Supporting Information

Solid-State Emission Enhancement via Molecular Engineering of Benzofuran Derivatives.

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Synthesis

General experimental methods

Unless otherwise stated, all the reactions were carried out under argon atmosphere with commercially available reagents and solvents. Anhydrous THF was obtained by distilling over sodium and benzophenone. The other reagent grade solvents were used without further purification. Melting points were obtained on a Start SMP melting point apparatus and they are uncorrected. Mass spectrometric (MS) measurements were recorded on a MALDI-TOF Bruker Biflex III instrument using a positive-ion mode. NMR spectra were recorded at 298 K on a NMR Bruker Avance III 300 spectrometer. Chemical shifts for $^{13}$C NMR spectra were recorded in parts per million using either the central peak of deuterated chloroform (77.23 ppm) or deuterated DMSO (39.51 ppm) as the internal standards. Proton NMR spectra were recorded in parts per million and they were referenced to the residual solvent proton according to the literature. Characteristic splitting patterns due to spin-spin coupling are expressed as follows: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet.

Benzofuran-2-carbaldehyde (8), diethyl benzylphosphonate (14), benzofuran-2-ylboronic acid (10), 5-bromofuran-2-carbaldehyde (11), benzofuran-2(3H)-one (15), and 2-phenylacetonitrile (13) were purchased from either Aldrich or Jansen and they were used as received.

Synthetic pathways to 1-7

Compounds 1-7 was prepared as indicated in scheme S1. Compound 1 was prepared in 70 % yield by McMurry coupling of 2-benzofuran carbaldehyde 8. The other molecules were prepared by Knoevenagel condensations or Wittig Horner reactions from the aldehydes 8 and 9. Aldehyde 9 was obtained in 78% yield by the Suzuki coupling between the boronic derivative of benzofuran 10 and the bromo-furaldehyde 11.

The Wittig-Horner reactions to obtain 3 and 5 were realized in THF at room temperature by adding a slight excess of tBuONa on a mixture of the stoichiometric amount of aldehyde 8 or 9 and phosphonate 14. The E isomers of 3 and 5 were isolated in 45 and 65 % yield respectively.
The Knoevenagel condensations between aldehyde 8 or 9 and acetonitrile derivatives 12 or 13 proceeded at room temperature in EtOH in presence of catalytic amount of tBuONa. After filtration of the precipitate and washing with a small amount of EtOH, compounds 2, 4, 6 and 7 were obtained as microcrystalline powders in range of 55 - 70 % yields. 2-Benzofuran acetonitrile 12 was obtained in one step by the condensation of the ylure 16 on the 2-coumaranone 15. The reaction proceeds rapidly in 15 min under microwave activation at 120°C in toluene to give 12 in 77% yield after a flash chromatography on silica gel.

Synthetic procedure and characterization of derivatives

5-(Benzofuran-2-yl)furan-2-carbaldehyde (9).

To a stirred solution of 5-bromofuran-2-carbaldehyde 11 (1.01 g, 5.76 mmol) in dioxane (200 mL) were added aqueous Na₂CO₃ (6.2 g, 58.50 mmol) and benzofuran-2-boronic acid 10 (1.14 g, 7.04 mmol). The mixture was then purged with argon for 30 min before adding tetrakis(triphenylphosphine)palladium(0) (1.39 mg, 1.21 mmol, 20 % mol) under a positive argon pressure. The reaction flask was sealed and heated to 110 °C for 12 h. The reaction mixture was then cooled to room temperature and the precipitate was filtered. The filtrate was evaporated in vacuo and the residue was extracted with EtOAc (100 mL). The organic layer was washed consecutively with concentrated sodium bicarbonate (3 x 50 mL) and brine (50 mL). It was then dried over magnesium sulfate, filtered, and concentrated in vacuo. The obtained residue was purified on silica gel using EtOAc/petroleum ether in different proportions to afford the title compound 9 as a yellow solid (1.17 g, 96%). M.p.: 137 – 139 °C. ¹H NMR (CDCl₃): δ 9.61 (s, 1H), 7.56 (dd, J = 7.7, 0.6 Hz, 1H), 7.45 (dd, J = 8.2, 0.6 Hz, 1H), 7.32 – 7.24 (m, 2H), 7.24 – 7.16 (m, 2H), 6.88 (d, J = 3.7 Hz, 1H). ¹³C NMR (CDCl₃): δ 177.2, 155.3, 152.4, 151.0, 146.1, 128.2, 125.9, 123.7, 123.0, 121.9, 111.4, 109.6, 105.6. HRMS (MALDI-TOF) calc’d for C₁₃H₈O₃: 212.0473; found: 212.0470.
Scheme S1. Synthetic pathways to 1-7

2-(Benzofuran-2-yl)acetonitrile (12).

