Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Reduction Potential Prediction of Some Aromatic Nitrogen Containing Molecules

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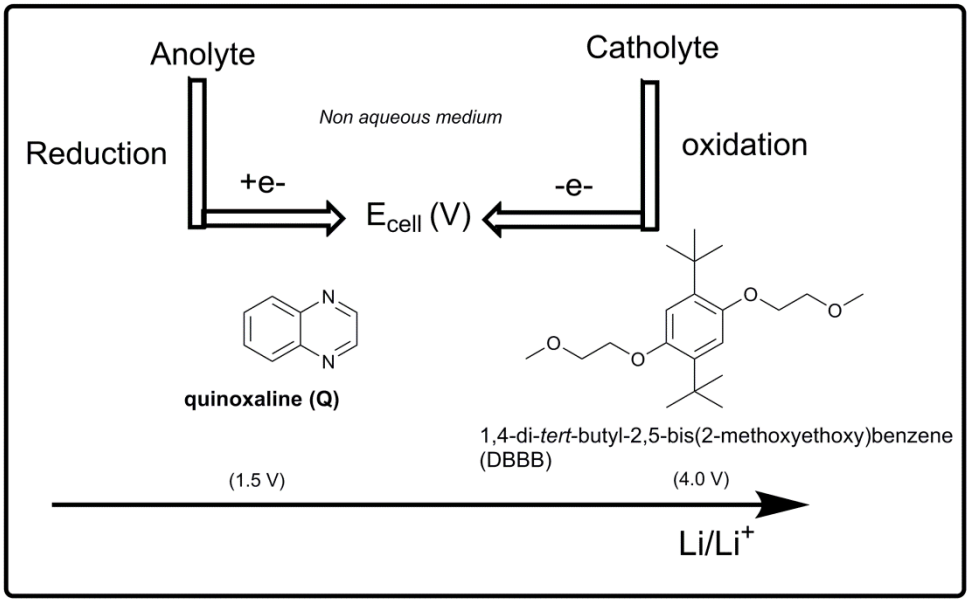


Scheme S1. A basic schematic of all organic redox battery with with an anolyte species of quinoxaline (1.5 V vs. Li/Li^+) and catholyte species of DBBB (4.0 V vs. Li/Li^+). The anticipated cell voltage is 2.5 V.

Table S1A. Comparison of computed gas phase free energy changes, solvation contributions and one electron reduction potentials using various theoretical methods. A 6-31+G(d) basis set is used for all density functional and Hartree Fock calculations.

Entry	Method	ΔG(gas), eV	ΔG(solvation), eV	E(Red1), vs. Li/Li^+
1	G4MP2	-0.87	-2.01[a]	1.64
2	B3LYP	-0.77	-2.01	1.55
3	B3PW91	-0.78	-2.06	1.60
4	M06-2X	-0.70	-2.07	1.54
5	wB97XD	-0.68	-2.08	1.52
6	PW91PW91	-0.89	-2.00	1.64
7	PBEPBE	-0.84	-2.00	1.60
8	PBE1PBE	-0.75	-2.06	1.57
9	HF	0.13	-2.11	0.74
10	PM3	-1.62	-2.38	2.76
11	PM6	-1.78	-2.38	2.92

Table S1B. Computed first and second redox potentials (V vs. Li/Li^+) of quinoxaline in the presence of various solvents. In the first strategy redox potentials were computed by optimizing the redox active molecules in the implicit solvent molecule. In the second strategy, optimization in the gas phase followed by a single point energy evaluation is performed.

Solvent (dielectric constant)	**Redox potential (V): optimization in solvent**	**Redox potential (V): optimization in gas phase and single point energy calculation in solvent**
water (ε=78.35)	1.53, 1.01	1.55, 1.00
dimethyl sulfoxide (ε=46.83)	1.50, 0.96	
methanol (ε=32.61)	1.48, 0.92	
acetone (ε=20.49)	1.44, 0.84	
diethyl ether (ε=4.21)	1.03, 0.06	
n-hexane (ε=1.88)	0.43, -0.01	
no solvent (ε=0)	-0.47	-0.47

