

Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
 Data File : BF102084.D
 Acq On : 16 Jan 2018 00:53
 Operator : SJ/JU
 Sample : J1122-24
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G-3

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-BF010918.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	4.934	480	484	493	rVB	228222	345245	7.66%	0.895%
2	5.340	547	553	556	rBV	3981665	4406451	97.80%	11.428%
3	6.363	720	727	730	rBV	3787098	4375757	97.12%	11.348%
4	6.492	744	749	752	rBV	4409791	4409245	97.87%	11.435%
5	6.722	784	788	791	rBV	1323422	1060382	23.54%	2.750%
6	6.881	810	815	818	rBV	3589968	3518205	78.09%	9.124%
7	7.286	878	884	887	rBV	2701062	2836529	62.96%	7.356%
8	7.369	894	898	901	rBV	50308	48306	1.07%	0.125%
9	8.004	1001	1006	1009	rBV	1490982	1337579	29.69%	3.469%
10	9.080	1183	1189	1192	rBV	4881411	4505366	100.00%	11.684%
11	9.475	1252	1256	1259	rBV	576626	494738	10.98%	1.283%
12	9.686	1289	1292	1296	rVB	205811	163696	3.63%	0.425%
13	9.751	1296	1303	1307	rBV2	1402595	1237224	27.46%	3.209%
14	9.957	1334	1338	1340	rBV2	48911	57686	1.28%	0.150%
15	10.010	1343	1347	1351	rBV2	47745	47896	1.06%	0.124%
16	10.186	1374	1377	1380	rVB	269238	194693	4.32%	0.505%
17	10.404	1409	1414	1417	rBV	63312	78881	1.75%	0.205%
18	10.539	1432	1437	1440	rBV	2130990	1939988	43.06%	5.031%
19	10.657	1454	1457	1466	rVB	210279	218548	4.85%	0.567%
20	11.104	1530	1533	1536	rBV	82844	65930	1.46%	0.171%
21	11.233	1551	1555	1560	rBV	1152265	994644	22.08%	2.580%
22	11.274	1560	1562	1568	rVB	69664	64744	1.44%	0.168%
23	11.451	1588	1592	1595	rBV	75630	74558	1.65%	0.193%
24	11.621	1618	1621	1624	rBV	144110	118758	2.64%	0.308%
25	11.763	1642	1645	1652	rBV	195621	205162	4.55%	0.532%
26	12.439	1757	1760	1763	rBV2	52425	66008	1.47%	0.171%
27	12.551	1776	1779	1782	rBV3	58521	65739	1.46%	0.170%
28	12.821	1820	1825	1828	rVB	2879484	2706825	60.08%	7.020%
29	13.027	1857	1860	1863	rBV5	35402	51786	1.15%	0.134%
30	13.710	1973	1976	1979	rBV	413975	383762	8.52%	0.995%
31	13.862	1998	2002	2005	rBV	1023380	930314	20.65%	2.413%
32	13.915	2009	2011	2014	rVB3	65945	69727	1.55%	0.181%
33	14.045	2030	2033	2038	rVB4	77582	91337	2.03%	0.237%
34	14.098	2039	2042	2044	rBV4	44839	49728	1.10%	0.129%

Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.215	2060	2062	2066	rBV4	59115	66958	1.49%	0.174%
36	14.345	2081	2084	2087	rVB2	110252	115933	2.57%	0.301%
37	14.392	2090	2092	2097	rVB3	68410	71460	1.59%	0.185%
38	14.468	2102	2105	2107	rBV2	45836	52043	1.16%	0.135%
39	14.874	2171	2174	2177	rBV4	52333	62928	1.40%	0.163%
40	15.280	2238	2243	2247	rBV	709159	839790	18.64%	2.178%
41	15.768	2322	2326	2332	rVB	100451	134373	2.98%	0.348%

