Development of intein-inspired amide cleavage chemical device

Chiaki Komiya†, Keisuke Aihara†, Ko Morishita, Hao Ding, Tsubasa Inokuma, Akira Shigenaga, Akira Otaka*

†Contributed equally

Institute of Biomedical Sciences and Graduate School of Pharmaceutical Sciences, Tokushima University, Shomachi, Tokushima 770-8505, Japan

E-mail:
aotaka@ph.tokushima-u.ac.jp

SUPPORTING INFORMATION

Content:
Copies of NMR spectra for all compounds ................................................................. p. S2
2-Nitrobenzyl \{2-[(tert-butoxycarbonyl)amino]ethyl\}ethylcarbamate

File \{LANDISK-AO\NMR\KOMIYA\ASN-DATA\2J\C051831DMSO\C051831-DMSO-100D\EG:20150615.ALS
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ProbeHD
Instrument
PulseProgram NON
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Solvent DMSO
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Window Exponential
RGain 21
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(8)-3-[(Allyloxy)carbonyl]amino]-2,2-dimethylsuccinic acid 4-(allyl)ester 8
(S)-4-(allyloxy)-2-[(allyloxy)carbonyl]amino]-3,3-dimethyl-4-oxobutanoic acid
Allyl (S)-2-{{(allyloxy)carbonyl}amino}-4-{{2-ethyl(2-nitrobenzyloxy carbonyl)aminoethyl}amino}-3,3-dimethyl-4-oxobutanoate 9a
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(S)-2-([(9H-Fluoren-9-yl)methoxycarbonyl]amino)-4-[(2-ethyl(2-nitrobenzyloxy carbonyl)amino)ethyl]amino)-3,3-dimethyl-4-oxobutanoic acid 10a
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- **Temp.**: 25.0 °C
- **Solvent**: CDCL3
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- **Window**: Exponential
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Allyl (S)-2-{[(allyloxy)carbonyl]amino}-4-{[2-(tert-butoxycarbonyl)(ethyl)aminoethyl]amino}-3,3-dimethyl-4-oxobutanoate 9b
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(S)-2-[(9H-Fluoren-9-yl)methoxycarbonyl]amino)-4-[(2-(tert-butoxycarbonyl)(ethyl)aminoethyl]amino]-3,3-dimethyl-4-oxobutanoic acid 10b
Nitrobenzyl [(2,4-dimethoxybenzyl)amino]ethyl)(ethyl)carbamate 14a
tert-Butyl [2-(4-dimethoxybenzyl)amino]ethyl(ethyl)carbamate 14b
Allyl (S)-2-[(allyloxy carbonyl) amino]-4-[(2,4-dimethoxybenzyl) (2-ethyl-2-nitrobenzyl oxycarbonyl aminoethyl) amino]-3,3-dimethyl-4-oxobutanoate 15
Allyl \((S)-3\text{-}(\text{allyloxy carbonyl})\text{amino}-4\text{-}([2,4\text{-} \text{dimethoxy benzyl}][2\text{-} \text{ethyl-2-nitrobenzyloxycarbonyl}
\text{amino})\text{ethyl}]\text{amino})\text{-}2,2\text{-} \text{dimethyl-4-oxobutanoate} \ 25
(S)-3-([(9H-Fluoren-9-yl)methoxycarbonyl]amino)-4-[(2,4-dimethoxybenzyl)[2-ethyl(2-nitrobenzyl oxycarbonyl)aminoethyl]amino]-2,2-dimethyl-4-oxobutanoic acid

S24
Allyl (S)-3-[(allyloxy carbonyl)amino]-4-[[2-ethyl(tert-butoxycarbonyl)aminoethyl][2,4-dimethoxybenzyl]amino]-2,2-dimethyl-4-oxobutanoate 26
(S)-3-[(9H-Fluoren-9-yl)methoxycarbonyl]amino)-4-[(2-ethyl(tert-butoxycarbonyl)aminoethyl)[2,4-dimethoxybenzyl]amino]-2,2-dimethyl-4-oxobutanoic acid 27
Allyl \( N^2\{-[(9H-\text{Fluoren}-9-\text{yl})\text{methoxy}]\text{carbonyl}\} - N^4\{-2\{-[(\text{tert-} \text{butoxycarbonyl})(\text{ethyl})\text{amino}]\text{ethyl}\}\} - N^1\{- (2,4\text{-dimethoxybenzyl})\} - \text{L-} \text{asparagine} \ 28
$N^2-[[9H-Fluoren-9-yl]methoxy]carbonyl]-N^4-[2-[(tert-butoxycarbonyl)(ethyl)amino]ethyl]-N^2-(2,4-dimethoxybenzyl)-L-asparagine 29$