

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
 Data File : BF087130.D
 Acq On : 18 May 2016 4:44
 Operator : UM/SJ
 Sample : H3085-04
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-CSPH3-13K

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-BF051716.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	1.724	10	12	47	rVB	3708743	7713368	100.00%	15.266%
2	3.244	142	145	154	rVB	78869	167334	2.17%	0.331%
3	4.718	272	274	290	rBV	1063439	1903984	24.68%	3.768%
4	5.187	312	315	317	rBV	4190395	4611768	59.79%	9.127%
5	5.587	347	350	355	rBV	108532	148094	1.92%	0.293%
6	6.261	406	409	411	rBV	4226801	4721815	61.22%	9.345%
7	6.364	416	418	420	rBV	4704192	4523143	58.64%	8.952%
8	6.593	435	438	440	rBV	777829	857856	11.12%	1.698%
9	6.741	449	451	454	rBV	2898674	3362584	43.59%	6.655%
10	7.164	485	488	491	rBV	2750758	2965860	38.45%	5.870%
11	7.873	548	550	553	rBV	913859	1074624	13.93%	2.127%
12	8.959	642	645	648	rBV	4385092	4386558	56.87%	8.682%
13	9.359	678	680	684	rBV	634038	595166	7.72%	1.178%
14	9.576	697	699	701	rBV	161293	148939	1.93%	0.295%
15	9.622	701	703	706	rBV2	982207	1204834	15.62%	2.385%
16	10.068	740	742	744	rVB	180615	173353	2.25%	0.343%
17	10.285	758	761	765	rBV	65178	115958	1.50%	0.229%
18	10.422	770	773	775	rBV	2753099	3253286	42.18%	6.439%
19	10.536	782	783	788	rVB	143764	226879	2.94%	0.449%
20	10.982	821	822	828	rVB	72111	117636	1.53%	0.233%
21	11.108	830	833	835	rBV	1025546	1194698	15.49%	2.364%
22	11.656	879	881	885	rBV	178509	187105	2.43%	0.370%
