

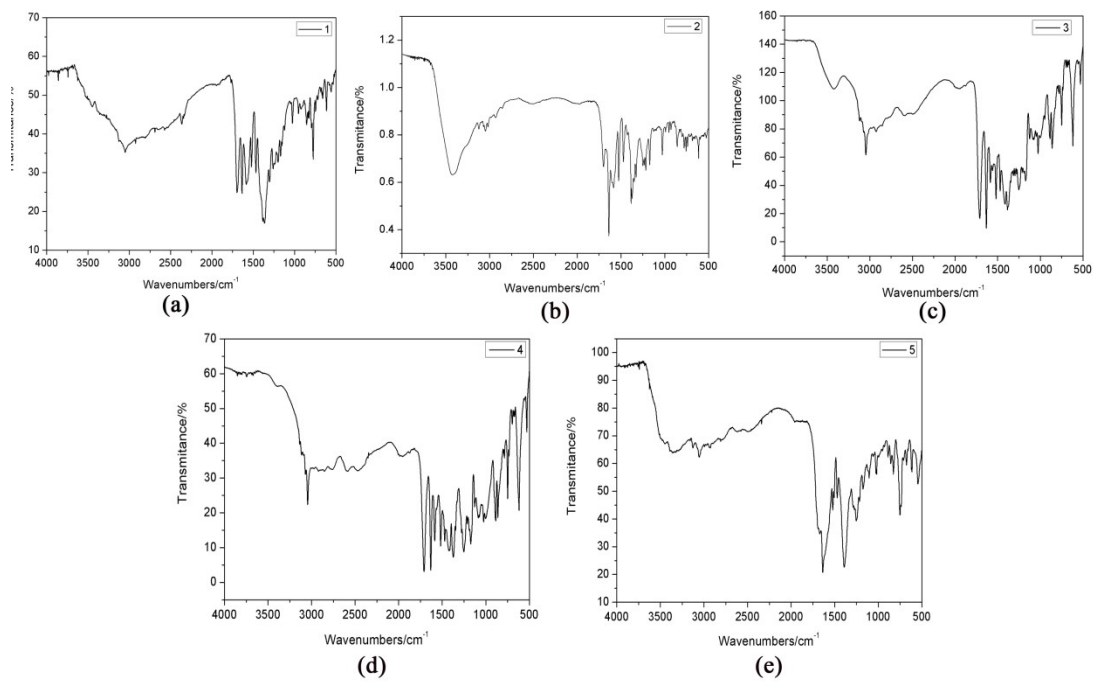
# Five novel supramolecular assemblies constructed from the thiazolothiazole extended viologen moiety

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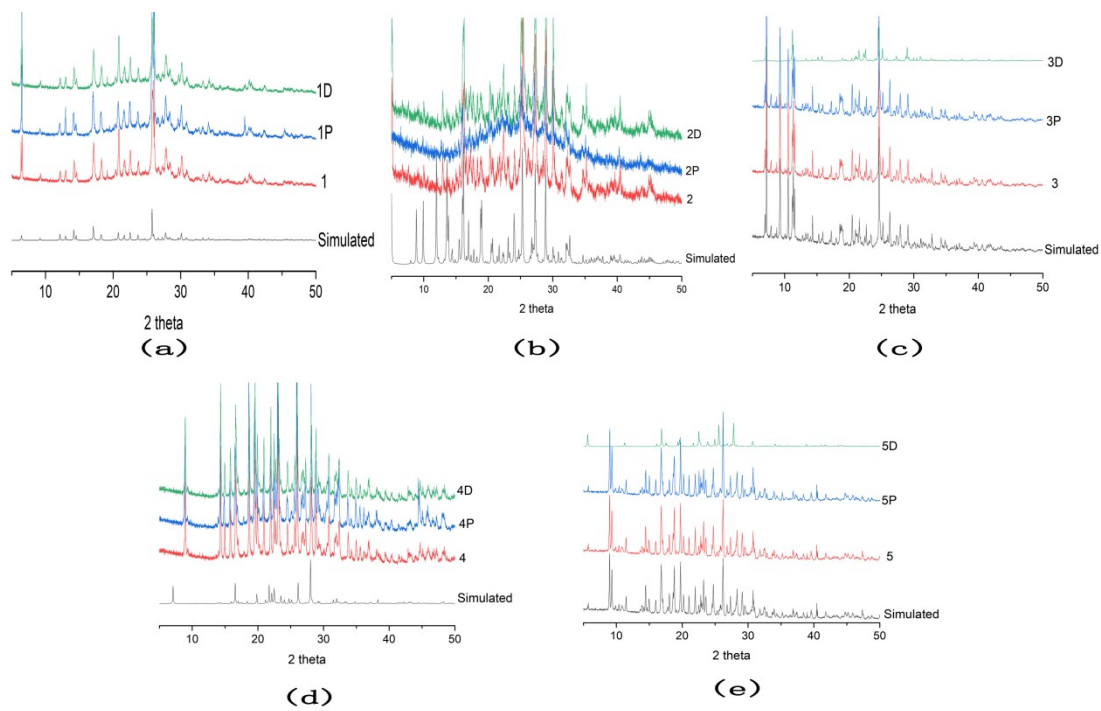
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**Table S1.** The hydrogen bond lengths (Å) in 1–5

