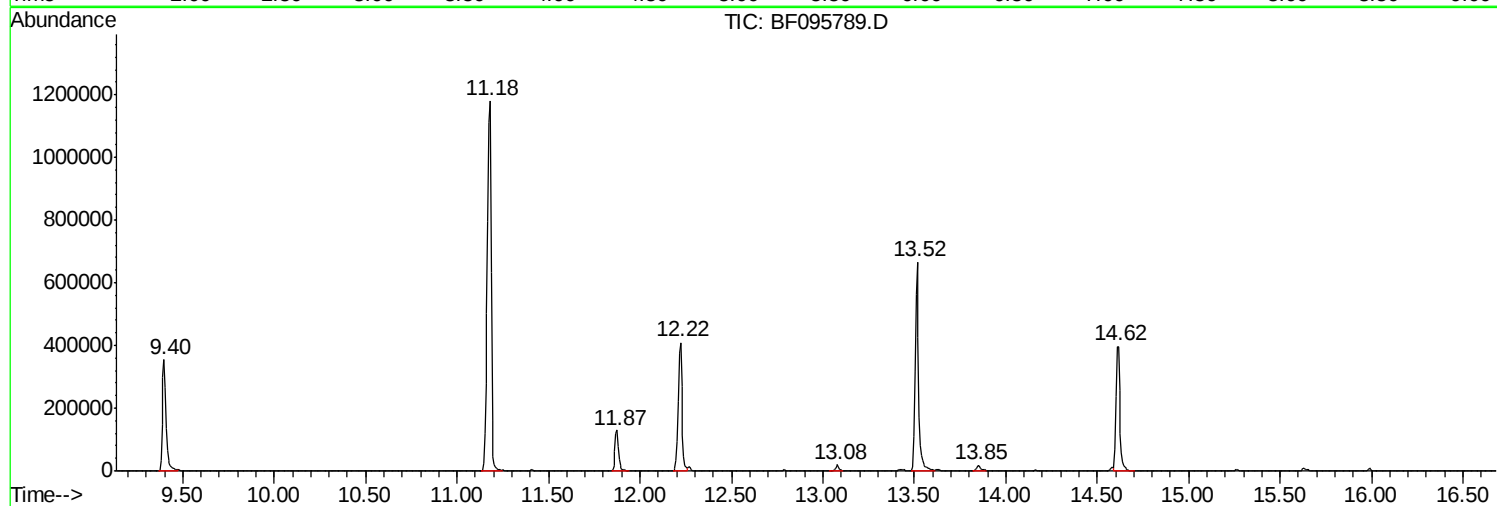
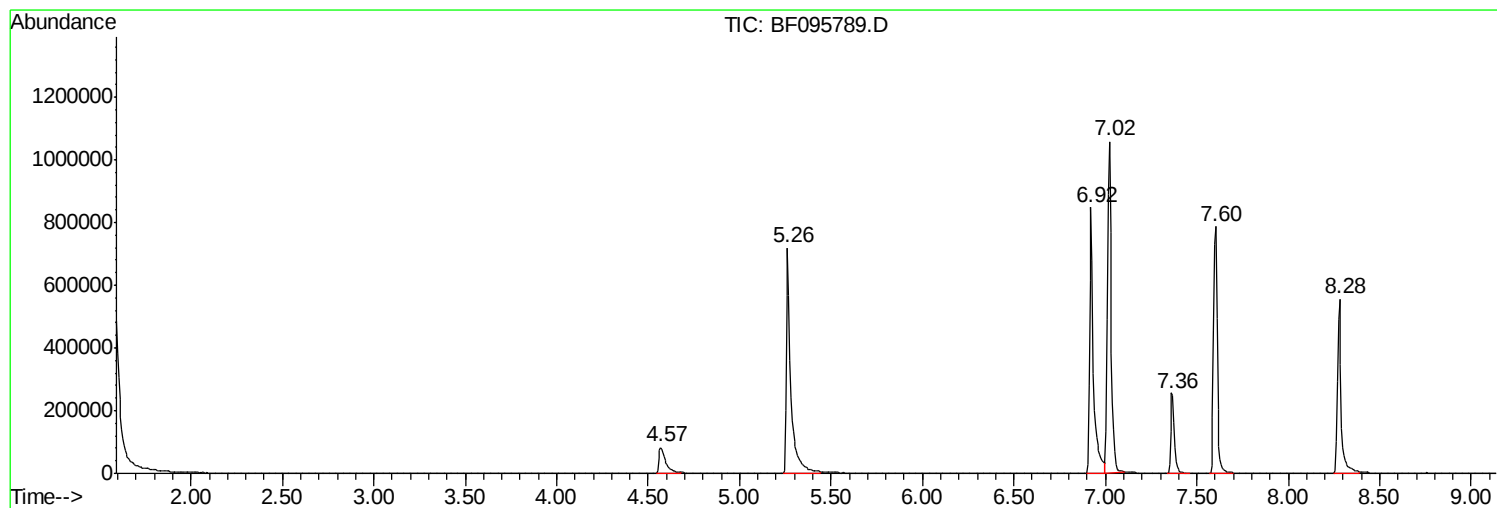
Sum of corrected areas: 13849035

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

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 : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

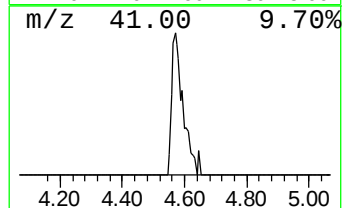
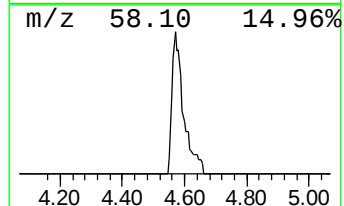
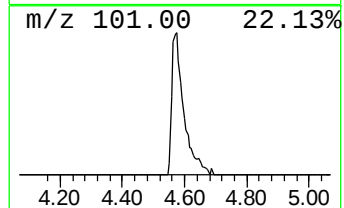
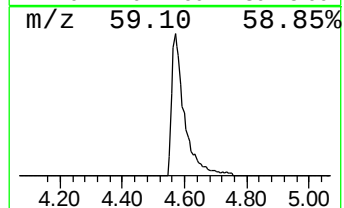
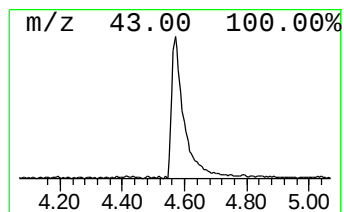
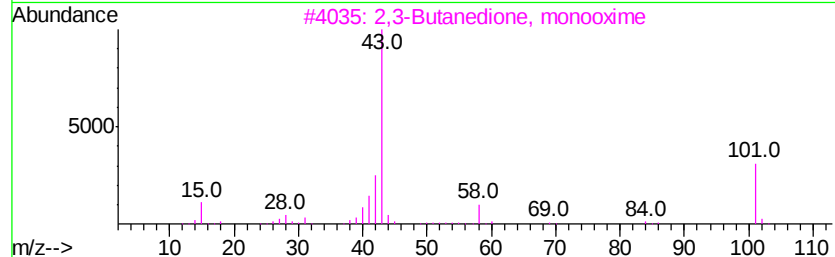
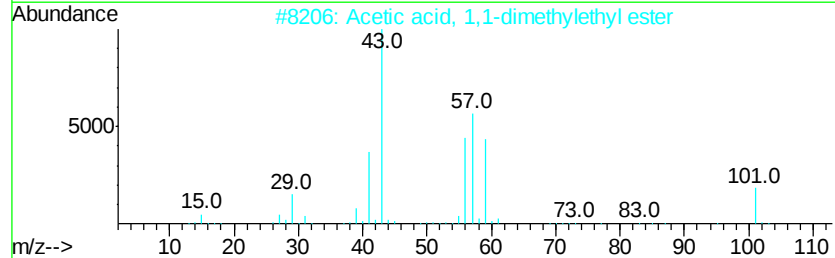
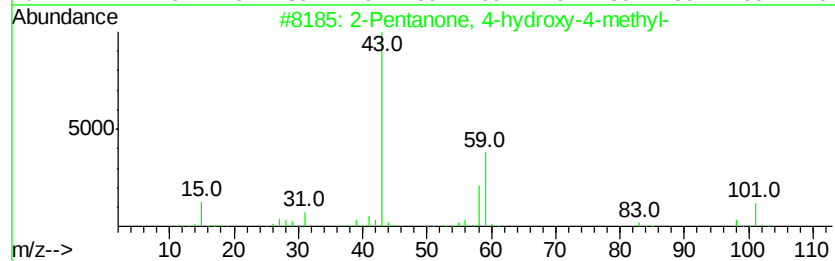
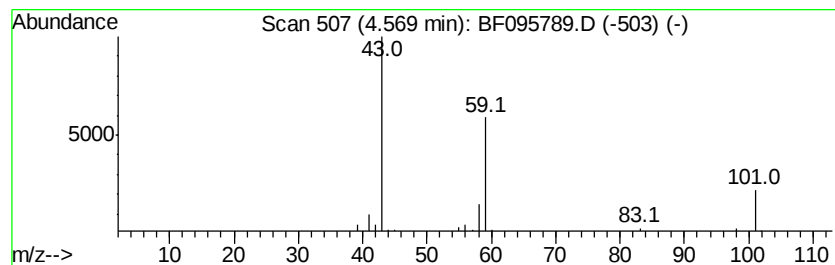
