Electronic Supplementary Information

Dual Responsive Salen-type Schiff Bases for the Effective Detection of L-Arginine *via* Static Quenching Mechanism.

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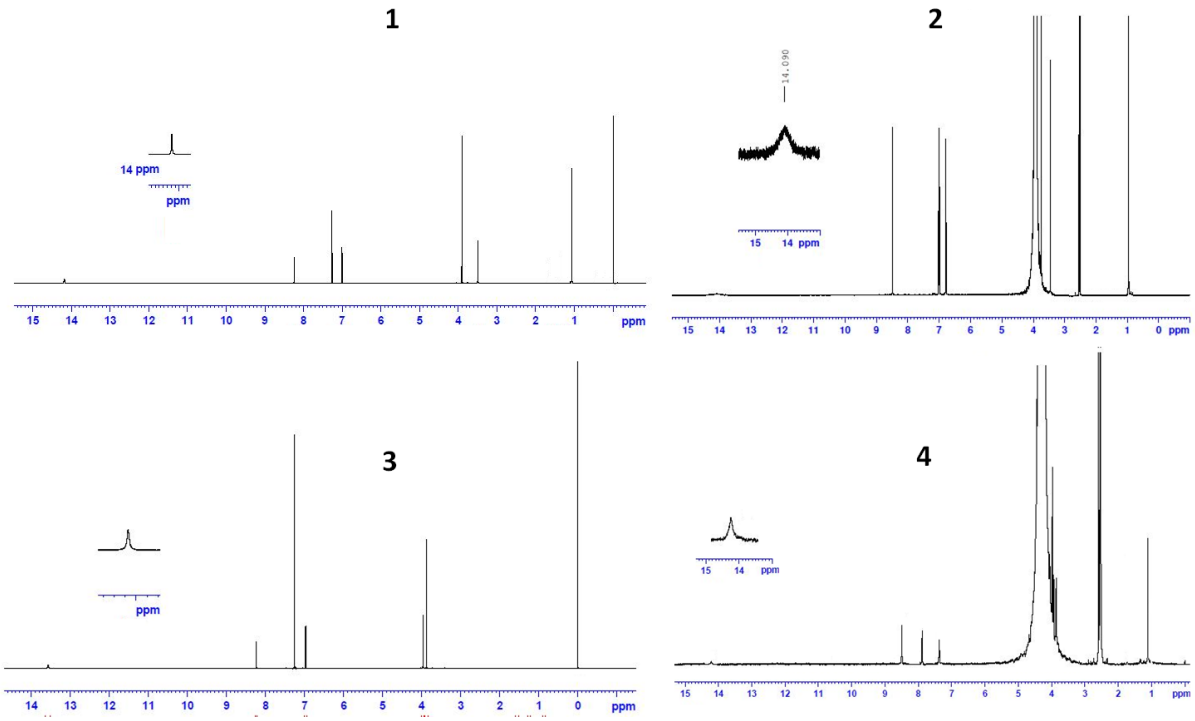

Figure S1. ^{1}H NMR spectra of sensors **1** to **4**.

