Supporting Information

Biosynthesis of Fe, Pd, and Fe-Pd bimetallic nanoparticles and their application as recyclable catalyst for [3 + 2] cycloaddition reaction: A comparative approach

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Characterization of nanoparticles

1. UV-vis spectra

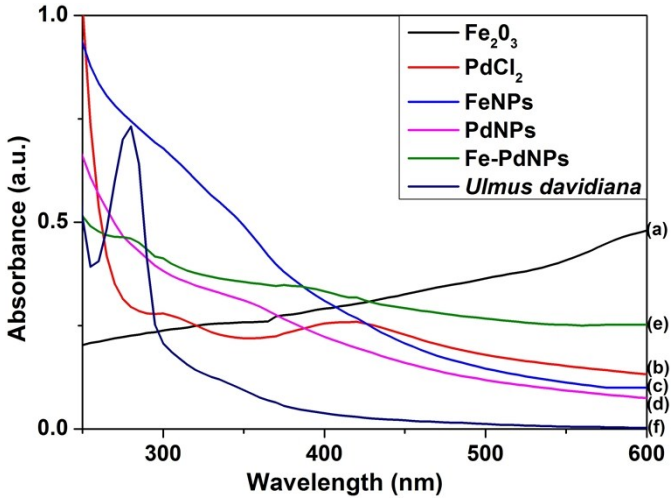


Fig. S1. UV-vis spectra of (a) Fe_2O_3, (b) $PdCl_2$, (c) FeNPs, (d) PdNPs, (e) Fe-PdNPs, and (f) *Ulmus davidiana* bark extract.

2. FTIR spectra.

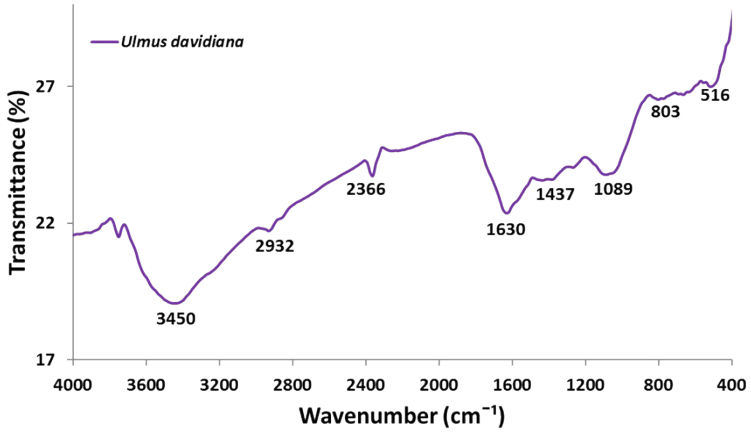


Fig. S2. FTIR spectum of *Ulmus davidiana* bark extract

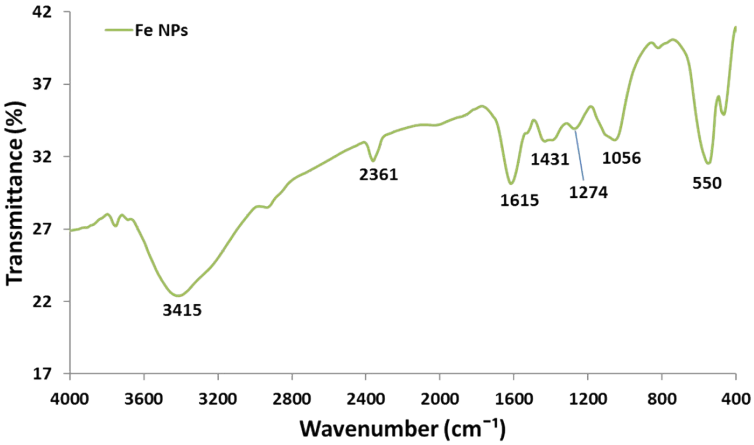


Fig. S3. FTIR spectum of FeNPs.