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	12.42 ng	222330	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

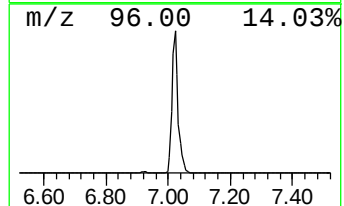
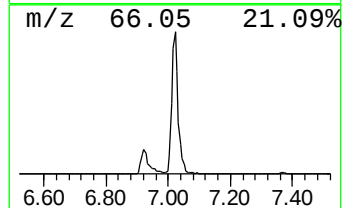
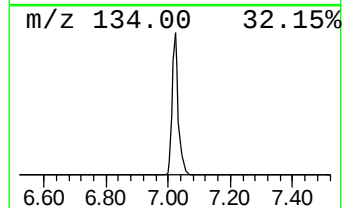
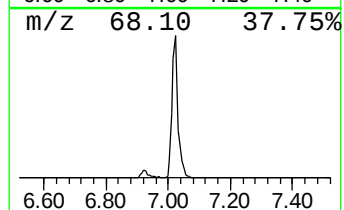
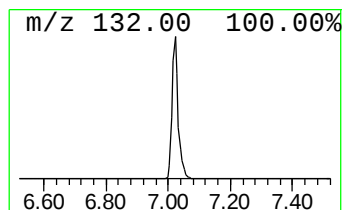
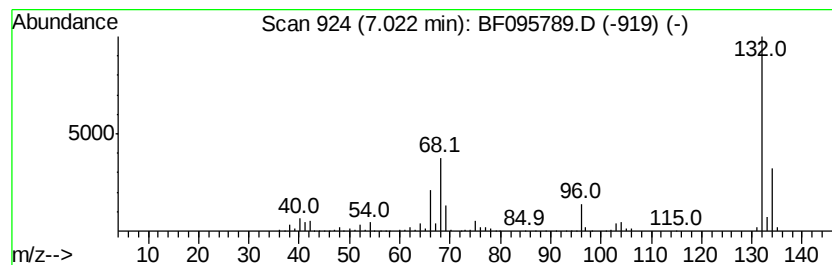
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	83.37 ng	1492350	1,4-Dichlorobenzene-d4	7.36

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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

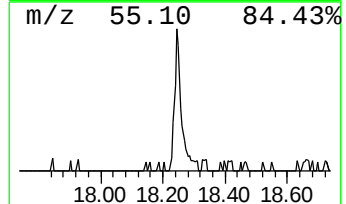
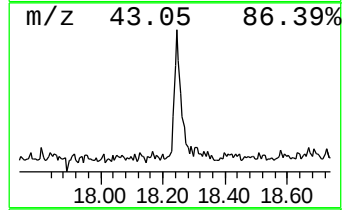
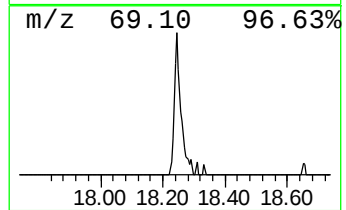
