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Elucidation of drug-like properties in metabolites of *Curcuma angustifolia* Roxb.

Irengbam Rocky Mangangcha[1], Vinay Shankar[2] and Heikham Evelin[3]*

[1]Department of Zoology, Deshbandhu College, University of Delhi, New Delhi 110019, India

[2]Department of Botany, Gaya College, Magadh University, Gaya, Bihar 823001, India

[3]Department of Botany, Rajiv Gandhi University, Doimukh, Arunachal Pradesh 791112, India

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Supplymentry Data

Supplementary Table — Physicochemical/drug likeness properties of the compounds (with highest concentration) identified from *C. angustifolia* Roxb.

Drug likeness	Metabolites					
	9,12-octadecadienoic acid	5-Hydroxymethyl furfural	n-Hexadecanoid acid	Terpineol	Cis-vaccenic acid	Coronarin E
Canonical SMILES	CCCCCC=CCC=CCC CCCCCC(=O)O	OCc1ccc(o1)C=O	CCCCCCCCCCC CCCCCC(=O)O	CC1=CCC(CC1)C (O)(C)C	CCCCCCC=CCCC CCCCCCC(=O)O	C=C1CCC2 C(C1C=Cc1cocc1) (C)CCCC2(C)C
Formula	C18H32O2	C6H6O3	C16H32O2	C10H18O	C18H34O2	C20H28O
MW	280.45	126.11	256.42	154.25	282.46	284.44
Heavy atoms	20	9	18	11	20	21
Aromatic heavy atoms	0	5	0	0	0	5
Fraction Csp3	0.72	0.17	0.94	0.8	0.83	0.6
Rotatable bonds	14	2	14	1	15	2
H-bond acceptors	2	3	2	1	2	1
H-bond donors	1	1	1	1	1	0
MR	89.46	30.22	80.8	48.8	89.94	90.87
TPSA	37.3	50.44	37.3	20.23	37.3	13.14
iLOGP	4.14	0.91	3.85	2.51	4.12	3.85
XLOGP3	6.98	-0.58	7.17	3.39	7.64	6.19
WLOGP	5.88	0.43	5.55	2.5	6.11	5.98
MLOGP	4.47	-1.06	4.19	2.3	4.57	4.52
Silicos-IT Log P	5.77	1.24	5.25	2.17	5.95	5.54

(*Contd.*)

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Consensus Log P	5.45	0.19	5.2	2.58	5.68	5.22
ESOL Log S	-5.05	-0.54	-5.02	-2.87	-5.41	-5.55
ESOL Solubility (mg/mL)	2.49E-03	3.67E+01	2.43E-03	2.10E-01	1.09E-03	8.06E-04
ESOL Solubility (mol/l)	8.87E-06	2.91E-01	9.49E-06	1.36E-03	3.85E-06	2.84E-06
ESOL Class	Moderately soluble	Very soluble	Moderately soluble	Soluble	Moderately soluble	Moderately soluble
Ali Log S	-7.58	-0.01	-7.77	-3.49	-8.26	-6.25
Ali Solubility (mg/mL)	7.42E-06	1.24E+02	4.31E-06	4.95E-02	1.54E-06	1.60E-04
Ali Solubility (mol/l)	2.64E-08	9.80E-01	1.68E-08	3.21E-04	5.46E-09	5.62E-07
Ali Class	Poorly soluble	Very soluble	Poorly soluble	Soluble	Poorly soluble	Poorly soluble
Silicos-IT LogSw	-4.67	-1.35	-5.31	-1.69	-5.39	-5.54
Silicos-IT Solubility (mg/mL)	5.93E-03	5.67E+00	1.25E-03	3.17E+00	1.14E-03	8.26E-04
Silicos-IT Solubility (mol/l)	2.11E-05	4.50E-02	4.88E-06	2.06E-02	4.04E-06	2.90E-06
Silicos-IT class	Moderately soluble	Soluble	Moderately soluble	Soluble	Moderately soluble	Moderately soluble
GI absorption	High	High	High	High	High	Low
BBB permeant	Yes	No	Yes	Yes	No	No
Pgp substrate	No	No	No	No	No	No
CYP1A2 inhibitor	Yes	No	Yes	No	Yes	No
CYP2C19 inhibitor	No	No	No	No	No	Yes
CYP2C9 inhibitor	Yes	No	Yes	No	Yes	Yes
CYP2D6 inhibitor	No	No	No	No	No	No
CYP3A4 inhibitor	No	No	No	No	No	No
log Kp (cm/s)	-3.05	-7.48	-2.77	-4.83	-2.6	-3.64
Lipinski violations	1	0	1	0	1	1
Ghose violations	1	3	0	1	1	1
Veber violations	1	0	1	0	1	0
Egan violations	1	0	0	0	1	1
Muegge violations	1	1	1	2	1	2
Bioavailability Score	0.85	0.55	0.85	0.55	0.85	0.55
PAINS alerts	0	0	0	0	0	0
Brenk alerts	1	1	0	1	1	1
Leadlikeness #violations	2	1	2	1	2	1
Synthetic Accessibility	3.1	2.25	2.31	3.24	3.07	4.85