Electronic Supplementary Material (ESI) for ChemComm.

Electronic supplementary information for:

Probing the Shape Space of Molecular Recognition via 2-Substituted Diarylamide Quasiracemates

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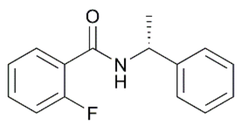
Electronic Supplementary Information

Table of Contents **Page**

S1. Experimental Details

Synthesis of (*S*)- and (*R*)-N-(2-substitutedbenzoyl)methylbenzylamine

General Considerations. All chemicals and solvents were purchased from the Aldrich Chemical Co. or Acros Chemicals and used as received without further purification unless stated otherwise. ^{1}H NMR and ^{13}C NMR spectral data were recorded with a 400 MHz Bruker Avance spectrometer using TopSpin v.3.2. They were referenced using the solvent residual signal as internal standard. The 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. The 2-substituted diarylamide derivatives for this study were prepared using a previously reported method starting from either the carboxylic acid or acid chloride.[1] The following general procedure, as described for (*R*)-N-(2-fluorobenzoyl)methylbenzylamine, was used to generate the homologous series of diarylamides.



(*R*)-N-(2-Fluorobenzoyl)methylbenzylamine

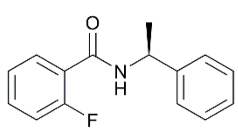
To a 25mL nitrogen purged 100-mL round-bottom flask containing a stir bar and 2-fluorobenzoic acid (0.8469 g, 6.00 mmol) at 0°C was added 2.2 mL of thionyl chloride (30.0 mmol). The reaction mixture was allowed to warm to room temperature and then refluxed for 2.5 hours to give a homogeneous yellow solution. Excess thionyl chloride was removed by washing the mixture with 15mL of hexanes and the mixture reduced using a mechanical diffusion pump to give a yellow solution. Without further purification, the acid chloride was treated with (*R*)-(+)-α-methylbenzylamine (1.7993 g, 14.8 mmol) dissolved in 5mL dichloromethane and stirred overnight at room temperature. The reaction mixture was then extracted in succession with 25 mL H_2O, 10 mL saturated $NaHCO_3$, 10 mL 4 M HCl, and 10 mL H_2O. The organic layer was dried using anhydrous magnesium sulfate and reduced under *vacuo* to give a solid colorless product (0.6413 g, 43.93% yield).

X-ray quality crystals were obtained *via* slow evaporation at room temperature using a 1:1 hexanes:dichloromethane solution.

Melting point 108-110°C.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.80 (br s, 1H, N-H), 7.57-7.24 (m, 9H, C_{Ar}-H), 5.12 (dq, *J* = 6.4 and 6.6 Hz, 1H, C_{sp3}-H), 1.43 (d, *J* = 6.4 Hz, 3H, CH_3)

^{13}C NMR (100 MHz, acetone-d_6): δ 163.1, 160.2-157.8 (d, *J* = 247.1 Hz), 144.6, 132.1-132.0 (d, *J* = 8.2 Hz), 129.9. 128.3, 126.7, 126.0, 124.8-124.6 (d, *J* = 15.3 Hz), 124.4-124.3 (d, *J* = 15.1 Hz), 116.1- 115.9 (d, *J* = 21.9 Hz), 48.6, 22.5.



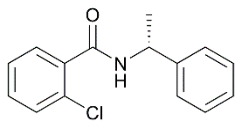
(*S*)-N-(2-Fluorobenzoyl)methylbenzylamine

Melting point 108-110°C, 85.89% yield.

1. S. L. Fomulu, M. S. Hendi, R. E. Davis and K. A. Wheeler, *Cryst. Growth Des*., 2002, **2**, 637.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.81-7.19 (m, 10H, N-H, C_{Ar}-H), 5.32 (dq, *J* = 7.1 and 7.2 Hz, 1H, C_{sp3}-H), 1.58 (d, *J* = 7.1, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 162.6, 161.2-158.8(d, *J* = 246.3 Hz), 144.4, 132.6-132.5 (d, *J* = 8.7 Hz), 130.8, 128.4, 126.8, 126.1, 124.5-124.4 (d, *J* = 3.4 Hz), 123.7-123.6 (d, *J* = 13.9 Hz), 116.0-115.8 (d, *J* = 23.3 Hz), 49.2, 21.8.

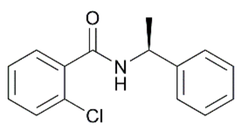


(*R*)-N-(2-Chlorobenzoyl)methylbenzylamine

Melting point 110-112°C, 68.25% yield.

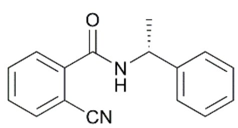
^{1}H NMR (400 MHz, acetone-d_6): δ 7.92 (br s, 1H, N-H), 7.52-7.24 (m, 9H, C_{Ar}-H), 5.29 (dq, *J* = 7.1 and 7.1 Hz, 1H, C_{sp3}-H), 1.57 (d, *J* = 7.1 Hz, 3H, CH_3)

^{13}C NMR (100 MHz, acetone-d_6): δ 165.5, 144.4, 137.3, 130.6, 130.5, 129.7, 129.0, 128.3, 126.9, 126.8, 126.2, 49.0, 21.7.



(*S*)-N-(2-Chlorobenzoyl)methylbenzylamine

Previously prepared by S. Fomulu with spectroscopic data provided in reference 1. Melting point 110-112°C

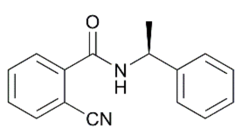


(*R*)-N-(2-Cyanobenzoyl)methylbenzylamine

Melting point 138-140°C, 84.11% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.28 (br s, 1H, N-H), 7.87-7.22 (m, 9H, C_{Ar}-H), 5.31 (dq, *J* = 7.1 and 7.1 Hz, 1H, C_{sp3}-H), 1.59 (d, *J* = 7.1 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 164.5, 144.1, 139.6, 133.9, 132.6, 130.7 128.4, 126.9, 126.2, 122.9, 117.3, 111.1, 49.2, 21.5.

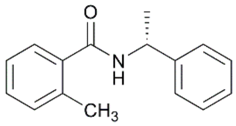


(*S*)-N-(2-Cyanobenzoyl)methylbenzylamine

Melting point 138-140°C, 34.58% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.23 (br s, 1H, N-H), 7.87-7.24 (m, 9H, C_{Ar}-H), 5.31 (dq, *J* = 7.1 and 7.1 Hz, 1H, C_{sp3}-H), 1.59 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 164.6, 144.1, 139.6, 133.9, 132.6, 130.7 128.4, 126.9, 126.3, 122.5, 117.3, 111.1, 49.3, 21.6.

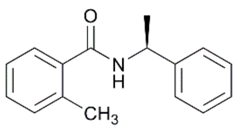


(*R*)-N-(2-Methylbenzoyl)methylbenzylamine

Melting point 110-112°C, 53.24% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.82 (br s, 1H, N-H), 7.50-7.12 (m, 9H, C_{Ar}-H), 5.29 (dq, *J* = 7.0 and 7.3 Hz, 1H, C_{sp3}-H), 2.36 (s, 3H, CH_3), 1.56 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.5, 144.9, 137.4, 135.7, 130.4, 129.2, 128.3, 126.9, 126.7, 126.2, 125.4, 48.7, 21.8, 19.0.

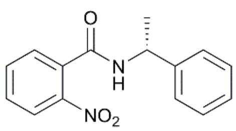


(*S*)-N-(2-Methylbenzoyl)methylbenzylamine

Melting point 110-112°C, 89.23% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.77 (br s, 1H, N-H), 7.50-7.17 (m, 9H, C_{Ar}-H), 5.30 (dq, *J* = 7.5 and 7.5 Hz, 1H, C_{sp3}-H), 2.36 (s, 3H, CH_3), 1.56 (d, *J* = 7.5 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.3, 144.8, 137.4, 135.7, 130.4, 129.2, 128.3, 126.9, 126.7, 126.2, 125.4, 48.6, 21.7, 18.9.

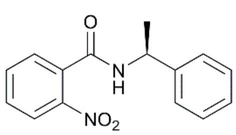


(*R*)-N-(2-Nitrobenzoyl)methylbenzylamine

Melting point 168-171°C, 30.44% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.17 (br s, 1H, N-H), 8.03-7.25 (m, 9H, C_{Ar}-H), 5.28 (dq, *J* = 7.0 and 7.2 Hz, 1H, C_{sp3}-H), 1.58 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 164.9, 147.4, 144.0, 142.2, 133.3, 130.4, 129.0, 128.3, 126.9, 126.2, 124.0, 49.0, 21.4.

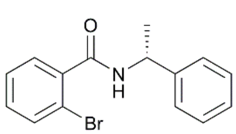


(*S*)-N-(2-Nitrobenzoyl)methylbenzylamine

Melting point 168-171°C, 82.78% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.19(br s, 1H, N-H), 8.03-7.25 (m, 9H, C_{Ar}-H), 5.28 (q, *J* = 7.0 and 7.2 Hz, 1H, C_{sp3}-H), 1.58 (d, *J* = 7.0 Hz, 3H, CH_3).

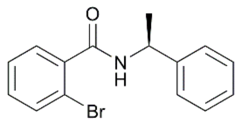
^{13}C NMR (100 MHz, acetone-d_6): δ 164.9, 148.0, 147.4, 144.0, 133.3, 130.4, 129.0, 128.3, 126.9, 126.3, 124.0, 49.0, 21.4.



(*R*)-N-(2-Bromobenzoyl)methylbenzylamine

Previously prepared by S. Fomulu with spectroscopic data provided in reference 1.

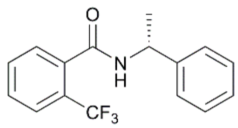
Melting point 117-121°C



(*S*)-N-(2-Bromobenzoyl)methylbenzylamine

Previously prepared by S. Fomulu with spectroscopic data provided in reference 1.

