

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
 Data File : BF098723.D
 Acq On : 23 Sep 2017 3:52
 Operator : SJ/JU
 Sample : I5340-03
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LT-TS-003

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-BF092117.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	2.257	25	29	46	rVB	97993	179147	5.09%	0.510%
2	2.381	47	50	58	rVB3	31223	47238	1.34%	0.134%
3	5.163	519	523	531	rVB	534486	637474	18.11%	1.815%
4	5.551	583	589	592	rBV	3458407	3442851	97.83%	9.800%
5	6.551	753	759	762	rBV	3275188	3457907	98.26%	9.843%
6	6.698	779	784	787	rBV	3738428	3519179	100.00%	10.018%
7	6.928	819	823	827	rVB	1191824	954154	27.11%	2.716%
8	7.087	846	850	853	rBV	3008981	2591192	73.63%	7.376%
9	7.492	913	919	922	rBV	2081319	2149813	61.09%	6.120%
10	7.551	924	929	933	rVB2	35270	39868	1.13%	0.113%
11	8.210	1037	1041	1044	rBV	1573966	1235753	35.11%	3.518%
12	9.286	1218	1224	1227	rBV	3826145	3443184	97.84%	9.801%
13	9.675	1286	1290	1293	rBV	603048	495213	14.07%	1.410%
14	9.886	1322	1326	1329	rBV	65273	49004	1.39%	0.139%
15	9.963	1335	1339	1343	rBV	1287989	1189512	33.80%	3.386%
16	10.386	1408	1411	1414	rVB	112561	89041	2.53%	0.253%
17	10.604	1442	1448	1451	rBV3	28053	45825	1.30%	0.130%
18	10.751	1467	1473	1476	rBV	1976545	1769477	50.28%	5.037%
19	10.857	1488	1491	1498	rBV2	112991	125858	3.58%	0.358%
20	11.310	1565	1568	1570	rBV	56948	49428	1.40%	0.141%
21	11.451	1588	1592	1595	rBV	1209533	988925	28.10%	2.815%
22	11.475	1595	1596	1598	rVB	100986	49900	1.42%	0.142%
23	11.927	1670	1673	1675	rBV	52718	46347	1.32%	0.132%
24	11.969	1675	1680	1689	rVB2	476683	491489	13.97%	1.399%
25	12.663	1794	1798	1807	rBV	222212	273302	7.77%	0.778%
26	12.751	1810	1813	1818	rBV2	168293	162355	4.61%	0.462%
27	12.892	1831	1837	1841	rBV	177203	174783	4.97%	0.498%
28	13.033	1857	1861	1865	rVB	2594204	2420495	68.78%	6.890%
29	13.233	1886	1895	1897	rBV4	31589	66823	1.90%	0.190%
30	13.916	2008	2011	2016	rBV2	344175	348044	9.89%	0.991%
31	14.092	2033	2041	2043	rBV	1001528	1030443	29.28%	2.933%
32	14.116	2043	2045	2053	rVB	102440	100916	2.87%	0.287%
33	14.245	2063	2067	2070	rBV3	37577	44709	1.27%	0.127%
34	14.551	2115	2119	2125	rBV	227583	248006	7.05%	0.706%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

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-BF092117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.863	2169	2172	2177	rBV4	32530	52941	1.50%	0.151%
36	14.939	2182	2185	2189	rBV	45275	50899	1.45%	0.145%
37	15.010	2194	2197	2202	rBV	230525	239399	6.80%	0.681%
38	15.139	2215	2219	2222	rBV	77040	114378	3.25%	0.326%
39	15.210	2227	2231	2232	rBV	127743	128641	3.66%	0.366%
40	15.233	2232	2235	2243	rVB2	402116	487636	13.86%	1.388%
41	15.451	2269	2272	2275	rBV	34888	45808	1.30%	0.130%
42	15.515	2280	2283	2289	rVB	48161	55601	1.58%	0.158%
43	15.586	2289	2295	2307	rVB	568864	816865	23.21%	2.325%
44	15.810	2330	2333	2338	rVB2	61624	82225	2.34%	0.234%
45	16.057	2370	2375	2379	rBV	137202	212937	6.05%	0.606%
46	16.104	2379	2383	2390	rVB2	123493	195408	5.55%	0.556%
47	16.486	2443	2448	2453	rVB6	90968	147953	4.20%	0.421%
48	16.886	2511	2516	2523	rBV5	47103	93234	2.65%	0.265%
49	17.198	2565	2569	2577	rVB3	50382	99098	2.82%	0.282%
50	17.280	2577	2583	2591	rBV3	51996	130523	3.71%	0.372%
51	17.698	2648	2654	2665	rBV5	97359	218203	6.20%	0.621%

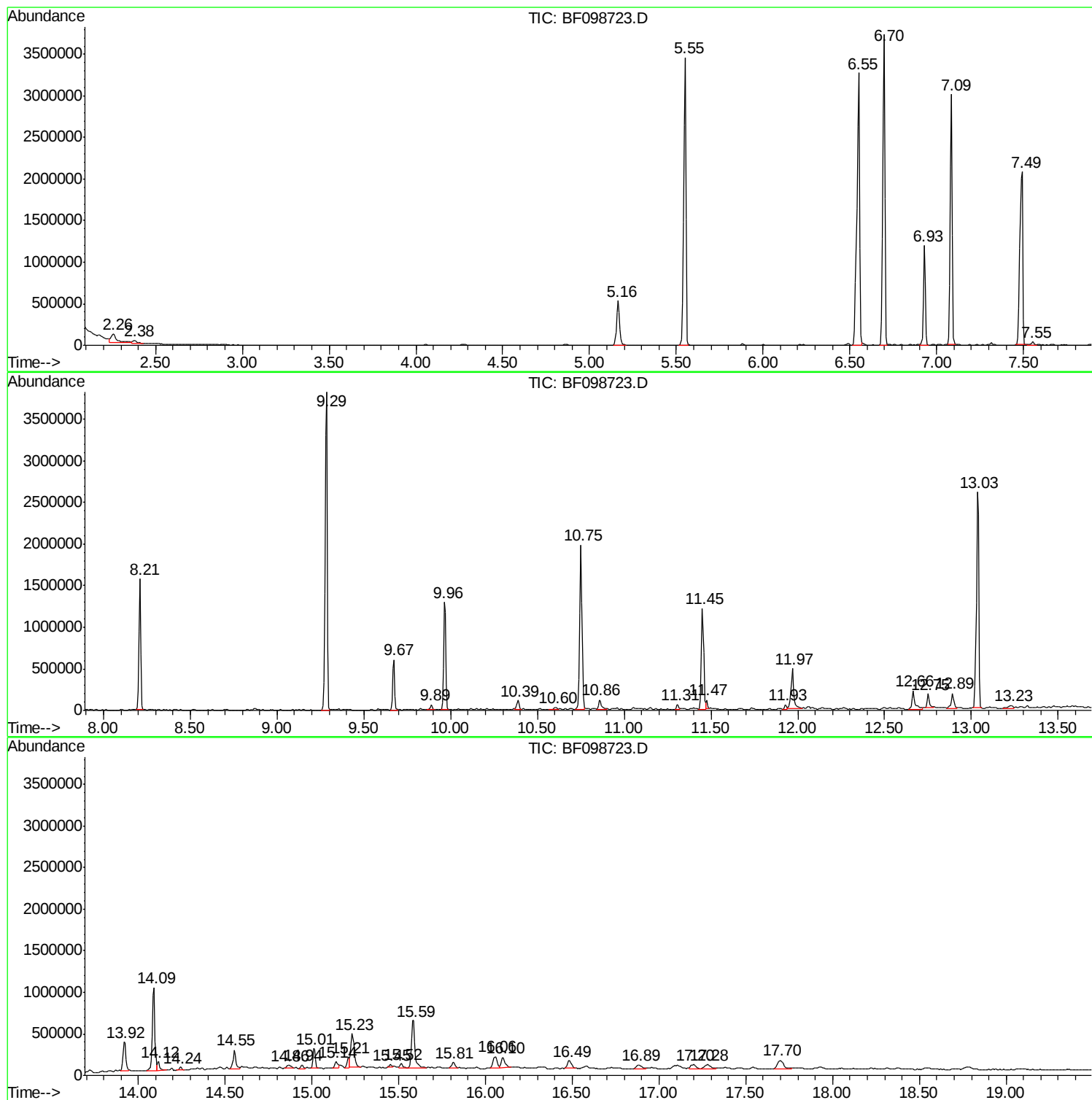
Sum of corrected areas: 35129404

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
LT-TS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

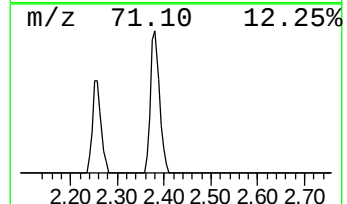
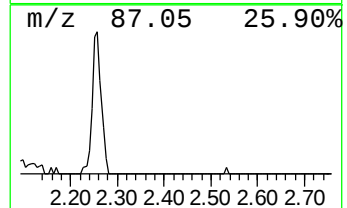
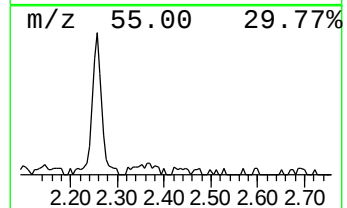
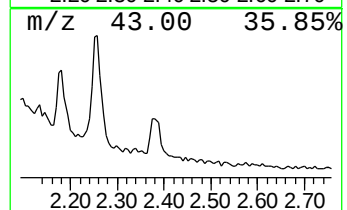
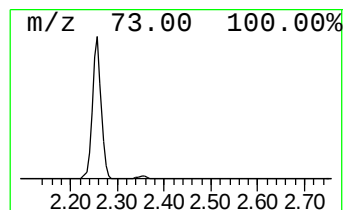
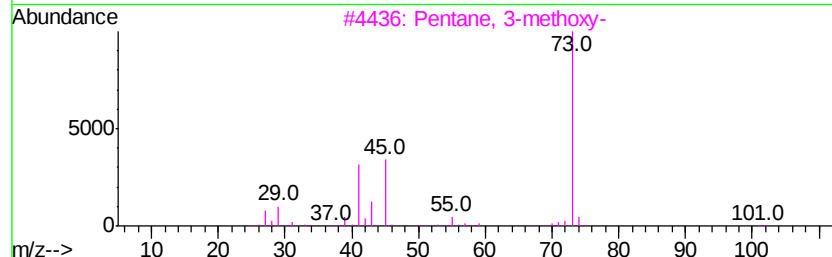
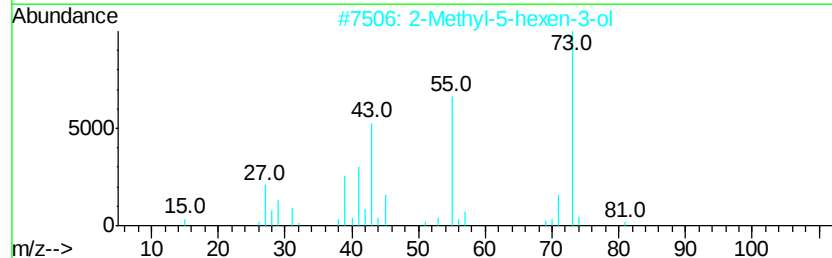
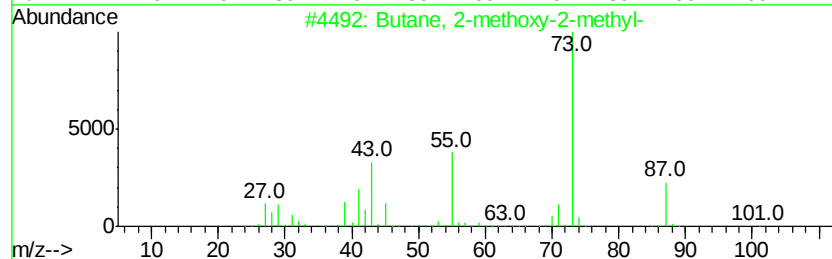
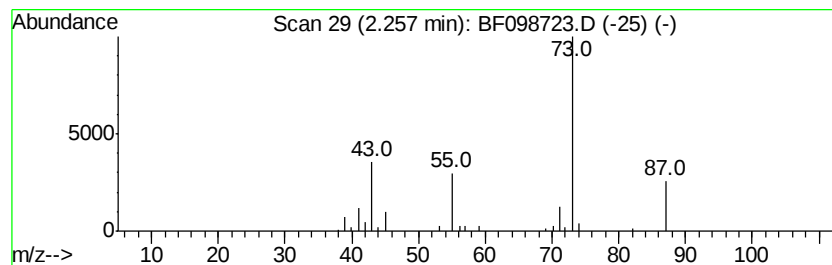
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	3.76 ng	179147	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

