Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

A Cu (II) complex of an imidazolium based ionic liquid: synthesis, X-ray structure and application in selective electrochemical sensing of guanine

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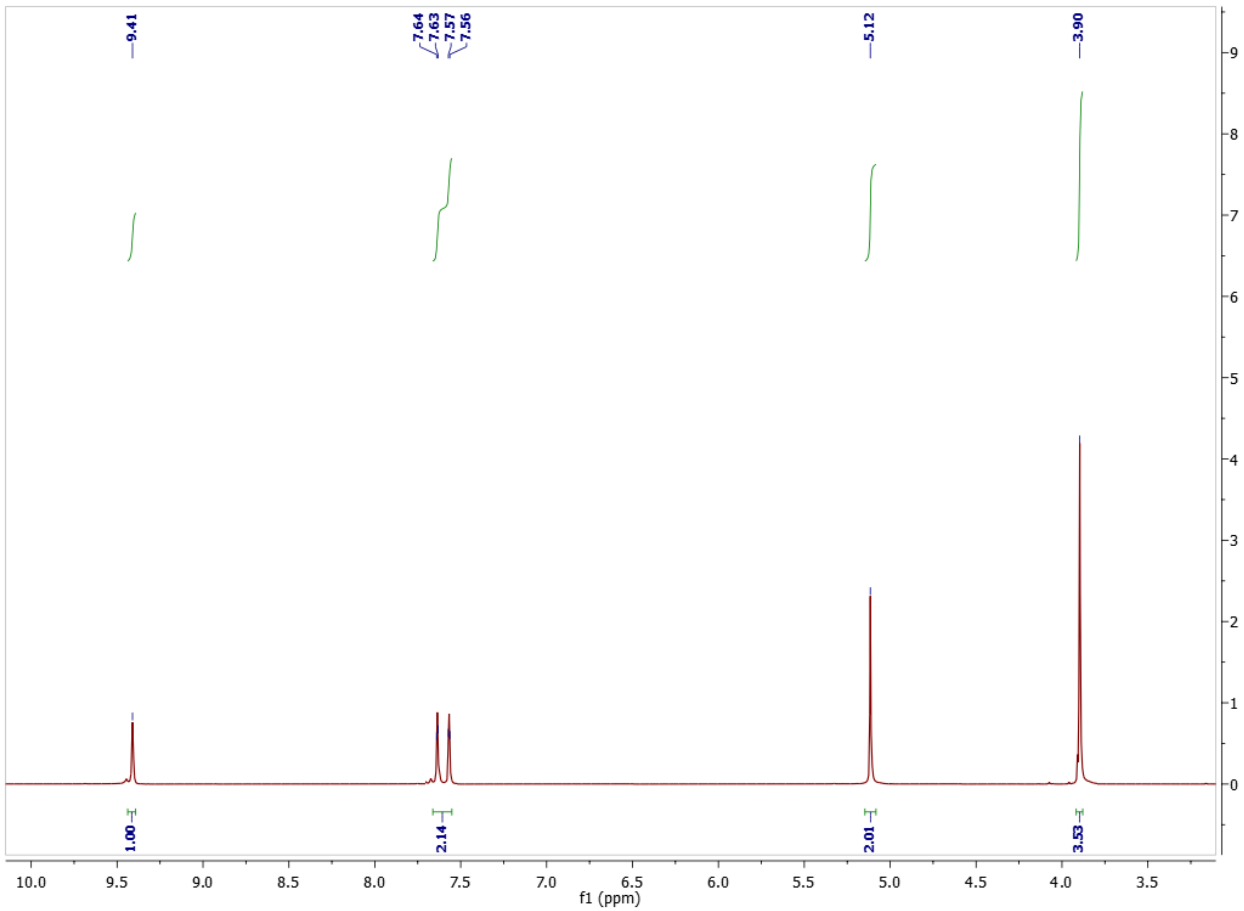

