

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
 Data File : BF101253.D
 Acq On : 8 Dec 2017 23:07
 Operator : SJ/JU
 Sample : I6717-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB-3(0-10)

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-BF113017.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	501	504	516	rBV	56416	76293	6.05%	0.675%
2	5.451	567	572	587	rBV	1111914	1067161	84.56%	9.445%
3	6.469	740	745	758	rVB	1111706	1129848	89.53%	10.000%
4	6.598	763	767	770	rBV	1209580	1131938	89.69%	10.018%
5	6.828	803	806	813	rBB	341438	266153	21.09%	2.356%
6	6.987	828	833	836	rBV	997403	891152	70.61%	7.887%
7	7.392	898	902	905	rBV	665635	634717	50.29%	5.618%
8	8.110	1021	1024	1027	rBV	428829	335344	26.57%	2.968%
9	9.186	1202	1207	1210	rBV	1555356	1262010	100.00%	11.170%
10	9.581	1270	1274	1277	rBV	139931	115314	9.14%	1.021%
11	9.786	1304	1309	1313	rBV	34567	26074	2.07%	0.231%
12	9.869	1319	1323	1326	rBV	407340	343270	27.20%	3.038%
13	9.898	1326	1328	1331	rVB	23034	15061	1.19%	0.133%
14	10.286	1391	1394	1397	rVB	39544	28078	2.22%	0.249%
