Minimal Catalytic Dissipative Assemblies via Cooperation of Amino acid, Nucleobase precursor and Cofactor

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Materials

1,3,5-triazine-2,4,6-triamine (**T**), 4-hydroxy-3-methoxybenzoic acid (**AR**), hemin (**Cf**), histidine, glacial acetic acid, HBTU and triethylamine were purchased from SRL Chemicals. 7-hydroxycoumarin, Nile red, Rhodamine 110, 1,3,5-trimethoxy benzene, hydrogen peroxide, HRP, 1,1,2,2 tetrachloroethane and all solvents were purchased from Sigma Aldrich Merck. Milli-Q water was used throughout the study.

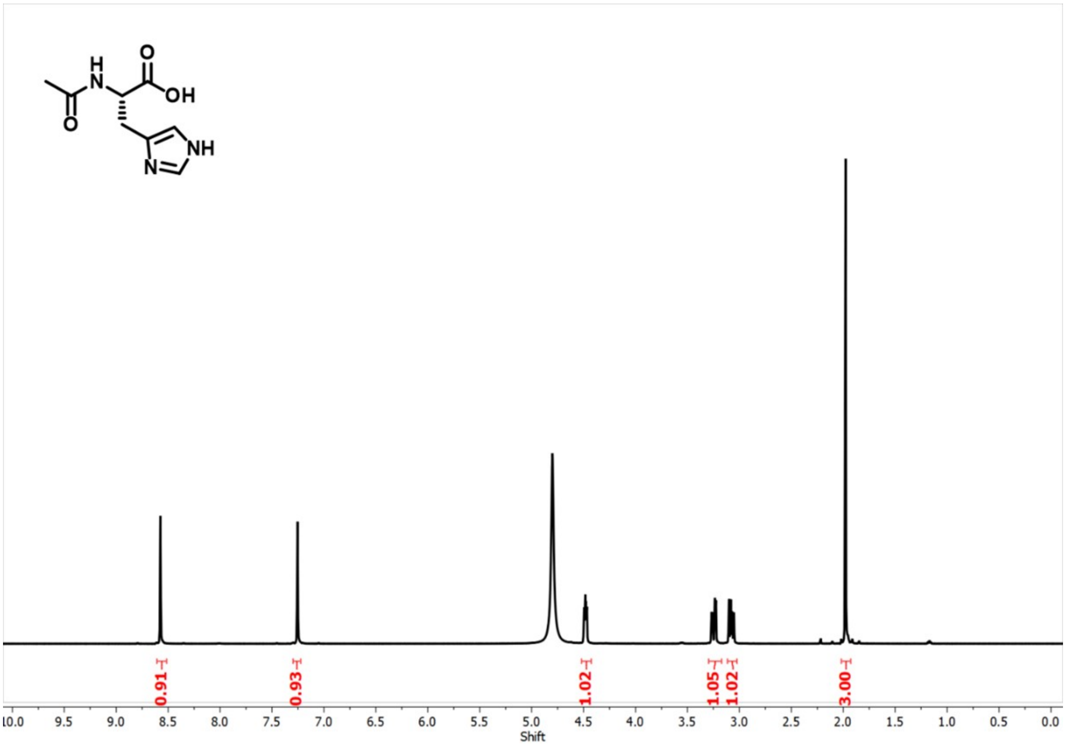
Synthesis

Synthesis and characterization of AA:

Step 1: Synthesis of N-acetylhistidine:

AA was synthesised by following previous literature.[1] Briefly, to a suspension of L-histidine (632 mg, 4.07 mmol) in glacial acetic acid (24 mL), acetic anhydride (0.4 mL, 440 mg, 4.32 mmol) was added. The solvent was evaporated After refluxing the reaction mixture for 15 h. The yellow oil formed was taken in H_2O (40 mL) and was extracted with $CHCl_3$. After evaporating the aqueous layer, the residue was dissolved in H_2O (15 mL) and was again evaporated twice. The oil was finally taken in H_2O (10 mL) and acetone (30 mL) was added afterwards. The mixture was kept at 0 °C overnight which led to the formation of a colourless precipitate. The precipitate was isolated and washed with a mixture of H_2O and acetone (3:7), only acetone (30 mL) and Et_2O (30 mL). Drying under high vacuum yielded N-acetylhistidine as a colourless solid.

^{1}H NMR (D_2O, 500 MHz) δ (ppm): 1.97 (s, 3H), 3.08 (dd, 1H), 3.25 (dd, 1H), 4.48 (dd, 1H), 7.25 (s, 1H), 8.57 (s, 1H).

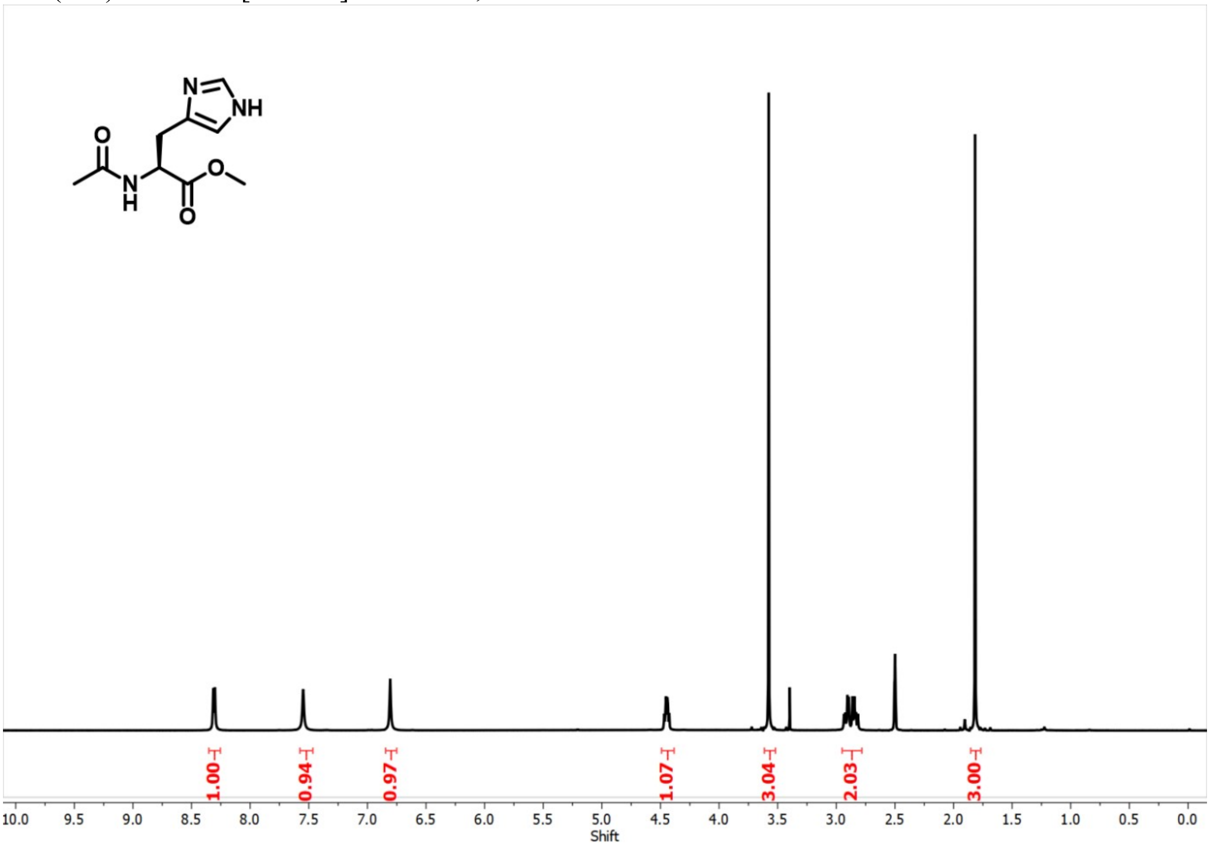


^{1}H NMR of **N-acetylhistidine**

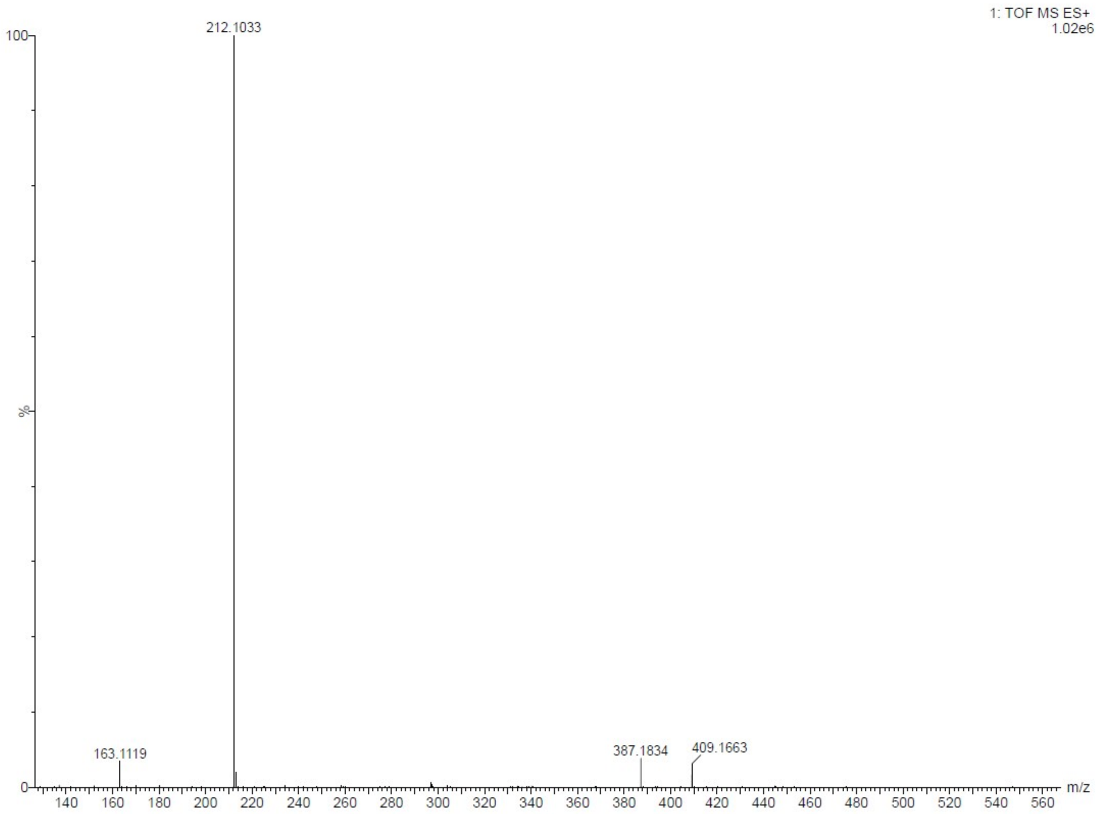
Step 2: Synthesis of N-acetyl histidine methyl ester (AA)

N-acetylhistidine (760 mg, 3.9 mmol) was taken in MeOH. The formed suspension was treated with thionyl chloride (1.25 mL, 2.03 g, 17.1 mmol) at 0 ˚C under N_2 atmosphere. The mixture was stirred for 16 h at room temperature. The solvent was evaporated, and the residue was taken in H_2O (50 mL) and solid $NaHCO_3$ was added to adjust the pH to 5. The oily residue formed after evaporation of the solvent was purified via column chromatography on silica gel (EtOAc/MeOH) to give N-acetyl histidine methyl ester (**AA**) as a colourless solid.

^{1}H NMR (DMSO-d_6, 500 MHz) δ (ppm): 1.81 (s, 3H), 2.82-2.93 (m, 2H), 3.57 (s, 3H), 4.42-4.47 (m, 1H), 6.81 (s, 1H), 7.54 (s, 1H), 8.31 (d, 1H).
ESI-MS (m/z) calcd. for [M + H^+]: 212.1030; found: 212.1033



^{1}H NMR of **N-acetyl histidine methyl ester (AA)**



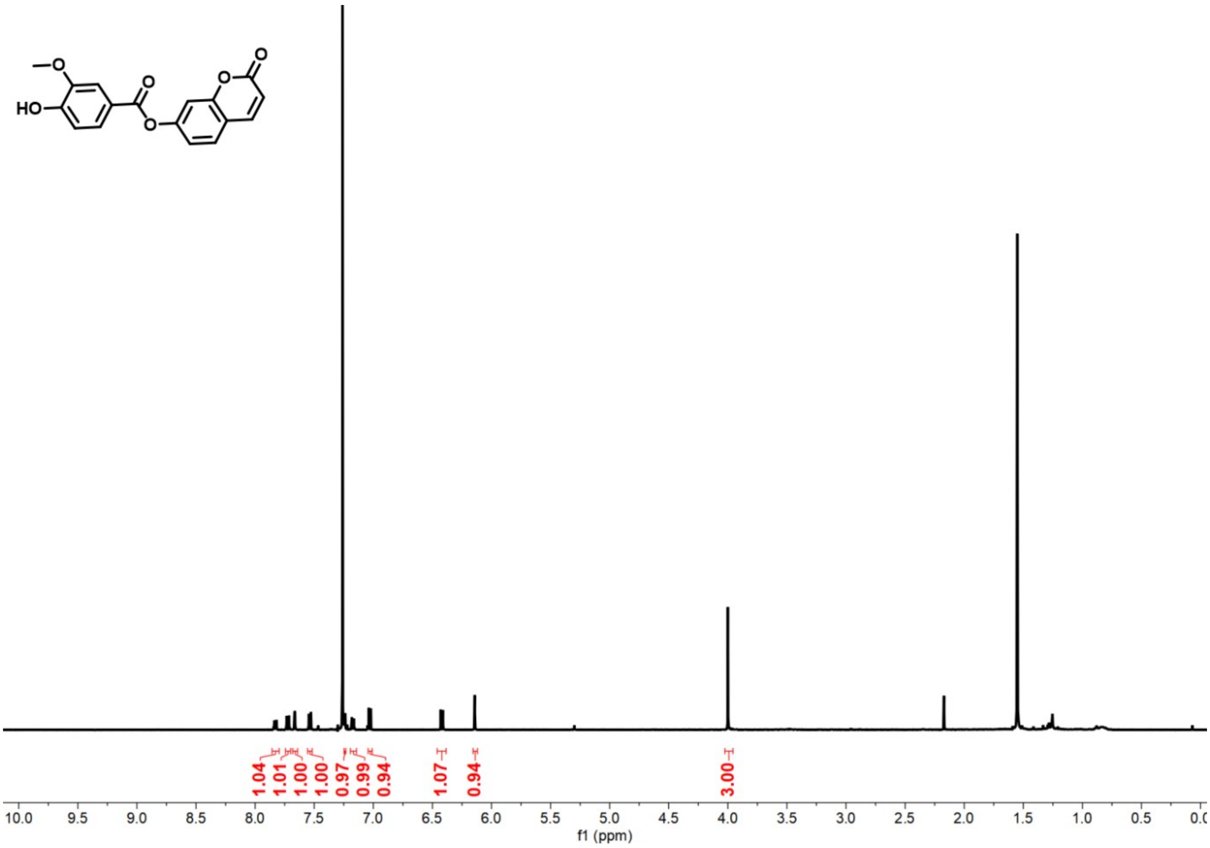
ESI-MS spectrum of **AA**

Synthesis and characterization of Pro-AR:

