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Supporting information for article:

The first example of stereoselective synthesis and crystal structure of spirobicycloquinazolinone based on ((ndash;)-fenchone and anthranilamide

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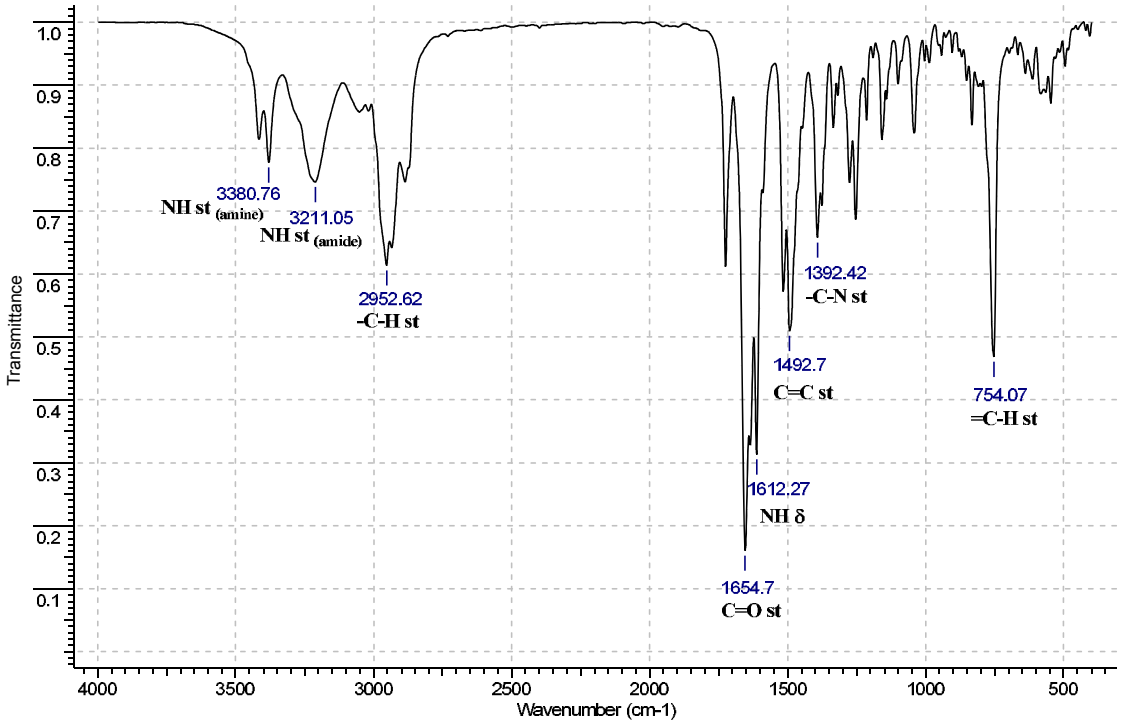

Figure S1 IR spectrum of compound **1**.

