**Supporting Information of** 

## 4-Dodecylbenzenesulfonic acid (DBSA) Promoted Solventfree Diversity-Oriented Synthesis of Primary Carbamates, S-Thiocarbamates and Ureas

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## 1. Experimental

## **1.1** General experimental methods

<sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded by BRUKER AVANCE DRX250 (250 MHz). The IR spectra were obtained on a Shimadzu FT-IR 8300. Mass spectra were analyzed by Shimadzu GC-MS QP 1000 EX. Elemental analysis was performed using Thermofinigan Flash EA-1112 CHNSO rapid elemental analyzer. Melting points were recorded by Electrothermal 9100 and the GallenKamp melting point apparatus and were uncorrected.

## 1.2 Chemicals

All starting materials and solvents were purified with appropriate purification techniques before use. Primary carbamates, *S*-thiocarbamates and ureas were prepared according to literature.





Figure S1. FT-IR spectra of Phenyl carbamate in KBr

Figure S2. <sup>13</sup>C-NMR spectra (63 MHz) of Phenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S3. <sup>1</sup>H-NMR spectra (250 MHz) of Phenyl carbamate in DMSO-*d*<sub>6</sub>







Figure S5. FT-IR spectra of 2-Methylphenyl carbamate in KBr



Figure S6. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Methylphenyl carbamate in DMSO-*d*<sub>6</sub>



18S



Figure S7. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Methylphenyl carbamate in DMSO-*d*<sub>6</sub>











Figure S10. <sup>13</sup>C-NMR spectra (63 MHz) of 3-Methylphenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S11. <sup>1</sup>H-NMR spectra (250 MHz) of 3-Methylphenyl carbamate in DMSO-*d*<sub>6</sub>







Figure S13. FT-IR spectra of 4-Methylphenyl carbamate in KBr



Figure S14. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Methylphenyl carbamate in DMSO- $d_6$ 



23S



Figure S15. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Methylphenyl carbamate in DMSO-*d*<sub>6</sub>











Figure S18. <sup>13</sup>C-NMR spectra (63 MHz) of 2,6-Dimethylphenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S19. <sup>1</sup>H-NMR spectra (250 MHz) of 2,6-Dimethylphenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S20. MS of 2,6-Dimethylphenyl carbamate



Figure S21. FT-IR spectra of 3,4-Dimethylphenyl carbamate in KBr



Figure S22. <sup>13</sup>C-NMR spectra (63 MHz) of 3,4-Dimethylphenyl carbamate in DMSO-*d*<sub>6</sub>





Figure S23. <sup>1</sup>H-NMR spectra (250 MHz) of 3,4-Dimethylphenyl carbamate in DMSO-*d*<sub>6</sub>







Figure S25. FT-IR spectra of 2-tert-Butyl-4-methylphenyl carbamate in KBr



Figure S26. <sup>13</sup>C-NMR spectra (63 MHz) of 2-tert-Butyl-4-methylphenyl carbamate in DMSO-d<sub>6</sub>



Figure S27. <sup>1</sup>H-NMR spectra (250 MHz) of 2-tert-Butyl-4-methylphenyl carbamate in DMSO-d<sub>6</sub>







Figure S29. FT-IR spectra of 4-Flourophenyl carbamate in KBr



Figure S30. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Flourophenyl carbamate in DMSO- $d_6$ 



Figure S31. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Flourophenyl carbamate in DMSO-d<sub>6</sub>







Figure S33. FT-IR spectra of 4-Chlorophenyl carbamate in KBr



Figure S34. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Chlorophenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S35. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Chlorophenyl carbamate in DMSO-*d*<sub>6</sub>






Figure S37. FT-IR spectra of 2-Chlorophenyl carbamate in KBr



Figure S38. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Chlorophenyl carbamate in DMSO-d<sub>6</sub>



Figure S39. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Chlorophenyl carbamate in DMSO- $d_6$ 







Figure S41. FT-IR spectra of 2,4-Dichlorophenyl carbamate in KBr



Figure S42. <sup>13</sup>C-NMR spectra (63 MHz) of 2,4-Dichlorophenyl carbamate in DMSO- $d_6$ 