15	10.663	1454	1458	1461	rBV	712829	629137	49.85%	5.568%
16	10.757	1472	1474	1479	rBV	29282	30966	2.45%	0.274%
17	11.357	1573	1576	1578	rBV	388640	315667	25.01%	2.794%
18	11.380	1578	1580	1584	rVB	149117	112815	8.94%	0.998%
19	11.433	1586	1589	1592	rVB	32893	24461	1.94%	0.216%
20	11.874	1658	1664	1665	rBV2	21841	28960	2.29%	0.256%
21	11.974	1677	1681	1683	rBV2	20797	22824	1.81%	0.202%
22	12.574	1780	1783	1787	rBV	187771	152004	12.04%	1.345%
23	12.757	1811	1814	1816	rVB	22313	18486	1.46%	0.164%
24	12.786	1816	1819	1820	rBV2	31251	28863	2.29%	0.255%
25	12.804	1820	1822	1825	rVB	148028	116443	9.23%	1.031%
26	12.945	1841	1846	1849	rBV	1108683	981655	77.79%	8.688%
27	13.027	1855	1860	1863	rBV4	10898	19146	1.52%	0.169%
28	13.198	1887	1889	1892	rVB	19732	16828	1.33%	0.149%
29	13.233	1892	1895	1898	rBV2	14606	19312	1.53%	0.171%
30	13.416	1922	1926	1930	rBV	147426	171151	13.56%	1.515%
31	13.451	1930	1932	1936	rVV	52472	50994	4.04%	0.451%
32	13.492	1936	1939	1944	rVB2	17612	19982	1.58%	0.177%
33	13.827	1990	1996	1999	rBV2	77153	89813	7.12%	0.795%
