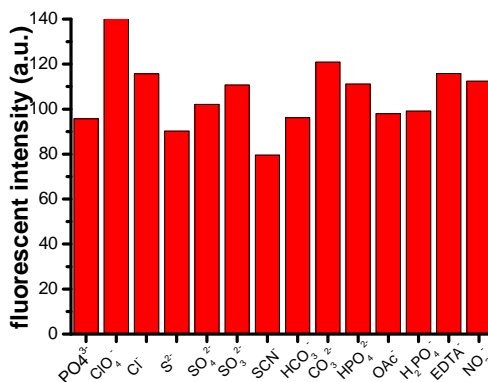


## Electronic Supplementary Information For

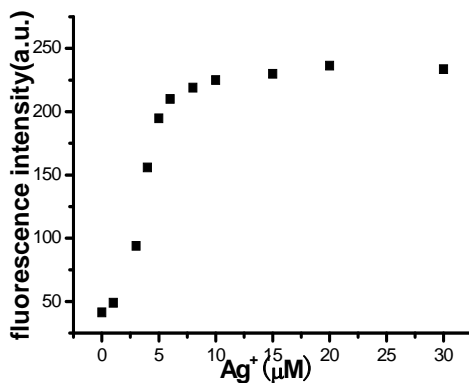
# Enhanced fluorescent chemosensor for $\text{Ag}^+$ in absolute aqueous solution and living cells: an experimental and theoretical study

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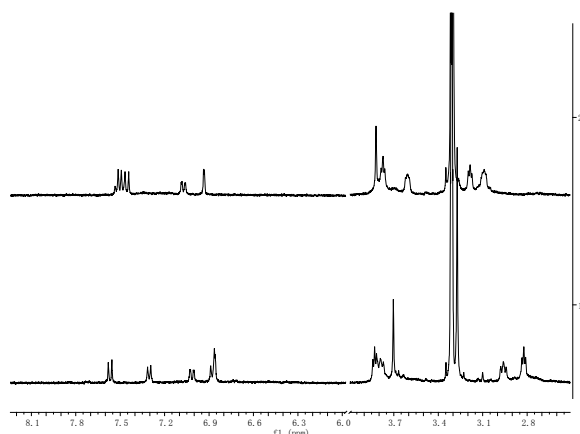
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Fax: +86-411-8498-6327; Tel: +86-411-8498-6306; E-mail [fanjl@dlut.edu.cn](mailto:fanjl@dlut.edu.cn); [pengxj@dlut.edu.cn](mailto:pengxj@dlut.edu.cn)



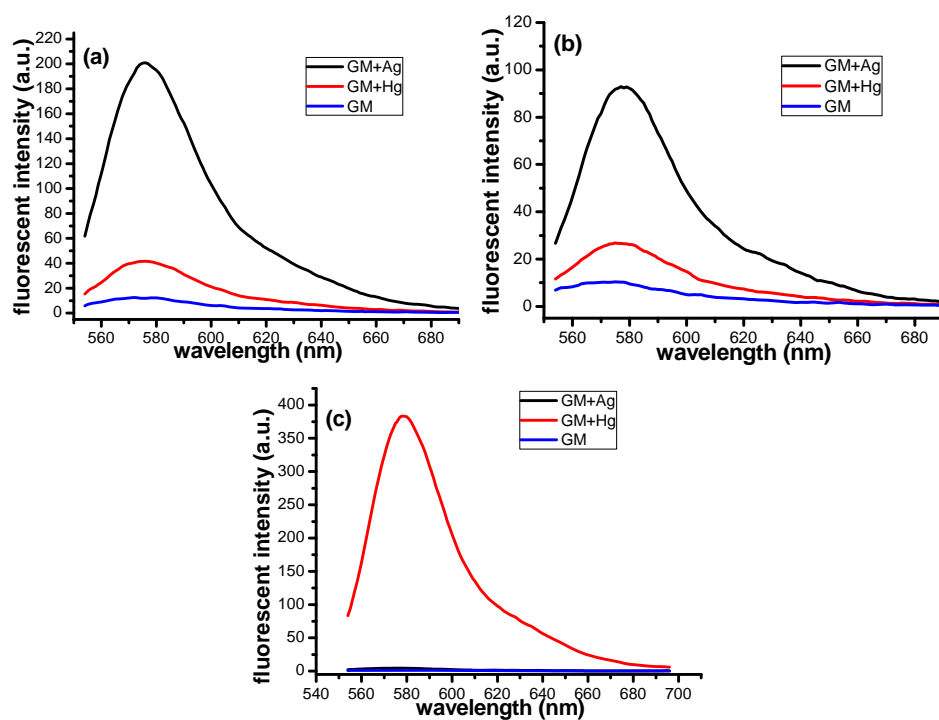
**Fig.S1** The fluorescence intensity at 578 nm of **RC-1**+ $\text{Ag}^+$  in the presence of different anions in HEPES buffer (20 mM HEPES, 100 mM  $\text{NaNO}_3$ , pH 7.4) solution. Excited: 545 nm



