

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
 Data File : BF104365.D
 Acq On : 9 Apr 2018 12:12
 Operator : JU/SJ
 Sample : J2148-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4C

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-BF040618.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	5.034	497	501	511	rVB	162344	246012	5.27%	0.600%
2	5.422	560	567	570	rBV	3734632	4403663	94.37%	10.735%
3	6.439	732	740	743	rBV	3615514	4415984	94.63%	10.765%
4	6.575	757	763	766	rBV	3861792	4452362	95.41%	10.854%
5	6.804	798	802	805	rBV	1088546	850365	18.22%	2.073%
6	6.963	824	829	832	rBV	3651202	3416039	73.20%	8.328%
7	7.375	892	899	901	rBV	2461279	2895805	62.06%	7.059%
8	8.086	1012	1020	1023	rBV	1388153	1169947	25.07%	2.852%
9	9.169	1198	1204	1207	rBV	4339747	4666440	100.00%	11.376%
10	9.369	1233	1238	1241	rBV	140168	110867	2.38%	0.270%
11	9.557	1266	1270	1273	rBV	404079	343100	7.35%	0.836%
12	9.769	1304	1306	1311	rVB	115432	98327	2.11%	0.240%
13	9.839	1311	1318	1322	rBV	1426107	1277781	27.38%	3.115%
14	10.274	1389	1392	1394	rVB	140159	118970	2.55%	0.290%
15	10.492	1424	1429	1432	rBV	53774	70553	1.51%	0.172%
16	10.633	1447	1453	1456	rBV	2779803	2957496	63.38%	7.210%
17	10.745	1469	1472	1482	rVB	158956	186751	4.00%	0.455%
18	11.192	1545	1548	1551	rBV2	94234	85016	1.82%	0.207%
19	11.221	1551	1553	1559	rVB	52980	56173	1.20%	0.137%
20	11.327	1567	1571	1574	rBV	1382344	1179568	25.28%	2.876%
21	11.351	1574	1575	1577	rVB	131539	60877	1.30%	0.148%
22	11.621	1618	1621	1624	rVB	77662	59920	1.28%	0.146%
23	11.857	1658	1661	1670	rBV2	601865	645678	13.84%	1.574%
24	12.027	1688	1690	1693	rVB2	51463	47194	1.01%	0.115%
25	12.074	1695	1698	1704	rVB7	52817	66674	1.43%	0.163%
26	12.186	1714	1717	1719	rBV	93807	84367	1.81%	0.206%
27	12.274	1730	1732	1735	rVB	83250	63897	1.37%	0.156%
