Supplementary materials for:

Molecular Recognition and Shape Studies of 3- and 4-Substituted Diarylamide Quasiracemates

Ali K. Brandt[1], Derek J. Boyle[1], Jacob P. Butler[1], Abigail R. Gillingham[1], Scott E. Penner[1], Jacqueline M. Spaniol[2], Alaina K. Stockdill[3], Morgan M. Vanderwall[1], Almat Yeraly[3], Diana R. Schepens[3]* and Kraig A. Wheeler[1]

1 Department of Chemistry, Whitworth University, 300 West Hawthorne Road, Spokane, Washington, 99251, USA.
2 Department of Chemistry, Eastern Illinois University, 600 Lincoln Avenue, Charleston, Illinois, 61920, USA
3 Department of Mathematics and Computer Science, Whitworth University, 300 West Hawthorne Road, Spokane, Washington, 99251, USA.
* Correspondence: dschepens@whitworth.edu (drs); kraigwheeler@whitworth.edu (kaw)

Supplementary Materials

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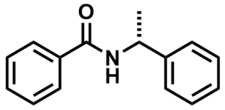
S1. Experimental Details

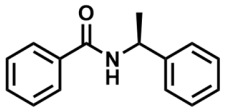
General Considerations: All chemicals and solvents were purchased from Acros Chemicals, the Aldrich Chemical Co., or VWR Scientific and used as received without further purification unless stated otherwise. ^{1}H NMR spectral data were recorded with a 400 MHz JEOL 400SS spectrometer using the Delta software (4.3.6.0). Spectral data are referenced using the solvent residual signal as internal standard and chemical shift values are expressed as δ values (ppm) and the value of coupling constants (*J*) in Hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; dd, doublet of doublets; t, triplet; q, quartet; m, multiplet; and br, broad.



(*R*)-N-(Benzoyl)methylbenzylamine - (*R*)-H

78.1% yield

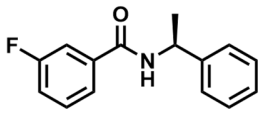
^{1}H NMR ($CDCl_3$): δ 7.80 -7.75 (m, 2H, H-C_{Ar}); 7.53-7.26 (m, 8H, H-C_{AR}); 6.32 (br d, *J* = 6.7 Hz, 1H, N-H); 5.35 (dq, *J* = 6.7 and 7.1 Hz, 1H, C_{sp3}-H); 1.62 (d, *J* = 7.1 Hz, 3H, -CH_3).



(*S*)-N-(Benzoyl)methylbenzylamine - (*S*)-H

75.4% yield

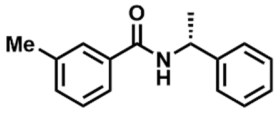
^{1}H NMR ($CDCl_3$): δ 7.81 - 7.75 (m, 2H, H-C_{Ar}); 7.52 - 7.26 (m, 8H, H-C_{Ar}); 6.34 (br d, *J* = 6.8 Hz, 1H, N-H); 5.35 (dq, *J* = 6.8 and 7.0 Hz, 1H, C_{sp3}-H); 1.62 (d, *J* = 7.0 Hz, 3H, H-CH_3).



(*S*)-N- (3-Fluorobenzoyl)methylbenzylamine - (*S*)-3-F

65.3% yield

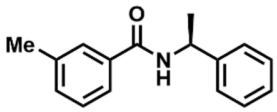
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.44 (m, 2H, C_{Ar}-H); 7.42-7.24 (m, 6H, C_{Ar}-H); 7.22-7.14 (m, 1H, C_{Ar}-H); 6.28 (br d, *J* = 6.6 Hz, 1H, N-H); 5.30 (dq, *J* = 6.6 and 6.9 Hz, 1H, C_{sp3}-H); 1.60 (d, *J* = 6.9 Hz, 3H, CH_3).



(*R*)-N-(3-Methylbenzoyl)methylbenzylamine - (*R*)-3-Me

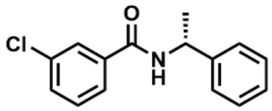
85.5% yield

'H NMR (400 MHz, $CDCl_3$): δ 7.58-7.52 (m, 2H, C_{Ar}-H); 7.40-7.31 (m, 4H, C_{Ar}-H); 7.29-7.27 (m, 3H, C_{Ar}-H); 6.35 (d, *J* = 6.4 Hz, 1H, N-H); 5.33 (dq, *J* = 6.4 and 6.8 Hz, 1H, C_{sp3}-H); 2.41 (s, 3H, CH_3); 1.59 (d, *J* = 6.8 Hz, 3H, CH_3).



(*S*)-N-(2-Methylbenzoyl)methylbenzylamine - (*S*)-3-Me

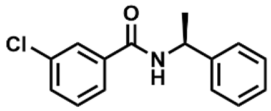
71.8% yield



(*R*)-N-(3-Chlorobenzoyl)methylbenzylamine - (*R*)-3-Cl

48.9% yield

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77-7.58 (m, 2H, C_{Ar}-H); 7.48-7.25 (m, 7H, C_{Ar}-H); 7.52-7.24 (m, 9H, C_{Ar}-H), 6.24 (br d, *J* = 6.6 Hz, 1H, N-H); 5.31 (dq, *J* = 6.6 and 7.1 Hz, 1H, C_{sp3}-H); 1.57 (d, *J* = 7.1 Hz, 3H, CH_3).

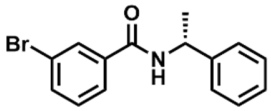


(*S*)-N-(3-Chlorobenzoyl)methylbenzylamine - (*S*)-3-Cl

61.5% yield

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.59 (m, 2H, C_{Ar}-H); 7.48-7.24 (m, 7H, C_{Ar}-H); 7.53-7.24 (m, 9H, C_{Ar}-H); 6.25 (br d, *J* = 6.5 Hz, 1H, N-H); 5.31 (dq, *J* = 6.5 and 7.1 Hz, 1H, C_{sp3}-H); 1.57 (d, *J* = 7.1 Hz, 3H, CH_3).

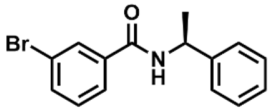
'H NMR (400 MHz, $CDCl_3$): δ 7.58-7.51 (m, 2H, C_{Ar}-H); 7.38-7.25 (m, 4H, C_{Ar}-H); 7.30-7.27 (m, 3H, C_{Ar}-H); 6.34 (br d, *J* = 6.4 Hz, 1H, N-H); 5.32 (dq, *J* = 6.4 and 6.9 Hz, 1H, C_{sp3}-H); 2.40 (s, 3H, CH_3); 1.58 (d, *J* = 6.9 Hz, 3H, CH_3).



(*R*)-N-(3-Bromobenzoyl)methylbenzylamine - (*R*)-3-Br

60.5% yield

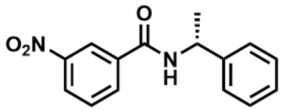
'H NMR (400 MHz, $CDCl_3$): δ 7.83-7.60 (m, 2H, C_{Ar}-H); 7.39-7.17 (m, 7H, C_{Ar}-H); 6.37 (d, *J* = 6.5 Hz, 1H, N-H); 5.28 (dq, *J* = 6.5 and 6.8 Hz, 1H, C_{sp3}-H); 1.57 (d, *J* = 6.8 Hz, 3H, CH_3).



(*S*)-N-(3-Bromobenzoyl)methylbenzylamine - (*S*)-3-Br

72.0% yield

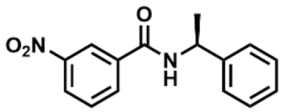
'H NMR (400 MHz, $CDCl_3$): δ 7.84-7.60 (m, 2H, C_{Ar}-H); 7.39-7.19 (m, 7H, C_{Ar}-H); 6.36 (d, *J* = 6.6 Hz, 1H, N-H); 5.27 (dq, *J* = 6.6 and 6.8 Hz, 1H, C_{sp3}-H); 1.58 (d, *J* = 6.8 Hz, 3H, CH_3)



(*R*)-N-(3-Nitrobenzoyl)methylbenzylamine - (*R*)-3-NO_2

88.1 % yield

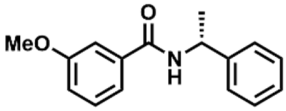
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70 (t, *J* = 1.8 Hz, 1H, C_{Ar}-H); 8.38-8.31 (m, 2H, C_{Ar}-H); 7.75 (t, *J* = 8.2 Hz, 1H, C_{Ar}-H); 7.46-7.18 (m, 5H, C_{Ar}-H); 6.39 (br d, *J* = 6.5 Hz, 1H, N-H); 5.31 (dq, *J* = 6.5 and 7.3 Hz, 1H, C_{sp3}-H); 1.56 (d, *J* = 7.3 Hz, 3H, CH_3).



(*S*)-N-(3-Nitrobenzoyl)methylbenzylamine - (*S*)-3-NO_2

92.4% yield

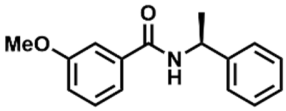
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (t, *J* = 1.7 Hz, 1H, C_{Ar}-H); 8.37-8.31 (m, 2H, C_{Ar}-H); 7.75 (t, *J* = 8.1 Hz, 1H, C_{Ar}-H); 7.45-7.17 (m, 5H, C_{Ar}-H); 6.36 (br d, *J* = 6.4 Hz, 1H, N-H); 5.31 (dq, *J* = 6.4 and 7.2 Hz, 1H, C_{sp3}-H); 1.56 (d, *J* = 7.2 Hz, 3H, CH_3).



(*R*)-N-(3-Methoxybenzoyl)methylbenzylamine - (*R*)-3-OMe

52.7% yield

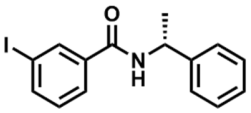
^{1}H NMR ($CDCl_3$): δ 7.43-7.24 (m, 7H, H-C_{Ar}); 6.95-6.88 (m, 2H, H-C_{Ar}); 6.29 (br d, *J* = 6.4 Hz, 1H, N-H); 5.33 (dq, *J* = 6.4 and 6.9 Hz, 1H, C_{sp3}-H); 3.83 (s, 3H, OCH_3); 1.62 (d, *J* = 6.9 Hz, 3H, CH_3).



(*S*)-N-(3-Methoxybenzoyl)methylbenzylamine - (*S*)-3-OMe

43.5% yield

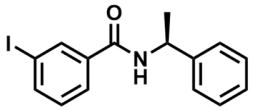
^{1}H NMR ($CDCl_3$): δ 7.44-7.24 (m, 7H, H-C_{Ar}); 6.95-6.87 (m, 2H, H-C_{Ar}); 6.29 (br d, *J* = 6.5 Hz, 1H, N-H); 5.33 (dq, *J* = 6.5 and 6.9 Hz, 1H, C_{sp3}-H); 3.83 (s, 3H, OCH_3); 1.62 (d, *J* = 6.9 Hz, 3H, CH_3).



(*R*)-N-(3-Iodobenzoyl)methylbenzylamine - (*R*)-3-I

68.6% yield

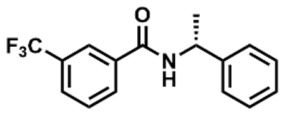
'H NMR (400 MHz, $CDCl_3$): δ 8.07-7.76 (m, 2H, C_{Ar}-H); 7.47-7.11 (m, 7H, C_{Ar}-H); 6.51 (br d, *J* = 6.4 Hz, 1 H, N-H); 5.28 (dq, J = 6.4 and 6.8 Hz, 1H, C_{sp3}-H); 1.57 (d, *J* = 6.8 Hz, 3H, CH_3).



(*S*)-N-(3-Iodobenzoyl)methylbenzylamine - (*S*)-3-I

50.3% yield

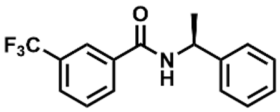
'H NMR (400 MHz, $CDCl_3$): δ 8.08-7.76 (m, 2H, C_{Ar}-H); 7.46-7.10 (m, 7H, C_{Ar}-H); 6.51 (br d, *J* = 6.5 Hz, 1 H, N-H); 5.28 (dq, J = 6.5 and 6.8 Hz, 1H, C_{sp3}-H); 1.57 (d, *J* = 6.8 Hz, 3H, CH_3).



(*R*)-N-(3-Trifluorobenzoyl)methylbenzylamine - (*R*)-3-CF_3

74.0% yield

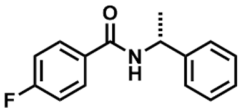
'H NMR (400 MHz, $CDCl_3$): δ 8.02 (s, 1H, C_{Ar}-H); 7.92 (d, *J* = 8.0 Hz, 1H, C_{Ar}-H); 7.70 (d, *J* = 7.2 Hz, 1H, C_{Ar}-H); 7.48 (t, *J* = 7.6 Hz, 1H, C_{Ar}-H); 7.39-7.23 (m, 3H, C_{Ar}-H); 6.38 (br d, *J* = 6.6, 1H, N-H); 5.29 (dq, *J* = 6.6 and 6.8 Hz, 1H, C_{sp3}-H); 1.57 (d, *J* = 6.8, 3H, CH_3).



(*S*)-N-(3-Trifluorobenzoyl)methylbenzylamine - (*S*)-3-CF_3

65.5% yield

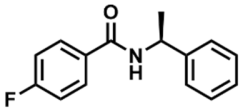
'H NMR (400 MHz, $CDCl_3$): δ 8.01 (s, 1H, C_{Ar}-H); 7.92 (d, *J* = 7.2 Hz, 1H, C_{Ar}-H); 7.72 (d, *J* = 7.2 Hz, 1H, C_{Ar}-H); 7.51 (d, *J* = 7.8 Hz, 1H, C_{Ar}-H); 7.46-7.22 (m, 3H, C_{Ar}-H); 6.59 (br d, *J* = 6.5 Hz, 1H, N-H); 5.31 (dq, *J* = 6.5 and 6.8 Hz, 1H, C_{sp3}-H); 1.59 (d, *J* = 6.8 Hz, 1H, CH_3).



(*R*)-N-(4-Fluorobenzoyl)methylbenzylamine - (*R*)-4-F

60.0% yield

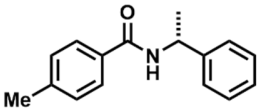
^{1}H NMR ($CDCl_3$): δ 7.81 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 7.45-7.30 (m, 5H, H-C_{Ar}); 7.13 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 6.38 (br d, *J* = 7.1 Hz, 1H, N-H); 5.35 (dq, *J* = 6.8 and 7.1 Hz, 1H, C_{sp3}-H); 1.64 (d, *J* = 6.8 Hz, 3H, CH_3).



(*S*)-N-(4-Fluorobenzoyl)methylbenzylamine - (*S*)-4-F

45.3% yield

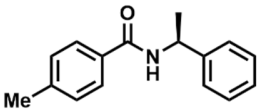
^{1}H NMR ($CDCl_3$): δ 7.80 (d, *J* = 8.3Hz, 2H, H-C_{Ar}); 7.43-7.29 (m, 5H, H-C_{Ar}); 7.12 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 6.37 (br d, *J* = 7.0 Hz, 1H, N-H); 5.35 (dq, *J* = 6.8 and 7.0 Hz, 1H, C_{sp3}-H); 1.64 (d, *J* = 6.8 Hz, 3H, CH_3).



(*R*)-N-(4-Methylbenzoyl)methylbenzylamine - (*R*)-4-Me

33.0% yield

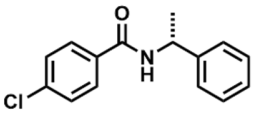
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.4 Hz, 2H, C_{Ar}-H), 7.43-7.25 (m, 7H, C_{Ar}-H); 6.30 (br d, *J* = 6.6 Hz, 1H, N-H); 5.31 (dq, *J* = 6.6 and 7.0 Hz, 1H, C_{sp3}-H), 2.40 (s, 3H, CH_3); 1.27 (d, *J* = 7.0 Hz, 3H, CH_3).



(*S*)-N-(4-Methylbenzoyl)methylbenzylamine - (*S*)-4-Me

56.9% yield

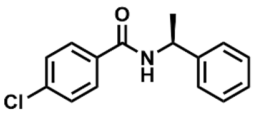
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.4 Hz, 2H, C_{Ar}-H), 7.44-7.23 (m, 7H, C_{Ar}-H); 6.31 (br d, *J* = 6.6 Hz, 1H, N-H); 5.32 (dq, *J* = 6.6 and 6.9 Hz, 1H, C_{sp3}-H), 2.40 (s, 3H, CH_3); 1.27 (d, *J* = 6.9 Hz, 3H, CH_3).



