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Efficient and Mild Microwave-Assisted Stepwise Functionalization of Naphthalenediimide with α -Amino Acids

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and

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goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

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C7 C 0.1471(2) 1.12636(19) 0.13912(12) 0.0160(3) Uani 1 1 d . . .
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C11 C -0.28322(19) 1.49006(18) 0.33079(12) 0.0142(3) Uani 1 1 d . . .
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C13 C -0.61401(19) 1.43127(19) 0.39748(12) 0.0154(3) Uani 1 1 d . . .
C14 C -0.43002(19) 1.61549(19) 0.39854(12) 0.0150(3) Uani 1 1 d . . .
C1' C 0.1923(2) 0.8167(2) -0.05835(13) 0.0178(3) Uani 1 1 d . . .
C2' C 0.26307(19) 0.85540(19) 0.04151(12) 0.0160(3) Uani 1 1 d . . .
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C3' C 0.3629(2) 0.6887(2) 0.11125(13) 0.0203(3) Uani 1 1 d . . .
H3'A H 0.3885 0.7222 0.1805 0.024 Uiso 1 1 calc R . . .
H3'B H 0.2840 0.6196 0.1324 0.024 Uiso 1 1 calc R . . .
C4' C 0.5365(2) 0.5749(2) 0.05188(12) 0.0178(3) Uani 1 1 d . . .
C5' C 0.6833(2) 0.6292(2) 0.03259(13) 0.0200(3) Uani 1 1 d . . .
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C6' C 0.8445(2) 0.5248(2) -0.02136(14) 0.0226(3) Uani 1 1 d . . .
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C7' C 0.8596(2) 0.3655(2) -0.05625(14) 0.0239(3) Uani 1 1 d . . .
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C8' C 0.7136(2) 0.3097(2) -0.03667(14) 0.0231(3) Uani 1 1 d . . .
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C9' C 0.5528(2) 0.4140(2) 0.01761(14) 0.0213(3) Uani 1 1 d . . .
H9' H 0.4541 0.3752 0.0312 0.026 Uiso 1 1 calc R . . .
C10' C 0.0097(3) 0.9364(3) -0.20209(17) 0.0363(4) Uani 1 1 d . . .
H10A H -0.0805 1.0463 -0.2271 0.054 Uiso 1 1 calc R . . .
H10B H -0.0445 0.8465 -0.1838 0.054 Uiso 1 1 calc R . . .
H10C H 0.1077 0.8994 -0.2614 0.054 Uiso 1 1 calc R . . .
C1'' C -0.8087(2) 1.60037(19) 0.59320(12) 0.0173(3) Uani 1 1 d . . .
C2'' C -0.73422(19) 1.69877(19) 0.49608(12) 0.0158(3) Uani 1 1 d . . .
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C3'' C -0.8786(2) 1.8206(2) 0.42452(13) 0.0193(3) Uani 1 1 d . . .
H3''A H -0.8202 1.8617 0.3556 0.023 Uiso 1 1 calc R . . .
H3''B H -0.9473 1.7538 0.4030 0.023 Uiso 1 1 calc R . . .
C4'' C -1.0068(2) 1.97786(19) 0.48290(12) 0.0167(3) Uani 1 1 d . . .
C5'' C -0.9503(2) 2.1121(2) 0.50094(13) 0.0197(3) Uani 1 1 d . . .
H5'' H -0.8309 2.1045 0.4768 0.024 Uiso 1 1 calc R . . .
C6'' C -1.0674(2) 2.2579(2) 0.55413(14) 0.0224(3) Uani 1 1 d . . .
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C7'' C -1.2418(2) 2.2692(2) 0.58955(14) 0.0227(3) Uani 1 1 d . . .
H7'' H -1.3215 2.3674 0.6266 0.027 Uiso 1 1 calc R . . .
C8'' C -1.2998(2) 2.1364(2) 0.57076(14) 0.0215(3) Uani 1 1 d . . .
H8'' H -1.4195 2.1448 0.5943 0.026 Uiso 1 1 calc R . . .
C9'' C -1.1827(2) 1.9910(2) 0.51745(13) 0.0200(3) Uani 1 1 d . . .
H9'' H -1.2229 1.9008 0.5047 0.024 Uiso 1 1 calc R . . .
C10'' C -0.7304(3) 1.3847(2) 0.74185(15) 0.0280(3) Uani 1 1 d . . .
H10D H -0.6246 1.3052 0.7760 0.042 Uiso 1 1 calc R . . .
H10E H -0.7935 1.3169 0.7168 0.042 Uiso 1 1 calc R . . .
H10F H -0.8097 1.4635 0.7965 0.042 Uiso 1 1 calc R . . .
N3 N -1.4736(4) 1.9749(3) 0.8260(2) 0.0569(7) Uani 1 1 d . . .
C15 C -1.3820(3) 1.6863(3) 0.72900(17) 0.0349(4) Uani 1 1 d . . .
H15A H -1.4213 1.7115 0.6543 0.052 Uiso 1 1 calc R . . .
H15B H -1.4377 1.6086 0.7731 0.052 Uiso 1 1 calc R . . .

H15C H -1.2519 1.6297 0.7236 0.052 Uiso 1 1 calc R . .
C16 C -1.4341(3) 1.8482(3) 0.78231(18) 0.0368(4) Uani 1 1 d . . .

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C16 0.0346(10) 0.0345(10) 0.0293(9) 0.0076(7) 0.0052(7) -0.0042(8)
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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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 O2 C7 1.2153(19) . ?
 O3 C13 1.2194(19) . ?
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