

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070716\
 Data File : BF088796.D
 Acq On : 7 Jul 2016 23:36
 Operator : UM/SJ
 Sample : H3889-03 20X
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-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-BF063016.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	1.827	19	21	68	rVB	1565965	4130454	100.00%	29.494%
2	5.313	324	326	329	rBV	91134	112107	2.71%	0.801%
3	5.564	346	348	364	rBV	19954	56425	1.37%	0.403%
4	6.364	416	418	422	rBV2	136298	143186	3.47%	1.022%
5	6.502	428	430	432	rBV	166108	133740	3.24%	0.955%
6	6.742	449	451	453	rBB	596054	515873	12.49%	3.684%
7	6.890	462	464	466	rBB	97793	102215	2.47%	0.730%
8	7.027	474	476	489	rBV	52133	69074	1.67%	0.493%
9	7.302	498	500	502	rVB	85430	77209	1.87%	0.551%
10	8.022	561	563	566	rBV	656251	626677	15.17%	4.475%
11	8.925	638	642	644	rBV2	59643	66441	1.61%	0.474%
12	9.108	655	658	660	rBV	105168	138266	3.35%	0.987%
13	9.633	702	704	706	rBB	110623	101215	2.45%	0.723%
14	9.782	714	717	719	rBV	499019	617864	14.96%	4.412%
15	10.559	783	785	788	rVB2	67043	69905	1.69%	0.499%
16	11.256	843	846	848	rVB	654779	580155	14.05%	4.143%
17	12.834	982	984	986	rBV	138707	121061	2.93%	0.864%
18	13.359	1027	1030	1034	rBV2	37411	51815	1.25%	0.370%
19	13.588	1048	1050	1053	rBV	46698	61391	1.49%	0.438%
20	13.794	1066	1068	1071	rVB	67675	72272	1.75%	0.516%
21	13.885	1073	1076	1078	rBV	458508	525946	12.73%	3.756%
22	14.011	1084	1087	1090	rBV	94073	130065	3.15%	0.929%