(*R*)-N-(4-Chlorobenzoyl)methylbenzylamine - (*R*)-4-Cl

77.0% yield

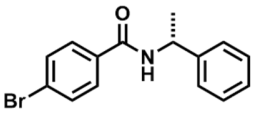
^{1}H NMR ($CDCl_3$): δ 7.71 (d, *J* = 8.6, 2H, H-C_{Ar}); 7.72-7.26 (m, 7H, H-C_{Ar}); 6.35 (br d, *J* = 6.5 Hz, 1H, N-H); 5.32 (dq, *J* = 6.5 and 6.8 Hz, 1H, C_{sp3}-H); 1.62 (d, *J* = 6.8 Hz, 3H, CH_3).



(*S*)-N-(4-Chlorobenzoyl)methylbenzylamine - (*S*)-4-Cl

67.4% yield

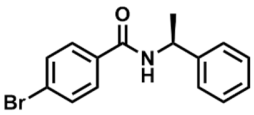
^{1}H NMR ($CDCl_3$): δ 7.71 (d, *J* = 8.6, 2H, H-C_{AR}); 7.51-7.37 (m, 7H, H-C_{Ar}); 6.32 (br d, *J* = 6.5 Hz, 1H, N-H); 5.34 (dq, *J* = 6.5 and 6.9 Hz, 1H, C_{sp3}-H); 1.62 (d, *J* = 6.9 Hz, 3H, CH_3).



(*R*)-N-(4-Bromobenzoyl)methylbenzylamine - (*R*)-4-Br

60.7% yield

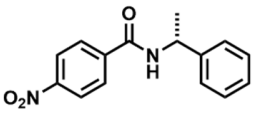
^{1}H NMR ($CDCl_3$): δ 7.60 (d, *J* = 8.6 Hz, 2H, H-C_{Ar}); 7.56 (d, *J* = 8.6 Hz, 2H, H-C_{Ar}); 7.38-7.36 (m, 5H, H-C_{Ar}); 6.34 (br d, *J* = 6.4 Hz, 1H, N-H); 5.32 (dq, *J* = 6.4 and 7.1 Hz, 1H, C_{sp3}-H); 1.62 (d, *J* = 7.1 Hz, 3H, CH_3).



(*S*)-N-(4-Bromobenzoyl)methylbenzylamine - (*S*)-4-Br

72.4% yield

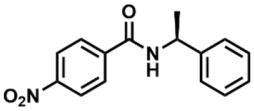
^{1}H NMR ($CDCl_3$): 7.61 (d, *J* = 8.6 Hz, 2H, H-C_{Ar}); 7.56 (d, *J* = 8.6 Hz, 2H, H-C_{Ar}); 7.38-7.34 (m, 5H, H-C_{Ar}); 6.33 (br d, *J* = 6.3 Hz, 1H, N-H); 5.32 (dq, *J* = 6.3 and 7.0 Hz, 1H, C_{sp3}-H); 1.61 (d, *J* = 7.0 Hz, 3H, CH_3).



(*R*)-N-(4-Nitrobenzoyl)methylbenzylamine - (*R*)-4-NO_2

72.9% yield

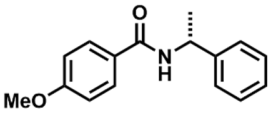
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (d, *J* = 8.5 Hz, 2H, C_{Ar}-H); 8.02 (d, *J* = 8.5 Hz, 2H, C_{Ar}-H); 7.45-7.21 (m, 5H, C_{Ar}-H); 6.39 (br d, *J* = 6.6 Hz, 1H, N-H); 5.35 (dq, *J* = 6.6 and 6.8 Hz, 1H, C_{sp3}-H), 1.66 (d, *J* = 6.8 Hz, 3H, CH_3).



(*S*)-N-(4-Nitrobenzoyl)methylbenzylamine - (*S*)-4-NO_2

84.0% yield

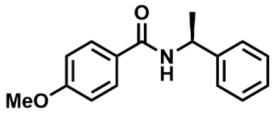
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54 (d, *J* = 8.4 Hz, 2H, C_{Ar}-H); 8.02 (d, *J* = 8.4 Hz, 2H, C_{Ar}-H); 7.45-7.20 (m, 5H, C_{Ar}-H); 6.38 (br d, *J* = 6.5 Hz, 1H, N-H); 5.35 (dq, *J* = 6.5 and 6.8 Hz, 1H, C_{sp3}-H), 1.65 (d, *J* = 6.8 Hz, 3H, CH_3).



(*R*)-N-(4-Methoxybenzoyl)methylbenzylamine - (*R*)-4-OMe

50.3% yield

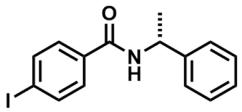
^{1}H NMR ($CDCl_3$): δ 7.75 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 7.41-7.28 (m, 5H, H-C_{Ar}); 6.92 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 6.34 (br d, *J* = 6.5 Hz, 1H, N-H); 5.33 (dq, *J* = 6.5 and 6.9 Hz, 1H, C_{sp3}-H); 3.84 (s, 3H, OCH_3) 1.62 (d, *J* = 6.9 Hz, 3H, CH_3).



(*S*)-N-(4-Methoxybenzoyl)methylbenzylamine - (*S*)-4-OMe

38.2% yield

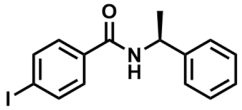
^{1}H NMR ($CDCl_3$): δ 7.74 (d, *J* = 8.7 Hz, 2H, H-C_{Ar}); 7.40 - 7.28 (m, 5H, H-C_{Ar}); 6.92 (d, *J* = 8.7 Hz, 2H, H-C_{Ar}); 6.36 (br d, *J* = 6.5 Hz, 1H, N-H); 5.33 (dq, *J* = 6.5 and 6.9 Hz, 1H, C_{sp3}-H); 3.85 (s, 3H, OCH_3) 1.62 (d, *J* = 6.9 Hz, 3H, CH_3).



(*R*)-N-(4-Iodobenzoyl)methylbenzylamine - (*R*)-4-I

62.9% yield

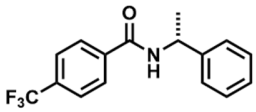
^{1}H NMR ($CDCl_3$): δ 7.80 (d, *J* = 8.3 Hz, 2H, H-C_{Ar}); 7.52 (d, *J* = 8.3 Hz, 2H, H-C_{Ar}); 7.41-7.30 (m, 5H, H-C_{Ar}); 6.32 (br d, *J* = 6.4 Hz, 1H, N-H); 5.34 (dq, *J* = 6.4 and 7.0 Hz, 1H, C_{sp3}-H); 1.65 (d, *J* = 7.0 Hz, 3H, H-CH_3).



(*S*)-N-(4-Iodobenzoyl)methylbenzylamine - (*S*)-4-I

55.1% yield

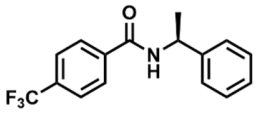
^{1}H NMR ($CDCl_3$): δ 7.81 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 7.51 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 7.44–7.29 (m, 5H, H-C_{Ar}); 6.38 (br d, *J* = 6.5 Hz, 1H, N-H); 5.35 (dq, *J* = 6.5 and 7.1 Hz, 1H, C_{sp3}-H); 1.64 (d, *J* = 7.1 Hz, 3H, CH_3).



(*R*)-N-(4-Trifluoromethylbenzoyl)methylbenzylamine - (*R*)-4-CF_3

87.0% yield

^{1}H NMR ($CDCl_3$): δ 7.90 (d, *J* = 8.3 Hz, 2H, H-C_{Ar}); 7.72 (d, *J* = 8.3 Hz, 2H, H-C_{Ar}); 7.44-7.31 (m, 5H, H-C_{Ar}); 6.35 (br d, *J* = 6.5 Hz, 1H, N-H); 5.37 (dq, *J* = 6.5 and 7.0 Hz, 1H, C_{sp3}-H); 1.66 (d, *J* = 7.0 Hz, 3H, CH_3).



(*S*)-N-(4-Trifluoromethylbenzoyl)methylbenzylamine - (*S*)-4-CF_3

74.8% yield

^{1}H NMR ($CDCl_3$): δ 7.91 (d, *J* = 8.4 Hz, 2H, H-C_{Ar}); 7.71 (d, *J* = 8.5 Hz, 2H, H-C_{Ar}); 7.45-7.31 (m, 5H, H-C_{Ar}); 6.36 (br d, *J* = 6.6 Hz, 1H, N-H); 5.35 (dq, *J* = 6.6 and 7.1 Hz, 1H, C_{sp3}-H); 1.65 (d, *J* = 7.1 Hz, 3H, CH_3).

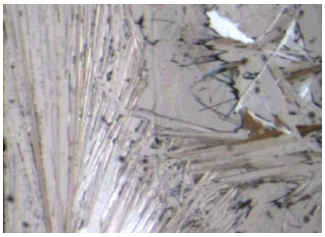
S2. Hot-Stage Microscopy

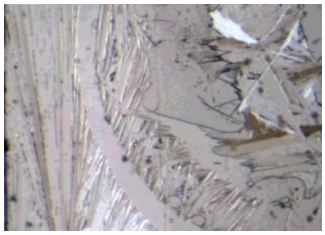
Hot-Stage Images of Racemic and Quasiracemic Pairs – 3-substituted diarylamides

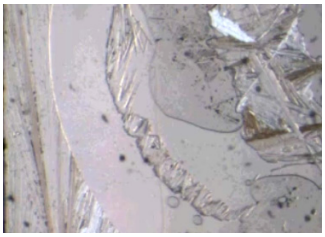
Racemic Mixtures

(*R*)-H (left)

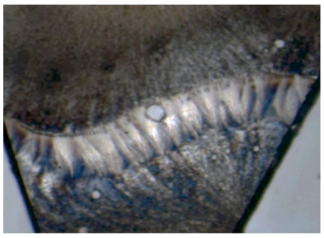
(*S*)-H (right)