23	12.696	969	972	974	rBV	3411379	4460274	57.83%	8.828%
24	13.645	1052	1055	1060	rBV2	45769	164267	2.13%	0.325%
25	13.725	1060	1062	1065	rBV	779739	920141	11.93%	1.821%
26	15.085	1179	1181	1187	rBV	623609	735444	9.53%	1.456%
27	15.348	1201	1204	1207	rVB	44005	79435	1.03%	0.157%
28	15.474	1213	1215	1221	rVB	57534	81653	1.06%	0.162%
29	15.828	1243	1246	1249	rBV	56517	103198	1.34%	0.204%
30	16.400	1291	1296	1300	rVB2	49800	141345	1.83%	0.280%
31	17.085	1352	1356	1362	rVB2	36821	107010	1.39%	0.212%
32	17.943	1426	1431	1437	rVB3	20253	79106	1.03%	0.157%

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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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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-BF051716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

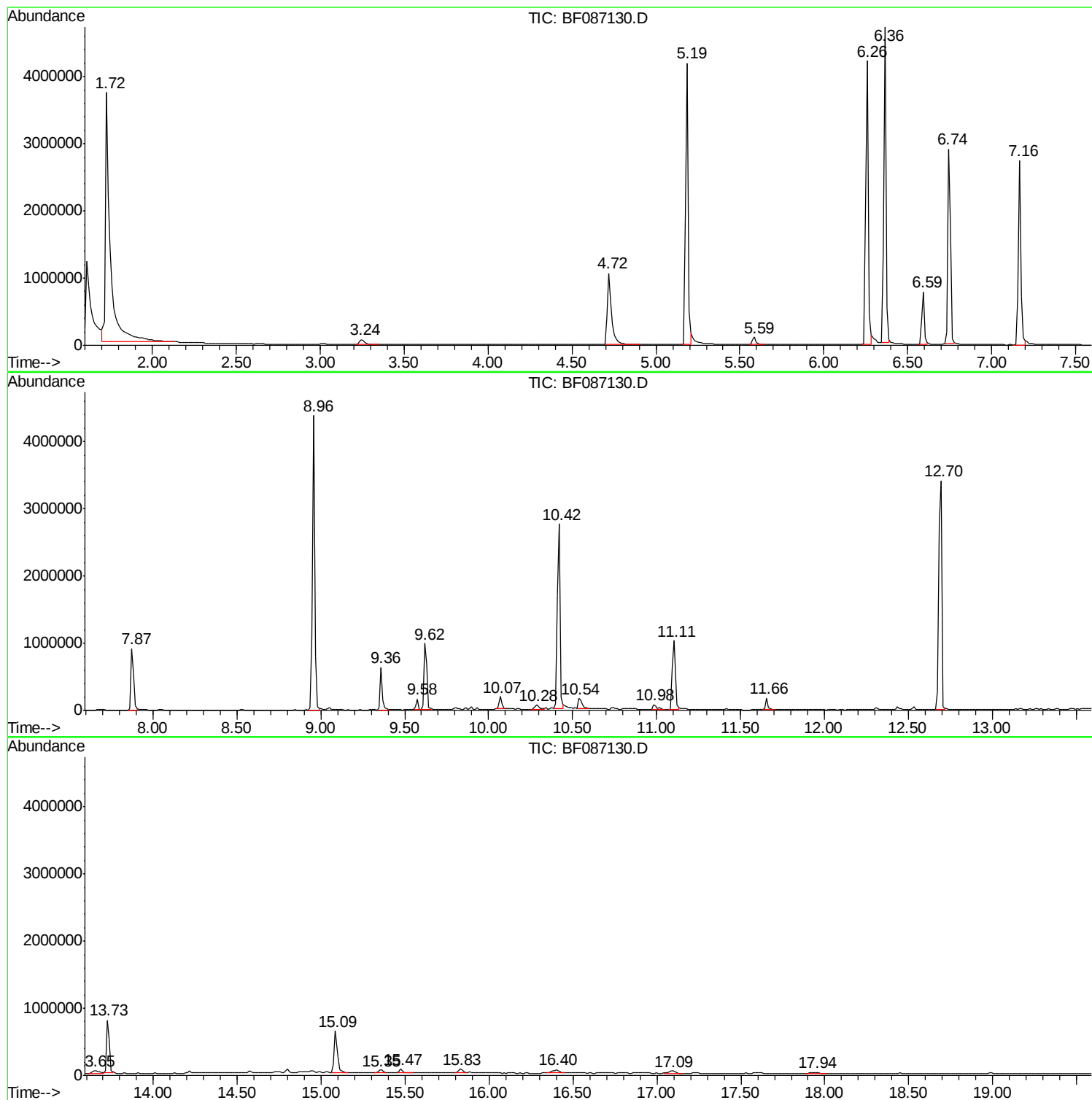
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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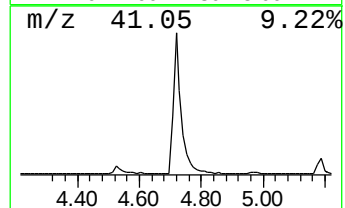
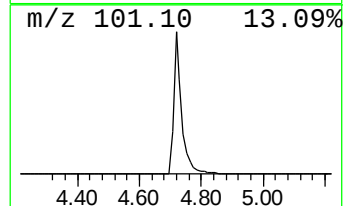
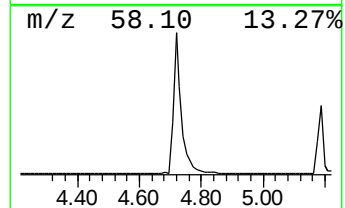
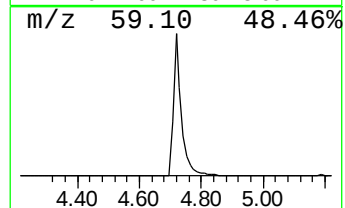
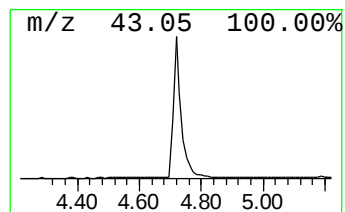
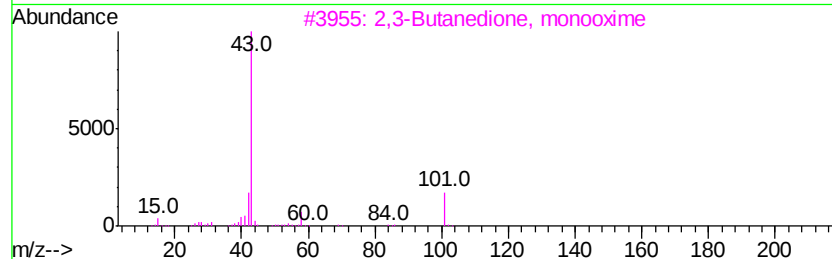
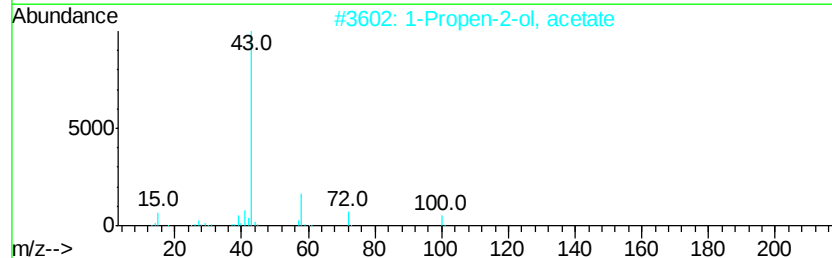
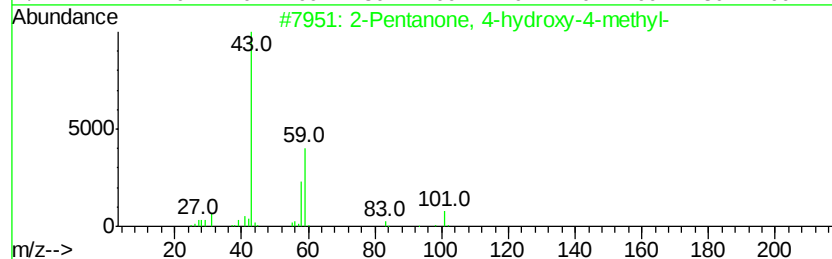
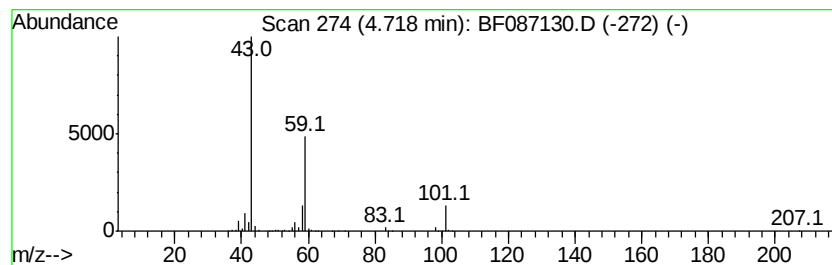
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	44.39 ng	1903980	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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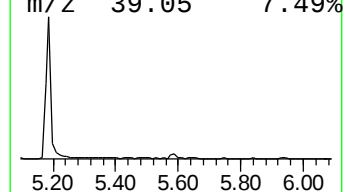