23	14.228	1101	1106	1109	rBV2	759644	969259	23.47%	6.921%
24	14.400	1118	1121	1126	rBV	154084	233707	5.66%	1.669%
25	14.594	1135	1138	1142	rBV	211179	255584	6.19%	1.825%
26	14.765	1150	1153	1160	rVB	181303	323815	7.84%	2.312%
27	14.982	1169	1172	1175	rBV	275735	362029	8.76%	2.585%
28	15.154	1184	1187	1190	rBV	245815	348259	8.43%	2.487%
29	15.268	1195	1197	1199	rVV	364557	402833	9.75%	2.876%
30	15.440	1208	1212	1222	rVB	241784	453328	10.98%	3.237%
31	15.600	1223	1226	1232	rBV	190980	352354	8.53%	2.516%
32	15.703	1232	1235	1237	rBV2	18129	44940	1.09%	0.321%
33	15.977	1256	1259	1267	rVB	195981	411285	9.96%	2.937%
34	16.137	1269	1273	1283	rVB	152530	339595	8.22%	2.425%

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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 >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.651	1314	1318	1324	rVB	71928	197115	4.77%	1.408%
36	16.777	1325	1329	1336	rVB	65863	171998	4.16%	1.228%
37	17.508	1387	1393	1403	rBV3	50255	286591	6.94%	2.046%
38	18.583	1477	1487	1503	rVB4	54048	348348	8.43%	2.487%

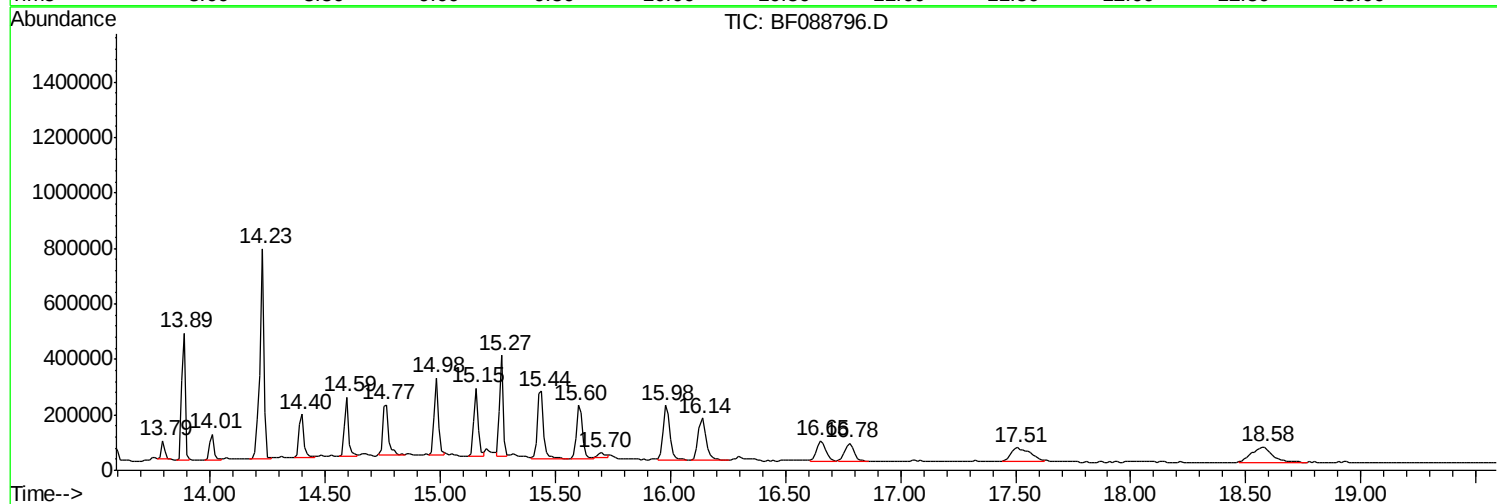
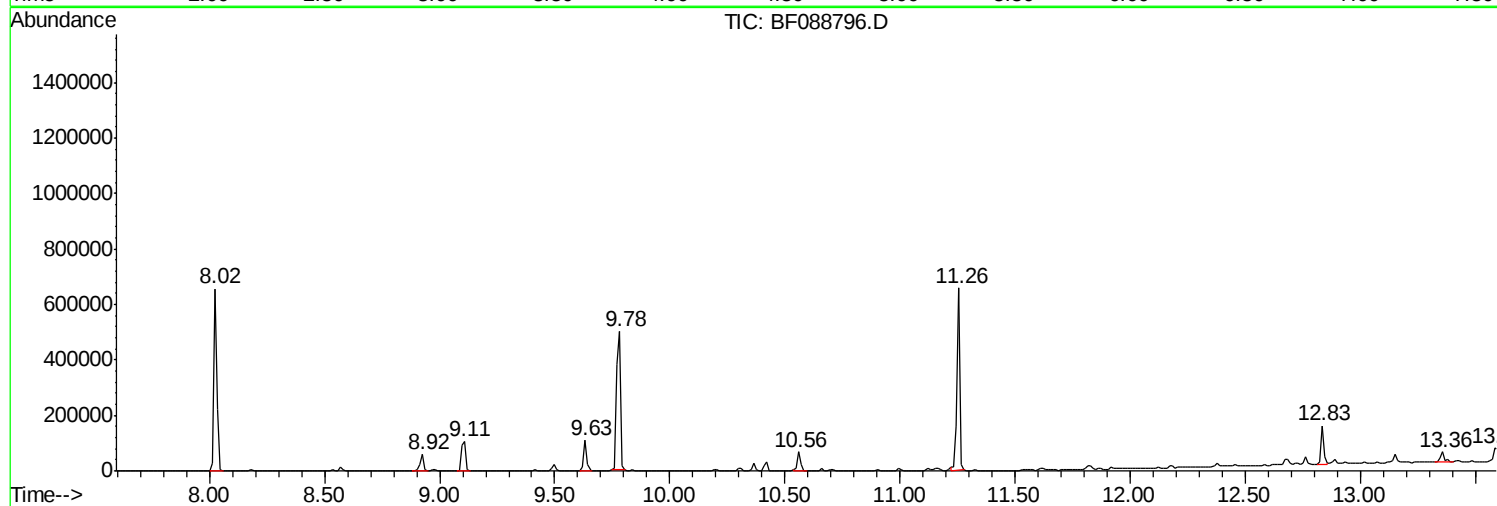
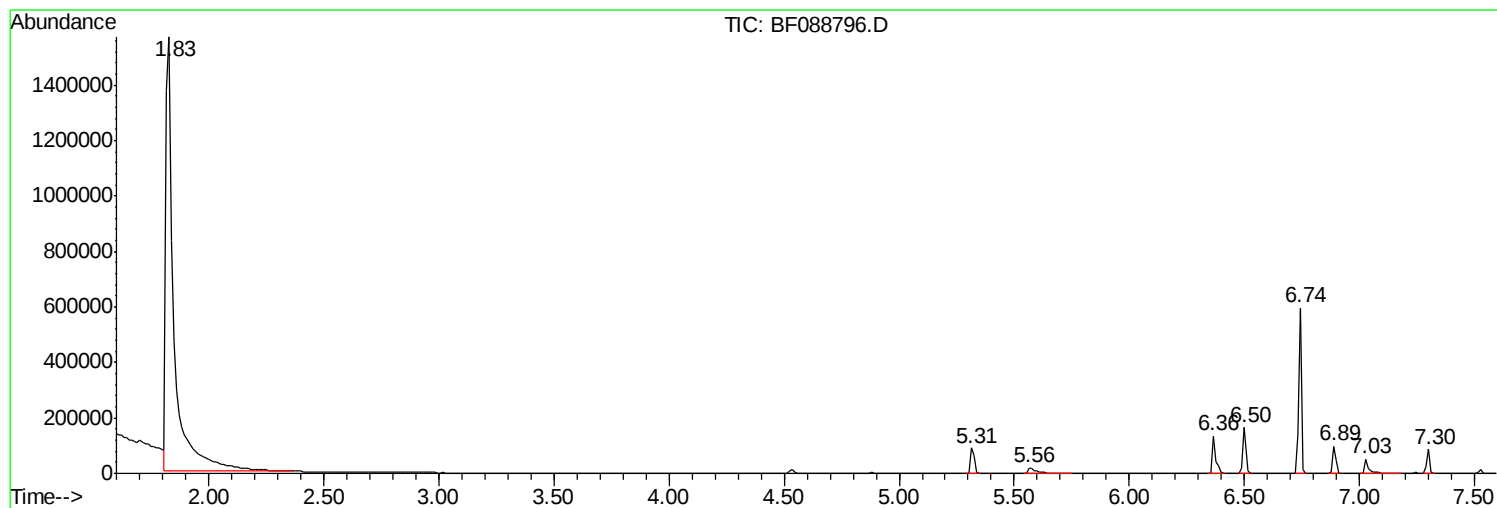
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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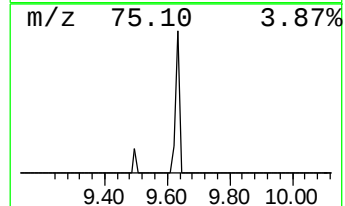
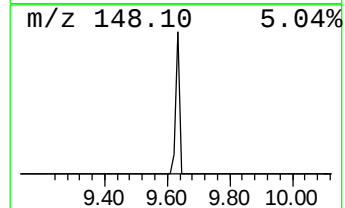
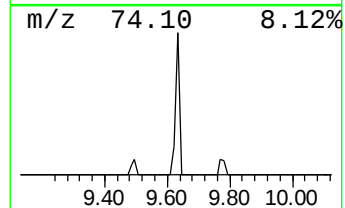
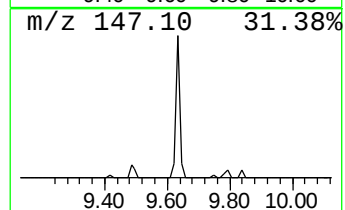
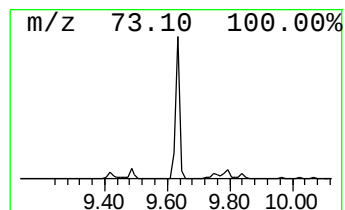
