

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
 Data File : BF103215.D
 Acq On : 26 Feb 2018 13:40
 Operator : SJ/JU
 Sample : J1652-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-2898

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-BF022218.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	2.163	5	13	23	rVB	1307311	1803978	36.75%	4.170%
2	5.116	512	515	530	rVB	198403	299504	6.10%	0.692%
3	5.498	575	580	583	rBV	4390263	4908329	100.00%	11.346%
4	6.510	746	752	755	rBV	3926117	4608428	93.89%	10.653%
5	6.645	770	775	778	rBV	4500233	4601371	93.75%	10.637%
6	6.869	809	813	821	rBV	1326512	1073426	21.87%	2.481%
7	7.028	835	840	843	rBV	3904467	3677352	74.92%	8.501%
8	7.440	904	910	913	rBV	2893807	3211088	65.42%	7.423%
9	8.151	1027	1031	1049	rVB	1513054	1388685	28.29%	3.210%
10	9.228	1209	1214	1217	rBV	4482214	4362469	88.88%	10.084%
11	9.298	1223	1226	1229	rVB	68722	57616	1.17%	0.133%
12	9.616	1275	1280	1288	rVB	273259	280840	5.72%	0.649%
13	9.828	1312	1316	1320	rVB	160530	126645	2.58%	0.293%
14	9.910	1326	1330	1334	rBV	1294850	1226580	24.99%	2.835%
15	10.328	1398	1401	1404	rVB	171854	133163	2.71%	0.308%
16	10.545	1432	1438	1440	rBV	40544	49253	1.00%	0.114%
