

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
 Data File : BF099562.D
 Acq On : 16 Oct 2017 23:40
 Operator : SJ/JU
 Sample : I5782-10
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S5(10-12)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	5.069	504	507	522	rBV	237428	326146	14.68%	1.717%
2	5.469	571	575	593	rBV	1935700	1866699	84.01%	9.828%
3	6.481	742	747	761	rBV	1823200	1954922	87.98%	10.292%
4	6.616	766	770	773	rBV	2181053	1924689	86.62%	10.133%
5	6.839	805	808	817	rVB	668824	609214	27.42%	3.207%
6	6.998	831	835	838	rBV	1819553	1532089	68.95%	8.066%
7	7.410	900	905	908	rBV	1265777	1154895	51.98%	6.080%
8	8.122	1023	1026	1030	rBV	916514	826555	37.20%	4.352%
9	9.198	1204	1209	1212	rBV	2588514	2222003	100.00%	11.698%
10	9.592	1272	1276	1286	rBV	637150	498051	22.41%	2.622%
11	9.880	1321	1325	1329	rBV	1057808	892933	40.19%	4.701%
12	10.592	1443	1446	1451	rBB	89689	68313	3.07%	0.360%
13	10.669	1455	1459	1474	rBV	1119664	1101346	49.57%	5.798%
14	11.369	1574	1578	1585	rBV	995120	820581	36.93%	4.320%
15	12.951	1843	1847	1850	rBV	1865265	1627683	73.25%	8.569%
16	13.833	1993	1997	2006	rBV2	36318	59761	2.69%	0.315%
17	14.015	2024	2028	2035	rBV	558680	546688	24.60%	2.878%
18	14.833	2164	2167	2171	rVB	34157	30614	1.38%	0.161%
19	15.092	2207	2211	2215	rBV	24720	25408	1.14%	0.134%
20	15.486	2271	2278	2288	rBV	441061	591244	26.61%	3.113%
21	15.898	2340	2348	2353	rBV	48391	75738	3.41%	0.399%
22	16.398	2427	2433	2440	rVB	44686	76664	3.45%	0.404%
23	16.980	2526	2532	2542	rVB2	33314	68812	3.10%	0.362%
24	17.668	2643	2649	2656	rVB3	24295	52018	2.34%	0.274%