28	12.539	1774	1777	1780	rBV	275934	213494	4.58%	0.520%
29	12.645	1792	1795	1800	rBV2	141304	149277	3.20%	0.364%
30	12.768	1813	1816	1819	rVB	229310	173400	3.72%	0.423%
31	12.921	1837	1842	1845	rBV	3509004	3572029	76.55%	8.708%
32	13.810	1990	1993	2003	rVB	461080	510941	10.95%	1.246%
33	13.968	2016	2020	2023	rBV	914285	893933	19.16%	2.179%
34	15.004	2194	2196	2205	rVB	128159	263556	5.65%	0.643%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.362	2255	2257	2260	rBV	81322	86825	1.86%	0.212%
36	15.433	2265	2269	2272	rBV	638895	733474	15.72%	1.788%
37	15.945	2353	2356	2365	rVB6	130177	247555	5.31%	0.603%
38	17.456	2609	2613	2620	rVB9	74354	145893	3.13%	0.356%

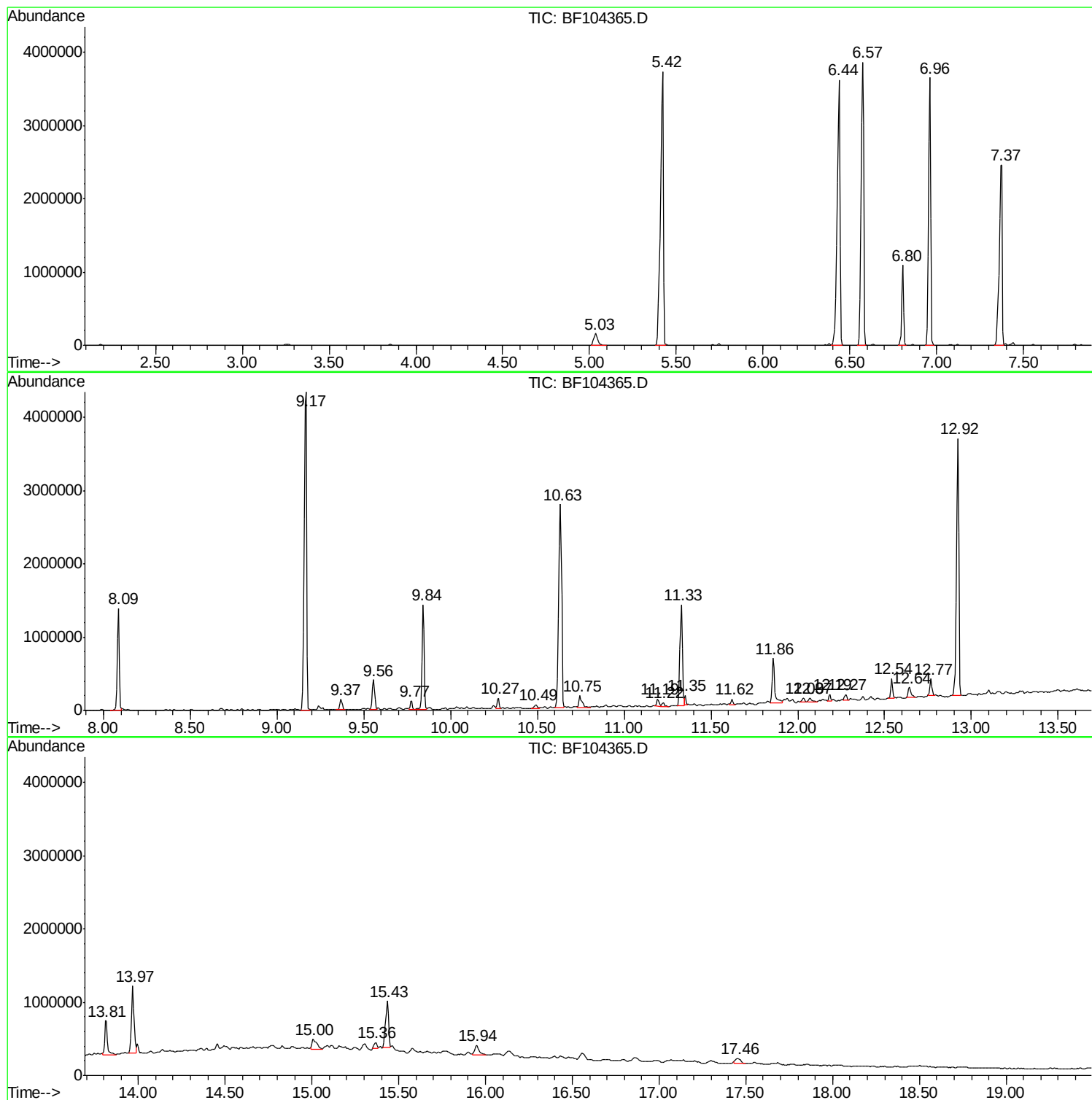
Sum of corrected areas: 41020203

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SB-4C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

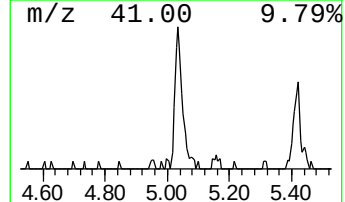
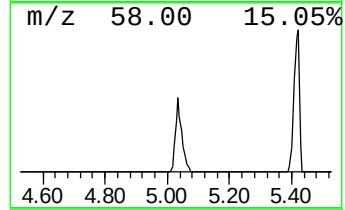