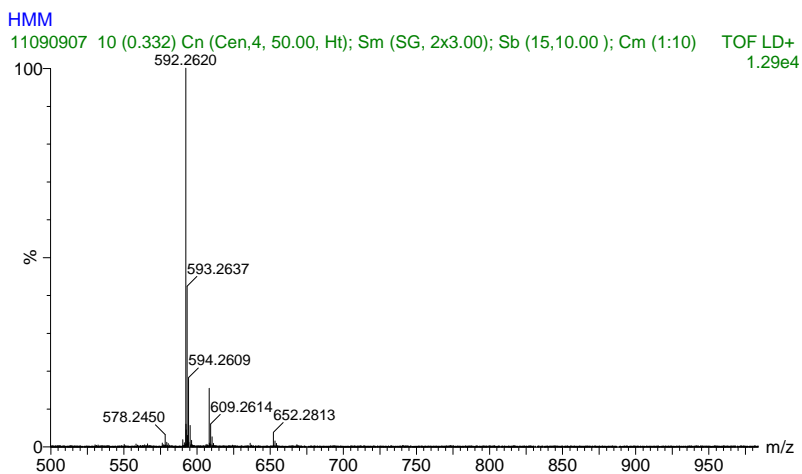
**Fig.S2** Fluorescence intensity profile of **RC-1** (5  $\mu\text{M}$ ) upon addition of  $\text{Ag}^+$  (1-30  $\mu\text{M}$ ). The intensity was taken at the peak height at 578 nm in HEPES buffer (20 mM HEPES, 100 mM  $\text{NaNO}_3$ , pH 7.4) solution. Excitation: 545 nm



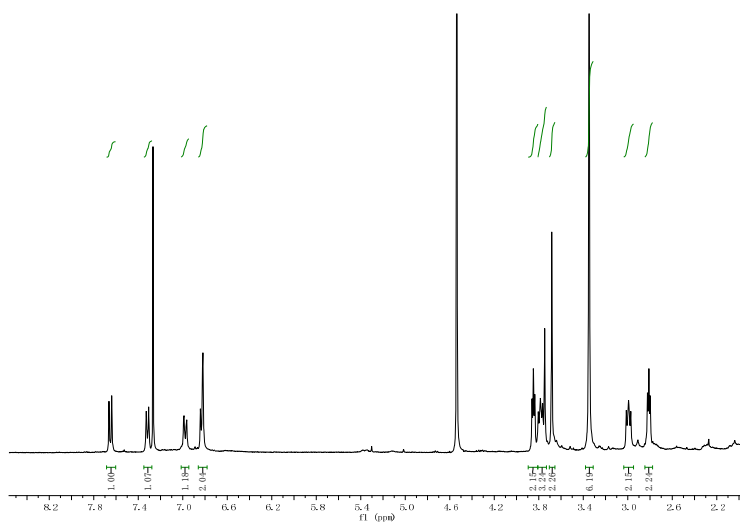
**Fig.S3.** Partial <sup>1</sup>H NMR (400 MHz) spectral changes of **RC-1** (10 mM) in CD<sub>3</sub>OD-D<sub>2</sub>O (1:1) upon addition of 1 equiv AgNO<sub>3</sub> at 298 K. Up: **RC-1**+Ag<sup>+</sup>; Below: **RC-1**



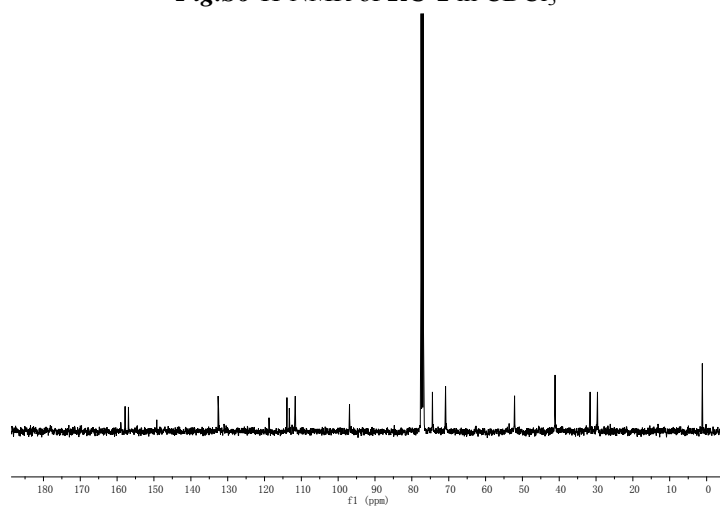
**Fig.S4** Fluorescence response of **RC-1** (5 μM) to Ag<sup>+</sup> (20 μM) and Hg<sup>2+</sup> (20 μM) in (a) HEPES buffer (20 mM HEPES, 100 mM NaNO<sub>3</sub>, pH 7.4) solution; (b) acetonitrile: HEPES = 1:1 buffer (20 mM HEPES, 100 mM NaNO<sub>3</sub>, pH 7.4) solution; (c) acetonitrile. Excitation: 545 nm.



**Fig.S5** TOF-MS of  $[RC-1]^+$  Calc. 592.2668; found 592.2620.



**Fig.S6**  $^1H$ -NMR of RC-1 in  $CDCl_3$



**Fig.S7.**  $^{13}C$ -NMR of RC-1 in  $CDCl_3$

DFT calculation of compound **RC-1**, **RC-1-Ag<sup>+</sup>**, **RC-1-Hg<sup>2+</sup>** in water and acetonitrile, respectively.

Compound **RC-1** in water (DFT B3LYP 6-31G(d))