25	18.492	2784	2789	2800	rVB5	14353	41158	1.85%	0.217%

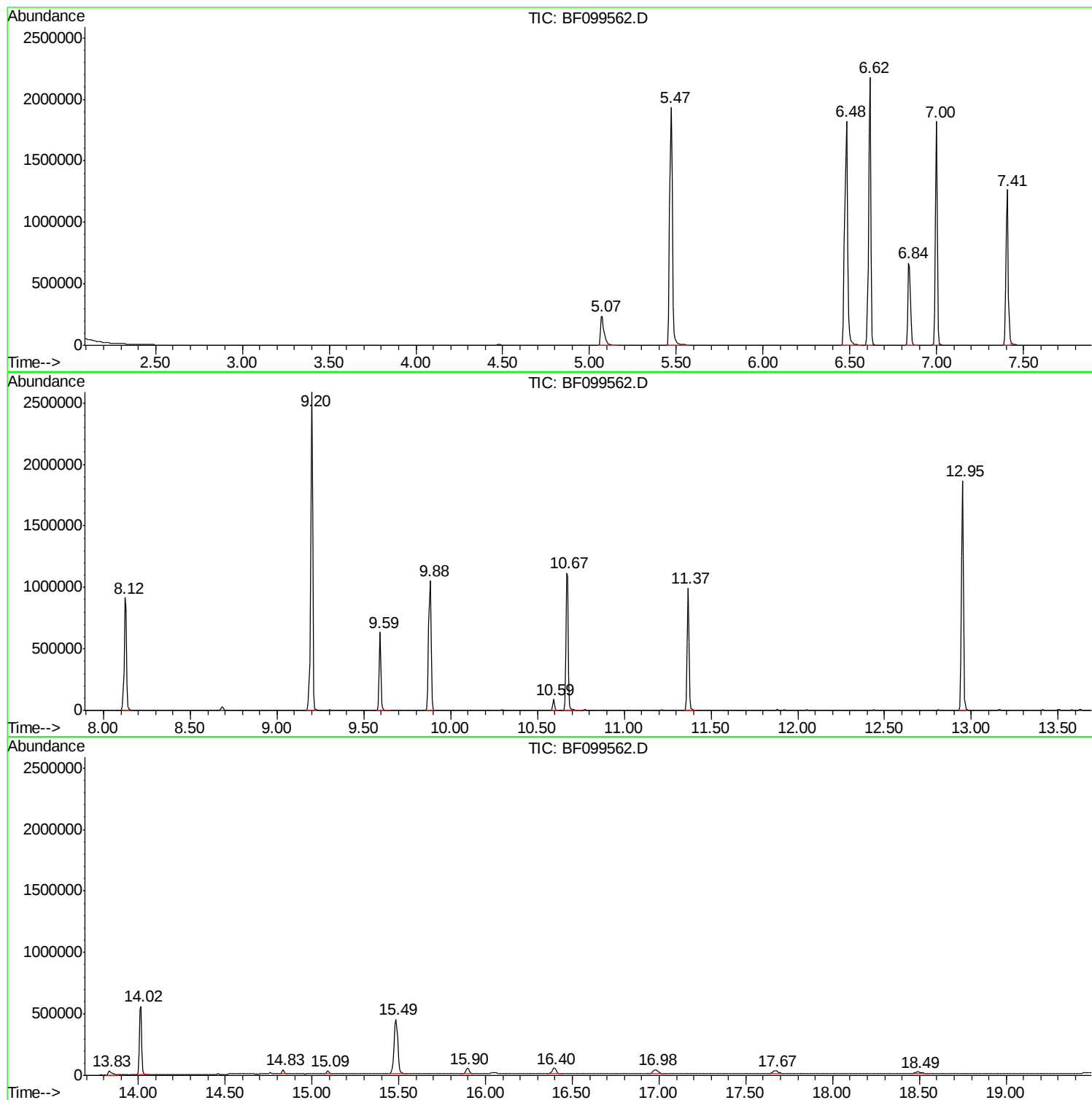
Sum of corrected areas: 18994224

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S5(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S5(10-12)

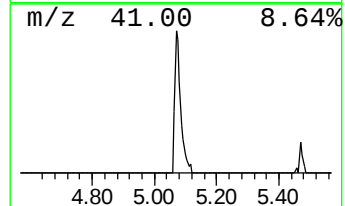
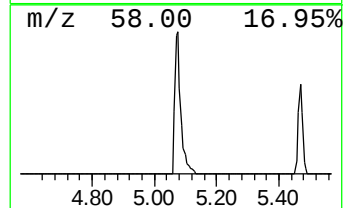
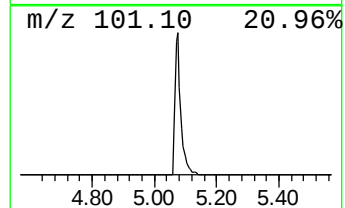
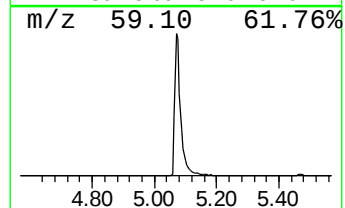
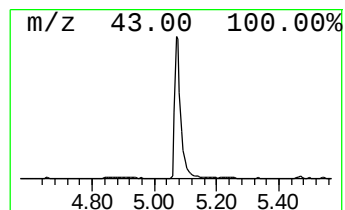
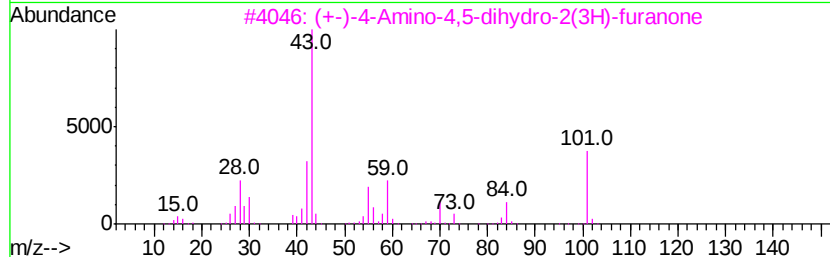
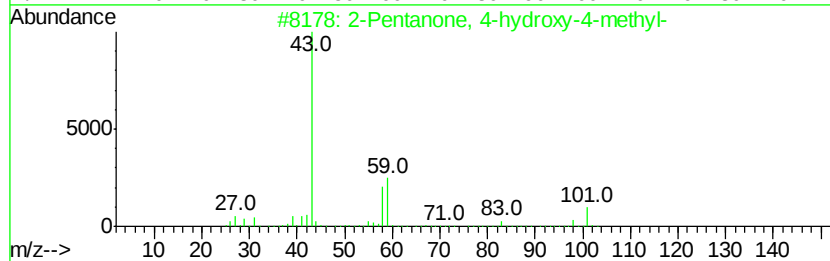
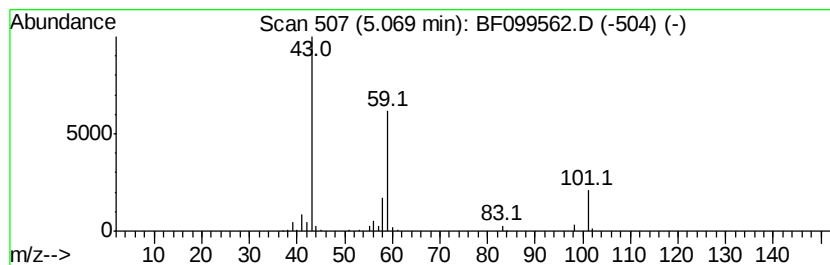
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.07	10.71 ng	326146	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	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\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S5(10-12)

