Birer-Williams et al., "A New Data Repository for Pharmacokinetic Natural Product-Drug Interactions: fr
Drug Metabolism and Disposition

Table S3. Data in the NaPDI Center repository on kratom (Mitragyna speciosa) as of April 2020

dy unique identi	Unique identifier	Natural product binomial	Experiment title	Experiment type name
NPDI-2a2LJw	NPDI-atzv7w	Mitragyna speciosa	Blood brain barrier t	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-_5ld1Q	Mitragyna speciosa	7-Hydroxymitragyni	In Vitro Transporter Inhibitio
NPDI-4xNSSg	NPDI-2HCqSQ	Mitragyna speciosa	Mitraphylline p-gp t	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-2VLnZA	Mitragyna speciosa	Mitragynine P-gp tra	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-iGAFkQ	Mitragyna speciosa	7-Hydroxymitragyni	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-mJ7zbw	Mitragyna speciosa	Inhibition of P-gp by	In Vitro Transporter Inhibitio
NPDI-4xNSSg	NPDI-ruor3g	Mitragyna speciosa	Mitraphylline P-gp t	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-TjrSew	Mitragyna speciosa	7-hyrdoxymitragyni	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-yG9O9A	Mitragyna speciosa	Mitragynine p-gp tra	In Vitro Transporter Kinetics
NPDI-6PgT2w	NPDI-FqB7Jg	Mitragyna speciosa	Kratom Metabolomi	Metabolomics
NPDI-9C7QHg	NPDI-3C6gmg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-3eovVg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-4_m2Gw	Mitragyna speciosa	Inhibition of UGT1A	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-4do0FA	Mitragyna speciosa	Inhibition of UGT1A	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-5VhYlA	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-9spGvg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-bX8XPA	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-ipamgg	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-Nl2Cww	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-NZQ3aw	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-pMOhyQ	Mitragyna speciosa	Inhibition of UGT in	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-Q5Hs5A	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-u96XKg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-Ve-SYA	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-ZTY8Qw	Mitragyna speciosa	Inhibition of UGT2B	In Vitro Enzyme Inhibition
NPDI-Algmhw	NPDI-_DqAGQ	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-_MysYg	Mitragyna speciosa	Mitragynine non-inc	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-_rs20g	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI--0S--Q	Mitragyna speciosa	Dimethyl sulfoxide r	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-5_pf-w	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-7sdBtQ	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-dQtQ2g	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-exquAQ	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-J0Eryw	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-LcX0tA	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-LD3MZA	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-sYa6vQ	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-Ww9TTQ	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-_xT8iQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-1t276A	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-1ZEwLw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction

NPDI-ct9Vuw	NPDI-20NK8g	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-2go-tA	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-32vFwA	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-3zWYhw	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-5qjXYw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-6g0qjA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-7AsxQw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-7mTHsg	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-8cNctg	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-8IvpNA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CeYlQA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CHz7Cw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CUKuJg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CyLsKQ	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-d5GHXw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-e6NVBw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-EAC81Q	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-ErfPVw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-feWibg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-FEZZeA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-GGux5Q	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-HcJ6bw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-iA1bqw	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-iaYQ2g	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-IczeVA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-JfsBYg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-jv2gJw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI--K-VUA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-l9MZKg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-lKNl2g	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-MbgjOA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Nhyfdg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-PBicLA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-poKS5A	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-PQ_z9Q	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Q_-B1A	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Q72VHA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-qToNMQ	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-r08Qaw	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-R0XxIA	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-R6WiQw	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-SIOBQQ	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-swW6FA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-SzdBUg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-tQOeEQ	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-tsaRoQ	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-u4e76g	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio

NPDI-ct9Vuw	NPDI-uo42Dw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-UwflXA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-v1ALwQ	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-vil20w	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-VRuDCg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-wkoAog	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI--Wn8sg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-wS5EeQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-WzrXMA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-X_71_g	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-x_T2_w	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-XaTzlQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-XY34BQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-y0jePg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-yHa9yA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Yic2CQ	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-ymobwA	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-YXF4Ww	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-Z3w0mg	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-z5snmg	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-ZI6hHA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-ZpaPqg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-d8OUzg	NPDI-4_UdSg	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-515DHw	Mitragyna speciosa	Inhibition kinetics of	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-71pBaQ	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-7-Gg-g	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-A66pwQ	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-bOmVTQ	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-EjMg0g	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI--jKvig	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-ksOM2w	Mitragyna speciosa	Inhibition kinetics of	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-o6FZsw	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-o8WmjA	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-ov597g	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-QbMPuw	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-sfeVpQ	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-Tr3Eyg	Mitragyna speciosa	Inhibition kinetics of	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-vr5BAA	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-XFPmtA	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-xK3lmw	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-Xrn4xQ	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-dIgOyA	NPDI-38uQKg	Mitragyna speciosa	Mitragynine metabc	In Vitro Enzyme Screen
NPDI-eReNjw	NPDI-_MFsyA	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-0hNq0Q	Mitragyna speciosa	Weak Inhibition of M	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-17YRkg	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-1Cjyxg	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-1vxnrQ	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition

NPDI-eReNjw	NPDI-2seH4Q	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-4AITQg	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-4HfEdA	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-5LuVNQ	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-7PU97Q	Mitragyna speciosa	Inhibition of Coryna	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-9xzv_Q	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-aGXuxA	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-aNb3lw	Mitragyna speciosa	Weak Inhibition of P	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-B_7tOA	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-BLzT_g	Mitragyna speciosa	Weak Inhibition of M	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-bXPXRQ	Mitragyna speciosa	Inhibition of Coryna	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-c_gPeA	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-cimaKA	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-DLH-JQ	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-eMZPbA	Mitragyna speciosa	Inhibition of 7-hydro	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-gxj_UA	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-iASYyA	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-J2PdQQ	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-JqmF7w	Mitragyna speciosa	Inhibition of Speciosc	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-K9DvIg	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-kew9FQ	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-laH1lA	Mitragyna speciosa	Weak Inhibition of M	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-o56vpA	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-olaGPQ	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-Oq9KmA	Mitragyna speciosa	Inhibition of Speciog	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-P2Nw6g	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-qMnZyA	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-QQeDSQ	Mitragyna speciosa	Inhibition of Speciog	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-qWS53g	Mitragyna speciosa	Inhibition of Coryna	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-s8ImuA	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-sN1pZA	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-t32_Ig	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-TTv3Iw	Mitragyna speciosa	Inhibition of Speciosc	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-Ua1CeQ	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-U-ajPw	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-ULP_qQ	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-V_oQog	Mitragyna speciosa	Weak Inhibition of P	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-WakYGw	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-WIpfxQ	Mitragyna speciosa	Inhibition of Speicog	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-wo-wRw	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-XeGihA	Mitragyna speciosa	Weak Inhibition of P	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-XQCOGw	Mitragyna speciosa	Inhibition of Speciosc	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-zKam8g	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-Zvn2gg	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-FfN_4A	NPDI-d5Gm3Q	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition
NPDI-FfN_4A	NPDI-MpwNXw	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition
NPDI-FfN_4A	NPDI-payj8A	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition

