

Supplementary Material to: More About Systematic Errors in Charge Density Studies

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Figure 1 shows the BayCoN plots for (ζ, I_o) , (ζ, I_c) , $(\zeta s.u.)$, and, where available, $(\zeta, \frac{\sin \theta}{\lambda})$ for data sets 1-20.

Figure 2 shows the probability density histograms and normal probability plots for the residuals of data sets 24-30.

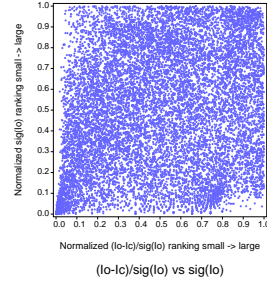
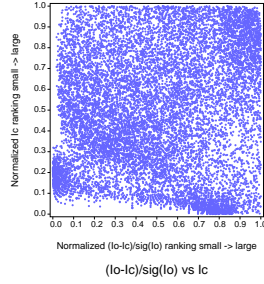
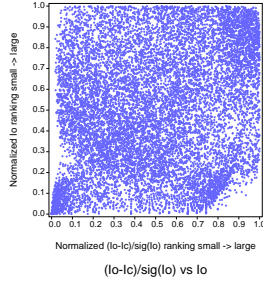
Figure 3 shows the BayCoN $(I_o, s.u.)$ plots for data sets 1-30.

Table 1 gives the χ_S^2 sums corresponding to the distributions $\chi_S^2(\zeta, I_o)$, $\chi_S^2(\zeta, I_c)$, $\chi_S^2(\zeta, s.u.)$, $\chi_S^2(\zeta, \frac{\sin \theta}{\lambda})$ of data sets 1-29, the meta residual values and the weighting scheme parameters.

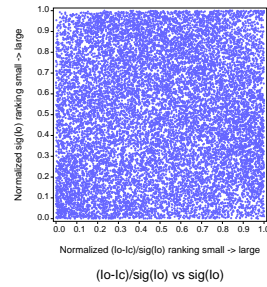
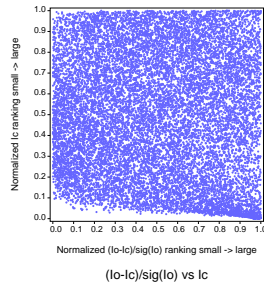
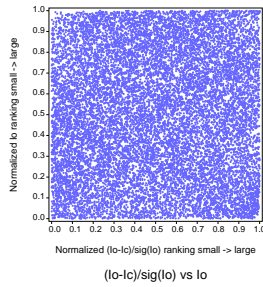
set no.

 (ζ, I_o)
(lo-ic)/sig(lo) vs lo (ζ, I_c)
(lo-ic)/sig(lo) vs ic $(\zeta, s.u.)$
(lo-ic)/sig(lo) vs sig(lo) $(\zeta, \frac{\sin \theta}{\lambda})$

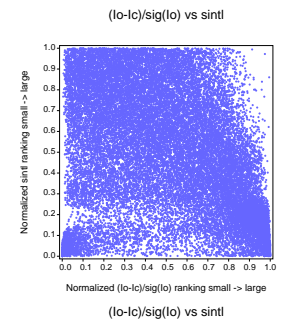
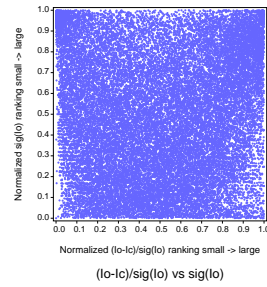
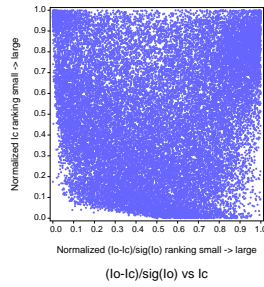
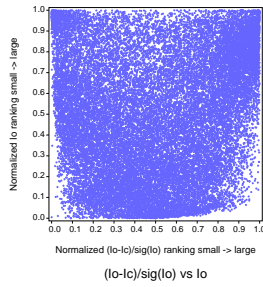
1



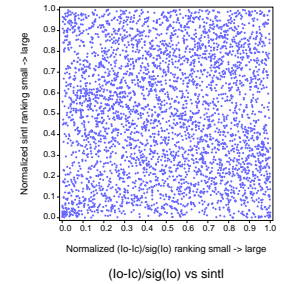
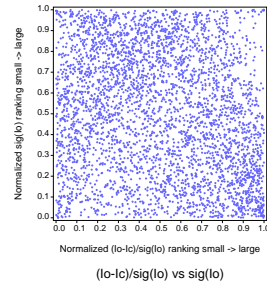
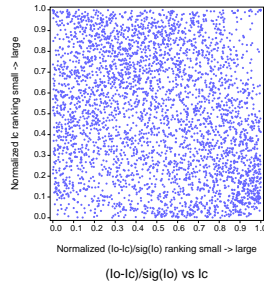
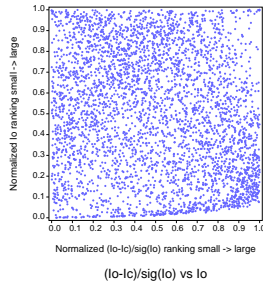
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3