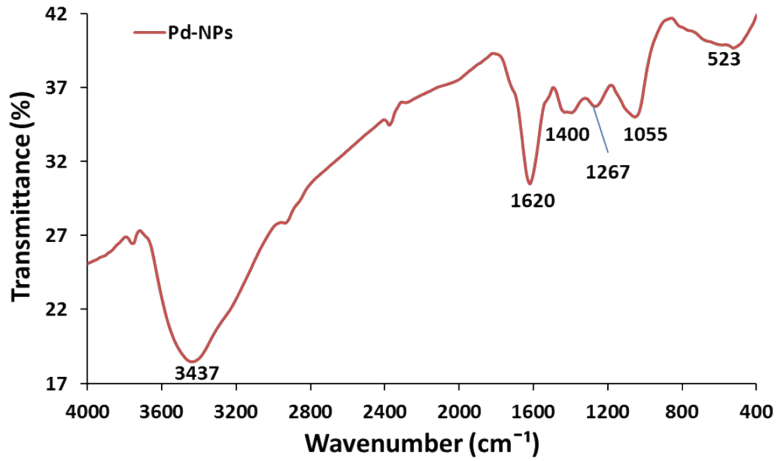


Fig. S4. FTIR spectum of PdNPs

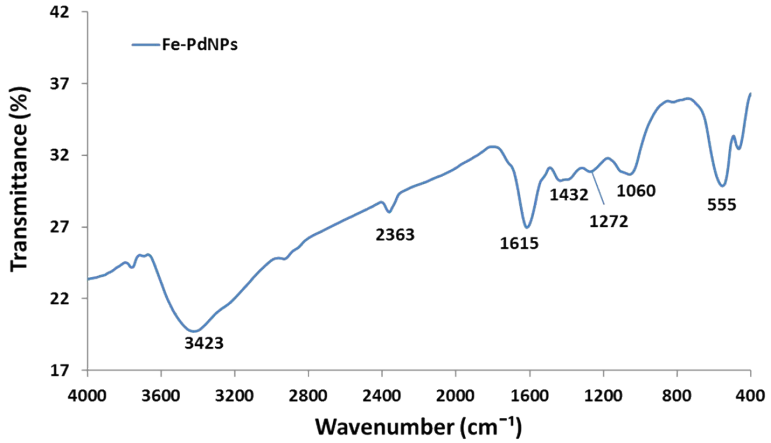
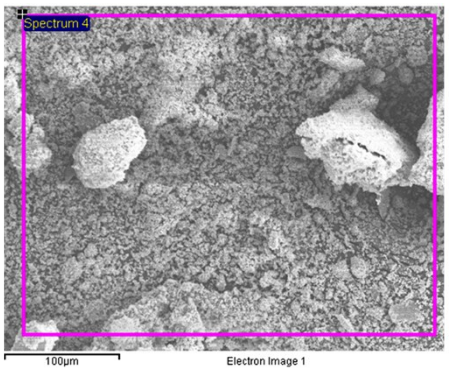


Fig. S5. FTIR spectum of Fe-PdNPs

3. EDS analysis



Element	Weight %	Atomic %
O K	15.26	41.47
Fe K	64.57	50.28
Pd L	20.18	8.25
Totals	100.00	

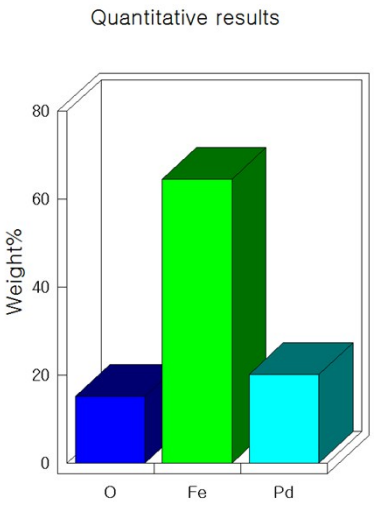


Fig. S6. Elemental abundance of Fe, O, and Pd in Fe-PdNPs by EDS.

