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Supporting Information

Access to enhanced catalytic core-shell CuO-Pd nanoparticles for the organic transformations

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1. Experimental section

Synthesis of CuO and Pd nanoparticles

A volume of 50 mL of the *C. rotundus* rhizome extract solution was added to 100 mL of an aqueous solution of 1.0 mmol $Cu(OAc)_2$. The mixture solution was then sonicated at 60 °C for 2 h. After 2 h, the color of the final solution changed to black, which indicated the formation of CuO nanoparticles. The synthesized nanoparticles were isolated by centrifugation and purified.

A volume of 50 mL of the *C. rotundus* rhizome extract solution was added to 100 mL of an aqueous solution of 1.0 mmol $PdCl_2$. The mixture solution was then sonicated at 60 °C for 2 h. After 2 h, the color of the final solution changed to dark brown, which indicated the formation of Pd nanoparticles. The synthesized nanoparticles were isolated by centrifugation and purified.

2. Characterization of nanoparticles

a. XPS spectra

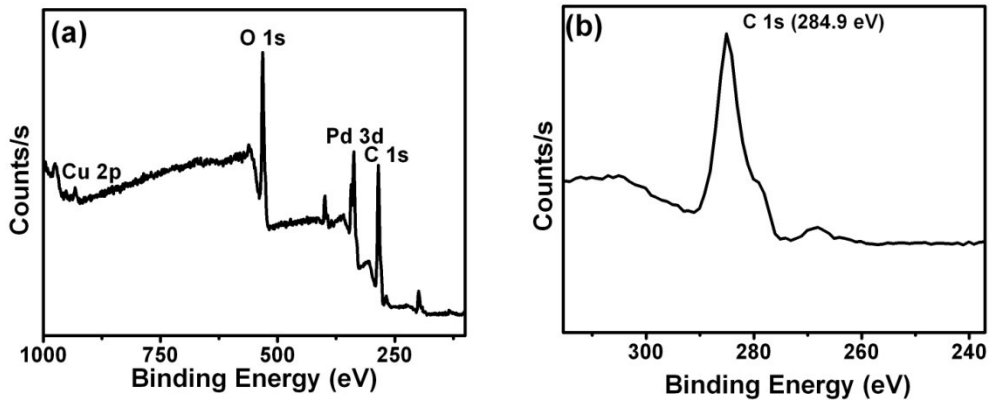

Fig. S1. (a) XPS full scan survey of CuO-Pd NPs, and (b) C 1s XPS spectra of CuO-Pd NPs.

b. HRTEM images of CuO-Pd NPs

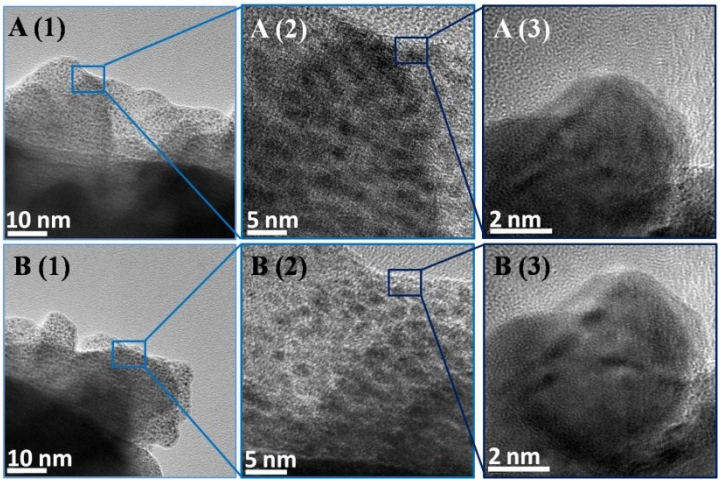

Fig. S2. HR-TEM images of CuO-Pd NPs at two different locations.

c. EDS peaks of CuO-Pd NPs

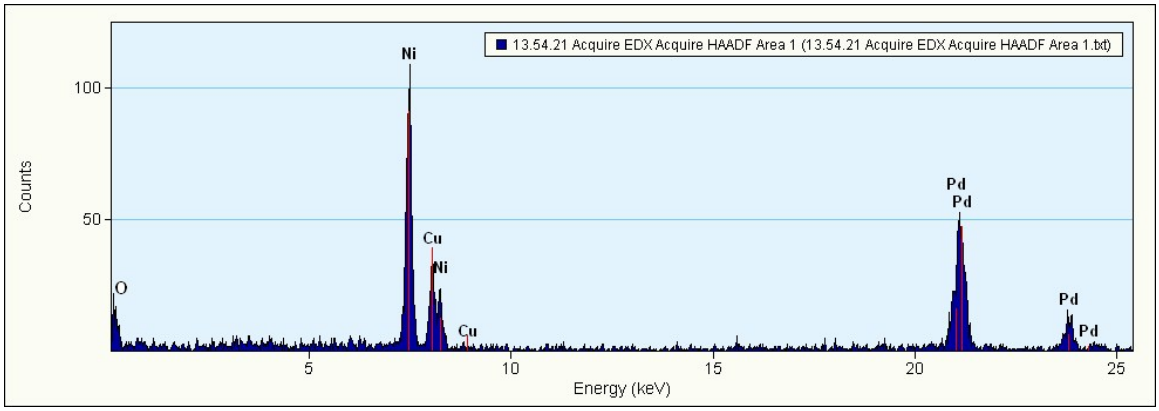

Fig. S3. EDS peaks of CuO-Pd NPs.

d. FTIR Spectra

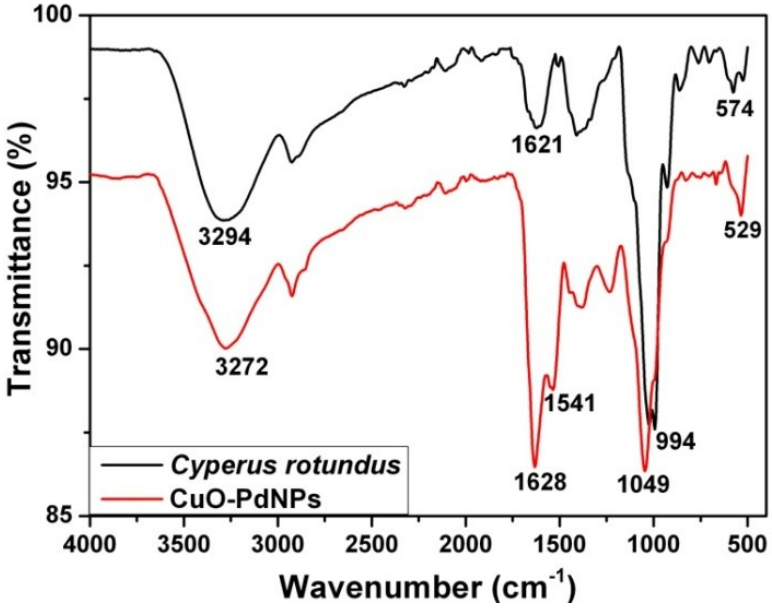

Fig. S4. FTIR spectra of CuO-Pd NPs and *Cyperus rotundus* rhizome extract.

e. Phytochemical constituents of *C. rotundus* extract.

