Supporting Information

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Synthesis, characterization, crystal structure and bioactivities of novel enamine and pyrrole derivatives endowed with acetylcholinesterase, α-glycosidase and human carbonic anhydrase inhibition effects

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Table of Contents **Page**

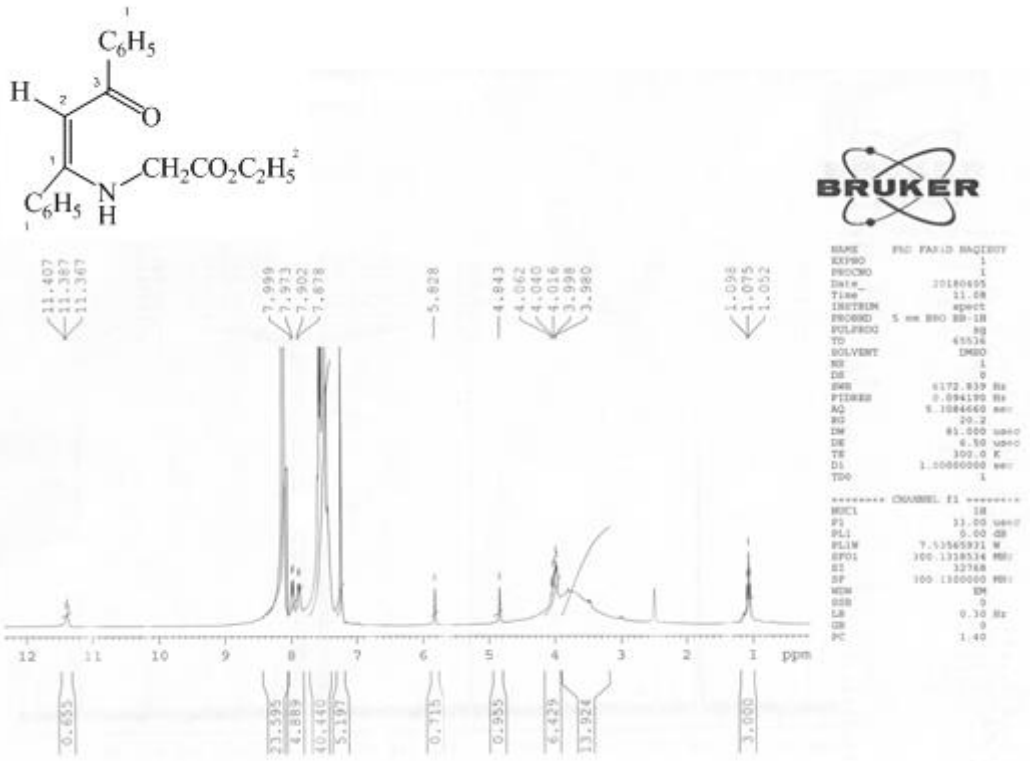

Figure S1: ^{1}H NMR (DMSO-*d*6) spectrum of compound 1

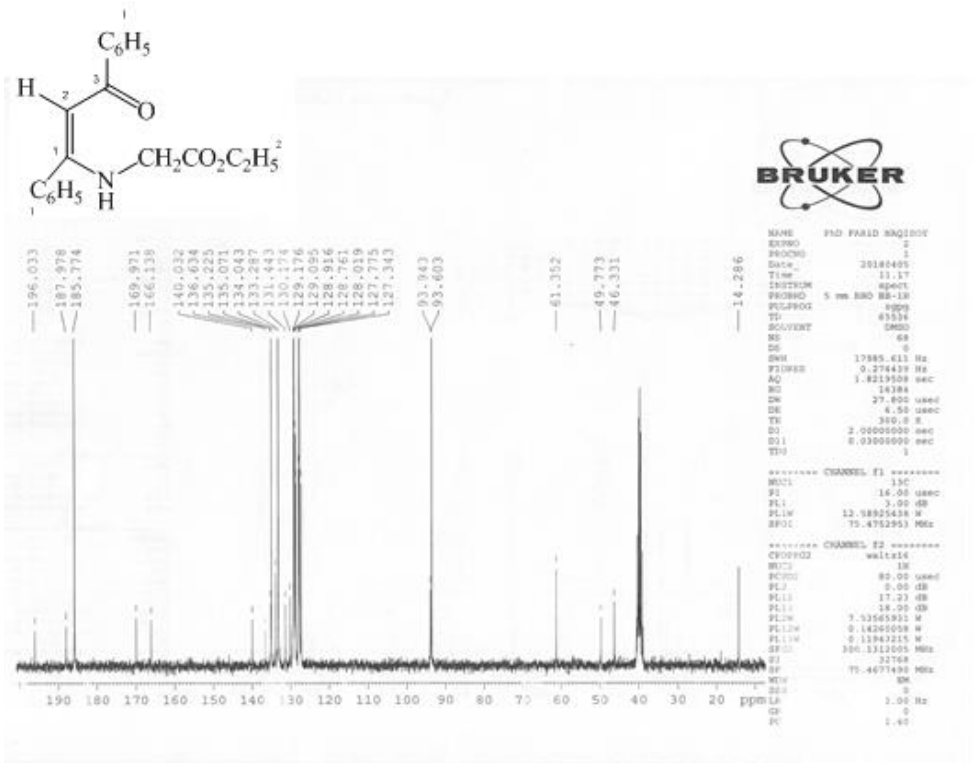

Figure S2: ^{13}C NMR (DMSO-*d*6) spectrum of compound 1

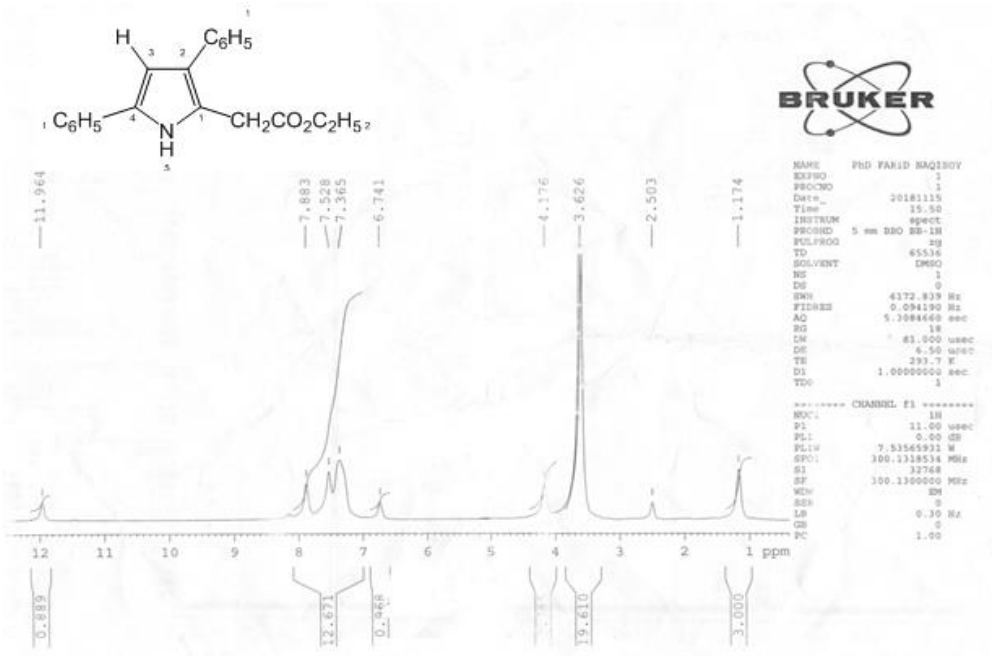

Figure S3: ^{1}H NMR (DMSO-*d*6) spectrum of compound 2

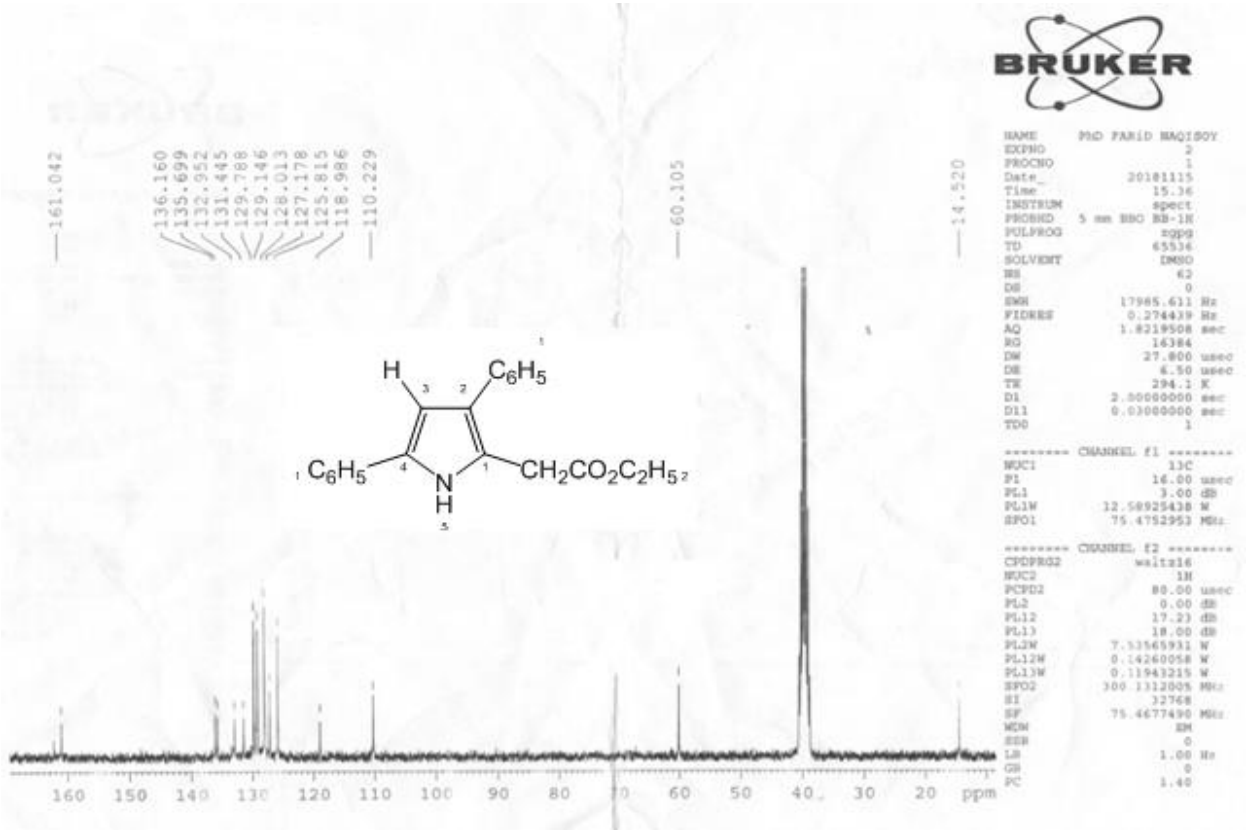