NPDI-FfN_4A	NPDI-TZxzig	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition
NPDI-JHPnhA	NPDI-4k7d3A	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-8GmUTQ	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-cxxGnA	Mitragyna speciosa	Control P-gp digoxin	In Vitro Transporter Kinetics
NPDI-JHPnhA	NPDI-DEOq7g	Mitragyna speciosa	Down regulation of	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-gdI_mg	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-GETspg	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-nWIYpA	Mitragyna speciosa	Down regulation of	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-U0t5zQ	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-Ue8YDg	Mitragyna speciosa	Permeability of mitr	In Vitro Transporter Kinetics
NPDI-JHPnhA	NPDI-WL-VKw	Mitragyna speciosa	Control inhibition of	In Vitro Transporter Inhibitio
NPDI-JHPnhA	NPDI-ye4dPw	Mitragyna speciosa	Down regulation of	In Vitro Transporter Inductio
NPDI-PSB8Vg	NPDI-79TG7g	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-Df2Xyw	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-FnVAqw	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-gWxQZg	Mitragyna speciosa	Inhibition of CYP2D6	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-H6ZqbA	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-jkwBEg	Mitragyna speciosa	Inhibition of CYP2C9	In Vitro Enzyme Inhibition
NPDI-vQCHYg	NPDI-XuAtuQ	Mitragyna speciosa	Characterization of I	Characterization of Material
NPDI-XtvOZQ	NPDI-_PhwAA	Mitragyna speciosa	Inhibition of CYP2D6	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-1tFkCA	Mitragyna speciosa	Inhibition of CYP2C9	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-d0noGQ	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-d-iKog	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-M8nR1A	Mitragyna speciosa	Enzyme kinetics of C	In Vitro Enzyme Kinetics
NPDI-XtvOZQ	NPDI-m-NOOw	Mitragyna speciosa	Enzyme kinetics of C	In Vitro Enzyme Kinetics
NPDI-XtvOZQ	NPDI-o-4ZoA	Mitragyna speciosa	Enzyme kinetics of C	In Vitro Enzyme Kinetics
NPDI-XtvOZQ	NPDI-v2Z25g	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-ypADxQ	Mitragyna speciosa	No inhibition of CYP	In Vitro Enzyme Inhibition
NPDI-Yknaag	NPDI-E56YVg	Mitragyna speciosa	Mitragynine Inhibiti	In Vitro Transporter Inhibitio
NPDI-Yknaag	NPDI-vs2diA	Mitragyna speciosa	R123 Transport Subs	In Vitro Transporter Kinetics

om Chemical Characterization to Clinical Studies",

Overall effect

In Vitro Transport
In Vitro Transporter Inhibition
In Vitro Transport
No In Vitro Transport Activity
No In Vitro Transport Activity
In Vitro Transporter Inhibition
In Vitro Transport
No In Vitro Transport Activity
No In Vitro Transport Activity

In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
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In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction

In Vitro Enzyme Induction
In Vitro Transporter Induction
In Vitro Enzyme Induction
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In Vitro Transporter Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
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In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Transporter Induction
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In Vitro Transporter Induction

In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Induction
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In Vitro Transporter Induction
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In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Detectable Metabolism
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition

In Vitro Enzyme Negligible Inhibition
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In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition

In Vitro Enzyme Inhibition
In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Transport
In Vitro Transporter Down Regulation
In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Transporter Down Regulation
In Vitro Transporter Induction
No In Vitro Transport Activity
In Vitro Transporter Inhibition
In Vitro Transporter Down Regulation
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition

In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Detectable Kinetic Metabolism
In Vitro Detectable Kinetic Metabolism
In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Transporter Inhibition
In Vitro Transport

Object compound name	Object metabolite compound name
mitragynine	
calcein-am	
mitraphylline	
mitragynine	
7-hydroxymitragynine	
calcein-am	
mitraphylline	
7-hydroxymitragynine	
mitragynine	
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide

midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
dextromethorphan	dextrorphan
dextromethorphan	dextrorphan
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
diclofenac	4'-hydroxydiclofenac
diclofenac	4'-hydroxydiclofenac
mitragynine	7-hydroxymitragynine
phenacetin	acetaminophen
diclofenac	4'-hydroxydiclofenac
dextromethorphan	dextrorphan
phenacetin	acetaminophen
phenacetin	acetaminophen

testosterone	6beta-hydroxytestosterone
dextromethorphan	dextrorphan
diclofenac	4'-hydroxydiclofenac
phenacetin	acetaminophen
midazolam	1'-hydroxymidazolam
testosterone	6beta-hydroxytestosterone
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
testosterone	6beta-hydroxytestosterone
amodiaquine	n-desethylamodiaquine
testosterone	6beta-hydroxytestosterone
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
diclofenac	4'-hydroxydiclofenac
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
testosterone	6beta-hydroxytestosterone
amodiaquine	n-desethylamodiaquine
amodiaquine	n-desethylamodiaquine
dextromethorphan	dextrorphan
midazolam	1'-hydroxymidazolam
phenacetin	acetaminophen
amodiaquine	n-desethylamodiaquine
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
testosterone	6beta-hydroxytestosterone
testosterone	6beta-hydroxytestosterone
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
amodiaquine	n-desethylamodiaquine
diclofenac	4'-hydroxydiclofenac
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
amodiaquine	n-desethylamodiaquine
dextromethorphan	dextrorphan
phenacetin	acetaminophen
midazolam	1'-hydroxymidazolam
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
amodiaquine	n-desethylamodiaquine
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
phenacetin	acetaminophen
diclofenac	4'-hydroxydiclofenac
3-cyano-7-ethoxycoumarin	3-cyano-7-hydroxycoumarin
3-cyano-7-ethoxycoumarin	3-cyano-7-hydroxycoumarin
3-[2-(n,n-diethyl-n-methylammoni	3-[2-(n,n-diethyl-n-methylammonium)ethyl]-