4. Thermogravimetric analyses

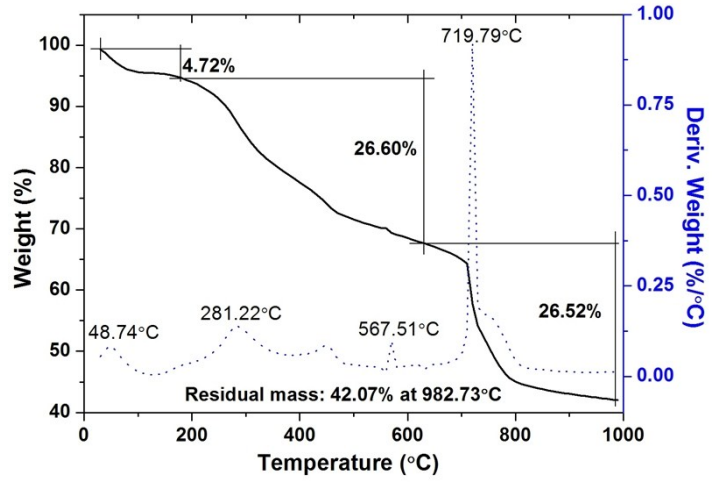


Fig. S7. TGA traces of FeNPs

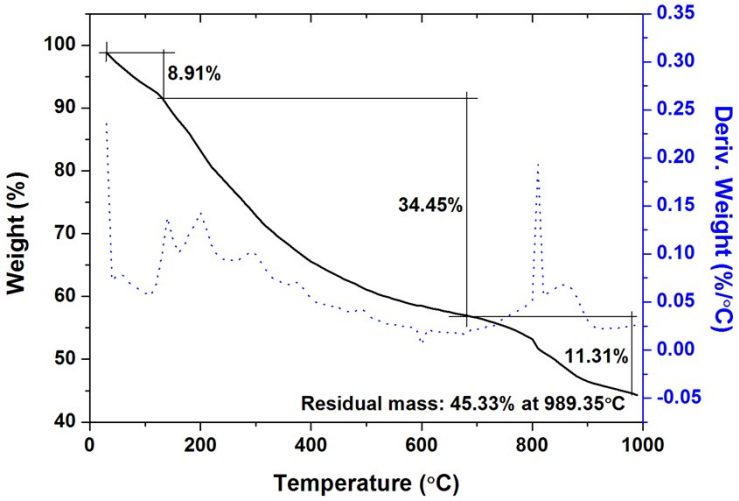


Fig. S8. TGA traces of PdNPs

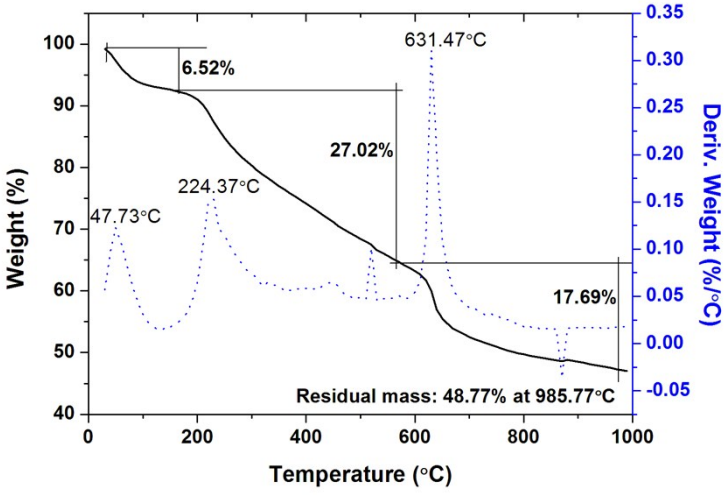


Fig. S9. TGA traces of Fe-PdNPs

5. SEM analysis

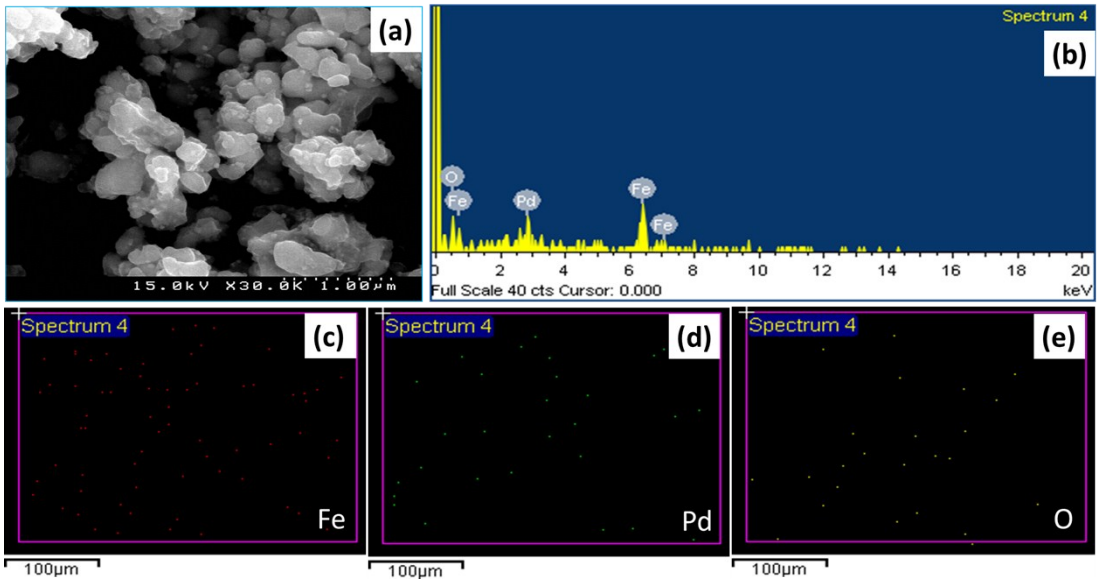


Fig. 10. (a) SEM image of the Fe-PdNPs at 1.00 µm, (b) EDS