34	14.004	2021	2026	2029	rBV2	346789	365629	28.97%	3.236%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.033	2029	2031	2033	rVB	57185	47506	3.76%	0.420%
36	14.098	2039	2042	2049	rBV7	29768	62854	4.98%	0.556%
37	14.392	2090	2092	2095	rVB2	16423	14773	1.17%	0.131%
38	14.739	2149	2151	2156	rVB4	31373	41700	3.30%	0.369%
39	14.827	2163	2166	2172	rBV	71319	78306	6.20%	0.693%
40	15.051	2200	2204	2206	rBV	48351	67547	5.35%	0.598%
41	15.351	2252	2255	2261	rVB	35067	49457	3.92%	0.438%
42	15.415	2263	2266	2270	rVB	42923	50982	4.04%	0.451%
43	15.480	2272	2277	2281	rBV	189077	242205	19.19%	2.144%
44	16.392	2430	2432	2438	rVB4	27850	40106	3.18%	0.355%
45	16.968	2526	2530	2536	rVB6	28373	65692	5.21%	0.581%

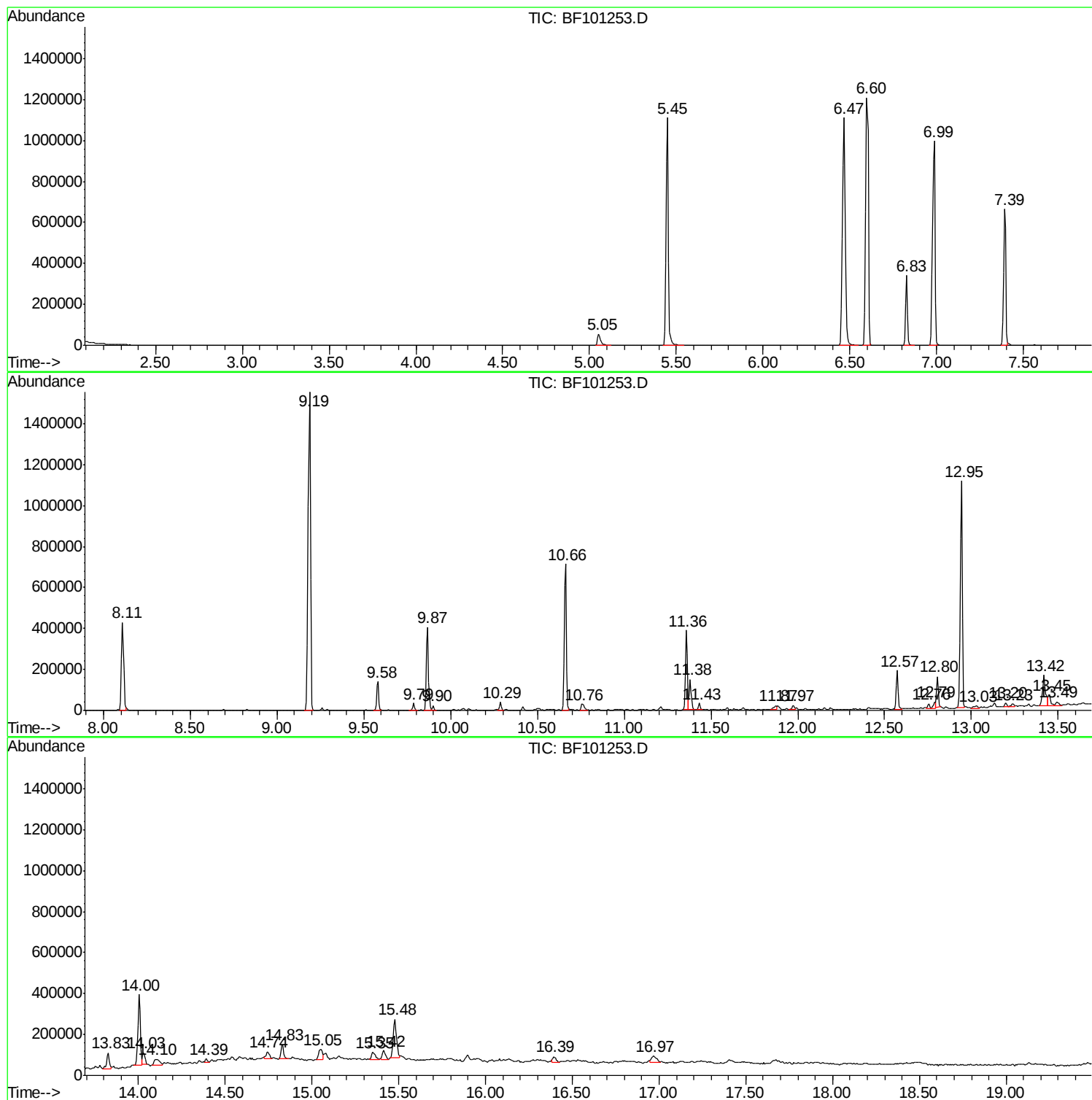
Sum of corrected areas: 11298677

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

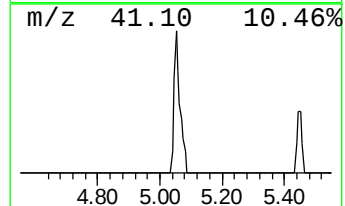
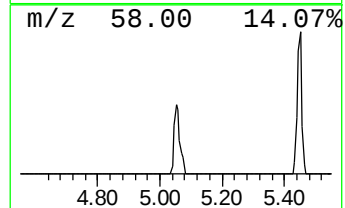
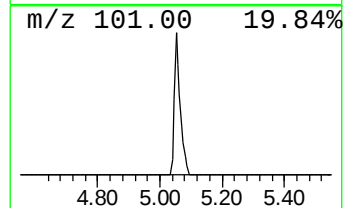
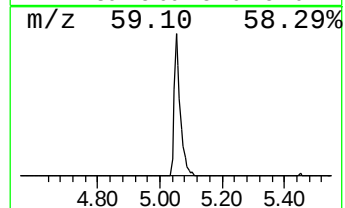
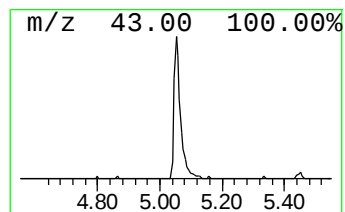
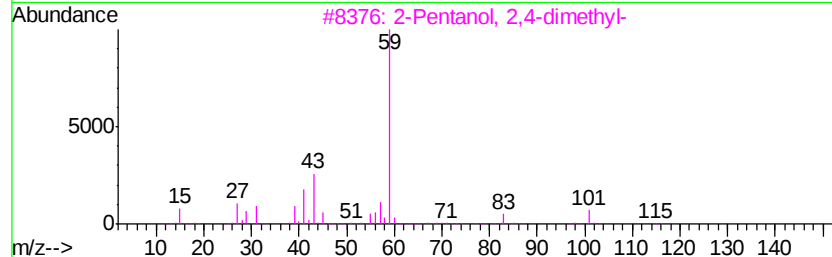
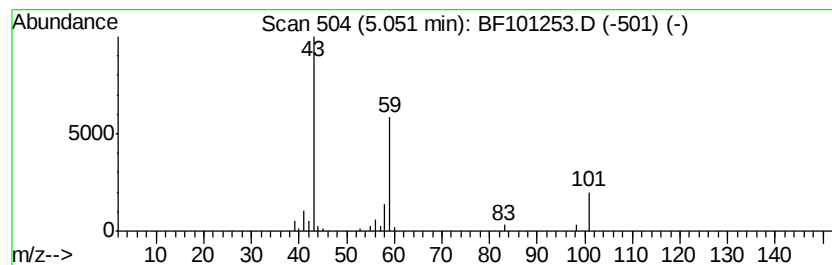
