

# **Electronic Supplementary Information**

# Water oxidation by a soluble iron(III)-cyclen complex: New findings

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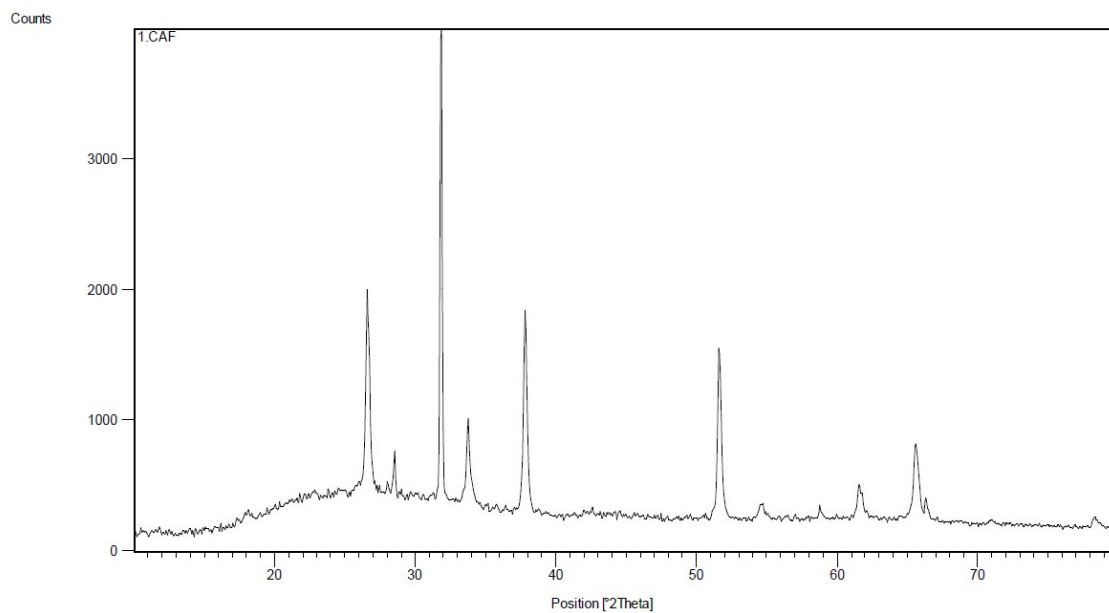
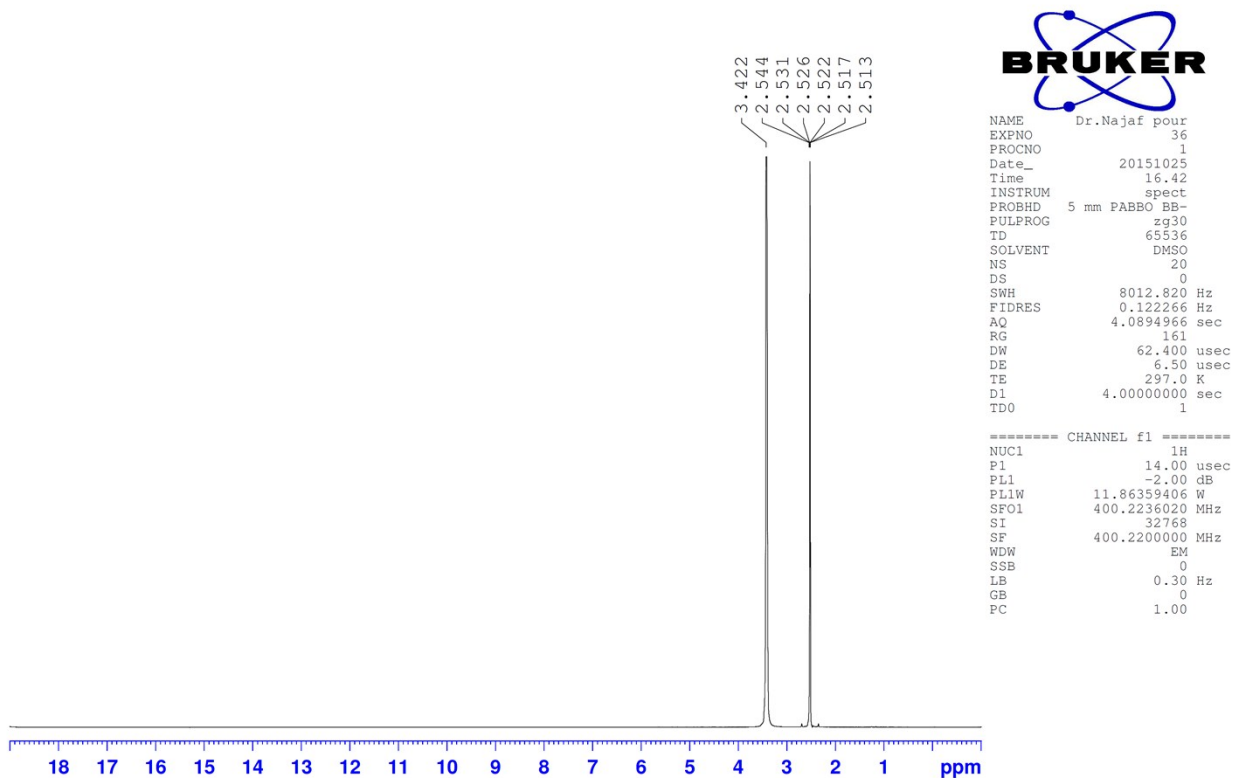