of the Fe-PdNPs and its elemental mapping (c) Fe, (d) Pd, and (e) O.

6. XPS analysis

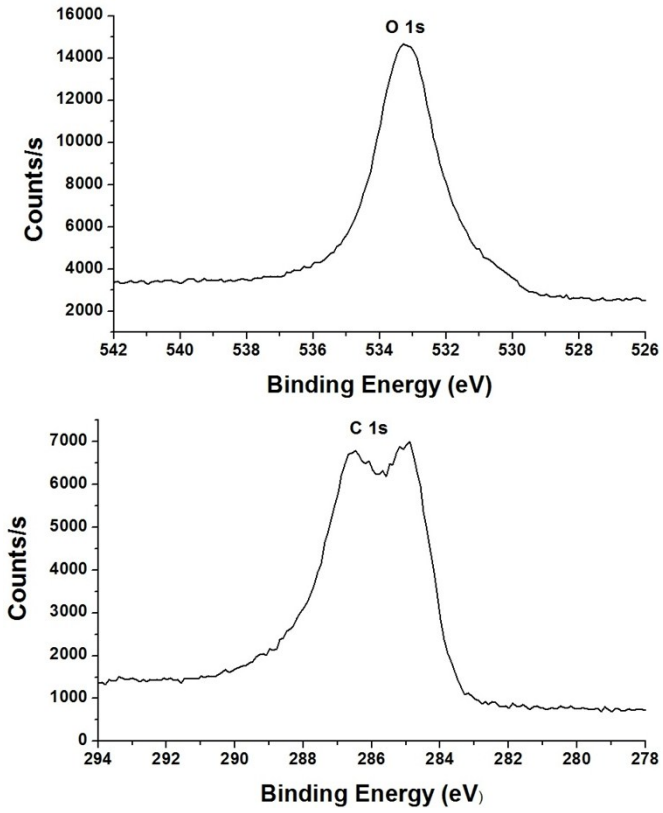


Fig. S11. XPS spectra of O 1s and C 1s of Fe-Pd NPs.

7. Recovery and reuse of catalyst

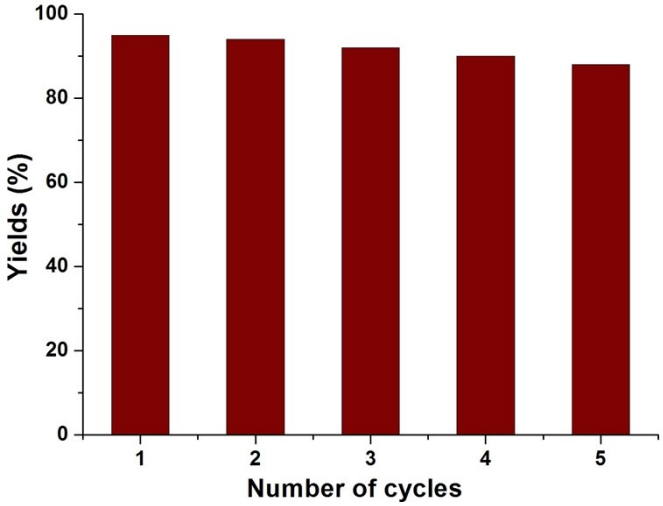


Fig. S12. Recovery and reuse of synthesized Fe-Pd bimetallic nanoparticles for the synthesis of compound **3.**