7-benzyloxy-4-(trifluoromethyl)-co 7-hydroxy-4-(trifluromethyl)-coumarin

digoxin

mitragynine
digoxin

luciferin 6â€™benzyl ether (luciferi luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
ethylene glycol ester of luciferin 6â luciferin
ethylene glycol ester of luciferin 6â luciferin
6â€™deoxyluciferin (luciferin h) luciferin
6â€™deoxyluciferin (luciferin h) luciferin

ethylene glycol ester of luciferin 6â luciferin
6â€™deoxyluciferin (luciferin h) luciferin
ethylene glycol ester of luciferin 6â luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
6â€™deoxyluciferin (luciferin h) luciferin
ethylene glycol ester of luciferin 6â luciferin
6â€™deoxyluciferin (luciferin h) luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
rhodamine 123
rhodamine 123

Precipitant compound name

7-hydroxymitragynine

mitragynine

7-hydroxymitragynine
buprenorphine
diclofenac
7-hydroxymitragynine
mitragynine
mitragynine
ketamine
ketamine
mitragynine
diclofenac
buprenorphine
7-hydroxymitragynine
diclofenac
ketamine
buprenorphine
dimethyl sulfoxide
mitragynine
dimethyl sulfoxide
dimethyl sulfoxide
mitragynine
mitragynine
dimethyl sulfoxide
dimethyl sulfoxide
mitragynine
mitragynine
mitragynine
mitragynine
mitragynine
mitragynine
speciogynine
isorotundifoline
mitragynine

rifampicin
mitragyna speciosa alkaloid rich fraction
omeprazole
rifampicin
paynantheine
7-hydroxymitragynine
corynoxine b
mitragynine
speciogynine
mitragyna speciosa alkaloid rich fraction
isospeciofoline
corynoxine
7betaâ€hydroxyâ€7hâ€mitraciliatine
methanolic extract of kratom
7-hydroxymitragynine
corynoxine
speciogynine
speciogynine
7-hydroxymitragynine
isorotundifoline
corynoxine
mitragyna speciosa alkaloid rich fraction
dexamethasone
omeprazole
paynantheine
paynantheine
isospeciofoline
corynoxine b
corynoxine
methanolic extract of kratom
methanolic extract of kratom
corynoxine b
7betaâ€hydroxyâ€7hâ€mitraciliatine
paynantheine
7betaâ€hydroxyâ€7hâ€mitraciliatine
methanolic extract of kratom
mitragynine
corynoxine b
paynantheine
corynoxine
corynoxine
speciogynine
mitragyna speciosa alkaloid rich fraction
mitragyna speciosa alkaloid rich fraction
corynoxine b
isospeciofoline
7betaâ€hydroxyâ€7hâ€mitraciliatine

isorotundifoline
mitragyna speciosa alkaloid rich fraction
isospeciofoline
mitragynine
7-hydroxymitragynine
isorotundifoline
isospeciofoline
7-hydroxymitragynine
7-hydroxymitragynine
dexamethasone
isospeciofoline
mitragynine
7betaâ€hydroxyâ€7hâ€mitraciliatine
mitragynine
7betaâ€hydroxyâ€7hâ€mitraciliatine
isorotundifoline
isorotundifoline
corynoxine b
methanolic extract of kratom
paynantheine
speciogynine
methanolic extract of kratom
mitragynine
mitragynine
methanolic extract of kratom
methanolic extract of kratom
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mitragynine
mitragynine

speciogynine
mitragynine
mitragynine
corynantheidine
7-hydroxymitragynine

speciociliatine
quinidine
paynantheine
alpha-naphthoflavone
corynantheidine
ketoconazole
corynantheidine
paynantheine
speciogynine
mitragynine
corynantheidine
mitragynine
7-hydroxymitragynine
7-hydroxymitragynine
7-hydroxymitragynine
(s)-(+)-n-3-benzylnirvanol
7-hydroxymitragynine
mitragynine
speciociliatine
paynantheine
ketoconazole
mitragynine
corynantheidine
7-hydroxymitragynine
speciogynine
speciogynine
corynantheidine
speciogynine
corynantheidine
montelukast
speciogynine
sulfaphenazole
speciociliatine
mitragynine
7-hydroxymitragynine
speciociliatine
paynantheine
paynantheine
speciogynine
paynantheine
paynantheine
speciociliatine
speciociliatine
speciociliatine
mitragynine
mitragynine
mitragynine

mitragynine
rifampicin
rifampicin

mitragynine
rifampicin
rifampicin
mitragynine
rifampicin

quinidine
quinidine
ketoconazole
methanolic extract of kratom
quinidine
methanolic extract of kratom
sulfaphenazole
methanolic extract of kratom

mitragynine
mitragynine
quinidine
ketoconazole

sulfaphenazole
mitragynine
mitragynine

Enzyme name

UGT2B7
UGT1A1
UGT1A1
UGT1A1
UGT1A1
UGT2B7
UGT2B7
UGT
UGT
UGT2B7
UGT
UGT
UGT
UGT1A1
UGT2B7
CYP1A2
CYP2D6
CYP3A4
CYP2D6
CYP3A4
CYP1A2
CYP3A4
CYP1A2
CYP1A2
CYP3A4
CYP1A2
CYP3A4
CYP2D6

CYP1A2
CYP3A4

CYP3A4

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CYP3A4

CYP1A2
CYP3A4
CYP3A
CYP3A
CYP2C9
CYP3A
CYP3A
CYP2C9
CYP3A
CYP2D6
CYP2D6
CYP2D6
CYP3A
CYP3A
CYP3A
CYP2D6
CYP3A
CYP3A
CYP2D6
CYP2C9
CYP2C9
CYP3A4
CYP1A2
CYP2C9
CYP2D6
CYP1A2
CYP1A2

