Supplementary Material: 5-[(3-Fluorophenyl)(2-hydroxy-6-oxocyclohex-1-en-1-yl)methyl]-6-hydroxy-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione

Assem Barakat, Hazem A. Ghabbour, Saleh Atef, Abdullah Mohammed Al-Majid, Mohammad Shahidul Islam, and M. Ali

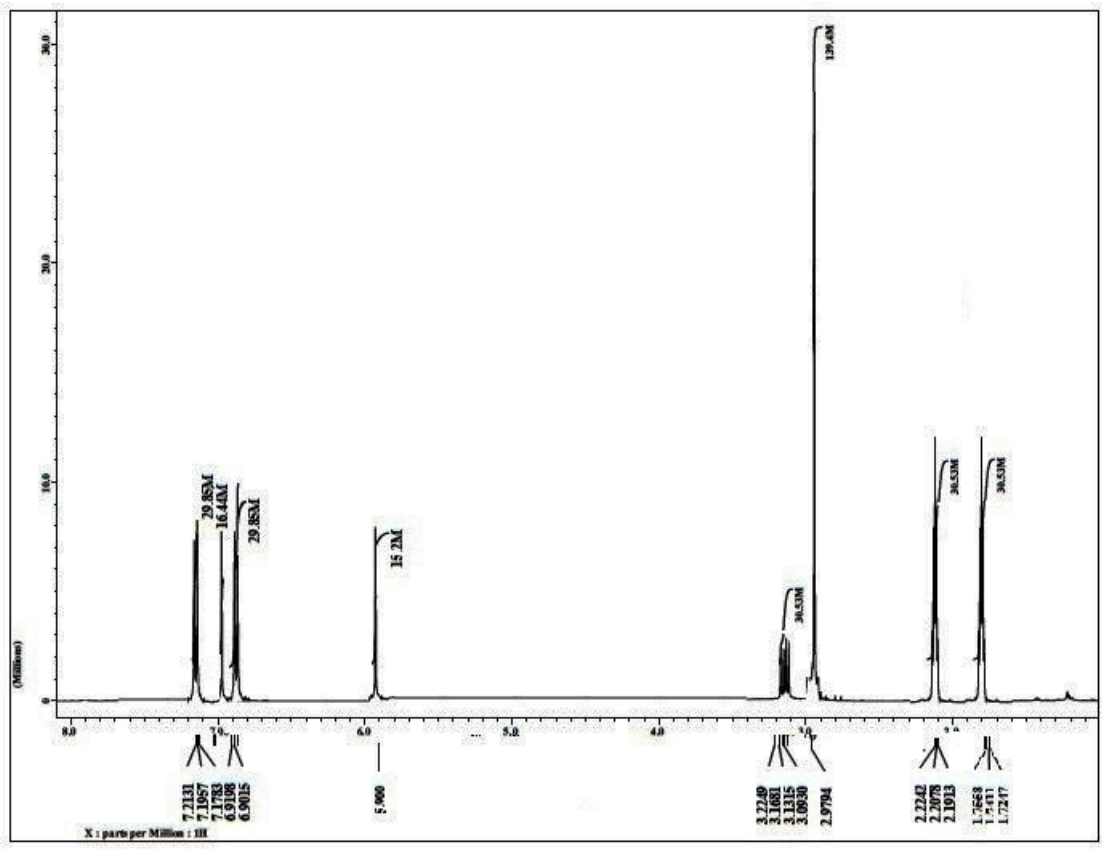

Figure S1: [1]H-NMR of the synthesized compound.

