Effect of the Dynamical Disorder on the Second-Order Nonlinear Optical Responses in Helicity-Encoded Polymer Strands

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Supporting Information

CONTENTS

Definition of the calculated NLO responses

HRS response

In the case of plane-polarized incident light and observation made perpendicular to the propagation plane without polarization analysis of the scattered beam, the second-order NLO response that can be extracted from HRS data reads:

$$\beta_{HRS}(-2\omega;\omega,\omega) = \sqrt{\left\{\left\langle\beta_{ZZZ}^2\right\rangle + \left\langle\beta_{XZZ}^2\right\rangle\right\}} \tag{1}$$

while the associated depolarization ratio (DR) is given by:

$$DR = \frac{\left\langle\beta_{ZZZ}^2\right\rangle}{\left\langle\beta_{XZZ}^2\right\rangle} \tag{2}$$

$\left\langle\beta_{ZZZ}^2\right\rangle$ and $\left\langle\beta_{XZZ}^2\right\rangle$ correspond to orientational averages of β tensor:

$$\begin{aligned}\left\langle\beta_{ZZZ}^2\right\rangle = {} & \frac{1}{7}\sum_{\zeta}^{x,y,z}\beta_{\zeta\zeta\zeta}^2 + \frac{4}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\eta}^2 + \frac{2}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\zeta}\beta_{\zeta\eta\eta} + \frac{4}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\eta\zeta\zeta}\beta_{\zeta\zeta\eta} + \frac{4}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\zeta}\beta_{\eta\eta\zeta} + \frac{1}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\eta\zeta\zeta}^2 \\ & + \frac{4}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\zeta\eta}\beta_{\eta\xi\xi} + \frac{1}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\eta\zeta\zeta}\beta_{\eta\xi\xi} + \frac{4}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\zeta\eta}\beta_{\xi\xi\eta} + \frac{2}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\eta\xi}^2 + \frac{4}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\eta\xi}\beta_{\eta\zeta\xi}\end{aligned} \tag{3}$$

$$\begin{aligned}\left\langle\beta_{XZZ}^2\right\rangle = {} & \frac{1}{35}\sum_{\zeta}^{x,y,z}\beta_{\zeta\zeta\zeta}^2 + \frac{4}{105}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\zeta}\beta_{\zeta\eta\eta} - \frac{2}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\zeta}\beta_{\eta\eta\zeta} + \frac{8}{105}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\eta}^2 + \frac{3}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\eta\eta}^2 - \frac{2}{35}\sum_{\zeta\neq\eta}^{x,y,z}\beta_{\zeta\zeta\eta}\beta_{\eta\zeta\zeta} \\ & + \frac{1}{35}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\eta\eta}\beta_{\zeta\xi\xi} - \frac{2}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\zeta\xi}\beta_{\eta\eta\xi} - \frac{2}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\zeta\eta}\beta_{\eta\xi\xi} + \frac{2}{35}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\eta\xi}^2 - \frac{2}{105}\sum_{\zeta\neq\eta\neq\xi}^{x,y,z}\beta_{\zeta\eta\xi}\beta_{\eta\zeta\xi}\end{aligned} \tag{4}$$

The depolarization ratio gives information on the geometry of the part of the molecule responsible for the NLO response (for an ideal D/A 1D system DR = 5, for an octupolar molecule, DR = 1.5 whereas for a Λ-shape molecule, the amplitude of DR depends on the angle between the chromophore as well as on the D/A groups [1]).

EFISHG response

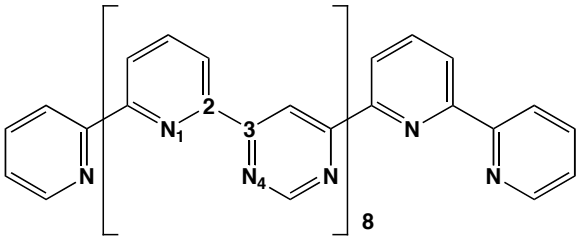
The EFISHG measurements give information on the projection of the vector part of β on the dipole moment vector:

$$\beta_{//}(-2\omega;\omega,\omega) = \beta_{//} = \frac{3}{5}\sum_{\zeta}^{x,y,z}\frac{\mu_\zeta}{\|\mu\|}\sum_{\eta}^{x,y,z}(\beta_{\zeta\eta\eta} + \beta_{\eta\zeta\eta} + \beta_{\eta\eta\zeta}) = \frac{3}{5}\sum_{\zeta}^{x,y,z}\frac{\mu_\zeta\beta_\zeta}{\|\mu\|} \tag{5}$$

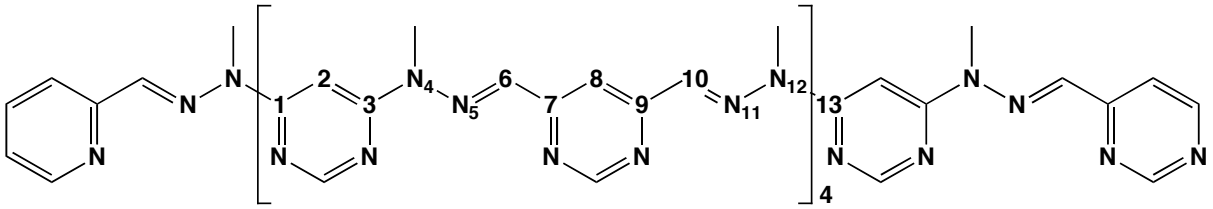
where $\|\mu\|$ is the norm of the dipole moment and μ_i and β_i the components of the μ and β vectors. The Taylor series expansion convention[2] was employed to define β while 1 a.u. of β = 3.6213 10^{-42} m^4 V^{-1} = 3.20636 10^{-53} C^3 m^3 J^{-2} = 8.6392 10^{-33} esu.

[1] M. Yang and B. Champagne, *J. Phys. Chem. A*, **2003**, *107*, 3942.
[2] Shelton, D.P.; Rice, J.E. *Chem. Rev.* **1994**, *94*, 3.

Atom labeling

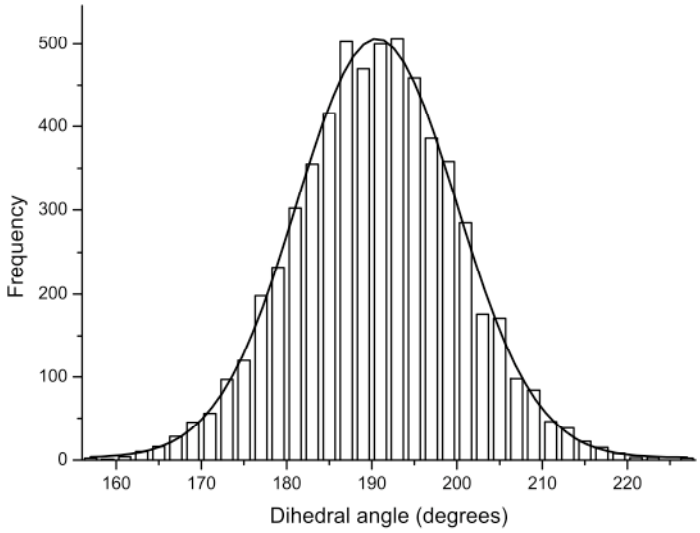


[S1] Atom labeling in the pyridine-pyrimidine foldamer.

