

Figure S2. ^1H NMR spectra of APTSPP in d_6 -DMSO.

Figure S2. ^1H NMR (d_6 -DMSO) δ : 8.95 (br, 2H, β -pyrrole), 8.82 (br, 6H, β -pyrrole), 8.16 (m, 6H, ortho triphenyl), 8.05 (m, 6H, meta triphenyl), 7.89 (br, 2H, 4-aminophenyl), 7.02 (br, 2H, 4-aminophenyl), 4.36 (s, 2H, amino), -2.87 (2H, pyrrole NH).

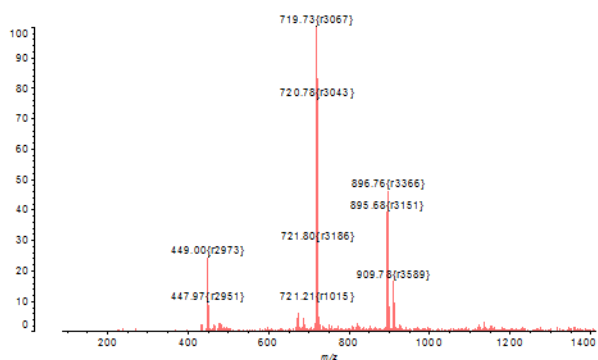


Figure S3. MALDI-TOF-MS of [6, 6]-phenyl- C_{61} -butyric acid.

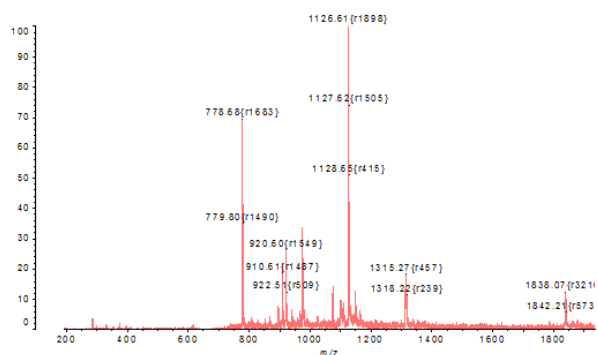


Figure S4. MALDI-TOF-MS of $\text{PC}_{61}\text{BA-APTSPP-Mn}$.

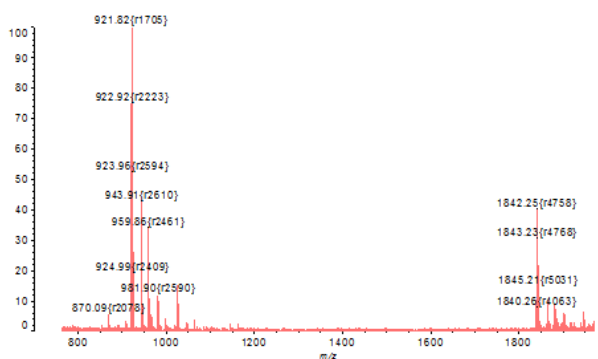


Figure S5. MALDI-TOF-MS of APTSPP-Mn.

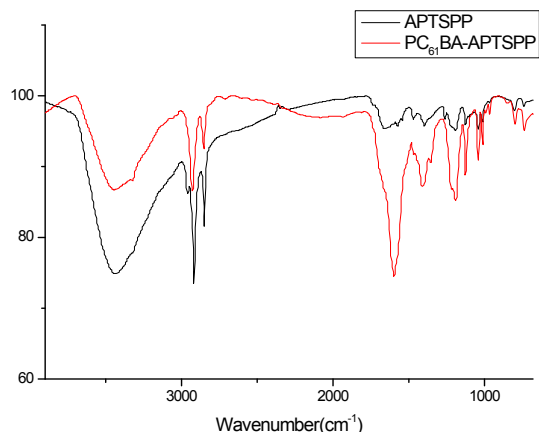


Figure S6. FTIR spectra of APTSPP and PC₆₁BA-APTSP.