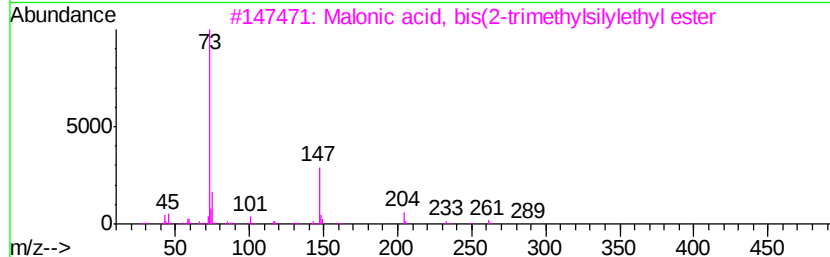
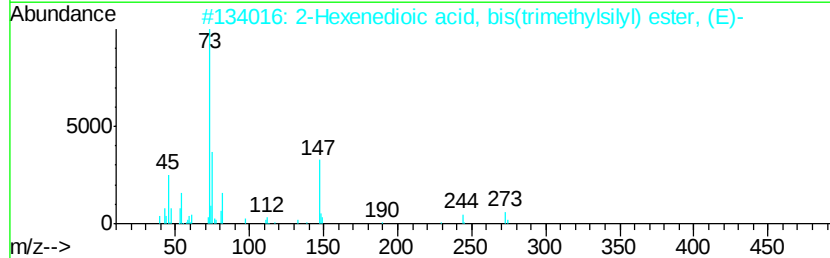
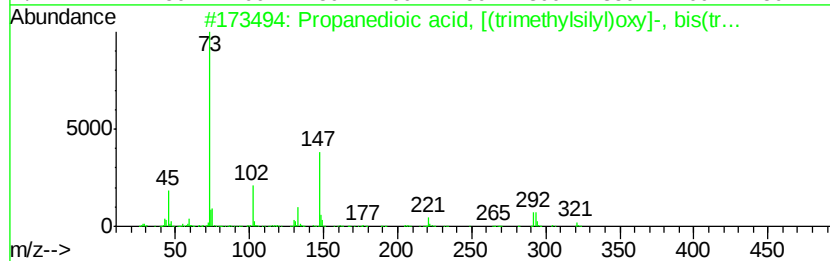
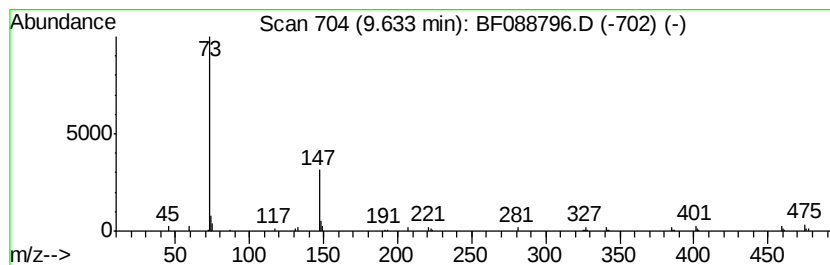
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown9.63 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	3.28 ng	101215	Acenaphthene-d10	9.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(tri...	336	C12H28O5Si3	038165-93-4	40
2		2-Hexenedioic acid, bis(trimethylsilyl) ester, (E)-	288	C12H24O4Si2	055494-10-5	40
3		Malonic acid, bis(2-trimethylsilylethyl) ester	304	C13H28O4Si2	090744-45-9	40
4		trans-3-Hexenedioic acid, bis(trimethylsilyl) ester, (E)-	288	C12H24O4Si2	1000078-95-4	33
5		2-Phenyl-2-trimethylsilyloxypropyl acetate	310	C15H26O3Si2	082326-12-3	33



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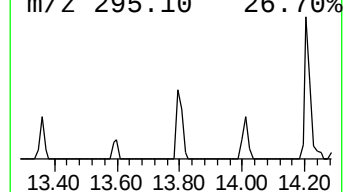
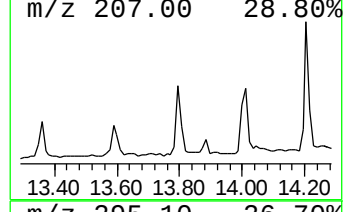
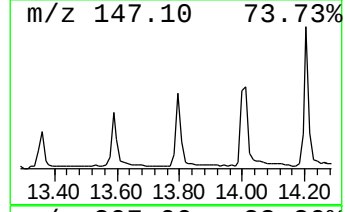
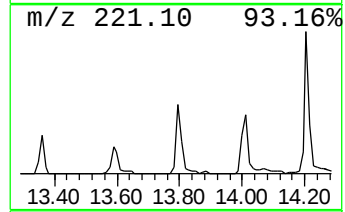
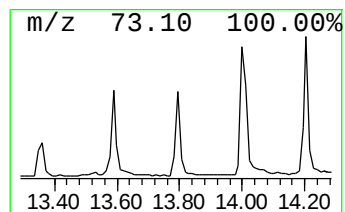
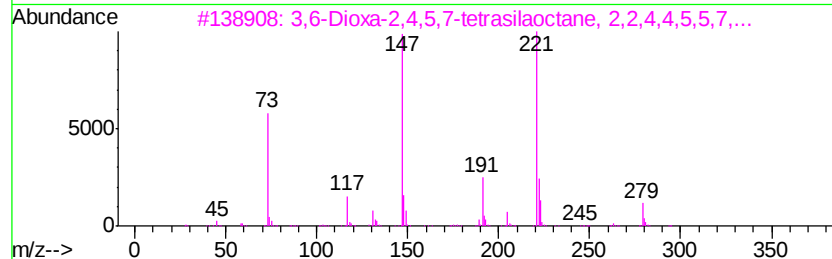
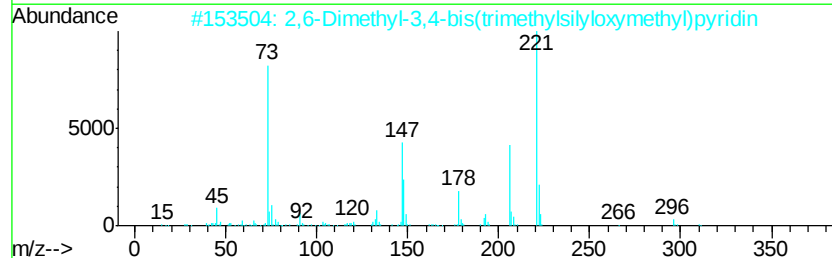
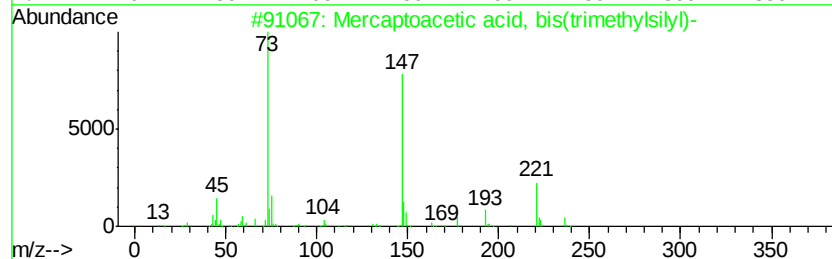
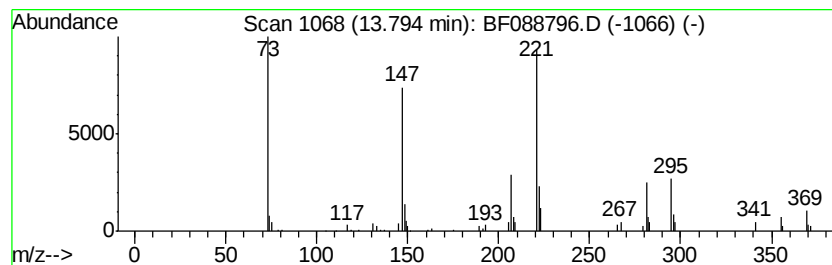
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown13.79 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.75 ng	72272	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	40
2		2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29N02Si2	1000079-52-1	37