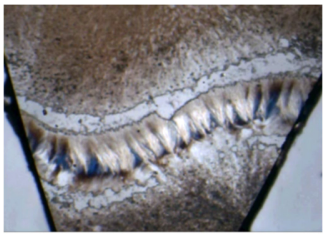

116.0°

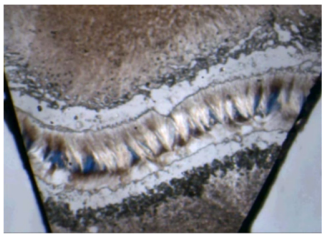

120.9°


126.1°

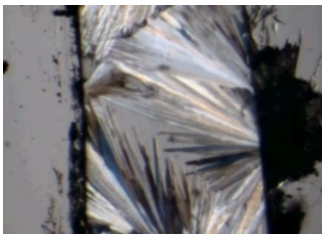
(*R*)-3-F
(*S*)-3-F

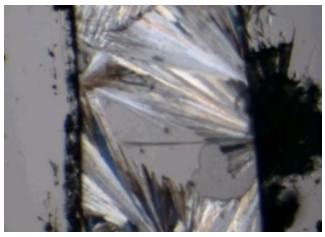

254.2°

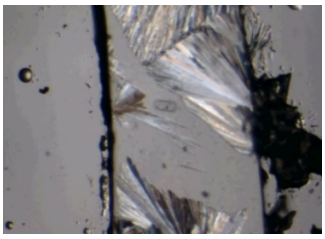

159.1°


163.3°

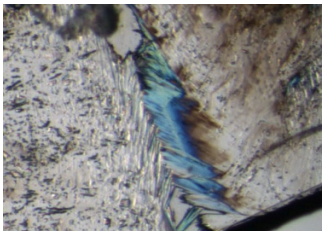
(*R*)-3-Me
(*S*)-3-Me

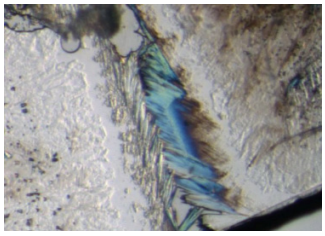

83.9°

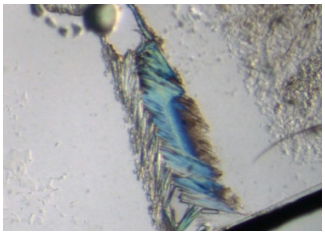

89.3°


105.3°

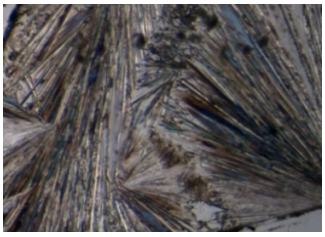
(*R*)-3-Cl
(*S*)-3-Cl

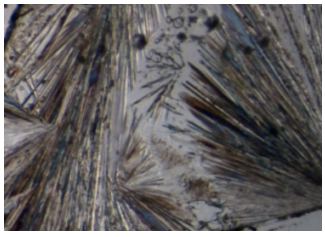

90.0°

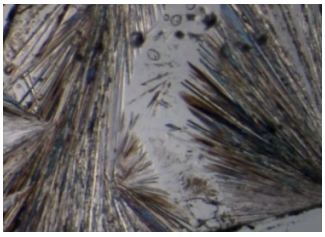

97.6°


101.7°

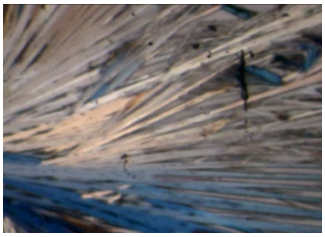
(*R*)-3-Br
(*S*)-3-Br

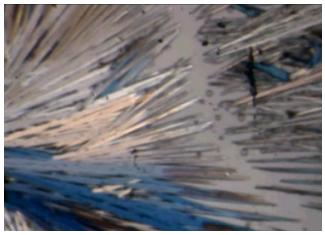

80.5°

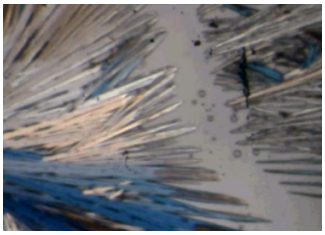

84.3°


85.5°

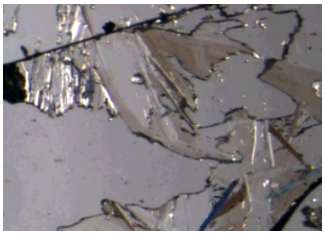
(*R*)-3-NO_2
(*S*)-3-NO_2

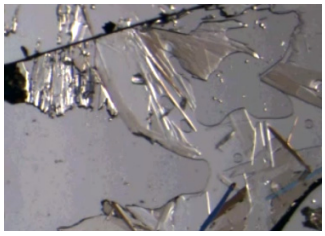

124.4°

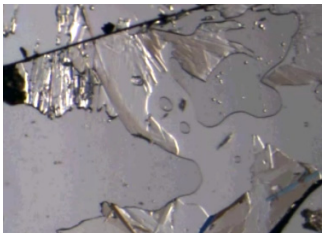

141.2°


145.0°

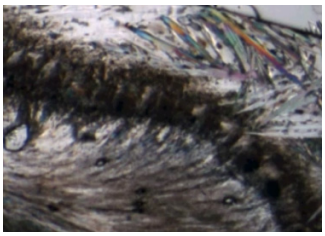
(*R*)-3-OMe
(*S*)-3-OMe

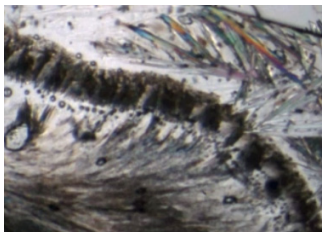

117.0°

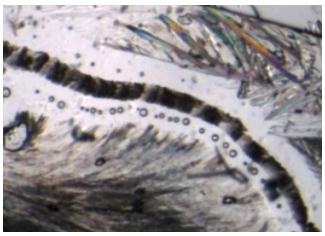

120.4°


134.2°

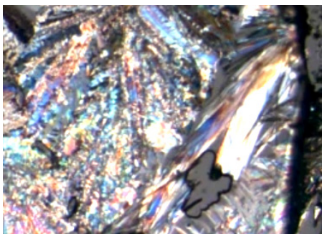
(*R*)-3-I
(*S*)-3-I

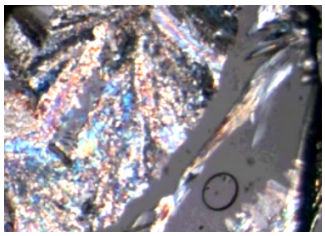

122.5°

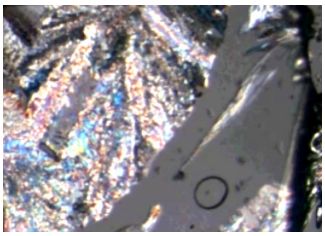

128.6°


132.4°

(*R*)-3-CF_3
(*S*)-3-CF_3


107.2°


130.1°

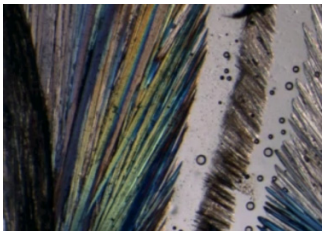

135.2°

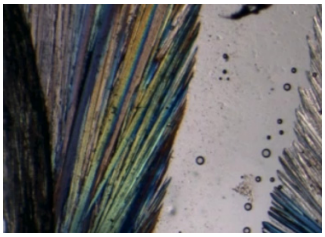
3-Hydrogen

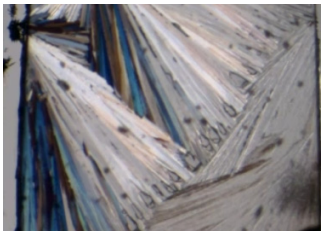
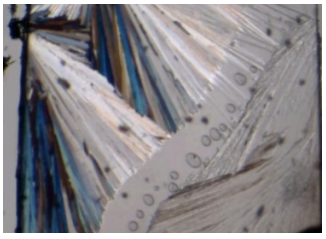
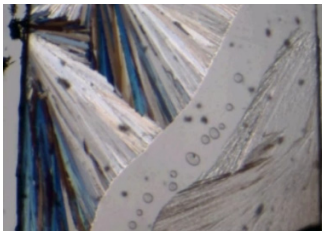
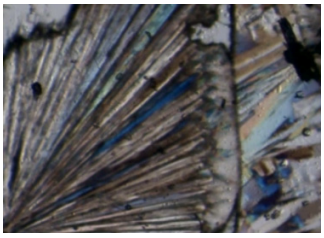
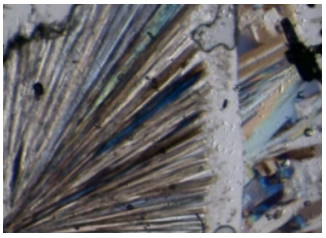
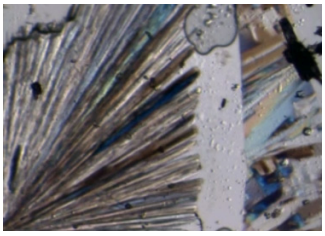
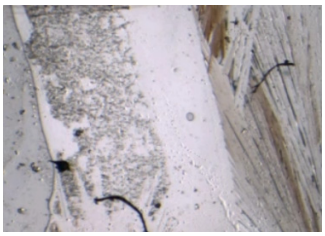
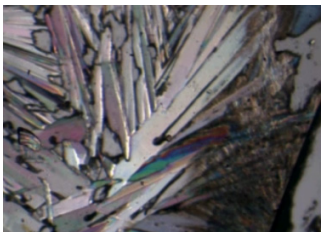
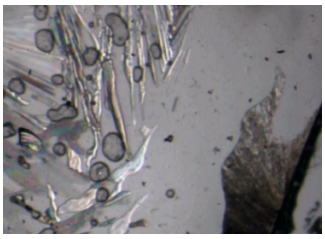
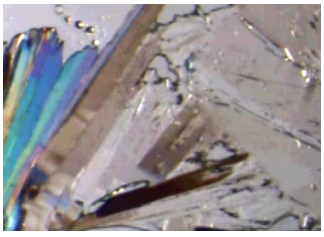
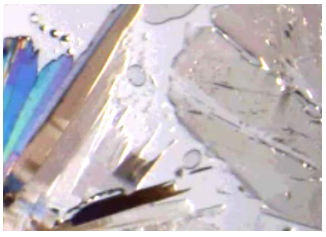
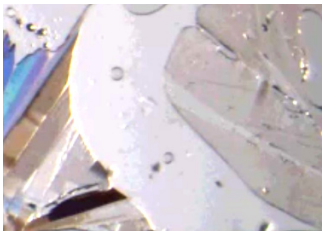
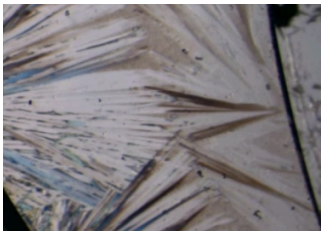
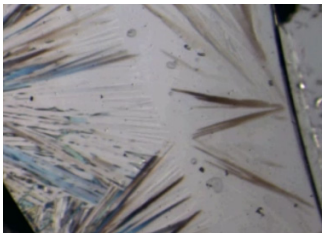
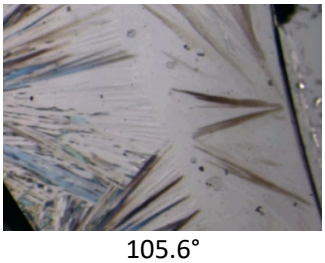
(*R*)-H
(left)

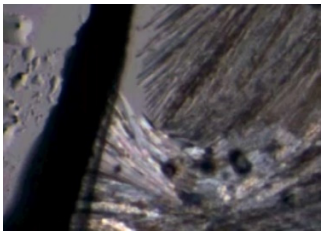
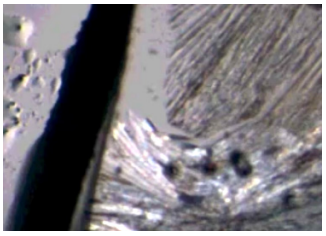
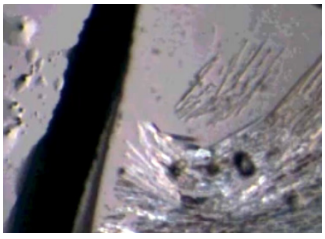
(*S*)-3-F
(right)


101.1°

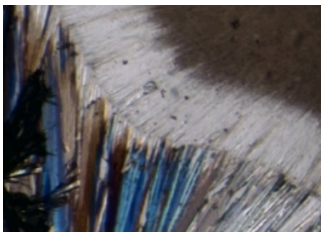
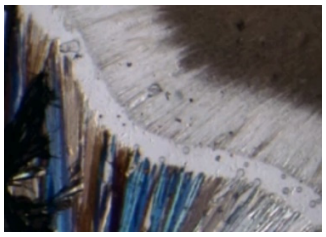
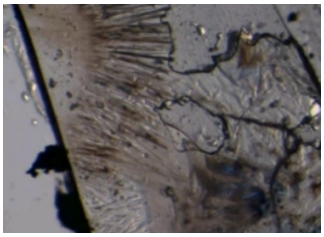
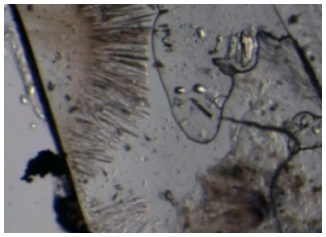
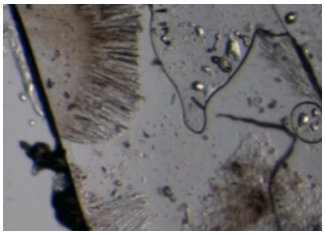
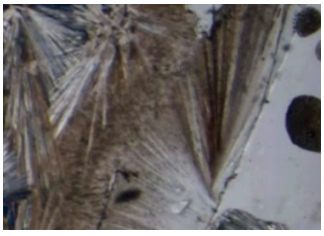
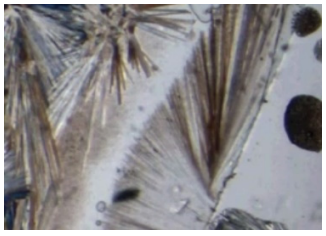
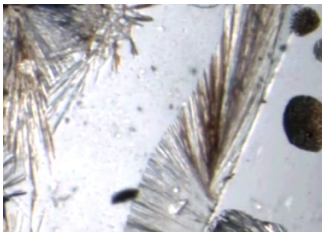
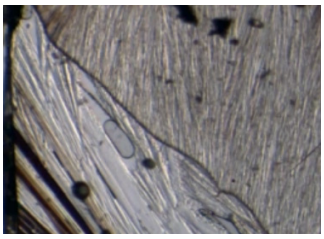
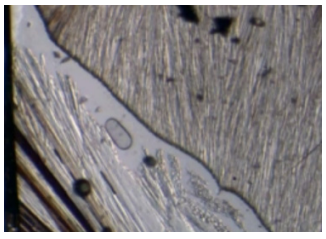
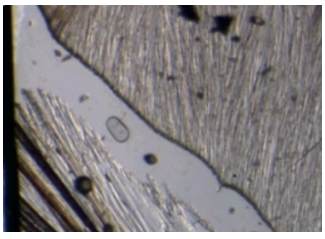

116.1°


118.4°

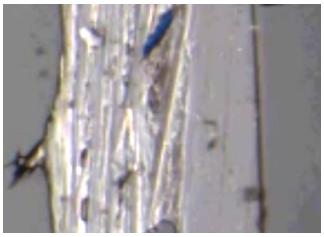
(*R*)-3-Me (*S*)-H	 96.1°	 102.0°	 105.7°
(*R*)-3-Cl (*S*)-3-H	 56.2°	 82.7°	 93.2°
(*R*)-H (*S*)-3-Br	 85.7°	 97.9°	 102.4°
(*R*)-H (*S*)-3-NO_2	 116.4°	 127.3°	 139.0°
(*R*)-H (*S*)-3-OMe	 101.4°	 111.5°	 113.6°
(*R*)-3-I (*S*)-H	 95.5°	 105.1°	 105.6°

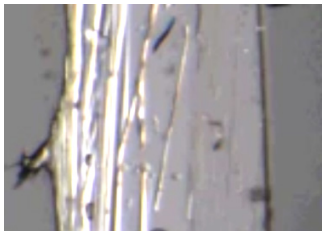
(*S*)-H (*R*)-3-CF_3	 105.3°	 112.1°	 116.6°

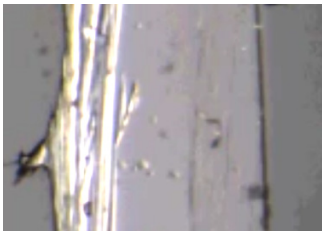
3-Fluoro

(*R*)-3-Me (*S*)-3-F	 97.0°	 101.3°	 112.0°
(*R*)-3-F (*S*)-3-Cl	 77.3°	 90.4°	 94.5°
(*R*)-3-Br (*S*)-3-F	 60.7°	 76.5°	 102.3°
(*R*)-3-F (*S*)-3-NO_2	 118.8°	 124.7°	 127.9°

