Synthesis, X-ray Crystal Structure, Hirshfeld Surface Analysis, and Molecular Docking Study of Novel Hepatitis B (HBV) Inhibitor: 8-Fluoro-5-(4-fluorobenzyl)-3-(2-methoxybenzyl)-3,5-dihydro-4H-pyrimido[5,4-b]indol-4-one

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SUPPORTING INFORMATION

Figure S1. UV/Vis spectrum of the title compound (3) (MeOH, M 0.0116 mmol/l, optical cell 1.0 cm)

Figure S2. IR spectrum of the title compound (**3**) (KBr pellet).

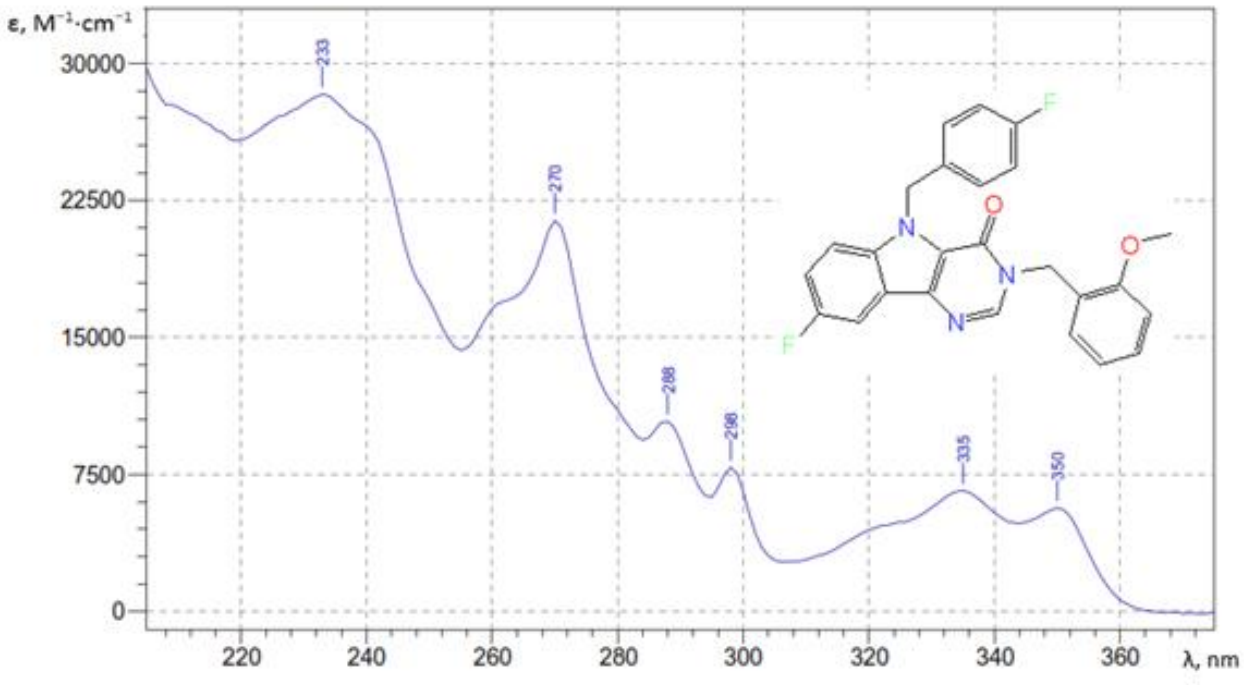
Figure S3. ^{19}F NMR (376.72 MHz, DMSO-d6) spectrum of the title compound (**3**).

Figure S4. ^{13}C NMR (75.48 MHz, DMSO-d6) spectrum of the title compound (**3**).

Figure S5. ^{1}H NMR (300.16 MHz, DMSO-d6) spectrum of the title compound (**3**).

Figure S6. LC/MS Data for Structural Determination of of the title compound (**3**).

