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Erratum

Erratum to "Photomodulation of conformational states of p-phenylazobenzyloxycarbonyl-L-proline and related peptides" [1] [J. Photochem. Photobiol. A: Chem., 105 (1997) 235–248] [2]

S. Rudolph-Böhner [a], M. Krüger [a], D. Oesterhelt [a], L. Moroder [a,*], T. Nägele [b], J. Wachtveitl [b]

[a] *Max-Planck-Institut für Biochemie, D-82152 Martinsried, Germany*

[b] *Institut für Medizinische Optik, Ludwig–Maximilian-Universität München, München, Germany*

The Publisher regrets that errors occurred in Tables 2–5 in the printed article. The corrected tables are printed on the following pages.

* Corresponding author.

[1] Presented at the International Meeting of Physical Chemistry on *Intra- and inter-molecular photoprocesses of conjugated molecules*, Riccione, Italy, July 14–18, 1996

[2] PII of original article: 1010-6030(96)04497-8.

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Table 2
^{1}H, ^{13}C chemical shifts and coupling constants of PZ-Pro-OH in DMSO-d_6

Residue	^{1}H	^{1}H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
trans-azo, *cis trans*-Pro before irradiation					
PZ1				*trans*-azo	122.5, 127.9, 128.2,
	trans-azo	7.92–7.84		C1, C2, 2′,	129.5, 131.5, 140.6,
	H3, 3′	m, 4H		C3, 3′ C4,	151.4, 151.3, 151.9
	H6, 6′			C5, C6, 6′	
				C7, 7′, C8	
	trans-azo	7.64–7.49			
	H2, 2′	m, 5H			
	H7, 7′				
	H8				
				CH_2–O	65.3
	CH_2–O	5.19, s, 2H		*trans*-azo-	
	trans-azo	5.21, d, 1H	$J=13.6$	*cis*, *trans*-	
	cis trans-Pro	5, 11, d, 1H	$J=13.6$	Pro	
				CO	153.5
					153.9
Pro 2	NH	–	–		–
	–COOH	12.65, br			
	α-CH			Cα	
	cis-Pro	4.29, dd	$J=3.5$, $J=9.0$	*cis*	58.4
	trans-Pro	4.19, dd	$J=3.2$, $J=8.7$	*trans*	59.0
	β-CH_2	2.31–2.16, m, β1		Cβ	
		1.98–1.79, m, β2		*cis*	30.4
				trans	29.4
	γ-CH_2	1.98–1.79, m		Cγ	
				cis	23.0
				trans	23.9
	δ-CH_2	3.53–3.37, m		Cδ	
				cis	46.8
				trans	46.2
				COOH	173.5
					173.9
trans cis-azo, *cis trans*-Pro after irradiation, 366 nm, 3 h					
PZ 1	*trans*-azo	7.92–7.84, m, 4H		*trans*/*cis*-azo	119.8, 120.0,
					120.1, 122.5,
	cis-azo	6.88–6.80, m, 4H		C1, C2, 2′,	127.2, 127.7,
	H3, 3′			C3, 3′, C4,	127.9, 128.2,
	H6, 6′			C5, C6, 6′,	128.9, 129.5,
				C7, 7′, C8,	131.6, 140.6,
					151.9, 152.8
	trans-azo	7.64–7.49, m, 5H			
	cis-azo	7.35–7.14, m, 5H			
	H2, 2′				
	H7, 7′, H8				
	CH_2–O			CH_2–O	
	trans-	5.19, s, 2H	$J=13.6$	*trans cis*-azo	65.2
	azo, *cis*	5.21, d, 1H	$J=13.6$		65.4
	trans-Pro	5.11, d, 1H		*cis trans*-Pro	
	cis-azo, *cis*	5.02, s, 2H	$J=13.7$		
	trans-Pro	5.02, d, 1H	$J=13.7$		
		4.96, d, 1H			
				CO	153.2, 153.4
Pro 2	NH	–	–		153.6, 153.8
	–COOH	12.65, br			
	α-CH			Cα	
	trans-azo,			*cis*	58.5
	cis-Pro	4.29, dd	$J=3.5$	*trans*	59.0
			$J=9.0$		
	trans-Pro	4.19, dd	$J=3.2$,		
			$J=8.7$		

(*continued*)

Table 2 (*continued*)