CYP3A5
CYP2D6
CYP2C9
CYP1A2
CYP3A5
CYP3A5
CYP2C19
CYP3A5
CYP2C8
CYP3A5
CYP2C9
CYP3A5
CYP2D6
CYP2C9
CYP2C19
CYP2C19
CYP3A5
CYP2C8
CYP2C8
CYP2D6
CYP3A5
CYP1A2
CYP2C8
CYP3A5
CYP2D6
CYP3A5
CYP3A5
CYP3A5
CYP2D6
CYP2C8
CYP2C9
CYP2C9
CYP3A5
CYP2C19
CYP2C8
CYP2D6
CYP1A2
CYP3A5
CYP2C19
CYP2C19
CYP2C8
CYP2C19
CYP1A2
CYP2C9
CYP2C19
CYP1A2
CYP2D6

CYP3A4

CYP3A4
CYP3A4
CYP2D6
CYP2D6
CYP2C9
CYP2C9

CYP2D6
CYP2C9
CYP2D6
CYP3A4
CYP3A4
CYP2C9
CYP2D6
CYP2C9
CYP3A4

Transporter name	Control data	Test system name	IC50 shift data
P-gp (ABCB1)	FALSE	Other cells	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
	FALSE		FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	TRUE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE

	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
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P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
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P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE

P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
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P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
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	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
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	FALSE	Not available	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
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P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE

Research organization's overall effect cutof	ditional informat
P < 0.001	
EC50 positive control verapamil (22.3Â± 1.4 Î¼M)	
ER of 2	
ER of 2	
2	
positive control verapamil (22.3Â± 1.4 Î¼M)	
ER of 2	
ER of 2	
ER of 2	
IC50 > 10 μM are low potential inhibitors. 1 μM < IC	
IC50 > 10 μM are low potential inhibitors. 1 μM < IC	
IC50 > 10 Î¼M are low potential inhibitors. 1 Î¼M < IC50 < 1	
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IC50 > 10 μM are low potential inhibitors. 1 μM < IC	
IC50 > 10 Î¼M are low potential inhibitors. 1 Î¼M < IC50 < 1	
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Not specified	Fig. 3. Positive cc
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IC50<10 µM for reversible inhibition and IC50s	
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50% inhibition at the highest tested concer	Three methanoli
IC50<10 µM for reversible inhibition and IC50s	
50% inhibition at the highest tested concentration	
IC50<10 µM for reversible inhibition and IC50s	
IC50<10 µM for reversible inhibition and IC50s	
N/A	
50% inhibition at the highest tested concer	Three methanoli
IC50<10 µM for reversible inhibition and IC50s	
50% inhibition at the highest tested concentration	
50% inhibition at the highest tested concer	Three methanoli
50% inhibition at the highest tested concentration	
N/A	
50% inhibition at the highest tested concentration	
IC50<10 µM for reversible inhibition and IC50s	
IC50<10 µM for reversible inhibition and IC50s	
IC50<10 µM for reversible inhibition and IC50s	

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p < 0.05 compared with control	
p < 0.05 compared with control	
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p < 0.05 compared with control	
p < 0.05 compared with control	
p < 0.05 compared with control	
p < 0.05 compared with control	
p < 0.05 compared with control	
(not provided)	
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p < 0.05 compared with control	
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	Comparison with
High probability of interaction if their IC50	values are less th
High probability of interaction if their IC50	values are less th
High probability of interaction if their IC50	Positive control
High probability of interaction if their IC50	Positive control
High probability of interaction if their IC50	Positive control
High probability of interaction if their IC50	values are less th
Unspecified	p<0.05 Values de
Unspecified	Positive control -

Experimental conditions comment

The amount of protein, the incubation time and the concentration of 4-MU used in the measurement of 4-MU glu
The amount of protein, the incubation time and the concentration of 4-MU used in the measurement of 4-MU glu
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Pooled human liver microsomes were purchased from Sigma-Aldrich; The enzyme activity assay mixture (250 Î¼L)
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The amount of protein, the incubation time and the concentration of 4-MU used in the measurement of 4-MU glu
ɔntrol: 50 uM omeprazole, ~4 ± 2 x 1012 copies

ɔntrols and results: CYP1A2: 50 uM omeprazole, mean ~1.2 ± 0.2-fold, n = 2 CYP2D6: 5uM quinidine,
e control used
ɔression of CYP3A4 was only slightly induced by mitragynine at all concentrations tested. Although this induction w

5 uM dexamethasone with ~1.6 ± 0.4 x 1013 copies

icle control used; unknown what solvent(s) and what % of those solvent(s) constituted the vehicle control.
icle control used; unknown what solvent(s) and what % of those solvent(s) constituted the vehicle control.
7â€benzyloxyâ€4â€(trifluoromethyl)coumarin (BFC) 2Î¼M was the fluorescent substrate used for CYP3A4 activity r

Positive control
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Positive control
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3â€Cyanoâ€7â€ethoxycoumarin (CEC) 1 Î¼M was the fluorescent substrate used for CYP1A2 activity measurement
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Positive control3â€Cyanoâ€7â€ethoxycoumarin (CEC) 1 Î¼M was the fluorescent substrate used for CYP1A2 activit
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7â€benzyloxyâ€4â€(trifluoromethyl)coumarin (BFC) 2Î¼M was the fluorescent substrate used for CYP3A4 activity r
A cocktail of probe substrates for CYP2C9 (diclofenac), CYP2D6 (dextromethorphan), and CYP3A (midazolam) was u
Methanol (0.8 % v/v) served as solvent control. 6',7'-Dihydroxybergamottin (1 and 2 ÂµM) served as a positive con
Methanol (0.8 % v/v) served as solvent control. Sulphaphenazole (1 ÂµM), quinidine (2 ÂµM), and ketoconazole (0
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Methanol (0.8 % v/v) served as solvent control. Quinidine (2 ÂµM) served as positive control inhibitors of CYP2D6 a
Methanol (0.8 % v/v) served as solvent control. Sulphaphenazole (1 ÂµM), quinidine (2 ÂµM), and ketoconazole (0
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Table S2