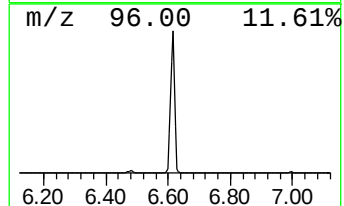
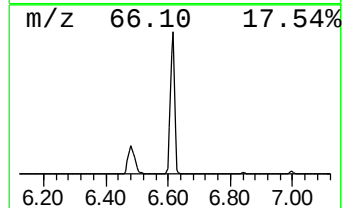
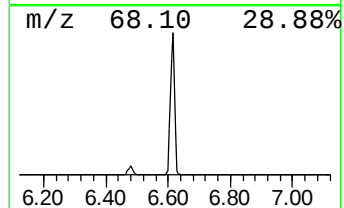
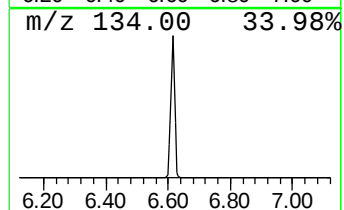
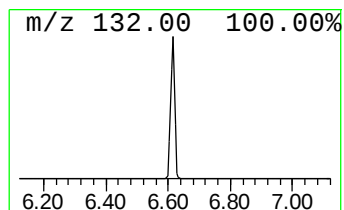
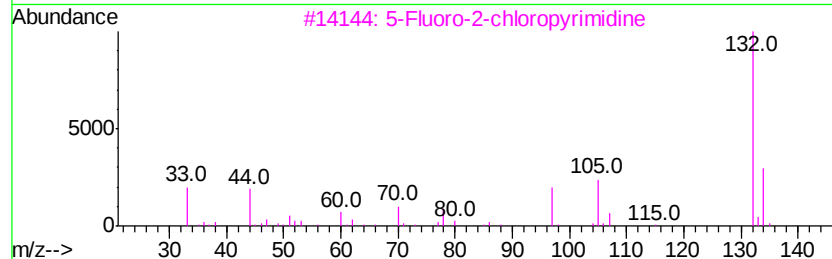
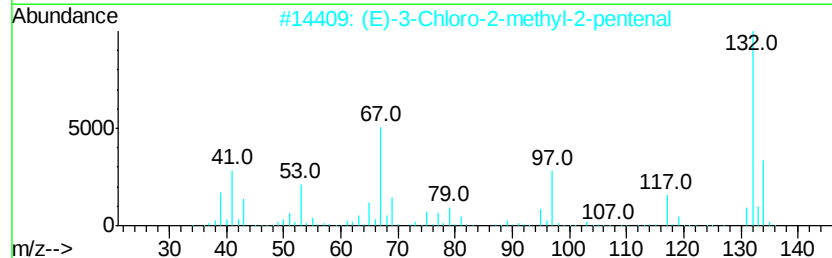
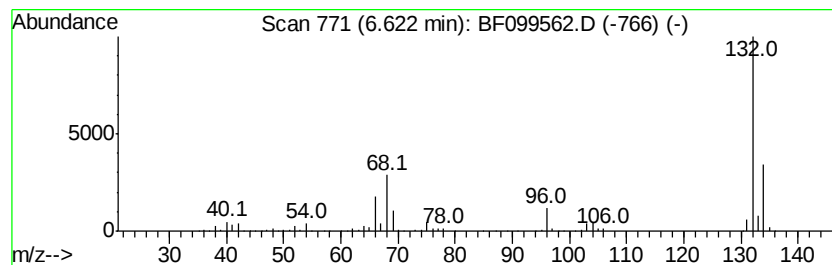
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	63.19 ng	1924690	1,4-Dichlorobenzene-d4	6.84

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

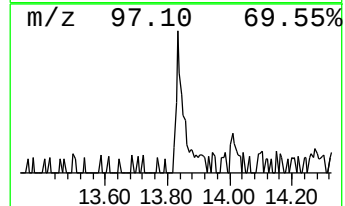
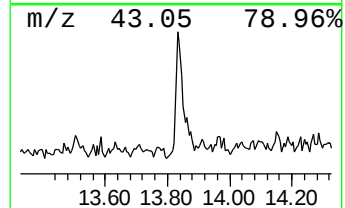
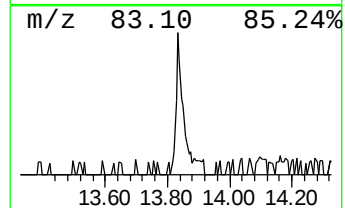
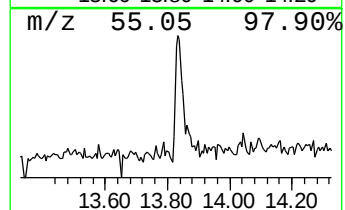
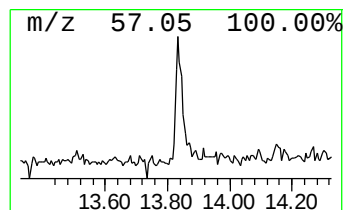
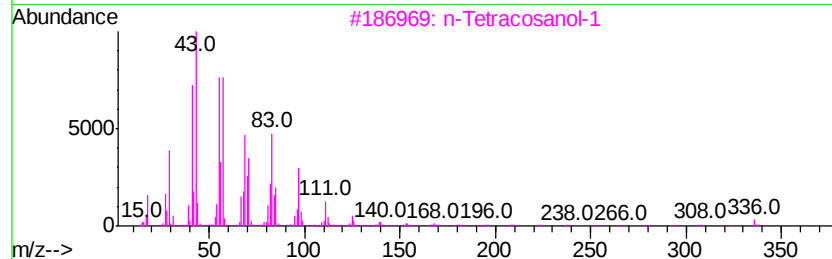
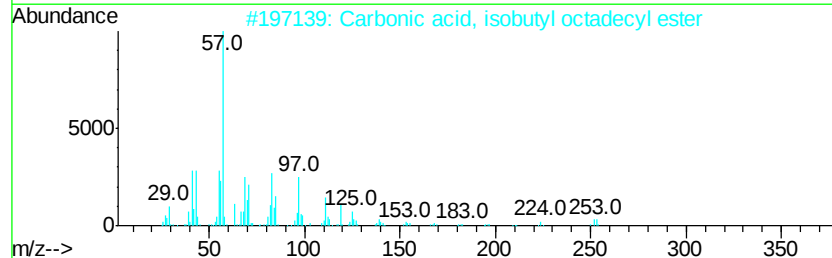