Melting point 117-121°C

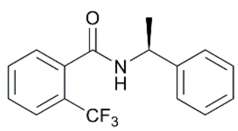


(*R*)-N-(2-Trifluorobenzoyl)methylbenzylamine

Melting point 140-143°C, 64.71% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.00 (br s, 1H, N-H), 7.77-7.25 (m, 9H, C_{Ar}-H), 5.29 (q, *J* = 7.0 and 7.0 Hz, 1H, C_{sp3}-H), 1.56 (d, *J* = 7.0 Hz, 3H, CH_3)

^{13}C NMR (100 MHz, acetone-d_6): δ 166.3, 144.2, 137.0, 132.1, 129.4, 128.5, 128.3, 126.9, 126.2, 126.1, 125.4, 122.7, 49.0, 21.5.

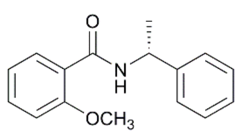


(*S*)-N-(2-Trifluorobenzoyl)methylbenzylamine

Melting point 140-143°C, 84.13% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.00 (br s, 1H, N-H), 7.77-7.25 (m, 9H, C_{Ar}-H), 5.30 (q, *J* = 7.0 and 7.0 Hz, 1H, C_{sp3}-H), 1.56 (d, *J*=7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 166.3, 144.2, 137.0, 132.1, 129.4, 128.5, 128.3, 127.2, 126.9, 126.2, 125.4, 122.7, 48.6, 21.5.

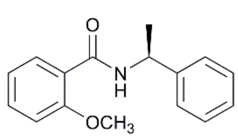


(*R*)-N-(2-Methoxybenzoyl)methylbenzylamine

Melting point 78-81°C, 86.85% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.34 (br s, 1H, N-H), 8.06-7.05 (m, 9H, C_{Ar}-H), 5.32 (dq, *J* = 7.0 and 7.5 Hz, 1H, C_{sp3}-H), 4.00 (s, 3H, O-CH_3), 1.56 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 163.8, 157.7, 144.8, 132.5, 131.5, 128.4, 126.8, 126.0, 122.4, 120.8, 111.9, 55.7, 48.9, 22.2.

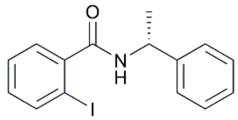


(*S*)-N-(2-Methoxybenzoyl)methylbenzylamine

Melting point 78-81°C, 75.82% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 8.42 (br d, J=6.72, N-H), 8.18-7.06 (m, 9H, C_{Ar}-H), 5.40 (dq, *J* = 7.0 and 7.1 Hz, 1H, C_{sp3}-H), 3.93 (s, 3H, O-CH_3), 1.61 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 163.7, 157.7, 144.8, 132.5, 131.5, 128.4, 126.8, 126.1, 122.4, 120.8, 111.8, 55.6, 48.9, 22.2.

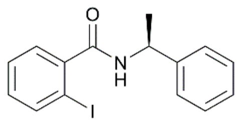


(*R*)-N-(2-Iodobenzoyl)methylbenzylamine

Melting point 137-140°C, 66.17% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.88-7.14 (m, 10H, N-H, C_{Ar}-H), 5.28 (dq, *J* = 7.0 and 7.5 Hz, 1H, C_{sp3}-H), 1.59 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 167.9, 144.1, 143.4, 139.4, 132.5, 130.4, 127.9, 127.8, 126.7, 126.3, 92.3, 48.8, 21.5.

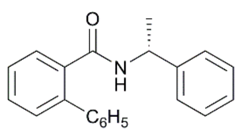


(*S*)-N-(2-Iodobenzoyl)methylbenzylamine

Melting point 137-140°C, 42.20% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.88-16 (m, 10H, N-H, C_{Ar}-H), 5.28 (dq, *J*=7.0 and 7.1 Hz, 1H), 1.59 (d, *J*=7.0, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.0, 144.2, 143.5, 139.5, 132.6, 130.5, 128.3, 128.0, 126.8, 126.3, 92.3, 48.9, 21.6.

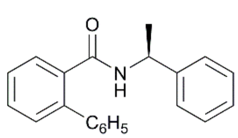


(*R*)-N-(2-Phenylbenzoyl)methylbenzylamine

Further purification of (*R*)-C_6H_5 was achieved by washing the sample with hexanes. Melting point 110-114°C, 63.24% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.52-7.16 (m, 13H, C_{Ar}-H), 5.07 (dq, *J* = 7.0 and 7.5 Hz, 1H, C_{sp3}-H), 1.27 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.2, 144.2, 140.6, 139.6, 137.5, 129.8, 129.3, 128.7, 128.1, 128.0, 127.2, 127.0, 126.5, 126.1, 48.6, 21.3, 13.4.

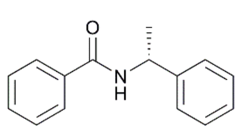


(*S*)-N-(2-Phenylbenzoyl)methylbenzylamine

Further purification of (*S*)-C_6H_5 was achieved by washing the sample with hexanes. Melting point 110-114°C, 19.78% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.52-7.16 (m, 13H, C_{Ar}-H), 5.07 (dq, *J* = 7.0 and 7.2 Hz, 1H, C_{sp3}-H), 1.27 (d, *J* = 7.0 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.2, 144.2, 140.7, 139.6, 137.5, 129.8, 129.3, 128.7, 128.2, 128.0, 127.2, 127.0, 126.6, 126.1, 48.6, 21.3, 13.4.

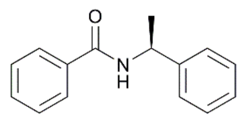


(*R*)-N-(Benzoyl)methylbenzylamine

Melting point 132-136°C, 68.38% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.80-7.75 (m, 2H, C_{Ar}-H), 7.53-7.26 (m, 8H, C_{Ar}-H), 5.35 (dq, *J* = 6.9 and 7.1 Hz, 1H, C_{sp3}-H), 1.62 (d, *J* = 7.1 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.2, 141.6, 134.6, 131.5, 128.8, 128.6, 127.5, 126.9, 126.3, 48.2, 21.7.



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

Melting point 132-136°C, 70.03% yield.

^{1}H NMR (400 MHz, acetone-d_6): δ 7.81-7.76 (m, 2H, C_{Ar}-H), 7.53-7.25 (m, 8H, C_{Ar}-H), 5.34 (dq, *J* = 7.0 and 7.1 Hz, 1H, C_{sp3}-H), 1.62 (d, *J* = 7.1 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, acetone-d_6): δ 168.2, 141.5, 134.6, 131.3, 128.7, 128.5, 127.5, 126.9, 126.3, 48.4, 21.7.

S2. Hot-Stage Microscopy

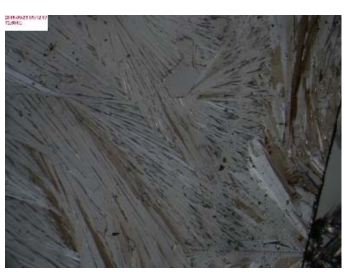
The hot-stage microscopy experiments were performed using an optical polarizing microscope (*Olympus SZX10*) equipped with an *Instec HCS 302* hot-stage connected to an *Instec mK2000* temperature controller. Micrographs were collected under a range of magnifications (3.0-6.3x) using an attached video camera. The hot-stage was controlled by the WINDV software package (V1.0.120820). Pairs of diarylamide components were analyzed for cocrystallization behavior. Samples were prepared using standard glass microscope slides and cover slips. The higher melting point component was delivered first by heating the sample to the melting point temperature drawing the sample under the cover slip. Upon cooling, the lower melting point component was then delivered in a similar fashion to create a contact interface between the two samples. These bimolecular samples were heated at a ramp rate of 2-5°C/min until complete melting of the sample occurred. All combinations (11 racemates and 55 quasiracemates) were processed using the video-assisted hot stage technique.

Hot-Stage Images of Racemic and Quasiracemic Pairs

Racemic Mixtures

(*R*)-H (left)

(*S*)-H (right)