17	10.698	1460	1464	1479	rBV	2057013	2193685	44.69%	5.071%
18	10.798	1479	1481	1486	rVV	98785	93830	1.91%	0.217%
19	11.398	1579	1583	1585	rBV	1052108	944248	19.24%	2.183%
20	11.422	1585	1587	1592	rVB	183039	155628	3.17%	0.360%
21	11.910	1666	1670	1672	rBV2	59318	77454	1.58%	0.179%
22	12.010	1684	1687	1696	rVB4	43871	74720	1.52%	0.173%
23	12.610	1786	1789	1795	rBV	317014	286125	5.83%	0.661%
24	12.786	1816	1819	1823	rVB	375979	335884	6.84%	0.776%
25	12.839	1823	1828	1831	rBV	290274	320576	6.53%	0.741%
26	12.863	1831	1832	1835	rVB	96771	67777	1.38%	0.157%
27	12.980	1847	1852	1856	rBV	2814920	2881055	58.70%	6.660%
28	13.157	1877	1882	1883	rBV3	34066	53761	1.10%	0.124%
29	13.492	1936	1939	1943	rBV	261728	242401	4.94%	0.560%
30	13.868	2000	2003	2011	rVB3	174339	235224	4.79%	0.544%
31	14.004	2023	2026	2028	rBV	88000	85750	1.75%	0.198%
32	14.039	2028	2032	2035	rVV2	899633	1050714	21.41%	2.429%
33	14.069	2035	2037	2040	rVB	162104	140876	2.87%	0.326%
34	14.186	2054	2057	2064	rVB2	61498	67420	1.37%	0.156%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.498	2107	2110	2116	rBV2	76755	100442	2.05%	0.232%
36	14.804	2159	2162	2164	rBV	65828	58065	1.18%	0.134%