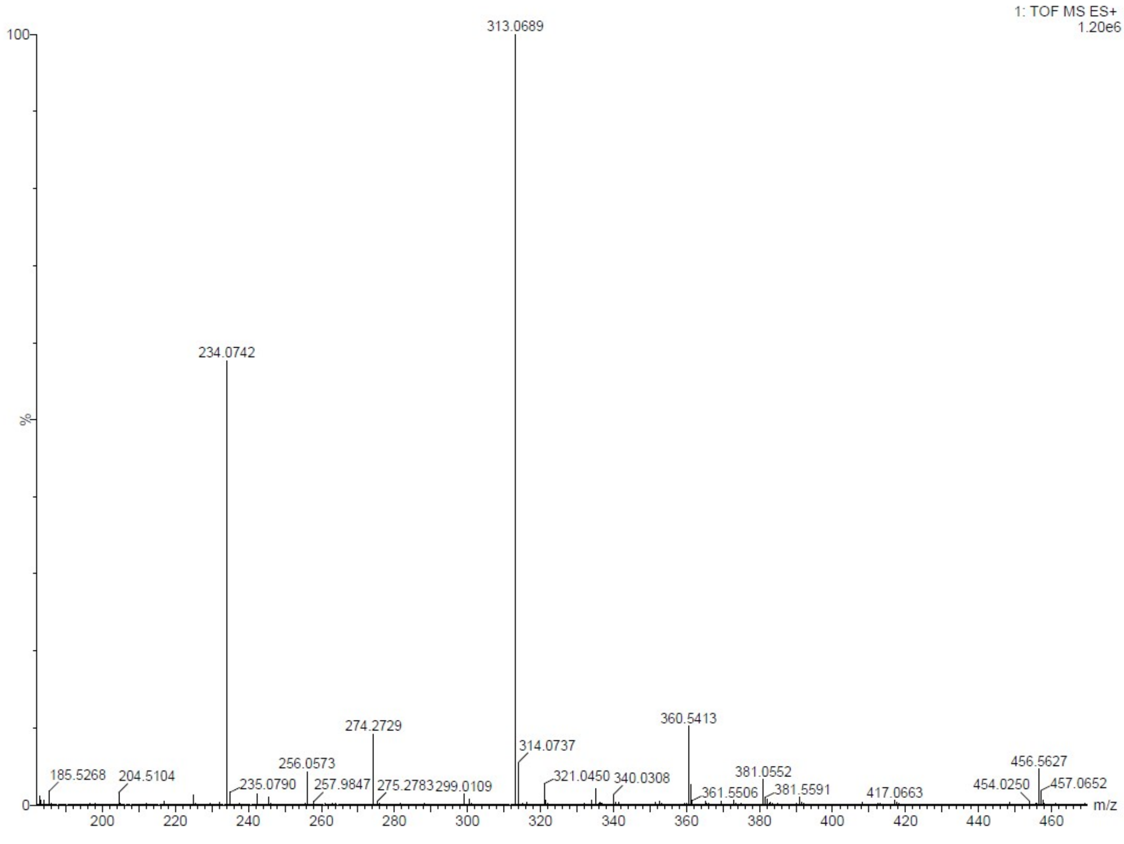
4-hydroxy-3-methoxybenzoic acid (**AR**, 1.0 g, 5.947 mmol) was taken along with 7 hydroxycoumarin (4.0 g, 23.6 mmol) in DCM. HBTU (13.53 g, 35.6 mmol) was added to the mixture which was kept for stirring under nitrogen atmosphere for 1 hour. Afterwards, triethylamine (4.96 ml, 35.58 mmol) was added and stirring was continued. The progress of the reaction was monitored with the help of thin layer chromatography. Upon completion of the reaction (~6 h), the solvent was removed in vacuo and ethyl acetate was added. The mixture was washed with brine and the organic layer was dried over Na_2SO_4. Column chromatography was performed with DCM as the eluent to obtain the pure product.

^1H NMR ($CDCl_3$, 500 MHz) δ (ppm): 3.99 (s, 3H), 6.14 (s, 1H), 6.41 (d, 1H), 7.02 (d, 1H), 7.17 (dd, 1H), 7.24 (d, 1H), 7.53 (d, 1H), 7.66 (d, 1H), 7.72 (d, 1H), 7.83 (dd, 1H).

ESI-MS (m/z) calcd. for [M + H^+]: 313.0707; found: 313.0689



[1]H NMR spectrum of **Pro-AR**



ESI-MS spectrum of **Pro-AR**

Experimental methods

Assembly Studies:

For gelation studies, **T** and **AR** were taken in a glass vial and required volume of H_2O and H_2O stock of **AA** (200mM) were added to the vial. The vials were heated to 80 °C to dissolve the compounds and afterwards, **Cf** (10mM, DMF stock) and H_2O_2 (1M stock) were added immediately. Inversion of the vial indicated the formation of the gels, and the lifetimes of the gel state were noted. Final solvent composition of all the system was 98.5:1.5 H_2O: DMF (v/v).

For the studies in presence of **Pro-AR**, required volume of **Pro-AR** (DMF stock, 800mM) of was added just after the addition of other components. Final solvent composition of the system was 97.25:2.75 H_2O: DMF (v/v).

NMR studies:

To characterize the synthesized compounds, all ^{1}H NMR spectra were recorded in Bruker (500 MHz) at 27 °C in respective solvents as mentioned in the synthesis and characterisation section.

NMR for binding of AR was carried out by preparing the gel in D_2O with different concentrations of AR (while the concentrations of rest of the components were same) in presence of 1,1,2,2 tetrachloroethane as an internal standard.

The time dependent NMR spectra of the dissipative samples were recorded in presence of **T** (50mM), **AR** (50mM), **AA** (10mM), **Cf** (150μM) and H_2O_2 (30mM) in D_2O (in presence of 1.5% DMF) at different time. The internal standard 1,1,2,2 tetrachloroethane (50mM) was taken into a capillary tube inside the NMR tube. The NMR of the ternary mixture (**T**+**AR**+**AA**) were recorded using the above-mentioned procedure with the internal standard. The standard plot of **AA** was done using different concentrations of **AA** in D_2O (in presence of 1.5% DMF) with internal standard. The peak area of **AA** was corrected with respect to standard following the peak at ~8.56 ppm.

Electrospray Ionization Mass Spectrometry (ESI-MS):

Mass spectra of the synthesized compounds and the oxidised product were recorded in Waters Xevo G2-XS QTof.

Transmission Electron Microscopy (TEM):

JEM-2100 plus microscopes were used to record the images. Samples were prepared by drop casting the diluted gel state or sol state on the TEM grid and allowing to adsorb for 60 s. Filter paper was used for wicking off excess solution and the samples were dried for few hours in vacuo at 4 °C before imaging.

Atomic Force Microscopy:

The gel sample was diluted (25 times diluted with respect to **T** or **AR** concentration) in MiliQ water and directly drop casted onto a silicon wafer and allowed to adsorb for 1 min. The excess solution was wicked off with a blotting paper and then the sample was kept in desiccator. Standard tapping mode probes were used for imaging the sample under ambient conditions using Oxford MFD-3D Infinity AFM.

Fluorescence:

Fluorescence spectra were recorded in Cary Agilent spectrofluorometer using a slit-width of 5 nm. For the time dependent fluorescence studies in presence of Rhodamine 110, 20 μM of dye was added to different vials containing the samples and were incubated for different times. Fluorescence spectra were recorded at different times from different vials. The samples were excited at 500 nm.

For monitoring the release of 7-hydroxy coumarin, the samples were excited at 330 nm.

Powder X-ray diffraction:

A Rigaku SmartLab powder X-ray diffractometer having Cu Kα = 1.54 Å radiation was used to perform the XRD measurements. Samples as xerogel (gel of ca. 2 min age) were prepared by plunging in liquid nitrogen, followed by drying by the process of lyophilization. The dried samples were then mounted on glass slides. The scanning window was fixed up from 5-45°.

UV Vis spectroscopy:

The UV-Vis measurements were carried out in Agilent Cary 3500 UV-Visible spectrophotometer. Samples were prepared using the same procedure as described before and were transferred to cells of 10 mm path length to perform the experiment.

CD spectroscopy:
CD spectra were recorded using a JASCO J-810 circular dichroism spectrometer fitted with a Peltier temperature controller to maintain the temperature of 25 °C. Gel samples were prepared (**T**=50 mM, **AR**=50 mM, **AA**=10 mM, **Cf**= 900 µM, H_2O_2=30 mM, final solvent composition was 98.5: 1.5 H_2O: DMF (v/v)) and diluted immediately to place into a quartz cuvette with 10 mm path length. Each spectrum was obtained by scanning wavelength from 500 nm to 200 nm at a scanning rate of 500 nm/min. Two successive wavelength scans were taken to average for each sample. CD spectra were also recorded for different control systems in same solvent system. Since we measuring induced CD signal (negative) of hemin (**Cf**) in presence of assembles, the concentration of **Cf** were kept high in every system (concentration of all other components were kept same).

Rheology:
MCR-102 rheometer from Anton Paar equipped with 25 mm cone plate (CP25-2, Anton Paar) geometry was used to characterize the viscoelastic behaviours at 25 °C. Strain sweep of the samples was performed by varying the strain from 0.01 % to 100 % at a fixed oscillatory frequency of 10 Hz and the linear viscoelastic regions (LVER) of the samples were determined. Mechanical strengths of the samples were determined from frequency sweep experiments carried out at a fixed strain of 0.1%. For the time dependent experiment, series of samples in vials were aged for different time intervals. Storage modulus (G') of each incubated sample was measured at fixed strain of 0.1 % and fixed oscillatory frequency of 1 Hz. The storage moduli were plotted against time. For comparison of gel strengths, the G' corresponding to the frequency of 1 Hz has been taken from the frequency sweeps of the different samples.

Confocal microscopy:
Nile red dye (1 µL, 1 mM) was added to 9 µL of the diluted samples and incubated for 10 min. The solution was then cast on a glass slide and was enclosed with a cover glass and excited by 561 nm laser line at an emission bandwidth of 570-670 nm. Confocal images were recorded at Olympus Laser Scanning Confocal System Model FV3000 (part of the Atomic Force Microscope with Rheological Measurement and Confocal Imaging Unit facility, supported by Swarnajayanti (SB/SJF/2020-21/08).

FTIR:
Solid-state FT-IR study were done after forming the samples (gel and individual components in same solvent system) followed by lyophilization and measured with a PerkinElmer Spectrum RX1 spectrophotometer by following the KBr disk technique.

HPLC:
HPLC was carried out with Waters HPLC system equipped with 1525 binary pump and 2998 photodiode array detector. For monitoring the consumption of **AR**, Atlantis C18 5µm 4.6 × 250 mm analytical HPLC column was used.
The flow rate was maintained at 0.7 mL/min with a gradient elution method by using 0.1% TFA containing acetonitrile and water as the mobile phase.
Oxidation of **AR**:
To monitor the oxidation of **AR** with time, samples were prepared in different vials and were incubated for different times. Samples were diluted at respective time before injection. The chromatograms were extracted at 260 nm to observe the decrease of **AR** peak with time. Standard plot was done using different concentrations of **AR** and the amount of **AR** consumption was determined. 1,3,5-trimethoxy benzene was used as the internal standard.
For the characterisation of oxidation products using HRP enzyme, the flow rate was maintained at 0.7 mL/min with a gradient elution method by using 0.1% formic acid containing water and 0.1% TFA containing acetonitrile as the mobile phase.
Hydrolysis of **Pro-AR**:

The hydrolysis of **Pro-AR** was monitored at 324 nm to observe the generation of fluorophore 7-hydroxycoumarin. The standard plot was done using different concentrations of 7-hydroxycoumarin to determine the amount of hydrolysed product. The rate was calculated for initial 30 minutes.

Binding of **AA**:

For calculating the amount of **AA** that was getting bound to the assemblies, Spherisorb 5µm ODS1 4.6×250mm analytical HPLC column was used. The dissipative self-assembled samples **T** (50 mM), **AR** (50 mM), **AA** (10mM), **Cf** (150 µM) and H_2O_2 (30 mM) incubated for different times were centrifuged and the supernatant was separated with the expectation that the supernatant will only have the unbound **AA**. The supernatant was injected in HPLC after dilution. The concentrations of the bound **AA** were calculated by subtracting the amount observed from HPLC at each time point from the total amount added i.e. 10mM. The chromatograms were extracted at 220 nm to find out the amount of **AA** present in the supernatant. Standard plot was done using different concentrations of **AA**.

Refuelling experiment:

Refuelling was done by adding 8.2 mM of **AR** after the mechanical strength showed a prominent decrease (~180 min). The system was heated for solubilization of the components and then set up for gelation and was followed by rheology measurements.

