Rational design, synthesis, and 2D-QSAR study of anti-oncological alkaloids against hepatoma and cervical carcinoma

Adel S. Girgis,ª Siva S. Panda,ª Marian N. Aziz,ª Peter J. Steel,ª C. Dennis Hall*ª and Alan R. Katritzkyª,ª

ªCenter for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, FL 32611-7200, USA. E-mail: charlesdennishall@gmail.com
ªPesticide Chemistry Department, National Research Centre, Dokki, Cairo 12622, Egypt
ªChemistry Department, University of Canterbury, Christchurch, New Zealand
ªDepartment of Chemistry, King Abdulaziz University, Jeddah, 21589, Saudi Arabia

Supplementary material

Figure captions

Figure S1. IR spectrum of compound 3.
Figure S2. IR spectrum of compound 11.
Figure S3. IR spectrum of compound 12.
Figure S4. IR spectrum of compound 13.
Figure S5. IR spectrum of compound 14.
Figure S6. IR spectrum of compound 15.
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Figure S28. $^{13}$C-NMR spectrum of compound 17.
Figure S29. $^{13}$C-NMR spectrum of compound 18.
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Figure S31. $^1$H, $^1$H-COSY spectrum of compound 14.
Figure S32A. $^1$H,$^{13}$C-Heteronuclear Single Quantum Coherence (HSQC) spectrum of compound 14 (full spectrum).
Figure S32B. $^1$H,$^{13}$C-Heteronuclear Single Quantum Coherence (HSQC) spectrum of compound 14 ($\delta_H = -0.4–4.1$, $\delta_C = 0–80$).
Figure S33. Dose-response curve for the synthesized compounds 11-19 against HeLa (cervical carcinoma) cell line.
Figure S34. Dose-response curve for the synthesized compounds 11-19 against HepG2 (liver carcinoma) cell line.
Figure S35. 3D-pharmacophore mapped on the synthesized compounds 11-19 against HeLa (cervical) tumor cell line.
Figure S36. 3D-pharmacophore mapped on the synthesized compounds 11-19 against HepG2 (liver) tumor cell line.
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Figure S6. IR spectrum of compound 15.
Figure S7. IR spectrum of compound 16.
**Figure S8.** IR spectrum of compound 17.
Figure S9. IR spectrum of compound 18.
Figure S10. IR spectrum of compound 19.
Figure S11. $^1$H-NMR spectrum of compound 3.
Figure S12. $^1$H-NMR spectrum of compound 11.
Figure S13. $^1$H-NMR spectrum of compound 12.
Figure S14. $^1$H-NMR spectrum of compound 13.
Figure S15. $^1$H-NMR spectrum of compound 14.
Figure S16. $^1$H-NMR spectrum of compound 15.
Figure S17. $^1$H-NMR spectrum of compound 16.
Figure S18. $^1$H-NMR spectrum of compound 17.
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Figure S32B. $^1$H,$^{13}$C-Heteronuclear Single Quantum Coherence (HSQC) spectrum of compound 14 ($\delta_H = -0.4-4.1$, $\delta_C = 0-80$).
IC₅₀ of compound 11 = 10.27 μg/ml (16.69 μM)

IC₅₀ of compound 12 = 8.26 μg/ml (12.71 μM)
IC_{50} of compound 13 = 2.50 µg/ml (4.87 µM)

IC_{50} of compound 14 = 3.15 µg/ml (5.75 µM)
Figure S33. Dose-response curve for the synthesized compounds 11-19 against HeLa (cervical carcinoma) cell line.
IC₅₀ of compound 11 = 2.17 µg/ml (3.53 µM)

IC₅₀ of compound 12 = 4.68 µg/ml (7.20 µM)

IC₅₀ of compound 13 = 5.60 µg/ml (10.90 µM)

IC₅₀ of compound 14 = 6.85 µg/ml (12.50 µM)
IC₅₀ of compound 15 = 9.02 µg/ml (18.42 µM)

IC₅₀ of compound 16 = 9.09 µg/ml (17.34 µM)
**IC₅₀ of compound 17 = 10.27 μg/ml (22.06 μM)**

- **Surviving fraction**
- **Concentration (μg/ml)**

**IC₅₀ of compound 18 = 8.17 μg/ml (17.04 μM)**

- **Surviving fraction**
- **Concentration (μg/ml)**
Figure S34. Dose-response curve for the synthesized compounds 11-19 against HepG2 (liver carcinoma) cell line.
Compound 13
Compound 15
Figure S35. 3D-pharmacophore mapped on the synthesized compounds 11-19 against HeLa (cervical) tumor cell line.
Figure S36. 3D-pharmacophore mapped on the synthesized compounds 11-19 against HepG2 (liver) tumor cell line.