4



5

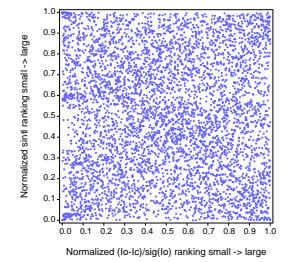
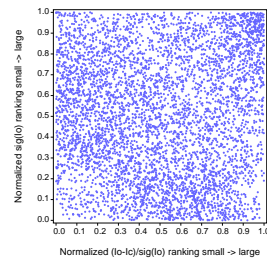
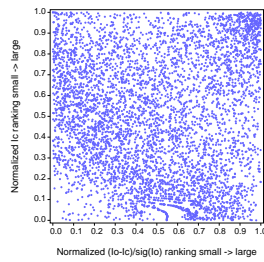
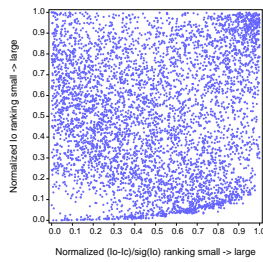


Fig. 1. BayCoN plots for datasets 1-5. Continuation of Figure on next page.

set no.

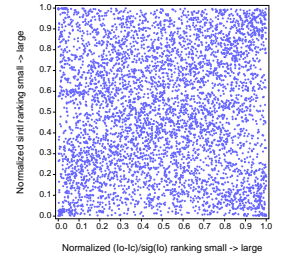
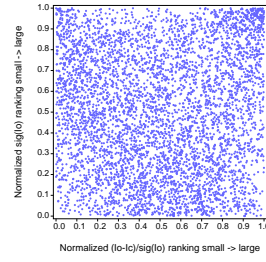
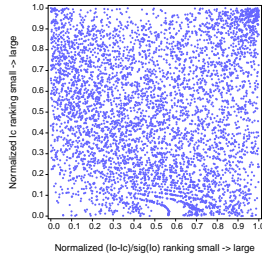
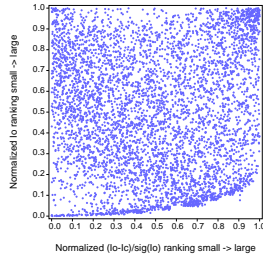
 (ζ, I_o)
 (lo-ic)/sig(lo) vs lo

 (ζ, I_c)
 (lo-ic)/sig(lo) vs ic

 $(\zeta, s.u.)$
 (lo-ic)/sig(lo) vs sig(lo)

 $(\zeta, \frac{\sin \theta}{\lambda})$
 (lo-ic)/sig(lo) vs sintl

6



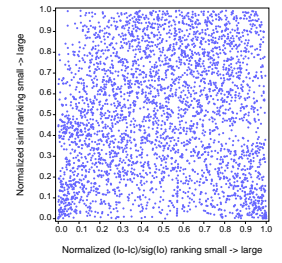
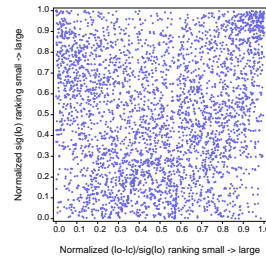
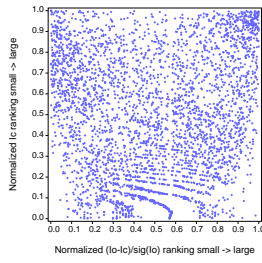
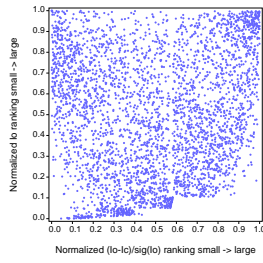
(lo-ic)/sig(lo) vs lo

(lo-ic)/sig(lo) vs ic

(lo-ic)/sig(lo) vs sig(lo)

(lo-ic)/sig(lo) vs sintl

7



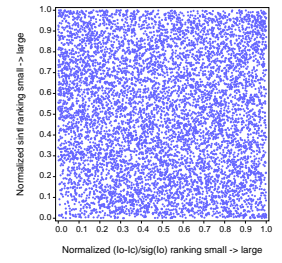
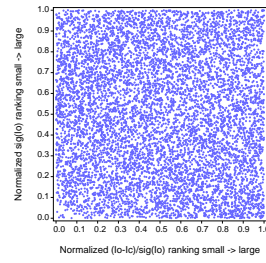
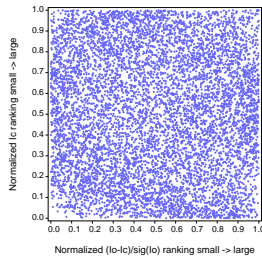
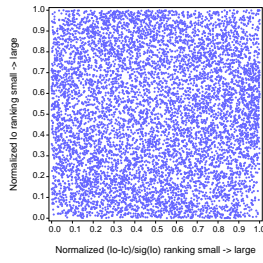
(lo-ic)/sig(lo) vs lo

(lo-ic)/sig(lo) vs ic

(lo-ic)/sig(lo) vs sig(lo)

(lo-ic)/sig(lo) vs sintl

8



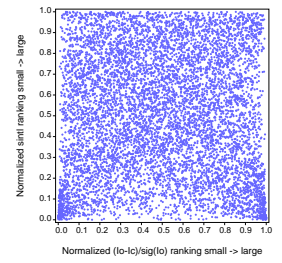
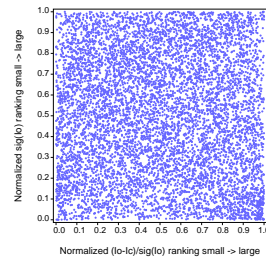
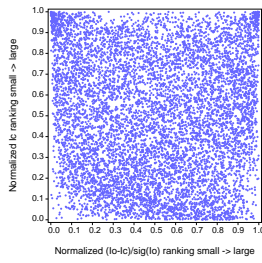
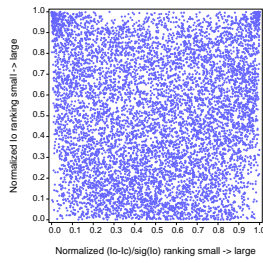
(lo-ic)/sig(lo) vs lo

