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Supporting information

Quantitative analysis of hydrogen and chalcogen bonds in two pyrimidine derivatives, potential DHFR inhibitors: an integrated crystallographic and theoretical study

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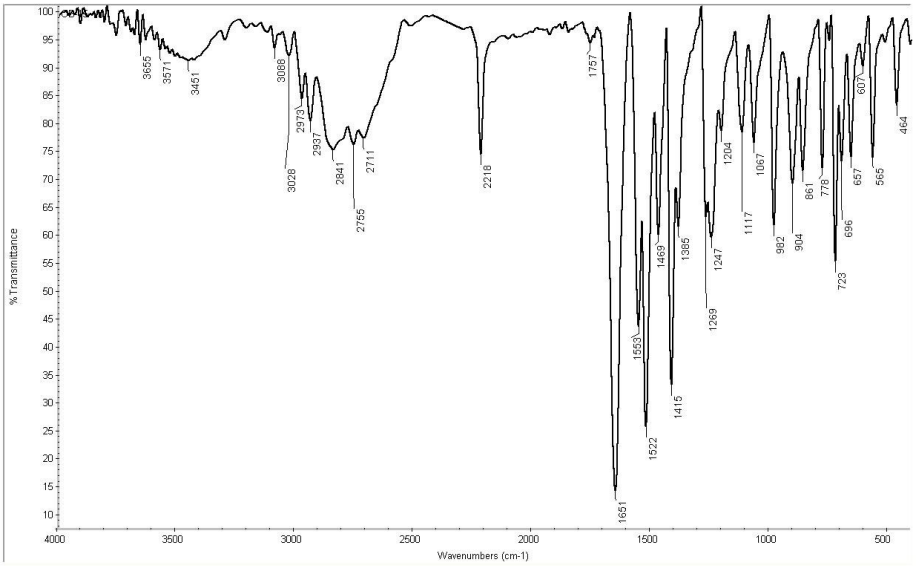
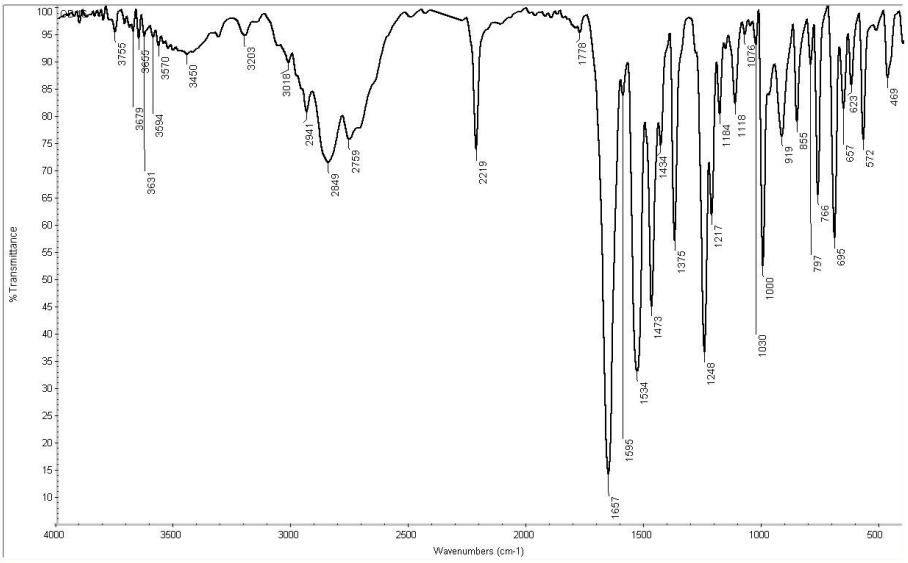


FT-IR spectrum for compound **1**.



FT-IR spectrum for compound **2**.