72.7°

122.2°

130.2°

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

76.4° | 95.6° | 99.2°

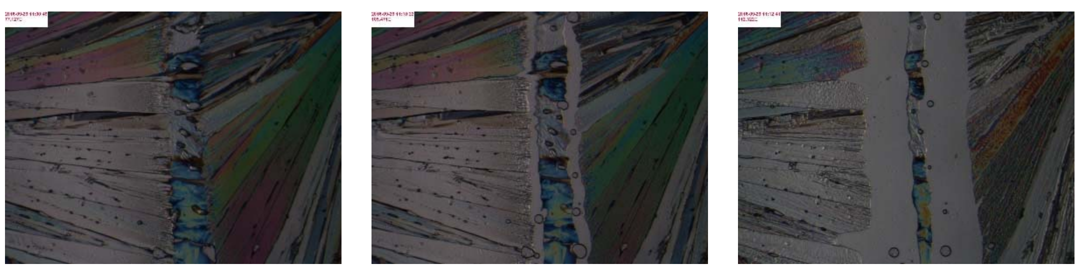
(*S*)-Cl
(*R*)-Cl

90.7° | 108.9° | 116.7°

(*S*)-CN
(*R*)-CN

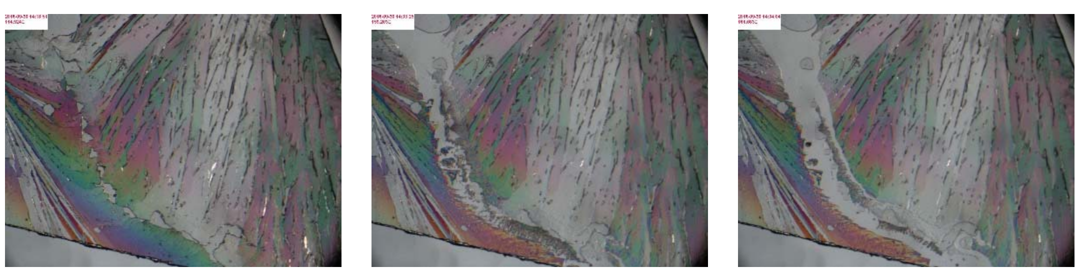
110.683° | 122.640° | 135.214°

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



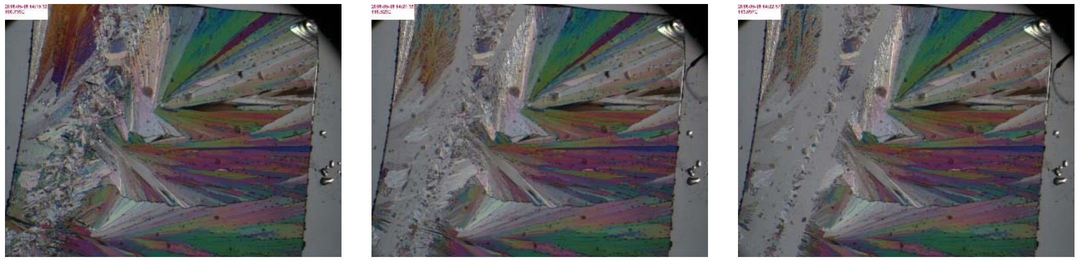
77.1° | 105.5° | 112.3°

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



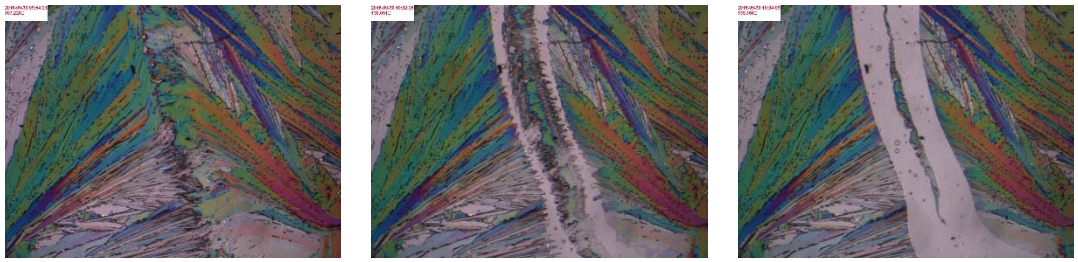
114.9° | 159.2° | 161.1°

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



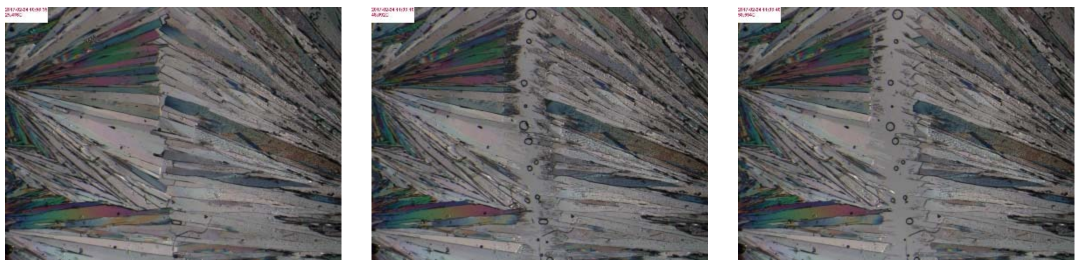
100.7° 110.5° 113.1°

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



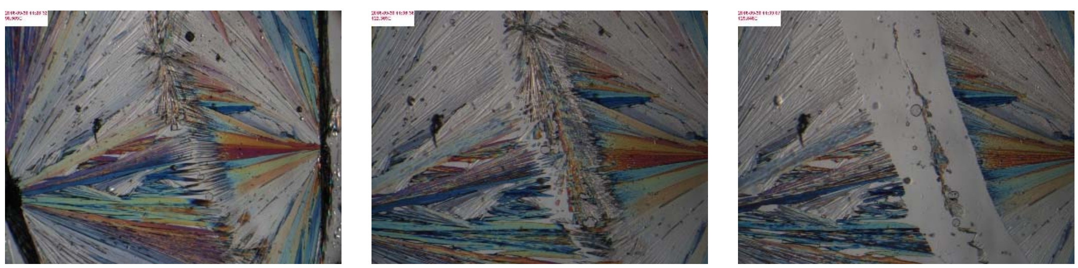
107.2° 130.1° 135.2°

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



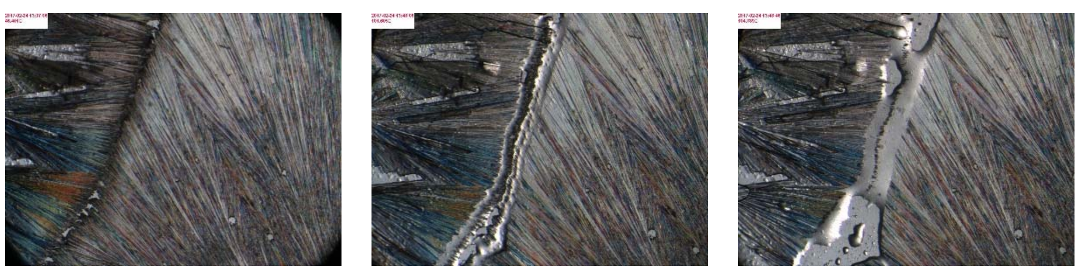
25.5° 48.1° 50.6°

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



98.5° 122.4° 129.8°

(*S*)-Phenyl
(*R*)-Phenyl



46.4° 101.6° 104.8°

Hydrogen

(*S*)-H
(left)

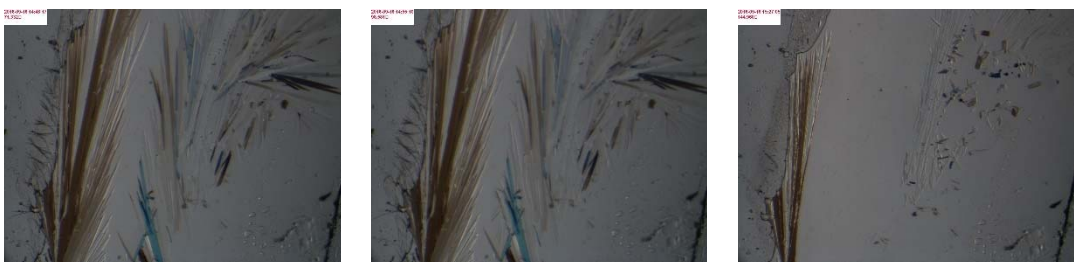
(*R*)-F
(right)

