

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
 Data File : BF102167.D
 Acq On : 17 Jan 2018 23:01
 Operator : SJ/JU
 Sample : J1145-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB-1(8-21.5)

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	474	484	492	rBV	180986	278467	7.58%	0.807%
2	5.334	547	552	555	rBV	3242421	3637932	99.00%	10.543%
3	6.363	721	727	731	rBV	3218535	3674623	100.00%	10.649%
4	6.492	744	749	752	rBV	3876651	3650477	99.34%	10.579%
5	6.722	784	788	791	rBV	1109558	920275	25.04%	2.667%
6	6.875	810	814	818	rBV	2889447	2734871	74.43%	7.926%
7	7.287	878	884	887	rBV	2238121	2282908	62.13%	6.616%
8	8.004	1001	1006	1012	rBV	1324620	1234842	33.60%	3.579%
9	8.422	1073	1077	1079	rBV	59576	53662	1.46%	0.156%
10	8.516	1089	1093	1096	rBV	470955	433509	11.80%	1.256%
11	8.557	1096	1100	1104	rVV	267884	228040	6.21%	0.661%
12	8.657	1110	1117	1120	rBV6	23315	54025	1.47%	0.157%
13	8.692	1120	1123	1125	rVB2	51879	52504	1.43%	0.152%
14	8.845	1145	1149	1152	rBV	155284	172401	4.69%	0.500%
15	8.875	1152	1154	1156	rBV2	70348	60875	1.66%	0.176%
16	8.922	1161	1162	1165	rVB	60332	45361	1.23%	0.131%
17	8.957	1165	1168	1172	rBV	133422	117455	3.20%	0.340%
18	8.998	1172	1175	1177	rBV	111214	87506	2.38%	0.254%
19	9.022	1177	1179	1182	rVB	257218	199548	5.43%	0.578%
20	9.081	1182	1189	1192	rBV	3729537	3283394	89.35%	9.515%
21	9.163	1199	1203	1207	rBV3	60346	92065	2.51%	0.267%
22	9.433	1246	1249	1252	rVB	920722	828827	22.56%	2.402%
23	9.475	1252	1256	1259	rVV	751708	706117	19.22%	2.046%
24	9.498	1259	1260	1264	rVB	99530	65668	1.79%	0.190%
25	9.539	1264	1267	1269	rVB	47457	39906	1.09%	0.116%
26	9.751	1300	1303	1307	rVB	1225985	1123021	30.56%	3.255%
27	10.010	1343	1347	1350	rVB2	44427	48071	1.31%	0.139%
28	10.245	1384	1387	1391	rBV	441352	376843	10.26%	1.092%
29	10.404	1409	1414	1417	rBV	29601	38577	1.05%	0.112%
30	10.469	1421	1425	1428	rBV	1025352	812036	22.10%	2.353%
31	10.545	1433	1438	1441	rBV	1811311	1788392	48.67%	5.183%
32	10.669	1454	1459	1467	rBV4	23452	37605	1.02%	0.109%
33	10.939	1502	1505	1508	rVB2	68419	57975	1.58%	0.168%
34	11.233	1550	1555	1559	rBV	1010185	863850	23.51%	2.503%

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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 >
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35	12.439	1757	1760	1763	rBV	54629	47295	1.29%	0.137%
36	12.669	1797	1799	1802	rVB	60200	46727	1.27%	0.135%
37	12.821	1820	1825	1828	rBV	2156245	1962078	53.40%	5.686%
38	13.298	1900	1906	1911	rBV	147304	220975	6.01%	0.640%
39	13.710	1973	1976	1983	rBV	306357	305842	8.32%	0.886%
40	13.868	1998	2003	2005	rBV	746433	774531	21.08%	2.245%
41	13.886	2005	2006	2009	rVB	82640	66532	1.81%	0.193%
42	13.980	2017	2022	2025	rBV6	22998	45086	1.23%	0.131%
43	14.392	2088	2092	2096	rBV4	35618	49750	1.35%	0.144%
44	14.874	2171	2174	2178	rBV	39104	47941	1.30%	0.139%
45	15.286	2238	2244	2248	rBV	624505	780632	21.24%	2.262%
46	15.768	2322	2326	2332	rVB3	48920	76896	2.09%	0.223%