(lo-ic)/sig(lo) vs ic

(lo-ic)/sig(lo) vs sig(lo)

(lo-ic)/sig(lo) vs sintl

9



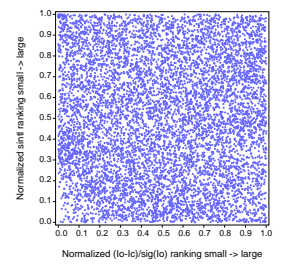
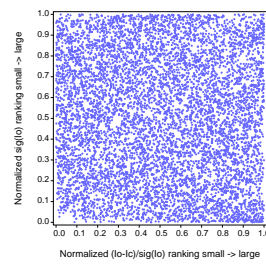
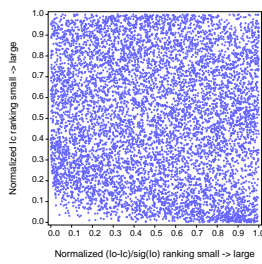
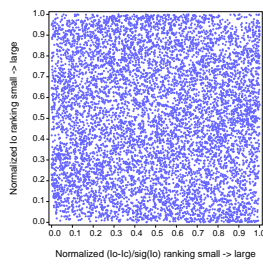
(lo-ic)/sig(lo) vs lo

(lo-ic)/sig(lo) vs ic

(lo-ic)/sig(lo) vs sig(lo)

(lo-ic)/sig(lo) vs sintl

10



(lo-ic)/sig(lo) vs lo

(lo-ic)/sig(lo) vs ic

(lo-ic)/sig(lo) vs sig(lo)

(lo-ic)/sig(lo) vs sintl

Fig. 1. BayCoN plots for datasets 6-10. Continuation of Figure on next page.

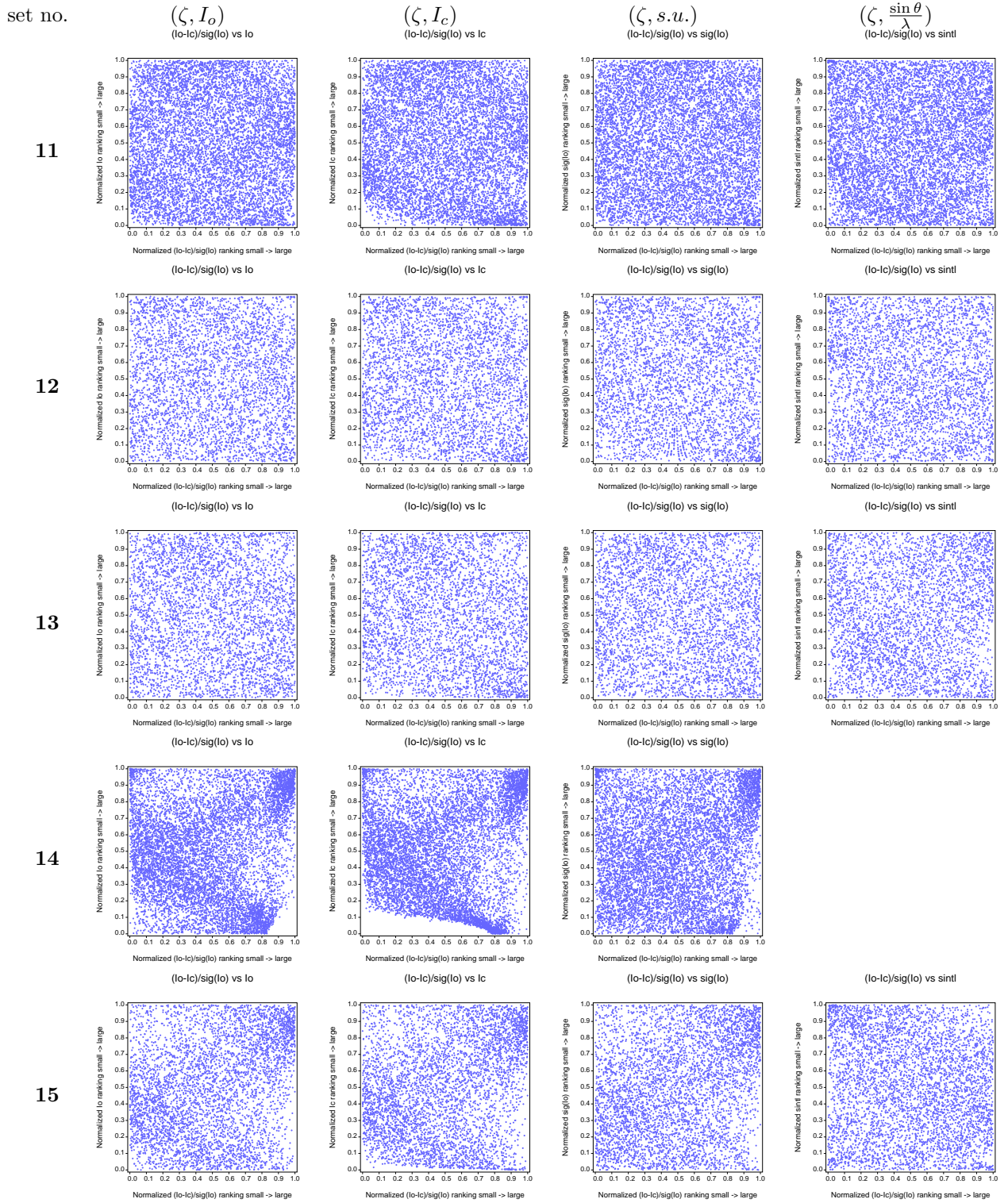


Fig. 1. BayCoN plots for datasets 11-15. Continuation of Figure on next page.