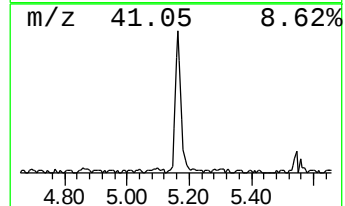
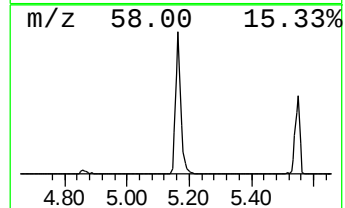
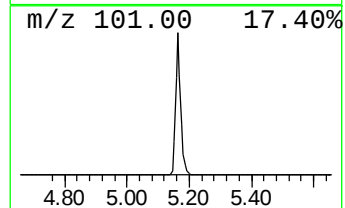
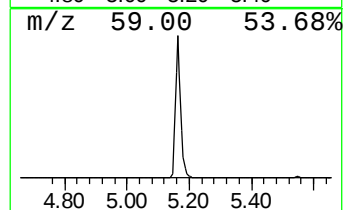
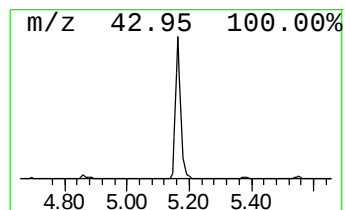
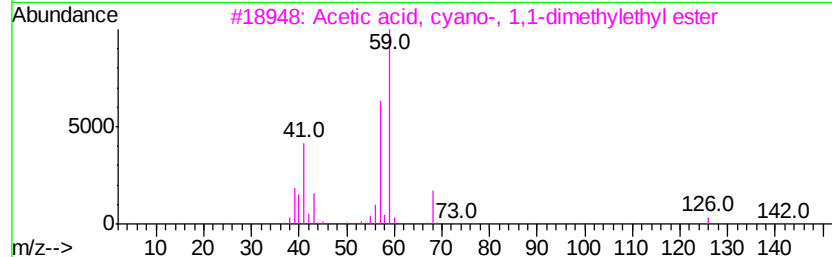
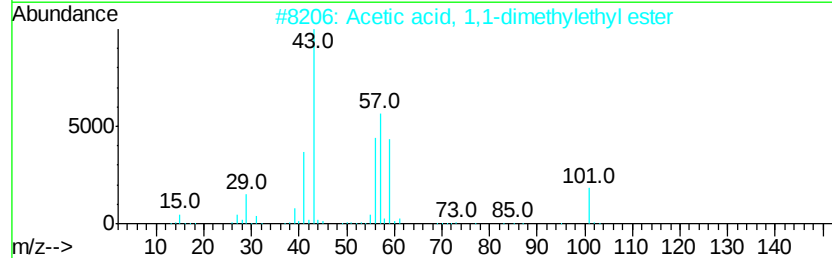
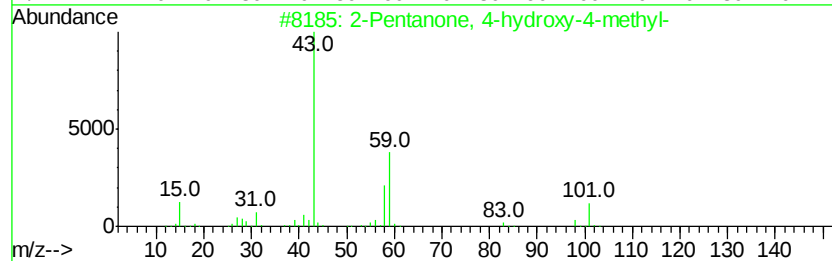
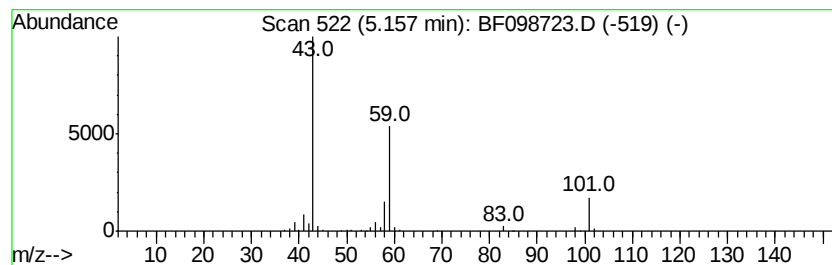
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	13.36 ng	637474	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

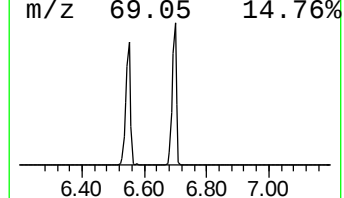
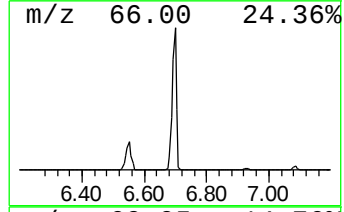
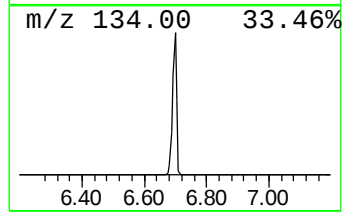
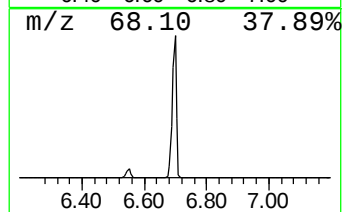
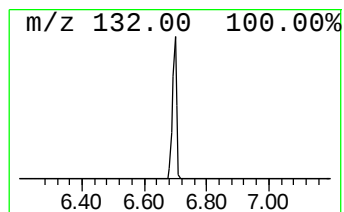
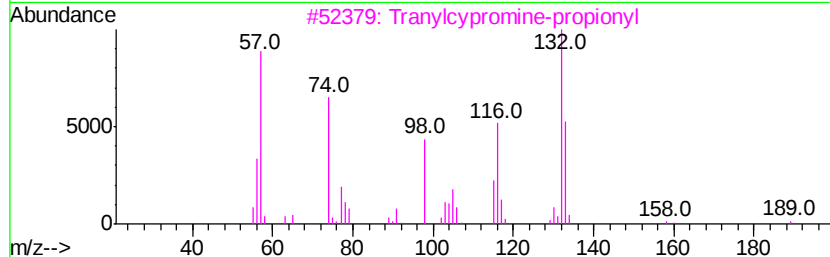
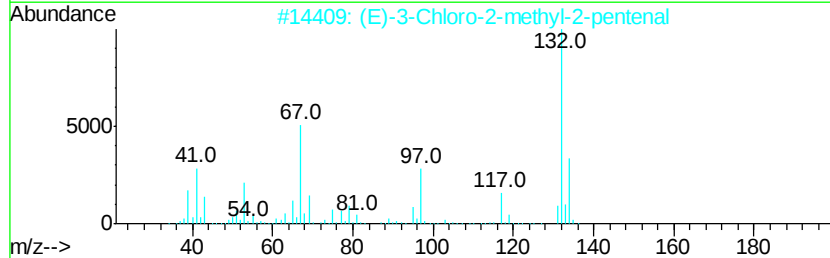
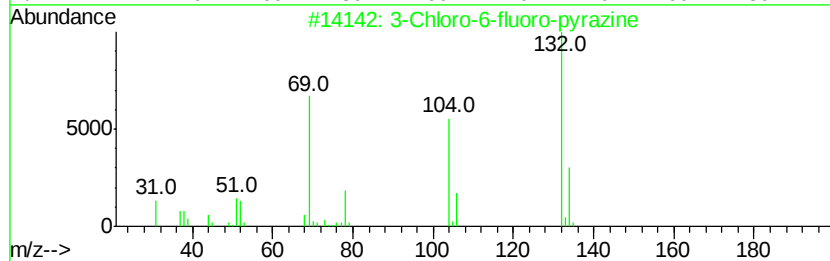
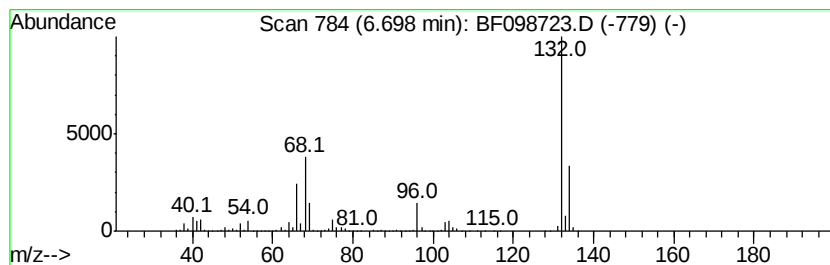
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	73.77 ng	3519180	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

