

## **Supplementary Material: More about residual values**

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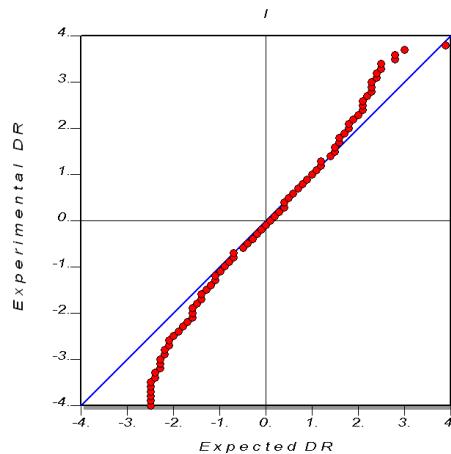
Table S1. Number of data set, *de facto* and predicted  $R$ -values for all observations included in the refinements, as well as  $R$ -values from the literature.

	$R_2^{act.}$	$R_2^{pred}$	$wR(F^2)^{act.}$ $w = 1/\sigma^2$	$wR(F^2)^{pred}$ $w = 1/\sigma^2$	$wR(F^2)^{act.}$ $w = 1/\hat{\sigma}^2$	$wR(F^2)^{pred}$ $w = 1/\hat{\sigma}^2$	$wR(F^2)^{Lit}$ $w = 1/\hat{\sigma}^2$
1	0.037	0.016	0.032	0.027	0.043	0.043	0.043
2	0.036	0.014	0.031	0.023	0.039	0.036	0.039
3	0.017	0.010	0.020	0.016	0.026	0.024	0.026
4	0.023	0.012	0.020	0.015	0.024	0.021	0.024
5	0.089	0.014	0.064	0.034	0.092	0.089	0.092
6	0.173	0.047	0.088	0.063	0.097	0.087	0.097