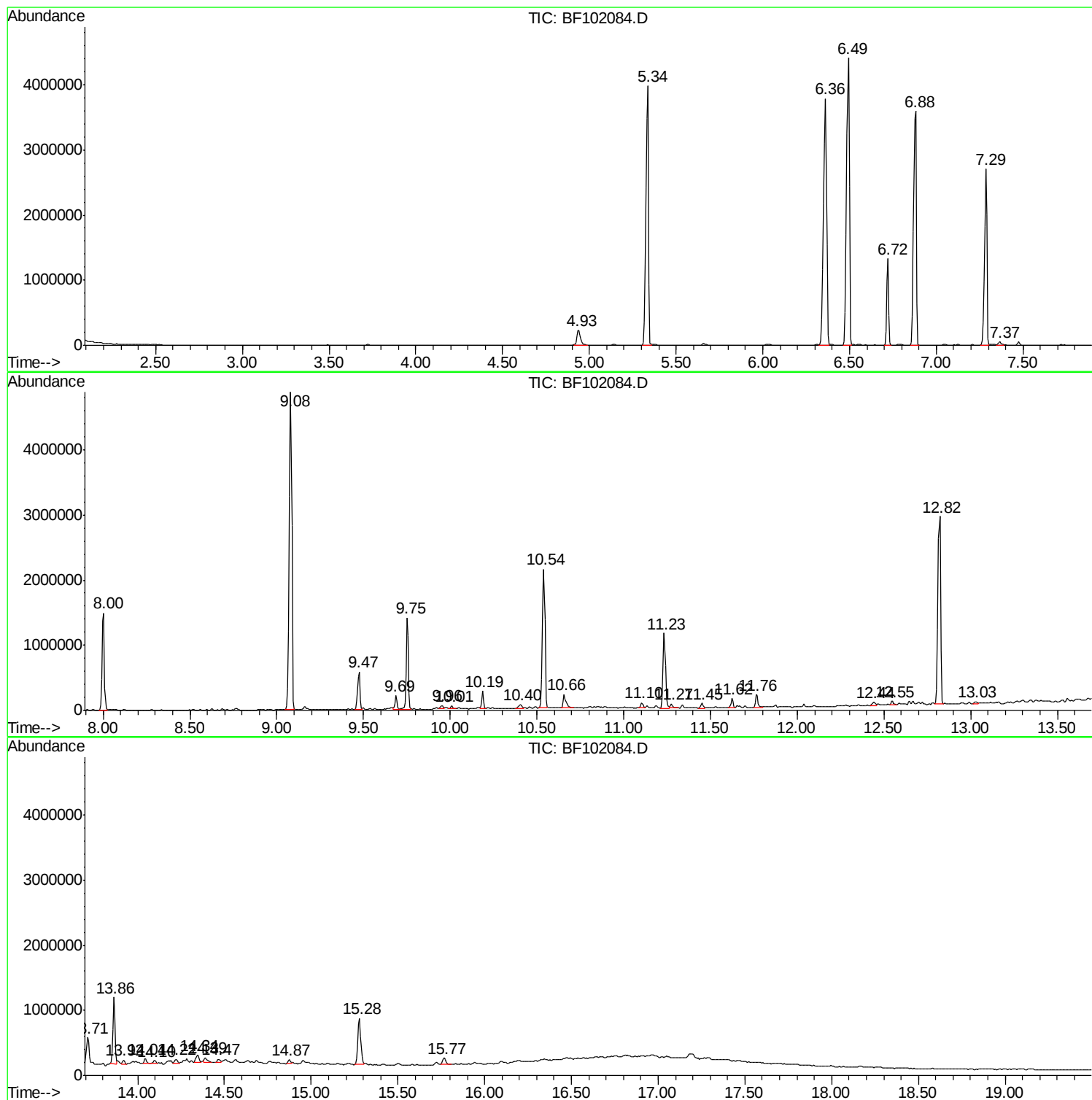
Sum of corrected areas: 38558922

Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
G-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

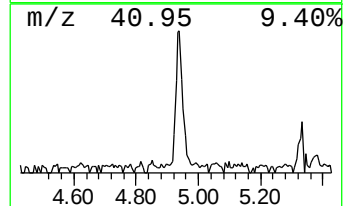
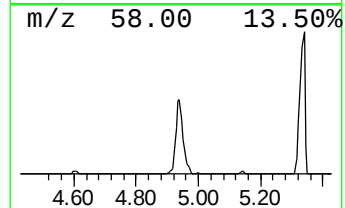
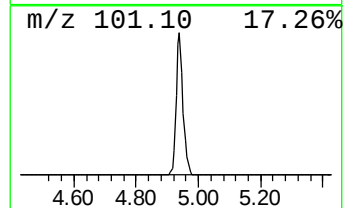
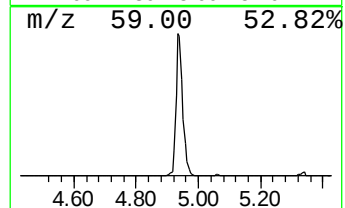
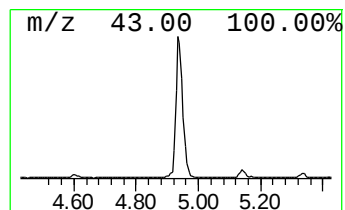
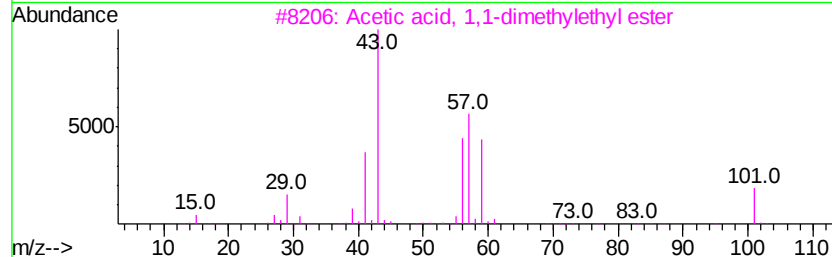
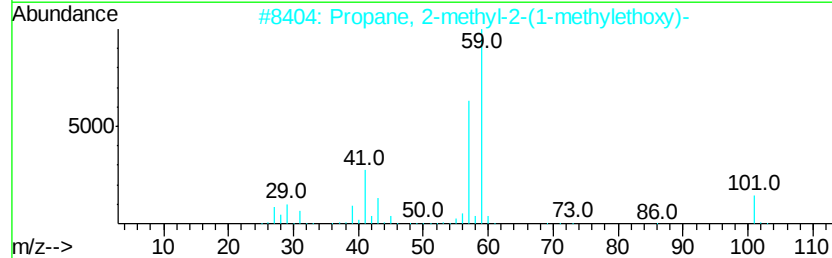
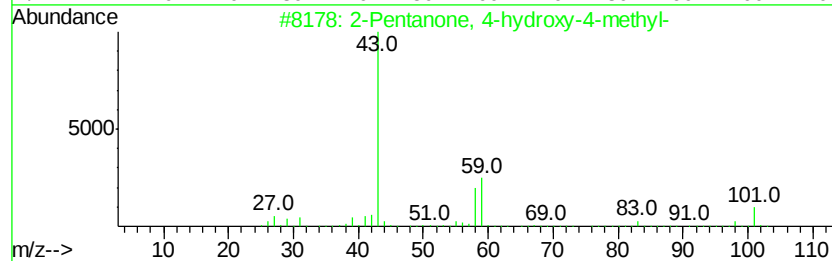
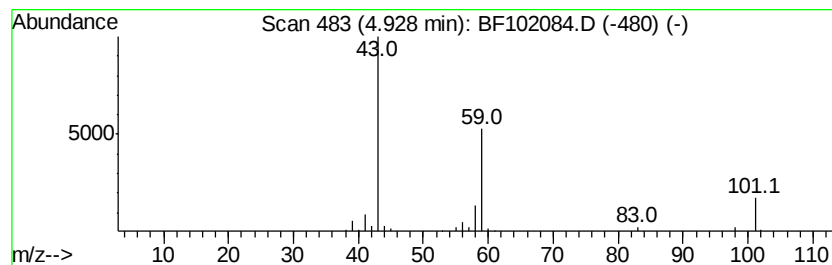
Instrument :
BNA_F
ClientSampleId :
G-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.93	6.51 ng	345245	1,4-Dichlorobenzene-d4	6.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-3