E(RB3LYP) -2469.009 a.u.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.09496100  | 4.06748400  | 0.40023100  |
| C | 2.69867200  | 3.76115600  | 0.26738900  |
| C | 2.27003500  | 2.47605300  | 0.06983200  |
| C | 3.17487400  | 1.37770700  | -0.02785200 |
| C | 4.55003700  | 1.70028000  | 0.16087100  |
| C | 5.00932100  | 2.98753500  | 0.36012000  |
| C | 2.79137000  | 0.02526600  | -0.23326600 |
| C | 3.81060000  | -0.96453500 | -0.23083800 |
| C | 5.16530100  | -0.58184000 | -0.00983900 |
| O | 5.49967500  | 0.72507500  | 0.17235900  |
| C | 3.60187900  | -2.34992600 | -0.49774200 |
| C | 4.62443300  | -3.26005600 | -0.47994900 |
| C | 5.97368300  | -2.85753900 | -0.19969500 |
| C | 6.21486300  | -1.47928500 | 0.01606000  |
| N | 4.51731200  | 5.34387200  | 0.57803500  |
| N | 6.98130900  | -3.76463500 | -0.16334500 |
| C | 8.35315200  | -3.32798300 | 0.09066500  |
| C | 6.72263600  | -5.18301200 | -0.41442900 |
| C | 5.93995200  | 5.62885600  | 0.75809400  |
| C | 3.56045100  | 6.45018200  | 0.62430700  |
| C | 1.37882100  | -0.33953500 | -0.44010400 |
| C | 0.59935000  | 0.27032600  | -1.44004200 |
| C | -0.72822700 | -0.07716200 | -1.64590800 |
| C | -1.37762900 | -1.03512200 | -0.82623500 |
| C | -0.58753500 | -1.64356000 | 0.18284300  |
| C | 0.74724800  | -1.31538300 | 0.35566300  |
| S | -5.87891200 | 0.24323000  | -3.16149600 |
| C | -5.94931100 | 1.93197600  | -2.43293800 |
| C | -6.92292700 | 2.10303400  | -1.27566500 |
| O | -6.36609100 | 1.52083600  | -0.10296800 |
| C | -7.29053100 | 1.45044300  | 0.97328600  |
| C | -6.56832500 | 1.07318100  | 2.24863200  |
| O | -6.07438600 | -0.25808000 | 2.17219100  |
| C | -5.50217100 | -0.67091200 | 3.40531900  |
| C | -4.90721600 | -2.06452300 | 3.28220000  |
| S | -3.41741400 | -2.18166900 | 2.20637700  |
| C | -4.19216300 | -2.69101600 | 0.61249400  |
| C | -3.21424100 | -2.67375100 | -0.57191400 |
| N | -2.72013100 | -1.35415500 | -0.98852700 |
| C | -3.47926300 | -0.66211200 | -2.04311100 |
| C | -5.00000300 | -0.72552800 | -1.86545900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.96290700  | 4.55037300  | 0.34167900  |
| H | 1.20709200  | 2.28413400  | -0.00163700 |
| H | 6.07253300  | 3.13204400  | 0.49040900  |
| H | 2.60206700  | -2.68995700 | -0.73555500 |
| H | 4.40389100  | -4.29614800 | -0.69775300 |
| H | 7.20831200  | -1.09180200 | 0.19286000  |
| H | 9.00748700  | -4.19737700 | 0.10091000  |
| H | 8.43388900  | -2.82545300 | 1.06061500  |
| H | 8.70384300  | -2.64140500 | -0.68825000 |
| H | 7.65236900  | -5.73589200 | -0.29529000 |
| H | 6.35206600  | -5.35067900 | -1.43176800 |
| H | 5.99345000  | -5.58554000 | 0.29591000  |
| H | 6.07404300  | 6.70059300  | 0.89056700  |
| H | 6.52050500  | 5.31450300  | -0.11626300 |
| H | 6.33861000  | 5.12019500  | 1.64297500  |
| H | 4.10951500  | 7.38661000  | 0.70194700  |
| H | 2.89322600  | 6.37028200  | 1.48976600  |
| H | 2.95309000  | 6.48635200  | -0.28546400 |
| H | 1.05442100  | 0.99690700  | -2.10576000 |
| H | -1.24825000 | 0.38817300  | -2.47179800 |
| H | -1.02372400 | -2.36260500 | 0.86356500  |
| H | 1.30009500  | -1.79338800 | 1.15809700  |
| H | -6.26325100 | 2.56977500  | -3.26406100 |
| H | -4.94666700 | 2.25063100  | -2.13376400 |
| H | -7.88917500 | 1.63871700  | -1.52067700 |
| H | -7.10202300 | 3.17836300  | -1.10846400 |
| H | -8.08301600 | 0.71875300  | 0.75422300  |
| H | -7.77106000 | 2.42832500  | 1.13171100  |
| H | -7.27679600 | 1.17011100  | 3.08639000  |
| H | -5.74184600 | 1.77809900  | 2.42781100  |
| H | -6.27635900 | -0.68794500 | 4.19121500  |
| H | -4.72606400 | 0.04093600  | 3.72543000  |
| H | -5.65403200 | -2.77756300 | 2.92186500  |
| H | -4.58925800 | -2.39415700 | 4.27501300  |
| H | -5.03945400 | -2.02958600 | 0.43684800  |
| H | -4.56834200 | -3.71316100 | 0.72361700  |
| H | -3.73310900 | -3.13220900 | -1.42251500 |
| H | -2.36488200 | -3.32764000 | -0.36445300 |
| H | -3.21502700 | -1.05439300 | -3.03754000 |
| H | -3.19163100 | 0.39050700  | -2.02263300 |
| H | -5.38270200 | -1.74228500 | -1.97400400 |
| H | -5.31112100 | -0.33258700 | -0.89778500 |

Compound **RC-1-Ag<sup>+</sup>** in water (DFT B3LYP 6-31G(d))  
E(RB3LYP) -1838.163 a.u.

