

Supporting Information

Synthesis of Ferrocene-based Saccharides and Their Anti-migration and Burning Rate

Catalytic Properties

Zain-ul-Abdin, Li Wang*, Haojie Yu*, Muhammad Saleem, Nasir M. Abbasi, Rizwan Ullah

Khan, Raja Summe Ullah, Muhammad Haroon

State Key Laboratory of Chemical Engineering, College of Chemical and Biological Engineering,

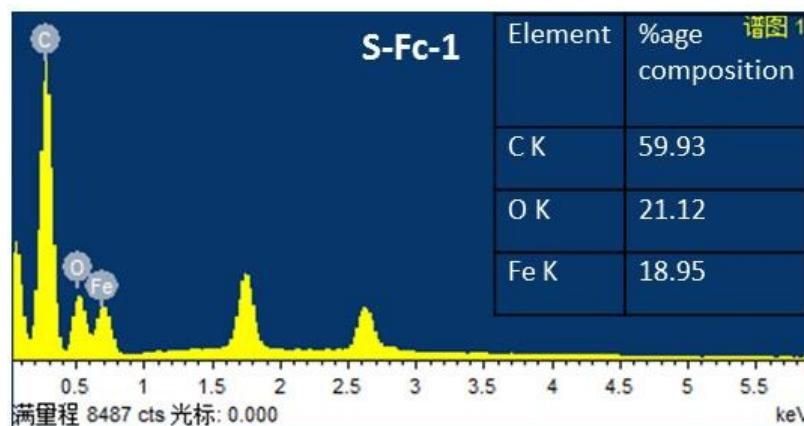
Zhejiang University, Hangzhou 310027, China

Table S1. Experimental detail for the synthesis of **S-Fcs**

| Sample | Saccharide (A) | | | Ferrocenecarbonyl chloride (B) | | | Mole ratio | NaH | | THF | Time | Temperature |
|----------|-------------------|------|---------------------|-----------------------------------|-------|---------------------|---------------|--------|-------|-----|------|-------------|
| | g | mmol | mol.L ⁻¹ | g | mmol | mol.L ⁻¹ | | g | mmol | | | |
| S-Fc-1* | 1.2000 | 6.66 | 0.09 | 11.5880 | 46.63 | 0.67 | 1 : 7 | 0.7996 | 33.33 | 70 | 10 | 66 |
| S-Fc-2* | 1.0000 | 2.92 | 0.10 | 6.5348 | 26.29 | 0.53 | 1 : 9 | 0.5608 | 23.37 | 50 | 10 | 66 |
| S-Fc-3* | 0.5000 | 0.99 | 0.03 | 2.9562 | 11.89 | 0.26 | 1 : 12 | 0.2616 | 10.90 | 45 | 10 | 66 |
| S-Fc-4** | 0.2780 | 1.71 | 0.06 | 1.2800 | 5.14 | 0.10 | 1 : 3 | 0.1233 | 5.14 | 50 | 10 | 66 |

*Calculations were done by taking molecular mass of the saccharides

**Calculations were done by taking mass of single repeating unit.



* Correspondence to Li Wang. E-mail: opl_wl@dial.zju.edu.cn and Haojie Yu. E-mail: hjyu@zju.edu.cn

Tel: +86-571-8795-3200; Fax: +86-571-8795-1612.