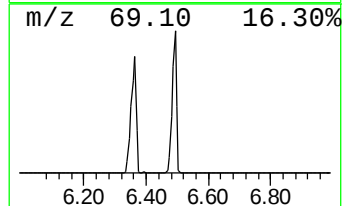
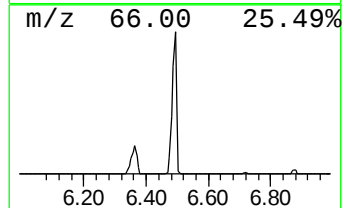
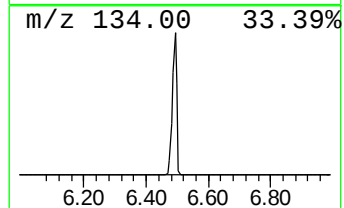
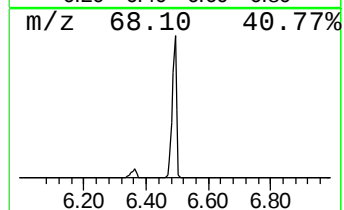
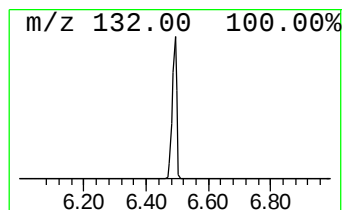
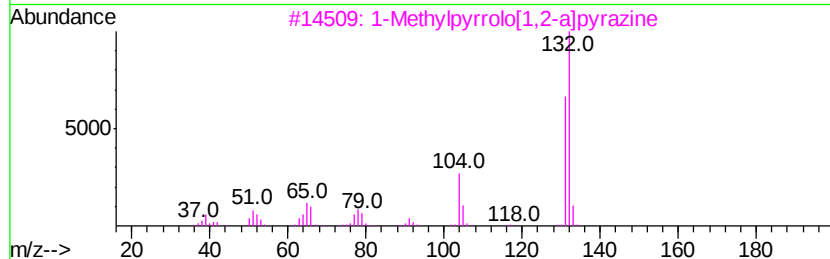
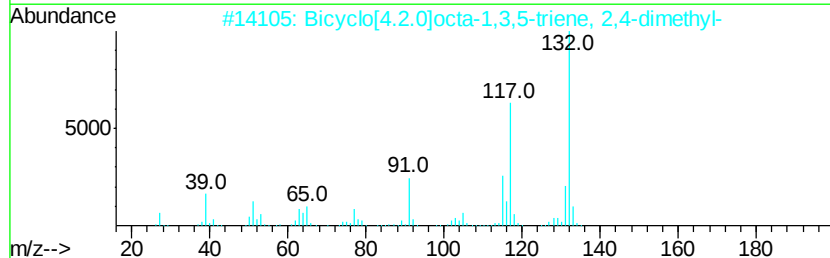
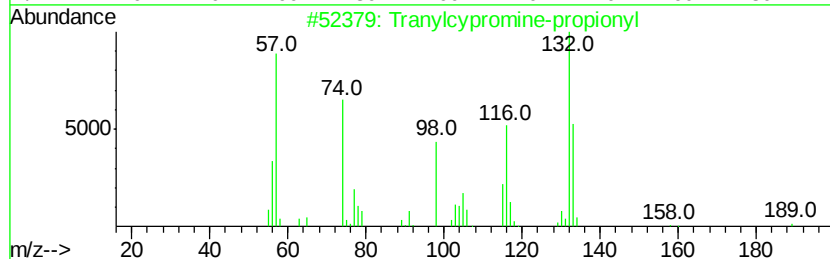
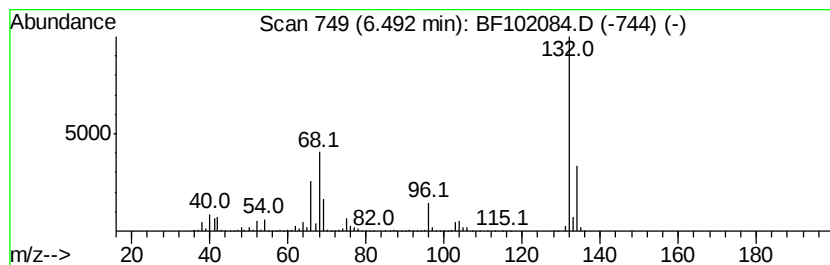
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	83.16 ng	4409250	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicvclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		1-Methvlpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	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 : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