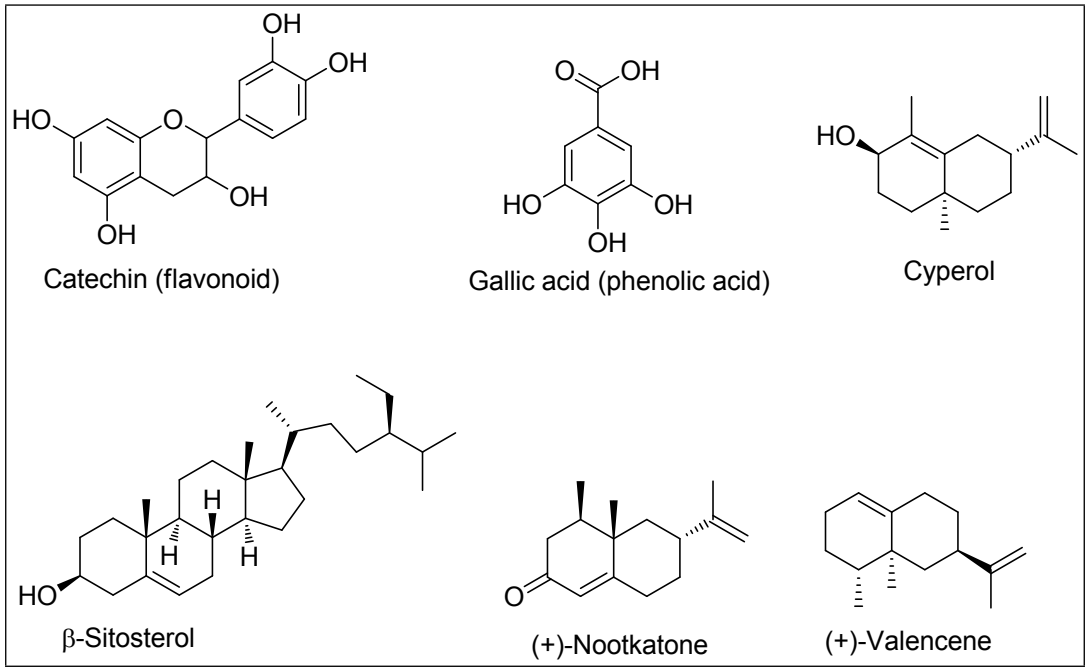

Fig. S5. Phytochemical constituents of *C. rotundus* extract.

f. UV-Vis spectra

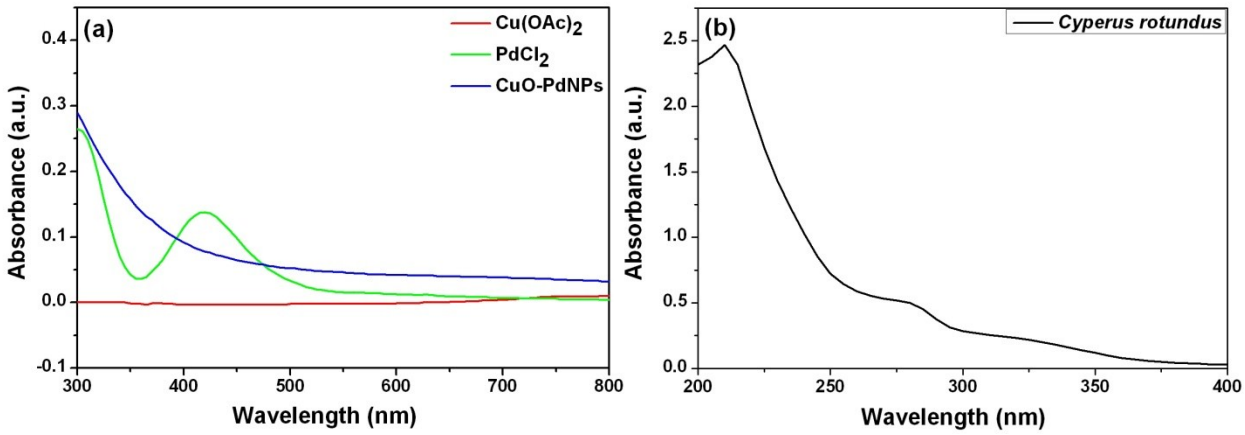

Fig. S6. UV-Vis spectra of (a) $Cu(OAc)_2$, $PdCl_2$, and CuO-Pd NPs and (b) *Cyperus rotundus*,.

g. DSC-TGA spectra

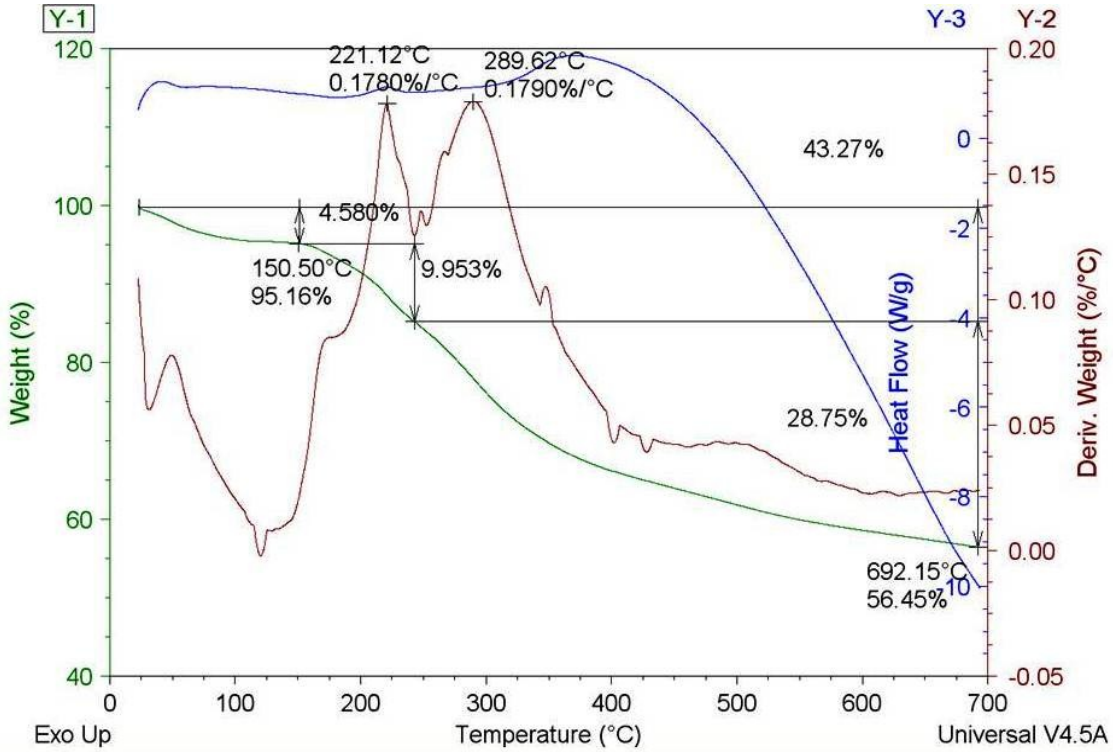

Fig. S7. DSC-TGA spectra of CuO-Pd NPs

h. Zeta potential distribution

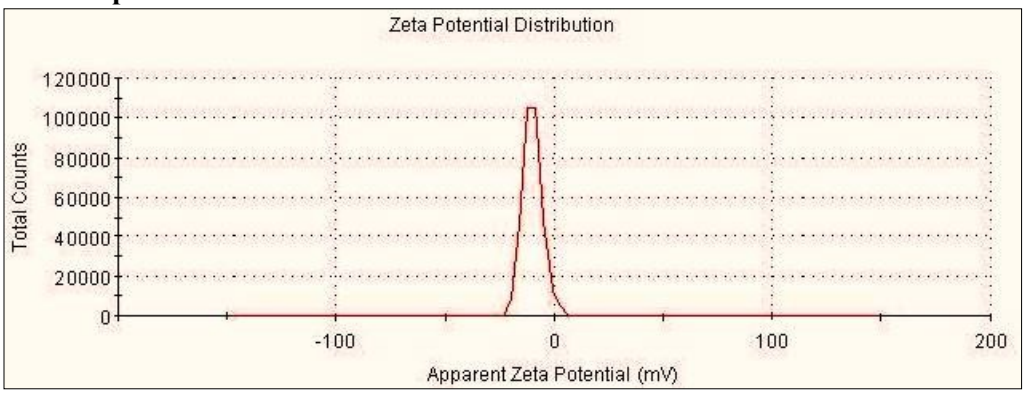

Fig. S8: Zeta potential (ZP) distribution of CuO-Pd NPs.

