

Supporting Information File 1
for
Strecker degradation of amino acids promoted by
a camphor-derived sulfonamide

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Experimental spectra for compound **2**: FTIR, NMR (¹H, ¹³C, DEPT, HMBC, HSQC, NOESY), ESIMS and the proposed fragmentation mechanism for **2** and **12**

Experimental Data

(3a*S*,6*S*,*Z*)-7-(((3a*S*,6*S*)-8,8-Dimethyl-2,2-dioxido-4,5,6,7-tetrahydro-3*H*-3a,6-methanobenzo[*c*]isothiazol-7-yl)imino)-8,8-dimethyl-4,5,6,7-tetrahydro-3*H*-3a,6-methanobenzo[*c*]isothiazole 2,2-dioxide (**2**).

Spectroscopic data

FTIR

The spectrum was obtained from KBr pellets using a JASCO FT/IR 4100 spectrometer.

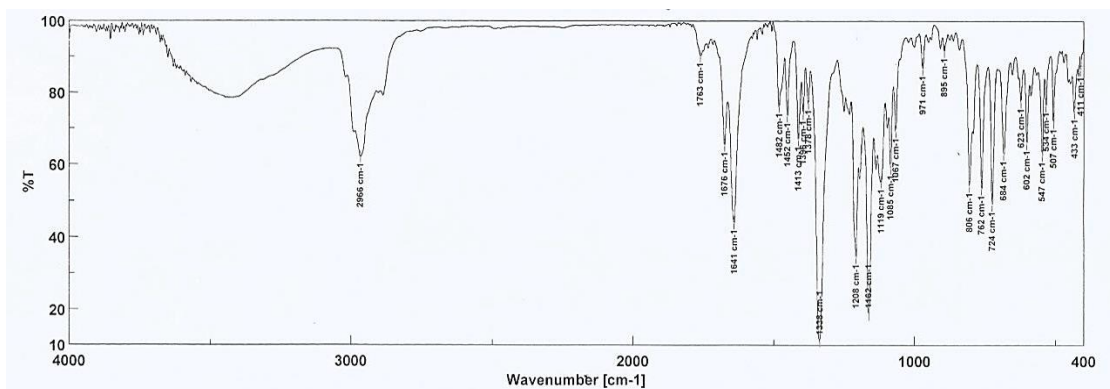


Figure S1: Spectrum of **2** (range 4000–400 cm⁻¹)

NMR

The spectra were obtained at 20 °C in CD₃CN using a Bruker Avance II⁺ 400 MHz spectrometer. The chemical shifts were referenced to TMS ($\delta = 0$ ppm).

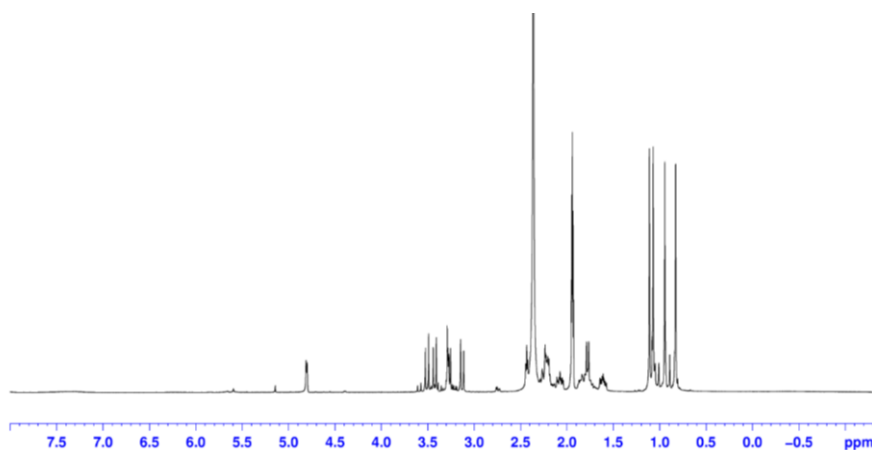


Figure S2: ¹H NMR spectrum of **2** obtained in CD₃CN at -20 °C.

