Supporting Information

Table S1. Crystal data and structure refinement for $[C_{16}PyO]$. H_2O.

Empirical formula	$C_{21}\ H_{39}\ N\ O_2$	
Formula weight	337.53	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.7504(8) Å	α= 90°.
	b = 7.9455(3) Å	β= 100.245(2)°.
	c = 13.4383(4) Å	γ = 90°.
Volume	2180.28(13) $Å^3$	
Z	4	
Density (calculated)	1.028 Mg/m^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	752	
Crystal size	0.20 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.00 to 25.06°.	
Index ranges	$-24 \le h \le 24$, $-9 \le k \le 9$, $-16 \le l \le 11$	
Reflections collected	17765	
Independent reflections	3846 [R(int) = 0.0905]	
Completeness to theta = 25.06°	99.5 %	
Absorption correction	Empirical	
Max. and min. transmission	0.96843 and 0.85753	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3846 / 0 / 225	
Goodness-of-fit on F^2	0.767	
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1068	
R indices (all data)	R1 = 0.1555, wR2 = 0.1543	
Largest diff. peak and hole	0.200 and -0.181 $e.Å^{-3}$	

Table S2. Selected bond distances [Å] and angles [°] for $[C_{16}PyO] \cdot H_2O$.

O(1)-C(3)	1.270(3)	H(2B)-O(2)-H(2C)	108(4)
O(2)-H(2B)	0.95(4)	C(1)-N(1)-C(5)	118.3(2)
O(2)-H(2C)	0.77(3)	C(1)-N(1)-C(6)	121.3(3)
N(1)-C(1)	1.335(3)	C(5)-N(1)-C(6)	120.2(2)
N(1)-C(5)	1.339(3)	N(1)-C(1)-C(2)	122.4(3)
N(1)-C(6)	1.479(3)	C(1)-C(2)-C(3)	122.0(3)
C(1)-C(2)	1.352(3)	O(1)-C(3)-C(2)	123.2(3)
C(2)-C(3)	1.411(4)	O(1)-C(3)-C(4)	123.5(3)
C(3)-C(4)	1.422(3)	C(2)-C(3)-C(4)	113.3(2)
C(4)-C(5)	1.352(3)	C(5)-C(4)-C(3)	121.7(3)
C(6)-C(7)	1.500(3)	N(1)-C(5)-C(4)	122.3(2)
C(7)-C(8)	1.522(3)	N(1)-C(6)-C(7)	115.3(2)
C(8)-C(9)	1.506(3)	C(6)-C(7)-C(8)	109.7(2)
C(9)-C(10)	1.522(3)	C(9)-C(8)-C(7)	115.8(2)
C(10)-C(11)	1.505(3)	C(8)-C(9)-C(10)	112.4(2)
C(11)-C(12)	1.515(3)	C(11)-C(10)-C(9)	115.9(2)
C(12)-C(13)	1.507(3)	C(10)-C(11)-C(12)	113.3(2)
C(13)-C(14)	1.511(3)	C(13)-C(12)-C(11)	115.1(2)
C(14)-C(15)	1.506(3)	C(12)-C(13)-C(14)	115.0(2)
C(15)-C(16)	1.504(3)	C(15)-C(14)-C(13)	115.2(2)
C(16)-C(17)	1.495(3)	C(16)-C(15)-C(14)	115.1(3)
C(17)-C(18)	1.502(3)	C(17)-C(16)-C(15)	115.9(3)
C(18)-C(19)	1.506(4)	C(16)-C(17)-C(18)	115.1(3)
C(19)-C(20)	1.486(4)	C(17)-C(18)-C(19)	116.1(3)
C(20)-C(21)	1.506(4)	C(20)-C(19)-C(18)	115.3(3)
		C(19)-C(20)-C(21)	116.3(3)

Symmetry transformations used to generate equivalent atoms:

Table S3. Crystal data and structure refinement for $[C_{16}PyOC_{16}]\ .\ H_2O$.