80.8° 95.8° 110.2°

(*S*)-Cl
(*R*)-H

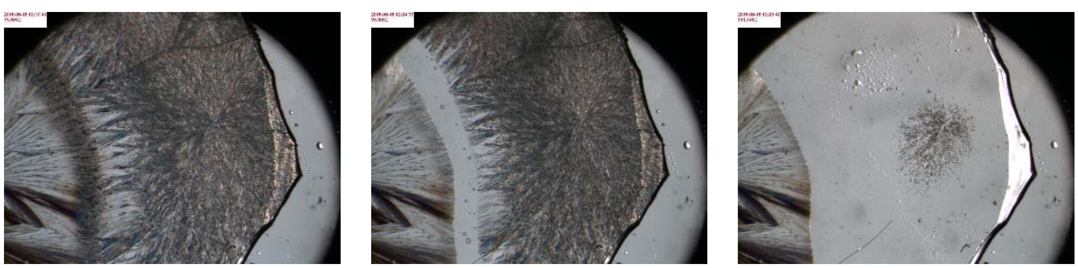
89.6° 110.3° 123.8°

(*S*)-H
(*R*)-CN



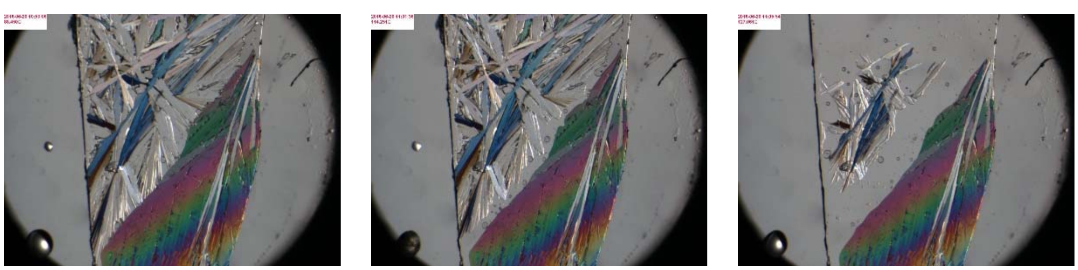
71.3° 98.6° 145.0°

(*R*)-H
(*S*)-Me



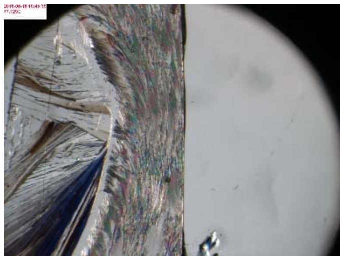
75.5° 95.9° 111.1°

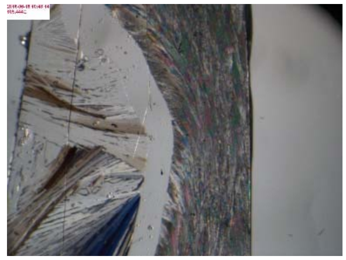
(*S*)-H
(*R*)- NO_2



88.5° 114.3° 127.1°

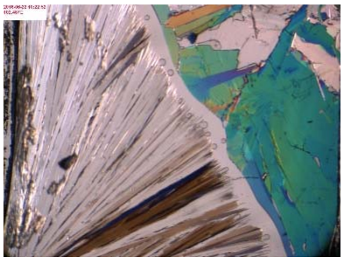
(*R*)-H
(*S*)-Br

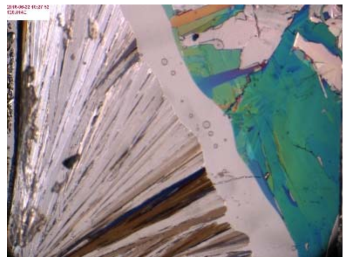

77.1°

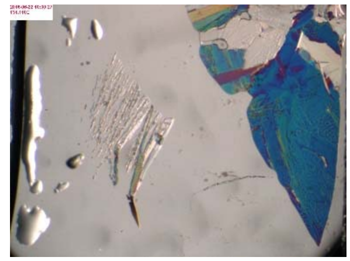

105.4°


121.9°

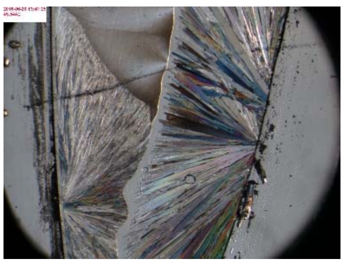
(*S*)-H
(*R*)-CF_3

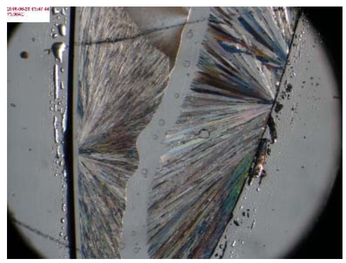

102.5°

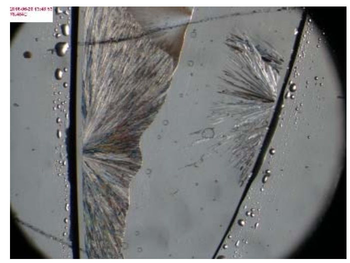

120.8°


131.1°

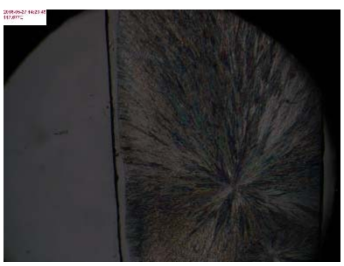
(*S*)-H
(*R*)-OMe

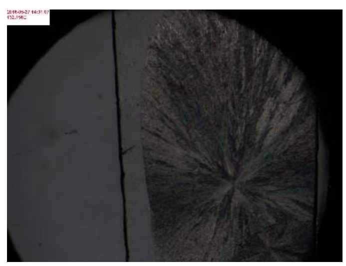

45.5°

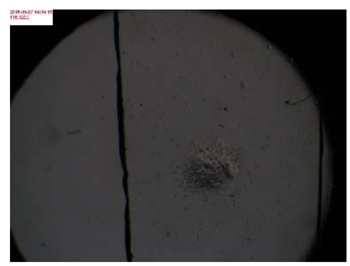

73.9°


78.5°

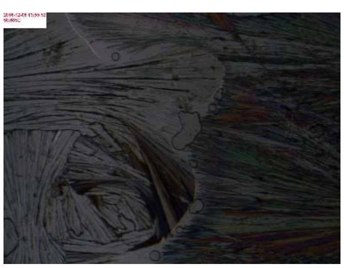
(*R*)-H
(*S*)-I

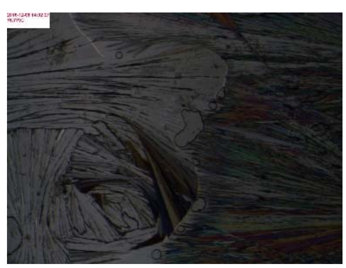

117.7°


132.2°


138.3°

(*R*)-H
(*S*)-Phenyl

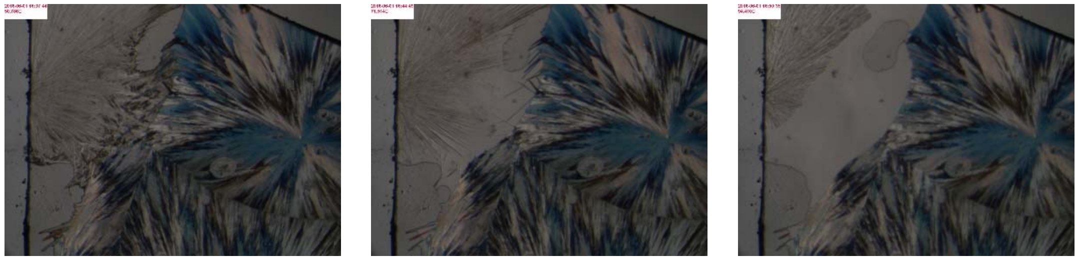

50.7°


76.8°


97.5°

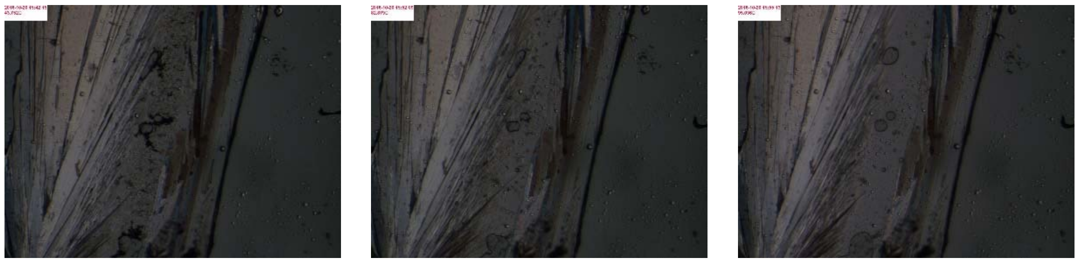
Fluoride

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



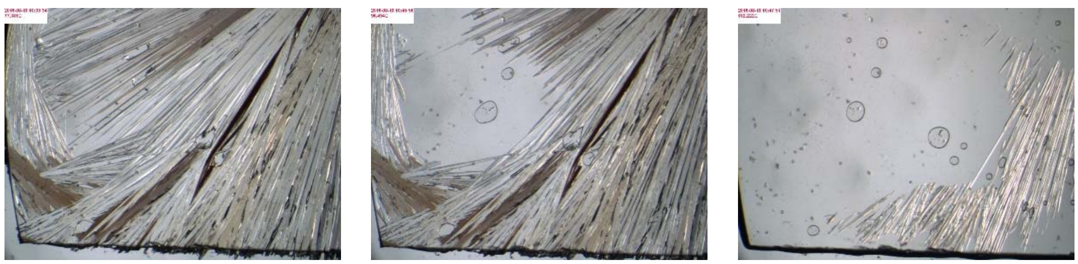
50.8° | 71.5° | 94.4°

(*S*)-F