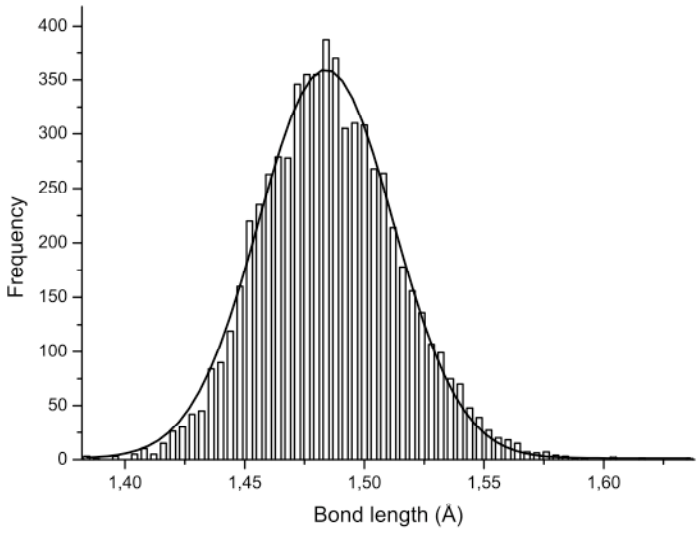


[S2] Atom labeling in the hydrazone-pyrimidine foldamer.

Geometrical parameters in the pyridine-pyrimidine foldamer

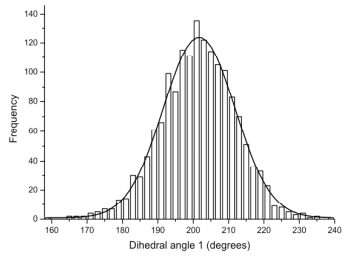


[S3] Distribution of the dihedral angles 1-2-3-4 in the pyridine-pyrimidine foldamer. Atom labeling refers to Figure S1. Mean value = 190.6°; Standard deviation σ = 18.8°; Correlation coefficient R^2 = 0.995.



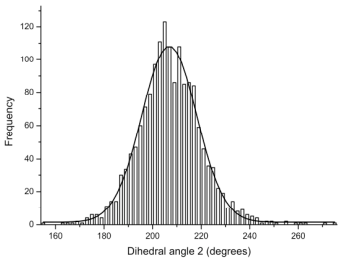
[S4] Distribution of the bond lengths 2-3 in the pyridine-pyrimidine foldamer. Atom labeling refers to Figure S1. Mean value = 1.484 Å; Standard deviation σ = 0.056 Å; Correlation coefficient R^2 = 0.992.

Geometrical parameters in the hydrazone-pyrimidine foldamer



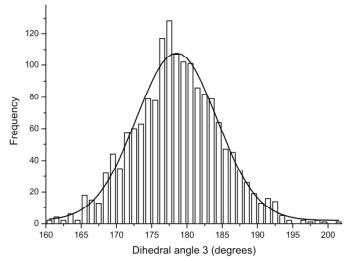
1-2-3-4

Mean = 201.7°
σ = 20.3°
R^2 = 0.989



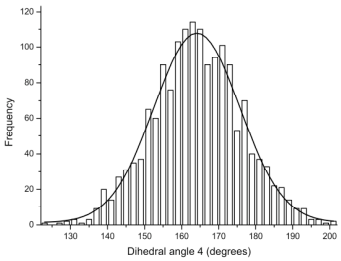
2-3-4-5

Mean = 206.9°
σ = 22.6°
R^2 = 0.983



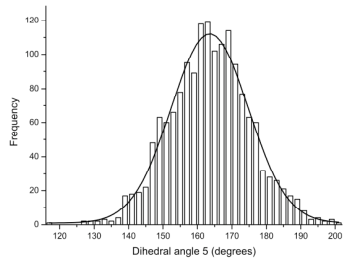
3-4-5-6

Mean = 178.5°
σ = 11.5°
R^2 = 0.970



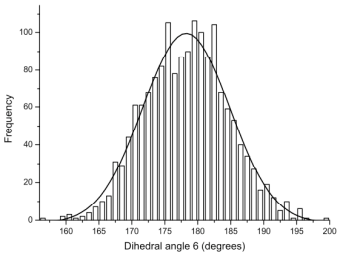
4-5-6-7

Mean = 164.1°
σ = 23.3°
R^2 = 0.971



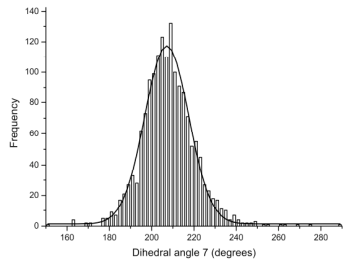
7-8-9-10

Mean = 163.6°
σ = 22.45°
R^2 = 0.979



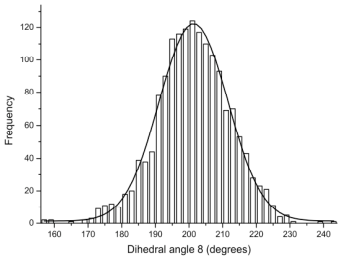
8-9-10-11

Mean = 178.2°
σ = 13.2°
R^2 = 0.968



9-10-11-12

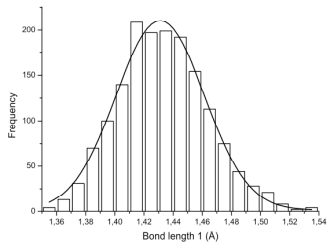
Mean = 207.1°
σ = 20.7°
R^2 = 0.984



10-11-12-13

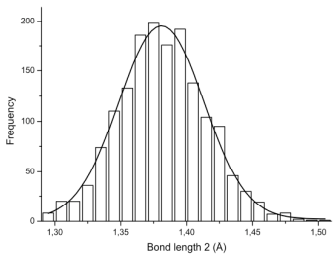
Mean = 201.4°
σ = 20.4°
R^2 = 0.989

[S5] Distribution of the dihedral angles in the hydrazone-pyrimidine foldamer. Atom labeling refers to Figure S1.