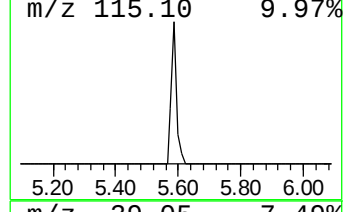
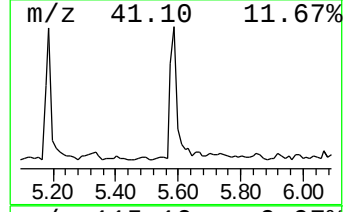
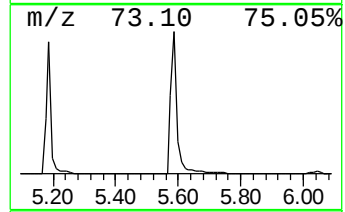
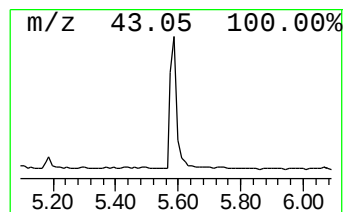
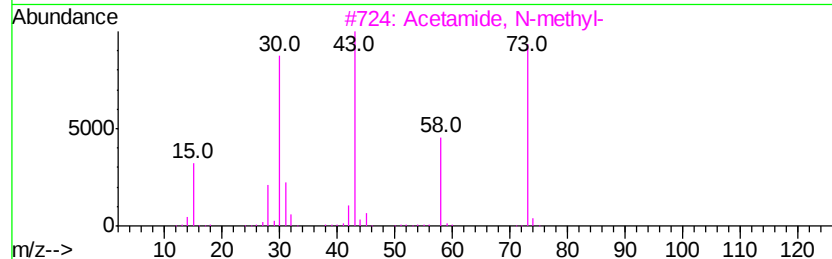
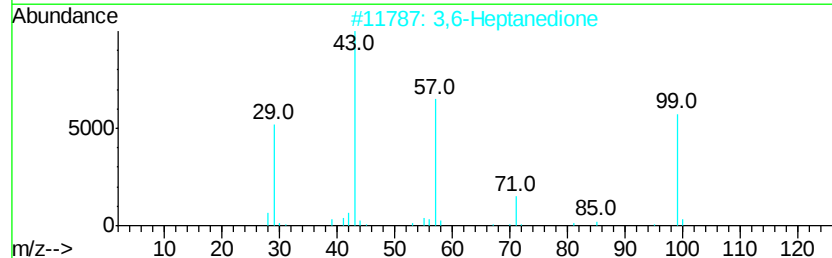
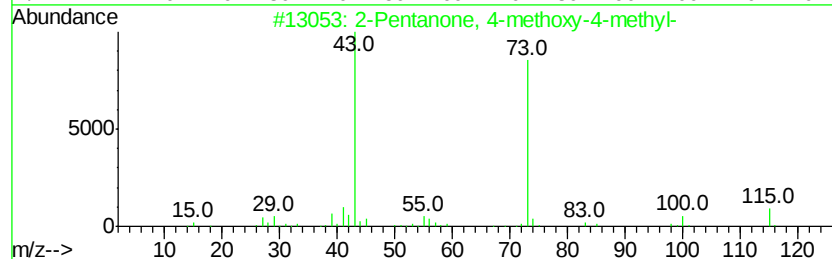
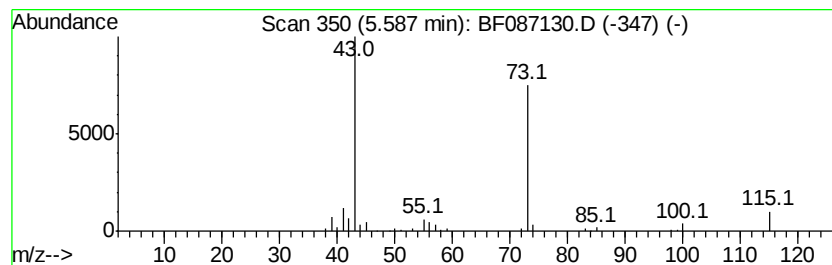
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	3.45 ng	148094	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			3,6-Heptanedione	128	C7H12O2	001703-51-1	23
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
5			N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12



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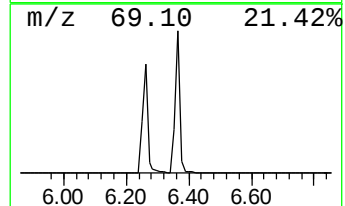
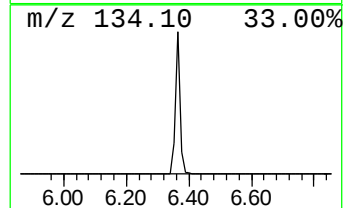
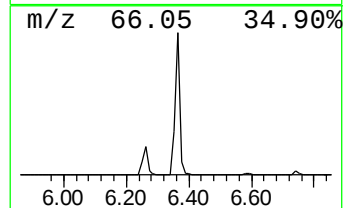
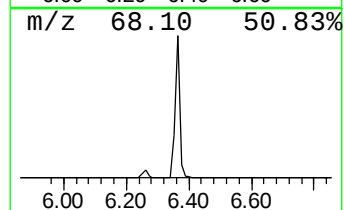
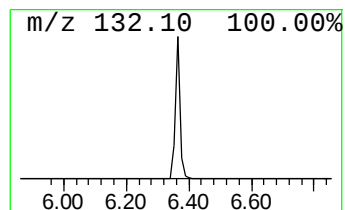
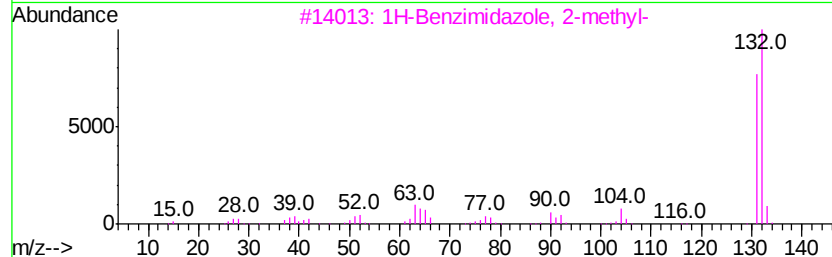
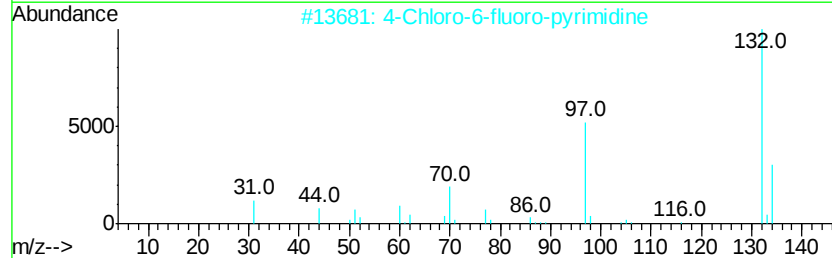
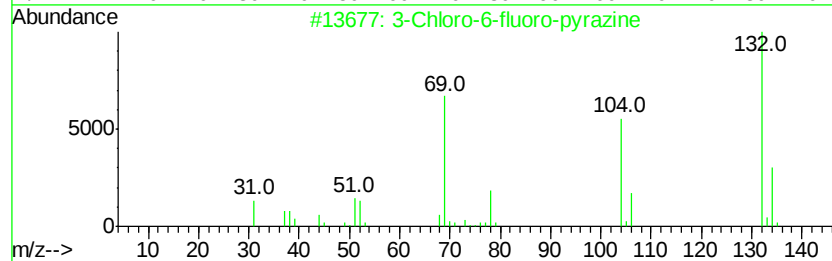
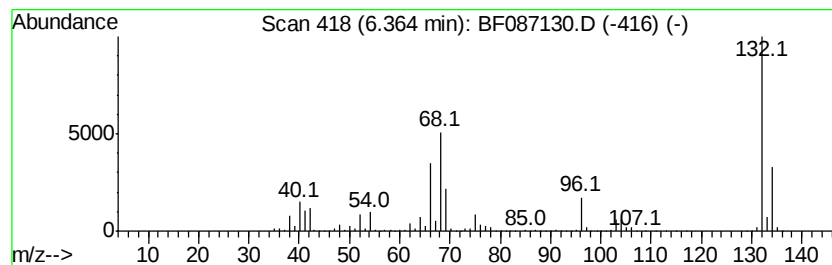
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	105.45 ng	4523140	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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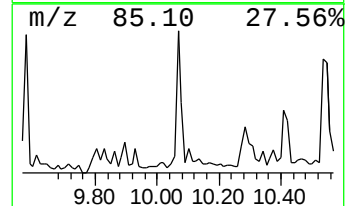
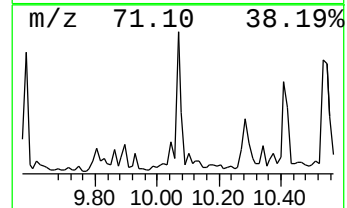
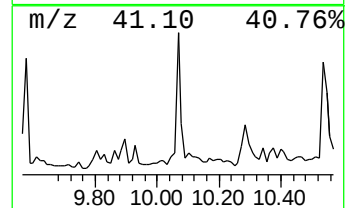
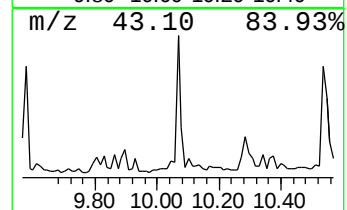
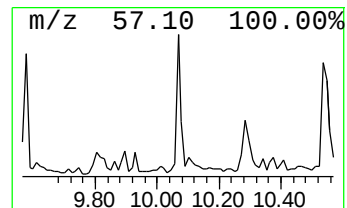
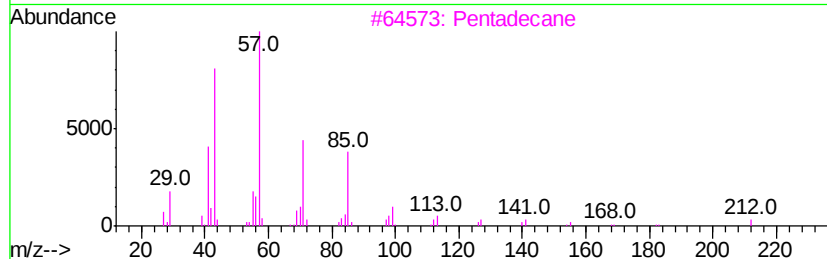