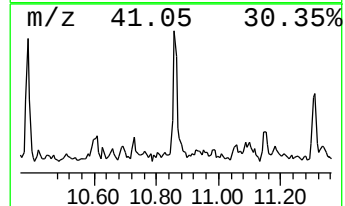
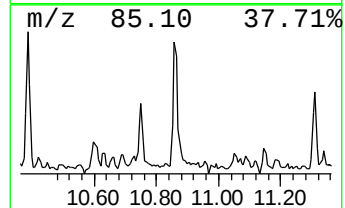
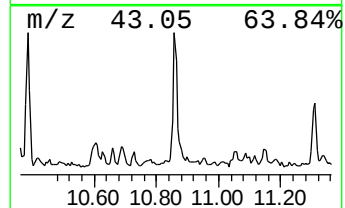
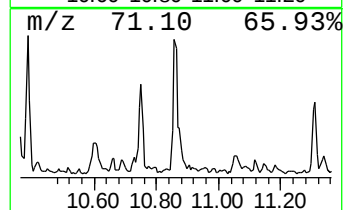
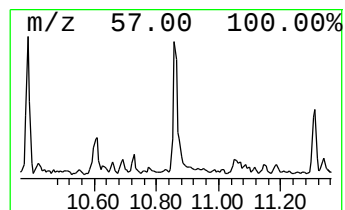
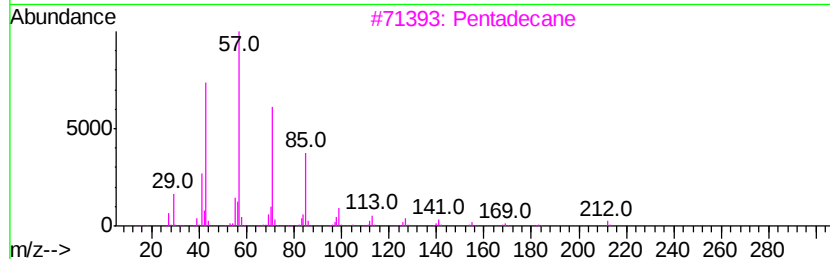
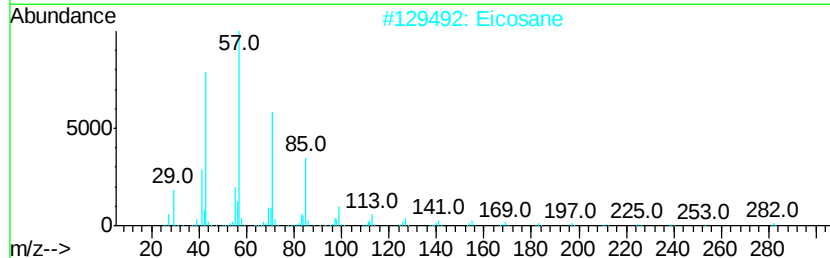
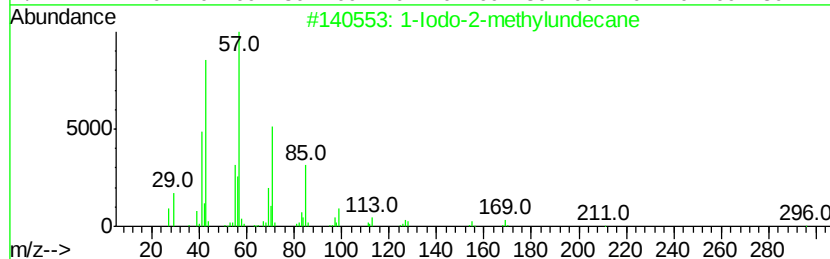
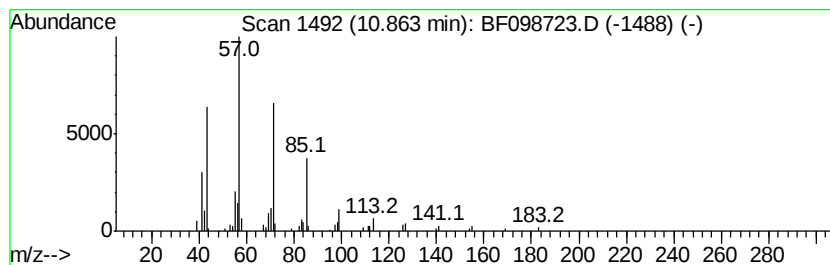
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Iodo-2-methylundecane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.55 ng	125858	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
2		Eicosane	282	C20H42	000112-95-8	86
3		Pentadecane	212	C15H32	000629-62-9	86
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

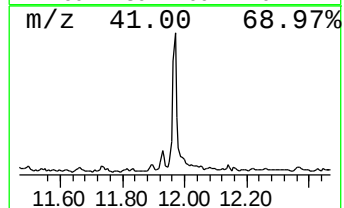
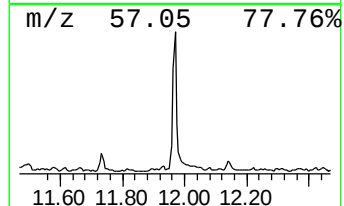
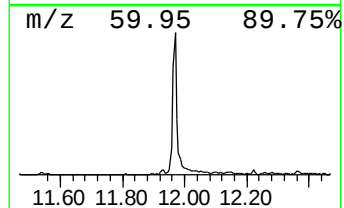
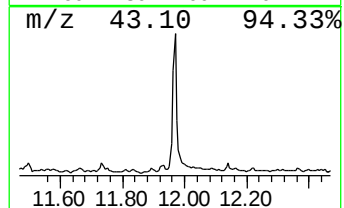
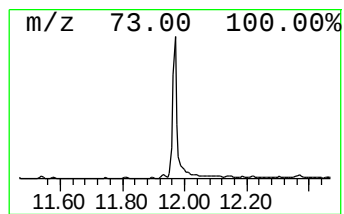
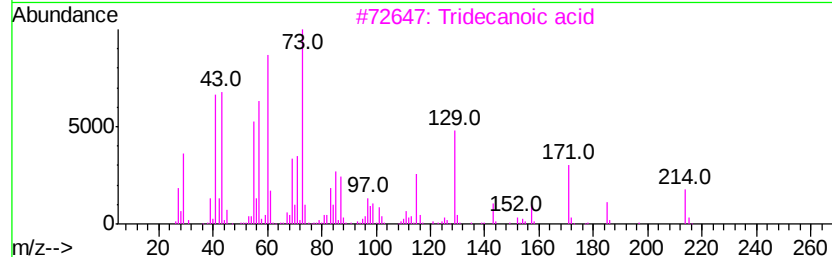
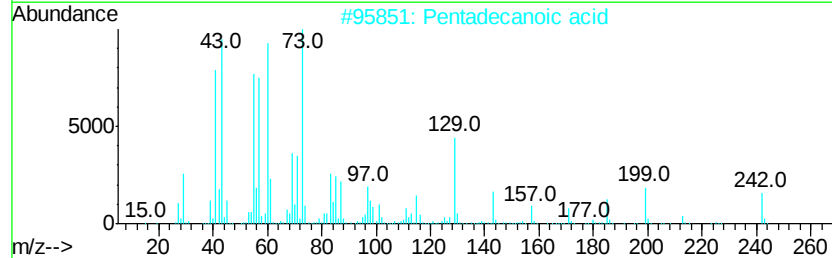
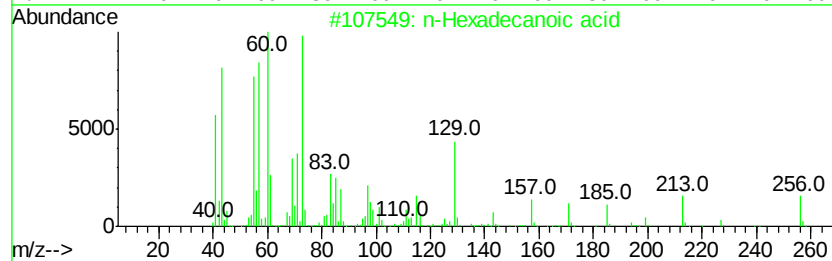
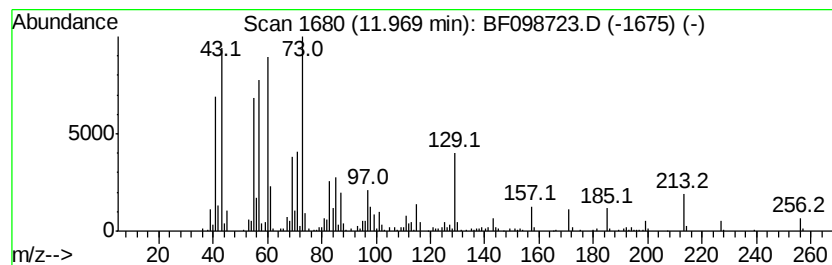
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	9.94 ng	491489	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