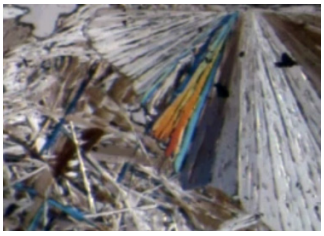
(*R*)-3-OMe
(*S*)-3-F

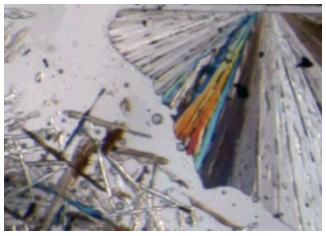

106.4°

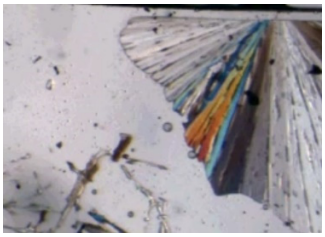

110.0°


114.5°

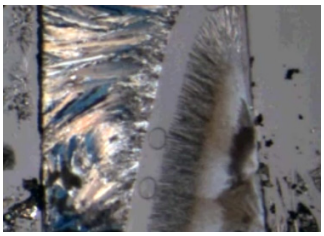
(*R*)-3-I
(*S*)-3-F

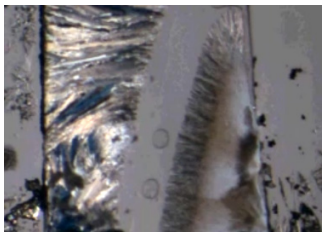

104.8°

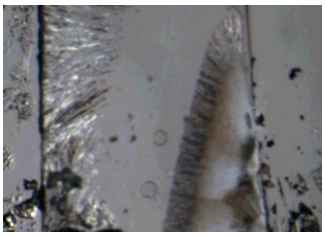

126.7°


130.2°

(*S*)-3-CF_3
(*R*)-3-F

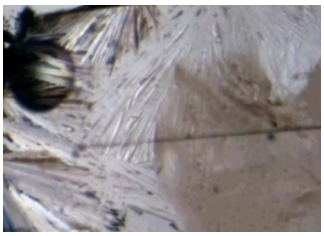

80.3°

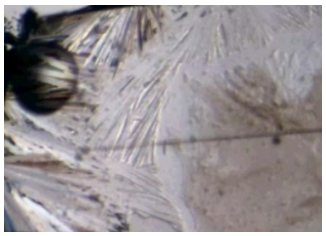

96.7°

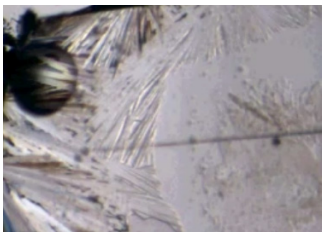

102.0°

3-Methyl

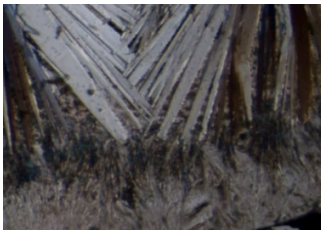
(*R*)-3-Me
(*S*)-3-Cl

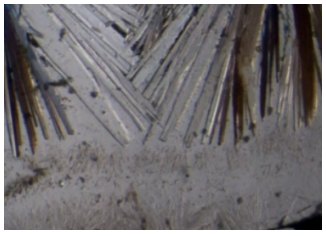

89.3°

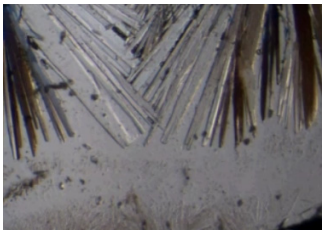

95.1°


98.3°

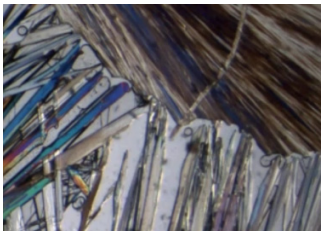
(*R*)-3-Br
(*S*)-3-Me

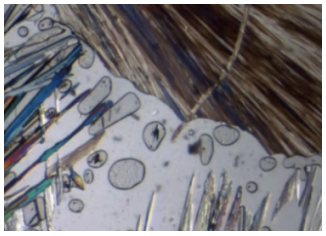

62.8°

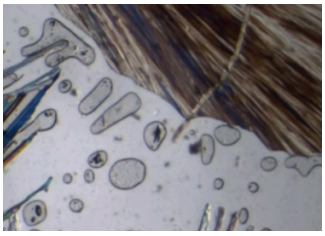

84.5°


85.0°

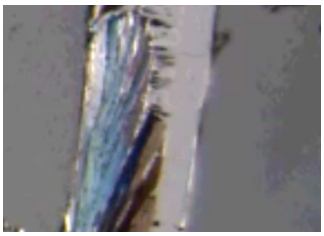
(*R*)-3-Me
(*S*)-3-NO_2

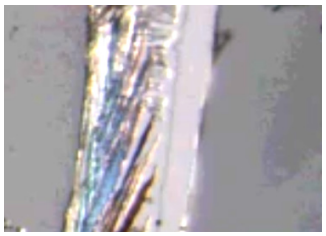

88.6°

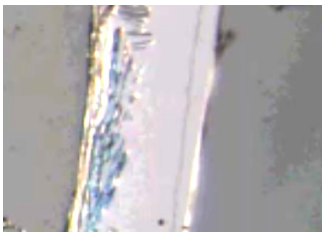

104.6°


110.2°

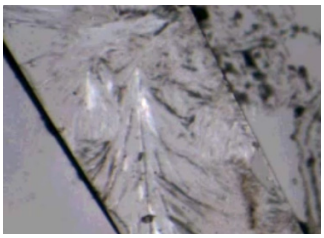
(*R*)-3-OMe
(*S*)-3-Me

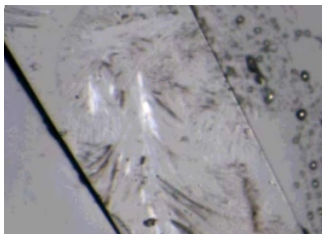

90.2°

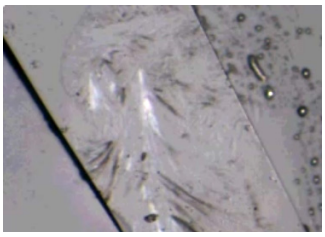

105.3°


106.8°

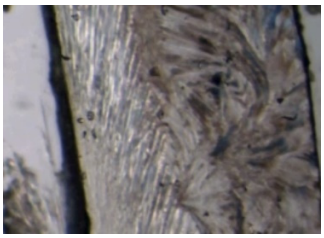
(*R*)-3-Me
(*S*)-3-I

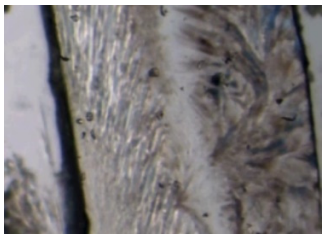

85.4°

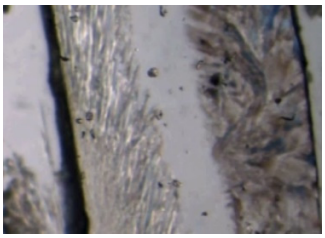

102.2°


108.1°

(*R*)-3-Me
(*S*)-3-CF_3

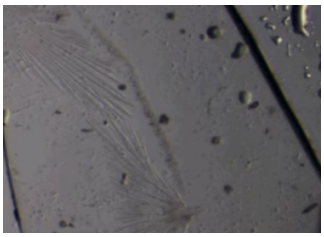

81.7°

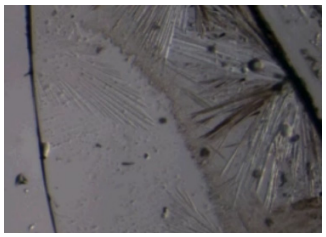

84.4°

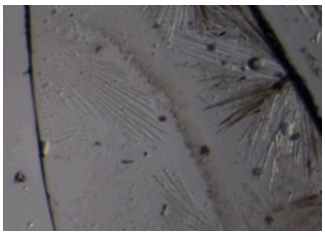

89.1°

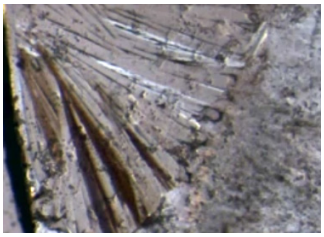
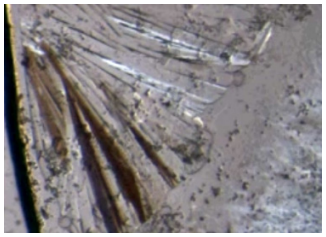
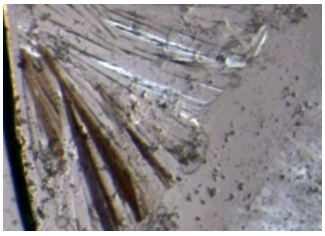
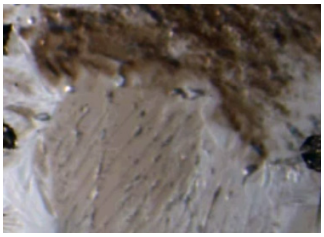
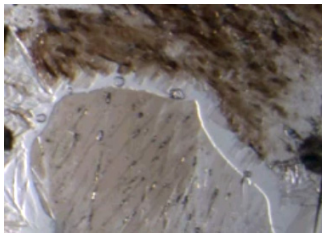
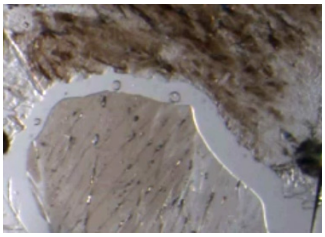
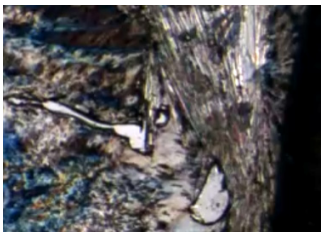
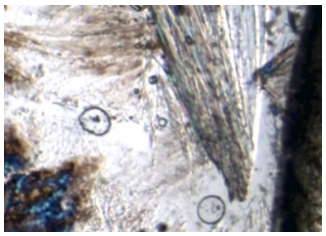
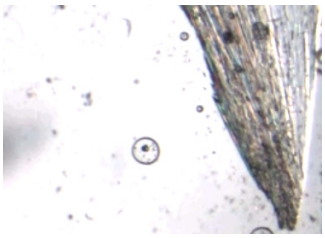
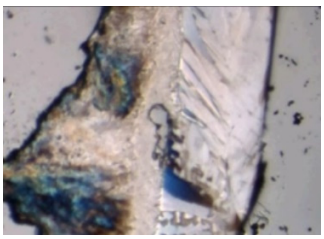
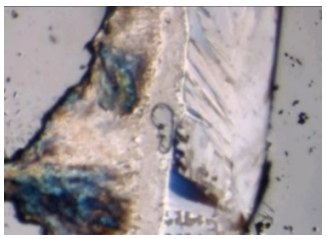
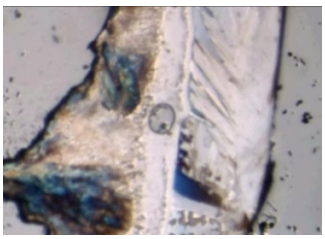
3-Chloro

(*R*)-3-Cl
(*S*)-3-Br

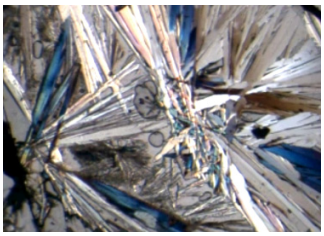
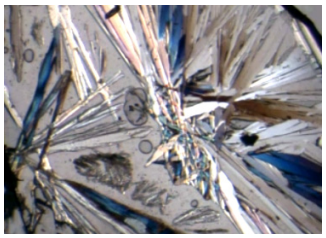
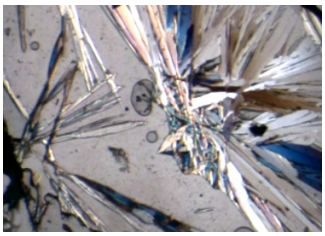

84.1°


91.2°

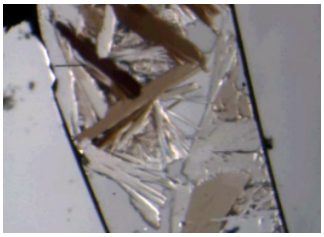

101.8°

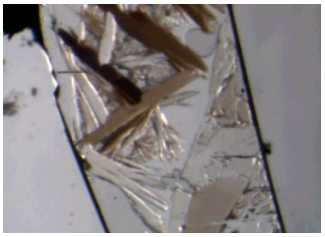
(*R*)-3-NO_2 (*S*)-3-Cl	 84.9°	 95.7°	 97.4°
(*R*)-3-Cl (*S*)-3-OMe	 69.2°	 90.5°	 96.0°
(*R*)-3-Cl (*S*)-3-I	 75.2°	 95.4°	 120.3°
(*R*)-3-Cl (*S*)-3-CF_3	 73.6°	 78.2°	 80.5°

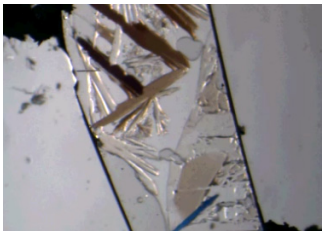
3-Bromo

(*R*)-3-NO_2 (*S*)-3-Br	 105.0°	 112.2°	 118.1°

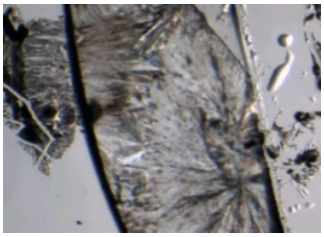
(*R*)-3-Br
(*S*)-3-OMe

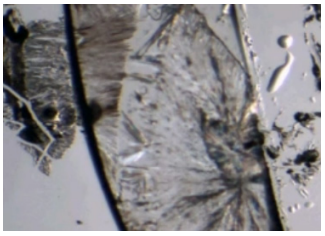

95.3°

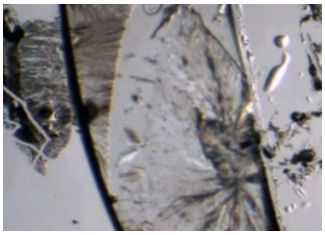

101.4°


107.1°

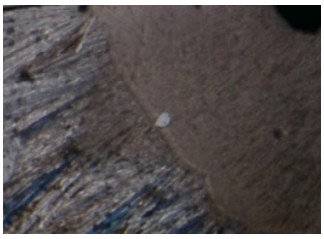
(*R*)-3-Br
(*S*)-3-I

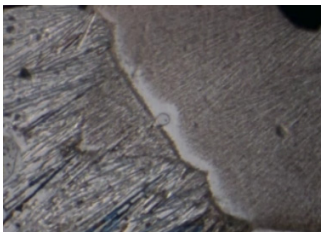

88.5°

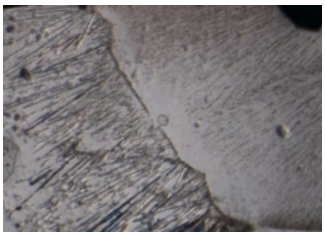

98.7°


104.3°

(*S*)-3-Br
(*R*)-3-CF_3

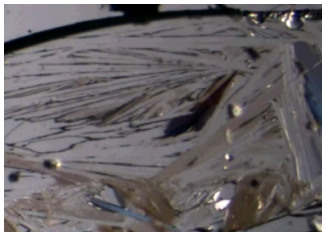

113.5°

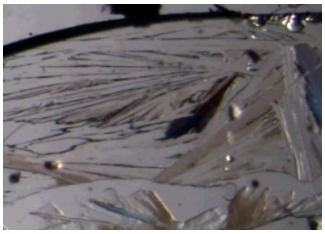

117.2°

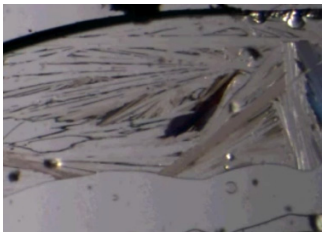

118.1°

3-Nitro

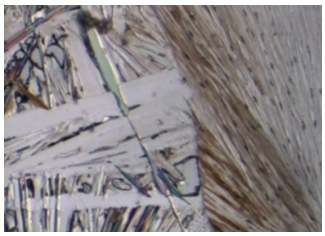
(*R*)-3-NO_2
(*S*)-3-OMe


70.5°

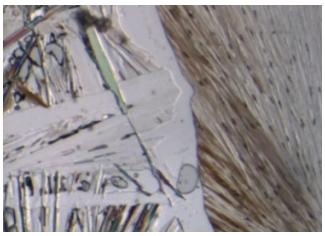

98.0°


100.3°

(*R*)-3-NO_2
(*S*)-3-I

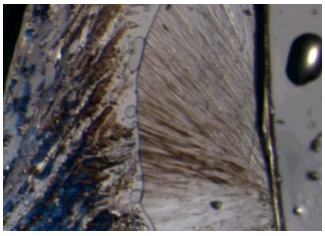

121.1°

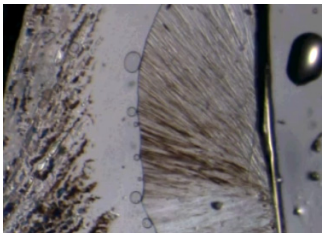

127.8°


131.3°

(*R*)-3-CF_3
(*S*)-3-NO_2

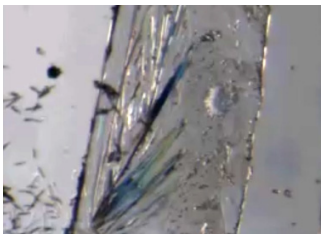

80.6°

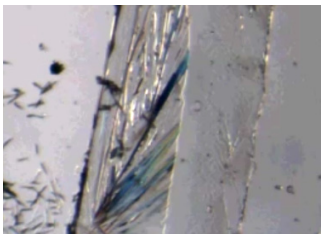

94.8°

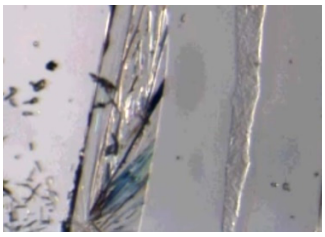

99.6°

3-Methoxy

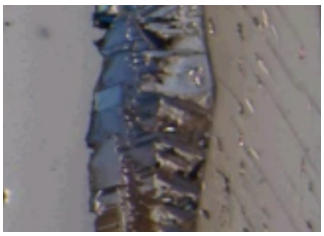
(*R*)-3-I
(*S*)-3-OMe

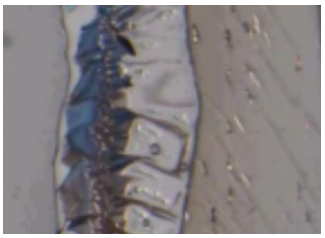

104.8°

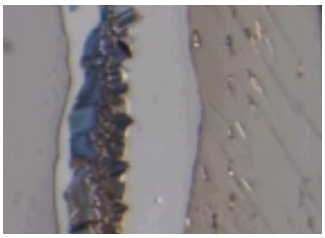

122.9°


135.0°

(*R*)-3-CF_3
(*S*)-3-OMe

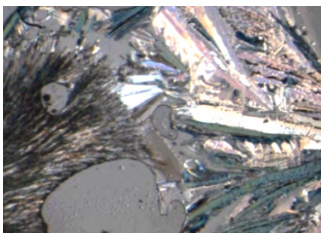

87.1°

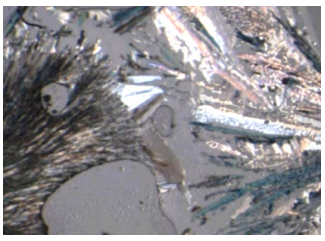

89.4°

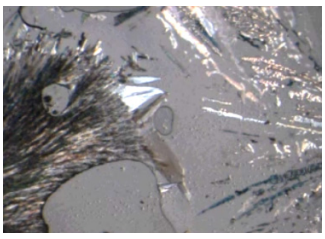

93.5°

3-Iodo

(*R*)-3-I
(*S*)-3-CF_3


87.2°


93.8°

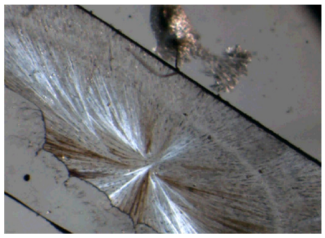

97.6°

Hot-Stage Images of Racemic and Quasiracemic Pairs – 4-substituted diarylamides

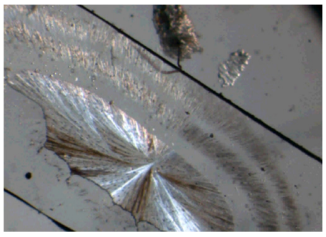
Racemic Mixtures

(*S*)-H (left)

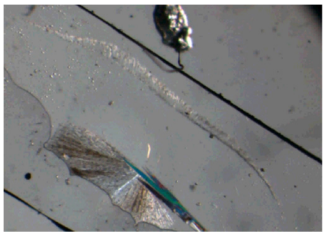
(*R*)-H (right)