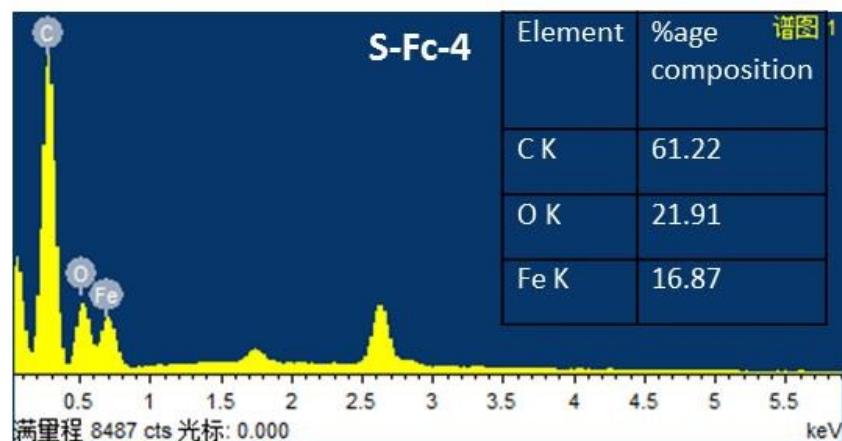
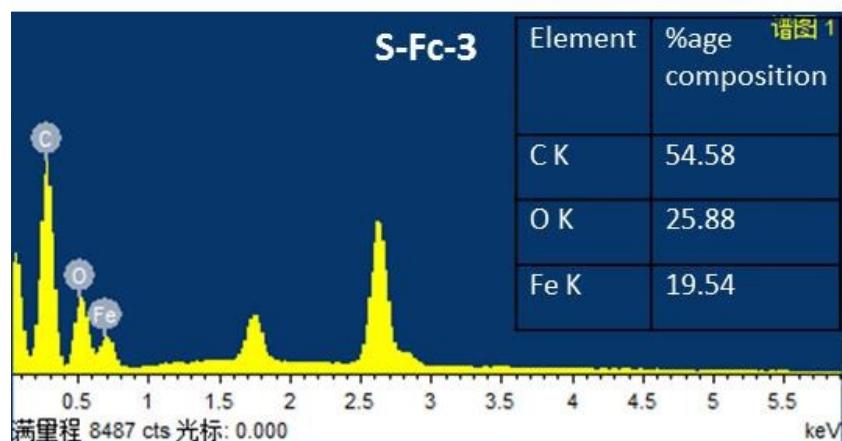
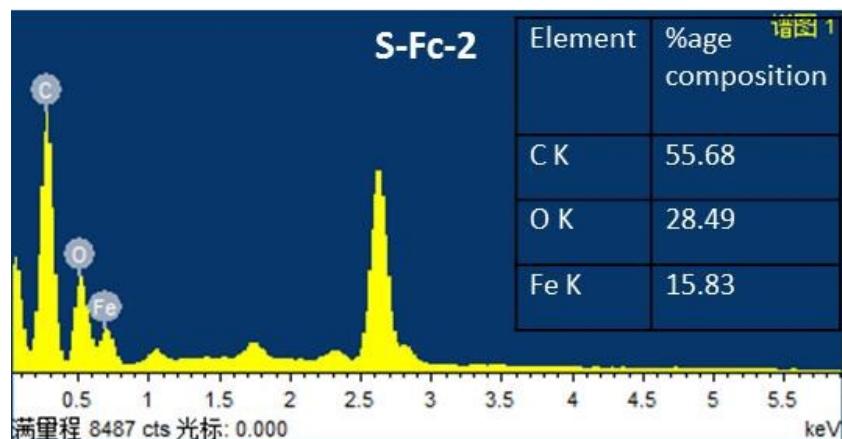


Figure S1. EDX spectra of S-Fcs.

Spectroscopic data of ferrocene-based saccharides (S-Fcs):

Data of **S-Fc-1**: ^1H NMR (600MHz, DMSO): δ ppm, 6.60 (d, 1H, **1**), 6.45 (d, 1H, **5**), 4.75 (m, 10H, **7**), 4.50 (m, 10H, **8**), 4.25 (m, 25H, **9**), 3.75 (t, 1H, **3**), 3.65 (t, 2H, **6**), 3.40 (t, 1H, **2**) and

2.90 (s, 1H, **4**). IR (KBr): cm^{-1} , 2847.57, 1710.81, 1474.66, 1122.64, 825.66 and 504.77. UV-Vis (0.012 mM solution in DCM): nm, 311 (charge transfer band), 264 and 232 ($\pi-\pi^*$ transitions).

Data of **S-Fc-2**: ^1H NMR (600MHz, DMSO): δ ppm, 6.60 (d, 2H, **1**), 6.45 (d, 2H, **5**), 4.75 (m, 16H, **7**), 4.50 (m, 16H, **8**), 4.25 (m, 40H, **9**), 3.65 (t, 4H, **6**), 3.50 (m, 4H, **2** and **3**) and 2.98 (m, 2H, **4**). IR (KBr): cm^{-1} , 2854.99, 1725.66, 1466.63, 1275.00, 1122.64, 825.70 and 482.49. UV-Vis (0.012 mM solution in DCM): nm, 312 (charge transfer band), 265 and 232 ($\pi-\pi^*$ transitions).

Data of **S-Fc-3**: ^1H NMR (600MHz, DMSO): δ ppm, 6.62 (d, 3H, **1**), 6.48 (d, 3H, **5**), 4.78 (m, 22H, **7**), 4.49 (m, 22H, **8**), 4.24 (m, 55H, **9**), 3.70 (t, 3H, **3**), 3.60 (m, 6H, **6**), 3.40 (m, 3H, **2**) and 2.90 (m, 3H, **4**). IR (KBr): cm^{-1} , 2847.57, 1710.82, 1458.38, 1275.25, 1130.83, 818.24 and 482.49. UV-Vis (0.012 mM solution in DCM): nm, 450 (d-d transitions), 312 (charge transfer band), 263 and 231 ($\pi-\pi^*$ transitions).