7	0.085	0.015	0.089	0.022	0.116	0.110	0.116
8	0.089	0.024	0.086	0.027	0.105	0.100	0.105
9	0.110	0.052	0.139	0.088	0.179	0.162	0.178
10	0.048	0.025	0.062	0.045	0.077	0.074	0.077
11	0.037	0.022	0.040	0.029	0.047	0.046	0.047
12	0.045	0.063	0.117	0.104	0.119	0.110	0.114
13	0.031	0.028	0.052	0.044	0.056	0.053	0.056
14	0.035	0.026	0.063	0.044	0.070	0.065	0.070
15	0.035	0.026	0.063	0.044	0.083	0.079	0.083
16	0.070	0.014	0.075	0.026	0.098	0.093	0.098
17	0.081	0.018	0.126	0.035	0.151	0.143	0.151
18	0.053	0.017	0.047	0.031	0.070	0.075	0.070
19	0.028	0.008	0.070	0.024	0.115	0.110	0.115
20	0.084	0.075	0.098	0.059	0.120	0.119	0.120
21	0.047	0.035	0.095	0.037	0.119	0.119	0.119
22	0.033	0.035	0.035	0.030	0.049	0.056	0.049
23	0.072	0.021	0.071	0.062	0.093	0.102	0.093
24	0.033	0.027	0.083	0.066	0.104	0.100	0.104