37	14.880	2173	2175	2180	rVB	61360	62498	1.27%	0.144%
38	15.098	2208	2212	2215	rBV	211674	300304	6.12%	0.694%
39	15.145	2218	2220	2223	rVB	78630	75326	1.53%	0.174%
40	15.410	2261	2265	2271	rVB	130635	180193	3.67%	0.417%
41	15.468	2272	2275	2281	rBV	131467	160849	3.28%	0.372%
42	15.539	2281	2287	2291	rBV	699515	1006100	20.50%	2.326%
43	15.968	2358	2360	2366	rVB2	73567	95793	1.95%	0.221%
44	17.615	2635	2640	2648	rVB2	43014	104056	2.12%	0.241%

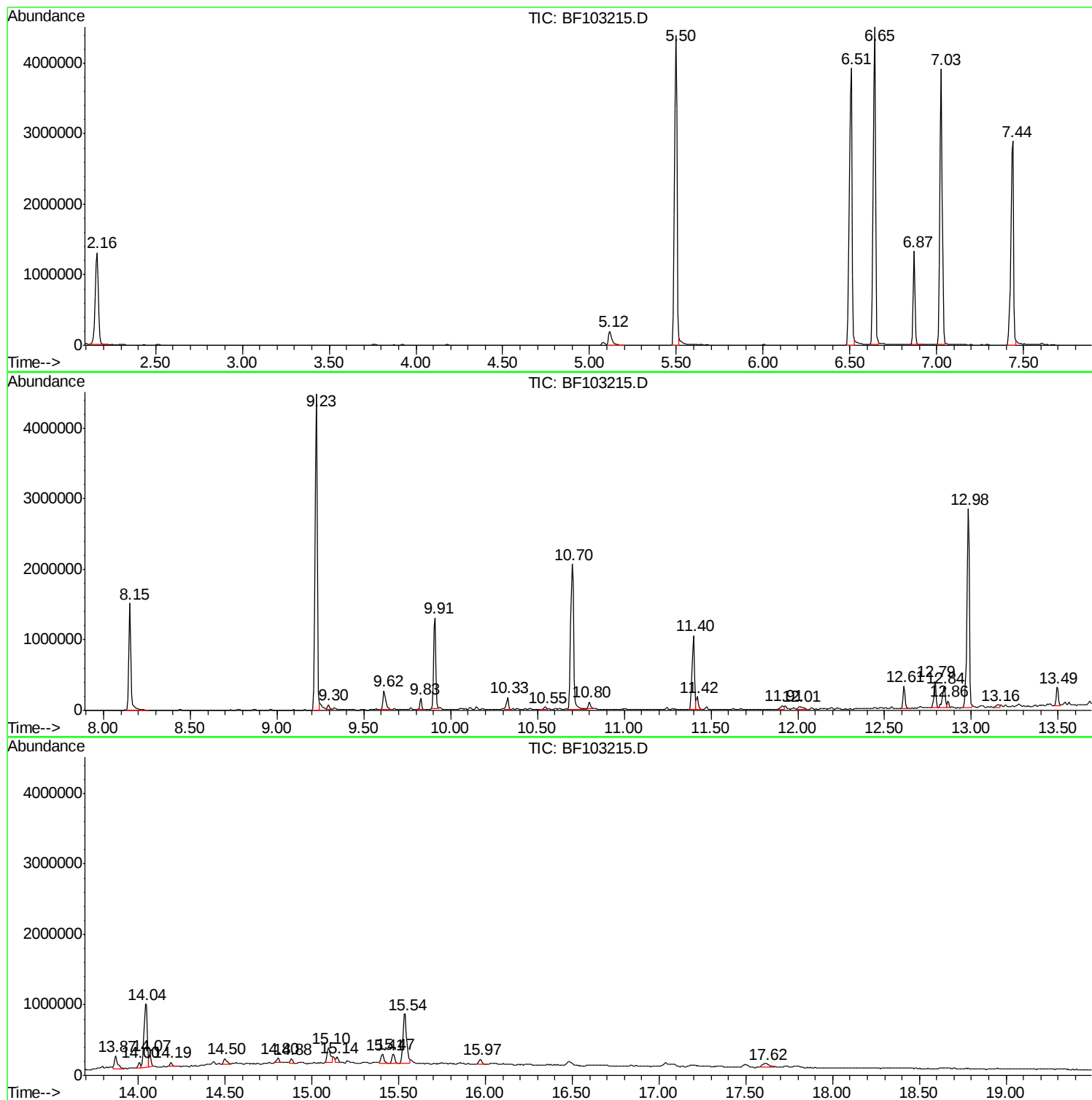
Sum of corrected areas: 43259481

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

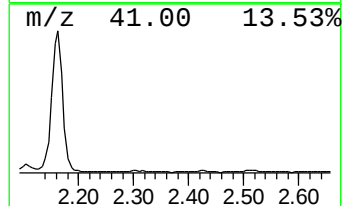
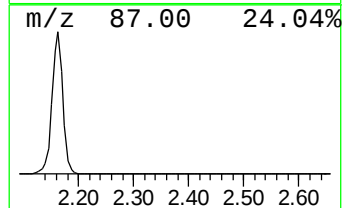
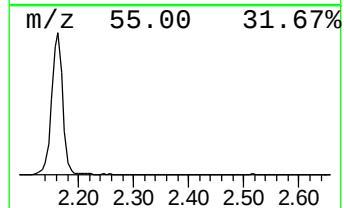
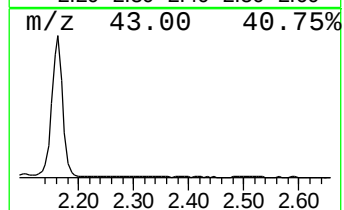
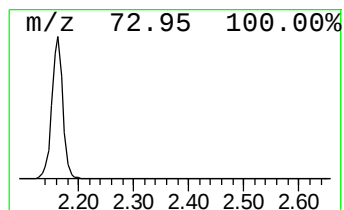
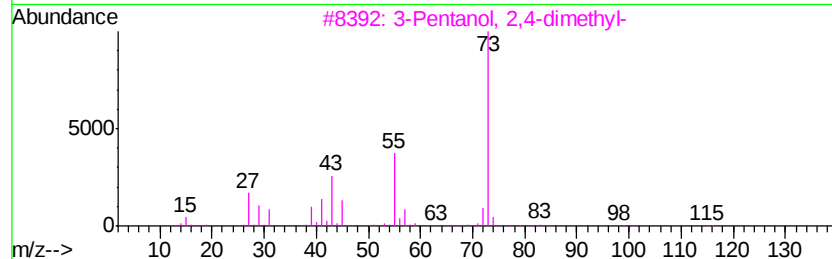
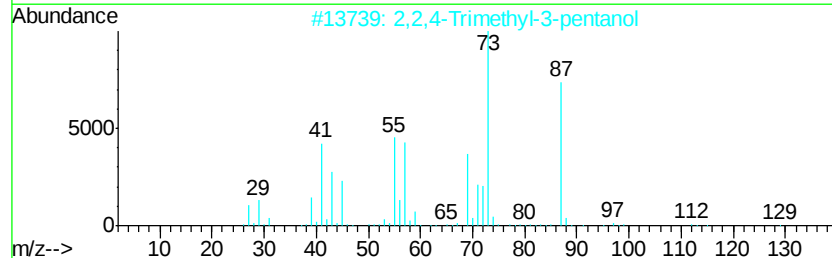
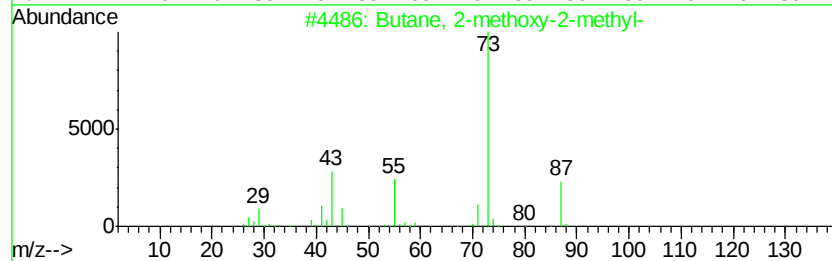
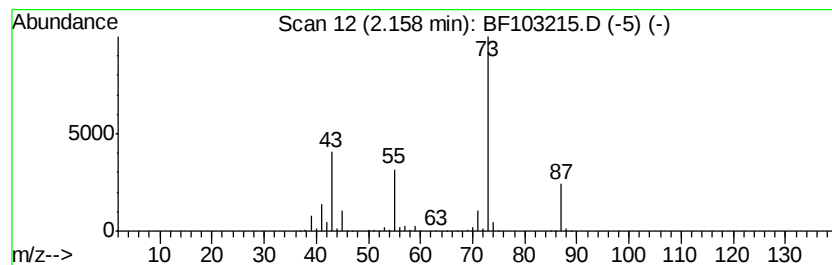
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	33.61 ng	1803980	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleID :
RT-2898

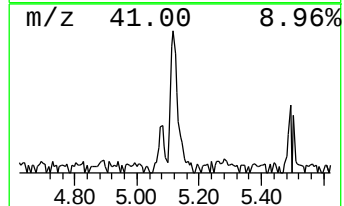
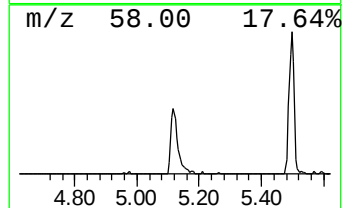