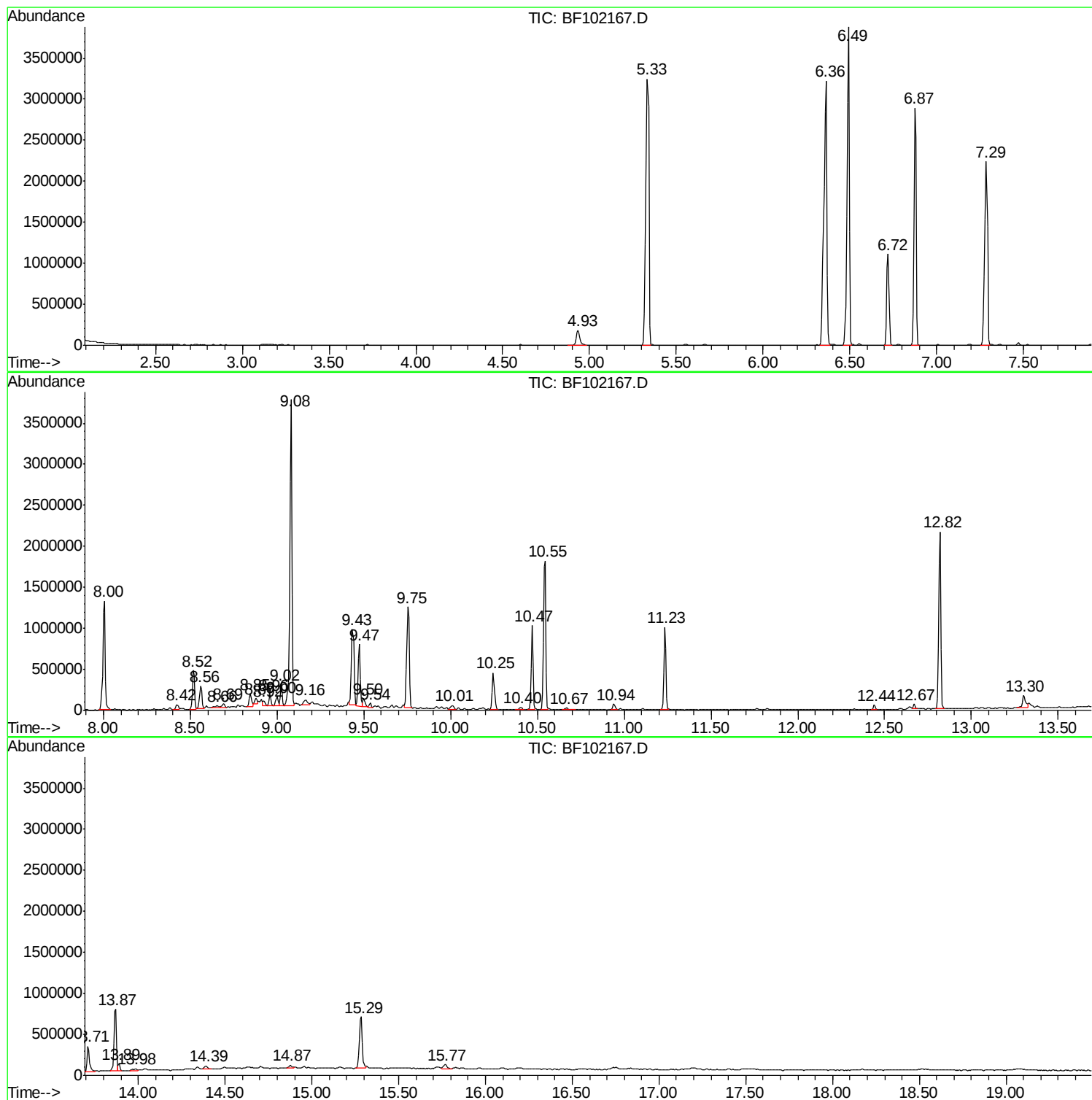
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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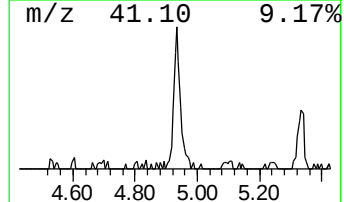
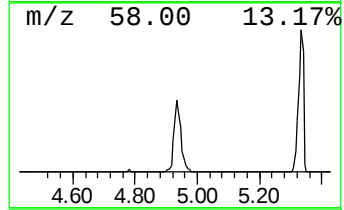
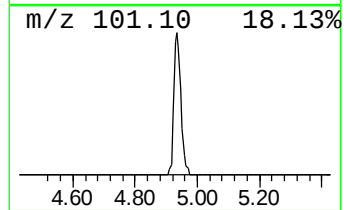
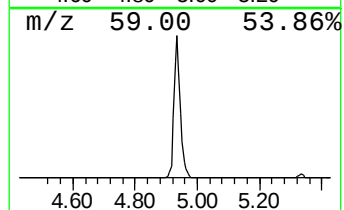
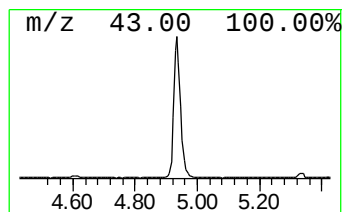
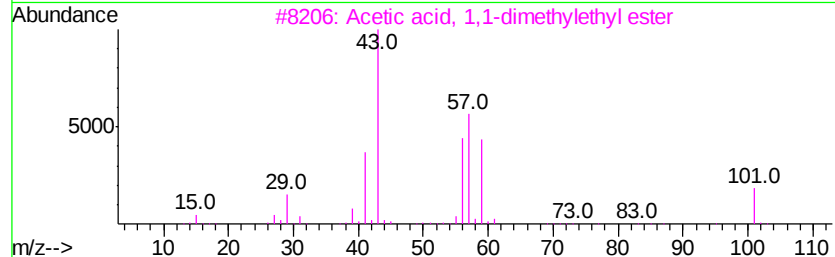
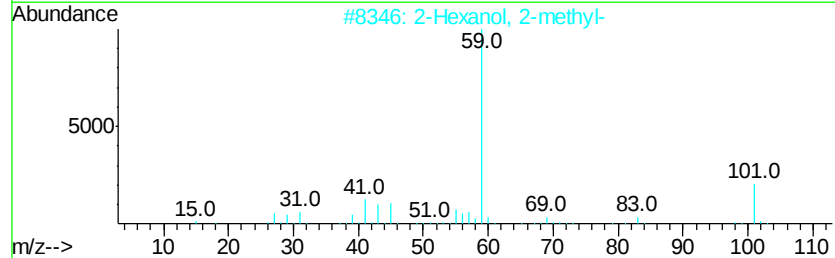
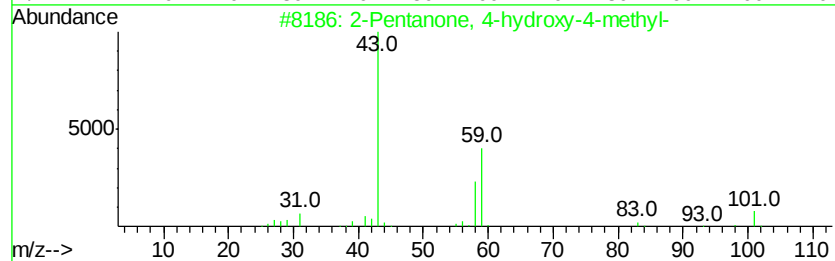
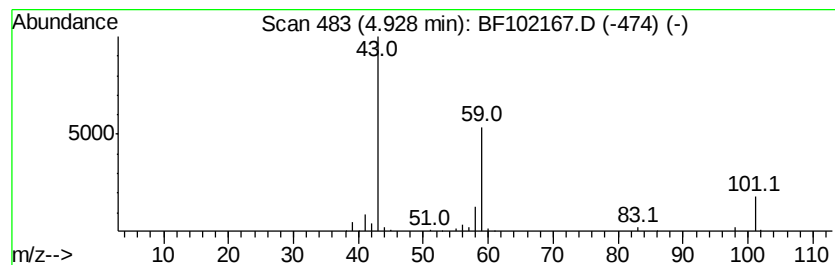
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.05 ng	278467	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	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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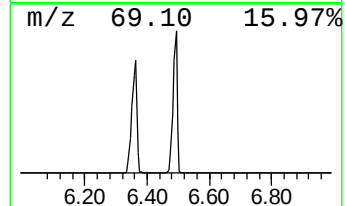
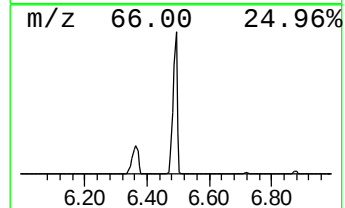
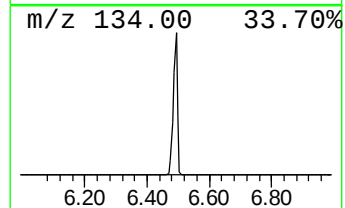
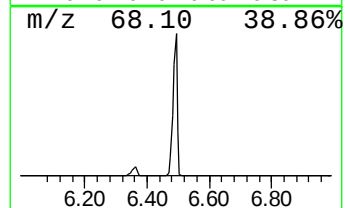
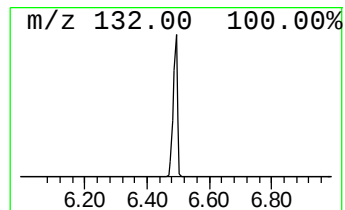
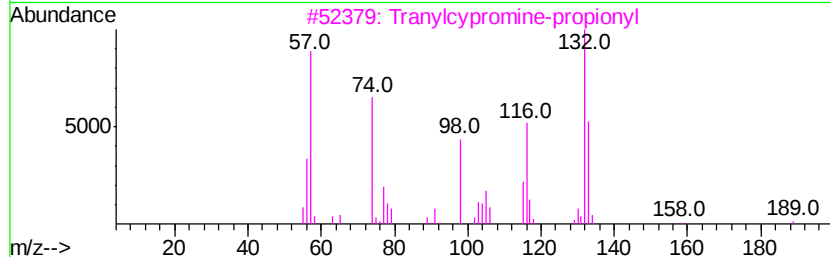
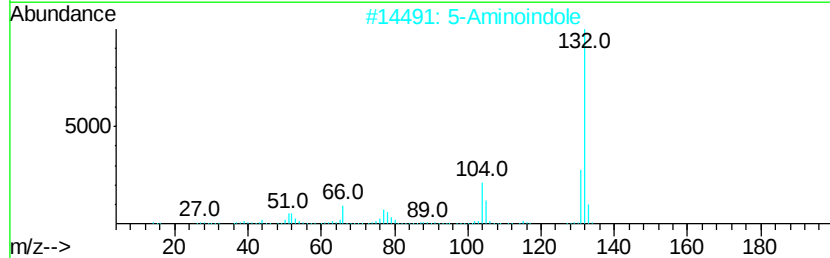
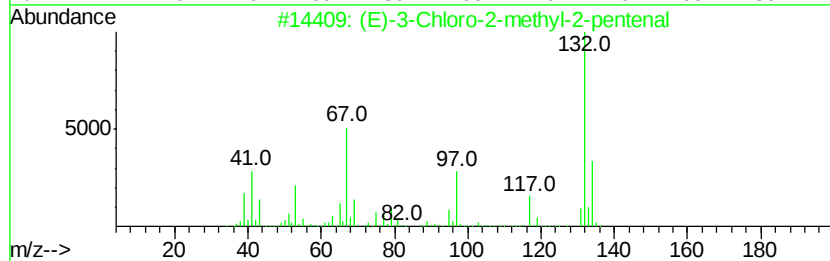
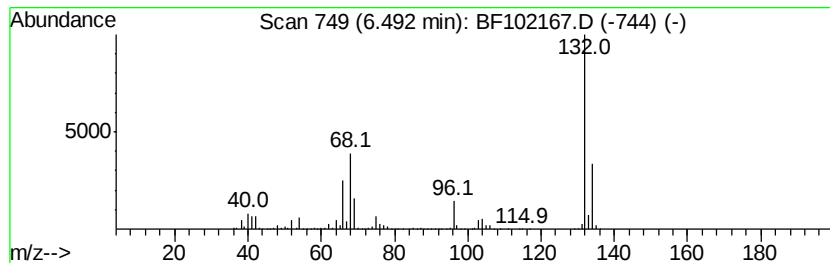
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	79.33 ng	3650480	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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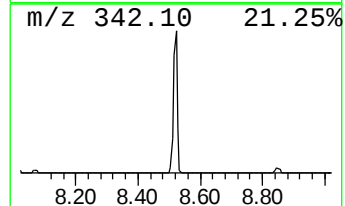
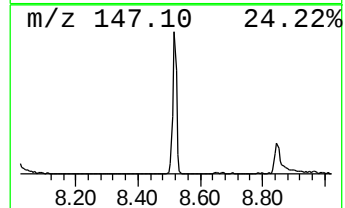
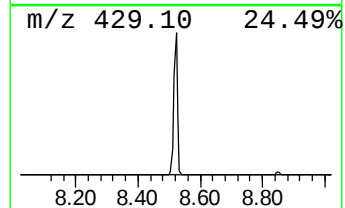
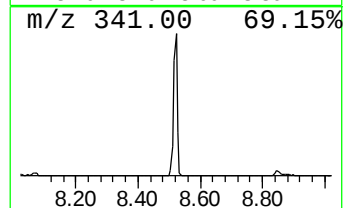
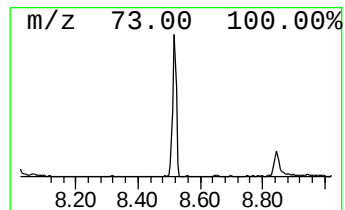
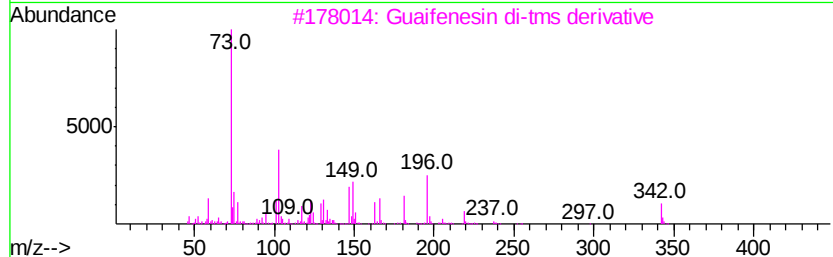
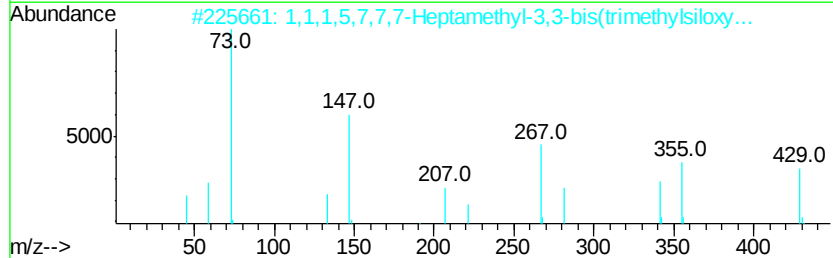
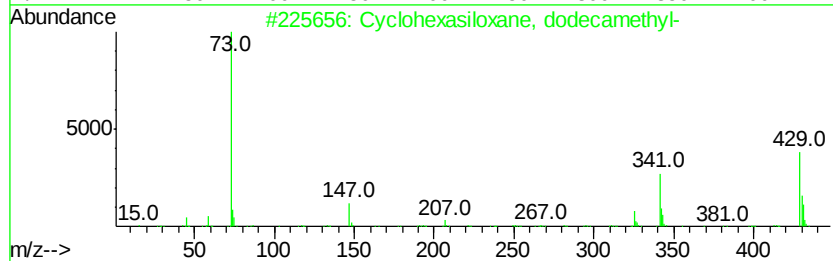
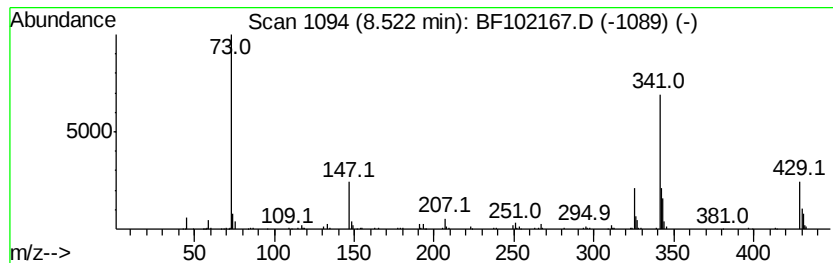
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexasiloxane, dodecane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	7.02 ng	433509	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32
3		Guaifenesin di-tms derivative	342	C16H30O4Si2	107966-19-8	17
4		2H-1,4-Benzodiazepin-2-one, 7-ch...	342	C18H19ClN2OSi	055299-24-6	12
5		Benzene, 1,2,3-tris[(trimethylsi...	342	C15H30O3Si3	017864-23-2	12