In Figure S6, compared with IR spectra of APTSPP, PC₆₁BA-APTSP showed much stronger absorption at 1598, 1407, 1189 cm⁻¹, which should belong to the characteristic absorption of PC₆₁BA (*J. Org. Chem., Vol.60, No. 3, 1995*). The other enhanced absorption may be attributed to the formation of conjugation system between PC₆₁BA and APTSPP, since IR absorption is generally strengthened after formation of conjugation system.

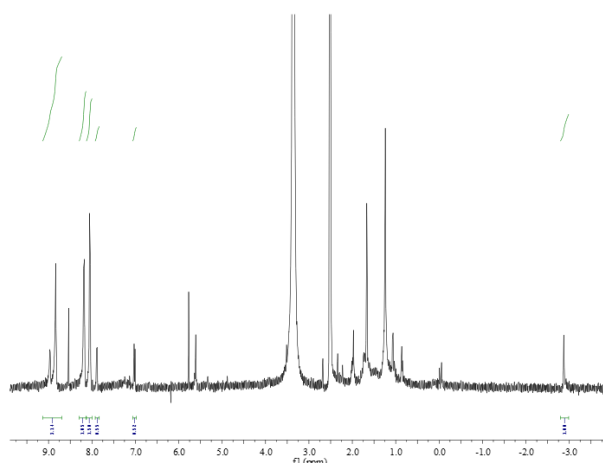


Figure S7. ¹H NMR spectrum of PC₆₁BA-APTSP in *d*₆-DMSO.

In Figure S7, ¹H NMR (*d*₆-DMSO)δ: 8.97 (br, 2H, β-pyrrole), 8.83 (br, 6H, β-pyrrole), 8.18 (m, 6H, ortho triphenyl), 8.05 (m, 6H, meta triphenyl), 7.89 (br, 2H, 4-aminophenyl), 7.02 (br, 2H, 4-aminophenyl), 5.77 (s, 2H, -CONH-), -2.87 (2H, pyrrole NH). Due to the overlapping between PC₆₁BA and APTSPP, it seems difficult to distinguish the chemical shift from the benzene ring of PC₆₁BA, but the chemical shift from alkane of PC₆₁BA can be found around δ 1.6-2.1 ppm.

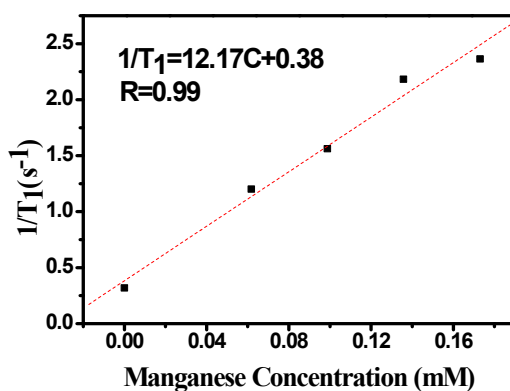


Figure S8. Linear relationship between T_1 relaxation rates ($1/T_1$) and manganese concentrations for PC₆₁BA-APTSPP-Mn in water at 3 T and 300 K.

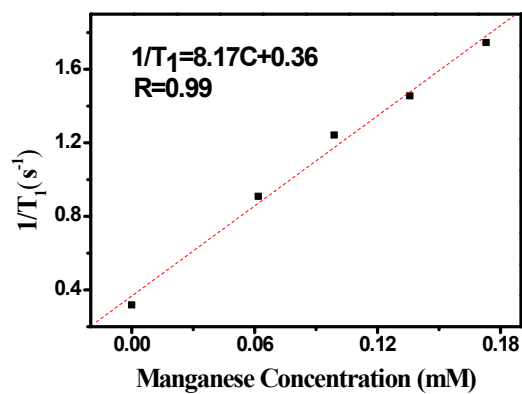


Figure S9. Linear relationship between T_1 relaxation rates ($1/T_1$) and manganese concentrations for APTSPP-Mn in water at 3 T and 300 K.