25	0.148	0.006	0.065	0.013	0.070	0.067	0.070
26	0.055	0.016	0.059	0.020	0.080	0.072	0.080
27	0.044	0.017	0.050	0.027	0.064	0.067	0.064
28	0.041	0.012	0.061	0.021	0.090	0.094	0.090
29	0.053	0.012	0.056	0.020	0.091	0.088	0.091
30	0.097	0.020	0.080	0.033	0.116	0.109	0.116
31	0.101	0.014	0.076	0.030	0.114	0.105	0.114
32	0.037	0.013	0.107	0.020	0.119	0.101	0.119
33	0.065	0.020	0.093	0.027	0.159	0.144	0.159
34	0.124	0.027	0.139	0.046	0.248	0.202	0.248
35	0.131	0.046	0.117	0.061	0.196	0.179	0.196
36	0.042	0.027	0.108	0.044	0.169	0.157	0.169
37	0.079	0.020	0.077	0.039	0.110	0.105	0.110

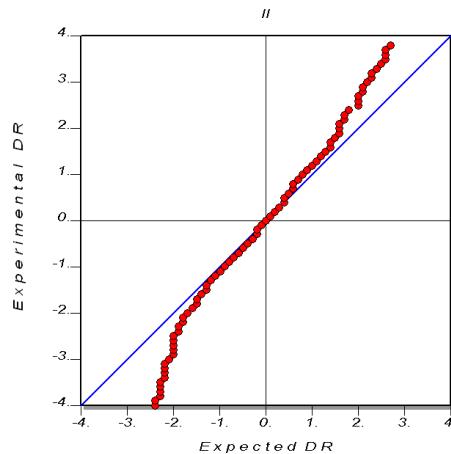
<sup>†</sup> References: (1-3) He *et al.* (2013), (4) Jennene Boukharrata *et al.* (2013), (5) Zhou *et al.* (2013), (6) Deng *et al.* (2013), (7-8) Wang *et al.