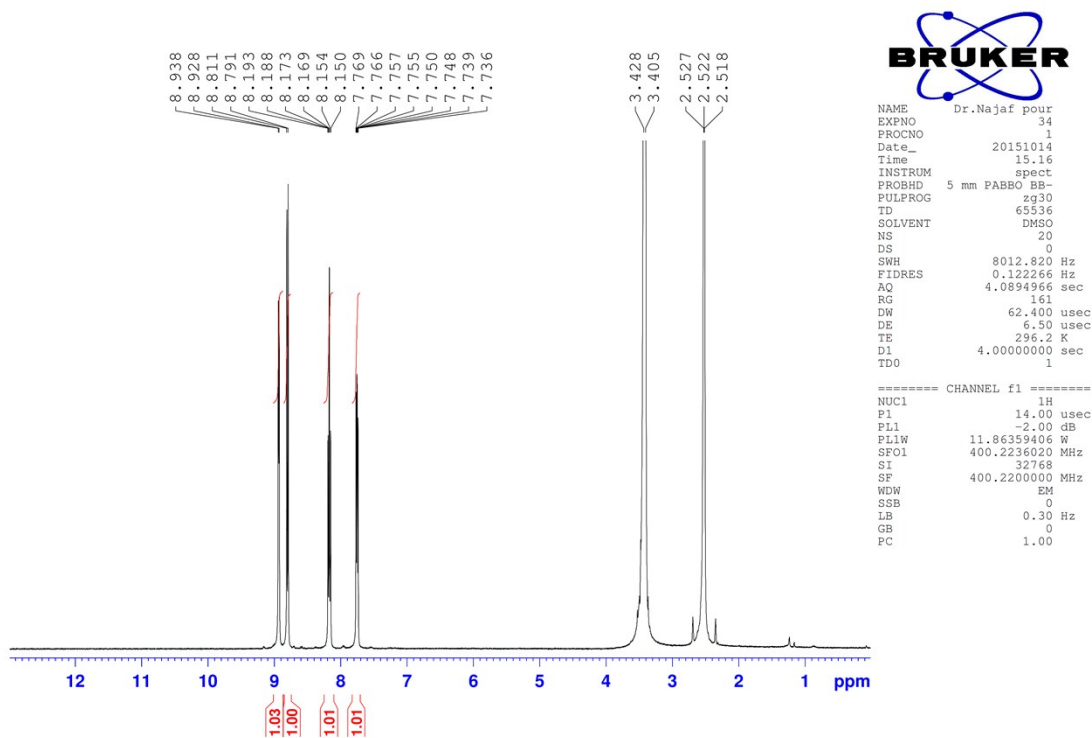


Fig. S1 XRD patterns for appeared film (**FTO-1**) electrode during 10 hours under water oxidation in 0.25 M phosphate buffer solution (pH = 11.0) in the bulk electrolysis of **1** at 1.5 V.

