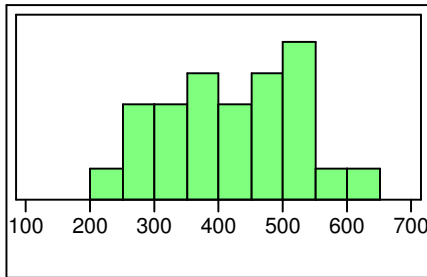


**C_thrombin
training set**

**Distributions
weight**



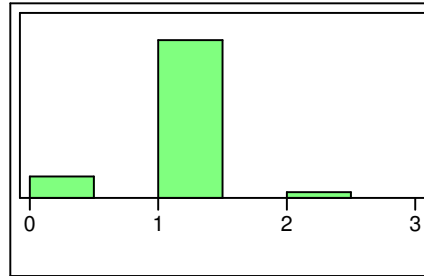
Quantiles

100.0%	maximum	614,80
99.5%		614,80
97.5%		614,80
90.0%		540,25
75.0%	quartile	504,14
50.0%	median	429,51
25.0%	quartile	328,88
10.0%		253,87
2.5%		209,25
0.5%		209,25
0.0%	minimum	209,25

Moments

Mean	415,80422
Std Dev	108,00678
Std Err Mean	21,601357
upper 95% Mean	460,38723
lower 95% Mean	371,22121
N	25

netcharge



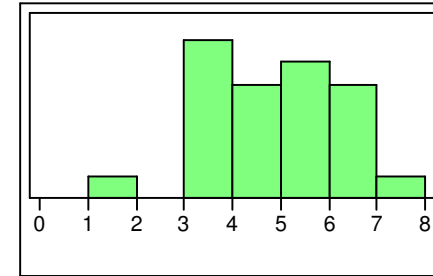
Quantiles

100.0%	maximum	2,0000
99.5%		2,0000
97.5%		2,0000
90.0%		1,0000
75.0%	quartile	1,0000
50.0%	median	1,0000
25.0%	quartile	1,0000
10.0%		0,0000
2.5%		0,0000
0.5%		0,0000
0.0%	minimum	0,0000

Moments

Mean	0,92
Std Dev	0,4
Std Err Mean	0,08
upper 95% Mean	1,0851119
lower 95% Mean	0,7548881
N	25

acceptors



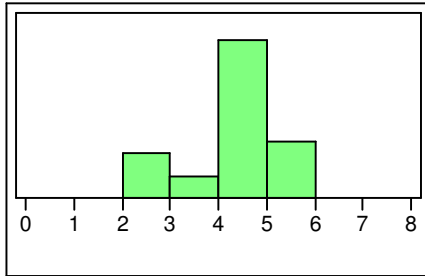
Quantiles

100.0%	maximum	7,0000
99.5%		7,0000
97.5%		7,0000
90.0%		6,0000
75.0%	quartile	5,5000
50.0%	median	4,0000
25.0%	quartile	3,0000
10.0%		3,0000
2.5%		1,0000
0.5%		1,0000
0.0%	minimum	1,0000

Moments

Mean	4,36
Std Dev	1,4106736
Std Err Mean	0,2821347
upper 95% Mean	4,9422974
lower 95% Mean	3,7777026
N	25

donors



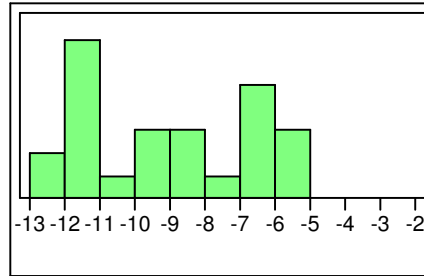
Quantiles

100.0%	maximum	5,0000
99.5%		5,0000
97.5%		5,0000
90.0%		5,0000
75.0%	quartile	4,0000
50.0%	median	4,0000
25.0%	quartile	3,5000
10.0%		2,0000
2.5%		2,0000
0.5%		2,0000
0.0%	minimum	2,0000

