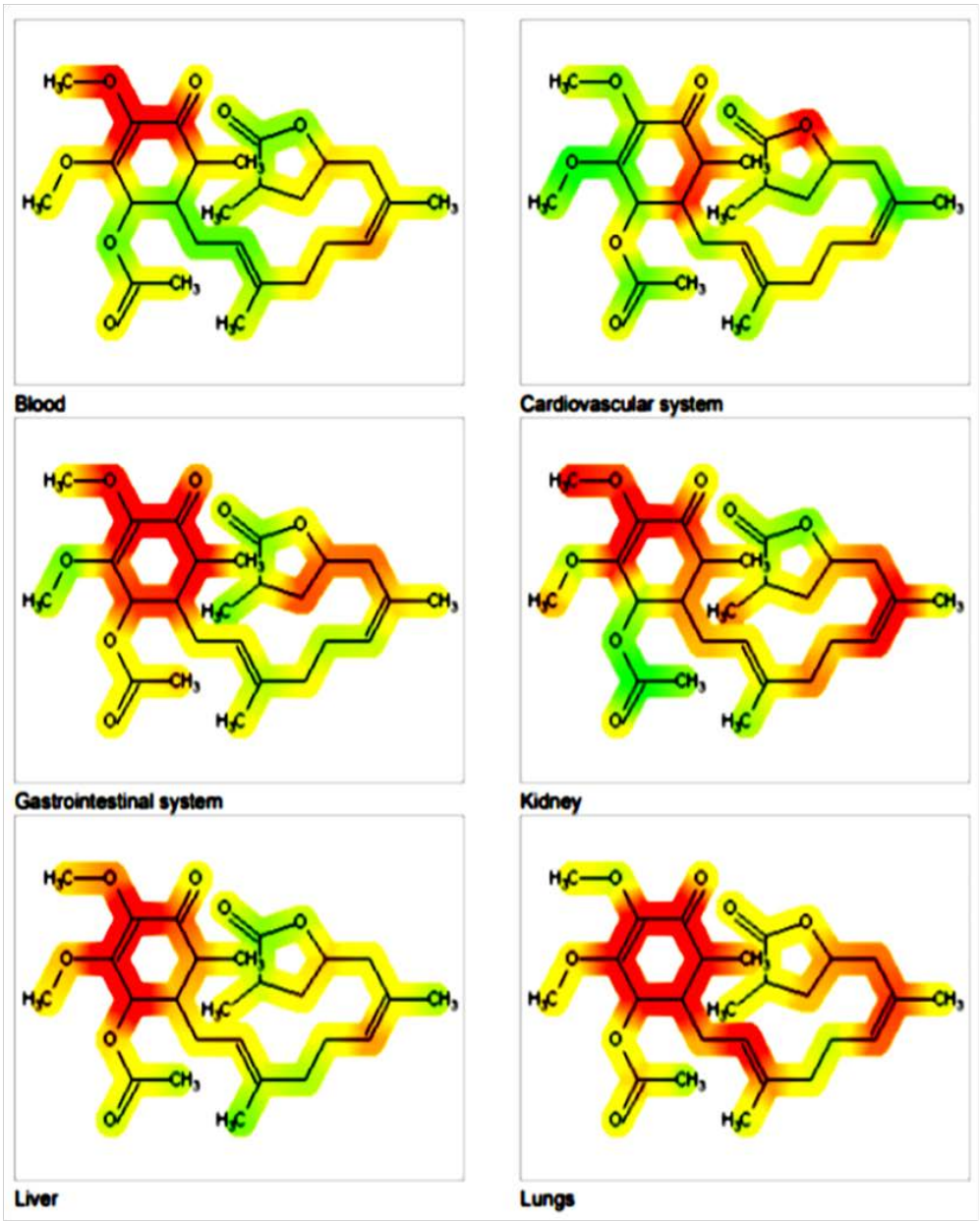
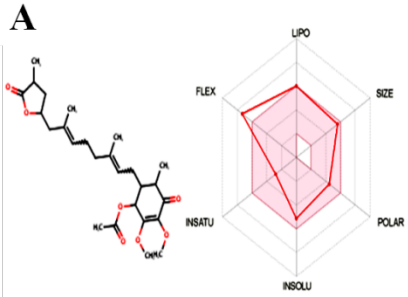