108.5°

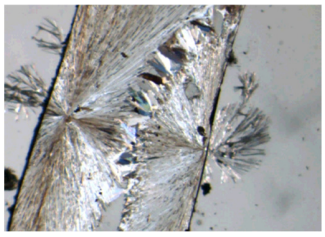


119.8°

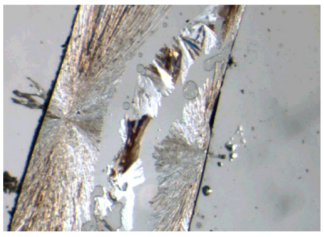


127.8°

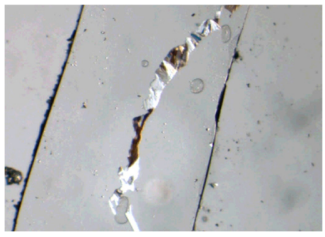
(*S*)-4-F
(*R*)-4-F



99.9°



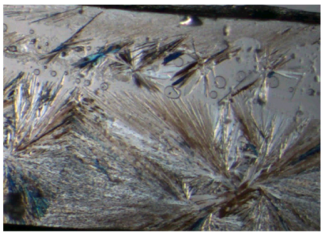
124.8°



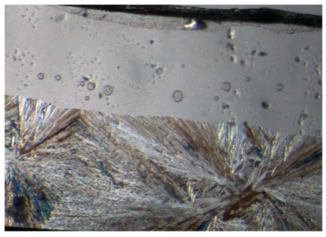
132.5°

(*R*)-4-Me
(*S*)-4-Me

103.3°

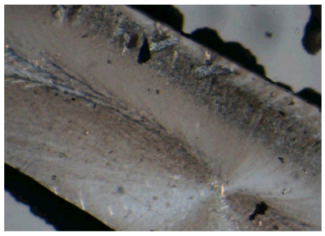


125.8°

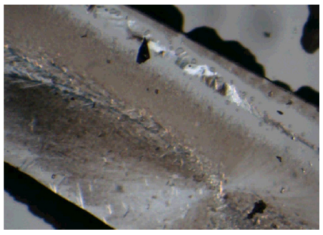


132.0°

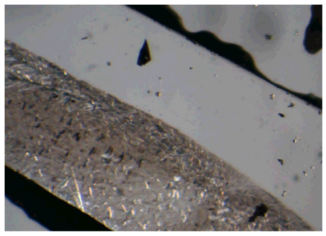
(*S*)-4-Cl
(*R*)-4-Cl



126.2°

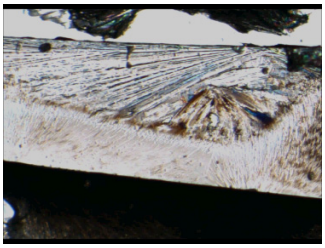


139.2°

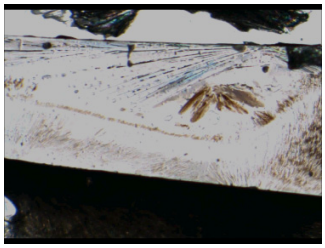


151.3°

(*R*)-4-Br
(*S*)-4-Br



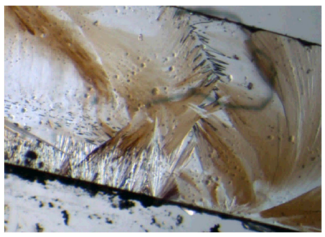
136.3°

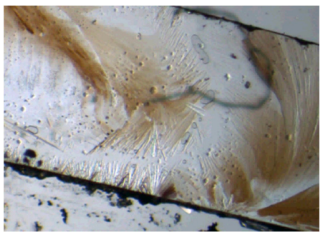


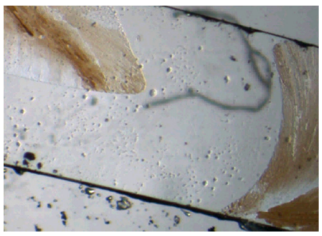
151.1°

169.1°

(*R*)-4-NO_2
(*S*)-4-NO_2


106.9°

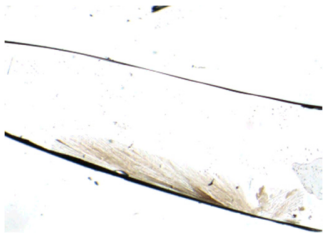

113.1°


142.0°

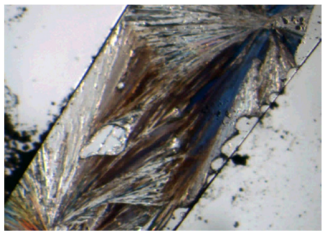
(*S*)-4-OMe
(*R*)-4-OMe

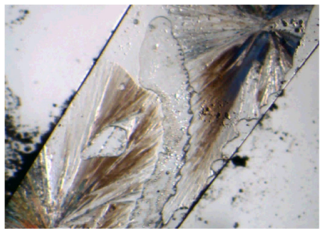

141.6°

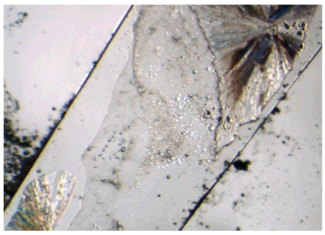

150.7°


156.3°

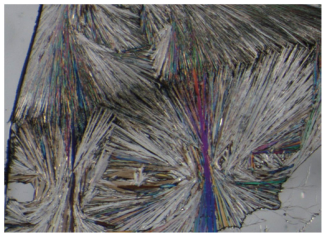
(*R*)-4-I
(*S*)-4-I

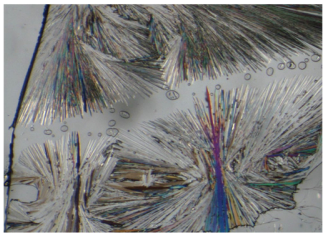

196.6°

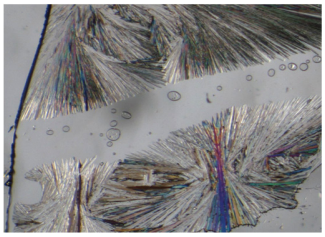

213.7°


229.7°

(*R*)-4-CF_3
(*S*)-4-CF_3


134.8°

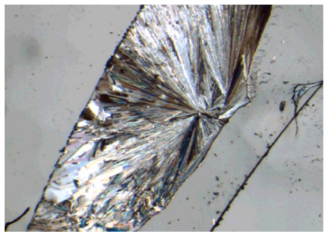

137.3°

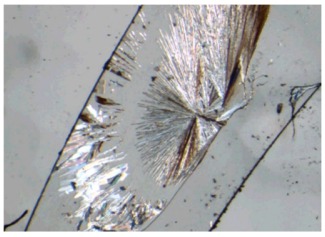

138.8°

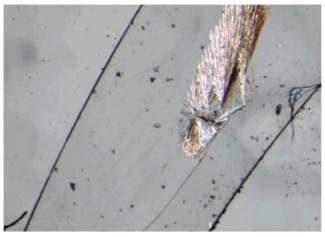
4-Hydrogen

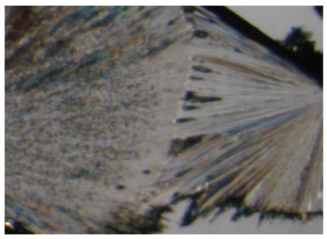
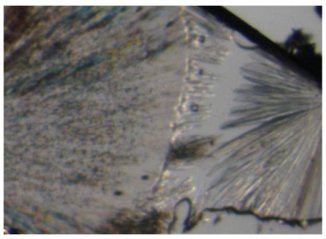
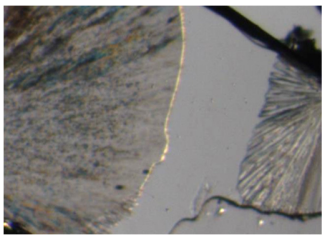
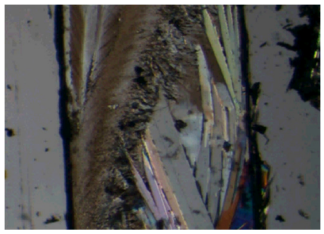
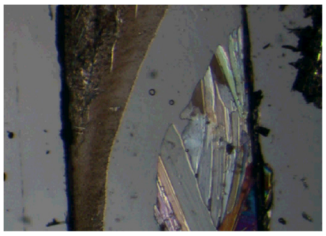
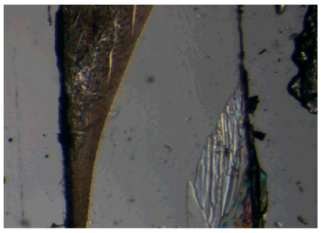
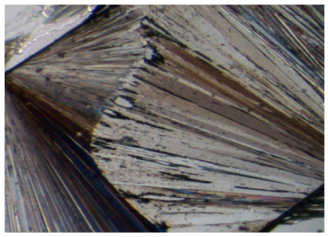
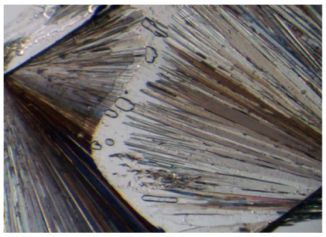
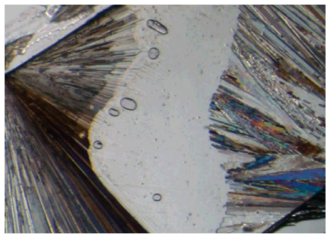
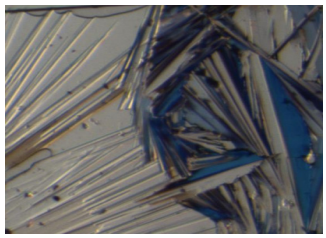
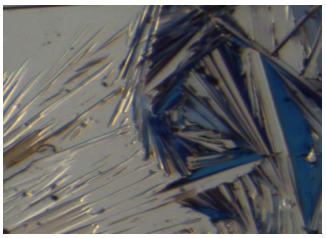
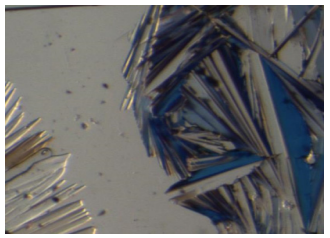
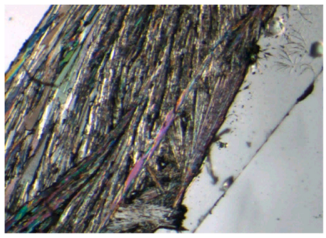
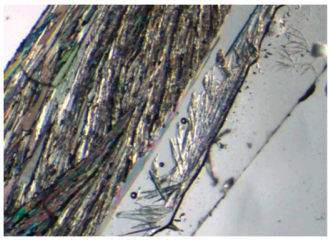
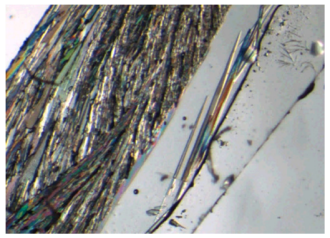
(*S*)-H
(left)

(*R*)-4-F
(right)

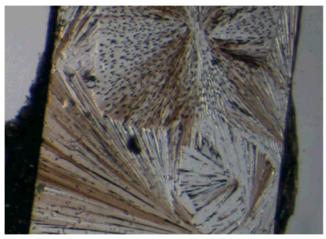

98.3°

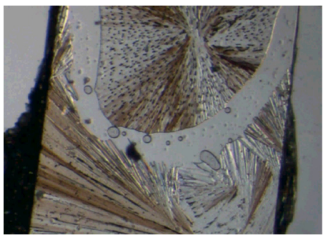

112.8°

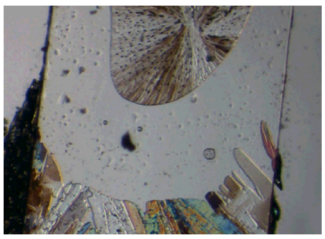

122.3°

(*R*)-H (*S*)-4-Me			
	101.1°	107.2°	111.8°
(*S*)-4-Cl (*R*)-H			
	89.6°	110.3°	123.8°
(*R*)-H (*S*)-4-Br			
	107.7°	119.5°	136.3°
(*S*)-H (*R*)-4-NO_2			
	96.3°	101.4°	104.2°
(*S*)-H (*R*)-4-OMe			
	102.5°	116.9°	121.1°
(*R*)-H (*S*)-4-I			
	117.7°	132.2°	138.3°