Figure S1: ^{1}H NMR spectrum of compound **1**

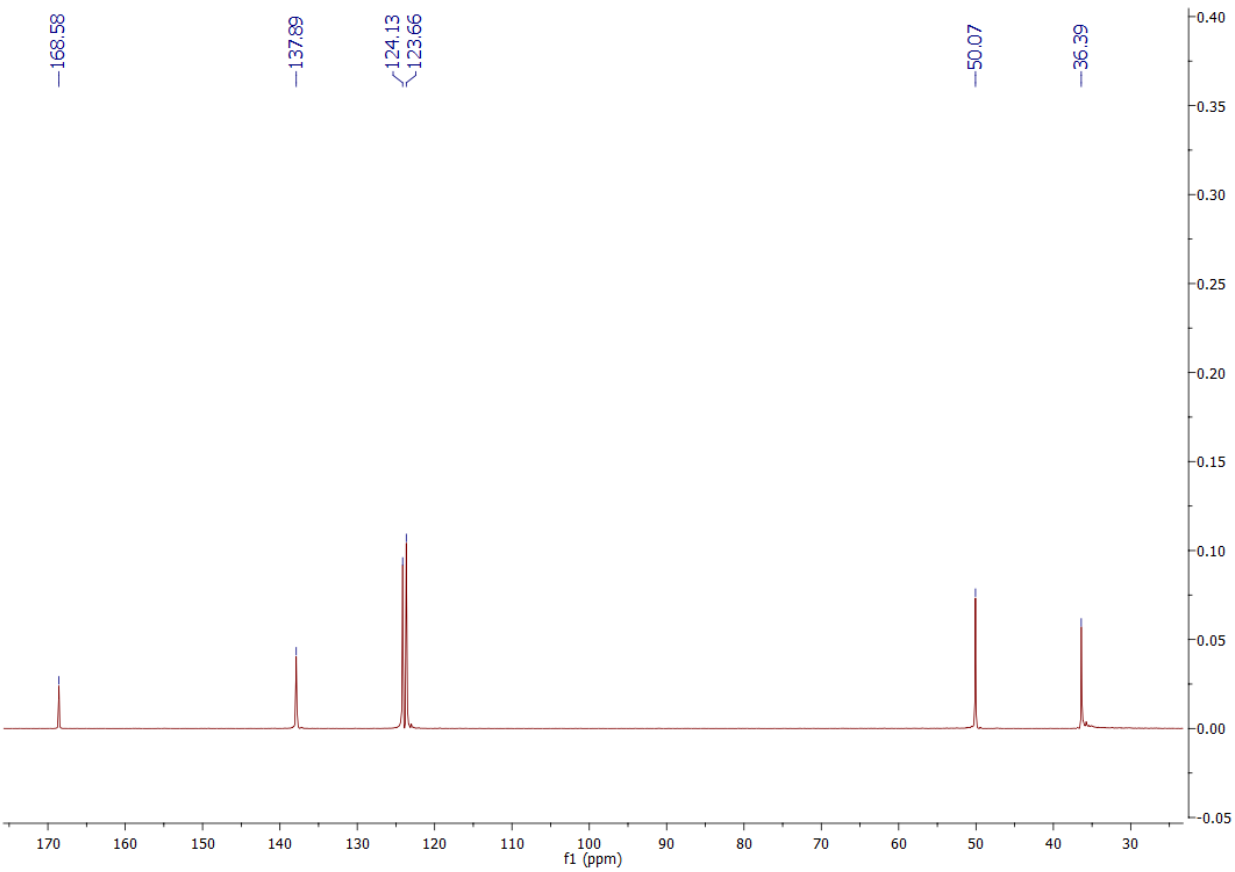

Figure S2: ^{13}C NMR spectrum of compound **1**

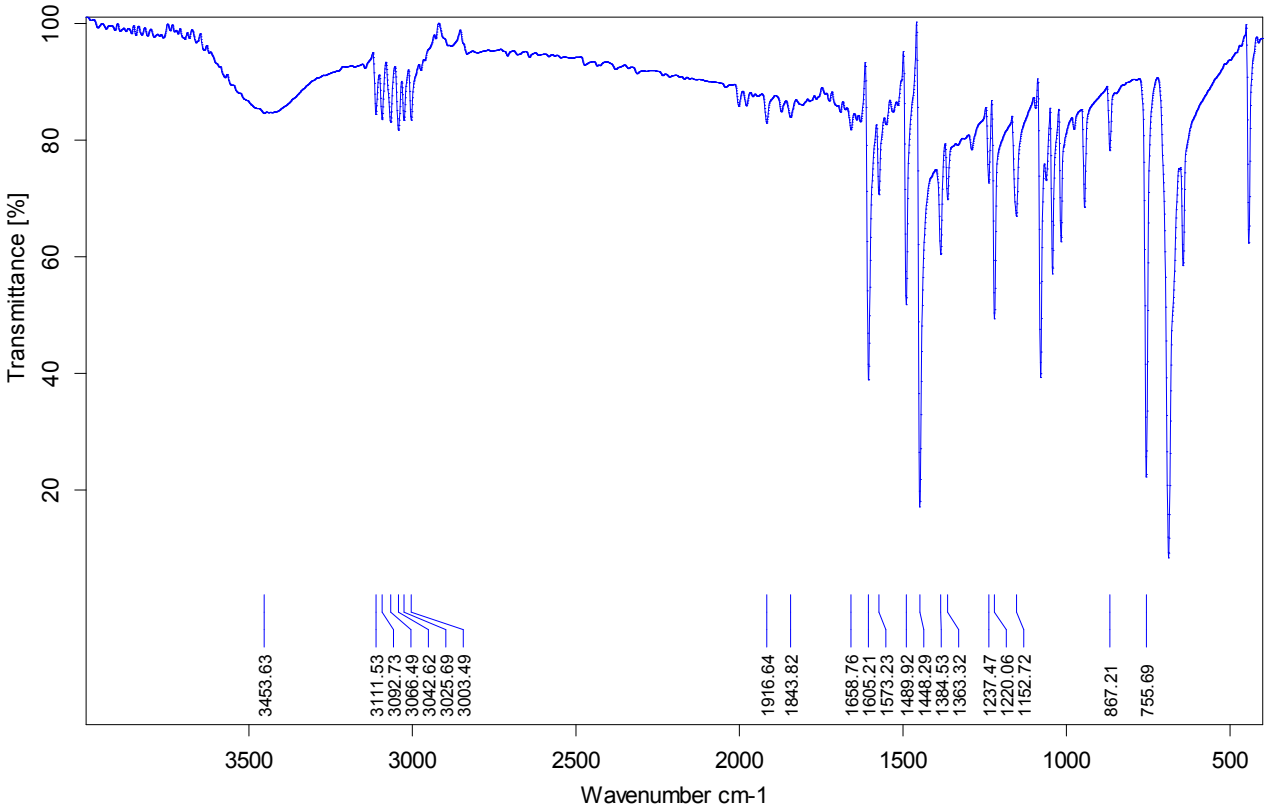

Figure S3. FT-IR spectra of Copper complex **R1**

Table S1: Crystal data and refinement parameters of compound R1

Compound	
Empirical Formula	C24 H34 Cl4 Cu2 N8 O30
M_w	1183.47
Temperature [K]	150(2) K
Crystal description	Needles, Bluish- green
Crystal System	Orthorhombic
Space group	Pnnm
a / [Å]	12.9191(5)
b / [Å]	14.6740(6)
c / [Å]	11.9279(4)
a/*β*/*γ* / [º]	90.00
V [Å^3]	2261.23(15)
Z	2
D_c [Mg m^{-3}]	1.738
μ / [mm^{-1}]	1.283
Reflections collected	37305
Data / restraints / parameters	2327 / 10 / 207
Unique reflections, [R_{int}]	2327 [0.0255]
GOF = S_{all}	1.047
Final *R* indices	
R_1, wR_2 [I>2σI]	0.0584, 0.1747
R_1, wR_2 (all data)	0.0644, 0.1814
Δρmax/Δρmin [Å^3]	0.986, -0.976