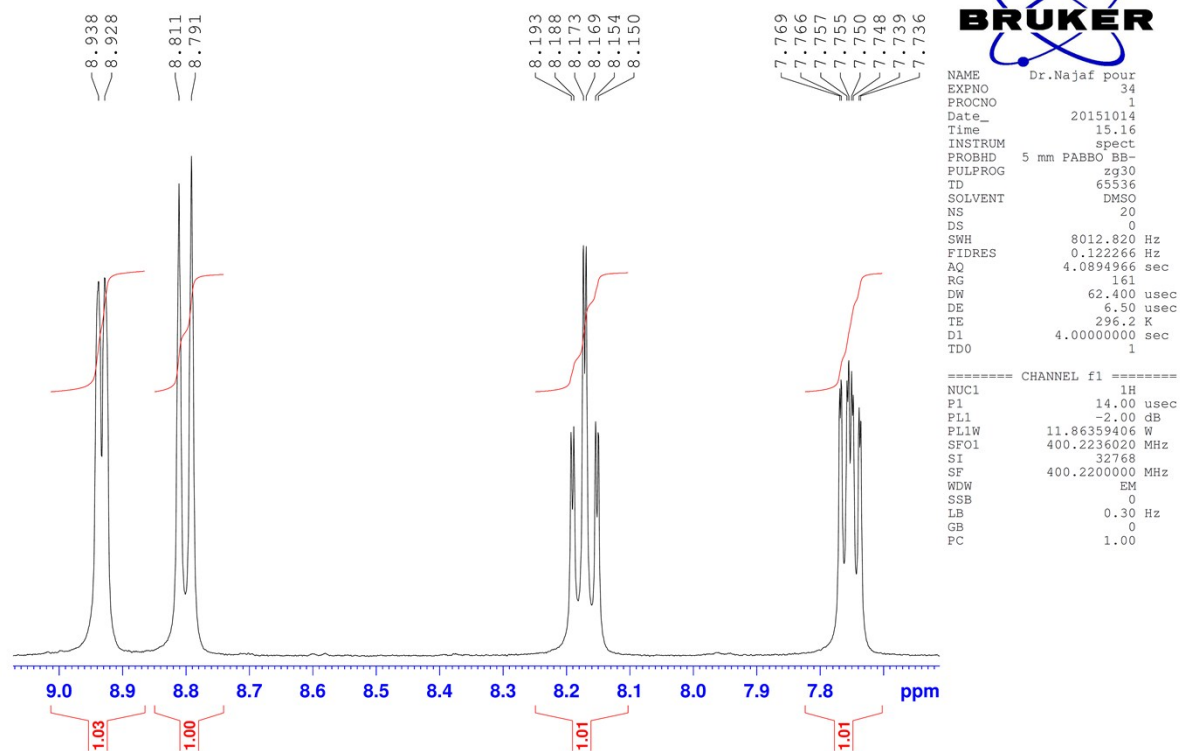


a



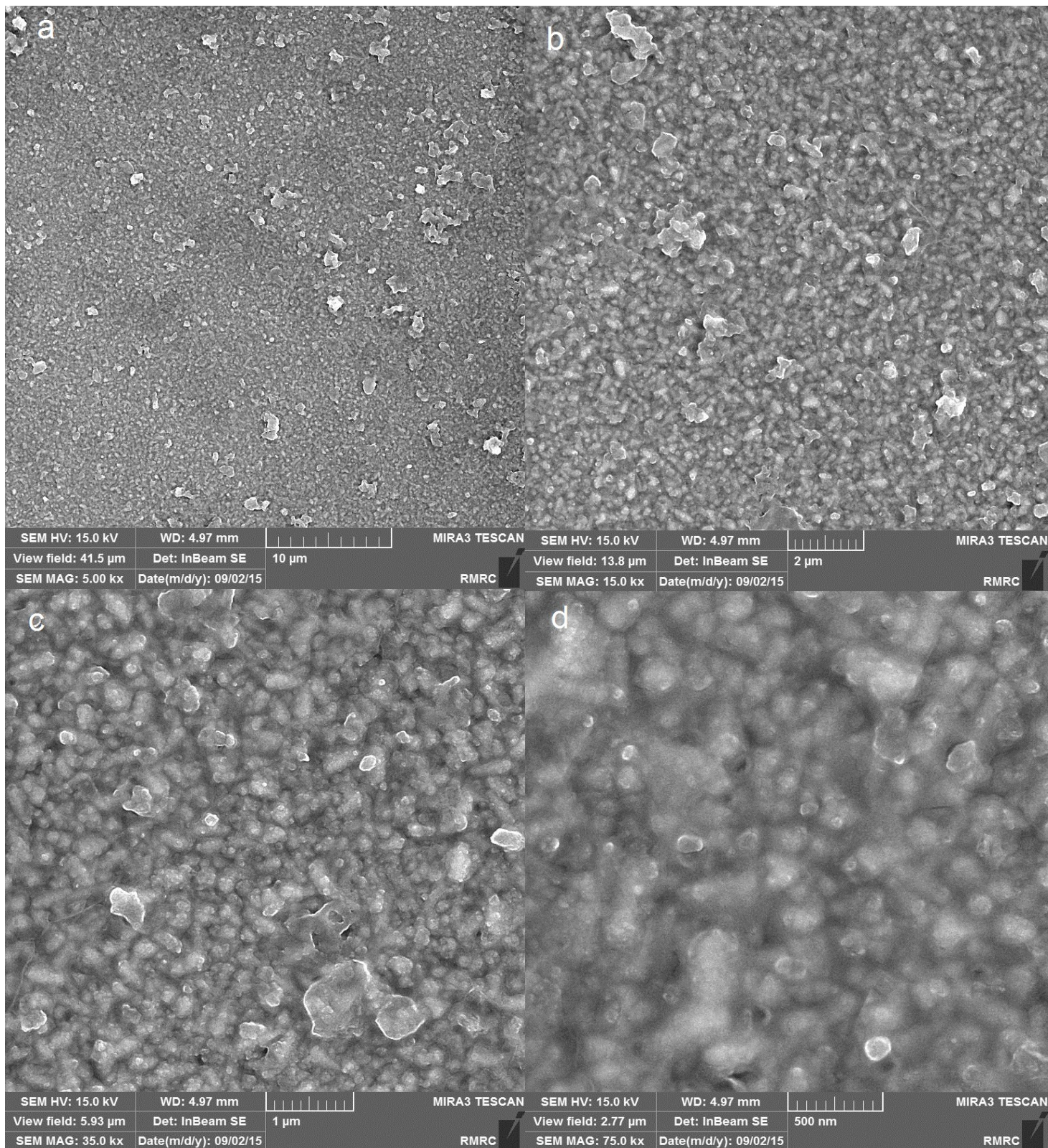
b

sample code: 1 in DMSO (safdari)



c

Fig. S2 <sup>1</sup>HNMR for cyclen (a) and the precipitated solid (b,c) after electrochemical reaction in DMSO.