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	35



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ClientSampled :
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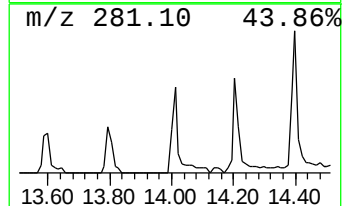
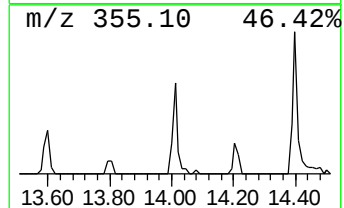
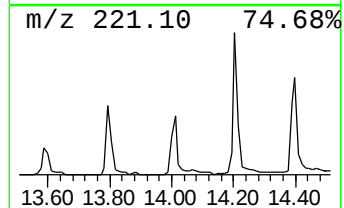
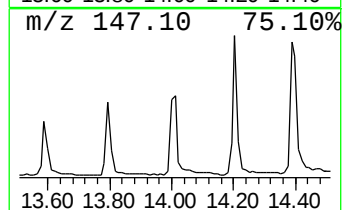
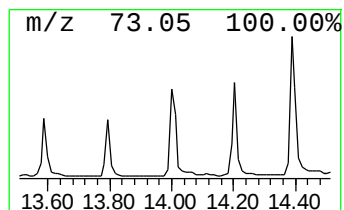
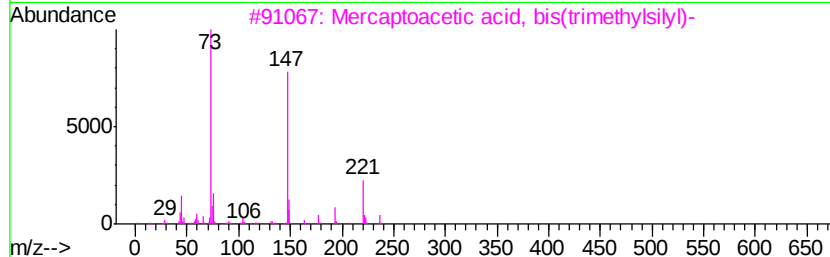
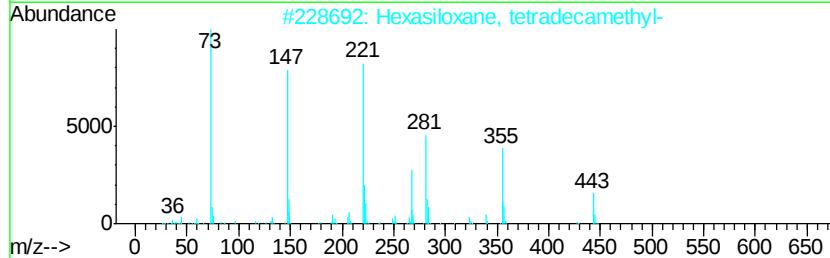
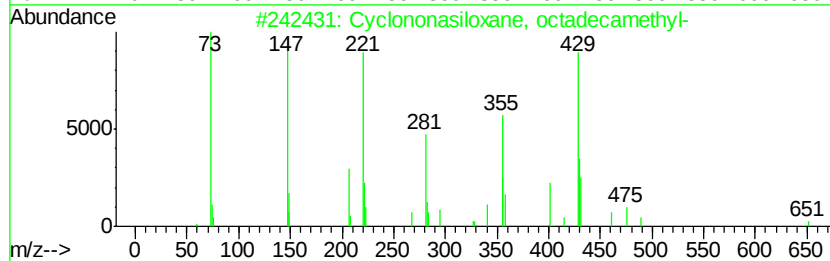
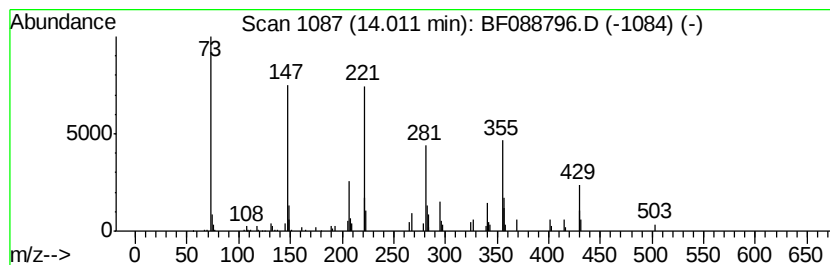
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	4.95 ng	130065	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	87
2		Hexasiloxane, tetradecamethyl-	458	C14H4205Si6	000107-52-8	74
3		Mercaptoacetic acid, bis(trimeth...	236	C8H2002SSi2	006398-62-5	37
4		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	37
5		2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48010Si9	145344-72-5	32



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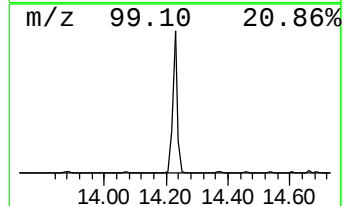
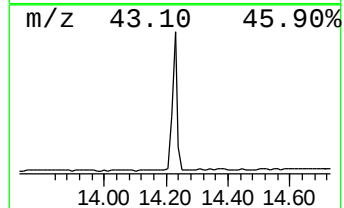
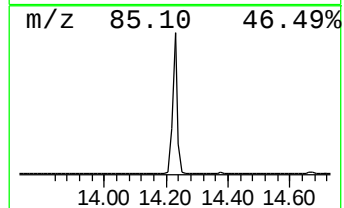
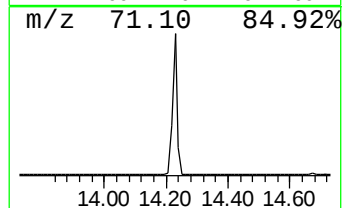
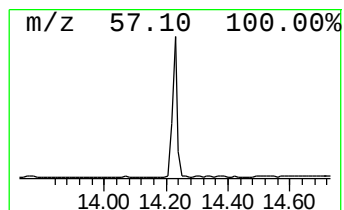
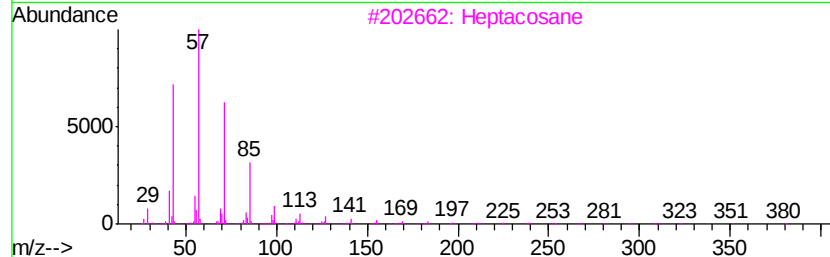
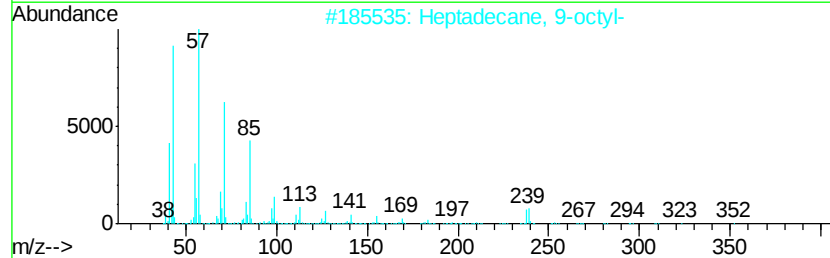
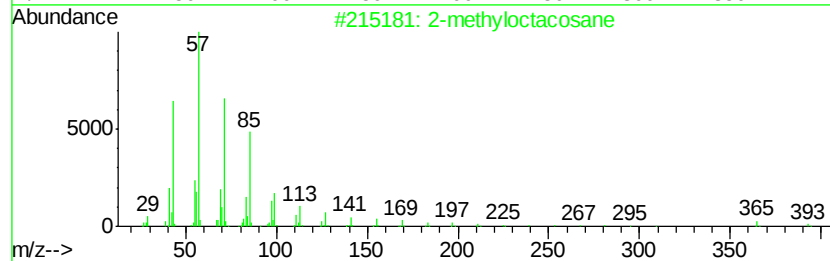
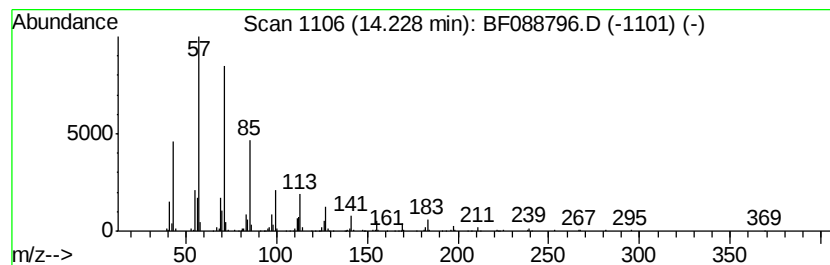
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-methyloctacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.23	36.86 ng	969259	Chrysene-d12		13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	90