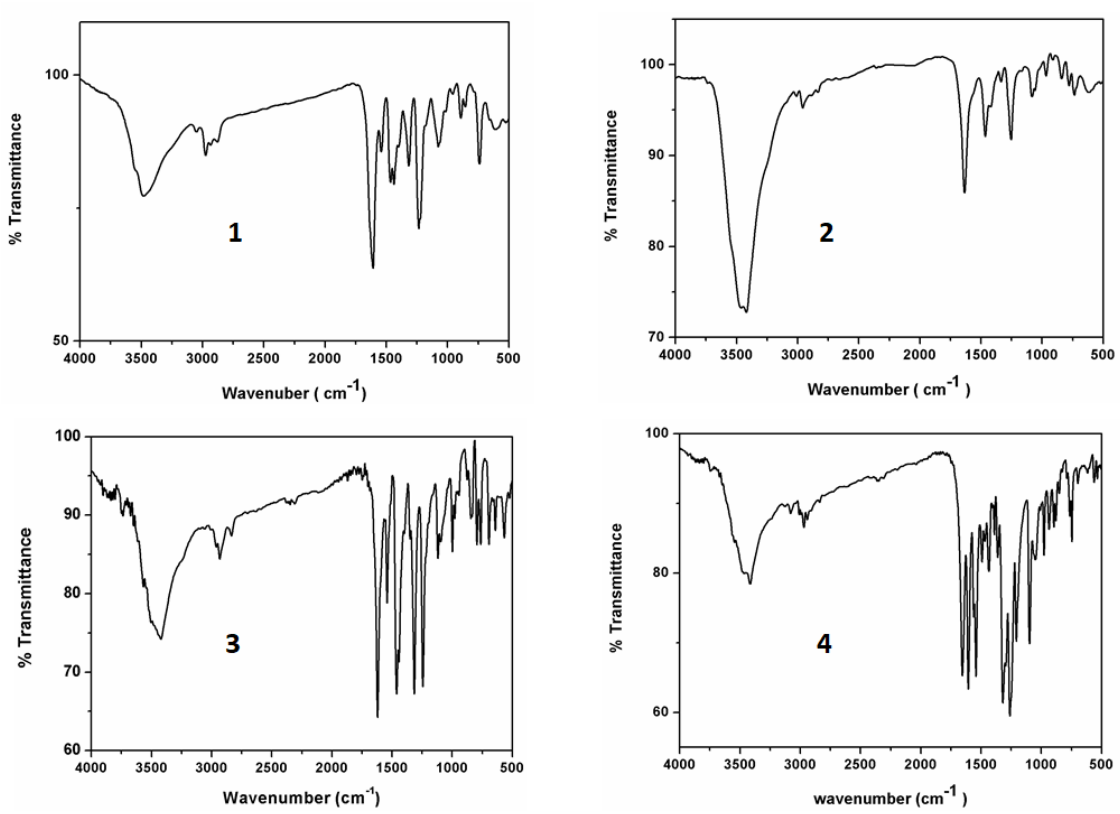

Figure S2. FT-IR spectra of sensors **1** to **4**.