(*R*)-CN



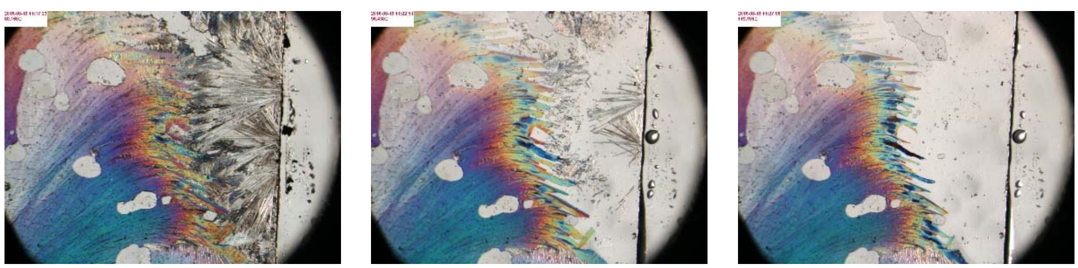
43.8° | 82.9° | 95.0°

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



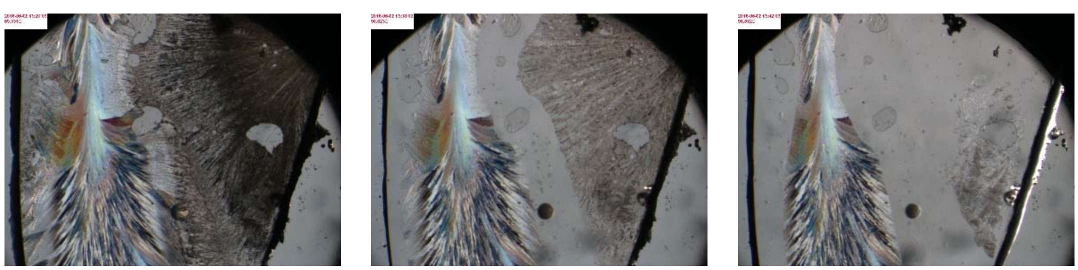
77.4° | 96.5° | 102.2°

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



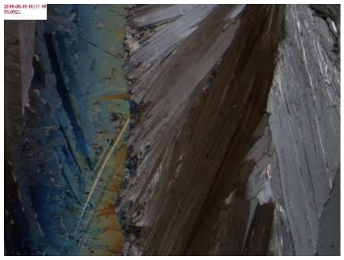
80.2° | 96.4° | 119.8°

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



69.3° | 90.8° | 98.9°

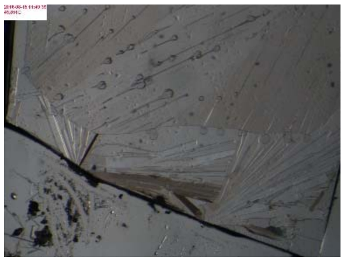
(S)-CF_3
(R)-F

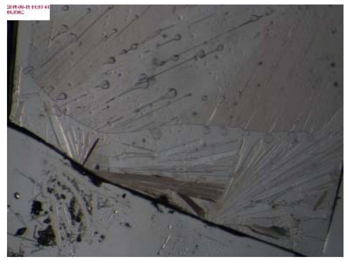

53.1°

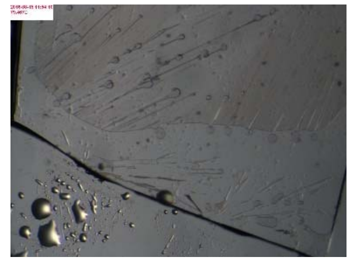

91.8°


97.8°

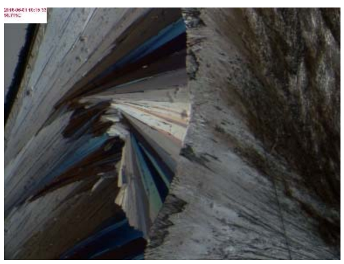
(S)-OMe
(R)-F


49.9°


61.8°


79.5°

(S)-I
(R)-F


58.7°


99.7°


102.5°

(R)-F
(S)-Phenyl

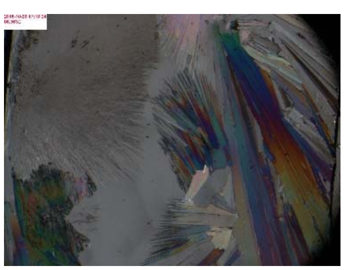

55.7°

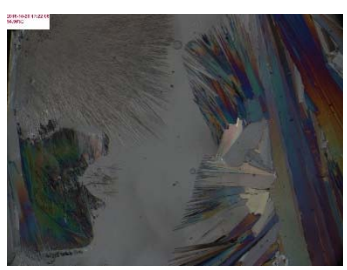

78.5°

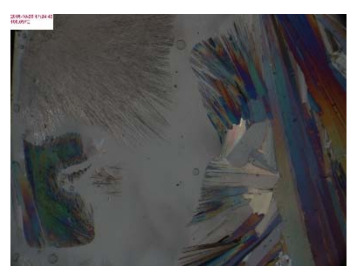

103.7°

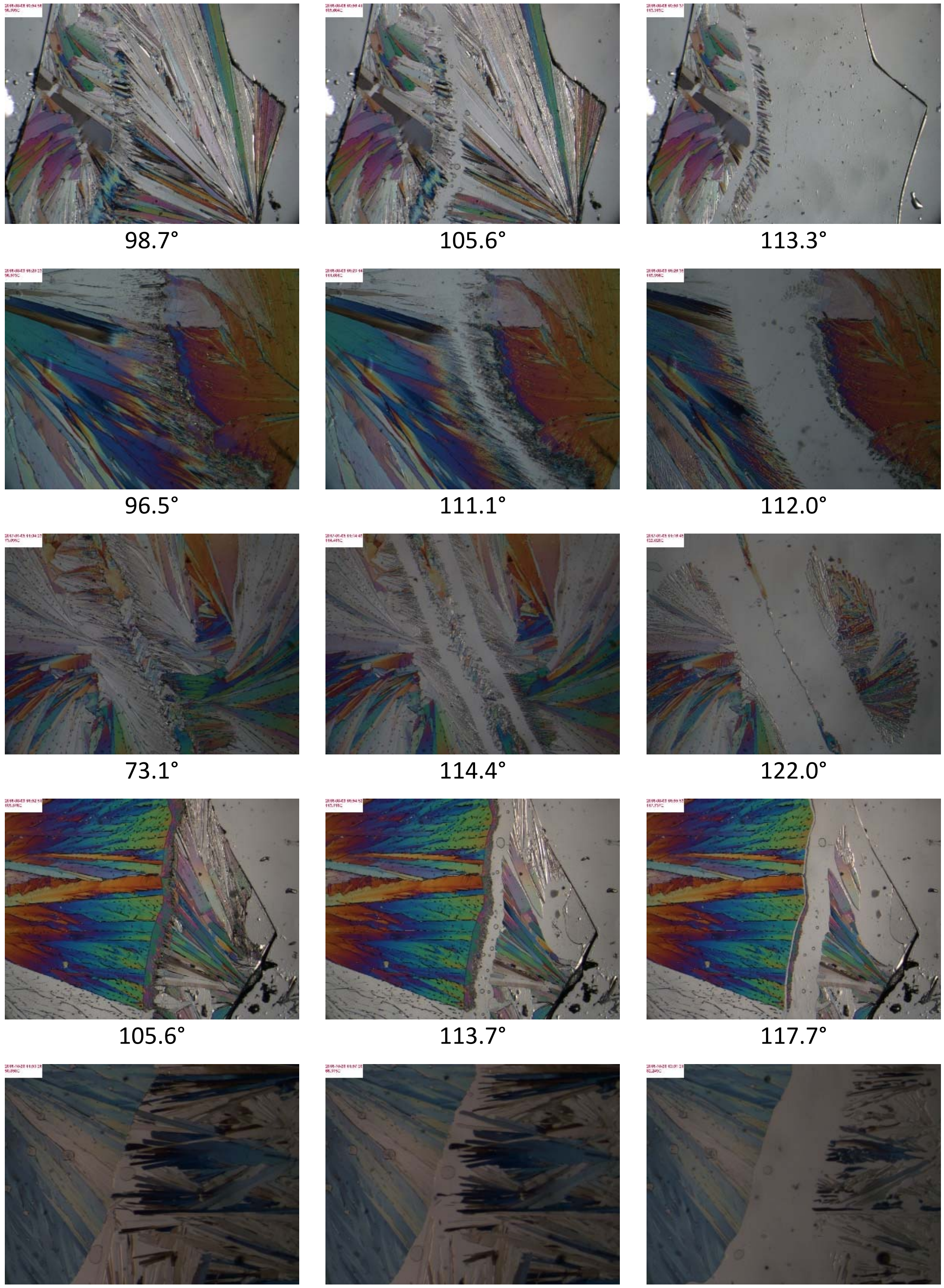
Chloride

(S)-Cl
(R)-CN


86.4°


95.0°


100.1°



(*S*)-Cl (*R*)-Me: 98.7°, 105.6°, 113.3°

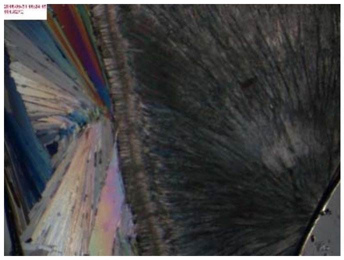
(*S*)-Cl (*R*)-Nitro: 96.5°, 111.1°, 112.0°

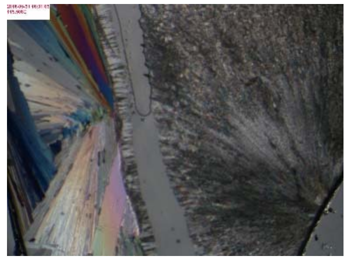
(*S*)-Cl (*R*)-Br: 73.1°, 114.4°, 122.0°

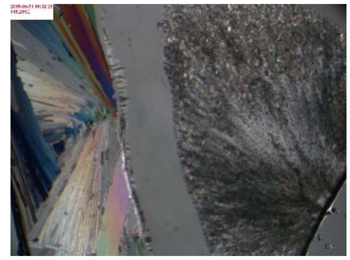
(*S*)-Cl (*R*)-CF_3: 105.6°, 113.7°, 117.7°