8. XPS spectra after recycled five times.

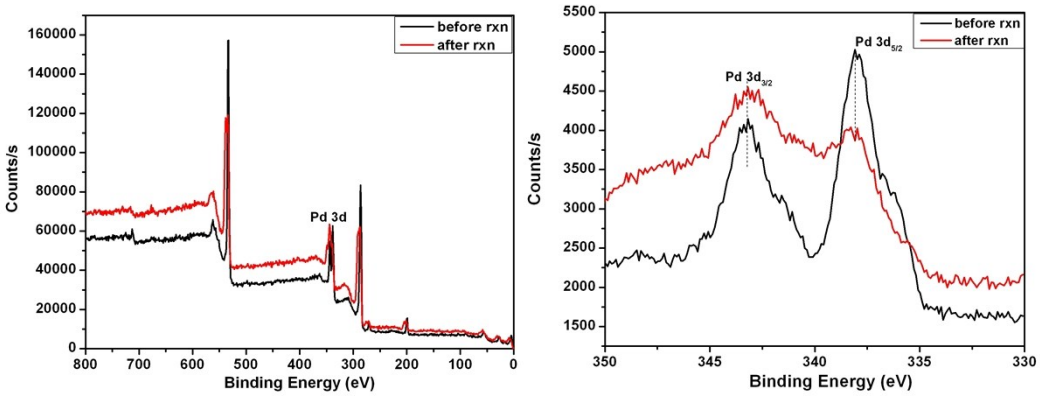


Fig. S13. XPS analysis to confirm the leaching of Pd from Fe-PdNPs before and after reaction.

9. XRD patterns of FePd-NPs after recycled five times.

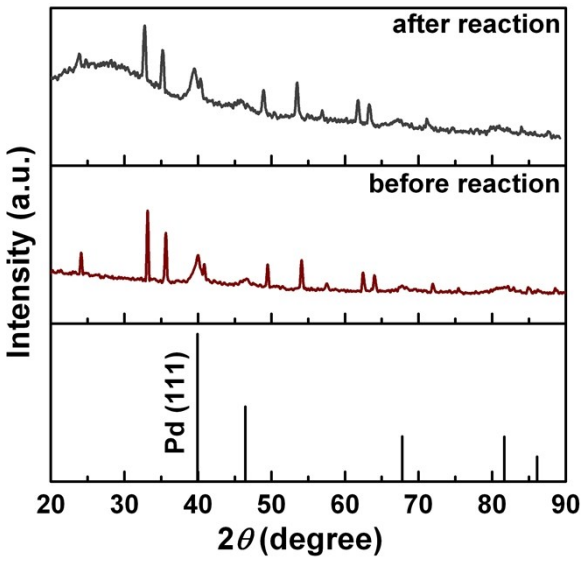


Fig. S14. XRD patterns of Fe-PdNPs before and after reaction.

10. Characterization of spectral data (3a-3l)

Methyl-5-hydroxy-2-methyl-3-(phenylcarbamoyl) naphtho [1,2-*b*]-furan-4-carboxylate (**3a**). Yellow solid; mp 237–238 ^{0}C; IR (KBr): 3398, 2926, 1672, 1649, 1533, 1441, 1378, 1343, 1311, 1255, 1170, 1110, 987, 765, 703 cm^{-1}; ^{1}H NMR (300 MHz, CDCl3/DMSO-d6, ratio 4 : 1) δ 11.60 (s, 1H), 9.44 (s, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.29 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.13–7.08 (m, 1H), 6.97–6.92 (m, 2H), 6.71 (dd, *J* = 7.5, 6.9 Hz, 1H), 3.29 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (75 MHz, CDCl3/DMSO-d6, ratio 4 : 1) δ 170.29, 163.68, 157.78, 53.84, 142.22, 138.76, 129.57, 128.29, 124.61, 124.08, 123.41, 123.15, 121.61, 119.00, 118.78, 117.24, 117.02, 98.72, 51.40, 12.64. HRMS: *m/z* [M+] calcd for $C_{22}H_{17}NO_5$ 375.1107; found: 375.1104.

