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Corrigendum

Corrigendum to "Matrix model to predict specific optical rotations of acyclic chiral molecules" [Tetrahedron 63 (2007) 2292–2314]

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Dear editor:

I appreciate one reader who found some errors in our paper entitled "Matrix model to predict specific optical rotations of acyclic chiral molecules" in *Tetrahedron* **2007**, 63, 2292–2314. The errors appeared in Table 3. The corrections are listed below:

Because of the errors, some det(D) and k_0 values in Table 4 should be corrected. However, all conclusions are not changed. The det(D) correction of **52** becomes +0.10 from −0.21 and the change leads to the k_0 values change from −0.45 to +0.095 and agreed well with the experimental result. The details are listed in the following table.

Table 3
Values of **m**, **r**, and **s** values for some selected substituents

R	Original **m** values	Corrected **m**
$-C_2H_5$	13.6	14.1
–n-Pr	14.0	14.5
–n-Bu	14.1	14.6
$-n-C_5H_{11}$	14.2	14.7

Table 4
Calculated values of det(D), experimental and computed $[\alpha]_D$ values (by DFT methods) of specific rotation and the values of k_0 from $[\alpha]_D$/det(D) for 90 example molecules

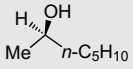
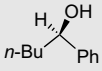
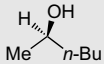
Structure no.	Structure	Original det(D)	Corrected det(D)	Original k_0	Corrected k_0
1		+16.16	+14.6	0.59	0.65
2		+14.98	+13.51	0.87	0.96
4		−27.18	−25.71	0.35	0.37
7		+31.23	+30.3	+0.66	+0.64
8		−14.46	−13.21	0.77	0.83

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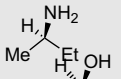
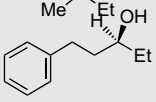
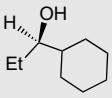
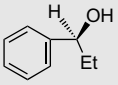
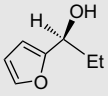
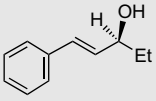
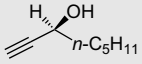
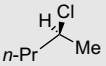
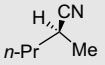
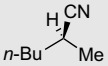
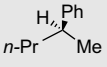
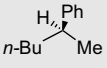
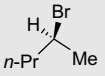
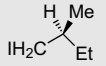
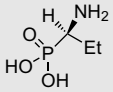
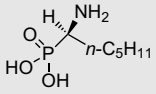
Table 4 (*continued*)

Structure no.	Structure	Original det(D)	Corrected det(D)	Original k_0	Corrected k_0
12		−11.02	−9.99	0.68	0.75
17		+4.97	+9.52	5.40	2.82
24		+5.98	+7.94	1.45	1.02
25		−32.16	−31.23	1.42	1.46
26		−18.96	−17.88	0.94	1.00
27		−5.14	−3.60	1.16	1.65
28		−31.41	−30.49	1.44 (PhH) 1.55 ($CHCl_3$)	1.48 (PhH) 1.59 ($CHCl_3$)
36		−29.53	−29.16	0.76	0.77
40		+8.21	+8.02	4.70	4.85
41		+8.06	+7.87	5.30	5.48
42		+12.64	+11.57	2.43	2.89
43		+11.79	+10.72	4.28	4.71
44		+11.57	+10.51	3.97	4.37
45		+6.57	+6.08	4.20	4.54
46		+6.18	+5.68	4.14	4.51
47		+6.08	+5.58	3.96	4.32
48		+14.67	14.74	1.80	1.80
49		+14.73	14.80	2.8	2.8
52		−0.21	+0.10	−0.45	+0.095

(*continued on next page*)

Table 4 (*continued*)

Structure no.	Structure	Original det(D)	Corrected det(D)	Original k_0	Corrected k_0
69		+1.75	+1.61	3.26	3.54
84		−96.02 (s_{NH2}=0) −96.67 (s_{NH2}=0.44)	−94.00 (s_{NH2}=0) −93.94 (s_{NH2}=0.44)	0.17 0.17	0.17 0.17
85		−259.5	157.76	0.16	0.16

Thus, some statements in the text should be revised. These are omitted here. I apologise for any inconvenience caused.