Supporting Information

Org. Commun. 14:3 (2021) 280-293

Synthesis of novel salicylic acid-pyrrolone conjugates and investigation of their cytotoxic and genotoxic effects in *Allium cepa* root tip cells

Mehmet Gümüş^{1,*}, Selin Can², H. Erhan Eroğlu^{2,*} and İrfan Koca³

¹Akdağmadeni Health College, Yozgat Bozok University, Yozgat, Türkiye ²Department of Biology, Faculty of Art & Sciences, Yozgat Bozok University, Yozgat, Türkiye ³Department of Chemistry, Faculty of Art & Sciences, Yozgat Bozok University, Yozgat, Türkiye

| Table of Contents | Page |
|--|------|
| General Procedure for the Synthesis of Novel Salicylic Acid Derived Compounds (7a-e) | 3 |
| Figure S1: HRMS spectra of 7a | 3 |
| Figure S2: ¹ H NMR spectra of 7a | 4 |
| Figure S3: ¹ H NMR spectra (AA'BB' system) of 7a | 4 |
| Figure S4: ¹³ C NMR spectra of 7a | 5 |
| Figure S5: HRMS spectra of 7b | 5 |
| Figure S6: ¹ H NMR spectra of 7b | 6 |
| Figure S7: ¹³ C NMR spectra of 7b | 6 |
| Figure S8: HRMS spectra of 7c | 7 |
| Figure S9: ¹ H NMR spectra of 7c | 7 |
| Figure S10: ¹³ C NMR spectra of 7c | 8 |
| Figure S11: HRMS spectra of 7d | 8 |
| | |

| Figure S12: ¹ H NMR spectra of 7d | 9 |
|--|----|
| Figure S23: ¹ H NMR spectra (AA'BB' system) of 7d | 9 |
| Figure S14: ¹ H NMR spectra of 7d | 10 |
| Figure S15: HRMS spectra of 7e | 10 |
| Figure S16: ₁ H NMR spectra of 7e | 11 |
| Figure S17: ¹³ C NMR spectra of 7e | 11 |
| | |

General Procedure for the Synthesis of Novel Salicylic Acid Derived Compounds (7a-e)

A mixture of furan-3-one **5** (10.0 mmol) and salicylic acid derivative **6** (10.0 mmol) in methanol (30 mL) was refluxed in the presence of catalytic amount of pyridine for 24 hours. The reaction was followed by TLC. After the solvent was removed under reduced pressure, the oily residue was treated with diethylether. The precipitated product was filtered off and purified by recrystallization or column chromatography methods. Butanol was used in recrystallization processes and chloroform:methanol solvent pair (10:1) was used in column chromatography processes (Yields: 74-83 %).

2-hydroxy-5-(2-hydroxy-2-(2-methoxy-2-oxoethyl)-4-(4-methoxybenzoyl)-5-(4-methoxy phenyl)-3-oxo-2,3-dihydro-1H-pyrrol-1-yl)benzoic acid (7a)