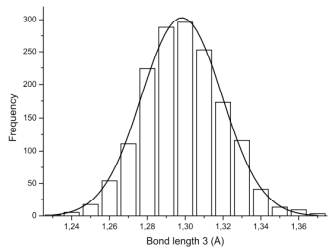
3-4

Mean = 1.431 Å
σ = 0.060 Å
R^2 = 0.989



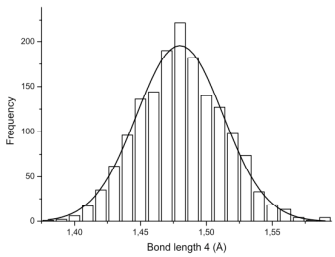
4-5

Mean = 1.381 Å
σ = 0.064 Å
R^2 = 0.986



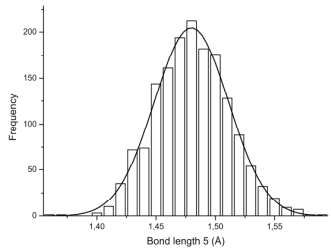
5-6

Mean = 1.298 Å
σ = 0.042 Å
R^2 = 0.994



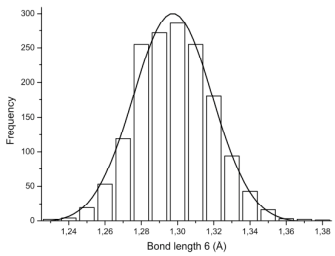
6-7

Mean = 1.480 Å
σ = 0.066 Å
R^2 = 0.983



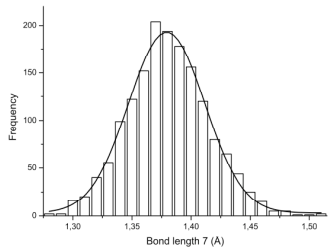
9-10

Mean = 1.480 Å
σ = 0.063 Å
R^2 = 0.991



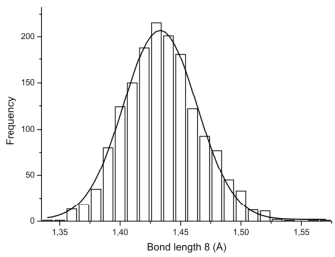
10-11

Mean = 1.297 Å
σ = 0.043 Å
R^2 = 0.989



11-12

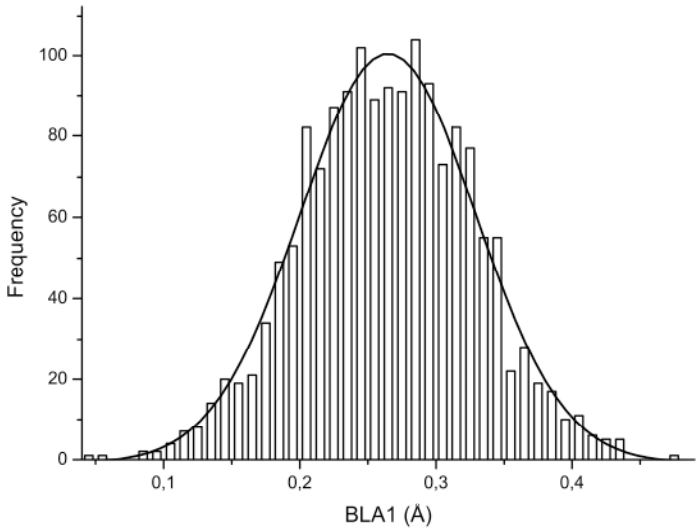
Mean = 1.379 Å
σ = 0.064 Å
R^2 = 0.992



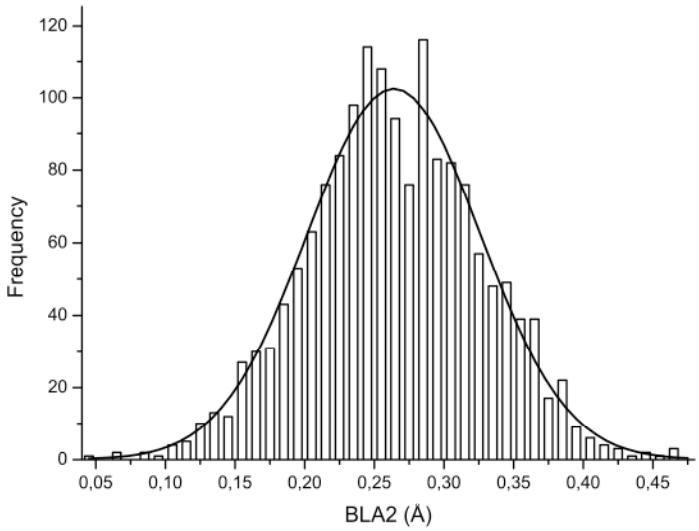
12-13

Mean = 1.433 Å
σ = 0.061 Å
R^2 = 0.990

[S6] Distribution of the bond lengths in the hydrazone-pyrimidine foldamer. Atom labeling refers to Figure S1.

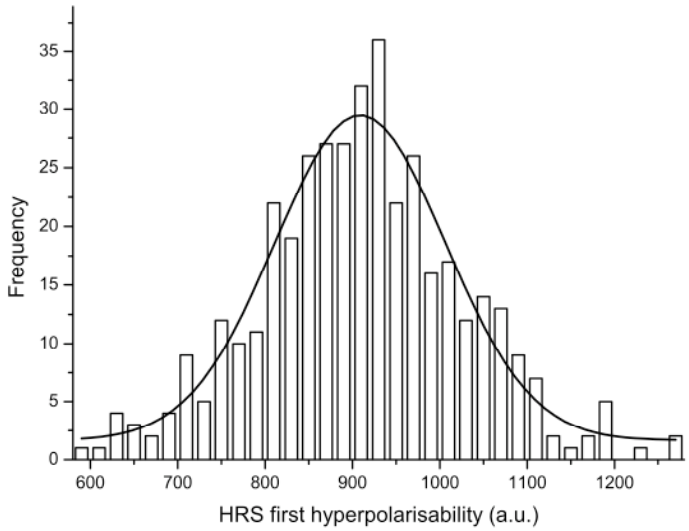


[S7] Distribution of the values of the bond length alternation (BLA1) in the hydrazone-pyrimidine foldamer. BLA1 = $d_{6\text{-}7} + d_{4\text{-}5} - 2d_{5\text{-}6}$ (atom labeling refers to Figure S1). Mean value = 0.265 Å; Standard deviation σ = 0.130 Å; Correlation coefficient R^2 = 0.975.

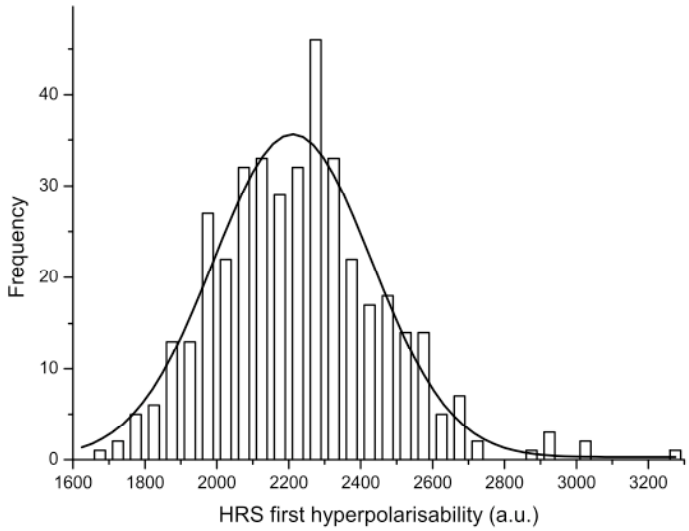


[S8] Distribution of the values of the bond length alternation (BLA2) in the hydrazone-pyrimidine foldamer. BLA2 = $d_{11\text{-}12} + d_{9\text{-}10} - 2d_{10\text{-}11}$ (atom labeling refers to Figure S1). Mean value = 0.264 Å; Standard deviation σ = 0.125 Å; Correlation coefficient R^2 = 0.968.