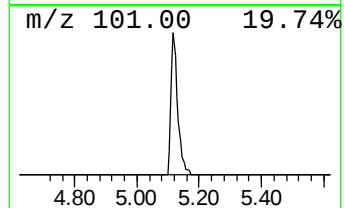
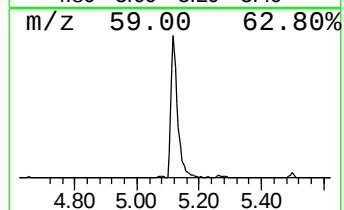
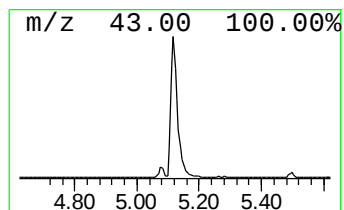
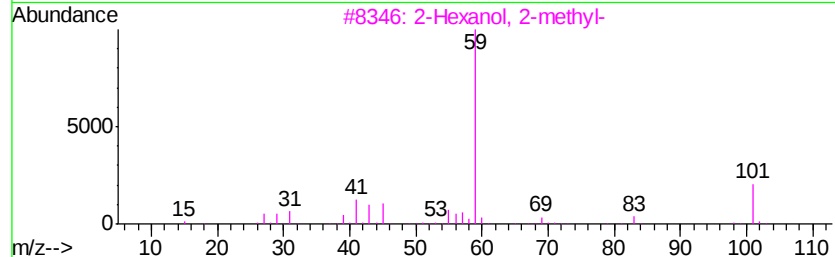
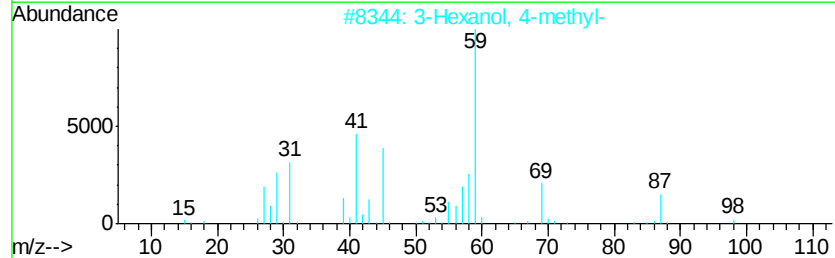
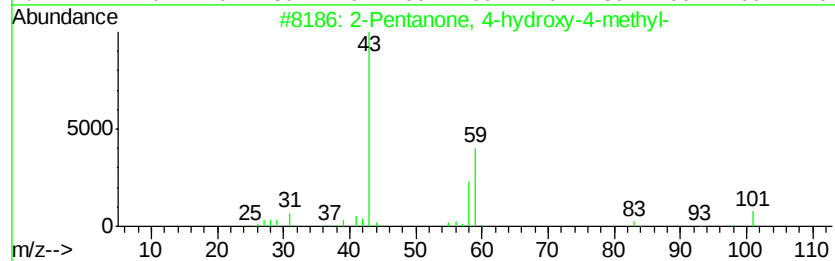
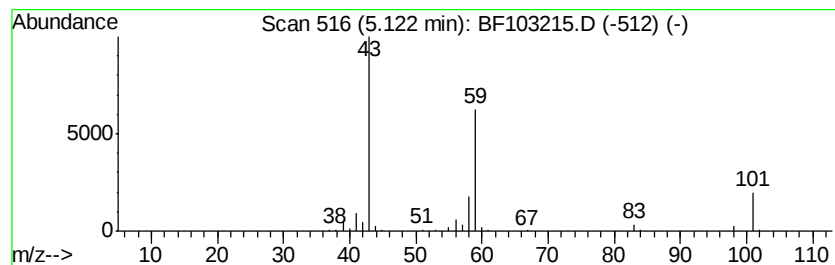
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	5.58 ng	299504	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

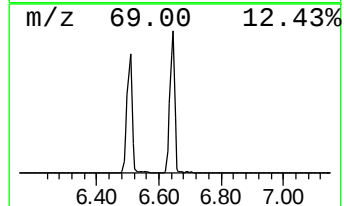
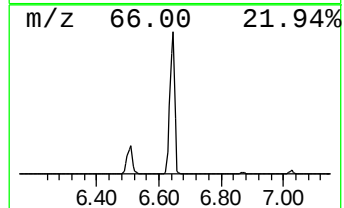
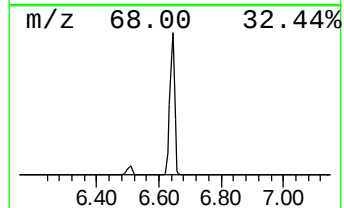
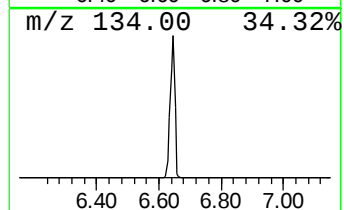
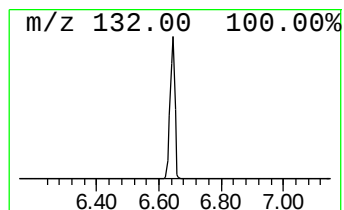
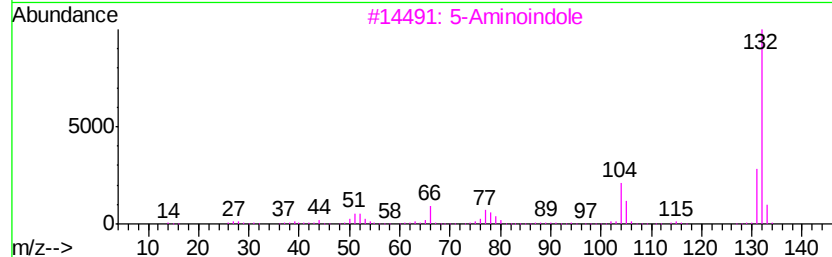
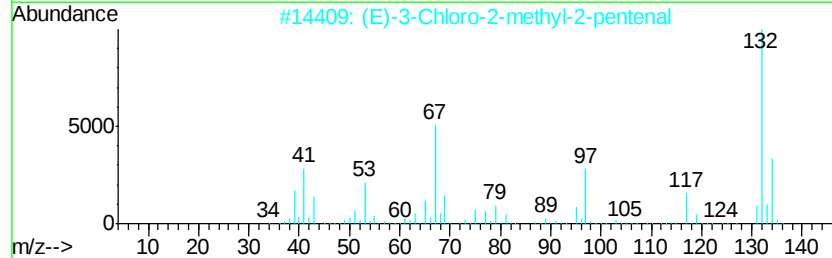
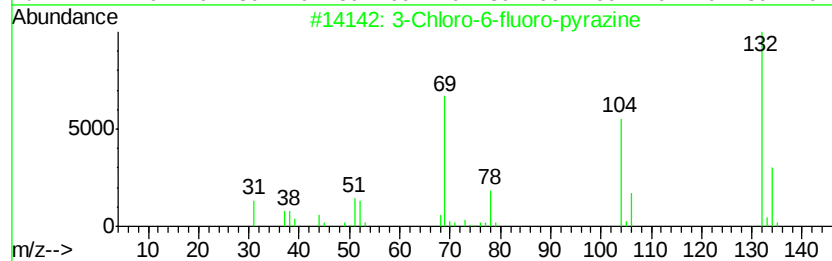
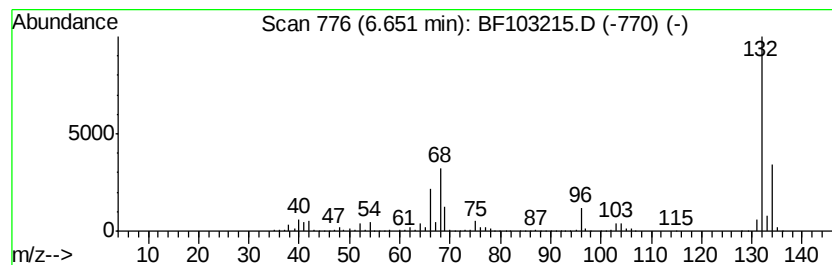
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	85.73 ng	4601370	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

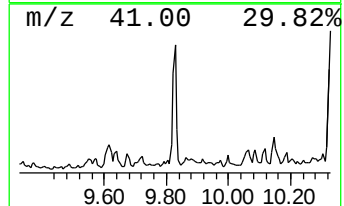
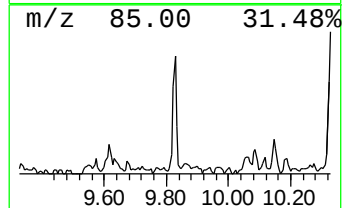
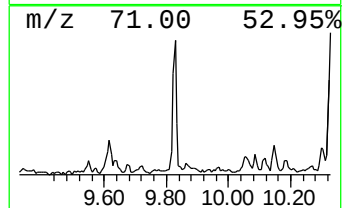
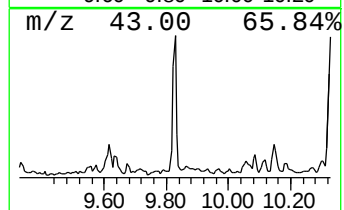
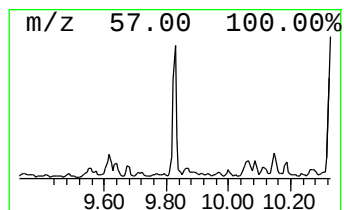
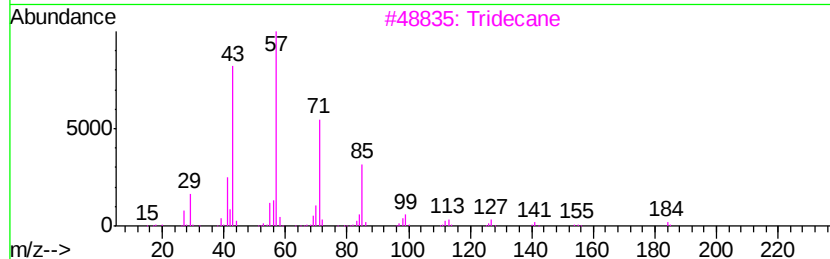
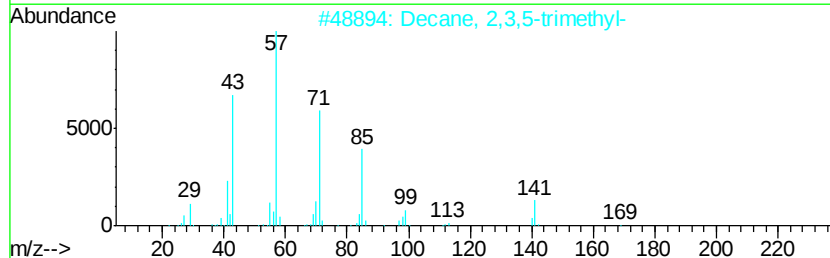