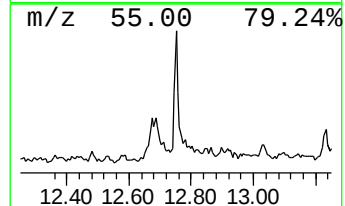
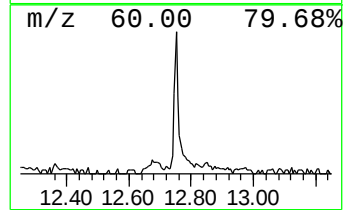
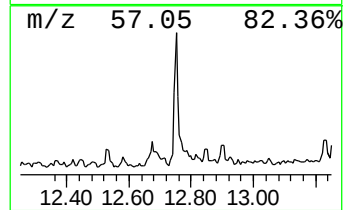
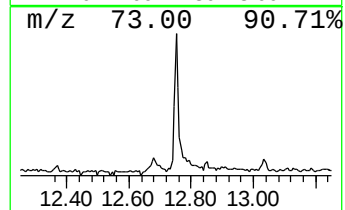
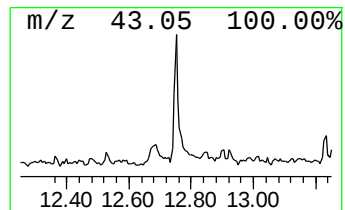
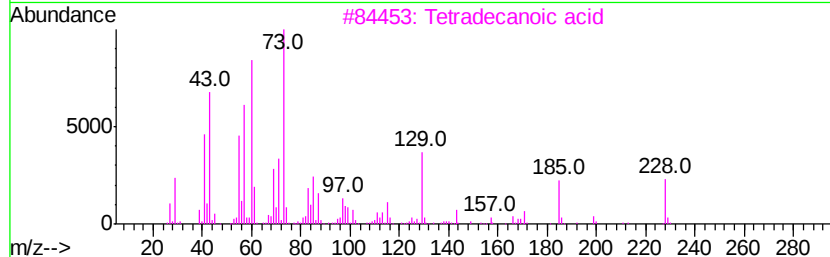
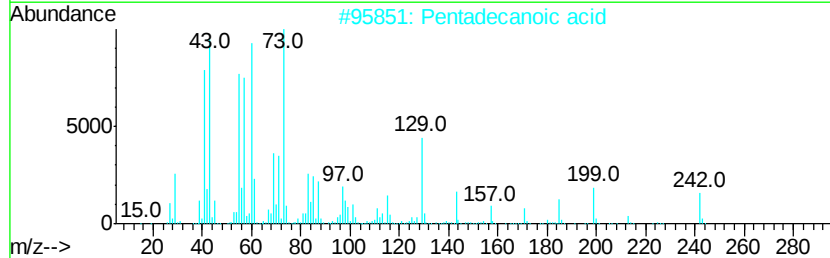
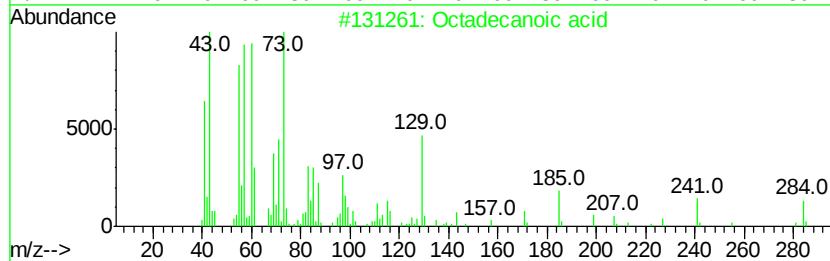
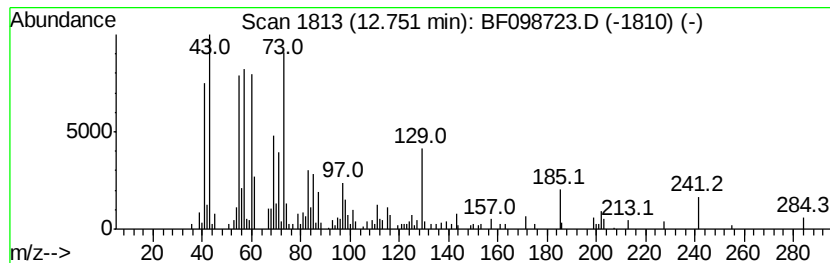
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	3.28 ng	162355	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Undecanoic acid	186	C11H22O2	000112-37-8	74
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

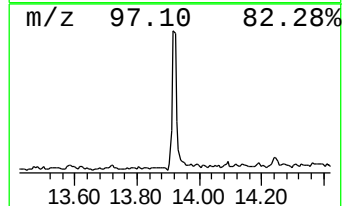
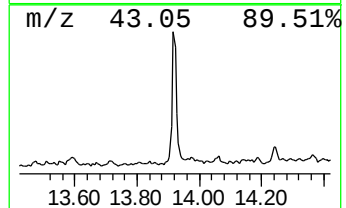
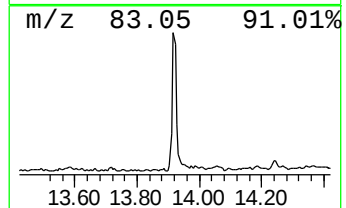
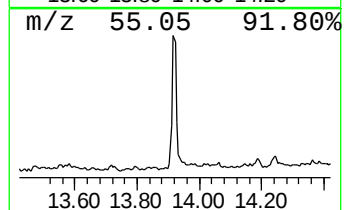
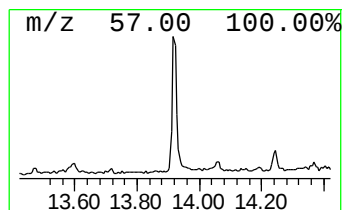
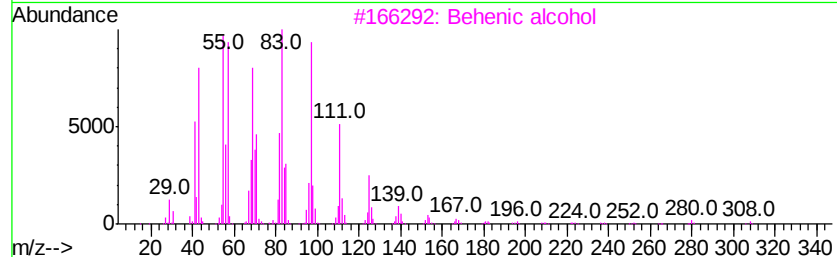
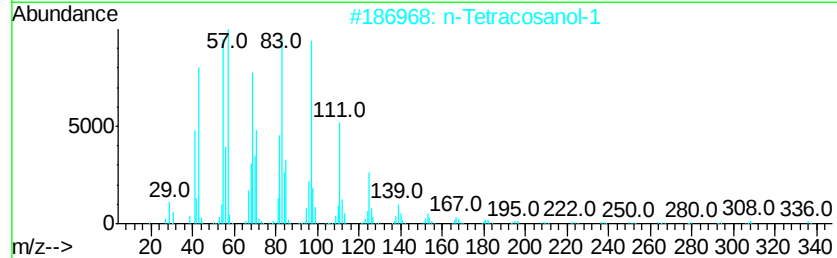
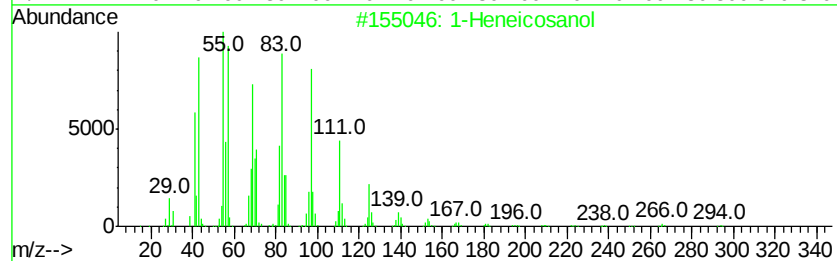
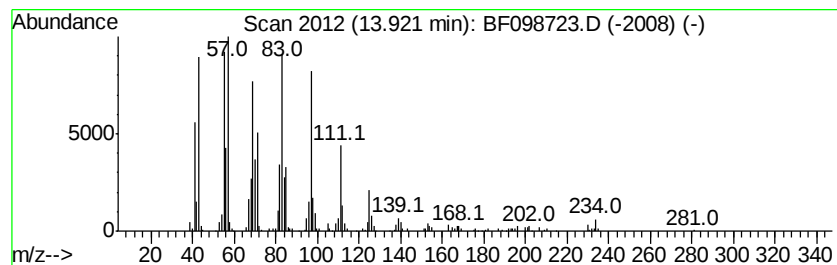
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	6.76 ng	348044	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

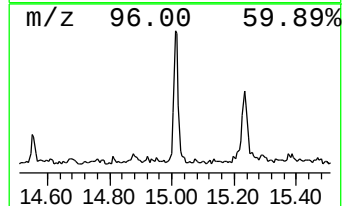
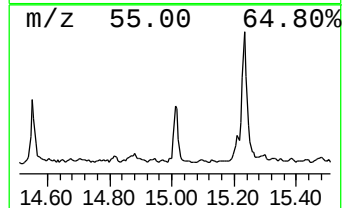
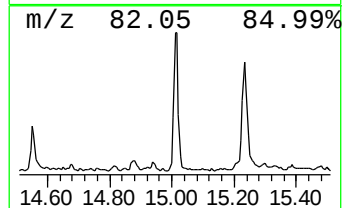
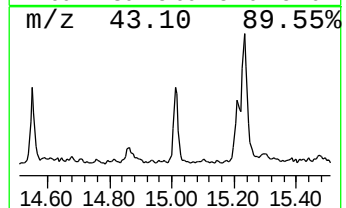
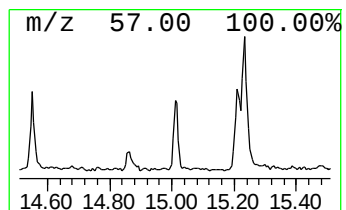
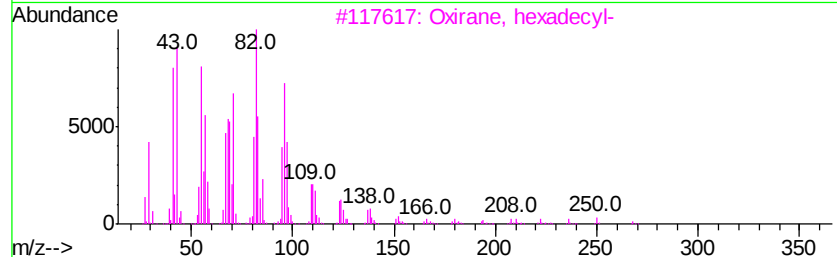
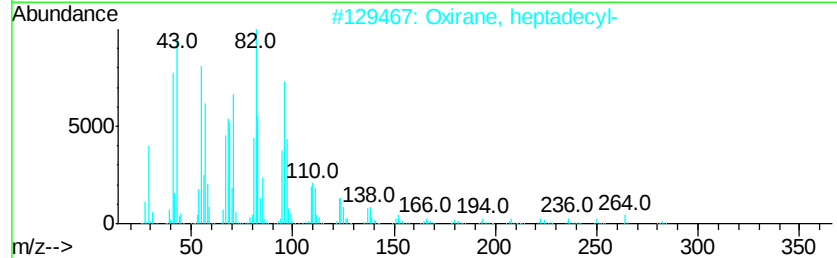
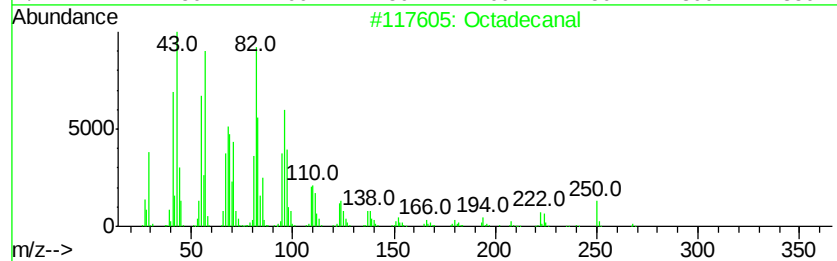
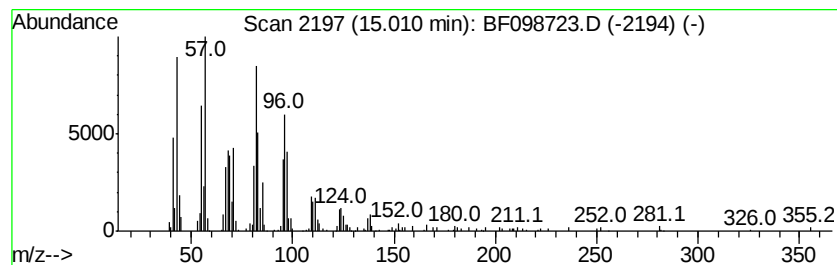
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	5.86 ng	239399	Perylene-d12	15.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	91
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
4			Hexadecanal	240	C16H32O	000629-80-1	87
5			16-Heptadecenal	252	C17H32O	1000144-57-9	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