* (2013), (9-10) Zhang *et al.* (2013), (11) Huang (2013), (12) Zhou & Wang (2013), (13) Wu & Jin (2013), (14) Luo (2013), (15-17) Krause *et al.* (2013), (18-19) Arkhipov *et al.* (2013), (20-21) Su *et al.* (2013), (22) Arderne (2013), (23-25) Bats *et al.* (2013), (26-27) Smith & Wermuth (2013a), (28-29) Smith & Wermuth (2013b), (30-31) Castillo *et al.* (2013), (32-36) Gomes *et al.* (2013), (37) Görbitz & Yadav (2013).

Fig. S1. Normal probability plots of all data sets 1 – 37 as obtained from the DRK-plot software implemented in WinGX (Farrugia, 2012).

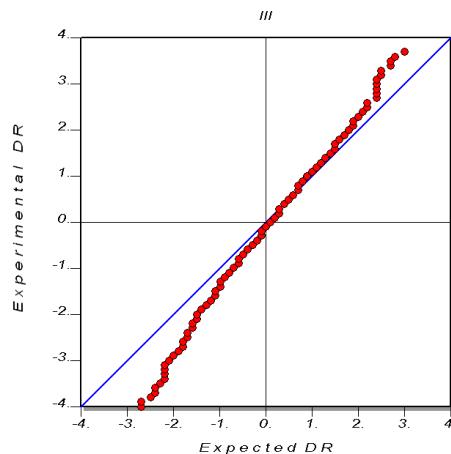
For more information on normal probability plots see Abrahams & Keve (1971).



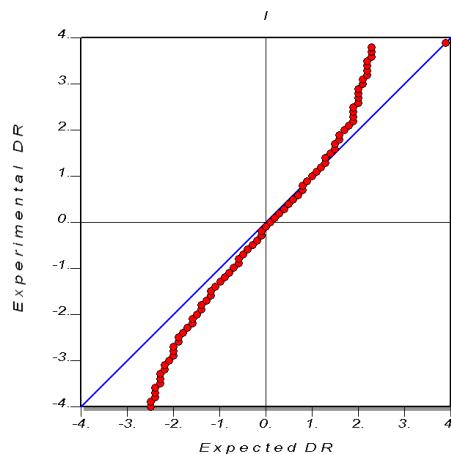
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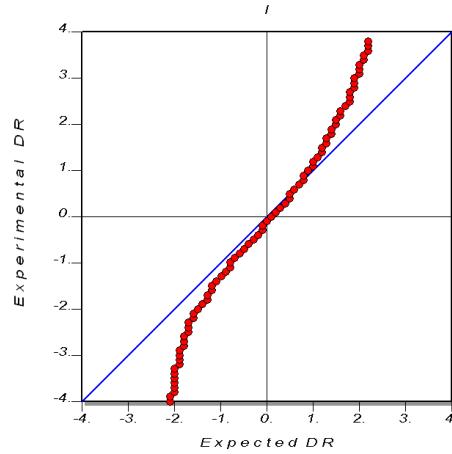