(*R*)-Cl (*S*)-OMe: 50.9°, 66.3°, 82.2°

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


101.8°


115.5°


118.2°

(*R*)-Cl
(*S*)-Phenyl

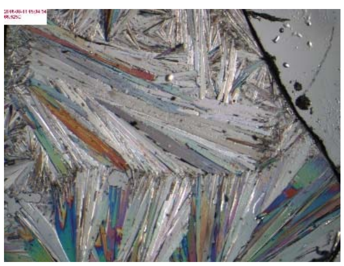

63.3°

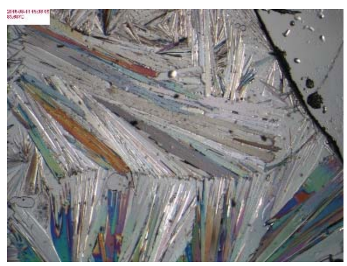

95.2°

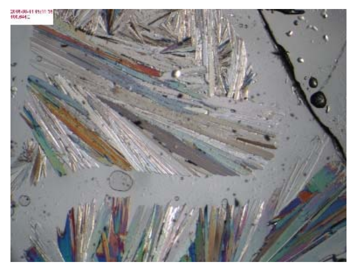

112.1°

Cyano

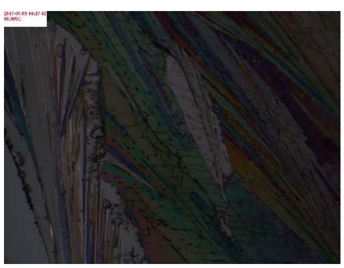
(*S*)-Me
(*R*)-CN

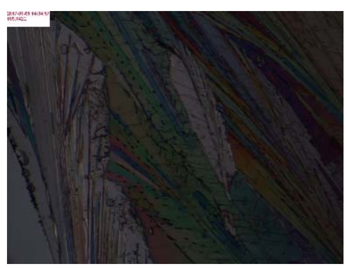

66.5°


83.7°


100.6°

(*R*)-CN
(*S*)-Nitro


80.9°


109.7°


121.7°

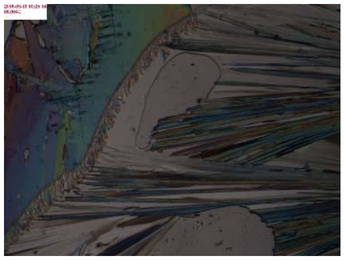
(*S*)-Br
(*R*)-CN

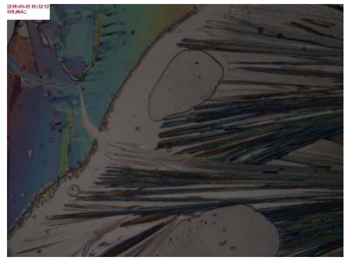

70.5°

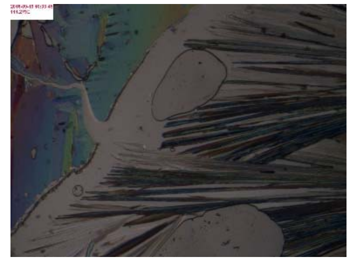

95.2°


99.1°

(*S*)-CF_3
(*R*)-CN

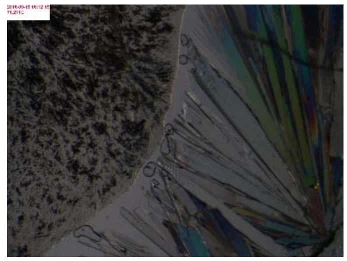

86.0°

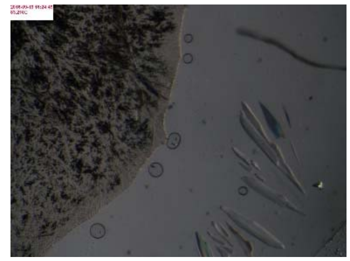

108.6°


111.3°

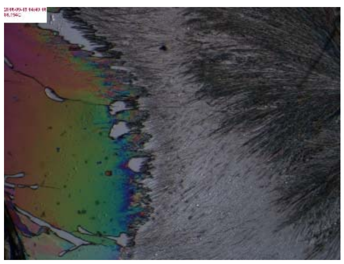
(*R*)-CN
(*S*)-OMe

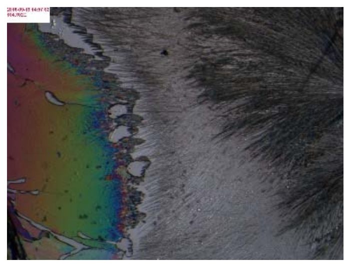

42.1°

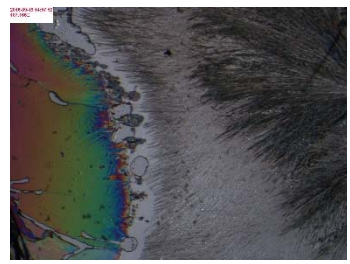

71.2°


83.2°

(*S*)-I
(*R*)-CN


81.2°


104.7°


107.2°

(*S*)-Phenyl
(*R*)-CN

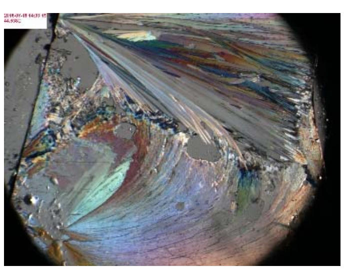

56.9°

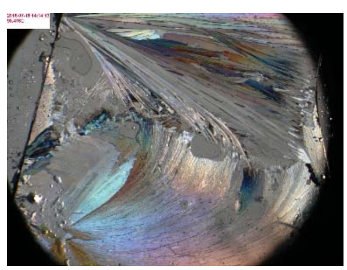

79.2°

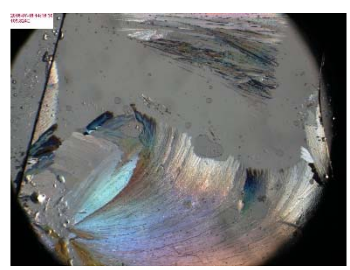

90.5°

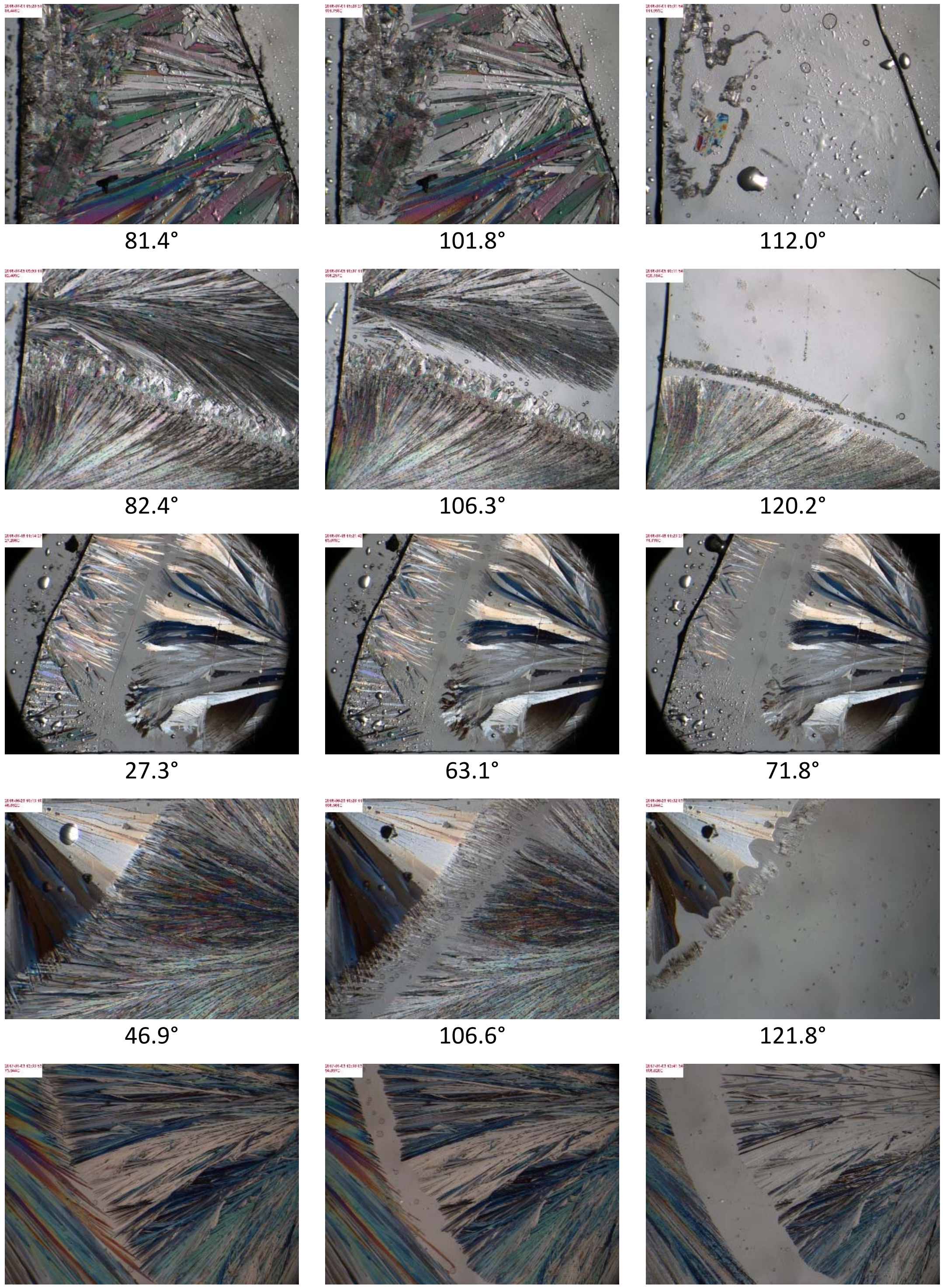
Methyl

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


44.5°


98.5°


109.8°



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

81.4° | 101.8° | 112.0°

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

82.4° | 106.3° | 120.2°

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

27.3° | 63.1° | 71.8°

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

46.9° | 106.6° | 121.8°

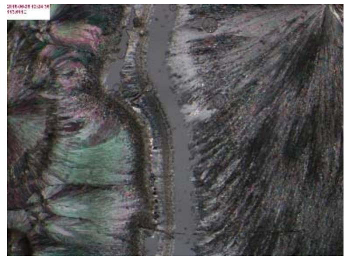
(*S*)-Me
(*R*)-Phenyl

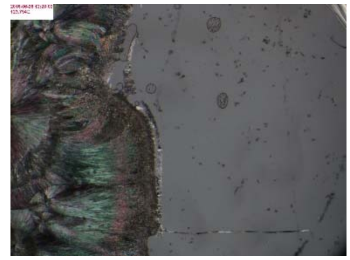
73.9° | 94.9° | 108.8°

Nitro

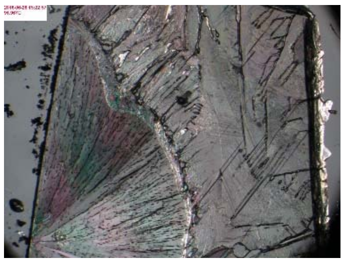
(R)-NO_2
(S)-Br

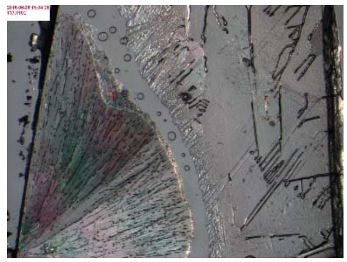

105.0°

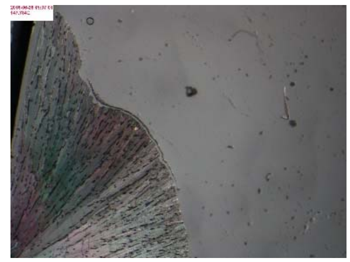

113.6°


123.8°