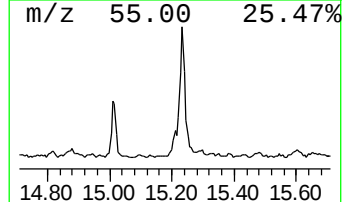
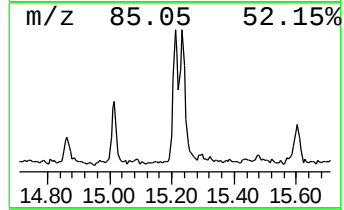
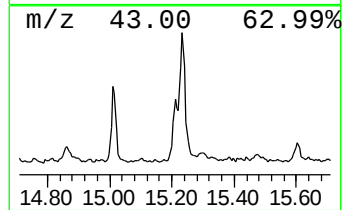
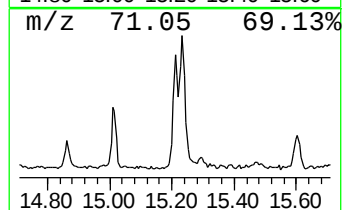
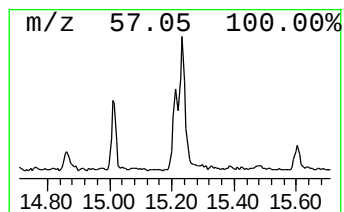
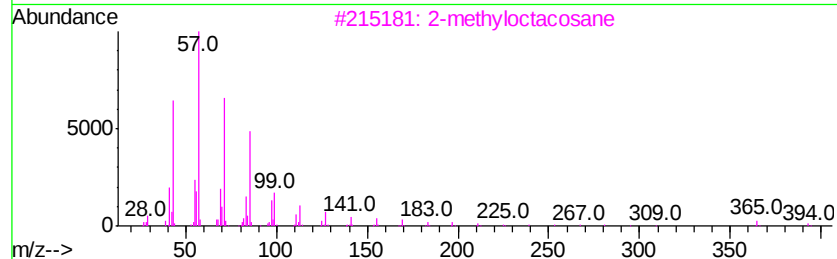
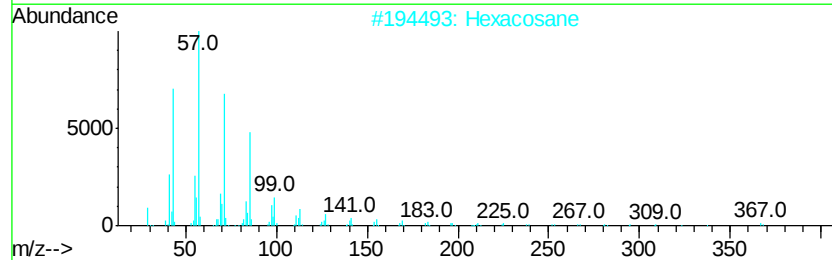
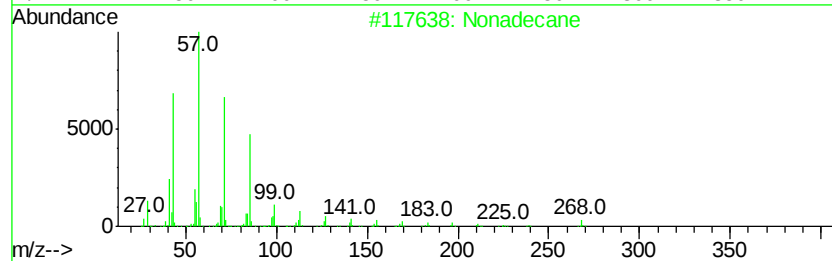
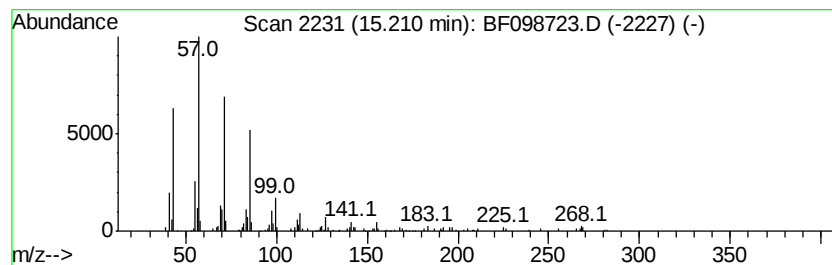
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	3.15 ng	128641	Perylene-d12	15.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Hexacosane	366	C26H54	000630-01-3	90
3			2-methyloctacosane	408	C29H60	1000376-72-8	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

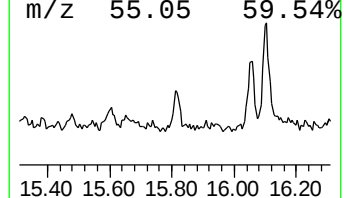
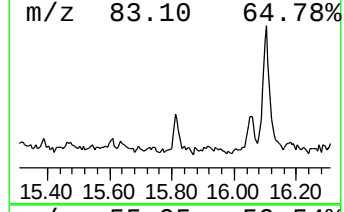
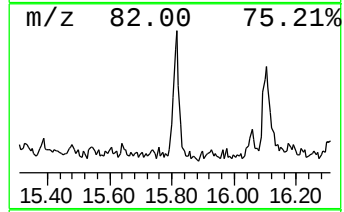
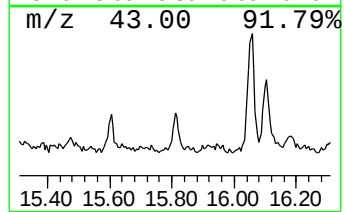
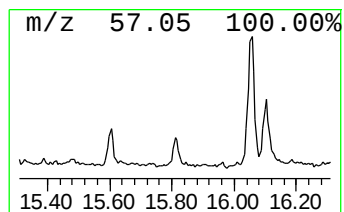
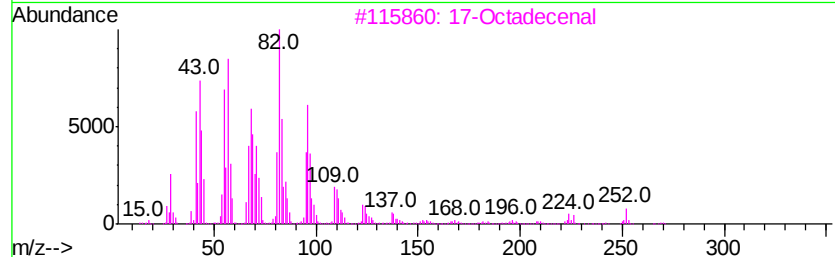
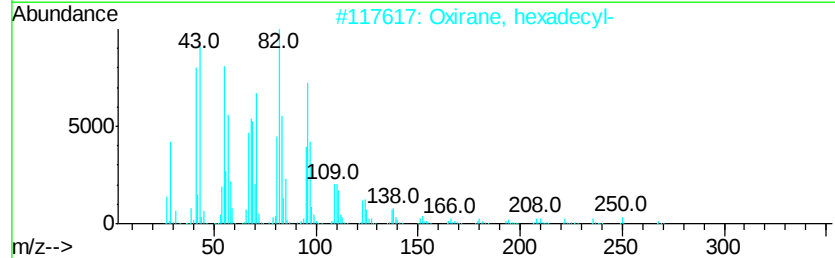
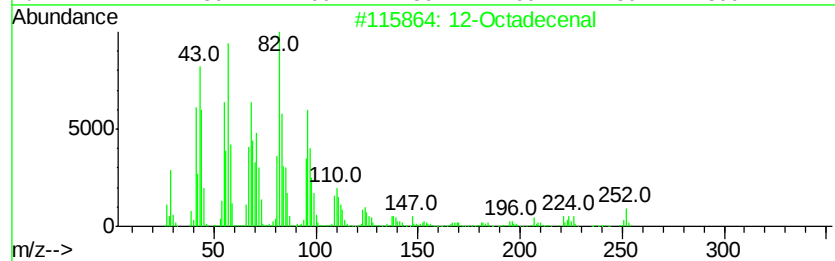
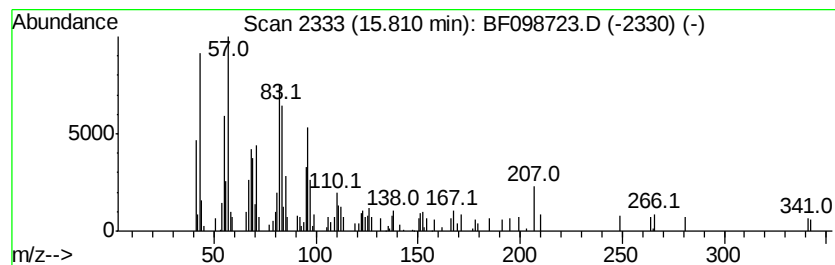
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 12-Octadecenal Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	2.01 ng	82225	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	12-Octadecenal	266	C18H34O	056554-91-7	83
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
3		17-Octadecenal	266	C18H34O	056554-86-0	64
4		1,19-Eicosadiene	278	C20H38	014811-95-1	62
5		18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

