Supporting information for:

WinPSSP: A revamp of the computer program *PSSP* and its performance solving the crystal structures of small organic compounds and solids of biological and pharmaceutical interest

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Table S1 Radiation type, wavelength and R_{wp} of the Le Bail fit of the materials **I** to **XVII** represented in Figure 4.

Compound	Radiation type	Wavelength (Å)	Le Bail fit R_{wp} (%)
I	Synchrotron	1.149901	7.06
II	Synchrotron	1.14970	6.54
III	Synchrotron	0.69940	7.52
IV	Synchrotron	0.699204	5.95
V	Synchrotron	1.149986	7.17
VI[a]	Synchrotron	1.150346	4.71
VI[b]	Synchrotron	1.149999	11.82
VII	Laboratory Cu Kα1	1.5406	3.93
VIII	Synchrotron	0.69847	5.41
IX	Synchrotron	0.700227	7.78
X	Synchrotron	0.699931	12.25
XI	Synchrotron	0.700227	7.12
XII	Synchrotron	0.6999311	5.50
XIII	Synchrotron	0.69993	3.41
XIV	Synchrotron	0.698697	5.95
XV	Synchrotron	0.700051	4.97
XVI	Synchrotron	0.700095	5.99
XVII	Laboratory Cu Kα1	1.5406	1.95

VI[a] corresponds to the orange polymorph, whereas VI[b] to the dark red polymorph.

S1. *WinPSSP* structure solution performance for the compounds I to XVII shown in Figure 4

Figures S1 to S18 show the graphs of the percentage of solutions in 20 runs *vs.* number of models per temperature. The fits shown were used to estimate the number of models per temperature required to solve the crystal structures 50% of the runs for each compound of Figure 4.

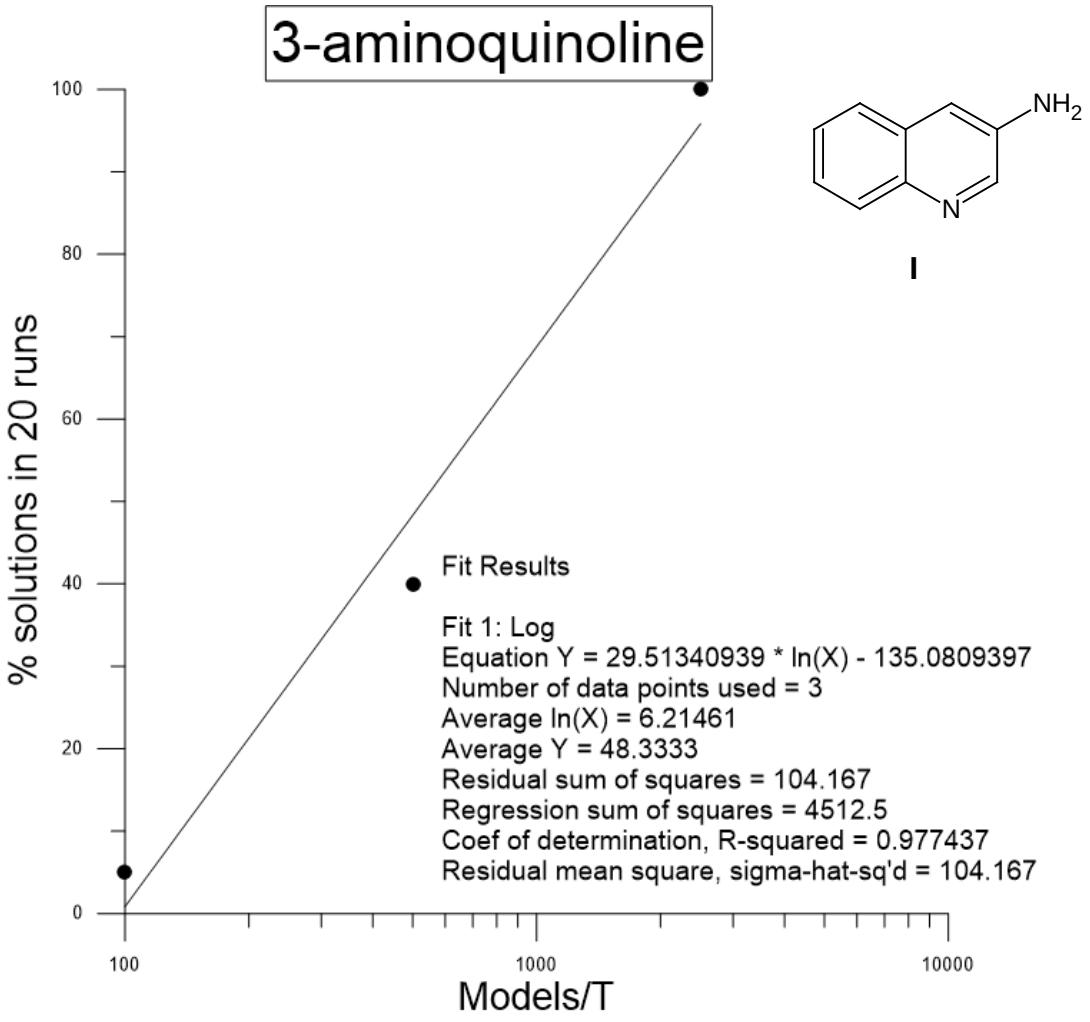

Figure S1 Percentage of 3-aminoquinoline (**I**) solutions in 20 simulated annealing runs using 100, 500 and 2,500 models per temperature, respectively. The crystal structure is solved 100% of times using 10,000 models/T. According to the fit shown in the figure, 529 models/T are estimated to produce 50% of solutions.

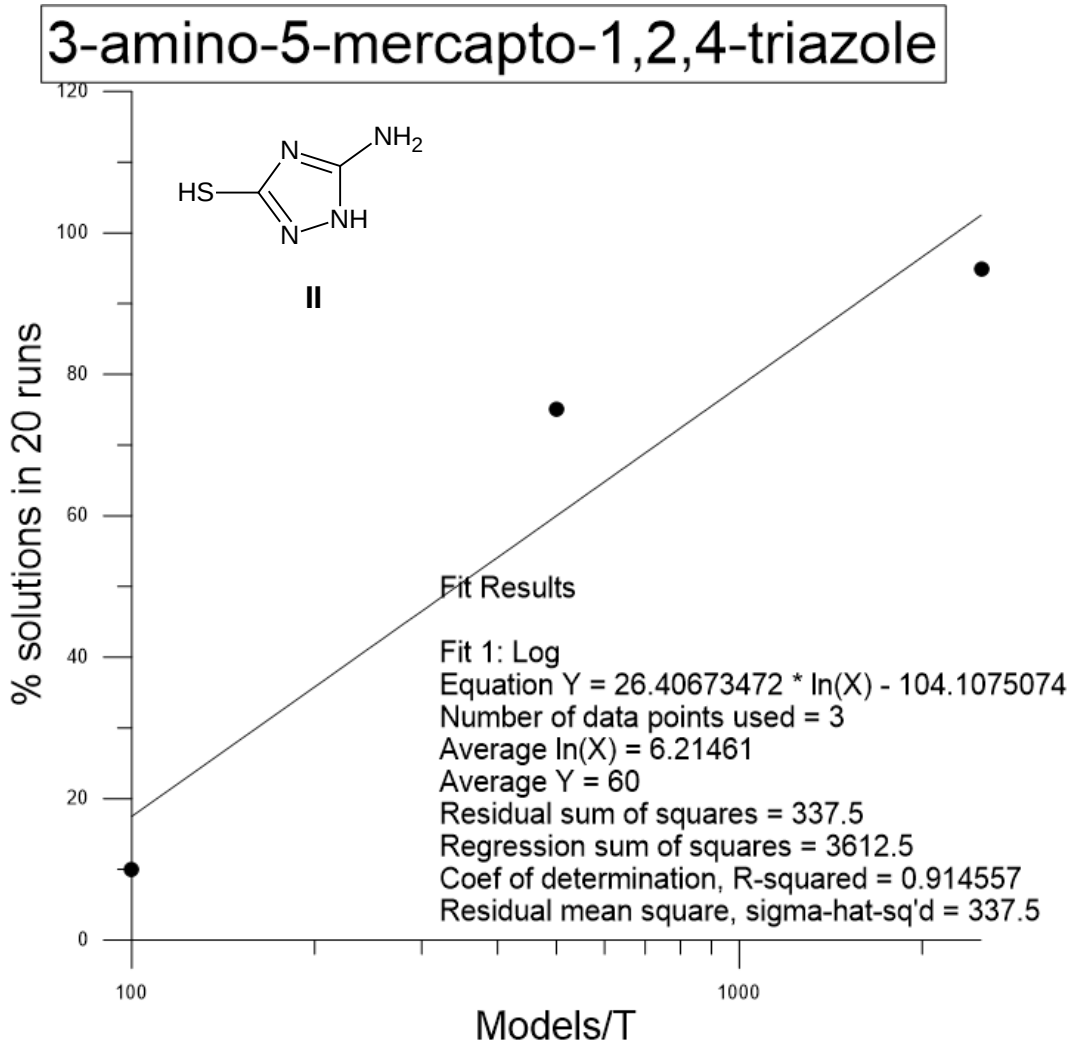

Figure S2 Percentage of 3-amino-5-mercapto-1,2,4-triazole (**II**) solutions in 20 simulated annealing runs using 100, 500 and 2,500 models per temperature, respectively. According to the fit shown in the figure, 342 models/T are estimated to produce 50% of solutions.

