



Supplementary Materials

Quinoline- and Benzoselenazole-Derived Unsymmetrical Squaraine Cyanine Dyes: Design, Synthesis, Photophysicochemical Features and Light-Triggerable Antiproliferative Effects against Breast Cancer Cell Lines

Eurico Lima ¹, Renato E. Boto ², Diana Ferreira ³, José R. Fernandes ¹, Paulo Almeida ²,

Luis F. V. Ferreira ³, Eliana B. Souto ^{4,5}, Amélia M. Silva ^{6,*} and Lucinda V. Reis ^{1,*}

- ¹ Chemistry Centre of Vila Real (CQ-VR), University of Trás-os-Montes and Alto Douro, Quinta de Prados, 5001-801 Vila Real, Portugal; eurico_lima@icloud.com (E.L.); jraf@utad.pt (J.R.F.)
- ² Health Sciences Research Centre (CICS-UBI), University of Beira Interior, Av. Infante D. Henrique, 6201-001 Covilhã, Portugal; rboto@ubi.pt (R.E.B.); pjsa@ubi.pt (P.A.)
- ³ Institute of Bioengineering and Biosciences (iBB), Higher Technical Institute, University of Lisbon, Av. Rovisco Pais, 1049-001 Lisbon, Portugal; diana.ferreira@det.uminho.pt (D.F.); luisfilipevf@ist.utl.pt (L.F.V.F.)
- ⁴ Department of Pharmaceutical Technology, Faculty of Pharmacy, University of Coimbra, Pólo das Ciências da Saúde, Azinhaga de Santa Comba, 3000-548 Coimbra, Portugal; ebsouto@ff.uc.pt
- ⁵ Centre of Biological Engineering (CEB), University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal
- ⁶ Department of Biology and Environment (DeBA), and Centre for Research and Technology of Agro-Environmental and Biological Sciences (CITAB-UTAD), University of Trás-os-Montes and Alto Douro, Quinta de Prados, 5001-801 Vila Real, Portugal
- * Correspondence: amsilva@utad.pt (A.M.S.); lucinda.reis@utad.pt (L.V.R.)

Received: 30 April 2020; Accepted: 8 June 2020; Published: date



Figure S1. NMR spectrum of compound 5 (600 MHz, CDCl₃, ppm). Residual solvent peaks: *Et₂O, **CH₃OH.



Figure S2 ¹³C NMR spectrum of compound 5 (150.90 MHz, CDCl3, ppm). Residual solvent peak: *Et₂O.



Figure S3. HRESI-TOFMS spectrum of compound 5.



Figure S4 1H NMR spectrum of dye 9 (600 MHz, CDCl3, ppm). Residual solvent peak: *CH3OH.



Figure S5.¹³C NMR spectrum of dye 9 (150.90 MHz, CDCl₃, ppm).



Figure S6. HRESI-TOFMS spectrum of dye 9.



Figure S7 1H NMR spectrum of dye 10 (400 MHz, CDCl3, ppm). Residual solvent peaks: *CH2Cl2, **CH3OH.



Figure S8 13C NMR spectrum of dye 10 (150.90 MHz, CDCl3, ppm). Residual solvent peaks: *Et2O, **CH2Cl2.



Figure S9. LRESI-TOFMS spectrum of dye 10.



Figure S10 ¹H NMR spectrum of dye 11 (600 MHz, DMSO-d6, ppm).







Figure S12. HRESI-TOFMS spectrum of dye 11.



Figure S13. NMR spectrum of dye 12 (600 MHz, DMSO-d6, ppm). Residual solvent peak: *CH2Cl2.



Figure S14. ¹³C NMR spectrum of dye 12 (150.90 MHz, DMSO-d6, ppm). Residual solvent peak: *CH2Cl2.

Mass Spectrum List Report Mass Spectrum Molecular Formula Report Analysis Info Electrospray (ESI)
Analysis Name D:\Data\AUTAD\LRLR14051014_000001.d Analysis Info Analysis Info Electrospray (ESI)
Analysis Name LRLR14051014_000001.d Sample Name Instrument apex-Qe Squaraine dye 12 Instrument apex-Qe Acquisition Parameter Capillary Exit 300.0 V Acquisition Parameter Capillary Exit 300.0 V Skimmer 1 20.0 V Skimmer 1 20.0 V Intens. x10⁸ 600.24826 Intens. x10⁸ LRLR14051014_000001.d: +MS 600.24826 1.0 1.0 0.8-0.6-0.8-598.24924 601.25178 0.4 0.2-596.25135 599.25281 602.24890 603.25239 0.6 ×108 LRLR14051014_000001.d: C 35 H 42 N 3 O Se .600.25 1.0 600.24876 0.8 0.4-0.6 598.24955 0.4 601.25212 0.2 0.2 597.25221 599.25291 602.24894 0.0 594.25472 300.12412 504 598 608 m/z 600 602 606 0.0 550 200 250 300 350 400 450 500 600 m/z Mass Spectrum Molecular Formula Report ----- +MS
 Meas.m/z
 #
 Formula
 Score
 m/z
 err [mDa]
 err [ppm]

 500.24826
 1
 C 35 H 42 N 3 O Se
 100.00
 600.24900
 0.50
 0.84

 2
 C 37 H 44 O 2 Se
 37.99
 600.25037
 1.85
 3.08
 mSigma rdb e⁻⁻Conf N-Rule 62.3 16.5 even ok 64.4 16.0 odd ok