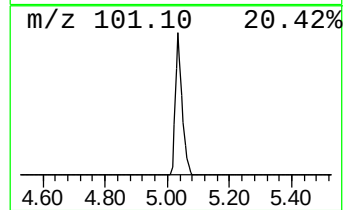
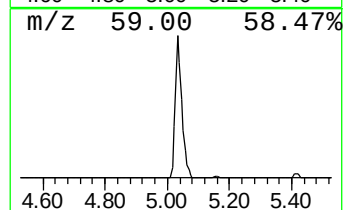
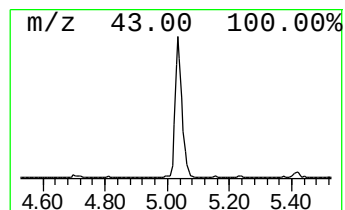
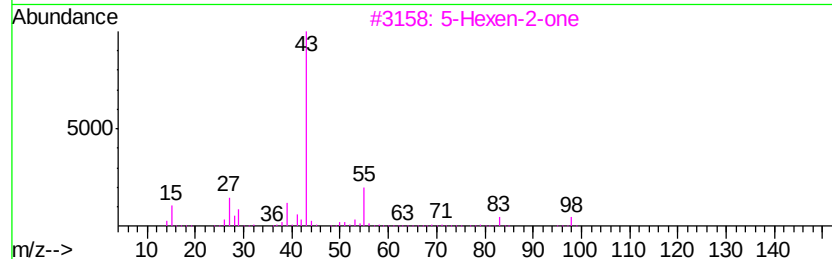
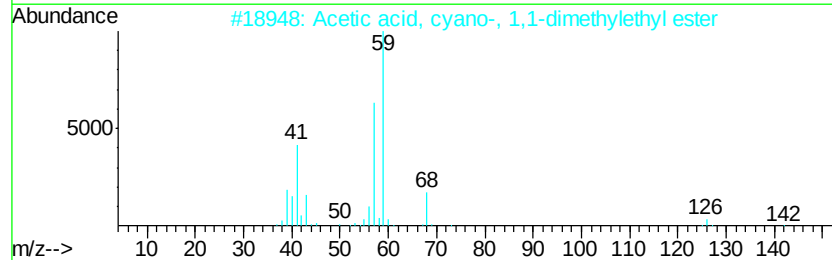
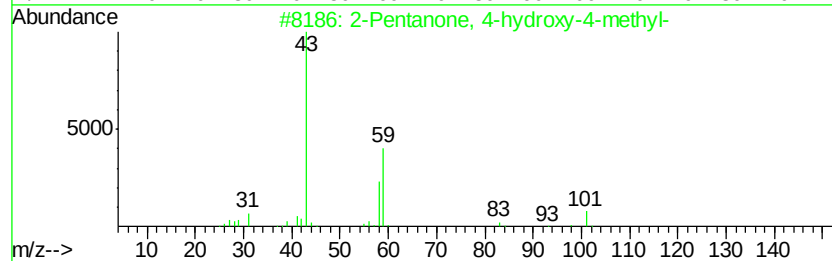
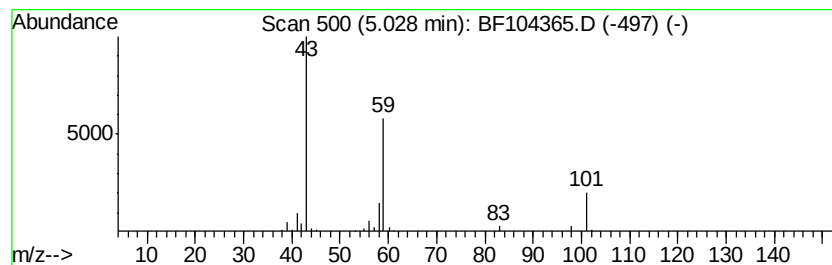
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.03	5.79 ng	246012	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

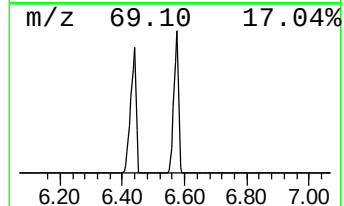
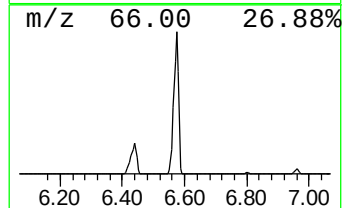
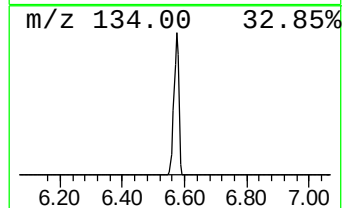
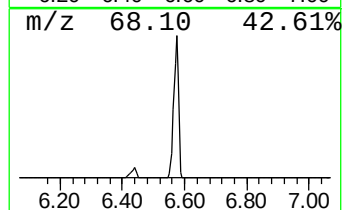
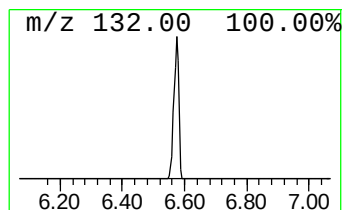
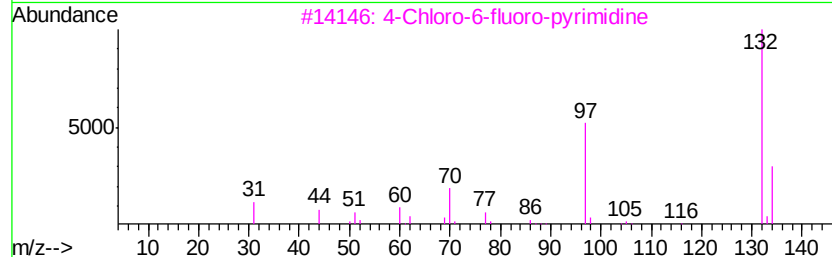
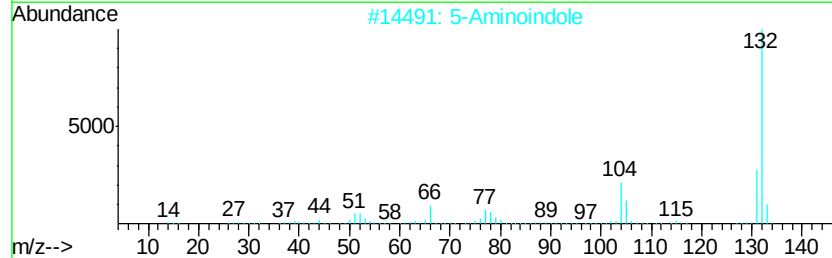
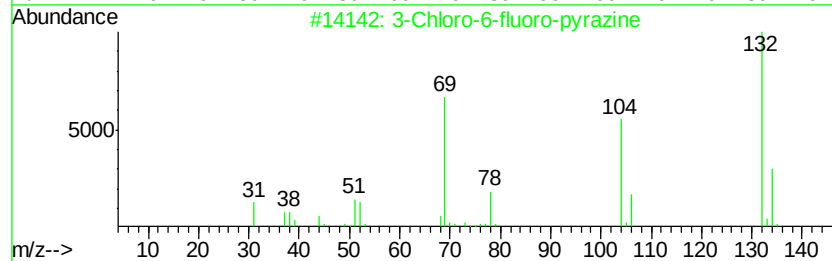
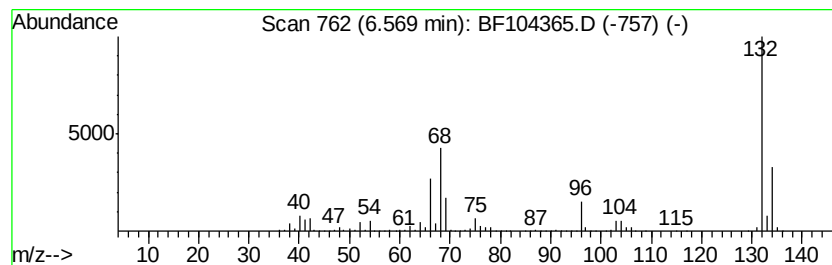
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	104.72 ng	4452360	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