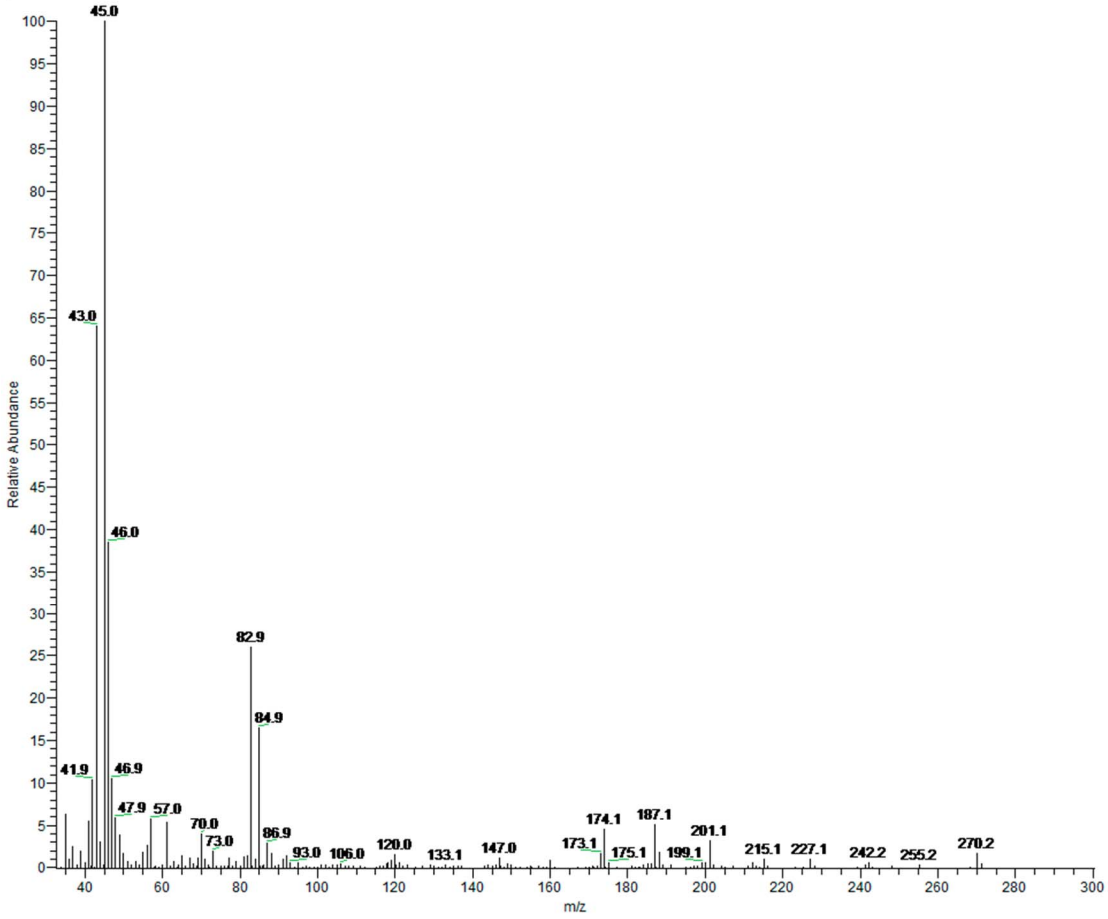

Figure S2 High-Resolution Mass Spectrum of compound **1**.

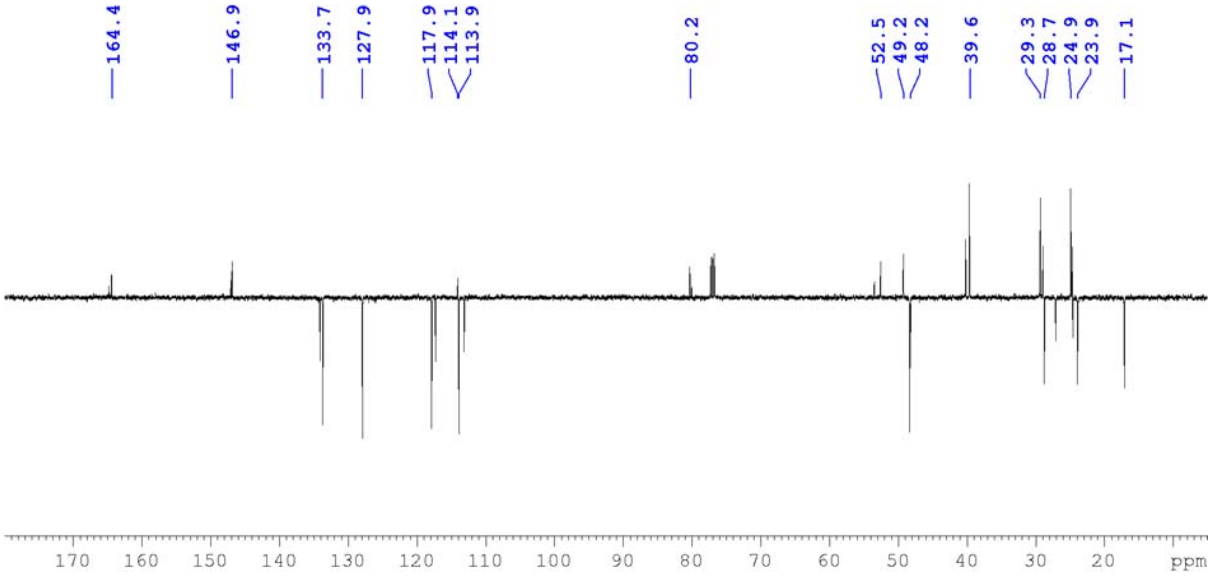

Figure S3 ^{13}C-NMR spectrum for compound **1** ($CDCl_3$, 125.76 MHz)