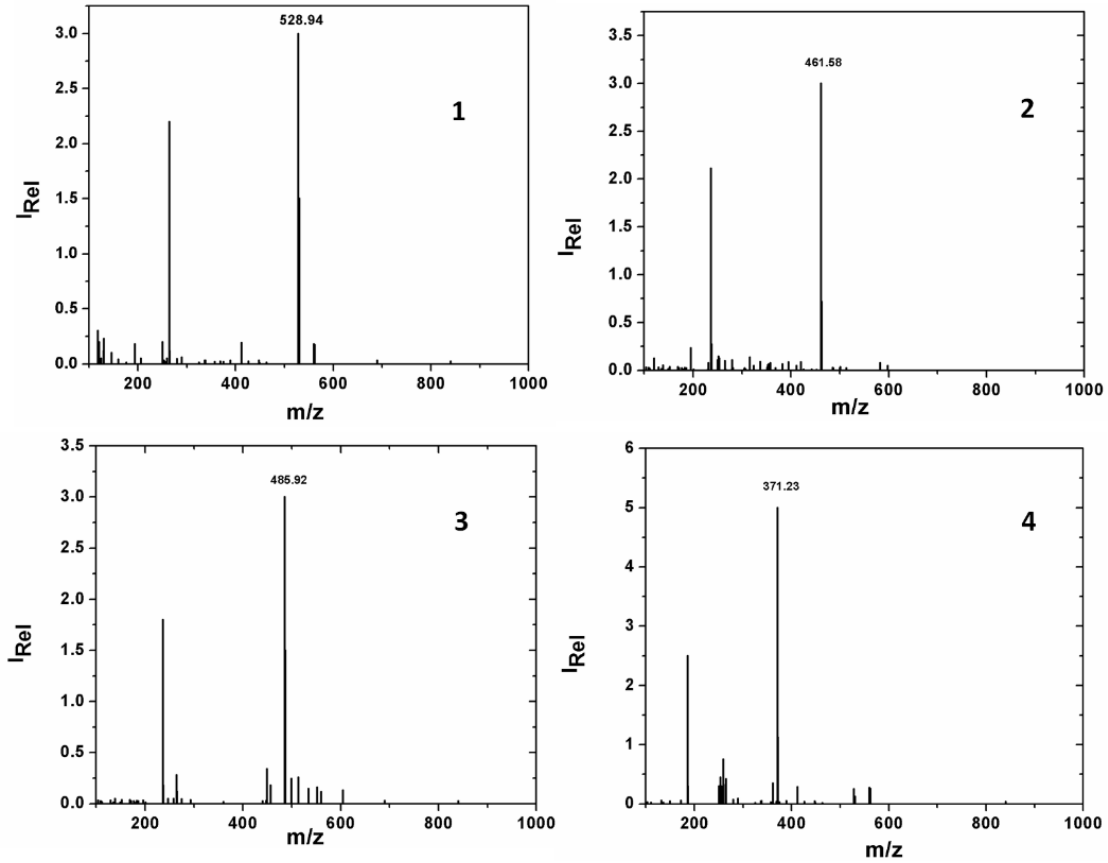

Figure S3. GC-MS data of sensors **1** to **4**.

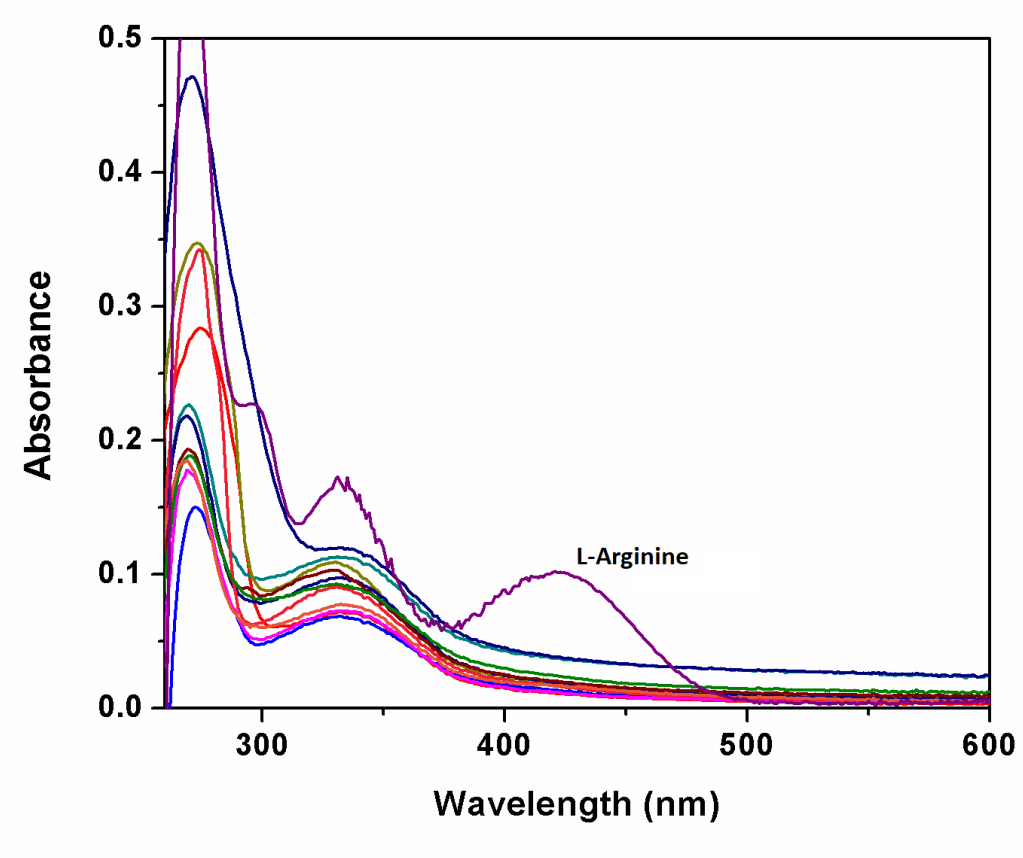

Figure S4. Absorption spectra of sensor **1** with five equivalents of various amino acids.

Table S1

Crystal data and structural refinement parameters of **2**.