Table S1: Average zeta potential calculation of CuO-Pd NPs

CuO-Pd NPs	T (°C)	ZP (mV)	Z-dev. (mV)
1	25	-9.8	4.40
2	25	-10.2	6.11
3	25	-9.82	5.52
	Avg.	-9.94	5.34
	Std Dev	0.225	0.869

i. AFM images

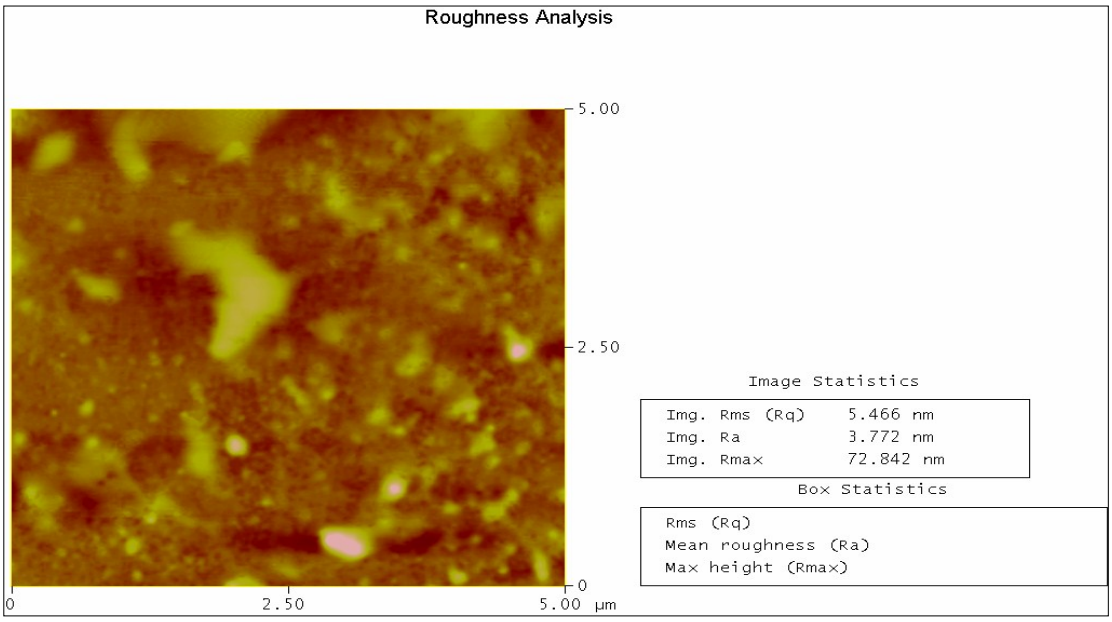

Fig. S9: Roughness analysis of CuO-Pd NPs at 5 µm^2.

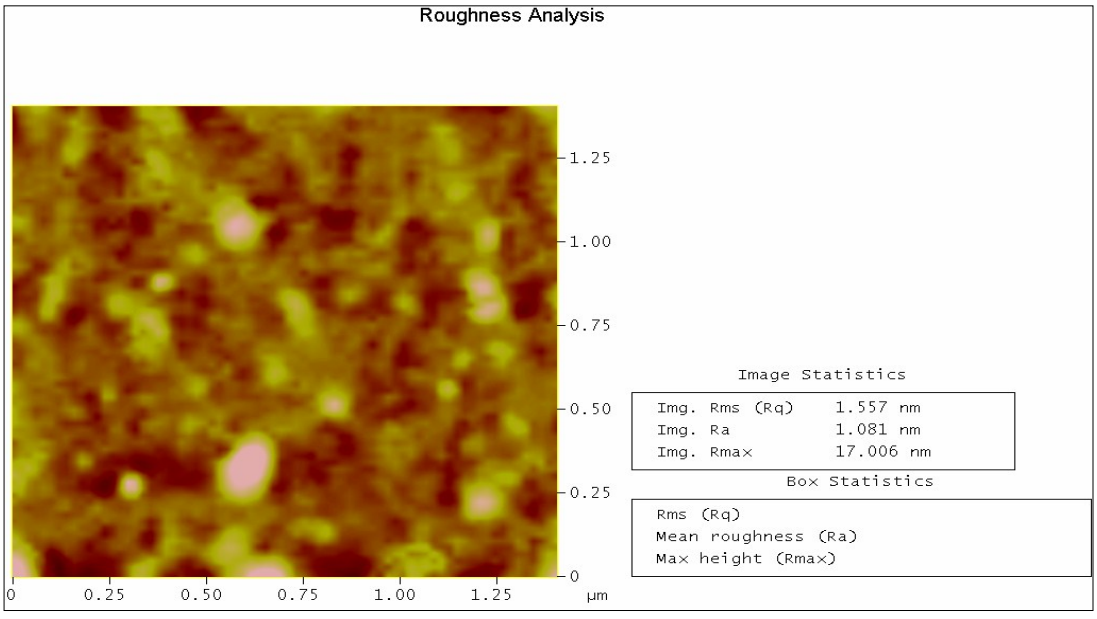

Fig. S10: Roughness analysis of CuO-Pd NPs at 1.3 µm^2.

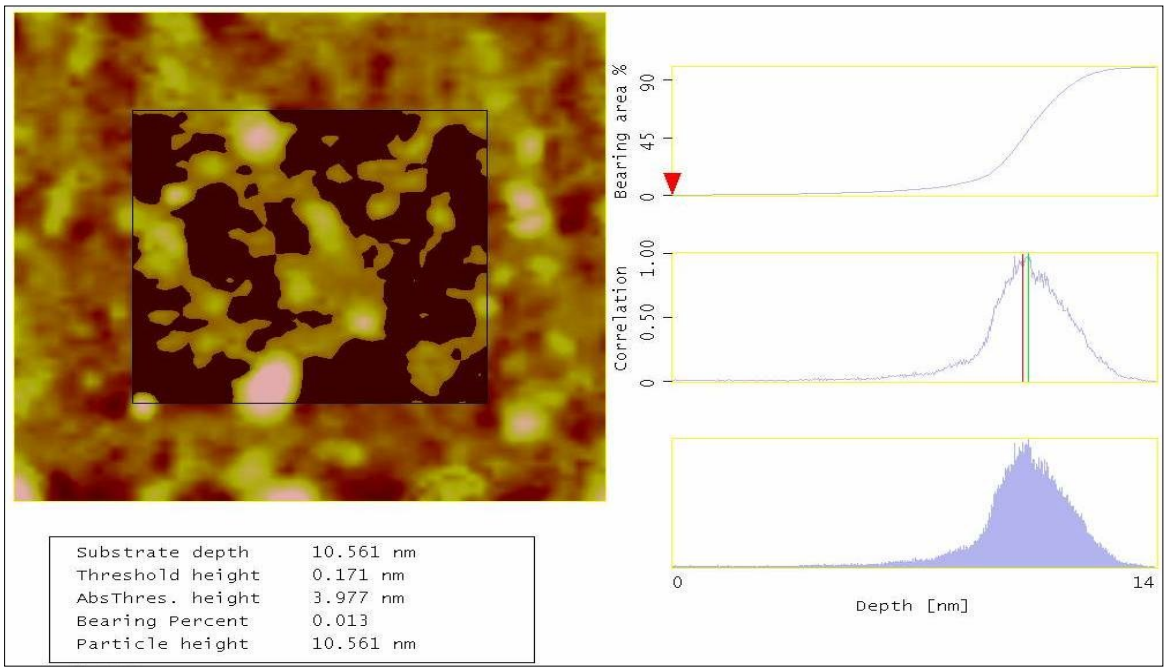

Fig. S11: Particle height of CuO-Pd NPs.