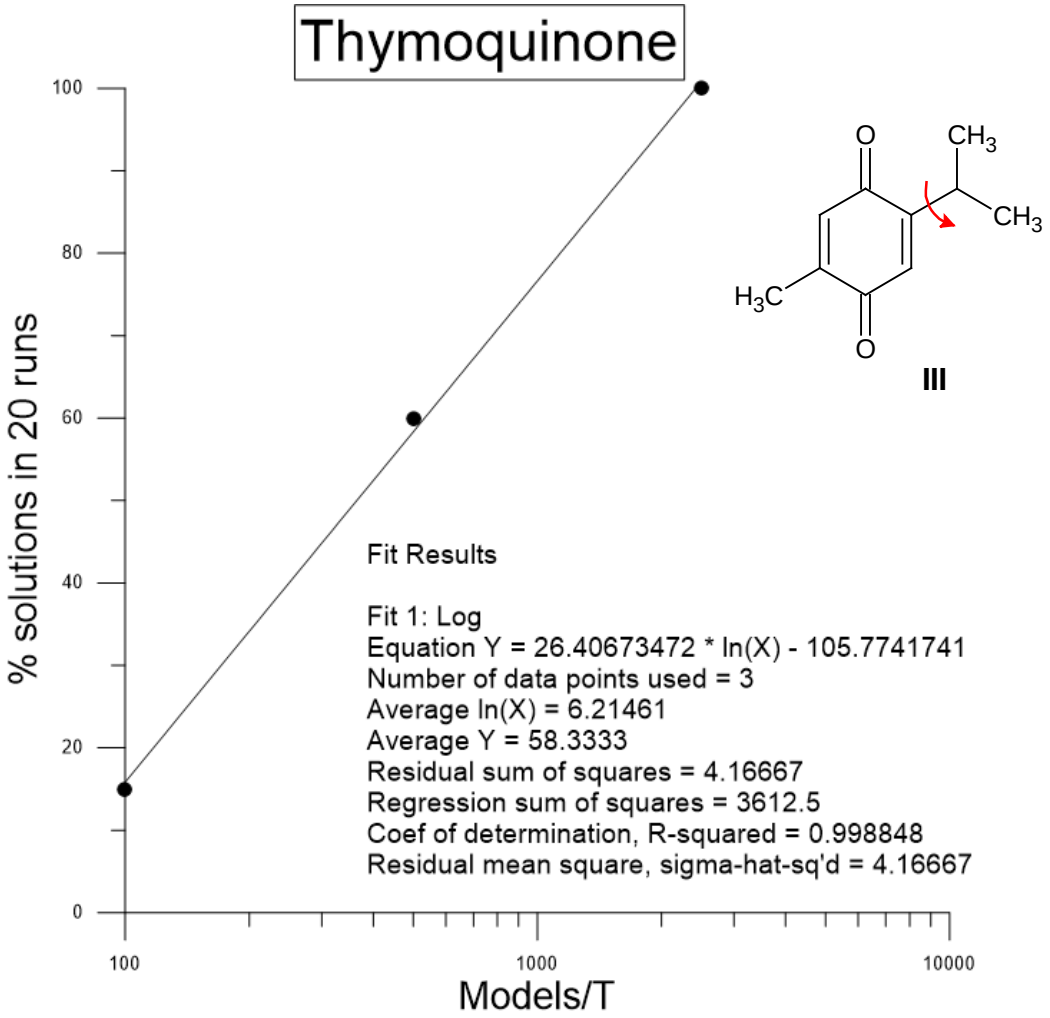

Figure S3 Percentage of thymoquinone (**III**) solutions in 20 simulated annealing runs using 100, 500 and 2,500 models per temperature, respectively. The crystal structure is solved 100% of times using 10,000 models/T. According to the fit shown in the figure, 365 models/T are estimated to produce 50% of solutions.

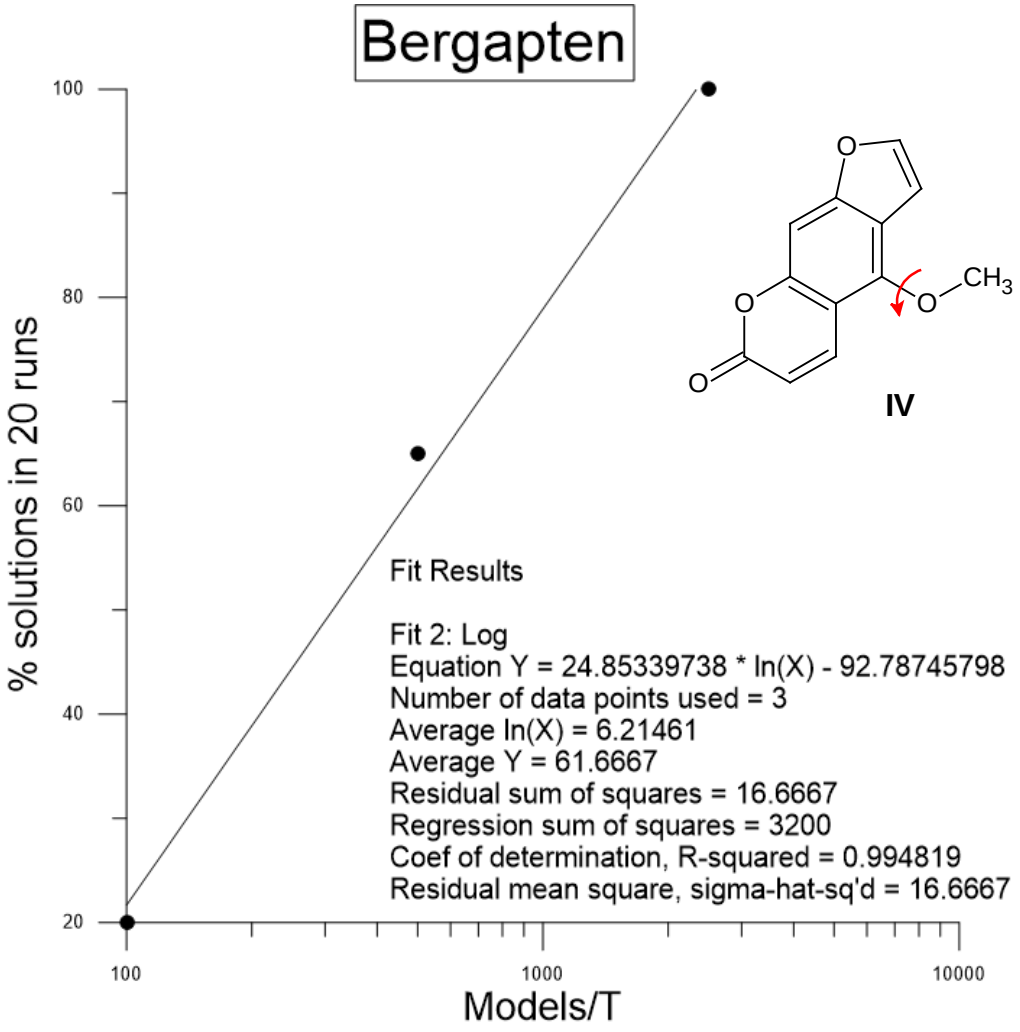

Figure S4 Percentage of bergapten (**IV**) solutions in 20 simulated annealing runs using 100, 500 and 2,500 models per temperature, respectively. According to the fit shown in the figure, 313 models/T are estimated to produce 50% of solutions.

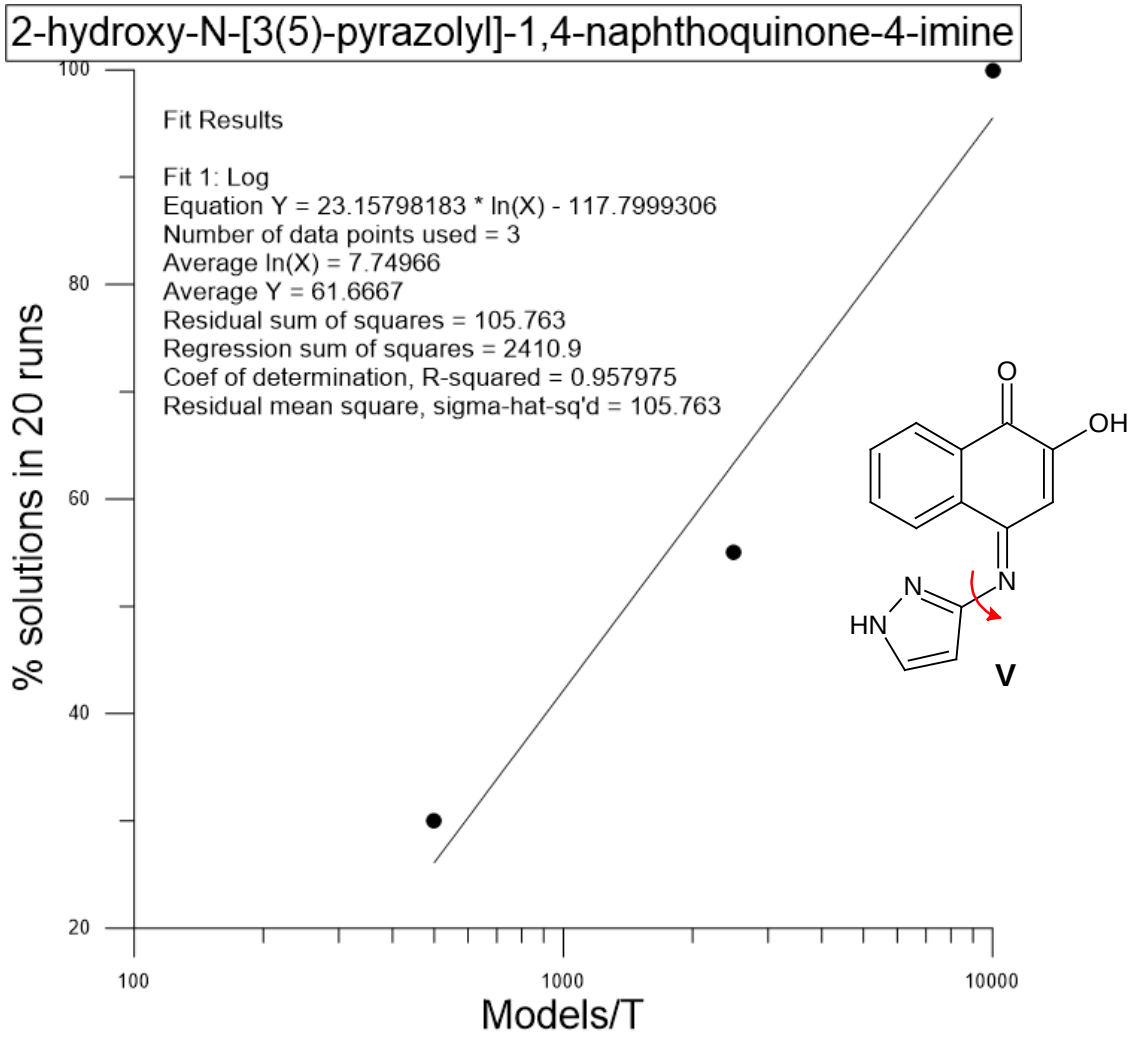

Figure S5 Percentage of 2-Hydroxy-N-[3(5)-pyrazolyl]-1,4-naphthoquinone-4-imine (**V**) solutions in 20 simulated annealing runs using 500; 2,500 and 10,000 models per temperature, respectively. According to the fit shown in the figure, 1,402 models/T are estimated to produce 50% of solutions.