Residue	^{1}H	^{1}H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
	cis-azo, *cis*-Pro	4.23, dd	$J=3.7$, $J=8.7$		
	trans-Pro	4.15, dd	$J=3.6$, $J=8.4$		
	β-CH_2	2.29–2.12, m, β1		Cβ	
	trans cis-azo-*cis* *trans*-Pro	1.98–1.74, m, β2		*cis*	30.4
				trans	29.3
	γ-CH_2	1.98–1.74, m		Cγ	
	trans cis-azo-*cis* *trans*-Pro			*cis*	23.0
				trans	23.9
	δ-CH_2	3.53–3.35, m		Cδ	
	trans cis-azo-*cis* *trans*-Pro			*cis*	46.8
				trans	46.2
				COOH	173.6
					173.9

Table 3
PZ-Pro-OH in DMSO-d_6 at 300 K

Before irradiation		
	trans-azo 97%	*cis*-azo < 3%
trans-Pro	**1**, 46%	**3** [a]
cis-Pro	**2**, 51%	**4** [a]
trans:*cis*-Pro ratio	47:53	[a]
After irradiation 366 nm		
	trans-azo 54%	*cis*-azo 46%
trans-Pro	**1**, 24%	**3**, 21%
cis-Pro	**2**, 29%	**4**, 26%
trans:*cis*-Pro ratio	47:53	47:53

[a] Quantification is not possible. **1**, *trans*-azo, *trans*-Pro-OH (tt); **2**, *trans*-azo, *cis*-Pro-OH (tc); **3**, *cis*-azo, *trans*-Pro-OH (ct); **4**, *cis*-azo, *cis*-Pro-OH (cc).

Table 4
^1H, ^{13}C chemical shifts and coupling constants of PZ-Pro–Phe-OH in DMSO-d_6

Residue	^1H	^1H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
trans-azo, *cis trans*-Pro before irradiation					
PZ 1				*trans*-azo	122.4, 122.5, 127.8,
	trans-azo	7.88–7,82		C1, C2, 2′	128.2, 129.5, 131.5,
	H3, 3′	m, 4H		C3, 3′, C4,	140.7, 151.2, 151.4,
	H6, 6′			C5, C6, 6′	151.9
				C7, 7′, C8	
	trans-azo	7.62–7.55			
	H2, 2′	m, 5H			
	H7, 7′				
	H8				
	CH_2–O			CH_2–O	
	trans-azo,			*trans*-azo,	65.2, 65.3
	trans-Pro	5.20, d, 1H	$J=14.4$	*cis trans*-Pro	
		5.15, d, 1H	$J=14.4$	Pro	
	cis-Pro	5.06, d, 1H	$J=13.8$		
		5.00, d, 1H	$J=13.8$		
				CO	153.7
Pro 2	NH	–	–		–
	α-CH	4.30–4.22, m, 2H		Cα	
	cis-Pro		$J=3.5, J=9.0$	*cis*	59.3
	trans-Pro		$J=3.2, J=8.7$	*trans*	59.7
	β-CH_2	2.16–1.98, m, β1		Cβ	
		1.82–1.66, m, β2		*cis*	31.0
				trans	29.7
	γ-CH_2	1.82–1.66, m		Cγ	
				cis	22.8
				trans	23.6
	δ-CH_2	3.51–3.38, m		Cδ	
				cis	47.1
				trans	46.5
				CO	171.8
					172.1
Phe 2	NH				
	cis-Pro	8.24, d 1H	$J=8.7$		
	trans-Pro	8.10, d, 1H	$J=7.7$		
	H2, H2′	7.26–7.10, m, 5H			126.3, 128.0, 129.0,
	H3, H3′				129.2, 137.6
	H4				
	α-CH			Cα	
	cis-Pro	4.49, m, 1H		*cis*	53.2
	trans-Pro	4,44, m, 1H		*trans*	53.4
	β-CH_2	3.08–3.00, m, β1		Cβ	36.5
		2.97–2.95, m, β2		*cis*	
				trans	
	COOH	12.68, br		COOH	172.7
					172.9
trans cis-azo, *cis trans*-Pro after irradiation, 366 nm, 3 h					
PZ 1	*trans*-azo	7.88–7.82 m, 4H		*trans cis*-	119.7, 119.9,
				azo	122.4, 122.5,
	cis-azo	6.87–6.73, m, 4H		C1, C2, 2′,	127.0, 127.1,
	H3, 3′			C3, 3′, C4,	127.7, 129,4
	H6, 6′			C5, C6, 6′,	131.5, 140.6,
				C7, 7′, C8	151.2, 151.9
	trans-azo	7.62–755, m, 5H			
	cis-azo	7.34–7.02, m, 5H			
	H2, 2′				
	H7, 7′, H8				

(*continued*)

Table 4 (*continued*)

