S7 Table. Pharmacological and ADME characterization of ML471.
For PK studies, rats (n = 2) were dosed with ML471 at 1 mg/kg i.v. or 10, 20 or 25 mg/kg p.o. and plasma and blood samples were collected for analysis. For blood to plasma ratio, rats (n = 2) were dosed with ML471 at 1 mg/kg and plasma and blood samples were collected for analysis.

PK analysis										
Route	**Dose**	**Matrix**	**AUC (INF)**	**T_{max}**	**C_{max}**	**$T_{1/2z}$**	**CL**	**Vss**	**Vz**	**%F**
	mg/kg		**(h*mM)**	**(h)**	**(nM)**	**(h)**	**(L/h/kg)**	**(L/kg)**	**(L/kg)**	
IV	1	Blood	21.00	0.17	1180	36.6	0.138	6.25	6.54	
IV	1	Plasma	0.70	0.08	1540	2.22	3.84	2.79	12.3	
PO	1	Blood	1.95	16.0	39.3	23.2				9.29
PO	1	Plasma	0.194	0.5	19.1	8.78				27.7
PO	10	Blood	13.15	6.0	261	29.5				9.56
PO	10	Plasma	1.74	0.38	196	9.15				25.2
PO	25	Blood	29.88	8.0	669	30.5				8.72
PO	25	Plasma	2.84	0.75	393	3.57				16.4

Blood to plasma ratio							
Time (h)	0.083	0.25	0.5	1	2	4	8
Mean blood to plasma ratio	0.8	1.5	2.1	5.5	17.8	48.9	113.9

ADME data			
Compound	AlogP/ TSPA	Solubility (μM)	Caco2 P_{app} ($x10^{-6}$ cm/s) (A to B; B to A)
ML471	-1.18/ 189	>100	7.6, 0.17, 1.3.