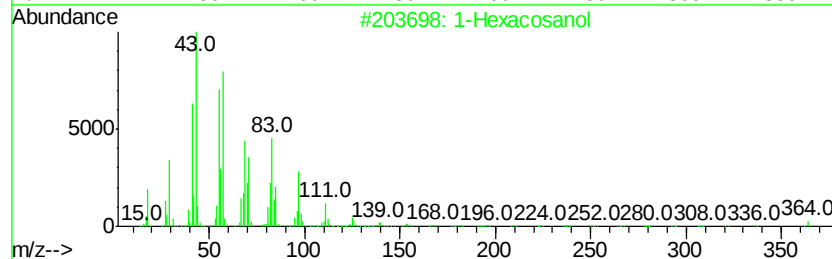
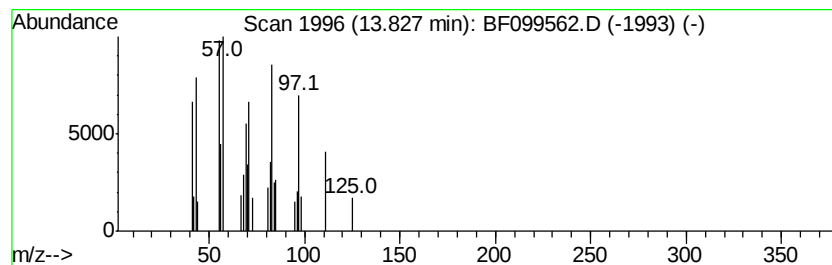
Instrument :
BNA_F
ClientSampleId :
S5(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.19 ng	59761	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexacosanol	382 C26H54O	000506-52-5	72
2	Carbonic acid, isobutyl octadecyl...	370 C23H46O3	1000314-61-5	58
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	53
4	2-Ethyl-1-dodecanol	214 C14H30O	019780-33-7	35
5	Cyclopentane, 1,1,3,4-tetramethy...	126 C9H18	020309-77-7	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S5(10-12)

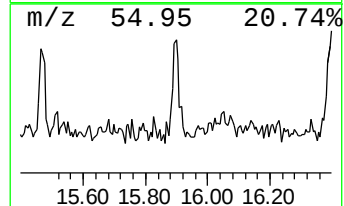
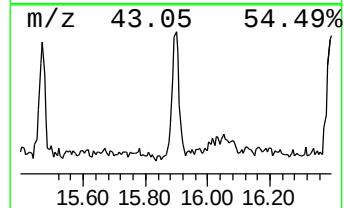
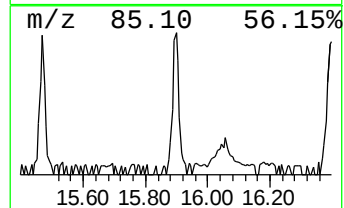
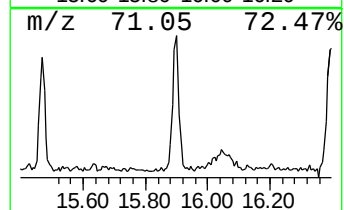
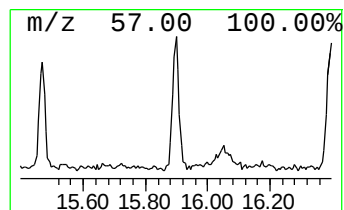
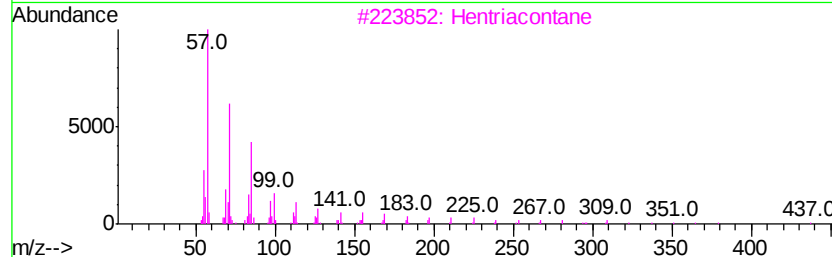