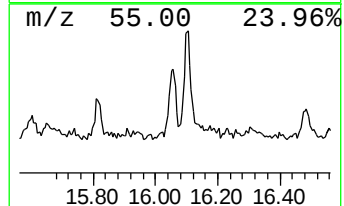
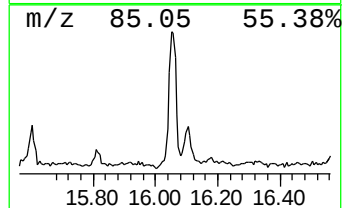
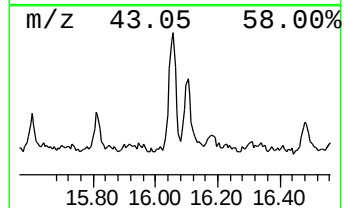
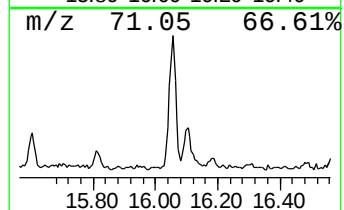
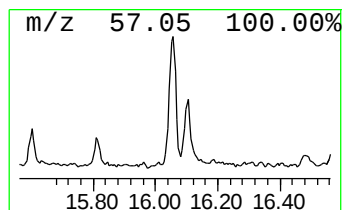
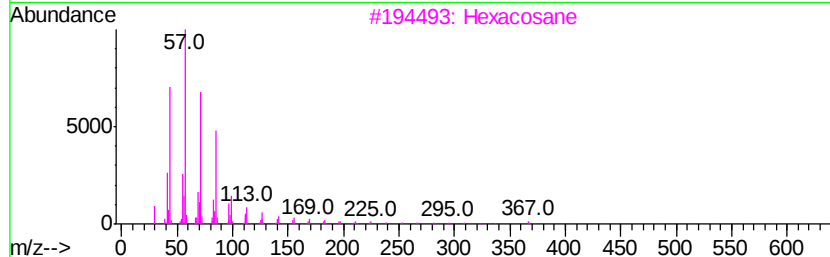
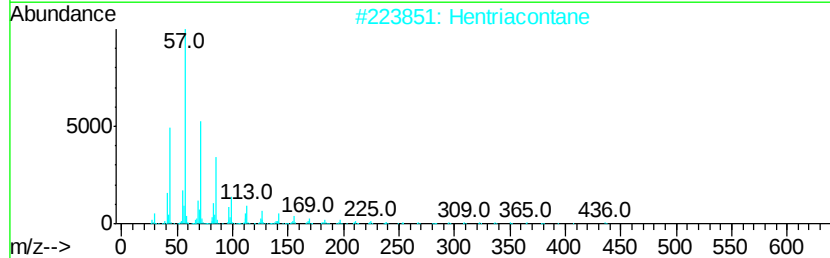
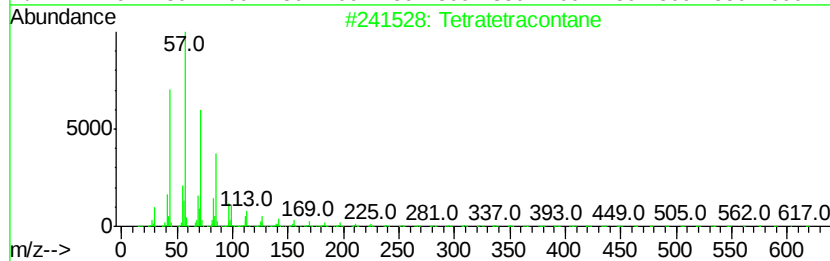
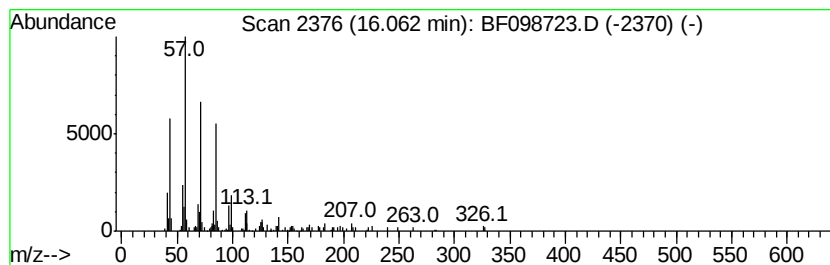
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	5.21 ng	212937	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

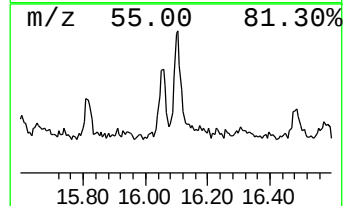
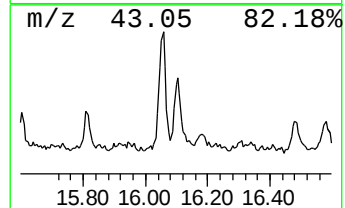
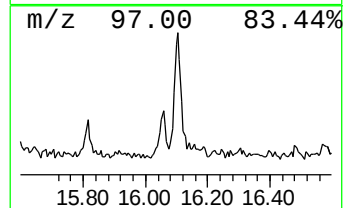
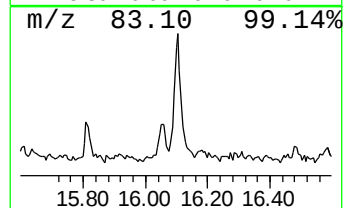
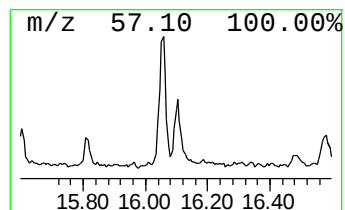
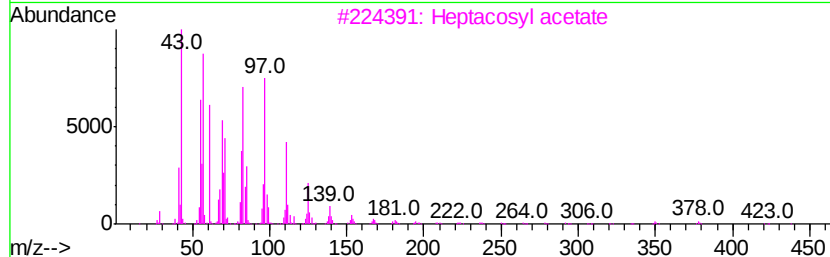
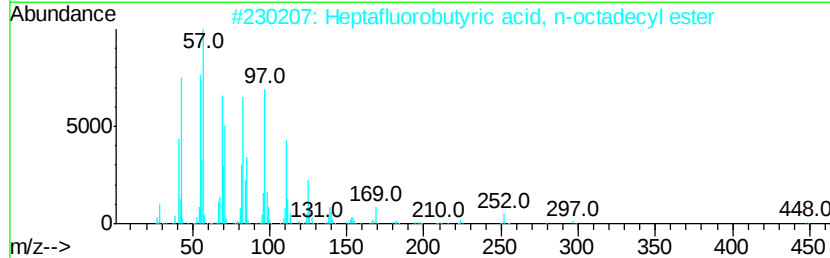
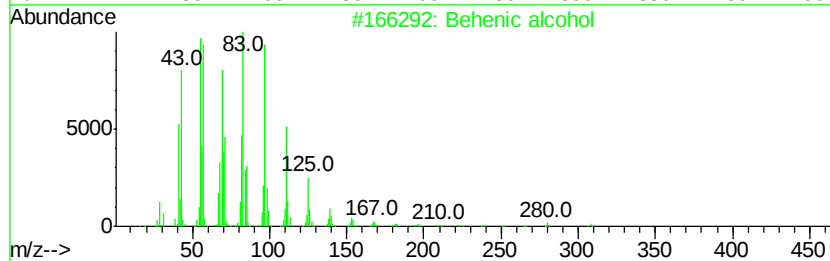
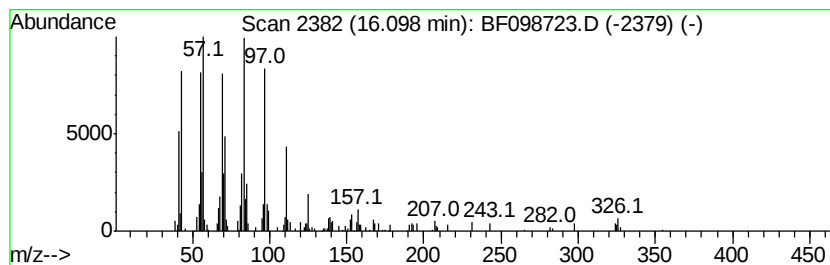
Instrument :
BNA_F
ClientSampleId :
LT-TS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Behenic alcohol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	4.78 ng	195408	Perylene-d12	15.59
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 70
2		Heptafluorobutyric acid, n-octadecyl ester	466 C22H37F7O2	000400-57-7 70
3		Heptacosyl acetate	438 C29H58O2	1000351-78-2 64
4		Octacosanol	410 C28H58O	000557-61-9 60
5		Octatriacontyl pentafluoropropio...	697 C41H77F5O2	1000351-89-1 58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

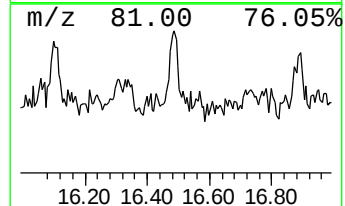
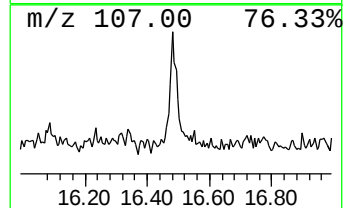
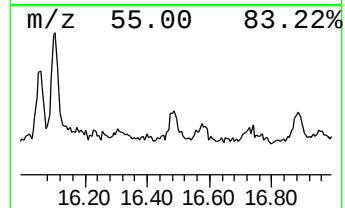
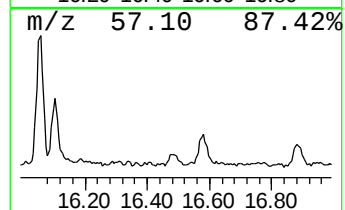
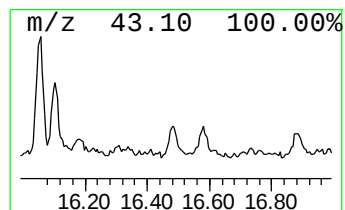
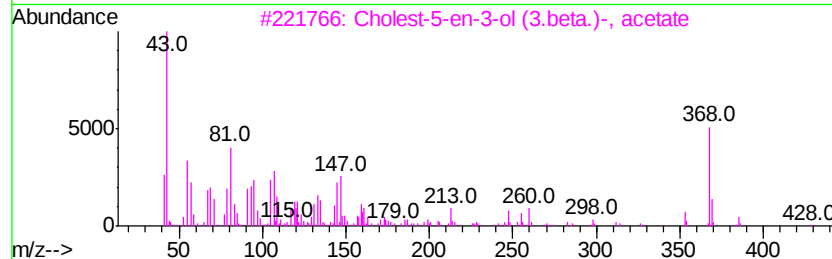
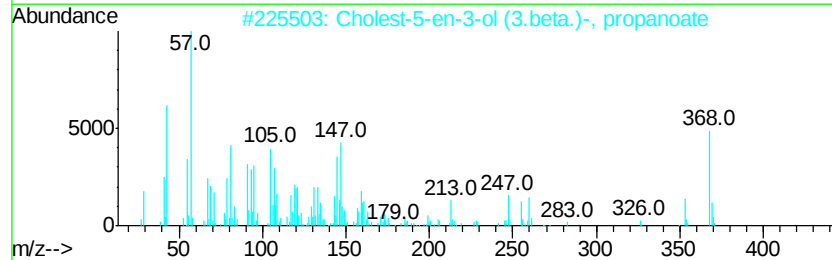
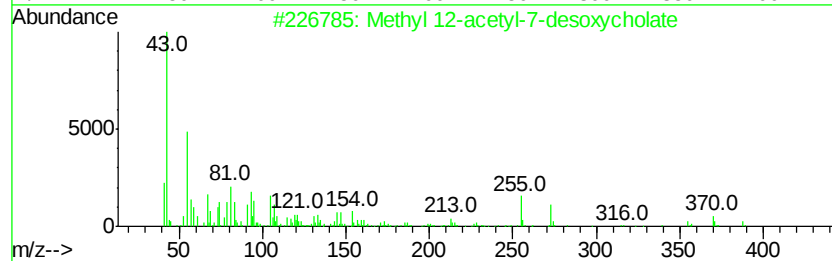
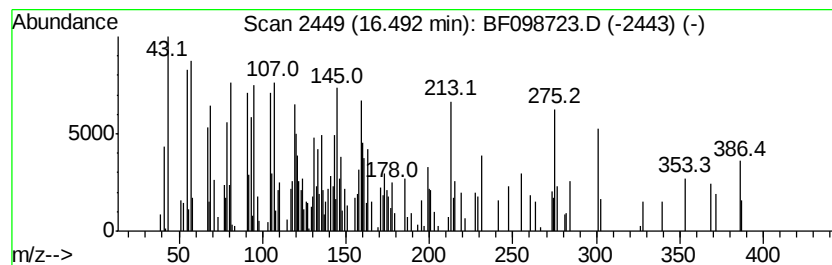
Instrument :
BNA_F
ClientSampleId :
LT-TS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown16.49 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.49	3.62 ng	147953	Perylene-d12	15.59		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl	12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	35
2	Cholest-5-en-3-ol (3.beta.)-, pr...		442	C30H50O2	000633-31-8	25
3	Cholest-5-en-3-ol (3.beta.)-, ac...		428	C29H48O2	000604-35-3	22
4	Cholest-5-en-3-ol (3.beta.)-, ca...		448	C28H45ClO2	007144-08-3	16
5	Cholesta-3,5-diene		368	C27H44	000747-90-0	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

