Data in Brief 6 (2016) 83–88

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Data analysis of "krokodil" samples obtained by street-like synthesis

João Filipe Neves [a], Emanuele Amorim Alves [b,c,d,*], José Xavier Soares [e], Sara Manuela Cravo [a], Artur M.S. Silva [f], Annibal Duarte Pereira Netto [g], Félix Carvalho [b], Ricardo Jorge Dinis-Oliveira [b,c,h,*], Carlos Manuel Afonso [a,i,**]

[a] Department of Chemical Sciences, Laboratory of Organic and Pharmaceutical Chemistry, Faculty of Pharmacy, University of Porto, Porto, Portugal
[b] UCIBIO-REQUIMTE, Laboratory of Toxicology, Department of Biological Sciences, Faculty of Pharmacy, University of Porto, Porto, Portugal
[c] Department of Legal Medicine and Forensic Sciences, Faculty of Medicine, University of Porto, Porto, Portugal
[d] EPSJV – Polytechnic School of Health Joaquim Venâncio, Oswaldo Cruz Foundation, Rio de Janeiro, Brazil
[e] LAQV-REQUIMTE, Department of Chemical Sciences, Laboratory of Applied Chemistry, Faculty of Pharmacy, University of Porto, Porto, Portugal
[f] Department of Chemistry and QOPNA, University of Aveiro, Campus Universitário de Santiago, Aveiro, Portugal
[g] Department of Analytical Chemistry, Chemistry Institute, Fluminense Federal University, Niterói, Brazil
[h] IINFACTS-Institute of Research and Advanced Training in Health Sciences and Technologies, Department of Sciences, University Institute of Health Sciences (IUCS), CESPU, CRL, Gandra, Portugal
[i] Interdisciplinary Center of Marine and Environmental Investigation (CIIMAR/CIMAR), Porto, Portugal

ARTICLE INFO

Article history:
Received 21 September 2015
Received in revised form
19 November 2015
Accepted 19 November 2015
Available online 28 November 2015

Keywords:
"Krokodil"
Street like synthesis
TLC profile
UV/Vis
^{1}H NMR
FTIR

ABSTRACT

The data described in this work is related to be the subject of an article in the Forensic Science International, titled: "The harmful chemistry behind "krokodil": street-like synthesis and product analysis" (http://dx.doi.org/10.1016/j.forsciint.2015.07.042) [1]. The data presented here provides additional description of the chemical profile of "krokodil". Physicochemical and organoleptic characteristics, TLC profile, UV/Vis, ^{1}H NMR and FTIR spectrum are presented. These data validate the proposed synthetic procedure and pathway and give further information about the contaminants present in "krokodil".

* Corresponding authors at: UCIBIO-REQUIMTE, Laboratory of Toxicology, Department of Biological Sciences, Faculty of Pharmacy, University of Porto, Porto, Portugal, Rua José Viterbo Ferreira no. 228 4050-313, Porto, Portugal. Tel.: +351 220428597.
** Corresponding author at: Department of Chemical Sciences, Laboratory of Organic and Pharmaceutical Chemistry, Faculty of Pharmacy, University of Porto.
E-mail addresses: manuhpa@hotmail.com (E.A. Alves), ricardinis@med.up.pt, ricardinis@sapo.pt (R.J. Dinis-Oliveira), cafonso@ff.up.pt (C.M. Afonso).

http://dx.doi.org/10.1016/j.dib.2015.11.046

Specifications Table

Subject area	*Chemistry*
More specific subject area	*Chemical profile data*
Type of data	*Figures*
How data was acquired	*UV analysis (Varian CARY 100 spectrophotometer from a range of 200 nm to 800 nm. Software: Cary Win UV, v. 3.0), FTIR analysis (Nicolet iS10 from Thermo Scientific. Smart OMNI-Transmisson accessory. Software OMNIC 8.3) and ^1H NMR analysis (Bruker DRX-300 spectrometer operating at 300.13 MHz for ^1H)*
Data format	*Analyzed data*
Experimental factors	*Additional chemical profile data from "krokodil" samples*
Experimental features	*Crude "krokodil" obtained using street-like synthesis and its extract after alkalization and organic extraction using ethyl acetate as solvent were analyzed*
Data source location	*Porto, Portugal*
Data accessibility	*Data is provided in this article*

Value of the data

- Detailed description of organoleptic properties and pH range of "krokodil" as well as the disclosure of UV/Vis and ^1H NMR spectra provide additional data to the establishment of the chemical profile of "krokodil".
- The description of the chemical profile of "krokodil" will eventually aid the competent authorities in dealing with this drug, in terms of identification and characterization.
- Further insight regarding the complex nature of "Krokodil" was revealed by TLC analysis and FTIR spectrum.

1. Data

Data presented here describes the additional chemical analysis of the "krokodil" samples obtained using the street-like synthesis. Physical and organoleptic characters, UV/Vis and ^1H NMR spectra were described on a "krokodil" sample freshly prepared (crude "krokodil"). Organic extract of "krokodil" (extracted "krokodil") was obtained after alkalization of the crude product and extraction using ethyl acetate. This organic extracts were analyzed by TLC, FTIR and ^1H NMR techniques.

2. Experimental design, materials and methods

The synthesis was carried out as described previously [1]. "Krokodil extract" samples were obtained by the treatment of 4 mL of crude "krokodil" with NaOH 20% (m/v) until alkalization, followed by extraction with ethyl acetate. The organic phases were gathered, dried over anhydrous sodium sulfate, filtered and concentered until dryness.

All pH measurements were made with a Model pH-meter GLP 22 (Crison, Allela, Spain).

UV/Vis spectra of water-diluted solutions of crude "krokodil" were recorded on a Varian CARY 100 spectrophotometer from a range of 200 nm to 800 nm (software: Cary Win UV, v. 3.0). ^1H NMR spectrum was recorded on a Bruker DRX-300 spectrometer (operating at 300 MHz for ^1H) using D_2O (Deutero GmbH) as solvent.