Table S1. Geometric parameters (Å, ◦) of the title compound (**3**)



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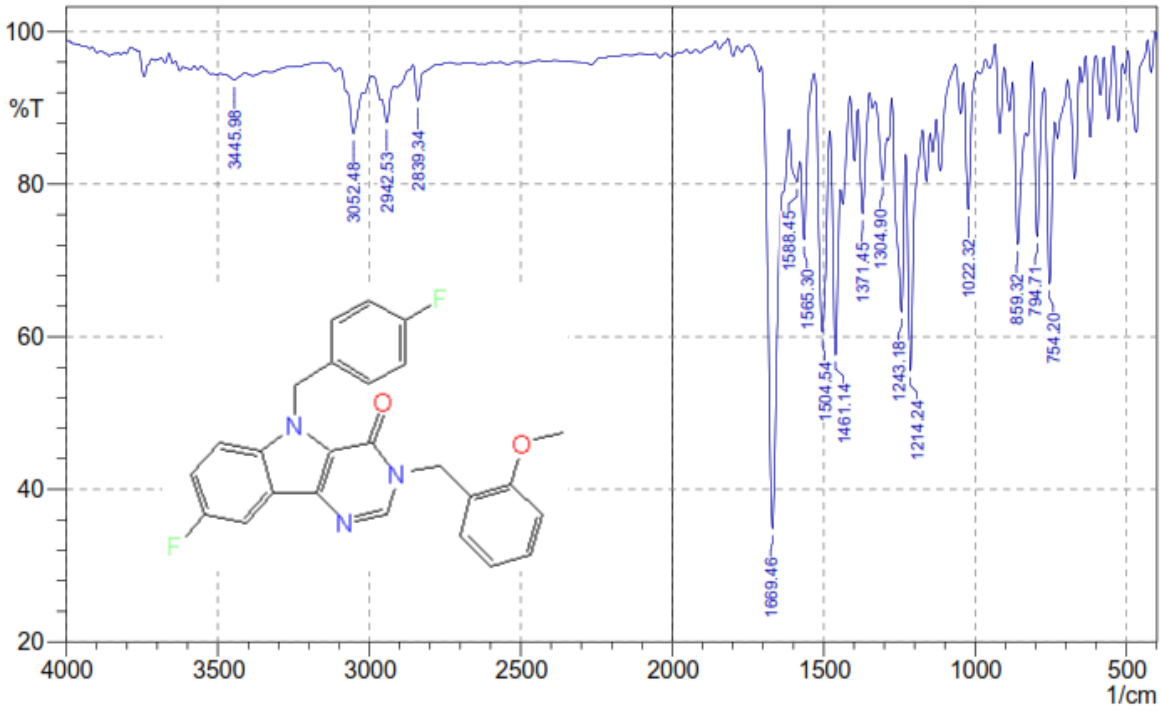
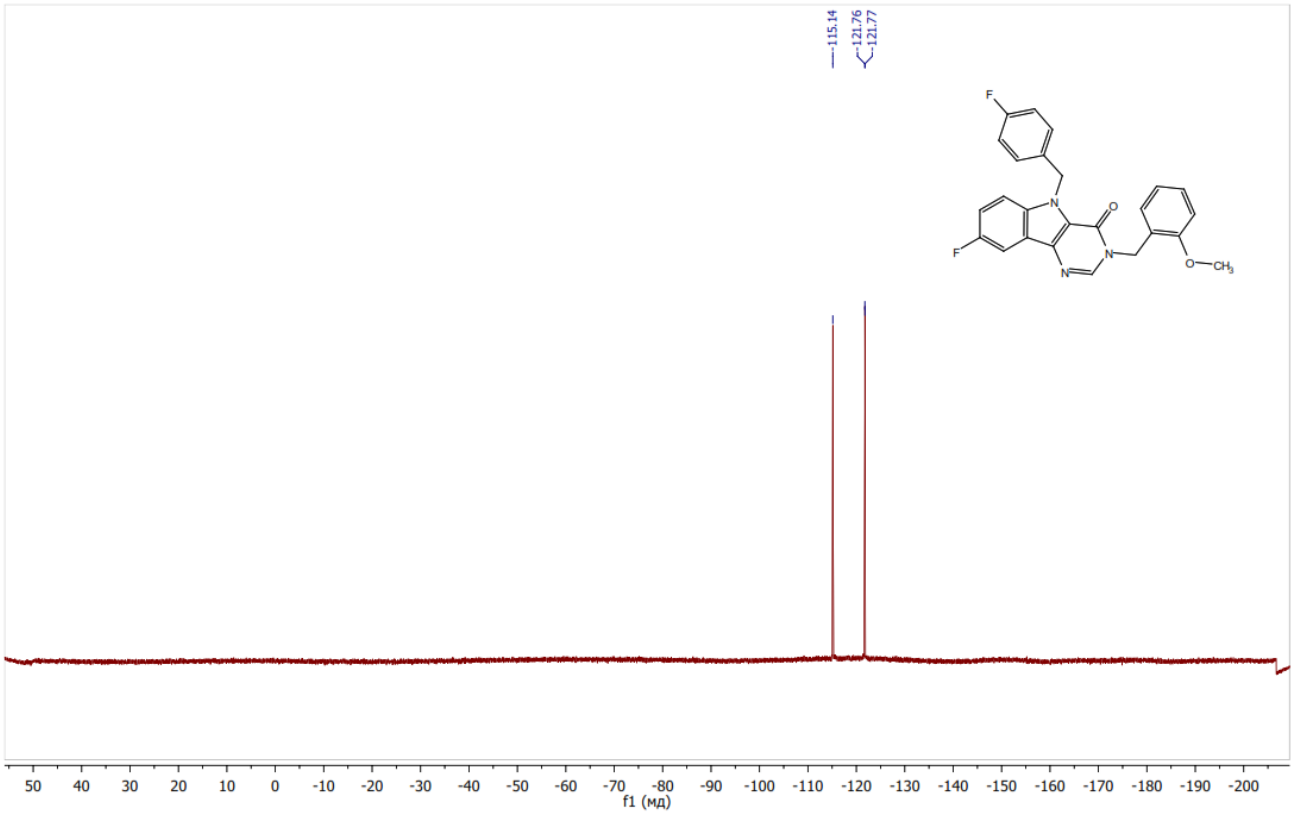