Figure S43. <sup>1</sup>H-NMR spectra (250 MHz) of 2,4-Dichlorophenyl carbamate in DMSO-*d*<sub>6</sub>





Figure S44. MS of 2,4-Dichlorophenyl carbamate

Figure S45. FT-IR spectra of 4-Bromophenyl carbamate in KBr



Figure S46. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Bromophenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S47. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Bromophenyl carbamate in DMSO-*d*<sub>6</sub>







Figure S49. FT-IR spectra of 2-Bromophenyl carbamate in KBr



Figure S50. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Bromophenyl carbamate in DMSO-*d*<sub>6</sub>





Figure S51. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Bromophenyl carbamate in DMSO-d<sub>6</sub>







Figure S53. FT-IR spectra of 4-Iodophenyl carbamate in KBr



Figure S54. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Iodophenyl carbamate in DMSO-d<sub>6</sub>







Figure S56. MS of 4-Iodophenyl carbamate



Figure S57. FT-IR spectra of 4-Methoxyphenyl carbamate in KBr



Figure S58. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Methoxyphenyl carbamate in DMSO- $d_6$ 



Figure S59. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Methoxyphenyl carbamate in DMSO- $d_6$ 







Figure S61. FT-IR spectra of O-4-Phenoxyphenyl carbamate in KBr



Figure S62. <sup>13</sup>C-NMR spectra (63 MHz) of *O*-4-Phenoxyphenyl carbamate in DMSO-*d*<sub>6</sub>



Figure S63. <sup>1</sup>H-NMR spectra (250 MHz) of O-4-Phenoxyphenyl carbamate in DMSO-d<sub>6</sub>







Figure S65. FT-IR spectra of Methyl carbamate in KBr



Figure S66. <sup>13</sup>C-NMR spectra (63 MHz) of Methyl carbamate in DMSO- $d_6$ 



Figure S67. <sup>1</sup>H-NMR spectra (250 MHz) of Methyl carbamate in DMSO-*d*<sub>6</sub>







Figure S69. FT-IR spectra of Ethyl carbamate in KBr



Figure S70. <sup>13</sup>C-NMR spectra (63 MHz) of Ethyl carbamate in DMSO-*d*<sub>6</sub>



Figure S71. <sup>1</sup>H-NMR spectra (250 MHz) of Ethyl carbamate in DMSO-*d*<sub>6</sub>







Figure S73. FT-IR spectra of 2-Propyl carbamate in KBr



Figure S74. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Propyl carbamate in DMSO-d<sub>6</sub>



Figure S75. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Propyl carbamate in DMSO-*d*<sub>6</sub>







Figure S77. FT-IR spectra of 1-Butyl carbamate in KBr



Figure S78. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Butyl carbamate in DMSO-*d*<sub>6</sub>



Figure S79. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Butyl carbamate in DMSO-*d*<sub>6</sub>







Figure S81. FT-IR spectra of 2-Butyl carbamate in KBr



Figure S82. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Butyl carbamate in DMSO- $d_6$ 



Figure S83. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Butyl carbamate in DMSO-*d*<sub>6</sub>







Figure S85. FT-IR spectra of tert-Butyl carbamate in KBr



Figure S86. <sup>13</sup>C-NMR spectra (63 MHz) of *tert*-Butyl carbamate in DMSO-*d*<sub>6</sub>



Figure S87. <sup>1</sup>H-NMR spectra (250 MHz) of *tert*-Butyl carbamate in DMSO-*d*<sub>6</sub>







Figure S89. FT-IR spectra of Cyclohexyl carbamate in KBr



Figure S90. <sup>13</sup>C-NMR spectra (63 MHz) of Cyclohexyl carbamate in DMSO- $d_6$ 



Figure S91. <sup>1</sup>H-NMR spectra (250 MHz) of Cyclohexyl carbamate in DMSO-*d*<sub>6</sub>







Figure S93. FT-IR spectra of (-)Menthyl carbamate in KBr



Figure S94. <sup>13</sup>C-NMR spectra (63 MHz) of (-)Menthyl carbamate in DMSO- $d_6$ 



Figure S95. <sup>1</sup>H-NMR spectra (250 MHz) of (-)Menthyl carbamate in DMSO-*d*<sub>6</sub>