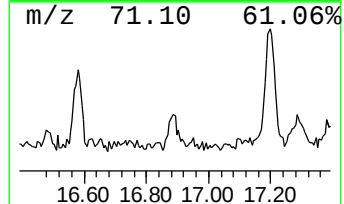
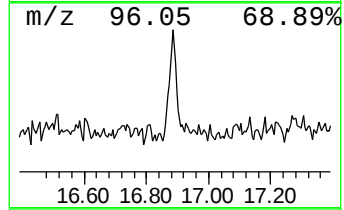
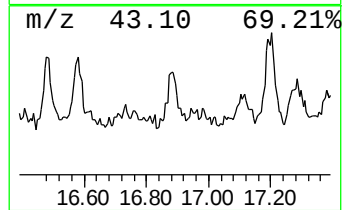
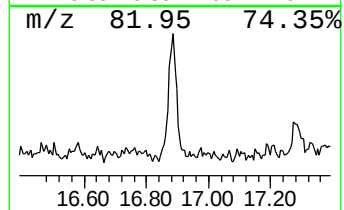
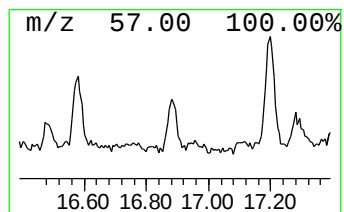
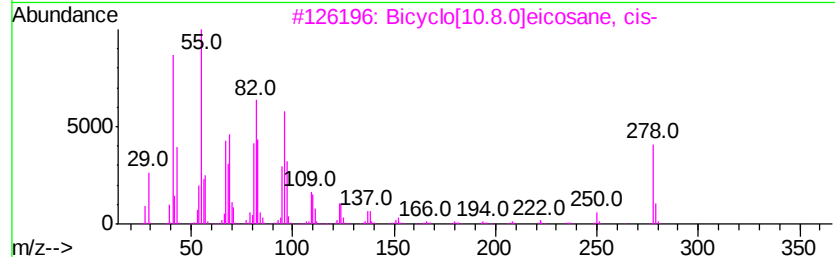
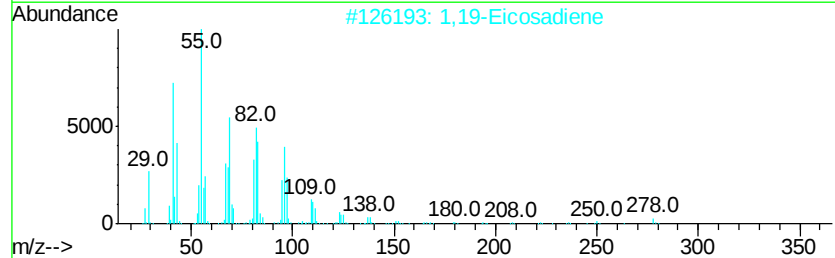
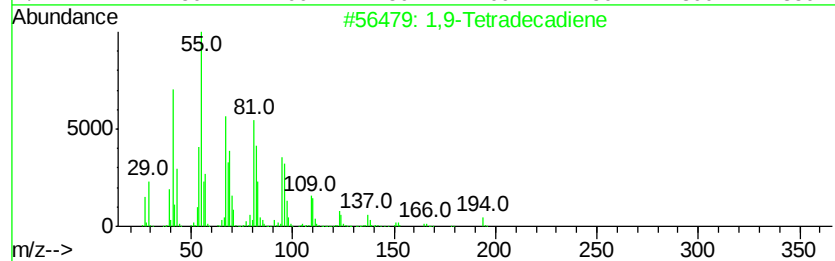
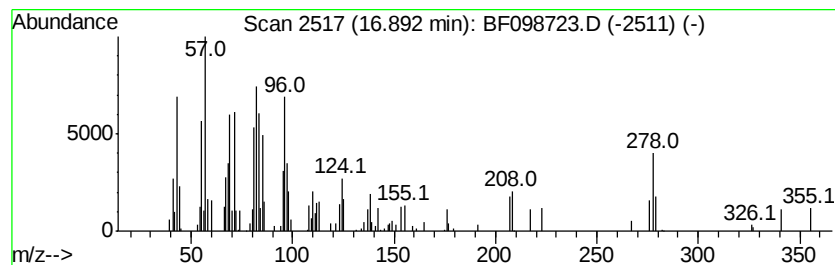
Instrument :
BNA_F
ClientSampleId :
LT-TS-003

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 1,9-Tetradecadiene Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.89	2.28 ng	93234	Perylene-d12	15.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,9-Tetradecadiene	194	C14H26	112929-06-3	64
2	1,19-Eicosadiene	278	C20H38	014811-95-1	60
3	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	58
4	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	58
5	Octanenitrile	125	C8H15N	000124-12-9	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

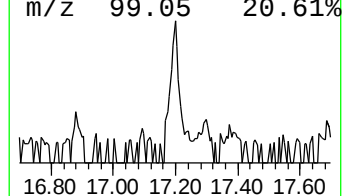
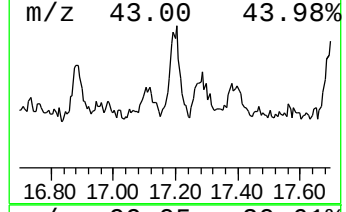
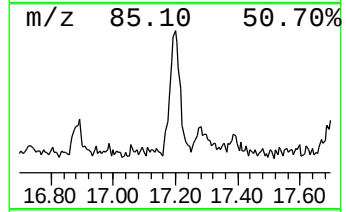
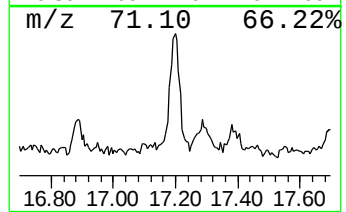
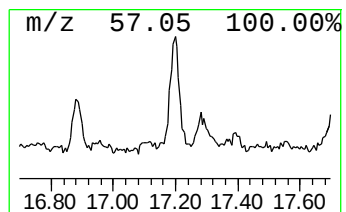
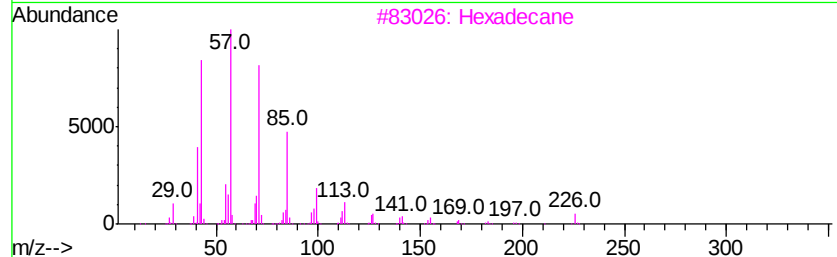
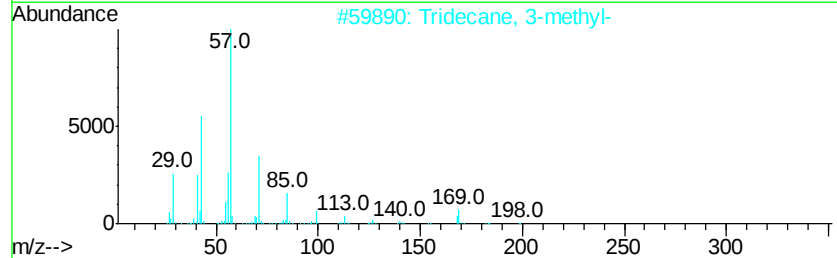
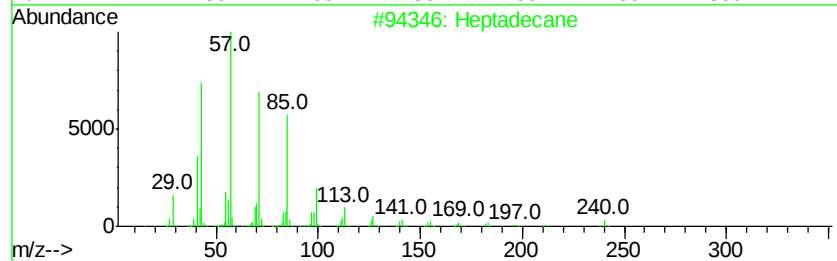
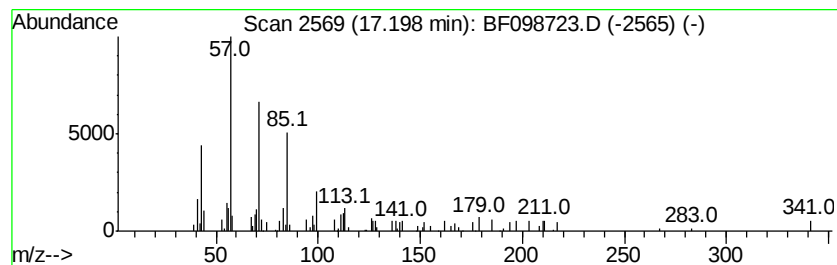
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Heptadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	2.43 ng	99098	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	80
2		Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
3		Hexadecane	226	C16H34	000544-76-3	72
4		5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	64
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