Methyl-5-hydroxy-2-methyl-3-(*o*-tolylcarbamoyl) naphtho[1,2-*b*]-furan-4-carboxylate (**3b**). Yellow solid; mp 237–237 ^{0}C; IR (KBr): 3392, 2922, 2854, 1646, 1513, 1442, 1344, 1236, 1161, 1109, 1052, 987, 735 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.24 (s, 1H), 9.67 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.44 (dd, *J* = 7.5, 7.2 Hz, 1H), 7.08 (dd, *J* = 7.2, 6.9 Hz, 2H), 6.95 (dd, *J* = 7.5, 6.9 Hz, 1H), 3.54 (s, 3H), 2.50 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 169.46, 162.69, 155.29, 154.48, 142.35, 136.30, 131.46, 130.60, 130.41, 126.07, 125.68, 125.26, 124.65, 124.43, 123.11, 122.02, 119.50, 118.53, 117.18, 101.27, 51.98, 18.25, 13.43. HRMS: *m/z* [M+] calcd for $C_{23}H_{19}NO_5$ 389.1263; found: 389.1261.

Methyl-5-hydroxy-3-((4-methoxyphenyl) carbamoyl)-2-methylnaphtho[1,2-*b*]furan-4-carboxylate (**3c**). Yellow solid; mp 225–226 ^{0}C; IR (KBr): 3407, 2922, 2852, 1736, 1665, 1513, 1447, 1345, 1279, 1243, 1165, 1111, 761 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.55 (s, 1H), 10.29 (s, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.81 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.71 (d, *J* = 9.0 Hz, 2H), 7.62 (dd, *J* = 7.8, 7.2 Hz, 1H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.75 (s, 3H), 3.62 (s, 3H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 169.63, 162.46, 155.85, 155.37, 154.42, 142.26, 132.66, 130.54, 125.71, 124.42, 123.20, 121.90, 120.62, 119.52, 118.23, 117.46, 113.99, 100.76, 55.21, 52.06, 13.14. HRMS: *m/z* [M+] calcd for $C_{23}H_{19}NO_6$ 405.1212; found: 405.1215.

Methyl-3-((2-chlorophenyl)carbamoyl)-5-hydroxy-2-methylnaphtho[1,2-*b*]furan-4-carboxylate (**3d**). Yellow solid; mp 180–181 ^{0}C; IR (KBr): 3398, 3062, 2953, 1662, 1586, 1515, 1442, 1345, 1247, 1167, 1109, 1056, 991, 759 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.49 (s, 1H), 10.06 (s, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 7.95–7.92 (m, 1H), 7.80 (t, *J* = 7.5 Hz, 1H), 7.61 (dd, *J* = 7.8, 7.5 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.42 (dd, *J* = 7.5, 6.9 Hz, 1H), 7.25 (dd, *J* = 7.5, 7.2 Hz, 1H), 3.75 (s, 3H), 2.69 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 169.51, 161.93, 155.61, 155.01, 142.37, 134.85, 130.46, 129.75, 127.55, 127.02, 126.66, 126.49, 125.69, 124.42, 123.14, 122.00, 119.49, 118.39, 116.73, 100.96, 51.87, 13.40. HRMS: *m/z* [M+] calcd for C22H16ClNO5 409.0717; found: 409.0716.

Methyl-3-(benzylcarbamoyl)-5-hydroxy-2-methyl naphtho[1,2-*b*]-furan-4-carboxylate (**3e**). Yellow solid; mp 185–186 ^{0}C; IR (KBr): 3304, 3064, 2924, 2855, 1644, 1534, 1447, 1345, 1250, 1168, 1116, 749, 699 cm^{-1}; ^{1}H NMR (300 MHz, CDCl3/DMSO-d6, ratio 1 : 1) δ 11.79 (s, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.08 (brs, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.53 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.38–7.16 (m, 6H), 4.48, (d, *J* = 6.0 Hz, 2H), 3.60 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, CDCl3/DMSO-d6, ratio 1 : 1) δ 170.37, 165.10, 157.53, 153.59, 142.31, 138.48, 129.49, 128.02, 127.45, 126.73, 124.54, 124.04, 123.39, 121.57, 119.03, 117.31, 116.41, 98.85, 50.86, 42.93, 12.66. HRMS: *m/z* [M+] calcd for $C_{23}H_{19}NO_5$ 389.1263; found: 389.1262.