Figure S4: ^{13}C NMR (DMSO-*d*6) spectrum of compound 2

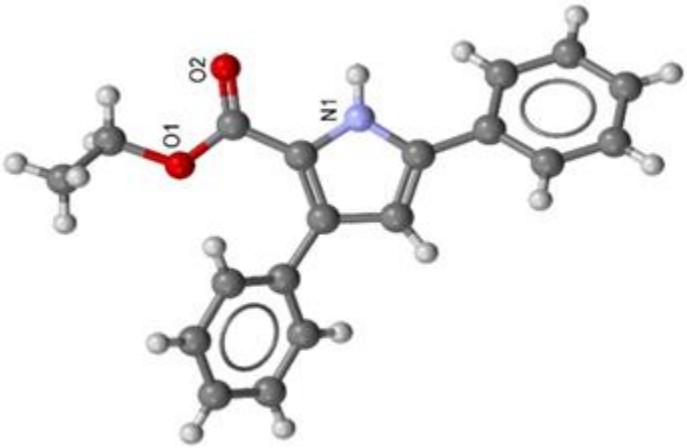

Figure S5: The molecular structure of the compound (2)

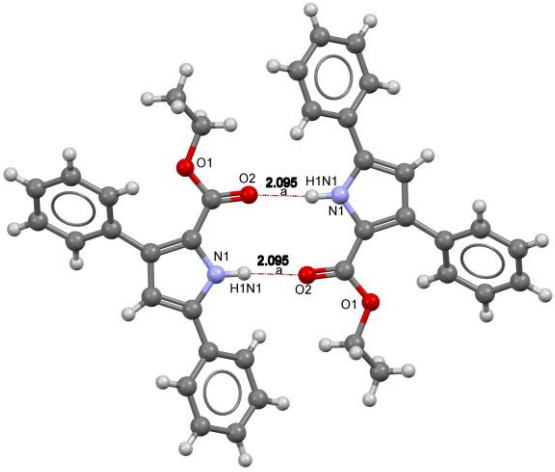

Figure S6: Packing diagram of the title compound. N—H···O hydrogen bonds are shown as dashed lines

Table S1: Crystal data and structure refinement for A_A.