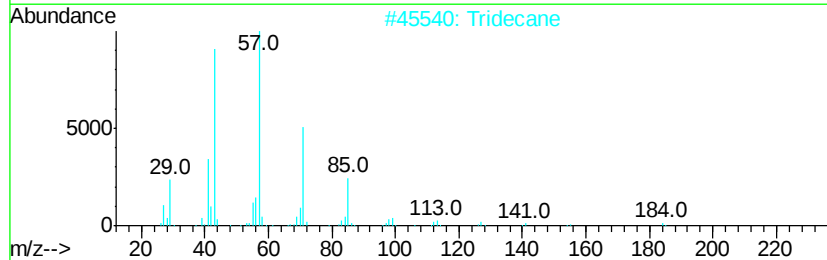
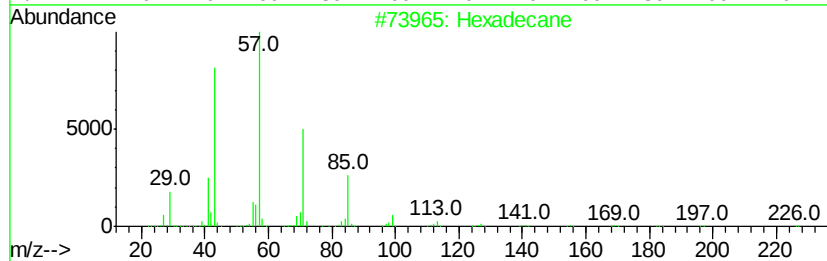
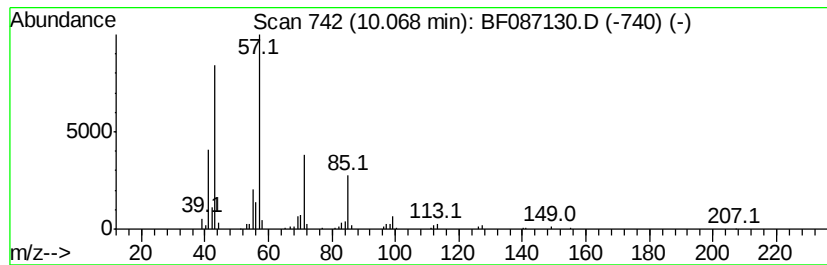
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.07	2.88 ng	173353	Acenaphthene-d10	9.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Tridecane	184 C13H28	000629-50-5	90
3	Pentadecane	212 C15H32	000629-62-9	86
4	Octadecane	254 C18H38	000593-45-3	86
5	Silane, trichlorooctadecyl-	386 C18H37Cl3Si	000112-04-9	86



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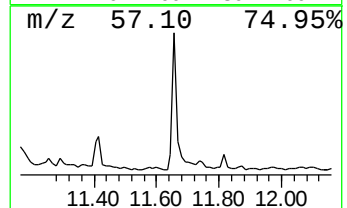
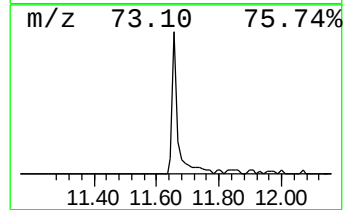
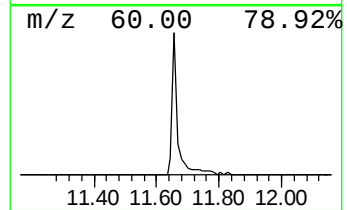
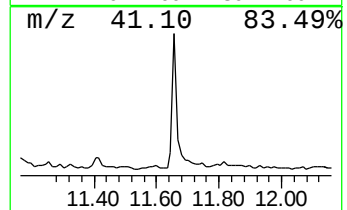
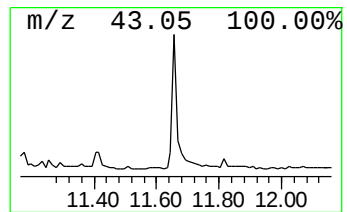
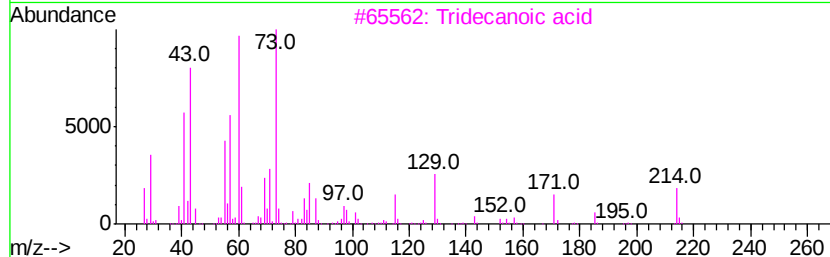
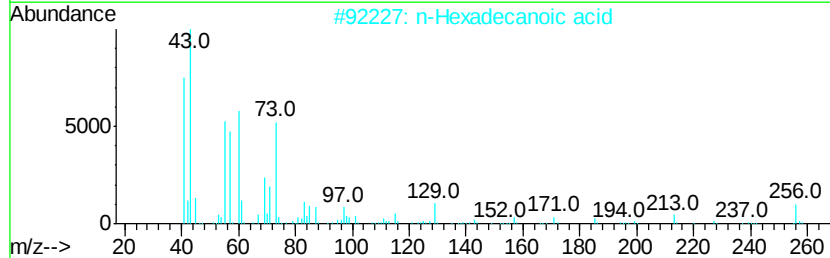
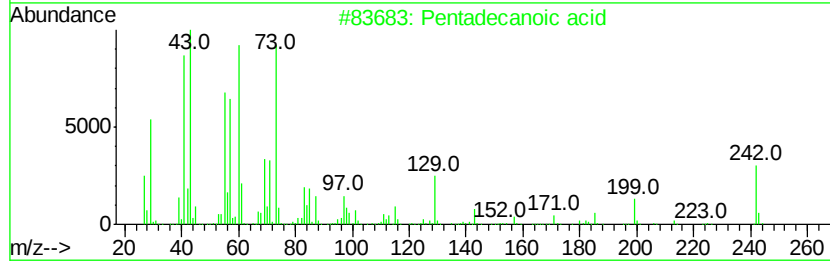
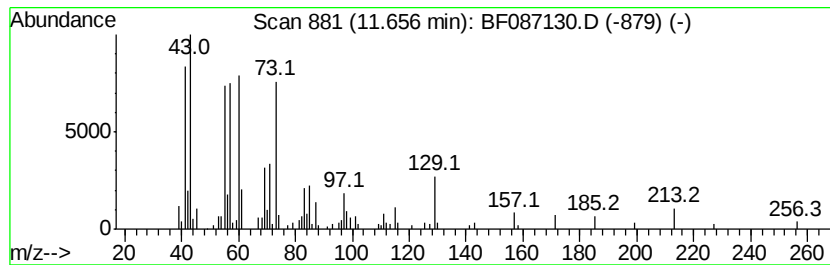
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 9 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.13 ng	187105	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Undecanoic acid	186	C11H22O2	000112-37-8	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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ALS Vial : 32 Sample Multiplier: 1

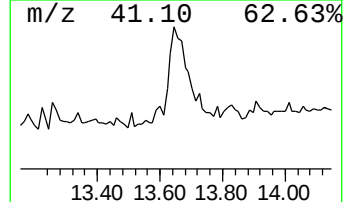
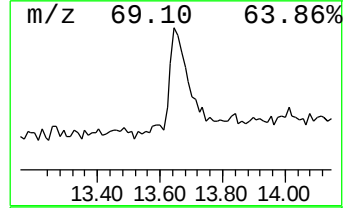
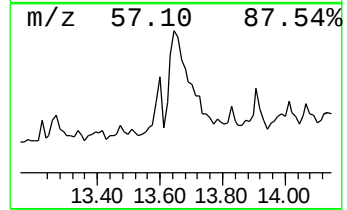
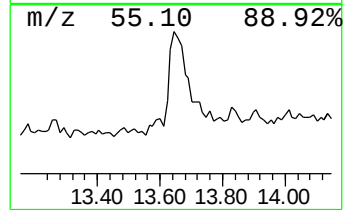
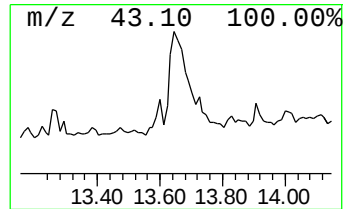
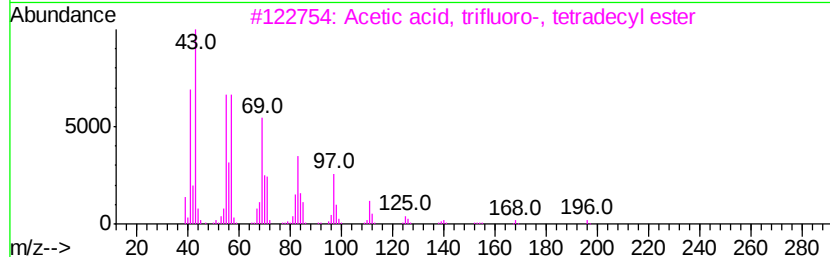
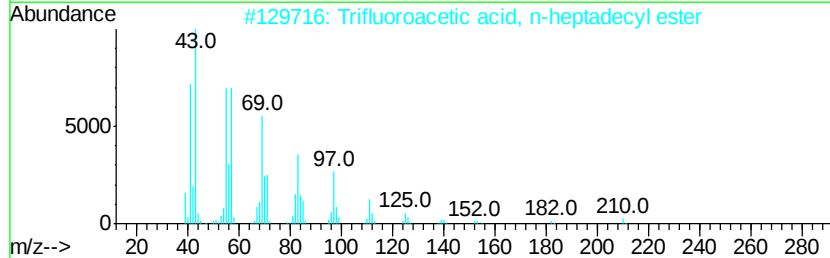