Table S2

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Table S2

Table S2

Table S2

Table S2

Positive controls sulfaphenazole, quinidine, and ketoconazole were purchased from Sigma Chemicals (St. Louis, US
M. speciosa methanolic extract was prepared in-house from the leaves of the plant. This assay was carried out usir
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ı Literature:A recent report [1] found that depending on source material, mitragyninewas detected in kratom (M. sp
Mitragynine was isolated in-house. This assay was carried out using the P450-Gloâ„¢ Screening Systems from Prom
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Positive inhibitors which are sulfaphenazole, quinidine and ketoconazole were purchased from Sigma Chemicals (S
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Positive inhibitors which are sulfaphenazole, quinidine and ketoconazole were purchased from Sigma Chemicals (S
Mitragynine was isolated in-house. This assay was carried out using the P450-Gloâ„¢ Screening Systems from Prom
Preincubated with KRB for 60 min
· verapamil (5 µM) ER of 7.4

Experimental results comment

positive control verapamil (22.3Â± 1.4 Î¼M)Fig 1S (with exact values in text pg 574)
p<0.001ER for 10 uM was 5.9 also significant(Table 4)
Results above for 5 uMER for 10 uM values reported: 1.1 N=3(Table 3)
ER for 10 uM also 1.2(Table 4)
positive control verapamil (22.3Â± 1.4 Î¼M) Fig 1S (with exact values in text pg 574)
ER for 10 uM is 3.4p<0.001(Table 3)
ER for 10 uM also 1.2(Table 3)
ER for 10 uM also 1.1(Table 4)

Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: 3 Â± 5%0.1 Î¼
The IC50 values were all greater than the highest concentrations used (IC50 > 1000 Î¼M) since inhibition at more t
Concentration ofÂ precipitant and % inhibition of UGT1A1 (values estimated from figure 4) (p < 0.05 for all values)
Concentration ofÂ precipitant and % inhibition of UGT1A1 (values estimated from figure 4)0.01 Î¼M: 6 Â± 1%0.1 Î¼
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more th
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more th
Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: -5 Â± 6%0.1 Î
The IC50 values were all greater than the highest concentrations used (IC50 > 1000 Î¼M) since inhibition at more tl
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more tha
Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: -1 Â± 3%0.1 Î
Concentration of precipitant and % inhibition of pooled human liver microsomes (values estimated from figure 3) (
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more tha
Concentration of precipitant and % inhibition of pooled human liver microsomes (values estimated from figure 3) (
The IC50 values were all greater than the highest concentrations used (IC50 > 1000 Î¼M) since inhibition at more t
Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: -8 Â± 4%0.1 Î
Figure 2. 3 copies, 0 copy number. Positive control: 50 uM omeprazole, ~4-6 x 1012 copies
"There was no significant change in the mRNA expression of CYP2D6 when the HepG2 cells were treated with mitr
Figure 3. P-value not reported.Â Positive controls and results: CYP1A2: 50 uM omeprazole, mean ~1.2Â Â± 0.2-fold
Fig. 2. Approximately ~1.2-1.5 x 1012 copies. No positive control used.
(Figure 2)The expression of CYP3A4 was only slightly induced by mitragynine at all concentrations tested. Although
68.5% of induction compared to positive control at [25 uM]
Figure 2. Approximately 4.9 Â± 0.3 x 1012 copies. Positive control: 5 uM dexamethasone with ~1.6Â Â± 0.4 x 1013
(Figure 4)
"The induction was only statistically significant at 25 lM and induction relative to omeprazole was approximately 4
"Mitragynine appeared to moderately induce the enzymatic activity of CYP3A4. The increase was gradual and the c
the protein expression of CYP1A2 showed an increased in relative values from 0.5uM onwards as compared to con
The protein expression of CYP3A4 was slightly induced after treatment with mitragynine, with higher relative prot
CYP2D6 protein expression was found to be increased within the range of 1-5 uM of mitragynine relative to the ur
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.57 Â± 0.03 fold (p < 0.01)1.1 Î¼M: 1.07
Estimated from Figure 3a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 6.2 Â± 0.4 fold (p < 0.01)1.1 Î¼M: 3.3 Â± 0.2
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.95 Â± 0.1 fold 1.1 Î¼M: 0.9 Â± 0.05 fold