Moments

Mean	3,8
Std Dev	0,9574271
Std Err Mean	0,1914854
upper 95% Mean	4,1952065
lower 95% Mean	3,4047935
N	25

thrombin_exper



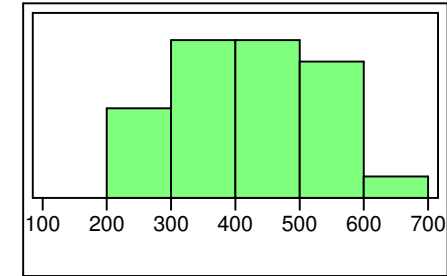
Quantiles

100.0%	maximum	-5,55
99.5%		-5,55
97.5%		-5,55
90.0%		-5,85
75.0%	quartile	-6,79
50.0%	median	-9,31
25.0%	quartile	-11,45
10.0%		-12,08
2.5%		-12,45
0.5%		-12,45
0.0%	minimum	-12,45

Moments

Mean	-9,122232
Std Dev	2,3496085
Std Err Mean	0,4699217
upper 95% Mean	-8,152362
lower 95% Mean	-10,0921
N	25

weight_CDK



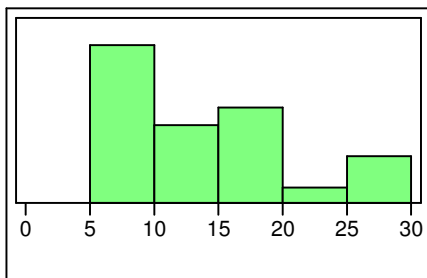
Quantiles

100.0%	maximum	614,26
99.5%		614,26
97.5%		614,26
90.0%		540,46
75.0%	quartile	504,25
50.0%	median	429,24
25.0%	quartile	328,64
10.0%		253,71
2.5%		210,10
0.5%		210,10
0.0%	minimum	210,10

Moments

Mean	415,70998
Std Dev	107,97955
Std Err Mean	21,595909
upper 95% Mean	460,28175
lower 95% Mean	371,13821
N	25

largestPiSystem



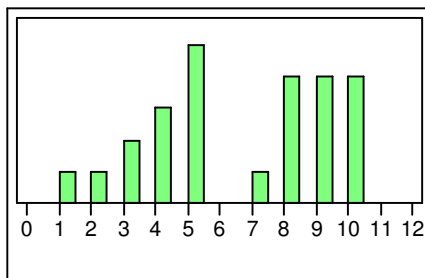
Quantiles

100.0%	maximum	25,000
99.5%		25,000
97.5%		25,000
90.0%		25,000
75.0%	quartile	19,000
50.0%	median	14,000
25.0%	quartile	7,000
10.0%		6,000
2.5%		5,000
0.5%		5,000
0.0%	minimum	5,000

Moments

Mean	13,2
Std Dev	6,5064071
Std Err Mean	1,3012814
upper 95% Mean	15,885713
lower 95% Mean	10,514287
N	25

hBondacceptors



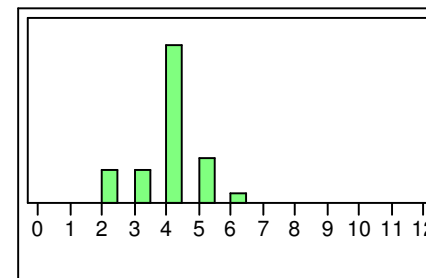
Quantiles

100.0%	maximum	10,000
99.5%		10,000
97.5%		10,000
90.0%		10,000
75.0%	quartile	9,000
50.0%	median	7,000
25.0%	quartile	4,000
10.0%		2,600
2.5%		1,000
0.5%		1,000
0.0%	minimum	1,000

Moments

Mean	6,44
Std Dev	2,8
Std Err Mean	0,56
upper 95% Mean	7,5957832
lower 95% Mean	5,2842168
N	25

hBondDonors



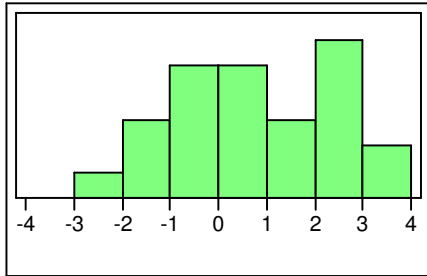
Quantiles

100.0%	maximum	6,0000
99.5%		6,0000
97.5%		6,0000
90.0%		5,0000
75.0%	quartile	4,0000
50.0%	median	4,0000
25.0%	quartile	3,5000
10.0%		2,0000
2.5%		2,0000
0.5%		2,0000
0.0%	minimum	2,0000