Residue	^{1}H	^{1}H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
	trans-azo, *trans*-Pro	5.20, d, 1H	$J=13.5$	*trans cis*-azo	64.9
		5.15, d, 1H	$J=13.5$	*cis trans*-	65.1
	cis-Pro	5.06, d, 1H	$J=13.8$	Pro	65.2
		5.00, d, 1H	$J=13.8$	CH_2–O	
	CH_2–O *cis*-azo, *trans*-Pro,	4.97, d, 1H	$J=13.2$		
		5.02, d, 1H	$J=13.2$		
	cis-Pro	5.00, d, 1H	$J=13.2$		
		5.05, d, 1H	$J=13.2$		
				CO	153.6
Pro 2	NH	–	–		–
	α-CH,			Cα	
	trans-azo, *cis trans*-Pro	4.29–4.23, m, 2H		*cis*	59.3
				trans	59.7
	cis-azo, *cis trans*-Pro	4.22–4.18, m, 2H			
	β-CH_2	2.15–1.94, m, β1		Cβ	
	trans cis-azo, *cis trans*-Pro	1.82–1.62, m, β2		*cis*	30.9
				trans	29.6
	γ-CH_2	1.82–1.62, m		Cγ	
	trans cis-azo, *cis trans*-Pro			*cis*	22.7
				trans	23.6
	δ-CH_2	3.51–3.39, m		Cδ	
	trans cis-azo, *cis trans*-Pro			*cis*	47.0
				trans	46.4
				CO	172.1
					172.0
Phe 2	NH *trans*-azo, *cis*-Pro	8.24, d, 1H	$J=8.7$		
	trans-Pro	8.10, d, 1H	$J=7.7$		
	cis-azo, *cis*-Pro	8.20, d, 1H	$J=8.3$		
	trans-Pro	8.08, d, 1H	$J=7.7$		
	H2, H2′ H3, H3′ H4	7.34–7.02 m, 5H			126.2, 128.0, 128.9, 129.1, 137.5
	α-CH			Cα	
	trans cis-azo, *cis trans*-Pro	4.29–4.23, m, 4H		*cis*	53.2
				trans	53.3
	β-CH_2	3.07–2.98, m, β1		Cβ	36.5
		2.97–2.81, m, β2		*cis*	
				trans	
	COOH	12.68, br		COOH	172.7

Table 5
^{1}H, ^{13}C chemical shifts and coupling constants of PZ-Pr–PHe–Gly-OH in DMSO-d_6

Residue	^{1}H	^{1}H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
trans-azo-*cis*, *trans*-Pro before irradiation					
PZ1				*trans*-azo	122.4, 122.5, 127.7,
	trans-azo	7.89–7,81		C1, C2,2′,	128.3, 129.5, 131.5,
	H3, 3′	m, 4H		C3, 3′, C4,	140.5, 140.7, 151.2,
	H6, 6′			C5, C6, 6′	151.9
				C7, 7′, C8	
	trans-azo	7.63–7.40			
	H2, 2′	m, 5H			
	H7, 7′				
	H8				
	CH_2–O			CH_2–O	
	trans-azo,			*trans*-azo,	65.1, 65.5
	trans-Pro	5.22, d, 1H	$J=13.5$	*cis trans*-	
		5.15, d, 1H	$J=13.5$	Pro	
	cis-Pro	5.03, d, 1H	$J=13.5$		
		4.98, d, 1H	$J=13.5$		
				CO	153.7
					154.4
Pro 2	NH	–	–		–
	α-CH			Cα	
	cis-Pro	4.25, dd, 1H	$J=2.9$, $J=9.3$	*cis*	60.2
	trans-Pro	4.12, dd, 1H	$J=2.6$, $J=8.7$	*trans*	59.4
	β-CH_2	2.13–1.93, m, β1		Cβ	
		1.79–1.62, m, β2		*cis*	31.0
				trans	29.6
	γ-CH_2	1.79–1.62, m		Cγ	
				cis	22.8
				trans	23.7
	δ-CH_2	3.51–3.37, m		Cδ	
				cis	47.6
				trans	46.5
				CO	171.0
					171.3
Phe 2	NH				
	cis-Pro	8.15, d, 1H	$J=8.0$		
	trans-Pro	8.04, d, 1H	$J=8.4$		
	H2, H2′	7.27–7.05, m, 5H			126.1, 127.9, 129.1,
	H3, H3′				129.2, 137.8
	H4				
	α-CH			Cα	53.5
	cis-Pro	4.62, m, 1H		*cis*	
	trans-Pro	4.55, m, 1H		*trans*	
	β-CH_2	3.09–2.99, m, β1		Cβ	
		2.85–2.80, m, β2		*cis*	37.4
				trans	37.1
				CO	171.5
Gly 3	NH				
	cis-Pro	8.25, t, 1H	$J=5.5$		
	trans-Pro	8.16, t, 1H	$J=5.2$		
	α-CH			Cα	40.7
	cis-Pro	3.75, d, 2H	$J=5.2$	*cis*	
	trans-Pro	3.77, d, 2H	$J=5.5$	*trans*	
	COOH	12.68		COOH	171.9
trans cis-azo, *cis trans*-Pro after irradiation, 366 nm, 3 h					
PZ 1	*trans*-azo	7.89–7.81 m, 4H		*trans cis*-	119.7, 119.9,
				azo	120.0, 122.4,
	cis-azo	6.83–6.76, m, 4H		C1, C2, 2′	122.5, 126.9,
	H3, 3′			C3, 3′ C4,	127.1, 127.7,
	H6, 6′			C5, C6, 6′,	129.4, 131.4,
				C7, 7′, C8	131.5, 137.8, 151.9