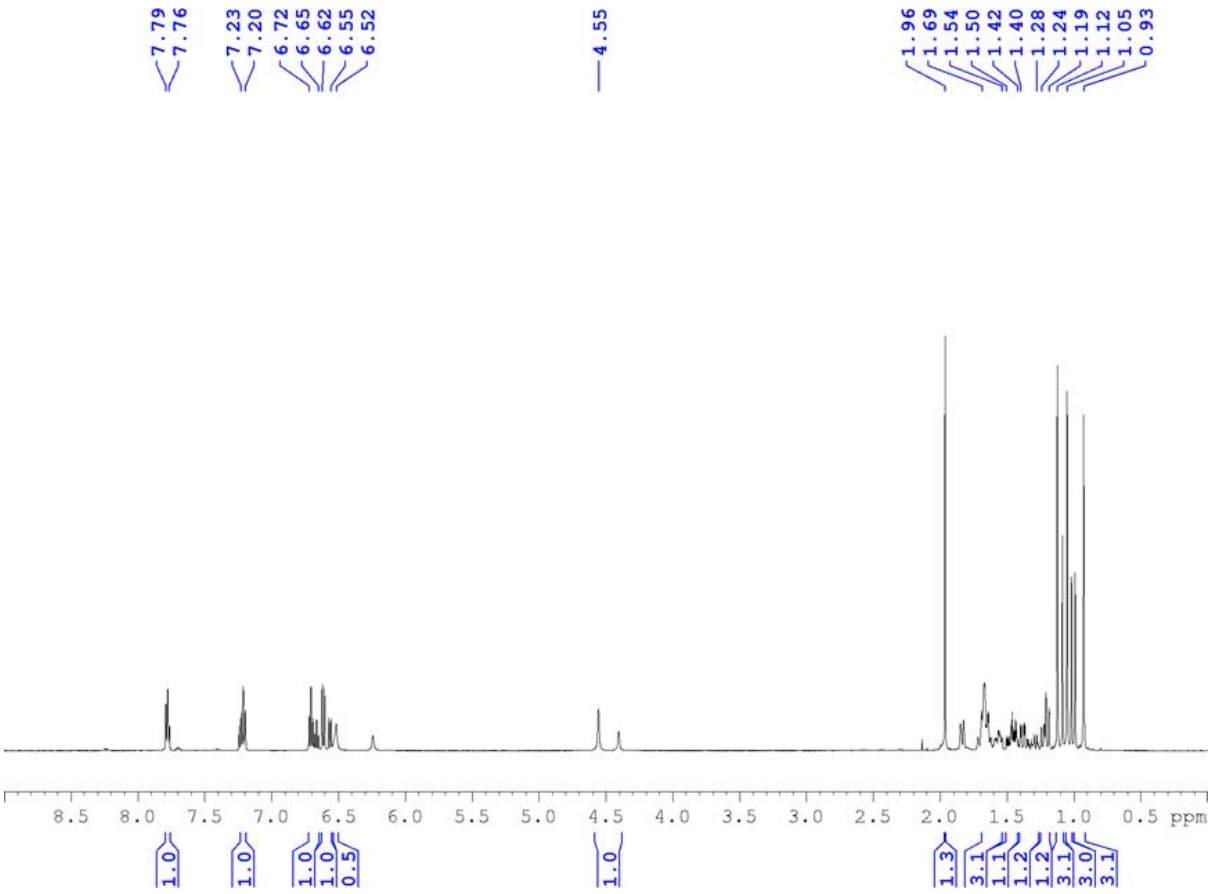

Figure S4 ^{1}H-NMR spectrum for compound **1** ($CDCl_3$, 400.13MHz)

Table S1 (1*R*,2*S*,4*S*)–1,3,3–trimethyl–1'H–spiro[bicyclo[2.2.1]heptane-2,2'-quinazolin]-4'(3'H)-one (**1**)

Crystal data	
Chemical formula	$C_{17}H_{22}N_2O$
M_r	270.36
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, *b*, *c* (Å)	11.8870 (5), 12.2535 (5), 27.7511 (11)
V (Å^3)	4042.2 (3)
Z	8
Radiation type	Mo *K*α