Table S2. Selected bond lengths and angles (Å,º) for compound R1

Bond lengths(Å)					
Cu(1)-O(1)	1.968(2)	Cu(1)-O(3)	2.163(5)	Cu(1)-Cu(1)#1	2.6416(11)
Cu(1)-O(2)#1	1.966(3)	Cu(1)-O(1)#3	1.968(2)	O(1)-C(6)	1.258(4)
O(2)-C(6)	1.255(4)	C(5)-C(6)	1.519(5)		
Bond angles(º)					
O(2)#1-Cu(1)-O(1)	168.48(11)	O(2)#2-Cu(1)-O(1)	89.12(12)	O(2)#1-Cu(1)-O(3)	92.57(11)
O(2)#1-Cu(1)-O(2)#2	88.69(16)	O(1)-Cu(1)-O(1)#3	90.78(15)	O(1)-Cu(1)-O(3)	98.83(11)
O(2)#1-Cu(1)-Cu(1)#1	85.46(7)	C(6)-O(1)-Cu(1)	123.5(2)	O(2)-C(6)-O(1)	127.0(3)

Table S3. Hydrogen bonding parameters (Å, º) of compound R1

D-H···A	D···A/ Å	H···A/ Å	D-H···A/º
C3-H3A...O1 [i]	3.277(4)	2.503(2)	140.9(2)
C4-H4B...O1 [i]	3.346(7)	2.465(2)	152.5(4)

Equivalent positions: (i) -x-1/2,+y-1/2,-z-1/2

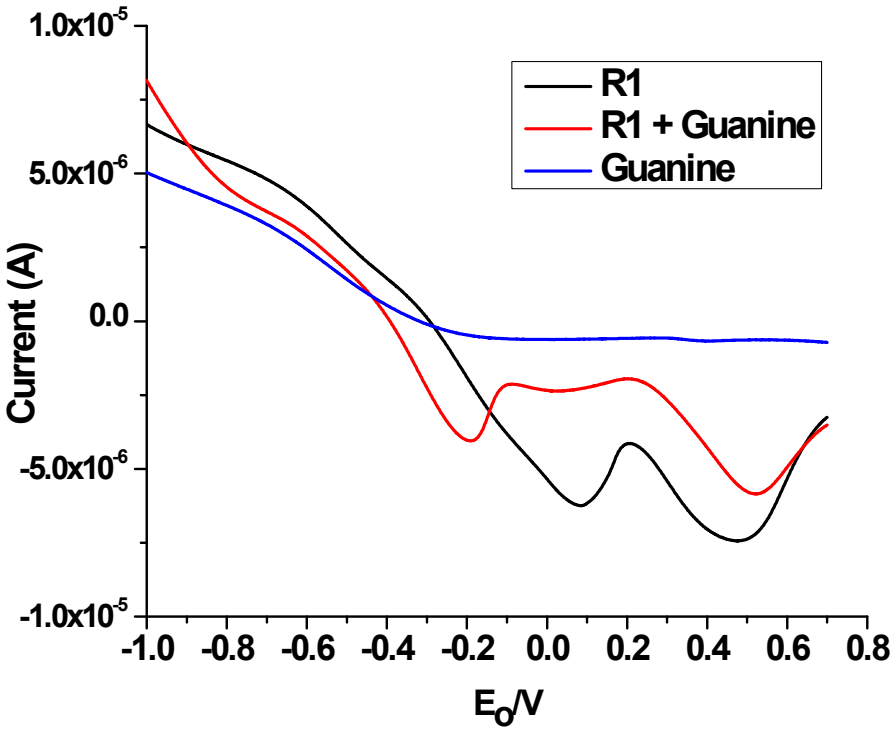

Figure S4. Comparison of LSV profile of complex **R1** (10 µM), Guanine and Change in LSV profile upon interaction with guanine in DMSO: H_2O (50:50)