Figure S2. IR spectrum of the title compound (**3**) (KBr pellet).



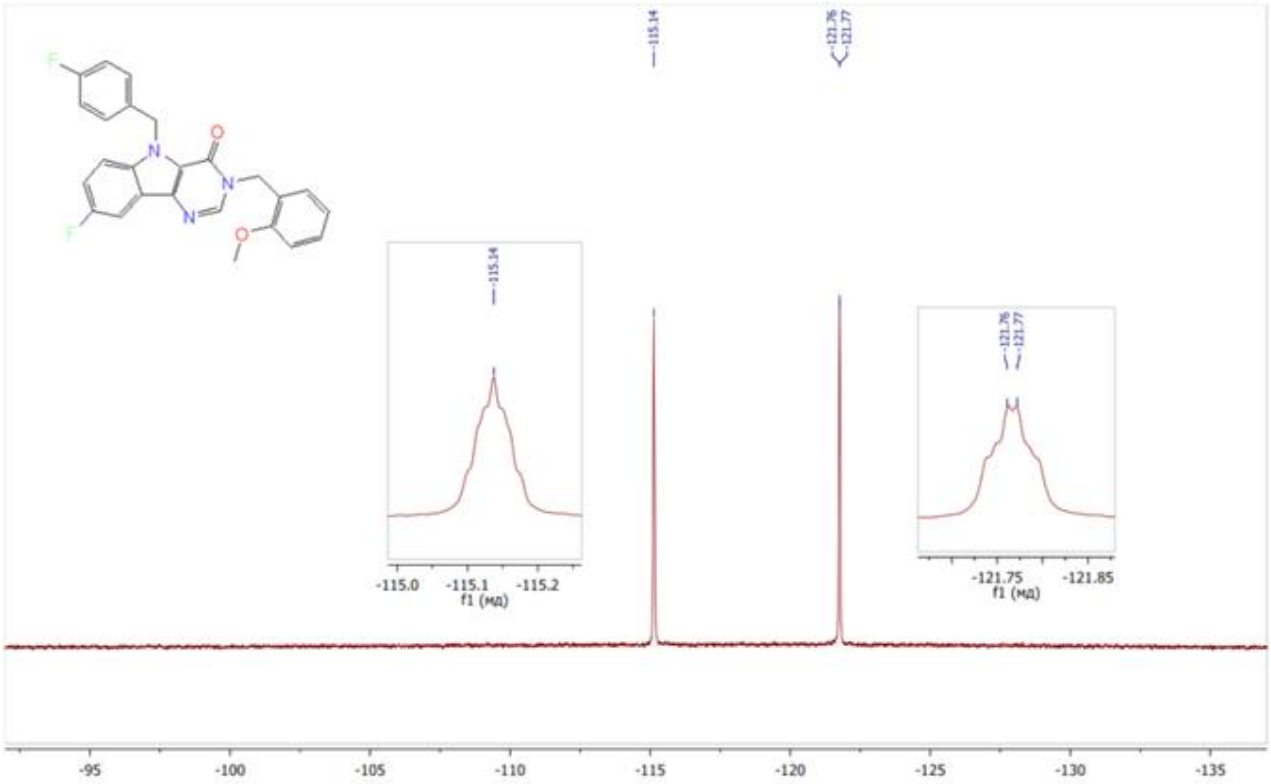


Figure S3. ^{19}F NMR (376.72 MHz, DMSO-d6) spectrum of the title compound (**3**).