To a solution of benzofuran-2(3H)-one 15 (500 mg, 3.73 mmol) in toluene (5 mL) was added (triphenylphosphoranylidene)acetonitrile 16 (1.22 g, 4.05 mmol). The mixture was irradiated in a CEM Discover microwave (300 W, 150°C, 5 bars) for 15 min. The solvent was then evaporated. The residue was
purified over silica gel (petroleum ether/methylene chloride 2/8) to give a white solid (450 mg, 77%). M.p.: 61-63°C. 1H NMR (CDCl3): 7.56 (dd, 1H, J=7.3 Hz, J=1.1 Hz), 7.46 (d, 1H, J=7.9 Hz), 7.35-7.21 (m, 2H), 6.75 (d, 1H, J=1.1 Hz), 3.92 (d, 2H, J=1.1 Hz). 13C NMR (CDCl3): 155.4, 146.1, 127.9, 125.0, 123.4, 121.2, 115.1, 111.3, 105.6, 18.2. HRMS (EI) calc’d for C10H7NO: 157.0528, found: 157.0525.

(E)-1,2-Di(benzofuran-2-yl)ethane (1).

To a solution of benzofuran-2-carbaldehyde (160 μL, 1.32 mmol) in THF (20 mL) was added titanium(IV) chloride (180 μL, 1.6 mmol) dropwise over a period of 30 min at −18 °C with stirring. The reaction was stirred for an additional 30 min. After the complete addition of TiCl4. Afterwards, zinc powder (210 mg, 3.2 mmol) was added in small portions over a period of 30 min. The mixture was stirred at −18°C for 30 min, warmed to room temperature, and then refluxed for 12 h. The reaction was quenched by adding ice water (100 mL). The resulting solid was dissolved in ethyl acetate and the insoluble inorganic material was filtered. The filtrate was evaporated and the residue was purified over silica gel (pentane / ethyl acetate 9/1) to give a white powder. The solid was recrystallized from ethanol to give colorless crystal (120 mg; 70 % yield). M.p.: 184 °C. 1H NMR (CDCl3): 7.61 (d, 2H, J=8.0 Hz), 7.53 (d, 2H, J=8.0 Hz), 7.40-7.23 (m, 6H), 6.82 (s, 2H). 13C NMR (CDCl3): 155.1, 154.9, 136.6, 130.2, 129.1, 125.0, 123.0, 121.0, 117.6, 111.0, 106.6. HRMS (FAB) calc’d for C18H12O2: 260.0837, found: 260.0833. Elemental analysis calc’d: C: 83.06; H: 4.65; found C: 83.09; H: 4.59. Previously published 2

General Wittig-Horner procedure

Under argon, NaO'Bu (1.1 equiv.) was added to an ice cooled stirred solution of diethyl benzylphosphonate (1 equiv.) and either 1 (450 mg, 3.08 mmol) or 2 (500 mg, 2.36 mmol) in anhydrous THF (25 mL). The reaction mixture was first allowed to stir at 0 °C for 1 h. Afterwards, it was stirred for 12 h and allowed to warm to room temperature. The solvent was removed in vacuo and the obtained residue was extracted with EtOAc (100 mL). The organic layer was washed consecutively with water (3 x 50 mL) and brine (50 mL). It was then dried over magnesium sulfate, filtered, and concentrated in vacuo. The product crystallized after the solvent was evaporated. The precipitate was collected by filtration, washed with small portions of cold ethanol, and then dried in high vacuo to afford the product as crystals.

(E)-2-Styrylbenzofuran (3).