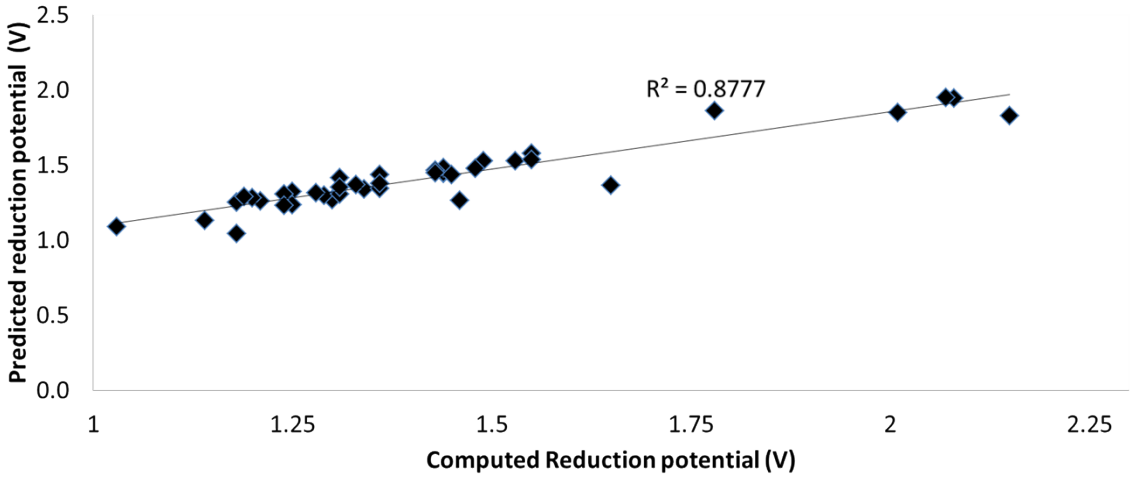
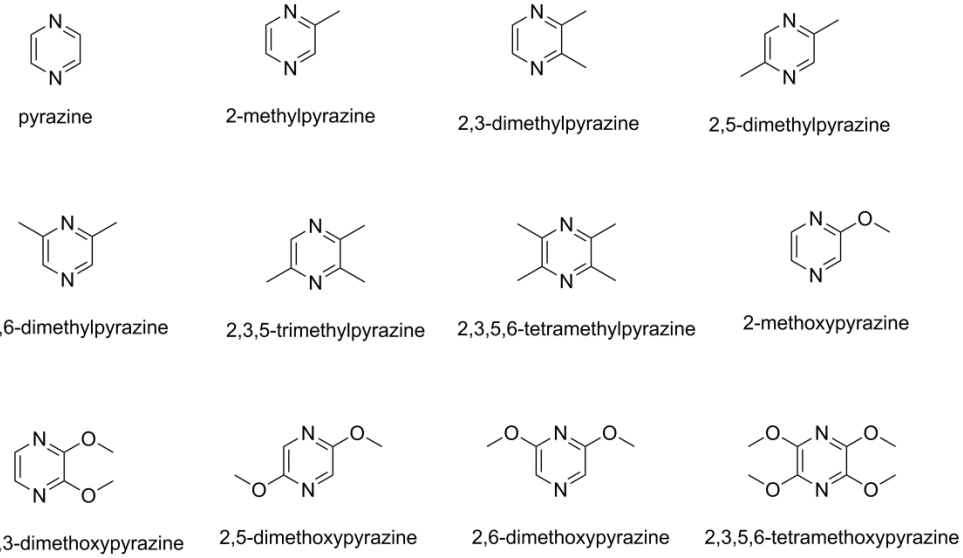


Figure S1. Computed reduction potentials using Eq. 3 vs. the predicted reduction potential using Eq. 8 for quinoxaline derivatives (data from Table 1)

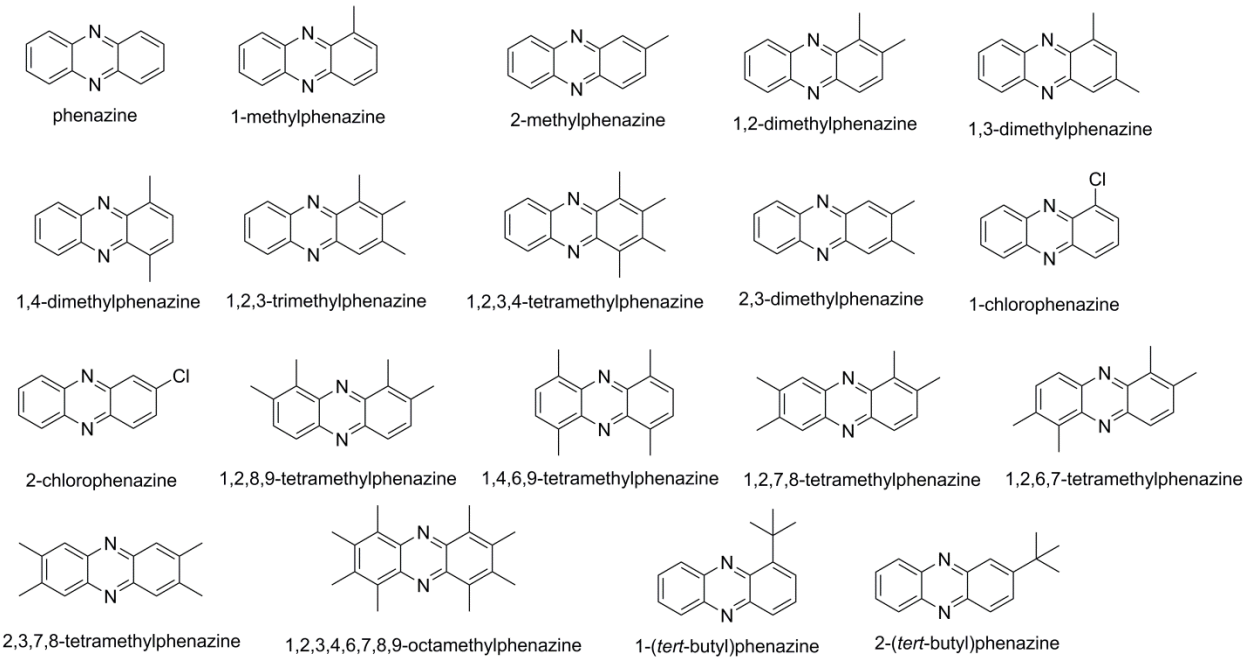
Table S22. Comparison of computed (using Eq. 3) vs predicted (using Eq. 8) reduction potential of various aromatic nitrogen containing molecules. Schematic representation of this data is shown in Figure 5.