Table S1. Topological parameters for intramolecular interactions in X-ray and optimized structues of **1** and **2** [ρ(r): electron density (e/Å^3), $\nabla^2\rho$(r): Laplacian of electron density (e/Å^5); V(r): potential energy density, G(r): kinetic energy density; H(r): total energy density; R_{ij}: bond path (Å), $De = -0.5\times V$(r) in kcal mol^{-1} and the values of V(r), G(r) and H(r) are expressed in kJ mol^{-1} bohr^{-3}]

Interaction	R_{ij}	ρ(r)	$\nabla^2\rho$(r)	V(r)	G(r)	H(r)	$\frac{-V(r)}{G(r)}$	D_e
1 (X-ray)								
C11–H11···C9	2.720	0.086	1.081	-20.3	24.9	4.6	0.82	2.4
1 (optimized)								
C11–H11···N2	3.009	0.093	1.189	-22.2	27.3	5.1	0.81	2.7
2 (X-ray, major disordered component)								
C11A–H111···C9	2.426	0.107	1.310	-27.9	31.8	3.9	0.88	3.3
2 (X-ray, minor disordered component)								
C11B–H112···C9	2.390	0.110	1.341	-28.8	32.6	3.9	0.88	3.4
2 (optimized)								
C11A–H111···C9	2.650	0.085	1.070	-21.5	25.3	3.8	0.85	2.6

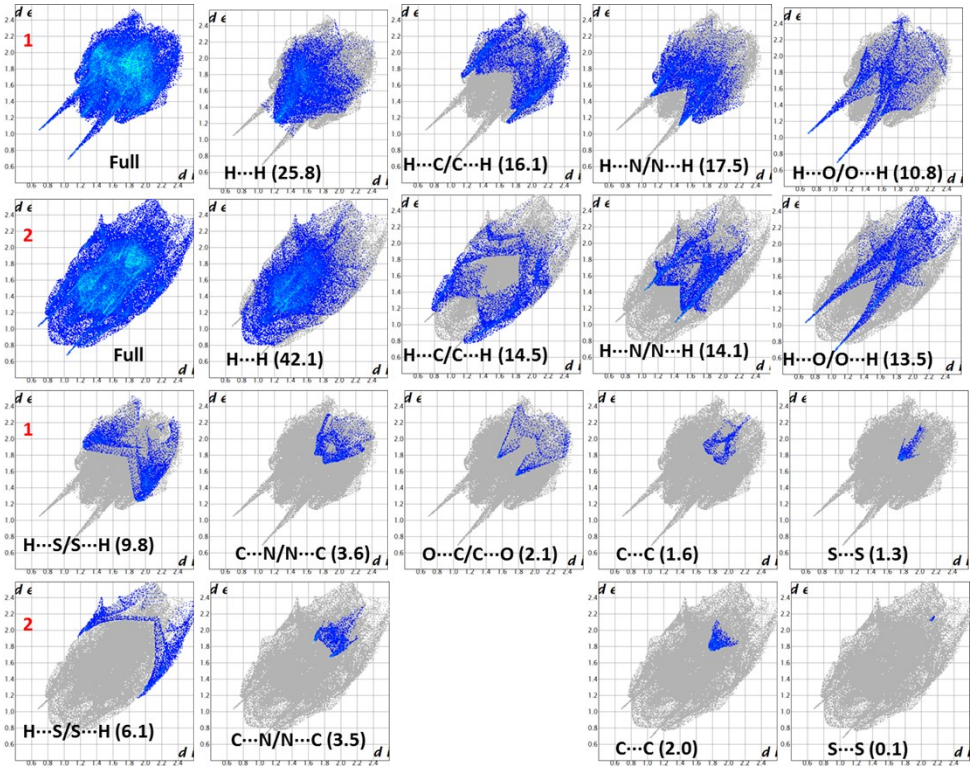


Fig. S1. 2D-fingerprint plots for various inter-contacts observed in **1** and **2**. The values in parenthesis corresponds to relative contribution to the total HS area.

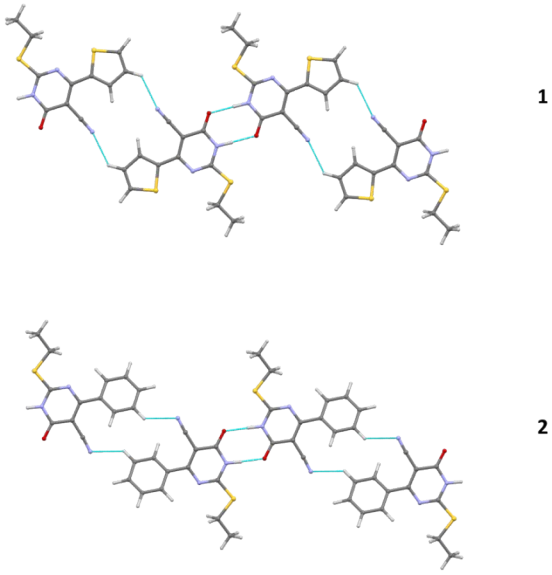


Fig. S2. 1D supramolecular construct observed in **1** and **2**.