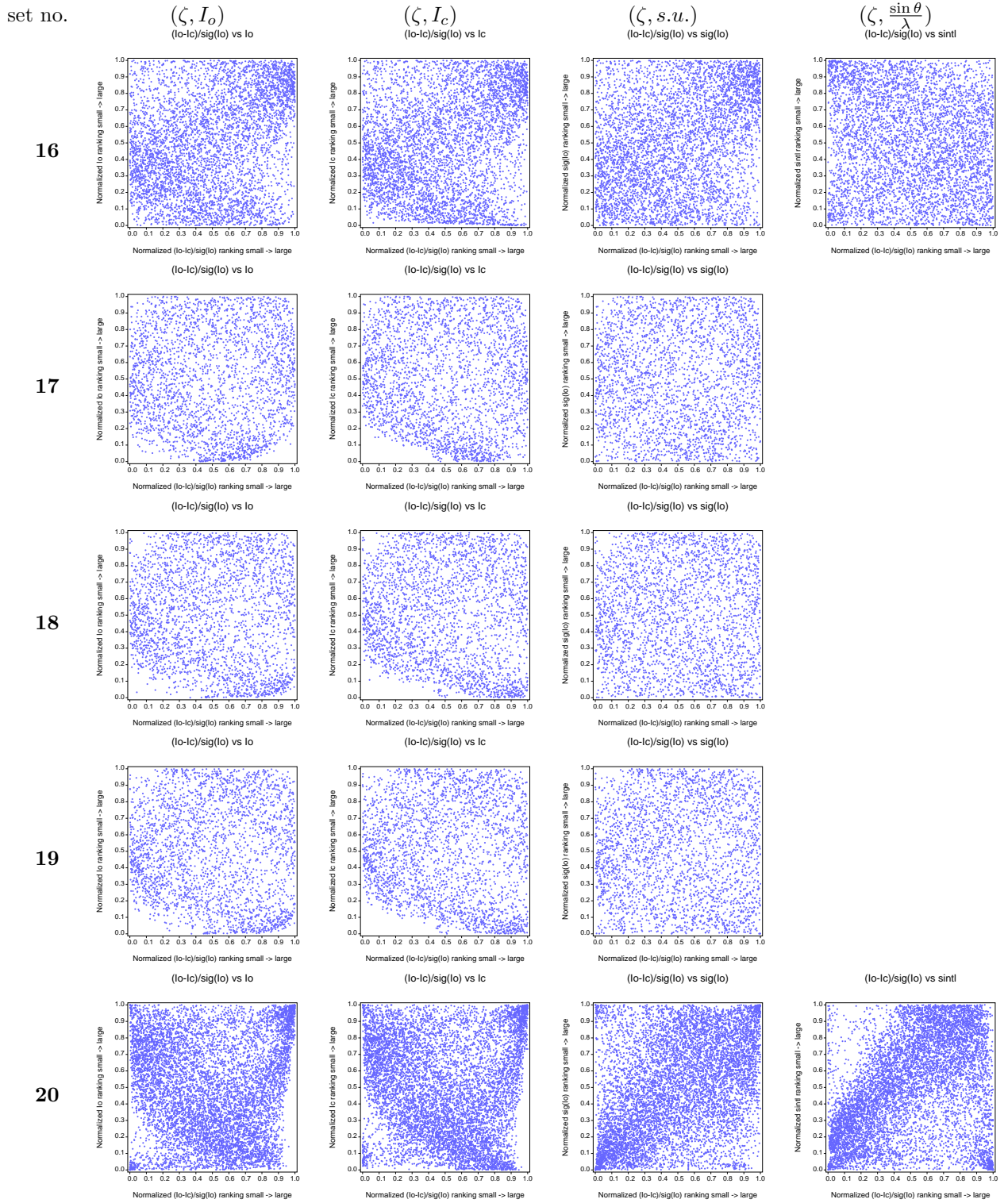


Fig. 1. BayCoN plots for datasets 16-20. Continuation of Figure on next page.