μ (mm^{-1})	0.06
Crystal size (mm)	0.60 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker *APEX*-II CCD
Absorption correction	Multi-scan *SADABS2008*/1
T_{min}, T_{max}	0.801, 0.939
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32223, 7494, 5139
R_{int}	0.053
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.178, 1.04
No. of reflections	7494
No. of parameters	361
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.27, −0.16
Absolute structure	Flack x determined using 1849 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	2.7 (5)

Computer programs: Bruker *APEX2*, Bruker *SAINT*, *SHELXS97* (Sheldrick, 2008), *SHELXL2014*/7 (Sheldrick, 2014), Bruker *SHELXTL*.

Table S2 Geometric parameters (Å, º)

O1—C11	1.244 (4)	O101—C111	1.250 (4)

N1—C11	1.337 (4)	N101—C111	1.327 (4)
N1—C2	1.471 (5)	N101—C102	1.469 (4)
N1—H1A	0.8600	N101—H10E	0.8600
C1—C6	1.505 (7)	C101—C108	1.489 (7)
C1—C7	1.529 (8)	C101—C106	1.546 (6)
C1—C8	1.532 (9)	C101—C102	1.556 (5)
C1—C2	1.573 (6)	C101—C107	1.557 (6)
N2—C13	1.378 (4)	N102—C113	1.383 (4)
N2—C2	1.437 (4)	N102—C102	1.447 (4)
N2—H2A	0.8600	N102—H10D	0.8600
C2—C3	1.603 (6)	C102—C103	1.603 (5)
C3—C10	1.508 (8)	C103—C109	1.543 (6)
C3—C9	1.526 (8)	C103—C104	1.546 (6)
C3—C4	1.612 (9)	C103—C110	1.563 (6)
C4—C5	1.450 (10)	C104—C105	1.520 (7)
C4—C7	1.530 (10)	C104—C107	1.538 (7)
C4—H4A	0.9800	C104—H10F	0.9800
C5—C6	1.561 (11)	C105—C106	1.497 (8)
C5—H5A	0.9700	C105—H10Q	0.9700
C5—H5B	0.9700	C105—H10R	0.9700
C6—H6A	0.9700	C106—H10O	0.9700
C6—H6B	0.9700	C106—H10P	0.9700
C7—H7A	0.9700	C107—H10G	0.9700
C7—H7B	0.9700	C107—H10H	0.9700
C8—H8A	0.9600	C108—H10I	0.9600
C8—H8B	0.9600	C108—H10J	0.9600

C8—H8C	0.9600	C108—H10K	0.9600
C9—H9A	0.9600	C109—H10L	0.9600
C9—H9B	0.9600	C109—H10M	0.9600
C9—H9C	0.9600	C109—H10N	0.9600
C10—H10A	0.9600	C110—H11E	0.9600
C10—H10B	0.9600	C110—H11F	0.9600
C10—H10C	0.9600	C110—H11G	0.9600
C11—C12	1.477 (5)	C111—C112	1.463 (4)
C12—C17	1.380 (5)	C112—C117	1.395 (5)
C12—C13	1.391 (5)	C112—C113	1.405 (5)
C13—C14	1.422 (5)	C113—C114	1.389 (5)
C14—C15	1.365 (6)	C114—C115	1.354 (6)
C14—H14A	0.9300	C114—H11A	0.9300
C15—C16	1.387 (7)	C115—C116	1.397 (6)
C15—H15A	0.9300	C115—H11D	0.9300
C16—C17	1.380 (6)	C116—C117	1.372 (5)
C16—H16A	0.9300	C116—H11C	0.9300
C17—H17A	0.9300	C117—H11B	0.9300
C11—N1—C2	126.3 (3)	C111—N101—C102	126.7 (3)
C11—N1—H1A	116.8	C111—N101—H10E	116.7
C2—N1—H1A	116.8	C102—N101—H10E	116.7
C6—C1—C7	102.7 (4)	C108—C101—C106	116.1 (4)
C6—C1—C8	114.1 (4)	C108—C101—C102	114.7 (3)
C7—C1—C8	115.3 (5)	C106—C101—C102	108.9 (3)
C6—C1—C2	110.3 (4)	C108—C101—C107	115.7 (4)
C7—C1—C2	100.1 (4)	C106—C101—C107	99.2 (3)