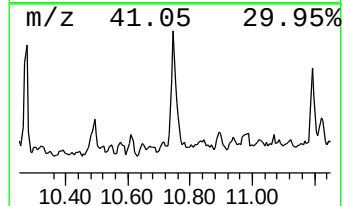
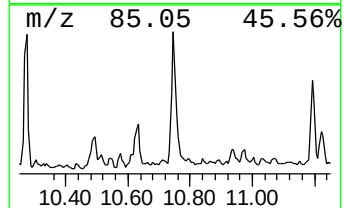
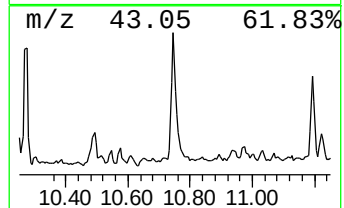
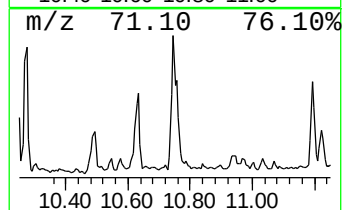
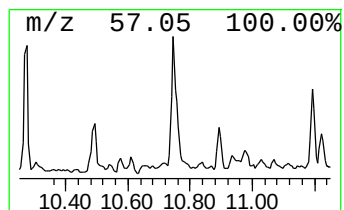
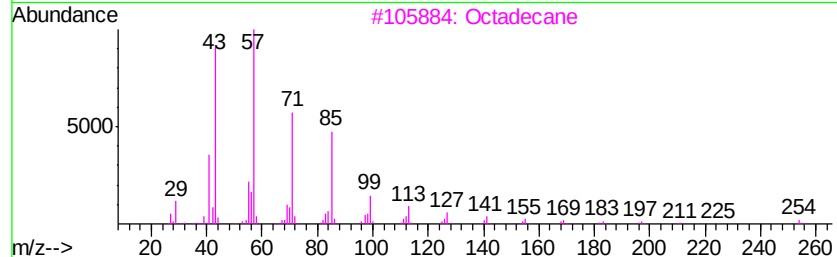
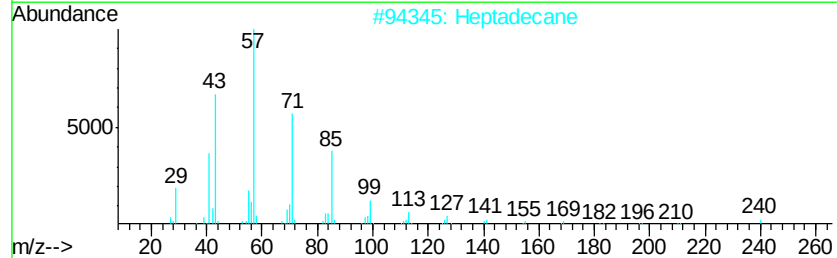
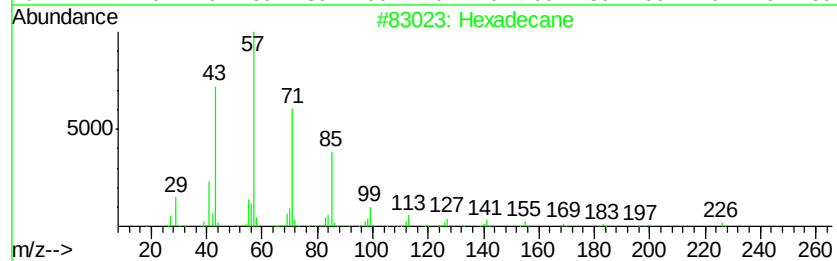
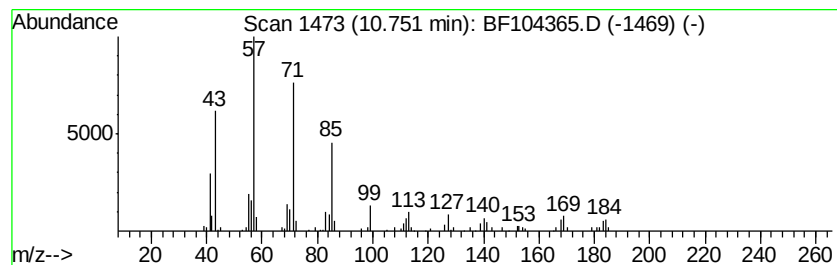
Instrument :
BNA_F
ClientSampleId :
SB-4C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.75	3.17 ng	186751	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Tetradecane	198	C14H30	000629-59-4	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

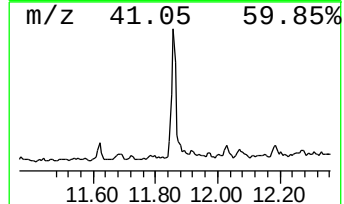
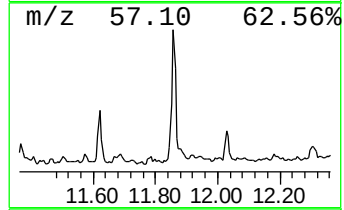
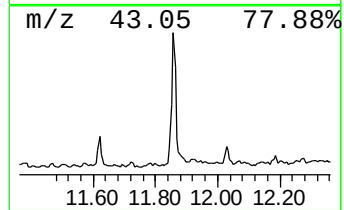
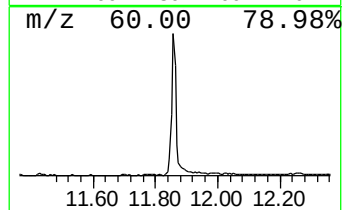
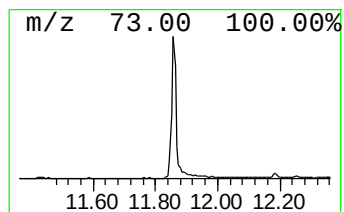
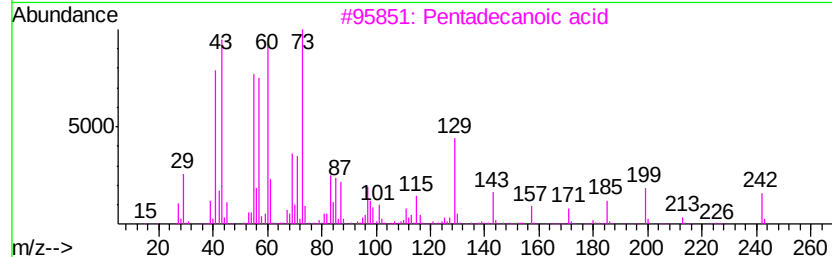