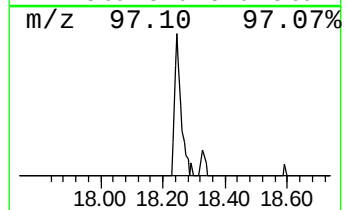
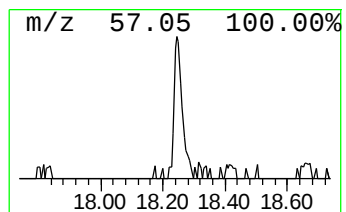
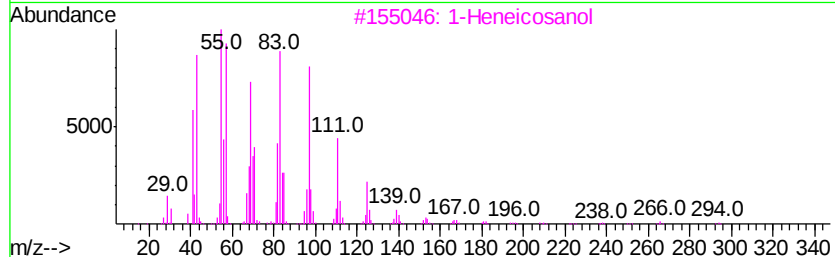
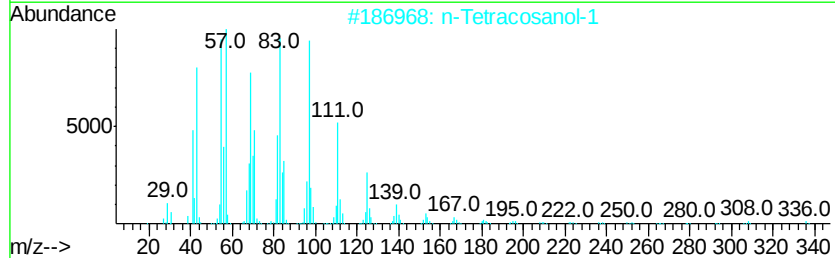
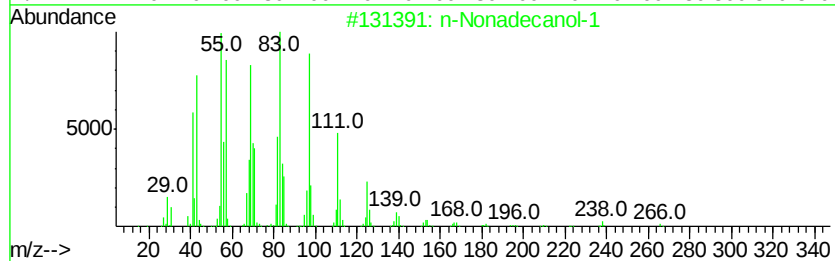
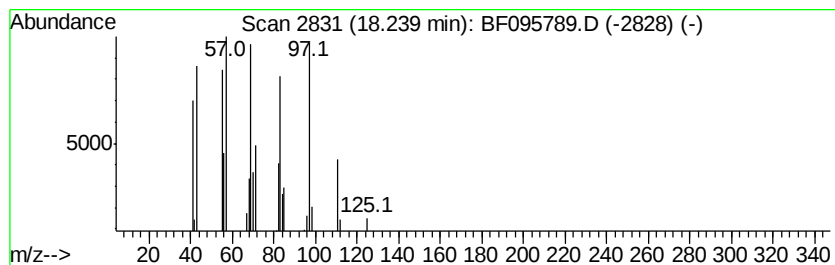
Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

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 4 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.24	3.06 ng	80718	Chrysene-d12	18.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

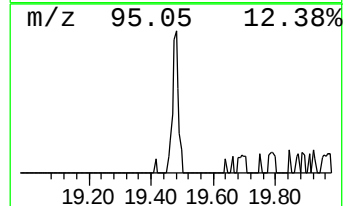
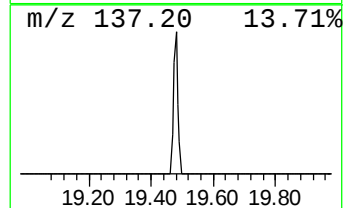
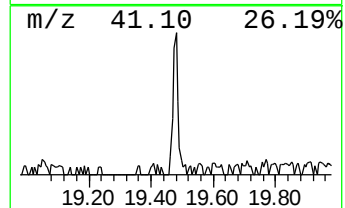
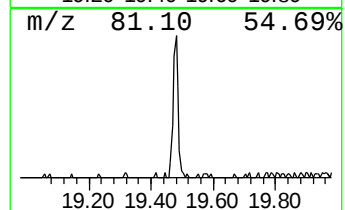
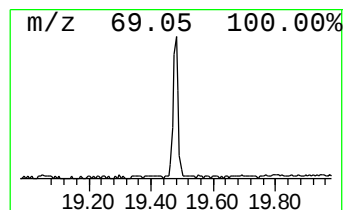