(*S*)-H
(*R*)-4-CF_3

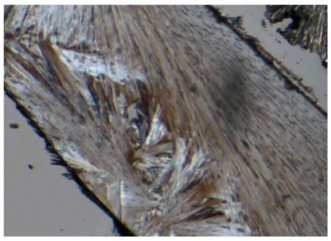

102.5°

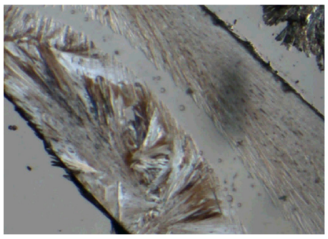

120.8°

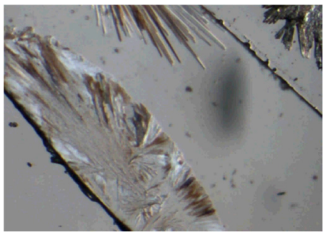

131.1°

3-Fluoro

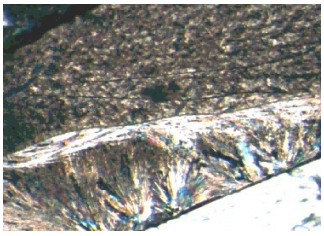
(*S*)-4-Me
(*R*)-4-F


99.6°

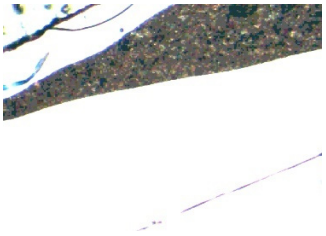

117.5°


126.7°

(*S*)-4-Cl
(*R*)-4-F

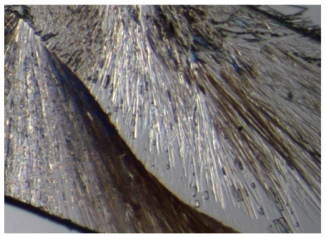

50.8°

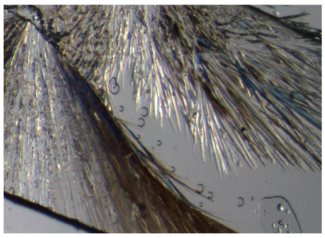

71.5°


94.4°

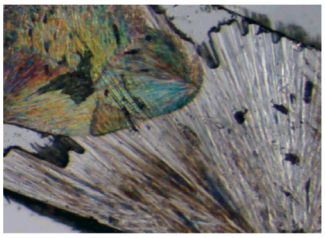
(*S*)-4-Br
(*R*)-4-F

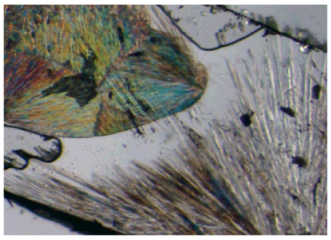

105.5°

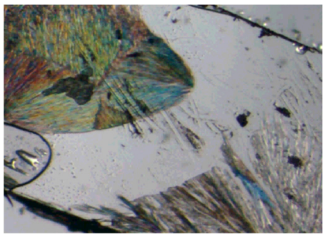

114.7°


119.4°

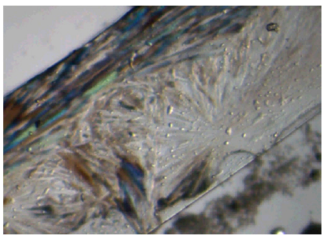
(*S*)-4-NO_2
(*R*)-4-F


80.2°

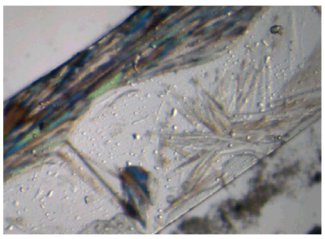

96.4°


119.8°

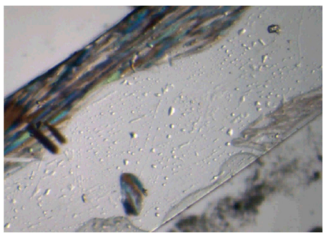
(*S*)-4-OMe
(*R*)-4-F



94.2°

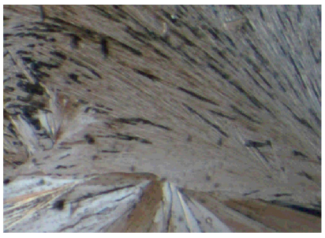


111.8°

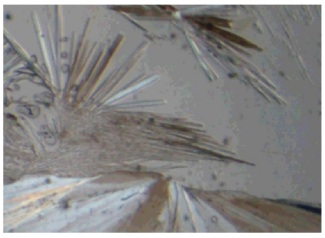


125.7°

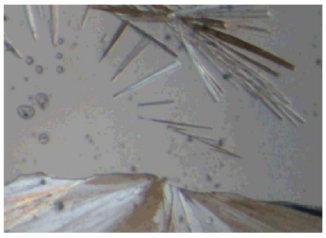
(*S*)-4-I
(*R*)-4-F



99.5°

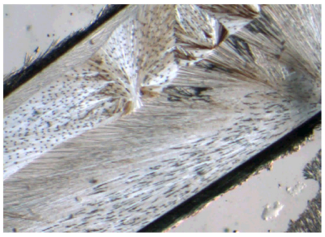


119.5°

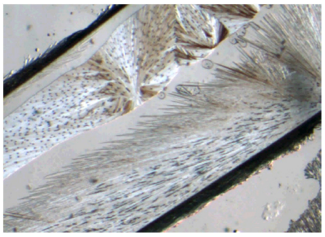


125.9°

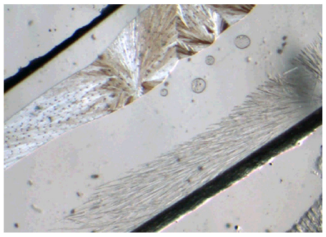
(*S*)-4-CF_3
(*R*)-4-F



97.3°



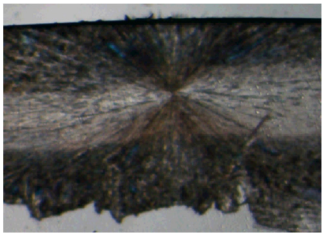
109.1°



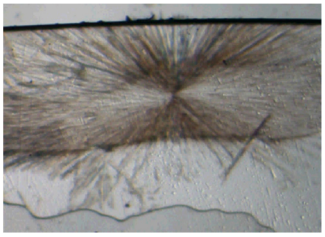
121.2°

4-Methyl

(*S*)-4-Cl
(*R*)-4-Me



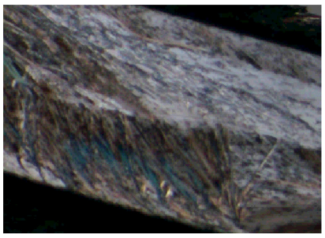
99.8°



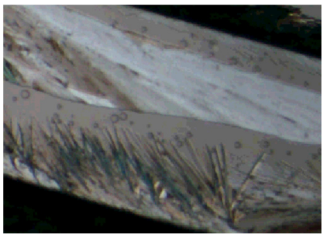
119.1°

140.7°

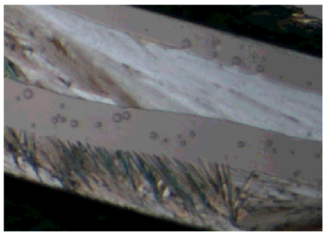
(*S*)-4-Br
(*R*)-4-Me



108.9°

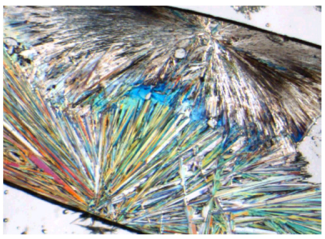


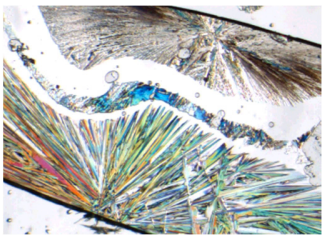
127.0°

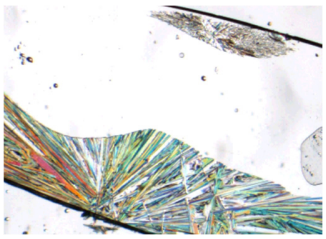


131.2°

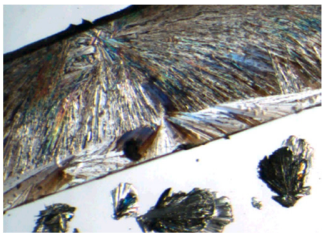
(*S*)-4-NO_2
(*R*)-4-Me

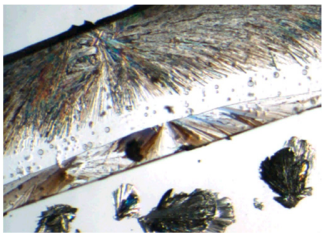

121.4°

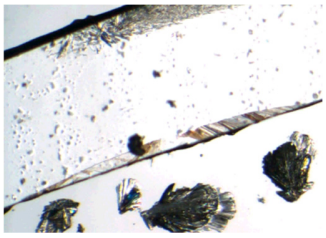

133.7°


144.7°

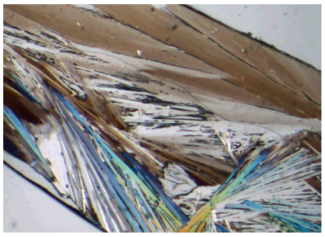
(*S*)-4-OMe
(*R*)-4-Me

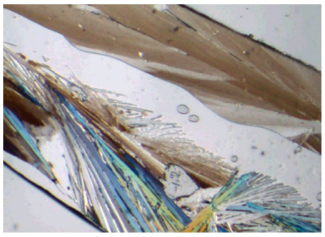

113.7°

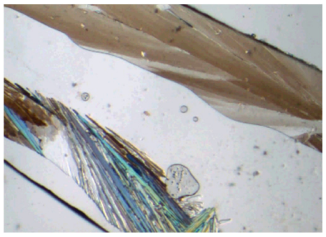

126.5°


144.9°

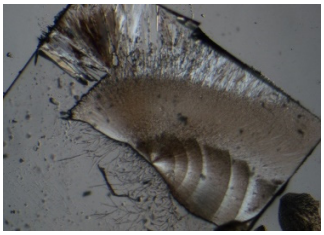
(*S*)-4-I
(*R*)-4-Me

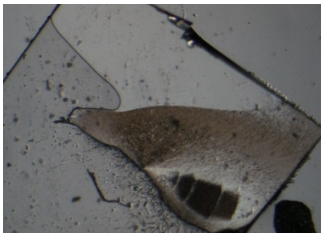

120.0°

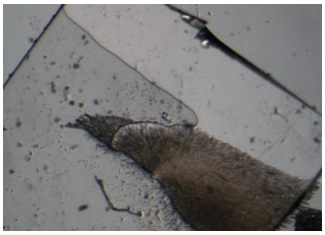

141.5°


145.3°

(*S*)-4-Me
(*R*)-4-CF_3

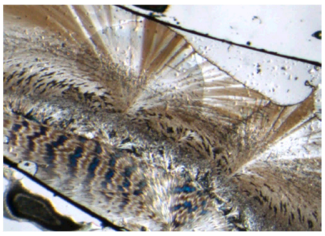

114.0°

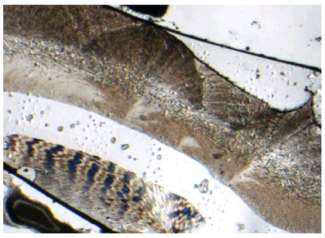

120.3°

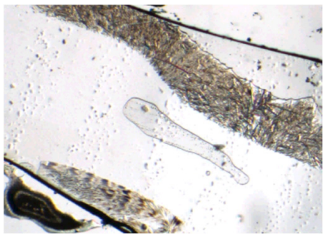

152.9°

4-Chloro

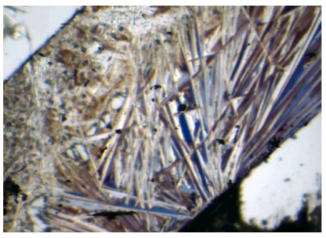
(*S*)-4-Cl
(*R*)-4-Br

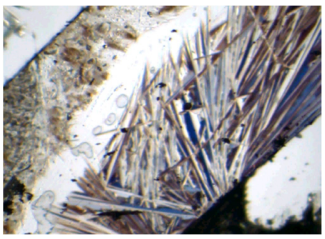

119.8°

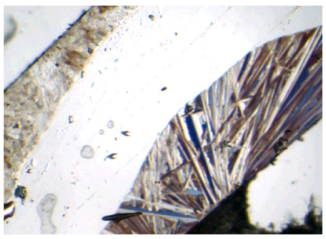

161.7°


146.1°

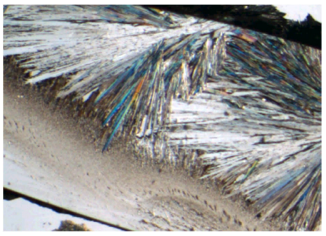
(*S*)-4-Cl
(*R*)-4-NO_2

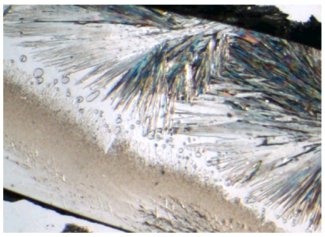

105.7°

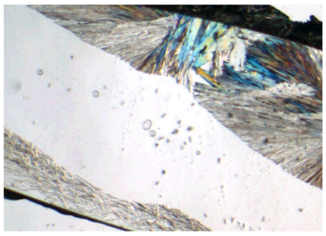

124.0°


147.1°

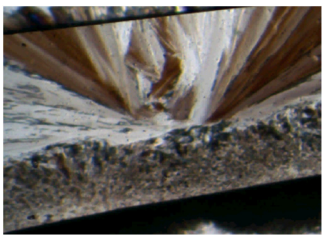
(*R*)-4-Cl
(*S*)-4-OMe

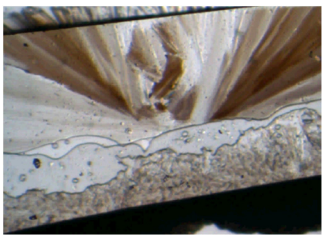

120.3°

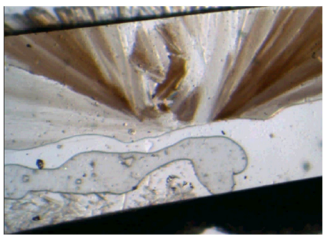

131.9°


152.2°

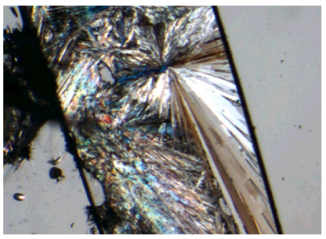
(*S*)-4-I
(*R*)-4-Cl

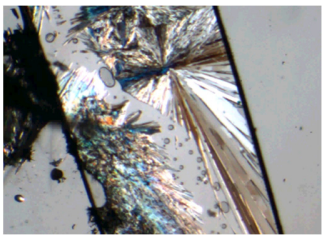

134.2°

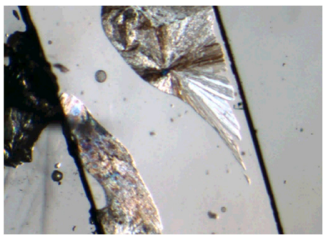

153.3°


158.0°

(*S*)-4-Cl
(*R*)-4-CF_3

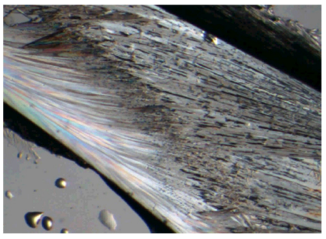

114.9°

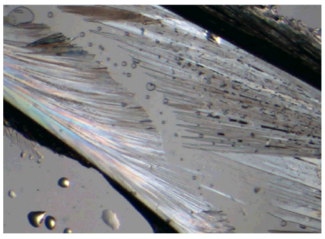

138.0°

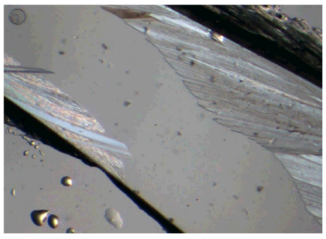

161.4°

4-Bromo

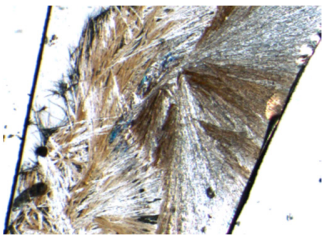
(*R*)-4-NO_2
(*S*)-4-Br

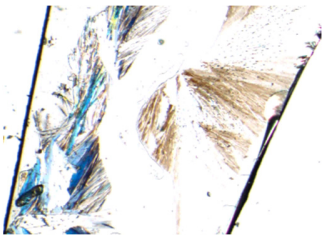

112.8°

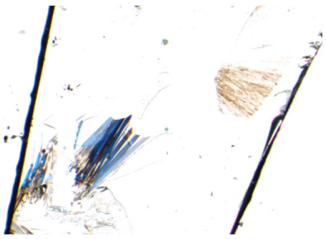

128.6°


147.0°

(*S*)-4-OMe
(*R*)-4-Br

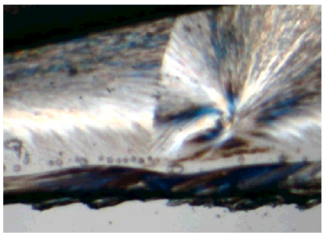

122.6°

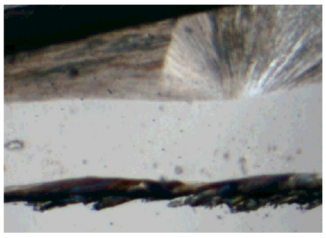

154.7°


164.4°

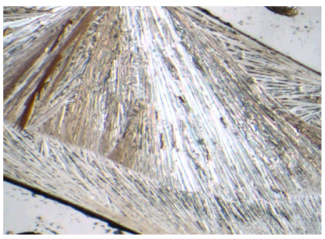
(*S*)-4-I
(*R*)-4-Br

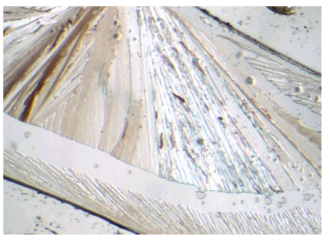

158.0°

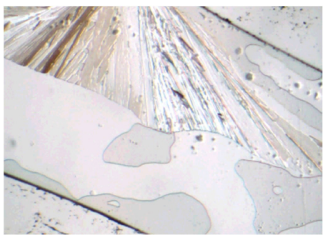

164.6°


179.3°

(*S*)-4-Br
(*R*)-4-CF_3

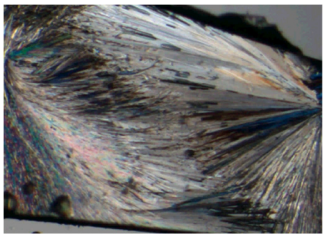

112.1°

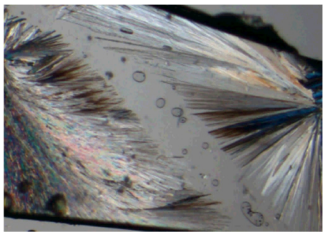

143.9°

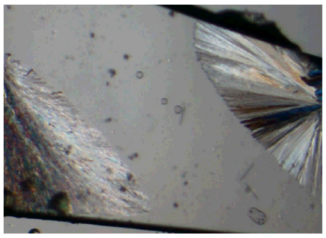

163.8°

4-Nitro

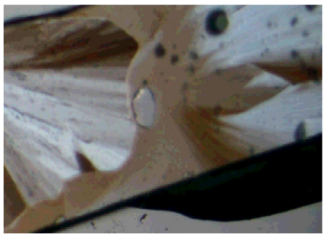
(*R*)-4-NO_2
(*S*)-4-OMe

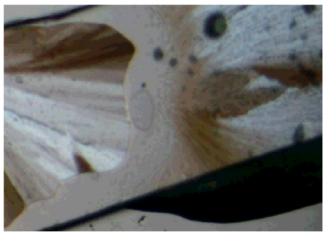

107.6°

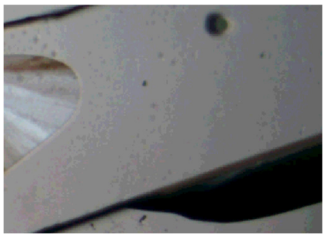

126.0°


146.4°

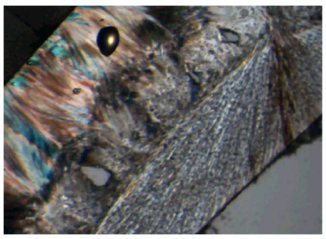
(*R*)-4-NO_2
(*S*)-4-I

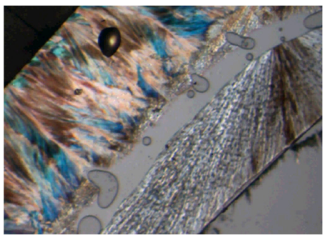

129.5°

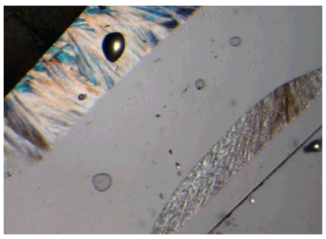

147.5°


207.4°

(*S*)-4-NO_2
(*R*)-4-CF_3

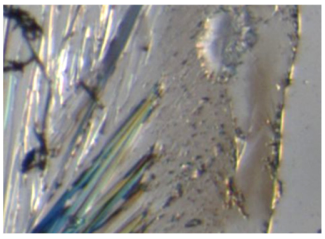

105.0°

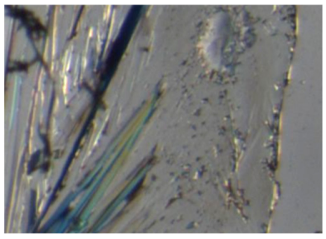

134.5°

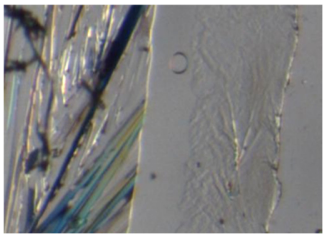

155.1°

4-Methoxy

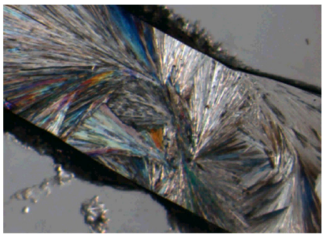
(*S*)-4-OMe
(*R*)-4-I

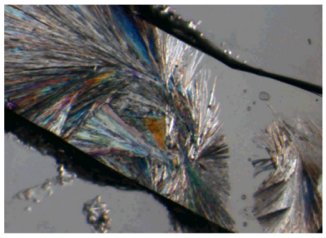

67.8°

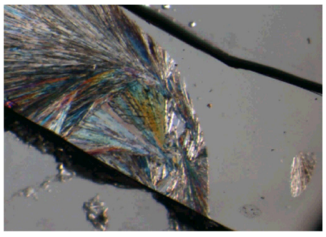

108.9°


122.8°

(*S*)-4-OMe
(*R*)-4-CF_3

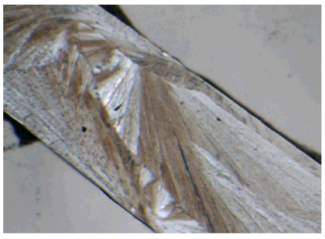

132.9°

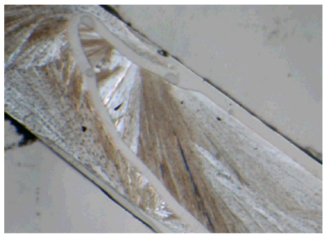

142.0°

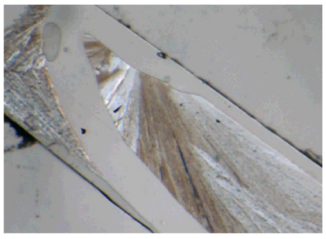

157.0°

4-Iodo

(*S*)-4-I
(*R*)-4-CF_3


138.6°


159.6°


164.4°

S3. X-ray Crystallography

Table S1. Crystallographic data for diarylamide quasiracemates and racemates.

	rac-H	(*R*)-H/(*S*)-3-F	*Rac*-3-F
Crystal data			
CCDC deposit no.	2111824	2111820	2111823
Empirical formula	$C_{15}H_{15}NO$	$C_{30}H_{29}FN_2O_2$	$C_{15}H_{14}FNO$
Crystal System, space group	Triclinic *P*-1 (no. 2)	Monoclinic $P2_1$ (no. 4)	Monoclinic $P2_1/c$ (no. 14)
M_r	225.28	468.55	243.27
a, Å	5.3257(2)	19.6145(8)	23.8795(7)
b, Å	15.3736(5)	5.2344(2)	5.2122(1)
c, Å	15.9929(5)	23.5535(10)	19.6496(6)
α, deg	64.793(1)	90	90
β, deg	85.938(1)	90.406(2)	90.415(1)
γ, deg	81.506(1)	90	90
V, (Å^3)	1171.69(7)	2418.18(17)	2445.62(11)
Z, *Z'*	4, 2	8, 2	8, 2
D_{calc} (g cm^{-3})	1.277	1.287	1.321
μ (mm^{-1}), rad. type	0.627, Cu $K\alpha$	0.689	0.783, Cu $K\alpha$
F_{000}	480	992	1024
temp (K)	100(2)	100(2)	100(2)
Crystal form, color	block, colorless	prism, colorless	needle, colorless
Crystal size, mm	0.26 x 0.24 x 0.20	0.39 x 0.8 x 0.33	0.17 x 0.06 x 0.03
Data collection			
Diffractometer	Bruker Apex II	Bruker D8 Venture	Bruker D8 Venture
T_{min}/T_{max}	0.687/0.753	0.661/0.754	0.689/0.753
No. of refls. (meas., uniq., and obs.)	15649/4230/3807	64624/9421/8391	23774/4473/3939
R_{int}	0.0381	0.0567	0.0440
θ_{max} (°)	68.23	72.36	68.31
Refinement			
$R/R^2\omega$ (obs data)	0.0466/0.1359	0.0534/0.1372	0.0325/0.0770