Moments

Mean	3,88
Std Dev	0,9712535
Std Err Mean	0,1942507
upper 95% Mean	4,2809137
lower 95% Mean	3,4790863
N	25

xlogP



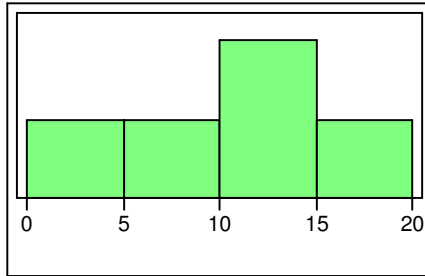
Quantiles

100.0%	maximum	3,745
99.5%		3,745
97.5%		3,745
90.0%		2,966
75.0%	quartile	2,216
50.0%	median	0,634
25.0%	quartile	-0,292
10.0%		-1,488
2.5%		-2,710
0.5%		-2,710
0.0%	minimum	-2,710

Moments

Mean	0,83732
Std Dev	1,6444489
Std Err Mean	0,3288898
upper 95% Mean	1,5161151
lower 95% Mean	0,1585249
N	25

rotatableBondsCount



Quantiles

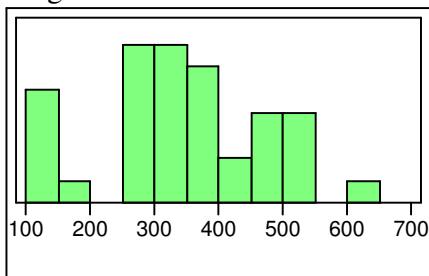
100.0%	maximum	18,000
99.5%		18,000
97.5%		18,000
90.0%		16,400
75.0%	quartile	14,000
50.0%	median	11,000
25.0%	quartile	5,000
10.0%		3,200
2.5%		2,000
0.5%		2,000
0.0%	minimum	2,000

Moments

Mean	9,92
Std Dev	4,9406477
Std Err Mean	0,9881295
upper 95% Mean	11,959399
lower 95% Mean	7,8806009
N	25

B_trypsin
training set

Distributions
weight



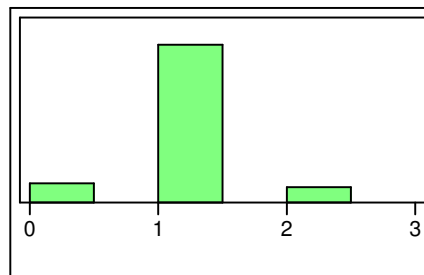
Quantiles

100.0%	maximum	601,71
99.5%		601,71
97.5%		601,71
90.0%		511,42
75.0%	quartile	453,55
50.0%	median	346,20
25.0%	quartile	254,27
10.0%		125,36
2.5%		108,16
0.5%		108,16
0.0%	minimum	108,16

Moments

Mean	341,45241
Std Dev	129,48485
Std Err Mean	21,287179
upper 95% Mean	384,62481
lower 95% Mean	298,28001
N	37

netcharge



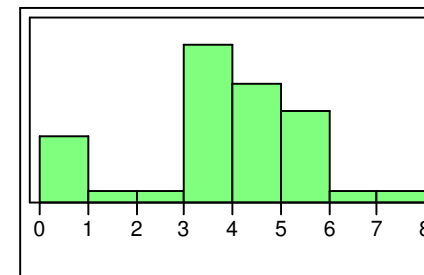
Quantiles

100.0%	maximum	2,0000
99.5%		2,0000
97.5%		2,0000
90.0%		1,2000
75.0%	quartile	1,0000
50.0%	median	1,0000
25.0%	quartile	1,0000
10.0%		0,0000
2.5%		0,0000
0.5%		0,0000
0.0%	minimum	0,0000

Moments

Mean	0,972973
Std Dev	0,4401065
Std Err Mean	0,0723531
upper 95% Mean	1,1197118
lower 95% Mean	0,8262342
N	37

acceptors



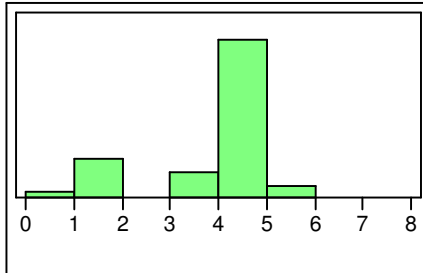
Quantiles

100.0%	maximum	7,0000
99.5%		7,0000
97.5%		7,0000
90.0%		5,0000
75.0%	quartile	4,5000
50.0%	median	3,0000
25.0%	quartile	3,0000
10.0%		0,0000
2.5%		0,0000
0.5%		0,0000
0.0%	minimum	0,0000