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	5.73 ng	76293	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		Silane, trimethyl-	74	C3H10Si	000993-07-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

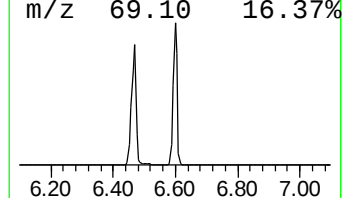
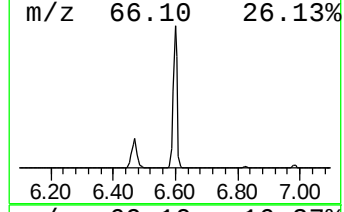
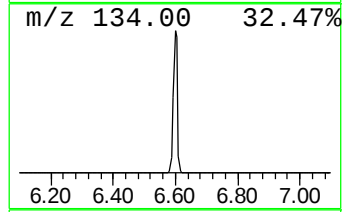
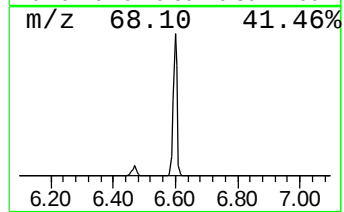
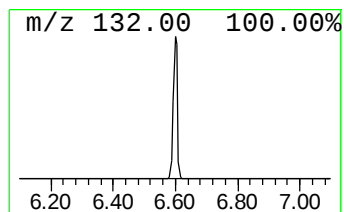
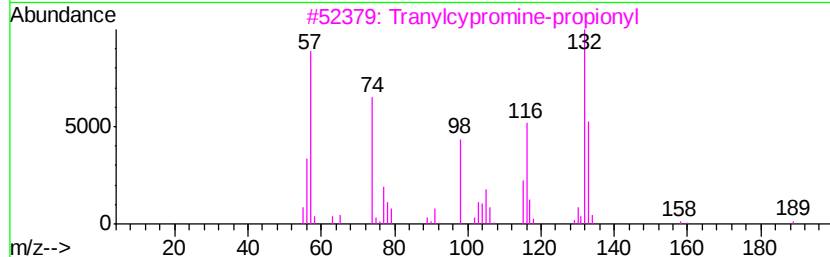
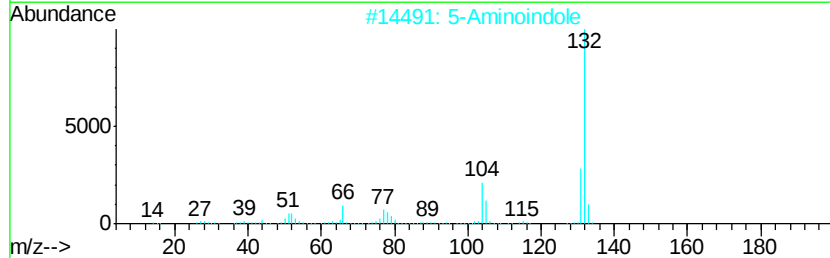
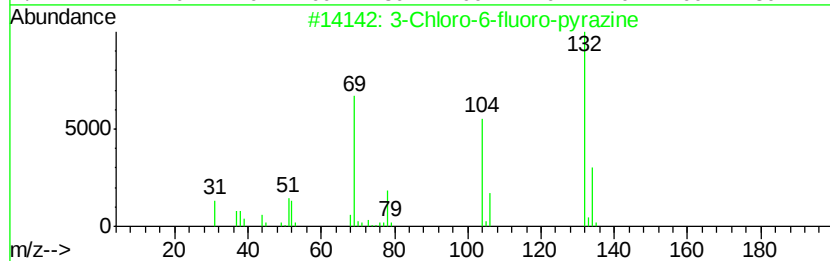
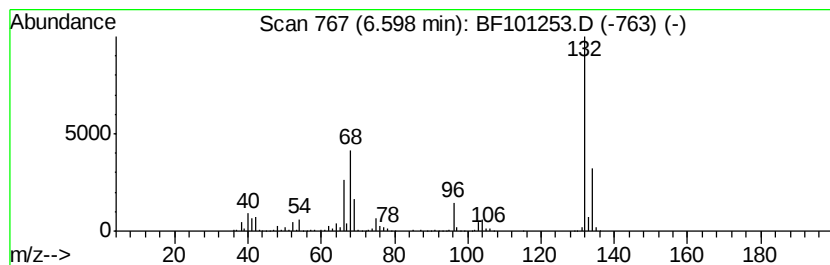
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	85.06 ng	1131940	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

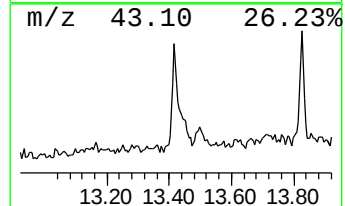
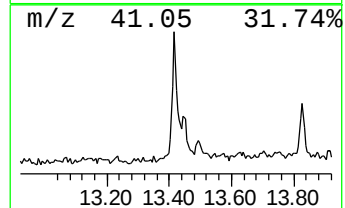
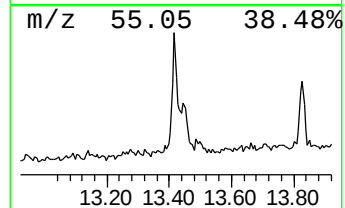
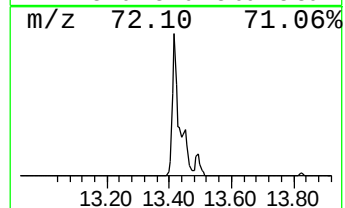
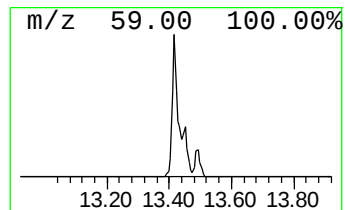
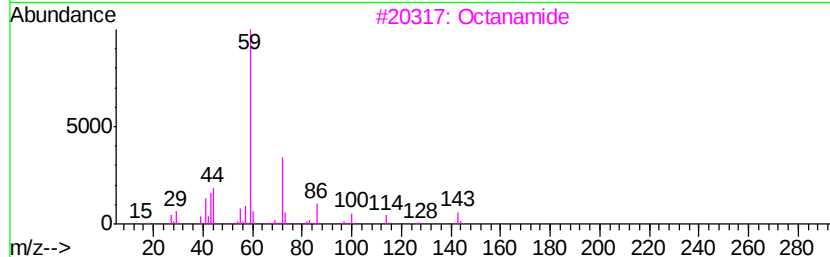
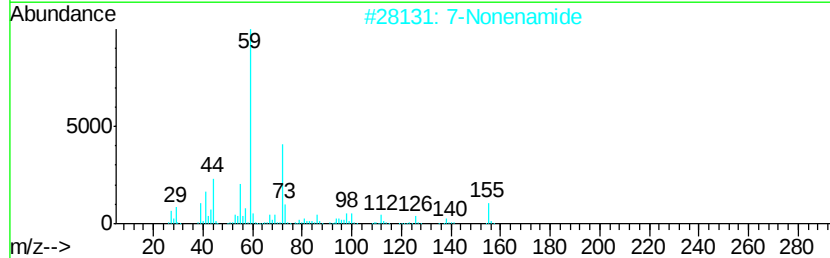
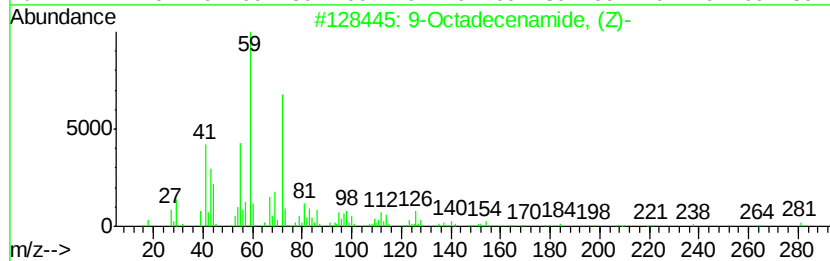
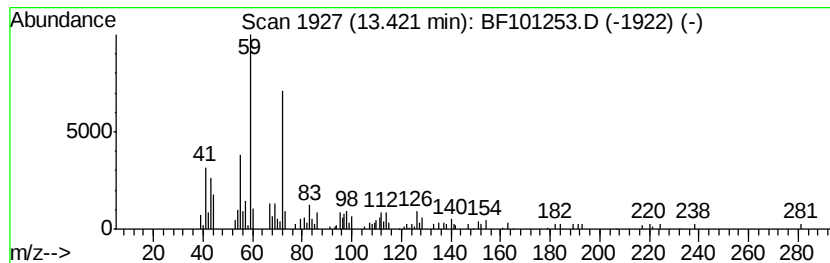