HRS First Hyperpolarizabilities

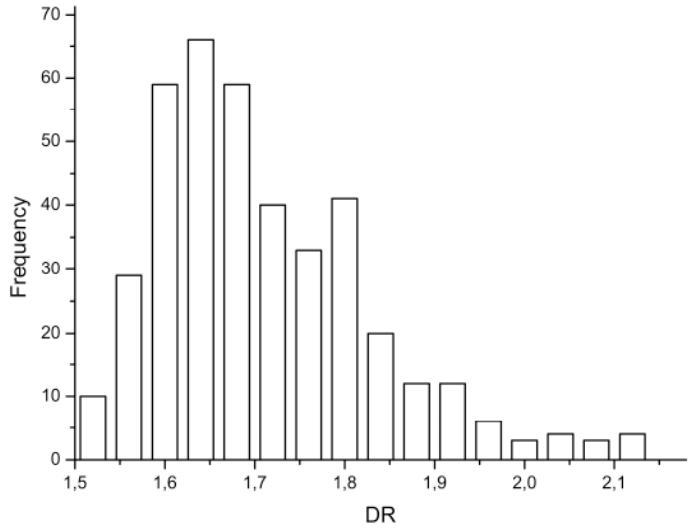


[S9] Distribution of the HRS first hyperpolarizability values in the pyridine-pyrimidine foldamer. Mean value = 909 a.u.; Standard deviation σ = 197 a.u.; Correlation coefficient R^2 = 0.929.

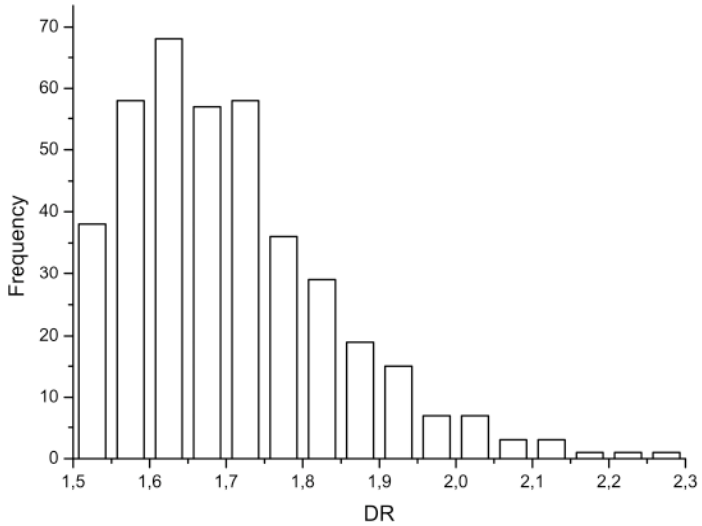


[S10] Distribution of the HRS first hyperpolarizability values in the hydrazone-pyrimidine foldamer. Mean value = 2211 a.u.; Standard deviation σ = 442 a.u.; Correlation coefficient R^2 = 0.934.

Depolarization Ratios

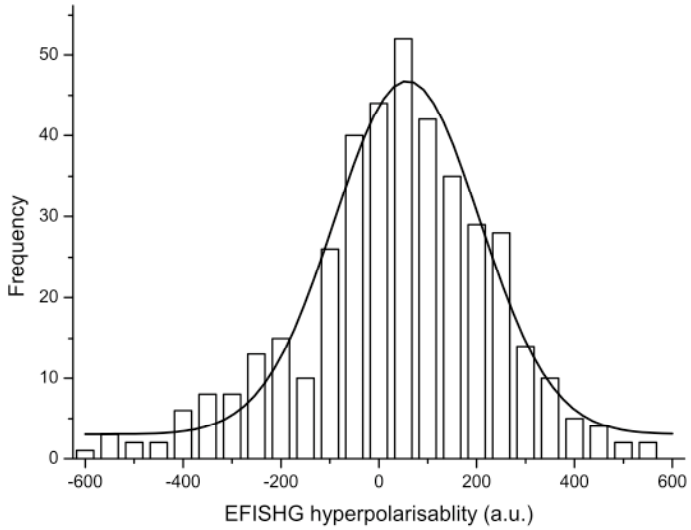


[S11] Distribution of the depolarization ratios in the pyridine-pyrimidine foldamer. Mean value = 1.669.

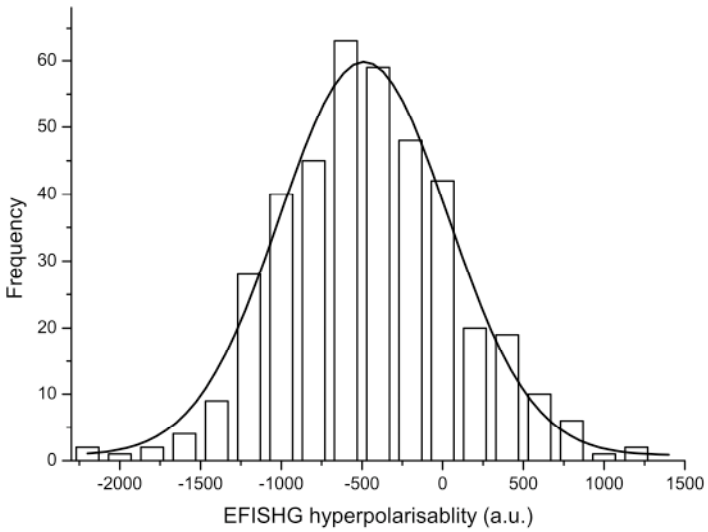


[S12] Distribution of the depolarization ratios in the hydrazone-pyrimidine foldamer. Mean value = 1.705.

EFISHG First Hyperpolarizabilities

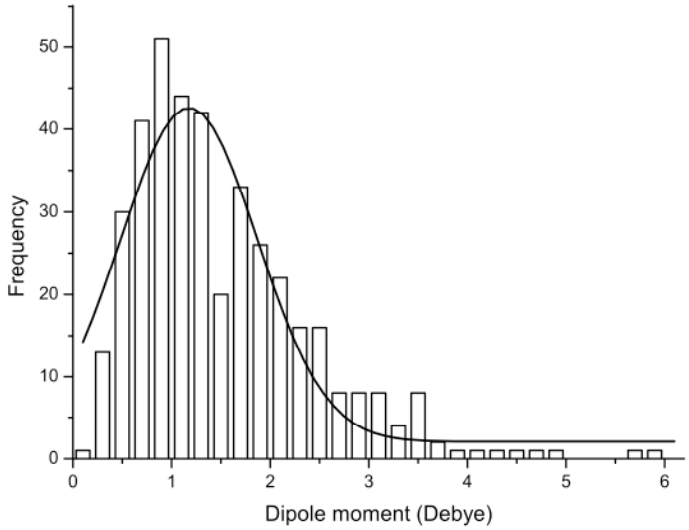


[S13] Distribution of the EFISHG first hyperpolarizability values in the pyridine-pyrimidine foldamer. Mean value = 58 a.u.; Standard deviation σ = 297 a.u.; Correlation coefficient R^2 = 0.955.