Identification code	A_A	
Empirical formula	C19 H17 N O2	
Formula weight	291.33	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.5340(6) Å	α= 90°.
	b = 7.5101(5) Å	β= 102.131(2)°.
	c = 20.2352(15) Å	γ = 90°.
Volume	1565.09(18) $Å^3$	
Z	4	
Density (calculated)	1.236 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	616	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	2.901 to 24.718°.	
Index ranges	-12<=h<=12, -8<=k<=8, -23<=l<=23	
Reflections collected	16631	
Independent reflections	2665 [R(int) = 0.0591]	
Completeness to theta = 24.718°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2665 / 0 / 200	
Goodness-of-fit on F^2	0.660	
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1325	
R indices (all data)	R1 = 0.0766, wR2 = 0.1492	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.153 and -0.145 $e.Å^{-3}$	

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for A_A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5347(2)	2645(3)	4437(1)	45(1)
O(1)	5695(2)	1009(3)	5686(1)	65(1)
O(2)	7217(2)	3003(3)	6119(1)	58(1)
C(1)	5318(2)	3740(3)	3900(1)	45(1)
C(2)	6243(2)	5038(3)	4103(1)	51(1)
C(3)	6854(2)	4734(3)	4780(1)	46(1)
C(4)	6270(2)	3223(3)	4981(1)	44(1)
C(5)	6353(2)	2296(3)	5616(1)	47(1)
C(6)	7380(3)	2205(5)	6780(1)	71(1)
C(7)	8722(4)	2454(7)	7131(2)	112(2)
C(8)	4403(2)	3534(3)	3250(1)	45(1)
C(9)	3213(3)	2705(4)	3203(1)	55(1)
C(10)	2344(3)	2596(4)	2590(2)	67(1)
C(11)	2637(3)	3338(4)	2018(1)	67(1)
C(12)	3814(3)	4164(4)	2058(1)	67(1)
C(13)	4689(3)	4262(4)	2665(1)	58(1)
C(14)	7884(3)	5910(4)	5156(1)	52(1)
C(15)	7767(3)	7742(4)	5074(2)	65(1)
C(16)	8740(4)	8868(5)	5394(2)	87(1)
C(17)	9845(4)	8185(6)	5800(2)	98(1)
C(18)	9989(3)	6375(6)	5880(2)	84(1)
C(19)	9016(3)	5238(5)	5561(1)	63(1)

Table S3: Bond lengths [Å] and angles [°] for A_A.

N(1)-C(1)	1.357(3)
N(1)-C(4)	1.378(3)
N(1)-H(1N1)	0.8998
O(1)-C(5)	1.215(3)
O(2)-C(5)	1.325(3)
O(2)-C(6)	1.443(3)
C(1)-C(2)	1.379(3)
C(1)-C(8)	1.467(3)
C(2)-C(3)	1.404(3)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.392(3)
C(3)-C(14)	1.479(3)
C(4)-C(5)	1.447(3)
C(6)-C(7)	1.456(4)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-C(9)	1.385(4)
C(8)-C(13)	1.394(3)
C(9)-C(10)	1.381(4)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.377(4)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.373(4)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.375(4)
C(12)-H(12A)	0.9300
C(13)-H(13A)	0.9300
C(14)-C(15)	1.388(4)
C(14)-C(19)	1.392(4)
C(15)-C(16)	1.381(4)
C(15)-H(15A)	0.9300
C(16)-C(17)	1.375(6)