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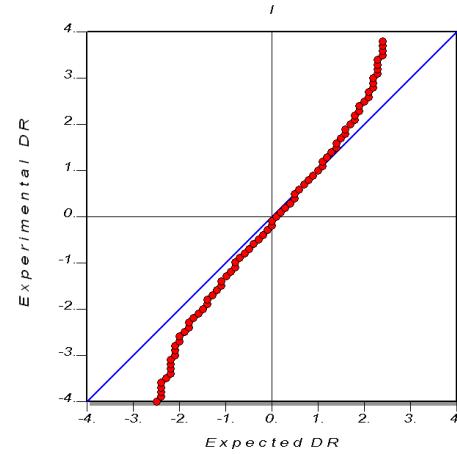
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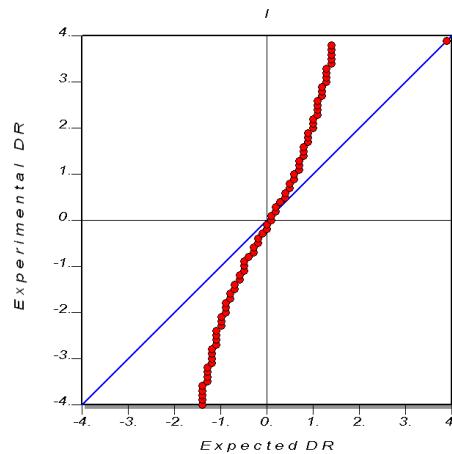
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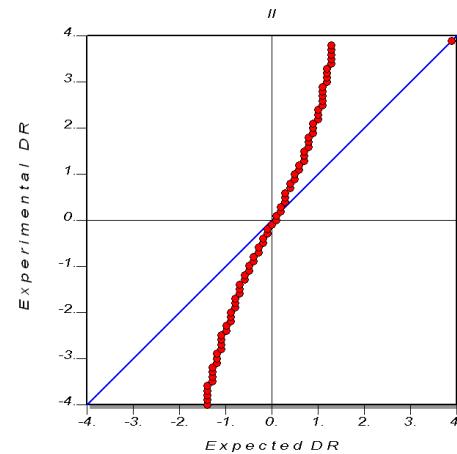
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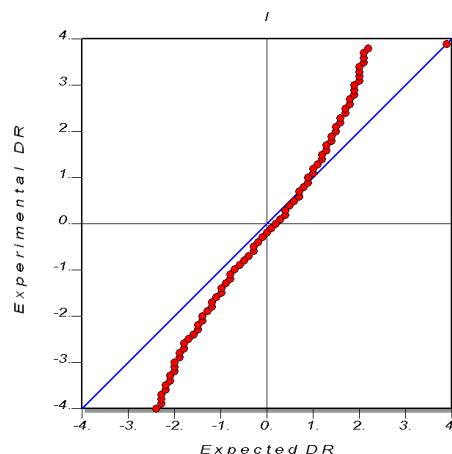
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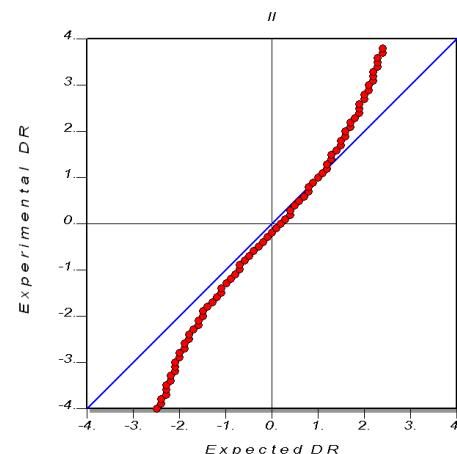
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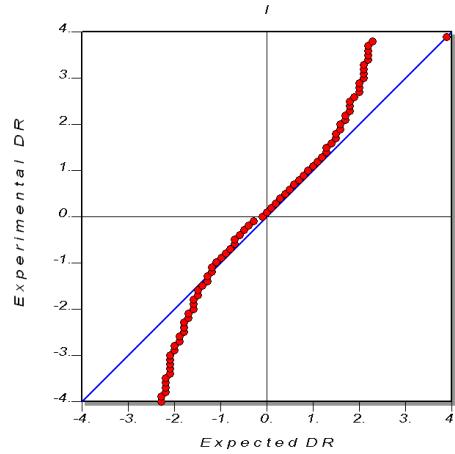
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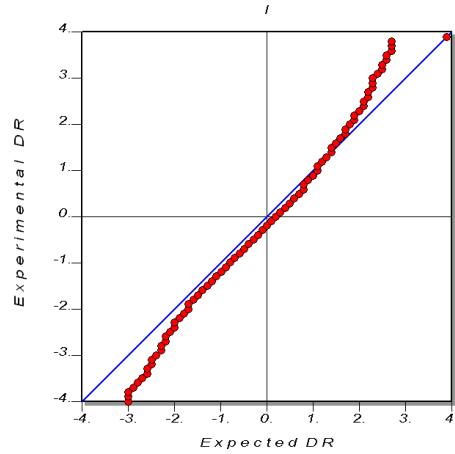
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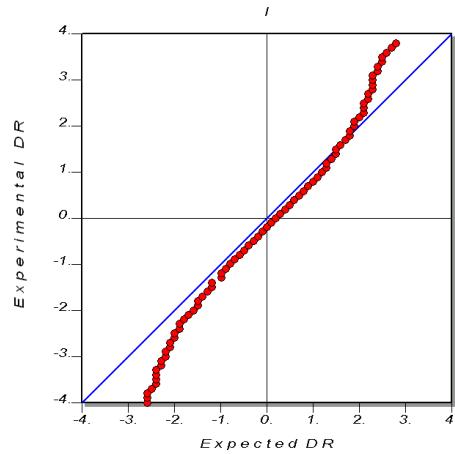