Empirical formula	$C_{37}\ H_{72}\ Br\ N\ O_2$	
Formula weight	642.87	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.1010(5) Å	α= 82.386(1)°.
	b = 8.7939(6) Å	β= 88.279(2)°.
	c = 33.018(2) Å	γ = 67.146(1)°.
Volume	1882.7(2) $Å^3$	
Z	2	
Density (calculated)	1.134 Mg/m^3	
Absorption coefficient	1.121 mm^{-1}	
F(000)	704	
Crystal size	0.50 x 0.30 x 0.20 mm^3	
Theta range for data collection	0.62 to 28.32°.	
Index ranges	$-9 \le h \le 9, -11 \le k \le 11, -43 \le l \le 44$	
Reflections collected	22009	
Independent reflections	9295 [R(int) = 0.0390]	
Completeness to theta = 28.32°	99.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.95251 and 0.76252	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9295 / 0 / 370	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.1231	
R indices (all data)	R1 = 0.0536, wR2 = 0.1287	
Largest diff. peak and hole	1.078 and -0.510 $e.Å^{-3}$	

Table S4. Selected bond distances [Å] and angles [°] for $[C_{16}PyOC_{16}]$. H_2O.

O(1)-C(3)	1.335(2)	C(3)-O(1)-C(6)	118.42(15)
O(1)-C(6)	1.467(2)	C(1)-N(1)-C(5)	119.72(17)
N(1)-C(1)	1.355(3)	C(1)-N(1)-C(22)	120.35(17)
N(1)-C(5)	1.368(3)	C(5)-N(1)-C(22)	119.51(17)
N(1)-C(22)	1.491(2)	N(1)-C(1)-C(2)	121.84(18)
C(1)-C(2)	1.376(3)	C(1)-C(2)-C(3)	118.99(18)
C(2)-C(3)	1.409(3)	O(1)-C(3)-C(4)	116.69(17)
C(3)-C(4)	1.406(3)	O(1)-C(3)-C(2)	124.93(18)
C(4)-C(5)	1.366(3)	C(4)-C(3)-C(2)	118.38(18)
C(6)-C(7)	1.518(3)	C(5)-C(4)-C(3)	119.97(18)
C(7)-C(8)	1.535(3)	C(4)-C(5)-N(1)	121.07(18)
C(8)-C(9)	1.532(3)	O(1)-C(6)-C(7)	107.31(16)
C(9)-C(10)	1.536(3)	C(6)-C(7)-C(8)	115.19(17)
C(10)-C(11)	1.527(3)	C(9)-C(8)-C(7)	114.69(17)
C(11)-C(12)	1.531(3)	C(8)-C(9)-C(10)	111.38(17)
C(12)-C(13)	1.529(3)	C(11)-C(10)-C(9)	114.61(17)
C(13)-C(14)	1.530(3)	C(10)-C(11)-C(12)	112.41(17)
C(14)-C(15)	1.527(3)	C(13)-C(12)-C(11)	114.09(17)
C(15)-C(16)	1.537(3)	C(12)-C(13)-C(14)	113.37(17)
C(16)-C(17)	1.529(3)	C(15)-C(14)-C(13)	113.45(17)
C(17)-C(18)	1.535(3)	C(14)-C(15)-C(16)	113.39(17)
C(18)-C(19)	1.529(3)	C(17)-C(16)-C(15)	113.43(17)
C(19)-C(20)	1.528(3)	C(16)-C(17)-C(18)	113.16(17)
C(20)-C(21)	1.530(3)	C(19)-C(18)-C(17)	113.71(17)
C(22)-C(23)	1.525(3)	C(20)-C(19)-C(18)	113.04(18)
C(23)-C(24)	1.531(3)	C(19)-C(20)-C(21)	113.7(2)
C(24)-C(25)	1.533(3)	N(1)-C(22)-C(23)	109.20(16)
C(25)-C(26)	1.526(3)	C(22)-C(23)-C(24)	115.92(17)
C(26)-C(27)	1.534(3)	C(23)-C(24)-C(25)	109.75(17)
C(27)-C(28)	1.527(3)	C(26)-C(25)-C(24)	115.64(17)
C(28)-C(29)	1.532(3)	C(25)-C(26)-C(27)	112.27(17)
C(29)-C(30)	1.528(3)	C(28)-C(27)-C(26)	113.89(17)
C(30)-C(31)	1.531(3)	C(27)-C(28)-C(29)	113.74(17)
C(31)-C(32)	1.529(3)	C(30)-C(29)-C(28)	113.53(17)
C(32)-C(33)	1.529(3)	C(29)-C(30)-C(31)	113.95(17)