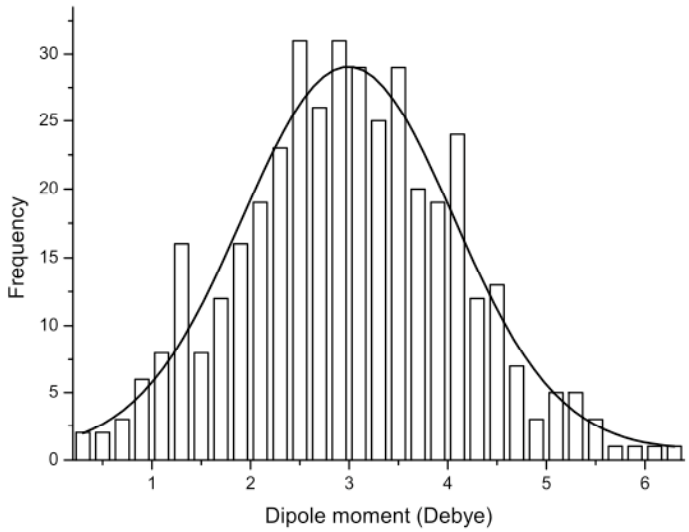


[S14] Distribution of the EFISHG first hyperpolarizability values in the hydrazone-pyrimidine foldamer. Mean value =-488 a.u.; Standard deviation σ = 1043 a.u.; Correlation coefficient R^2 = 0.978.

Dipole moments

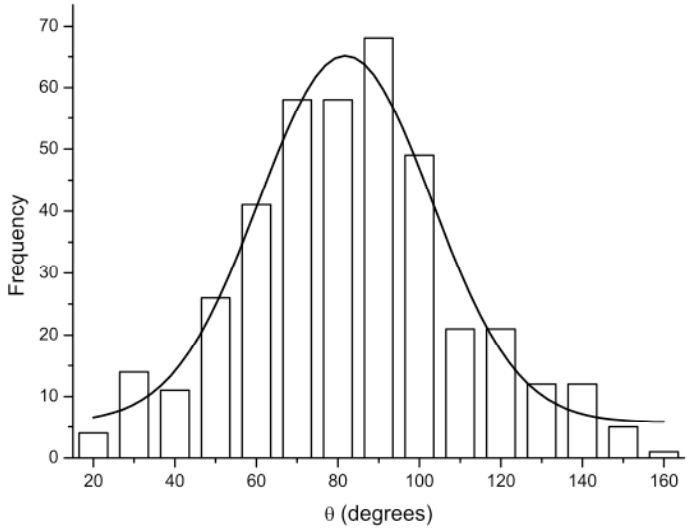


[S15] Distribution of the dipole moments in the pyridine-pyrimidine foldamer. Mean value = 1.177 D; Standard deviation σ = 1.389 D; Correlation coefficient R^2 = 0.871.

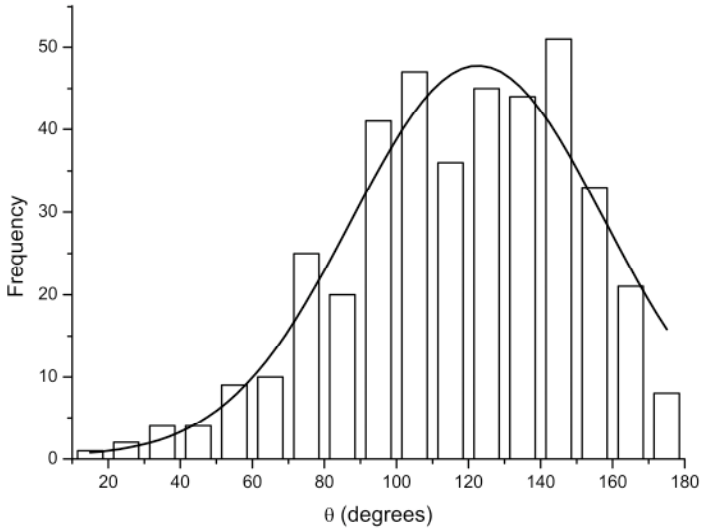


[S16] Distribution of dipole moments in the hydrazone-pyrimidine foldamer. Mean value = 2.991 D; Standard deviation σ = 2.141 D; Correlation coefficient R^2 = 0.934.