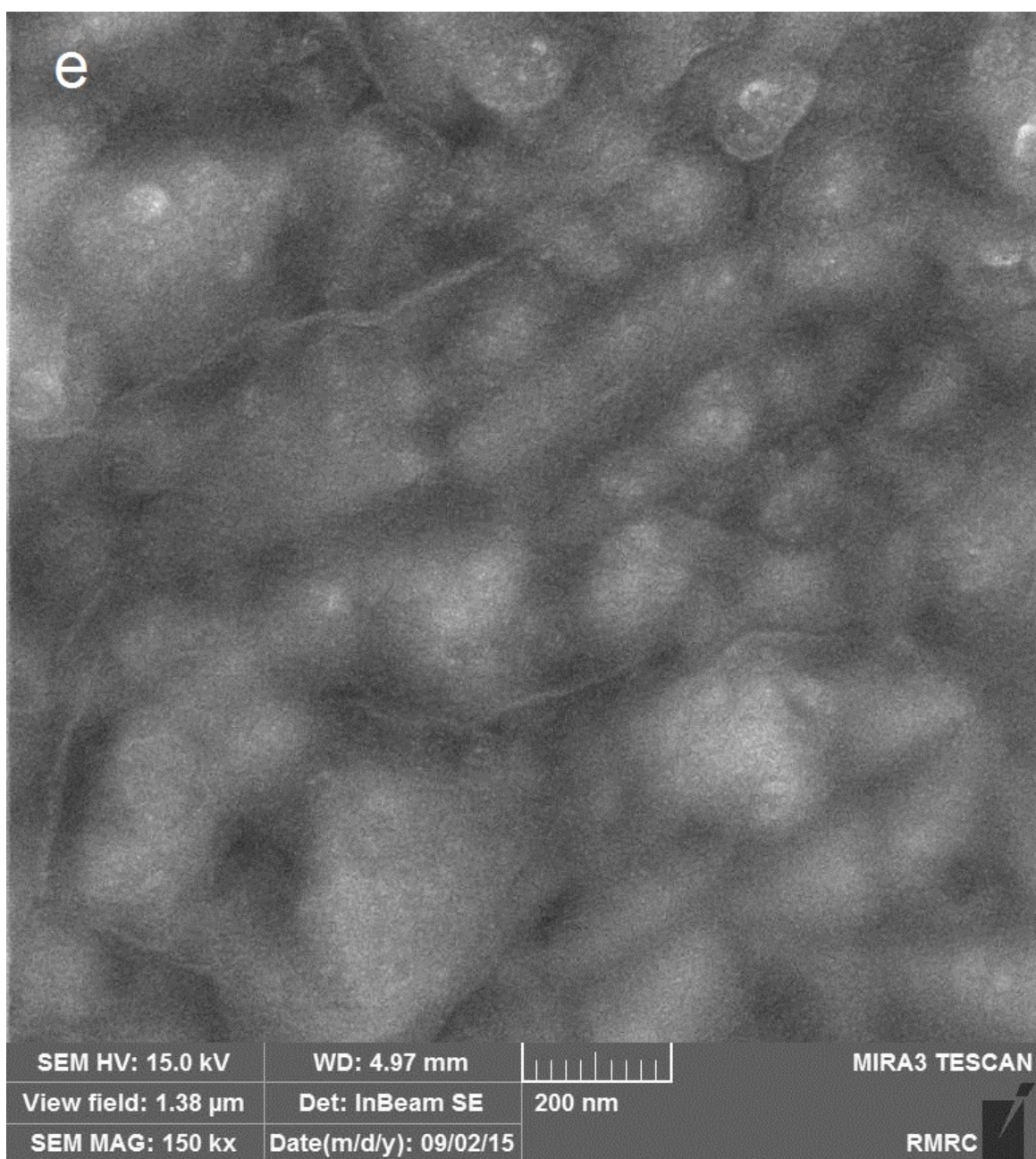


Fig. S3 SEM images for appeared film (**FTO-1**) electrode during 10 hours under water oxidation in 0.25 M phosphate buffer solution (pH = 11.0) in the bulk electrolysis of **1** at 1.5 V (a-e).