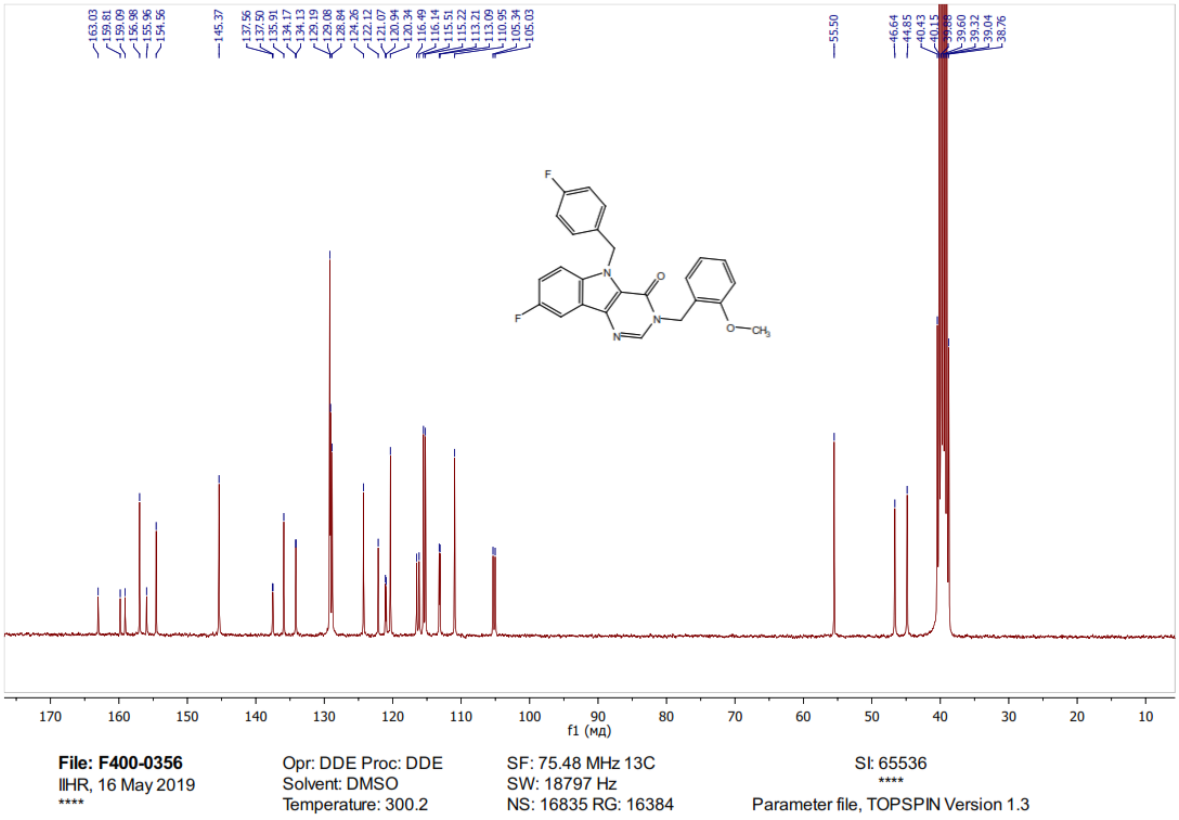


Figure S4. ^{13}C NMR (75.48 MHz, DMSO-d6) spectrum of the title compound (**3**).