| Compound 1     |       |                |       |
|----------------|-------|----------------|-------|
| O(1)-H···O(2)  | 2.257 | O(1)-H···O(4)  | 1.769 |
| C(21)-H···O(2) | 2.706 | O(8)-H···O(3)  | 1.991 |
| C(2)-H···O(4)  | 2.431 | C(22)-H···O(4) | 3.320 |
| C(4)-H···O(6)  | 2.275 | O(7)-H···O(4)  | 2.886 |
| C(5)-H···O(2)  | 2.190 | O(7)-H···O(3)  | 1.972 |
| Compound 2     |       |                |       |
| O(1)-H···O(29) | 1.911 | O(1)-H···O(30) | 2.994 |
| O(2)-H···O(10) | 1.904 | O(2)-H···O(27) | 2.621 |
| C(3)-H···O(30) | 2.959 | C(37)-H···O(4) | 3.140 |
| O(5)-H···O(15) | 3.284 | C(34)-H···O(7) | 2.912 |
| O(7)-H···O(4)  | 1.930 | C(25)-H···O(8) | 2.587 |
| C(36)-H···O(8) | 2.259 | O(10)-H···O(1) | 2.484 |
| O(15)-H···O(5) | 3.166 | O(3)-H···O(24) | 2.620 |
| O(27)-H···O(2) | 2.625 | O(29)-H···O(1) | 1.903 |
| Compound 3     |       |                |       |
| O(1)-H···O(3)  | 1.791 | C(3)-H···O(2)  | 3.355 |
| C(5)-H···O(6)  | 2.395 | O(4)-H···O(5)  | 1.498 |
| C(6)-H···O(6)  | 3.138 | O(7)-H···O(8)  | 1.979 |
| O(8)-H···O(6)  | 2.879 | C(16)-H···O(3) | 2.675 |
| C(16)-H···O(4) | 2.707 |                |       |
| Compound 4     |       |                |       |
| C(7)-H···O(1)  | 2.385 | C(2)-H···O(1)  | 2.792 |
| O(2)-H···O(7)  | 1.781 | C(5)-H···O(3)  | 2.461 |
| O(4)-H···O(5)  | 1.842 | C(19)-H···O(5) | 2.400 |
| C(4)-H···O(7)  | 3.101 | C(3)-H···O(7)  | 2.755 |
| C(4)-H···O(8)  | 3.129 |                |       |
| Compound 5     |       |                |       |
| O(4)-H···O(1)  | 1.699 | C(5)-H···O(2)  | 2.431 |
| O(2)-H···O(4)  | 2.812 | C(2)-H···O(2)  | 3.137 |
| O(3)-H···O(5)  | 1.960 | O(5)-H···O(2)  | 1.946 |
| C(14)-H···O(3) | 3.039 | C(7)-H···O(3)  | 3.034 |