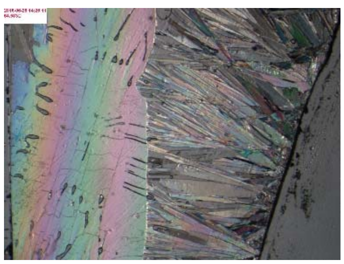
(S)-NO_2
(R)-CF_3

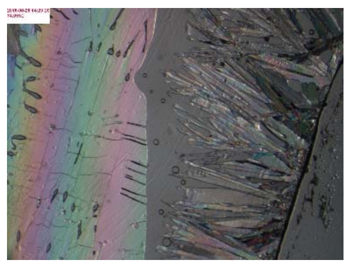

92.0°

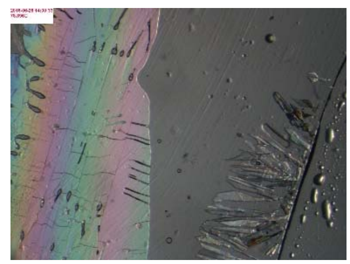

137.7°


147.8°

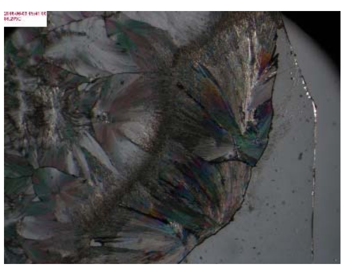
(R)-NO_2
(S)-OMe


64.6°


74.1°


78.9°

(R)-NO_2
(S)-I

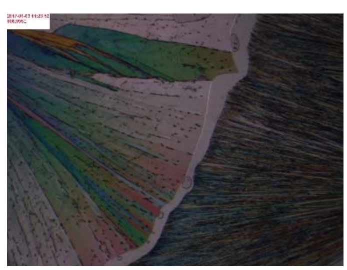

81.3°


118.3°


128.6°

(S)-NO_2
(R)-Phenyl

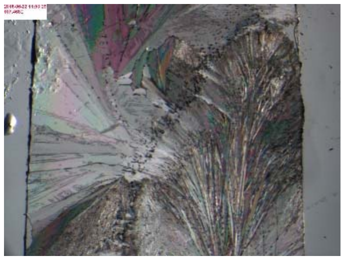

60.4°


107.0°

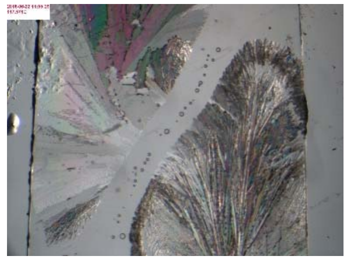

113.1°

Bromide

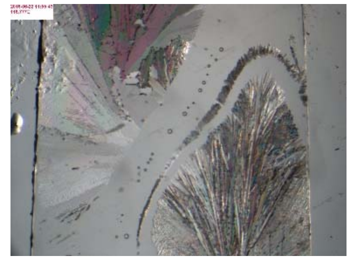
(*S*)-Br
(*R*)-CF_3



107.5°

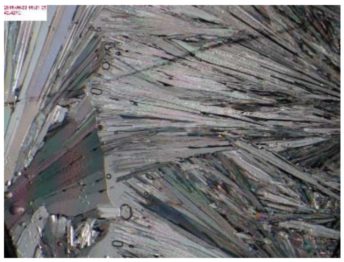


117.6°

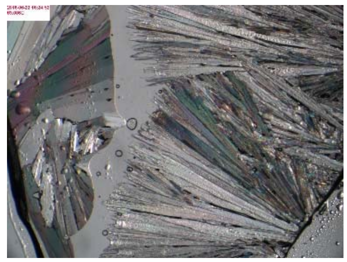


118.8°

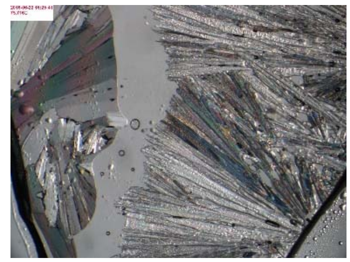
(*S*)-OMe
(*R*)-Br



42.4°

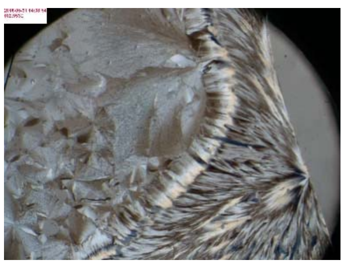


69.1°

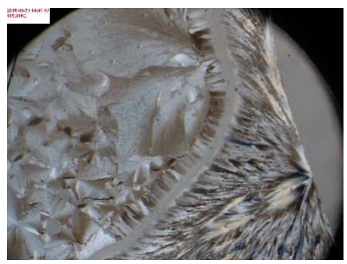


75.7°

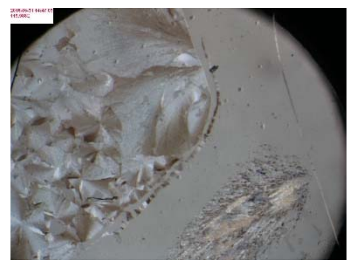
(*S*)-I
(*R*)-Br



103.0°



109.8°



112.0°

(*S*)-Br
(*R*)-Phenyl

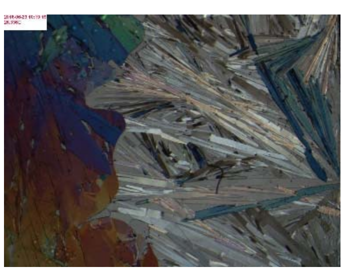
74.6°

97.1°

111.9°

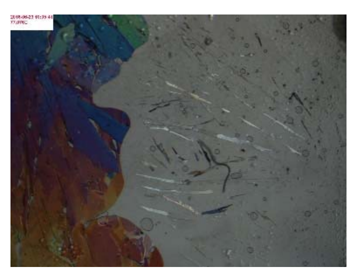
Trifluoromethyl

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



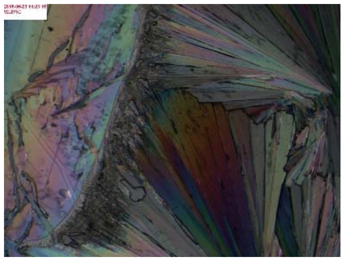
26.3°

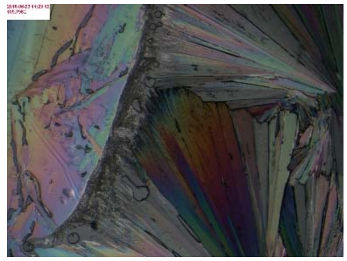
65.4°

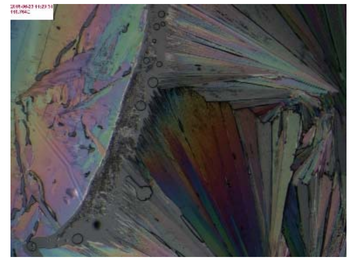


77.1°

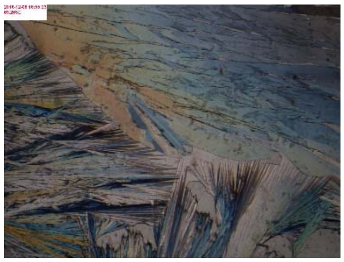
(*S*)-I
(*R*)-CF_3


92.3°

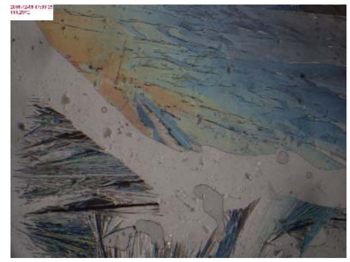

109.8°


110.8°

(*S*)-Phenyl
(*R*)-CF_3


69.3°


95.4°


111.3°

Methoxy

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


42.3°


73.1°


105.5°

(*R*)-Phenyl
(*S*)-OMe

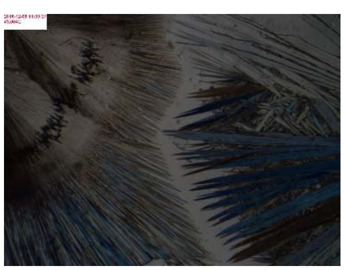

31.0°

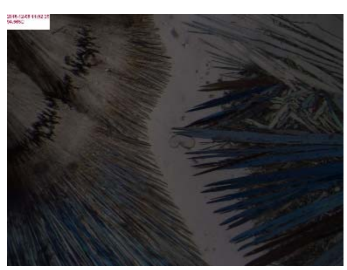

60.2°


78.4°

Iodide

(*R*)-I
(*S*)-Phenyl


43.0°


94.6°

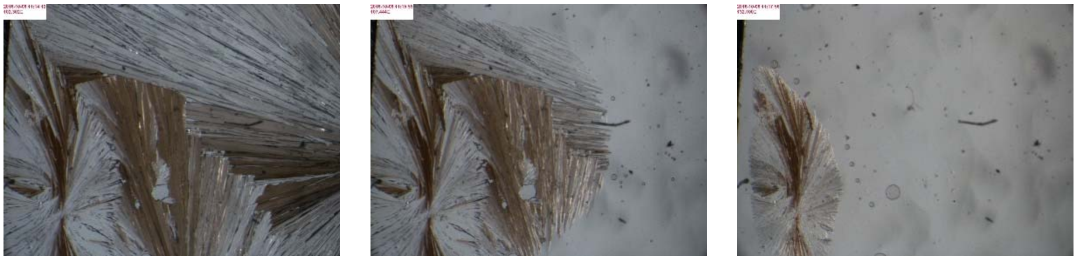

111.6°

Hot Stage Images of Same Handed Homochiral Diarylamide Derivatives

Hydrogen

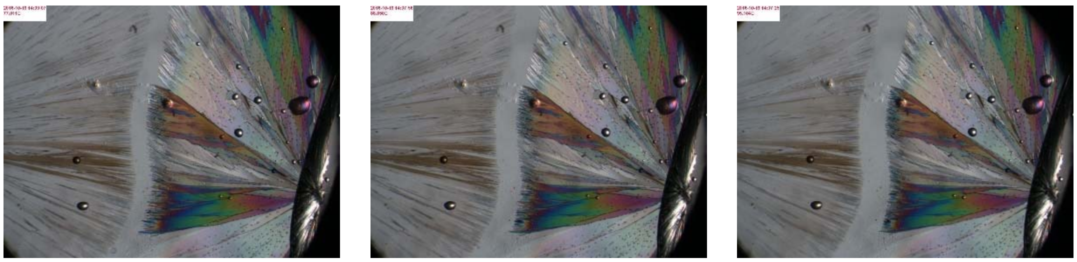
(*R*)-H (left)

(*R*)-F (right)