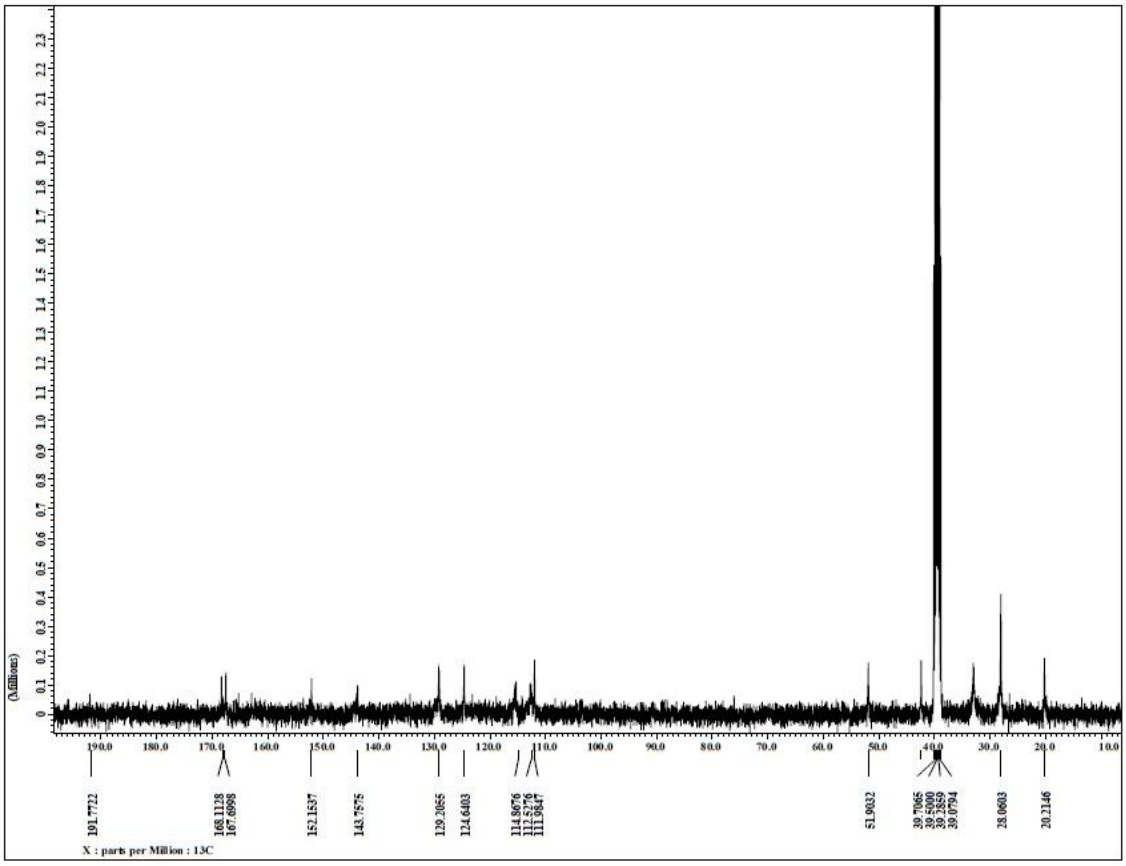

Figure S2: ^{13}C-NMR of the synthesized compound.