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90
3	Heptacosane		380	C27H56	000593-49-7	90
4	Hexacosane		366	C26H54	000630-01-3	86
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	86



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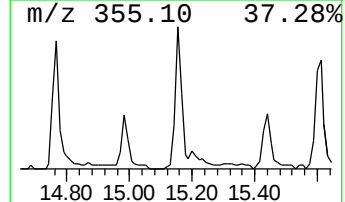
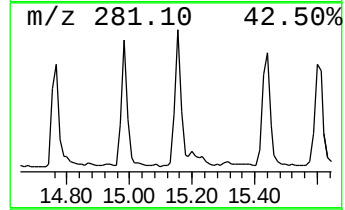
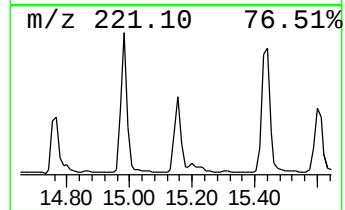
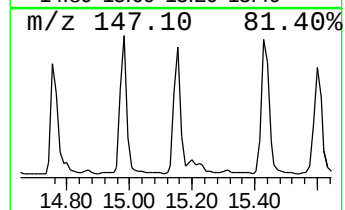
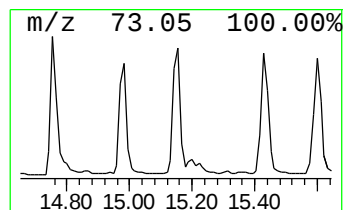
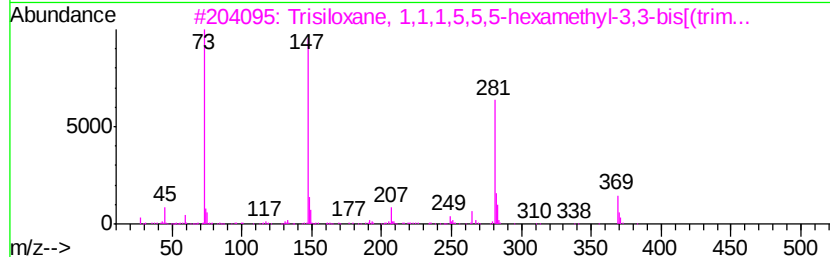
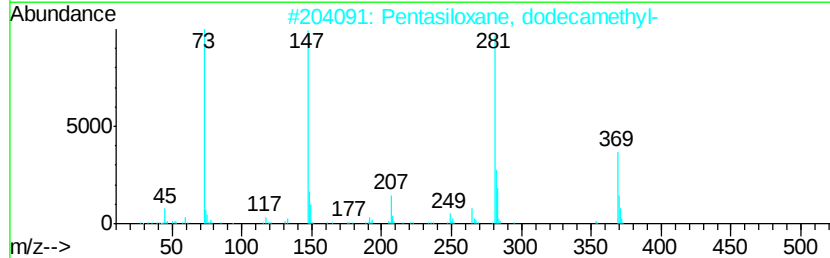
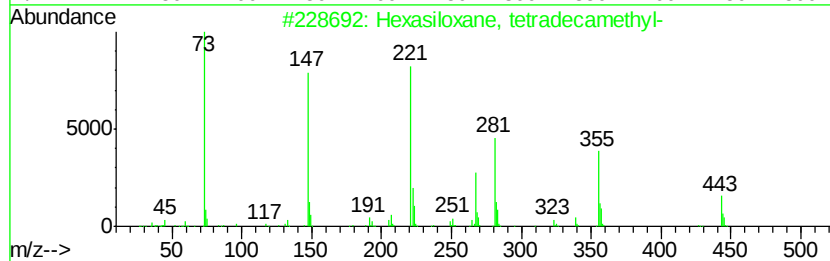
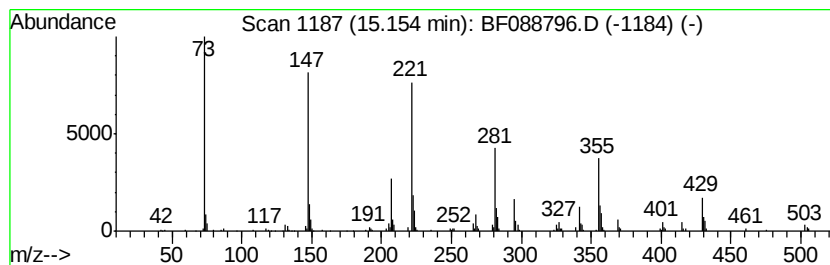
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexasiloxane, tetradecamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	17.29 ng	348259	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	41
3		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	38
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	35
5		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
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Acq On : 7 Jul 2016 23:36
Operator : UM/SJ
Sample : H3889-03 20X
Misc :
ALS Vial : 26 Sample Multiplier: 1

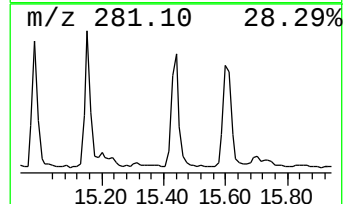
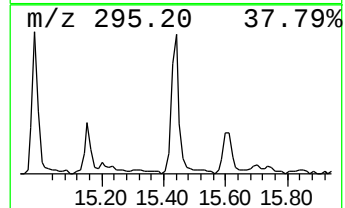
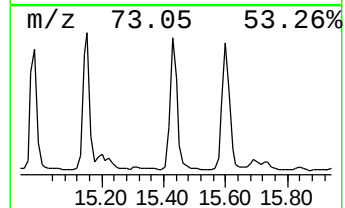
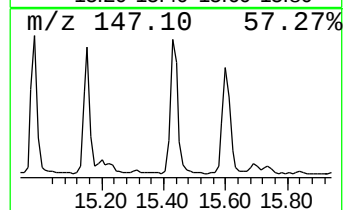
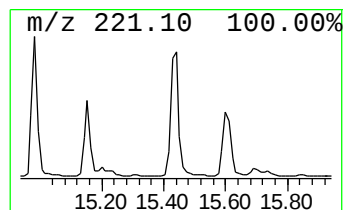
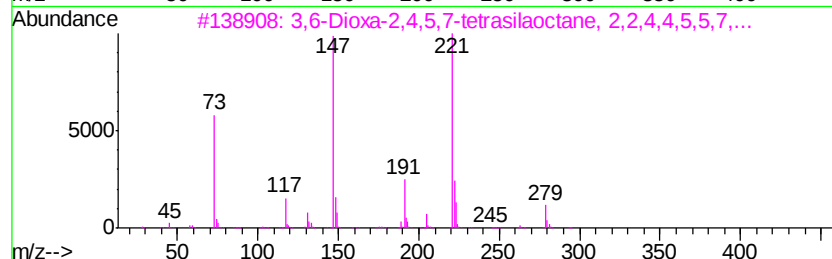