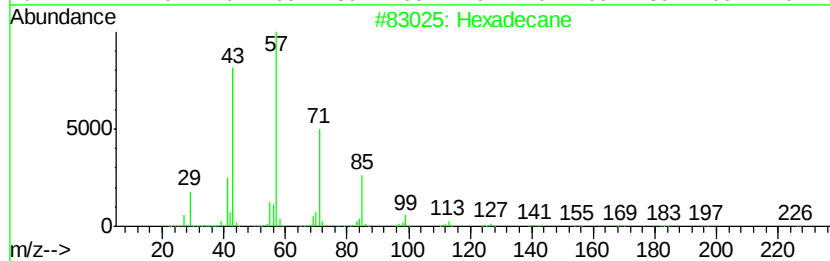
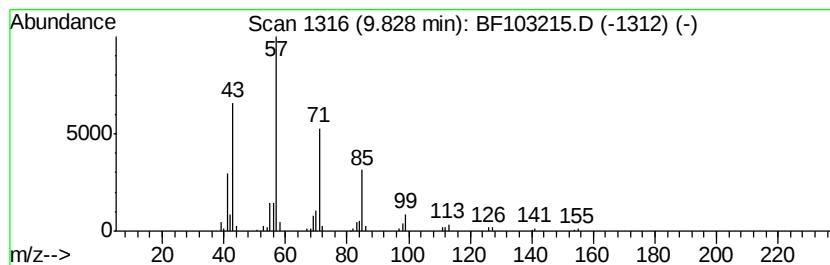
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.07 ng	126645	Acenaphthene-d10	9.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	86
3	Tridecane		184	C13H28	000629-50-5	83
4	Pentadecane		212	C15H32	000629-62-9	83
5	Tridecane, 6-methyl-		198	C14H30	013287-21-3	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

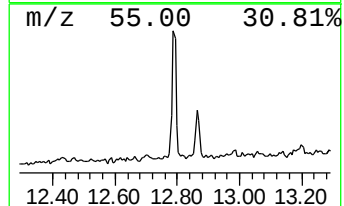
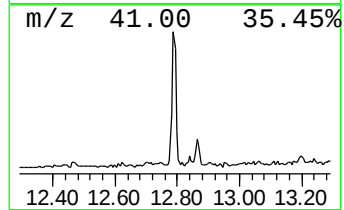
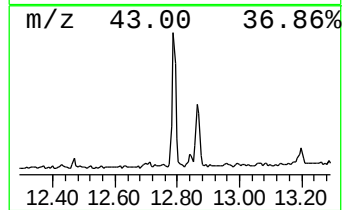
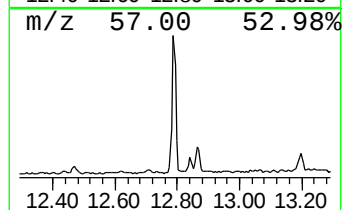
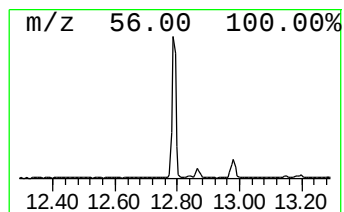
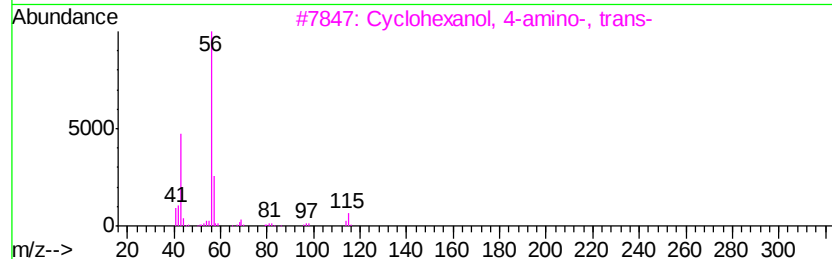
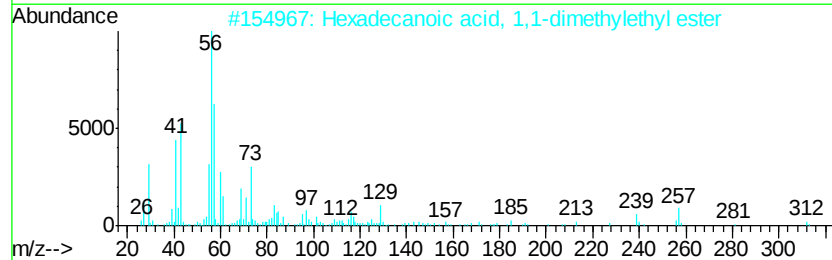
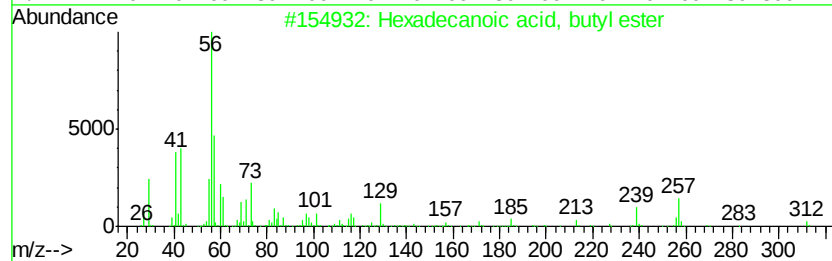
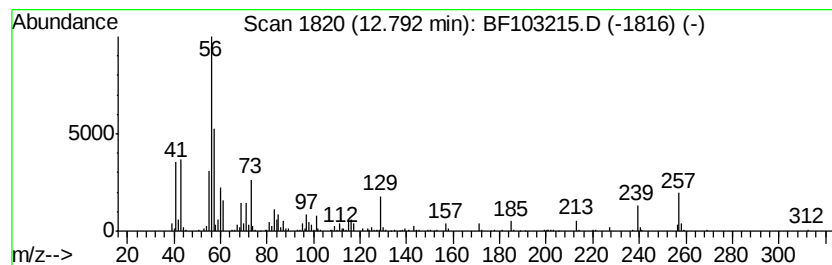
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	6.39 ng	335884	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
4		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

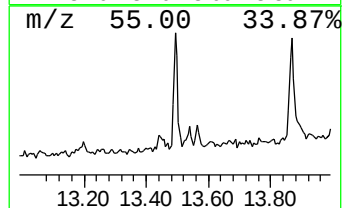
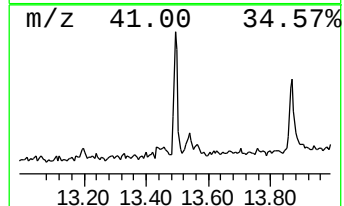
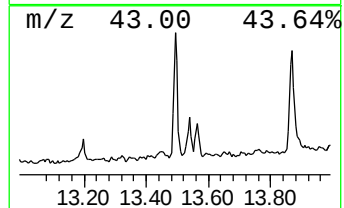
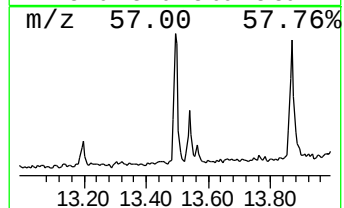
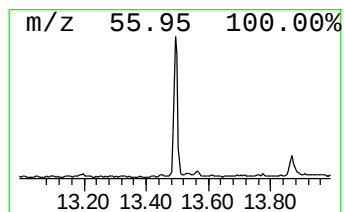
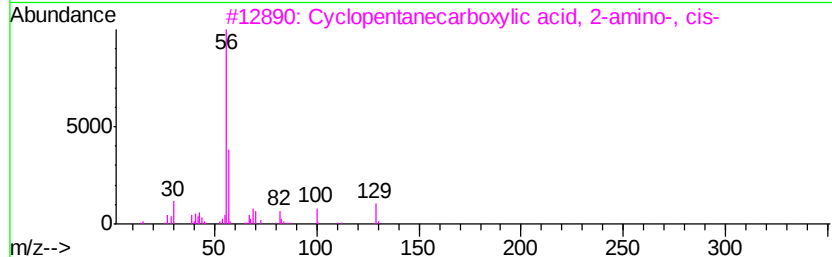