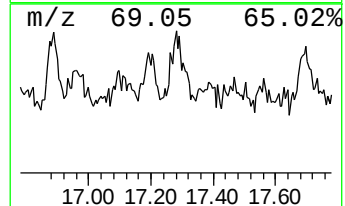
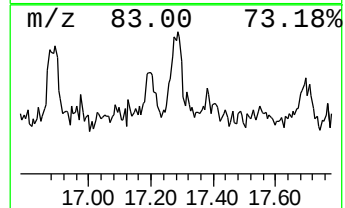
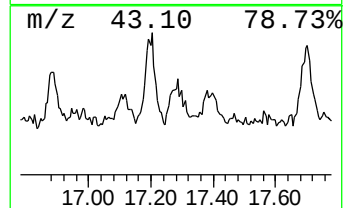
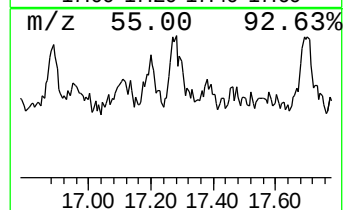
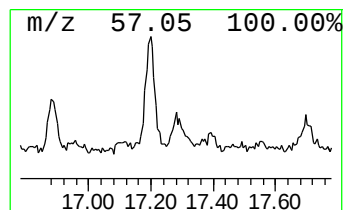
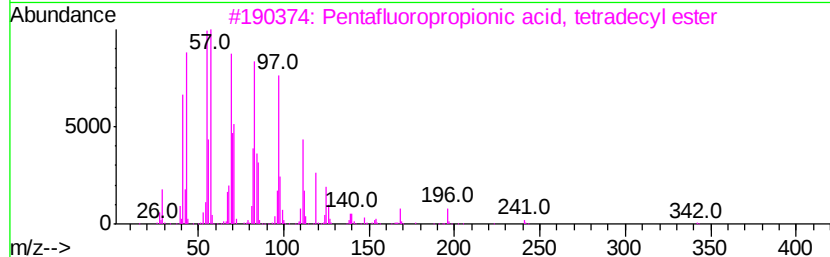
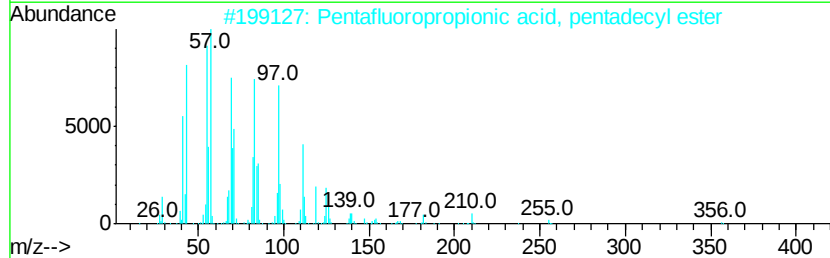
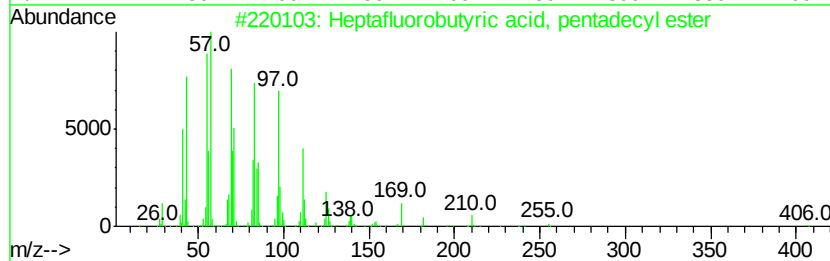
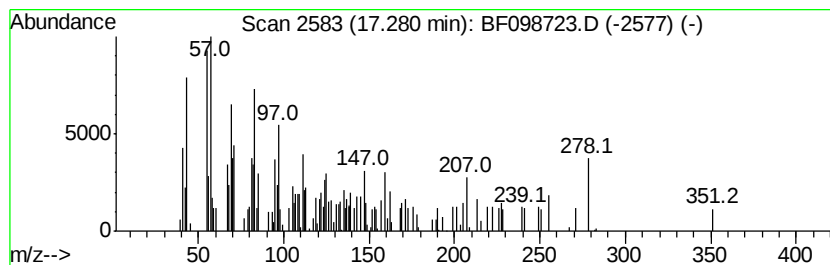
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.28 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	3.20 ng	130523	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	49
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	49
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	49
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	49
5		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098723.D
Acq On : 23 Sep 2017 3:52
Operator : SJ/JU
Sample : I5340-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LT-TS-003

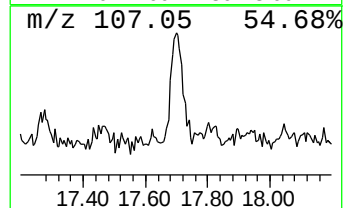
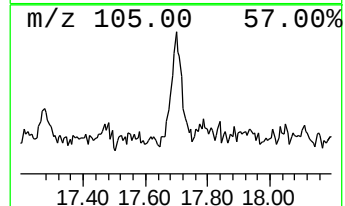
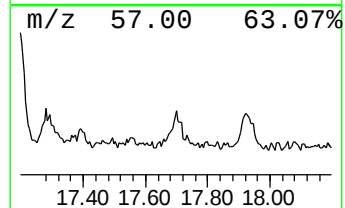
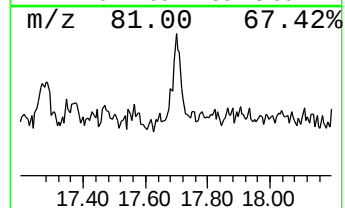
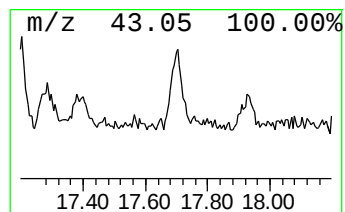
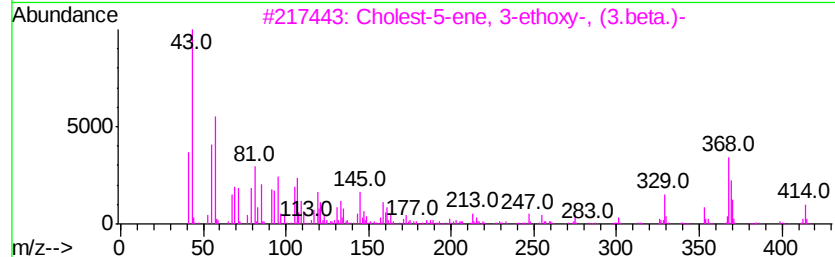
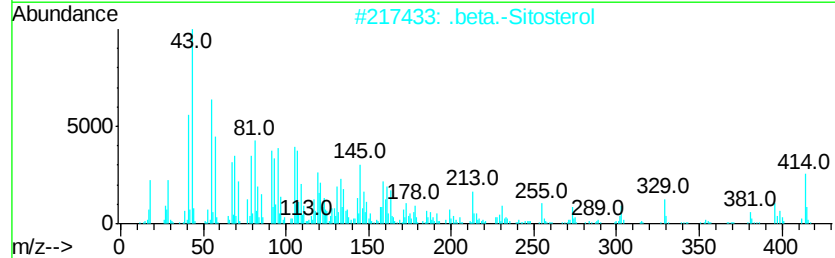
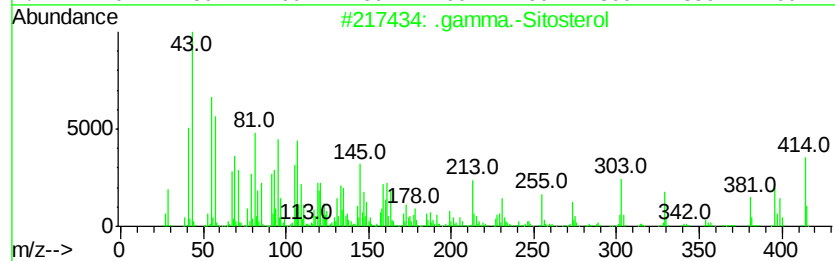
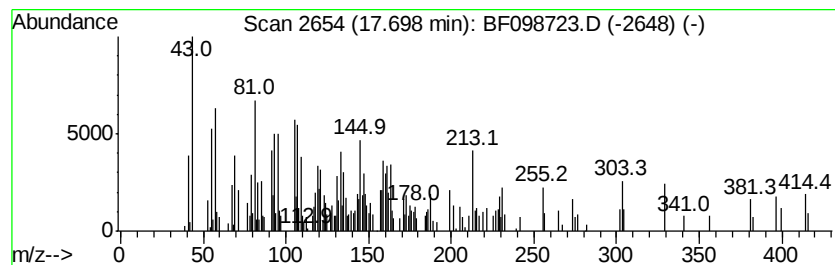
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .gamma.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	5.34 ng	218203	Perylene-d12	15.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2			.beta.-Sitosterol	414	C29H50O	000083-46-5	96
3			Cholest-5-ene, 3-ethoxy-, (3.beta....	414	C29H50O	000986-19-6	46
4			Ursodeoxycholic acid	392	C24H40O4	000128-13-2	42
5			Chenodioli	392	C24H40O4	000474-25-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
 Data File : BF098723.D
 Acq On : 23 Sep 2017 3:52
 Operator : SJ/JU
 Sample : I5340-03
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LT-TS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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
Butane, 2-methoxy...	2.26	3.8	ng	179147	1	6.93	954154	20.0
2-Pentanone, 4-hy...	5.16	13.4	ng	637474	1	6.93	954154	20.0
unknown6.70	6.70	73.8	ng	3519180	1	6.93	954154	20.0
1-Iodo-2-methylun...	10.86	2.5	ng	125858	4	11.45	988925	20.0
n-Hexadecanoic acid	11.97	9.9	ng	491489	4	11.45	988925	20.0
Octadecanoic acid	12.75	3.3	ng	162355	4	11.45	988925	20.0
1-Heneicosanol	13.92	6.8	ng	348044	5	14.09	1030440	20.0
Octadecanal	15.01	5.9	ng	239399	6	15.59	816865	20.0
Nonadecane	15.21	3.1	ng	128641	6	15.59	816865	20.0
12-Octadecenal	15.81	2.0	ng	82225	6	15.59	816865	20.0
Tetratetracontane	16.06	5.2	ng	212937	6	15.59	816865	20.0
Behenic alcohol	16.10	4.8	ng	195408	6	15.59	816865	20.0
unknown16.49	16.49	3.6	ng	147953	6	15.59	816865	20.0
1,9-Tetradecadiene	16.89	2.3	ng	93234	6	15.59	816865	20.0
Heptadecane	17.20	2.4	ng	99098	6	15.59	816865	20.0
unknown17.28	17.28	3.2	ng	130523	6	15.59	816865	20.0
.gamma.-Sitosterol	17.70	5.3	ng	218203	6	15.59	816865	20.0