**S2 Table.** Crystal data and structure refinement for the TABA.

|  |  |
| --- | --- |
| Empirical formula | C13H12O8 |
| Formula weight | 296.23 |
| Crystal system | Triclinic |
| Space group |  |
| a/Å | 8.3990(11) |
| b/Å | 8.4870(8) |
| c/Å | 9.8050(11) |
| α/° | 87.999(7) |
| β/° | 82.508(6) |
| γ/° | 88.714(7) |
| Volume/Å3 | 692.42(14) |
| Z | 2 |
| ρcalc/g.cm-3 | 1.421 |
| μ/mm‑1 | 0.120 |
| F(000) | 308.0 |
| Radiation | MoKα (λ = 0.71073) |
| 2θ range for data collection/º | 6.274 to 53.48 |
| Reflections collected | 2915 |
| Independent reflections | 2915 [Rint = 0.038] |
| Data/restraints/parameters | 2915/0/193 |
| Goodness-of-fit on F2 | 1.028 |
| Final R indexes [I > 2σ (I)] | R1 = 0.0479, wR2 = 0.1313 |
| Final R indexes [all data] | R1 = 0.0621, wR2 = 0.1417 |
| Largest diff. peak/hole / e Å-3 | 0.30/-0.23 |