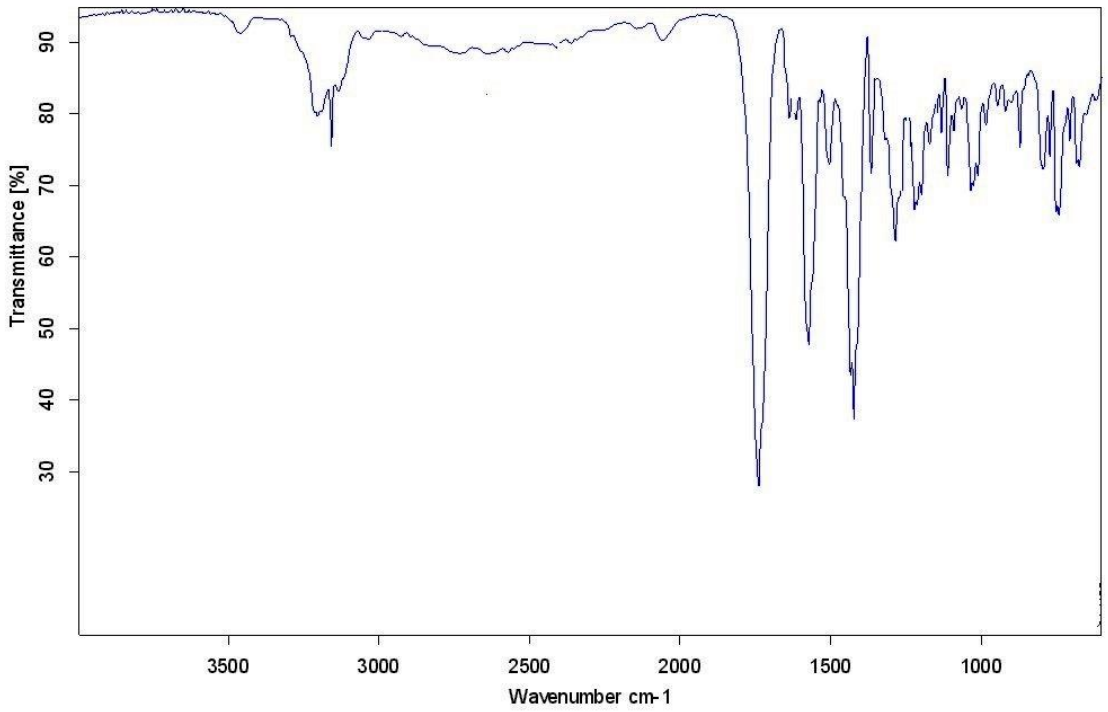

Figure S3. IR of the synthesized compound.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
F1	−0.1311 (3)	0.12942 (12)	0.3160 (2)	0.0268 (9)	0.778 (6)
O1	−0.1376 (3)	0.49915 (10)	0.17784 (18)	0.0198 (7)	
O2	−0.3832 (3)	0.50065 (11)	−0.22786 (18)	0.0221 (7)	
O3	−0.4913 (3)	0.32129 (10)	−0.01902 (18)	0.0180 (7)	
O4	−0.2015 (3)	0.44261 (11)	0.42059 (19)	0.0218 (7)	
O5	−0.5745 (3)	0.29161 (10)	0.16814 (17)	0.0171 (7)	
N1	−0.2673 (3)	0.50110 (12)	−0.0237 (2)	0.0159 (8)	
N2	−0.4507 (3)	0.41503 (12)	−0.1169 (2)	0.0158 (8)	
C1	−0.2331 (4)	0.46947 (15)	0.0903 (3)	0.0149 (9)	
C2	−0.1828 (4)	0.56528 (15)	−0.0338 (3)	0.0215 (11)	
C3	−0.3671 (4)	0.47398 (15)	−0.1286 (3)	0.0173 (10)	
C4	−0.5697 (4)	0.38617 (16)	−0.2250 (3)	0.0231 (11)	
C5	−0.4144 (4)	0.37952 (15)	−0.0090 (3)	0.0145 (10)	
C6	−0.3054 (4)	0.40434 (14)	0.0944 (3)	0.0145 (10)	
C7	−0.2445 (4)	0.36448 (15)	0.2113 (3)	0.0160 (9)	
C8	−0.3717 (4)	0.36353 (14)	0.2939 (2)	0.0133 (9)	
C9	−0.3402 (4)	0.40279 (14)	0.3957 (3)	0.0148 (10)	
C10	−0.4570 (4)	0.40460 (15)	0.4807 (3)	0.0171 (10)	
C11	−0.5606 (4)	0.34067 (15)	0.4765 (3)	0.0204 (11)	
C12	−0.6518 (4)	0.32336 (15)	0.3464 (2)	0.0166 (10)	
C13	−0.5291 (4)	0.32517 (14)	0.2640 (3)	0.0149 (10)	
C14	−0.1736 (4)	0.29498 (15)	0.1897 (3)	0.0152 (9)	
C15	−0.1866 (4)	0.24102 (15)	0.2640 (3)	0.0179 (10)	
C16	−0.1126 (4)	0.18100 (16)	0.2452 (3)	0.0217 (11)	
C17	−0.0245 (4)	0.17065 (16)	0.1568 (3)	0.0209 (10)	
C18	−0.0094 (4)	0.22481 (17)	0.0846 (3)	0.0236 (11)	
C19	−0.0831 (4)	0.28576 (16)	0.1007 (3)	0.0206 (10)	
F1X	0.0702 (17)	0.2128 (9)	0.0030 (15)	0.043 (4)	0.222 (6)
O1W	−0.1452 (3)	−0.00941 (11)	1.12439 (19)	0.0253 (8)	
H1O3	−0.522 (5)	0.3070 (19)	0.059 (4)	0.063 (12)*	
H2B	−0.27100	0.59860	−0.06230	0.0320*	
H2C	−0.11020	0.56120	−0.08990	0.0320*	
H2A	−0.11180	0.57810	0.04410	0.0320*	
H4A	−0.66950	0.36690	−0.20320	0.0350*	
H4B	−0.50900	0.35220	−0.25800	0.0350*	
H4C	−0.60820	0.42050	−0.28430	0.0350*	
H7A	−0.14160	0.38880	0.25780	0.0190*	
H10A	−0.53750	0.44190	0.45990	0.0200*	
H10B	−0.38640	0.41160	0.56250	0.0200*	
H11A	−0.64740	0.34600	0.52330	0.0250*	
H11B	−0.48240	0.30460	0.51200	0.0250*	
H12A	−0.70240	0.27910	0.34400	0.0200*	
H12B	−0.74680	0.35470	0.31700	0.0200*	
H15A	−0.24460	0.24550	0.32540	0.0210*	
H17A	0.02280	0.12920	0.14590	0.0250*	
H18A	0.026 (10)	0.215 (4)	0.013 (8)	0.0320*	0.778 (6)
H19A	−0.07180	0.32130	0.05070	0.0250*	
H1O4	−0.189 (5)	0.468 (2)	0.499 (4)	0.061 (12)*	
H16	−0.08 (3)	0.142 (6)	0.302 (14)	0.0520*	0.222 (6)
H2OW	−0.236 (7)	−0.001 (3)	1.181 (5)	0.13 (2)*	
H1OW	−0.0176 (19)	−0.015 (3)	1.165 (5)	0.13 (2)*	