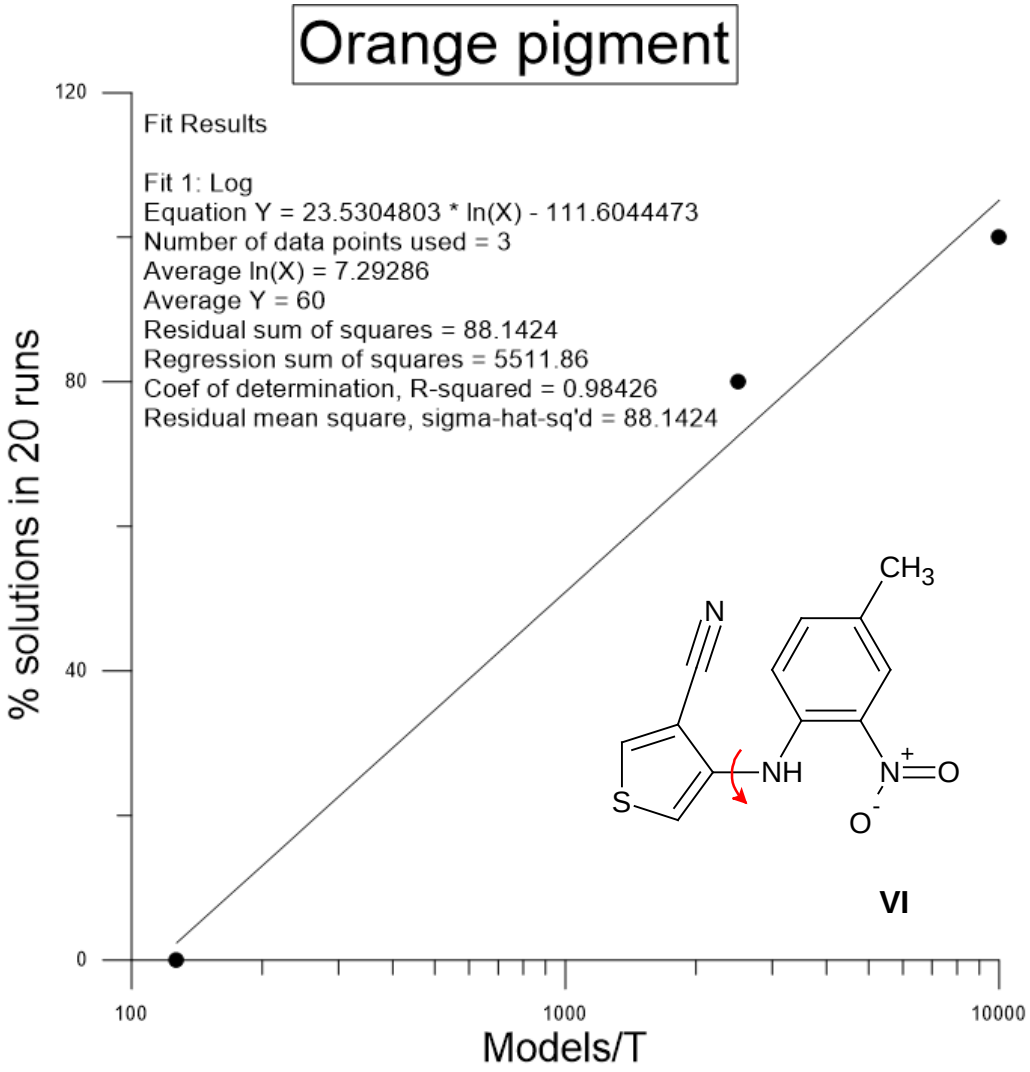

Figure S6 Percentage of solutions for 5-methyl-2-[(2-nitro-4-methylphenyl)amino]-3-thiophenecarbonitrile (**VI**), orange polymorph, in 20 simulated annealing runs using 127; 2,500 and 10,000 models per temperature, respectively. According to the fit shown in the figure, 961 models/T are estimated to produce 50% of solutions.

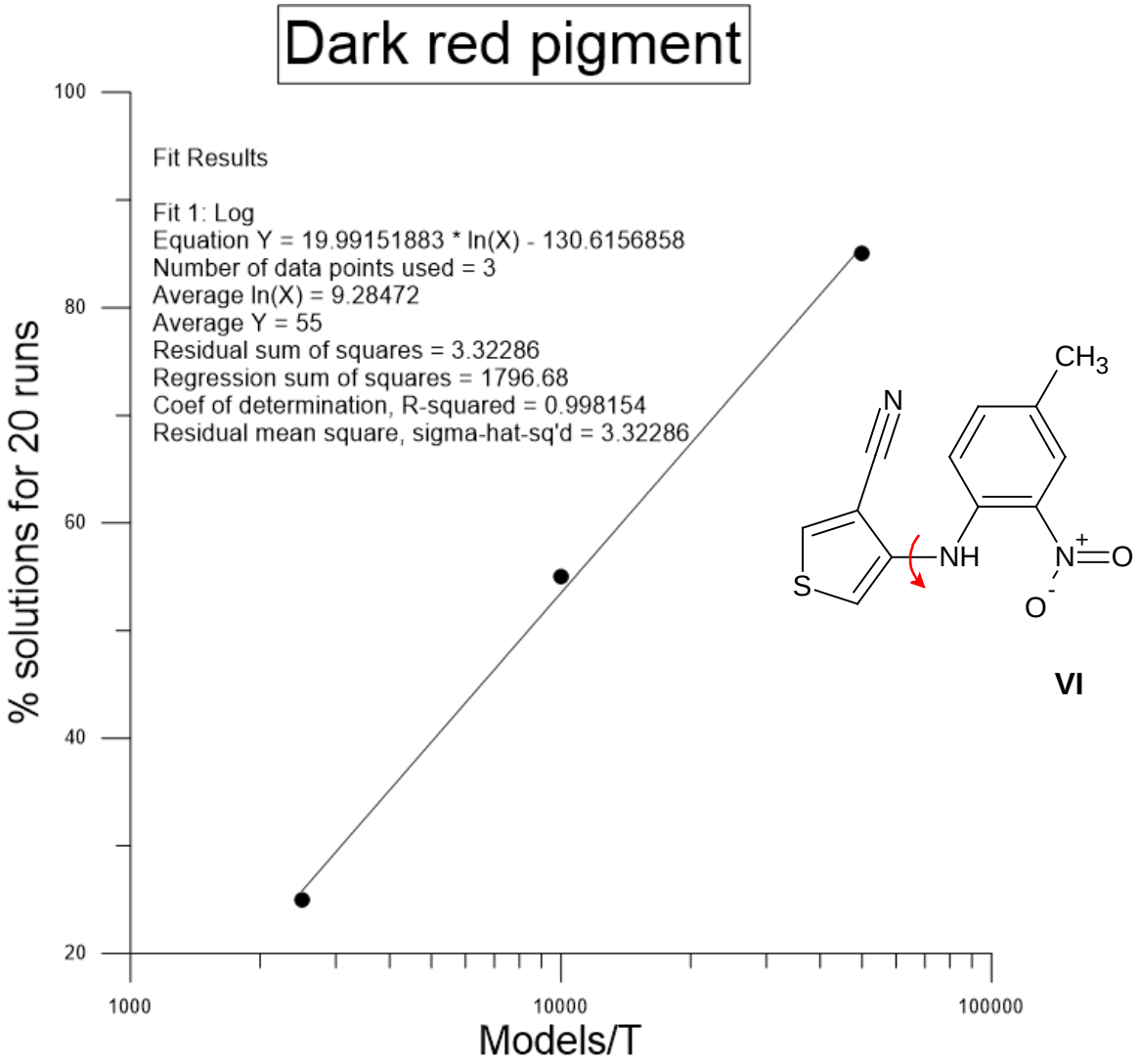

Figure S7 Percentage of solutions for 5-methyl-2-[(2-nitro-4-methylphenyl)amino]-3-thiophenecarbonitrile (**VI**), dark red polymorph, in 20 simulated annealing runs using 2,500, 10,000 and 50,000 models per temperature, respectively. According to the fit shown in the figure, 8,389 models/T are estimated to produce 50% of solutions.

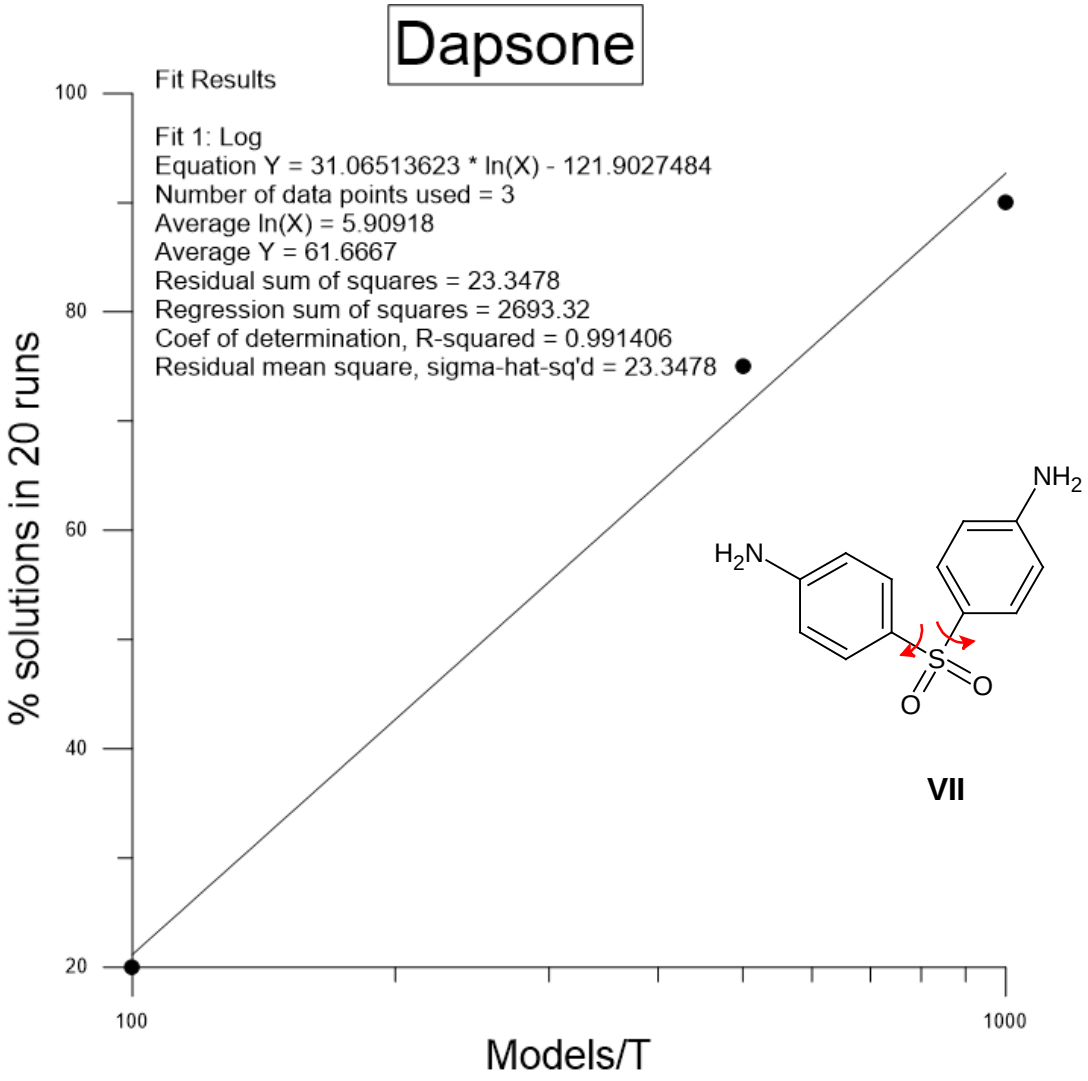

Figure S8 Percentage of dapsone (**VII**) solutions in 20 simulated annealing runs using 100, 500 and 1,000 models per temperature, respectively. According to the fit shown in the figure, 253 models/T are estimated to produce 50% of solutions.