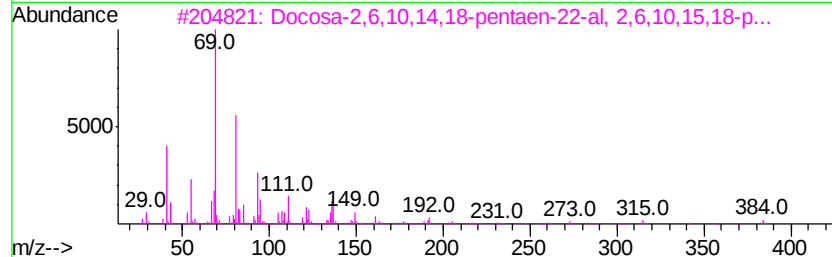
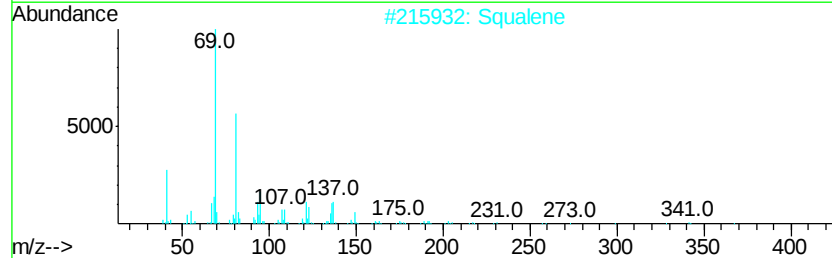
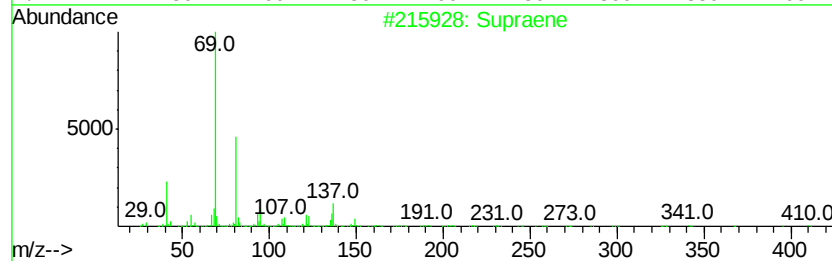
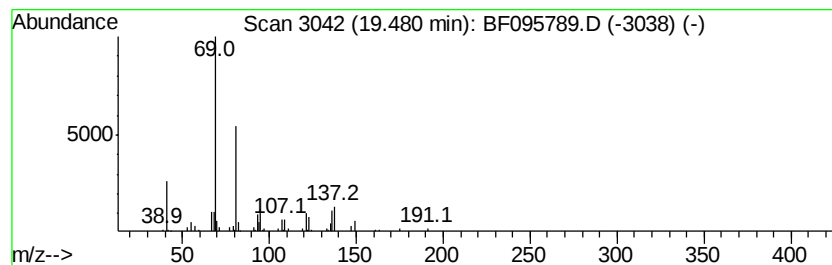
Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

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 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.48	3.79 ng	84796	Perylene-d12	20.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene		410 C30H50	007683-64-9 91
2	Squalene		410 C30H50	000111-02-4 91
3	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 90
4	Farnesol (E), methyl ether		236 C16H28O	1000352-67-3 72
5	Trifluoroacetyl-lavandulol		250 C12H17F3O2	028673-24-7 64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