Compound	**2**
Empirical formula	$C_{21}H_{26}N_2O_4$
Formula weight	370.44
Color	Yellow
Crystal system	Monoclinic
Space group	$P2_1/n$
Cell parameters	
a (Å)	15.1698(10)
b (Å)	6.9547(4)
c (Å)	19.5022(12)
α (°)	90
β (°)	93.802(3)
γ (°)	90
Volume V (Å^3)	2053.0(2)
Z	4
Calculated density (ρ) (Mg m^{-3})	1.198
Absorption coefficient, μ (mm^{-1})	0.083
F(000)	792
Crystal size mm^3	0.30 x 0.20 x 0.20
θ(°) range for data collection	2.69 to 28.35
Limiting indices	-20≤h≤20, -9≤k≤9, -26≤l≤24
Reflections collected	24051
Unique Reflections (R_{int})	5084(0.0485)
Absorption correction	Semi-empirical from equivalents
Maximum and minimum transmission	0.995 and 0.982
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5084/ 3 / 245
Goodness-of-fit on F^2	0.879
Final R indices [I > 2σ (I)]	R_1= 0.0604, wR_2 = 0.1659
R indices (all data)	R_1= 0.1547, wR_2 = 0.2384
Largest difference peak and hole (e Å^{-3})	0.264 and -0.206

$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$ $\quad wR_2 = [\Sigma w(F_o^2-F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

Table S2

Intramolecular hydrogen bonding interactions in **2**.

Hydrogen bonding interactions				
D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (°)
O(2)–H(2)···N(1)[a]	0.82	1.86	2.59	147
O(3)–H(3)···N(2)[a]	0.82	1.87	2.59	147
C(11)–H(11A)···N(2)[b]	0.96	2.58	2.90	115

Equivalent position codes : a = 1/2-x, -1/2+y, 1/2-z; b = -1+x, -1+y, z.
D, Donor; A, acceptor.

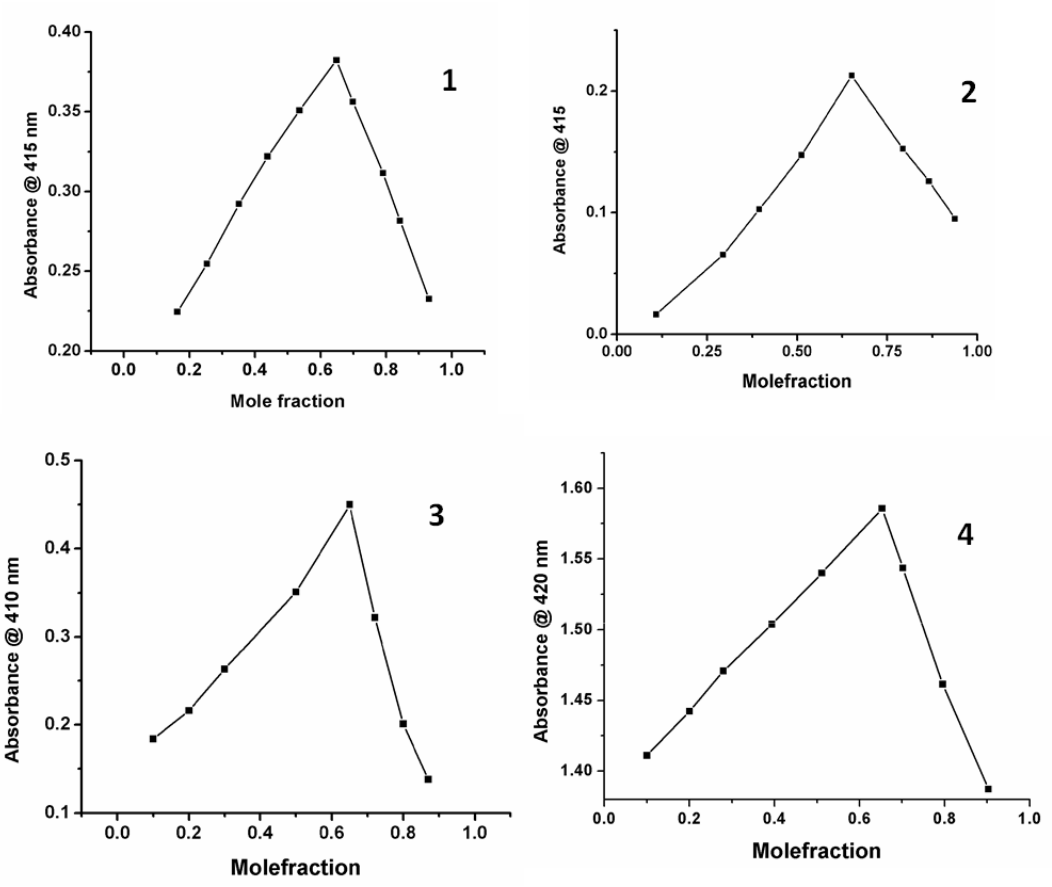

Figure S5. Jobs plot of sensors **1** to **4** showing 1:2 complex formation between the sensor and the analyte.