Probability of effect on:

Blood	**0.93**
Cardiovascular system	**0.99**
Gastrointestinal system	**0.99**
Kidney	**0.88**
Liver	**0.78**
Lungs	**0.89**

Supplementary Figure 1

A



SMILES COC1=C(OC)C(=O)C(C(C1OC(=O)C)CC=C(CCC=C(CC1OC(=O)C(C1)C)C)C)C

Physicochemical Properties	
Formula	C26H38O7
Molecular weight	462.58 g/mol
Num. heavy atoms	33
Num. arom. heavy atoms	0
Fraction Csp3	0.65
Num. rotatable bonds	11
Num. H-bond acceptors	7
Num. H-bond donors	0
Molar Refractivity	126.39
TPSA	88.13 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	4.34
Log $P_{o/w}$ (XLOGP3)	5.01
Log $P_{o/w}$ (WLOGP)	4.66
Log $P_{o/w}$ (MLOGP)	2.20
Log $P_{o/w}$ (SILICOS-IT)	4.97
Consensus Log $P_{o/w}$	4.24

Water Solubility	
Log *S* (ESOL)	-5.14
Solubility	3.36e-03 mg/ml ; 7.27e-06 mol/l
Class	Moderately soluble
Log *S* (Ali)	-6.60
Solubility	1.16e-04 mg/ml ; 2.51e-07 mol/l
Class	Poorly soluble
Log *S* (SILICOS-IT)	-4.53
Solubility	1.35e-02 mg/ml ; 2.92e-05 mol/l
Class	Moderately soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-5.56 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: #atoms>70
Veber	No; 1 violation: Rotors>10
Egan	Yes
Muegge	No; 1 violation: XLOGP3>5
Bioavailability Score	0.56
Medicinal Chemistry	
PAINS	0 alert
Brenk	2 alerts: isolated_alkene, more_than_2_esters
Leadlikeness	No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5
Synthetic accessibility	5.84

B

Property	Model Name	Predicted Value	Unit
Toxicity	AMES toxicity	No	Categorical (Yes/No)
Toxicity	Max. tolerated dose (human)	0.092	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	No	Categorical (Yes/No)
Toxicity	hERG II inhibitor	No	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	1.935	Numeric (mol/kg)
Toxicity	Oral Rat Acute Toxicity (LOAEL)	0.491	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	No	Categorical (Yes/No)
Toxicity	Skin Sensitisation	No	Categorical (Yes/No)
Toxicity	*T. Pyriformis* toxicity	0.393	Numeric (log ug/L
Toxicity	Minnow toxicity	-0.077	Numeric (log mM)

C

Species/Administration route	LD50 (mg/kg)	Reliability (RI)
Mouse/Intraperitoneal	270	Borderline(0.39)
Mouse/Oral	3700	Not Reliable(0.21)
Mouse/Intravenous	55	Borderline(0.39)
Mouse/Subcutaneous	250	Not Reliable(0.24)
Rat/Intraperitoneal	680	Borderline(0.46)
Rat/Oral	3400	Not Reliable(0.27)

D

77% probability that compound belongs to any of above categories

84% probability that LD50 =< 5000 mg/kg
92% probability that LD50 > 300 mg/kg

Probabilities of LD50 (mg/kg) ranges:

=< 5	=< 50	=< 300	=< 2000	=< 5000
0.005	0.022	0.083	0.498	0.838
> 50	**> 50**	**> 300**	**> 2000**	**> 5000**
0.995	0.978	0.917	0.502	0.162

Supplementary Figure 2