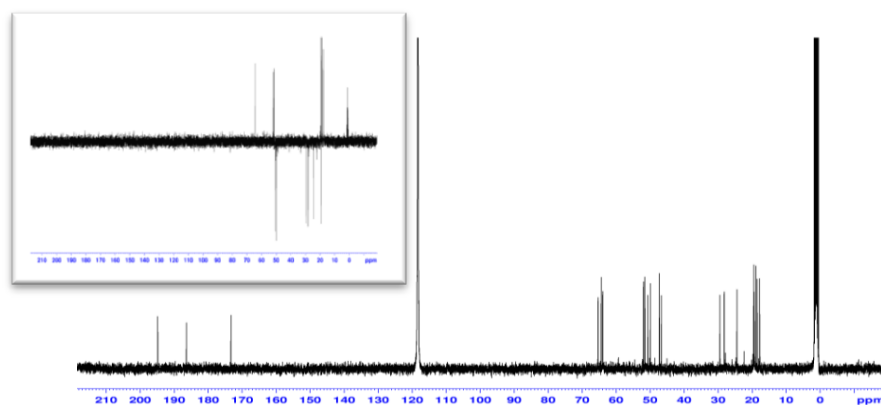


Figure S3: ^{13}C NMR spectrum and DEPT (insert) of **2** obtained in CD_3CN at -20°C .

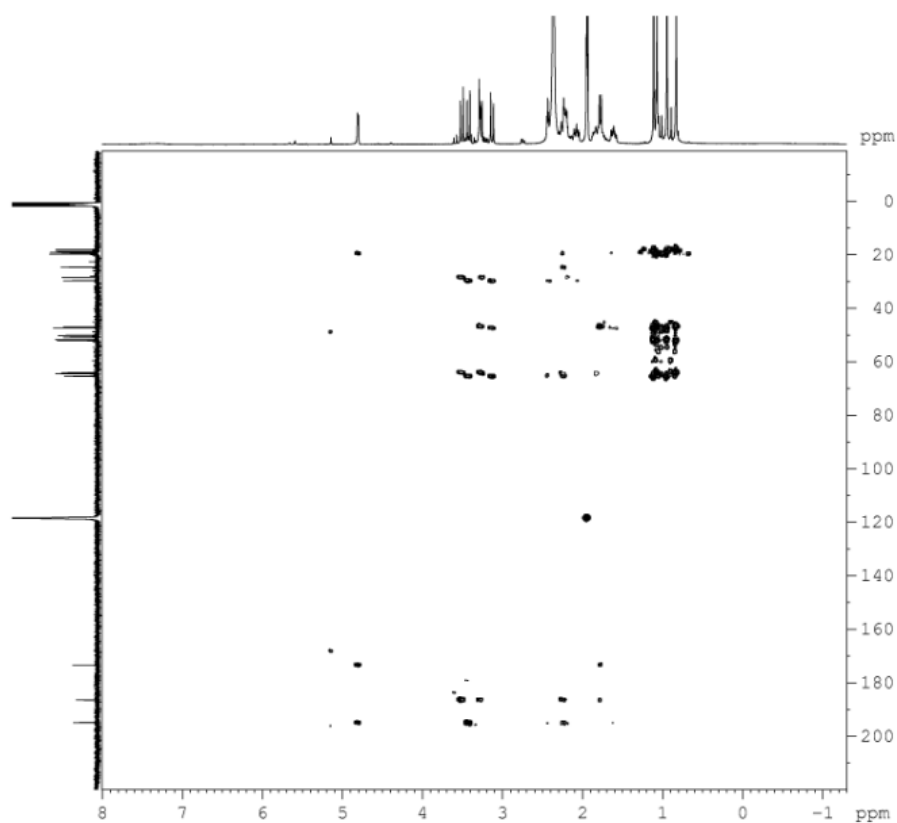


Figure S4: HMBC of **2** obtained in CD_3CN at -20°C .