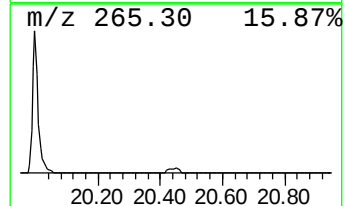
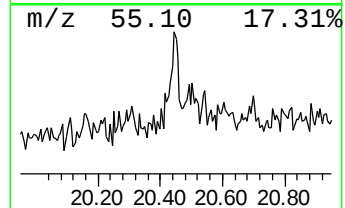
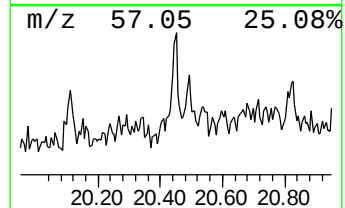
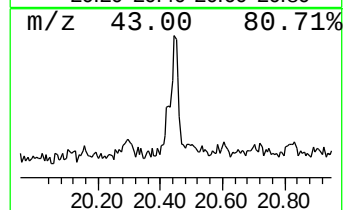
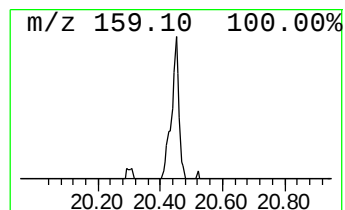
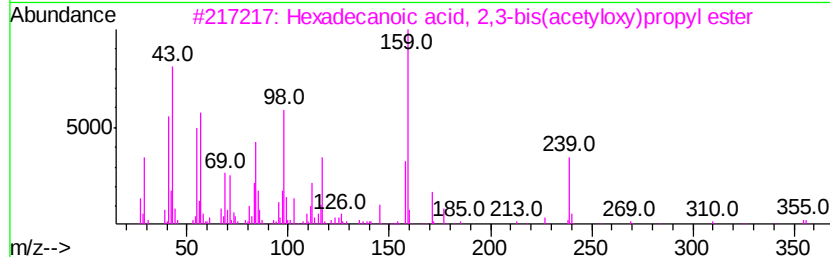
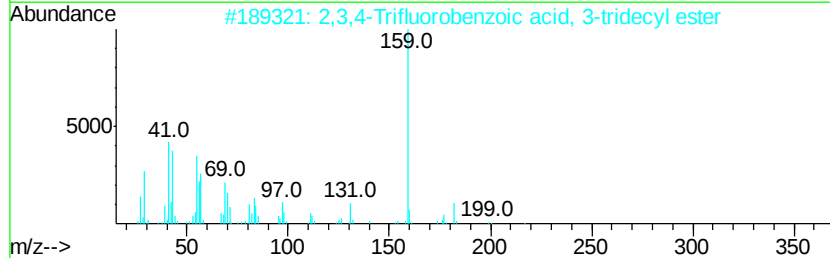
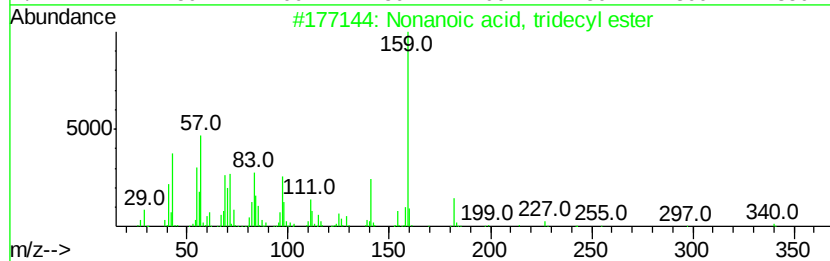
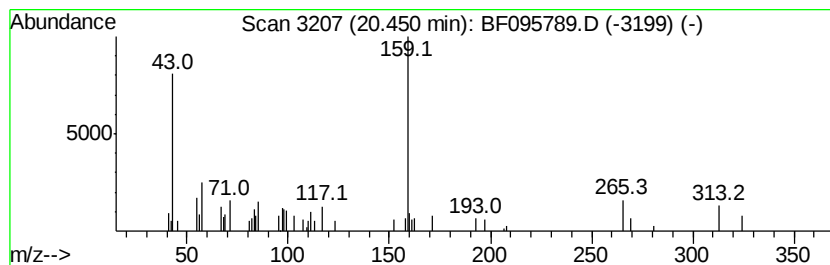
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonanoic acid, tridecyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.45	2.44 ng	54615	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid, tridecyl ester	340	C22H44O2	1000340-28-0	53
2		2,3,4-Trifluorobenzoic acid, 3-t...	358	C20H29F3O2	1000280-61-8	53
3		Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	50
4		2,4-Difluorobenzoic acid, heptad...	396	C24H38F2O2	1000338-79-5	50
5		2,4-Difluorobenzoic acid, nonade...	424	C26H42F2O2	1000338-79-7	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095789.D
Acq On : 8 Jun 2017 18:22
Operator : SJ/MA
Sample : I3559-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.57	12.4	ng	222330	1	7.36	357988	20.0
unknown7.02	7.02	83.4	ng	1492350	1	7.36	357988	20.0
n-Nonadecanol-1	18.24	3.1	ng	80718	5	18.33	526964	20.0
Supraene	19.48	3.8	ng	84796	6	20.00	447837	20.0
Nonanoic acid, tr...	20.45	2.4	ng	54615	6	20.00	447837	20.0