Angles between the dipole moment and the β vector

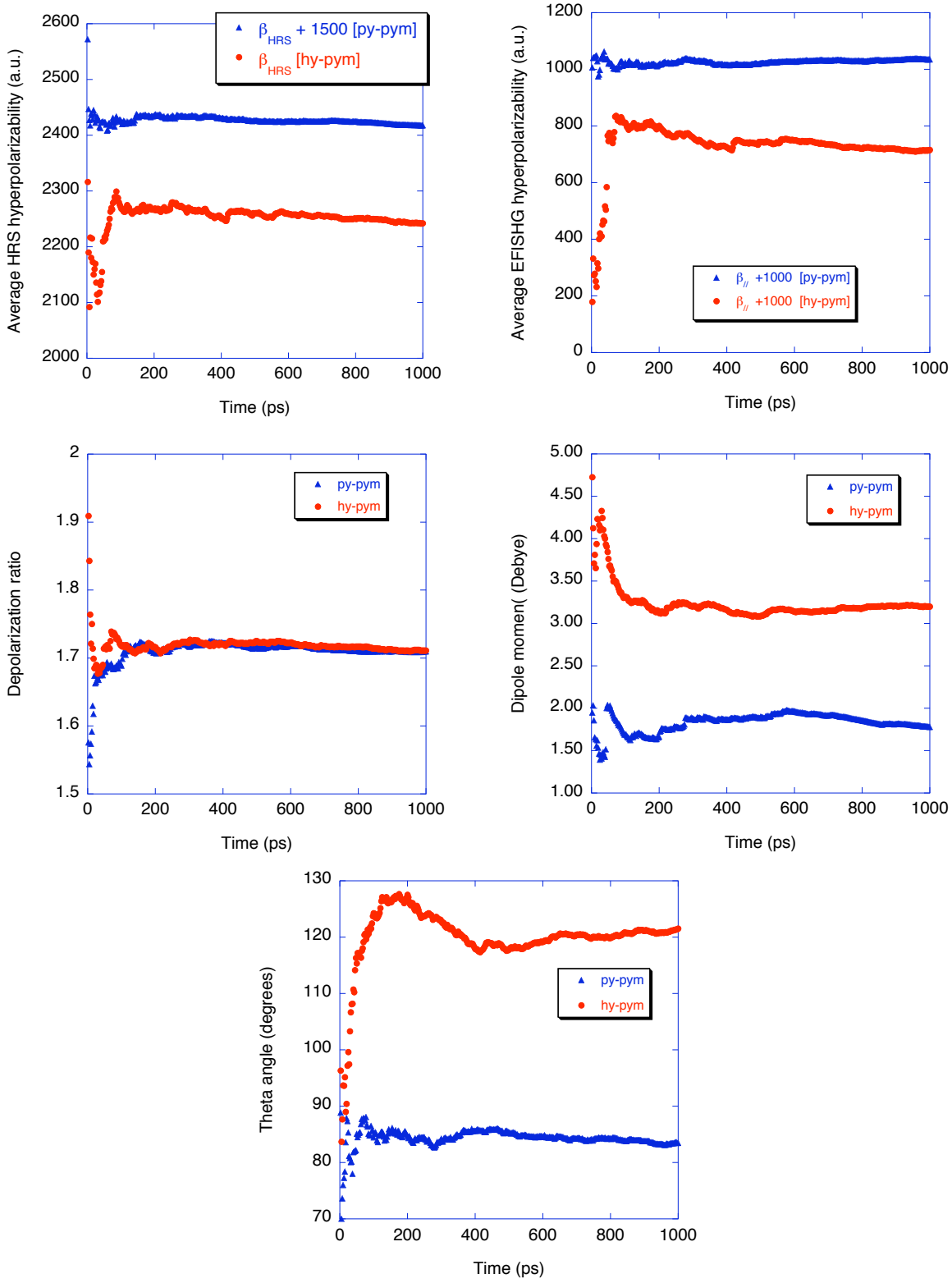


[S17] Distribution of the angles between the dipole moment and the β vector in the pyridine-pyrimidine foldamer. Mean value = 81.9°; Standard deviation σ = 42.3°; Correlation coefficient R^2 = 0.956.



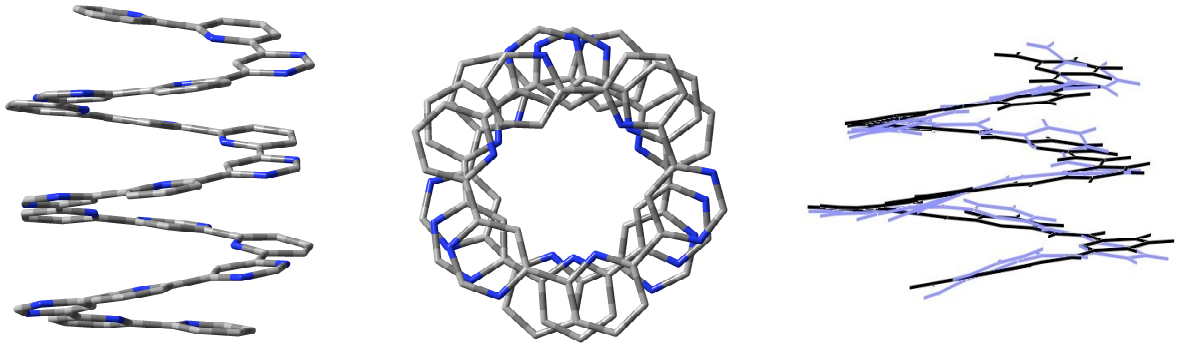
[S18] Distribution of the angles between the dipole moment and the β vector in the hydrazone-pyrimidine foldamer. Mean value = 122.6°; standard deviation σ = 70.0°; Correlation coefficient R^2 = 0.905.

Time evolution of the average NLO properties



[S19] Evolution of HRS (β_{HRS} and depolarization ratio) and EFISHG ($\beta_{//}$, dipole moment (μ), and angle between the μ and β vectors) quantities as a function of the number of points in the simulation, demonstrating that they converge when considering a 1 ns dynamics with 0.5 fs time step.

Molecular Structures



(a) **(b)** **(c)**

[S20] side (a) and top (b) views of the pyridine-pyrimidine crystal structure; (c): superimposition of the crystal structure (blue) with the structure optimized using the MMFF94 force field (black). RMS calculated on the differences in the Cartesian coordinates of all atoms = 0.4017.

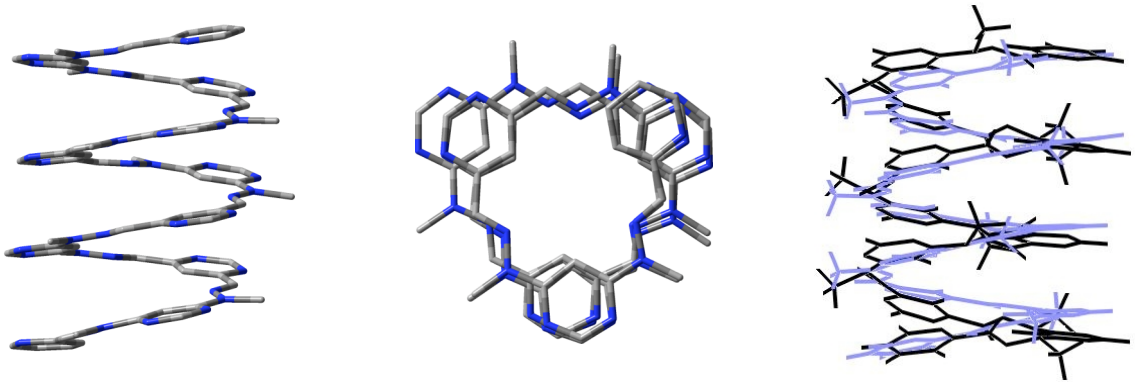
[S21] Structure of the pyridine-pyrimidine foldamer optimized at the MMFF94 level.

N	-0.40200	0.00400	-1.25800
C	-0.81500	-0.02000	0.02700
C	0.02800	0.15500	1.11500
C	1.38300	0.36700	0.87600
C	1.84600	0.39300	-0.43500
C	0.92500	0.19900	-1.45600
C	1.34800	0.19000	-2.86700
N	2.52100	0.60000	-3.24500
N	2.75100	0.52500	-4.60000
C	2.01200	1.46200	-5.45700
C	4.11900	0.41300	-5.00700
N	4.46500	0.71100	-6.27600
C	5.75000	0.55100	-6.60200
N	6.72800	0.11400	-5.80300
C	6.38500	-0.19400	-4.53600
C	5.07300	-0.04600	-4.10900
N	7.39000	-0.63800	-3.62000
C	8.55600	-1.19000	-4.32100
N	6.95800	-1.26900	-2.47400
C	7.78900	-1.21800	-1.47900
C	7.50000	-1.82100	-0.16500
N	8.56900	-1.90800	0.65800
C	8.33600	-2.48100	1.84400
N	7.15400	-2.92500	2.28400
C	6.12700	-2.77900	1.42000
C	6.23400	-2.23500	0.16300
C	4.82300	-3.24600	1.92400
N	3.71100	-2.80500	1.42300
N	2.57300	-3.37300	1.94400
C	2.16600	-2.95700	3.28900
C	1.45800	-3.46500	1.05100
N	0.21500	-3.65800	1.52900
C	-0.76100	-3.78200	0.62000
N	-0.63500	-3.73000	-0.71100