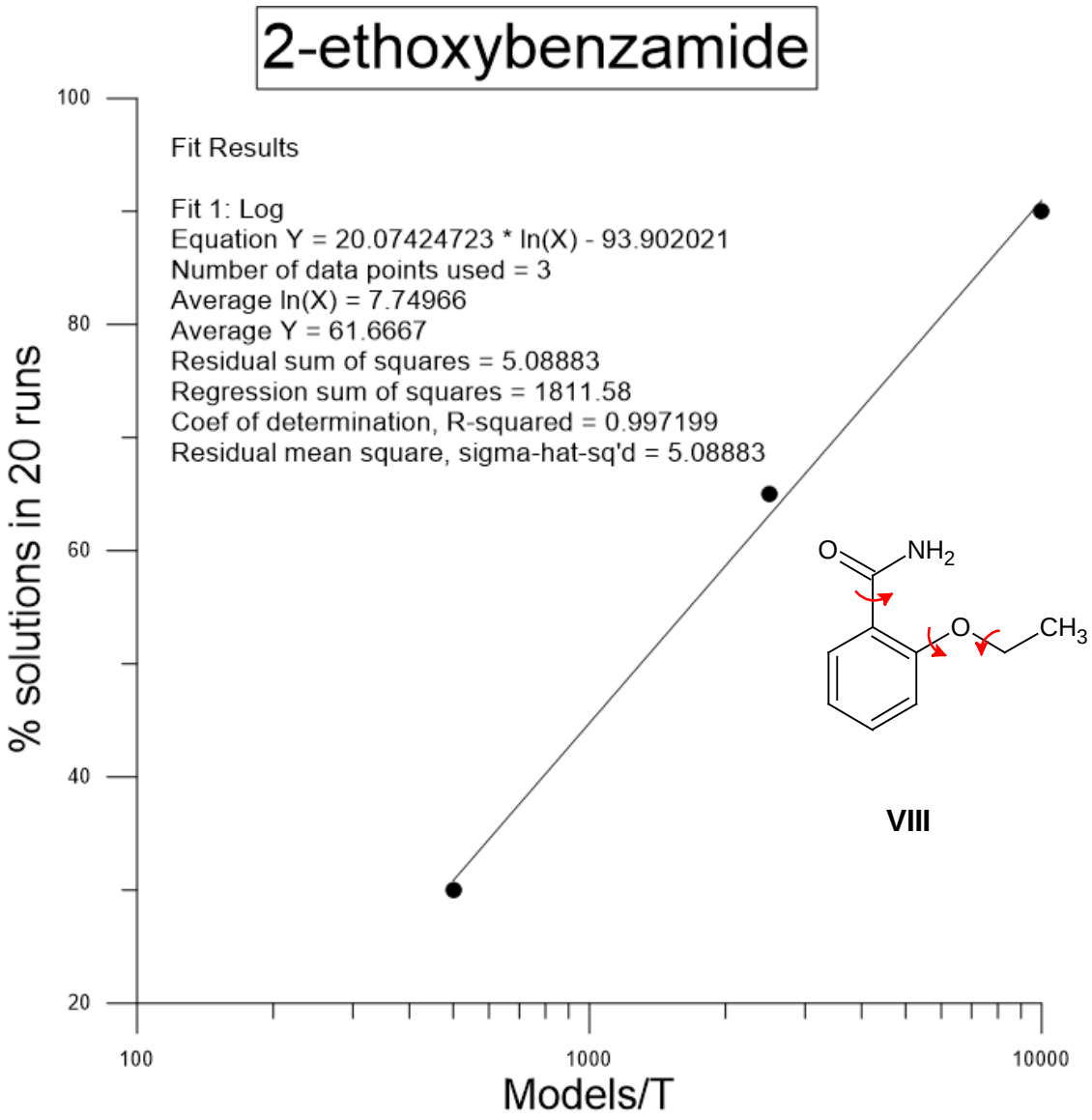

Figure S9 Percentage of solutions for 2-ethoxybenzamide (**VIII**) in 20 simulated annealing runs using 500; 2,500 and 10,000 models per temperature, respectively. According to the fit shown in the figure, 1,298 models/T are estimated to produce 50% of solutions.

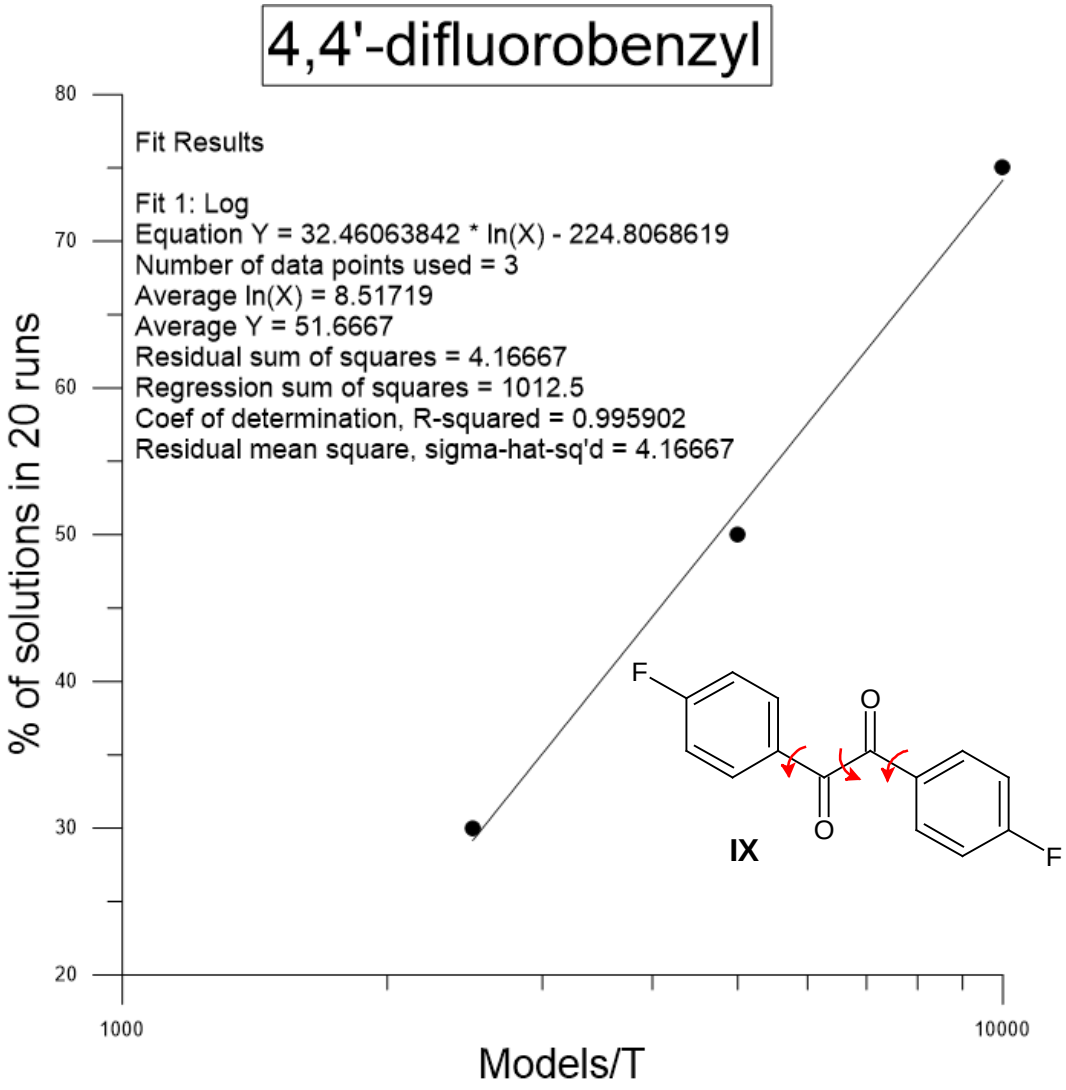

Figure S10 Percentage of solutions for 4,4'-difluorobenzyl (**IX**) in 20 simulated annealing runs using 2,500; 5,000 and 10,000 models per temperature, respectively. According to the fit shown in the figure, 4,750 models/T are estimated to produce 50% of solutions.