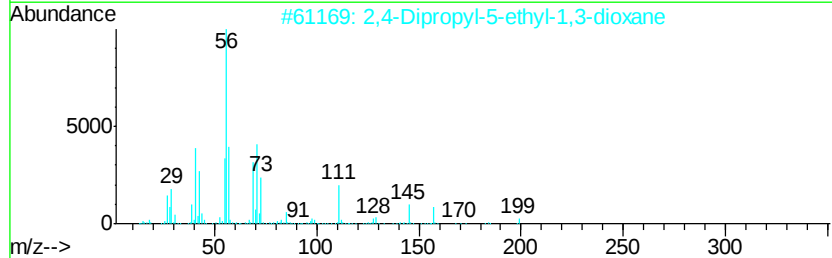
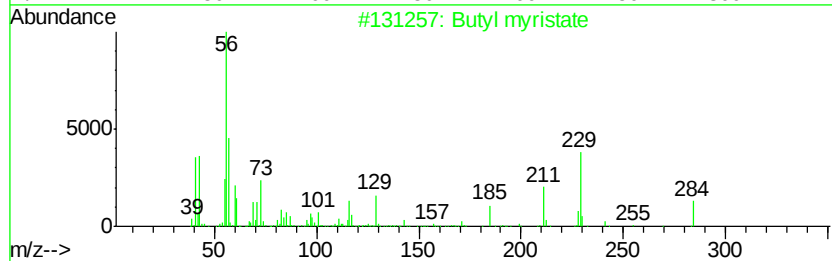
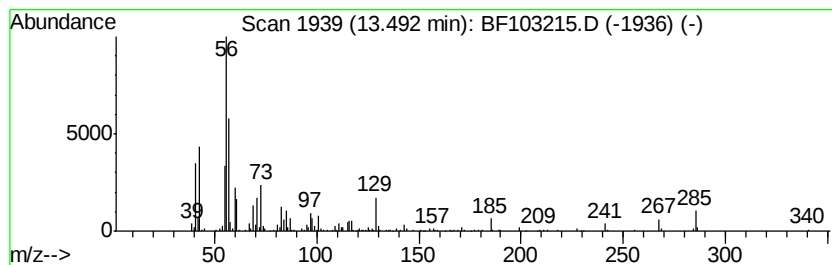
Instrument :
BNA_F
ClientSampleId :
RT-2898

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	4.61 ng	242401	Chrysene-d12	14.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	86
2	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	50
3	Cyclopentanecarboxylic acid, 2-amino-	129	C6H11NO2	037910-65-9	43
4	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	43
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

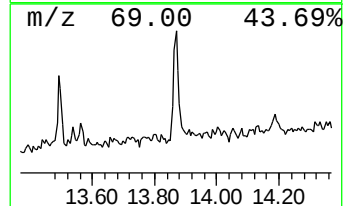
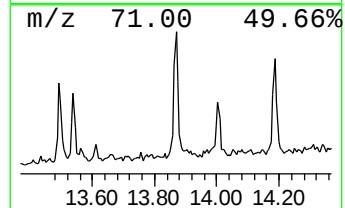
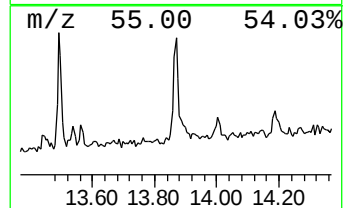
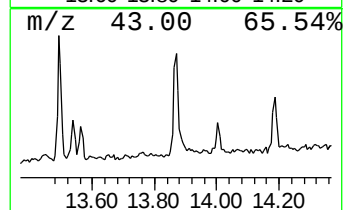
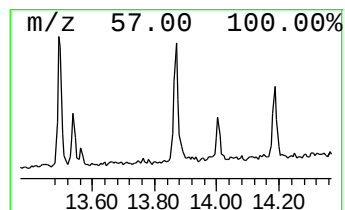
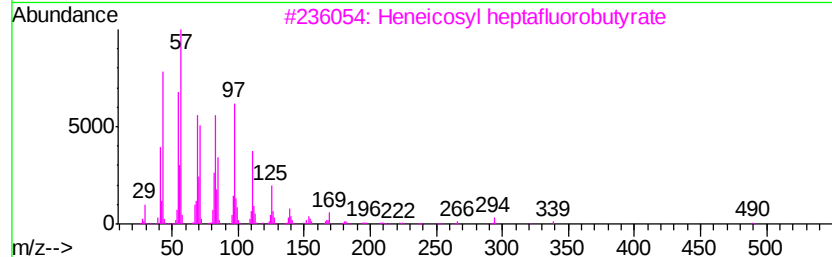
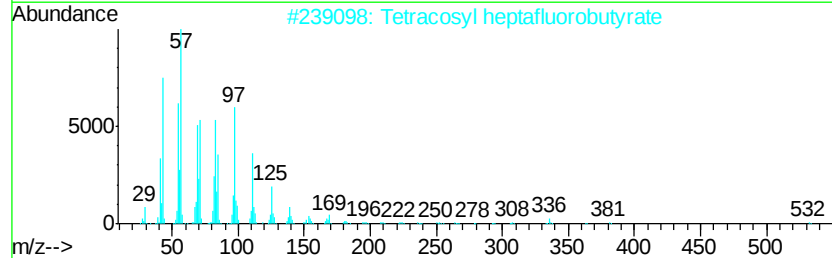
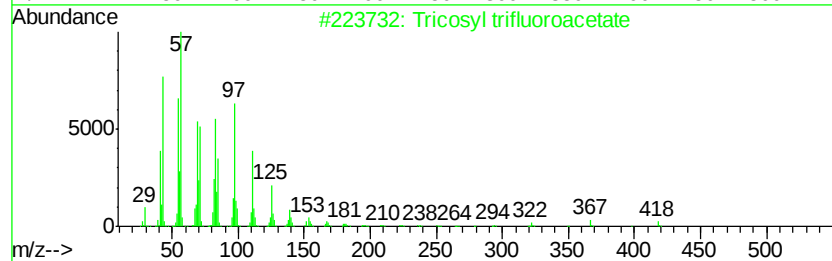
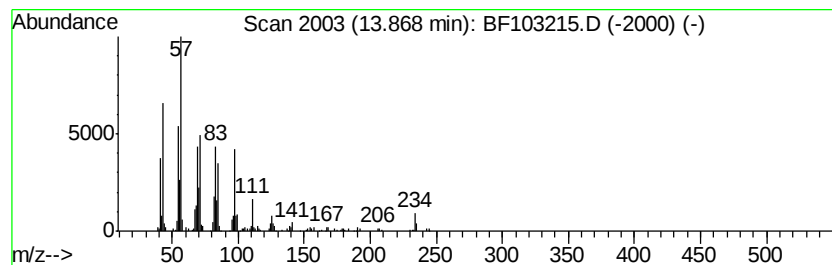
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tricosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.48 ng	235224	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
2		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