C(33)-C(34)	1.529(3)	C(32)-C(31)-C(30)	113.48(17)
C(34)-C(35)	1.530(3)	C(31)-C(32)-C(33)	114.21(17)
C(35)-C(36)	1.523(3)	C(34)-C(33)-C(32)	113.27(17)
C(36)-C(37)	1.529(3)	C(33)-C(34)-C(35)	113.99(17)
		C(36)-C(35)-C(34)	113.31(18)
		C(35)-C(36)-C(37)	113.55(19)

Symmetry transformations used to generate equivalent atoms:

Table S5. Crystal data and structure refinement for $[C_{16}PyOH][Cl]\cdot H_2O$.

Empirical formula	$C_{21}H_{38}ClNO_2$	
Formula weight	355.97	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-(1)	
Unit cell dimensions	a = 5.0633(2) Å	α= 92.227(2)°.
	b = 7.8476(3) Å	β= 93.436(2)°.
	c = 28.8648(9) Å	γ = 102.045(2)°.
Volume	1118.12(7) $Å^3$	
Z	2	
Density (calculated)	1.057 Mg/m^3	
Absorption coefficient	0.178 mm^{-1}	
F(000)	392	
Crystal size	2.00 x 1.50 x 0.50 mm^3	
Theta range for data collection	0.71 to 28.04°.	
Index ranges	$-6 \le h \le 6, -10 \le k \le 10, -37 \le l \le 37$	
Reflections collected	16173	
Independent reflections	5404 [R(int) = 0.0342]	
Completeness to theta = 28.04□	99.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5404 / 0 / 229	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1710	
R indices (all data)	R1 = 0.0983, wR2 = 0.1997	
Largest diff. peak and hole	0.343 and -0.393 e. $Å^{-3}$.	

Table S6. Selected bond distances [Å] and angles [°] for $[C_{16}PyOH][Cl] \cdot H_2O$.

C(5)-N(1)	1.482(2)	C(5)-C(6)-C(7)	110.89(16)
C(5)-C(6)	1.500(3)	C(3)-C(4)-C(21)	119.52(18)
C(6)-C(7)	1.518(3)	N(1)-C(3)-C(4)	121.74(18)
C(4)-C(3)	1.360(3)	C(2)-C(1)-C(21)	119.43(18)
C(4)-C(21)	1.392(3)	N(1)-C(2)-C(1)	121.49(18)
C(3)-N(1)	1.338(2)	C(9)-C(10)-C(11)	114.41(17)
C(1)-C(2)	1.366(3)	C(8)-C(7)-C(6)	114.34(16)
C(1)-C(21)	1.382(3)	C(12)-C(11)-C(10)	114.78(17)
C(2)-N(1)	1.349(2)	C(7)-C(8)-C(9)	113.97(17)
C(10)-C(9)	1.503(3)	C(10)-C(9)-C(8)	114.59(17)
C(10)-C(11)	1.517(3)	C(15)-C(16)-C(17)	115.30(17)
C(7)-C(8)	1.508(3)	C(15)-C(14)-C(13)	114.79(17)
C(11)-C(12)	1.509(3)	C(11)-C(12)-C(13)	114.51(17)
C(8)-C(9)	1.519(3)	C(12)-C(13)-C(14)	114.32(17)
C(16)-C(15)	1.503(3)	C(16)-C(15)-C(14)	114.93(17)
C(16)-C(17)	1.511(3)	C(18)-C(17)-C(16)	114.82(17)
C(14)-C(15)	1.514(3)	C(17)-C(18)-C(19)	115.34(18)
C(14)-C(13)	1.513(3)	C(20)-C(19)-C(18)	114.1(2)
C(12)-C(13)	1.513(3)	C(3)-N(1)-C(2)	119.37(16)
C(17)-C(18)	1.502(3)	C(3)-N(1)-C(5)	120.12(16)
C(18)-C(19)	1.504(3)	C(2)-N(1)-C(5)	120.50(16)
C(20)-C(19)	1.502(3)	O(1)-C(21)-C(1)	118.49(17)
C(21)-O(1)	1.328(2)	O(1)-C(21)-C(4)	123.10(18)
		C(1)-C(21)-C(4)	118.40(17)