Species	**Computed reduction potential (Eq. 3), V vs. Li/Li^+**	**Predicted reduction potential (Eq. 8), V vs. Li/Li^+**
Quinoxaline	1.55	1.58
Pyrazine	1.10	1.07
Phenazine	2.01	1.90
Bipyridine	1.31	1.18
Pyridine	0.45	0.62
Pyrimidine	0.84	0.92
Pyridazine	1.06	1.05
Quinoline	1.04	1.02
Isoquinoline	0.98	1.01

(a)


pyrazine
2-methylpyrazine
2,3-dimethylpyrazine
2,5-dimethylpyrazine
2,6-dimethylpyrazine
2,3,5-trimethylpyrazine
2,3,5,6-tetramethylpyrazine
2-methoxypyrazine
2,3-dimethoxypyrazine
2,5-dimethoxypyrazine
2,6-dimethoxypyrazine
2,3,5,6-tetramethoxypyrazine

(b)


phenazine
1-methylphenazine
2-methylphenazine
1,2-dimethylphenazine
1,3-dimethylphenazine
1,4-dimethylphenazine
1,2,3-trimethylphenazine
1,2,3,4-tetramethylphenazine
2,3-dimethylphenazine
1-chlorophenazine
2-chlorophenazine
1,2,8,9-tetramethylphenazine
1,4,6,9-tetramethylphenazine
1,2,7,8-tetramethylphenazine
1,2,6,7-tetramethylphenazine
2,3,7,8-tetramethylphenazine
1,2,3,4,6,7,8,9-octamethylphenazine
1-(*tert*-butyl)phenazine
2-(*tert*-butyl)phenazine

(c)

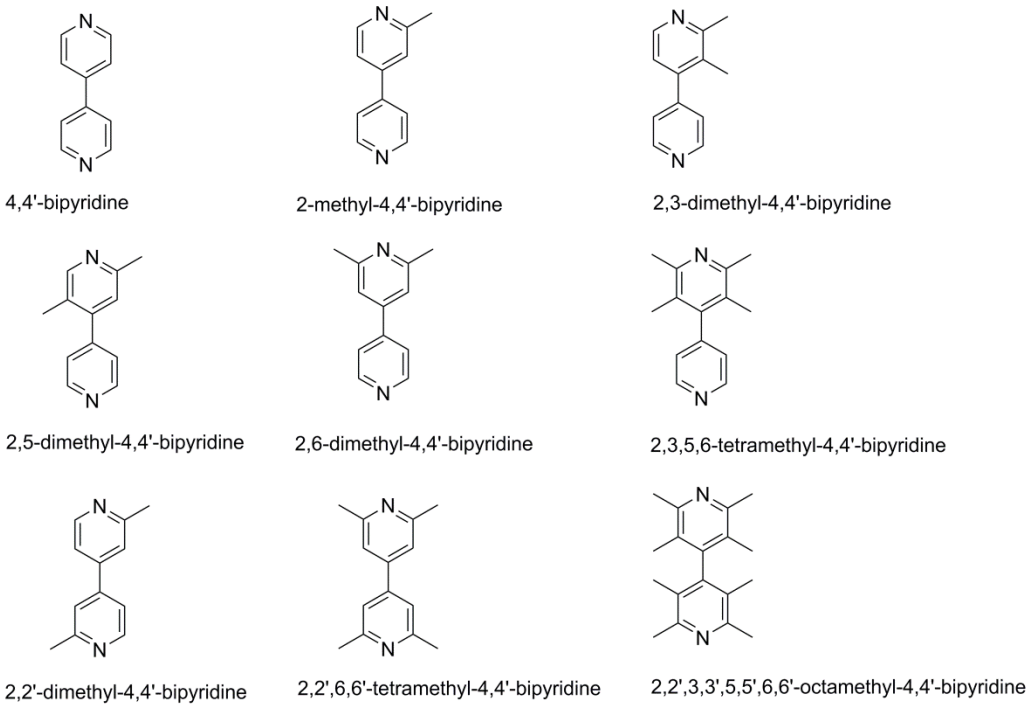


Figure S2. (a): Selected pyrazine (b) phenazine and (c) bipyridine molecules.