Computational study:

All computational calculations were done using the ORCA 5.0.3 quantum mechanical programme suite.[2] Unconstrained geometry optimizations were done employing the BP86[3] generalized gradient approximation (GGA) functional, along with D3BJ [4] empirical dispersion correction to precisely account for non-covalent interactions such as π-π stacking and hydrogen bonding. A double-ζ quality split-valence def2-SVP basis set was applied to all atoms. The density-fitting resolution of identity (RI) approximation, paired with the auxiliary Coulomb-fitting basis set def2/J, was used to enhance computational efficiency. Tight convergence criteria (energy tolerance of $1 \times 10-8$ Hartree) were adhered for all self-consistent field (SCF) calculations. Finally, energies of the optimized geometries were refined with single-point calculations using the B3LYP-D3BJ[5] functional, augmented with empirical dispersion correction, and the double-ζ quality split-valence def2-SVP basis set on all atoms using CPCM[6] solvent model and water (ε= 80.4, refractive index = 1.33) as solvent. Binding Energies (B.E.) were calculated using the following equation (i),

$$BE = \frac{Energy(higher\ conformer) - n * Energy(monomer)}{n} \quad \text{......(i)}$$

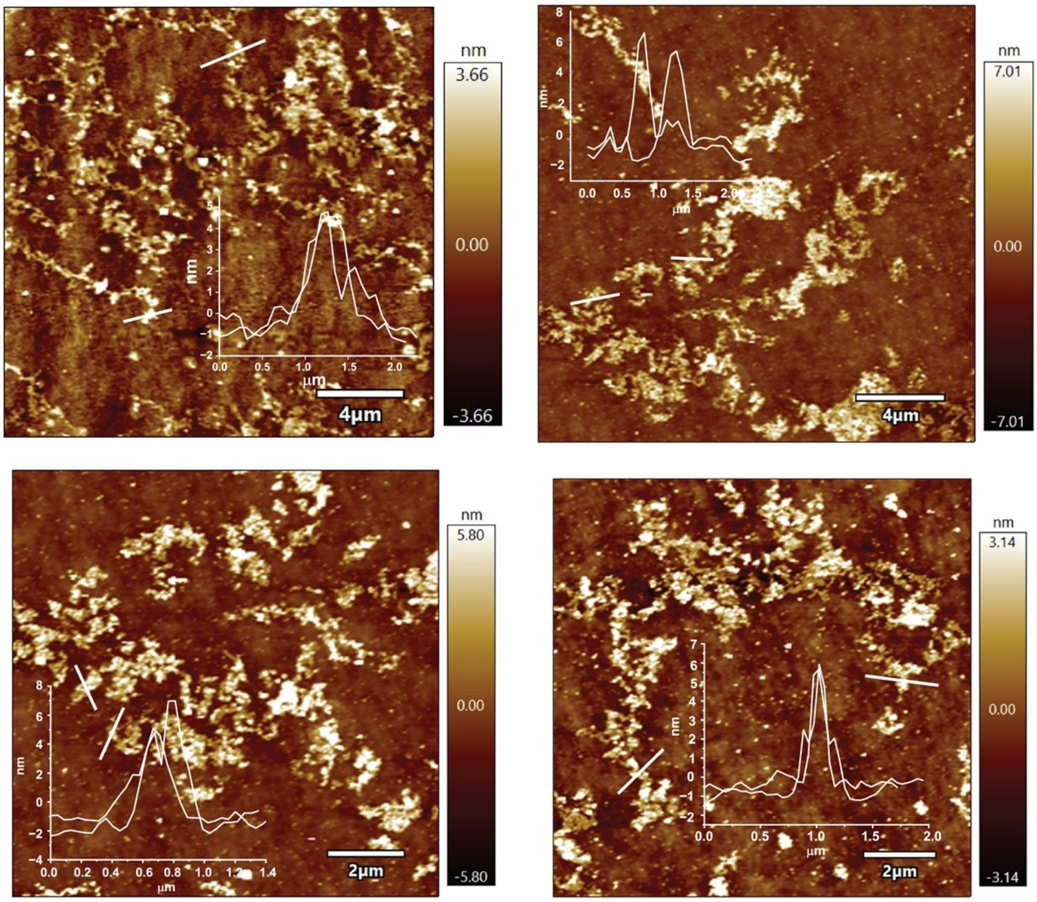


Figure S1. Representative AFM images and corresponding height profile of the diluted system containing **T** (50 mM), **AR** (50 mM), **AA** (10mM), **Cf** (150 μM) and H_2O_2 (30 mM) at 10 min

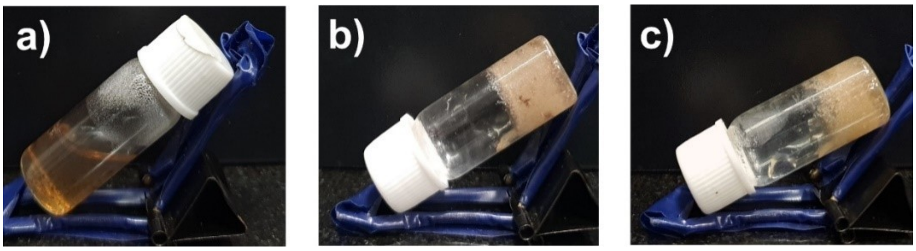


Figure S2. Representative vial images of a system containing **T** (50 mM), **AR** (50 mM), **Cf** (150 μM) and H_2O_2 (30 mM) at (a) ≈ 0 min, (b) 2 min and (c) 12 h, final solvent composition was 98.5: 1.5 H_2O: DMF (v/v).

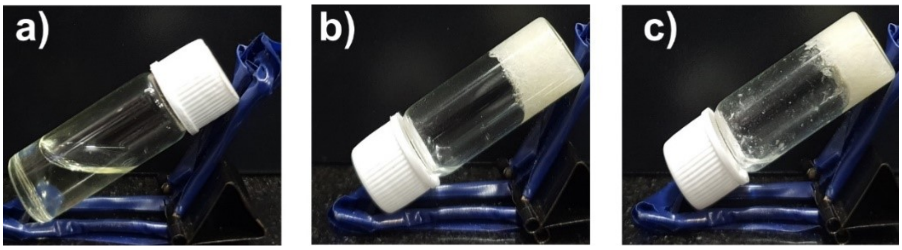


Figure S3. Representative vial images of the sample containing **T** (50 mM), **AR** (50 mM), **AA** (10 mM) and H_2O_2 (30 mM) at (a) ≈ 0 min, (b) 2 min and c) 12 h, final solvent composition was 98.5: 1.5 H_2O: DMF (v/v).

Figure S4. Representative vial image of a sample containing **T** (50 mM) and **AR** (50 mM) after 12h, final solvent composition was 98.5:1.5 H_2O: DMF (v/v).

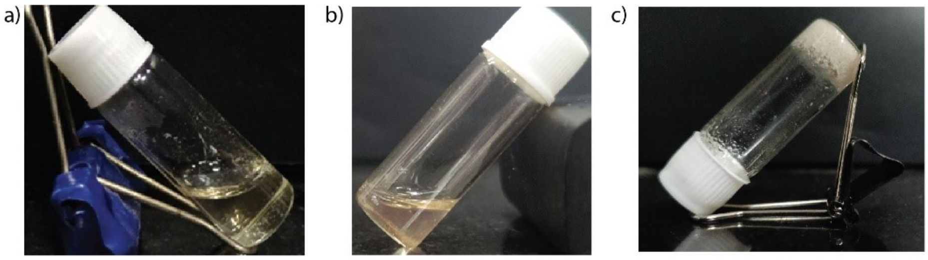


Figure S5. Representative vial images of a sample containing a) **T** (50 mM), **AA** (10 mM), **Cf** (150 μM) and H_2O_2 (30 mM) at 30min and b) **AR** (50 mM), **AA** (10 mM), **Cf** (150 μM) and H_2O_2 (30 mM) at 30min, c) **T** (50 mM), **AR** (50 mM), **AA** (10 mM), **Cf** (150 μM) at 6h; final solvent composition was 98.5:1.5 H_2O: DMF (v/v).

Concentration variation of different components	**T**	10mM	50mM	70mM	50mM	50mM	50mM	50mM	50mM	50mM
	AR	50mM	50mM	50mM	50mM	50mM	50mM	50mM	10mM	70mM
	AA	10mM	10mM	10mM	1mM	20mM	10mM	10mM	10mM	10mM
	Cf	150μM	150μM	150μM	150μM	150μM	10μM	300μM	150μM	150μM
	H_2O_2	30mM	30mM	30mM	30mM	30mM	30mM	30mM	30mM	30mM
	Lifetime (min)	No aggregation	150±15	360±40	Kinetically stable co-assembly	60±6	Kinetically stable co-assembly	90±12	No aggregation	240±60

pH variation	Concentration of components **T**(50mM) **AR**(50mM) **AA**(10mM) **Cf**(150μM) H_2O_2(30mM)			
	Lifetime (min)	pH=2	pH=5	pH≥7
		210±80	150±15	No aggregation

Figure S6. Behavior of the co-assembled systems having varying concentrations of **T**, **AR**, **AA** and **Cf** and at varying pH.

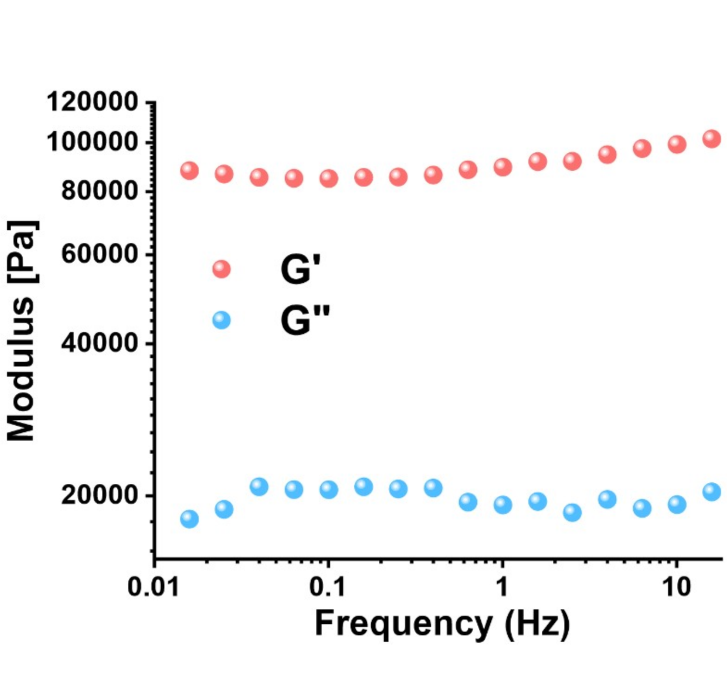


Figure S7. Frequency sweep of the dissipative self-assembled gel containing **T** (50 mM), **AR** (50 mM), **AA** (10 mM), **Cf** (150 μM) and H_2O_2 (30 mM) at t =2 min.

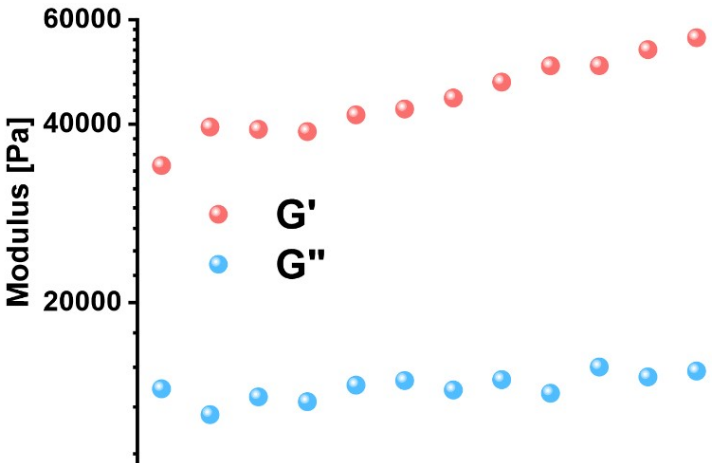


Figure S8. Frequency sweep of the gel containing **T** (50 mM), **AR** (50 mM), **AA** (10 mM) and H_2O_2 (30 mM) at t =10 min.

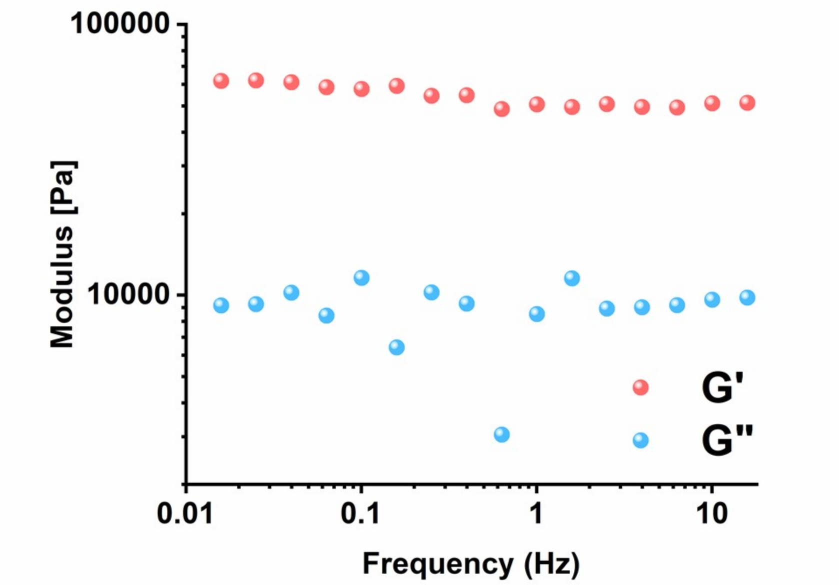


Figure S9. Frequency sweep of the gel containing **T** (50 mM), **AR** (50 mM), **Cf** (150 µM) and H_2O_2 (30 mM) at t =2 min.

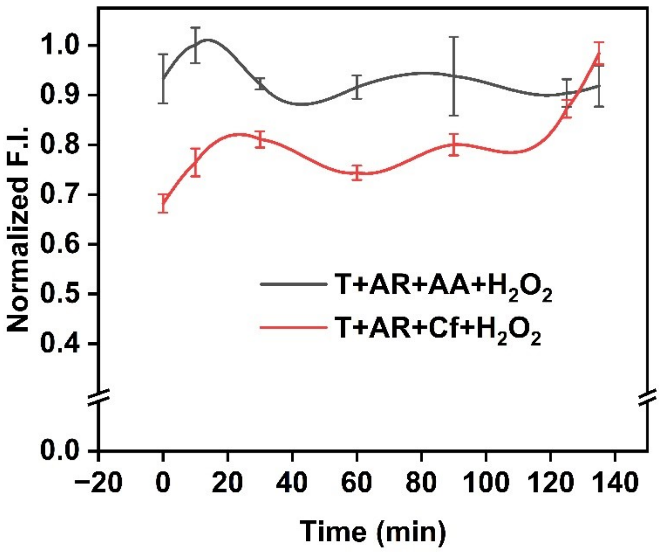


Figure S10: Time dependent fluorescence intensities of Rhodamine 110 in different systems.