Positive controlEstimated from Figure 2a***P<0.001
Estimated from Figure 4bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 0.45 Â± 0.06 fold (p < 0.01)3.3 Î¼g/m
Positive control***P<0.001
Positive controlEstimated from Figure 2b***P<0.001
Estimated from Figure 4aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.3 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.2 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 2.0 Â± (
Estimated from Figure 2b***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 1.8 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.1 Â± 0.(
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p <0.01)1.1 Î¼M: 1.3 Â± 0.1
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p < 0.01)1.1 Î¼M: 1.5 Â± 0.1
Estimated from Figure 2bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.0 Â± 0.05 fold (p < 0.05)3.3 Î¼g/ml
Estimated from Figure 3a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 3.4 Â± 0.3 fold (p < 0.05)1.1 Î¼M: 2.1 Â± 0.2
Estimated from Figure 2b***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.0 Â± 0.(
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.9 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.6 Â± (
Estimated from Figure 4a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.2 Â± 0.1 fold (p < 0.01)3.3 Î¼g/ml: 1.4
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.3 Â± 0.1 fold (p < 0.01)1.1 Î¼M: 1.7 Â± 0.1
Estimated from Figure 4aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.2 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.7 Â±0
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.2 Â± 0.1 fold1.1 Î¼M: 1.0 Â± 0.05 fold
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.05 Â± 0.1 fold 1.1 Î¼M: 1.0 Â± 0.05 fold
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.05 fold (p < 0.01)1.1 Î¼M: 1.3 Â±
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.3 Â± (
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.8 Â± 0.4 fold (p < 0.05)1.1 Î¼M: 2.7 Â± (
Estimated from Figure 4a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.7 Â± 0.3 fold (p < 0.001)3.3 Î¼g/ml: 1
Positive controlEstimated from Figure 4a*** P<0.001
Positive controlEstimated from Figure 3b***P<0.001
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.0 Â± 0.05 fold 1.1 Î¼M: 0.9 Â± 0.1 fold
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.85 Â± 0.05 fold1.1 Î¼M: 0.80 Â± 0.05 fo
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.6 Â± 0.1
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.8 Â± 0.3 fold (p < 0.05)1.1 Î¼M: 2.3 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.1 Â± (
Estimated from Figure 3a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 3.4 Â± 0.4 fold (p < 0.05)3.3 Î¼g/ml: 1.6
Estimated from Figure 2aMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 1.9 Â± 0.1 fold (p < 0.05)3.3 Î¼g/ml:
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.9 Â± (
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.3 Â± 0.4 fold (p < 0.05)1.1 Î¼M: 1.5 Â± (
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.8 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.1 Â± (
Estimated from Figure 3bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.5 Â± 0.3 fold (p < 0.05)3.3 Î¼g/ml:
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.6 Â± 0.3 fold (p < 0.01)1.1 Î¼M: 1.8 Â± (
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.7 Â± 0.2
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.7 Â± 0.4 fold (p < 0.05)1.1 Î¼M: 1.8 Â± (
Estimated from Figure 4b*** p < 0.001 for 10Â Î¼M (see above)3.3 Î¼M: 0.51 Â± 0.04 fold (p < 0.05)1.1 Î¼M: 1.01 A
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.5 Â± 0.5 fold (p < 0.01)1.1 Î¼M: 1.0 Â± (
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.5 Â± 0.3 fold (p < 0.01)1.1 Î¼M: 1.5 Â± (
Estimated from Figure 3a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 4.4 Â± 0.9 fold (p < 0.01)3.3 Î¼g/ml: 1.9
Estimated from Figure 3bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 3.6 Â± 0.5 fold (p < 0.01)3.3 Î¼g/ml:
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.2 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.0 Â± (
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.3 Â± (
Estimated from Figure 4aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.6 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.2 Â± (

Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.4 Â± 0.0
Estimated from Figure 2aMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.0 Â± 0.3 fold (p < 0.05)3.3 Î¼g/ml:
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.9 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.4 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.3 Â± 0.3 fold1.1 Î¼M: 0.9 Â± 0.1 fold
Estimated from Figure 3bMeasurement forÂ 10Â Î¼M (see above)3.3 Î¼M: 2.2 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.7 Â±
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.1 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.3 fold (p < 0.05)1.1 Î¼M: 1.2 Â± (
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.47 Â± 0.06 fold (p < 0.01)1.1 Î¼M: 1.06
Estimated from Figure 3a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 5.2 Â± 0.7 fold (p < 0.01)1.1 Î¼M: 3.8 Â± 0.7
Positive controlEstimated from Figure 4b*** P<0.001
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.57 Â± 0.04 fold (p < 0.05)1.1 Î¼M: 1.02
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.60 Â± 0.05 fold (p < 0.05)1.1 Î¼M: 1.00
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.53 Â± 0.07 fold (p < 0.01)1.1 Î¼M: 0.97
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.2 Â± 0.5 fold (p < 0.01)1.1 Î¼M: 2.3 Â± (
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.6 Â± 0.25 fold (p < 0.05)1.1 Î¼M: 1.0 Â±
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.3 Â± 0.2 fold1.1 Î¼M: 1.0Â± 0.05 fold
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.55 Â± 0.06 fold (p < 0.05)1.1 Î¼M: 1.03
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.58 Â± 0.03 fold (p < 0.05)1.1 Î¼M: 0.97
Estimated from Figure 4bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 0.50 Â± 0.02 fold (p < 0.01)3.3 Î¼g/m
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.57 Â± 0.08 fold (p < 0.05)1.1 Î¼M: 1.05
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.7 Â± 0.6 fold (p < 0.01)1.1 Î¼M: 2.2 Â±0
Estimated from Figure 2bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.0 Â± 0.05 fold (p < 0.05)3.3 Î¼g/ml
A 7-fold shift in IC50was observed towards CYP3A activity in HLM, 18.9 Â±1.8 vs. 2.6 Â±0.3 ÂµM, in absence and pr
The KIand kinactvalues for mitragynine towards CYP3A activity in HLM were 4.1 Â±Â 0.7 ÂµM and 0.051 Â± 0.002 r
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
A 7-fold shift in IC50was observed towards CYP3A activity in HIM, 21.9 Â±2.7 vs. 3.2 Â±0.3 ÂµM, in absence and pr
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
A 7-fold shift in IC50was observed towards CYP3A activity in HLM, 18.9 Â±1.8 vs. 2.6 Â±0.3 ÂµM, in presence and a
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
Mitragynine was shown to be a strong competitive inhibitor of CYP2D6 activity, with a Kiof 0.97 Â±Â 0.07 ÂµM, 1.2
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
A 7-fold shift in IC50was observed towards CYP3A activity in HIM, 21.9 Â±2.7 vs. 3.2 Â±0.3 ÂµM, in presence and al
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP3A activity in HIM. Mitragynin
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
The KIand kinactvalues for mitragynine towards CYP3A activity in HIM were 4.5 Â±Â 1.1 ÂµM and 0.072 Â± 0.006 m
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP3A activity in HIM. Mitragynin
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
% remaining was inferred from panel A of Fig 5 where the total contribution of each enzyme to MTG metabolism is
% result estimated from Figure S2 at around 30 ÂµM
% result estimated from Figure 2 at around 30 ÂµM
% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM
% result estimated from Figure S4 at around 100 ÂµM

% result estimated from Figure S3 at around 100 ÂµM

% result estimated from Figure S5 at around 100 ÂµM

% result estimated from Figure 3 at around 100 ÂµM

% result estimated from Figure 3 at around 30 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
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% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM
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% result estimated from Figure S4 at around 100 ÂµM

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% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure S3 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM

% result estimated from Figure 2 at around 30 ÂµM
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% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
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% result estimated from Figure 3 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM

% result estimated from Figure S2 at around 30 ÂµM

% result estimated from Figure S3 at around 100 ÂµM
% result estimated from Figure 2
% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S3 at around 100 ÂµM
% result estimated from Figure S3 at around 30 ÂµM
% result estimated from Figure S3
IC50 was not determined because inhibition was < 50%.Tranylcypromine was used as a positive control.(Table 2, Fi
Furafylline is used as the positive control(Table 2, Figure 2)
Quinidine was used as the positive control(Table 2, Figure 2)

Ketoconazole was used as the positive control.(Table 2, Figure 2)

Mean taken from text. SD estimated from Figure 3a.