Symmetry transformations used to generate equivalent atoms:

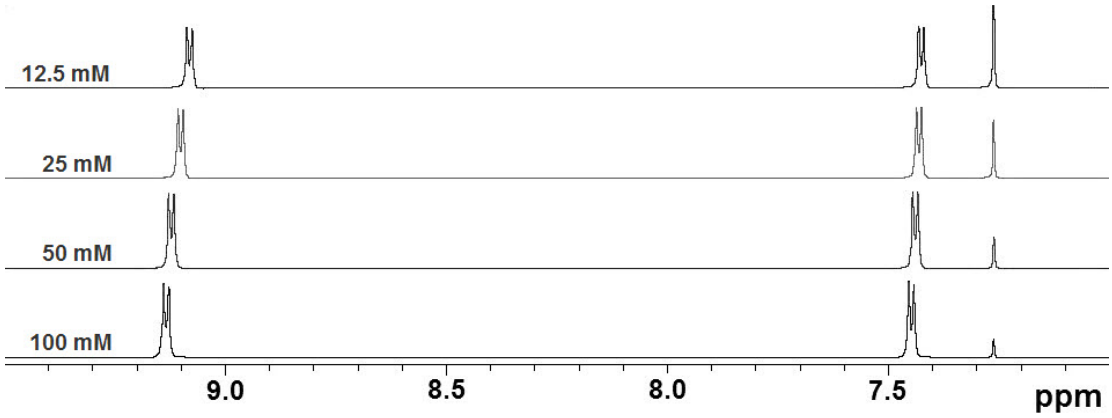

Figure S1. ^{1}H-NMR spectra of $[C_{16}PyOC_{16}][Br]$ at different concentrations in $CDCl_3$ at 298 K.