Colorless crystals 45 % yield). M.p.: 120 – 122 °C. 1H NMR (CDCl3): δ 7.54 (d, J = 7.4 Hz, 3H), 7.48 (d, J = 8.0 Hz, 1H), 7.42 – 7.17 (m, 6H), 7.01 (d, J = 16.2 Hz, 1H), 6.68 (s, 1H). 13C NMR (CDCl3): δ 155.1, 154.9, 136.6, 130.2, 129.1, 128.8, 128.1, 126.7, 124.6, 122.9, 120.8, 116.4, 110.9, 105.2. MALDI-TOF-
MS: \textit{m/z} = 286.1 [M]⁺. HRMS (\textit{m/z}, FAB⁺) calc’d for C₁₆H₁₂O: 220.0888; found: 220.0884. Elemental analysis calc’d: C: 87.25; H: 5.49; found C: 87.07; H: 5.49. Previously published.³

\textit{(E)-2-}(5-Styrylfuran-2-yl)benzofuran (5).

Colorless crystals (65% yield). M.p.: 104 -105 °C. \textit{¹H} NMR (CDCl₃): \(\delta\) 7.63 – 7.60 (m, 1H), 7.54-7.52 (m, 3H), 7.39 (t, \(J = 7.5\) Hz, 2H), 7.35 – 7.24 (m, 3H), 7.19 (d, \(J = 16.3\) Hz, 1H), 7.04 (s, 1H), 6.94 (d, \(J = 3.5\) Hz, 1H). \textit{¹³C} NMR (CDCl₃): \(\delta\) 154.8, 153.9, 148.0, 145.6, 136.9, 128.9, 128.9, 128.2, 127.9, 126.6, 124.6, 123.3, 121.1, 116.0, 111.2, 110.9, 110.0, 101.5. MALDI-TOF-MS: \textit{m/z} = 286.1 \([\text{M}]^+\). HRMS (\textit{m/z}, FAB⁺) calc’d for C₂₀H₁₄O₂: 286.0994; found: 286.0989. Elemental analysis calc’d: C: 83.90; H: 4.93; found C: 83.25; H: 4.95.

\textit{General Knoevenagel condensations procedure}

A mixture of aldehyde (4 mmol for 1 or 2 mmol for 2), carbonitrile derivative (1.1 equiv.) and a catalytic amount of NaO\textit{t}Bu (10% mol.) was stirred in ethanol (10 mL) for 12 h at room temperature. The resulting precipitate was filtered. It was then washed with distilled water and cold ethanol. Afterwards, it was dried in high \textit{vacuo} to afford coloured crystals.

\textit{(E)-2,3-}(Benzofuran-2-yl)acrylonitrile (2). Yellow solid (70% yield). M.p.: 143 – 145 °C. \textit{¹H} NMR (CDCl₃): 7.69-7.57 (m, 4H), 7.52-7.25 (m, 6H), 7.12 (s, 1H). \textit{¹³C} NMR (CDCl₃): 155.7, 155.5, 151.0, 150.9, 128.6, 128.2, 127.3, 126.2, 125.9, 123.8, 123.7, 122.1, 121.8, 115.6, 112.6, 111.6, 111.8, 111.1, 107.5, 100.9. HRMS (FAB) calc’d for C₁₉H₁₁NO: 285.0790, found: 285.0783. Elemental analysis calc’d: C: 79.99; H: 3.89; N: 4.91 found C: 79.24; H: 3.88; N: 4.83.

\textit{(Z)-3-}(Benzofuran-2-yl)-2-phenylacrylonitrile (4).

Yellow pale solid (77% yield). M.p.: 105-107°C. \textit{¹H} NMR (CDCl₃): 7.66 (d, 2H, \(J=8.0\) Hz), 7.60 (d, 1H, \(J=8.0\) Hz), 7.51 (d, 1H, \(J=8.4\) Hz), 7.48-7.30 (m, 6H), 7.22 (d, 1H, \(J=8.4\) Hz). \textit{¹³C} NMR (CDCl₃): 155.2, 151.2, 133.5, 129.5, 129.2, 128.1 (2), 126.9, 125.9, 123.7, 122.0, 117.4, 111.6, 111.2, 110.9. HRMS (FAB) calc’d for C₁₉H₁₁NO: 245.0845, found: 245.0840. Elemental analysis calc’d: C: 83.25; H: 4.52; N: 5.71 found C: 83.65; H: 4.57; N: 5.83.

\textit{(Z)-3-}(5-(Benzofuran-2-yl)furan-2-yl)-2-phenylacrylonitrile (6).