|   |            |            |             |
|---|------------|------------|-------------|
| C | 4.90038100 | 3.99561900 | -0.37467600 |
| C | 3.49514500 | 3.77856600 | -0.10214500 |
| C | 2.99043500 | 2.50843500 | 0.08099100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.82163000  | 1.34048000  | 0.00985900  |
| C | 5.21544600  | 1.58575800  | -0.23637800 |
| C | 5.75163000  | 2.84899200  | -0.42670500 |
| C | 3.35818800  | 0.00786900  | 0.19858800  |
| C | 4.29458900  | -1.06275500 | 0.14373200  |
| C | 5.68429000  | -0.78705000 | -0.09326300 |
| O | 6.11513300  | 0.52386200  | -0.28047700 |
| C | 3.95224200  | -2.45044600 | 0.27562300  |
| C | 4.90140500  | -3.44832300 | 0.20577900  |
| C | 6.29984100  | -3.14051400 | -0.00748000 |
| C | 6.66103600  | -1.76695800 | -0.16488400 |
| N | 5.39397700  | 5.25605500  | -0.56452100 |
| N | 7.23817800  | -4.13272400 | -0.06640000 |
| C | 8.66046200  | -3.80268700 | -0.29025100 |
| C | 6.85213900  | -5.55220300 | 0.08292800  |
| C | 6.83243000  | 5.46260300  | -0.82892200 |
| C | 4.50635900  | 6.43674700  | -0.49812100 |
| C | 1.91209600  | -0.26339000 | 0.44999500  |
| C | 0.94105300  | 0.02126800  | -0.53779600 |
| C | -0.41584400 | -0.23329300 | -0.29749700 |
| C | -0.84715800 | -0.76178200 | 0.93798800  |
| C | 0.12057700  | -1.05610300 | 1.92197200  |
| C | 1.48279200  | -0.80977100 | 1.67795000  |
| S | -4.47669900 | -3.72427700 | -1.22856100 |
| C | -4.21836300 | -2.51359900 | -2.67095800 |
| C | -5.36205800 | -1.53391900 | -2.91851000 |
| O | -5.24999700 | -0.36856500 | -2.01827200 |
| C | -6.42387000 | 0.51670400  | -2.10186600 |
| C | -5.99751000 | 1.94652100  | -1.78739700 |
| O | -5.40218000 | 2.07316700  | -0.44753300 |
| C | -6.30148300 | 2.38694800  | 0.67877500  |
| C | -6.18147100 | 1.35946600  | 1.80830300  |
| S | -4.40659200 | 1.31214200  | 2.51774800  |
| C | -4.14953200 | -0.54959800 | 2.86530300  |
| C | -2.69899000 | -0.98072000 | 2.58182600  |
| N | -2.28268500 | -1.03425500 | 1.13337300  |
| C | -2.62635300 | -2.35458700 | 0.45585300  |
| C | -4.13394800 | -2.58312700 | 0.24812400  |
| H | 2.82292900  | 4.62443900  | -0.03184300 |
| H | 1.93472300  | 2.38732000  | 0.29710200  |
| H | 6.81538600  | 2.93437100  | -0.60565100 |
| H | 2.91289300  | -2.72144400 | 0.42420700  |
| H | 4.58605100  | -4.47908600 | 0.30680000  |
| H | 7.68304200  | -1.46230600 | -0.34752500 |
| H | 9.24896200  | -4.72074100 | -0.28045100 |
| H | 9.04199300  | -3.14203300 | 0.49871400  |
| H | 8.80599200  | -3.31047400 | -1.26067300 |
| H | 7.74514800  | -6.17354100 | 0.00665400  |
| H | 6.15321300  | -5.86045600 | -0.70453700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.38845600  | -5.73802800 | 1.05960100  |
| H  | 7.02457200  | 6.52785500  | -0.96162200 |
| H  | 7.14542400  | 4.94052600  | -1.74215000 |
| H  | 7.44533400  | 5.10417400  | 0.00825500  |
| H  | 5.09286200  | 7.33413000  | -0.69829000 |
| H  | 4.05200700  | 6.53940000  | 0.49533500  |
| H  | 3.70787400  | 6.37621200  | -1.24764300 |
| H  | 1.24472700  | 0.43106300  | -1.49681400 |
| H  | -1.14083000 | -0.01322900 | -1.07889400 |
| H  | -0.16453700 | -1.48379400 | 2.87683600  |
| H  | 2.20869000  | -1.03476200 | 2.45438200  |
| H  | -4.10674800 | -3.16524400 | -3.54337700 |
| H  | -3.27537500 | -1.97758800 | -2.52443800 |
| H  | -6.33413900 | -2.02286500 | -2.76620600 |
| H  | -5.31093400 | -1.16896400 | -3.95626000 |
| H  | -7.19508900 | 0.15652200  | -1.40727100 |
| H  | -6.83478500 | 0.50069300  | -3.12190200 |
| H  | -6.85440000 | 2.62495400  | -1.88188700 |
| H  | -5.21190600 | 2.26391500  | -2.47987400 |
| H  | -7.34017200 | 2.39678500  | 0.32507800  |
| H  | -6.04309900 | 3.39243700  | 1.03040500  |
| H  | -6.42265100 | 0.35370800  | 1.45458000  |
| H  | -6.86082600 | 1.63071800  | 2.62065300  |
| H  | -4.88505700 | -1.09937700 | 2.27773500  |
| H  | -4.35538400 | -0.71311600 | 3.92608300  |
| H  | -2.55419900 | -1.96895400 | 3.04598200  |
| H  | -2.03405200 | -0.28168200 | 3.09697000  |
| H  | -2.19500100 | -3.18504100 | 1.03583700  |
| H  | -2.12324000 | -2.33652800 | -0.51400500 |
| H  | -4.60517700 | -3.07659100 | 1.10151600  |
| H  | -4.65809700 | -1.65007700 | 0.03352000  |
| Ag | -3.51568900 | 0.66252600  | -0.11955900 |