Table S2. Atomic displacement parameters (Å^2).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0286 (15)	0.0178 (15)	0.0367 (16)	0.0076 (11)	0.0133 (12)	0.0135 (11)
O1	0.0198 (11)	0.0211 (12)	0.0155 (12)	−0.0033 (10)	−0.0014 (10)	−0.0013 (10)
O2	0.0233 (12)	0.0296 (13)	0.0141 (12)	0.0039 (10)	0.0058 (10)	0.0071 (10)
O3	0.0211 (11)	0.0197 (13)	0.0125 (12)	−0.0059 (10)	0.0030 (9)	−0.0016 (10)
O4	0.0229 (12)	0.0233 (13)	0.0195 (12)	−0.0095 (10)	0.0057 (10)	−0.0068 (10)
O5	0.0210 (11)	0.0168 (12)	0.0139 (12)	−0.0014 (9)	0.0050 (9)	−0.0024 (10)
N1	0.0157 (13)	0.0165 (14)	0.0149 (13)	−0.0006 (11)	0.0028 (11)	0.0010 (11)
N2	0.0156 (13)	0.0197 (15)	0.0106 (14)	−0.0010 (11)	0.0004 (11)	−0.0006 (11)
C1	0.0135 (15)	0.0170 (17)	0.0143 (16)	0.0058 (13)	0.0038 (13)	0.0026 (14)
C2	0.0239 (18)	0.0191 (19)	0.0217 (18)	−0.0027 (15)	0.0061 (15)	0.0031 (14)
C3	0.0156 (16)	0.0224 (19)	0.0146 (18)	0.0060 (14)	0.0050 (14)	0.0006 (14)
C4	0.0254 (18)	0.030 (2)	0.0118 (17)	−0.0019 (15)	0.0004 (14)	−0.0015 (14)
C5	0.0146 (16)	0.0163 (18)	0.0137 (16)	0.0014 (14)	0.0056 (13)	0.0006 (13)
C6	0.0141 (16)	0.0171 (18)	0.0121 (16)	0.0008 (13)	0.0026 (13)	−0.0003 (13)
C7	0.0160 (16)	0.0165 (17)	0.0138 (16)	−0.0039 (13)	0.0004 (13)	−0.0013 (13)
C8	0.0195 (16)	0.0108 (16)	0.0089 (15)	0.0027 (13)	0.0023 (13)	0.0037 (13)
C9	0.0123 (16)	0.0130 (17)	0.0173 (17)	0.0015 (13)	0.0002 (13)	0.0045 (13)
C10	0.0204 (17)	0.0190 (18)	0.0110 (16)	0.0023 (14)	0.0022 (14)	−0.0006 (13)
C11	0.0244 (18)	0.0214 (19)	0.0164 (18)	−0.0027 (14)	0.0068 (15)	−0.0005 (14)
C12	0.0177 (16)	0.0190 (18)	0.0141 (16)	−0.0042 (14)	0.0061 (13)	−0.0010 (13)
C13	0.0189 (16)	0.0104 (17)	0.0136 (17)	0.0063 (13)	0.0006 (13)	0.0037 (13)
C14	0.0102 (15)	0.0181 (18)	0.0149 (16)	−0.0019 (13)	−0.0016 (13)	0.0001 (13)
C15	0.0147 (16)	0.0215 (18)	0.0169 (17)	0.0027 (14)	0.0028 (14)	0.0008 (14)
C16	0.0178 (17)	0.0191 (19)	0.0245 (19)	−0.0001 (15)	−0.0019 (15)	0.0026 (15)
C17	0.0132 (16)	0.0223 (19)	0.0252 (19)	0.0055 (14)	0.0007 (14)	−0.0035 (15)
C18	0.0195 (18)	0.031 (2)	0.021 (2)	0.0040 (15)	0.0061 (16)	−0.0024 (16)
C19	0.0189 (17)	0.0218 (19)	0.0209 (18)	0.0007 (15)	0.0048 (14)	0.0023 (14)
F1X	0.036 (8)	0.060 (7)	0.042 (6)	0.029 (6)	0.027 (6)	0.008 (5)
O1W	**0.0237 (13)**	**0.0301 (14)**	**0.0219 (13)**	**0.0037 (11)**	**0.0051 (11)**	**0.0043 (10)**

Table S3. Geometric parameters (Å, °).