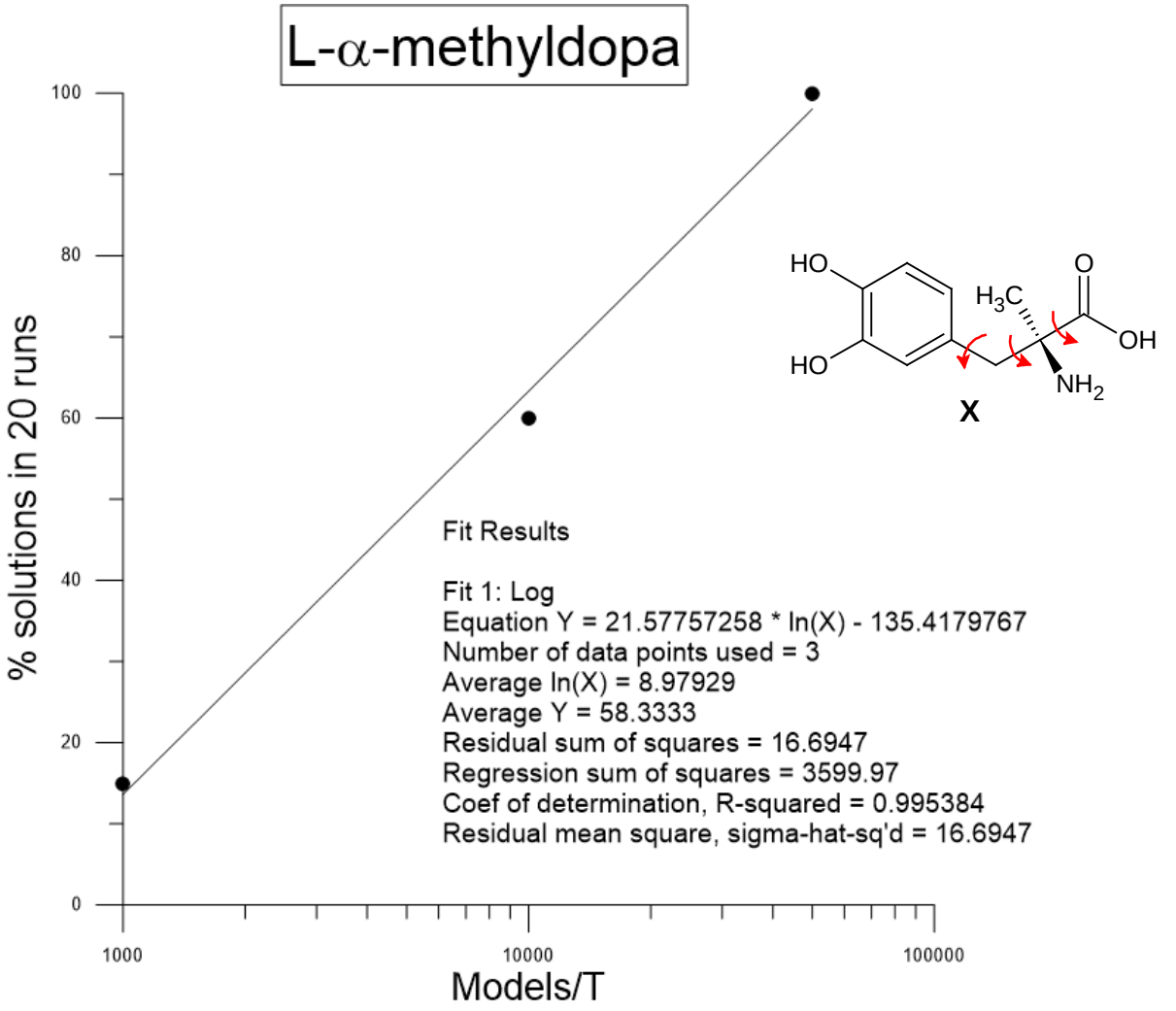

Figure S11 Percentage of solutions for L-α-methyldopa (**X**) in 20 simulated annealing runs using 1,000; 10,000 and 50,000 models per temperature, respectively. According to the fit shown in the figure, 5,394 models/T are estimated to produce 50% of solutions.

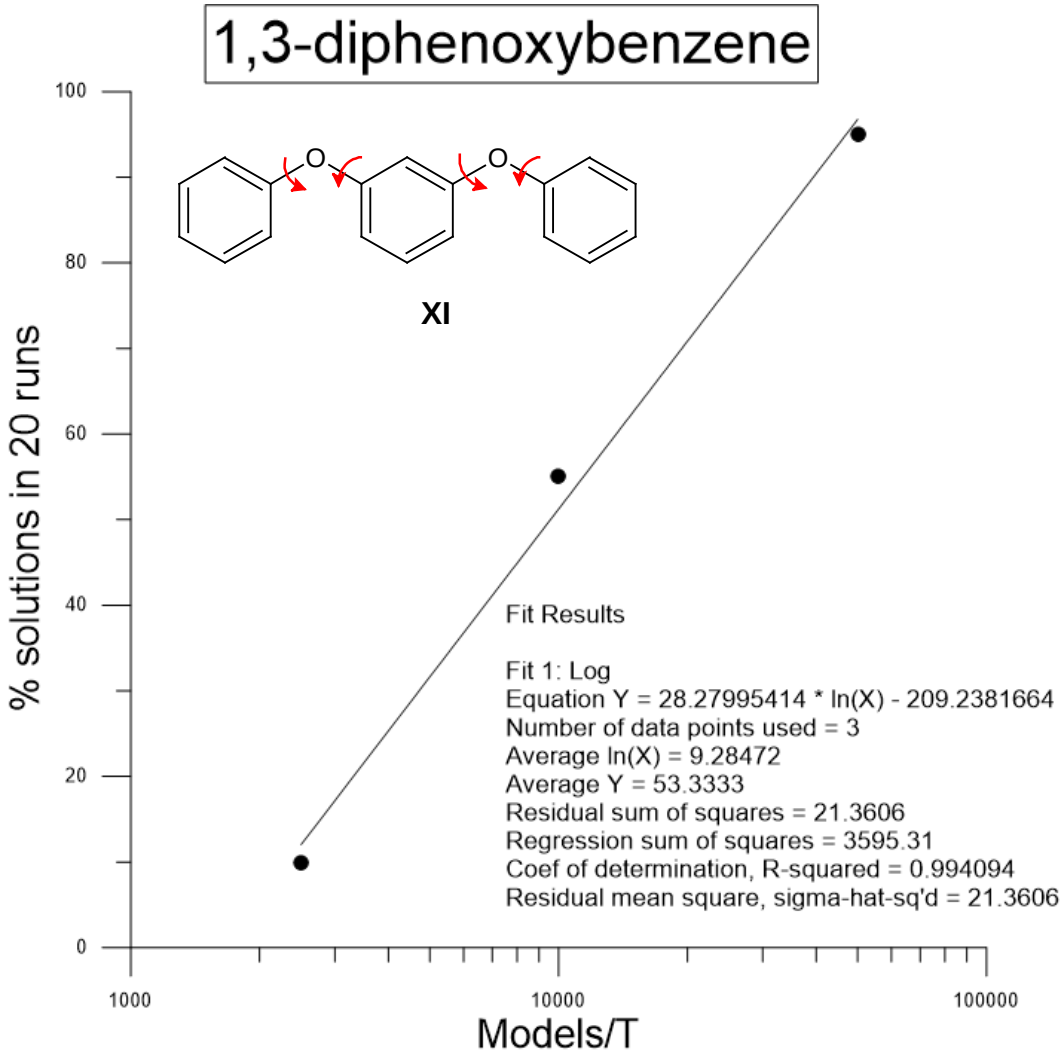

Figure S12 Percentage of solutions for 1,3-diphenoxybenzene (**XI**) in 20 simulated annealing runs using 2,500; 10,000 and 50,000 models per temperature, respectively. According to the fit shown in the figure, 9,574 models/T are estimated to produce 50% of solutions.

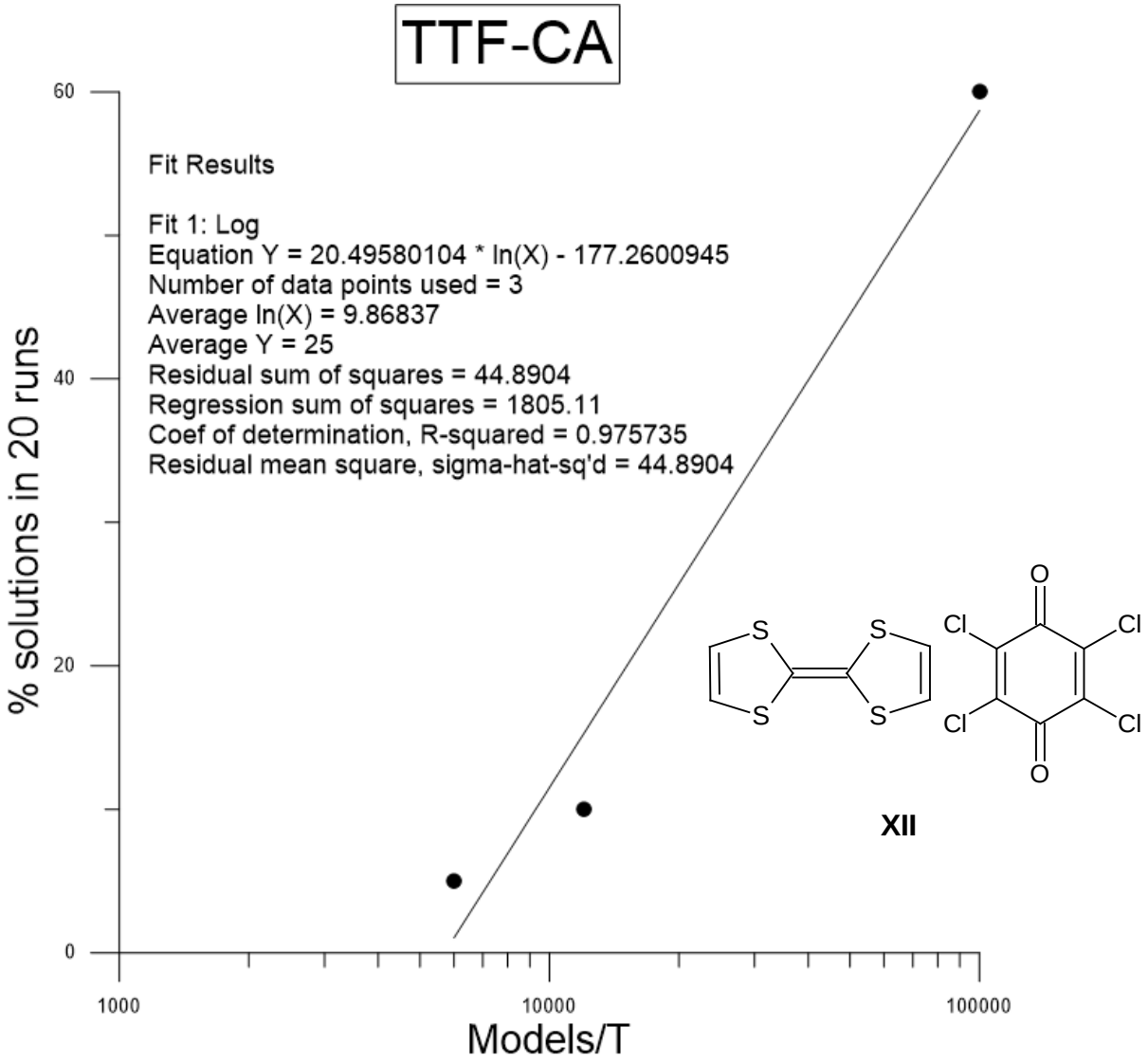

Figure S13 Percentage of solutions for tetrathiafulvalene chloranil, black polymorph (**XII**) in 20 simulated annealing runs using 6,000; 12,000 and 100,000 models per temperature, respectively. According to the fit shown in the figure, 65,390 models/T are estimated to produce 50% of solutions.