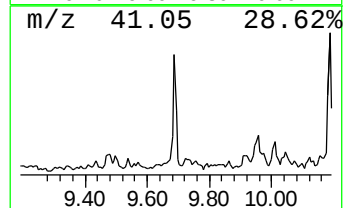
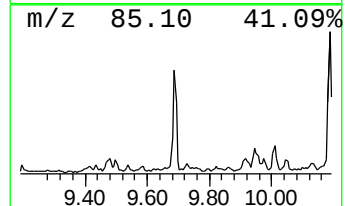
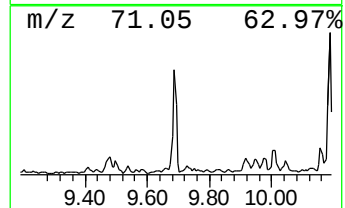
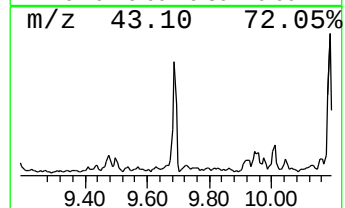
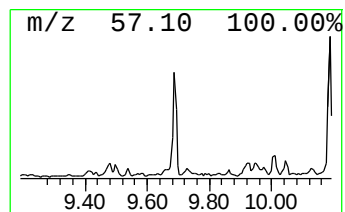
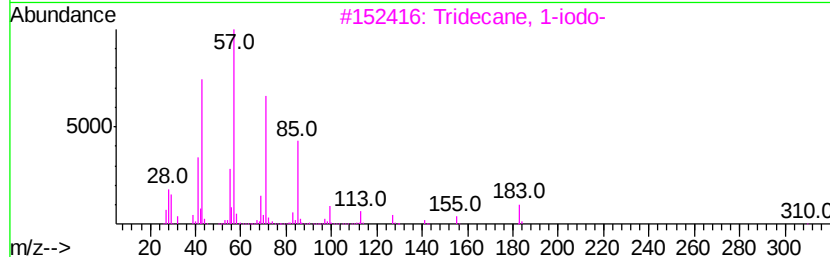
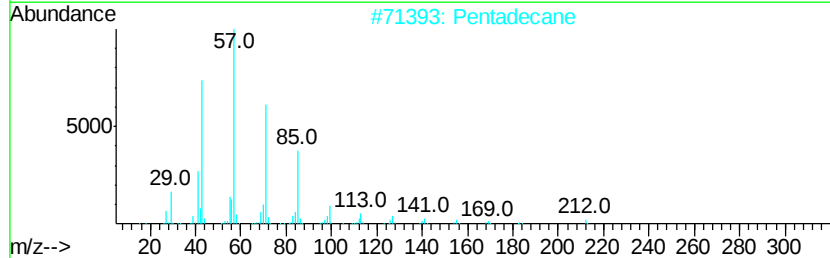
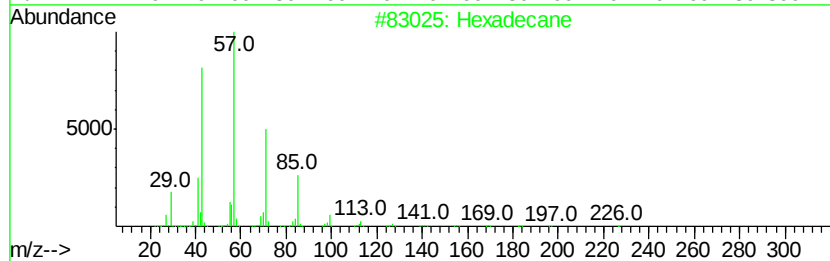
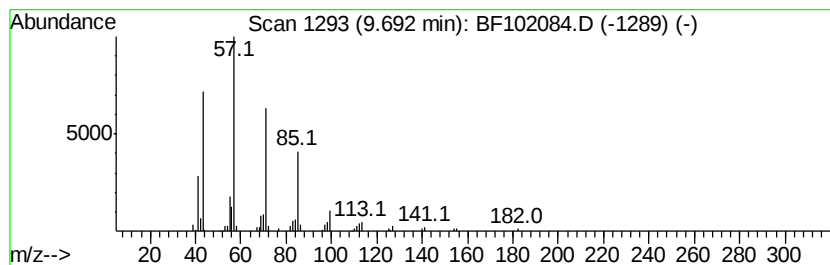
Instrument :
BNA_F
ClientSampleId :
G-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
9.69	2.65 ng	163696	Acenaphthene-d10		9.75		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Pentadecane	212	C15H32	000629-62-9	90
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
4			3-Hexanone, 2,2-dimethyl-	128	C8H16O	005405-79-8	50
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	47



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

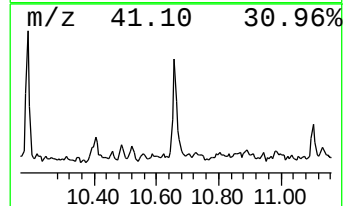
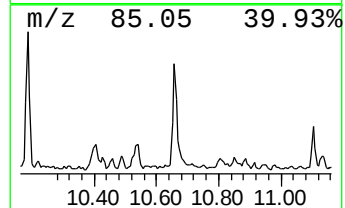
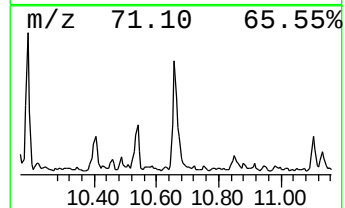
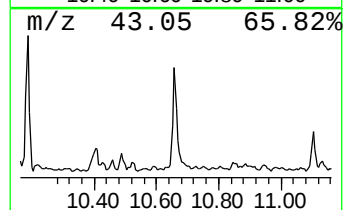
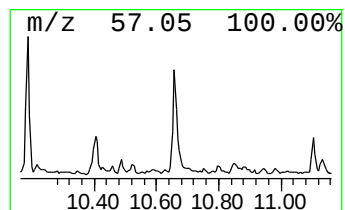
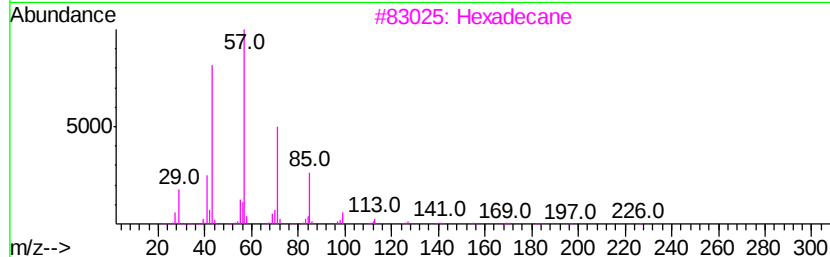
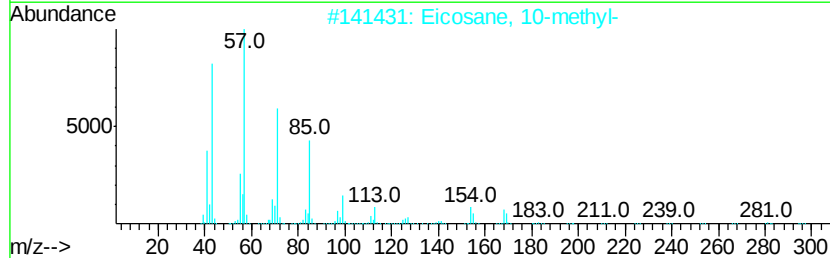
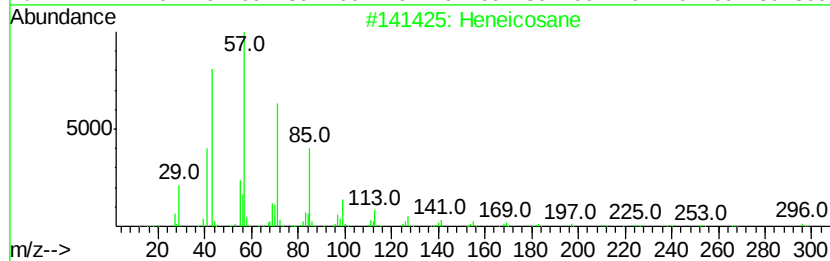
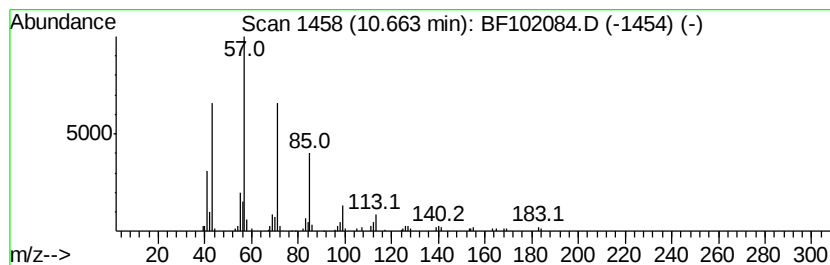
Instrument :
BNA_F
ClientSampleId :
G-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.66	4.39 ng	218548	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
5	Tetradecane	198	C14H30	000629-59-4	87



Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-3

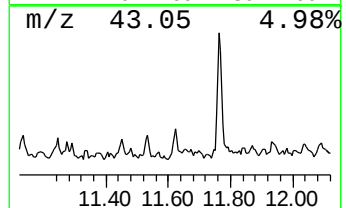
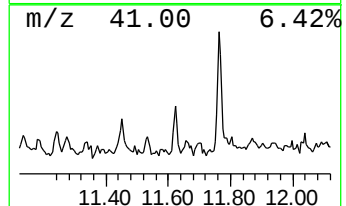
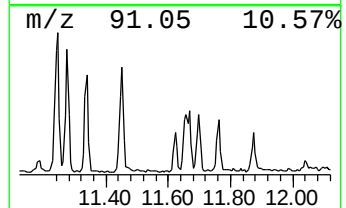
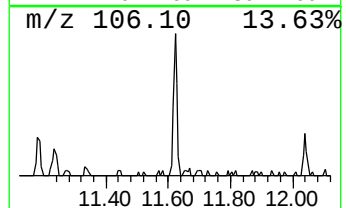
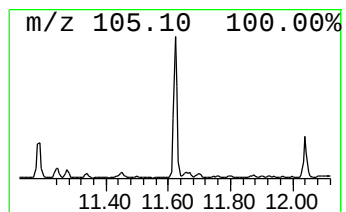
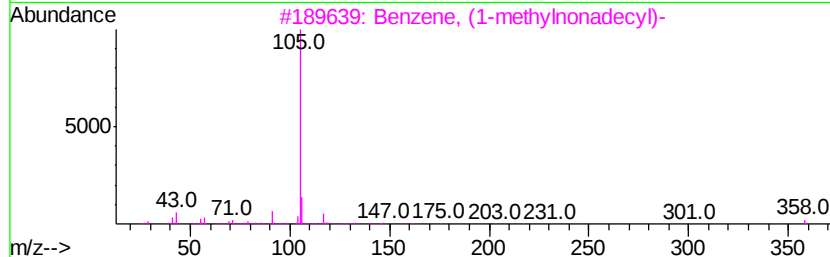
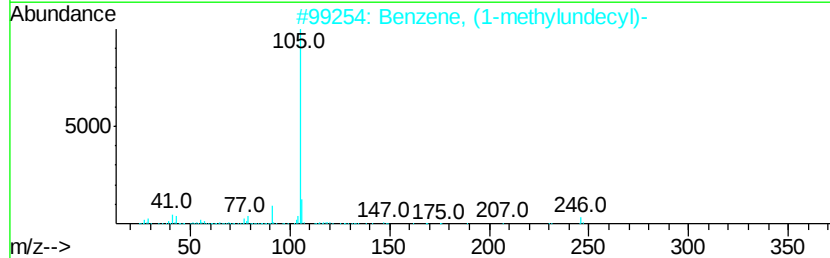
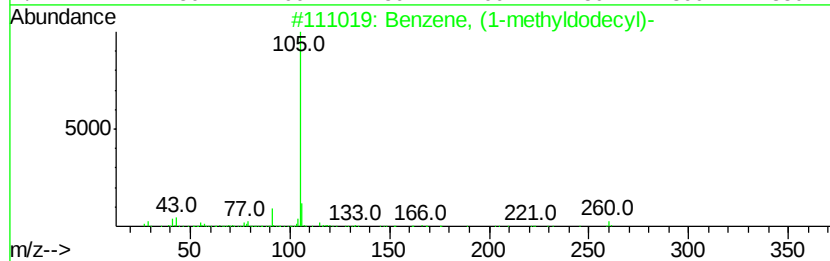
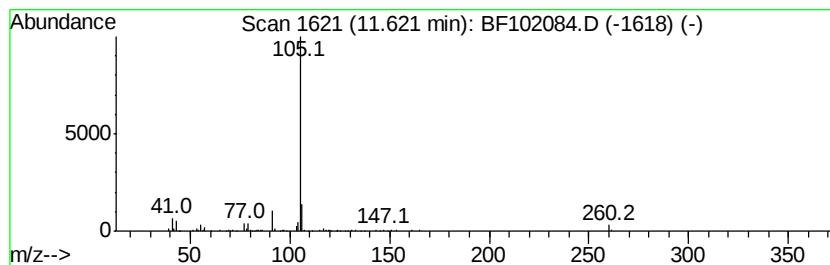
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, (1-methyldodecyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.39 ng	118758	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	90
2		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
3		Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	64
4		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	64
5		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64



Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

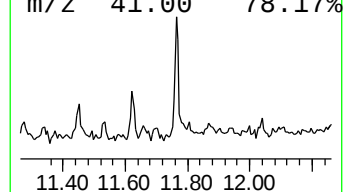
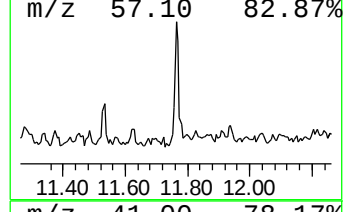
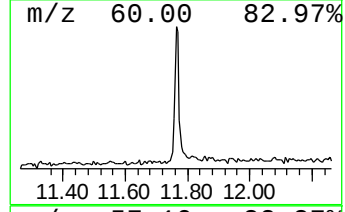
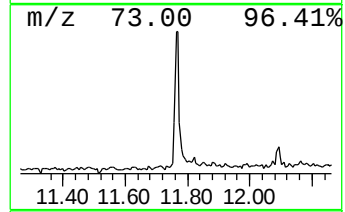
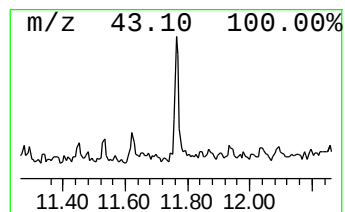
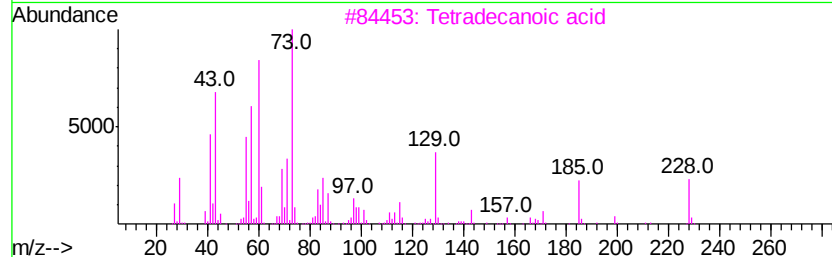
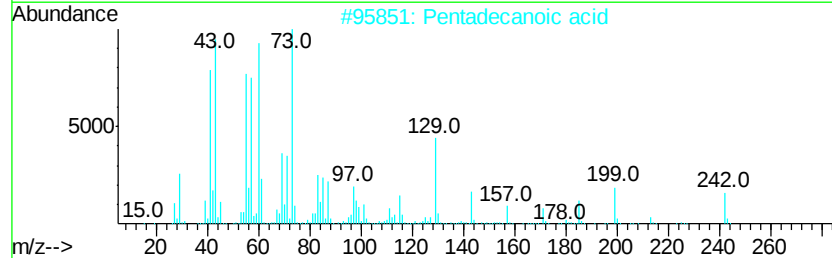
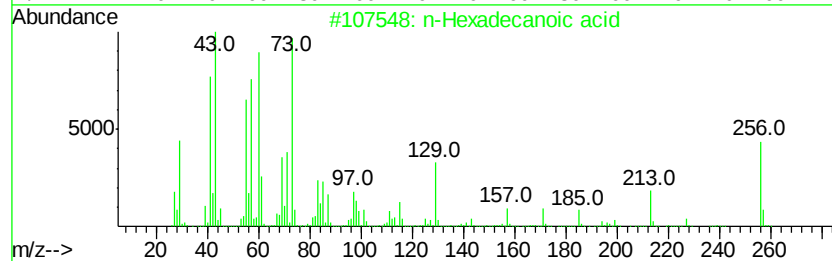
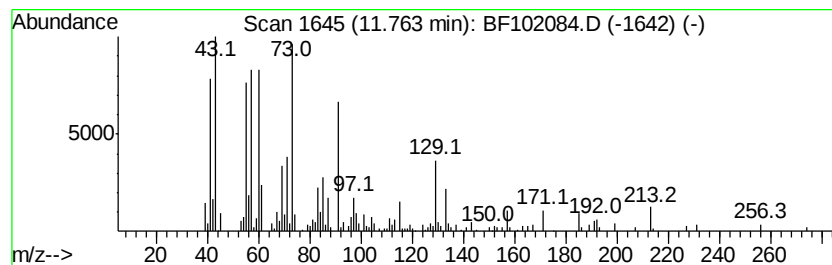
Instrument :
BNA_F
ClientSampleId :
G-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.76	4.13 ng	205162	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-3

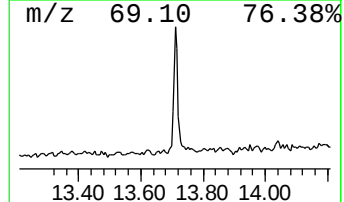
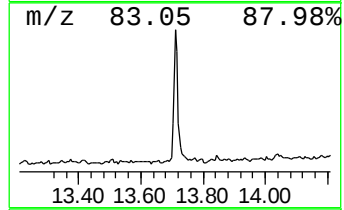
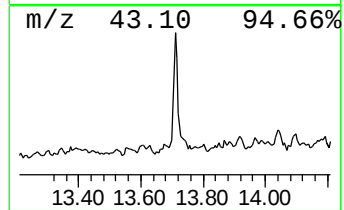
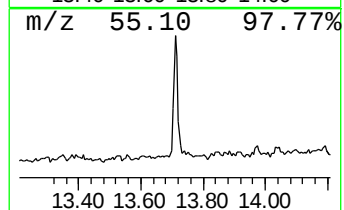
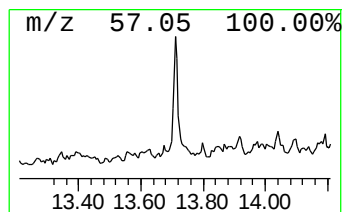
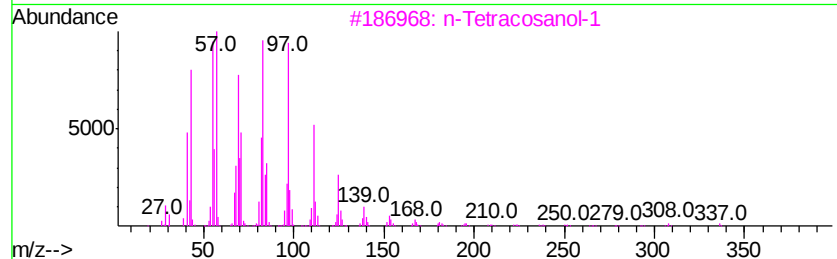
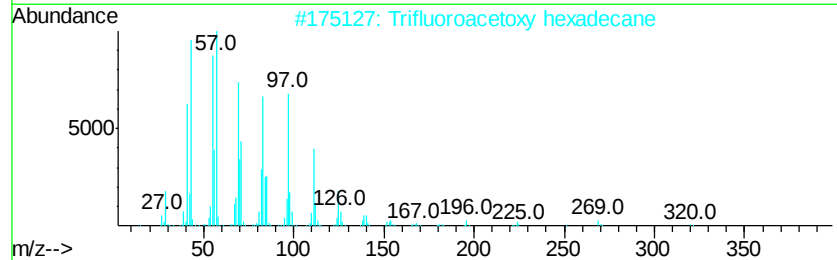
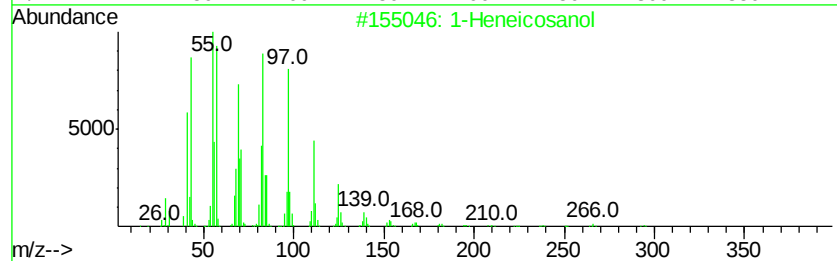
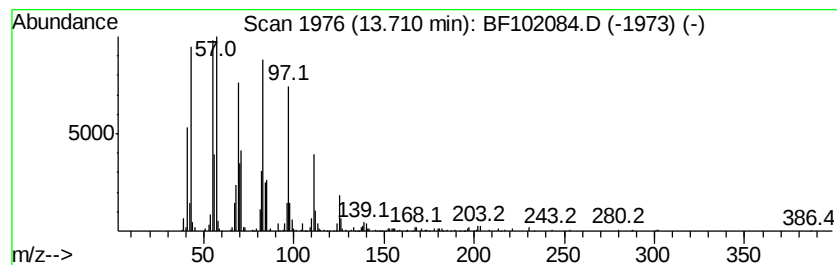
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	8.25 ng	383762	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-3