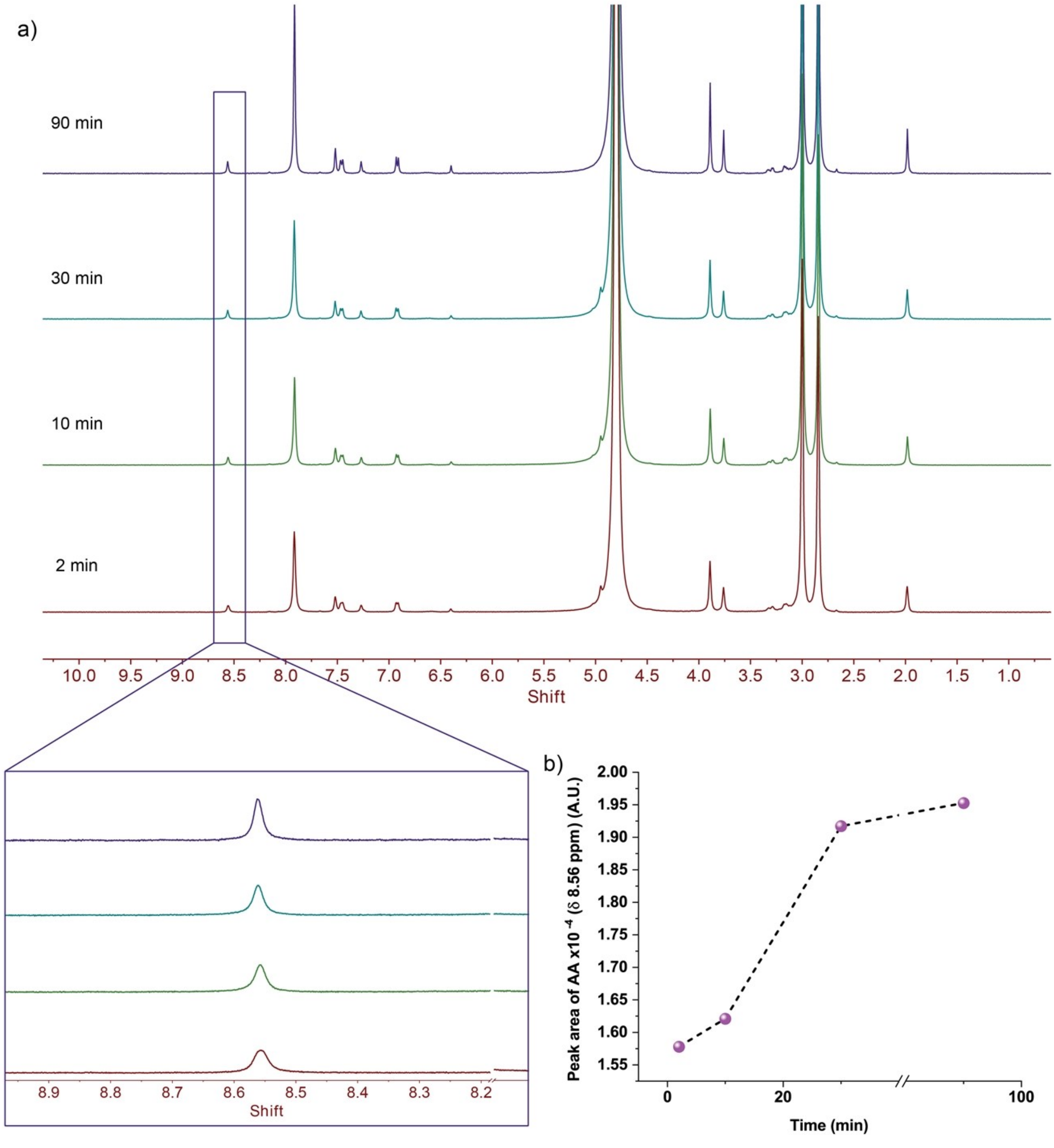


Figure S11: a) Time dependent [1]H-NMR spectra of the dissipative self-assembled system (**T**+**AR**+**AA**+**Cf**+H_2O_2). b) Peak area of the 8.56 ppm peak of **AA** (shown as zoomed) with time.

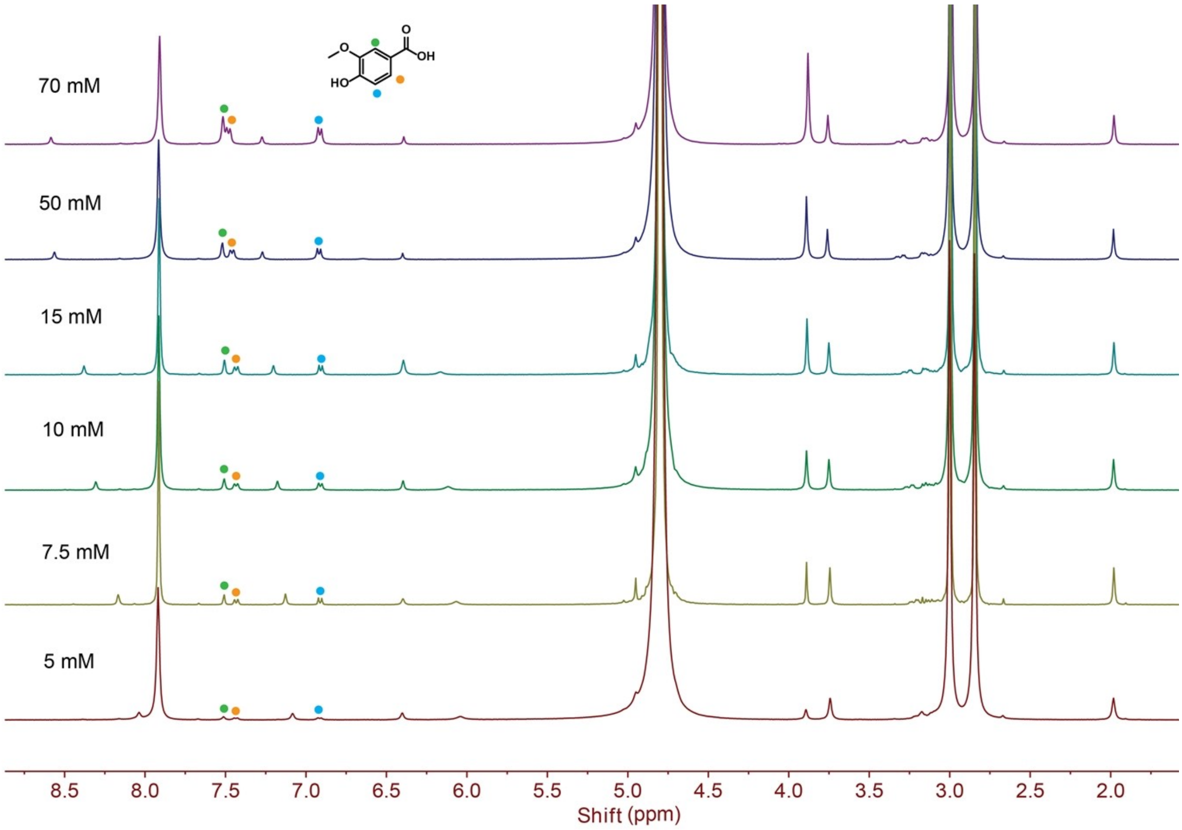


Figure S12: ^{1}H-NMR spectra at age of 10 min of the co-assembled system (**T**+**AR**+**AA**+**Cf**+H_2O_2) with different concentrations of **AR**.

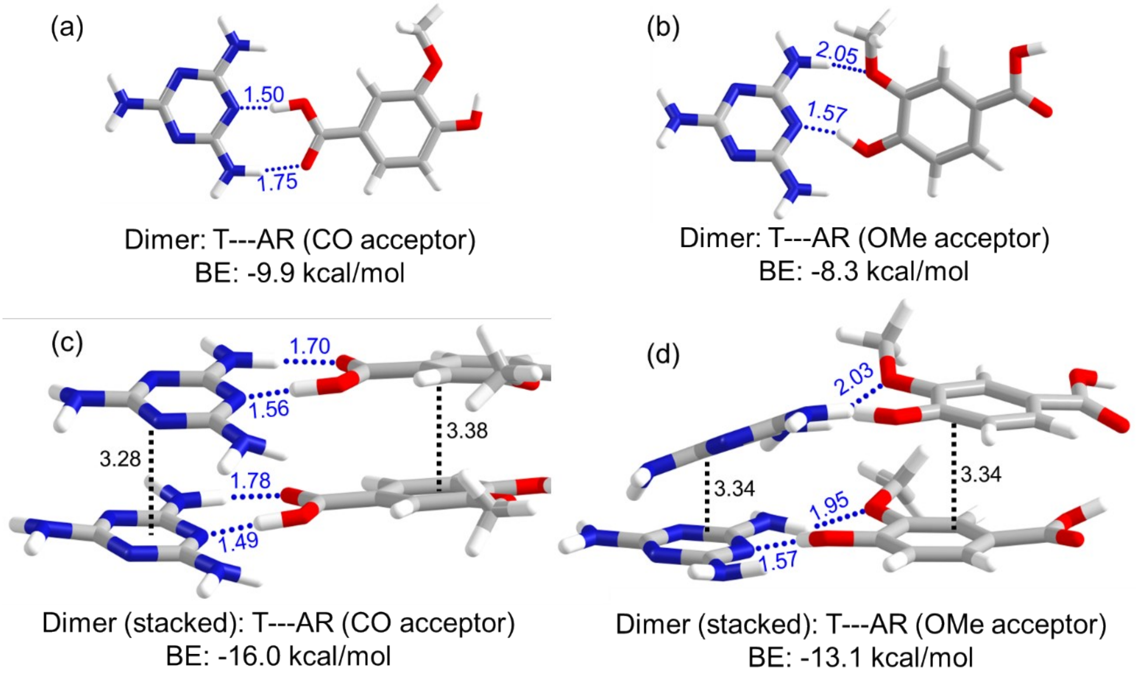


Figure S13. Optimized geometries of computational models with different interaction modes between **T** and **AR**: (a) dimer with CO as H-bond acceptor, (b) dimer with OMe as H-bond acceptor, (c) parallel stacked-dimer with CO as H-bond acceptor and (d) parallel stacked-dimer with OMe as H-bond acceptor. Distances shown are in units of Å; blue colored: H-bond, black colored: π- π stacking distance.

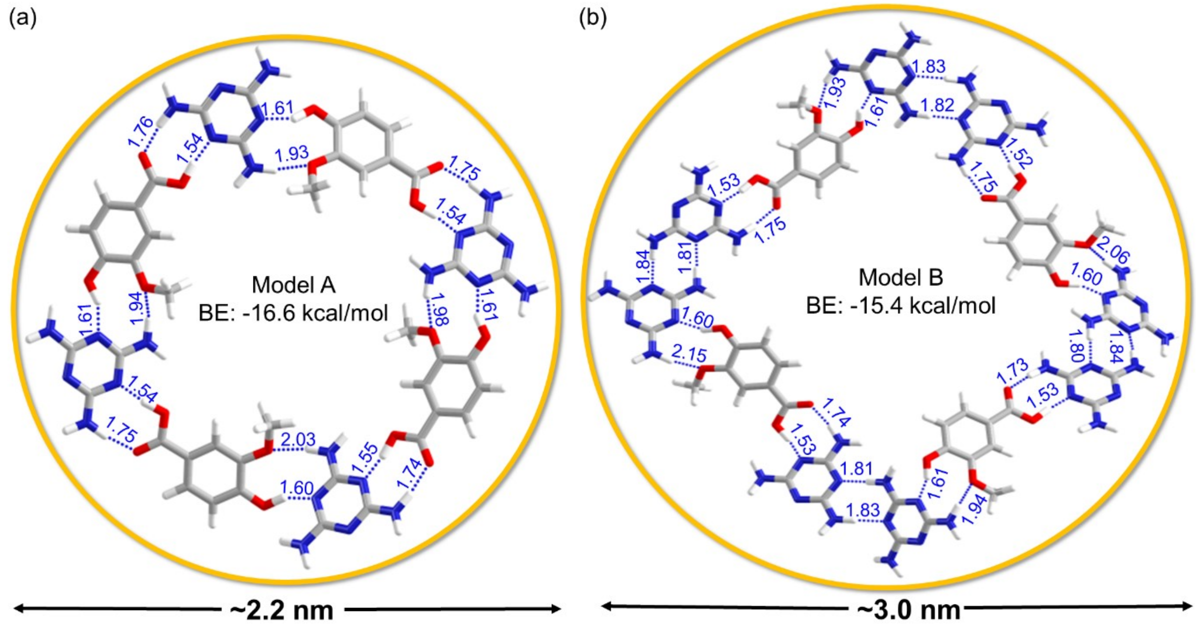


Figure S14. Proposed cyclic rosette geometries: (a) Model A and (b) Model B for **T** and **AR** assembly guided through H-bond networks and its calculated diameter. Energetically, Model A is preferred over Model B and preferably leads to self-assembled structures.

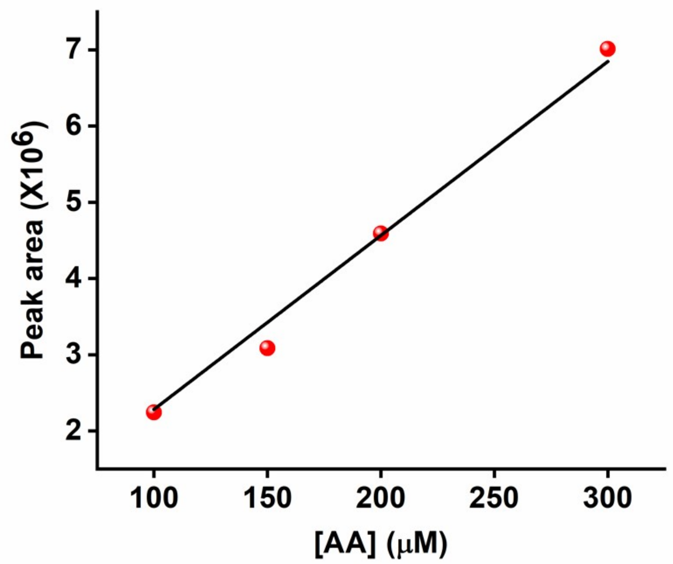


Figure S15: Standard plot of **AA** (λ=220 nm) obtained from HPLC.