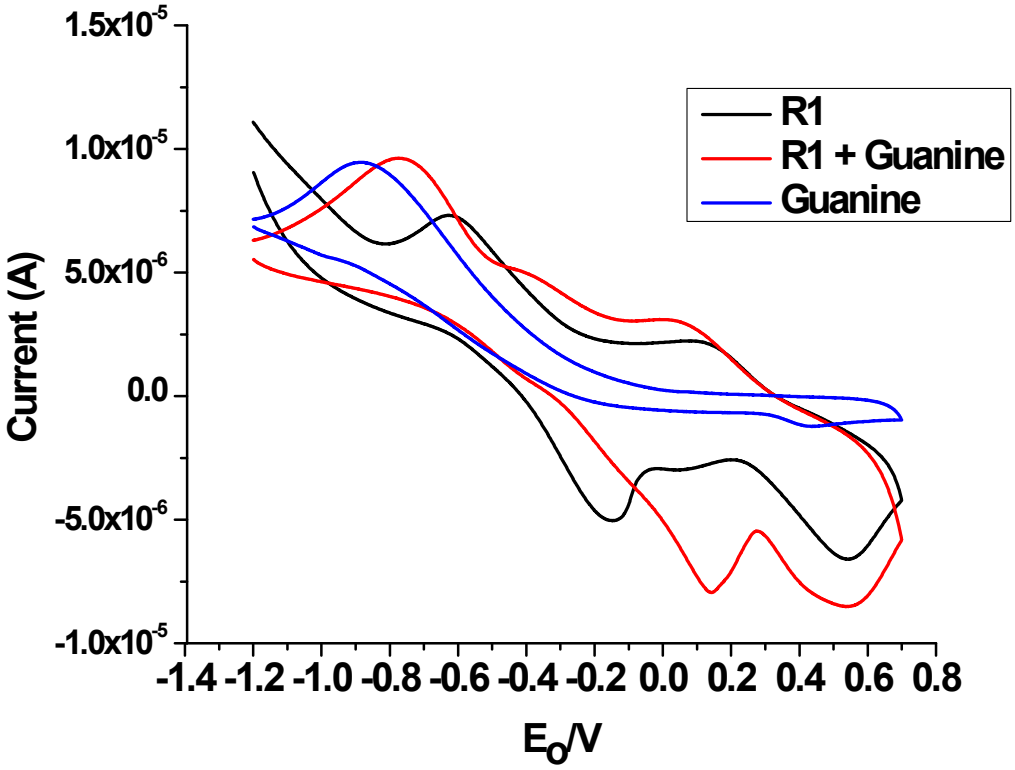

Figure S5. Comparison of CV profile of complex **R1** (10 μM), Guanine and Change in cyclic voltametry profile upon interaction with guanine in DMSO: H_2O (50:50)