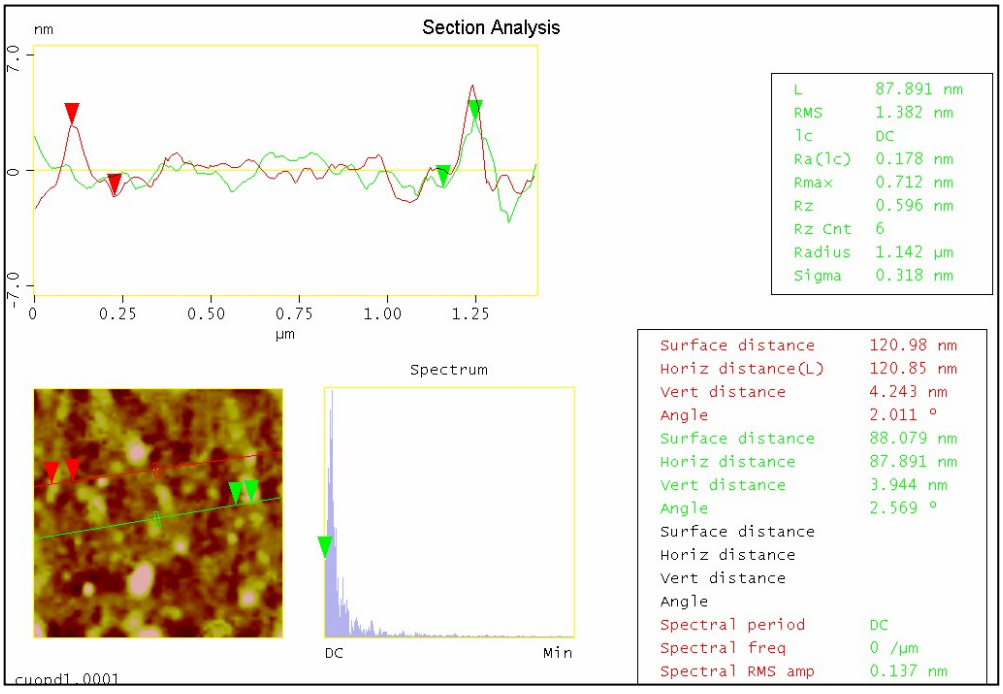

Fig. S12: Section analysis of CuO-Pd NPs.

j. XRD patterns after 5th cycle

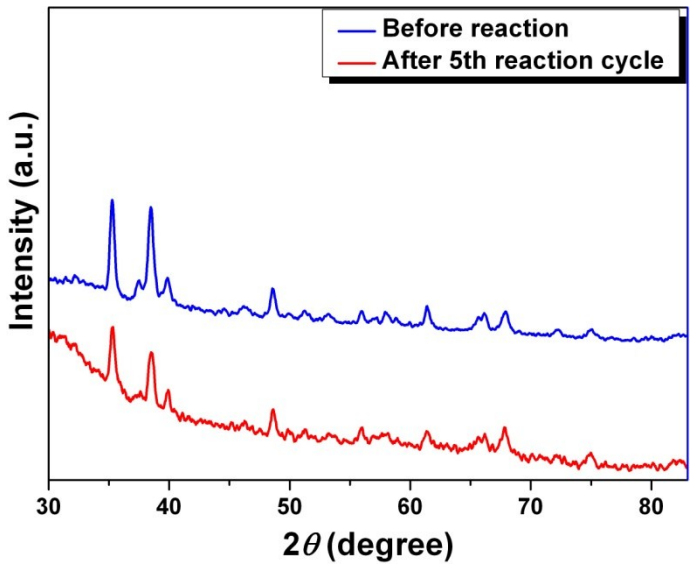

Fig. S13: XRD patterns of CuO-Pd NPs before and after recycling for five times.

3. Characterization spectral data (4a-4e) [1], (6a-6e)[1], and (9a-9e)

2,3-Diphenyl-2,3-dihydroquinazolin-4(1*H*)-one (4a). Yield: 97%; yellow solid; mp 205-206 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.77 (1H, d, *J*=7.8 Hz), 7.64 (1H, s), 7.42-7.18 (11H, m), 6.79 (1H, d, *J*=8.1 Hz), 6.74 (1H, t, *J*=7.2 Hz), 6.30 (1H, s); ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.2, 146.5, 140.7, 140.6, 133.7, 128.5, 128.3, 128.2, 127.9, 126.5, 126.2, 125.9, 117.4, 115.3, 114.7, 72.6; IR (KBr) 3427, 3294, 3061, 2832, 1633, 1511, 1392, 1332, 1257, 1158, 1025, 754 cm^{-1}; HRMS *m/z* (M$^+$) calcd for $C_{20}H_{16}N_2O$: 300.1263. Found: 300.1265.

2-(4-Methoxyphenyl)-3-m-tolyl-2,3-dihydroquinazolin-4(1*H*)-one (4b). Yield: 92%; yellow solid; mp 209-210 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.75 (1H, d, *J*=7.5 Hz), 7.54 (1H, s), 7.33-7.19 (5H, m), 7.14 (1H, s), 7.03 (2H, t, *J*=8.7 Hz), 6.88-6.85 (2H, m), 6.77 (1H, t, *J*=8.1 Hz), 6.22 (1H, s), 3.71 (3H, s), 2.27 (3H, s); ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.2, 159.0, 146.5, 140.8, 137.8, 133.6, 132.7, 128.3, 127.9, 127.8, 126.8, 126.6, 123.2, 117.4, 115.4, 114.7, 113.6, 72.3, 55.0, 20.8; IR (KBr) 3424, 3301, 2961, 2833, 1634, 1507, 1393, 1301, 1248, 1170, 1026, 830, 766 cm^{-1}; HRMS *m/z* (M$^+$) calcd for $C_{22}H_{20}N_2O_2$: 344.1525. Found: 344.1525.

3-(4-Isopropylphenyl)-2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4c). Yield: 95%; yellow solid; mp 171-172 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.75 (1H, d, *J*=7.5 Hz), 7.55 (1H, s), 7.32-7.21 (7H, m), 6.86 (2H, d, *J*=8.4 Hz), 6.74 (2H, t, *J*=8.4 Hz), 6.19 (1H, s), 3.70 (3H, s), 2.91-2.82 (1H, m), 1.19 (6H, d, *J*=6.9 Hz); ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.1, 159.05, 146.4, 145.9, 138.6, 133.5, 132.8, 127.8, 127.6, 126.3, 125.9, 117.3, 115.4, 114.7, 113.6, 72.2, 54.9, 32.9, 23.7; IR (KBr) 3420, 3298, 2956, 1630, 1508, 1392, 1332, 1249, 1177, 1027, 833, 700 cm^{-1}; HRMS *m/z* (M$^+$) calcd for $C_{24}H_{24}N_2O_2$: 372.1838. Found: 372.1840.

3-(4-Fluorophenyl)-2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4d). Yield: 94%; yellow solid; mp 259-260 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.74 (1H, d, *J*=7.8 Hz), 7.49 (1H, s), 7.29-7.12 (7H, m), 6.86 (2H, d, *J*=8.7 Hz), 6.76 (2H, t, *J*=7.8 Hz), 6.23 (1H, s), 3.70 (3H, s); ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.5, 159.2, 146.8, 133.7, 132.2, 128.8, 128.7, 128.09, 127.9, 117.4, 115.4, 115.1, 115.0, 114.6, 113.6, 72.6, 55.0; IR (KBr) 3427, 3302, 1643, 1504, 1390, 1305, 1245, 1026, 994, 832, 760 cm^{-1}; HRMS *m/z* (M$^+$) calcd for $C_{21}H_{17}FN_2O_2$: 348.1274. Found: 348.1272.