$R/R^2\omega$ (all data)	0.0502/0.1383	0.0592/0.1439	0.0395/0.0809
S	1.170	1.032	1.045
No. of refls.	4230	9421	4473
No. of parameters	315	666	353
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.310/-0.206	0.621/-0.259	0.199/-0.201
flack	-	0.08(8)	-

Table S1. Crystallographic Data for Diarylamide Quasiracemates and Racemates. (Continued)

	rac-3-Cl	(*R*)-3-Cl/(*S*)-3-Me	*rac*-3-Me
Crystal data			
CCDC deposit no.	2111822	2111817	2111826
Empirical formula	$C_{15}H_{14}ClNO$	$C_{31}H_{31}ClN_2O_2$	$C_{16}H_{17}NO$
Crystal System, space group	Orthorhombic *Pbca* (no. 61)	Orthorhombic $P2_12_12_1$ (no. 19)	Tetragonal $P4_2/n$ (no. 86)
M_r	259.72	499.03	239.30
a, Å	10.2810(3)	9.9288(3)	224232(5)
b, Å	9.9520(3)	10.2423(3)	22.4232(5)
c, Å	25.9574(8)	26.1270(7)	5.1912(2)
α, deg	90	90	90
β, deg	90	90	90
γ, deg	90	90	90
V, (Å^3)	2655.874(14)	2656.95(13)	2610(15)
Z, *Z'*	8, 1	4, 1	8, 1
D_{calc} (g cm^{-3})	1.299	1.248	1.218
μ (mm^{-1}), rad. type	2.432, Cu $K\alpha$	1.506, Cu $K\alpha$	0.590, Cu $K\alpha$
F_{000}	1088	1056	1024
temp (K)	100(2)	100(2)	100(2)
Crystal form, color	block, colorless	needle, colorless	needle, colorless
Crystal size, mm	0.26 x 0.18 x 0.11	0.21 x 0.04 x 0.02	0.22 x 0.06 x 0.02
Data collection			
Diffractometer	Bruker Apex II	Bruker D8 Venture	Bruker D8 Venture
T_{min}/T_{max}	0.635/0.753	0.681/0.753	0.693/0.754
No. of refls. (meas., uniq., and obs.)	11017/2429/2227	81064/4867/4562	16133/2675/2318
R_{int}	0.0350	0.0616	0.0426
θ_{max} (°)	68.25	68.23	74.40
Refinement			
$R/R^2\omega$ (obs data)	0.0339/00860	0.0364/0.0921	0.0418/0.1083
$R/R^2\omega$ (all data)	0.0366/0.0880	0.0397/0.0948	0.0496/0.1143
S	1.062	1.026	1.050
No. of refls.	2429	4867	2675
No. of parameters	213	484	168
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.302/-0.220	0.482/-0.247	0.499/-0.221
flack	-	0.062(4)	-

Table S1. Crystallographic Data for Diarylamide Quasiracemates and Racemates. (Continued)

	rac-3-Br	(*R*)-3-Br/(*S*)-3-CF_3	*rac*-3-CF_3
Crystal data			
CCDC deposit no.	2111821	2111816	2111825
Empirical formula	$C_{15}H_{14}BrNO$	$C_{31}H_{28}BrF_3N_2O_2$	$C_{16}H_{14}F_3NO$
Crystal System, space group	Monoclinic $P2_1/c$ (no. 14)	Monoclinic $P2_1$ (no. 4)	Monoclinic $P2_1/c$ (no. 14)
M_r	304.18	597.46	293.28
a, Å	12.0922(8)	9.3990(8)	24.6609(11)
b, Å	5.0801(3)	5.8355(5)	5.8339(3)
c, Å	21.6705(14)	24.4782(14)	9.4777(4)
α, deg	90	90	90
β, deg	98.83693)	93.306(6)	93.863(2)
γ, deg	90	90	90
V, (Å^3)	1315.41(14)	1340.34(14)	1360.45(11)
Z, *Z'*	4, 1	2, 1	4, 1
D_{calc} (g cm^{-3})	1.536	1.480	1.432
μ (mm^{-1}), rad. type	4.146, Cu $K\alpha$	2.545, Cu $K\alpha$	1.005, Cu $K\alpha$
F_{000}	616	612	608
temp (K)	100(2)	100(2)	100(2)
Crystal form, color	needle, colorless	block, colorless	block, colorless
Crystal size, mm	0.26 x 0.06 x 0.05	0.25 x 0.25 x 0.09	0.25 x 0.16 x 0.10
Data collection			
Diffractometer	Bruker D8 Venture	Bruker Apex II	Bruker Apex II
T_{min}/T_{max}	0.566/0.753	0.623/0.753	0.640/0.753
No. of refls. (meas., uniq., and obs.)	17437/2395/2224	18045/4872/4714	34741/2439/2310
R_{int}	0.0587	0.0327	0.0353
θ_{max} (°)	68.22	69.018	68.46
Refinement			
$R/R^2\omega$ (obs data)	0.0248/0.0593	0.0258/0.0658	0.0365/0.0862
$R/R^2\omega$ (all data)	0.0280/0.0613	0.0271/0.0671	0.0381/0.0870
S	1.064	1.047	1.171
No. of refls.	2395	4872	2439
No. of parameters	167	354	191
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.450/-0.292	0.258/-0.249	0.240/-0.217
flack	-	0.041(6)	-

Table S1. Crystallographic Data for Diarylamide Quasiracemates and Racemates. (Continued)

	rac-H	(*R*)-H/(*S*)-4-F	*rac*-4-F
Crystal data			
CCDC deposit no.	2111824	2111819	2111828
Empirical formula	$C_{15}H_{15}NO$	$C_{30}H_{29}FN_2O_2$	$C_{15}H_{14}FNO_2$
Crystal System, space group	Triclinic *P*-1 (no. 2)	Monoclinic $P2_1$ (no. 4)	Monoclinic $P2_1/c$ (no. 14)
M_r	225.28	468.55	243.27
a, Å	5.3257(2)	9.6630(4)	11.4913(4)
b, Å	15.3736(5)	11.6828(6))	11.7383(5)
c, Å	15.9929(5)	11.4711(5)	9.6372(4)
α, deg	64.793(1)	90	90
β, deg	85.938(1)	106.186(2)	106.175(3)
γ, deg	81.506(1)	90	90
V, (Å^3)	1171.69(7)	1243.65(10)	1248.49(9)
Z, *Z'*	4, 2	2, 1	4, 1
D_{calc} (g cm^{-3})	1.277	1.251	1.294
μ (mm^{-1}), rad. type	0.627, Cu $K\alpha$	0.670, Cu $K\alpha$	0.747, Cu $K\alpha$
F_{000}	480	496	512
temp (K)	100(2)	100(2)	100(2)
Crystal form, color	block, colorless	needle, colorless	blade, colorless
Crystal size, mm	0.26 x 0.24 x 0.20	0.23 x 0.12 x 0.04	0.27 x 0.07 x 0.04
Data collection			
Diffractometer	Bruker Apex II	Bruker Apex II	Bruker Apex II
T_{min}/T_{max}	0.687/0.753	0.670/0.753	0.677/0.753
No. of refls. (meas., uniq., and obs.)	15649/4230/3807	19000/4178/3090	9413/2269/1680
R_{int}	0.0381	0.0679	0.0515
θ_{max} (°)	68.23	68.22	68.24
Refinement			
R/R^2_ω (obs data)	0.0466/0.1359	0.0514/0.1258	0.0509/0.1207
R/R^2_ω (all data)	0.0502/0.1383	0.0751/0.1395	0.0719/0.1321
S	1.170	1.026	1.036
No. of refls.	4230	4178	2269
No. of parameters	315	324	167
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.310/-0.206	0.220/-0.226	0.191/-0.333
flack	-	0.1(2)	-

Table S1. Crystallographic Data for Diarylamide Quasiracemates and Racemates. (Continued)

	rac-4-Me[1]	(*R*)-4-Me/(*S*)-4-NO_2[1]	*rac*-4-NO_2[1]
Crystal data			
CCDC deposit no.	ISACEK	ISACUA	ISACOU
Empirical formula	$C_{16}H_{17}NO$	$C_{31}H_{31}N_3O_4$	$C_{15}H_{14}N_2O_3$
Crystal System, space group	Orthorhombic *Pca*2_1 (no. 29)	Monoclinic *P*2_1 (no. 4)	Monoclinic *P*2_1/*n* (no. 14)
M_r	478.64	574.46	270.29
a, Å	12.332(1)	9.4413(9)	11.8850(1)
b, Å	9.731(1)	5.9721(7)	5.4550(1)
c, Å	22.926(1)	23.294(3)	40.4438(6)
α, deg	90	90	90
β, deg	90	93.670(9)	95.367(1)
γ, deg	90	90	90
V, (Å^3)	2751.18	1316.35	2610.58
Z, *Z'*	8, 1	2, 1	8, 2
D_{calc} (g cm^{-3})	1.155	1.286	1.375
μ (mm^{-1}), rad. type			
F_{000}			
temp (K)			
Crystal form, color			
Crystal size, mm			
Data collection			
Diffractometer			
T_{min}/T_{max}			
No. of refls. (meas., uniq., and obs.)			
R_{int}			
θ_{max} (°)			
Refinement			
R/R^2_ω (obs data)			
R/R^2_ω (all data)			
S			
No. of refls.			
No. of parameters			
$\Delta\rho_{max/min}$ (e·Å^{-3})			
flack			

[1]. Hendi, M.S.; Hooter, P.; Davis, R.E.; Lynch, V.M.; Wheeler, K.A. Cryst.Growth Des. **2004**, *4*, 95-101.