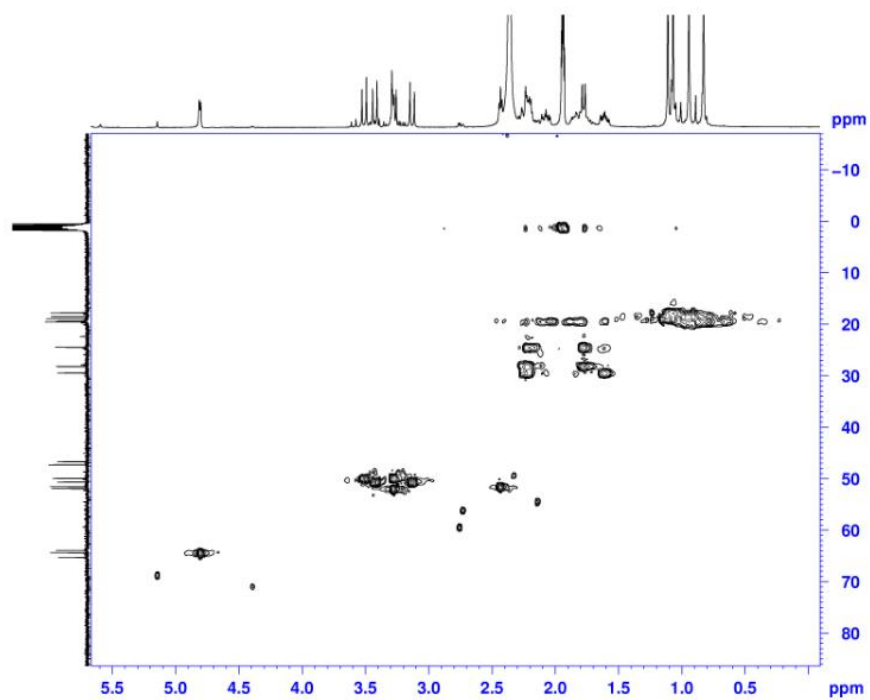


Figure S5: HSQC of **2** obtained in CD₃CN at -20 °C.