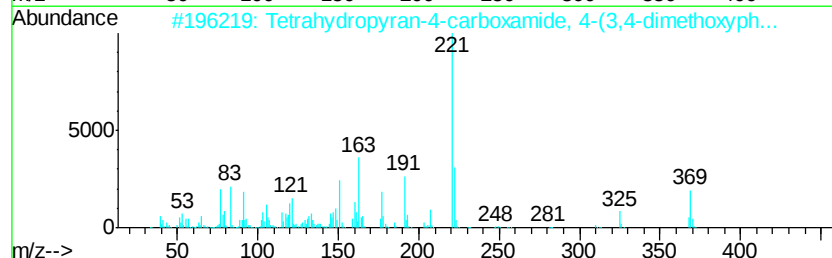
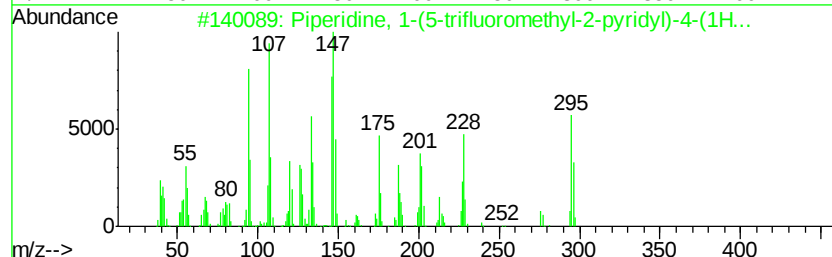
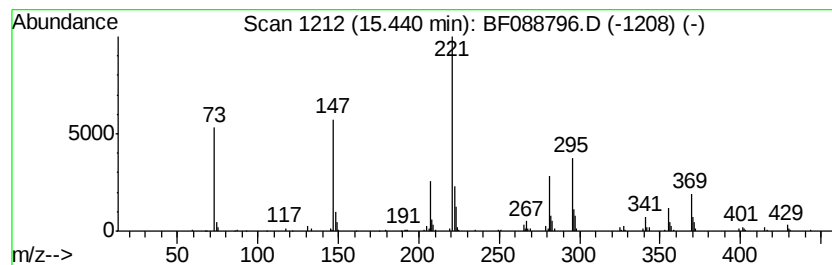
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Piperidine, 1-(5-trifluoromethyl-2-pyridyl)-4-(1H... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.44	22.51 ng	453328	Perylene-d12	15.27		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Piperidine, 1-(5-trifluoromethyl-2-pyridyl)-4-(1H-tetrahydropyran-4-carboxamide, 4-(3,4-dimethoxyphenyl)-2-oxo-2-(hydroxymethyl)-1,2,3,4-tetrahydro-1,2,3,4-benzoxazin-6-yl)-1,2,3,				



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070716\
Data File : BF088796.D
Acq On : 7 Jul 2016 23:36
Operator : UM/SJ
Sample : H3889-03 20X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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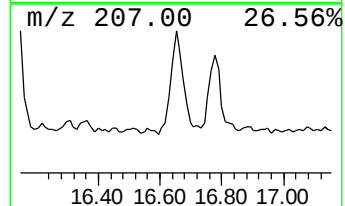
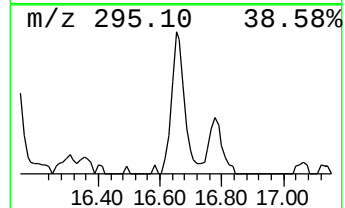
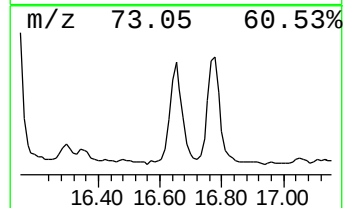
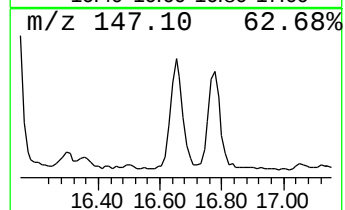
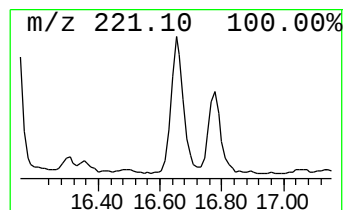
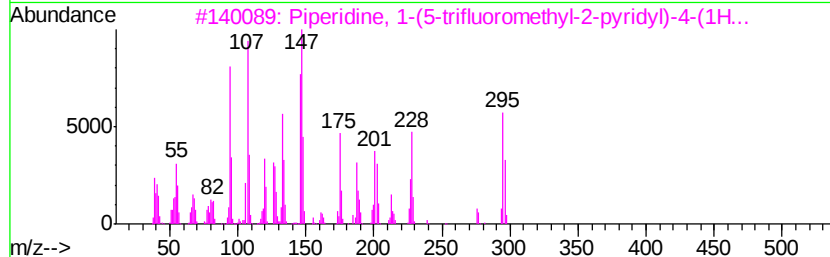
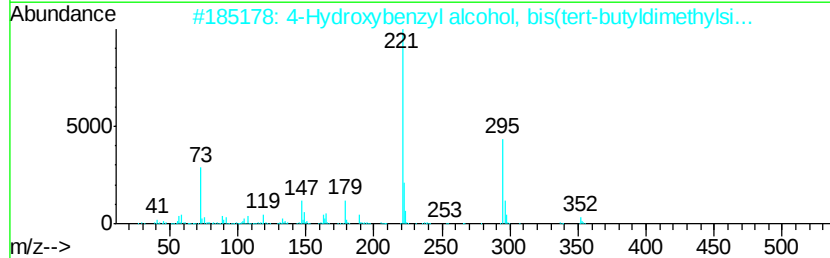
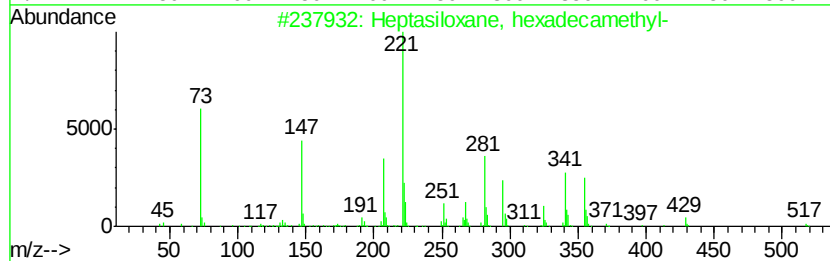
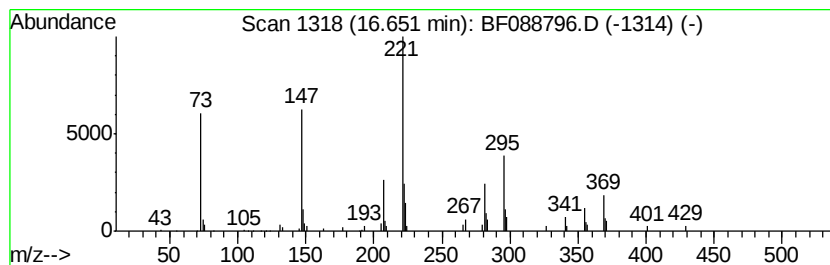
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Heptasiloxane, hexadecamethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	9.79 ng	197115	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	53
2		4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	38