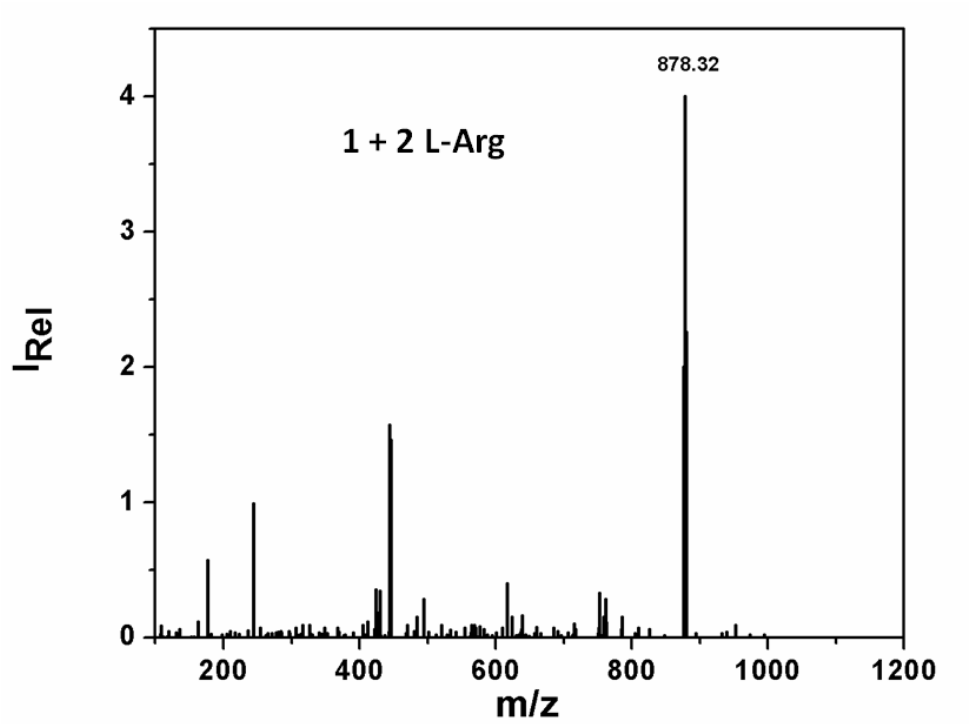

Figure S6. Mass spectrum of **1** + 2 L-Arginine.

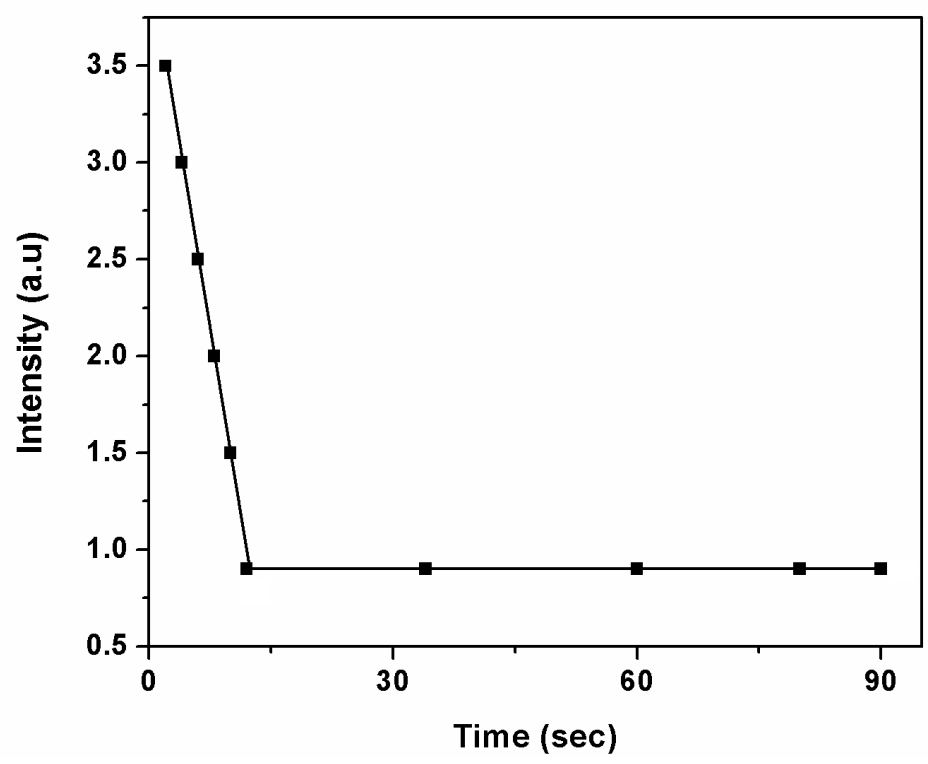

Figure S7. Fluorometric response time of the sensor **4** towards L-Arginine.

