

Chemical analysis, toxicity and *in silico* carcinogenic potential of the Pataqueira essential oil (*Conobea scoparioides* Cham. & Schldl.) native to the Amazon region, Brazil

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Conobea scoparioides is popularly known as pataqueira, is an aromatic plant native to the Amazon widely used by the traditional population to combat cavities and polyneuritis caused by vitamin B1 deficiency, it is also used in the treatment of leishmaniasis and trypanosomiasis and has antimicrobial action (COSTA et al., 2014). Although the plant is widely used, aspects about its toxicity and carcinogenic potential are little known, so the objective of this work was to evaluate the chemical profile, toxicity and *in silico* carcinogenic potential of the essential oil of pataqueira and its constituents. The leaves were collected in March 2015, in Santarem / PA. The plant material (400g of leaves) was dehydrated at 40 ° C for 48h. The extraction of the essential oil was carried out in a Clevenger type hydrodistiller, using 150g of macerated dry leaves; the extraction occurred for 3h at 110 ± 10 ° C. The chemical evaluation was performed by GC-MS. The toxicological potential of the sample was determined by the *Artemia salina* lethality test (MAYORGA et al., 2010). Studies predictive of oral toxicity in rats (ToxOR), fish toxicity (ToxFS) and carcinogenicity of the compounds were determined using Protox servers (DRWAL et al., 2014) and Admet-SAR (CHENG et al., 2012). The yield of essential oil was 1.3%. Chemical analysis showed the presence of five constituents in the essential oil, with thymol and methylthymol being the major compounds (59.9% and 34.6%, respectively); the other components were: α -felandren (3.4%), 3-octanone (1.2%) and p-cymene (0.7%). The toxicity test against *Artemia salina* showed that the sample showed high toxicity (LC₅₀ 4.49 $\mu\text{g}\cdot\text{mL}^{-1}$). ToxOR analysis showed thymol and methylthymol presented toxicity grade III (moderate) (640mg/ kg and 880mg/ kg, respectively), p-cymene is noteworthy for its grade I toxicity (high toxicity) (3 mg / kg), 3-octanone and α -phellandrene presented low toxicity (6,430 mg / kg and 5,700 mg / kg, respectively). The analysis ToxFS, demonstrated that all the compounds showed high toxicity and the evaluation of the carcinogenic potential indicated the p-cimeno and α -felandreno as potential carcinogenic agents. Considering that the test with *A. salina* has a correlation with biological activities of medical interest, the essential oil of pataqueira has demonstrated potential for development of products for therapeutic purposes, however, the toxicological aspects should be considered for the standardization of safe dosages for its use in herbal products.

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