F1—C16	1.341 (4)	C11—C12	1.520 (4)
F1X—C18	1.266 (16)	C12—C13	1.504 (4)
O1—C1	1.242 (4)	C14—C19	1.388 (5)
O2—C3	1.229 (4)	C14—C15	1.392 (4)
O3—C5	1.306 (4)	C15—C16	1.375 (4)
O4—C9	1.324 (4)	C16—C17	1.372 (5)
O5—C13	1.257 (4)	C17—C18	1.384 (5)
O3—H1O3	1.02 (4)	C18—C19	1.383 (5)
O4—H1O4	1.01 (4)	C2—H2C	0.9600
O1W—H1OW	1.00 (3)	C2—H2A	0.9600
O1W—H2OW	1.09 (6)	C2—H2B	0.9600
N1—C1	1.411 (4)	C4—H4C	0.9600
N1—C2	1.465 (4)	C4—H4B	0.9600
N1—C3	1.370 (4)	C4—H4A	0.9600
N2—C4	1.470 (4)	C7—H7A	0.9800
N2—C5	1.388 (4)	C10—H10A	0.9700
N2—C3	1.374 (4)	C10—H10B	0.9700
C1—C6	1.429 (4)	C11—H11B	0.9700
C5—C6	1.369 (5)	C11—H11A	0.9700
C6—C7	1.526 (5)	C12—H12B	0.9700
C7—C14	1.542 (4)	C12—H12A	0.9700
C7—C8	1.534 (4)	C15—H15A	0.9300
C8—C13	1.425 (4)	C16—H16	1.01 (15)