C	0.61000	-3.53800	-1.18900
C	1.68000	-3.40500	-0.31700
N	0.85200	-3.43500	-2.59700
C	-0.28300	-3.90600	-3.39300
N	2.11900	-3.79000	-3.00000
C	2.53500	-3.25500	-4.10600
C	3.89500	-3.50900	-4.62100
N	4.08700	-3.18900	-5.91700
C	5.31400	-3.43800	-6.38900
N	6.33900	-3.95500	-5.70000
C	6.07800	-4.22400	-4.40300
C	4.86200	-4.02800	-3.79700
C	7.21400	-4.76800	-3.63400
N	7.23000	-4.73600	-2.33700
N	8.31000	-5.32900	-1.72700
C	9.62000	-4.68900	-1.87100
C	8.07500	-5.79100	-0.39200
N	9.09400	-5.96200	0.47000
C	8.77700	-6.42600	1.68500
N	7.55500	-6.74300	2.13300
C	6.53700	-6.58200	1.26800
C	6.77800	-6.10000	-0.01100
N	5.18900	-6.86300	1.65700
C	5.11900	-7.70600	2.85300
N	4.32800	-7.13800	0.62100
C	3.07200	-6.89900	0.83900
C	2.05700	-7.09200	-0.21500
N	0.78500	-7.19600	0.22500
C	-0.13100	-7.39600	-0.73100
N	0.10200	-7.48200	-2.04700
C	1.39300	-7.34100	-2.41100
C	2.43200	-7.14900	-1.53400
C	1.64700	-7.41400	-3.86300
N	2.76000	-6.99200	-4.37800
N	2.90100	-7.16400	-5.73600
C	2.05000	-6.36700	-6.62400
C	4.25200	-7.24200	-6.20400
N	4.57000	-6.89900	-7.46700
C	5.85500	-7.03800	-7.81700
N	6.85700	-7.48400	-7.05000
C	6.53800	-7.82700	-5.78800
C	5.23100	-7.70900	-5.33900
N	7.55200	-8.26600	-4.87700
C	8.72000	-8.80700	-5.57600
N	7.10600	-8.94700	-3.76900
C	7.83800	-8.80700	-2.70800
C	7.45300	-9.42400	-1.42600
N	8.47000	-9.61100	-0.55800
C	8.13300	-10.19300	0.59800
N	6.90800	-10.60500	0.94300
C	5.93600	-10.35800	0.03700
C	6.14500	-9.77200	-1.18500
C	4.58900	-10.78900	0.45500
N	3.50900	-10.42600	-0.16800
N	2.34200	-10.93800	0.35500
C	1.93400	-10.51100	1.69900
C	1.22300	-11.03300	-0.53100
N	-0.01600	-11.19500	-0.02300
C	-1.01700	-11.30800	-0.90100
N	-0.91700	-11.27300	-2.23200
C	0.32000	-11.12100	-2.74500
C	1.41800	-10.99900	-1.90400
N	0.49500	-11.03800	-4.16400

C	-0.62100	-11.67000	-4.88000
N	1.76400	-11.28500	-4.63800
C	2.03800	-10.72800	-5.77900
C	3.34500	-10.88400	-6.44000
N	3.38200	-10.47700	-7.73300
C	4.57400	-10.58400	-8.35700
C	5.71900	-11.08700	-7.75700
C	5.64400	-11.50700	-6.43300
C	4.43400	-11.40900	-5.75600
H	-1.87700	-0.19500	0.16800
H	-0.36000	0.11400	2.12600
H	2.07600	0.49100	1.70300
H	2.89900	0.54000	-0.65000
H	0.59900	-0.18500	-3.58800
H	6.02800	0.80200	-7.62000
H	4.79500	-0.28800	-3.09200
H	9.30200	-1.57300	-3.61800
H	8.27400	-2.02000	-4.97700
H	9.06000	-0.41700	-4.91400
H	8.76800	-0.71200	-1.56300
H	9.18300	-2.59100	2.51300
H	5.39600	-2.14700	-0.51300
H	4.85000	-3.98200	2.74700
H	1.48100	-3.68400	3.74000
H	3.03300	-2.89400	3.95600
H	1.69000	-1.97000	3.27300
H	-1.76200	-3.94100	1.00500
H	2.67800	-3.24900	-0.70400
H	-0.07900	-3.81000	-4.46400
H	-0.50500	-4.95900	-3.19400
H	-1.17900	-3.30500	-3.19400
H	1.90300	-2.58300	-4.71300
H	5.49500	-3.19800	-7.43100
H	4.68000	-4.26600	-2.76000
H	8.03900	-5.20400	-4.22500
H	9.77800	-4.34400	-2.89900
H	9.71600	-3.81800	-1.21500
H	10.43000	-5.39500	-1.65500
H	9.59700	-6.56000	2.38200
H	5.95900	-5.96700	-0.70500
H	4.07900	-7.90800	3.13200
H	5.60900	-8.67200	2.69200
H	5.57800	-7.20700	3.71400
H	2.69900	-6.53800	1.81400
H	-1.16100	-7.49800	-0.41000
H	3.45700	-7.04900	-1.85600
H	0.84000	-7.85100	-4.47700
H	2.00000	-6.81300	-7.62400
H	1.02100	-6.32800	-6.25100
H	2.40800	-5.33600	-6.70600
H	6.11100	-6.75800	-8.83300
H	4.97200	-7.98500	-4.32600
H	9.48300	-9.13700	-4.86200
H	8.45000	-9.67300	-6.19200
H	9.19500	-8.04700	-6.20600
H	8.77900	-8.22900	-2.71100
H	8.92700	-10.35200	1.31900
H	5.34900	-9.59300	-1.89300
H	4.55700	-11.45000	1.34000
H	1.28800	-11.26000	2.17000
H	2.79900	-10.39100	2.36100
H	1.41200	-9.54800	1.67400
H	-2.01200	-11.44100	-0.49100

H	2.41100	-10.87400	-2.31500
H	-1.56900	-11.16100	-4.66800
H	-0.47900	-11.61000	-5.96400
H	-0.70900	-12.73100	-4.61900
H	1.30000	-10.10800	-6.32000
H	4.59000	-10.23800	-9.38600
H	6.65300	-11.13700	-8.30600
H	6.52400	-11.89100	-5.92500
H	4.35000	-11.71400	-4.71800
H	0.96800	1.55000	-5.13600
H	2.45200	2.46500	-5.41900
H	1.98400	1.11400	-6.49600



(a) **(b)** **(c)**

[S22] side (a) and top (b) views of the hydrazone-pyrimidine crystal structure; (c): superimposition of the crystal structure (blue) with the structure optimized using the MMFF94 force field (black). RMS calculated on the differences in the Cartesian coordinates of all atoms = 0.9722.

[S23] Structure of the hydrazone-pyrimidine foldamer optimized at the MMFF94 level.