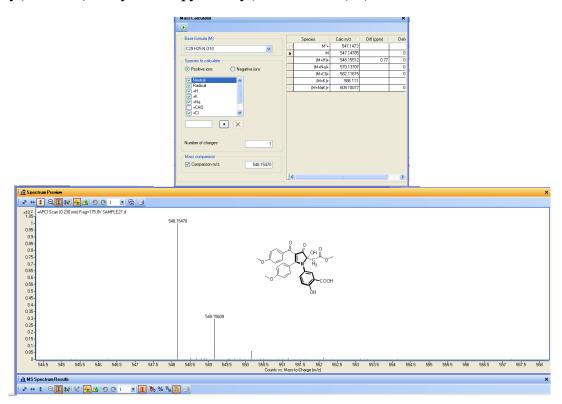


Figure S3: HRMS spectra of 7a

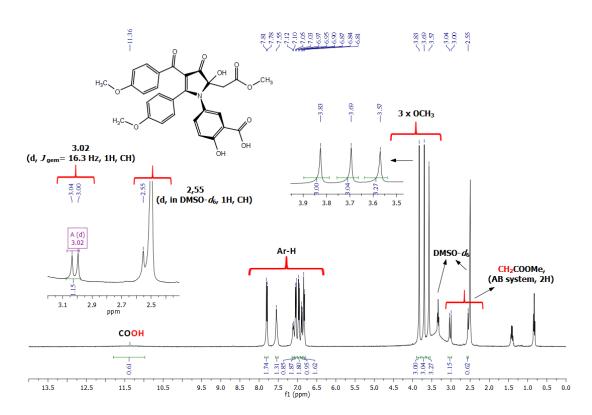


Figure S4: ¹H NMR spectra of 7a

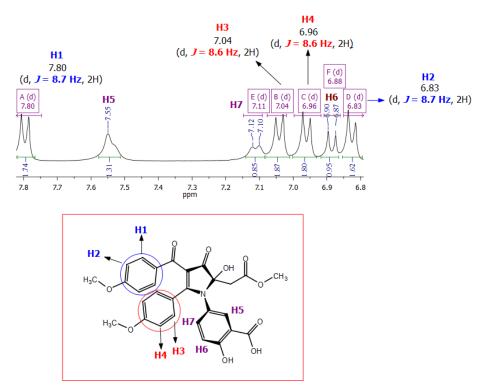


Figure S5: ¹H NMR spectra (AA'BB' system) of 7a

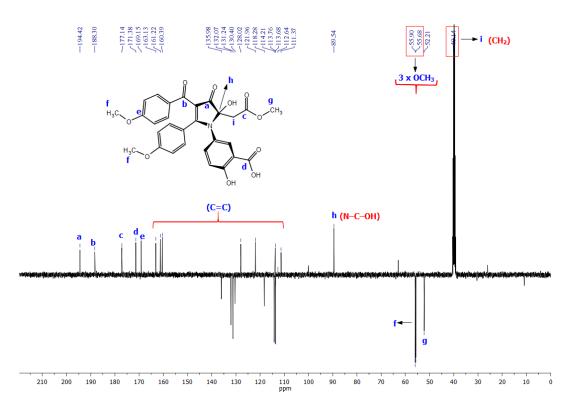


Figure S6: ¹³C NMR spectra of 7a

 $5-(2-(2-ethoxy-2-oxoethyl)-2-hydroxy-4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-3-oxo-2, \\ 3-dihydro-1H-pyrrol-1-yl)-2-hydroxybenzoic\ acid\ (7b)$

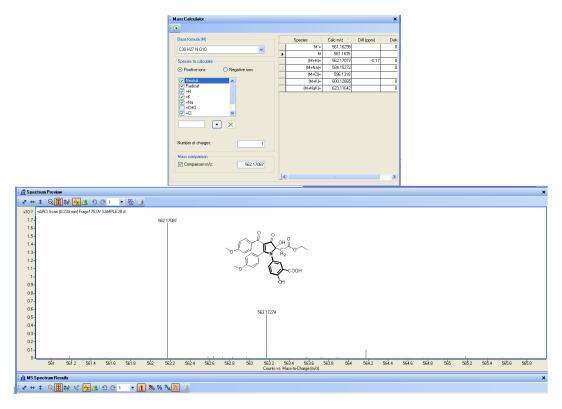


Figure S7: HRMS spectra of 7b

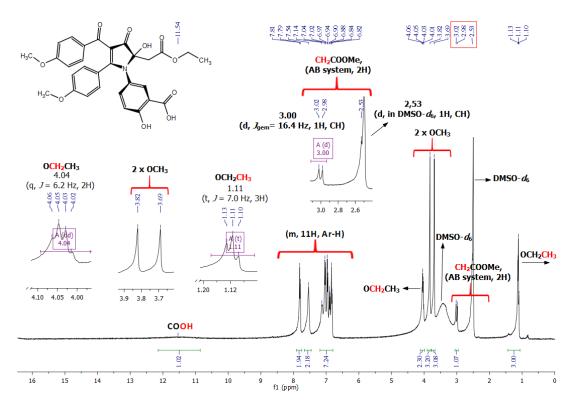


Figure S8: ¹H NMR spectra of 7b

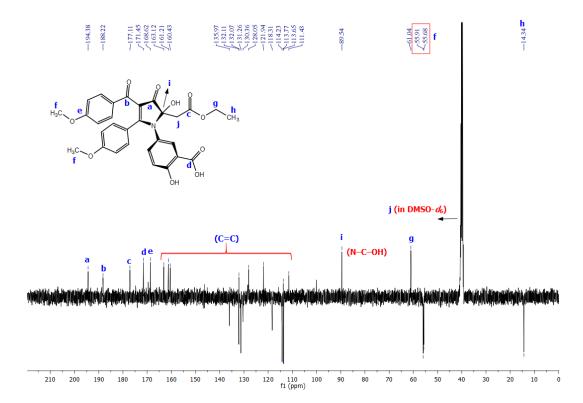


Figure S9: ¹³C NMR spectra of 7b

2-hydroxy-4-(2-hydroxy-2-(2-methoxy-2-oxoethyl)-4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1H-pyrrol-1-yl)benzoic acid (7c)

