Electronic Supplementary Material (ESI) for RSC Advances.

Discovery of NAD(P)H:quinone oxidoreductase 1 (NQO1) inhibitors with novel chemical scaffolds by shape-based virtual screening combined with cascade docking

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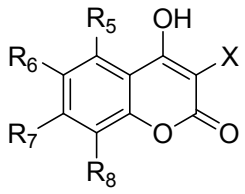
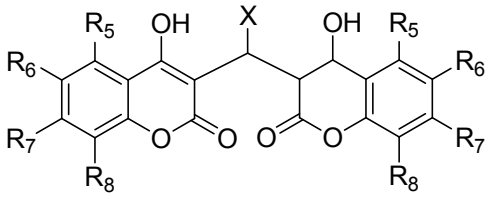
Table S1

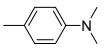
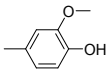
Structures of NQO1 inhibitors used to develop the active set for ROCS model and docking model. (Biological values used in this study were from references 1 and 2).



AS



S

Cmpd	R5	R6	R7	R8	X	pIC_{50} (M)
S1	H	H	H	H	H	6.39
S2	H	CH_3	H	H	H	5.25
S3	OCH_3	H	H	H	H	7.42
S4	H	OCH_3	H	H	H	5.48
S5	H	F	H	H	H	5.80
S6	H	CH_3	CH_3	H	H	6.63
S7	H	H	7,8-C_4H_4		H	6.43
S8	H	H	CH_3	CH_3	H	7.02
S9	H	H	OH	H	H	6.46
S10	H	H	H	H		5.30
S11	H	H	H	H		5.23
S12	H	H	H	H		6.19

AS1	H	CH_3	CH_3	H	1-naphthyl	5.96
AS2	H	CH_3	CH_3	H	2-naphthyl	6.78
AS3	H	H	7,8-C_4H_4		2-naphthyl	6.59
AS4	5,6-C_4H_4		H	H	1-naphthyl	6.21
AS5	5,6-C_4H_4		H	H	Phenyl	6.33
AS6	H	CH_3	CH_3	H	3,4-dimethyl phenyl	6.72

Reference

[1] K.A. Nolan, H. Zhao, P.F. Faulder, A.D. Frenkel, D.J. Timson, D. Siegel, D. Ross, T.R. Burke Jr, I.J. Stratford, R.A. Bryce, Coumarin-based inhibitors of human NAD(P)H: quinone oxidoreductase-1. Identification, structure–activity, off-target effects and in vitro human pancreatic cancer toxicity, J. Med. Chem. 50 (2007) 6316-6325.

[2] K.A. Nolan, J.R. Doncaster, M.S. Dunstan, K.A. Scott, A.D. Frenkel, D. Siegel, R.A. Bryce, Synthesis and biological evaluation of coumarin-based inhibitors of NAD(P)H: quinone oxidoreductase-1 (NQO1), J. Med. Chem. 52 (2009) 7142-7156.