2,3-Bis(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4e). Yield: 96%; yellow solid; mp 227-228 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.74 (1H, d, *J*=7.8 Hz), 7.44 (1H, s), 7.31-7.23 (3H, m), 7.15 (2H, d, *J*=8.7 Hz), 6.89-

6.84 (4H, m) 6.75 (2H, t, *J*=7.8 Hz), 6.16 (1H, s), 3.73 (3H, s), 3.70 (3H, s); ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.3,159.1, 157.2, 146.6, 133.5, 132.7, 127.9, 127.8, 127.4, 117.3, 115.2, 114.6, 113.7, 113.6, 72.8, 55.1, 55.0; IR (KBr) 3426, 2936, 2837, 1636, 1510, 1394, 1441,1243,1174,1025, 996, 830, 762 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_20N_2O_3$: 360.1474. Found: 360.1477.

3'-Phenyl-1'*H*-spiro[indoline-3,2'-quinazoline]-2,4'(3'*H*)-dione (6a). Yield: 98%; yellow solid; mp 264-266 ^{o}C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.39 (1H, s), 7.68 (1H, d, *J*=7.5 Hz), 7.60 (1H, s), 7.53 (1H, d, *J*=7.5 Hz), 7.30 (1H, t, *J*=7.8 Hz) 7.24-7.12 (4H, m), 7.01-6.98 (2H, m), 6.92 (1H, t, *J*=7.5 Hz), 6.78-6.70 (2H, m), 6.64 (1H, d, *J*=7.5 Hz); ^{13}C NMR (75 MHz, DMSO-d_6) δ 175.6, 163.8, 146.3, 141.4, 138.3, 134.2, 134.0, 129.9, 129.7, 129.2, 128.3, 127.9, 118.4,115.0,114.6, 114.1, 112.6, 76.8; IR (KBr) 3447, 3303, 1721, 1644, 1615, 1486, 1358, 1194, 1105, 1012, 964, 865, 752 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{15}N_3O_2$: 341.1164. Found: 341.1161.

3'-*m*-Tolyl-1'*H*-spiro[indoline-3,2'-quinazoline]-2,4'(3'*H*)-dione (6b). Yield: 95%; yellow solid; mp 274-276 ^{o}C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.40 (1H, s), 7.66 (1H, d, *J*=7.8 Hz), 7.59 (1H, s), 7.53 (1H, d, *J*=7.2 Hz), 7.30 (1H, t, *J*=7.8 Hz), 7.15 (1H, t, *J*=7.5 Hz), 7.07 (1H, t, *J*=7.2 Hz), 6.98-6.90 (3H, m), 6.82 (1H, s), 6.75 (1H, t, *J*=8.4 Hz), 6.70 (1H, d, *J*=8.1 Hz), 6.64 (1H, d, *J*=7.5 Hz), 2.15 (3H, s); ^{13}C NMR (75 MHz, DMSO-d_6) δ 174.3, 163.9, 146.5, 143.6, 138.3, 134.1, 131.4, 128.8, 128.7, 127.9, 127.1, 126.6, 123.1, 118.2, 115.1, 114.6, 109.3, 76.6, 21.2; IR (KBr) 3298, 3206, 3093, 1724, 1643, 1616, 1485, 1361, 1236, 1193, 1100, 1048, 963, 751 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{17}N_3O_2$: 355.1321. Found: 355.1318.

3'-(4-Isopropylphenyl)-1'*H*-spiro[indoline-3,2'-quinazoline]-2,4'(3'*H*)-dione (6c). Yield: 98%; yellow solid; mp 276-278 ^{o}C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.36 (1H, s), 7.66 (1H, d, *J*=7.5 Hz), 7.56 (1H, s), 7.52 (1H, d, *J*=7.5 Hz), 7.29 (1H, t, *J*=8.1 Hz), 7.15 (1H, t, *J*=7.5 Hz), 7.08-6.87 (5H, m), 6.77-6.63 (3H, m), 2.79-2.73 (1H, m),1.09 (6H, d, *J*=6.9 Hz); ^{13}C NMR (75 MHz, DMSO-d_6) δ 175.3, 163.6, 147.4, 146.0, 141.5, 135.6, 133.5, 130.6, 129.0, 127.5,127.4, 126.3, 126.2, 122.1,117.6, 114.5,114.0, 110.0, 76.3, 32.7, 23.6, 23.5; IR (KBr) 3311, 3066, 2961, 1725, 1632, 1511, 1484, 1359, 1214, 1190, 1105, 1051, 955, 817, 752 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{24}H_{21}N_3O_2$: 383.1634. Found: 383.1630.

3'-(4-Fluorophenyl)-1'*H*-spiro[indoline-3,2'-quinazoline]-2,4'(3'*H*)-dione (6d). Yield: 93%; yellow solid; mp 295-296 ^{o}C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.47 (1H, s), 7.67 (2H, t, *J*=3.3 Hz), 7.59 (1H, d, *J*=10.5 Hz), 7.31 (1H, t, *J*=7.2 Hz), 7.18 (1H, t, *J*=7.5 Hz), 7.09-6.92 (5H, m), 6.78-6.65 (3H, m); ^{13}C NMR (75 MHz, DMSO-d_6) δ 175.4, 163.9, 146.3, 141.4, 134.4, 134.3, 134.1, 129.8, 129.7, 127.9, 118.4, 116.2, 115.9, 114.8, 114.6, 114.2, 112.6, 76.9; IR (KBr) 3272, 3066, 1726, 1642, 1616, 1509, 1483, 1360, 1328, 1221, 1197, 1154, 1099, 961, 827, 750 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{14}FN_3O_2$: 359.1070. Found: 359.1068.

3'-Benzyl-1'*H*-spiro[indoline-3,2'-quinazoline]-2,4'(3'*H*)-dione (6e). Yield: 96%; yellow solid; mp 210-211 ^{o}C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.34 (1H, s), 7.72 (1H, d, *J*=7.8 Hz), 7.45 (1H, s), 7.36-7.24 (3H, m), 7.17-7.15 (3H, m), 6.93-6.88 (3H, m), 6.83 (1H, d, *J*=7.8 Hz), 6.76 (1H, t, *J*=7.5 Hz), 6.67 (1H, d, *J*=7.5 Hz), 4.48 (1H, d, *J*=15.3 Hz), 4.15 (1H, d, *J*=15.3 Hz); ^{13}C NMR (75 MHz, DMSO-d_6) δ 175.4, 164.5, 146.4, 142.9, 137.8, 133.8, 131.7, 128.2, 127.8, 127.2, 126.8, 126.7, 122.4, 118.1, 115.1, 114.4, 110.9, 75.5, 46.3; IR (KBr) 3297, 3090, 2944, 1727, 1625, 1483, 1383, 1323, 1242, 1191, 968. 750 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{17}N_3O_2$: 355.1321. Found: 355.1318.

6-Amino-1,3-dimethyl-5-(2-phenyl-4*H*-chromen-4-yl)pyrimidine-2,4(1*H*,3*H*)-dione (9a). Yield: 87%; red solid; mp 146-148 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (2H, d, *J*=6.3 Hz), 7.38-7.31 (3H, m), 7.15 (1H, t, *J*=7.8 Hz), 7.07-6.94 (3H, m), 5.55 (1H, d, *J*=3.0 Hz), 5.39 (1H, d, *J*=3.9 Hz), 4.86 (2H, s), 3.30 (3H, s), 3.28 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.8, 151.4, 151.0, 149.2, 133.2, 128.8, 128.7, 128.3, 128.1, 124.3, 124.2, 121.2, 116.3, 98.9, 92.4, 29.1, 28.8, 28.4; IR (KBr) 3340, 3215, 1735, 1692, 1581, 1488, 1315, 1187, 1110, 1041, 916, 756, 502 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{19}N_3O_3$: 361.1426. Found: 361.1430.

