Supplemental Data for:

Cytochrome P450 binding and bioactivation of tumor-targeted duocarmycin agents

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Table S1. Crystallographic data for ICT2700 and ICT2726 small molecule structures.

	ICT2700	**ICT2726**
Empirical formula	$C_{21}H_{18}ClN_3O_2$	$C_{20}H_{14}ClFN_2O_2$
Formula weight	379.83	368.78
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1$	$P2_12_12_1$
a (Å)	13.0404(4)	5.4139(2)
b (Å)	5.13720(10)	14.3526(6)
c (Å)	14.6273(4)	21.0329(8)
α (°)	90	90
β (°)	115.747(2)	90
γ (°)	90	90
V (Å^3)	882.62(4)	1634.33(11)
Z	2	4
Temperature (K)	173(2)	173(2)
Calc. density (g cm^{-3})	1.429	1.499
Absorption coefficient (mm^{-1})	2.11	2.325
Theta range for data collection (°)	3.35 to 66.32	3.37 to 66.36
Index ranges	$-15 \leq h \leq 13$ $-6 \leq k \leq 5$ $-17 \leq l \leq 17$	$-6 \leq h \leq 5$ $-16 \leq k \leq 16$ $-20 \leq l \leq 24$
Reflections collected	23078	4974
Independent reflections	2880	2573
Refinement method	Full-matrix least squares on F2	Full-matrix least squares on F2
Data/ restraints/ parameters	2880/1.022/318	2573/0.994/292
Goodness-of-fit on F^2	1.022	0.994
Final R indices [I>2sigma(I)]	R = 0.0526, wR = 0.1182	R = 0.0342, wR = 0.0796
R indices (all data)	R = 0.0826, wR = 0.1337	R = 0.0391, wR = 0.0817

Table S2. LC-MS gradient method

Run Time = 30 min

Injection Vol = 10 µl

Flow rate = 0.30 ml/min

Time (min)	% Solvent A (90% H_2O, 10% Acetonitrile, 0.1% furfuryl alcohol)	% Solvent B (90% Acetonitrile, 10% H_2O, 0.1% furfuryl alcohol)
0	60	40
15	40	60
25	0	100
26	60	40

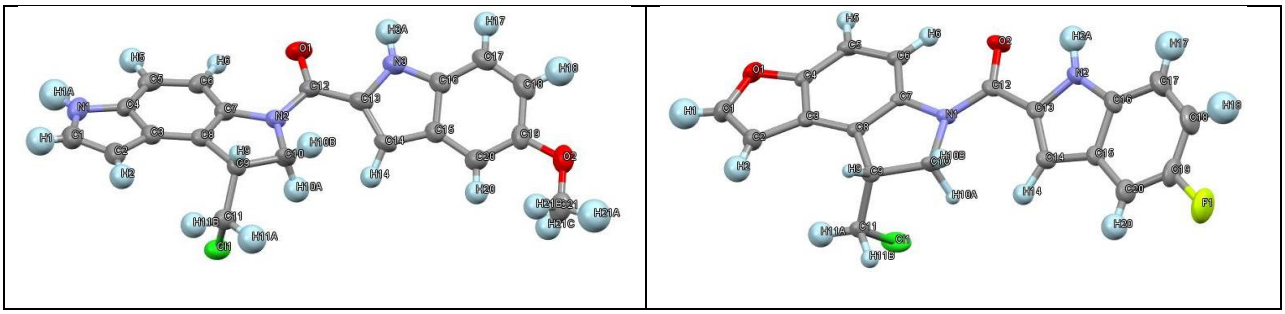

Figure S1. Structures of (*R*)-ICT2700 and (*R*)-ICT2726 as determined by single molecule X-ray crystallography. Thermal ellipsoids drawn at 50% probability level.