Orange solid (60 % yield). M.p: 135 – 137 °C. \textit{¹H} NMR (CDCl₃): 7.68 (d, 2H, \(J=8.0\) Hz), 7.63 (d, 1H, \(J=7.4\) Hz), 7.51 (d, 1H, \(J=8.0\) Hz), 7.49-7.20 (m, 8H), 6.96 (d, 1H, \(J=3.6\) Hz). \textit{¹³C} NMR CDCl₃): 155.1, 150.2, 148.0, 146.9, 133.7, 129.1 (2), 128.5, 126.7, 125.6, 125.2, 123.5, 121.6, 117.8, 117.5, 111.2, 110.2,
Orange solid (55% Yield). M.p: 195-197 °C. $^1$H NMR (CDCl$_3$): 7.65-7.58 (m, 3H), 7.51 (d, 1H, $J$=8.0 Hz), 7.47 (d, 1H, $J$=8.0 Hz), 7.36-7.23 (m, 5H), 7.14 (d, 1H, $J$=3.7 Hz), 7.07 (s, 1H), 6.97 (d, 1H, $J$=3.7 Hz). $^{13}$C NMR (CDCl$_3$): 155.3, 155.2, 151.1, 149.9, 148.7, 146.7, 128.7, 128.5, 125.8, 125.4, 124.4, 123.6, 123.5, 121.7, 121.6, 118.9, 116.0, 111.2, 111.0, 110.3, 106.6, 104.7, 98.0. HRMS (FAB) calc’d for C$_{23}$H$_{13}$NO$_3$: 351.0895, found: 351.0897. Elemental analysis calc’d: C: 78.62; H: 3.73; N: 3.99 found C: 78.84; H: 3.82; N: 3.65.

**Structure refinement and crystal data**

Single crystals suitable for X-ray diffraction analyses were obtained for all the compounds by the slow evaporation of ethanol – chloroform solution. The data collection details are found in Tables 1 and 2.

X-ray single-crystal diffraction data were collected on an Agilent SuperNova diffractometer equipped with Atlas CCD detector and mirror monochromated micro-focus Cu-K$_\alpha$ radiation ($\lambda$ = 1.54184 Å) for compounds 1-5, and on a BRUKER KappaCCD diffractometer, equipped with a graphite monochromator utilizing MoK$_\alpha$ radiation ($\lambda$ = 0.71073Å) for compounds 6, 7. The structures were solved by direct methods and refined on F$^2$ by full matrix least-squares techniques using SHELX (G.M. Sheldrick, 1997, 2013, 2016) package. All non-hydrogen atoms were refined anisotropically and the H atoms were included in the calculation without refinement. Multiscan empirical absorption was corrected by SADABS program (Sheldrick, Bruker, 2008) for 6, 7, and using CrysAlisPro program (CrysAlisPro, Agilent Technologies, V1.171.38.41r, 2015) for 1-5.
Table S1. Crystallographic data of 1, 2, 3, and 4.

|             | 1            | 2            | 3            | 4            |
|-------------|--------------|--------------|--------------|--------------|
| Formula     | C_{18}H_{12}O_{2} | C_{19}H_{11}NO_{2} | C_{16}H_{12}O_{2} | C_{17}H_{11}NO_{2} |
| M           | 260.28       | 285.29       | 220.26       | 245.27       |
| T (K)       | 150          | 293          | 150          | 150          |
| Crystal system | Monoclinic  | Monoclinic  | Monoclinic  | Monoclinic  |
|             | P2_{1}       | Pc           | P2_{1}/c     | P_{n}        |
| Unit cell: a (Å) | 6.4009(2)   | 5.8430(2)   | 13.4246(5)  | 3.8218(2)   |
| b (Å)       | 7.3211(3)   | 3.9026(2)   | 5.6336(2)   | 5.7496(3)   |
| c (Å)       | 13.9114(6)  | 30.318(2)   | 7.7042(3)   | 27.2500(13) |
| α (°)       | 90          | 90          | 90          | 90          |
| β (°)       | 100.161(4)  | 94.535(4)   | 90.883(3)   | 93.862(5)   |
| γ (°)       | 90          | 90          | 90          | 90          |
| Volume (Å³) | 641.69(4)   | 689.18(6)   | 582.59(4)   | 597.43(5)   |
| Z           | 2           | 2           | 2           | 2           |
| Calc’d density | 1.347       | 1.375       | 1.256       | 1.363       |
| F(000)      | 272         | 296         | 232         | 256         |
| θ range (°) | 3.23 to 76.19 | 5.86 to 76.21 | 3.292 to 76.493 | 3.25 to 76.12 |
| Limiting indices | -8<h<8     | -7<h<7      | -15<h<16    | -4<h<4      |
|             | -8<k<9      | -4<k<4      | -6<k<6      | -6<k<6      |
|             | -17<l<17    | -33<l<37    | -8<l<9      | -24<l<33    |
| Reflection coll. | 3840        | 2870        | 4158        | 2149        |
| Unique      | 2178        | 1873        | 1179        | 1194        |
| R (int)     | 0.0203      | 0.0142      | 0.0164      | 0.0137      |
| Final R indices, | [I>2sigma(I)], R1 | 0.0326    | 0.0498      | 0.0663      | 0.0390      |
|             | wR2         | 0.0922      | 0.1352      | 0.1626      | 0.0991      |
| R indices (all data), R1 | 0.0344 | 0.0547 | 0.0683 | 0.0429 |
|             | wR2         | 0.0934      | 0.1484      | 0.1637      | 0.1018      |
| Largest diff. | 0.158    | 0.253       | 0.396       | 0.196       |
| Peak and hole (e Å⁻³) | -0.159 | -0.252 | -0.181 | -0.220 |
| CCDC number | 1856854     | 1856855     | 1856856     | 1856857     |
Table S2. Crystallographic data of 5, 6, and 7.