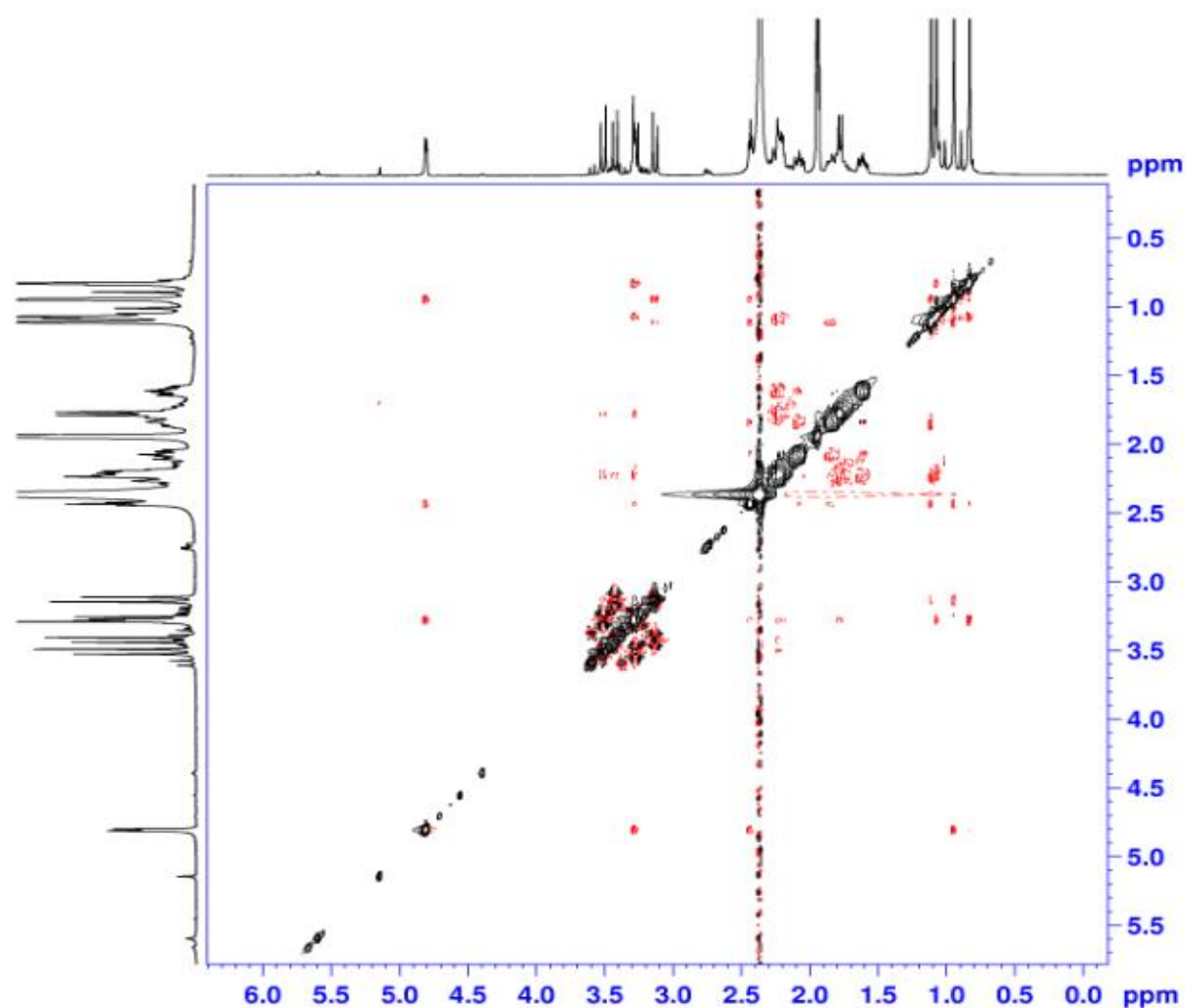


Figure S6: NOESY of **2** obtained in CD₃CN at –20 °C.

ESI-MS

Data for **2**

LRESI mass spectrum and tandem mass experiments were carried out on a LCQ Fleet mass spectrometer operated in the ESI positive ion mode (Thermo Scientific), with the following optimized parameters: ion spray voltage, +4.5 kV; capillary voltage, 16 V; tube lens offset, –63 V; sheath gas (N₂), 80 arbitrary units; auxiliary gas, 5 arbitrary units; capillary temperature, 250 °C. The spectra were recorded in the range 100–1500 Da. Spectrum typically corresponds to the average of 20–35 scans. Tandem mass spectrum was obtained with an isolation window of 2 Da, a 30% relative collision energy and with an activation energy of 30 ms. HRESI mass spectrum was obtained on a UHR-QqTOF Impact II (Bruker Daltonics) operating in the high resolution mode.

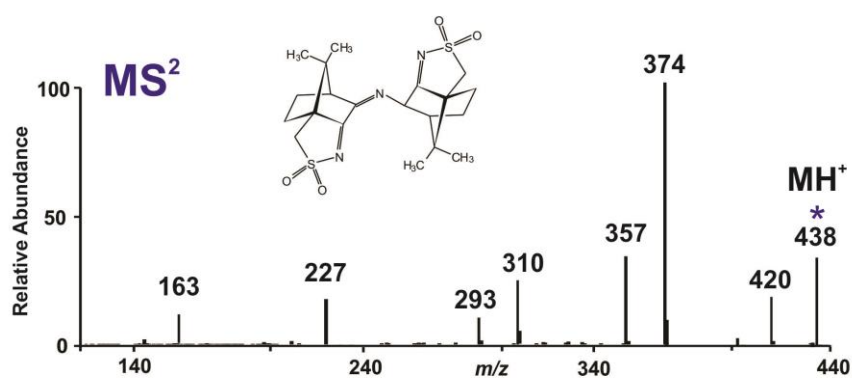


Figure S7: ESI tandem mass spectrum of the protonated molecule of **2**.