C8—C1—C2	113.1 (4)	C102—C101—C107	100.2 (3)
C13—N2—C2	121.7 (3)	C113—N102—C102	121.2 (3)
C13—N2—H2A	119.2	C113—N102—H10D	119.4
C2—N2—H2A	119.2	C102—N102—H10D	119.4
N2—C2—N1	106.7 (3)	N102—C102—N101	105.9 (3)
N2—C2—C1	111.4 (3)	N102—C102—C101	111.8 (3)
N1—C2—C1	109.8 (3)	N101—C102—C101	109.4 (3)
N2—C2—C3	114.7 (3)	N102—C102—C103	115.5 (3)
N1—C2—C3	111.8 (3)	N101—C102—C103	111.8 (3)
C1—C2—C3	102.5 (3)	C101—C102—C103	102.4 (3)
C10—C3—C9	107.4 (5)	C109—C103—C104	113.2 (4)
C10—C3—C2	111.2 (4)	C109—C103—C110	107.3 (4)
C9—C3—C2	112.5 (4)	C104—C103—C110	108.2 (4)
C10—C3—C4	116.5 (5)	C109—C103—C102	113.2 (3)
C9—C3—C4	109.2 (5)	C104—C103—C102	102.7 (3)
C2—C3—C4	100.0 (4)	C110—C103—C102	112.2 (3)
C5—C4—C7	102.8 (7)	C105—C104—C103	110.3 (4)
C5—C4—C3	108.4 (6)	C105—C104—C107	100.1 (4)
C7—C4—C3	102.9 (4)	C103—C104—C107	102.0 (3)
C5—C4—H4A	113.8	C105—C104—H10F	114.3
C7—C4—H4A	113.8	C103—C104—H10F	114.3
C3—C4—H4A	113.8	C107—C104—H10F	114.3
C4—C5—C6	103.7 (6)	C106—C105—C104	103.8 (4)
C4—C5—H5A	111.0	C106—C105—H10Q	111.0
C6—C5—H5A	111.0	C104—C105—H10Q	111.0
C4—C5—H5B	111.0	C106—C105—H10R	111.0

C6—C5—H5B	111.0	C104—C105—H10R	111.0
H5A—C5—H5B	109.0	H10Q—C105—H10R	109.0
C1—C6—C5	102.5 (5)	C105—C106—C101	105.7 (4)
C1—C6—H6A	111.3	C105—C106—H10O	110.6
C5—C6—H6A	111.3	C101—C106—H10O	110.6
C1—C6—H6B	111.3	C105—C106—H10P	110.6
C5—C6—H6B	111.3	C101—C106—H10P	110.6
H6A—C6—H6B	109.2	H10O—C106—H10P	108.7
C1—C7—C4	93.7 (5)	C101—C107—C104	94.9 (3)
C1—C7—H7A	113.0	C101—C107—H10G	112.8
C4—C7—H7A	113.0	C104—C107—H10G	112.8
C1—C7—H7B	113.0	C101—C107—H10H	112.8
C4—C7—H7B	113.0	C104—C107—H10H	112.8
H7A—C7—H7B	110.4	H10G—C107—H10H	110.2
C1—C8—H8A	109.5	C101—C108—H10I	109.5
C1—C8—H8B	109.5	C101—C108—H10J	109.5
H8A—C8—H8B	109.5	H10I—C108—H10J	109.5
C1—C8—H8C	109.5	C101—C108—H10K	109.5
H8A—C8—H8C	109.5	H10I—C108—H10K	109.5
H8B—C8—H8C	109.5	H10J—C108—H10K	109.5
C3—C9—H9A	109.5	C103—C109—H10L	109.5
C3—C9—H9B	109.5	C103—C109—H10M	109.5
H9A—C9—H9B	109.5	H10L—C109—H10M	109.5
C3—C9—H9C	109.5	C103—C109—H10N	109.5
H9A—C9—H9C	109.5	H10L—C109—H10N	109.5
H9B—C9—H9C	109.5	H10M—C109—H10N	109.5