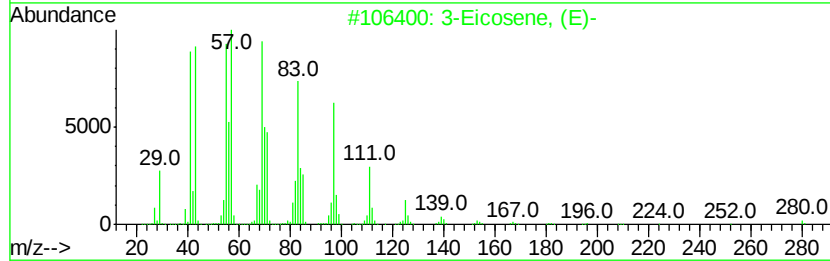
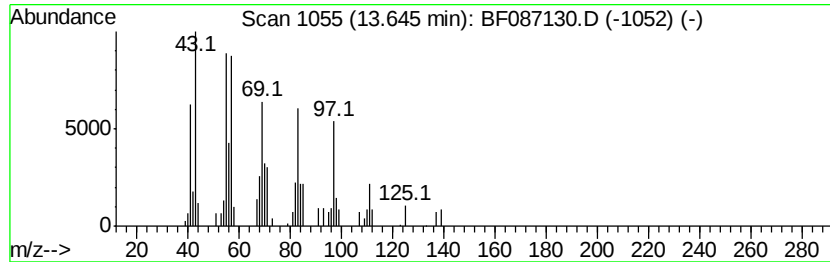
Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-13K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.65	3.57 ng	164267	Chrysene-d12	13.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
3	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-13K

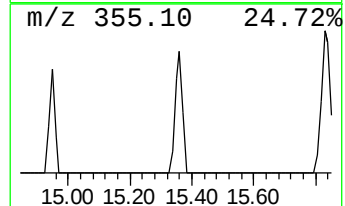
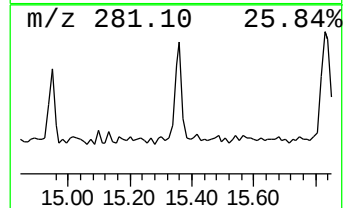
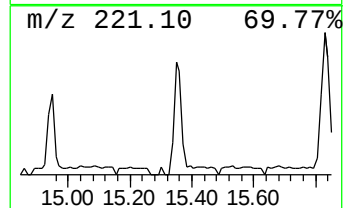
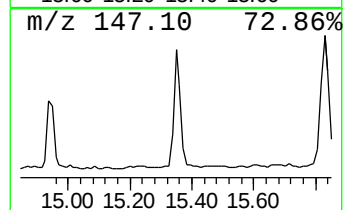
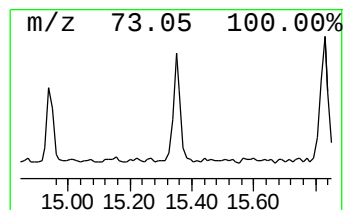
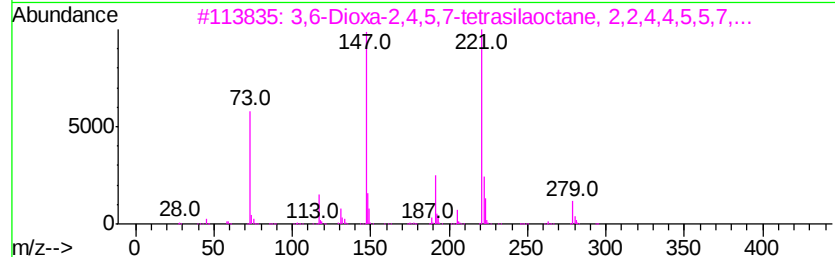
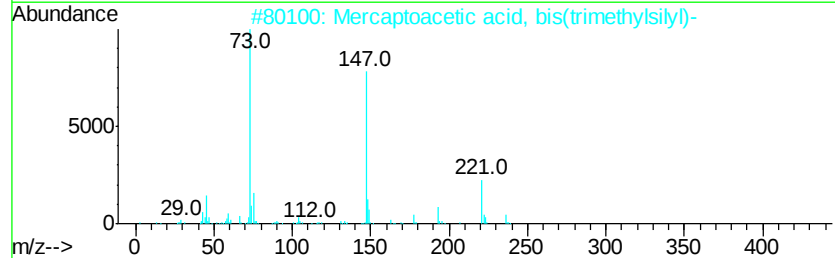
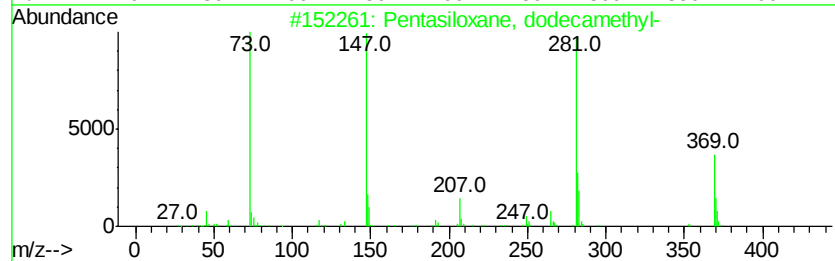
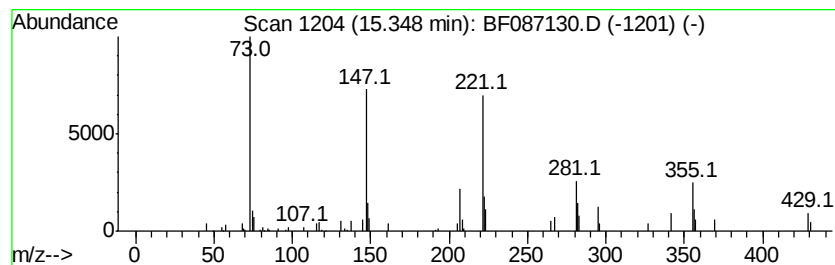
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.35 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	2.16 ng	79435	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27
2		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	25
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
4		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	12
5		2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	12



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
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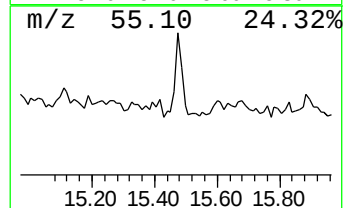
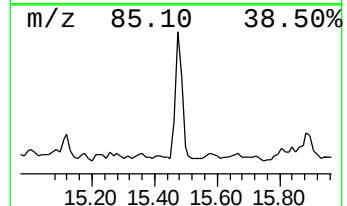
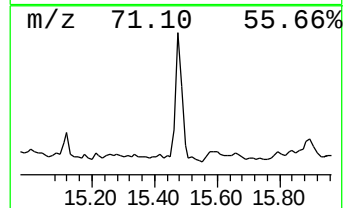
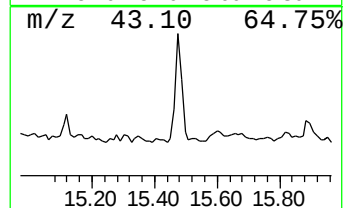
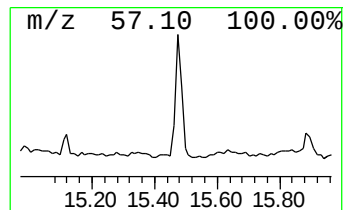
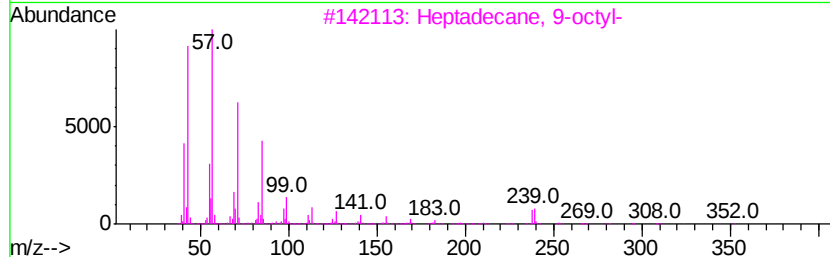
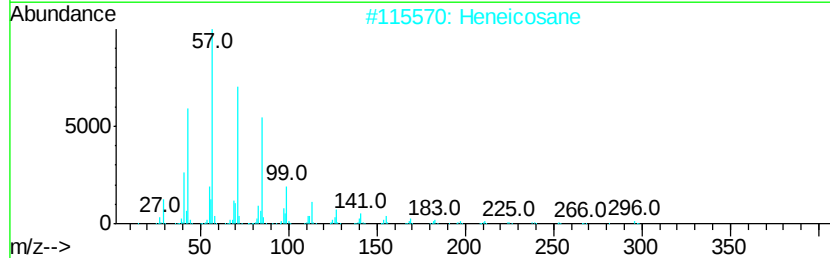