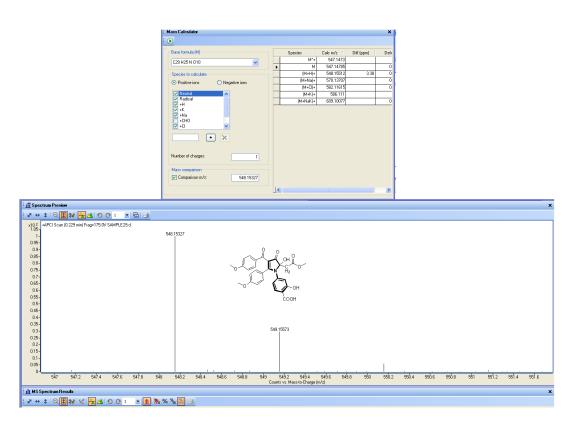


Figure S10: HRMS spectra of 7c

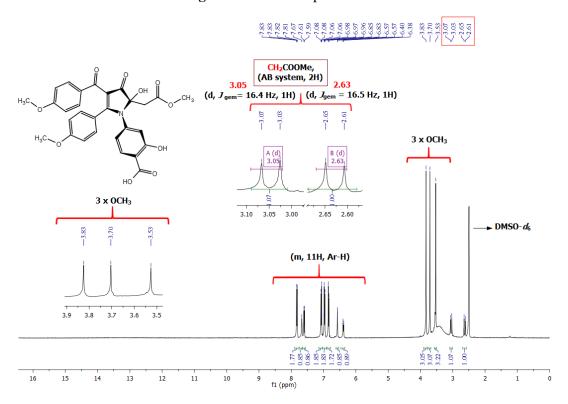


Figure S11: ¹H NMR spectra of 7c

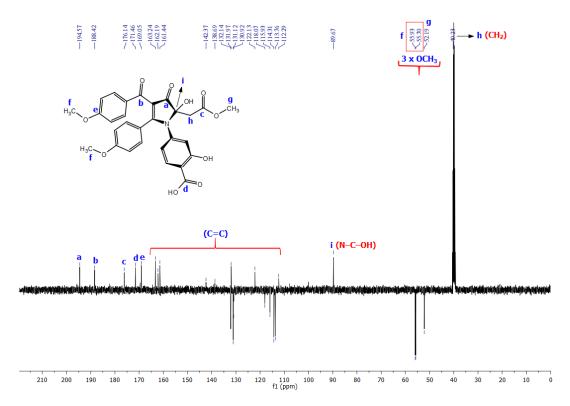


Figure S12: ¹³C NMR spectra of 7c

 $4-(2-(2-ethoxy-2-oxoethyl)-2-hydroxy-4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-3-oxo-2, \\ 3-dihydro-1H-pyrrol-1-yl)-2-hydroxybenzoic\ acid\ (7d)$

