**Supplementary table S1**

Supplementary data associated with this article can be found in the attached file. These data include IR, 1H-NMR, 13C-NMR and HR-MS spectra of the synthesized compounds (**2** and **4a-i**).

1H-NMR (δ, ppm and *J*, Hz): 12.19 (1H, *b*, NH), 8.07 (1H, *dd*, 3*J*=8.0, 4*J*=1.0, Ar-H), 7.75 (1H, *ddd*, 3*J*1=3*J*2=7.5, 4*J*=1.5, Ar-H), 7.56 (1H, *d,* 3*J*=8.0, Ar-H), 7.44 (1H, 3*J*=8.0, Ar-H).

 (**4a-i**)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Position | **4a**  R=4Br | **4b**  R=4Cl | **4c**  R=3Cl | **4d**  R=2Cl | **4e**  R=4OMe | **4f**  R=4Me | **4g**  R=2Me | **4h**  R=4H | **4i**  R=4NO2 |
| 2a | 2.56 | 2.56 | 2.55 | 2.57 | 2.55 | 2.55 | 2.57 | 2.58 | 2.57 |
| 6 | 8.10 | 8.11 | 8.09 | 8.12 | 8.10 | 8.10 | 8.12 | 8.10 | 8.10 |
| 7 | 7.51 | 7.51 | 7.51 | 7.51 | 7.51 | 7.51 | 7.51 | 7.51 | 7.52 |
| 8 | 7.83 | 7.83 | 7.83 | 7.83 | 7.83 | 7.83 | 7.83 | 7.83 | 7.84 |
| 9 | 7.64 | 7.64 | 7.63 | 7.63 | 7.63 | 7.63 | 7.63 | 7.64 | 7.64 |
| 11 | 4.98 | 4.98 | 4.97 | 5.08 | 4.95 | 4.96 | 5.03 | 4.98 | 5.04 |
| 13 | 10.60 | 10.61 | 10.67 | 10.11 | 10.31 | 10.38 | 9.83 | 10.48 | 11.09 |
| 15 | 7.58 | 7.64 | 7.80 | - | 7.50 | 7.48 | - | 7.60 | 7.85 |
| 16 | 7.52 | 7.39 | - | 7.53 | 6.90 | 7.14 | 7.40 | 7.33 | 8.23 |
| 17 | - | - | 7.15 | 7.23 | - | - | 7.11 | 7.08 | - |
| 18 | 7.52 | 7.39 | 7.37 | 7.34 | 6.90 | 7.14 | 7.18 | 7.33 | 8.23 |
| 19 | 7.58 | 7.64 | 7.45 | 7.71 | 7.50 | 7.48 | 7.24 | 7.60 | 7.85 |
| Other | - | - | - | - | 3.73  (H17a) | 2.26  (H17a) | 2.26  (H15a) | - | - |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Position | **4a**  R=4Br | **4b**  R=4Cl | **4c**  R=3Cl | **4d**  R=2Cl | **4e**  R=4OMe | **4f**  R=4Me | **4g**  R=2Me | **4h**  R=4H | **4i**  R=4NO2 |
| 2 | 155.8 | 155.8 | 155.8 | 155.8 | 155.9 | 155.9 | 155.9 | 155.9 | 155.8 |
| 2a | 23.5 | 23.5 | 23.5 | 23.4 | 23.4 | 23.5 | 23.4 | 23.4 | 23.5 |
| 4 | 161.7 | 161.7 | 161.7 | 161.7 | 161.7 | 161.7 | 161.7 | 161.7 | 161.7 |
| 5 | 120.1 | 120.1 | 120.1 | 120.2 | 120.1 | 120.1 | 120.2 | 120.1 | 120.0 |
| 6 | 126.6 | 126.6 | 126.6 | 126.7 | 126.6 | 126.6 | 126.7 | 126.6 | 126.6 |
| 7 | 127.1 | 127.1 | 127.1 | 127.1 | 127.1 | 127.1 | 127.1 | 127.1 | 127.1 |
| 8 | 135.0 | 135.0 | 135.1 | 135.0 | 135.0 | 135.0 | 135.0 | 135.0 | 135.1 |
| 9 | 126.9 | 126.8 | 126.9 | 126.9 | 126.8 | 126.8 | 126.8 | 126.9 | 126.9 |
| 10 | 147.6 | 147.6 | 147.6 | 147.6 | 147.6 | 147.6 | 147.6 | 147.6 | 147.6 |
| 11 | 47.5 | 47.5 | 47.6 | 47.0 | 47.3 | 47.4 | 47.0 | 47.4 | 47.8 |
| 12 | 166.2 | 166.2 | 165.5 | 166.7 | 165.4 | 165.7 | 166.1 | 166.0 | 167.2 |
| 14 | 138.4 | 138.0 | 140.5 | 134.8 | 132.2 | 133.0 | 136.2 | 139.1 | 145.2 |
| 15 | 115.7 | 121.2 | 119.2 | 127.2 | 121.2 | 119.6 | 132.4 | 119.6 | 119.5 |
| 16 | 132.2 | 127.7 | 133.6 | 128.0 | 114.4 | 129.7 | 130.9 | 129.3 | 125.6 |
| 17 | 121.6 | 129.2 | 123.8 | 130.1 | 160.0 | 136.6 | 126.5 | 124.1 | 143.0 |
| 18 | 132.2 | 127.7 | 131.1 | 126.7 | 114.4 | 129.7 | 126.0 | 129.3 | 125.6 |
| 19 | 115.7 | 121.2 | 118.0 | 120.2 | 121.2 | 119.6 | 125.5 | 119.6 | 119.5 |
| Other | - | - | - | - | 55.7  C17a | 20.9  C17a | 18.3  C15a | - | - |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound | NH | C=O | C=C | Other |
| **2** | 3404 | 1655 | 1607 1564 1468 | 775 692 664 |
| **4a** | 3310 3281 | 1686 1647 | 1595 1543 1470 | 773 692 656 |
| **4b** | 3312 3283 | 1686 1647 | 1591 1547 1470 | 771 681 662 |
| **4c** | 3318 3285 | 1692 1647 | 1593 1553 1477 | 772 683 656 |
| **4d** | 3204 | 1682 1665 | 1605 1541 1476 | 781 754 687 |
| **4e** | 3277 | 1676 1643 | 1597 1533 1470 | 770 691 656 |
| **4f** | 3312 | 1670 1667 | 1595 1537 1470 | 772 656 |
| **4g** | 3246 | 1682 1653 | 1599 1539 1468 | 781 748 658 |
| **4h** | 3279 | 1684 1651 | 1595 1549 1469 | 779 748 691 |
| **4i** | 3283 3227 | 1694 1641 | 1612 1589 1570 1470 | 775 692 658 |