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	9.36 ng	171151	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2		7-Nonenamide	155	C9H17NO	090949-53-4	72
3		Octanamide	143	C8H17NO	000629-01-6	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Nonanamide	157	C9H19NO	001120-07-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

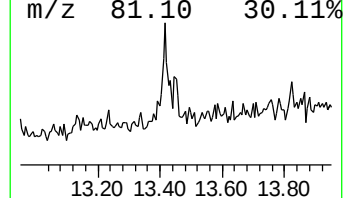
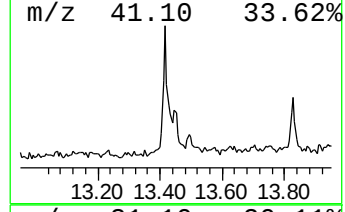
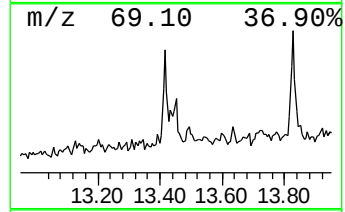
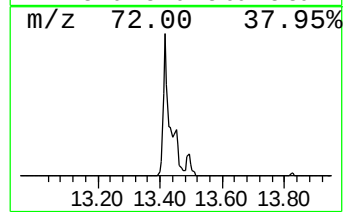
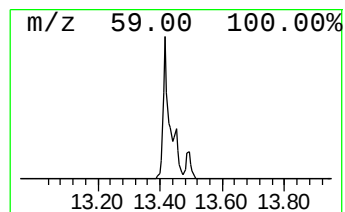
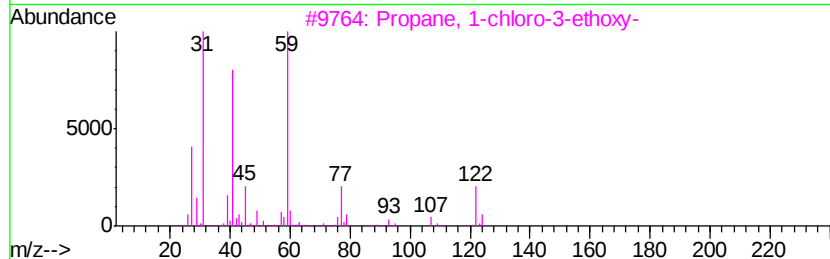
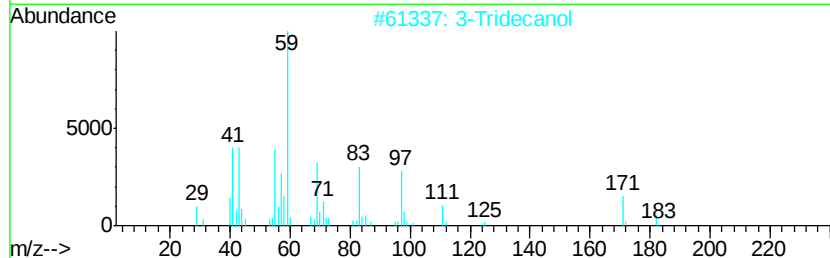
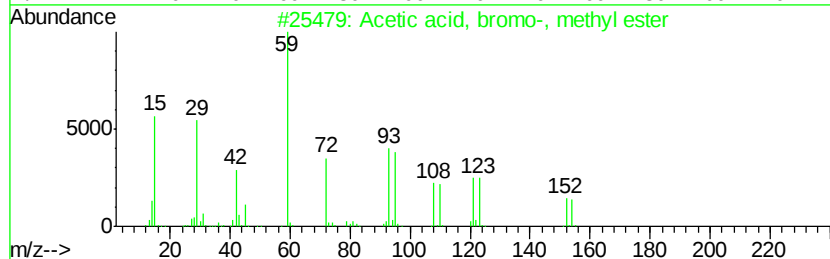
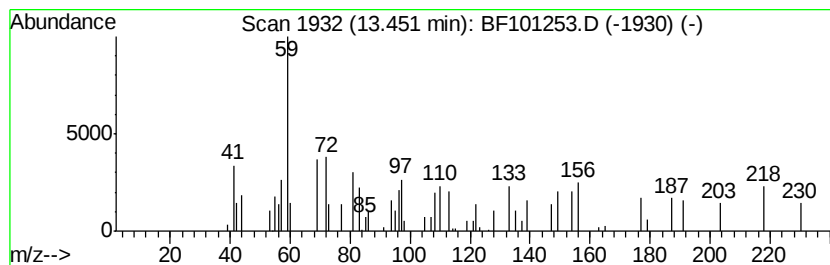
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.45 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.79 ng	50994	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, bromo-, methyl ester	152	C3H5BrO2	000096-32-2	23
2		3-Tridecanol	200	C13H28O	010289-68-6	14
3		Propane, 1-chloro-3-ethoxy-	122	C5H11ClO	036865-38-0	14
4		Tetradecanamide	227	C14H29NO	000638-58-4	14
