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Correction: Mechanochemical enzymatic resolution of *N*-benzylated-β^3-amino esters

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Correction

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The original published Tables 1–4 and Supporting Information File 1 contain some incorrect values. In this Correction article the whole corrected Tables are given. The positions of the correted values are described in detail in the paragraphs below.

In Table 1 in entry 5 the yield (column 3) has been corrected.

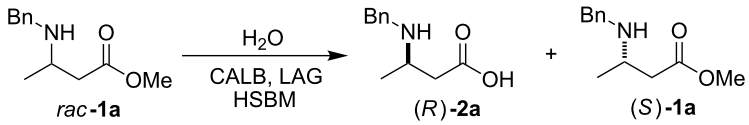
In Table 2 in entry 4 the ee value of (*S*)-**1** (column 5), and in entry 6 the yield (column 4) have been corrected.

In Table 3 entry 1 the ee of (*S*)-**1a** (column 4), in entry 2 the yield (column 3) and the *c* value (column 6), and in entry 3 the *c* value (column 6) have been corrected.

In Table 4 in entry 3 the yield (column 3) has been corrected.

A corrected version of Supporting Information File 1 is also part of this Correction. The new Supporting Information File 1 is the complete file with the corrections marked in yellow color.

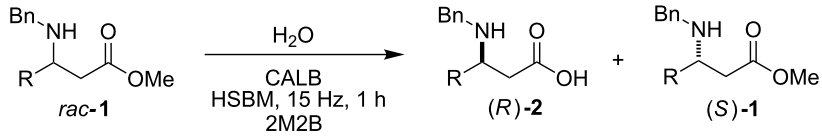
Table 1: Search of the best parameters in the enzymatic enantioselective hydrolysis of *rac*-**1a** under ball milling.



entry[a]	LAG additive[b]	yield (%)[c] (*S*)-**1a**/(*R*)-**2a**	time (h)	ee (*S*)-**1a** (%)[d]	ee (*R*)-**2a** (%)[d]	c^e (%)	E^f
1[g]	2M2B	51/49	0.5	99	80	55	46
2	2M2B	70/30	0.5	89	77	54	23
3	**2M2B**	**51/49**	**1**	**99**	**95**	**51**	**>200**
4	AcOEt	86/13	1	69	95	42	81
5	IPA	80/20	1	48	95	34	63
6	CH_3CN	65/29	1	65	95	41	77
7	hexane	40/60	1	97	86	53	55
8	–	58/41	1	95	92	51	89
9[g]	–	58/42	1	93	86	52	45
10[h]	–	68/31	1	74	80	48	20

[a]Reactions were carried out with 0.5 equivalents of water and 15 Hz of frequency. [b]0.2 mL of LAG additive was used. [c]Determined after purification by flash chromatography. [d]Determined by HPLC with chiral stationary phase. [e]Calculated from $c = ee_s/(ee_s + ee_p)$.
[f]$E = \ln[1 - c(1 + ee_p)]/\ln[1 - c(1 - ee_p)]$. [g]25 Hz of frequency was used. [h]0.25 equivalents of water were used.

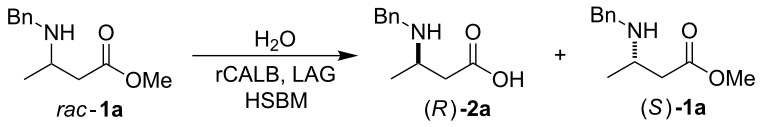
Table 2: Substrate scope for the enzymatic resolution of *N*-benzylated-β^3-amino esters.