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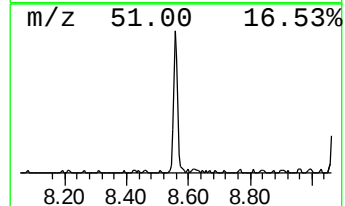
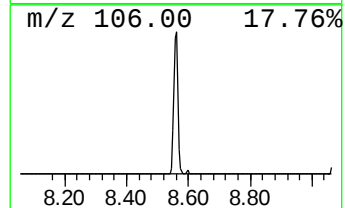
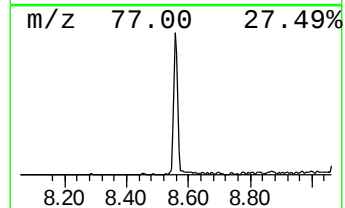
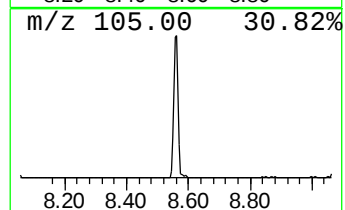
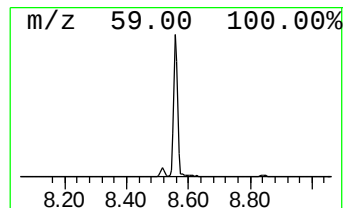
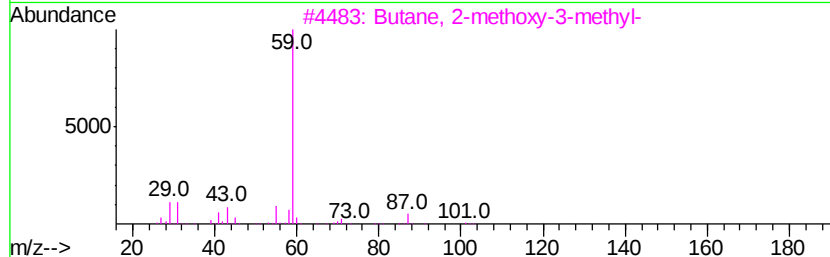
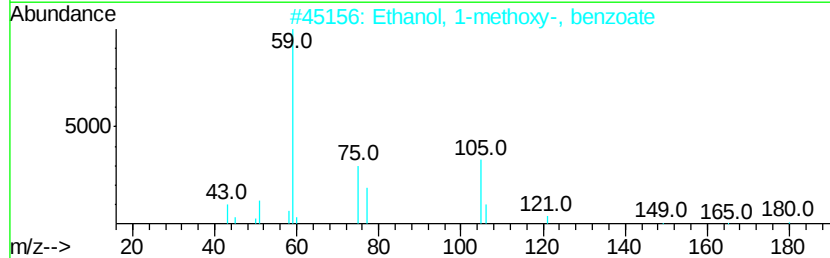
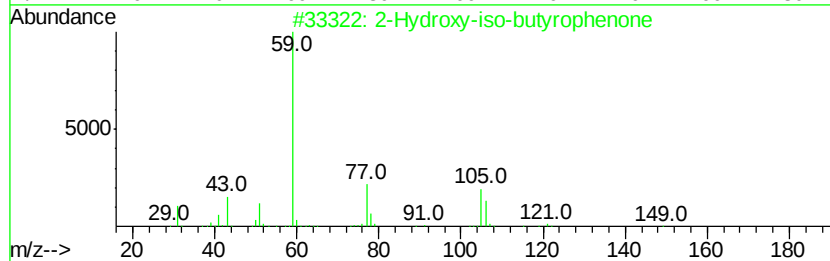
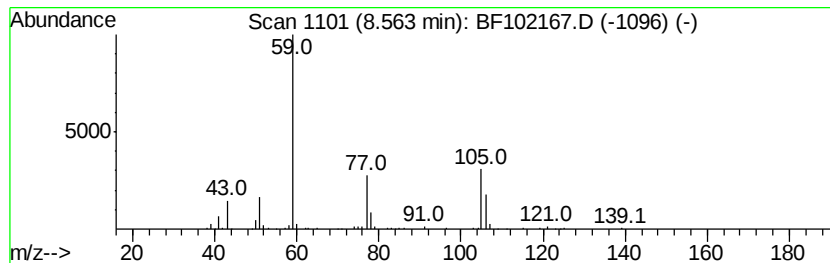
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Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	3.69 ng	228040	Napthalene-d8	8.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3		Butane, 2-methoxy-3-methyl-	102	C6H14O	062016-49-3	32
4		Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	10
5		Acetamide, 2,2'-thiobis-	148	C4H8N2O2S	014618-65-6	7