C(16)-H(16A)	0.9300
C(17)-C(18)	1.374(6)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.384(4)
C(18)-H(18A)	0.9300
C(19)-H(19A)	0.9300
C(1)-N(1)-C(4)	110.1(2)
C(1)-N(1)-H(1N1)	126.9
C(4)-N(1)-H(1N1)	123.0
C(5)-O(2)-C(6)	118.2(2)
N(1)-C(1)-C(2)	107.1(2)
N(1)-C(1)-C(8)	123.6(2)
C(2)-C(1)-C(8)	129.2(2)
C(1)-C(2)-C(3)	109.0(2)
C(1)-C(2)-H(2A)	125.5
C(3)-C(2)-H(2A)	125.5
C(4)-C(3)-C(2)	106.1(2)
C(4)-C(3)-C(14)	131.1(2)
C(2)-C(3)-C(14)	122.7(2)
N(1)-C(4)-C(3)	107.7(2)
N(1)-C(4)-C(5)	117.3(2)
C(3)-C(4)-C(5)	134.7(2)
O(1)-C(5)-O(2)	123.1(2)
O(1)-C(5)-C(4)	123.8(2)
O(2)-C(5)-C(4)	113.1(2)
O(2)-C(6)-C(7)	108.3(3)
O(2)-C(6)-H(6A)	110.0
C(7)-C(6)-H(6A)	110.0
O(2)-C(6)-H(6B)	110.0
C(7)-C(6)-H(6B)	110.0
H(6A)-C(6)-H(6B)	108.4
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5

C(9)-C(8)-C(13)	118.2(2)
C(9)-C(8)-C(1)	121.6(2)
C(13)-C(8)-C(1)	120.1(2)
C(10)-C(9)-C(8)	120.5(3)
C(10)-C(9)-H(9A)	119.7
C(8)-C(9)-H(9A)	119.7
C(11)-C(10)-C(9)	120.5(3)
C(11)-C(10)-H(10A)	119.7
C(9)-C(10)-H(10A)	119.7
C(10)-C(11)-C(12)	119.5(3)
C(10)-C(11)-H(11A)	120.2
C(12)-C(11)-H(11A)	120.2
C(13)-C(12)-C(11)	120.3(3)
C(13)-C(12)-H(12A)	119.9
C(11)-C(12)-H(12A)	119.9
C(12)-C(13)-C(8)	121.0(3)
C(12)-C(13)-H(13A)	119.5
C(8)-C(13)-H(13A)	119.5
C(15)-C(14)-C(19)	118.2(3)
C(15)-C(14)-C(3)	119.5(3)
C(19)-C(14)-C(3)	122.1(3)
C(16)-C(15)-C(14)	120.8(3)
C(16)-C(15)-H(15A)	119.6
C(14)-C(15)-H(15A)	119.6
C(17)-C(16)-C(15)	120.2(4)
C(17)-C(16)-H(16A)	119.9
C(15)-C(16)-H(16A)	119.9
C(16)-C(17)-C(18)	119.9(3)
C(16)-C(17)-H(17A)	120.1
C(18)-C(17)-H(17A)	120.1
C(17)-C(18)-C(19)	120.2(4)
C(17)-C(18)-H(18A)	119.9
C(19)-C(18)-H(18A)	119.9
C(18)-C(19)-C(14)	120.6(3)
C(18)-C(19)-H(19A)	119.7
C(14)-C(19)-H(19A)	119.7

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for A_A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	52(1)	40(1)	42(1)	0(1)	6(1)	-10(1)
O(1)	87(1)	53(1)	52(1)	6(1)	5(1)	-25(1)
O(2)	63(1)	64(1)	42(1)	5(1)	-3(1)	-17(1)
C(1)	55(1)	43(1)	38(1)	0(1)	12(1)	0(1)
C(2)	64(2)	46(1)	44(1)	2(1)	17(1)	-13(1)
C(3)	49(1)	48(1)	42(1)	-4(1)	12(1)	-7(1)
C(4)	47(1)	43(1)	41(1)	-2(1)	7(1)	-6(1)
C(5)	51(1)	41(1)	46(1)	-2(1)	6(1)	-4(1)
C(6)	88(2)	76(2)	43(2)	9(2)	0(2)	-2(2)
C(7)	91(3)	143(4)	81(3)	23(3)	-29(2)	-10(3)
C(8)	57(2)	39(1)	40(1)	-2(1)	7(1)	2(1)
C(9)	55(2)	61(2)	45(2)	4(1)	5(1)	0(1)
C(10)	55(2)	77(2)	62(2)	-2(2)	-3(1)	3(2)
C(11)	78(2)	70(2)	45(2)	-4(2)	-7(1)	21(2)
C(12)	91(2)	67(2)	41(2)	1(1)	13(2)	4(2)
C(13)	76(2)	57(2)	42(2)	-4(1)	14(1)	-7(1)
C(14)	57(2)	59(2)	43(1)	-10(1)	20(1)	-19(1)
C(15)	77(2)	57(2)	66(2)	-10(2)	28(2)	-23(2)
C(16)	108(3)	71(2)	92(3)	-23(2)	41(2)	-43(2)
C(17)	94(3)	120(4)	86(3)	-42(3)	29(2)	-66(3)
C(18)	62(2)	122(3)	66(2)	-19(2)	12(2)	-31(2)
C(19)	57(2)	79(2)	54(2)	-8(2)	13(1)	-20(2)