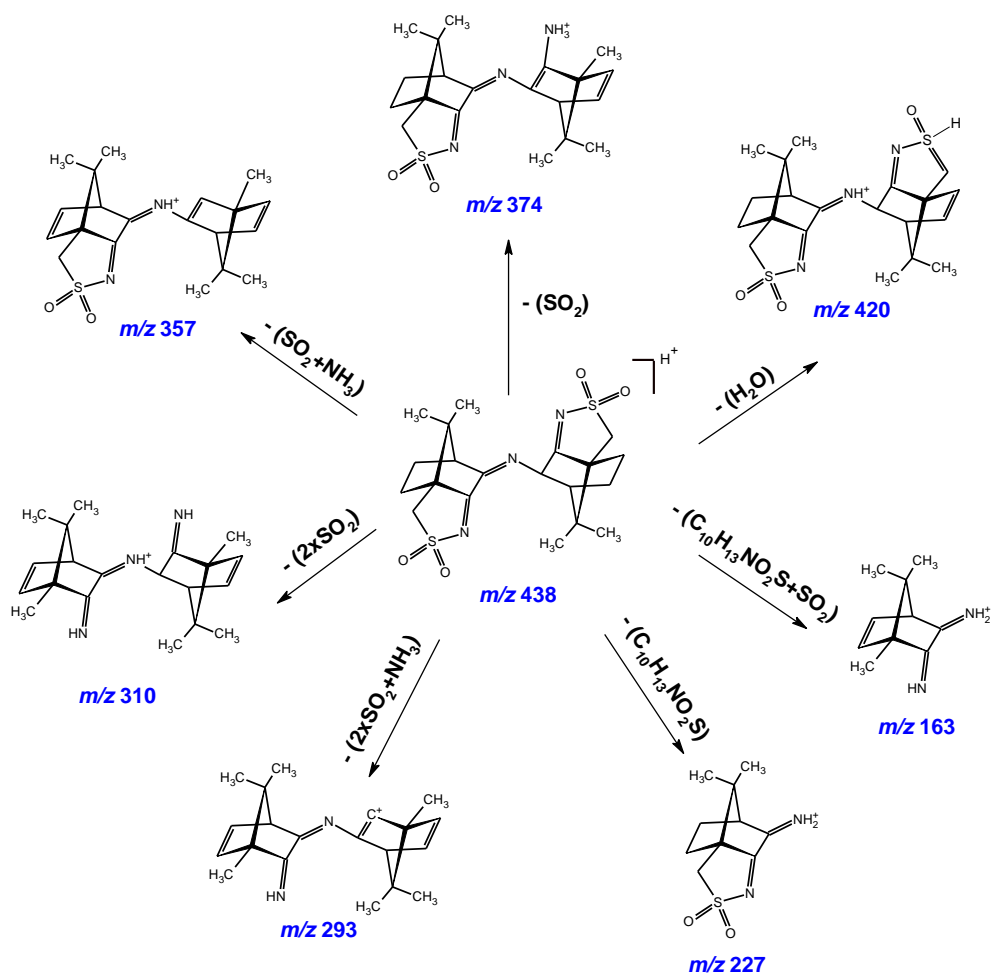


Figure S8: Proposed fragmentation mechanism for the precursor ion *m/z* 438.