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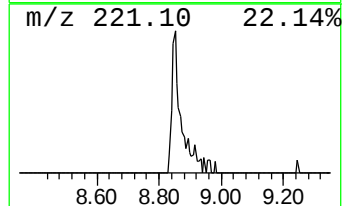
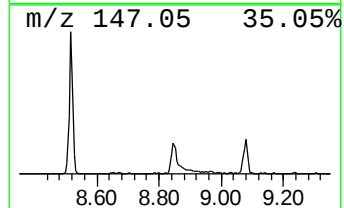
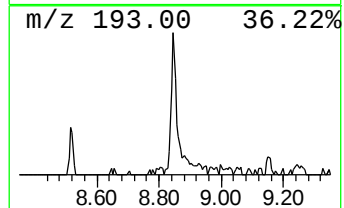
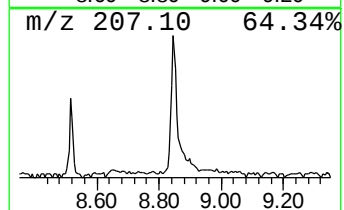
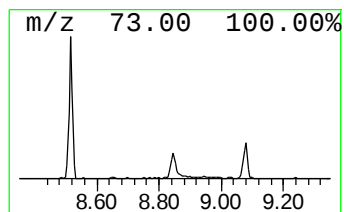
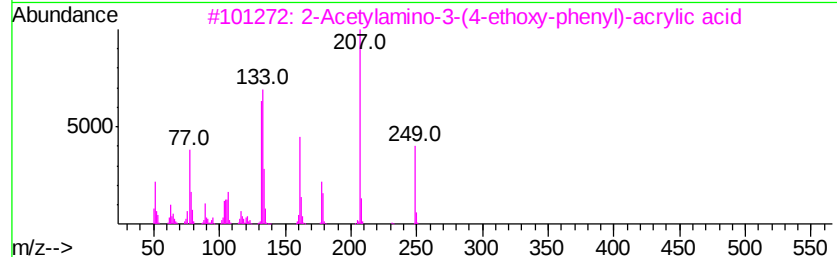
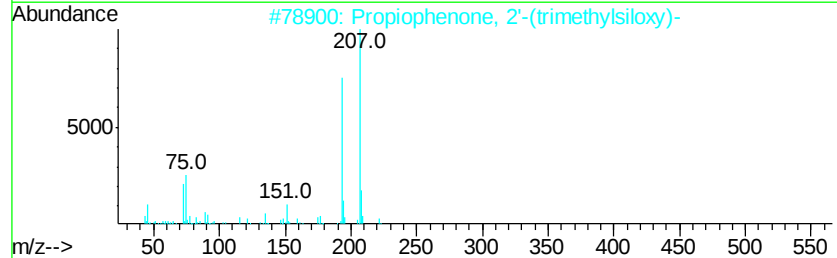
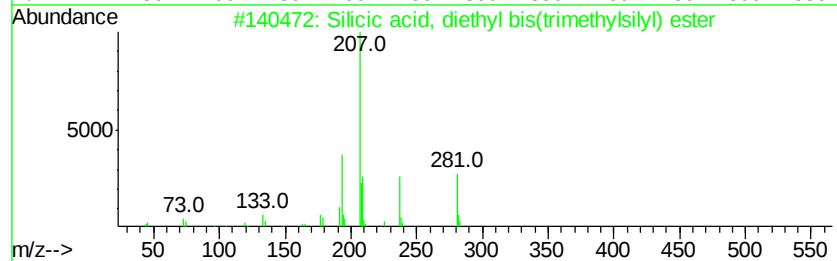
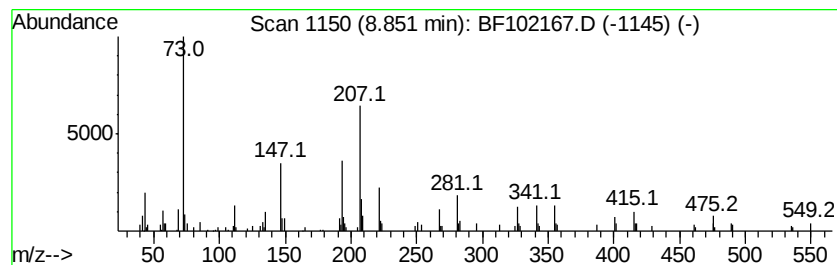
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.85 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	2.79 ng	172401	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silicic acid, diethyl bis(trimet...	296	C10H28O4Si3	003555-45-1	38
2		Propiophenone, 2'-(trimethylsilo...	222	C12H18O2Si	033342-87-9	38
3		2-Acetylmino-3-(4-ethoxy-phenyl...	249	C13H15NO4	325482-56-2	38
4		Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	35
5		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	35



Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102167.D
Acq On : 17 Jan 2018 23:01
Operator : SJ/JU
Sample : J1145-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-1(8-21.5)

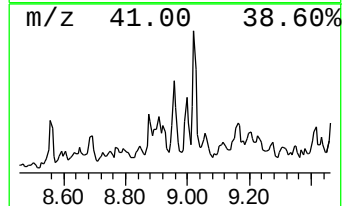
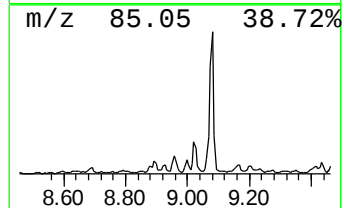
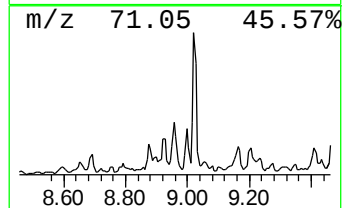
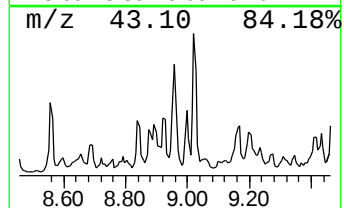
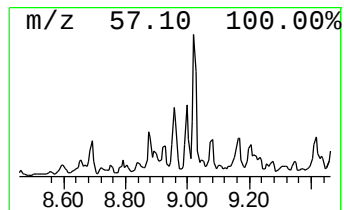
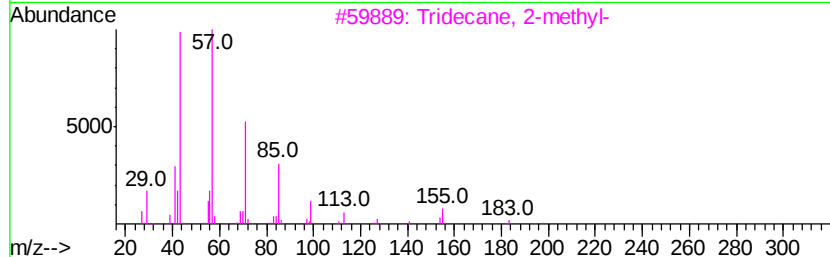
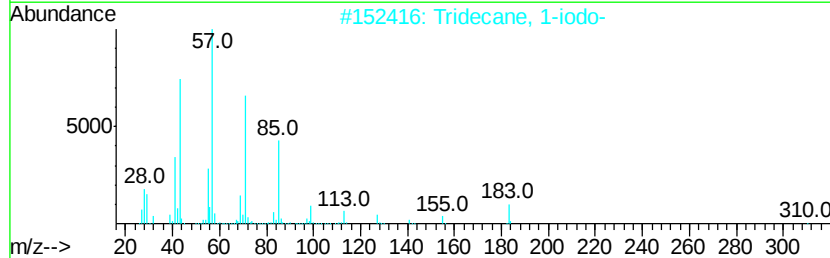
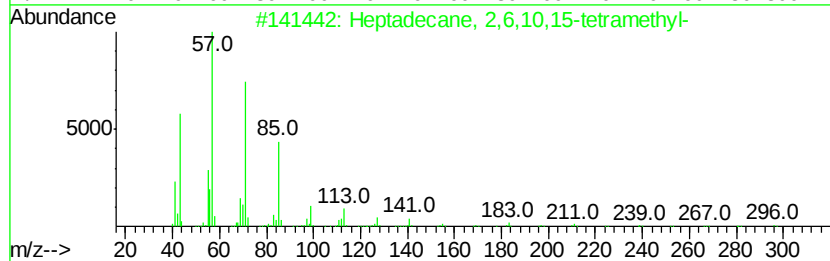
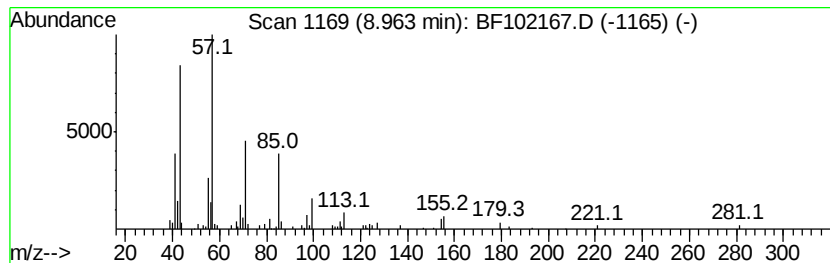
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	2.09 ng	117455	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3		Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
4		Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	76
5		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	72



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
Data File : BF102167.D
Acq On : 17 Jan 2018 23:01
Operator : SJ/JU
Sample : J1145-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB-1(8-21.5)