Figure S98. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Phenethyl carbamate in DMSO-*d*<sub>6</sub>





Figure S99. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Phenethyl carbamate in DMSO-d<sub>6</sub>






Figure S101. FT-IR spectra of 1-Phenethyl carbamate in KBr

Figure S102. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Phenethyl carbamate in DMSO- $d_6$ 





Figure S103. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Phenethyl carbamate in DMSO-d<sub>6</sub>







Figure S105. FT-IR spectra of Naphthalen-1-yl carbamate in KBr

Figure S106. <sup>13</sup>C-NMR spectra (63 MHz) of Naphthalen-1-yl carbamate in DMSO-d<sub>6</sub>





Figure S107. <sup>1</sup>H-NMR spectra (250 MHz) of Naphthalen-1-yl carbamate in DMSO-d<sub>6</sub>







Figure S109. FT-IR spectra of Naphthalen-2-yl carbamate in KBr

Figure S110. <sup>13</sup>C-NMR spectra (63 MHz) of Naphthalen-2-yl carbamate in DMSO-d<sub>6</sub>





Figure S111. <sup>1</sup>H-NMR spectra (250 MHz) of Naphthalen-2-yl carbamate in DMSO-d<sub>6</sub>





Figure S113. FT-IR spectra of Allyl carbamate in KBr



Figure S114. <sup>13</sup>C-NMR spectra (63 MHz) of Allyl carbamate in DMSO-d<sub>6</sub>



Figure S115. <sup>1</sup>H-NMR spectra (250 MHz) of Allyl carbamate in DMSO-*d*<sub>6</sub>







Figure S117. FT-IR spectra of Phenyl S-thiocarbamate in KBr



Figure S118. <sup>13</sup>C-NMR spectra (63 MHz) of Phenyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S119. <sup>1</sup>H-NMR spectra (250 MHz) of Phenyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S120. MS of Phenyl S-thiocarbamate



Figure S121. FT-IR spectra of 4-Methylphenyl S-thiocarbamate in KBr



Figure S123. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Methylphenyl S-thiocarbamate in DMSO-d<sub>6</sub>

0.0

5.0

10.0 ppm (t1)







Figure S125. FT-IR spectra of 4-Chlorophenyl S-thiocarbamate in KBr



Figure S126. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Chlorophenyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S127. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Chlorophenyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S129. FT-IR spectra of 4-Bromophenyl S-thiocarbamate in KBr



Figure S130. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Bromophenyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S131. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Bromophenyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S133. FT-IR spectra of 4-Methoxyphenyl S-thiocarbamate in KBr



Figure S134. <sup>13</sup>C-NMR spectra (63 MHz) of 4-Methoxyphenyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S135. <sup>1</sup>H-NMR spectra (250 MHz) of 4-Methoxyphenyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S136. MS of 4-Methoxyphenyl S-thiocarbamate



Figure S137. FT-IR spectra of Naphthalen-2-yl S-thiocarbamate in KBr



Figure S138. <sup>13</sup>C-NMR spectra (63 MHz) of Naphthalen-2-yl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S139. <sup>1</sup>H-NMR spectra (250 MHz) of Naphthalen-2-yl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S141. FT-IR spectra of Ethyl S-thiocarbamate in KBr



Figure S142. <sup>13</sup>C-NMR spectra (63 MHz) of Ethyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S143. <sup>1</sup>H-NMR spectra (250 MHz) of Ethyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S145. FT-IR spectra of Propyl S-thiocarbamate in KBr



Figure S146. <sup>13</sup>C-NMR spectra (63 MHz) of Propyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S147. <sup>1</sup>H-NMR spectra (250 MHz) of Propyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S149. FT-IR spectra of 1-Butyl S-thiocarbamate in KBr



Figure S150. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Butyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S151. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Butyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S153. FT-IR spectra of 1-Pentyl S-thiocarbamate in KBr



Figure S154. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Pentyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S155. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Pentyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S161. FT-IR spectra of 1-Octyl S-thiocarbamate in KBr



Figure S162. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Octyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S163. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Octyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S165. FT-IR spectra of 2-Butyl S-thiocarbamate in KBr