C3—C10—H10A	109.5	C103—C110—H11E	109.5
C3—C10—H10B	109.5	C103—C110—H11F	109.5
H10A—C10—H10B	109.5	H11E—C110—H11F	109.5
C3—C10—H10C	109.5	C103—C110—H11G	109.5
H10A—C10—H10C	109.5	H11E—C110—H11G	109.5
H10B—C10—H10C	109.5	H11F—C110—H11G	109.5
O1—C11—N1	121.9 (3)	O101—C111—N101	121.6 (3)
O1—C11—C12	121.5 (3)	O101—C111—C112	122.0 (3)
N1—C11—C12	116.6 (3)	N101—C111—C112	116.3 (3)
C17—C12—C13	120.5 (3)	C117—C112—C113	119.3 (3)
C17—C12—C11	121.6 (3)	C117—C112—C111	121.9 (3)
C13—C12—C11	117.8 (3)	C113—C112—C111	118.8 (3)
N2—C13—C12	119.8 (3)	N102—C113—C114	123.0 (3)
N2—C13—C14	121.5 (3)	N102—C113—C112	118.0 (3)
C12—C13—C14	118.6 (3)	C114—C113—C112	118.8 (3)
C15—C14—C13	119.0 (4)	C115—C114—C113	120.9 (3)
C15—C14—H14A	120.5	C115—C114—H11A	119.5
C13—C14—H14A	120.5	C113—C114—H11A	119.5
C14—C15—C16	122.6 (4)	C114—C115—C116	121.1 (3)
C14—C15—H15A	118.7	C114—C115—H11D	119.4
C16—C15—H15A	118.7	C116—C115—H11D	119.4
C17—C16—C15	118.1 (4)	C117—C116—C115	118.8 (4)
C17—C16—H16A	121.0	C117—C116—H11C	120.6
C15—C16—H16A	121.0	C115—C116—H11C	120.6
C16—C17—C12	121.3 (4)	C116—C117—C112	121.0 (3)
C16—C17—H17A	119.3	C116—C117—H11B	119.5

C12—C17—H17A	119.3	C112—C117—H11B	119.5
C13—N2—C2—N1	−38.8 (4)	C113—N102—C102—N101	−42.0 (4)
C13—N2—C2—C1	−158.6 (3)	C113—N102—C102—C101	−161.0 (3)
C13—N2—C2—C3	85.6 (4)	C113—N102—C102—C103	82.4 (4)
C11—N1—C2—N2	30.5 (5)	C111—N101—C102—N102	32.0 (4)
C11—N1—C2—C1	151.3 (3)	C111—N101—C102—C101	152.6 (3)
C11—N1—C2—C3	−95.7 (4)	C111—N101—C102—C103	−94.6 (4)
C6—C1—C2—N2	−58.2 (5)	C108—C101—C102—N102	73.4 (4)
C7—C1—C2—N2	−166.0 (4)	C106—C101—C102—N102	−58.5 (4)
C8—C1—C2—N2	70.9 (5)	C107—C101—C102—N102	−162.0 (3)
C6—C1—C2—N1	−176.2 (4)	C108—C101—C102—N101	−43.6 (5)
C7—C1—C2—N1	76.1 (4)	C106—C101—C102—N101	−175.5 (3)
C8—C1—C2—N1	−47.0 (5)	C107—C101—C102—N101	81.0 (3)
C6—C1—C2—C3	64.9 (5)	C108—C101—C102—C103	−162.3 (4)
C7—C1—C2—C3	−42.8 (4)	C106—C101—C102—C103	65.7 (4)
C8—C1—C2—C3	−166.0 (4)	C107—C101—C102—C103	−37.7 (3)
N2—C2—C3—C10	4.4 (6)	N102—C102—C103—C109	2.3 (5)
N1—C2—C3—C10	126.0 (5)	N101—C102—C103—C109	123.5 (4)
C1—C2—C3—C10	−116.5 (5)	C101—C102—C103—C109	−119.4 (4)
N2—C2—C3—C9	−116.2 (5)	N102—C102—C103—C104	124.8 (3)
N1—C2—C3—C9	5.4 (6)	N101—C102—C103—C104	−114.0 (3)
C1—C2—C3—C9	123.0 (5)	C101—C102—C103—C104	3.1 (3)
N2—C2—C3—C4	128.0 (4)	N102—C102—C103—C110	−119.3 (4)
N1—C2—C3—C4	−110.4 (4)	N101—C102—C103—C110	1.9 (4)
C1—C2—C3—C4	7.2 (4)	C101—C102—C103—C110	119.0 (4)
C10—C3—C4—C5	42.1 (8)	C109—C103—C104—C105	50.1 (5)