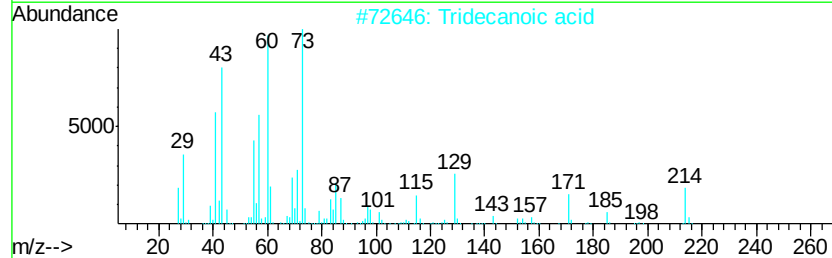
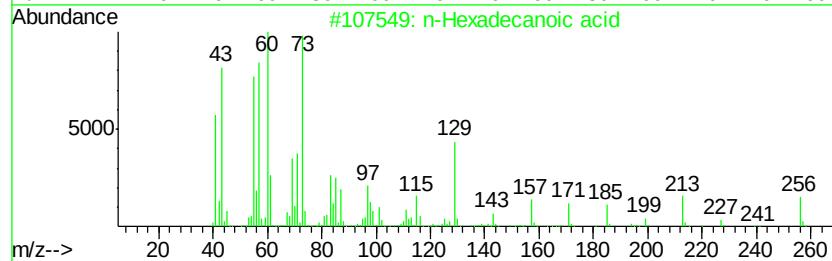
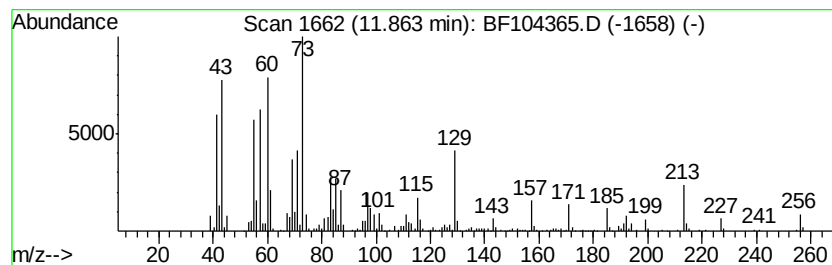
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	10.95 ng	645678	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

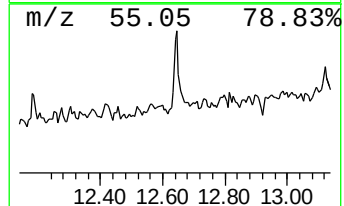
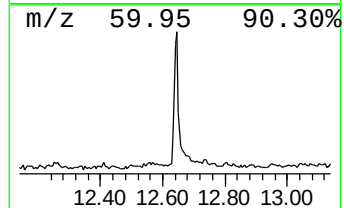
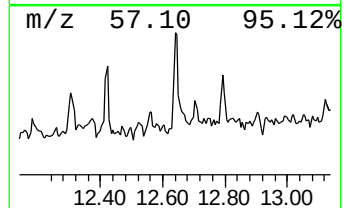
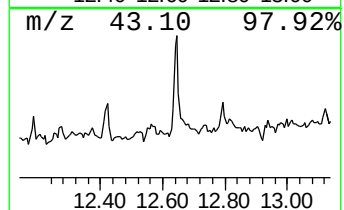
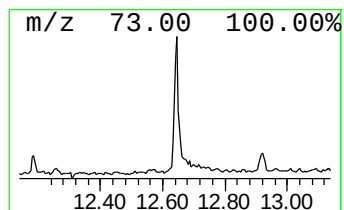
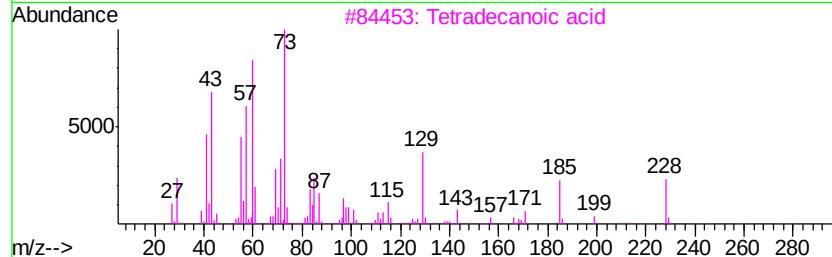
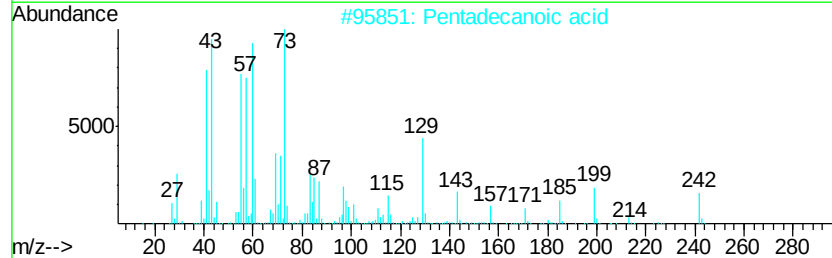
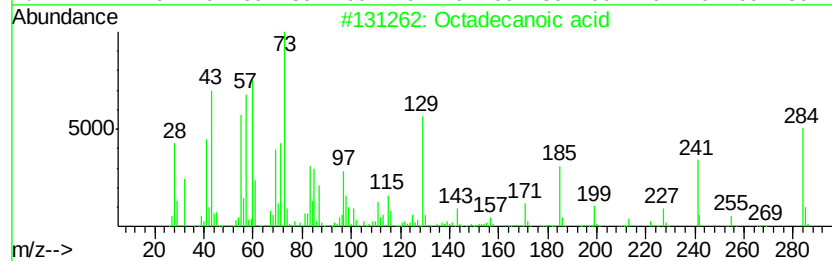
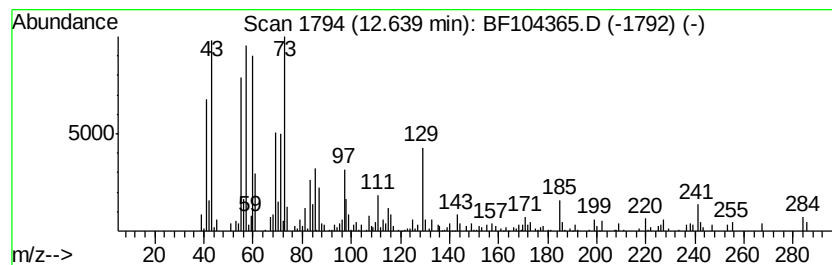
Instrument :
BNA_F
ClientSampleId :
SB-4C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.64	2.53 ng	149277	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

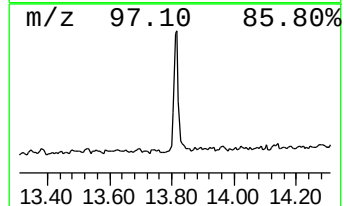
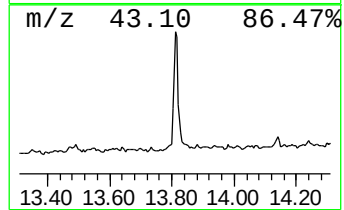
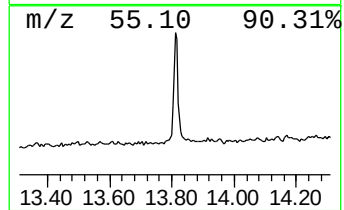