Estimate from Fig 3a

Figure 2a for Papp ratio

% Inhibition mean taken from text. SD estimated from Figure 3b.
Positive control
% enzyme inhibition versus precipitant concentration:Values estimated from Figure 1d. In some cases, SEM could r
Positive control
% enzyme inhibition versus precipitant concentration:Values estimated from Figure 1d. In some cases, SEM could r
Positive control
IC50 not determined due to the less than 50% of inhibition.% enzyme inhibition versus precipitant concentration:V
peciosa) products at a concentration range between 1 and 6% of leaf content (10 to 60 mg/g) and that 7-hydroxymi
IC50 values from Table 1, Ki values from Table 3% enzyme inhibition versus precipitant concentration:Values estim
IC50 values from Table 1, Ki values from Table 3% enzyme inhibition versus precipitant concentration:Values estim
Positive controlIC50 values from Table 1% enzyme inhibition versus precipitant concentration:Values estimated frc
Positive controlIC50 values from Table 1% enzyme inhibition versus precipitant concentration:Values estimated frc
Km and Vmax from Table 2
Km and Vmax from Table 2
Km and Vmax from Table 2
Positive controlIC50 values from Table 1% enzyme inhibition versus precipitant concentration:Values estimated frc
IC50 values from Table 1, Ki values from Table 3% enzyme inhibition versus precipitant concentration:Values estim
Results for Mitragynine+R123 were statistically significant ($p<0.05$) vs R123 alone. Values from Fig. 5
Values from Fig 5

Internal: Additional comments

Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32
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Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32
han 50% did not occur at the highest concentration.Concentration of precipitant and % inhibition of pooled human
an 50% did not occur at the highest concentration.Concentration ofÂ precipitant and % inhibition of pooled human
Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32
p<0.05 for all values)0.01 Î¼M: 27 Â± 2%0.1 Î¼M: 39 Â± 1% 1 Î¼M: 43 Â± 3% 10 Î¼M: 55 Â± 1% 100 Î¼M: 61 Â± 2%
an 50% did not occur at the highest concentration.Concentration ofÂ precipitant and % inhibition of pooled human
p<0.05 for all values)0.01 Î¼M: 8 Â± 3%0.1 Î¼M: 9 Â± 2% 1 Î¼M: 20 Â± 1% 10 Î¼M: 21 Â± 1% 100 Î¼M: 41 Â± 1%10
Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32
Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32
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, n = 2 CYP2D6: 5uM quinidine, mean ~1.2Â Â± 0.1 fold, n = 2 CYP3A4: 5uM dexamethasone, mean ~1.2Â Â± 0.1 fo

this induction was statistically significant within the range of 1-5 uM of mitragynine, the induction relative to dexa
Mitragynine appeared to induce the mRNA expression of CYP1A2 in a concentration-dependent manner; significar
copies

0.7% (Fig. 4a)."
changes in the enzymatic activity were minimal. The greatest increase in CYP3A4 enzymatic activity, approximately
How to enter results?
ein expression at concentrations of 0.1uM and above, with the highest induction occurring at 0.5 uM relative to un
ntreated control. [...] Although the corresponding mRNA expression of CYP2D6 did show slight increase in the mRN
Â± 0.03 fold
2 fold (p < 0.05)
d

ıl: 0.95 Â± 0.06 fold

0.05 fold
0.1 fold (p < 0.05)
)5 fold
fold
l fold
: 1.1 Â± 0.05 fold
2 fold
)5 fold
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1 Â±0.2 fold
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ł
ŧ 0.1 fold
0.1 fold
0.6 fold (p < 0.05)
.5 Â± 0.1 fold

ɔld
l fold
0.4 fold (p < 0.05)
0.05 fold
5 Â± 0.2 fold
1.2 Â± 0.1 fold
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1.2 Â± 0.05 fold
0.2 fold
2 fold
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Â± 0.04 fold
0.1 fold
0.1 fold
9 Â± 0.2 fold
2.1 Â± 0.1 fold (p < 0.05)
0.1 fold
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0.1 fold

)5 fold
1.2 Â± 0.05 fold
0.1 fold

± 0.2 fold
0.1 fold
0.05 fold
 Â± 0.05 fold
 fold (p < 0.05)

 Â± 0.06 fold
 Â± 0.10 fold
 Â± 0.07 fold
0.5 fold (p < 0.05)
± 0.05 fold

 Â± 0.03 fold
 Â± 0.08 fold
ıl: 1.03 Â± 0.07 fold
 Â± 0.04 fold
).1 fold (p < 0.05)
: 1.1 Â± 0.05 fold
esenceÂ of NADPH, respectively. [IC50values (Mean Â± SEM) were determined using nonlinear least-squares regre
nin-1, 4.0 Â±Â 0.5 ÂµM and 0.057 Â± 0.002 min-1, and 5.9 Â±Â 0.9 ÂµM and 0.17 Â± 0.01 min-1, respectively, for t
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
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bsence of NADPH, respectively. [IC50values (Mean Â± SEM) were determined using nonlinear least-squares regres
, paroxetine (0.25 and 0.5 ÂµM), and 6',7'-dihydroxybergamottin (1 and 2 ÂµM) served as positive control inhibitor
!5 Â±Â 0.09 ÂµM, and 0.95 Â± 0.11 ÂµM, respectively, for three individual experiments. [Ki(Mean Â± SEM) values w
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
bsence ofÂ NADPH, respectively. [IC50values (Mean Â± SEM) were determined using nonlinear least-squares regre
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
e at 10 ÂµM inhibited CYP3A activity by 44%. Kratom extracts at 20 Âµg/mLÂ inhibited CYP3A activity by 82-90%.
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
nin-1, 6.0 Â±Â 0.5 ÂµM and 0.074 Â± 0.002 min-1, and 7.3 Â±Â 2.5 ÂµM and 0.17 Â± 0.02 min-1, respectively, for th
e at 10 ÂµM inhibited CYP3A activity by 44%. Kratom extracts at 20 Âµg/mLÂ inhibited CYP3A activity by 82-90%.
, paroxetine (0.25 and 0.5 ÂµM), and 6',7'-dihydroxybergamottin (1 and 2 ÂµM) served as positive control inhibitor
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s shown. Note that other reactions besides 7-OH-MTG were also included in the total contribution of metabolism c