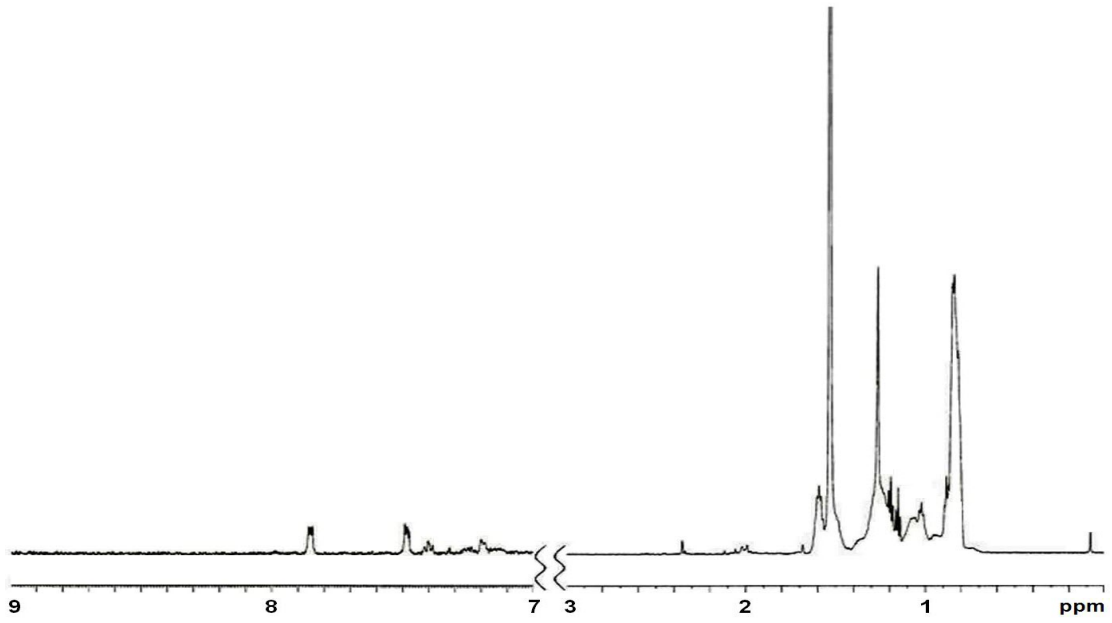

Figure S2. ^{1}H-NMR spectrum of AuNPs in CD_2Cl_2.

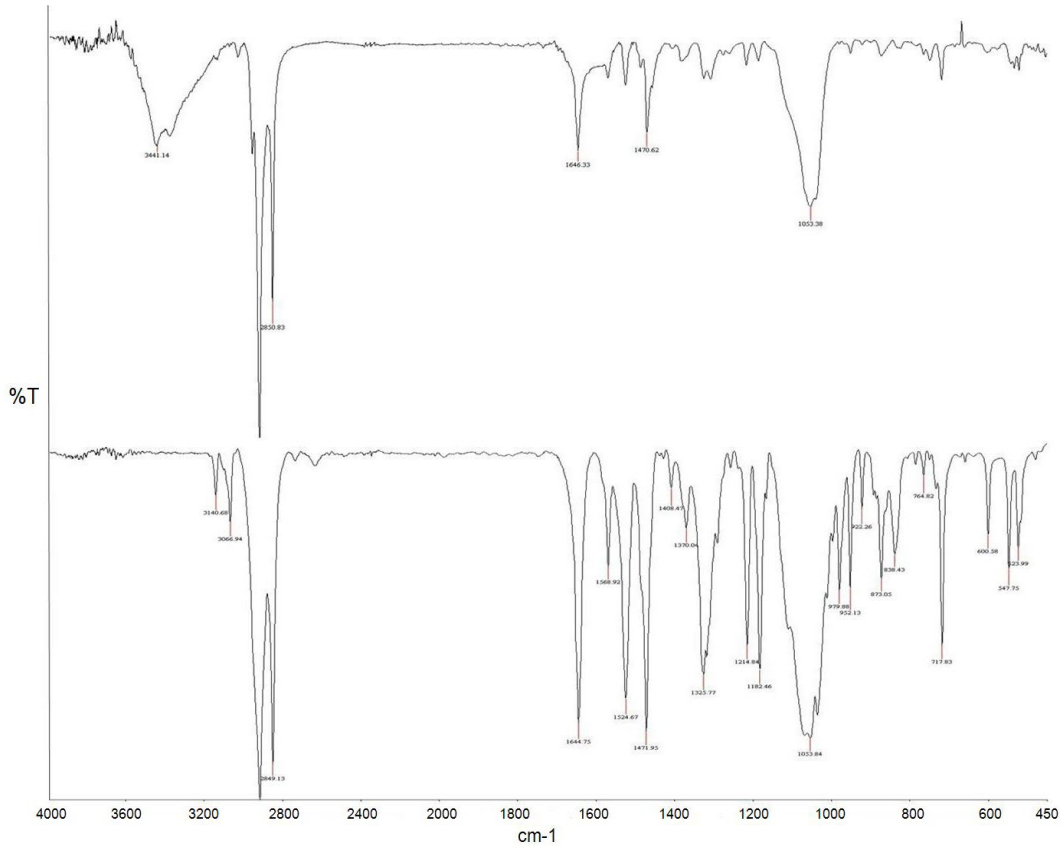

Figure S3. FT-IR spectra of AuNPs (top) and free stabilizer $[C_{16}PyOC_{16}][BF_4]$ (bottom).