3		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	86
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	86
5		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

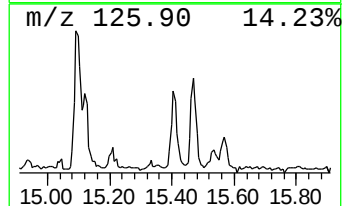
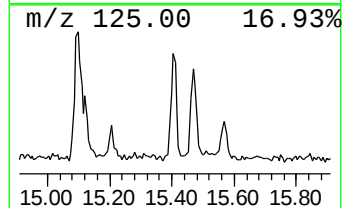
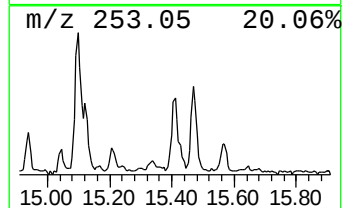
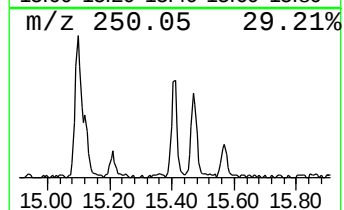
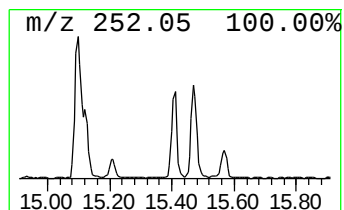
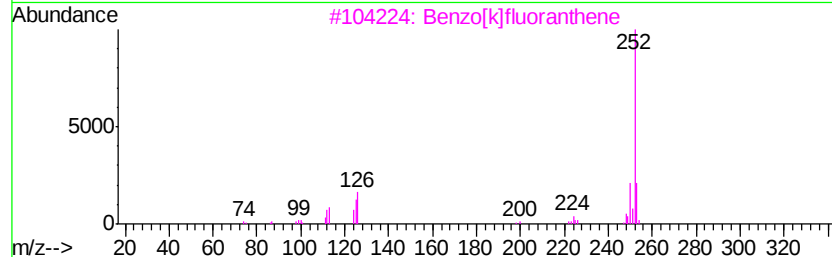
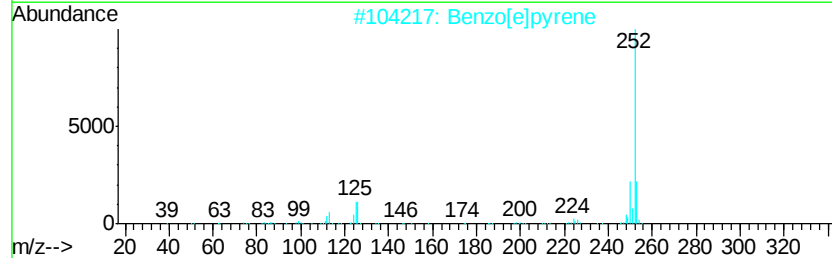
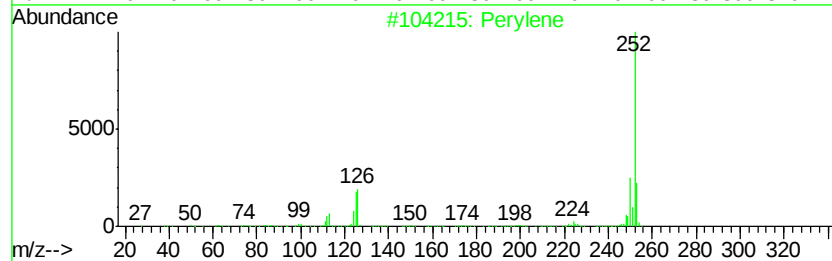
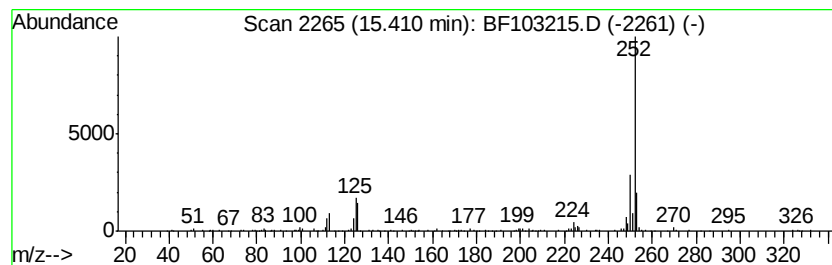
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	3.58 ng	180193	Perylene-d12	15.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	97
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	95
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

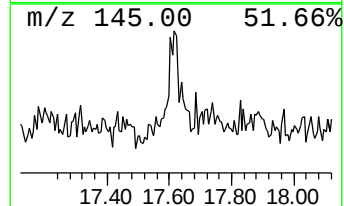
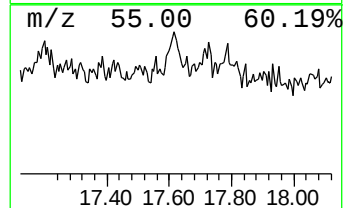
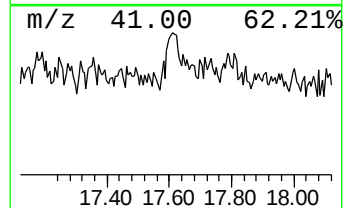
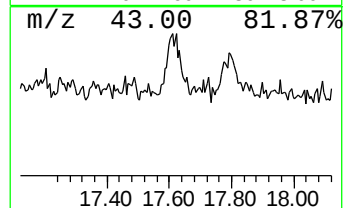
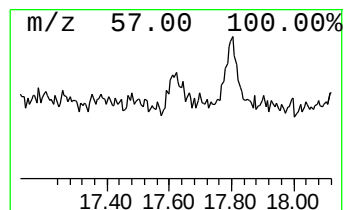
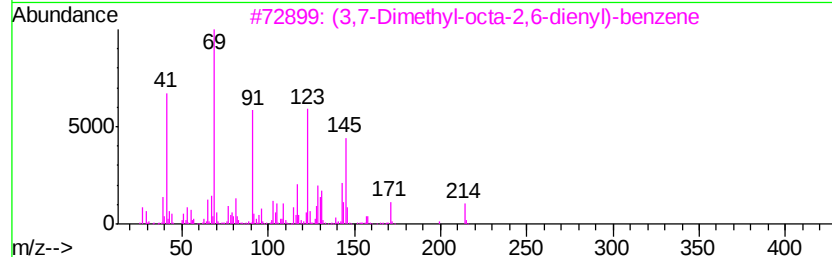
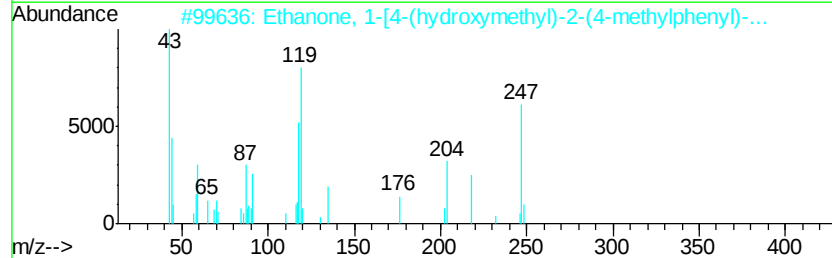
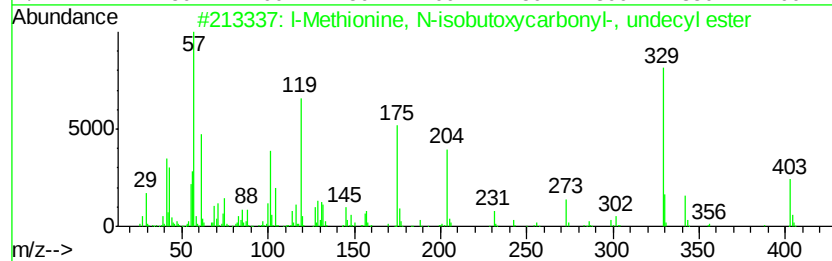
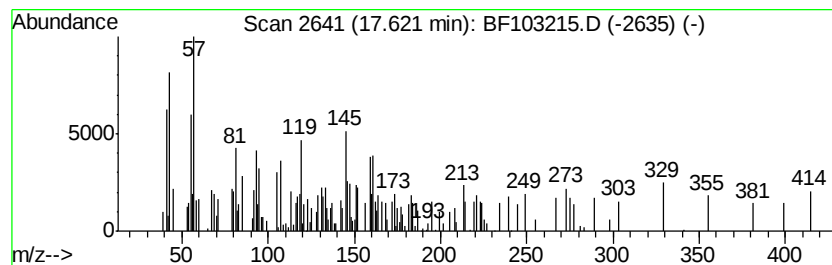