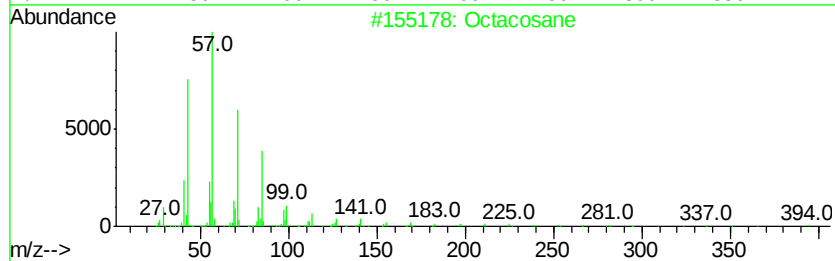
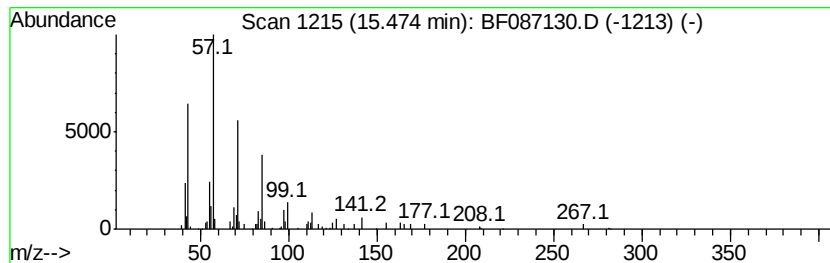
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ClientSampleId :
VITALE-FILL-CSPH3-13K

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.		
15.47	2.22 ng	81653	Perylene-d12		15.09		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VITALE-FILL-CSPH3-13K

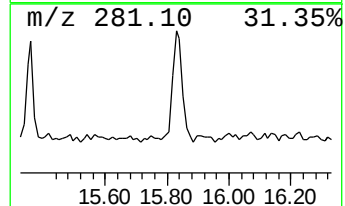
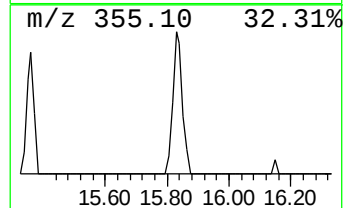
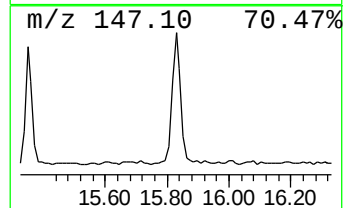
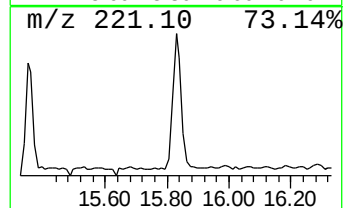
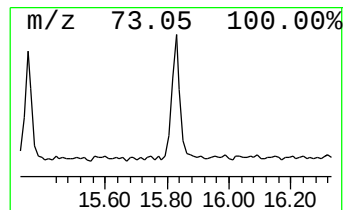
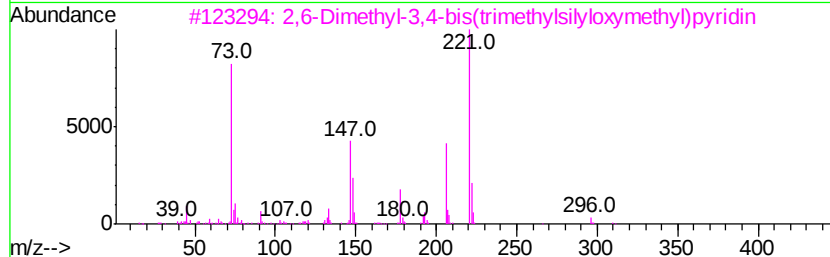
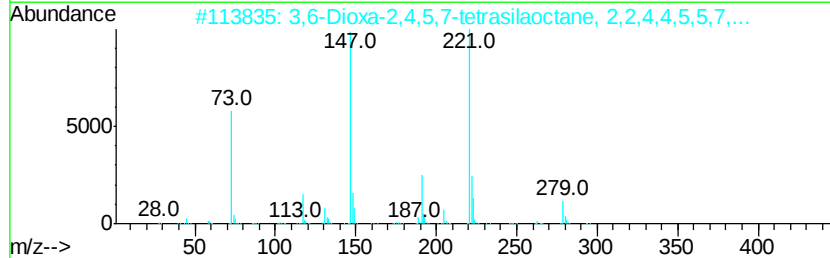
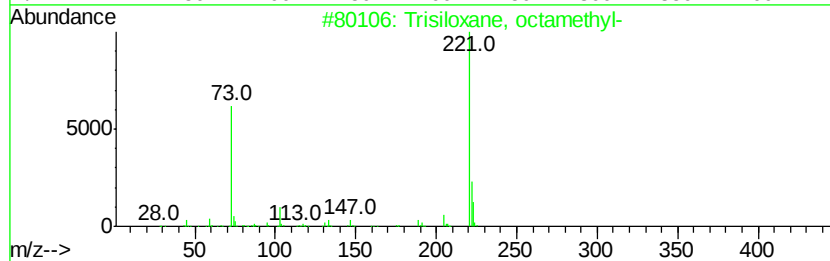
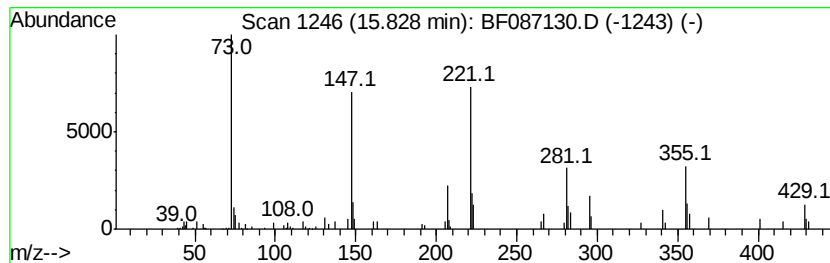
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown15.83 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.81 ng	103198	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	35
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	28
3		2,6-Dimethyl-3,4-bis(trimethylsilyl)...	311	C15H29N02Si2	1000079-52-1	23
4		2(3H)-Thiazolethione, 3-ethyl-4-...	221	C11H11NS2	055976-02-8	16
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VITALE-FILL-CSPH3-13K

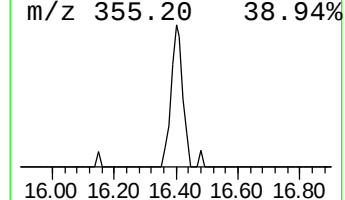
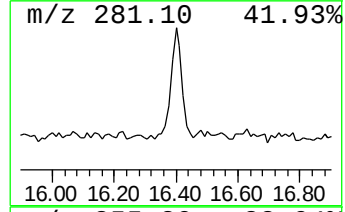
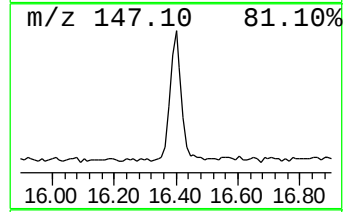
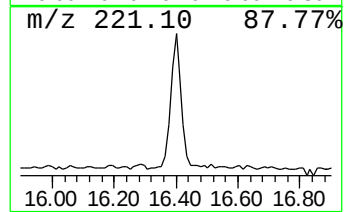
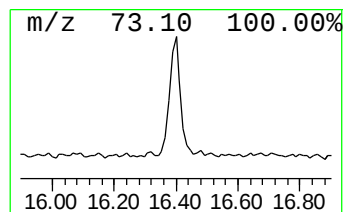
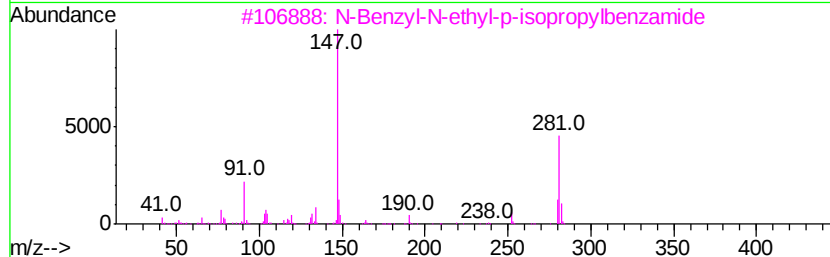
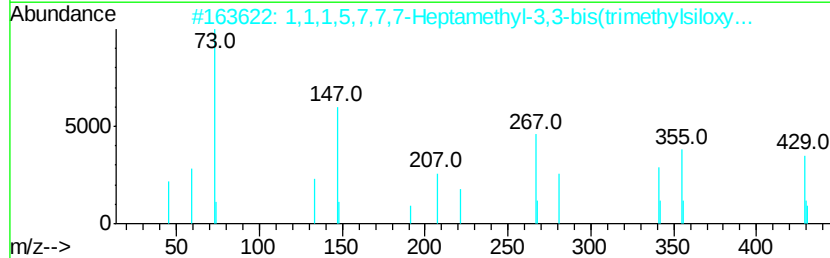
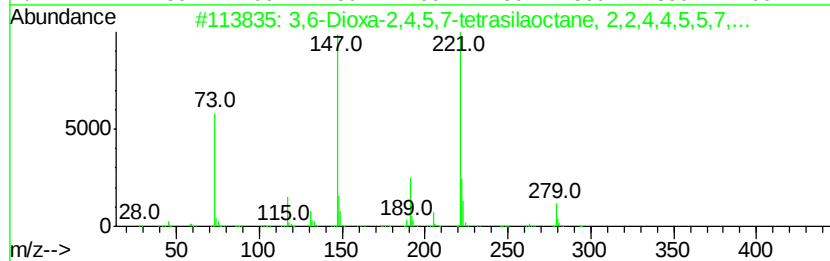