Compound **RC-1-Hg<sup>2+</sup>** in water (DFT B3LYP 6-31G(d))  
E(RB3LYP) -1735.017 a.u.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.47735200 | -3.03024900 | -0.18834400 |
| C | -5.18781600 | -3.40598800 | 0.34706100  |
| C | -4.20623600 | -2.46341100 | 0.57857900  |
| C | -4.39755100 | -1.06918900 | 0.29565900  |
| C | -5.71029800 | -0.71910900 | -0.16801900 |
| C | -6.71634800 | -1.64134000 | -0.41375000 |
| C | -3.40825000 | -0.05161600 | 0.48414200  |
| C | -3.77673600 | 1.30745900  | 0.21630100  |
| C | -5.12028700 | 1.62796200  | -0.17270100 |
| O | -6.05390800 | 0.61485600  | -0.37167200 |
| C | -2.87838300 | 2.42641500  | 0.26500800  |
| C | -3.29737600 | 3.72232800  | 0.04192000  |
| C | -4.67841600 | 4.02171300  | -0.26243100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.57569500 | 2.91936100  | -0.39473500 |
| N | -7.43742600 | -3.96987700 | -0.44829900 |
| N | -5.10064000 | 5.31158400  | -0.43693300 |
| C | -6.51213300 | 5.59568800  | -0.76369300 |
| C | -4.15747100 | 6.44178200  | -0.30431600 |
| C | -8.75944800 | -3.56097700 | -0.96298000 |
| C | -7.17715100 | -5.40471800 | -0.20913100 |
| C | -2.04183400 | -0.37698400 | 0.95318400  |
| C | -1.25617800 | -1.39388400 | 0.34841600  |
| C | 0.05412900  | -1.65121500 | 0.76461500  |
| C | 0.65587300  | -0.90277700 | 1.81838100  |
| C | -0.15155000 | 0.08099700  | 2.45887100  |
| C | -1.45543500 | 0.33933400  | 2.02772300  |
| S | 4.75469700  | 1.94453700  | 2.78270800  |
| C | 4.05796400  | 2.79298400  | 1.22831500  |
| C | 4.99337000  | 2.78719000  | 0.02300500  |
| O | 4.92983400  | 1.48088900  | -0.65992900 |
| C | 6.08102100  | 1.18636300  | -1.52776700 |
| C | 5.59109500  | 0.44206100  | -2.76681000 |
| O | 4.80510400  | -0.75376400 | -2.42829500 |
| C | 5.52320400  | -2.02040500 | -2.21228500 |
| C | 5.41801400  | -2.50415700 | -0.76505400 |
| S | 3.59900500  | -2.84116700 | -0.29853000 |
| C | 3.75970000  | -2.92637200 | 1.59686000  |
| C | 2.48069500  | -2.51318900 | 2.35156600  |
| N | 2.00111500  | -1.12178800 | 2.19280900  |
| C | 2.70755700  | -0.05826800 | 2.94769400  |
| C | 4.17781900  | 0.15350100  | 2.50860700  |
| H | -4.98442900 | -4.44225900 | 0.58652200  |
| H | -3.26554700 | -2.78857300 | 1.00637000  |
| H | -7.67146100 | -1.27468200 | -0.76645100 |
| H | -1.82891800 | 2.24918800  | 0.46638300  |
| H | -2.56887800 | 4.52210300  | 0.08834600  |
| H | -6.61209700 | 3.05627700  | -0.67431100 |
| H | -6.65521500 | 6.67456500  | -0.83518300 |
| H | -7.18332400 | 5.21143200  | 0.01520200  |
| H | -6.79687600 | 5.14641400  | -1.72411300 |
| H | -4.70093000 | 7.37730300  | -0.44317800 |
| H | -3.36327600 | 6.39241700  | -1.06018000 |
| H | -3.69612700 | 6.45958400  | 0.69089400  |
| H | -9.37714100 | -4.44692000 | -1.11485500 |
| H | -8.66603000 | -3.03868700 | -1.92392100 |
| H | -9.27531100 | -2.90011300 | -0.25409500 |
| H | -8.04307200 | -5.98297800 | -0.53411400 |
| H | -7.00787500 | -5.60978600 | 0.85579500  |
| H | -6.30452700 | -5.74930200 | -0.77744300 |
| H | -1.64926900 | -1.94907100 | -0.49856200 |
| H | 0.63145000  | -2.40230700 | 0.23485300  |
| H | 0.22238000  | 0.62612900  | 3.31784700  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.04365000 | 1.07779000  | 2.56487700  |
| H  | 3.87074600  | 3.82646900  | 1.53536100  |
| H  | 3.09659700  | 2.33297000  | 0.97357800  |
| H  | 6.02679100  | 2.98249800  | 0.33574000  |
| H  | 4.68624400  | 3.56568600  | -0.69126600 |
| H  | 6.80650400  | 0.59647500  | -0.95310700 |
| H  | 6.56181100  | 2.11841900  | -1.85379900 |
| H  | 6.44187600  | 0.16419200  | -3.40159300 |
| H  | 4.90746700  | 1.07479800  | -3.34034400 |
| H  | 6.58269500  | -1.88968400 | -2.46642200 |
| H  | 5.08756900  | -2.75075400 | -2.90280200 |
| H  | 5.80951300  | -1.76184000 | -0.06503100 |
| H  | 5.96715200  | -3.44276900 | -0.64980900 |
| H  | 4.61823700  | -2.31404100 | 1.87235900  |
| H  | 3.98334800  | -3.96906400 | 1.84074800  |
| H  | 2.69475200  | -2.69094800 | 3.41938700  |
| H  | 1.66807100  | -3.19512900 | 2.08637800  |
| H  | 2.67602700  | -0.25153000 | 4.03236400  |
| H  | 2.17296900  | 0.87611700  | 2.76996600  |
| H  | 4.87950400  | -0.45294500 | 3.08684300  |
| H  | 4.31480200  | -0.04738300 | 1.44699000  |
| Hg | 2.66609500  | -0.02271300 | -1.10475400 |