Table S3

Life time of sensors with and without analyte showing static quenching.

Compounds	Average Lifetime (ns)
Sensor **1**	1.40
Sensor **1 + L-Ar**	1.52
Sensor **2**	0.95
Sensor **2 + L-Ar**	0.91
Sensor **3**	0.62
Sensor **3 + L-Ar**	0.68
Sensor **4**	1.25
Sensor **4 + L-Ar**	1.49

Table S3

K_{SV} values as obtained from Stern-Volmer plots and quantum yield measurements against standard quinine sulphate for **1**-**4**.

Sensor	**1**	**2**	**3**	**4**
$K_{SV}(10^4)$	11.43	6.42	6.89	13.85
Φ	0.107	0.274	0.110	0.386

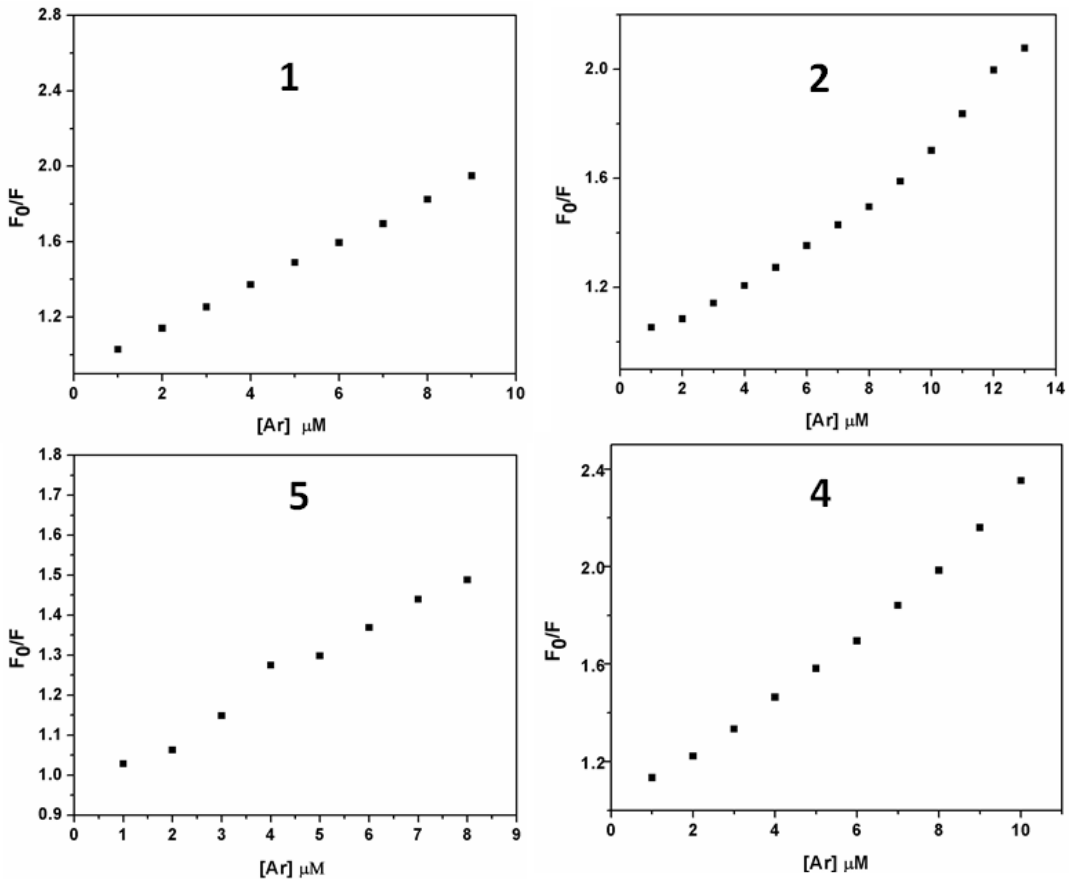

Figure S8. Stern-Volmer plots for sensors **1** to **4**.