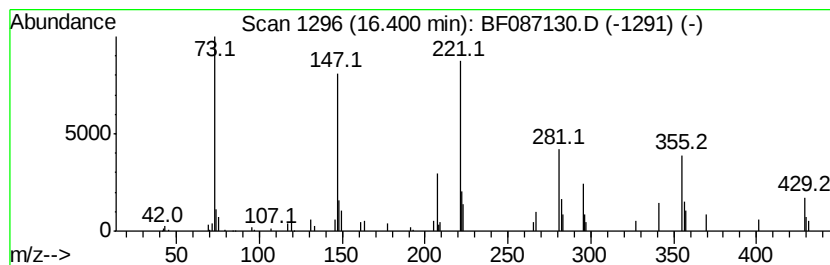
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown16.40 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	3.84 ng	141345	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
2			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	37
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VITALE-FILL-CSPH3-13K

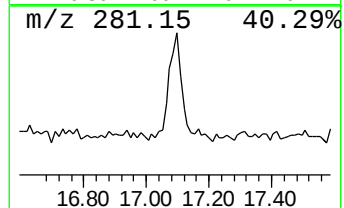
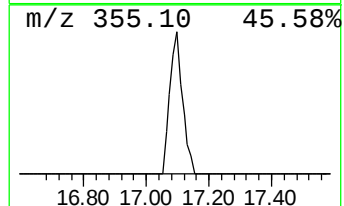
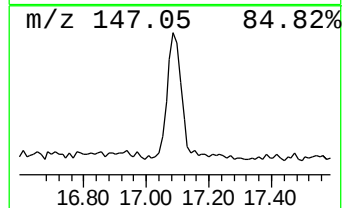
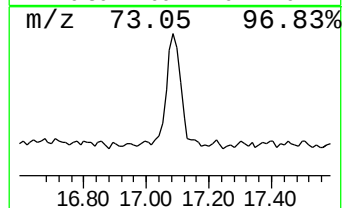
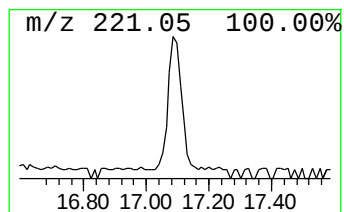
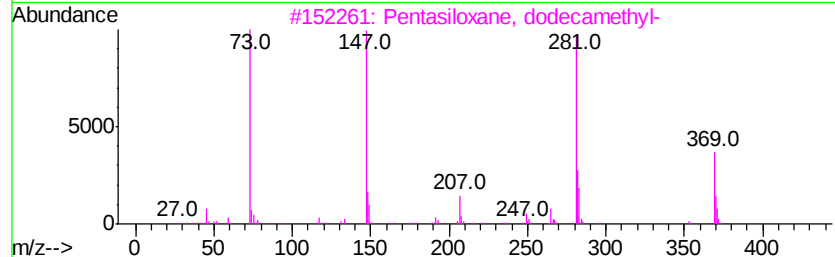
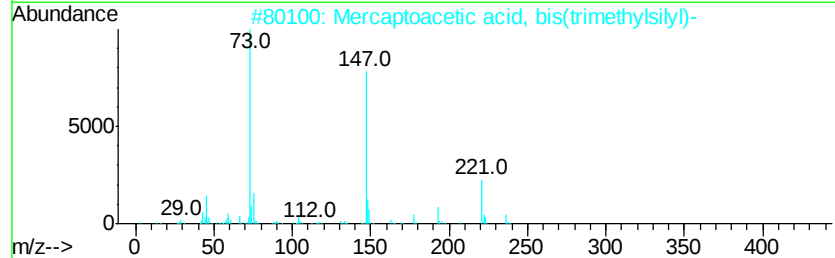
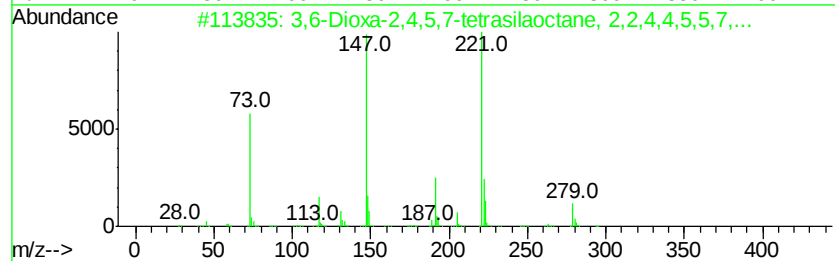
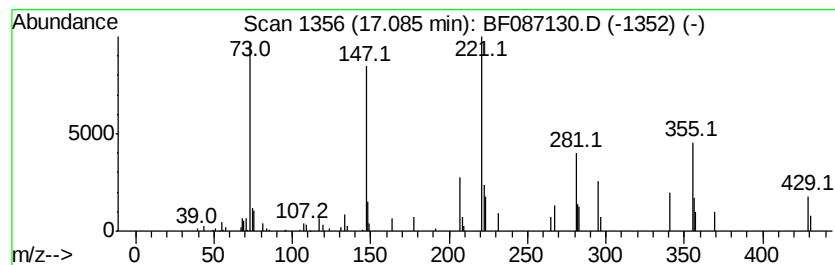
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown17.09 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	2.91 ng	107010	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	43
2		Mercaptoacetic acid, bis(trimeth...	236	C8H2002SSi2	006398-62-5	37
3		Pentasiloxane, dodecamethyl-	384	C12H3604Si5	000141-63-9	27
4		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H3604Si5	003555-47-3	27
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

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ClientSampleId :
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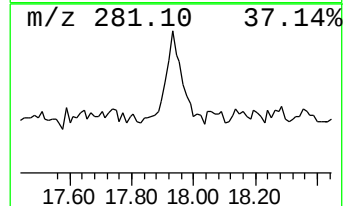
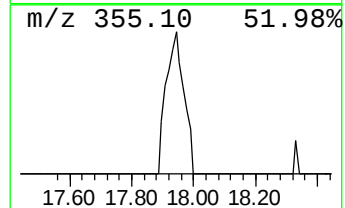
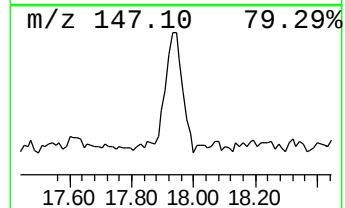
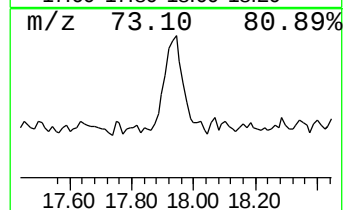
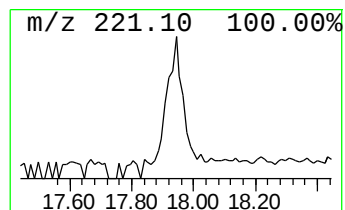