C8—C9	1.373 (4)	C17—H17A	0.9300
C9—C10	1.491 (5)	C18—H18A	0.95 (9)
C10—C11	1.512 (4)	C19—H19A	0.9300
C5—O3—H1O3	112 (2)	F1X—C18—C17	114.7 (9)
C9—O4—H1O4	113 (2)	F1X—C18—C19	124.4 (9)
H2OW—O1W—H1OW	118 (4)	C17—C18—C19	120.9 (3)
C2—N1—C3	116.9 (2)	C14—C19—C18	121.5 (3)
C1—N1—C3	124.3 (3)	N1—C2—H2A	109.00
C1—N1—C2	118.7 (2)	N1—C2—H2B	109.00
C3—N2—C4	118.5 (2)	H2A—C2—H2B	110.00
C3—N2—C5	121.9 (3)	H2A—C2—H2C	109.00
C4—N2—C5	119.4 (2)	H2B—C2—H2C	109.00
O1—C1—N1	117.7 (3)	N1—C2—H2C	109.00
O1—C1—C6	125.3 (3)	N2—C4—H4B	109.00
N1—C1—C6	117.0 (3)	N2—C4—H4C	110.00
O2—C3—N2	121.3 (3)	N2—C4—H4A	109.00
N1—C3—N2	116.2 (3)	H4A—C4—H4C	110.00
O2—C3—N1	122.5 (3)	H4B—C4—H4C	109.00
O3—C5—C6	125.3 (3)	H4A—C4—H4B	109.00
O3—C5—N2	113.0 (3)	C8—C7—H7A	105.00
N2—C5—C6	121.7 (3)	C14—C7—H7A	105.00
C5—C6—C7	123.9 (3)	C6—C7—H7A	105.00
C1—C6—C5	118.3 (3)	C9—C10—H10B	109.00
C1—C6—C7	117.7 (3)	C11—C10—H10A	109.00
C6—C7—C8	115.5 (3)	C9—C10—H10A	109.00
C6—C7—C14	112.4 (3)	H10A—C10—H10B	108.00
C8—C7—C14	113.8 (3)	C11—C10—H10B	109.00
C7—C8—C9	120.2 (3)	C10—C11—H11A	110.00
C7—C8—C13	121.3 (2)	C10—C11—H11B	110.00
C9—C8—C13	118.4 (3)	C12—C11—H11B	110.00
C8—C9—C10	123.5 (3)	H11A—C11—H11B	108.00
O4—C9—C10	116.9 (3)	C12—C11—H11A	110.00
O4—C9—C8	119.6 (3)	C11—C12—H12B	109.00
C9—C10—C11	111.9 (3)	C13—C12—H12A	109.00
C10—C11—C12	110.2 (3)	C13—C12—H12B	109.00
C11—C12—C13	112.5 (3)	H12A—C12—H12B	108.00
C8—C13—C12	121.1 (3)	C11—C12—H12A	109.00
O5—C13—C12	116.2 (3)	C16—C15—H15A	120.00
O5—C13—C8	122.7 (3)	C14—C15—H15A	120.00
C7—C14—C15	121.3 (3)	C15—C16—H16	129 (9)
C15—C14—C19	118.0 (3)	C17—C16—H16	105 (11)
C7—C14—C19	120.5 (3)	C18—C17—H17A	122.00
C14—C15—C16	119.1 (3)	C16—C17—H17A	122.00
F1—C16—C15	117.8 (3)	C17—C18—H18A	116 (5)
C15—C16—C17	123.8 (3)	C19—C18—H18A	121 (5)
F1—C16—C17	118.4 (3)	C14—C19—H19A	119.00
C16—C17—C18	116.8 (3)	C18—C19—H19A	119.00
C2—N1—C1—O1	2.7 (4)	C14—C7—C8—C9	124.9 (3)
C2—N1—C1—C6	−174.6 (3)	C14—C7—C8—C13	−58.6 (4)
C3—N1—C1—O1	178.7 (3)	C6—C7—C14—C15	−150.2 (3)
C3—N1—C1—C6	1.3 (4)	C6—C7—C14—C19	34.7 (4)
C1—N1—C3—O2	−174.3 (3)	C8—C7—C14—C15	−16.5 (4)
C1—N1—C3—N2	6.3 (4)	C8—C7—C14—C19	168.4 (3)
C2—N1—C3—O2	1.7 (4)	C7—C8—C9—O4	1.6 (4)
C2—N1—C3—N2	−177.7 (3)	C7—C8—C9—C10	−179.8 (3)
C4—N2—C3—O2	−3.8 (4)	C13—C8—C9—O4	−175.1 (3)
C4—N2—C3—N1	175.6 (3)	C13—C8—C9—C10	3.6 (4)
C5—N2—C3—O2	170.6 (3)	C7—C8—C13—O5	−1.8 (4)

C5—N2—C3—N1	−10.0 (4)	C7—C8—C13—C12	178.8 (3)
C3—N2—C5—O3	−172.6 (3)	C9—C8—C13—O5	174.8 (3)
C3—N2—C5—C6	6.1 (5)	C9—C8—C13—C12	−4.6 (4)
C4—N2—C5—O3	1.7 (4)	O4—C9—C10—C11	−156.2 (3)
C4—N2—C5—C6	−179.6 (3)	C8—C9—C10—C11	25.2 (4)
O1—C1—C6—C5	177.3 (3)	C9—C10—C11—C12	−50.8 (3)
O1—C1—C6—C7	−7.5 (5)	C10—C11—C12—C13	50.1 (3)
N1—C1—C6—C5	−5.6 (4)	C11—C12—C13—O5	157.5 (3)
N1—C1—C6—C7	169.6 (3)	C11—C12—C13—C8	−23.1 (4)
O3—C5—C6—C1	−179.4 (3)	C7—C14—C15—C16	−176.4 (3)
O3—C5—C6—C7	5.7 (5)	C19—C14—C15—C16	−1.1 (5)
N2—C5—C6—C1	2.1 (5)	C7—C14—C19—C18	176.1 (3)
N2—C5—C6—C7	−172.8 (3)	C15—C14—C19—C18	0.8 (5)
C1—C6—C7—C8	101.3 (3)	C14—C15—C16—F1	−178.3 (3)
C1—C6—C7—C14	−125.9 (3)	C14—C15—C16—C17	0.3 (5)
C5—C6—C7—C8	−83.8 (4)	F1—C16—C17—C18	179.4 (3)
C5—C6—C7—C14	49.0 (4)	C15—C16—C17—C18	0.8 (5)
C6—C7—C8—C9	−102.9 (3)	C16—C17—C18—C19	−1.1 (5)
C6—C7—C8—C13	73.6 (4)	C17—C18—C19—C14	0.4 (5)