Methyl-5-hydroxy-2-phenyl-3-(phenylcarbamoyl) naphtho[1,2-b]-furan-4-carboxylate (**3f**). Yellow solid; mp 241–242 ^{0}C; IR (KBr): 3411, 2925, 1658, 1599, 1538, 1444, 1349, 1251, 1156, 1110, 762, 688 cm^{-1}; ^{1}H NMR (300MHz, DMSO-d6) δ 12.02 (brs, 1H), 10.63 (s, 1H), 8.41 (d, *J* = 8.4 Hz, 2H), 7.99 (d, *J* = 7.2 Hz, 2H), 7.89 (t, *J* = 7.5 Hz, 1H), 7.77 (d, *J* = 7.8 Hz, 2H), 7.70 (dd, *J* = 8.1, 7.2 Hz, 1H), 7.52 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.12 (dd, J = 7.5, 7.2 Hz, 1H), 3.61 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 169.90, 163.36, 157.23, 152.09, 142.82, 139.42, 130.96, 129.42, 129.32, 129.12, 129.02, 126.51, 126.13, 124.58, 123.74, 123.40, 122.62, 120.13, 119.19, 118.69, 116.92, 100.16, 52.20. HRMS: *m/z* [M+] calcd for $C_{27}H_{19}NO_5$ 437.1263; found: 437.1266.

Phenyl-5-hydroxy-2-methyl-3-(phenylcarbamoyl) naphtho[1,2-*b*]-furan-4-carboxylate (**3g**). Yellow solid; mp 295–296 ^{0}C; IR (KBr): 3410, 3270, 3057, 2986, 1710, 1663, 1587, 1532, 1497, 1438, 1353, 1263, 1195, 1142, 1092, 896, 743, 697 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.30 (s, 1H), 10.50 (s, 1H), 8.38 (d, *J* = 8.1 Hz, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 7.82 (dd, *J* = 7.8, 7.5 Hz, 1H), 7.63 (dd, *J* = 7.8, 7.5 Hz, 1H), 7.55 (d, J = 7.8 Hz, 2H), 7.25–7.14 (m, 7H), 6.70 (t, *J* = 7.2 Hz, 1H), 2.62 (s, 3H); ^{13}C NMR (75MHz, DMSOd6) δ 167.84, 162.80, 156.19, 154.91, 149.64, 142.57, 139.13, 130.70, 129.11, 128.45, 126.09, 125.84, 124.54, 123.36, 122.17, 122.0, 119.60, 119.45, 118.21, 117.44, 115.34, 101.05, 13.36. HRMS: *m/z* [M+] calcd for $C_{27}H_{19}NO_5$ 437.1263; found: 437.1261.

Phenyl-5-hydroxy-2-methyl-3-(*o*-tolylcarbamoyl) naphtho[1,2-*b*]-furan-4-carboxylate (**3h**). Yellow solid; mp 195–196 ^{0}C; IR (KBr): 3374, 3056, 2986, 2926, 1710, 1672, 1599, 1431, 1357, 1265, 1191, 1146, 1100, 895, 833, 739, 600 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.14 (s, 1H), 9.77 (s, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 8.1 Hz, 1H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.65 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.34–7.25 (m, 5H), 7.21–7.13 (m, 2H), 7.04 (dd, *J* = 7.2, 6.6 Hz, 1H), 6.96 (dd, *J* = 7.5, 6.9 Hz, 1H), 2.73 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 167.40, 162.54, 155.25, 154.42, 149.80, 142.48, 135.81, 131.35, 130.12, 129.89, 128.84, 125.81, 125.40, 125.22, 124.94, 124.83, 124.25, 123.05, 122.10, 121.92, 119.27, 118.47, 116.94, 101.54, 17.67, 13.28. HRMS: *m/z* [M+] calcd for $C_{28}H_{21}NO_5$ 451.1420; found: 451.1417.

Phenyl-5-hydroxy-3-((4-methoxyphenyl) carbamoyl)-2-methylnaphtho[1,2-*b*]furan-4-carboxylate (**3i**). Yellow solid; mp 276–277 ^{0}C; IR (KBr): 3334, 3058, 2953, 2856, 1668, 1643, 1512, 1413, 1354, 1264, 1103, 1031, 895, 744 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.26 (brs, 1H), 10.06 (s, 1H), 8.42 (d, J = 7.5 Hz, 1H), 8.21 (d, J = 7.2 Hz, 1H), 7.82 (dd, J = 7.5, 7.2 Hz, 1H), 7.63 (dd, J = 8.1, 6.9 Hz, 1H), 7.40 (d, J = 5.7 Hz, 2H), 7.25 (d, J = 5.7 Hz, 2H), 7.18–7.15 (m, 3H), 6.77–6.75 (m, 2H), 3.72 (s, 3H), 2.62 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 167.58, 162.14, 155.99, 155.29, 154.36, 149.50, 142.37, 132.02, 130.24, 128.66, 125.59, 125.38, 124.19, 123.20, 121.94, 121.59, 120.94, 119.22, 118.07, 117.33, 113.43, 100.93, 55.06, 12.81. HRMS: *m/z* [M+] calcd for $C_{28}H_{21}NO_6$ 467.1369; found: 467.1366.