Moments

Mean	3,3243243
Std Dev	1,7329175
Std Err Mean	0,2848899
upper 95% Mean	3,9021078
lower 95% Mean	2,7465409
N	37

donors



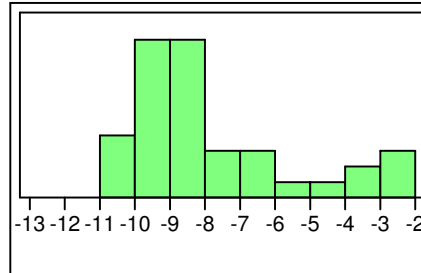
Quantiles

100.0%	maximum	5,0000
99.5%		5,0000
97.5%		5,0000
90.0%		4,0000
75.0%	quartile	4,0000
50.0%	median	4,0000
25.0%	quartile	3,0000
10.0%		1,0000
2.5%		0,0000
0.5%		0,0000
0.0%	minimum	0,0000

Moments

Mean	3,3513514
Std Dev	1,2956383
Std Err Mean	0,2130016
upper 95% Mean	3,7833387
lower 95% Mean	2,919364
N	37

trypsin_exper



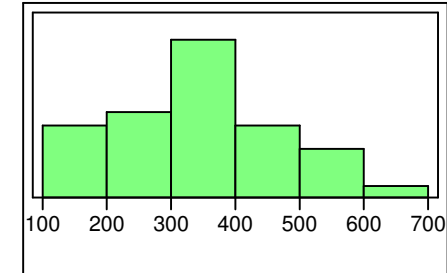
Quantiles

100.0%	maximum	-2,30
99.5%		-2,30
97.5%		-2,30
90.0%		-3,59
75.0%	quartile	-6,59
50.0%	median	-8,41
25.0%	quartile	-9,54
10.0%		-10,11
2.5%		-10,71
0.5%		-10,71
0.0%	minimum	-10,71

Moments

Mean	-7,807631
Std Dev	2,3617876
Std Err Mean	0,3882755
upper 95% Mean	-7,020172
lower 95% Mean	-8,595091
N	37

weight_CDK



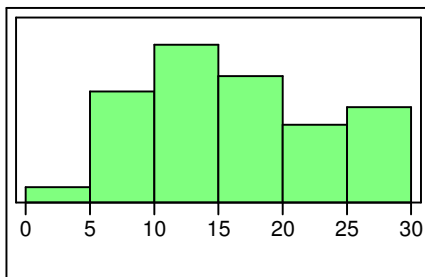
Quantiles

100.0%	maximum	601,26
99.5%		601,26
97.5%		601,26
90.0%		511,00
75.0%	quartile	453,17
50.0%	median	345,04
25.0%	quartile	254,10
10.0%		125,28
2.5%		108,08
0.5%		108,08
0.0%	minimum	108,08

Moments

Mean	341,09054
Std Dev	129,35869
Std Err Mean	21,266438
upper 95% Mean	384,22088
lower 95% Mean	297,96021
N	37

largestPiSystem



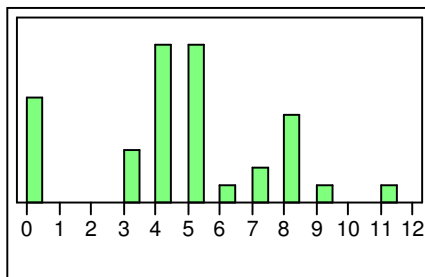
Quantiles

100.0%	maximum	26,000
99.5%		26,000
97.5%		26,000
90.0%		25,000
75.0%	quartile	20,000
50.0%	median	15,000
25.0%	quartile	11,500
10.0%		6,000
2.5%		0,000
0.5%		0,000
0.0%	minimum	0,000

Moments

Mean	15,540541
Std Dev	6,8377815
Std Err Mean	1,1241243
upper 95% Mean	17,82037
lower 95% Mean	13,260711
N	37

hBondacceptors



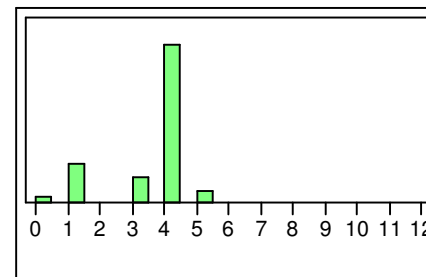
Quantiles

100.0%	maximum	11,000
99.5%		11,000
97.5%		11,000
90.0%		8,000
75.0%	quartile	6,500
50.0%	median	5,000
25.0%	quartile	3,500
10.0%		0,000
2.5%		0,000
0.5%		0,000
0.0%	minimum	0,000