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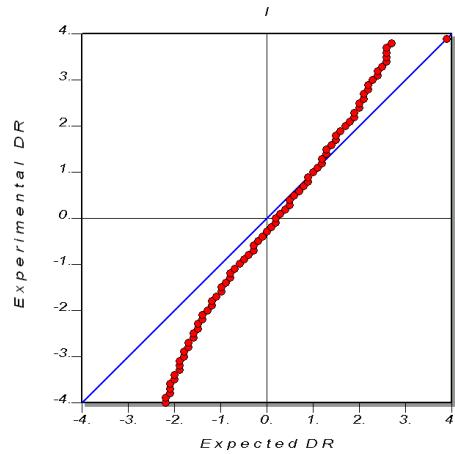
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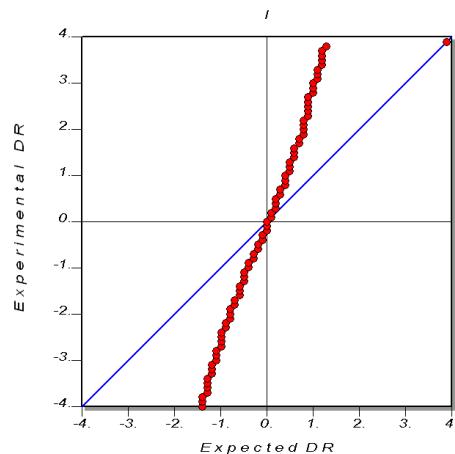
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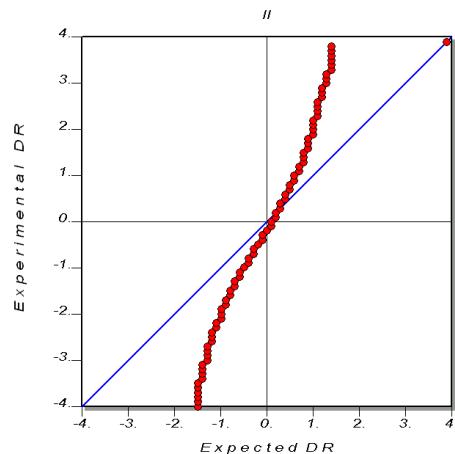
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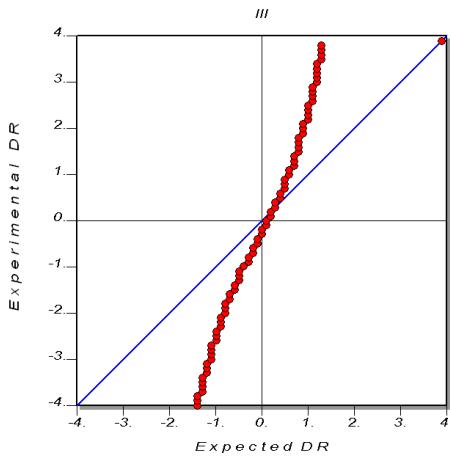
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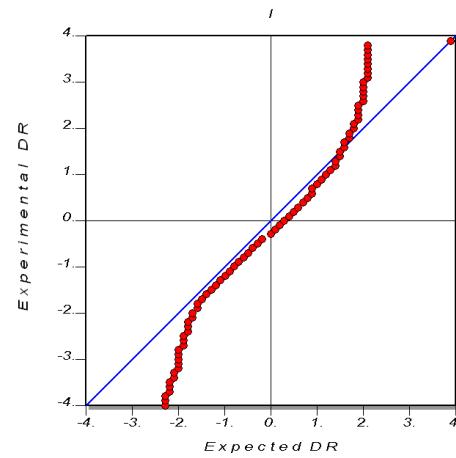
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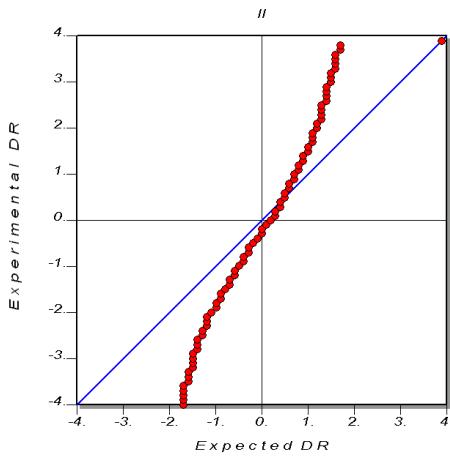
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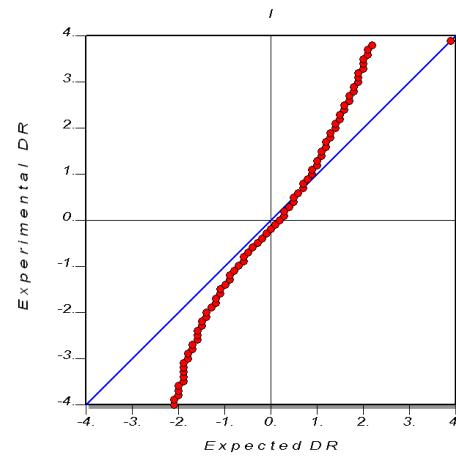
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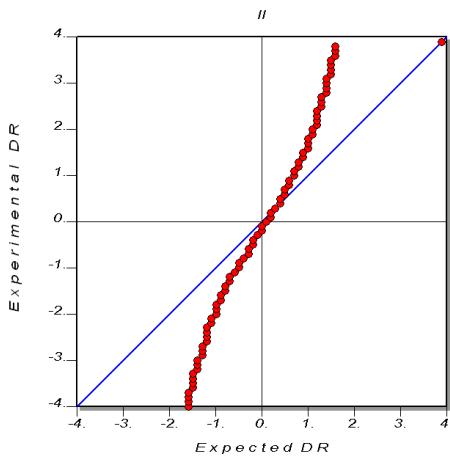