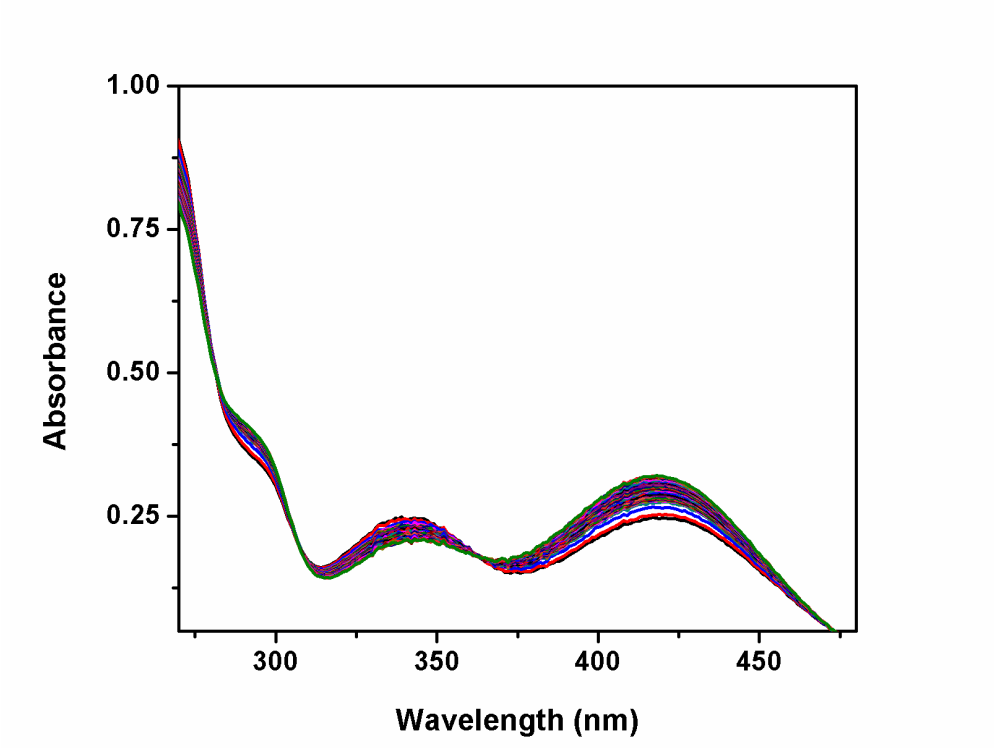

Figure S9. Absorption titration of **1** with guanidine.

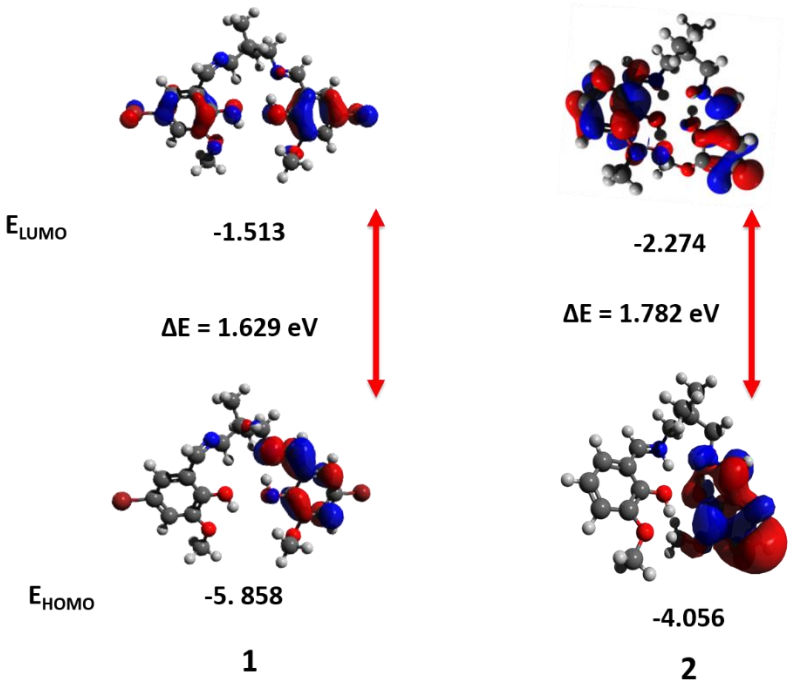

Figure S10. HOMO-LUMO plots of DFT optimized structures of **1** and **2** with the associated energy gaps.