Phenyl-3-((2-chlorophenyl)carbamoyl)-5-hydroxy-2-methylnaphtho[1,2-b]furan-4-carboxylate (**3j**). Yellow solid; mp 255–256 ^{0}C; IR (KBr): 3401, 3315, 3207, 3057, 2923, 1667, 1583, 1517, 1481, 1436, 1349, 1263, 1194, 1097, 741, 703 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.28 (s, 1H), 9.89 (s, 1H), 8.43 (d, J = 8.1 Hz, 1H), 8.21 (d, J = 7.8 Hz, 1H), 7.83 (dd, J = 7.5, 7.2 Hz, 1H), 7.64 (dd, J = 7.5, 7.2 Hz, 1H), 7.43–7.28 (m, 7H), 7.15–7.04 (m, 2H), 2.75 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 167.45, 162.63, 155.76, 154.85, 149.62, 142.43, 134.35, 130.21, 128.99, 128.87, 126.80, 126.50, 126.01, 125.81, 125.42, 124.22, 123.11, 122.00, 121.78, 119.24, 118.22, 116.55, 115.06, 101.07, 13.20. HRMS: *m/z* [M+] calcd for $C_{27}H_{18}ClNO_5$ 471.0874; found: 471.0873.

Phenyl-3-(benzylcarbamoyl)-5-hydroxy-2-methyl naphtho[1,2-*b*]furan-4-carboxylate (**3k**). Yellow solid; mp 225–226 ^{0}C; IR (KBr): 3324, 3061, 2924, 2855, 1659, 1533, 1449, 1344, 1265, 1232, 1193, 1028, 738, 700 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.16 (s, 1H), 8.91 (t, J = 5.4 Hz, 1H), 8.37 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.1 Hz, 1H), 7.81 (dd, J = 7.8, 7.2 Hz, 1H), 7.62 (dd, J = 7.8, 7.5 Hz, 1H), 7.54–7.49 (m, 2H), 7.38–7.33 (m, 3H), 7.29–7.24 (m, 3H), 7.21–7.17 (m, 2H), 4.12 (d, J = 5.4 Hz, 2H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6) δ 167.72, 164.08, 155.64, 154.43, 149.94, 142.55, 139.02, 130.59, 129.50, 128.35, 127.57, 127.33, 126.95, 126.36, 125.78, 124.52, 123.27, 122.12, 119.59, 118.46, 116.86, 101.47, 42.55, 13.34. HRMS: *m/z* [M+] calcd for $C_{28}H_{21}NO_5$ 451.1420; found: 451.1419.

Phenyl-5-hydroxy-2-phenyl-3-(phenylcarbamoyl) naphtho[1,2-b]-furan-4-carboxylate (**3l**). Yellow solid; mp > 300 ^{0}C; IR (KBr): 3426, 3389, 2925, 1644, 1534, 1489, 1442, 1261, 1142, 1028, 760, 687 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d6) δ 11.75 (brs, 1H), 10.54 (s, 1H), 8.46 (d, J = 8.4 Hz, 1H), 8.41 (d, J = 8.1 Hz, 1H), 7.98 (d, J = 6.9Hz, 2H), 7.90 (t, J = 7.5Hz, 1H), 7.69 (dd, J = 7.8, 7.2 Hz, 1H), 7.51–7.44 (m, 5H), 7.21–7.08 (m, 6H), 6.97 (dd, J = 7.2, 6.6 Hz, 1H), 6.82–6.80 (m, 1H); ^{13}C NMR (75MHz, DMSO-d6) δ 168.01, 162.80, 157.45, 152.15, 149.18, 142.87, 138.88, 130.73, 129.07, 128.67 (Ar-4C), 128.02, 126.17, 126.05, 125.72, 124.40, 123.40, 123.03, 122.58, 121.73, 119.84, 119.17, 118.59, 116.93, 115.11, 100.25. HRMS: *m/z* [M+] calcd for $C_{32}H_{21}NO_5$ 499.1420; found: 499.1422.