|                  | 5       | 6       | 7       |
|------------------|---------|---------|---------|
| Formula          | C_{20}H_{14}O_{2} | C_{21}H_{13}NO_{2} | C_{23}H_{13}NO_{3} |
| M                | 286.31  | 311.32  | 351.34  |
| T (K)            | 150     | 293     | 293     |
| Crystal system   | Orthorhombic | Orthorhombic | Orthorhombic |
| Space group      | P na21  | P bca   | P2_{1} 2_{1} |
| Unit cell: a (Å) | 11.0189(3) | 7.3530(10) | 6.2228(6) |
| b (Å)            | 5.6659(2) | 13.0226(9) | 16.253(1) |
| c (Å)            | 46.0573(15) | 32.757(4)  | 17.111(1) |
| α (°)            | 90      | 90      | 90      |
| β (°)            | 90      | 90      | 90      |
| γ (°)            | 90      | 90      | 90      |
| Volume (Å³)      | 2875.45(16) | 3136.7(6)  | 1730.6(2) |
| Z                | 8       | 8       | 4       |
| Calc’d density   | 1.323   | 1.319   | 1.348   |
| F(000)           | 1200    | 1296    | 728     |
| θ range (°)      | 7.88 to 77.09 | 4.00 to 27.56 | 3.51 to 27.49 |
| Limiting indices | -13<h<13 | -8<h<9  | -7<h<8  |
|                  | -6<k<7  | -11<k<16| -20<k<21|
|                  | -57<l<57| -42<l<39| -22<l<20|
| Reflection coll. | 28174   | 21470   | 22183   |
| Unique           | 5865    | 3530    | 2273    |
| R (int)          | 0.0336  | 0.0802  | 0.0637  |
| Final R indices, |         |         |         |
| | [I>2sigma(I)], R1 | 0.0288  | 0.0470  | 0.0398  |
| | wR2     | 0.0699  | 0.0868  | 0.0714  |
| | R indices (all data), R1 | 0.0308  | 0.1783  | 0.0897  |
| | wR2     | 0.0722  | 0.1106  | 0.086   |
| Largest diff.    | 0.158   | 0.137   | 0.125   |
| Peak and hole (e Å⁻³) | -0.155 | -0.201  | -0.155  |
| CCDC number      | 1856858 | 1856859 | 1856860 |
Table S3: HOMO and LUMO energy levels, theoretical bandgap $\Delta E$, and cyclic voltammetry data$^d$ of compounds 1-7.

