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Modified-amino acid/peptide pyrimidine analogs: Synthesis, structural characterization and DFT study of N-(pyrimidyl) gabapentine and N-(pyrimidyl)baclofen

by

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Compound 1

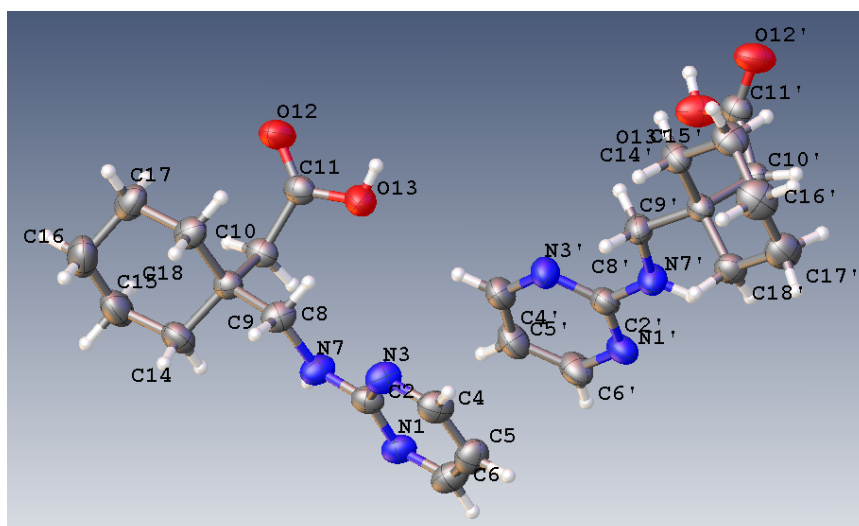


Fig. S1. ORTEP plot of compound 1 with atom numbering scheme

Table S1 Hydrogen Bonds for 1.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O13	H13	N1 ¹	0.82	1.85	2.664(4)	170.5
O13	H13	N7 ¹	0.82	3.07	3.739(4)	141.0
N7	H7	O12 ²	0.86	2.19	3.032(4)	167.3
N7	H7	O13 ²	0.86	3.20	3.739(4)	123.5
C4	H4	O13 ³	0.93	2.58	3.463(4)	158.6
C5	H5	O13 ¹²	0.93	2.95	3.741(5)	143.9
C6	H6	N3 ⁴	0.93	2.81	3.439(4)	125.6
C6	H6	N3 ¹²	0.93	2.72	3.489(4)	140.8
C8	H8B	N1 ⁵	0.97	3.05	3.859(4)	141.3
C10	H10A	O12 ²	0.97	2.93	3.754(4)	144.0
C14	H14B	O12 ²	0.97	2.78	3.691(5)	157.6

C17	H17B	O12	0.97	2.82	3.471(5)	124.8
C18	H18A	O12 ³	0.97	3.01	3.899(4)	152.2
O13'	H13'	N1 ¹⁶	0.82	1.85	2.653(4)	164.9
O13'	H13'	N7 ¹⁶	0.82	3.10	3.741(4)	136.7
N7'	H7'	O12 ¹⁷	0.86	2.18	3.029(4)	167.3
N7'	H7'	O13 ¹⁷	0.86	3.20	3.741(4)	123.3
C4'	H4'	O13	0.93	2.59	3.468(4)	158.4
C5'	H5'	O13 ²	0.93	2.94	3.737(5)	144.3
C6'	H6'	N3 ²	0.93	2.70	3.471(4)	141.4
C6'	H6'	N3 ¹²	0.93	2.82	3.439(4)	124.8
C8'	H8'A	N1 ¹¹	0.97	3.05	3.859(4)	142.1
C10'	H10D	O12 ¹⁷	0.97	2.92	3.742(4)	143.8
C14'	H14D	O12 ¹³	0.97	3.01	3.897(4)	153.0
C15'	H15C	O12 ¹	0.97	2.84	3.481(5)	124.6
C18'	H18D	O12 ¹⁷	0.97	2.74	3.660(4)	158.6

Symmetry codes: ¹+X,1-Y,-1/2+Z; ²+X,1-Y,1/2+Z; ³+X,1+Y,+Z; ⁴+X,2-Y,1/2+Z; ⁵+X,2-Y,-1/2+Z; ⁶+X,-Y,-1/2+Z; ⁷+X,-Y,1/2+Z

