

Supplementary Data. NMR data of CpaA product *cyclo*-acetoacetyl-L-tryptophan (cAATrp)

No.	¹³ C		¹ H (multi., <i>J</i> in Hz)	HMBC
	δ ppm		δ ppm	
2	174.7			
3	100.7			
4	194.7			
5	63.0	59.8*	4.11 (1H, dd., <i>J</i> =3.4, 10.3)	C-2, -3, -4, -8
6	185.5	189.0*		
7	19.7	20.4*	2.47 (3H,s)	C-3, -6
8	28.3		2.83 (1H, dd., <i>J</i> =10.3, 14.9)	C-5, -9, -17
			3.45 (1H, dd., <i>J</i> =3.4, 14.9)	C-10, -17
9	110.9			
10	122.9		7.06 (1H, s)	C-9, -12, -17
12	136.5			
13	111.5		7.38 (1H, br. d., <i>J</i> =8.1)	C-15, -17
14	122.7		7.22 (1H, t-like, <i>J</i> =8.1)	C-12, -16
15	120.1		7.14 (1H, t-like, <i>J</i> =7.4)	C-13, -17
16	118.7		7.61 (1H, br. d., <i>J</i> =7.4)	C-9, -12, -14
17	127.0			
(NH)			5.93	
(NH)			8.12	

¹H (500 MHz, CDCl₃) and ¹³C (125 MHz, CDCl₃) NMR data were measured by JOEL ECA-500 spectrometer. *Minor abundance due to tautomerization.

HMBC correlation of cAATrp and its tautomerization