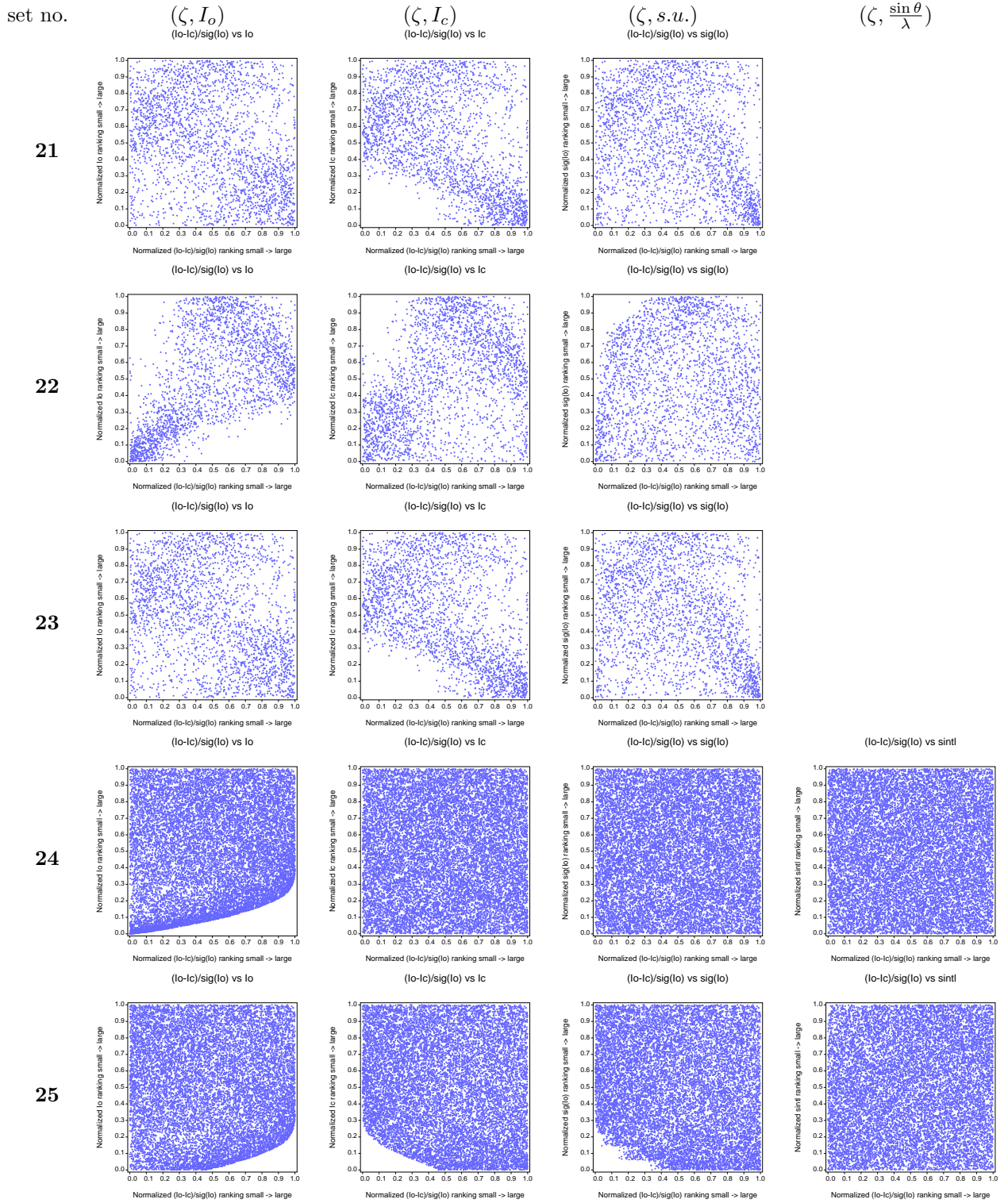


Fig. 1. BayCoN plots for datasets 21-25. Artificial data sets start with no. 24. Continuation of Figure on next page.