6-Amino-1,3-dimethyl-5-(6-methyl-2-phenyl-4*H*-chromen-4-yl)pyrimidine-2,4(1*H*,3*H*)-dione (9b). Yield: 85%; red solid; mp 151-153 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (2H, d, *J*=7.8 Hz), 7.36-7.28 (3H, m), 6.96-6.86 (3H, m), 5.53 (1H, d, *J*=3.6 Hz), 5.37 (1H, d, *J*=4.2 Hz), 4.80 (2H, s), 3.33 (3H, s), 3.29 (3H, s), 2.20 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.8, 151.4, 151.1, 149.3, 149.0, 133.7, 133.4, 128.9, 128.8, 128.7, 128.3, 124.4, 120.8, 116.0,

98.7, 92.6, 29.2, 28.7, 28.4, 20.6; IR (KBr) 3337, 3213, 1735, 1693, 1583, 1492, 1374, 1125, 1043, 1012, 942, 760, 506 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{21}N_3O_3$: 375.1583. Found: 375.1579.

6-Amino-1,3-dimethyl-5-(8-methyl-2-phenyl-4*H*-chromen-4-yl)pyrimidine-2,4(1*H*,3*H*)-dione (9c). Yield: 85%; red solid; mp 150-152 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.68 (2H, d, *J*=7.8 Hz), 7.40-7.33 (3H, m), 7.03 (1H, d, *J*=6.9 Hz), 6.95-6.86 (2H, m), 5.62 (1H, d, *J*=3.6 Hz), 5.45 (1H, d, *J*=3.9 Hz), 4.63 (2H, s), 3.37 (3H, s), 3.30 (3H, s), 2.39 (3H, s); ^{13}C NMR (75MHz, $CDCl_3$) δ 162.8, 151.2, 151.1, 149.4, 149.2, 133.6, 129.5, 128.7, 128.5, 126.4, 125.6, 124.4, 123.7, 120.9, 99.0, 93.0, 29.5, 28.7, 28.5, 16.0; IR (KBr) 3337, 3220, 1691, 1585, 1497, 1445, 1375, 1262, 1174, 1099, 1088, 763, 699, 507 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{21}N_3O_3$: 375.1583. Found: 375.1582.

6-Amino-1,3-dimethyl-5-(3-methyl-2-phenyl-4*H*-chromen-4-yl)pyrimidine-2,4(1*H*,3*H*)-dione (9d). Yield: 84%; red solid; mp 153-155 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.44 (2H, d, *J*=6.3 Hz), 7.40-7.35 (3H, m), 7.10 (2H, d, *J*=6.9 Hz), 6.96 (1H, t, *J*=7.2 Hz), 6.89 (1H, d, *J*=8.4 Hz), 5.45 (1H, s), 4.89 (2H, s), 3.35 (3H, s), 3.34 (3H, s), 1.69 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 151.2, 151.1, 151.0, 145.3, 134.4, 128.8, 128.7, 128.5, 128.1, 127.8, 123.8, 121.7, 115.6, 107.3, 91.9, 34.7, 28.8, 28.5, 16.8; IR (KBr) 3334, 3207, 1689, 1584, 1489, 1239, 1193, 1094, 1062, 910, 702, 506 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{21}N_3O_3$: 375.1583. Found: 375.1585.

6-Amino-5-(6-bromo-2-phenyl-4*H*-chromen-4-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (9e). Yield: 81%; red solid; mp 159-161 ^oC; ^1H NMR (600 MHz, $CDCl_3$) δ 7.59 (2H, d, *J*=7.2 Hz), 7.33-7.28 (3H, m), 7.22 (1H, dd, *J*=9.0, 1.8 Hz), 7.16 (1H, s), 6.87 (1H, d, *J*=9.0 Hz), 5.55 (1H, s), 5.37 (1H, d, *J*=4.2 Hz), 4.58 (2H, s), 3.34 (3H, s), 3.28 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 151.3, 151.0, 150.3, 149.4, 132.9, 131.4, 131.2, 129.0, 128.5, 124.4, 123.7, 118.1, 116.5, 98.7, 92.4, 29.2, 28.7, 28.5; IR (KBr) 3336, 3208, 1690, 1586, 1490, 1241, 1195, 1097, 1082, 915, 701, 505 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{18}BrN_3O_3$: 439.0532. Found: 439.0529.

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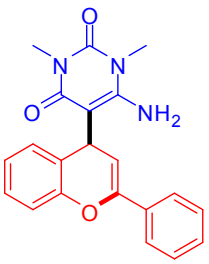
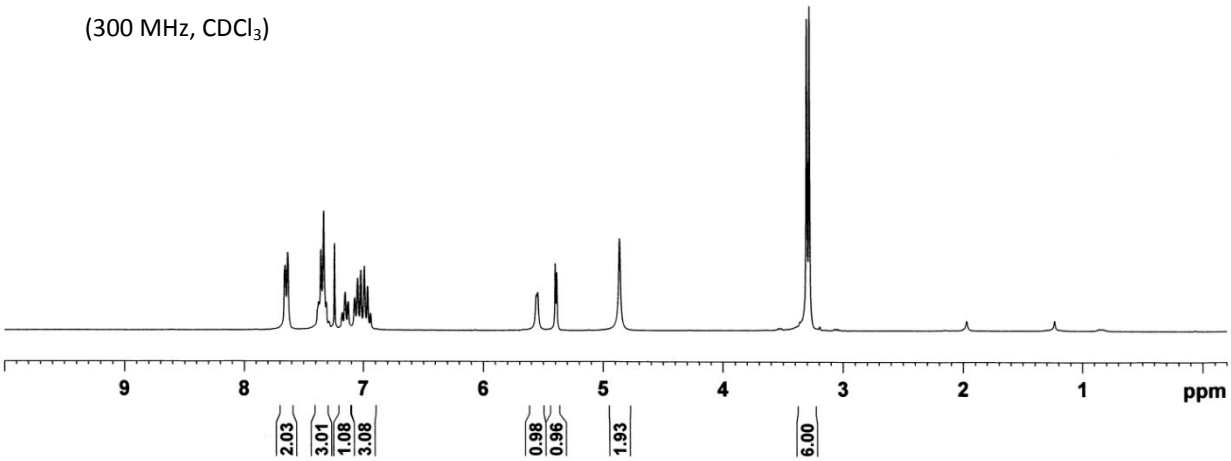
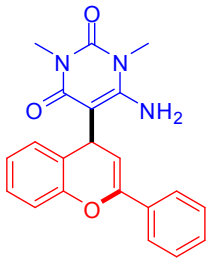
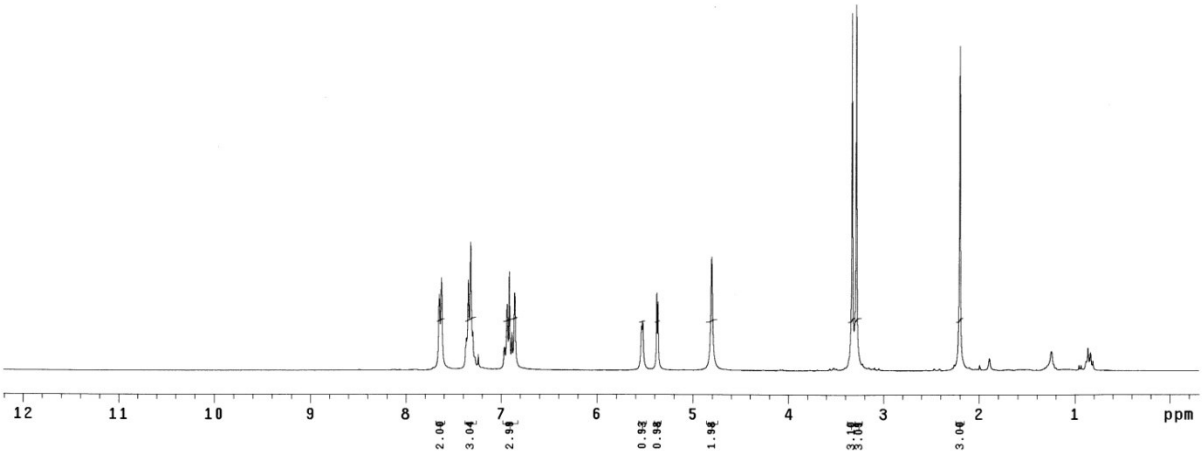