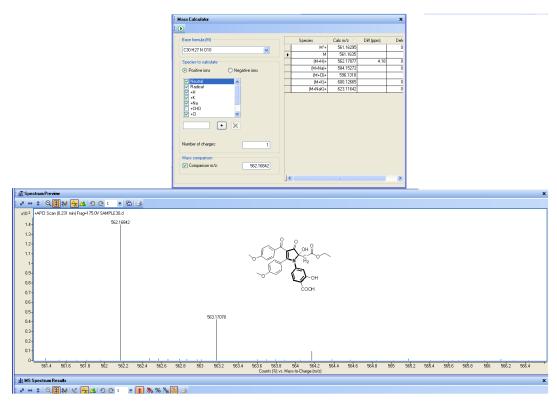


Figure S13: HRMS spectra of 7d

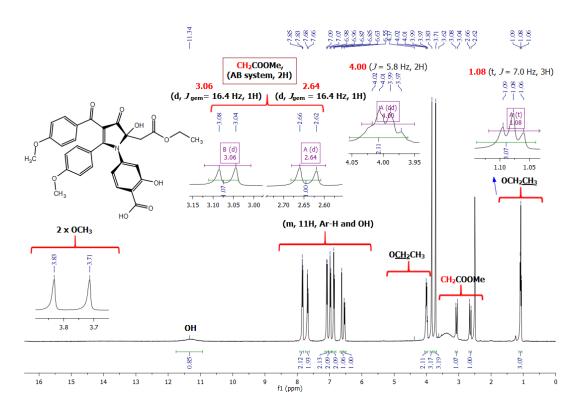


Figure S14: ¹H NMR spectra of 7d

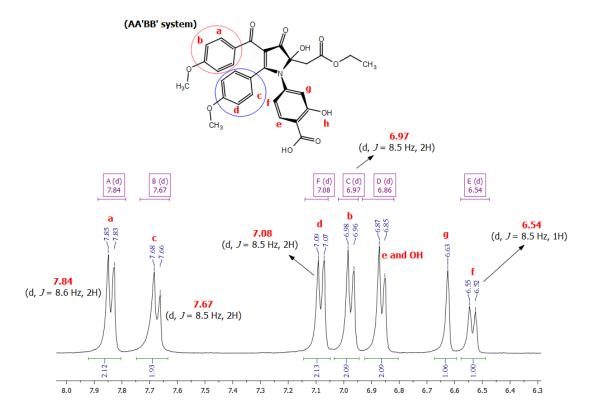


Figure S15: ¹H NMR spectra (AA'BB' system) of 7d

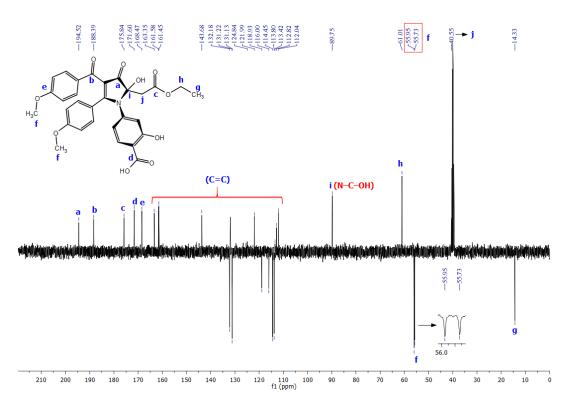


Figure S16: ¹H NMR spectra of 7d

 $4-(4-(ethoxycarbonyl)-2-hydroxy-2-(2-methoxy-2-oxoethyl)-5-(4-methoxyphenyl)-3-oxo-2, 3-dihydro-1H-pyrrol-1-yl)-2-hydroxybenzoic\ acid\ (7e)$

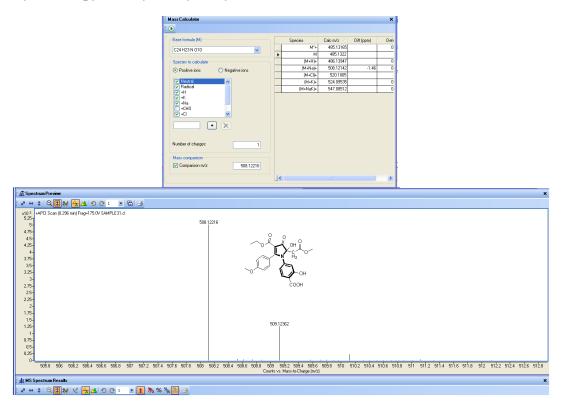


Figure S17: HRMS spectra of 7e

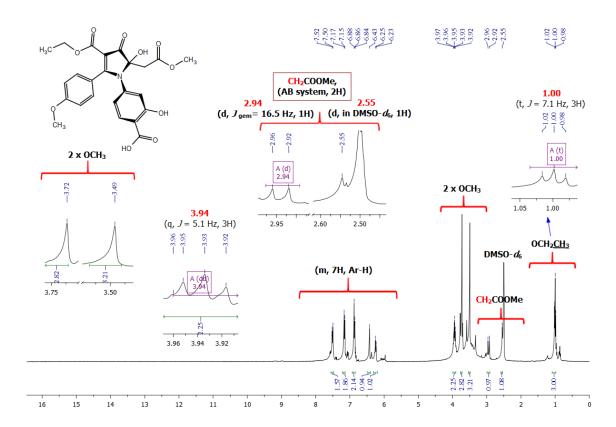


Figure S18: ¹H NMR spectra of 7e

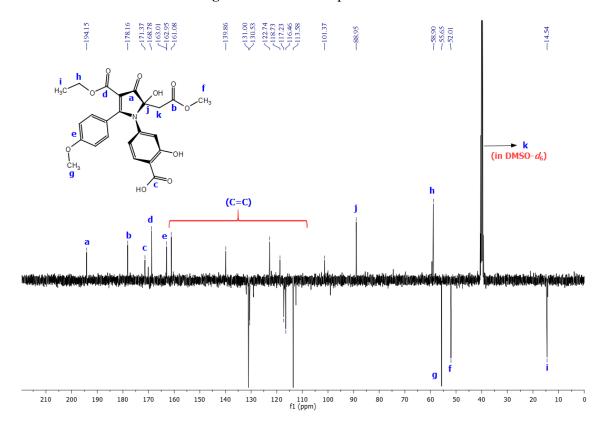


Figure S19: ¹³C NMR spectra of 7e