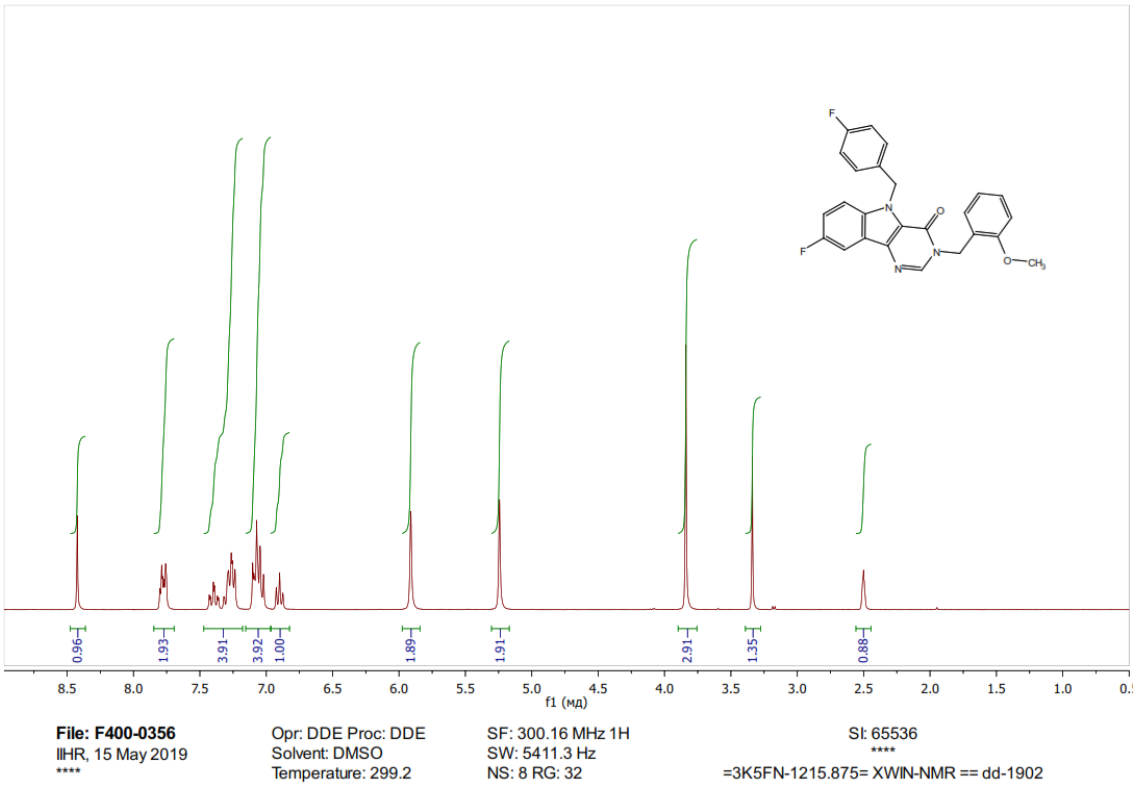


Figure S5. ^{1}H NMR (300.16 MHz, DMSO-d6) spectrum of the title compound (**3**).