Compound **RC-1** in acetonitrile (DFT B3LYP 6-31G(d))  
E(RB3LYP) -2469.008 a.u.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.09517800  | 4.06761500  | 0.40024300  |
| C | 2.69894400  | 3.76079600  | 0.26850700  |
| C | 2.27060200  | 2.47555600  | 0.07107900  |
| C | 3.17575200  | 1.37758100  | -0.02753800 |
| C | 4.55085400  | 1.70054900  | 0.16063400  |
| C | 5.00982000  | 2.98798700  | 0.35967700  |
| C | 2.79243100  | 0.02497500  | -0.23288600 |
| C | 3.81212100  | -0.96451900 | -0.23049500 |
| C | 5.16671800  | -0.58135900 | -0.01001200 |
| O | 5.50082900  | 0.72567000  | 0.17186000  |
| C | 3.60385100  | -2.34989500 | -0.49754900 |
| C | 4.62675000  | -3.25968900 | -0.48016800 |
| C | 5.97590300  | -2.85675300 | -0.20034300 |
| C | 6.21662800  | -1.47847400 | 0.01542600  |
| N | 4.51726400  | 5.34426300  | 0.57752300  |
| N | 6.98397100  | -3.76353700 | -0.16452000 |
| C | 8.35573100  | -3.32633700 | 0.08870600  |
| C | 6.72581000  | -5.18188500 | -0.41610300 |
| C | 5.93999400  | 5.62987000  | 0.75563100  |
| C | 3.55993600  | 6.45005200  | 0.62529100  |
| C | 1.38017500  | -0.33998600 | -0.43979200 |
| C | 0.60034600  | 0.27087600  | -1.43894600 |
| C | -0.72713100 | -0.07646400 | -1.64490600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.37654800 | -1.03506500 | -0.82579100 |
| C | -0.58610100 | -1.64453000 | 0.18251600  |
| C | 0.74870600  | -1.31673100 | 0.35509700  |
| S | -5.87728600 | 0.24118700  | -3.16390200 |
| C | -5.95844400 | 1.92912900  | -2.43474500 |
| C | -6.93482800 | 2.09421000  | -1.27890300 |
| O | -6.37570300 | 1.51562100  | -0.10566500 |
| C | -7.30014700 | 1.44030700  | 0.97005100  |
| C | -6.57609500 | 1.06881700  | 2.24604200  |
| O | -6.07602800 | -0.26018000 | 2.17245000  |
| C | -5.49983300 | -0.66636800 | 3.40586200  |
| C | -4.90134100 | -2.05891900 | 3.28756200  |
| S | -3.41314800 | -2.17761300 | 2.21003700  |
| C | -4.19160700 | -2.68391000 | 0.61710900  |
| C | -3.21502800 | -2.67122300 | -0.56846300 |
| N | -2.71864900 | -1.35372200 | -0.98845900 |
| C | -3.47812900 | -0.66081100 | -2.04229700 |
| C | -4.99891500 | -0.72453300 | -1.86517200 |
| H | 1.96290100  | 4.54968900  | 0.34359900  |
| H | 1.20767300  | 2.28317000  | 0.00067600  |
| H | 6.07302000  | 3.13276400  | 0.48972600  |
| H | 2.60409200  | -2.69016000 | -0.73525900 |
| H | 4.40650100  | -4.29579800 | -0.69819300 |
| H | 7.20998100  | -1.09053700 | 0.19174800  |
| H | 9.01041800  | -4.19547500 | 0.09887200  |
| H | 8.43683700  | -2.82363300 | 1.05854900  |
| H | 8.70588500  | -2.63980700 | -0.69051900 |
| H | 7.65577700  | -5.73450600 | -0.29741300 |
| H | 6.35511000  | -5.34938100 | -1.43344300 |
| H | 5.99695900  | -5.58504400 | 0.29424200  |
| H | 6.07399700  | 6.70184700  | 0.88639000  |
| H | 6.51963200  | 5.31449500  | -0.11897900 |
| H | 6.33991600  | 5.12260600  | 1.64077900  |
| H | 4.10855400  | 7.38670800  | 0.70333000  |
| H | 2.89334300  | 6.36923100  | 1.49115800  |
| H | 2.95191300  | 6.48673000  | -0.28404800 |
| H | 1.05534200  | 0.99801500  | -2.10412600 |
| H | -1.24736500 | 0.38945600  | -2.47032400 |
| H | -1.02231400 | -2.36357500 | 0.86318200  |
| H | 1.30165500  | -1.79534700 | 1.15710500  |
| H | -6.27478200 | 2.56523100  | -3.26628600 |
| H | -4.95825300 | 2.25364600  | -2.13367100 |
| H | -7.89781900 | 1.62385500  | -1.52528100 |
| H | -7.12085600 | 3.16846900  | -1.11196500 |
| H | -8.08798200 | 0.70348600  | 0.75139600  |
| H | -7.78682800 | 2.41536800  | 1.12739400  |
| H | -7.28494500 | 1.16409400  | 3.08376100  |
| H | -5.75293700 | 1.77801600  | 2.42357500  |
| H | -6.27229500 | -0.68228200 | 4.19357500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.72496800 | 0.04893600  | 3.72121400  |
| H | -5.64716200 | -2.77551300 | 2.93216000  |
| H | -4.58046000 | -2.38324800 | 4.28122400  |
| H | -5.03620000 | -2.01885100 | 0.44234400  |
| H | -4.57194800 | -3.70448200 | 0.72901800  |
| H | -3.73584900 | -3.13016000 | -1.41760900 |
| H | -2.36681300 | -3.32659100 | -0.36084600 |
| H | -3.21352200 | -1.05216200 | -3.03700700 |
| H | -3.19081900 | 0.39187700  | -2.02087500 |
| H | -5.38118600 | -1.74165000 | -1.97177700 |
| H | -5.31075100 | -0.32980900 | -0.89845800 |