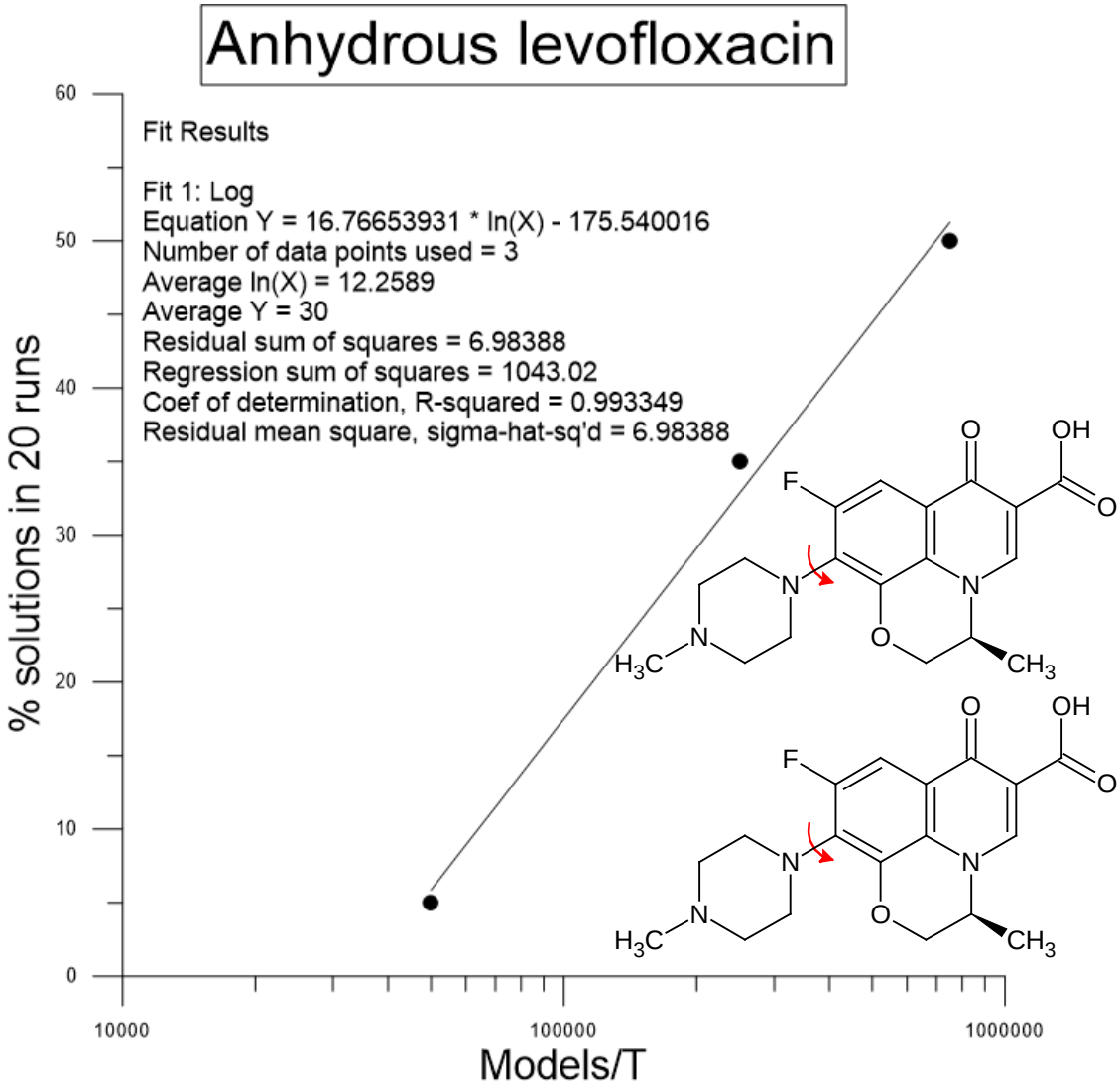

Figure S14 Percentage of solutions for anhydrous levofloxacin (**XIII**) in 20 simulated annealing runs using 50,000; 250,000 and 750,000 models per temperature, respectively. According to the fit shown in the figure, 695,109 models/T are estimated to produce 50% of solutions.

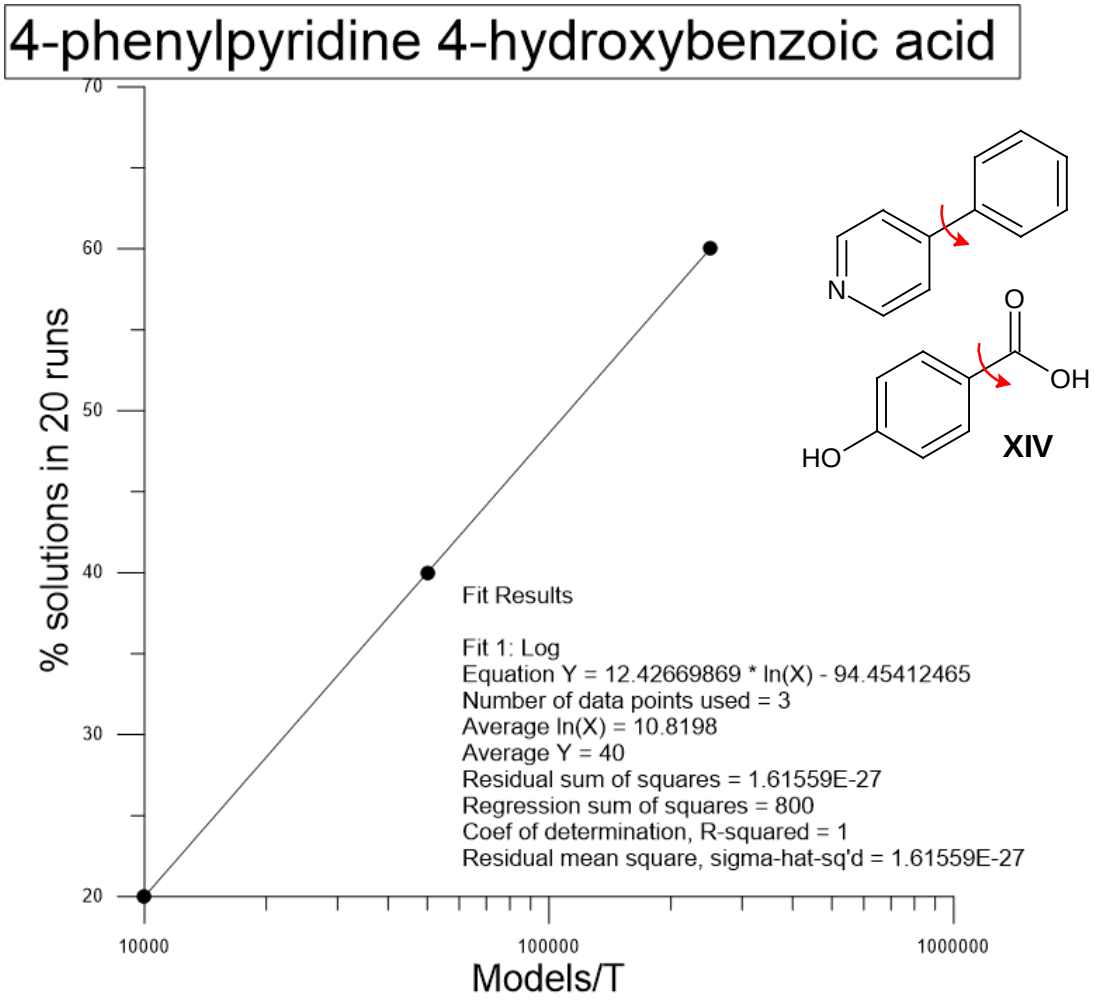

Figure S15 Percentage of solutions for 4-phenylpyridine 4-hydroxybenzoic acid 1:1 co-crystal (**XIV**) in 20 simulated annealing runs using 10,000; 50,000 and 250,000 models per temperature, respectively. According to the fit shown in the figure, 111,803 models/T are estimated to produce 50% of solutions.