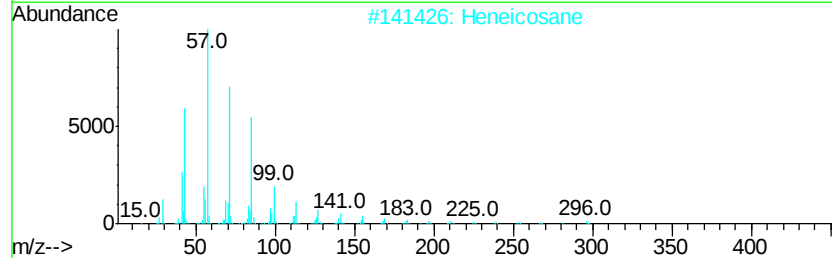
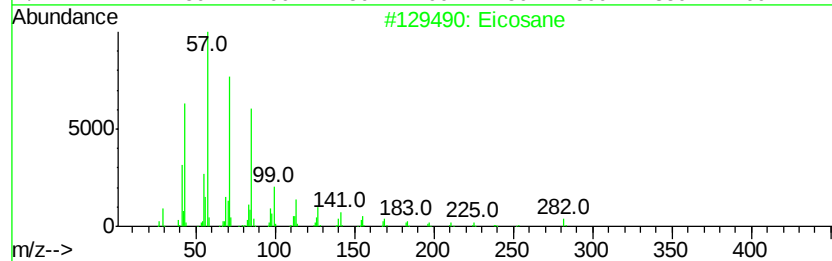
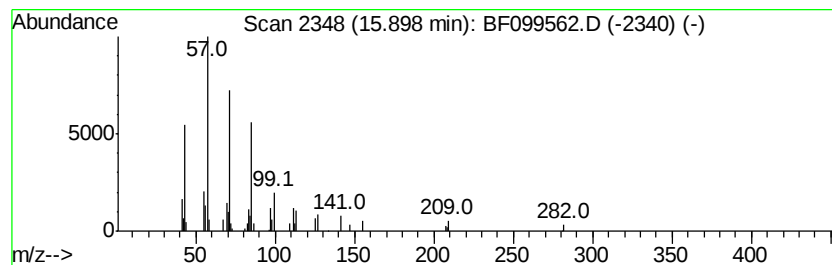
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	2.56 ng	75738	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	96
2	Heneicosane		296	C21H44	000629-94-7	90
3	Hentriacontane		437	C31H64	000630-04-6	87
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
5	Triacontane		422	C30H62	000638-68-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S5(10-12)

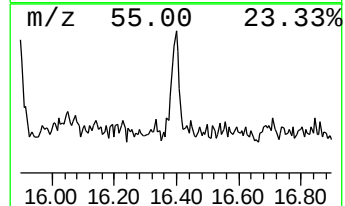
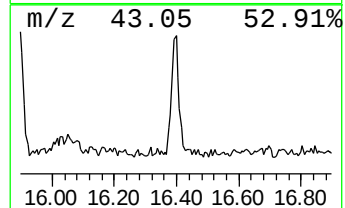
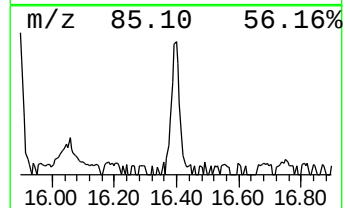
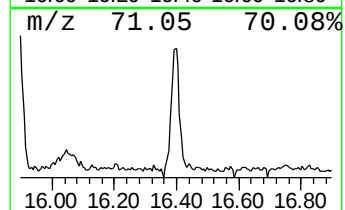
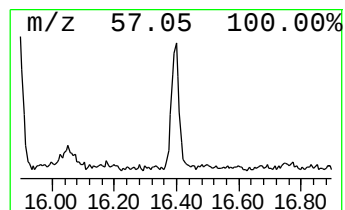
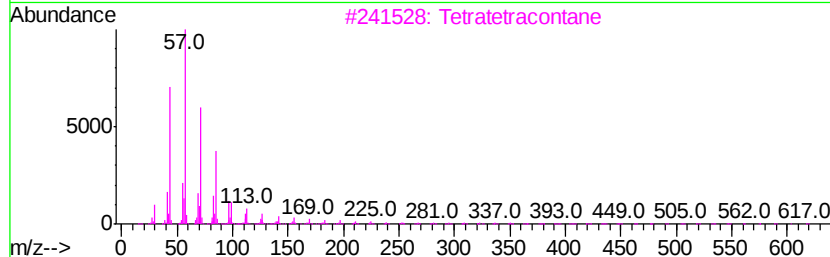
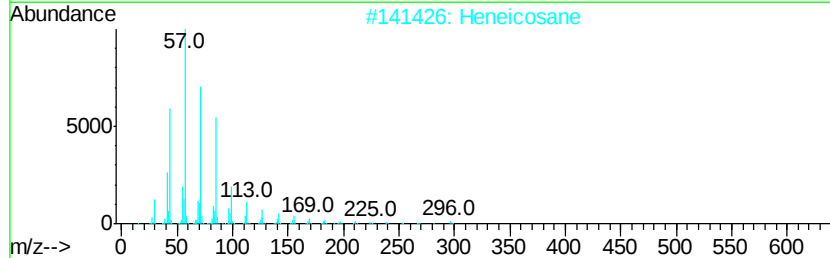