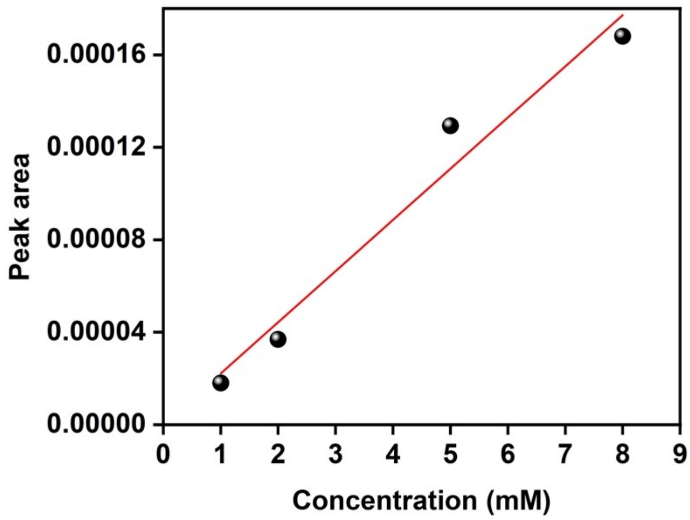


Figure S16: Standard plot of **AA** obtained from ^{1}H-NMR**.**

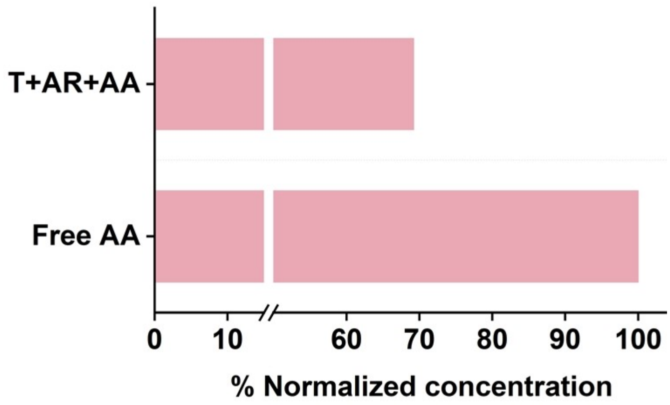


Figure S17: % concentration decrease of **AA** obtained from [1]H-NMR.

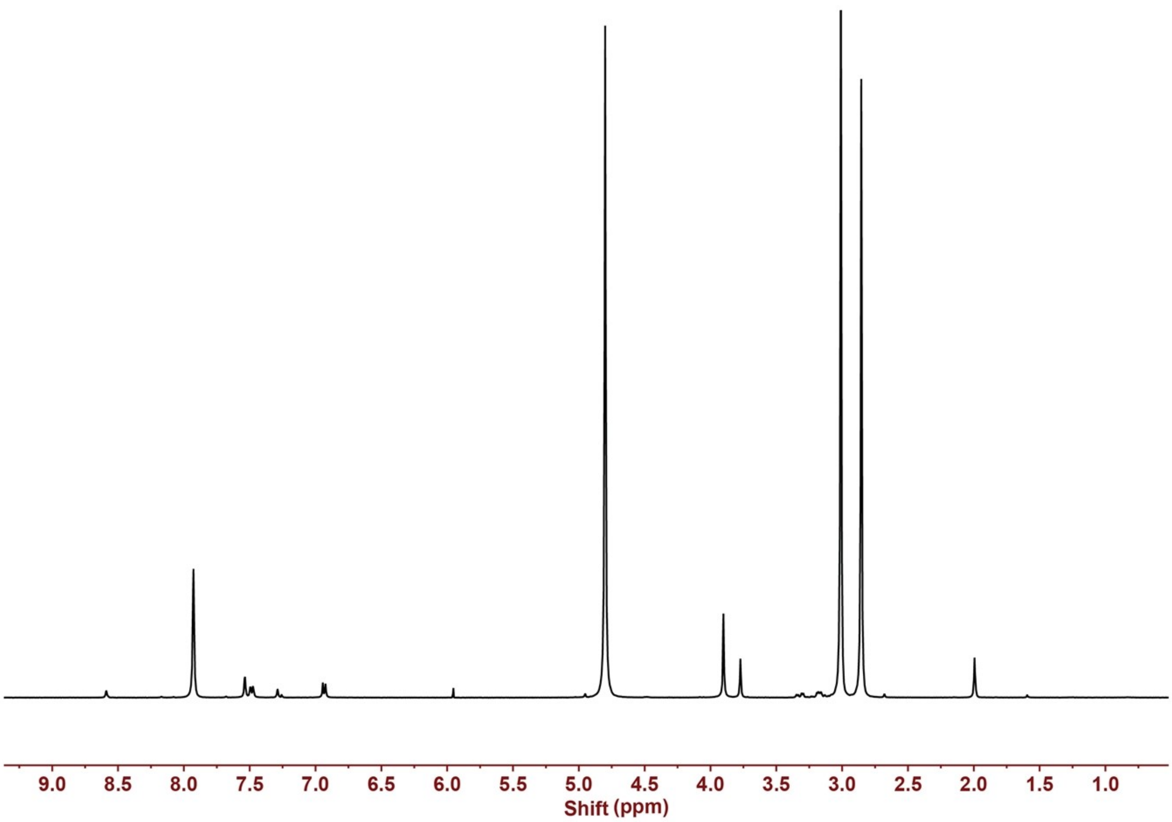


Figure S18: Representative ^{1}H-NMR spectra of **T**+**AR**+**AA** in D_2O (in presence of 1.5% DMF).

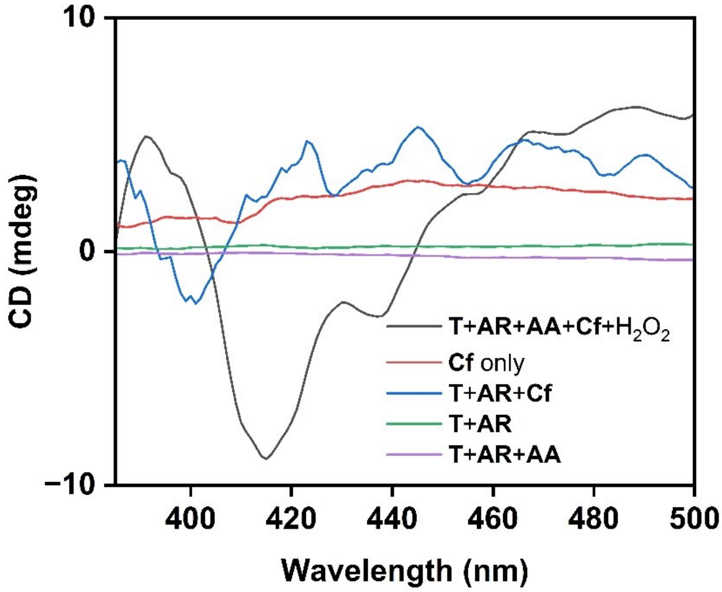


Figure S19: CD spectra of different systems ([**T**]=50 mM, [**AR**]=50 mM, [**AA**]=10 mM, [**Cf**]=900 μM, [H_2O_2] =30 mM).

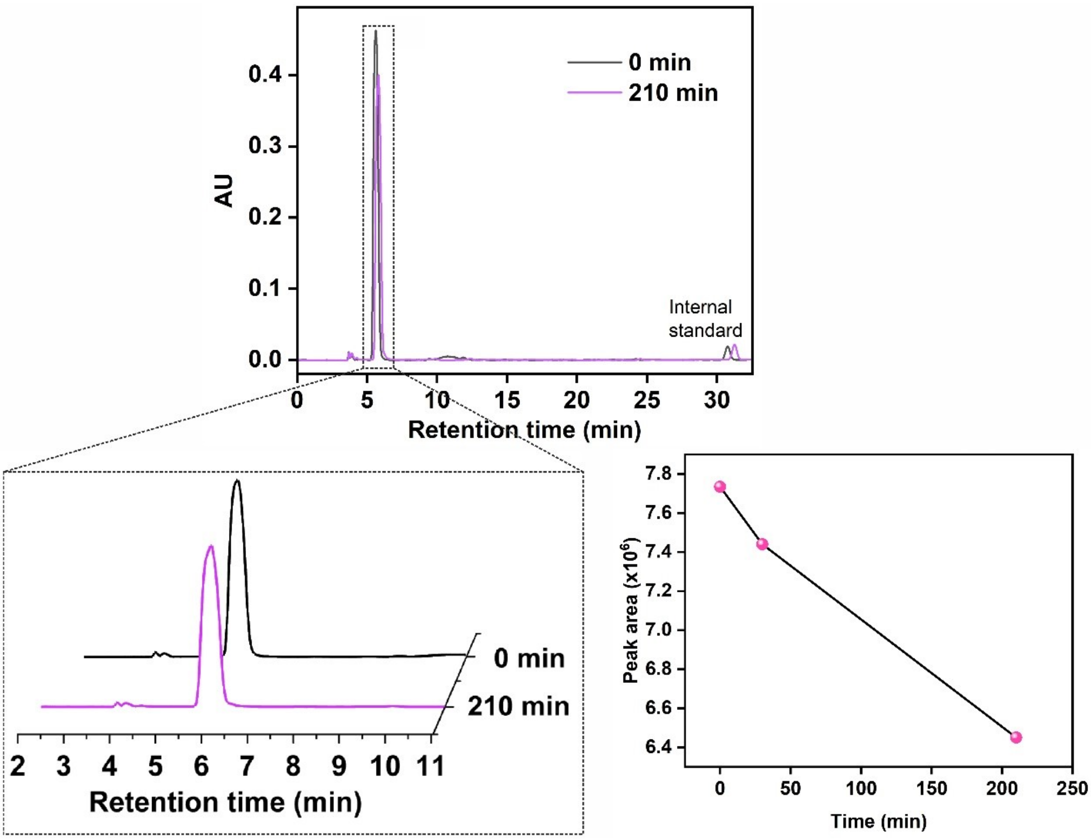


Figure S20: Full HPLC chromatogram and the peak area decrease showing the consumption of **AR** with time.

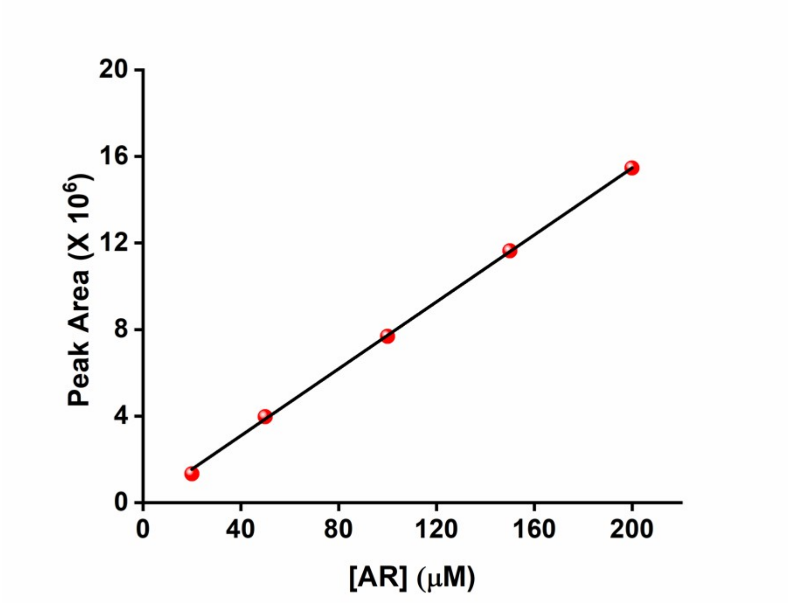


Figure S21. Standard plot of **AR** (λ=260 nm) obtained from HPLC**.**

Figure S22. Representative vial image of a sample containing **T** (50 mM), **AR** (41.8 mM) **AA** (10 mM), **Cf** (150 μM) and H_2O_2 (30 mM) at 10min

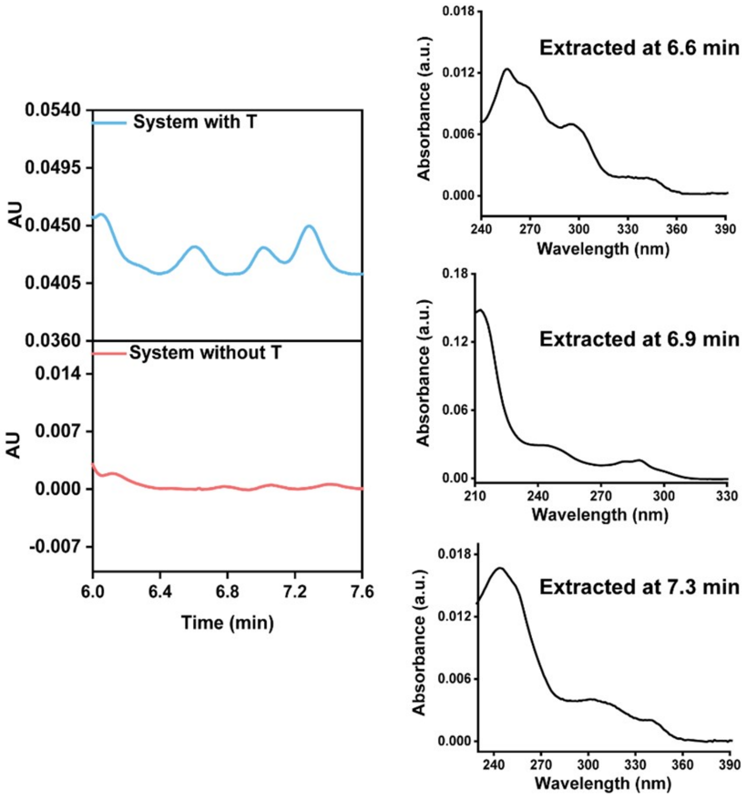


Figure S23. HPLC chromatograms (λ=254 nm) of the samples in presence and absence of **T** after 3.5 h and the UV-Vis spectra of the different peaks generated in presence of **T**. (Solvent system: 0.1% TFA containing acetonitrile-water)

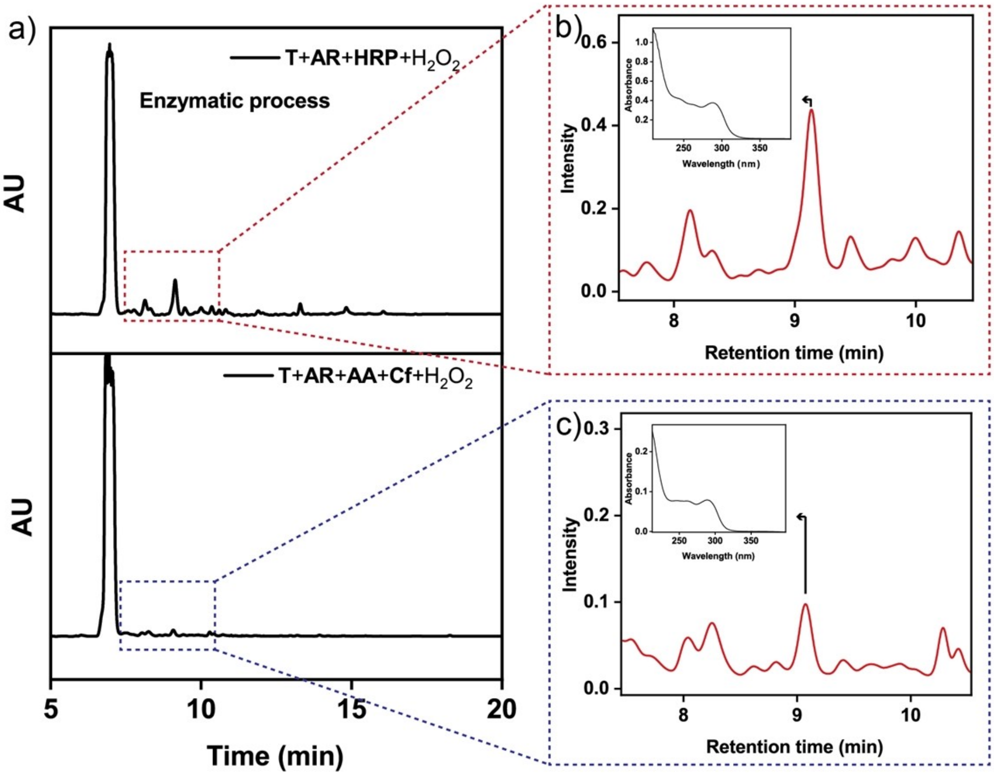


Figure S24. a) Full HPLC chromatograms (λ= 254 nm) and corresponding UV-Vis spectra (inset) of the oxidation products of **AR** in zoomed images (b) in presence of horseradish peroxidase (HRP, 50 μM) and H_2O_2 (30 mM) and (c) co-assembled system (**T**+**AR**+**AA**+**Cf**+H_2O_2) (Solvent system: 0.1% formic acid containing water-0.1% TFA containing acetonitrile).