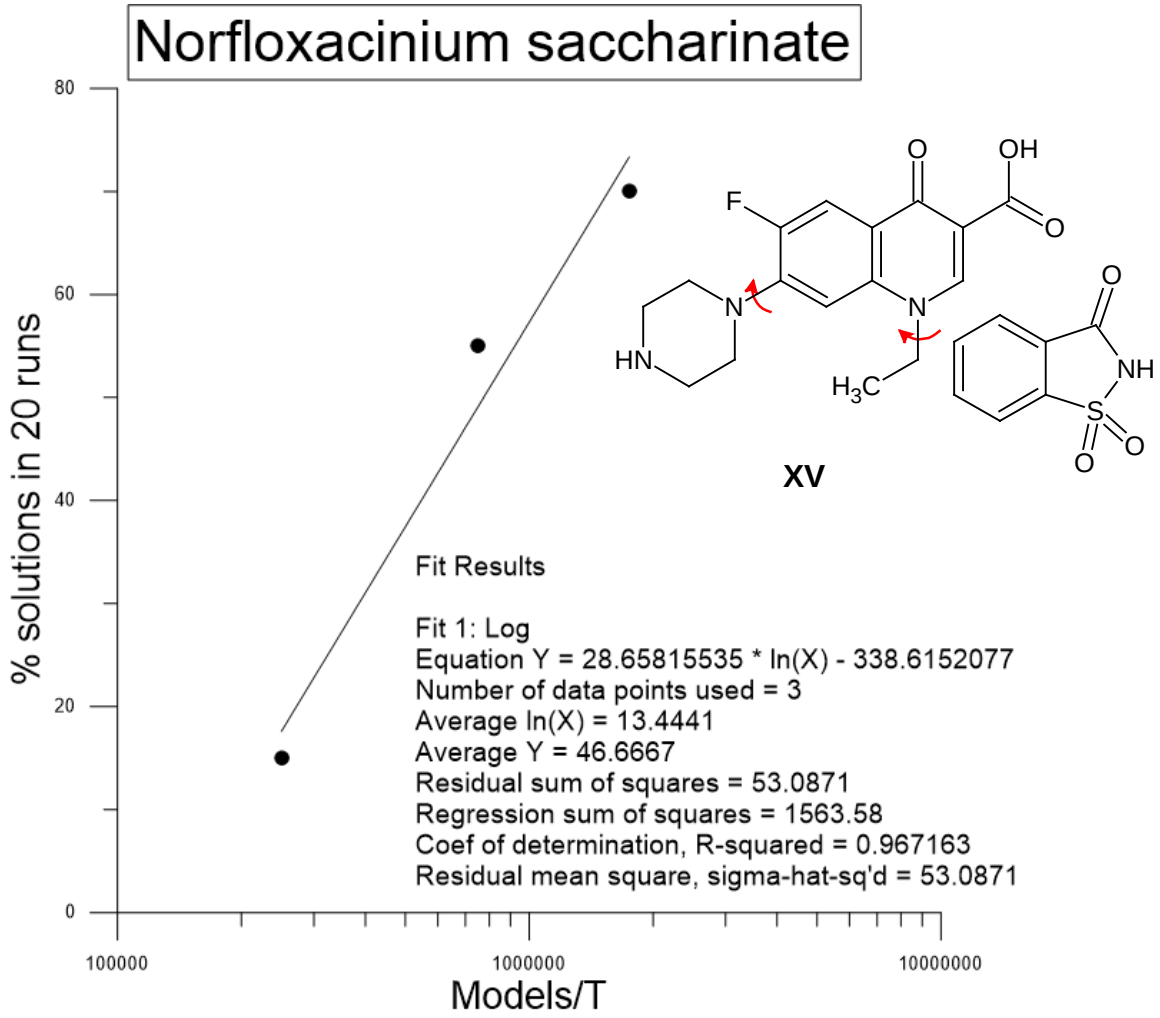

Figure S16 Percentage of solutions for norfloxacinium saccharinate (**XV**) in 20 simulated annealing runs using 250,000; 750,000 and 1,750,000 models per temperature, respectively. According to the fit shown in the figure, 774,808 models/T are estimated to produce 50% of solutions.

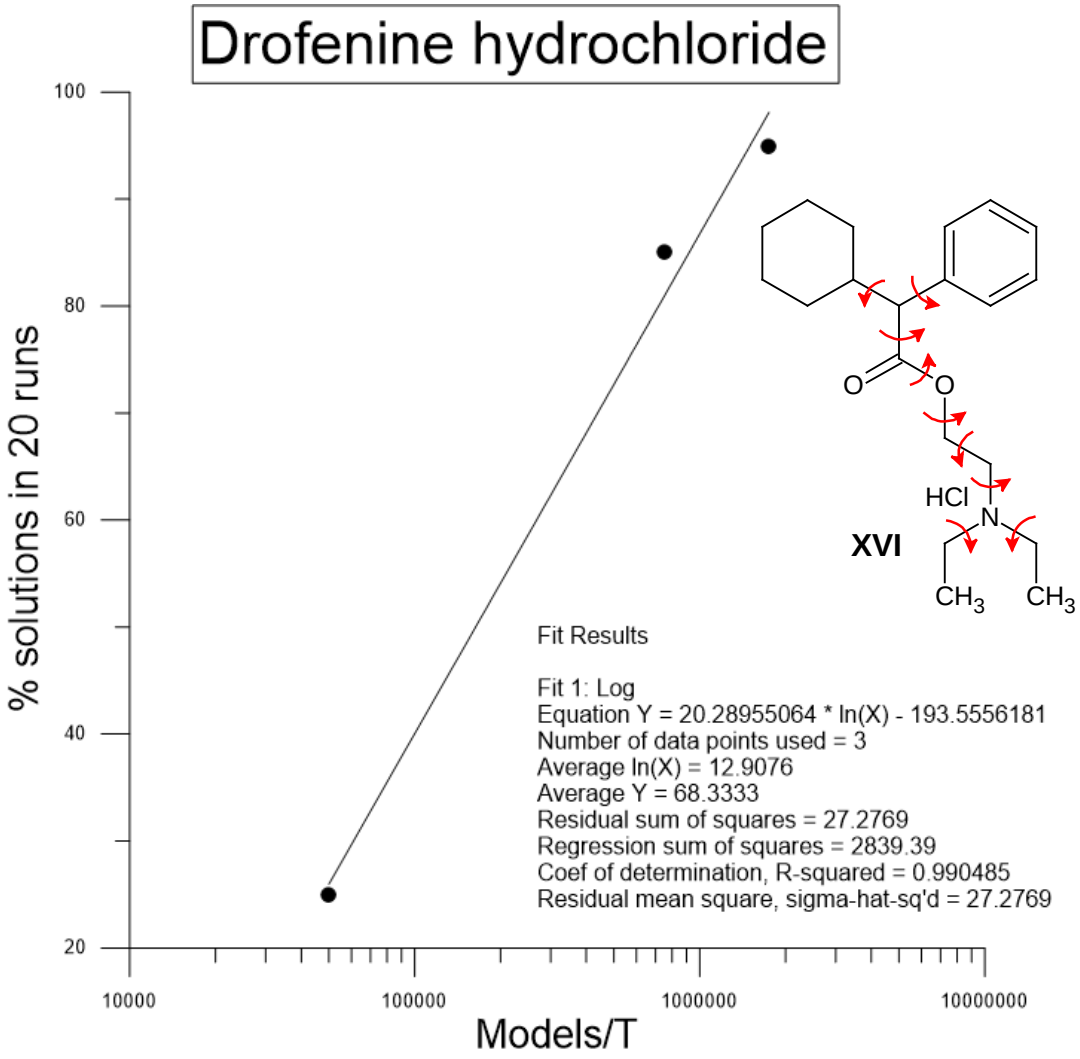

Figure S17 Percentage of solutions for drofenine hydrochloride (**XVI**) in 20 simulated annealing runs using 50,000; 750,000 and 1,750,000 models per temperature, respectively. According to the fit shown in the figure, 163,406 models/T are estimated to produce 50% of solutions.

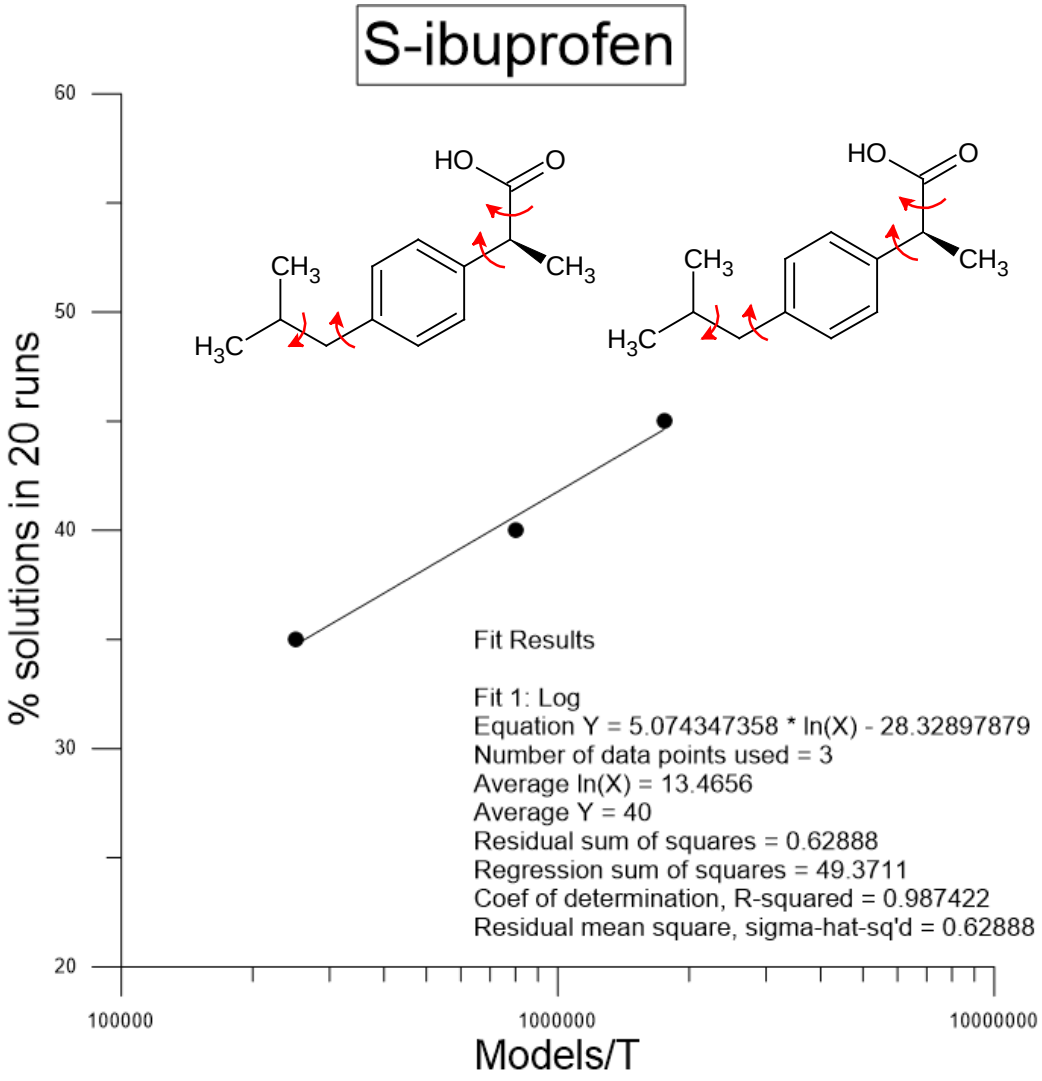

Figure S18 Percentage of solutions for S-ibuprofen (**XVII**) in 20 simulated annealing runs using 250,000; 800,000 and 1,750,000 models per temperature, respectively. According to the fit shown in the figure, 5.1×10^6 models/T are estimated to produce 50% of solutions.