5		2,11-Dimethyl-2,11-dodecanediol	230	C14H30O2	022092-59-7	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

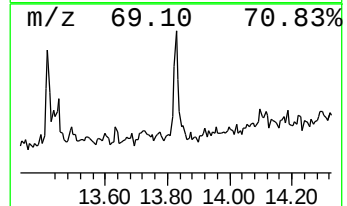
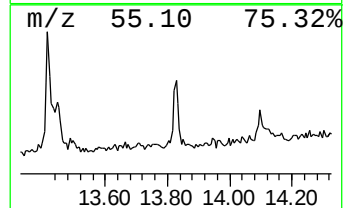
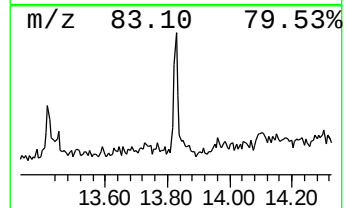
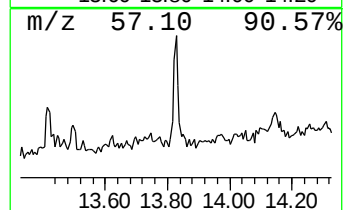
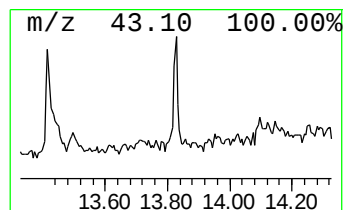
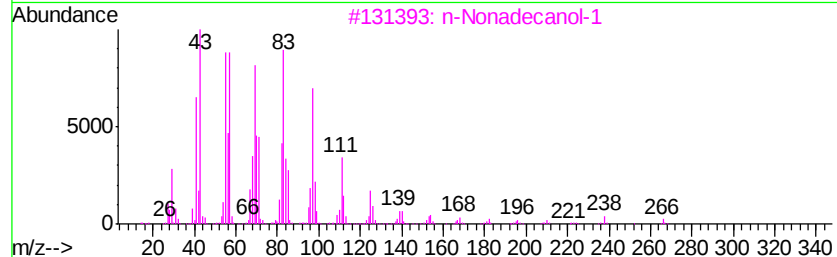
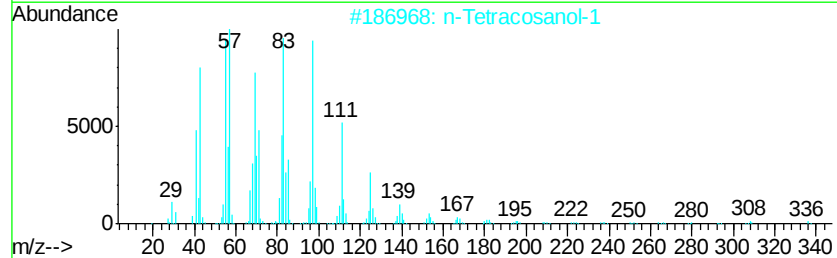
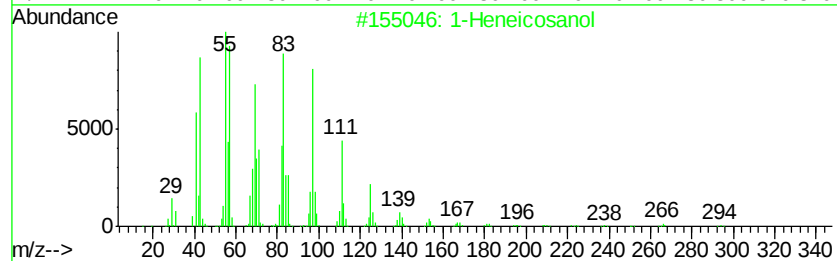
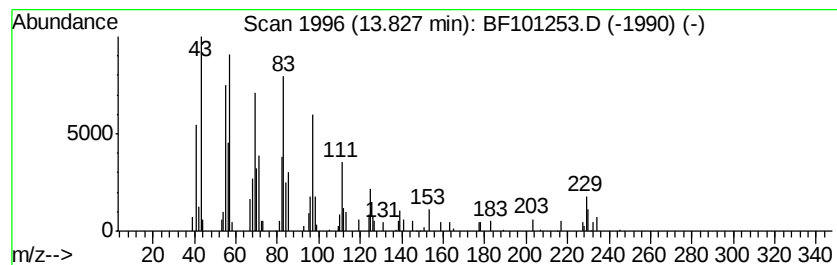
Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.83	4.91 ng	89813	Chrysene-d12		14.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Heptafluorobutyrlic acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

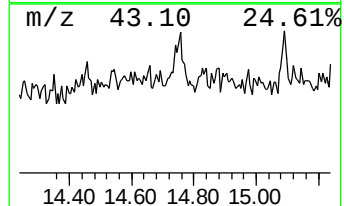
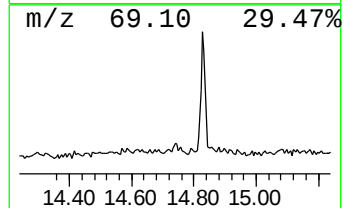
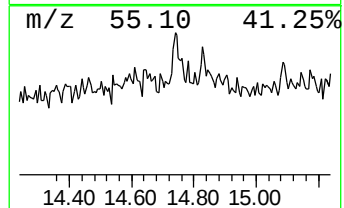
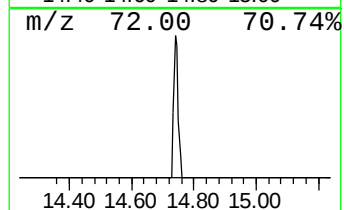
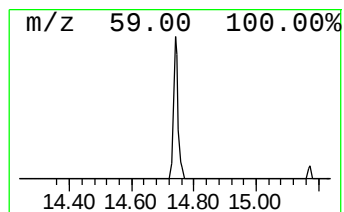
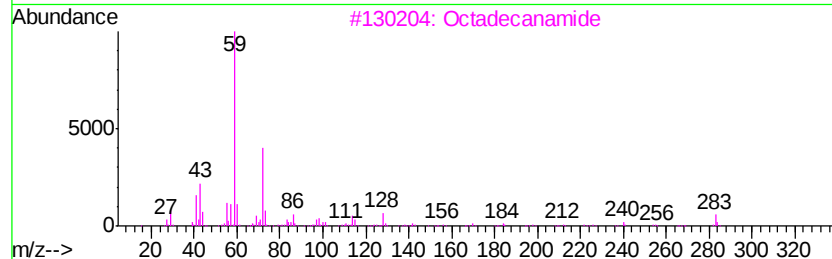
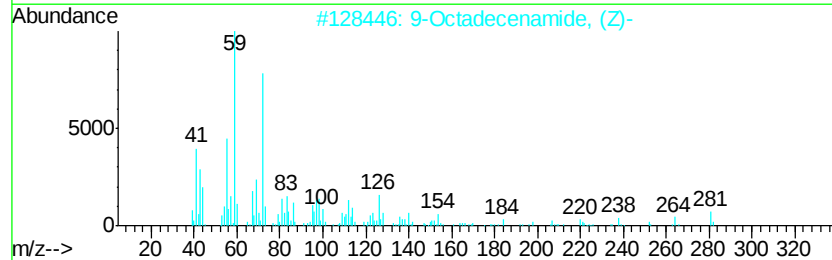
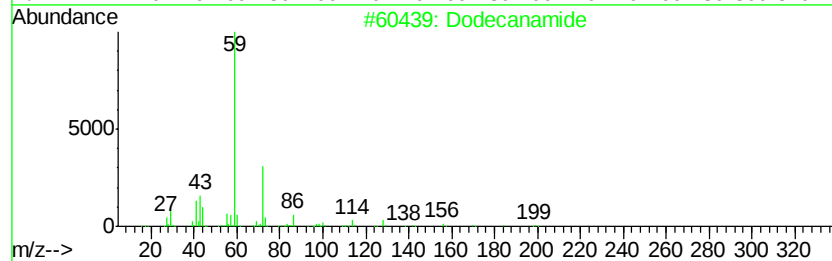
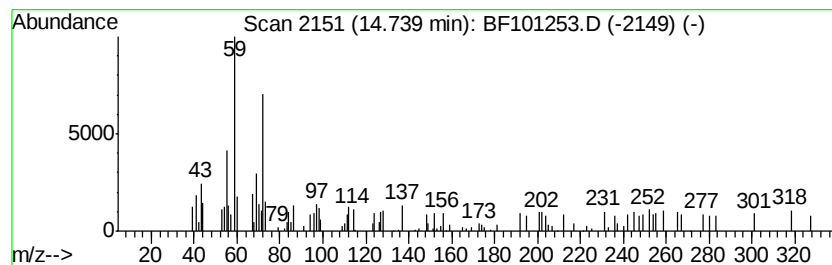