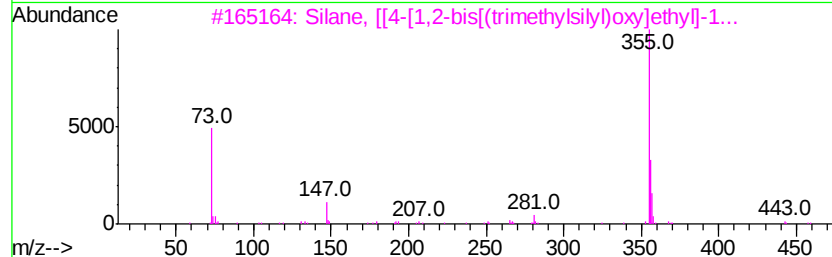
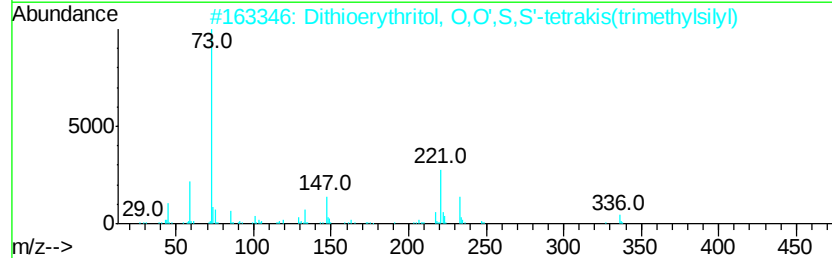
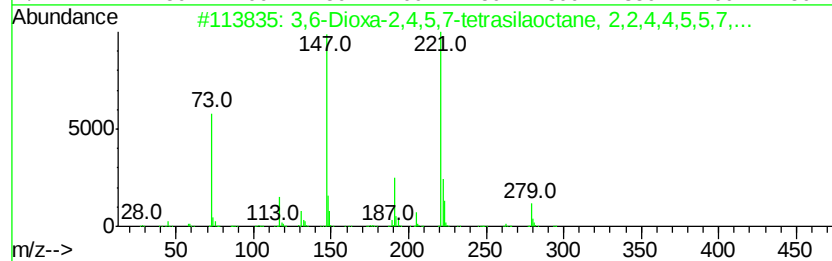
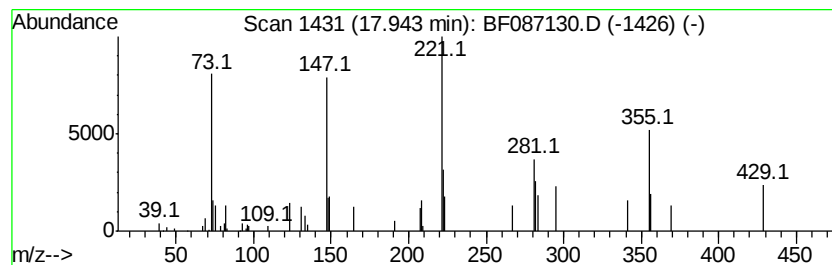
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown17.94 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	2.15 ng	79106	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	37
2			Dithioerythritol, 0,0',S,S'-tetr...	442	C16H4202S2Si4	1000079-30-7	25
3			Silane, [[4-[1,2-bis[(trimethyls...	458	C20H4204Si4	056114-62-6	25
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H3604Si5	003555-47-3	22
5			1,1,1,3,5,5,7,7,7-Nonamethyl-3-(...	384	C12H3604Si5	038146-99-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087130.D
Acq On : 18 May 2016 4:44
Operator : UM/SJ
Sample : H3085-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-13K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.72	44.4	ng	1903980	1	6.59	857856	20.0
2-Pentanone, 4-me...	5.59	3.5	ng	148094	1	6.59	857856	20.0
unknown6.36	6.36	105.5	ng	4523140	1	6.59	857856	20.0
Hexadecane	10.07	2.9	ng	173353	3	9.62	1204830	20.0
Pentadecanoic acid	11.66	3.1	ng	187105	4	11.11	1194700	20.0
3-Eicosene, (E)-	13.65	3.6	ng	164267	5	13.73	920141	20.0
unknown15.35	15.35	2.2	ng	79435	6	15.09	735444	20.0
Octacosane	15.47	2.2	ng	81653	6	15.09	735444	20.0
unknown15.83	15.83	2.8	ng	103198	6	15.09	735444	20.0
unknown16.40	16.40	3.8	ng	141345	6	15.09	735444	20.0
unknown17.09	17.09	2.9	ng	107010	6	15.09	735444	20.0
unknown17.94	17.94	2.1	ng	79106	6	15.09	735444	20.0