Compound **RC-1-Ag<sup>+</sup>** in acetonitrile (DFT B3LYP 6-31G(d))  
E(RB3LYP) -1838.159 a.u.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.24367400  | 3.86895600  | -0.36340100 |
| C | 3.82795400  | 3.76525900  | -0.07799400 |
| C | 3.22268500  | 2.53939000  | 0.10110800  |
| C | 3.95512800  | 1.30812900  | 0.01223700  |
| C | 5.36166800  | 1.44033600  | -0.24952000 |
| C | 5.99745600  | 2.65692500  | -0.43605000 |
| C | 3.38733000  | 0.01664300  | 0.19655900  |
| C | 4.23055000  | -1.12682700 | 0.11943700  |
| C | 5.63542300  | -0.96463900 | -0.13354400 |
| O | 6.17011600  | 0.30831300  | -0.31438200 |
| C | 3.77551300  | -2.48231400 | 0.24497500  |
| C | 4.63752400  | -3.55455700 | 0.15471600  |
| C | 6.05427300  | -3.36168200 | -0.07320000 |
| C | 6.52672300  | -2.02132700 | -0.22463900 |
| N | 5.83749600  | 5.08640300  | -0.54592600 |
| N | 6.90549100  | -4.42820400 | -0.14979200 |
| C | 8.34686900  | -4.21690800 | -0.39383900 |
| C | 6.40448900  | -5.81134300 | 0.00040900  |
| C | 7.28571100  | 5.17592200  | -0.82230700 |
| C | 5.05075100  | 6.33527600  | -0.45876800 |
| C | 1.92775300  | -0.13773300 | 0.47314900  |
| C | 0.96713000  | 0.21622400  | -0.49976700 |
| C | -0.40364700 | 0.06596700  | -0.23565200 |
| C | -0.84823200 | -0.42415100 | 1.00620500  |
| C | 0.10941200  | -0.77882100 | 1.98127000  |
| C | 1.48094300  | -0.63960200 | 1.71567200  |
| S | -4.55466900 | -3.85656300 | -0.17229500 |
| C | -4.37648200 | -3.11612200 | -1.91361600 |
| C | -5.52718200 | -2.22371100 | -2.37020800 |
| O | -5.36020300 | -0.85062000 | -1.85021600 |
| C | -6.53744300 | -0.00694400 | -2.11949100 |
| C | -6.09561800 | 1.44663500  | -2.24682700 |
| O | -5.43313400 | 1.93689600  | -1.02745500 |
| C | -6.25765800 | 2.62678700  | -0.01801100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.12317000 | 1.98109200  | 1.36370800  |
| S | -4.32797200 | 2.07785700  | 2.01377900  |
| C | -4.10449300 | 0.36948300  | 2.84117200  |
| C | -2.68013000 | -0.18092000 | 2.65047300  |
| N | -2.29480500 | -0.60924100 | 1.25033200  |
| C | -2.64678000 | -2.06013600 | 0.94499800  |
| C | -4.15889200 | -2.33708800 | 0.89233400  |
| H | 3.22833700  | 4.66286600  | 0.00519700  |
| H | 2.16266400  | 2.50346700  | 0.32701600  |
| H | 7.06228000  | 2.65673600  | -0.62817500 |
| H | 2.71909500  | -2.66755800 | 0.40471900  |
| H | 4.23909100  | -4.55663900 | 0.25028100  |
| H | 7.56865000  | -1.80047100 | -0.41595000 |
| H | 8.85305300  | -5.18244800 | -0.41855800 |
| H | 8.79826400  | -3.61222700 | 0.40315700  |
| H | 8.51719500  | -3.71479500 | -1.35491300 |
| H | 7.24496000  | -6.50328100 | -0.06473500 |
| H | 5.68977300  | -6.06530300 | -0.79252000 |
| H | 5.91888600  | -5.95442800 | 0.97343400  |
| H | 7.56677600  | 6.22334300  | -0.93728100 |
| H | 7.54518000  | 4.64676300  | -1.74823600 |
| H | 7.87318200  | 4.75077400  | 0.00167600  |
| H | 5.70773800  | 7.18394200  | -0.65209900 |
| H | 4.61270200  | 6.46194200  | 0.53924600  |
| H | 4.24536100  | 6.35079300  | -1.20320300 |
| H | 1.28634300  | 0.59682300  | -1.46580000 |
| H | -1.12371200 | 0.33941900  | -1.00375900 |
| H | -0.19930800 | -1.16497900 | 2.94767700  |
| H | 2.20148900  | -0.91033200 | 2.48230600  |
| H | -4.32271000 | -3.99392400 | -2.56545900 |
| H | -3.42198400 | -2.58477400 | -1.98263500 |
| H | -6.49139400 | -2.62823100 | -2.03298700 |
| H | -5.53258700 | -2.17208200 | -3.47014700 |
| H | -7.26826800 | -0.14226400 | -1.31046600 |
| H | -7.00371500 | -0.30597200 | -3.06953200 |
| H | -6.95711800 | 2.08209700  | -2.48656500 |
| H | -5.34788100 | 1.54333400  | -3.03998300 |
| H | -7.31132300 | 2.58665100  | -0.32147000 |
| H | -5.93893400 | 3.67526900  | 0.00149700  |
| H | -6.40482400 | 0.92557500  | 1.33205400  |
| H | -6.76584200 | 2.50679200  | 2.07482400  |
| H | -4.87577600 | -0.29125100 | 2.44359500  |
| H | -4.27740900 | 0.50271300  | 3.91219400  |
| H | -2.56774500 | -1.03092800 | 3.34130600  |
| H | -1.96835500 | 0.58686800  | 2.96835700  |
| H | -2.17055000 | -2.72126900 | 1.68513500  |
| H | -2.19684100 | -2.27743400 | -0.02790900 |
| H | -4.57862300 | -2.56192000 | 1.87581900  |
| H | -4.70832300 | -1.50701600 | 0.44393400  |