C	-0.01500	-0.24700	-0.34900
C	-0.74200	0.94000	-0.41000
C	-2.12200	0.88400	-0.53200
C	-2.71800	-0.36200	-0.59500
N	-2.03900	-1.53000	-0.54500
C	-0.68300	-1.47300	-0.41500
N	1.38500	-2.70500	-0.14500
C	0.03800	-2.76700	-0.34600
C	-0.61400	-3.99100	-0.48300
C	0.12300	-5.16800	-0.42300
C	1.49600	-5.10200	-0.22000
C	2.10600	-3.85800	-0.07500
C	4.13400	-2.48600	0.45800
C	3.56300	-3.71000	0.15300
N	4.32000	-4.82800	0.04400
C	5.63600	-4.68000	0.23400
N	6.27700	-3.53700	0.50900
C	5.50700	-2.43000	0.63100
N	5.40200	-0.10800	1.28300
C	6.20000	-1.16100	0.95600
C	7.58600	-1.03300	0.93000
C	8.16200	0.19700	1.23000
C	7.34400	1.27200	1.56200
C	5.96400	1.09300	1.59300
C	3.68500	1.92400	2.20300
C	5.02400	2.17800	1.95800
N	5.52600	3.43200	2.03700
C	4.65900	4.40200	2.35100
N	3.34700	4.25700	2.58200
C	2.86400	2.99400	2.51800
N	1.00100	1.51700	2.90800
C	1.42100	2.80600	2.79700
C	0.53100	3.86600	2.93500
C	-0.81300	3.59900	3.17900
C	-1.23900	2.27800	3.29100
C	-0.31000	1.25100	3.16200

C	0.29500	-1.16800	3.35300
C	-0.67300	-0.18100	3.27700
N	-1.99100	-0.48500	3.28800
C	-2.29600	-1.78900	3.34800
N	-1.43200	-2.81200	3.41500
C	-0.11900	-2.48700	3.42500
N	2.14900	-3.24200	3.73900
C	0.85500	-3.59800	3.51600
C	0.49100	-4.93500	3.38200
C	1.47300	-5.91800	3.45600
C	2.79700	-5.54800	3.67200
C	3.11100	-4.20000	3.82300
C	4.74300	-2.39400	4.39600
C	4.48800	-3.71800	4.07900
N	5.49000	-4.62400	3.98600
C	6.72900	-4.16000	4.19600
N	7.07300	-2.90100	4.49600
C	6.05800	-2.01300	4.60400
N	5.37200	0.19900	5.27700
C	6.41200	-0.61800	4.95800
C	7.72200	-0.15200	4.97000
C	7.96700	1.18000	5.28800
C	6.90000	2.01700	5.60000
C	5.60800	1.50000	5.60100
C	3.17900	1.72700	6.14800
C	4.41800	2.31000	5.94800
N	4.59100	3.64800	6.05900
C	3.49800	4.36400	6.35400
N	2.26100	3.89100	6.55600
C	2.11000	2.55000	6.46000
N	0.66900	0.64500	6.78800
C	0.75700	2.00000	6.70600
C	-0.37100	2.80300	6.85200
C	-1.61000	2.20400	7.06000
C	-1.69700	0.81700	7.13000
C	-0.53900	0.05600	7.00300
C	0.64800	-2.13800	7.16600
C	-0.53500	-1.42300	7.09100
N	-1.73500	-2.04800	7.09400
C	-1.70600	-3.38600	7.15800
N	-0.61600	-4.16200	7.22200
C	0.57400	-3.51900	7.23900
N	2.95100	-3.68600	7.62100
C	1.79300	-4.35200	7.35800
C	1.77600	-5.73700	7.22500
C	2.96800	-6.44600	7.34100
C	4.15200	-5.75900	7.59300
C	4.11700	-4.37500	7.73600
C	5.22900	-2.21900	8.34400
C	5.32300	-3.56300	8.02400
N	6.52100	-4.18900	7.96000
C	7.59900	-3.43100	8.19900
N	7.60600	-2.13100	8.51800
C	6.39900	-1.52400	8.59600
N	5.16700	0.43900	9.27000
C	6.38500	-0.08900	8.96700
C	7.53800	0.68800	9.01000
C	7.43900	2.03400	9.34600
C	6.19100	2.57500	9.63900
C	5.06700	1.75500	9.60200
C	2.63800	1.38000	10.08400
C	3.70600	2.24700	9.91900
N	3.55000	3.58600	10.04300

C	2.31200	4.01800	10.31100
N	1.22500	3.25800	10.49200
C	1.39900	1.92000	10.38100
N	0.42800	-0.27600	10.66800
C	0.20700	1.06600	10.60000
C	-1.07500	1.59500	10.73700
C	-2.15000	0.73500	10.93100
C	-1.92300	-0.63500	10.99000
C	-0.62300	-1.12100	10.86100
N	-1.36300	-3.42300	11.05400
C	-1.10000	-4.74800	11.10300
C	0.17200	-5.28800	11.04500
C	1.24400	-4.41600	10.92800
C	1.00400	-3.04500	10.86700
C	-0.30800	-2.56900	10.92800
H	1.06500	-0.21000	-0.23900
H	-0.23000	1.89500	-0.34600
H	-2.71800	1.78800	-0.57200
H	-3.79600	-0.45900	-0.68900
H	-1.68800	-4.02800	-0.63900
H	2.08100	-6.01500	-0.16700
H	3.52100	-1.59700	0.55700
H	6.24500	-5.57400	0.15300
H	8.21600	-1.88000	0.67400
H	7.78200	2.23500	1.80700
H	3.29300	0.91400	2.15300
H	5.05700	5.40900	2.42000
H	0.87500	4.89200	2.85200
H	-2.28300	2.05500	3.48900
H	1.34900	-0.91500	3.35200
H	-3.35000	-2.04200	3.34200
H	-0.54500	-5.20900	3.20900
H	3.57200	-6.30500	3.73200
H	3.93500	-1.67600	4.47700
H	7.53700	-4.87900	4.11500
H	8.54600	-0.81400	4.72200
H	7.07800	3.05700	5.85200
H	3.04900	0.65300	6.06500
H	3.62800	5.43800	6.43700
H	-0.29000	3.88400	6.79500
H	-2.65600	0.33700	7.29700
H	1.60600	-1.63100	7.17300
H	-2.66500	-3.89300	7.15900
H	0.84700	-6.26000	7.02100
H	5.08900	-6.30100	7.67900
H	4.26600	-1.72200	8.39200
H	8.56500	-3.92100	8.13000
H	8.50500	0.25700	8.77000
H	6.10200	3.62600	9.90000
H	2.76800	0.30800	9.98300
H	2.17600	5.09100	10.39300
H	-1.24000	2.66700	10.68500
H	-2.75400	-1.31800	11.13800
H	-1.97300	-5.38900	11.19400
H	0.32300	-6.36000	11.08500
H	2.26100	-4.79400	10.86700
H	1.83800	-2.35800	10.76000
H	9.24200	0.31600	1.21100
H	-0.37100	-6.12900	-0.53200
H	8.98300	1.56400	5.29200
H	8.32700	2.65900	9.37600
H	-1.52300	4.41300	3.28800
H	1.20800	-6.96500	3.34300

H	-2.50200	2.81400	7.16800
H	-3.15700	1.12800	11.03400
H	2.97600	-7.52700	7.22900