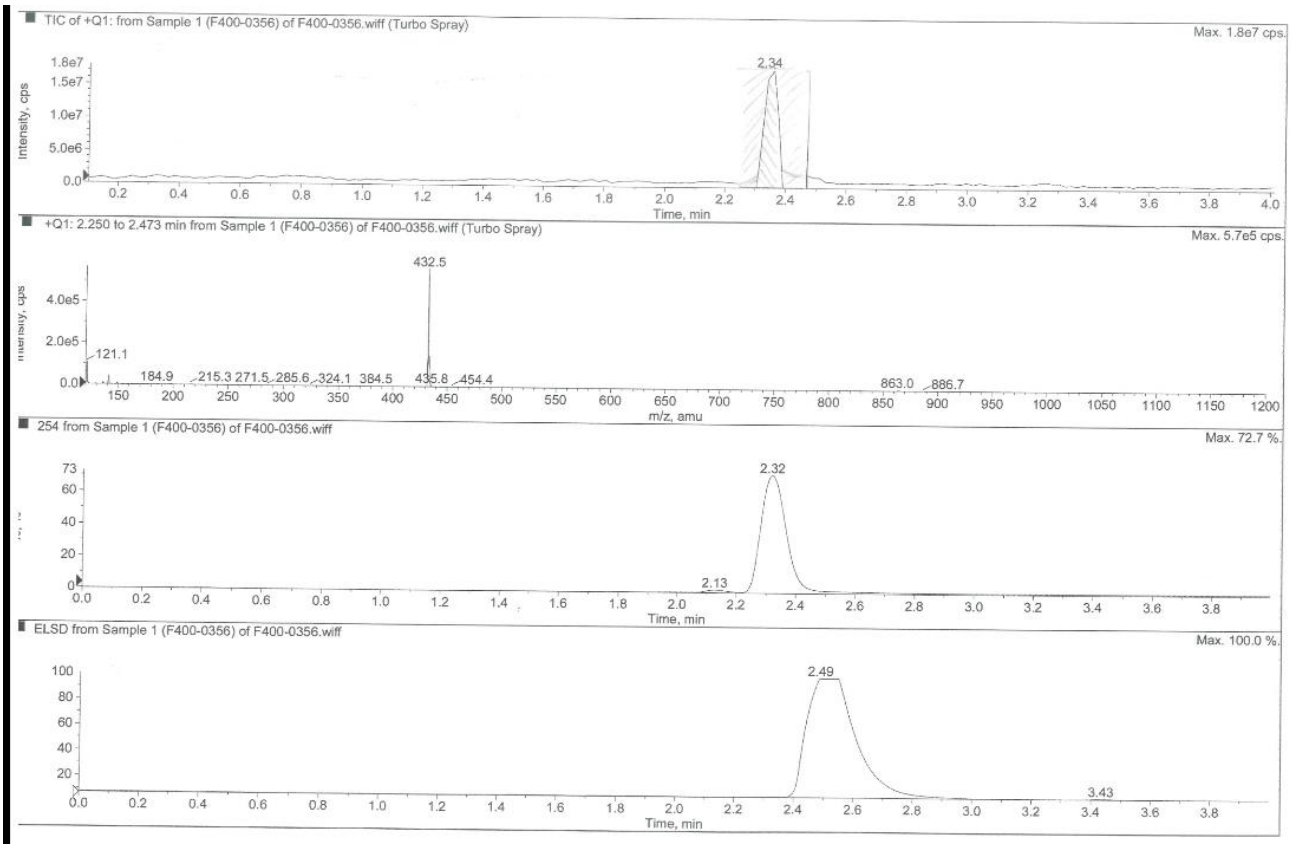


Figure S6. LC/MS Data for Structural Determination of of the title compound (**3**).

