



STRUCTURAL
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Supporting information for article:

Structural and thermodynamic analysis of interactions between death-associated protein kinase 1 and anthraquinones

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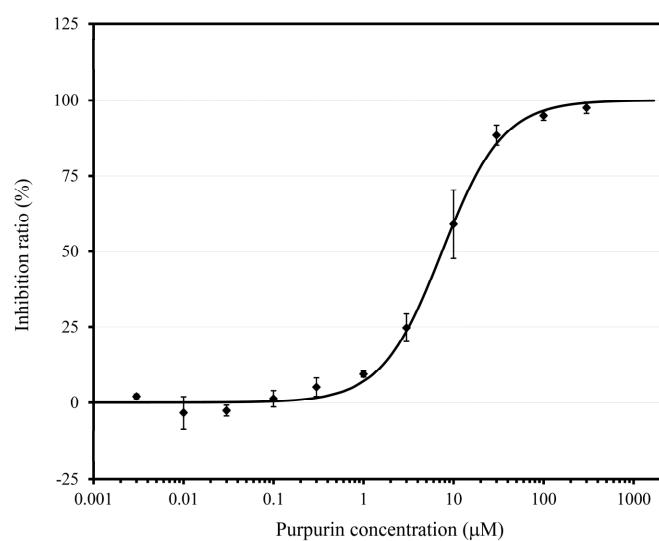
Table S1 IC₅₀ values determined using Fluorospark® Kinase/ADP and EnzyChrom™ ADP.

Compound	IC ₅₀ (μ M)	
	Fluorospark® Kinase/ADP	EnzyChrom™ ADP
	Multi-Assay Kit	Assay Kit
Emodin	N.D.	N.D.
Physcion	N.D.	N.D.
Rhein	N.D.	N.D.
Aloe emodin	N.D.	N.D.
Chrysophanol	N.D.	N.D.
Chrysazin	N.D.	N.D.
Purpurin	0.89 ± 0.035	13 ± 8.8
Quinizarin	N.D.	N.D.
Leucoquinizarin	N.D.	>300
Alizarin	3.6 ± 0.15	19 ± 10
Anthrarufin	>120	N.D.
Quinalizarin	11 ± 0.87	76 ± 70
Isopurpurin	29 ± 0.36	220 ± 110
Alizarin safirol SE	31 ± 0.24	240 ± 73
Nuclear fast red	9.6 ± 0.26	53 ± 48
Diacerein	N.D.	N.D.
Daunorubicin	18 ± 0.35	100 ± 80
# r^2		0.973

r^2 was calculated using the values of the compounds purpurin, alizarin, quinalizarin, isopurpurin, alizarin safirol SE, nuclear fast red and daunorubicin.

Table S2 IC₅₀ values of the tested compounds against the binding of ANS to DAPK1.

Compound	IC ₅₀ (μ M)
Physcion	N.D.
Rhein	110 ± 23
Aloe emodin	95 ± 41
Chrysophanol	>300
Chrysazin	>300
Purpurin	6.1 ± 1.4
Quinizarin	>300
Leucoquinizarin	N.D.
Alizarin	9.1 ± 0.016
Anthrarufin	N.D.
Quinalizarin	5.8 ± 1.5
Isopurpurin	29 ± 1.9

**Figure S1** Semilog plot of the ANS competitive assay of purpurin.

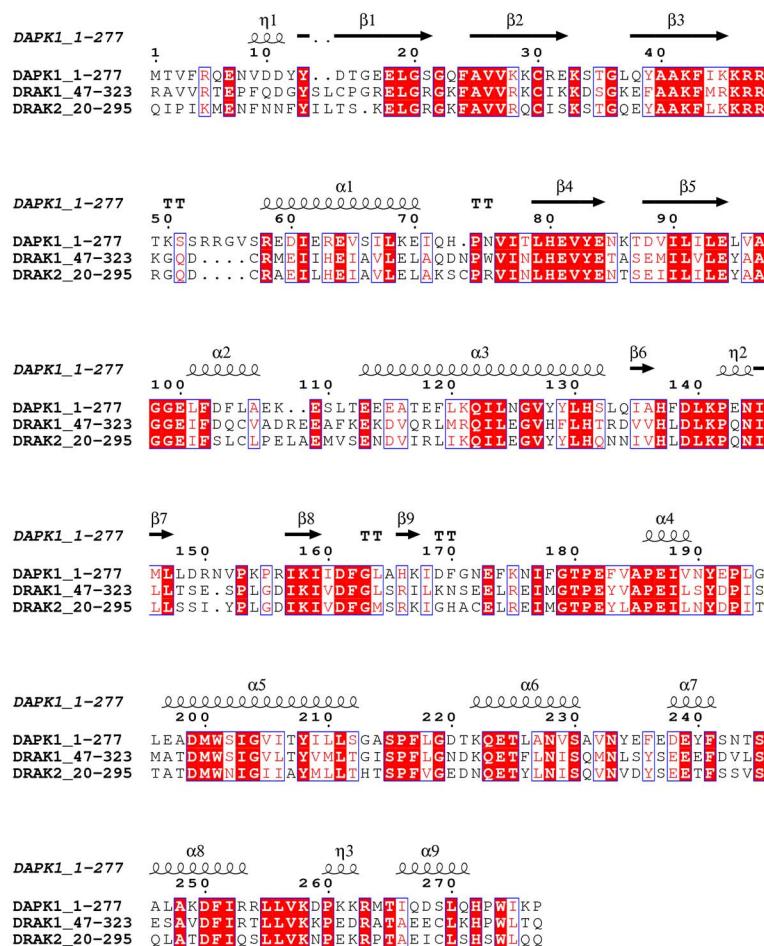


Figure S2 Sequence alignment of DAPK1, DRAK1 and DRAK2.