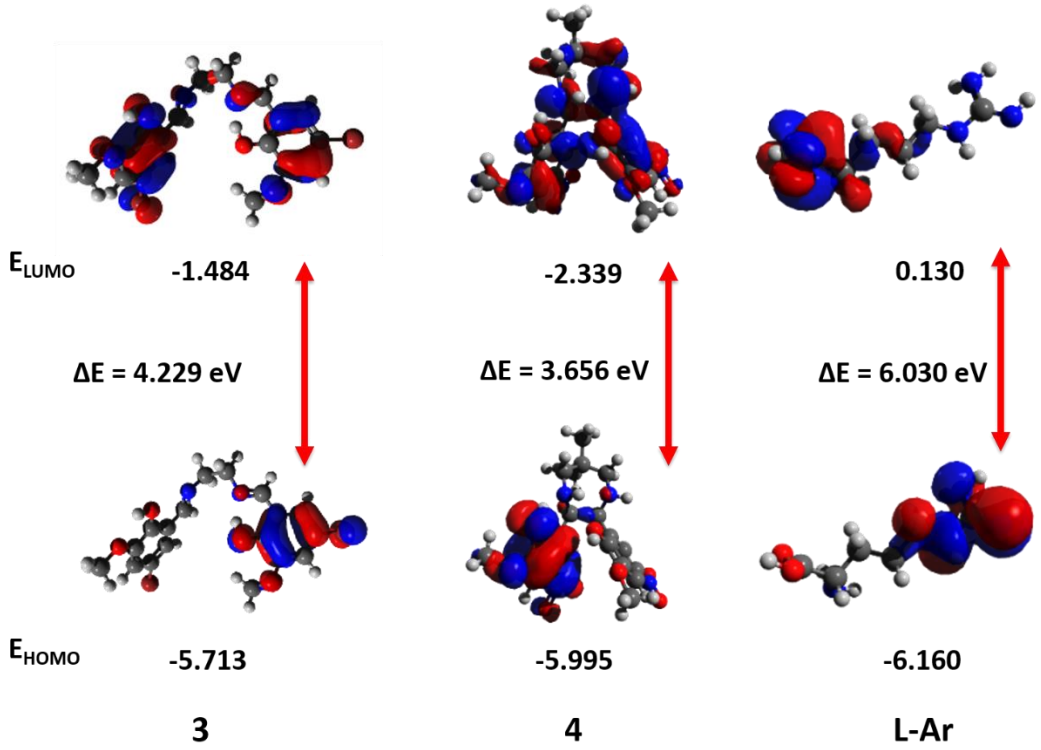

Figure S11. HOMO-LUMO plots of DFT optimized structures of **3, 4** and **L-Ar** with the associated energy gaps.

Frontier orbital compositional analysis

Frontier orbital calculations were performed using Mulliken method as employed in multiwfn program version 3.3.9.[1] In the case of **1**, HOMO is on one of the benzene rings 73.15% with a little contribution from the azomethine group of the same side (19.13%). But the LUMO is evenly distributed among the two sides with phenolic groups having the highest contribution of about 86.65%. For **2**, HOMO is on the benzene ring of one side with a contribution of about 79.37% and on the methoxy oxygen group (15.44%). In the case of **3**, the trend is similar with the HOMO being concentrated on one of the benzene ring (75.68%) and azomethine nitrogen atom (19.15%) and the LUMO on phenolic moieties (82.27%) on either side with a slight contribution form bromine atoms (9.19%). In **4**, HOMO is mainly concentrated on of the benzene rings with a cumulative contribution of about 88.96% and there is some share from the oxygen atoms of the nitro group (7.21%) while LUMO is concentrated on phenolic moieties on either side with a total contribution of about 76.58%. In the case of L-Arginine, the HOMO is concentrated on the nitrogen atoms of the amine side with a cumulative contribution of about 85.51% and the LUMO is on the acidic part oxygen atoms with a total of about 79.10%.

Reference

1. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.