**S4 Table. Structures of inactive D series phthalazinone derivatives.** n.d. = not determined. a. Data from [28]. b. Data from [37]. c. Single determination.

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| --- | --- | --- | --- | --- |
|  | | | | |
| **Cmpd** | **R** | **X** | ***Ki,app* (nM)** | |
| **C*p*IMPDH** | ***Ba*IMPDH** |
| **D1** | 4-OMePh | H | 1000 ± 200 a | 1800 ± 30 b |
| **D20** | 3-OMePh | H | >5000 a | 11000 c |
| **D21** | 2-OMePh | H | >5000 a | n.d. |
| **D24** | 4-ClPh | H | 230 ± 50 a | 300 ± 100 b |
| **D27** | 3,4-diClPh | H | 55 ± 6 a | 280 c |
| **D29** | 4-BrPh | H | 130 ± 30 a | 80 ± 20 b |
| **D30** | 4-FPh | H | >5000 a | 7300 c |
| **D31** | 3-Cl,4-BrPh | H | 30 ± 1 a | 270 ± 100 b |
| **D41** | 2-Naphthyl | H | 61 ± 4 a | 80 ± 30 b |
| **D45** | 3-CF3,4-BrPh | H | 24 ± 2 a | 6500 c |
| **D48** | 3-CF3,4-ClPh | H | 13 ± 1 a | 4000 ± 1000 b |
| **D50** | 3-CF3, 4-CNPh | H | 54 ± 5 a | 1800 ± 200 |
| **D59** | 3-CF3, 4-BrPh | H | 32 ± 6 a | 770 c |
| **D61** |  | H | 90 ± 20 a | 290 ± 40 b |
| **D67** |  | H | 20 ± 5 a | 470 ± 10 b |
| **D69** | 3-OMe,4-ClPh | H | 31 ± 2 a | 120 ± 10 b |
| **D73** |  | H | 4 ± 1 a | 50 ± 20 b |
| **D85** | 3-OMe,4-ClPh | Me | 44 ± 3 **b** | 60 ± 10 b |
| **D87** |  | OH | 30 ± 10 **b** | 30 ± 10 b |