Electronic Supplementary Material (ESI) for RSC Advances.

FACILE, HIGH-YIELDING PREPARATION OF PYRROLIDINIUM, PIPERIDINIUM, MORPHOLINIUM AND 2,3-DIHYDRO-1*H*-ISOINDOLINIUM SALTS AND IONIC LIQUIDS FROM SECONDARY AMINES

Supplementary Information

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CALCULATION OF OVERALL "GREENNESS" SCORE

EHS Scores for the chemicals used

CHEMICAL	HEALTH	SAFETY	ENVIRON.	EHS SCORE[a]
K_2CO_3	7	10	10	8.9
$LiNTf_2$	4	10	7	6.5
$Br(CH_2)_4Br$	4	10	10	7.4
$Br(CH_2)_5Br$	10	10	10	10
$\{Br(CH_2)_2\}_2O$	7	10	10	8.9
o-$C_6H_4(CH_2Br)_2$	4	10	10	7.4
$HN(C_2H_5)_2$	7	4	10	6.5
$HN(C_3H_7)_2$	7	4	10	6.5
$HN(C_4H_9)_2$	7	4	10	6.5
$HN(C_2H_5)(C_4H_9)$	7	4	10	6.5
$HN(CH_3)(C_4H_9)$	7	4	10	6.5
Pyrrolidine	7	4	10	6.5
Piperidine	4	4	10	5.4
Morpholine	7	7	10	7.9
Formaldehyde	1	10	1	2.2
C_4H_9Br	10	4	4	5.4
CH_3CO_2H	4	7	10	6.5
Zinc	10	1	1	2.2
$NaBH_4$	4	4	10	5.4

[a] Determined by the geometric mean of the Health, Safety, and Environmental scores.

Assessment of Chemistry scores

	For the new method:	For Scheme 4:
Work-up	10	7
Co-reagents	4	4
Other issues	10	10
Stoichiometry	7	1
Clean Chemistry score	7.3	4.1

Calculation of Overall "Greenness" scores

For the synthesis of **15** (*N*-butyl-*N*-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide):

For the new method:

Overall EHS $= (EHS(K_2CO_3) \times EHS(HN(CH_3)(C_4H_9)) \times EHS(Br(CH_2)_4Br) \times EHS(LiNTf_2))^{1/4}$

$= (8.9 \times 6.5 \times 7.4 \times 6.5)^{1/4}$

$= 7.3$

Overall "greenness" score $= (EHS \times \text{Clean Chemistry})^{1/2}$

$= (7.3 \times 7.3)^{1/2}$

$= 7.3$

For Scheme 4 (method 1 in step 1):

Overall EHS $= (EHS(\text{pyrrolidine}) \times EHS(Zn) \times EHS(\text{formaldehyde}) \times EHS(CH_3CO_2H) \times EHS(C_4H_9Br) \times EHS(LiNTf_2))^{1/6}$

$= (6.5 \times 2.2 \times 2.2 \times 6.5 \times 5.4 \times 6.5)^{1/6}$

$= 4.4$

Overall "greenness" score $= (EHS \times \text{Clean Chemistry})^{1/2}$

$= (4.1 \times 4.4)^{1/2}$

$= 4.2$

For Scheme 4 (method 2 in step 1):

Overall EHS = (EHS(pyrrolidine) × EHS(formaldehyde) × EHS($NaBH_4$) × EHS(C_4H_9Br) × EHS($LiNTf_2$))$^{1/5}$

= $(6.5 \times 2.2 \times 5.4 \times 5.4 \times 6.5)^{1/5}$

= 4.9

Overall "greenness" score = (EHS × Clean Chemistry)$^{1/2}$

= $(4.9 \times 4.1)^{1/2}$

= 4.5