Table S5: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for A_A.

	x	y	z	U(eq)
H(1N1)	4865	1662	4449	54
H(2A)	6433	5966	3835	61
H(6A)	7176	945	6737	86
H(6B)	6799	2762	7032	86
H(7A)	8822	2076	7593	168
H(7B)	8949	3690	7120	168
H(7C)	9282	1761	6914	168
H(9A)	2997	2218	3587	66
H(10A)	1554	2016	2563	80
H(11A)	2042	3281	1607	81
H(12A)	4020	4658	1672	80
H(13A)	5484	4822	2686	70
H(15A)	7025	8216	4799	78
H(16A)	8647	10093	5336	105
H(17A)	10494	8947	6020	118
H(18A)	10742	5912	6148	100
H(19A)	9120	4014	5619	76

Table S6: Torsion angles [°] for A_A.

C(4)-N(1)-C(1)-C(2)	0.3(3)
C(4)-N(1)-C(1)-C(8)	-177.4(2)
N(1)-C(1)-C(2)-C(3)	-0.1(3)
C(8)-C(1)-C(2)-C(3)	177.4(2)
C(1)-C(2)-C(3)-C(4)	-0.2(3)
C(1)-C(2)-C(3)-C(14)	-179.0(2)
C(1)-N(1)-C(4)-C(3)	-0.5(3)
C(1)-N(1)-C(4)-C(5)	174.7(2)
C(2)-C(3)-C(4)-N(1)	0.4(3)
C(14)-C(3)-C(4)-N(1)	179.1(3)
C(2)-C(3)-C(4)-C(5)	-173.5(3)
C(14)-C(3)-C(4)-C(5)	5.1(5)
C(6)-O(2)-C(5)-O(1)	-0.2(4)
C(6)-O(2)-C(5)-C(4)	179.4(2)
N(1)-C(4)-C(5)-O(1)	3.0(4)
C(3)-C(4)-C(5)-O(1)	176.5(3)
N(1)-C(4)-C(5)-O(2)	-176.6(2)
C(3)-C(4)-C(5)-O(2)	-3.1(4)
C(5)-O(2)-C(6)-C(7)	149.2(3)
N(1)-C(1)-C(8)-C(9)	25.6(4)
C(2)-C(1)-C(8)-C(9)	-151.5(3)
N(1)-C(1)-C(8)-C(13)	-157.8(2)
C(2)-C(1)-C(8)-C(13)	25.0(4)
C(13)-C(8)-C(9)-C(10)	0.6(4)
C(1)-C(8)-C(9)-C(10)	177.2(3)
C(8)-C(9)-C(10)-C(11)	-1.2(5)
C(9)-C(10)-C(11)-C(12)	1.2(5)
C(10)-C(11)-C(12)-C(13)	-0.6(5)
C(11)-C(12)-C(13)-C(8)	-0.1(5)
C(9)-C(8)-C(13)-C(12)	0.1(4)
C(1)-C(8)-C(13)-C(12)	-176.6(3)
C(4)-C(3)-C(14)-C(15)	-137.8(3)
C(2)-C(3)-C(14)-C(15)	40.7(4)
C(4)-C(3)-C(14)-C(19)	46.2(4)
C(2)-C(3)-C(14)-C(19)	-135.3(3)

C(19)-C(14)-C(15)-C(16)	-1.0(4)
C(3)-C(14)-C(15)-C(16)	-177.1(3)
C(14)-C(15)-C(16)-C(17)	0.2(5)
C(15)-C(16)-C(17)-C(18)	0.8(6)
C(16)-C(17)-C(18)-C(19)	-1.0(6)
C(17)-C(18)-C(19)-C(14)	0.2(5)
C(15)-C(14)-C(19)-C(18)	0.8(4)
C(3)-C(14)-C(19)-C(18)	176.8(3)

Symmetry transformations used to generate equivalent atoms:

Table S7: Hydrogen bonds for A_A [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N1)...O(1)#1	0.90	2.09	2.947(3)	158.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1