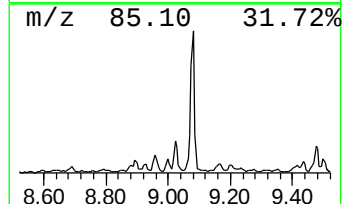
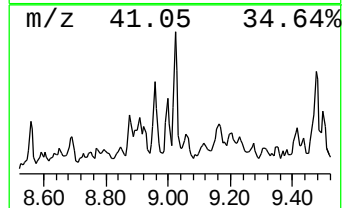
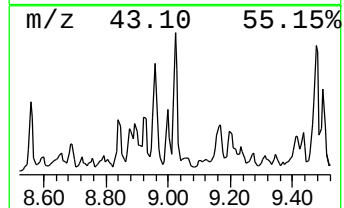
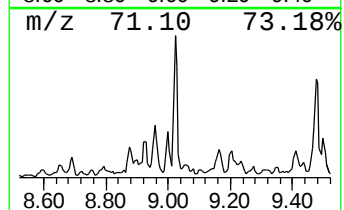
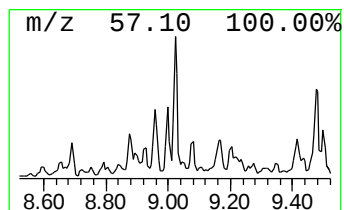
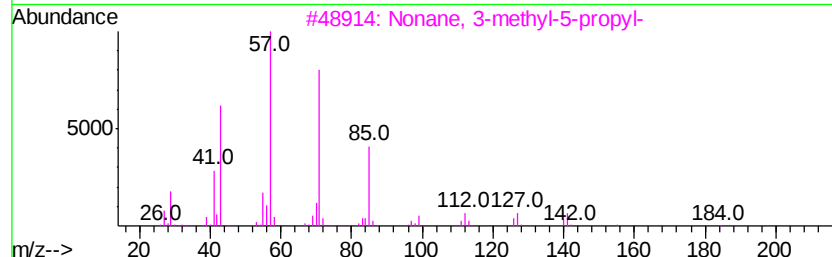
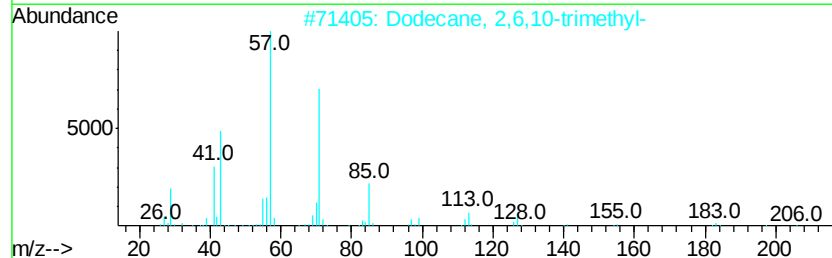
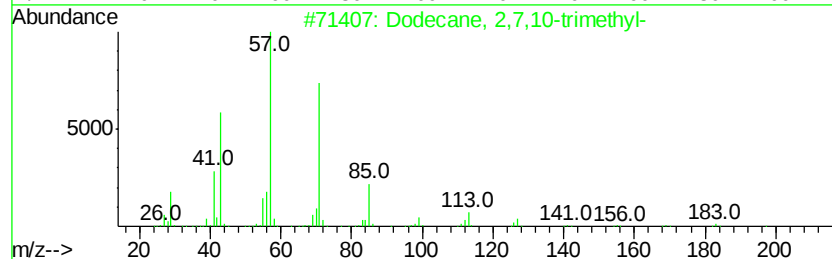
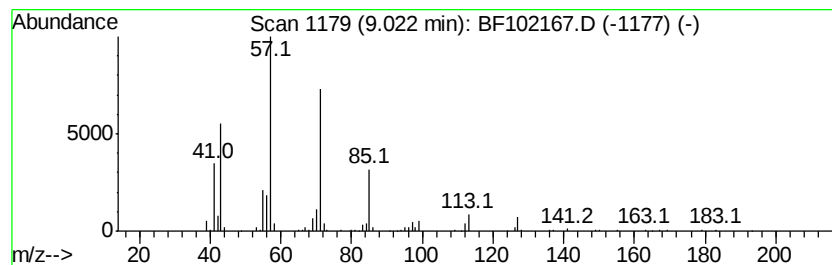
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2,7,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	3.55 ng	199548	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	91
2		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	90
3		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	78
4		Octadecane	254	C18H38	000593-45-3	72
5		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	64



Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
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Acq On : 17 Jan 2018 23:01
Operator : SJ/JU
Sample : J1145-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

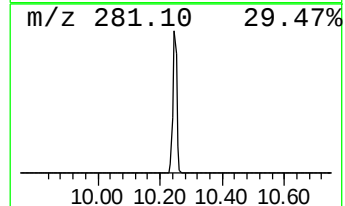
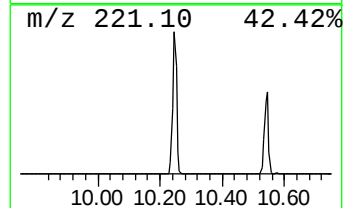
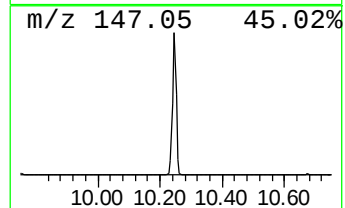
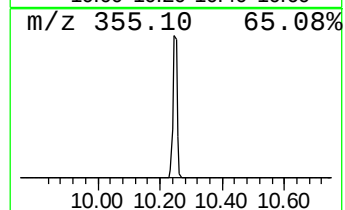
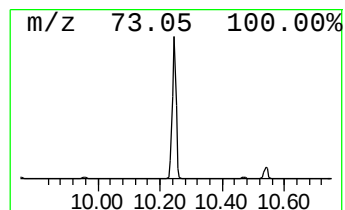
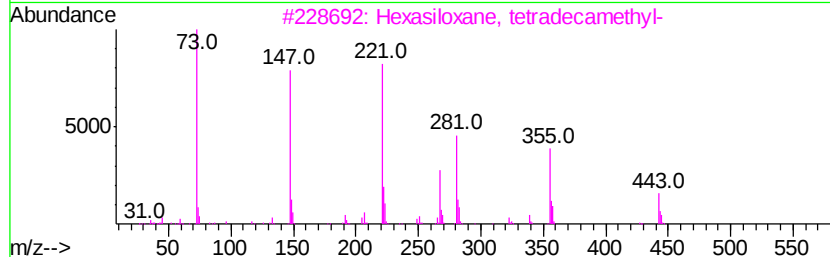
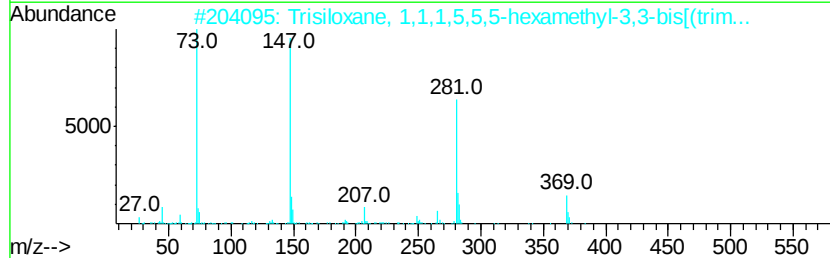
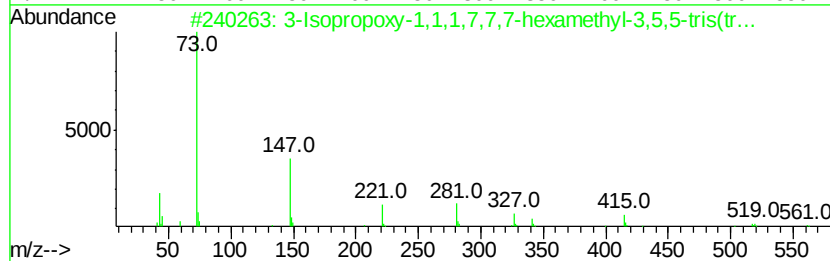
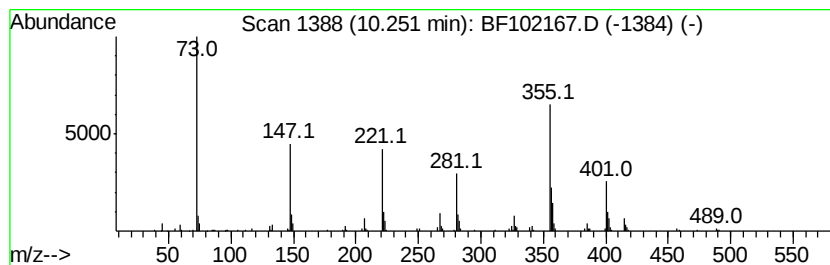
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PB-1(8-21.5)

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 unknown10.25 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.25	6.71 ng	376843	Acenaphthene-d10	9.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	37
2	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	32
3	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	28
4	Benzoic acid, 2,5-bis(trimethyls...	370	C16H30O4Si3	003618-20-0	25
5	Silane, 1,6-heptadiyne-1,7-diylb...	236	C13H24Si2	041268-43-3	25