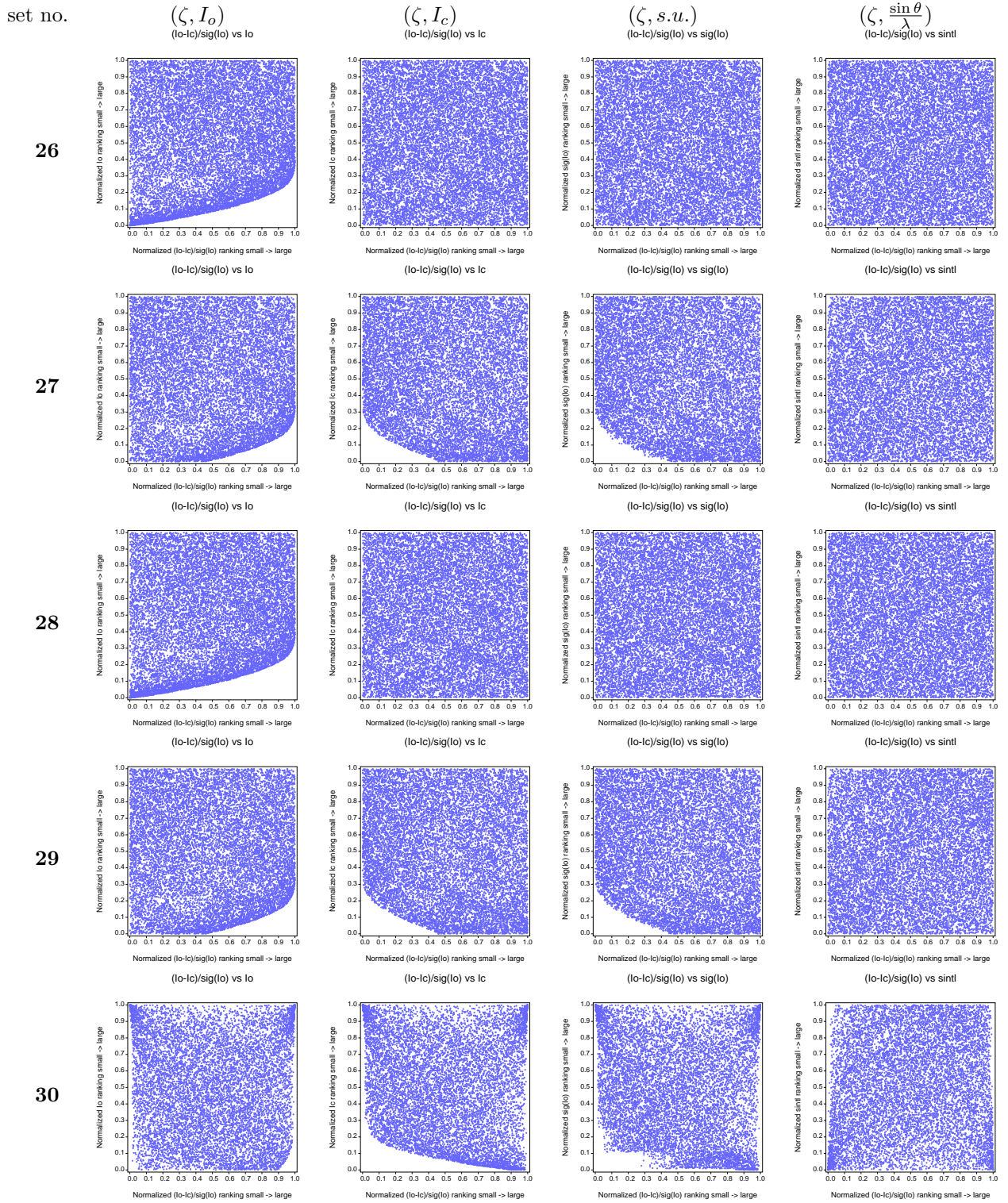


Fig. 1. BayCoN plots for datasets 26-30.