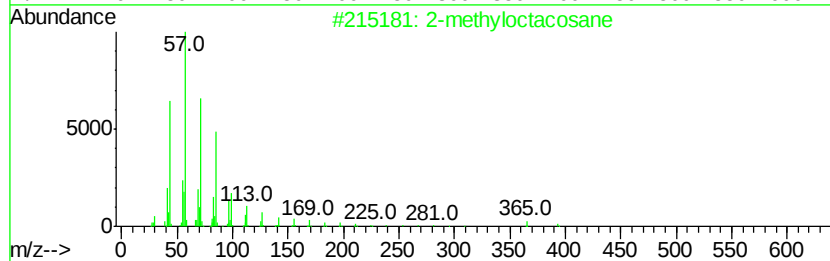
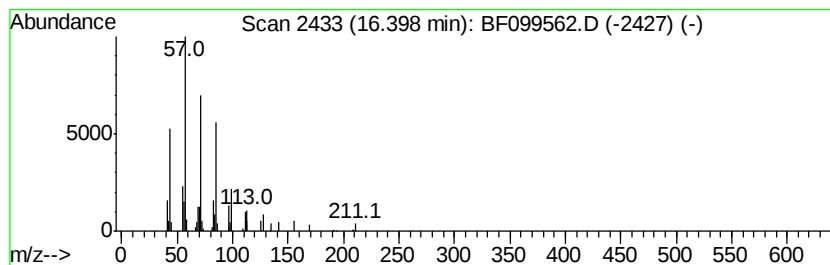
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.59 ng	76664	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tetratetracontane	619	C44H90	007098-22-8	87
4		Triacontane	422	C30H62	000638-68-6	86
5		10-Methylnonadecane	282	C20H42	056862-62-5	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099562.D
Acq On : 16 Oct 2017 23:40
Operator : SJ/JU
Sample : I5782-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S5(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.07	10.7	ng	326146	1	6.84	609214	20.0
unknown6.62	6.62	63.2	ng	1924690	1	6.84	609214	20.0
1-Hexacosanol	13.83	2.2	ng	59761	5	14.02	546688	20.0
Eicosane	15.90	2.6	ng	75738	6	15.49	591244	20.0
2-methyloctacosane	16.40	2.6	ng	76664	6	15.49	591244	20.0