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
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Operator : SJ/JU
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Misc :
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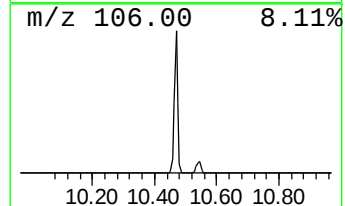
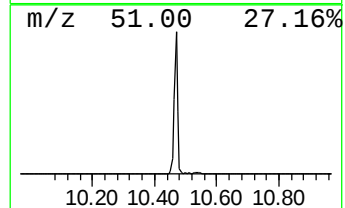
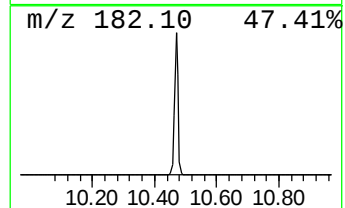
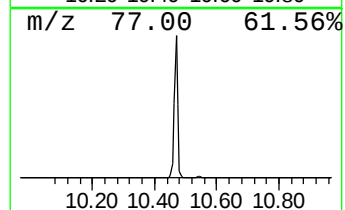
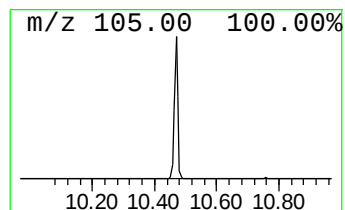
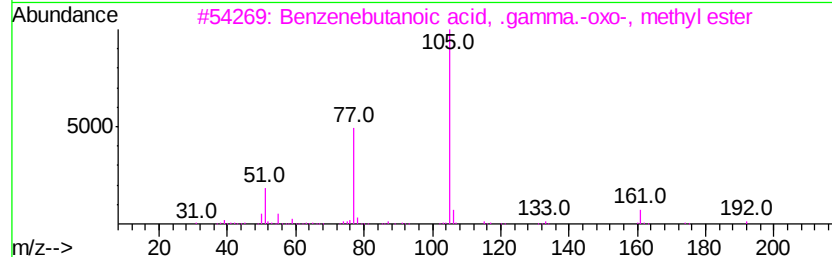
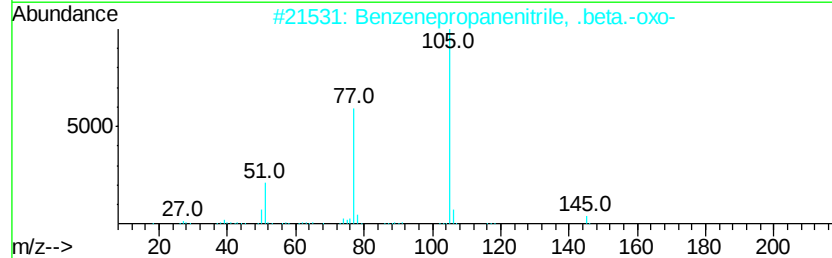
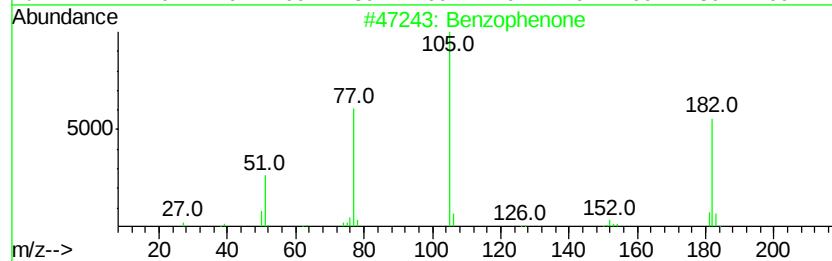
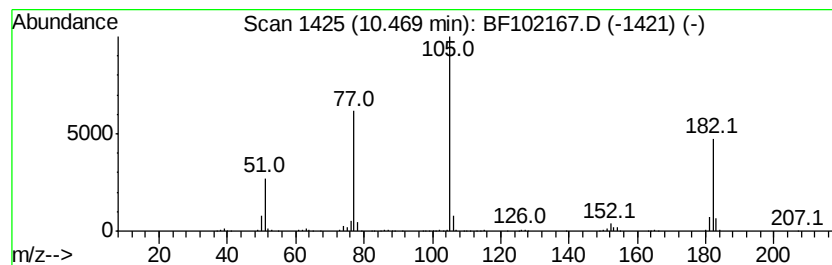
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ClientSampleId :
PB-1(8-21.5)

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 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	14.46 ng	812036	Acenaphthene-d10	9.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Benzenepropanenitrile, .beta.-oxo-	145 C9H7NO	000614-16-4 47
3		Benzenebutanoic acid, .gamma.-ox...	192 C11H12O3	025333-24-8 47
4		Vinyl benzoate	148 C9H8O2	000769-78-8 47
5		1-Propanone, 2-bromo-1-phenyl-	212 C9H9BrO	002114-00-3 47



Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102167.D
Acq On : 17 Jan 2018 23:01
Operator : SJ/JU
Sample : J1145-02
Misc :
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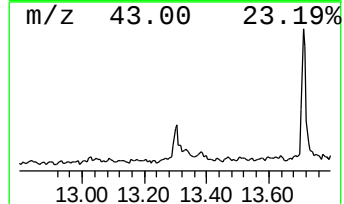
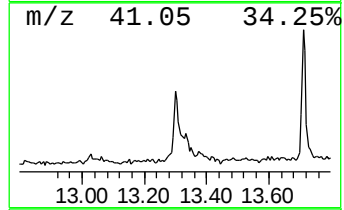
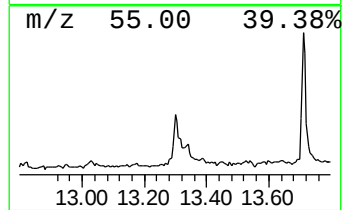
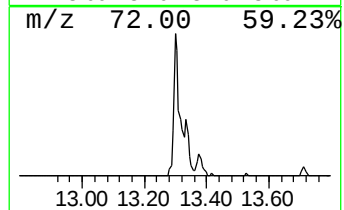
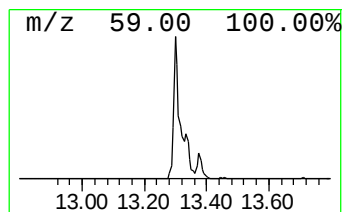
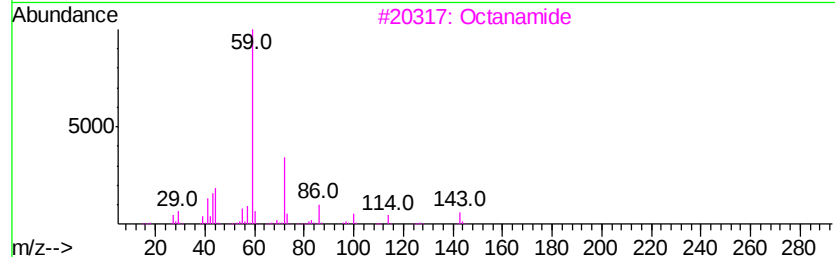
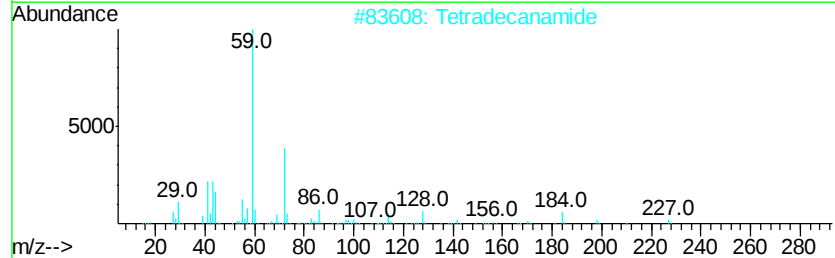
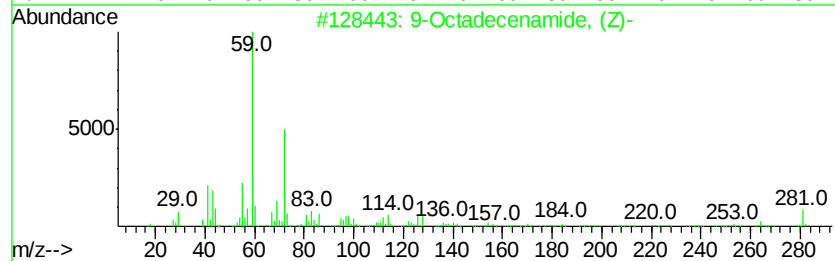
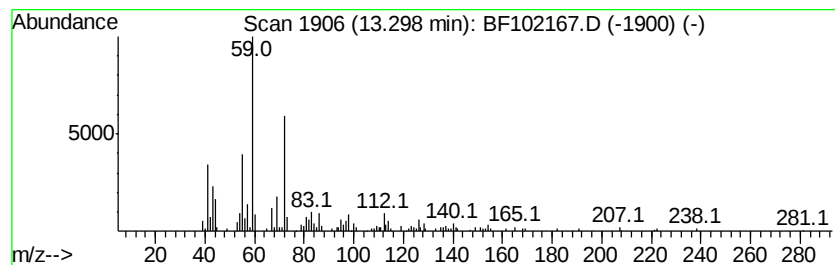
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.30	5.71 ng	220975	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Hexadecanamide	255	C16H33NO	000629-54-9	53
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
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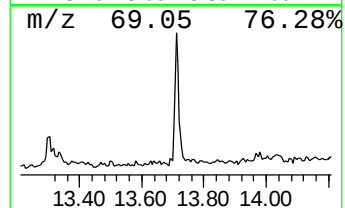
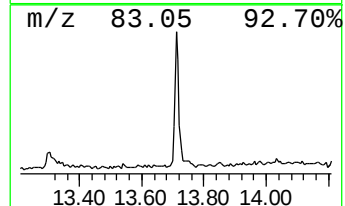
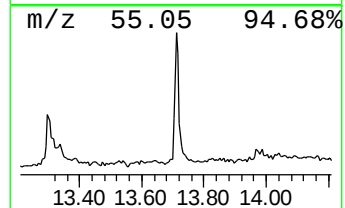
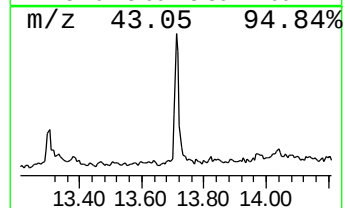
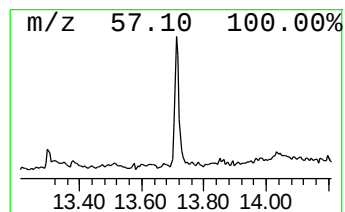
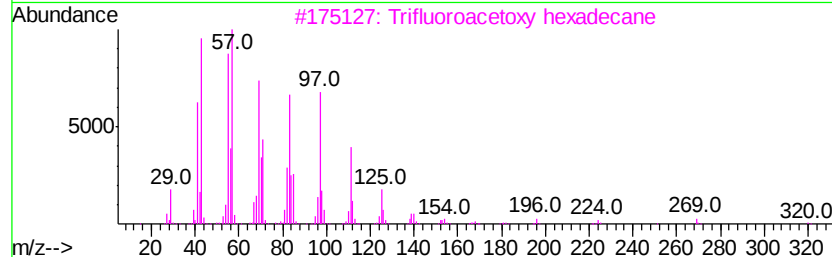
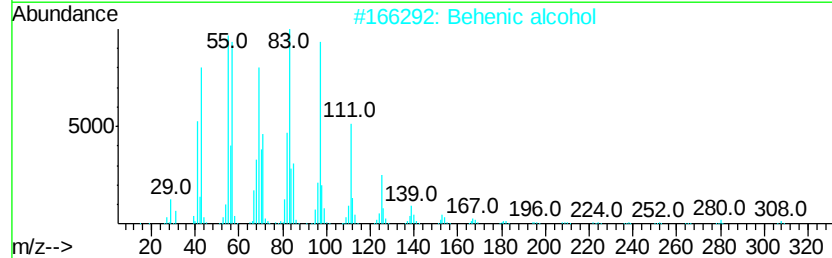
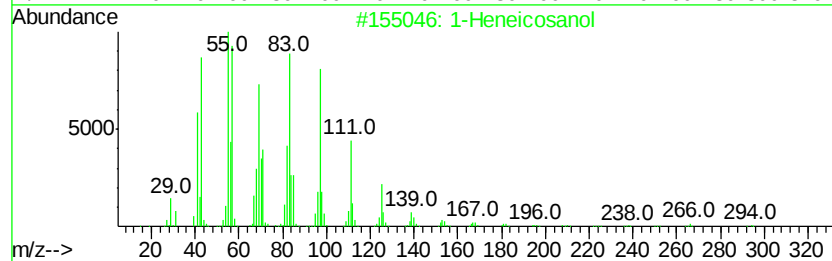
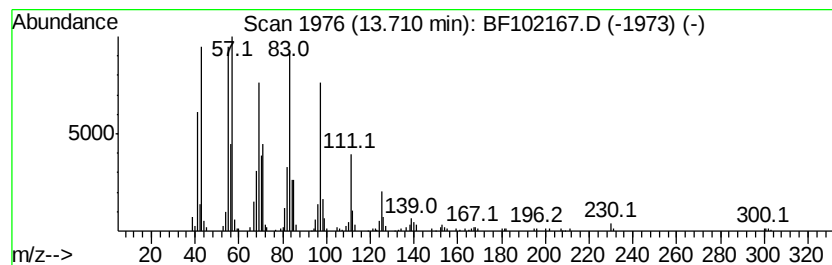
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ClientSampleId :
PB-1(8-21.5)

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 12 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.71	7.90 ng	305842	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
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 Acq On : 17 Jan 2018 23:01
 Operator : SJ/JU
 Sample : J1145-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 PB-1(8-21.5)

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
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unknown6.49	6.49	79.3	ng	3650480	1	6.72	920275	20.0
Cyclohexasiloxane...	8.52	7.0	ng	433509	2	8.00	1234840	20.0
2-Hydroxy-iso-but...	8.56	3.7	ng	228040	2	8.00	1234840	20.0
unknown8.85	8.85	2.8	ng	172401	2	8.00	1234840	20.0
Heptadecane, 2,6,...	8.96	2.1	ng	117455	3	9.75	1123020	20.0
Dodecane, 2,7,10-...	9.02	3.5	ng	199548	3	9.75	1123020	20.0
unknown10.25	10.25	6.7	ng	376843	3	9.75	1123020	20.0
Benzophenone	10.47	14.5	ng	812036	3	9.75	1123020	20.0
9-Octadecenamide,...	13.30	5.7	ng	220975	5	13.87	774531	20.0
1-Heneicosanol	13.71	7.9	ng	305842	5	13.87	774531	20.0