**C:\Users\cce\Desktop\Sebastião\Fig 1S.tifAdditional file 1**

**Figure S1** 1H NMR spectrum (400 MHz) of (A) MeOH in methanol-*d*4 and KH4PO4 solution in D2O; pH 6; (B) EtOAc in CDCl3 and (C) CH2Cl2 in CDCl3. The signals at *δ* 1.60 and *δ* 2.30 ppm are characteristics of *β-*CH2 and *α*-CH2 of saturated fatty acids. Signals of unsaturated fats acids at *δ* 2.07 and *δ* 5.35 ppm. The aromatic compounds appeared between *δ* 7.0 and 8.0 ppm.



**Figure S2** Chromatogram of the F5 which was obtained by gas chromatography coupled to mass spectrometry. The main substance, identified as ketamine, was ionized by electron impact at 70 eV.

|  |  |
| --- | --- |
| Coding name sub-fraction | Substances |
| F1 | Nonanoic acid, 9-oxo-methyl ester; Palmitic acid methyl ester; Oleic acid methyl ester; Stearic acid methyl ester |
| F2 | Nonanoic acid, 9-oxo-methyl ester; Palmitic acid methyl ester; Oleic acid methyl ester; Stearic acid methyl ester; *cis*-Vaccenic acid |
| F7 | Benzeneacetic acid; 2,5-Dihydroxyphenylacetic acid; 1,9-Decadiyne; Benzeneacetic acid, 10-undecenyl ester; Palmitic acid |
| F8 | Linolelaidic acid, methyl ester; Palmitic acid |
| F9 | Palmitic acid; Oleic acid methyl ester; *cis*-vaccenic acid |

**Table S1**  Substances present in the ethyl acetate sub-fractions identified by GC/MS.

**Table S2** 1H and 13C NMR spectral data and 1H-1H COSY; 1H-13C HSQC and 1H-13C HMBC of F5 and its correlations to structure ketamine.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Position | *δ* 1Ha | *δ* 13Cb | COSY | HMBC |
| 1 | - | 208.9 | - | - |
| 2 | - | 70.6 | - | - |
| 3 | 1.83, 2.93 | 38.4 | H-4 | C-2, C-4,C-5, C-1’ |
| 4 | 1.74 | 21.8 | H-3, H-5 | C-5 |
| 5 | 1.86, 2.04 | 28.7 | H-6 | C-4 |
| 6 | 2.52 | 39.8 | H-5 | C-1 |
| 1’ | - | 135.6 | - | - |
| 2’ | - | 134.0 | - | - |
| 3’ | 7.38 | 131.4 | H-4’ | C-5’ |
| 4’ | 7.29 | 129.4 | H-3’, H-5’ | C-2’, C-6’ |
| 5’ | 7.35 | 127.0 | H-6’ | C-1’, C-3’ |
| 6’ | 7.60 | 129.8 | H-5’ | C-4’, C-2’ |
| NCH3 | 2.14 | 28.8 | - | C-2 |

a 1H determined from HSQC experiment.

b 13C determined from HSQC and HMBC experiments.



# Figure S3 Key HMBC and 1H–1H COSY correlations of ketamine.

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**Figure S4** The 1H–1H COSY spectrum of F5 in CDCl3 at 400 MHz.

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**Figure S54** The1H-13C HSQC spectrum of F5 in CDCl3 at 400 and 100 MHz.

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**Figure S6** The1H-13C HMBC spectrum of F5 in CDCl3 at 400 and 100 MHz.



**Figure S7** Chromatogram of EtOAcF5, obtained by UHPLC / MS monitored by ultraviolet light (A) and monitored by positive mode electrospray ionization (B). Spotlight figure spectral profiles fragments obtained in MS/MS mode positive ionization for ions *m/z* = 238 Da (A- EtOAc fraction and B- Ketamine reference) and *m/z* = 240 (C- EtOAc fraction and D- Ketamine reference). m/z = 238 Da [M + H]+, m/z = 240.10 Da [M + 37Cl]+



**Figure S8** Proposal of ions after fragmentation the ion *m/z* 238.17 Da, monitored by positive mode electrospray ionization at retention time 2.24 min.