S2. Examples of crystallographic information file "*filename*.cif" files

S2.1. Crystallographic information file for 3-amino-5-mercapto-1,2,4-triazole

```
##########################################################################
   3-amino-5-mercapto-1,2,4-triazole in P21/c
##########################################################################
data_3-amino-5-mercapto-1,2,4-triazole
_symmetry_cell_setting Monoclinic
_symmetry_space_group_name_H-M 'P21/c'
_space_group_IT_number '14'
_cell_length_a 3.998577
_cell_length_b 12.379599
_cell_length_c 9.846816
_cell_angle_alpha 90.000000
_cell_angle_beta 102.1314
_cell_angle_gamma 90.000000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 1.654714 0.874686 0.453026
C2 C 1.227021 0.624719 0.375448
N3 N 1.364551 0.717644 0.324658
N4 N 1.265262 0.624785 0.517124
C5 C 1.491872 0.776182 0.443699
N6 N 1.427151 0.717183 0.559994
S7 S 1.038344 0.526811 0.265731
```

S2.2. Crystallographic information file for the compound (X), L-α-methyldopa

```
##########################################################################
    L-alpha-methyldopa
##########################################################################
data_L-alpha-methyldopa
_symmetry_cell_setting Orthorhombic
_symmetry_space_group_name_H-M 'P212121'
_space_group_IT_number '19'
_cell_length_a 17.986700
_cell_length_b 9.508800
_cell_length_c 5.881000
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 90.000000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.505529 0.515636 0.362770
C2 C 0.565935 0.603892 0.326046
```

```
C3 C 0.620422 0.622557 0.489535
C4 C 0.615335 0.549446 0.695405
C5 C 0.554283 0.463270 0.734260
C6 C 0.500100 0.445999 0.569308
C7 C 0.447488 0.491864 0.180156
C8 C 0.386003 0.604072 0.165888
C9 C 0.314567 0.549920 0.275407
C10 C 0.370927 0.650496 -0.080237
O11 O 0.387813 0.770866 -0.137093
O12 O 0.338845 0.558726 -0.205613
O13 O 0.681181 0.709115 0.459593
O14 O 0.671726 0.566818 0.850021
N15 N 0.410621 0.731018 0.299073
```

S2.3. Crystallographic information file for the compound (VII), dapsone

```
#####################################################################
 DAPSONE
#####################################################################
data_DAPSONE
_symmetry_space_group_name_H-M 'P 21 21 21'
_cell_length_a 25.515924
_cell_length_b 8.054261
_cell_length_c 5.756876
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 90.000000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
O1 O 0.587935 0.671652 1.320657
O2 O 0.661944 0.863291 1.279965
S3 S 0.625739 0.756835 1.172530
C4 C 0.537633 0.839872 0.922944
C5 C 0.591486 0.867478 0.960418
C6 C 0.659693 0.601721 1.022710
C7 C 0.638991 0.442651 0.996945
C8 C 0.710228 0.645764 0.932144
C9 C 0.513769 0.923235 0.747088
C10 C 0.618794 0.974365 0.812160
C11 C 0.667995 0.322569 0.883718
C12 C 0.738073 0.521558 0.811193
C13 C 0.717020 0.361401 0.786802
C14 C 0.592939 1.051398 0.636117
C15 C 0.540437 1.025748 0.591198
N16 N 0.746506 0.240530 0.670480
N17 N 0.516210 1.107474 0.409316
```

S2.4. Crystallographic information file for the compound (XVII), *S*-Ibuprofen

```
##################################################################################
   S-Ibuprofen
##################################################################################
data_ S-Ibuprofen
_symmetry_cell_setting Monoclinic
_symmetry_space_group_name_H-M 'P21'
_space_group_IT_number '4'
_cell_length_a 12.453100
_cell_length_b 8.022770
_cell_length_c 13.527460
_cell_angle_alpha 90.000000
_cell_angle_beta 112.932098
_cell_angle_gamma 90.000000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
O1 O -0.029982 0.507898 0.958857
C2 C 0.353594 0.853135 0.991545
C3 C 0.628220 0.966443 1.155780
C4 C 0.287550 0.706875 0.972099
C5 C 0.439163 1.116447 1.096501
C6 C 0.063416 0.511315 0.934241
C7 C 0.372761 0.948749 1.082595
C8 C 0.564353 1.109723 1.174580
O9 O 0.051876 0.540233 0.842794
C10 C 0.244392 0.653854 1.043830
C11 C 0.175806 0.487767 1.024282
C12 C 0.327619 0.890461 1.153864
C13 C 0.266023 0.747374 1.134913
C14 C 0.575533 1.108183 1.288387
C15 C 0.241672 0.336968 1.006574
O16 O 1.079774 1.119455 0.793083
C17 C 0.732672 0.847050 0.548703
C18 C 0.612039 0.456468 0.464120
C19 C 0.822788 0.943653 0.541557
C20 C 0.652895 0.619073 0.631025
C21 C 1.054806 1.172780 0.693555
C22 C 0.754043 0.732126 0.631148
C23 C 0.649388 0.449842 0.581803
O24 O 1.058687 1.320503 0.676916
C25 C 0.931743 0.929852 0.617165
C26 C 1.030160 1.042614 0.611560
C27 C 0.866061 0.721950 0.706729
C28 C 0.951541 0.818387 0.699801
C29 C 0.573798 0.330541 0.609739
C30 C 1.141056 0.948907 0.621405
```

S3. Examples of Cartesian coordinates "*filename*.xyz" files

S3.1. Cartesian coordinates file for the compound (X), L-α-methyldopa

15
XYZ file for : L-alpha-methyldopa

C	-2.92683	-0.33652	-1.29794
C	-0.59832	0.61706	-1.23973
C	0.77760	-1.47577	-1.01569
C	-2.58949	2.00444	-0.44751
C	-1.97633	0.59865	-0.55449
C	1.79304	-2.21266	-0.42951
C	0.47950	-0.20073	-0.55867
C	2.53932	-1.68590	0.61700
C	1.21089	0.31371	0.50526
C	2.22600	-0.41231	1.10416
N	-1.80782	0.05340	0.83875
O	-2.97914	2.51510	-1.55452
O	-2.70536	2.51432	0.66634
O	3.58259	-2.35562	1.20544
O	2.97436	0.06281	2.16111

S3.2. Cartesian coordinates file for the compound (VII), dapsone

17
XYZ file for : DAPSONE

O	0.32992	2.52851	0.94838
O	-0.28585	0.84772	2.62144
S	-0.00317	1.19460	1.23286
C	-2.53836	0.85574	-1.82059
C	-3.40819	-0.14850	-1.45286
C	3.03217	-0.23638	-1.03843
C	-1.52971	1.28684	-1.01788
C	1.94860	0.48811	-0.51467
C	3.42977	-1.40523	-0.15859
C	-3.26058	-0.65169	-0.15913
C	-1.37274	0.72923	0.25466
C	-2.25524	-0.28380	0.67785
C	1.30833	0.15606	0.72629
C	2.79309	-1.68968	1.08498
C	1.72380	-0.92274	1.50481
N	-4.41774	-0.54700	-2.31256
N	4.50587	-2.20180	-0.57656

S3.3. Cartesian coordinates file for the compound (XVII), *S*-Ibuprofen, Z'=2

30
XYZ file for : S-ibuprofen

O	-7.26735	0.26375	-3.22224
O	-6.79638	2.34415	-2.70363
O	7.28304	-1.90782	2.47459
O	6.76048	-0.31830	3.89542

C	-6.30520	2.60733	-5.63478
C	-5.86953	1.46957	-4.70605
C	0.88591	3.03062	-4.85569
C	-3.57316	0.46938	-4.57877
C	-4.37651	1.51467	-4.29651
C	0.71791	1.64281	-4.33759
C	-2.23875	0.48173	-4.16274
C	2.04477	1.05575	-4.07128
C	-6.68247	1.42752	-3.48661
C	-3.84891	2.58360	-3.60798
C	-1.70693	1.57883	-3.49424
C	-2.55720	2.62267	-3.22250
C	-0.19556	1.58608	-3.14253
C	6.63918	-1.47332	3.55291
C	2.12630	-2.49095	3.06319
C	3.41403	-2.83547	3.26622
C	0.17700	-0.81618	3.29384
C	1.62647	-1.30751	3.54906
C	5.75889	-2.44778	4.20512
C	4.29046	-2.02535	3.95249
C	-0.87555	-1.56367	4.06806
C	2.49662	-0.49667	4.26938
C	3.83548	-0.85666	4.44744
C	-0.33177	-2.78475	4.72791
C	6.11875	-2.63183	5.68273
C	-1.55003	-0.72219	5.07476

S4. Examples of Le Bail fit files (first 10 lines for brevity)

S4.1. GSAS Le Bail fit file (*filename*.rfl) for the compound (X), L-α-methyldopa

H	K	L	M	sth/lam	TTH	FWHM	FoSq	sig	Fobs	obs	phase
2	0	0	2	0.0555987	4.4513	0.0468	2.839E+03	880.	53.285	0	0.000
1	1	0	4	0.0594806	4.7634	0.0447	48.9	16.2	6.995	0	0.000
2	1	0	4	0.0765269	6.1332	0.0364	1.617E+03	502.	40.208	0	0.000
1	0	1	4	0.0894550	7.1728	0.0283	383.	120.	19.563	0	0.000
0	1	1	4	0.0999727	8.0117	0.0681	258.	80.9	16.058	0	0.000
3	1	0	4	0.0985920	7.9053	0.0369	114.	36.3	10.674	0	0.000
0	2	0	2	0.1051693	8.4266	0.0862	845.	263.	29.065	0	0.000
1	1	1	8	0.1037658	8.3185	0.0560	170.	53.8	13.053	0	0.000
2	0	1	4	0.1015904	8.1471	0.0353	1.039E+04	3.219E+03	101.922	0	0.000

…

S4.2. FULLPROF Le Bail fit file (*filename*.hkl) for the compound (II), 3-amino-5-mercapto-1,2,4-triazole

>Phase no.: 1 phase 1: 50 reflections, N&T: 0 0.00 (The # of eff. reflections may be lower)
! SPGR: P 21/a; CELL: 9.84981 12.38257 3.99943 90.00000 102.16579 90.00000

Code	h	k	l	Mult	D(A)	2T	HW	Iobs	Icalc	io-ic
1	1	1	0	4	7.601019	8.675	0.030896	308.7	308.6	0.0
1	0	2	0	2	6.191260	10.655	0.029225	49.5	49.5	-0.1
1	1	2	0	4	5.207597	12.675	0.036441	222.0	222.0	0.0

```
  1   2   0   0    2  4.814293   13.716  0.042440    34.7    34.7     0.0
  1   2   1   0    4  4.487082   14.721  0.049069   356.3   356.1     0.2
  1   0   0   1    2  3.909580   16.910  0.065129    22.1    22.1     0.0
  1   2   2   0    4  3.800510   17.399  0.068909   778.5   778.3     0.2
…
```