3		Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	38
4		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15N03	024451-17-0	23
5		Acetamide, 2-(5,7-dimethyl-[1,2,...	389	C21H19N5OS	1000304-63-9	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070716\
Data File : BF088796.D
Acq On : 7 Jul 2016 23:36
Operator : UM/SJ
Sample : H3889-03 20X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-3

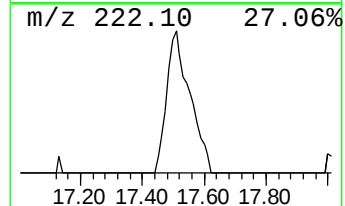
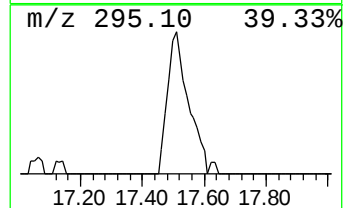
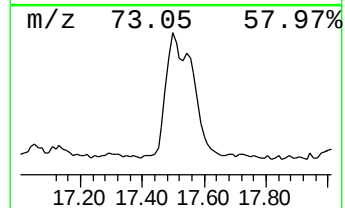
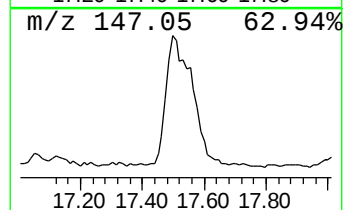
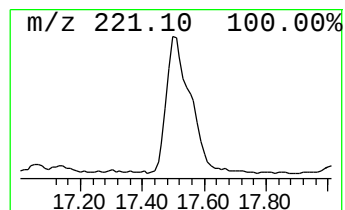
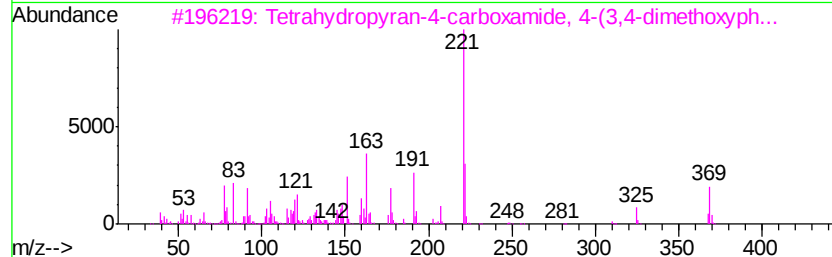
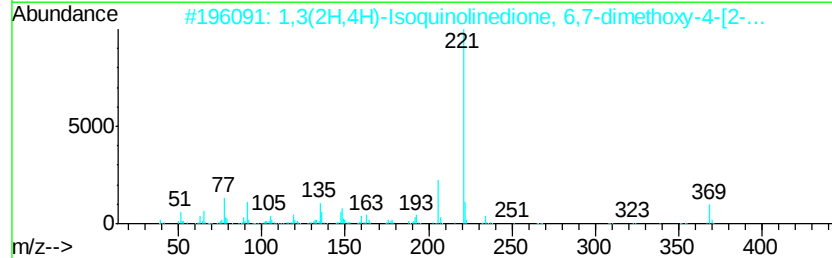
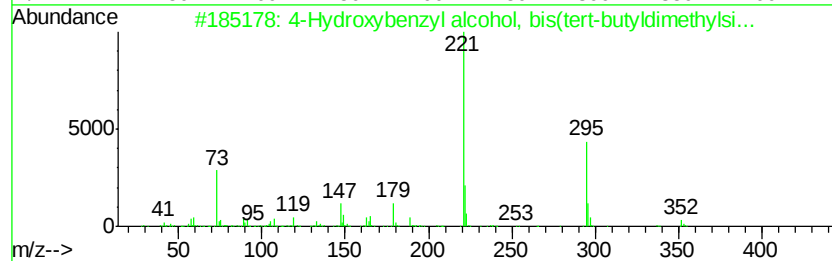
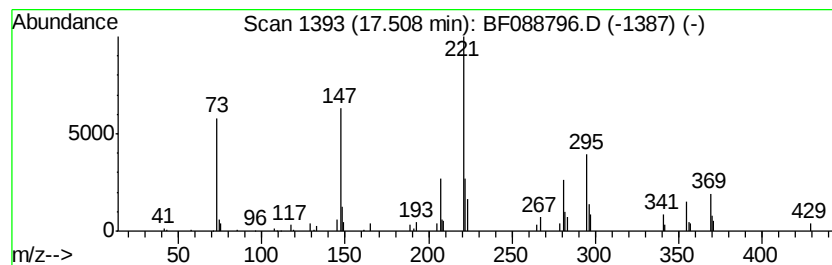
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.51 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.51	14.23 ng	286591	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	37
2		1,3(2H,4H)-Isoquinolinedione, 6,...	369	C20H19N06	1000115-82-7	35
3		Tetrahydropyran-4-carboxamide, 4...	369	C22H27N04	1000310-01-9	35
4		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	32
5		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15N03	024451-17-0	23



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070716\
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Sample : H3889-03 20X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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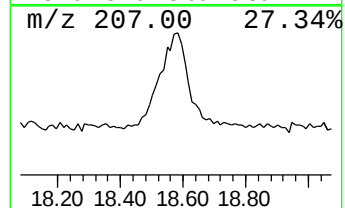