| Compounds | HOMO$^a$ (eV) | LUMO$^a$ (eV) | $\Delta E_{\text{the}}^a$ (eV) | $E_{\text{aix}}^b$ (V) | HOMO$^c$ (eV) | $E_{\text{red}}^b$ (V) | LUMO$^d$ (eV) | $\Delta E_{\text{elec}}^e$ (eV) |
|-----------|---------------|---------------|-----------------|---------|---------------|---------|---------------|-----------------|
| 1         | -5.21         | -1.81         | 3.40            | 1.17    | -5.86         | -2.00   | -2.96         | 2.78            |
| 2         | -5.56         | -2.44         | 3.12            | 1.57    | -6.16         | -1.41   | -3.46         | 2.65            |
| 3         | -5.32         | -1.60         | 3.72            | 1.26    | -5.96         | -       | -             | -               |
| 4         | -5.72         | -2.31         | 3.35            | 1.75    | -5.67         | -1.62   | -3.27         |                 |
| 5         | -5.00         | -1.72         | 3.28            | 1.02    | -5.76         | -       | -             | -               |
| 6         | -5.39         | -2.34         | 3.05            | 1.30    | -5.94         | -1.60   | -3.32         | 2.83            |
| 7         | -5.30         | -2.48         | 2.82            | 1.24    | -5.92         | -1.43   | -3.43         | 2.48            |

$^a$B3LYP/6-31G(d,p), $^b$10$^{-3}$ mol L$^{-1}$ 0.1 M Bu4NPF6/ CH2Cl2, v = 100 mV s$^{-1}$, ref SCE, $^c$HOMO = -(E onset,ox vs Fc+/Fc + 5.1), $^d$LUMO = -(E onset,red vs Fc+/Fc + 5.1), $^e$$\Delta E_{\text{elec}} = E_{\text{HOMO}} - E_{\text{LUMO}}$.

Figure S1: Representation of the optimized HOMO and LUMO orbitals of compounds 1-7.
Figure S2: CV traces of compounds 1 (black), 2 (blue) and 7 (red), $10^{-3}$ mol.l$^{-1}$ in 0.1M Bu$_4$NPF$_6$/CH$_2$Cl$_2$, $v = 100$ mV s$^{-1}$, ref SCE.
Figure S3. $^1$H NMR spectrum of 1 in CDCl$_3$. 
Figure S4. $^{13}$C NMR spectrum of 1 in CDCl$_3$. 
Figure S5. $^1$H NMR spectrum of 2 in CDCl$_3$. 
Figure S6. $^{13}$C NMR spectrum of 2 in CDCl$_3$. 
Figure S7. $^1$H NMR spectrum of 3 in CDCl$_3$. 
Figure S8. $^{13}$C NMR spectrum of 3 in CDCl$_3$. 
Figure S9. $^1$H NMR spectrum of 4 in CDCl$_3$. 
Figure S10. $^{13}$C NMR spectrum of 4 in CDCl$_3$. 
Figure S11. $^1$H NMR spectrum of 5 in CDCl$_3$. 
Figure S12. $^{13}$C NMR spectrum of 5 in CDCl$_3$. 
Figure S13. $^1$H NMR spectrum of 6 in CDCl$_3$. 
Figure S14. $^{13}$C NMR spectrum of 6 in CDCl$_3$. 
Figure S15. $^1$H NMR spectrum of 7 in CDCl$_3$. 
Figure S16. $^{13}$C NMR spectrum of 7 in CDCl$_3$. 
Figure S17: MALDI-ToF spectrum of compound 1

Chemical Formula: C_{18}H_{12}O_{2}

Exact Mass: 260.0837
Figure S18: HRMS spectrum (Fab) of compound 1
Figure S19: MALDI-TOF spectrum of compound 2

Chemical Formula: C_{19}H_{12}NO_{2}

Exact Mass: 285.0790
Figure S20: HRSM spectrum (Fab) of compound 2
Figure S21: MALDI-TOF spectrum of compound 3

Chemical Formula: C₁₆H₁₂O
Exact Mass: 220.0888
Molecular Weight: 220.2710
Figure S22: HRMS spectrum of compound 3
Figure S23: MALDI-TOF spectrum of compound 4
Figure S24: HRMS spectrum of compound 4

Chemical Formula: C_{17}H_{11}NO
Exact Mass: 245.0841
Figure S25: MALDI-TOF spectrum of compound 5
Figure S26: HRMS spectrum of compound 5
Figure S29: MALDI-TOF spectrum of compound 6

Chemical Formula: C_{21}H_{13}NO_2
Exact Mass: 311.0946
Molecular Weight: 311.3400
Figure S30: HRMS spectra of compound 6

Chemical Formula: C_{21}H_{13}NO_{2}
Exact Mass: 311.0946
Figure S31: MALDI-TOF spectrum of compound 7

Chemical Formula: \( \text{C}_{23}\text{H}_{13}\text{NO}_3 \)
Exact Mass: 351.0895
Figure S33: HRMS spectrum (FAB) of compound 7

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