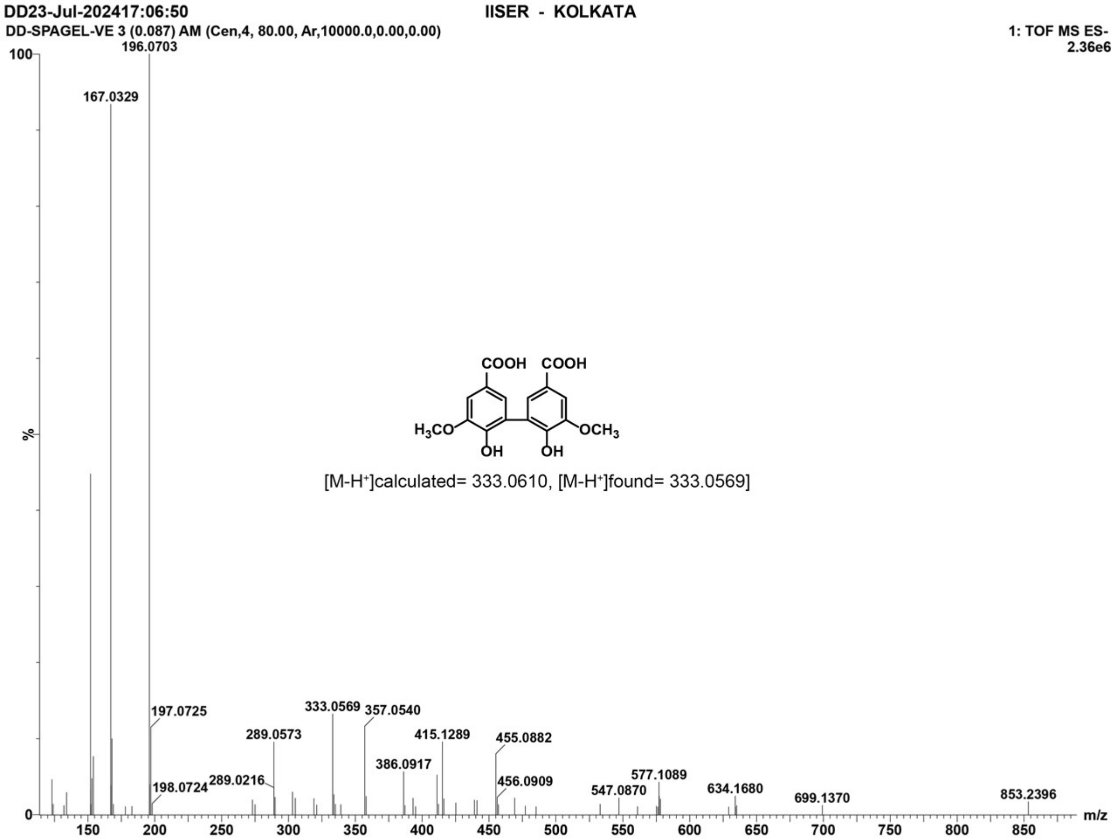


Figure S25: HRMS spectrum of the dissipative system (**T**+**AR**+**AA**+**Cf**+H_2O_2).

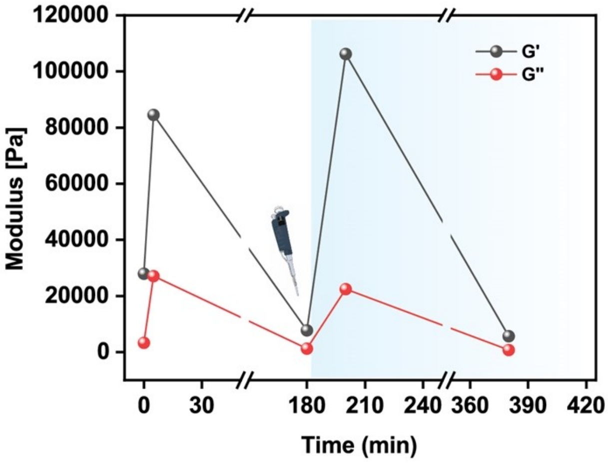


Figure S26. Rheology showing an additional cycle of dissipative (dis)assembly fueled by addition of **AR** after the first cycle.

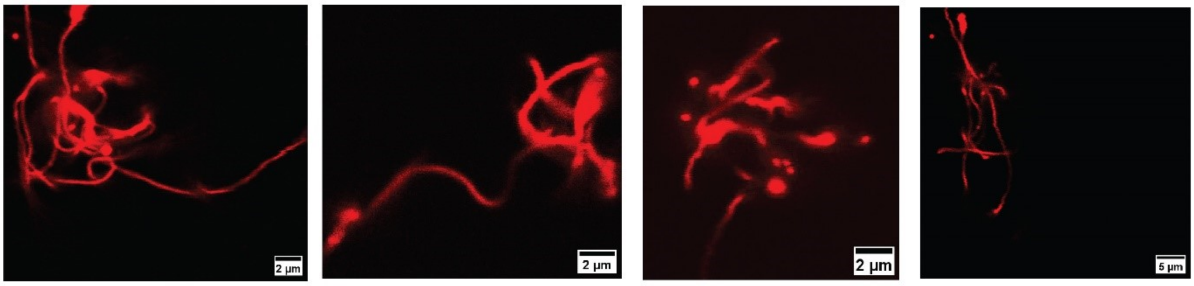


Figure S27. Representative CLSM images of the dissipative assemblies at t=2 min incubated with Nile red.

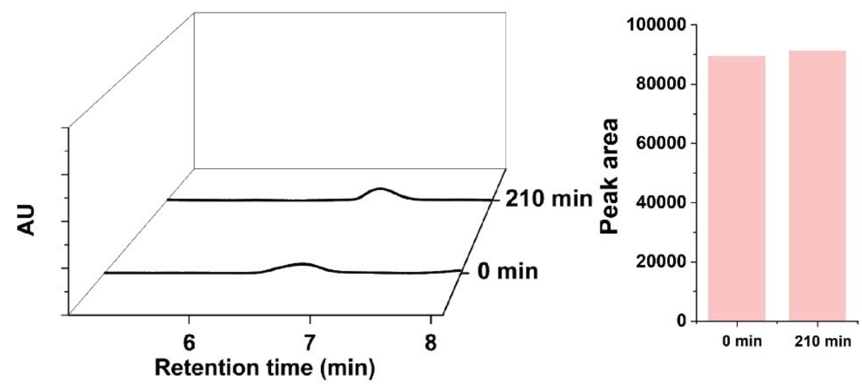


Figure S28: HPLC chromatograms showing negligible generation of 7-hydroxycoumarin from **Pro-AR** at pH 5.32.

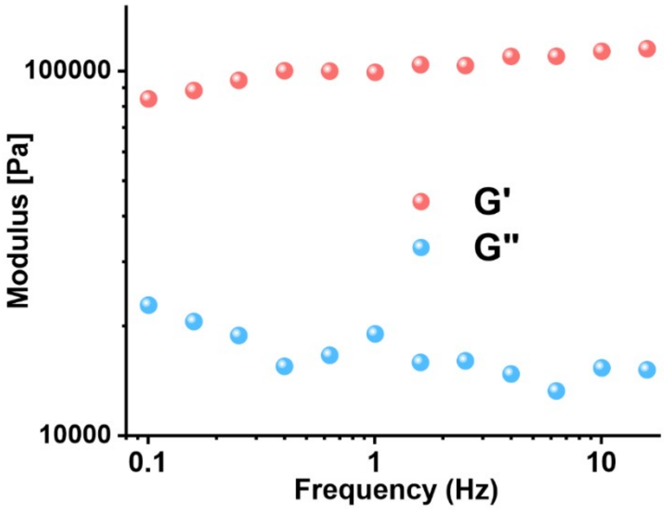


Figure S29. Frequency sweep of the gel containing **T** (50 mM), **AR** (50 mM), **AA** (10 mM), **Cf** (150 μM), H_2O_2 (30 mM) and **Pro-AR** (10 mM) at t=2 min.

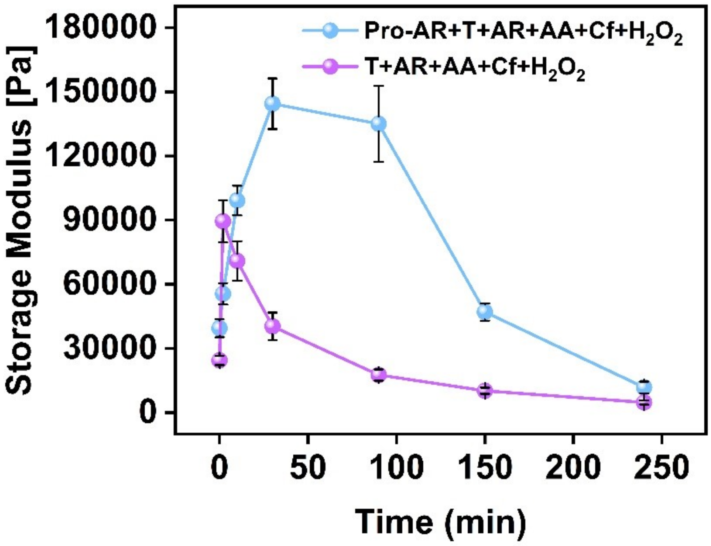


Figure S30. Time dependent changes of storage modulus in the dissipative self-assembled systems in the presence and absence of **Pro-AR**.

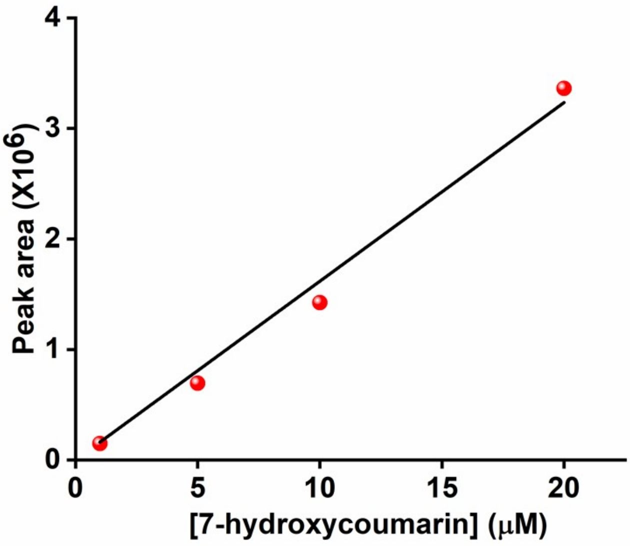


Figure S31. Standard plot (λ=324 nm) of 7-hydroxycoumarin obtained from HPLC.

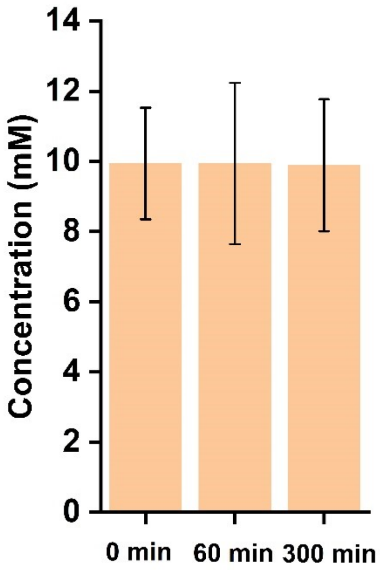


Figure S32. Bar diagram of concentration of **AA** in the system (**T**+**AR**+**AA**+**Cf**+H_2O_2) with time.

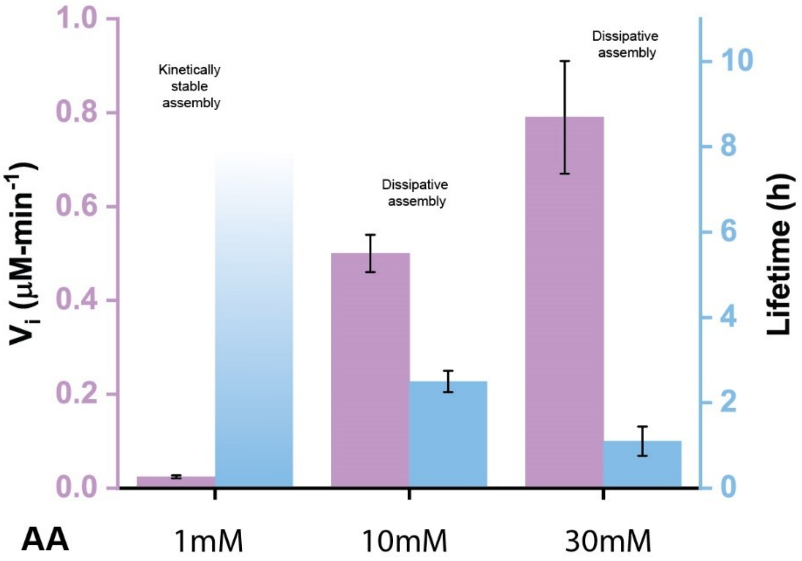


Figure S33. Bar diagram of rate of hydrolysis of **Pro-AR** with different concentrations of **AA** (**T**=50 mM, **AR**=50 mM, **Cf**=150 µM, H_2O_2=30 mM)**.** The kinetically stable co-assembly shown with a fading bar implies a lifetime of more than 48 h.