(continued)

Table 5 (*continued*)

Residue	^{1}H	^{1}H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
	trans-azo	7.63–7.55, m, 5H			
	cis-azo	7.33–7.03, m, 5H			
	H2, 2′				
	H7, 7′, H8				
	trans-azo,			*trans cis*-	
	trans-Pro	5.22, d, 1H	$J=13.5$	azo,	64.9
		5.15, d, 1H	$J=13.5$	*cis trans*-	65.1
	cis-Pro	5.03, d, 1H	$J=13.5$	Pro,	65.5
		4.98, d, 1H	$J=13.5$	CH_2–O	
	CH_2–O				
	cis-azo,				
	trans-Pro,	4.97, d, 1H	$J=13.1$		
		5.04, d, 1H	$J=13.1$		
	cis-Pro	4.88, d, 1H	$J=13.5$		
		4.77, d, 1H	$J=13.5$		
				CO	153.7
					154.4
	NH	–	–		–
	α-CH			Cα	
	trans-azo,			*cis*	59.4
	cis-Pro	4.25, dd, 1H	$J=2.9$, $J=9.3$	*trans*	60.2
	trans-Pro	4.12, dd, 1H	$J=2.6$, $J=8.7$		
	cis-azo,				
	cis-Pro	4.18, dd, 1H	$J=2.9$, $J=9.3$		
	trans-Pro	4.12, dd, 1H	$J=2.5$, $J=8.7$		
	β-CH_2	2.12–1.90, m, β1		Cβ	
	trans cis-	1.77–1.58, m, β2		*cis*	31.0
	azo, *cis*			*trans*	29.5
	trans-Pro				
	γ-CH_2	1.77–1.58, m		Cγ	
	trans cis-			*cis*	22.7
	azo, *cis*			*trans*	23.6
	trans-Pro				
	δ-CH_2	3.51–3.39, m		Cδ	
	trans cis-			*cis*	47.1
	azo, *cis*			*trans*	46.5
	trans-Pro				
				COOH	171.2
					171.4
Phe 2	NH				
	trans-azo,				
	cis-Pro	8.15, d 1H	$J=8.0$		
	trans-Pro	8.04, d, 1H	$J=8.4$		
	cis-azo,				
	cis-Pro	8.10, d, 1H	$J=8.7$		
	trans-Pro	8.00, d, 1H	$J=8.4$		
	H2, H2′	7.33–7.03, m, 5H			126.1, 127.8, 129.0,
	H3, H3′				129.1, 137.7
	H4				
	α-CH			Cα	
	trans cis-	4.65–4.50, m, 4H		*cis*	53.4
	azo,			*trans*	53.5
	cis trans-Pro				
	β-CH_2	3.12–2.94, m, β1		Cβ	
		2.88–2.74, m, β2		*cis*	37.4
				trans	37.1
				CO	171.4
					171.6

(*continued*)

Table 5 (*continued*)

Residue	^{1}H	^{1}H chemical shift (ppm)	Coupling constants (Hz)	^{13}C	^{13}C chemical shift (ppm)
Gly 3	NH				
	trans-azo,				
	cis-Pro	8.25, t, 1H	$J=5.5$		
	trans-Pro	8.16, t, 1H	$J=5.2$		
	cis-azo	8.22, t, 1H	$J=5.5$		
	cis-Pro	8.13, t, 1H	overlap		
	trans-Pro				
	α-CH			Cα	40.6
	trans-azo,			*cis*	
	cis-Pro	3.75, d, 2H	$J=5.2$	*trans*	
	trans-Pro	3.77, d, 2H	$J=5.5$		
	cis-azo	3.73, d, 2H	$J=5.5$		
	cis-Pro	3.77, d, 2H	$J=6.1$		
	trans-Pro				
	COOH	12.68		COOH	171.9