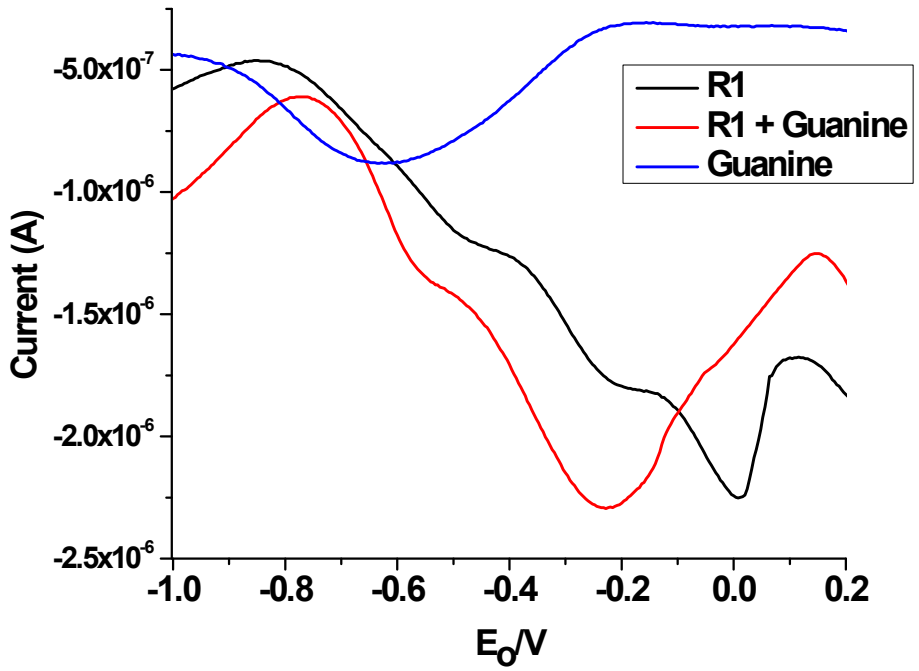

Figure S6. Comparison of DPV profile of complex **R1** (10 μM), Guanine and Change in DPV profile upon interaction with guanine in DMSO: H_2O (50:50)

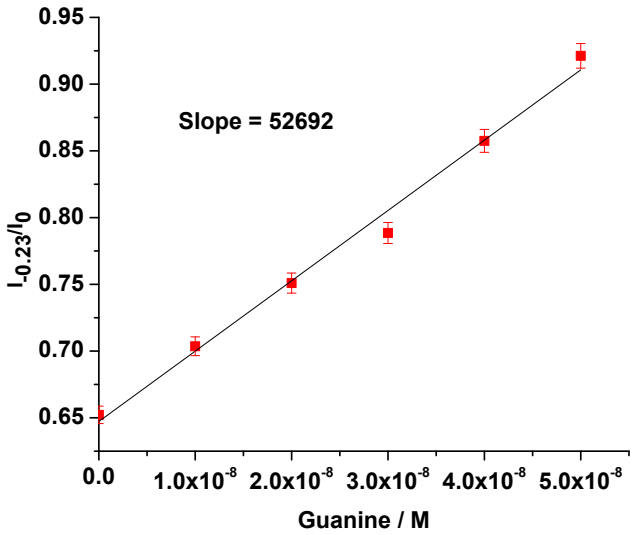

Figure S7. Calibration curve concentration of guanine and $I_{-0.23}/I_0$ in case Differential Pulse Voltammetry titration

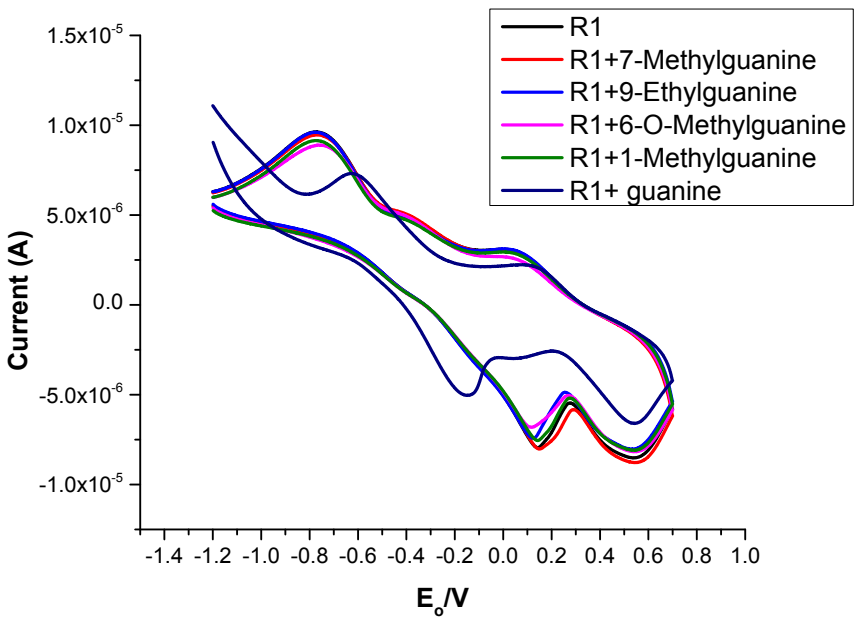

Figure S8. Changes in the CV profile of **R1** (10 μM) upon addition of various derivatives of guanine (20 μM) in DMSO: H_2O (50:50)

