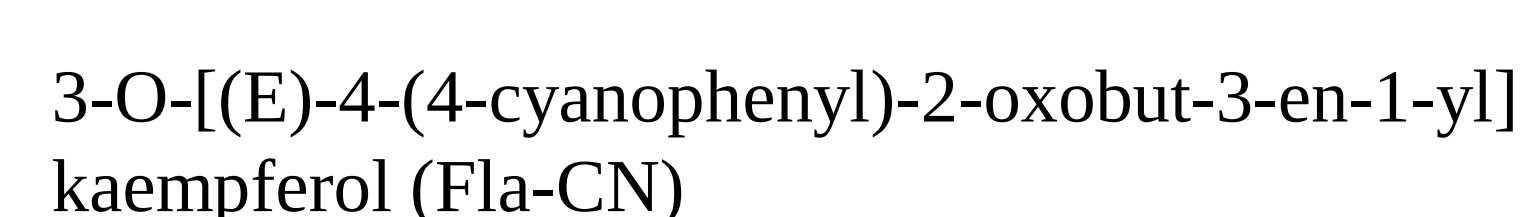


4-5 October 2023



We focus ourselves on the extension of the antidiabetic molecular library built from molecules elucidated from plants of the African flora in the purpose to design potential anti-drugs. Therefore, a molecular library of 28 flavonoids has been obtained from the following species: *Erythrina mildbraedii*, *Dorstenia psilurus*, *Ceiba pentandra*, *Bauhinia megalandra*, *Pueraria lobata* and *Rhus verniciflua*, *Stelechocarpus*, *Cauliflorus*, *Chorisia Crispiflora*, *Bombax ceiba* and *Arbutus unedol*). 5,3'-dihydroxy-7,4',5'-trimethoxyisoflavone or vavain isolated from methanol extract of *Ceiba pentandra* bark after a characterization of spectral data analysis (1D, 2D, 3D NMR) has been added to the said molecular data. A rapid strident screening analysis of the molecular library extended using sucessively the rules of lipinski, oprea and verdonk has involved the following parameters: molecular weight (MW), hydrogen bond acceptor (HBA), hydrogen bond donor (HBD) and skin permeability parameter (LogKp). Unfortunately, none of our molecules has not satisfied these series of the required conditions. The examination of the permeability, absorption and distribution of the molecules in the body (using blood brain barrier (BBB), number or rotatable bond (NRB), polar surface area (PSA)...) has been done. But, none of molecules explored met the mandatory constraints. In the whole, we concluded that all the molecules of our extended library have predicted not to be drug-likeness.

Addition of vavain isolated from ceiba pentadra bark

Nie *et al.*, 2020

Isoxazole derivative

Better than Fla-CN (valuable compound

for anti-diabetic drug discovery)