igure 2)

not be estimated from the provided figure. 0.01 Âµg/mL: 18 Â± Unknown%0.1 Âµg/mL: 11 Â± 4%1 Âµg/mL: 9Â± 0%

not be estimated from the provided figure. 0.01 Âµg/mL: 25 Â± Unknown%0.1 Âµg/mL: 21 Â± Unknown%1 Âµg/mL

values estimated from Figure 1d. In some cases, SEM could not be estimated from the provided figure. 0.01 Âµg/mL
itragynine levels ranged from 0.01 to 0.04% (0.1 to 0.4 mg/g). Thus, the reported values we have provided a
ated from Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 43 Â± Unknown
ated from Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: -5 Â± 2%0.2 Î¼M
om Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 47 Â± Unknown%0.2 Î¼
om Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 37 Â± Unknown%0.2 Î¼

om Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 38 Â± Unknown%0.2 Î¼
ated from Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: -24 Â± 0%0.2 Î¼

Study title
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Characterization of Kratom material
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P-glycoprotein interactions of novel psychoactive substances - Stimulation of ATP consumption and transport acro
P-glycoprotein interactions of novel psychoactive substances - Stimulation of ATP consumption and transport acro

Study URL

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ated IC50 shift experimen	Related control data experiment ID
NPDI--0S--Q	
NPDI-dQtQ2g	
NPDI-_DqAGQ	
NPDI-exquAQ	
NPDI-exquAQ	
NPDI-_rs20g	
NPDI-_rs20g	
NPDI-_rs20g	

NPDI-EjMg0g

NPDI-o8WmjA

NPDI-4_UdSg
NPDI-XFPmtA

NPDI-A66pwQ

NPDI--jKvig
NPDI-Xrn4xQ
NPDI-xK3lmw

NPDI-5LuVNQ
NPDI-t32_Ig
NPDI-4AITQg
NPDI-5LuVNQ
NPDI-5LuVNQ

NPDI-9xzv_Q

NPDI-t32_Ig

NPDI-kew9FQ

NPDI-gxj_UA
NPDI-9xzv_Q
NPDI-s8ImuA
NPDI-9xzv_Q
NPDI-t32_Ig
NPDI-kew9FQ
NPDI-4AITQg
NPDI-t32_Ig
NPDI-gxj_UA

NPDI-9xzv_Q
NPDI-s8ImuA
NPDI-s8ImuA
NPDI-4AITQg

NPDI-5LuVNQ
NPDI-s8ImuA
NPDI-kew9FQ
NPDI-4AITQg
NPDI-9xzv_Q
NPDI-9xzv_Q
NPDI-kew9FQ
NPDI-4AITQg

NPDI-t32_Ig

NPDI-kew9FQ
NPDI-gxj_UA
NPDI-s8ImuA
NPDI-4AITQg
NPDI-5LuVNQ
NPDI-kew9FQ
NPDI-gxj_UA
NPDI-gxj_UA
NPDI-s8ImuA
NPDI-gxj_UA
NPDI-5LuVNQ
NPDI-t32_Ig

NPDI-cxxGnA

NPDI-vs2diA

Control data for experiment ID	Quantified metabolite ID
NPDI-7sdBtQ	
NPDI-LD3MZA	
NPDI-_MysYg	
NPDI-5_pf-w	
NPDI-LcX0tA	

80

37

NPDI-17YRkg

NPDI-_MFsyA

NPDI-qMnZyA

NPDI-eMZPbA

NPDI-olaGPQ

NPDI-o56vpA

NPDI-bXPXRQ

NPDI-Ue8YDg

247

NPDI-E56YVg

Quantified metabolite name	Quantified metabolite InChI	ntified metabolite concept ID (or

berberine	YBHILYKTIRIUTE-UHFFFAOYS/	19012197

(-)-epigallocatechin gallate

rotundifoline	IXWWTVSMMIIIFZ-LWWKTLCYSA-N

ntified metabolite enantiomer of compo	Object metabolite compound ID
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Object metabolite compound InChI **al: Object metabolite compound con**

ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
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JAQUASYNZVUNQP-PVAVHDDUSA-N
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QHSMEGADRFZVNE-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
JAQUASYNZVUNQP-PVAVHDDUSA-N
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IJQYTHQDUDCJEQ-UHFFFAOYSA-N

CCKWMCUOHJAVOL-UHFFFAOYSA-N	InChi Key generated by ChemDraw 17
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
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IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
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IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin

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Precipitant compound unique ingredient identifier	mpound international chem
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	LELBFTMXCIIKKX-QVRQZEMU
	RYENLSMHLCNXJT-CYXFISRXS
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	RYENLSMHLCNXJT-CYXFISRXS
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	LELBFTMXCIIKKX-QVRQZEMU
	YQEZLKZALYSWHR-UHFFFAO
	YQEZLKZALYSWHR-UHFFFAO
	LELBFTMXCIIKKX-QVRQZEMU
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	RMRJXGBAOAMLHD-IHFGGW
	RYENLSMHLCNXJT-CYXFISRXS
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	YQEZLKZALYSWHR-UHFFFAO
	RMRJXGBAOAMLHD-IHFGGW
	IAZDPXIOMUYVGZ-UHFFFAO
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LELBFTMXCIIKKX-QVRQZEMU

Precipitant compound description

SA-N

JSA-N

SA-N
VKQSA-N
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SA-N
JSA-N
JSA-N
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JSA-N

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JSA-N
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Internal: Precipitant compound comment	recipitant compound concept ID (omop
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	1124300

Often refers to the leaves of M. speciosa

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Often refers to the leaves of M. speciosa

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26 R60L0SM5BC
14 144O8QL0L1
26 R60L0SM5BC
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26 R60L0SM5BC
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107

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94
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XKFSBWQWNMZWFA-UHFFFAOYSA-N	
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