Moments

Mean	4,5945946
Std Dev	2,7432691
Std Err Mean	0,4509907
upper 95% Mean	5,5092461
lower 95% Mean	3,6799431
N	37

hBondDonors



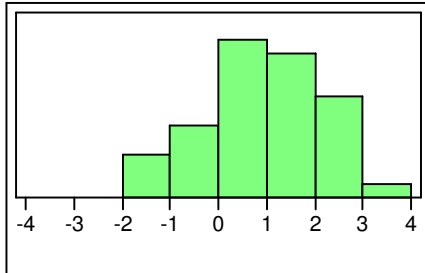
Quantiles

100.0%	maximum	5,0000
99.5%		5,0000
97.5%		5,0000
90.0%		4,0000
75.0%	quartile	4,0000
50.0%	median	4,0000
25.0%	quartile	3,0000
10.0%		1,0000
2.5%		0,0000
0.5%		0,0000
0.0%	minimum	0,0000

Moments

Mean	3,3513514
Std Dev	1,2956383
Std Err Mean	0,2130016
upper 95% Mean	3,7833387
lower 95% Mean	2,919364
N	37

xlogP



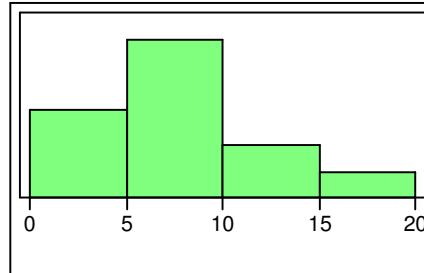
Quantiles

100.0%	maximum	3,196
99.5%		3,196
97.5%		3,196
90.0%		2,752
75.0%	quartile	1,879
50.0%	median	0,994
25.0%	quartile	0,273
10.0%		-0,996
2.5%		-1,882
0.5%		-1,882
0.0%	minimum	-1,882

Moments

Mean	1,0060541
Std Dev	1,2543043
Std Err Mean	0,2062063
upper 95% Mean	1,4242599
lower 95% Mean	0,5878482
N	37

rotatableBondsCount



Quantiles

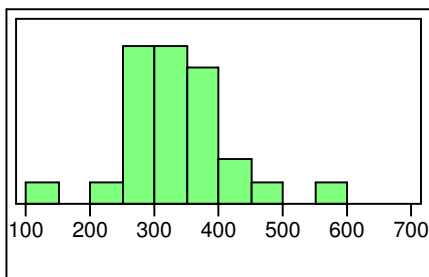
100.0%	maximum	19,000
99.5%		19,000
97.5%		19,000
90.0%		12,600
75.0%	quartile	9,500
50.0%	median	6,000
25.0%	quartile	4,000
10.0%		2,000
2.5%		2,000
0.5%		2,000
0.0%	minimum	2,000

Moments

Mean	7,1351351
Std Dev	4,0425663
Std Err Mean	0,6645938
upper 95% Mean	8,4829938
lower 95% Mean	5,7872764
N	37

A_urokinase
training set

**Distributions
weight**



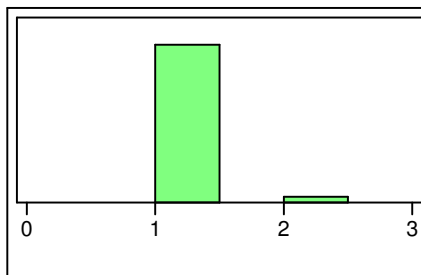
Quantiles

100.0%	maximum	554,64
99.5%		554,64
97.5%		554,64
90.0%		457,52
75.0%	quartile	383,95
50.0%	median	333,39
25.0%	quartile	278,56
10.0%		246,49
2.5%		121,16
0.5%		121,16
0.0%	minimum	121,16