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.28 ng	41700	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanamide	199	C12H25NO	001120-16-7	53
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	50
3		Octadecanamide	283	C18H37NO	000124-26-5	50
4		7-Nonenamide	155	C9H17NO	090949-53-4	47
5		Methaniminium, N,N-dimethyl-, [[...	252	C14H24N2O2	1000142-12-3	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

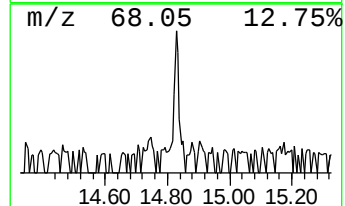
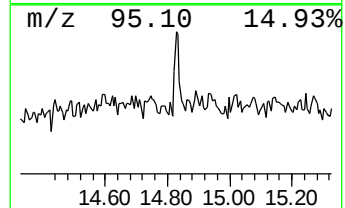
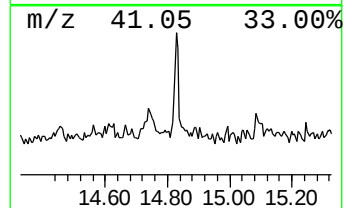
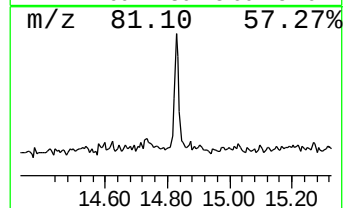
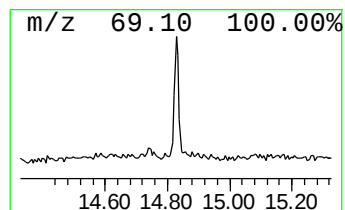
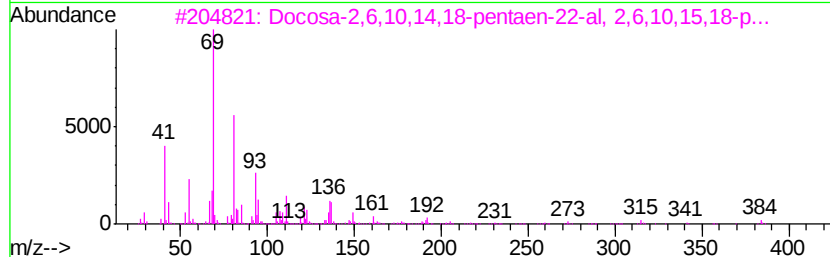
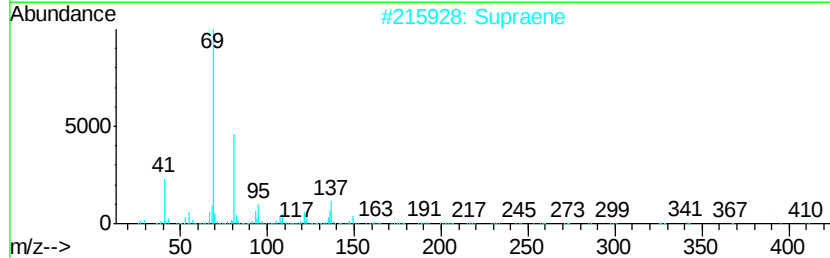
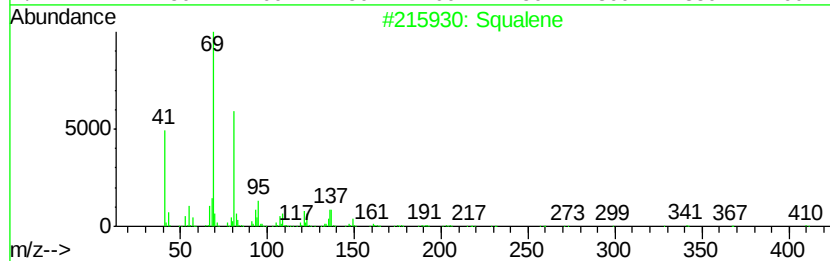
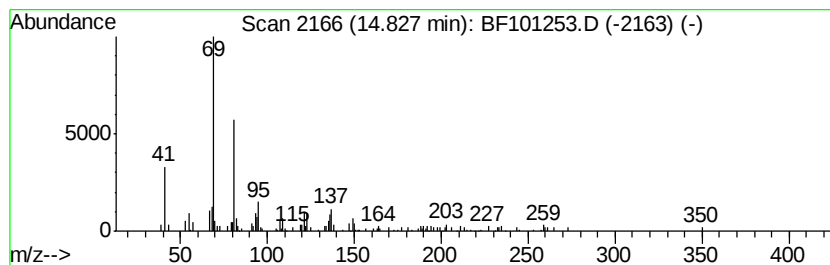
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	6.47 ng	78306	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	83
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

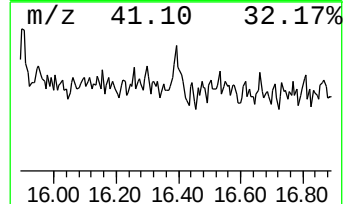
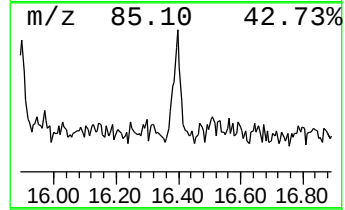
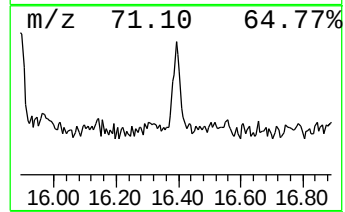
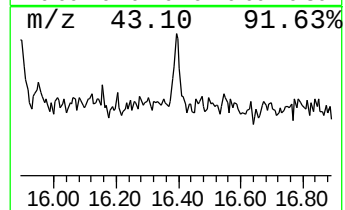
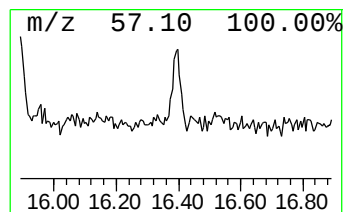