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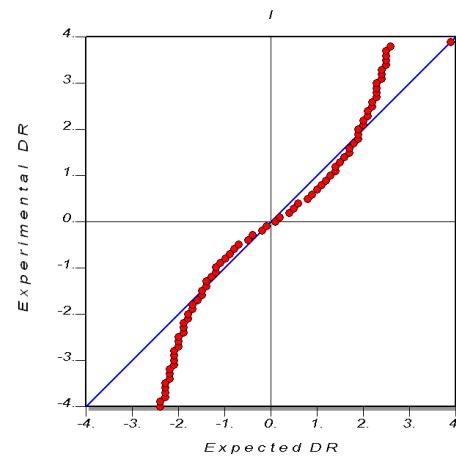
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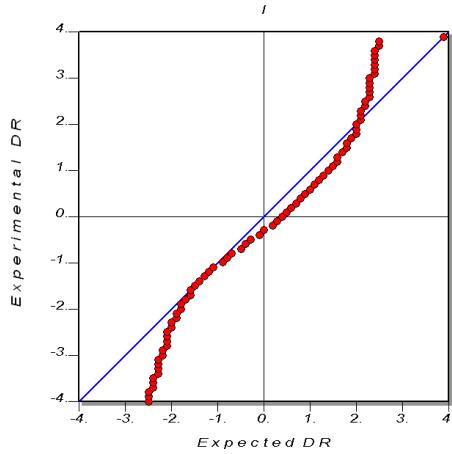
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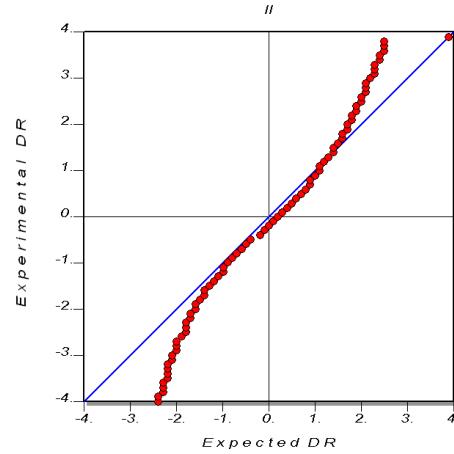
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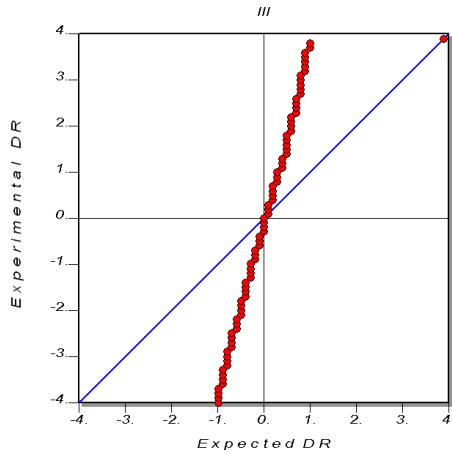
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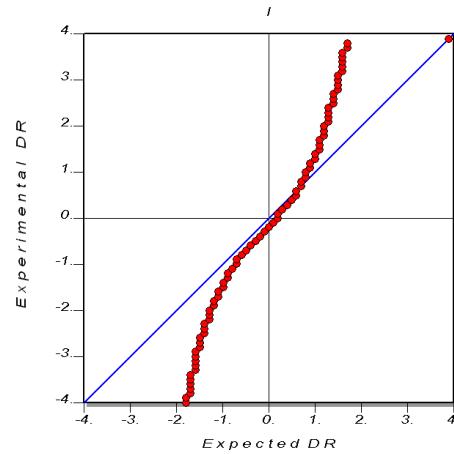
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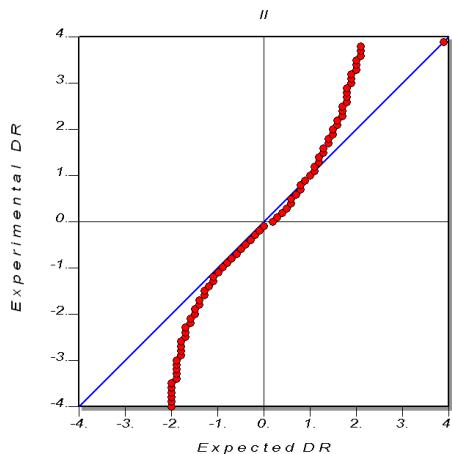
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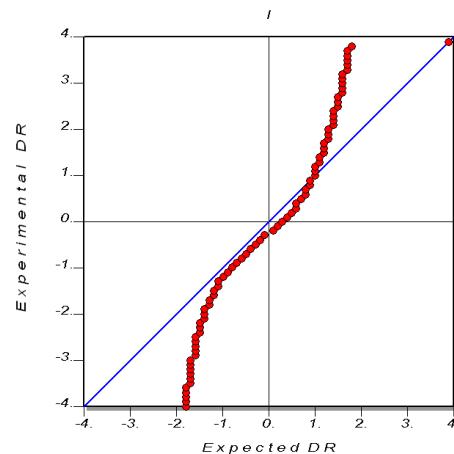
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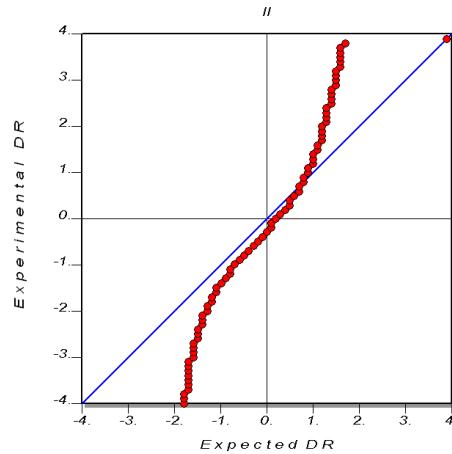
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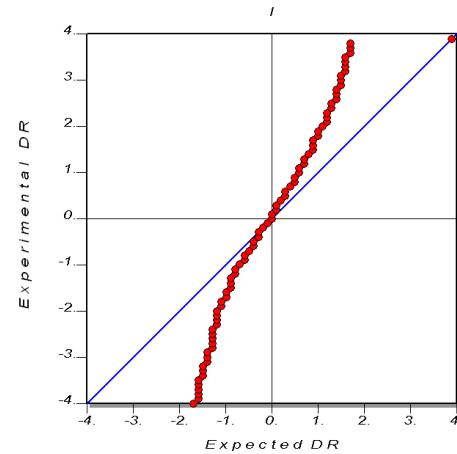