Ag                    -3.56707300    0.64498000    -0.37447200

Compound **RC-1-Hg<sup>2+</sup>** in acetonitrile (DFT B3LYP 6-31G(d))  
E(RB3LYP) -1734.995 a.u.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.92022500  | 3.73083100  | -0.03365200 |
| C | 4.50892300  | 3.67654600  | 0.28500400  |
| C | 3.84286400  | 2.47300100  | 0.37749800  |
| C | 4.50526500  | 1.21755400  | 0.16397200  |
| C | 5.90987500  | 1.29836900  | -0.12647300 |
| C | 6.60568900  | 2.49193200  | -0.22897800 |
| C | 3.87101700  | -0.05312000 | 0.25111500  |
| C | 4.64700700  | -1.22825100 | 0.05656400  |
| C | 6.05097500  | -1.11854100 | -0.22955400 |
| O | 6.65159200  | 0.13495700  | -0.31465800 |
| C | 4.12152600  | -2.56340400 | 0.08644300  |
| C | 4.91851700  | -3.66764000 | -0.12971800 |
| C | 6.33432200  | -3.52987100 | -0.40135000 |
| C | 6.87677200  | -2.20848800 | -0.44962600 |
| N | 6.57233400  | 4.92748100  | -0.13598100 |
| N | 7.12042900  | -4.62742700 | -0.61270400 |
| C | 8.56010200  | -4.46945500 | -0.90371600 |
| C | 6.54976200  | -5.99054700 | -0.56360300 |
| C | 8.01359900  | 4.96694400  | -0.45705500 |
| C | 5.85588200  | 6.20317300  | 0.07911400  |
| C | 2.40462100  | -0.13852300 | 0.52535400  |
| C | 1.47883100  | 0.33547300  | -0.42633600 |
| C | 0.09590400  | 0.29181200  | -0.17549800 |
| C | -0.40090900 | -0.21014400 | 1.04222400  |
| C | 0.53032000  | -0.68789000 | 1.99675800  |
| C | 1.90999400  | -0.66511400 | 1.73858700  |
| S | -4.46649900 | -3.43069300 | 1.72374500  |
| C | -4.48511200 | -3.33369600 | -0.17450700 |
| C | -5.72553800 | -2.70324800 | -0.80536000 |
| O | -5.60431100 | -1.22804900 | -0.88317200 |
| C | -6.88526000 | -0.52913600 | -1.10570900 |
| C | -6.65370800 | 0.65357200  | -2.04087400 |
| O | -5.60723900 | 1.55582800  | -1.53506600 |
| C | -6.01169600 | 2.76074000  | -0.79041300 |
| C | -5.56176400 | 2.72305600  | 0.67309900  |
| S | -3.65674300 | 2.65683200  | 0.80339000  |
| C | -3.42676600 | 1.63655300  | 2.39647900  |
| C | -2.07749800 | 0.89976400  | 2.41493300  |
| N | -1.85288800 | -0.17636600 | 1.37083000  |
| C | -2.30347500 | -1.56681800 | 1.79272400  |
| C | -3.79569500 | -1.70895600 | 2.17118500  |
| H | 3.96116900  | 4.59375800  | 0.46006300  |
| H | 2.78821500  | 2.47236400  | 0.62945900  |
| H | 7.66358500  | 2.45343000  | -0.45272000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.06281900  | -2.70494100 | 0.27485000  |
| H  | 4.46919100  | -4.65227800 | -0.10137100 |
| H  | 7.92237100  | -2.02719700 | -0.66108700 |
| H  | 9.01058300  | -5.45352600 | -1.03691200 |
| H  | 9.07727500  | -3.96347300 | -0.07849100 |
| H  | 8.71746400  | -3.89159600 | -1.82358200 |
| H  | 7.34516800  | -6.71590800 | -0.73807400 |
| H  | 5.78331200  | -6.12992100 | -1.33625400 |
| H  | 6.10547700  | -6.20004000 | 0.41716800  |
| H  | 8.34059300  | 6.00546800  | -0.51809400 |
| H  | 8.21669300  | 4.48613500  | -1.42241000 |
| H  | 8.60673300  | 4.46408300  | 0.31773400  |
| H  | 6.55537300  | 7.03008200  | -0.04845600 |
| H  | 5.44009900  | 6.26107700  | 1.09265800  |
| H  | 5.04127700  | 6.32908500  | -0.64485900 |
| H  | 1.83143900  | 0.73512200  | -1.37295600 |
| H  | -0.55992800 | 0.67424000  | -0.94659000 |
| H  | 0.19422900  | -1.06803000 | 2.95666900  |
| H  | 2.59924200  | -1.02738800 | 2.49615000  |
| H  | -4.42503000 | -4.37927300 | -0.49236100 |
| H  | -3.56803500 | -2.83529000 | -0.50758900 |
| H  | -6.62136400 | -2.95125000 | -0.22363900 |
| H  | -5.85097500 | -3.08007000 | -1.83038000 |
| H  | -7.27959200 | -0.21484200 | -0.13208500 |
| H  | -7.60161300 | -1.21224600 | -1.57949100 |
| H  | -7.59068200 | 1.20429100  | -2.18803100 |
| H  | -6.28984100 | 0.30122800  | -3.01097700 |
| H  | -7.10430700 | 2.85594300  | -0.81884100 |
| H  | -5.57343400 | 3.61696300  | -1.31414800 |
| H  | -5.96036100 | 1.84768600  | 1.19098000  |
| H  | -5.89498500 | 3.63053800  | 1.18288500  |
| H  | -4.28176900 | 0.96730000  | 2.49227400  |
| H  | -3.44005500 | 2.34210300  | 3.23117100  |
| H  | -1.96021900 | 0.46737200  | 3.42159700  |
| H  | -1.27956000 | 1.63913000  | 2.29604100  |
| H  | -1.70969900 | -1.92097800 | 2.64656700  |
| H  | -2.06465700 | -2.21537900 | 0.94472000  |
| H  | -3.94763300 | -1.62763000 | 3.25084500  |
| H  | -4.45896300 | -0.99736900 | 1.68432300  |
| Hg | -3.48505800 | 0.18483000  | -0.90855700 |