Table S1. Crystallographic Data for Diarylamide Quasiracemates and Racemates. (Continued)

	rac-4-Br	(*R*)-4-Br/(*S*)-4-OCH_3	*rac*-4-OCH_3
Crystal data			
CCDC deposit no.	2111827	2111818	2111829
Empirical formula	$C_{15}H_{14}BrNO$	$C_{31}H_{31}BrN_2O_3$	$C_{16}H_{17}NO_2$
Crystal System, space group	Monoclinic $P2_1/c$ (no. 14)	Monoclinic $C2$ (no. 5)	Monoclinic $C2/c$ (no. 15)
M_r	304.18	559.49	255.30
a, Å	11.7790(3)	20.4363(12)	20.524(3)
b, Å	11.9146(3)	5.2417(3)	5.2239(5)
c, Å	9.7984(2)	24.4632(14)	24.426(3)
α, deg	90	90	90
β, deg	102.518(2)	94.410(3)	93.260(8)
γ, deg	90	90	90
V, (Å^3)	1342.44(6)	2612.8(3)	2614.7(5)
Z, *Z'*	4, 1	4, 1	8, 1
D_{calc} (g cm^{-3})	1.505	1.422	1.297
μ (mm^{-1}), rad. type	4.063, Cu $K\alpha$	2.429, Cu $K\alpha$	0.682, Cu $K\alpha$
F_{000}	616	1160	1088
temp (K)	100(2)	100(2)	100(2)
Crystal form, color	needle, colorless	needle, colorless	needle, colorless
Crystal size, mm	0.25 x 0.07 x 0.04	0.34 x 0.07 x 0.06	0.19 x 0.04 x 0.02
Data collection			
Diffractometer	Bruker Apex II	Bruker Apex II	Bruker Apex II
T_{min}/T_{max}	0.677/0.753	0.526/0.753	0.678/0.753
No. of refls. (meas., uniq., and obs.)	9079/2432/2194	20609/4825/3810	13710/2357/1909
R_{int}	0.0285	0.0551	0.0608
θ_{max} (°)	68.25	68.30	68.24
Refinement			
$R/R^2\omega$ (obs data)	0.0258/0.0651	0.0467/0.1173	0.0476/0.1216
$R/R^2\omega$ (all data)	0.0294/0.0668	0.0486/0.1182	0.0596/0.1272
S	1.056	1.083	1.108
No. of refls.	2432	4719	2357
No. of parameters	167	343	177
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.352/-0.324	1.158/-0.496	0.235/-0.216
flack	-	0.001(12)	-

Table S2. Hydrogen Bond Parameters for Diarylamide Crystal Structures.

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
rac-H	N1A–H1A···O1A^{i}	0.83(2)	2.33(2)	3.1093(14)	156.5(18)
	N1B–H1B···O1B^{ii}	0.84(2)	2.34(2)	3.1173(17)	153.7(18)
(*S*)-H/(*R*)-3-F	N1A–H1A···O1A^{iii}	0.88(5)	2.21(5)	3.050(5)	159(4)
	N1B–H1B···O1B^{iii}	0.86(6)	2.21(5)	3.031(5)	166(4)
	N1C–H1C···O1C^{iv}	0.87(5)	2.18(5)	3.031(4)	163(4)
	N1D–H1D···O1D^{iv}	0.86(5)	2.22(6)	3.044(5)	160(4)
rac-3-F	N1A–H1A···O1^{iv}	0.865(17)	2.176(17)	3.0030(14)	160.0(14)
	N1B–H1B···O1B^{iii}	0.861(17)	2.194(17)	3.0283(14)	163.3(14)
rac-3-Cl	N1–H1···O1^{iv}	0.83(4)	2.04(2)	2.855(3)	170(3)
(*R*)-3-Cl/(*S*)-3-Me	N1A–H1A···O1B^{v}	0.89(4)	1.95(4)	2.838(3)	172(3)
	N1B–H1B···O1A^{i}	0.83(4)	2.04(4)	2.855(3)	170(3)
rac-3-Me	N1–H1···O1^{vi}	0.86(2)	2.21(2)	3.0467(15)	161.5(16)
rac-3-Br	N1–H1···O1^{iii}	0.83(3)	2.13(3)	2.923(2)	159(2)
(*R*)-3-Br/(*S*)-3-CF_3	N1A–H1A···O1B^{vii}	0.81(4)	2.17(4)	2.954(3)	162(4)
	N1B–H1B···O1A^{v}	0.85(4)	2.10(4)	2.928(3)	163(3)
rac-3-CF_3	N1–H1···O1^{viii}	0.85(2)	2.13(2)	2.9478(17)	160.0(16)
(*S*)-H/(*R*)-4-F	N1A–H1A···O1B^{ix}	0.86(3)	2.13(3)	2.948(6)	159(5)
	N1B–H1B···O1A^{x}	0.85(3)	2.12(3)	2.954(6)	164(5)
rac-4-F	N1–H1···O1^{xi}	0.86(3)	2.09(3)	2.933(2)	167(2)
rac-4-Br	N1A–H1A···O1^{xi}	0.80(3)	2.15(3)	2.924(2)	165(2)
(S)-4-Br/(*R*)-4-OMe	N1A–H1A···O1A^{ix}	0.79(8)	2.29(9)	3.050(8)	161(8)
	N1B–H1B···O1B^{iv}	0.81(9)	2.27(9)	3.043(7)	162(8)
rac-4-OMe	N1A–H1A···O1^{iv}	0.87(2)	2.19(2)	3.025(2)	159(2)

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) *x*, *y*+1, *z*; (iv) *x*, *y*-1, *z*; (v) *x*, *y*, *z*; (vi) *x*, *y*, *z*+1; (vii) *x*+1, *y*, *z*; (viii) *x*, -*y*+0.5, *z*-0.5; (*ix*) 2-*x*, *y*-3/2, 2-*z*; (*x*) 3-*x*, *y*+1/2, 1-*z*; (*xi*) *x*, -*y*+1/2, *z*+1/2

S4. Hirschfeld Surface Analyses

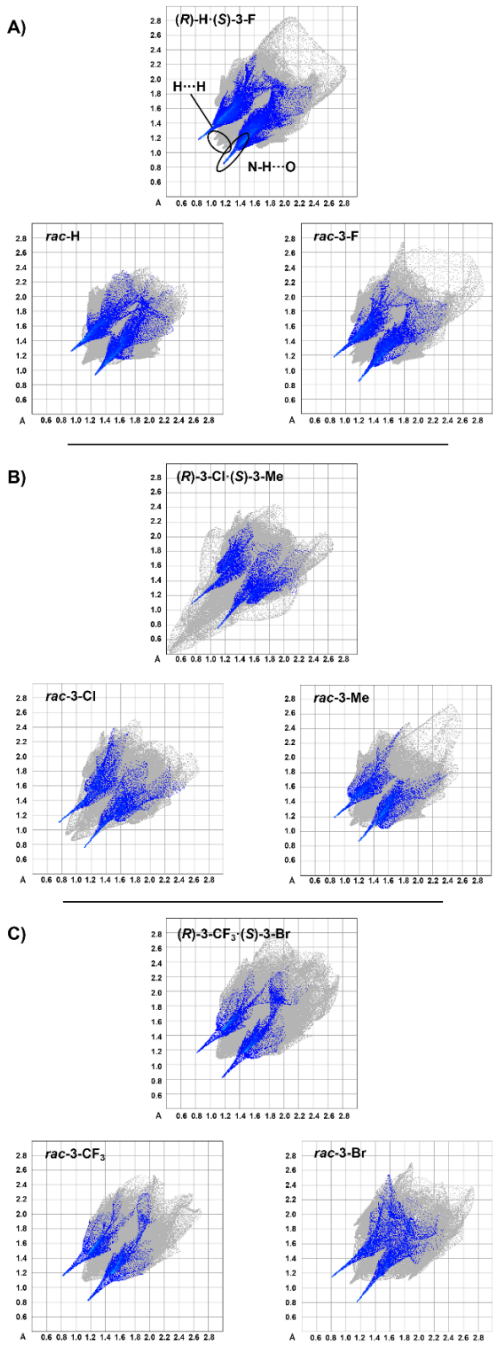


Figure S1. Hirshfeld fingerprint plots for the A) *rac*-3-H, (*R*)-3-H·(*S*)-3-F, *rac*-3-F, B) *rac*-3-Cl, (*R*)-3-Cl·(*S*)-3-Me, *rac*-3-Me, and C) *rac*-3-CF_3, (*R*)-3-CF_3·(*S*)-3-Br, *rac*-3-Br 3-substituted diarylamide systems highlighting H···H and O···H contacts. Highlighted blue regions indicate O/H contributions to the surface.

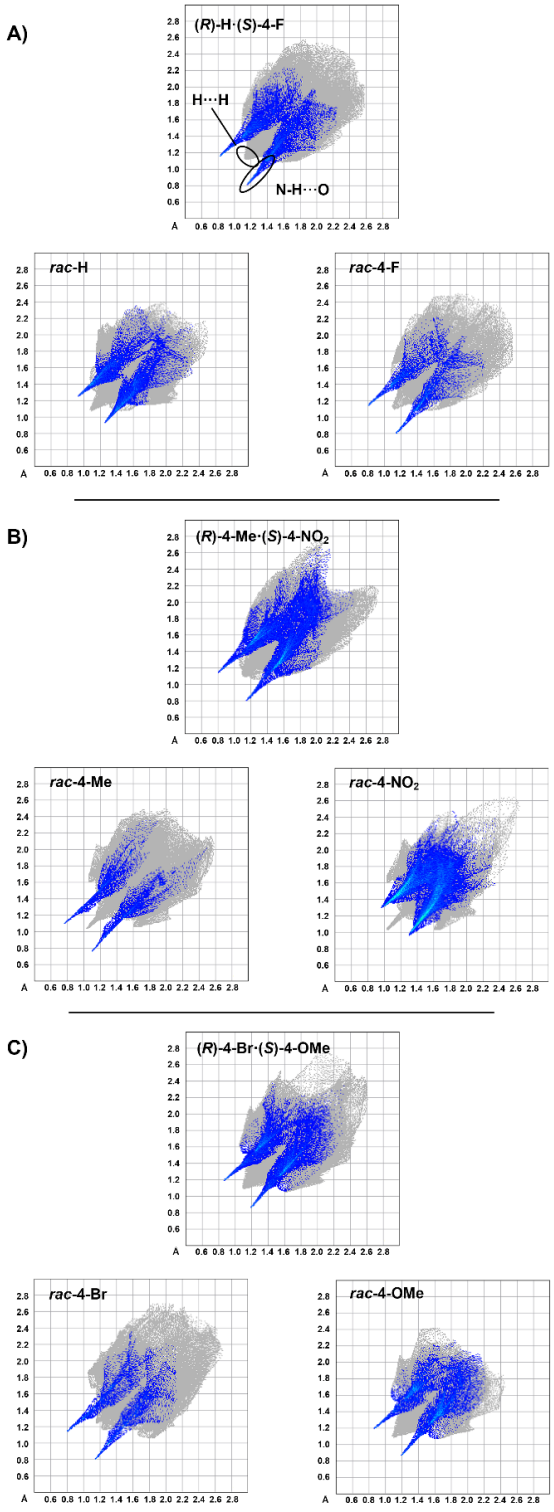


Figure S2. Hirshfeld fingerprint plots for the A) *rac*-4-H, (*R*)-4-H·(*S*)-4-F, *rac*-4-F, B) *rac*-4-Me, (*R*)-4-Me·(*S*)-4-NO_2, *rac*-4-NO_2, and C) *rac*-4-Br, (*R*)-4-Br·(*S*)-3-OMe, *rac*-4-OMe 4-substituted diarylamide systems highlighting H···H and O···H contacts. Highlighted blue regions indicate the O/H contributions to the surface.

S5. Molecular Volume and Shape Difference Determinations

Compound Name	CSD reference codes*	V_{vdW} (Å^3) (eq 1)	V_{vdW} (Å^3) VABC	V_{vdW} (Å^3) TSAR
Acetamide	ACEMID07	52.18	60.30	48.04
Acetic acid	ACETAC09	49.71	58.09	46.48
n-Butane	DUCKOB07	65.94	77.74	59.34
cis-Butene	WUBLUD	62.98	75.10	52.56
Cyclohexane	CYCHEX	87.97	99.98	77.93
Cyclohexanol	QQQEJV08	94.14	108.77	84.87
Cyclohexene	COVJON	83.08	97.34	74.27
Cyclopentane	ZZZVYE01	73.86	82.68	66.14
Methanol	METHOL04	31.99	34.64	28.91
Octanol	ZZZVYK01	133.24	155.72	118.90
Propanoic acid	PRONAC	66.50	75.39	58.81
t-Butanol	VATSAK02	74.14	86.53	66.32
trans-Butene	WUBMAK	62.05	75.10	56.53
Trimethylamine	CEKGUU06	62.64	71.44	55.69
Acetophenone	ACETPH	110.42	121.91	100.08
Anthracene	ANTCEN23	158.89	162.48	120.08
Benzene	BENZENE26	73.67	81.17	58.13
Benzophenone	BPHENO19	161.96	177.23	138.62
Biphenyl	BIPHEN04	143.87	153.78	108.33
Ethylamine	DEBLAYX	47.78	54.15	43.55
Ethylenediamine	ETDIAM18	59.41	65.14	52.72
Formamide	FORMAM02	38.39	43.00	31.11
Piperazine	KOXDOTX	80.30	87.38	71.53
Imidazole	IMAZOL14	58.26	53.91	45.65
Phenol	PHENOL03	84.01	89.96	76.38
Quinoline	WADTOMX	113.97	115.52	86.84
Styrene	ZZZTKA02	102.28	113.12	77.13
Toluene	TOLUEN	90.01	98.46	82.38
1,2-Dichlorobenzene	ABUMIT	105.87	111.59	90.60
1-Methylnaphthalene	SAHWOQ	131.75	139.12	120.53
1,3,5-Trimethylbenzene	TUYPEJ	118.03	133.05	106.85
1,2,4,5-Tetrafluorobenzene	FACJAU01	99.81	105.44	87.17
Benzonitrile	AYELIZ	93.25	104.19	73.88
Chrysene	CRYSEN02	201.00	203.13	150.18
Cycloheptane	UNIDUR	97.45	117.27	90.71
Diisopropylether	DEWPIF	104.65	121.12	94.16

m-Dibromobenzene	SOFVUG02	114.20	119.73	99.27
Methtbutylether	CEZSEF	89.65	103.83	79.76
m-Nitrophenol	MNPHOL20	108.08	115.90	99.94
Nitrobenzene	NITRBE01	99.99	107.11	79.06
N-Methylmorpholine	ULOKEL	93.04	102.47	83.53
o-Nitrotoluene	MOVVOJ	114.17	124.40	105.82
p-Dichlorobenzene	DCLBEN06	106.46	111.59	90.10
Perylene	PERLEN08	216.14	211.83	162.13
Thiophene	DOYBUQ01	57.66	67.72	57.87
3-Methylindole	GIYKUU	116.94	118.16	108.49
1-Naphthol	NAPHOL	130.32	130.61	114.56
2-Naphthol	GIYBIZ	126.66	130.61	114.84
2-Methylfuran	ZOGQUK	74.77	75.30	59.54
3,4-Dinitrophenol	XIHNOS	132.63	162.46	122.52
1,3,5-Trihydroybenzene	PHGLOH03	99.93	107.54	92.21
Anthraquinone	ANTQUO05	176.33	188.32	132.75
Antipyrine	ANTPYR	163.14	169.90	148.03
a-Terpineol	VUYHAA	149.05	175.31	129.57
Barbital	DETBAA12	151.94	175.02	127.37
Dibenzothiophene	DBZTHP01	140.40	149.03	120.03
Dimethylformamide	KOSSOK	68.00	77.60	57.63
Dimethyloxalate	DMEOXA	94.07	107.63	85.99
Ephedrine	EPHEDH02	152.49	170.14	128.64
Ethylbenzoate	WAWFOP	131.25	148.00	120.81
Eucalyptol	MOFPAY	143.06	165.59	130.19
Formic acid	FORMAC01	36.41	40.80	30.25
Furfural	ZOGQEU	79.79	81.45	62.31
Gallic acid	IJUMEG	127.55	139.78	102.22
Hydroquinone	HYQUIN06	92.26	98.75	83.25
Valeric acid	VALRAC	87.47	109.98	85.35
Isoforone	AFOGUAX	131.00	155.38	117.38
Maleic anhydride	MLEICA01	73.57	83.85	62.64
Methadone	METHAD01	286.70	326.59	251.75
Nitrofurazone	WEVEU02	144.84	155.04	116.54
Octanoic acid	DIKCUW	136.61	161.87	120.16
o-Phthalic acid	PHTHAC04	130.58	145.65	105.75
Phenytoin	PHYDAN03	204.74	227.61	182.95
Resorcinol	RESORA03	92.70	98.75	84.21
Salicilic acid	SALIAC16	112.93	122.20	87.35
Succinic acid	SUCACB16	93.01	107.63	78.01
Thymine	THYMIN03	98.86	114.35	79.00

Trifluoromethylbenzene	OHAQOD	107.42	116.67	104.80
Trimethylamine	CEKGUU01	62.93	71.44	55.69
Triphenylphosphine oxide	TPEPHO05	236.35	255.00	210.47
Water	AFIDIE	17.24	17.35	14.20

*CSD reference codes used to retrieve structural data and determine V_{vdW} ($Å^3$) (Eq 1) values.

The computer code developed to determine molecular volume (V_{vdW}) and the shape space differences ($\%V_{vdW}$) of pairs of diarylamides can be found at https://github.com/dschepens/MDPI-Crystals.