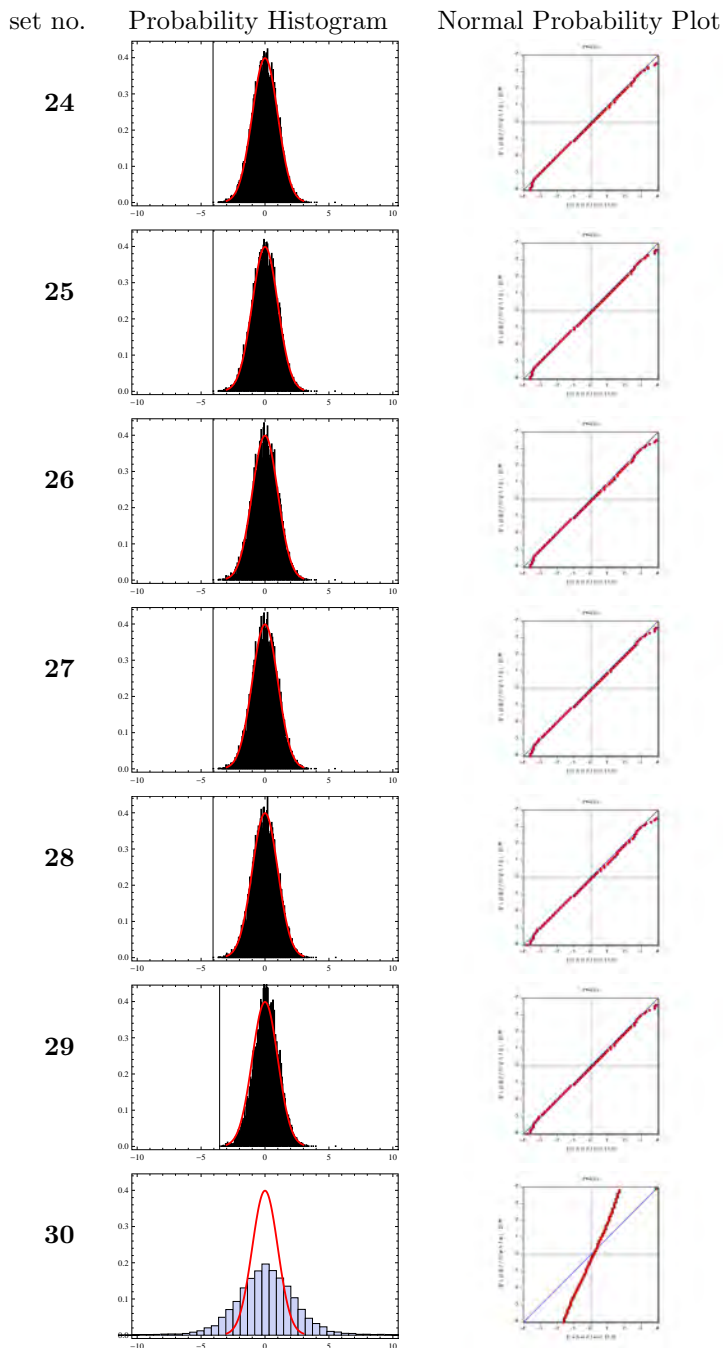
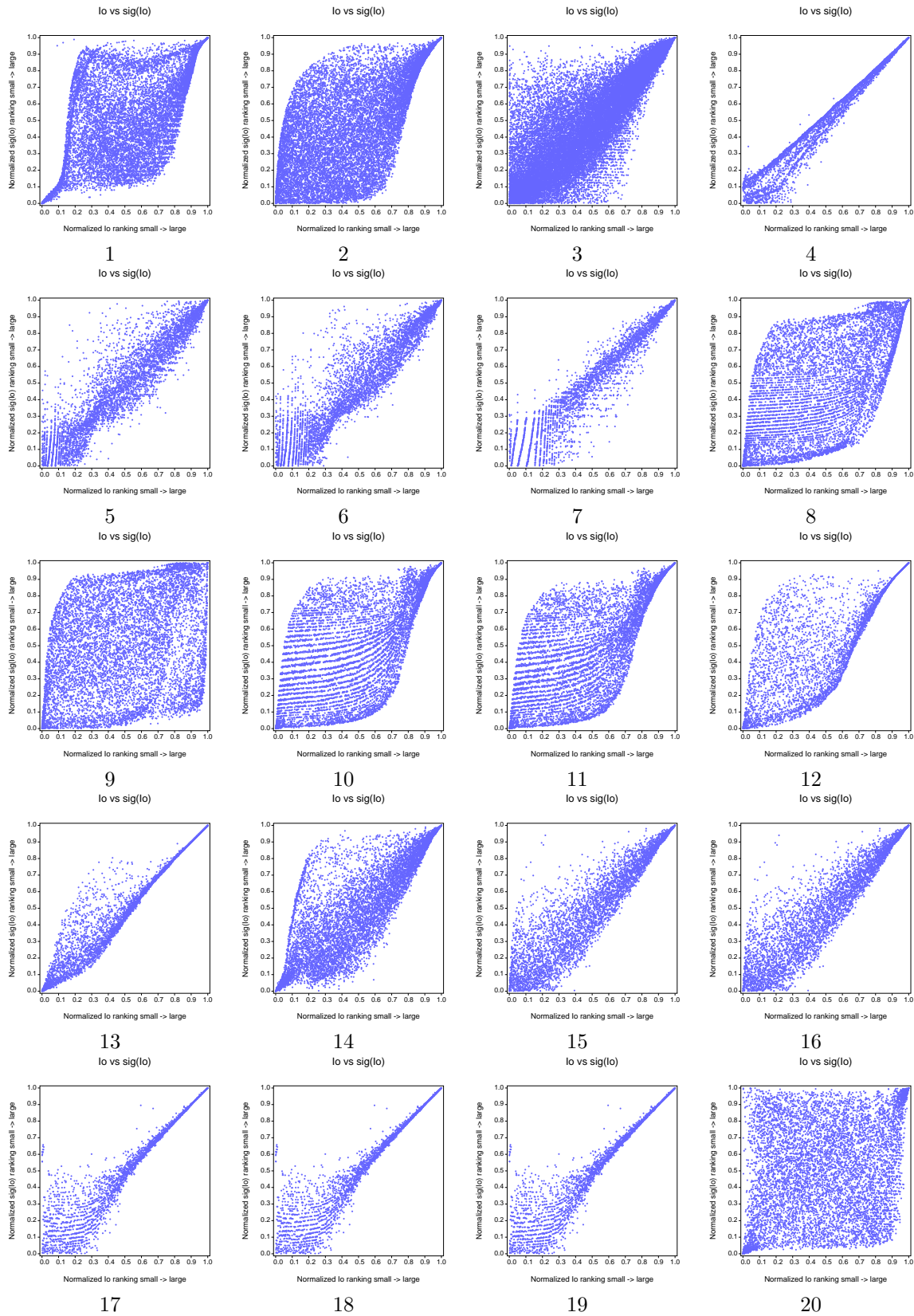