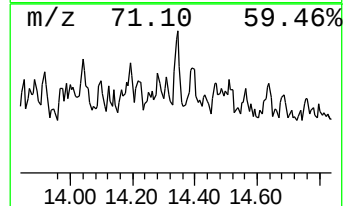
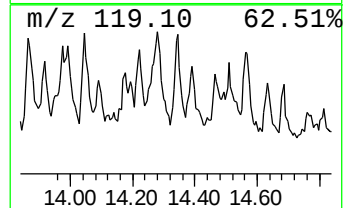
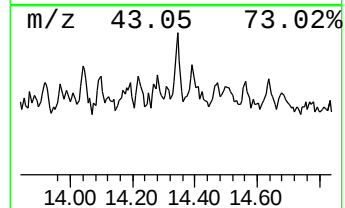
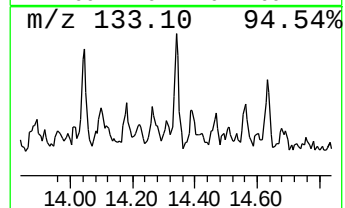
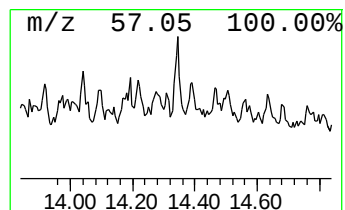
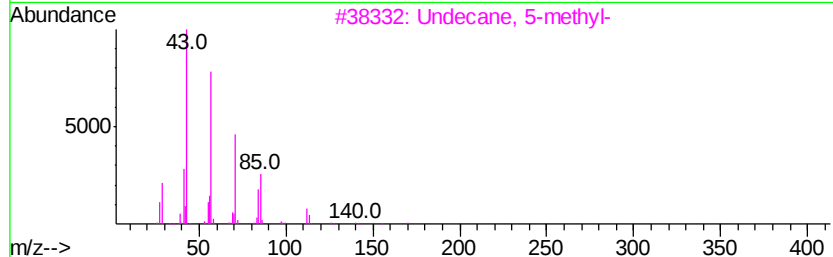
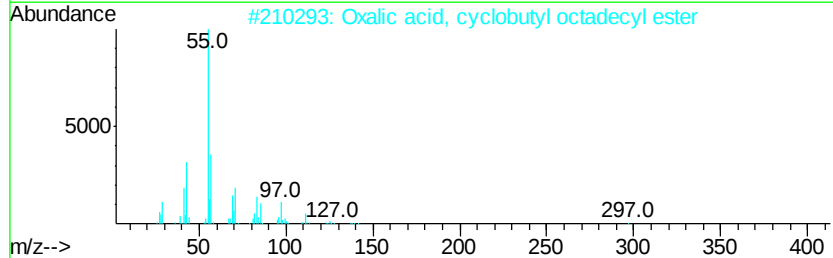
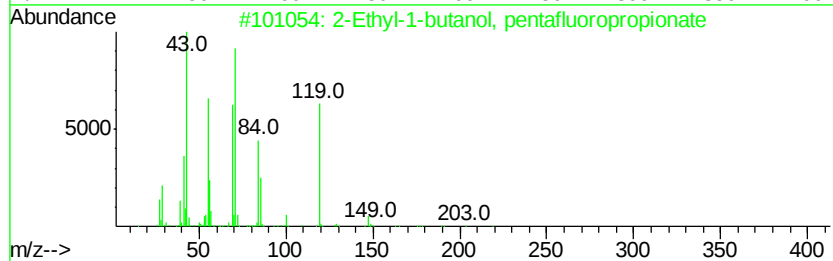
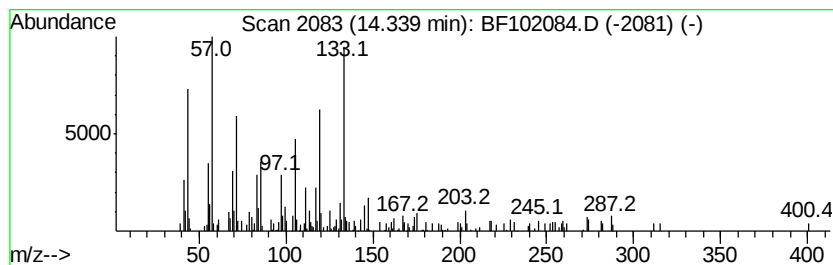
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.34 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.49 ng	115933	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Ethyl-1-butanol, pentafluoropr...	248	C9H13F5O2	1000352-36-5	38
2		Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	22
3		Undecane, 5-methyl-	170	C12H26	001632-70-8	22
4		Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	22
5		Tridecane	184	C13H28	000629-50-5	20