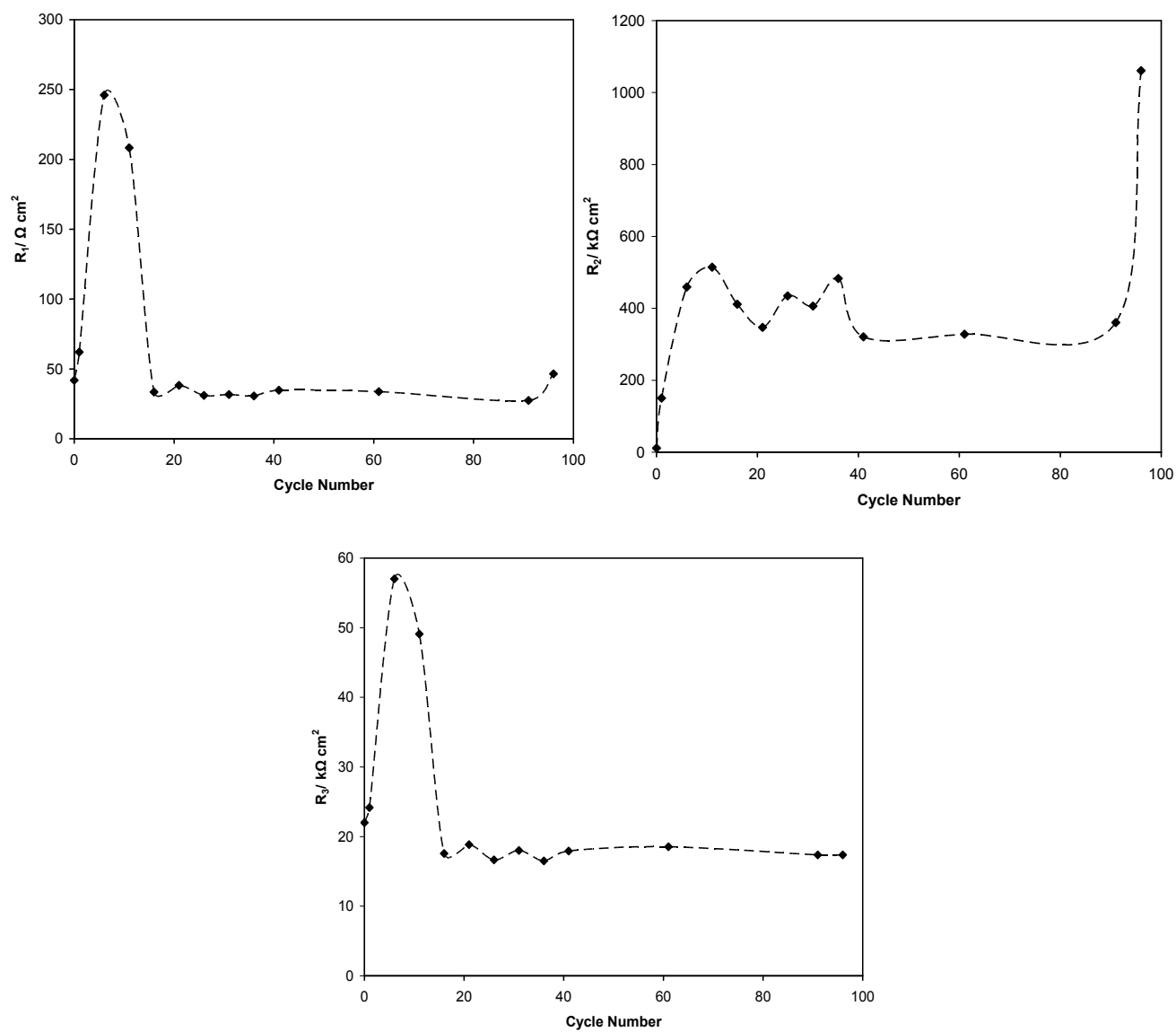


Fig. S4 Variation of  $R_1$ ,  $R_2$ , and  $R_3$  values with cycle number

Table S1: Equivalent circuit parameters obtained by fitting EIS experimental spectra recorded at various cycle number in LiClO<sub>4</sub> containing **1** solution on FTO electrode.