Data of **S-Fc-4**: ^1H NMR (600MHz, DMSO): δ ppm, 6.65 (d, 1H, **1**), 6.50 (d, 1H, **5**), 4.74 (m, 6H, **7**), 4.49 (m, 6H, **8**), 4.23 (m, 15H, **9**), 3.63 (t, 2H, **6**), 3.42 (m, 2H, **2** and **3**) and 2.96 (m, 1H, **4**). IR (KBr): cm^{-1} , 2847.57, 1710.81, 1474.06, 1283.50, 1107.80, 825.66 and 489.91. UV-Vis (0.012 mM solution in DCM): nm, 453 (d-d transitions), 312 (charge transfer band), 262 and 230 ($\pi-\pi^*$ transitions).

Table S2. The detail of samples preparation for UV-Vis absorption studies

| Sample | Amount of sample | | Solvent | Volume of | Concentration |
|---------------|------------------|---------|---------|-----------|---------------|
| | mg | mmol | | | |
| S-Fc-1 | 0.2 | 0.00012 | DCM | 10 | 0.012 |
| S-Fc-2 | 0.3 | 0.00012 | DCM | 10 | 0.012 |
| S-Fc-3 | 0.3 | 0.00012 | DCM | 10 | 0.012 |
| S-Fc-4 | 0.1 | 0.00012 | DCM | 10 | 0.012 |

Table S3. The detail of samples preparation for CV studies

| Ferrocene-based saccharides | Amount of sample | | | Amount of electrolyte (Bu_4NBF_4) | | | *Volume of solution mL |
|-----------------------------|------------------|-------|----------------------|---|------|----------------------|---------------------------|
| | mg | mmol | mmol.L ⁻¹ | mg | mmol | mmol.L ⁻¹ | |
| S-Fc-1 | 6.2 | 0.005 | 0.50 | 329.3 | 1.0 | 100 | 10 |
| S-Fc-2 | 10.6 | 0.005 | 0.50 | 329.3 | 1.0 | 100 | 10 |
| S-Fc-3 | 14.2 | 0.005 | 0.50 | 329.3 | 1.0 | 100 | 10 |
| S-Fc-4 | 4.2 | 0.005 | 0.50 | 329.3 | 1.0 | 100 | 10 |

*Solvents used for the preparation of solution were DCM, CHCl_3 and DMSO.

Table S4. The detail of samples preparation for anti-migration studies

| Sample | Ammonium perchlorate | | Burning rate catalyst | | Hydroxyl terminated polybutadiene | | Isophorone diisocyanate | |
|-----------|----------------------|-------|-----------------------|------|-----------------------------------|-------|-------------------------|-------|
| | g | Wt. % | g | Wt. | g | Wt. % | g | Wt. % |
| S-Fc-1 | 1.9149 | 69.08 | 0.0820 | 2.95 | 0.5820 | 20.99 | 0.1930 | 6.96 |
| S-Fc-2 | 1.9238 | 70.97 | 0.0885 | 3.26 | 0.5302 | 16.56 | 0.1680 | 6.20 |
| S-Fc-3 | 1.9551 | 71.64 | 0.0792 | 2.90 | 0.5215 | 19.11 | 0.1731 | 6.34 |
| S-Fc-4 | 1.9923 | 71.32 | 0.0821 | 2.94 | 0.5210 | 18.65 | 0.1980 | 7.05 |
| Ferrocene | 1.9400 | 70.11 | 0.0820 | 2.96 | 0.5650 | 20.41 | 0.1801 | 6.50 |
| Catocene | 1.9152 | 70.34 | 0.0899 | 3.30 | 0.5465 | 20.07 | 0.1711 | 6.28 |
| Blank | 21.1605 | 71.93 | - | - | 6.2619 | 21.28 | 1.9971 | 6.79 |

Table S5. The detail of samples preparation for TG and DTG analysis

| Sample | Sample Code | S-Fcs | AP | Total amount | Wt.% of S-Fcs | Sample used |
|--------|--------------------|-------|------|--------------|---------------|-------------|
| 1 | AP+ 5 Wt.% S-Fc-1 | 1.5 | 28.5 | 30.0 | 5.0 | 3.2 |
| 2 | AP + 5 Wt.% S-Fc-2 | 1.5 | 28.5 | 30.0 | 5.0 | 2.8 |
| 3 | AP + 5 Wt.% S-Fc-3 | 1.5 | 28.5 | 30.0 | 5.0 | 3.6 |
| 4 | AP + 5 Wt.% S-Fc-4 | 1.0 | 19.0 | 20.0 | 5.0 | 3.7 |

| | | | | | | |
|---|---------------------------|-----|------|------|-----|-----|
| 5 | AP + 1 Wt.% S-Fc-4 | 0.3 | 29.7 | 30.0 | 1.0 | 3.1 |
| 6 | AP + 2 Wt.% S-Fc-4 | 0.6 | 29.4 | 30.0 | 2.0 | 2.9 |
| 7 | AP + 3 Wt.% S-Fc-4 | 0.9 | 29.1 | 30.0 | 3.0 | 2.9 |
| 8 | AP + 4 Wt.% S-Fc-4 | 1.2 | 28.8 | 30.0 | 4.0 | 2.8 |