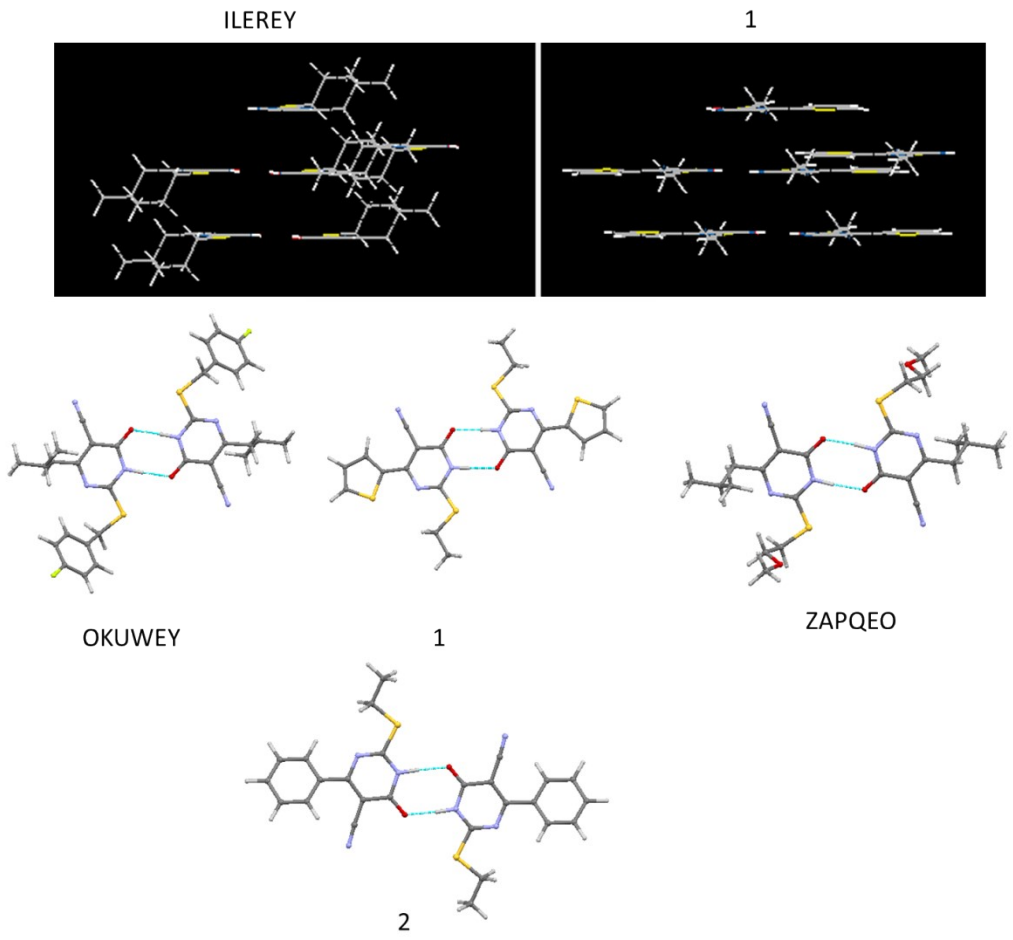


Fig. S3. Supramolecular constructs observed in **1**, **2** and their closely related structures.