**Fig. S1.** IR for 1-5.



**Fig. S2.** The PXR D spectra before and after irradiation for 1-5.

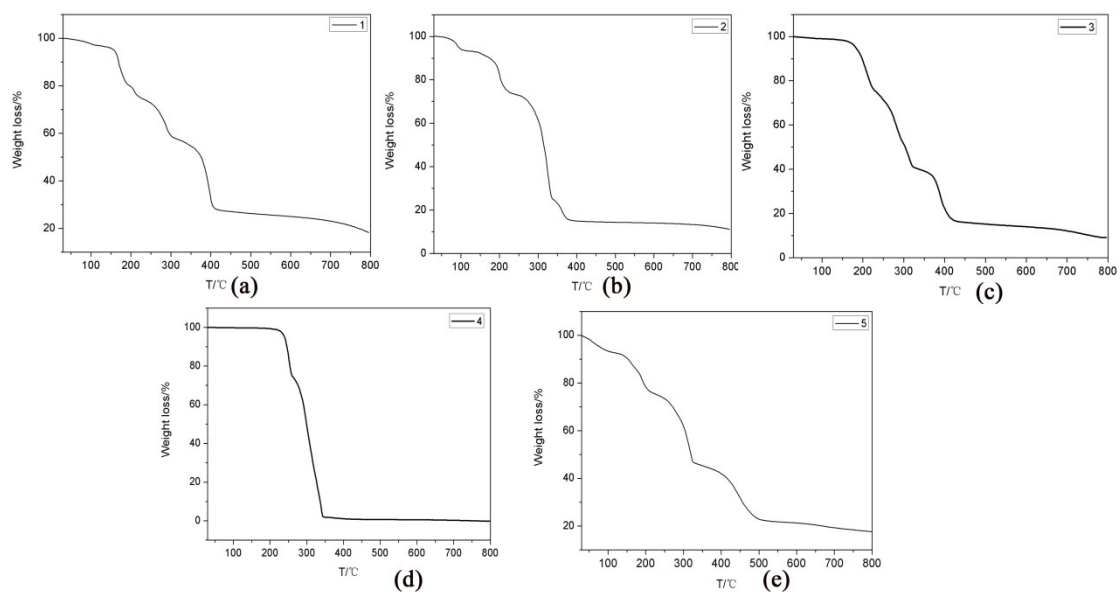


Fig. S3. TG for 1-5.

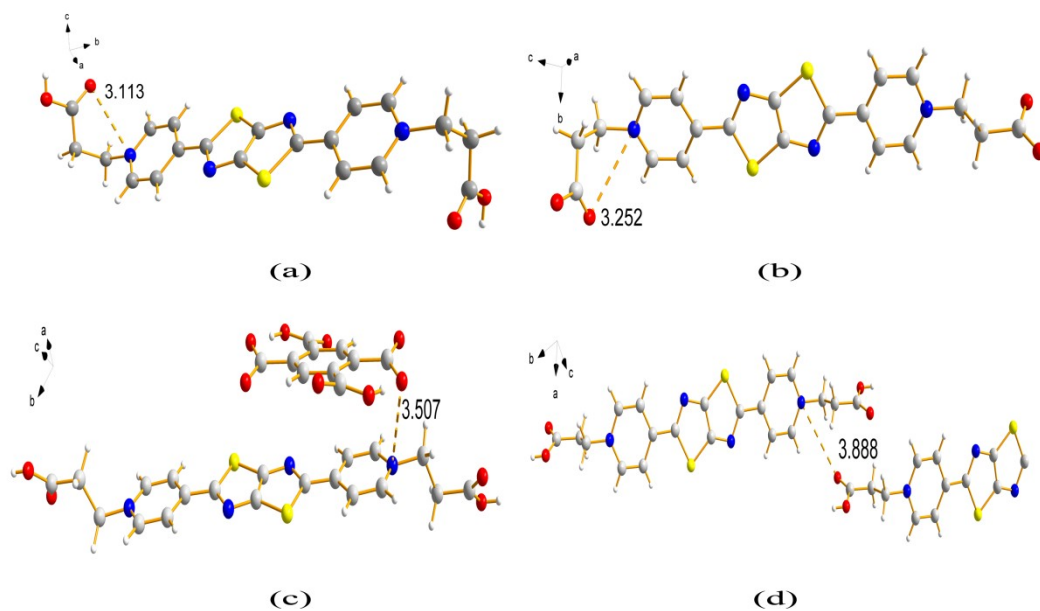


Fig. S4 The N...O distance for 1-4

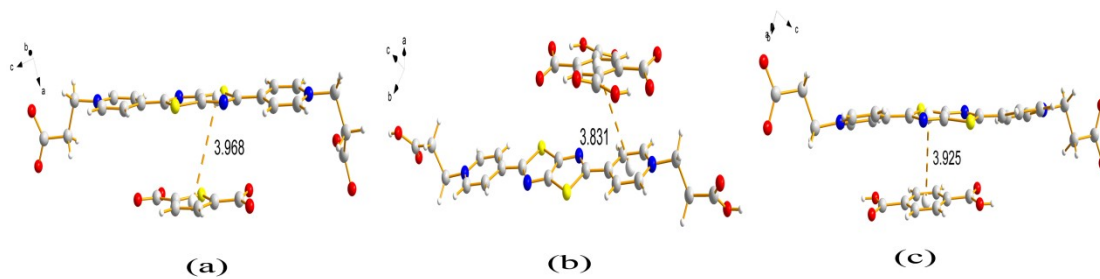


Fig. S5 The  $\pi \cdots \pi$  distance for 2 (a), 3 (b) and 5 (c)