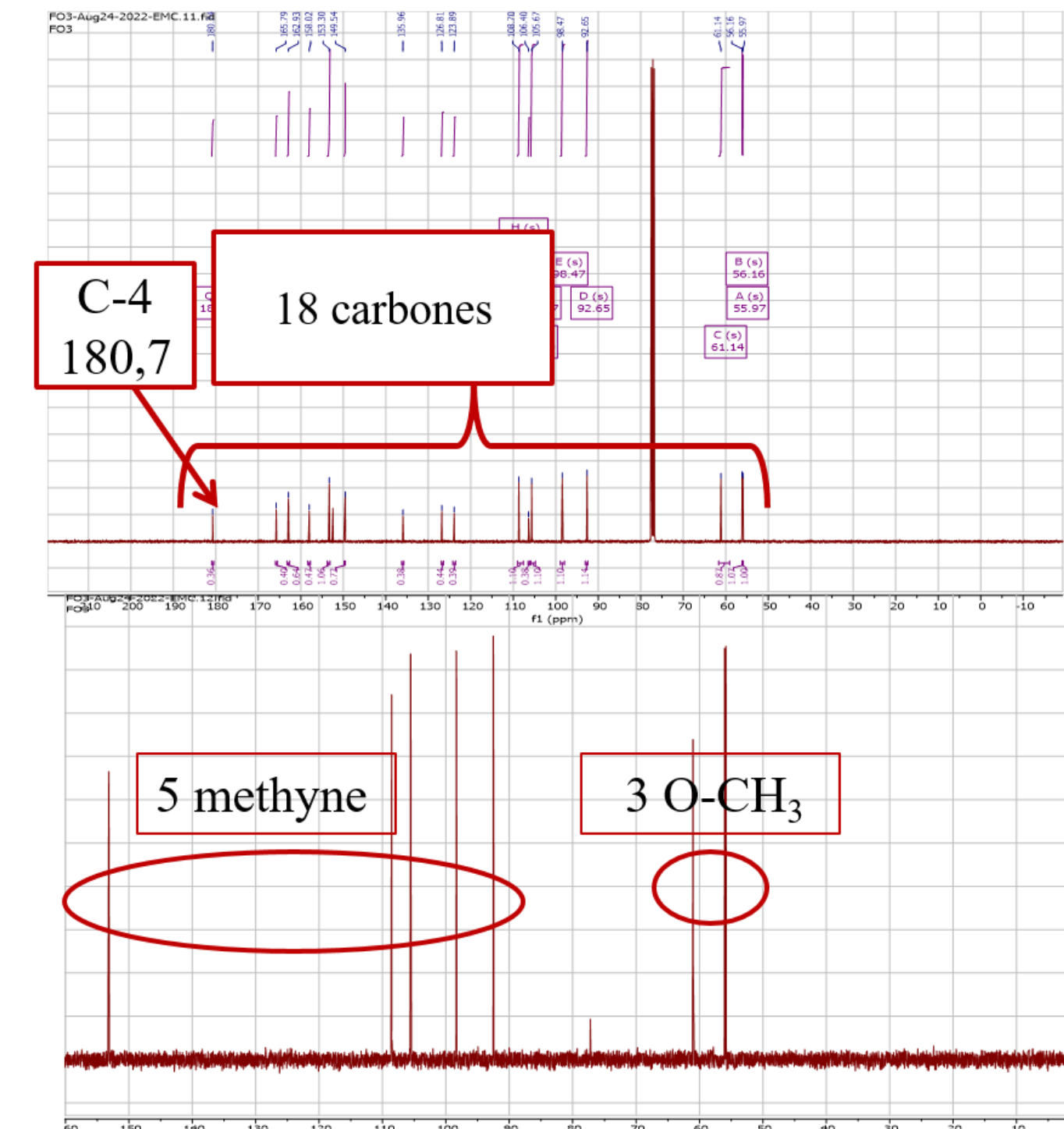
PO3-Aug24-2022-EMC-10.F16
PO3

The figure displays the ^1H NMR spectrum of compound 3, recorded in CDCl_3 . The spectrum shows peaks in the aromatic region (6.20-6.85 ppm) and the aliphatic region (3.88-4.01 ppm). Two chemical structures of compound 3 are provided: one with protons labeled A through H, and another with protons labeled 1 through 8. The assignments are as follows:

- Aromatic protons (6.20-6.85 ppm):**
 - 6.72 and 6.74 ppm: assigned to protons A and B.
 - 6.39 and 6.41 ppm: assigned to protons D and C.
 - 6.38 ppm: assigned to proton E.
 - 6.39 ppm: assigned to proton F.
 - 6.41 ppm: assigned to proton G.
 - 6.43 ppm: assigned to proton H.
- Aliphatic protons (3.88-4.01 ppm):**
 - 3.88, 3.91, and 3.93 ppm: assigned to the three $\text{O}-\text{CH}_3$ groups.
 - 3.85 ppm: assigned to the OH group.

The spectrum also shows a solvent peak for CDCl_3 at 7.26 ppm and a reference peak for TMS at 0 ppm.

Spectrum of RMN ^1H (500Hz; CDCl_3) de FO_3



Spectrum RMN
 ^{13}C (125 MHz ;
 CDCl_3) of FO_3

Spectrum DEPT-
135 (125 MHz;
CDCl₃) of FO₃

The aim of our work was to extend a bank of anti-diabetic molecules extracted from African flora and to investigate potential anti-diabetic drugs. The expansion of the library was done by carrying out a phytochemical study on *Ceiba pentandra* barks, from this study, nine (9) compounds were isolated and purified using chromatographic techniques (CC, TLC). We found that none of the molecules qualified as lead compounds in the drug discovery process. However, we project to characterise the other compounds and to search for flavonoids, to confirm in vivo and in vitro pharmacokinetic profiles in order to converge towards a concrete pharmacodynamics specification and to study the interaction between these 29 ligands and an anti-diabetic protein.

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Adjahonoun E., Ake A., (1989). Contribution au recensement des plantes médicinales de Côte d'Ivoire. Centre National de floristique 04, B.P.232 Abidjan. Copyright Université d'Abidjan.

Adjahonoun J, Ahyi R, Assi A., Baniakina J., Chibon P., Cusset G., Doulou V., Enzanza A., Eymé J, Goudoté E, Keita A, Mbemba C, Mollet J, Moutsamboté J, Mpati J, Sita P., (1988). Médecine traditionnelle et pharmacopée. Contribution aux études ethnobotaniques et floristiques en République Populaire du Congo. Agence de Coopération Culturelle et Technique. Congo. Pp. 338- 403.

Ake Assi, Abeye, Guinko S, Guinget R, Bangavou Y., (1980). Contribution à l'identification et au recensement des plantes utilisées dans la médecine traditionnelle et la pharmacopée en République Centrafricaine. 2ème édition, AC.C.T. Pp. 327- 400

Descripteur	Description	Intervalle	Norme	Molécule
NRB	Nombre de liaison rotative	0 - 8	$NBR \leq 10$	Toutes les molécules respectent la norme
PSA	Surface polaire	65.75- 264.02	$PSA \leq 140$	5 (17N, 18N, 26N, 27N, 28N) ne respectent pas la norme
LogKp	Traverser la barrière membranaire	- 7.026 à -2.234	$LogKp > -2.5 \text{ cm/s}$	5N, 6N, 12N, et 13N ne pourront pas traverser
Log BB	Traverser la barrière hémato encéphalique	- 4.52 à -0.88	-3 et 1	17N, 18N, 27N et 28N ne pourront pas traverser

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Descripteur	Description	Intervalle	Norme	Molécule
Caco-2	Absorption gastro-intestinale	65,75 – 264,02	Caco-2 > 500 nm/s	1N, 5N, 6N, 12N, 13N, e 16N pourront être absorbés
Log HERG	Toxicité cardiaque	-6.189 à -4.681	Log HERG < -5	17N, 18N, 19N, 20N, 23N et 24N non toxique
Score de biodisponibilité	Fraction de médicament dans la circulation sanguine	0.17 – 0.55	0.11 – 0.85	Toutes les molécules sont bio-disponibles
Log S	Solubilité dans le sang	-8.615 à -2.467	-6 et 0.5	62.52% solubles

High-speed screening

Absorption