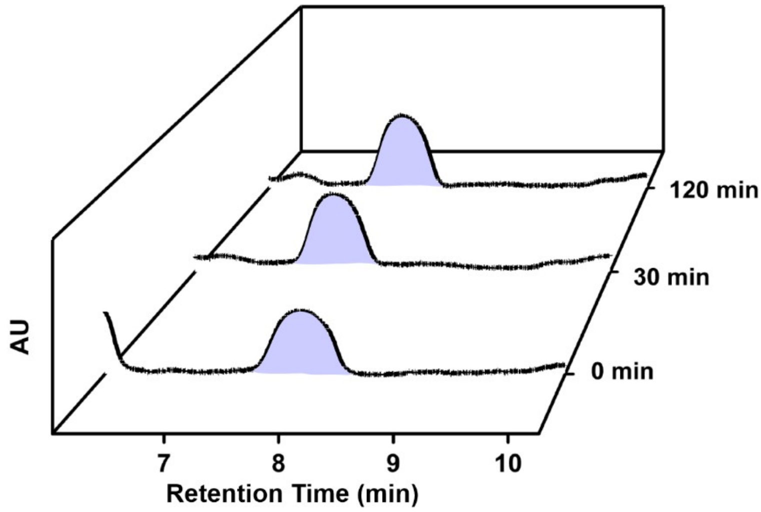


Figure S34. HPLC chromatograms showing the release of 7-hydroxycoumarin due to the hydrolysis of **Pro-AR** (10 mM) in presence of **AA** (10 mM), **AR** (50 mM), **Cf** (150 μM) and H_2O_2 (30 mM) in absence of **T** (**AA**+**AR**+**Cf**+**Pro-AR**+H_2O_2, no assemblies).

XYZ coordinates of optimized geometries:

T (triazine amine)

N	0.007015000	0.003081000	-0.018862000
H	-0.455577000	0.760117000	-0.515383000
H	0.472396000	-0.753081000	-0.514111000
C	0.003392000	0.001646000	1.343376000
N	0.631796000	-1.026155000	1.953746000
C	0.589445000	-0.964587000	3.302185000
N	1.204625000	-1.971053000	3.983543000
H	1.663159000	-2.714463000	3.463269000
H	1.194694000	-1.959800000	5.000121000
N	-0.003760000	-0.001722000	4.040076000
C	-0.593405000	0.962827000	3.301392000
N	-0.628302000	1.027734000	1.952991000
N	-1.211382000	1.968088000	3.981959000
H	-1.667107000	2.712566000	3.460708000
H	-1.206987000	1.954802000	4.998539000

AR

C	-0.019740000	-0.038563000	2.341274000
C	0.103215000	-0.738205000	3.566438000
H	0.276488000	-1.820381000	3.537643000
C	-0.241749000	1.349395000	2.345882000
H	-0.334065000	1.874780000	1.385102000
C	-0.340436000	2.033232000	3.564581000
H	-0.514717000	3.122109000	3.579003000
C	-0.220159000	1.350631000	4.787285000
O	-0.306625000	1.960418000	5.996772000
H	-0.460177000	2.912701000	5.846852000
C	0.005924000	-0.060385000	4.788143000
O	0.109751000	-0.634834000	6.016559000
C	0.339325000	-2.032021000	6.072550000
H	1.297043000	-2.313004000	5.579070000
H	-0.487347000	-2.606097000	5.596313000
H	0.392974000	-2.296560000	7.144616000
C	0.079995000	-0.730573000	1.031489000
O	-0.013921000	-0.191515000	-0.061349000
O	0.294447000	-2.075059000	1.155417000
H	0.340291000	-2.407298000	0.233165000

Dimer: T---AR (CO acceptor)

C	-7.525850000	9.405421000	29.775336000
N	-8.478740000	9.279166000	28.829006000
C	-9.740188000	9.224569000	29.301455000
N	-10.735321000	9.095443000	28.384638000
H	-10.497836000	9.068966000	27.395999000
H	-11.701868000	9.072015000	28.700044000
N	-10.120365000	9.280692000	30.601271000
C	-9.098686000	9.409300000	31.461996000
N	-7.790300000	9.479051000	31.114683000
N	-9.388436000	9.482753000	32.788984000

H	-8.637224000	9.526606000	33.475553000
H	-10.358634000	9.387110000	33.078944000
N	-6.235416000	9.465115000	29.404103000
H	-5.486347000	9.535332000	30.129661000
H	-6.031235000	9.397227000	28.409148000
C	-3.869045000	9.805713000	33.839565000
C	-4.331033000	9.924343000	35.172877000
H	-5.412873000	9.942646000	35.353749000
C	-2.486479000	9.781843000	33.576729000
H	-2.158773000	9.689670000	32.531656000
C	-1.558473000	9.874100000	34.623285000
H	-0.474936000	9.856940000	34.436929000
C	-2.007794000	9.992095000	35.947478000
O	-1.136149000	10.083928000	36.980829000
H	-1.689081000	10.155211000	37.790050000
C	-3.407175000	10.016448000	36.214514000
O	-3.696777000	10.135136000	37.553908000
C	-4.828778000	9.705853000	32.700825000
O	-4.430430000	9.606975000	31.527937000
O	-6.105916000	9.733730000	33.048016000
H	-6.744608000	9.641113000	32.179866000
C	-5.060986000	10.176655000	37.938072000
H	-5.584588000	11.047599000	37.484660000
H	-5.594645000	9.245500000	37.644052000
H	-5.077833000	10.273986000	39.039199000

Dimer: T---AR (OMe acceptor)

C	-3.366906000	11.596324000	22.785845000
C	-4.656318000	11.424033000	22.228882000
H	-4.766811000	11.464226000	21.138385000
C	-3.205510000	11.539975000	24.184598000
H	-2.197468000	11.674218000	24.602318000
C	-4.310890000	11.326399000	25.010428000
H	-4.207430000	11.288601000	26.104892000
C	-5.610214000	11.163925000	24.477052000
O	-6.635137000	10.975600000	25.314590000
H	-7.599498000	10.993805000	24.896677000
C	-5.761783000	11.201423000	23.054379000
O	-7.044725000	11.013204000	22.585009000
C	-2.175074000	11.836798000	21.940852000
O	-1.032741000	11.990026000	22.350042000
O	-2.467158000	11.875057000	20.602832000
H	-1.603106000	12.037045000	20.167119000
C	-7.319902000	11.402358000	21.246320000
H	-7.017870000	12.456910000	21.065759000
H	-6.802234000	10.750523000	20.507614000
H	-8.413839000	11.303084000	21.116722000
H	-10.288762000	9.342763000	22.468256000
H	-8.614012000	9.742599000	22.939422000
N	-9.622668000	9.756622000	23.116469000
C	-10.088748000	10.607452000	24.066147000
N	-11.416891000	10.785931000	24.172424000
C	-11.784706000	11.633836000	25.160822000
N	-13.116003000	11.862082000	25.305999000

H	-13.772883000	11.361136000	24.712521000
H	-13.436301000	12.461389000	26.062972000
N	-10.959478000	12.278871000	26.015860000
C	-9.653798000	12.024464000	25.818862000
H	-9.086452000	13.173021000	27.413582000
H	-7.763244000	12.342909000	26.556408000
N	-8.745453000	12.625325000	26.626812000
N	-9.160161000	11.205346000	24.852736000

Stacked-Dimer: T---AR (CO acceptor)

C	-5.597481000	6.590501000	24.345933000
C	-4.681145000	7.077350000	25.307965000
H	-5.067468000	7.456496000	26.261626000
C	-5.126909000	6.114588000	23.106984000
H	-5.865507000	5.763322000	22.374067000
C	-3.757408000	6.101490000	22.821916000
H	-3.371291000	5.740675000	21.858069000
C	-2.842241000	6.587894000	23.767267000
O	-1.515472000	6.613789000	23.501671000
H	-1.093347000	7.090771000	24.249745000
C	-3.317635000	7.084059000	25.013091000
O	-2.311452000	7.553352000	25.825030000
C	-7.060150000	6.557206000	24.604142000
O	-7.859343000	6.185591000	23.732340000
O	-7.434449000	6.923327000	25.831699000
H	-8.475648000	6.749745000	25.949419000
C	-2.681645000	8.120335000	27.067581000
H	-3.399847000	8.957240000	26.925435000
H	-3.145934000	7.361710000	27.736752000
H	-1.755689000	8.506176000	27.530650000
H	-11.289935000	6.212385000	23.391580000
H	-9.556086000	6.137566000	23.879962000
N	-10.576782000	6.132592000	24.114515000
C	-10.960477000	6.402860000	25.370951000
N	-12.278066000	6.539400000	25.638556000
C	-12.562877000	6.867749000	26.907803000
N	-13.874384000	7.157431000	27.189591000
H	-14.565871000	6.813419000	26.522957000
H	-14.132534000	7.194994000	28.175822000
N	-11.686849000	6.976429000	27.932044000
C	-10.408709000	6.804412000	27.565744000
H	-9.777007000	6.975594000	29.495410000
H	-8.513277000	6.614649000	28.339027000
N	-9.447890000	6.978211000	28.530068000
N	-9.978489000	6.523045000	26.316945000
C	-4.544747000	9.770730000	23.255436000
C	-3.945914000	10.348717000	24.399959000
H	-4.597502000	10.709081000	25.205962000
C	-3.737990000	9.317085000	22.197907000
H	-4.231775000	8.880295000	21.319232000
C	-2.340575000	9.389867000	22.284194000
H	-1.692722000	9.006688000	21.483800000
C	-1.740224000	9.917517000	23.435682000
O	-0.389348000	9.949326000	23.578523000

H	-0.229043000	10.407076000	24.433465000
C	-2.557164000	10.425390000	24.482662000
O	-1.833867000	10.942372000	25.539222000
C	-6.023892000	9.586580000	23.189987000
O	-6.590300000	9.174242000	22.164709000
O	-6.645692000	9.887064000	24.317989000
H	-7.701509000	9.670225000	24.257920000
C	-2.517518000	11.783272000	26.455325000
H	-3.047319000	12.606861000	25.928344000
H	-3.259961000	11.218154000	27.062171000
H	-1.752166000	12.206301000	27.132237000
H	-10.013399000	9.014459000	21.283134000
H	-8.367558000	9.067464000	22.029319000
N	-9.409567000	9.100337000	22.097746000
C	-9.995652000	9.264154000	23.296628000
N	-11.342810000	9.275837000	23.384800000
C	-11.824767000	9.433123000	24.635332000
N	-13.180479000	9.498905000	24.779452000
H	-13.721609000	9.160305000	23.984016000
H	-13.537263000	9.282870000	25.713489000
N	-11.093077000	9.537189000	25.771957000
C	-9.766786000	9.506356000	25.578485000
H	-9.383975000	9.397040000	27.563562000
H	-8.001671000	9.221357000	26.532500000
N	-8.943115000	9.601293000	26.664941000
N	-9.165387000	9.401249000	24.370034000

Stacked-Dimer: T---AR (OMe acceptor)

C	-9.049842000	8.626469000	11.057856000
C	-7.809197000	8.824142000	11.699193000
H	-6.905982000	8.466239000	11.192349000
C	-10.233289000	9.031809000	11.703072000
H	-11.193598000	8.847421000	11.201118000
C	-10.173218000	9.625560000	12.964322000
H	-11.085069000	9.938175000	13.493538000
C	-8.942576000	9.824966000	13.626588000
O	-8.956789000	10.364007000	14.856790000
H	-8.084561000	10.793207000	15.205999000
C	-7.748024000	9.406775000	12.969400000
O	-6.564365000	9.572302000	13.672150000
C	-9.150631000	7.858857000	9.789758000
O	-10.204125000	7.498753000	9.282790000
O	-7.935464000	7.535449000	9.268223000
H	-8.081889000	6.761217000	8.671332000
C	-5.410200000	8.932225000	13.140496000
H	-5.605699000	7.858130000	12.940833000
H	-5.066314000	9.414208000	12.198606000
H	-4.619854000	9.025193000	13.909834000
H	-4.142199000	11.433293000	15.752903000
H	-5.543569000	10.949447000	14.767044000
N	-5.138161000	11.238098000	15.663953000
C	-5.982764000	11.835889000	16.555000000
N	-5.455004000	12.376863000	17.663365000
C	-6.373745000	12.829340000	18.544539000

N	-5.903084000	13.358548000	19.702661000
H	-4.897708000	13.410062000	19.849399000
H	-6.553663000	13.765876000	20.369887000
N	-7.717068000	12.791984000	18.388223000
C	-8.127956000	12.266067000	17.215439000
H	-10.083635000	12.369452000	17.748907000
H	-9.762421000	11.610961000	16.187283000
N	-9.458424000	12.216908000	16.959594000
N	-7.297843000	11.789163000	16.250887000
C	-7.744075000	5.142278000	11.390197000
C	-6.980071000	5.435370000	12.545848000
H	-5.894556000	5.275656000	12.519225000
C	-9.143064000	5.314329000	11.426063000
H	-9.732258000	5.088683000	10.527178000
C	-9.762138000	5.805293000	12.575288000
H	-10.849093000	5.961941000	12.610351000
C	-9.012603000	6.165952000	13.717750000
O	-9.639503000	6.671789000	14.777083000
H	-9.063841000	7.068765000	15.568900000
C	-7.598636000	5.952396000	13.684788000
O	-6.919439000	6.312986000	14.829949000
C	-7.100391000	4.743631000	10.124962000
O	-7.633764000	4.754930000	9.016074000
O	-5.793624000	4.377200000	10.269860000
H	-5.487315000	4.183713000	9.357505000
C	-5.673270000	5.681928000	15.095152000
H	-5.768763000	4.576357000	15.038160000
H	-4.877505000	6.008361000	14.388519000
H	-5.389314000	5.985529000	16.120000000
H	-5.996123000	9.269083000	16.741979000
H	-6.735295000	8.019968000	15.752318000
N	-6.680537000	8.516196000	16.649112000
C	-7.858833000	8.665518000	17.307036000
N	-7.929527000	9.568710000	18.300941000
C	-9.148203000	9.683643000	18.873038000
N	-9.281363000	10.628456000	19.850671000
H	-8.628632000	11.422733000	19.795707000
H	-10.236733000	10.810423000	20.158256000
N	-10.247150000	8.962953000	18.556898000
C	-10.060833000	8.072821000	17.564600000
H	-12.031090000	7.569026000	17.557034000
H	-11.057021000	6.816063000	16.285064000
N	-11.120733000	7.315207000	17.177820000
N	-8.886858000	7.871634000	16.910763000

Model A

N	0.081104000	-0.497040000	0.614357000
H	-0.931436000	-0.450514000	0.762472000
H	0.478715000	-0.566920000	-0.319886000
C	0.910331000	-0.193255000	1.641359000
N	2.228556000	-0.109880000	1.395057000
C	2.995242000	0.180485000	2.468356000
N	4.324204000	0.289272000	2.315881000
H	4.702891000	0.162136000	1.379215000