Figure S166. <sup>13</sup>C-NMR spectra (63 MHz) of 2-Butyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S167. <sup>1</sup>H-NMR spectra (250 MHz) of 2-Butyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S168. MS of 2-Butyl S-thiocarbamate



Figure S169. FT-IR spectra of tert-Butyl S-thiocarbamate in KBr



Figure S170. <sup>13</sup>C-NMR spectra (63 MHz) of tert-Butyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S171. <sup>1</sup>H-NMR spectra (250 MHz) of tert-Butyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S173. FT-IR spectra of Benzyl S-thiocarbamate in KBr



Figure S174. <sup>13</sup>C-NMR spectra (63 MHz) of Benzyl S-thiocarbamate in DMSO-d<sub>6</sub>



Figure S175. <sup>1</sup>H-NMR spectra (250 MHz) of Benzyl S-thiocarbamate in DMSO-d<sub>6</sub>







Figure S177. FT-IR spectra of 1-Phenylurea in KBr


Figure S178. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Phenylurea in DMSO-*d*<sub>6</sub>



Figure S179. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Phenylurea in DMSO-*d*<sub>6</sub>







Figure S181. FT-IR spectra of 1-(4-Methylphenyl)urea in KBr



Figure S182. <sup>13</sup>C-NMR spectra (63 MHz) of 1-(4-Methylphenyl)urea in DMSO-d<sub>6</sub>



Figure S183. <sup>1</sup>H-NMR spectra (250 MHz) of 1-(4-Methylphenyl)urea in DMSO-d<sub>6</sub>







Figure S185. FT-IR spectra of 1-(4-Chlorophenyl)urea in KBr



Figure S186. <sup>13</sup>C-NMR spectra (63 MHz) of 1-(4-Chlorophenyl)urea in DMSO-d<sub>6</sub>



Figure S187. <sup>1</sup>H-NMR spectra (250 MHz) of 1-(4-Chlorophenyl)urea in DMSO-d<sub>6</sub>







Figure S189. FT-IR spectra of 1-(3-Bromophenyl)urea in KBr



Figure S190. <sup>13</sup>C-NMR spectra (63 MHz) of 1-(3-Bromophenyl)urea in DMSO-d<sub>6</sub>



Figure S191. <sup>1</sup>H-NMR spectra (250 MHz) of 1-(3-Bromophenyl)urea in DMSO-d<sub>6</sub>







Figure S193. FT-IR spectra of 1-(4-Methoxyphenyl)urea in KBr



Figure S194. <sup>13</sup>C-NMR spectra (63 MHz) of 1-(4-Methoxyphenyl)urea in DMSO-d<sub>6</sub>



Figure S195. <sup>1</sup>H-NMR spectra (250 MHz) of 1-(4-Methoxyphenyl)urea in DMSO-d<sub>6</sub>







Figure S197. FT-IR spectra of 1-(4-(Dimethylamino)phenyl)urea in KBr



Figure S198. <sup>13</sup>C-NMR spectra (63 MHz) of 1-(4-(Dimethylamino)phenyl)urea in DMSO- $d_6$ 



Figure S199. <sup>1</sup>H-NMR spectra (250 MHz) of 1-(4-(Dimethylamino)phenyl)urea in DMSO-d<sub>6</sub>







Figure S201. FT-IR spectra of 1-Butylurea in KBr



Figure S202. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Butylurea in DMSO-*d*<sub>6</sub>



Figure S203. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Butylurea in DMSO-*d*<sub>6</sub>



Figure S205. FT-IR spectra of 1,1-Dimethylurea in KBr



Figure S207. <sup>1</sup>H-NMR spectra (250 MHz) of 1,1-Dimethylurea in DMSO- $d_6$ .







Figure S209. FT-IR spectra of 1-Benzylurea in KBr



Figure S210. <sup>13</sup>C-NMR spectra (63 MHz) of 1-Benzylurea in DMSO-d<sub>6</sub>



Figure S211. <sup>1</sup>H-NMR spectra (250 MHz) of 1-Benzylurea in DMSO-*d*<sub>6</sub>



Figure S212. MS of 1-Benzylurea