Data for **12**

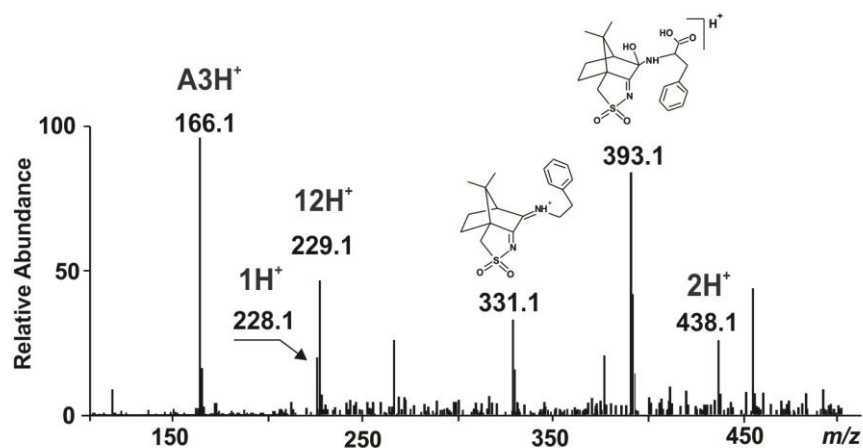


Figure S9: ESI tandem mass spectrum of the reaction mixture after 1 h reaction showing protonated phenylalanine, **A3**; oxoimine, **1**; the proposed intermediate **12** (Figure 11 in the manuscript) and the final product **2**. Other intermediates were identified and their formula assigned to the corresponding mass.

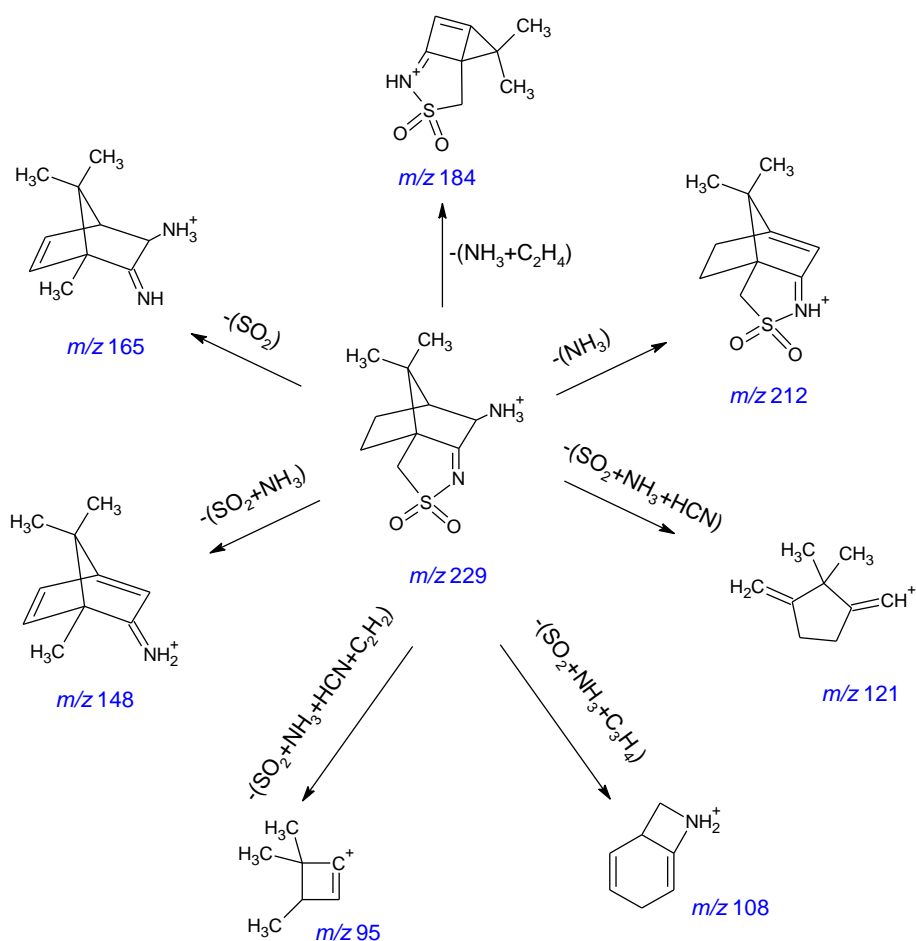


Figure S10: Proposed fragmentation mechanism for intermediate **12** (m/z 229).