C9—C3—C4—C5	164.0 (6)	C110—C103—C104—C105	168.9 (4)
C2—C3—C4—C5	−77.8 (6)	C102—C103—C104—C105	−72.3 (4)
C10—C3—C4—C7	150.5 (5)	C109—C103—C104—C107	155.8 (4)
C9—C3—C4—C7	−87.6 (6)	C110—C103—C104—C107	−85.4 (4)
C2—C3—C4—C7	30.7 (5)	C102—C103—C104—C107	33.4 (4)
C7—C4—C5—C6	−37.9 (7)	C103—C104—C105—C106	68.3 (5)
C3—C4—C5—C6	70.7 (8)	C107—C104—C105—C106	−38.7 (5)
C7—C1—C6—C5	31.7 (6)	C104—C105—C106—C101	4.0 (5)
C8—C1—C6—C5	157.2 (6)	C108—C101—C106—C105	156.1 (4)
C2—C1—C6—C5	−74.3 (6)	C102—C101—C106—C105	−72.7 (5)
C4—C5—C6—C1	3.7 (8)	C107—C101—C106—C105	31.5 (5)
C6—C1—C7—C4	−52.7 (5)	C108—C101—C107—C104	−178.3 (4)
C8—C1—C7—C4	−177.4 (4)	C106—C101—C107—C104	−53.4 (4)
C2—C1—C7—C4	61.0 (4)	C102—C101—C107—C104	57.8 (3)
C5—C4—C7—C1	55.9 (5)	C105—C104—C107—C101	57.1 (4)
C3—C4—C7—C1	−56.8 (5)	C103—C104—C107—C101	−56.3 (4)
C2—N1—C11—O1	171.8 (3)	C102—N101—C111—O101	175.9 (3)
C2—N1—C11—C12	−8.9 (5)	C102—N101—C111—C112	−7.7 (5)
O1—C11—C12—C17	−5.4 (5)	O101—C111—C112—C117	−12.5 (5)
N1—C11—C12—C17	175.3 (3)	N101—C111—C112—C117	171.2 (3)
O1—C11—C12—C13	171.2 (3)	O101—C111—C112—C113	165.6 (3)
N1—C11—C12—C13	−8.1 (4)	N101—C111—C112—C113	−10.8 (4)
C2—N2—C13—C12	26.8 (5)	C102—N102—C113—C114	−155.5 (3)
C2—N2—C13—C14	−157.4 (4)	C102—N102—C113—C112	28.9 (4)
C17—C12—C13—N2	176.2 (3)	C117—C112—C113—N102	178.7 (3)
C11—C12—C13—N2	−0.5 (5)	C111—C112—C113—N102	0.6 (4)

C17—C12—C13—C14	0.3 (5)	C117—C112—C113—C114	2.8 (5)
C11—C12—C13—C14	−176.4 (3)	C111—C112—C113—C114	−175.3 (3)
N2—C13—C14—C15	−176.3 (4)	N102—C113—C114—C115	−178.4 (4)
C12—C13—C14—C15	−0.5 (6)	C112—C113—C114—C115	−2.8 (5)
C13—C14—C15—C16	−0.3 (7)	C113—C114—C115—C116	0.7 (6)
C14—C15—C16—C17	1.3 (8)	C114—C115—C116—C117	1.5 (6)
C15—C16—C17—C12	−1.4 (7)	C115—C116—C117—C112	−1.4 (6)
C13—C12—C17—C16	0.7 (6)	C113—C112—C117—C116	−0.8 (5)
C11—C12—C17—C16	177.3 (4)	C111—C112—C117—C116	177.3 (3)

Table S3 Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	∠*D*—H···*A* (°)
N1—H1A···O101	0.86	2.19	2.989 (3)	154.7
N101—H10E···O1	0.86	2.15	2.942 (3)	153.4
N102—H10D···O101^{i}	0.86	2.72	3.372 (4)	134.0
C114—H11A···O1^{i}	0.93	2.73	3.453 (4)	135.2
C114—H11A···O101^{i}	0.93	2.70	3.508 (5)	145.8

Symmetry code(s): (i) –*x* + 2, *y* − 1/2, −*z* + 1/2.