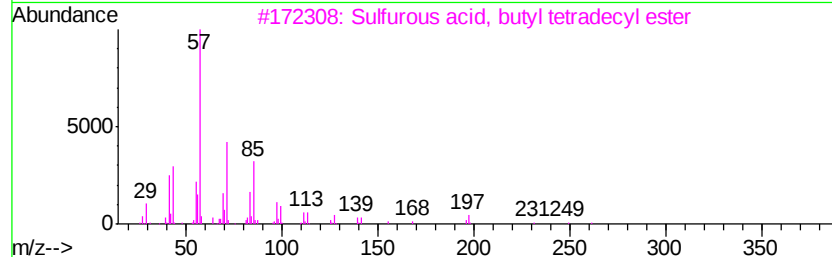
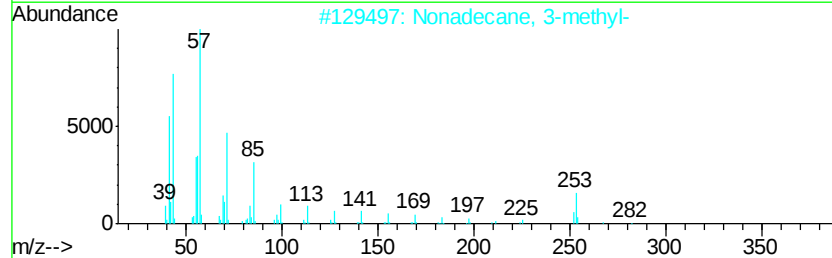
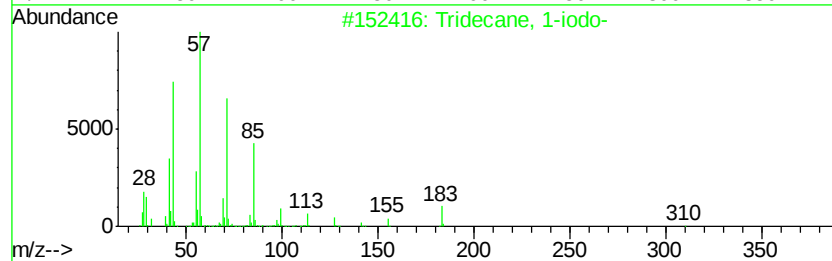
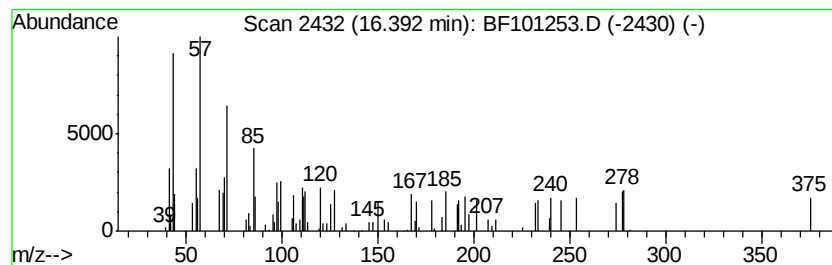
Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	3.31 ng	40106	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tridecane, 1-iodo-	310 C13H27I	035599-77-0 10
2		Nonadecane, 3-methyl-	282 C20H42	006418-45-7 10
3		Sulfurous acid, butyl tetradecyl...	334 C18H38O3S	1000309-18-1 10
4		Pentadecane	212 C15H32	000629-62-9 10
5		Docosane, 11-butyl-	366 C26H54	013475-76-8 10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101253.D
Acq On : 8 Dec 2017 23:07
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	5.7	ng	76293	1	6.83	266153	20.0
unknown6.60	6.60	85.1	ng	1131940	1	6.83	266153	20.0
9-Octadecenamide, ...	13.42	9.4	ng	171151	5	14.00	365629	20.0
unknown13.45	13.45	2.8	ng	50994	5	14.00	365629	20.0
1-Heneicosanol	13.83	4.9	ng	89813	5	14.00	365629	20.0
Dodecanamide	14.74	2.3	ng	41700	5	14.00	365629	20.0
Squalene	14.83	6.5	ng	78306	6	15.48	242205	20.0
unknown16.39	16.39	3.3	ng	40106	6	15.48	242205	20.0