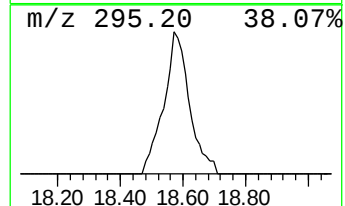
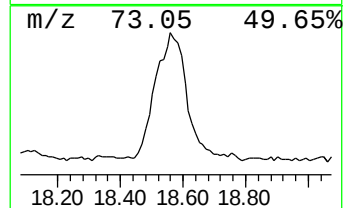
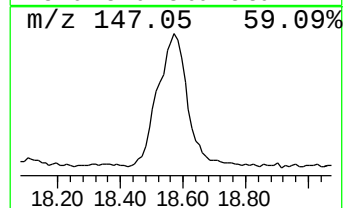
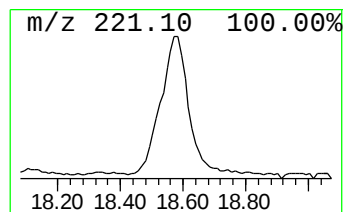
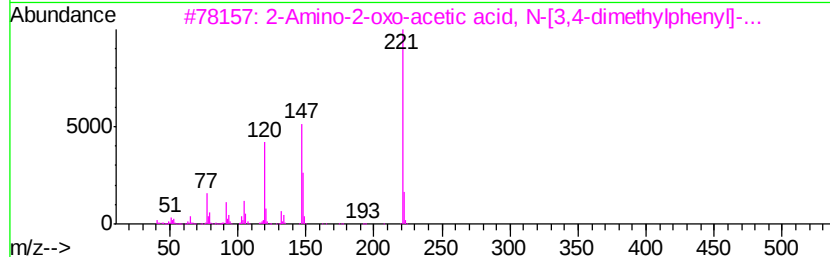
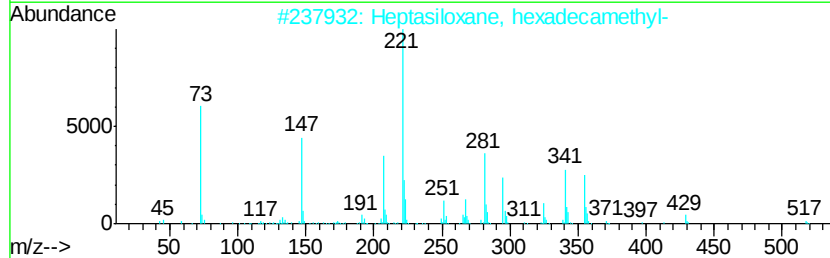
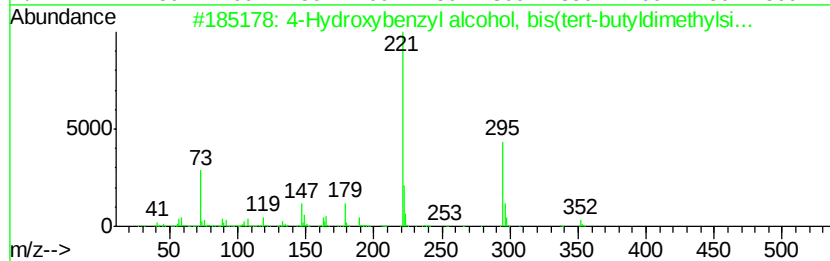
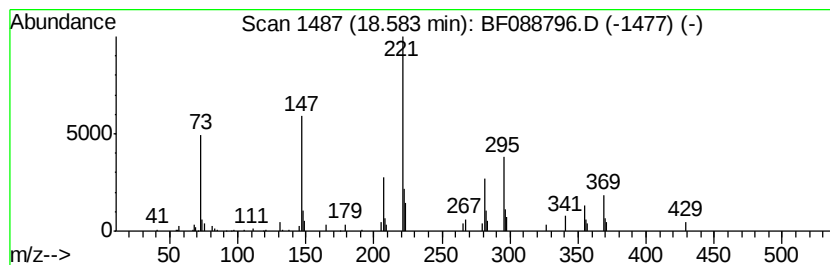
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.58 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	17.29 ng	348348	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	47
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
3		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15N03	024451-17-0	37
4		Tetrahydropyran-4-carboxamide, 4...	369	C22H27N04	1000310-01-9	35
5		Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070716\
Data File : BF088796.D
Acq On : 7 Jul 2016 23:36
Operator : UM/SJ
Sample : H3889-03 20X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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unknown13.79	13.79	2.8	ng	72272	5	13.89	525946	20.0
Cyclononasiloxane...	14.01	5.0	ng	130065	5	13.89	525946	20.0
2-methyloctacosane	14.23	36.9	ng	969259	5	13.89	525946	20.0
Hexasiloxane, tet...	15.15	17.3	ng	348259	6	15.27	402833	20.0
Piperidine, 1-(5-...	15.44	22.5	ng	453328	6	15.27	402833	20.0
Heptasiloxane, he...	16.65	9.8	ng	197115	6	15.27	402833	20.0
unknown17.51	17.51	14.2	ng	286591	6	15.27	402833	20.0
unknown18.58	18.58	17.3	ng	348348	6	15.27	402833	20.0