H	4.916741000	0.578484000	3.128755000	C	5.928271000	1.046612000	7.015168000
N	2.504575000	0.378180000	3.730095000	C	5.354732000	0.731785000	8.267911000
C	1.165062000	0.298797000	3.866472000	H	4.320402000	0.366880000	8.287055000
N	0.321523000	0.002604000	2.855861000	C	7.254799000	1.516867000	6.964369000
N	0.627223000	0.535674000	5.085783000	H	7.690595000	1.752283000	5.983032000
H	-0.385959000	0.411156000	5.194638000	C	7.991101000	1.671639000	8.141667000
H	1.236084000	0.786772000	5.862712000	H	9.028956000	2.035848000	8.122887000
C	-5.632248000	-0.817203000	4.636788000	C	7.440803000	1.349535000	9.402933000
C	-4.353480000	-0.933347000	5.226701000	O	8.196157000	1.503695000	10.498985000
H	-4.290345000	-1.252027000	6.274735000	H	7.801908000	1.132167000	11.388411000
C	-5.733773000	-0.416171000	3.289975000	C	6.092413000	0.876498000	9.446068000
H	-6.734061000	-0.337560000	2.840857000	O	5.597526000	0.573624000	10.700082000
C	-4.583477000	-0.122701000	2.553822000	C	4.463403000	-0.280637000	10.765078000
H	-4.643583000	0.195832000	1.502675000	H	4.627847000	-1.209543000	10.177193000
C	-3.295243000	-0.230118000	3.126260000	H	3.541465000	0.220085000	10.393467000
O	-2.225229000	0.060846000	2.377437000	H	4.330859000	-0.537985000	11.832848000
H	-1.292047000	-0.013381000	2.831618000	C	5.158185000	0.874523000	5.754232000
C	-3.201534000	-0.651282000	4.488604000	O	5.677810000	1.045685000	4.638875000
O	-1.920510000	-0.761602000	4.999908000	O	3.888666000	0.519553000	5.926335000
C	-1.730529000	-1.636432000	6.105720000	H	3.394609000	0.463331000	4.987845000
H	-2.168166000	-2.637049000	5.900425000	C	8.279029000	-0.574988000	15.307518000
H	-2.179691000	-1.233444000	7.040729000	N	9.293880000	-0.611891000	14.416810000
H	-0.636414000	-1.729207000	6.241557000	C	9.026994000	-0.055209000	13.223942000
C	-6.866255000	-1.102601000	5.416293000	N	9.991597000	-0.061973000	12.274648000
O	-7.992592000	-1.087525000	4.892475000	H	10.904961000	-0.443514000	12.510155000
O	-6.658983000	-1.368451000	6.702602000	H	9.817166000	0.418313000	11.386399000
H	-7.591020000	-1.454025000	7.207022000	N	7.842980000	0.524349000	12.873759000

C	6.894491000	0.529562000	13.831534000	H	4.862597000	-1.851920000	20.148235000
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N	5.712864000	1.127889000	13.539877000	H	2.739285000	-2.195568000	21.498911000
H	4.954173000	1.091812000	14.219070000	C	1.448475000	-1.366266000	19.989330000
H	5.544495000	1.379860000	12.560580000	O	0.359919000	-1.567592000	20.742025000
N	8.452667000	-1.119942000	16.520980000	H	-0.548449000	-1.251925000	20.343005000
H	7.660093000	-1.130830000	17.204965000	C	1.396931000	-0.783969000	18.684700000
H	9.347049000	-1.567723000	16.712290000	O	0.136204000	-0.446990000	18.228643000
H	-11.210519000	-1.982158000	5.991146000	C	5.073172000	-0.782383000	17.692825000
H	-9.465153000	-1.602523000	5.708269000	O	6.176320000	-1.157019000	18.124284000
N	-10.263656000	-1.844524000	6.340120000	O	4.907264000	-0.199810000	16.509280000
C	-10.103351000	-1.735293000	7.668719000	H	5.833844000	-0.137829000	15.995547000
N	-11.174088000	-1.877378000	8.479433000	C	0.048773000	0.507846000	17.179489000
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N	-11.944942000	-1.876769000	10.665659000	H	0.425272000	0.103339000	16.213316000
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H	-11.795702000	-1.619874000	11.645824000	H	-3.230954000	-1.445147000	17.377525000
N	-9.697717000	-1.462625000	10.331896000	H	-1.563068000	-1.447736000	18.018329000
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H	-7.352980000	-0.948402000	10.945939000	C	-3.018427000	-0.989562000	19.370539000
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N	-7.462127000	-1.025022000	9.927580000	C	-4.725083000	-0.318375000	20.769077000
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C	3.821719000	-0.968048000	18.474096000	H	-6.671761000	-0.072940000	20.103860000
C	2.567348000	-0.581888000	17.949252000	H	-6.326512000	0.301430000	21.841021000
H	2.538362000	-0.129450000	16.950226000	N	-3.887207000	-0.182523000	21.820194000
C	3.880636000	-1.554702000	19.753573000	C	-2.600816000	-0.472897000	21.565016000

H	-2.041472000	-0.145443000	23.505107000
H	-0.738935000	-0.678582000	22.412220000
N	-1.701350000	-0.367647000	22.572069000
N	-2.106433000	-0.861678000	20.355639000
C	-7.851513000	-0.690418000	16.270242000
C	-7.297004000	-1.204031000	15.075881000
H	-6.262749000	-1.569846000	15.095514000
C	-9.180387000	-0.222526000	16.265079000
H	-9.599884000	0.170616000	17.202052000
C	-9.937036000	-0.259231000	15.091472000
H	-10.976288000	0.100419000	15.069464000
C	-9.399514000	-0.764182000	13.885320000
O	-10.164948000	-0.781254000	12.788489000
H	-9.720260000	-1.102059000	11.904345000
C	-8.052031000	-1.240440000	13.901380000
O	-7.574226000	-1.729044000	12.698365000
C	-6.488684000	-2.647229000	12.744921000
H	-6.703894000	-3.481797000	13.446406000
H	-5.538056000	-2.156596000	13.051725000
H	-6.375081000	-3.043082000	11.718091000
C	-7.053115000	-0.623886000	17.523004000
O	-7.533136000	-0.191247000	18.584165000
O	-5.801318000	-1.055123000	17.406423000
H	-5.282313000	-0.923293000	18.324145000

Model B

C	2.779822000	9.746789000	20.030603000
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C	3.851331000	10.179002000	18.045948000
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H	5.720922000	11.110296000	17.906321000
H	4.902255000	10.603970000	16.373172000
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C	1.763980000	9.288341000	18.015224000
N	1.675696000	9.301986000	19.368369000
N	0.680788000	8.819753000	17.338860000
H	-0.098247000	8.408839000	17.851206000
H	0.740706000	8.738628000	16.326629000
N	2.730562000	9.728605000	21.374427000
H	1.914888000	9.273372000	21.849185000
H	3.534382000	10.070486000	21.896376000
C	-1.838795000	7.882096000	22.282331000
C	-3.032654000	7.916170000	21.526184000
H	-2.980721000	8.294672000	20.498061000
C	-1.873085000	7.395709000	23.603056000
H	-0.938403000	7.379280000	24.181374000
C	-3.078279000	6.954075000	24.156486000
H	-3.127096000	6.571323000	25.186856000
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C	-4.241678000	7.485417000	22.080835000
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C	-0.554751000	8.365491000	21.706583000

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O	-0.614114000	8.696629000	20.421733000	N	-9.909572000	9.916264000	29.518399000
H	0.353142000	8.973549000	20.064121000	C	-9.018891000	9.967761000	30.518288000
C	-5.501372000	8.252016000	20.201790000	N	-7.675161000	9.854190000	30.376753000
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H	-6.562831000	8.257873000	19.891042000	H	-10.491539000	10.149467000	31.927203000
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H	-7.323141000	6.455907000	21.260668000	H	-5.301154000	9.370026000	29.806049000
N	-8.295918000	6.765629000	21.331244000	H	-5.534691000	9.307318000	28.020629000
C	-8.632920000	7.523230000	22.408514000	C	-4.405970000	9.145188000	33.758913000
N	-9.806013000	8.186029000	22.375952000	C	-5.004038000	9.517189000	34.984238000
C	-10.074903000	8.884411000	23.498036000	H	-5.982338000	10.013320000	34.956928000
N	-11.253250000	9.573128000	23.525522000	C	-3.146848000	8.512871000	33.774174000
H	-11.766450000	9.650975000	22.648867000	H	-2.689999000	8.233630000	32.814008000
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N	-9.299675000	8.951262000	24.602229000	H	-1.523092000	7.752550000	35.017192000
C	-8.133242000	8.257627000	24.533411000	C	-3.089842000	8.604164000	36.223663000
H	-7.552345000	8.787149000	26.470927000	O	-2.436509000	8.325602000	37.356123000
H	-6.459396000	7.694237000	25.509699000	H	-2.901897000	8.574252000	38.253866000
N	-7.302096000	8.274121000	25.585691000	C	-4.361924000	9.255573000	36.196588000
N	-7.759785000	7.537935000	23.438618000	O	-4.887136000	9.597276000	37.430324000
C	-7.226726000	9.636857000	29.109645000	C	-5.093577000	9.389174000	32.462626000
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C	-9.369703000	9.723844000	28.289000000	O	-6.304209000	9.926807000	32.568420000
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H	-5.491118000	11.540630000	36.934457000	N	8.342067000	11.911620000	20.872010000
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H	-6.018169000	10.871016000	38.535267000	H	10.390154000	12.808918000	21.923906000
H	-6.133055000	8.472171000	40.618747000	H	10.831058000	13.951937000	20.610991000
H	-5.330000000	8.585881000	39.019244000	N	10.222930000	13.239501000	21.007074000
N	-5.295653000	8.508134000	40.042458000	N	8.955920000	13.369224000	19.069270000
C	-4.095066000	8.629494000	40.657384000	H	15.013522000	9.650569000	27.380511000
N	-4.075695000	8.657970000	42.006340000	H	16.676056000	9.524000000	27.981075000
C	-2.840293000	8.732373000	42.537458000	N	15.674050000	9.418727000	28.120537000
N	-2.751019000	8.745517000	43.899945000	C	15.223977000	9.089369000	29.360781000
H	-3.616614000	8.869117000	44.422670000	N	13.878857000	9.012572000	29.520013000
H	-1.870084000	9.034274000	44.322355000	C	13.448363000	8.693749000	30.772740000
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C	-1.801710000	8.757871000	40.497909000	H	11.469983000	8.827625000	30.170092000
H	0.260272000	8.787553000	40.214883000	H	11.779476000	8.333763000	31.881131000
H	-0.791163000	8.680110000	38.741491000	N	14.283708000	8.461829000	31.809437000
N	-0.684637000	8.800469000	39.753110000	C	15.612387000	8.541349000	31.528473000
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H	6.702897000	13.267831000	16.774923000	H	17.461802000	8.430234000	32.339878000
H	8.175951000	14.212028000	16.892155000	N	16.472432000	8.287767000	32.535260000
N	7.629841000	13.400010000	17.176370000	N	16.134362000	8.858045000	30.317665000
C	7.866742000	12.903550000	18.426739000	C	10.285108000	9.960740000	26.489854000
N	6.998743000	11.979543000	18.893310000	C	10.880025000	10.365492000	25.273213000
C	7.260498000	11.520421000	20.145254000	H	11.974916000	10.358818000	25.201547000
N	6.415999000	10.631099000	20.693479000	C	8.880766000	9.962756000	26.602810000
H	5.490014000	10.432840000	20.231863000	H	8.432756000	9.645361000	27.555106000
H	6.596544000	10.366468000	21.666320000	C	8.087305000	10.359586000	25.524319000

H	6.989375000	10.362135000	25.591822000	H	13.498583000	8.869384000	39.219974000
C	8.661569000	10.769015000	24.299105000	H	15.010022000	8.115527000	39.790496000
O	7.855607000	11.134855000	23.296475000	C	8.046976000	9.642332000	38.295969000
H	8.307079000	11.442720000	22.409144000	C	9.145268000	8.917274000	38.812276000
C	10.087436000	10.769924000	24.196144000	H	8.961407000	8.216459000	39.635851000
O	10.598470000	11.188304000	22.980904000	C	8.258280000	10.552788000	37.242485000
C	11.921491000	10.789149000	22.648899000	H	7.395313000	11.109206000	36.850008000
H	12.043215000	9.689059000	22.751576000	C	9.538787000	10.729386000	36.711719000
H	12.683454000	11.294660000	23.283520000	H	9.723310000	11.428964000	35.883001000
H	12.076818000	11.084486000	21.594050000	C	10.648030000	10.006352000	37.205978000
C	11.111906000	9.549022000	27.655458000	O	11.852053000	10.207052000	36.654664000
O	10.592831000	9.207187000	28.732224000	H	12.606904000	9.546527000	36.940556000
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H	12.948789000	9.314230000	28.340962000	O	11.546079000	8.429076000	38.747208000
N	13.527208000	8.875362000	34.528247000	C	11.336150000	7.268267000	39.536626000
H	12.728592000	9.455374000	34.804268000	H	10.666499000	6.546534000	39.019862000
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C	14.322515000	8.432933000	35.514126000	H	12.332048000	6.808662000	39.681258000
N	15.457283000	7.759594000	35.188503000	C	6.677283000	9.457860000	38.847431000
C	16.195354000	7.336026000	36.237658000	O	5.700346000	10.079557000	38.395177000
N	17.343188000	6.655500000	35.950164000	O	6.594054000	8.587123000	39.846123000
H	17.462799000	6.284673000	35.008965000	H	5.588082000	8.528674000	40.206153000
H	17.825976000	6.205917000	36.726407000	H	2.270558000	10.136614000	39.085746000
N	15.918735000	7.539941000	37.541661000	H	4.049031000	9.870044000	38.940695000
C	14.783845000	8.234012000	37.761435000	N	3.118977000	9.650837000	39.369415000
N	13.948503000	8.684328000	36.798829000	C	3.066304000	8.859919000	40.456341000
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C	1.923639000	7.845747000	42.170030000
N	0.766012000	7.632610000	42.825369000
H	-0.131512000	8.069799000	42.502439000
H	0.797600000	6.988595000	43.613703000
N	3.041214000	7.256953000	42.664327000
C	4.160687000	7.517592000	41.975599000
H	5.298165000	6.371848000	43.239026000
H	6.196615000	7.151751000	41.924490000
N	5.319429000	6.946783000	42.400349000
N	4.239680000	8.313015000	40.879766000

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