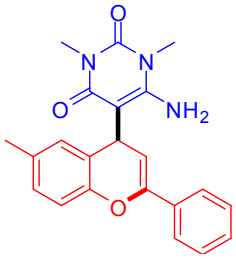
^{1}H NMR of **9a**
(300 MHz, $CDCl_3$)



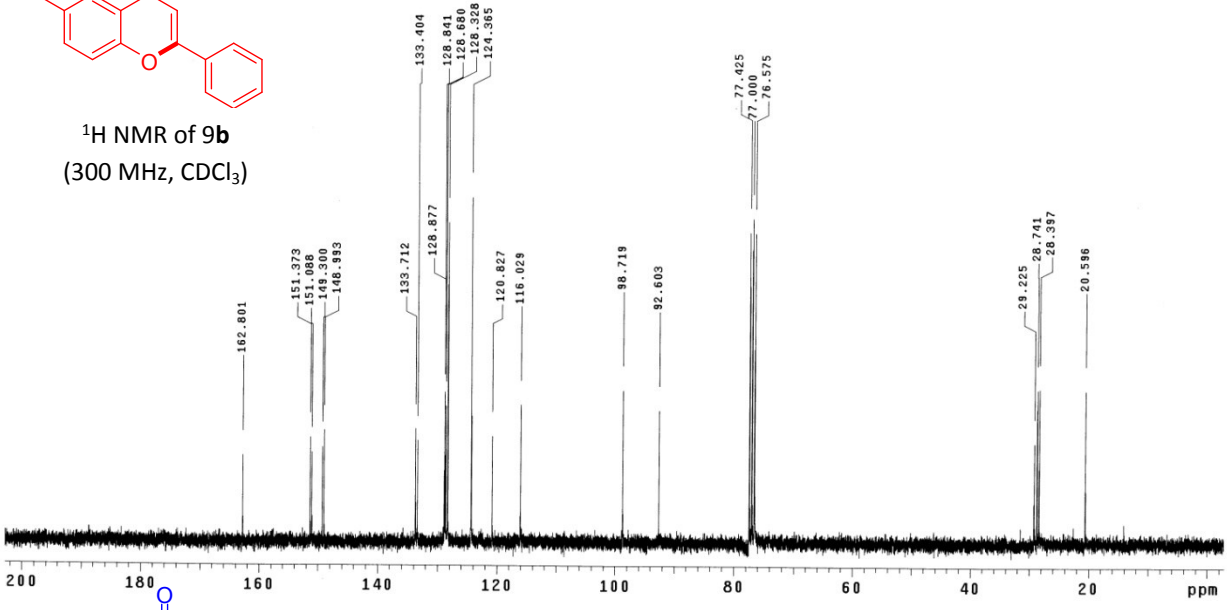


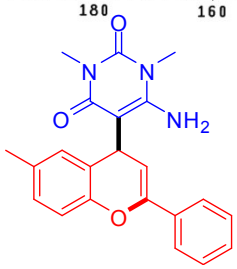
^{13}C NMR of **9a**
(75 MHz, $CDCl_3$)



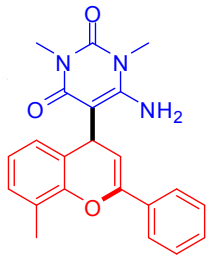


^{1}H NMR of 9**b**
(300 MHz, $CDCl_3$)

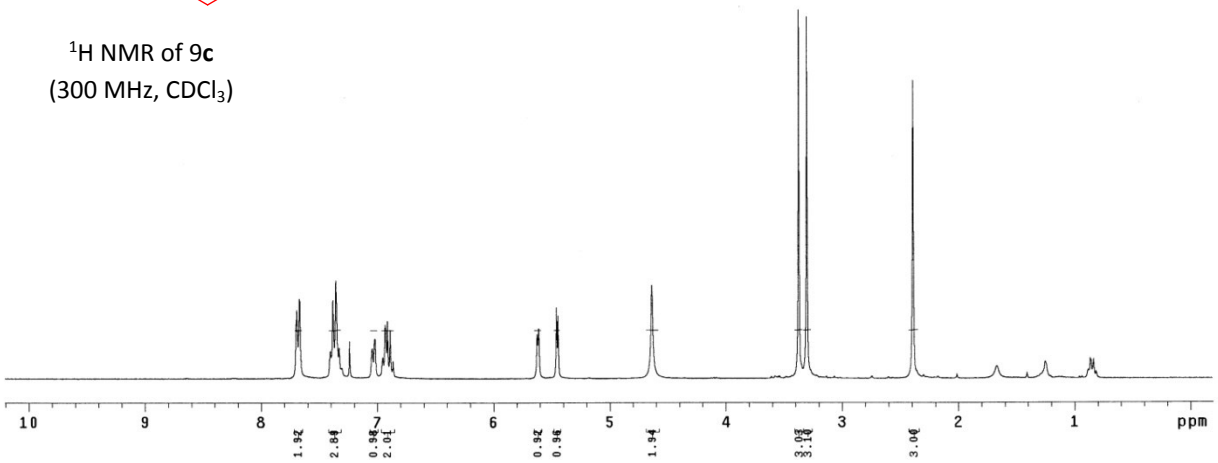


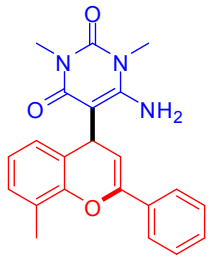


^{13}C NMR of **9b**
(75 MHz, $CDCl_3$)

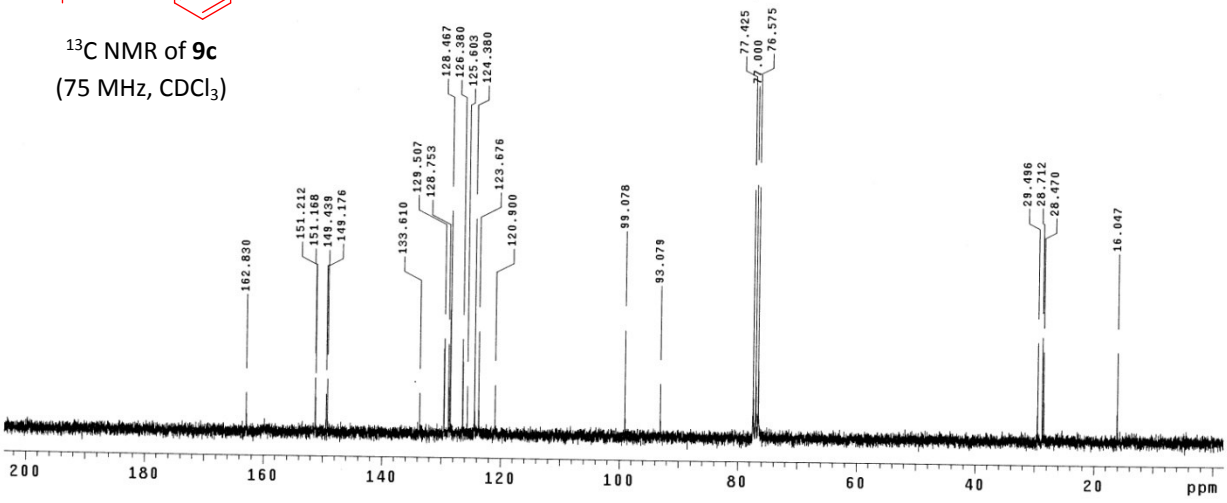


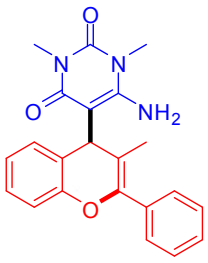
^{1}H NMR of 9**c**
(300 MHz, $CDCl_3$)