Data Path : U:\HPCHEM1\BNA F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

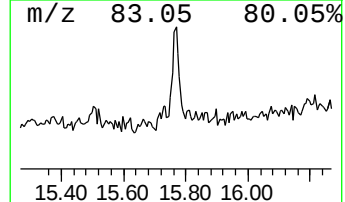
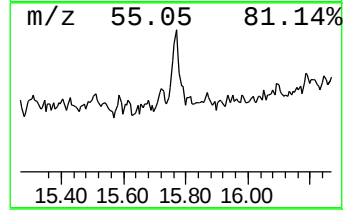
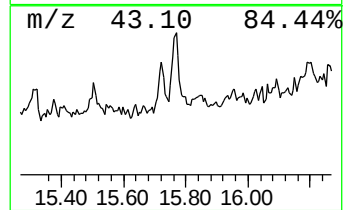
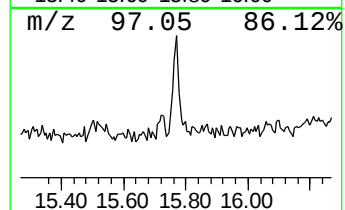
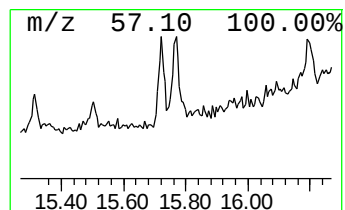
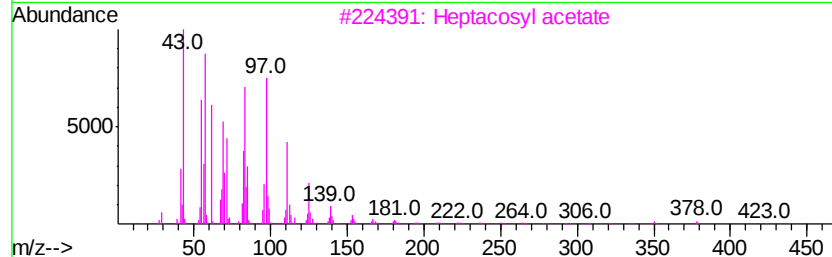
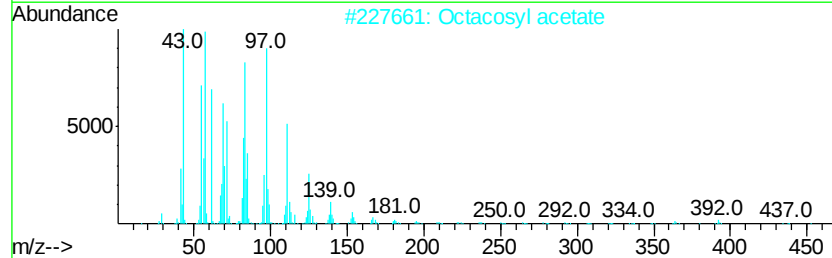
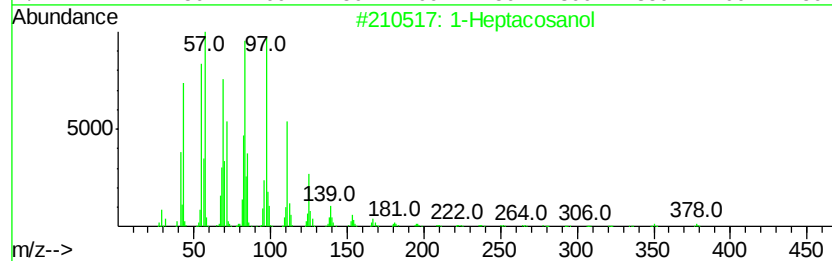
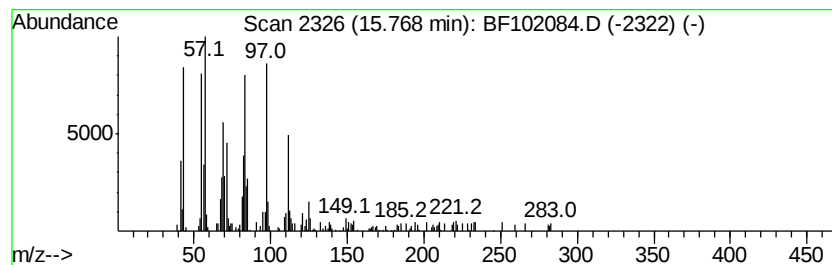
Instrument :
BNA_F
ClientSampled :
G-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.77	3.20 ng	134373	Perylene-d12	15.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Octacosyl acetate	452	C30H60O2	018206-97-8	91
3	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
4	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	74
5	Behenic alcohol	326	C22H46O	000661-19-8	74



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011518\
Data File : BF102084.D
Acq On : 16 Jan 2018 00:53
Operator : SJ/JU
Sample : J1122-24
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	6.5	ng	345245	1	6.72	1060380	20.0
unknown6.49	6.49	83.2	ng	4409250	1	6.72	1060380	20.0
Hexadecane	9.69	2.6	ng	163696	3	9.75	1237220	20.0
Heneicosane	10.66	4.4	ng	218548	4	11.23	994644	20.0
Benzene, (1-methy...	11.62	2.4	ng	118758	4	11.23	994644	20.0
n-Hexadecanoic acid	11.76	4.1	ng	205162	4	11.23	994644	20.0
1-Heneicosanol	13.71	8.3	ng	383762	5	13.86	930314	20.0
unknown14.34	14.34	2.5	ng	115933	5	13.86	930314	20.0
1-Heptacosanol	15.77	3.2	ng	134373	6	15.28	839790	20.0