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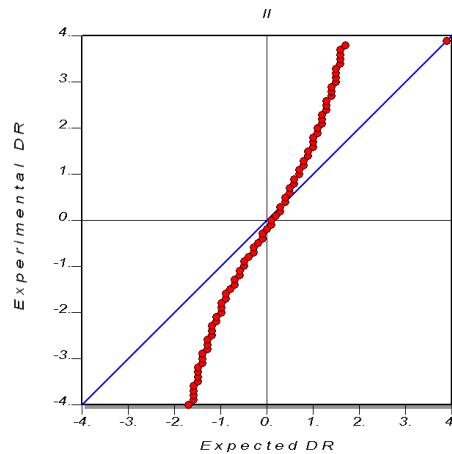
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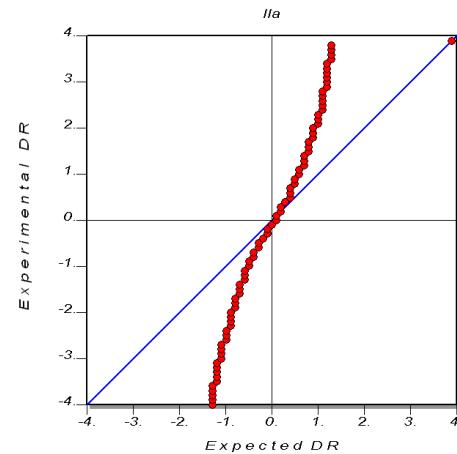
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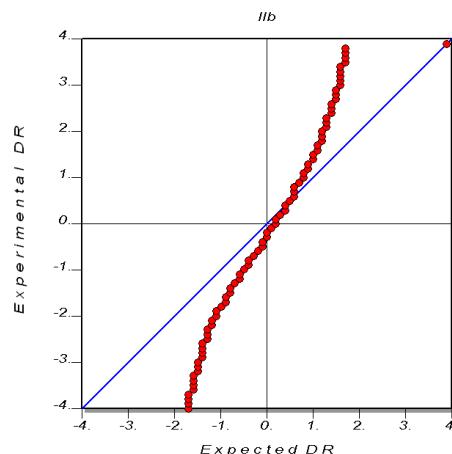
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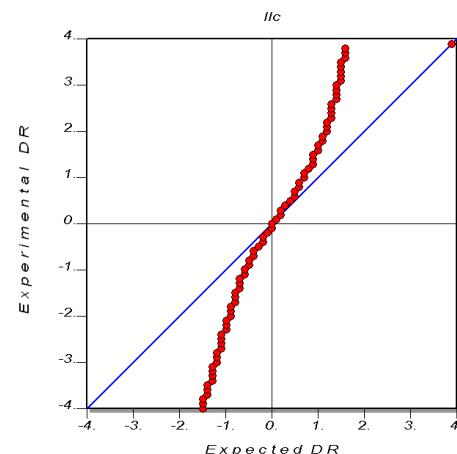
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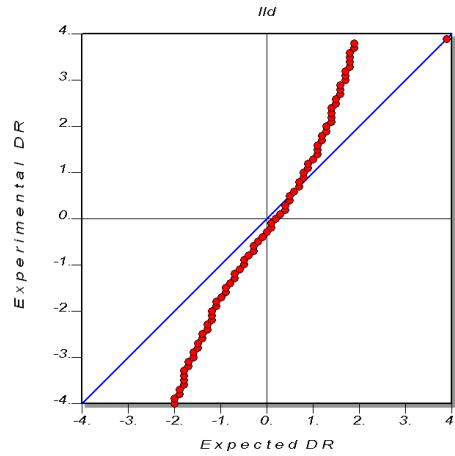
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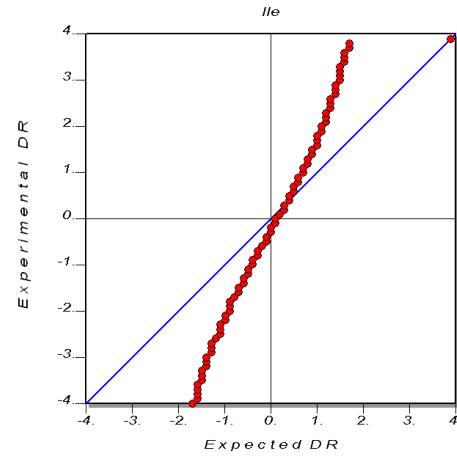
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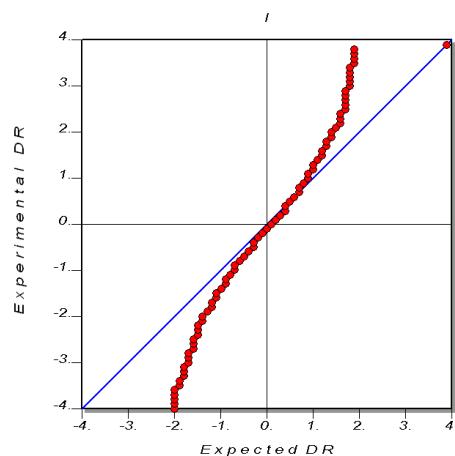
Data set no. 34



Data set no. 35



Data set no. 36



Data set no. 37

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