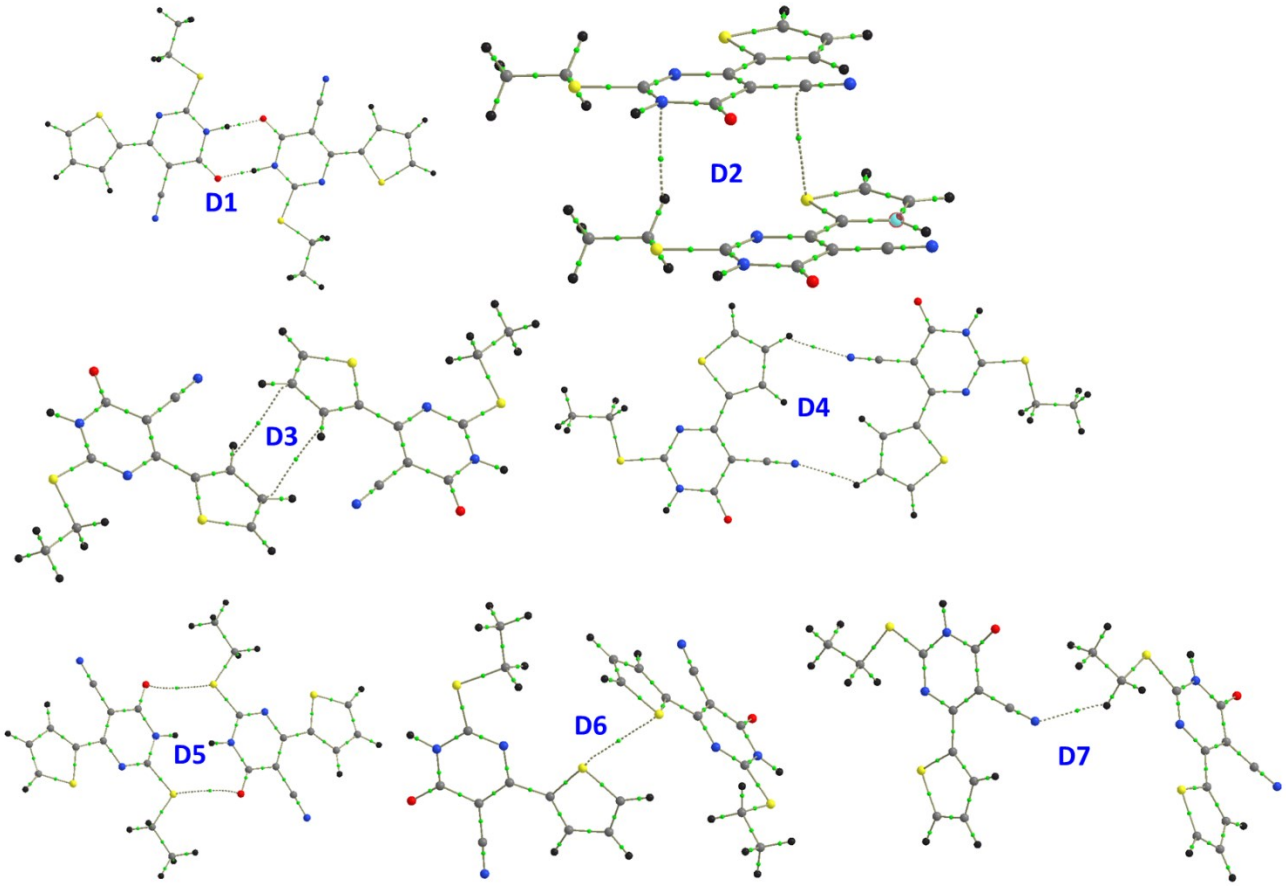


Fig. S4. Molecular graphs showing intermolecular interactions in different dimers observed in **1**.