Moments

Mean	335,68962
Std Dev	87,581293
Std Err Mean	17,176105
upper 95% Mean	371,06447
lower 95% Mean	300,31477
N	26

netcharge



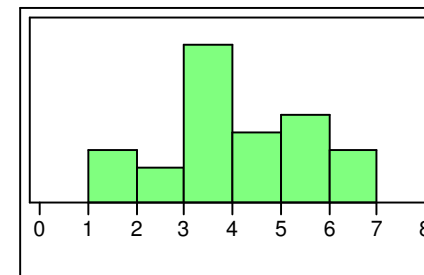
Quantiles

100.0%	maximum	2,0000
99.5%		2,0000
97.5%		2,0000
90.0%		1,0000
75.0%	quartile	1,0000
50.0%	median	1,0000
25.0%	quartile	1,0000
10.0%		1,0000
2.5%		1,0000
0.5%		1,0000
0.0%	minimum	1,0000

Moments

Mean	1,0384615
Std Dev	0,1961161
Std Err Mean	0,0384615
upper 95% Mean	1,1176746
lower 95% Mean	0,9592485
N	26

acceptors



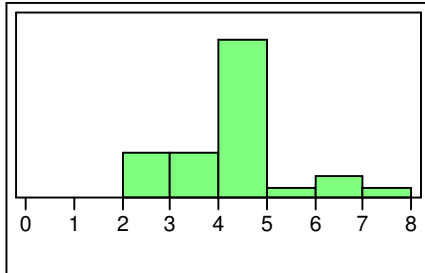
Quantiles

100.0%	maximum	6,0000
99.5%		6,0000
97.5%		6,0000
90.0%		6,0000
75.0%	quartile	5,0000
50.0%	median	3,0000
25.0%	quartile	3,0000
10.0%		1,0000
2.5%		1,0000
0.5%		1,0000
0.0%	minimum	1,0000

Moments

Mean	3,5769231
Std Dev	1,5012815
Std Err Mean	0,2944255
upper 95% Mean	4,1833038
lower 95% Mean	2,9705424
N	26

donors



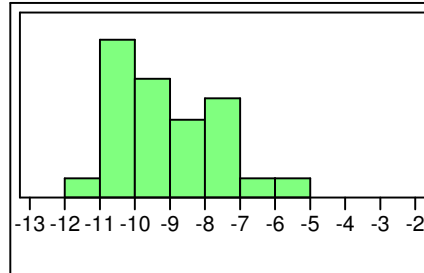
Quantiles

100.0%	maximum	7,0000
99.5%		7,0000
97.5%		7,0000
90.0%		6,0000
75.0%	quartile	4,0000
50.0%	median	4,0000
25.0%	quartile	3,0000
10.0%		2,0000
2.5%		2,0000
0.5%		2,0000
0.0%	minimum	2,0000

Moments

Mean	3,8461538
Std Dev	1,2228592
Std Err Mean	0,2398224
upper 95% Mean	4,3400774
lower 95% Mean	3,3522303
N	26

uPA_exper



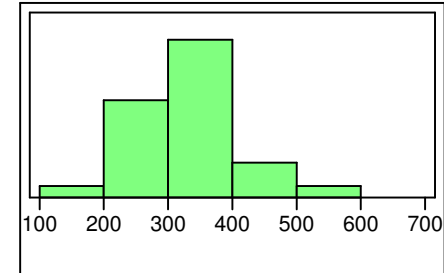
Quantiles

100.0%	maximum	-5,47
99.5%		-5,47
97.5%		-5,47
90.0%		-6,75
75.0%	quartile	-7,35
50.0%	median	-9,30
25.0%	quartile	-10,17
10.0%		-10,60
2.5%		-11,18
0.5%		-11,18
0.0%	minimum	-11,18

Moments

Mean	-8,910829
Std Dev	1,5403823
Std Err Mean	0,3020938
upper 95% Mean	-8,288655
lower 95% Mean	-9,533003
N	26

weight_CDK



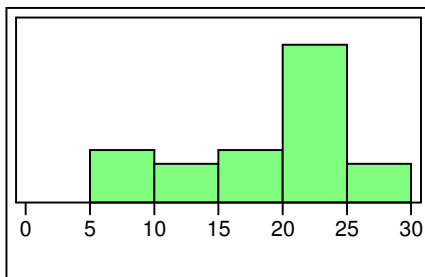
Quantiles

100.0%	maximum	554,21
99.5%		554,21
97.5%		554,21
90.0%		457,17
75.0%	quartile	383,69
50.0%	median	333,15
25.0%	quartile	278,37
10.0%		246,19
2.5%		121,08
0.5%		121,08
0.0%	minimum	121,08