Fig. 2. Probability density histograms (left column) with ideal probability density function (red line, corresponding to a normal distribution, $\mu = 0$, $\sigma = 1$) and normal probability plots (right column) of the artificial data sets 24-30.

Fig. 3. BayCoN ($I_o, s.u.$) plots for datasets 1-20. Continuation of Figure on next page.

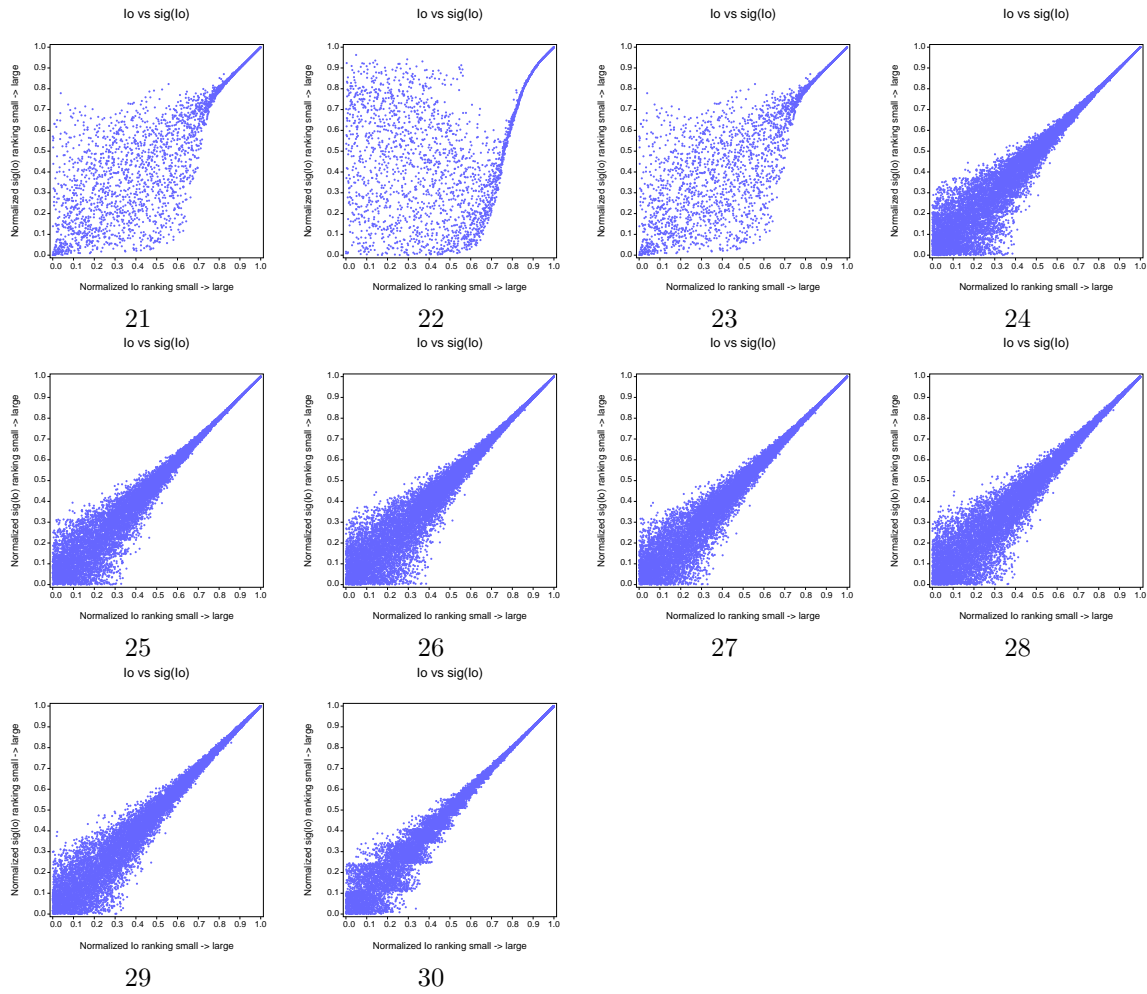


Fig. 3. BayCoN ($I_o, s.u.$) plots for datasets 21-30.

Table 1. *Chi-square residual sums for data sets 1-29.*

data set no.	$\chi_S^2(\zeta, I_o)$	$\chi_S^2(\zeta, I_c)$	$\chi_S^2(\zeta, s.u.)$	$\chi_S^2(\zeta, \frac{\sin \theta}{\lambda})$	R^{meta}	weighting scheme
1	2901.36	3180.98	2272.82	—	0.805	$7/\sigma^2(F_o)$
2	291.60	1434.91	398.34	—	0.087	$1/(1.101 \sigma^2(F_o^2))$
3	6857.72	6986.23	3432.13	10673.5	0.710	$1/\sigma^2(F_o)$
4	431.17	433.00	388.73	212.59	0.277	$1/\sigma^2(F_o)$
5	979.15	1026.15	587.91	239.90	0.161	$1/\sigma^2(F_o)$
6	837.37	827.65	488.36	354.82	0.215	$1/\sigma^2(F_o)$
7	1166.85	1021.82	738.52	539.03	0.395	$1/\sigma^2(F_o)$
8	266.04	315.96	137.82	170.39	0.124	$1/(\sigma^2(F_o^2) + (0.006F_o^2)^2 + 0.008F_o^2)$
9	249.31	295.23	129.68	155.65	0.099	$1/(\sigma^2(F_o^2) + (0.006F_o^2)^2 + 0.012F_o^2)$
10	174.38	409.99	145.03	219.74	0.103	$1/(\sigma^2(F_o^2) + (0.008F_o^2)^2 + 0.012F_o^2)$
11	219.54	466.17	132.79	181.77	0.131	$1/(\sigma^2(F_o^2) + (0.012F_o^2)^2 + 0.015F_o^2)$
12	145.67	205.69	184.38	144.35	0.163	$1/(\sigma^2(F_o^2) + (0.005F_o^2)^2 + 0.006F_o^2)$
13	137.50	243.59	162.36	289.10	0.054	$1/(\sigma^2(F_o^2) + (0.015F_o^2)^2 + 0.056F_o^2)$
14	2823.28	4278.34	1363.67	—	0.500	$1/\sigma^2(F_o)$
15	937.71	973.60	653.23	286.66	0.267	$1/\sigma^2(F_o^2)$
16	975.08	1007.54	704.52	306.17	0.254	$1/\sigma^2(F_o^2)$
17	423.88	501.89	186.31	—	0.578	$1/(3.68 \sigma^2(F_o^2) + 0.001(F_o^2)^2)$
18	401.4	534.48	170.69	—	0.163	$1/(3.68 \sigma^2(F_o^2) + 0.001(F_o^2)^2)$
19	452.75	578.17	176.58	—	0.160	$1/(3.68 \sigma^2(F_o^2) + 0.001(F_o^2)^2)$
20	2168.19	2397.94	2180.9	3283.80	0.579	$1/\sigma^2(F_o)$
21	627.82	1403.16	753.52	—	0.402	$1/(\sigma^2(F_o) + 0.004(F_o^2))$
22	2336.25	1107.85	498.39	—	0.164	$1/(\sigma^2(F_o) + 0.004(F_o^2))$
23	627.82	1403.16	753.52	—	0.402	$1/(\sigma^2(F_o) + 0.004(F_o^2))$
24	2705.82	118.49	116.04	66.95	0.006	$1/\sigma^2(F_o^2)$
25	955.16	928.46	827.35	135.25	-0.027	$1/\sigma^2(F_o^2)$
26	2754.3	107.33	105.34	69.80	0.003	$1/\sigma^2(F_o^2)$
27	946.88	943.35	919.57	144.42	-0.028	$1/\sigma^2(F_o^2)$
28	2790.63	115.88	118.01	61.72	0.003	$1/\sigma^2(F_o^2)$
29	904.55	964.39	943.94	149.49	-0.029	$1/\sigma^2(F_o^2)$