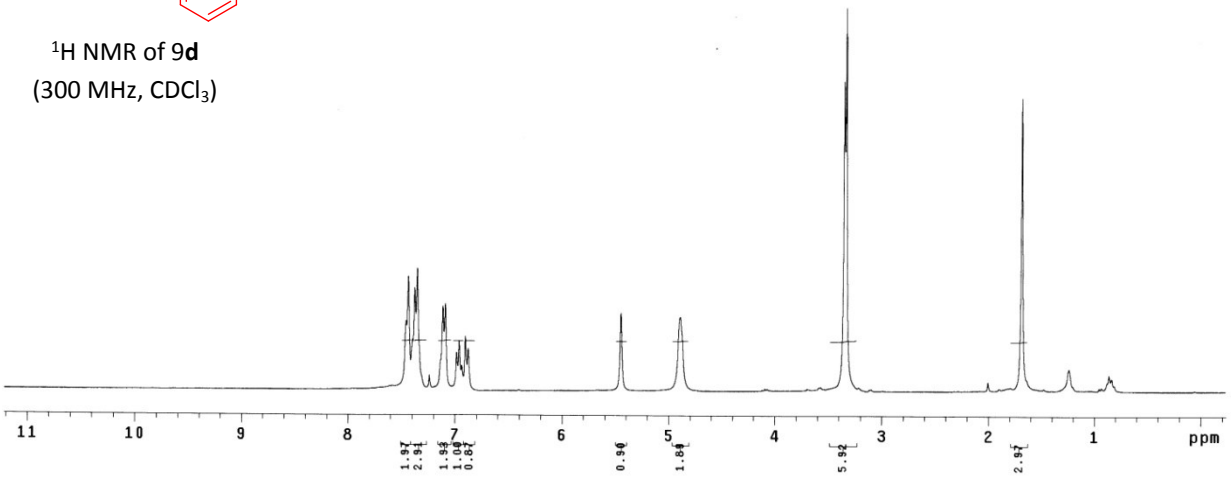


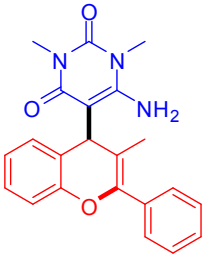
^{13}C NMR of **9c**
(75 MHz, $CDCl_3$)



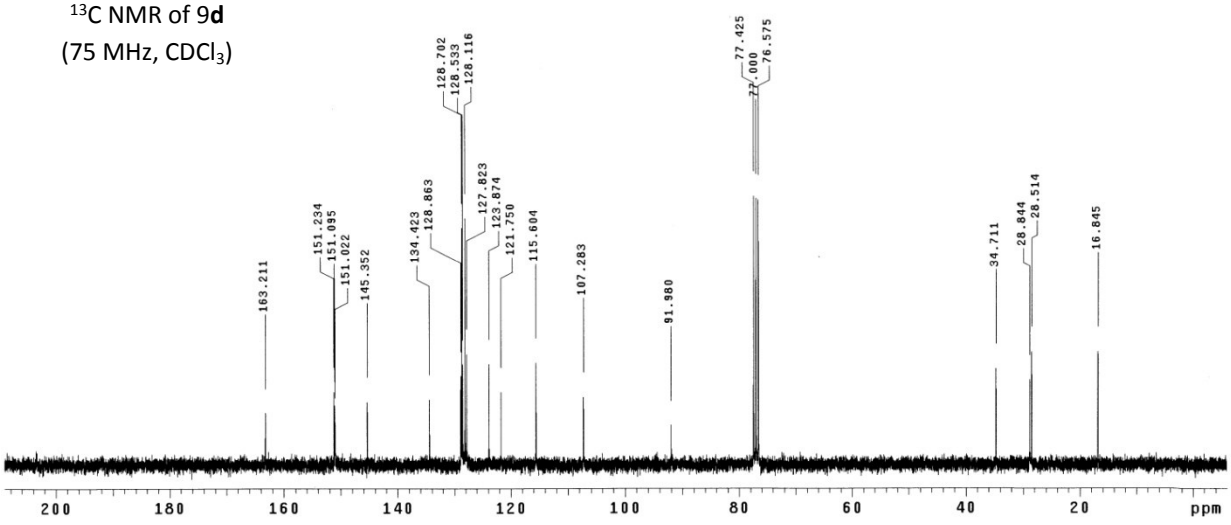


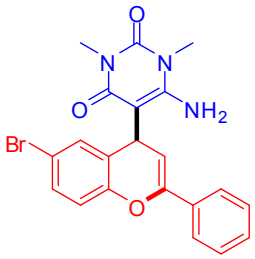
^{1}H NMR of 9**d**
(300 MHz, $CDCl_3$)



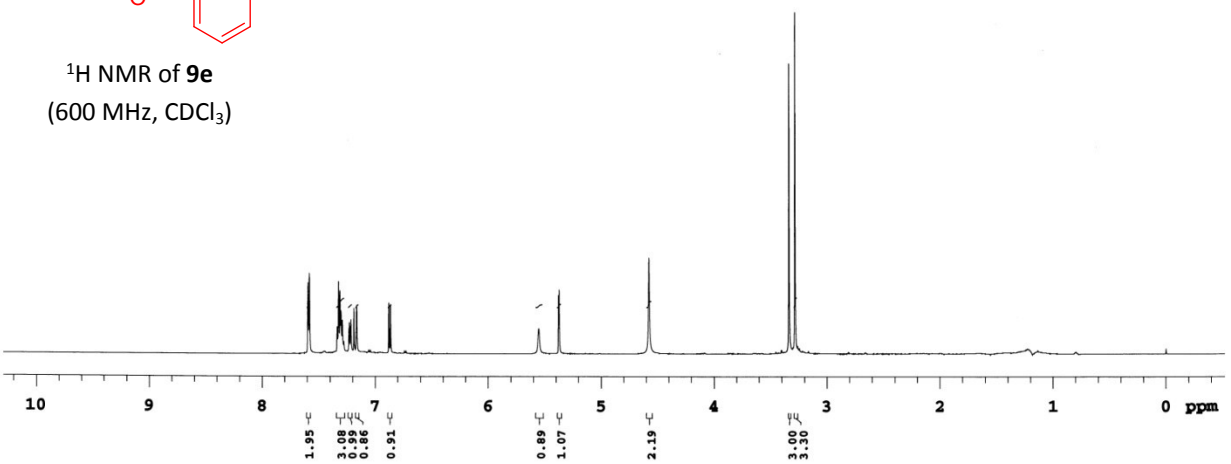


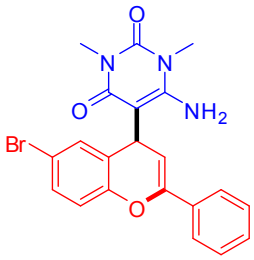
^{13}C NMR of 9**d**
(75 MHz, $CDCl_3$)





^{1}H NMR of **9e**
(600 MHz, $CDCl_3$)





^{13}C NMR of **9e**
(150 MHz, $CDCl_3$)