entry[a]	*rac*	R	yield (%)[b] (*S*)-**1**/(*R*)-**2**	ee[c] (*S*)-**1**(%)	$[\alpha]_D^{25}$[d]	ee[c] (*R*)-**2**(%)	$[\alpha]_D^{25}$[e]	c^f (%)	E[g]	absolute configuration[h]
1	**1b**	CH_3-(CH_2)-	51/49	91	4.5	97	−36.5	48	>200	*R*
2	**1c**	CH_3-$(CH_2)_2$-	53/43	84	2.1	98	−45.2	46	>200	*R*
3	**1d**	CH_3-$(CH_2)_3$-	68/29	23	2.0	94	−35.3	20	40	*R*
4	**1e**	CH_3-$(CH_2)_4$-	74/24	16	0.2	94	−40.0	15	38	*R*
5	**1f**	CH_3-$(CH_2)_5$-	79/18	13	0.8	91	−39.7	13	24	*R*
6[i]	**1g**	Ph	90/10	18	3.4	83	−35.0	18	13	*S*
7[i]	**1h**	4-MeO-Ph	89/10	1	−0.5	80	−31.7	1	9	*S*
8	**1i**	*t*-Bu	89/4	4	−0.6	94	12.8	4	34	*S*

[a]Reactions were carried out with 0.5 equivalents of water and 0.2 mL of 2M2B at 15 Hz during 1 h. [b]Determined after purification by flash chromatography. [c]Determined by HPLC with chiral stationary phase. [d] $c = 0.33$ in CH_3Cl. [e]$c = 0.33$ in MeOH. [f]Calculated from $c = ee_s/(ee_s + ee_p)$.
[g]$E = \ln[1 - c(1 + ee_p)]/\ln[1 - c(1 - ee_p)]$. [h]Assigned by chemical correlation and by HPLC with chiral stationary phase. [i]0.75 equivalents of water were used.

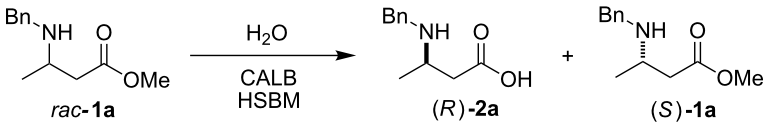
Table 3: Recycling capacity of immobilized CALB under HSBM conditions.



entry[a]	Recycling cycle	yield (%)[b] (*S*)-**1a**/(*R*)-**2a**	ee[c] (*S*)-**1a** (%)	ee[c] (*R*)-**2a** (%)	*c*[d] (%)	*E*[e]
1	–	51/49	99	95	51	>200
2	1	65/35	35	88	28	22
3	2	80/20	6	80	7	10
4	3	100/0	0	–	–	–

[a]Reactions were carried out with 0.5 equivalents of water and 0.2 mL of 2M2B at 15 Hz during 1 h. [b]Determined after purification by flash chromatography. [c]Determined by HPLC with chiral stationary phase. [d]Calculated from $c = ee_s/(ee_s + ee_p)$. [e]$E = \ln[1 - c(1 + ee_p)]/\ln[1 - c(1 - ee_p)]$.

Table 4: Scaling-up of the enzymatic hydrolysis reaction under ball-milling using substrate *rac*-**1a**.



entry[a]	catalyst/substrate (equiv) [b]	yield (%)[c] (*S*)-**1a**/(*R*)-**2a**	ee[d] (*S*)-**1a** (%)	ee[d] (*R*)-**2a** (%)	*c*[e] (%)	*E*[f]
1[g]	1/1	51/49	>99	95	51	>200
2	1/3	52/48	62	93	40	52
3	1/6	61/38	53	93	36	47
4	1/9	59/40	49	94	34	53

[a]Reactions were carried out with 0.5 equivalents of water at 15 Hz during 1 h. [b]1 equivalent of enzyme = 40 mg; 1 equivalent of susbtrate = 82 mg. [c]Determined after purification by flash chromatography. [d]Determined by HPLC with chiral stationary phase. [e]Calculated from $c = ee_s/(ee_s + ee_p)$. [f]$E = \ln[1 - c(1 + ee_p)]/\ln[1 - c(1 - ee_p)]$. [g]0.2 mL of LAG were used.

Supporting Information

Supporting Information File 1

Experimental section, NMR spectra, chromatograms and X-ray diffraction data.
[http://www.beilstein-journals.org/bjoc/content/supplementary/1860-5397-13-210-S1.pdf]

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