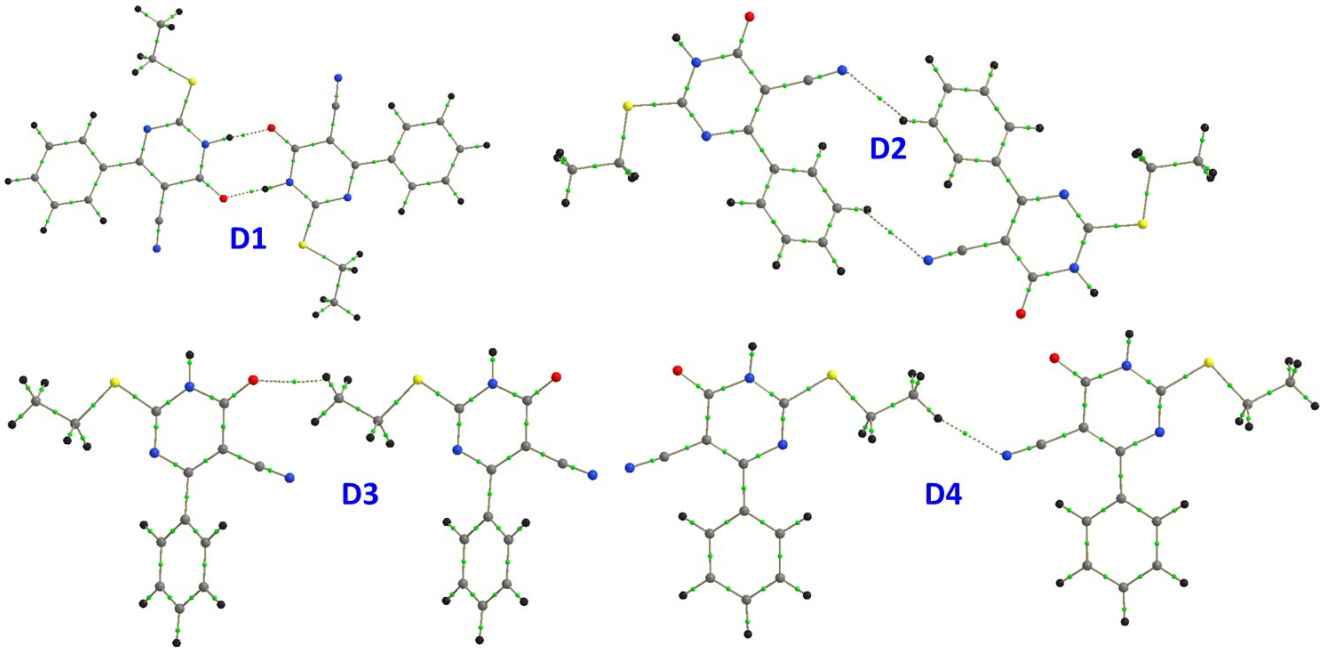


Fig. S5. Molecular graphs showing intermolecular interactions in different dimers observed in **2** (major disordered component).

Checkcif reports

Compound 1:

Datablock: shelx

```
Bond precision:      C-C = 0.0020 A              Wavelength=1.54184
Cell:        a=14.5546(2)   b=4.9907(5)     c=17.1813(3)
             alpha=90       beta=113.268(2) gamma=90
Temperature: 160 K
                    Calculated                      Reported
Volume              1146.51(12)                     1146.50(12)
Space group         P 21/n                          P 21/n
Hall group          -P 2yn                          -P 2yn
Moiety formula      C11 H9 N3 O S2                  ?
Sum formula         C11 H9 N3 O S2                  C11 H9 N3 O S2
Mr                  263.33                          263.33
Dx,g cm-3           1.526                           1.526
Z                   4                               4
Mu (mm-1)           4.102                           4.102
F000                544.0                           544.0
F000'               547.95
h,k,lmax            18,6,21                         18,6,21
Nref                2336                            2336
Tmin,Tmax           0.726,0.884                     0.745,0.908
Tmin'               0.658
Correction method= # Reported T Limits: Tmin=0.745
Tmax=0.908 AbsCorr = ANALYTICAL
Data completeness= 1.000       Theta(max)= 74.466
R(reflections)= 0.0249( 2147)     wR2(reflections)= 0.0687( 2336)
S = 1.064             Npar= 159
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	3 Report

Alert level G

PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		6 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.9 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		9 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		3 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

```
   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Compound 2:

Datablock: shelx

```
Bond precision:      C-C = 0.0019 A              Wavelength=1.54184
Cell:         a=4.6908(2)     b=9.2376(3)    c=14.6613(3)
              alpha=94.308(2) beta=93.766(2) gamma=100.924(3)
Temperature: 160 K
                    Calculated                      Reported
Volume              619.95(4)                       619.95(4)
Space group         P -1                            P -1
Hall group          -P 1                            -P 1
Moiety formula      C13 H11 N3 O S                  ?
Sum formula         C13 H11 N3 O S                  C13 H11 N3 O S
Mr                  257.31                          257.31
Dx,g cm-3           1.378                           1.378
Z                   2                               2
Mu (mm-1)           2.248                           2.248
F000                268.0                           268.0
F000'               269.37
h,k,lmax            5,11,18                         5,11,18
Nref                2528                            2524
Tmin,Tmax           0.922,0.956                     0.848,0.960
Tmin'               0.747
Correction method= # Reported T Limits: Tmin=0.848
Tmax=0.960 AbsCorr = ANALYTICAL
Data completeness= 0.998        Theta(max)= 74.464
R(reflections)= 0.0327( 2219)      wR2(reflections)= 0.0888( 2524)
S = 1.024              Npar= 205
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for S1 --C2 . 5.3 s.u.

Alert level G

PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 22% Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 5
Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5
Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

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2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