Table S1. Geometric parameters (Å, ◦) of the compound (**3**).

Atom	Bond Length/Angle	Atom	Bond Length/Angle
F1—C9	1.358 (5)	C6—C7	1.389 (5)
F2—C15	1.366 (5)	C7—C8	1.372 (5)
O1—C2	1.221 (5)	C8—C9	1.395 (6)
O2—C24	1.362 (5)	C9—C10	1.340 (6)
O2—C25	1.425 (5)	C11—C12	1.503 (5)
N1—C1	1.369 (5)	C12—C13	1.394 (5)
N1—C2	1.400 (5)	C12—C17	1.386 (5)
N1—C18	1.460 (4)	C13—C14	1.372 (6)
N2—C1	1.289 (5)	C14—C15	1.359 (6)
N2—C4	1.375 (5)	C15—C16	1.364 (6)

N3—C3	1.385 (5)	C16—C17	1.380 (6)
N3—C6	1.395 (5)	C18—C19	1.508 (5)
N3—C11	1.449 (5)	C19—C20	1.367 (6)
C2—C3	1.427 (5)	C19—C24	1.397 (5)
C3—C4	1.377 (5)	C20—C21	1.377 (6)
C4—C5	1.430 (5)	C21—C22	1.359 (6)
C5—C6	1.401 (5)	C22—C23	1.365 (6)
C5—C10	1.407 (5)	C23—C24	1.379 (6)

C24—O2—C25	118.7 (4)	F1—C9—C8	117.0 (4)
C1—N1—C2	123.2 (4)	C10—C9—F1	118.8 (5)
C1—N1—C18	119.3 (4)	C10—C9—C8	124.2 (4)
C2—N1—C18	117.5 (3)	C9—C10—C5	116.7 (4)
C1—N2—C4	113.3 (4)	N3—C11—C12	113.3 (3)
C3—N3—C6	106.8 (3)	C13—C12—C11	120.7 (4)
C3—N3—C11	126.1 (3)	C17—C12—C11	121.7 (4)
C6—N3—C11	126.8 (3)	C17—C12—C13	117.6 (4)
N2—C1—N1	126.7 (4)	C14—C13—C12	121.9 (4)
O1—C2—N1	121.4 (4)	C15—C14—C13	118.2 (4)
O1—C2—C3	128.1 (5)	C14—C15—F2	119.4 (4)
N1—C2—C3	110.4 (4)	C14—C15—C16	122.5 (5)
N3—C3—C2	127.5 (4)	C16—C15—F2	118.0 (4)
C4—C3—N3	110.2 (4)	C15—C16—C17	118.9 (4)
C4—C3—C2	122.3 (4)	C16—C17—C12	120.9 (4)
N2—C4—C3	124.0 (4)	N1—C18—C19	113.8 (3)
N2—C4—C5	128.6 (4)	C20—C19—C18	123.4 (4)
C3—C4—C5	107.4 (4)	C20—C19—C24	118.6 (4)
C6—C5—C4	106.1 (3)	C24—C19—C18	118.0 (4)
C6—C5—C10	120.0 (4)	C19—C20—C21	120.6 (4)

C10—C5—C4	133.8 (4)	C22—C21—C20	120.3 (5)
N3—C6—C5	109.5 (3)	C21—C22—C23	120.6 (5)
C7—C6—N3	128.9 (4)	C22—C23—C24	119.5 (5)
C7—C6—C5	121.6 (4)	O2—C24—C19	115.1 (4)
C8—C7—C6	117.5 (4)	O2—C24—C23	124.5 (4)
C7—C8—C9	119.9 (4)	C23—C24—C19	120.4 (4)