| <i>Cycle Number</i> | $Y_0 \times 10^{-5}$<br>( $\Omega^{-1} s^n cm^{-2}$ ) | $n$  | $R_1$<br>( $\Omega cm^2$ ) | $C_1 \times 10^{-5}$<br>( $F.cm^{-2}$ ) | $Y_0 \times 10^{-5}$<br>( $\Omega^{-1} s^n cm^{-2}$ ) | $n$  | $R_2$<br>( $\Omega cm^2$ ) | $C_2 \times 10^{-5}$<br>( $F.cm^{-2}$ ) | $Y_0 \times 10^{-6}$<br>( $\Omega^{-1} s^n cm^{-2}$ ) | $n$  | $R_3$<br>( $\Omega cm^2$ ) |
|---------------------|-------------------------------------------------------|------|----------------------------|-----------------------------------------|-------------------------------------------------------|------|----------------------------|-----------------------------------------|-------------------------------------------------------|------|----------------------------|
| 0                   | 0.379                                                 | 0.99 | 41.89                      | 0.347                                   | 0.841                                                 | 0.94 | 109930                     | 0.834                                   | 2.87                                                  | 0.74 | 22.00                      |
| 1                   | 0.952                                                 | 0.99 | 62.12                      | 0.883                                   | 0.677                                                 | 0.96 | 149199                     | 0.677                                   | 3.91                                                  | 0.72 | 24.18                      |
| 6                   | 1.14                                                  | 0.99 | 246                        | 1.07                                    | 0.415                                                 | 0.95 | 431580                     | 0.426                                   | 0.827                                                 | 0.37 | 57.02                      |
| 11                  | 1.11                                                  | 0.98 | 208                        | 9.79                                    | 0.464                                                 | 0.95 | 483430                     | 0.485                                   | 0.601                                                 | 0.41 | 49.10                      |
| 16                  | 1.94                                                  | 0.99 | 33.43                      | 1.80                                    | 1.59                                                  | 0.95 | 406310                     | 1.75                                    | 1.20                                                  | 0.80 | 17.57                      |
| 21                  | 2.22                                                  | 0.99 | 38.28                      | 2.07                                    | 1.52                                                  | 0.95 | 341060                     | 1.65                                    | 1.35                                                  | 0.77 | 18.85                      |
| 26                  | 2.07                                                  | 0.99 | 30.98                      | 1.92                                    | 1.64                                                  | 0.95 | 414940                     | 1.82                                    | 0.777                                                 | 0.83 | 16.66                      |
| 31                  | 2.00                                                  | 0.99 | 31.61                      | 1.86                                    | 1.64                                                  | 0.94 | 385290                     | 1.85                                    | 1.06                                                  | 0.78 | 18.00                      |
| 36                  | 1.95                                                  | 0.99 | 30.67                      | 1.81                                    | 1.70                                                  | 0.94 | 433350                     | 1.94                                    | 0.830                                                 | 0.83 | 16.51                      |
| 41                  | 2.05                                                  | 0.99 | 34.7                       | 1.90                                    | 1.75                                                  | 0.93 | 318490                     | 1.98                                    | 0.960                                                 | 0.8  | 17.94                      |
| 61                  | 1.96                                                  | 0.99 | 33.76                      | 1.82                                    | 1.88                                                  | 0.92 | 324370                     | 2.19                                    | 1.05                                                  | 0.79 | 18.53                      |
| 91                  | 1.69                                                  | 0.99 | 27.47                      | 1.56                                    | 2.20                                                  | 0.90 | 376610                     | 2.77                                    | 0.740                                                 | 0.83 | 17.38                      |
| 96                  | 2.27                                                  | 0.95 | 46.46                      | 1.58                                    | 1.28                                                  | 0.93 | 1022000                    | 1.56                                    | 0.831                                                 | 0.82 | 17.36                      |