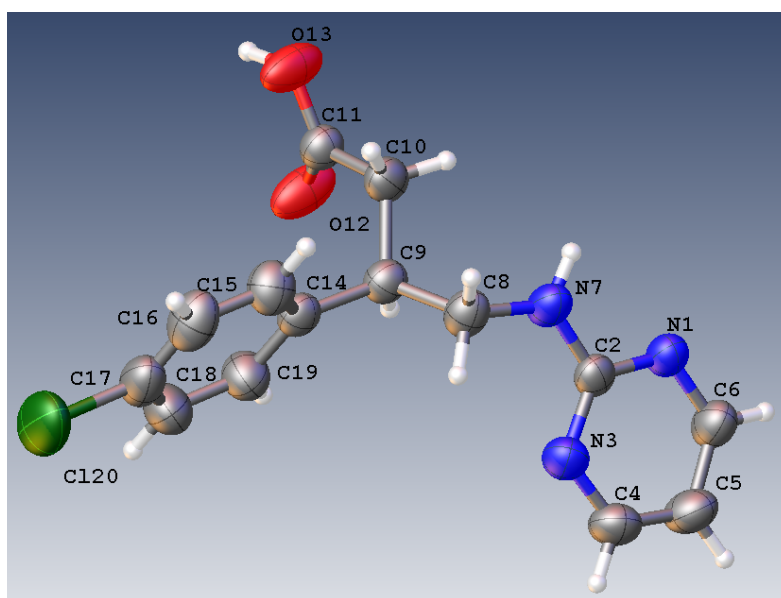


Fig. S2. ORTEP plot of compound **2** with atom numbering scheme

Table S2 Hydrogen Bonds for **2**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N7	H7	O12 ¹	0.86	2.14	2.922(2)	150.3
O13	H13	N1 ²	0.96(4)	1.68(4)	2.633(2)	170(3)

Symmetry codes: ¹3/2-X,1/2+Y,1/2-Z; ²3/2-X,-1/2+Y,1/2-Z

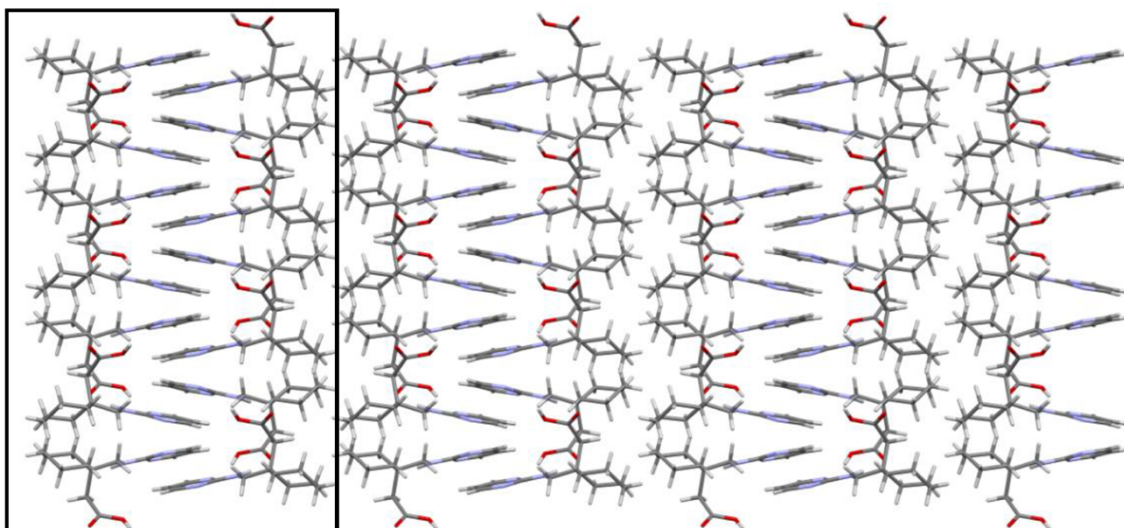


Fig. S3. Packing of compound 1

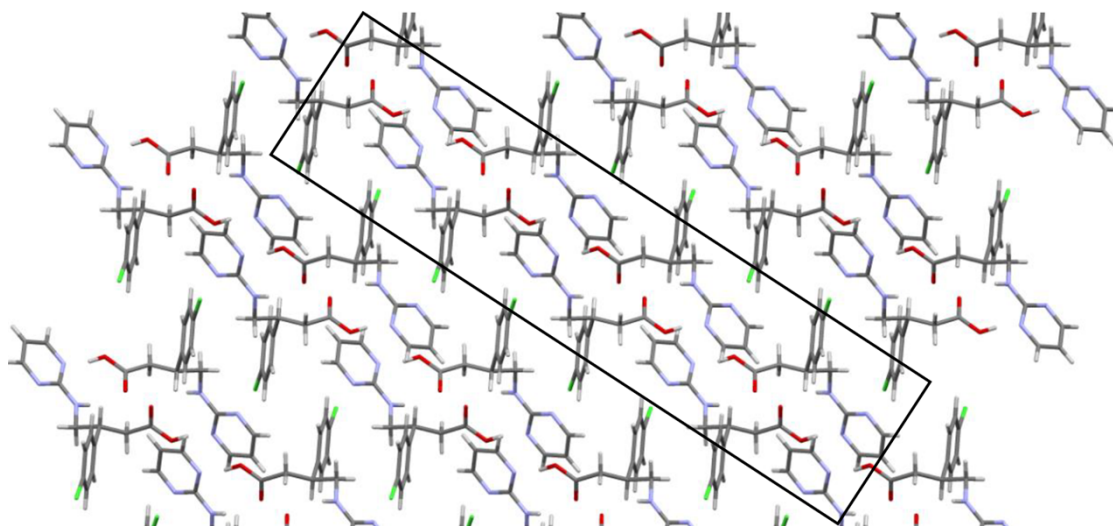


Fig. S4. 3D packing of compound 2