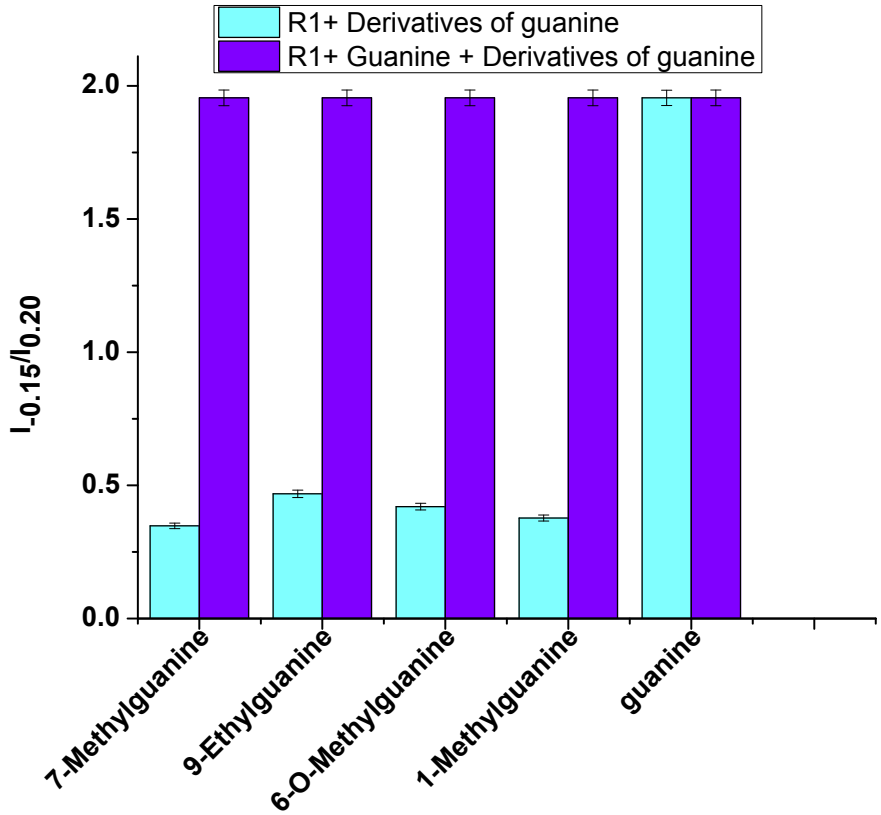

Figure S9. Change in reduction potential of **R1** in CV profile upon addition of guanine in presence of various interfering species

Table S4: Comparison of binding ability of different receptors with guanine

S. No	Receptor	Analytical method	Detection limit	Reference
1.	Cobalt(II) phthalocyanine-modified carbon paste electrode	DPV	550 nM	1
2.	Cobalt hexacyanoferrate	CV	340 nM	2
3.	β-Cyclodextrin incorporated carbon nanotube	DPV	200 nM	3
4.	Aptamers	Fluorescence	6.7 μM	4
5.	Carbon ionic liquid-modified electrode	CV	78.7 nM	5
6.	Carbon screen-printed electrode	DPV	200 nM	6
7.	Cu(II) complex of imidazolium ionic liquid (present work)	DPV, CV	45 nM	-

References:

1. A. Abbaspour, M. A. Mehrgardi and R. Kia, *J. Electroanal.Chem.,* 2004, **568**, 261.
2. A. Abbaspour and M. A. Mehrgardi, *Anal. Chem*. 2004, **76**, 5690.

3. Z. Wang, S. Xiao and Y. Chen, *J. Electroanal. Chem*. 2006, **589**, 237.
4. X. Fan, F. Lin, Y. Zhang, J. Zhao, H. Li and S. Yao, *New J.Chem,* 2012, **36**, 2260–2265.
5. W. Sun, Y. Li, Y. Duan and K. Jiao, *Biosens. Bioelectron*. 2008, **24**, 988.
6. A. Abbaspour, L. Baramakeh and S. M. Nabavizadeh, *Electrochim. Acta*, 2007, **52**, 4798.