Moments

Mean	335,40148
Std Dev	87,508706
Std Err Mean	17,161869
upper 95% Mean	370,74701
lower 95% Mean	300,05595
N	26

largestPiSystem



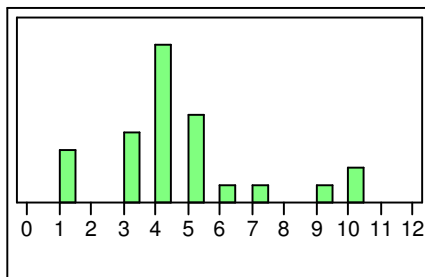
Quantiles

100.0%	maximum	25,000
99.5%		25,000
97.5%		25,000
90.0%		25,000
75.0%	quartile	22,000
50.0%	median	20,000
25.0%	quartile	13,750
10.0%		9,000
2.5%		9,000
0.5%		9,000
0.0%	minimum	9,000

Moments

Mean	18,538462
Std Dev	5,3608266
Std Err Mean	1,0513446
upper 95% Mean	20,703746
lower 95% Mean	16,373177
N	26

hBondacceptors



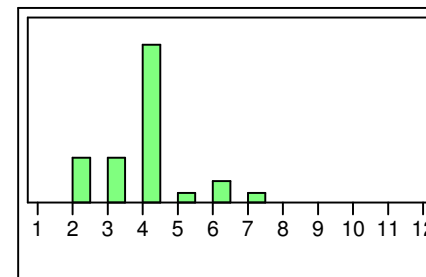
Quantiles

100.0%	maximum	10,000
99.5%		10,000
97.5%		10,000
90.0%		10,000
75.0%	quartile	5,000
50.0%	median	4,000
25.0%	quartile	3,000
10.0%		1,000
2.5%		1,000
0.5%		1,000
0.0%	minimum	1,000

Moments

Mean	4,5384615
Std Dev	2,3533936
Std Err Mean	0,4615385
upper 95% Mean	5,4890178
lower 95% Mean	3,5879053
N	26

hBondDonors



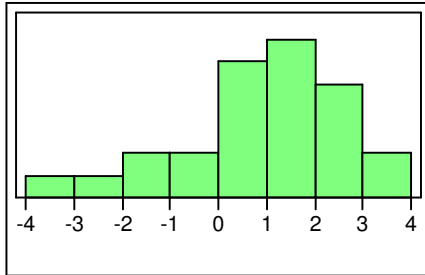
Quantiles

100.0%	maximum	7,0000
99.5%		7,0000
97.5%		7,0000
90.0%		7,0000
75.0%	quartile	4,0000
50.0%	median	4,0000
25.0%	quartile	3,0000
10.0%		2,0000
2.5%		2,0000
0.5%		2,0000
0.0%	minimum	2,0000

Moments

Mean	3,8461538
Std Dev	1,2228592
Std Err Mean	0,2398224
upper 95% Mean	4,3400774
lower 95% Mean	3,3522303
N	26

xlogP



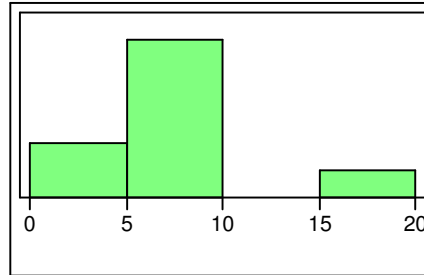
Quantiles

100.0%	maximum	3,993
99.5%		3,993
97.5%		3,993
90.0%		2,928
75.0%	quartile	2,155
50.0%	median	1,124
25.0%	quartile	0,183
10.0%		-2,042
2.5%		-3,177
0.5%		-3,177
0.0%	minimum	-3,177

Moments

Mean	0,8630385
Std Dev	1,7336221
Std Err Mean	0,3399913
upper 95% Mean	1,5632636
lower 95% Mean	0,1628133
N	26

rotatableBondsCount



Quantiles

100.0%	maximum	18,000
99.5%		18,000
97.5%		18,000
90.0%		15,600
75.0%	quartile	7,250
50.0%	median	6,000
25.0%	quartile	4,750
10.0%		3,400
2.5%		2,000
0.5%		2,000
0.0%	minimum	2,000

Moments

Mean	6,9615385
Std Dev	3,9847787
Std Err Mean	0,7814794
upper 95% Mean	8,5710254
lower 95% Mean	5,3520515
N	26