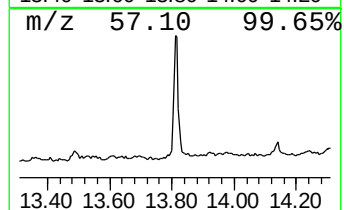
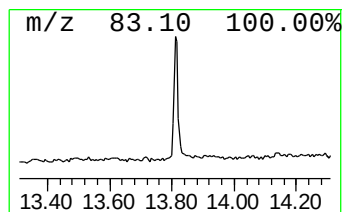
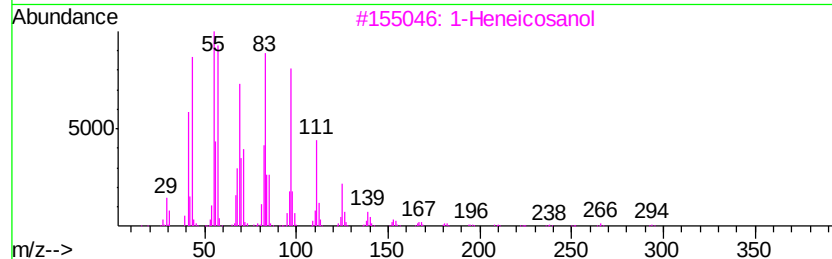
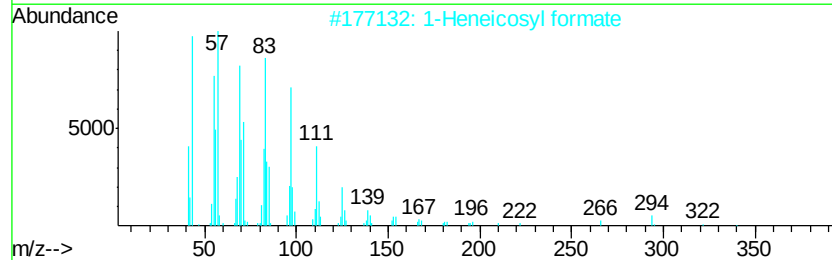
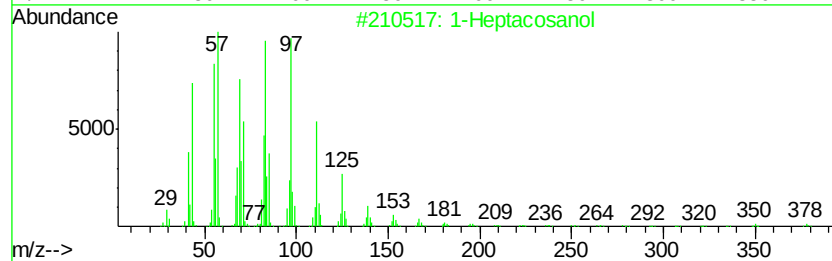
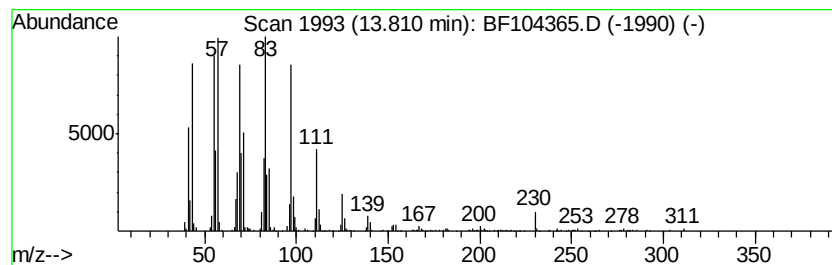
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	11.43 ng	510941	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	94
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

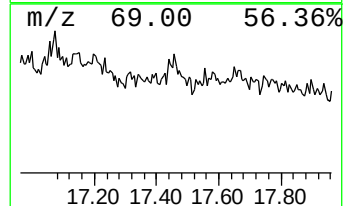
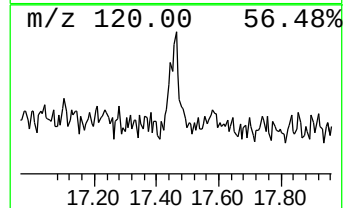
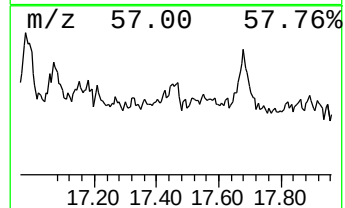
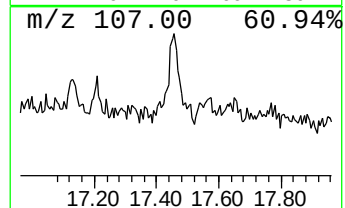
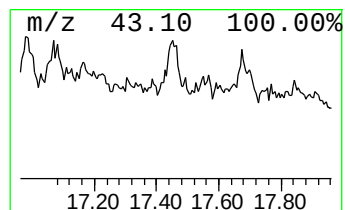
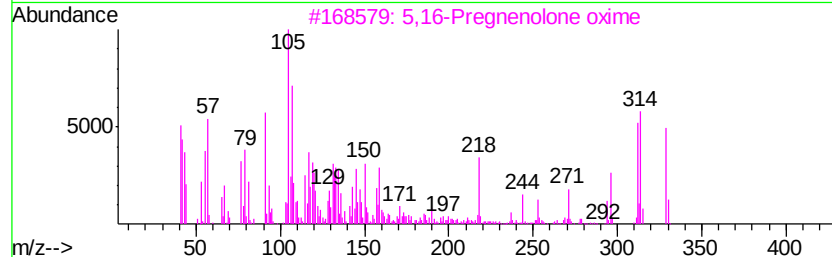
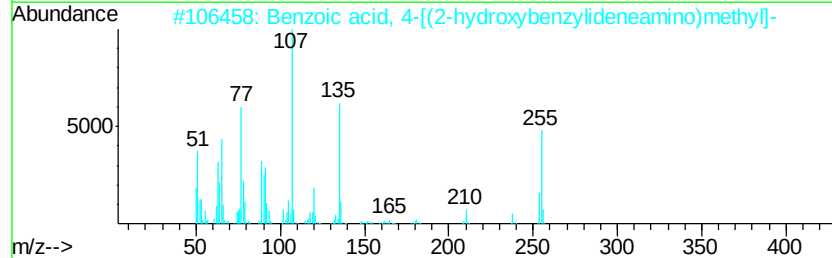
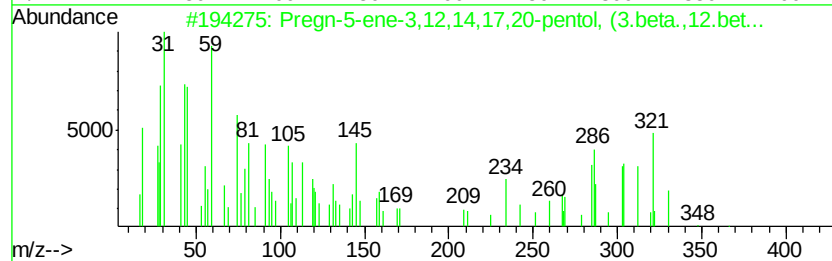
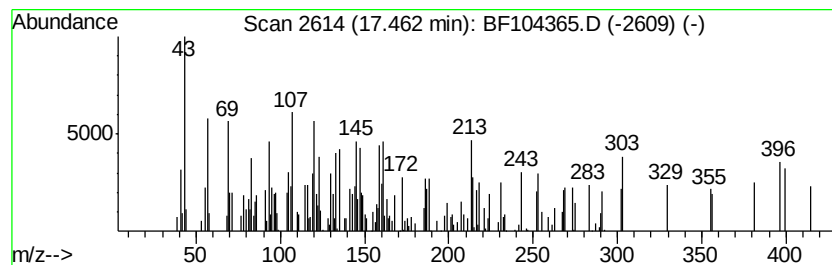
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.46 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	3.98 ng	145893	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pregn-5-ene-3,12,14,17,20-pentol...	366	C21H34O5	028417-32-5	20
2		Benzoic acid, 4-[(2-hydroxybenzy...	255	C15H13NO3	058469-81-1	11
3		5,16-Pregnenolone oxime	329	C21H31NO2	001045-71-2	10
4		Pyroqallol, tris(trifluoroacetate)	414	C12H3F9O6	1000375-76-9	9
5		Hydrazine, 1-(4-methoxyphenyl)-2...	329	C15H15N5O4	051808-28-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104365.D
Acq On : 9 Apr 2018 12:12
Operator : JU/SJ
Sample : J2148-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.03	5.8	ng	246012	1	6.80	850365	20.0
unknown6.57	6.57	104.7	ng	4452360	1	6.80	850365	20.0
Hexadecane	10.75	3.2	ng	186751	4	11.33	1179570	20.0
n-Hexadecanoic acid	11.86	10.9	ng	645678	4	11.33	1179570	20.0
Octadecanoic acid	12.64	2.5	ng	149277	4	11.33	1179570	20.0
1-Heptacosanol	13.81	11.4	ng	510941	5	13.97	893933	20.0
unknown17.46	17.46	4.0	ng	145893	6	15.43	733474	20.0