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.62 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	2.07 ng	104056	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	l-Methionine, N-isobutoxycarbonyl...	403	C21H41N04S	1000314-68-4	12
2		Ethanone, 1-[4-(hydroxymethyl)-2...	247	C13H13N02S	067387-03-5	11
3		(3,7-Dimethyl-octa-2,6-dienvl)-b...	214	C16H22	021488-83-5	10
4		Mestanolone	304	C20H32O2	000521-11-9	9
5		Tetradecylbis(trifluoromethyl)ph...	398	C16H29F6PS	146920-12-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103215.D
Acq On : 26 Feb 2018 13:40
Operator : SJ/JU
Sample : J1652-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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...	2.16	33.6	ng	1803980	1	6.87	1073430	20.0
2-Pentanone, 4-hy...	5.12	5.6	ng	299504	1	6.87	1073430	20.0
unknown6.65	6.65	85.7	ng	4601370	1	6.87	1073430	20.0
Hexadecane	9.83	2.1	ng	126645	3	9.91	1226580	20.0
Hexadecanoic acid...	12.79	6.4	ng	335884	5	14.05	1050710	20.0
Butyl myristate	13.49	4.6	ng	242401	5	14.05	1050710	20.0
Tricosyl trifluor...	13.87	4.5	ng	235224	5	14.05	1050710	20.0
Perylene	15.41	3.6	ng	180193	6	15.54	1006100	20.0
unknown17.62	17.62	2.1	ng	104056	6	15.54	1006100	20.0