102.3° 107.4° 132.1°

(*S*)-Cl
(*S*)-H



77.0° 88.9° 95.1°

(*R*)-H
(*R*)-CN

86.6° 122.5° 130.3°

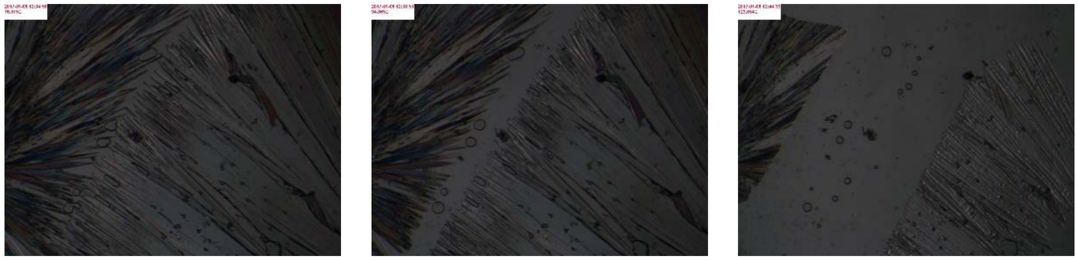
(*S*)-H
(*S*)-Me

90.2° 102.4° 109.0°

(*S*)-NO_2
(*S*)-H

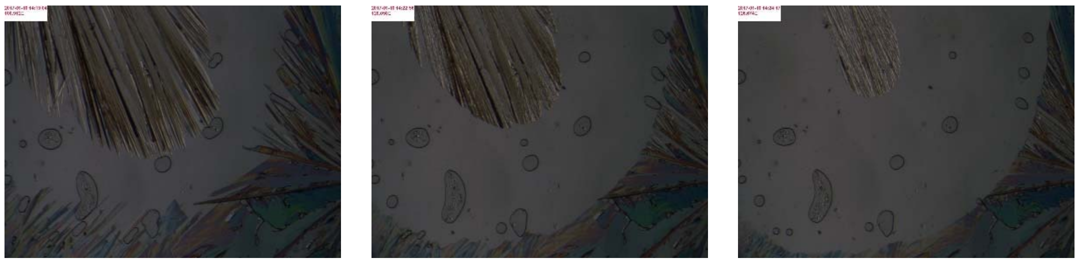
93.5° 118.3° 135.4°

(*S*)-H
(*S*)-Br



76.5° 94.9° 123.1°

(*S*)-H
(*S*)-CF_3



100.9° 120.1° 126.7°

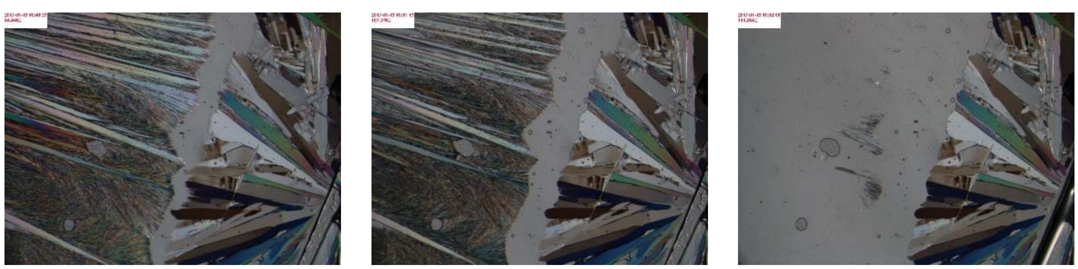
(*S*)-OMe
(*S*)-H

62.2° 78.2° 80.1°

(*S*)-I
(*S*)-H

90.1° 126.4° 132.2°

(*R*)-Phenyl
(*R*)-H



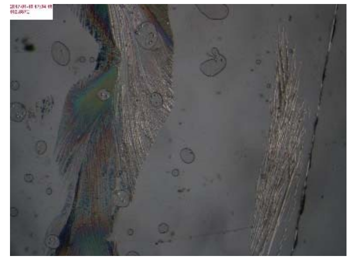
84.0° 107.4° 111.9°

Fluoride

(S)-Cl
(S)-F


65.6°

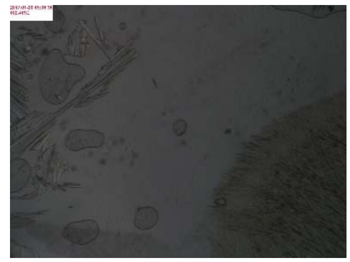

90.3°


102.9°

(R)-F
(R)-CN


89.9°

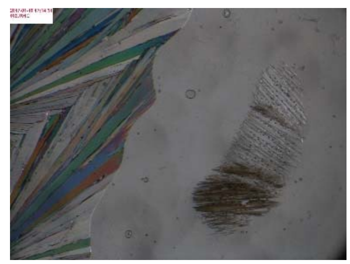

100.5°


102.4°

(S)-Me
(S)-F

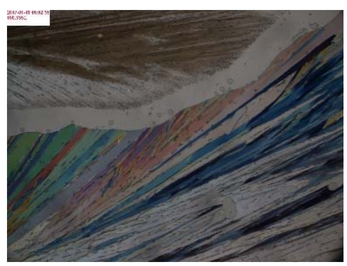

64.4°

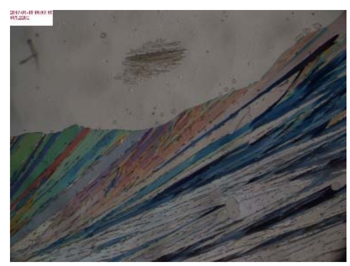

87.8°


102.7°

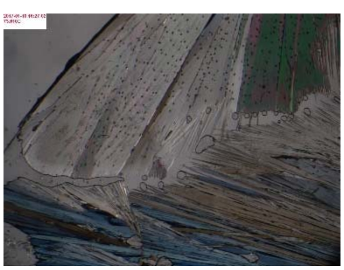
(S)-F
(S)-NO_2


72.4°

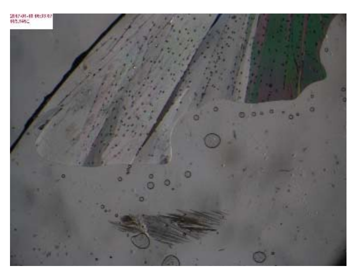

100.3°


103.2°

(S)-Br
(S)-F


73.6°

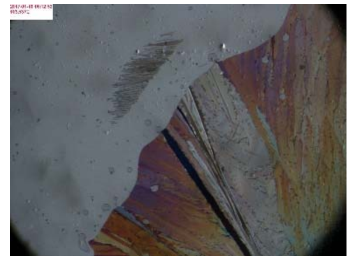

100.2°


103.7°

(*S*)-F
(*S*)-CF_3

62.4°

97.9°



103.5°

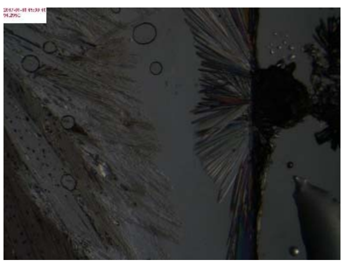
(*S*)-F
(*S*)-OMe

55.1°

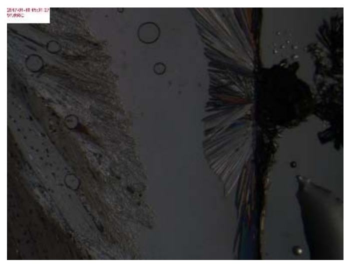
75.6°

78.3°

(*S*)-F
(*S*)-I



91.3°

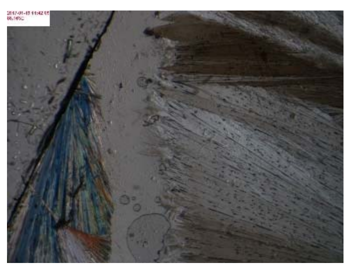


97.7°

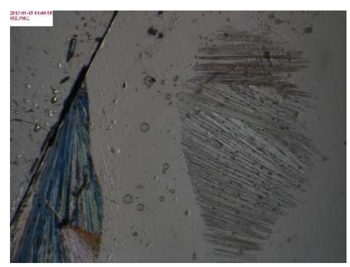
103.6°

(*R*)-Phenyl
(*R*)-F

75.9°



88.2°



102.8°

Chloride

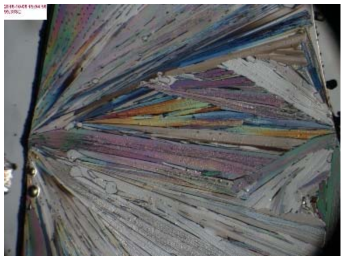
(*R*)-Cl
(*R*)-CN

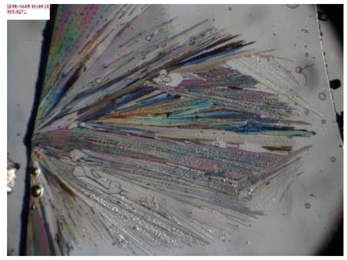
78.5°

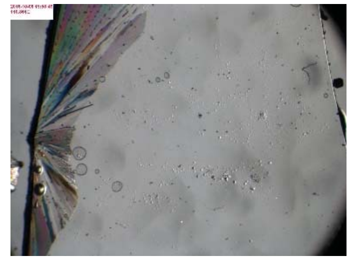
113.7°

119.3°

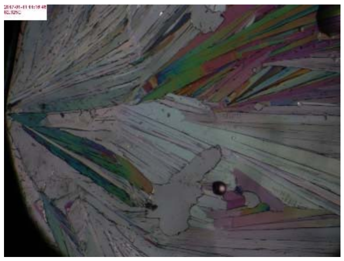
(*S*)-Cl
(*S*)-Me


99.4°

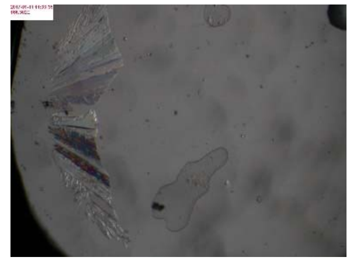

103.5°


110.9°

(*S*)-NO_2
(*S*)-Cl

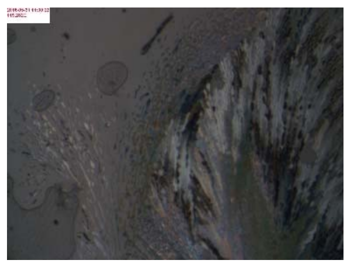

82.2°


122.6°


166.3°

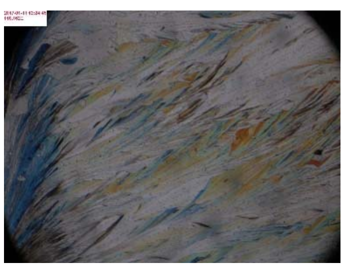
(*R*)-Cl
(*R*)-Br


112.7°

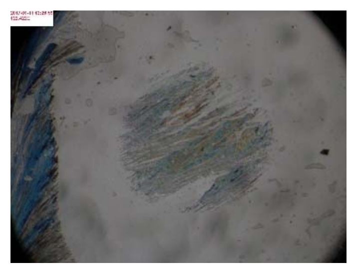

119.3°


121.0°

(*S*)-CF_3
(*S*)-Cl

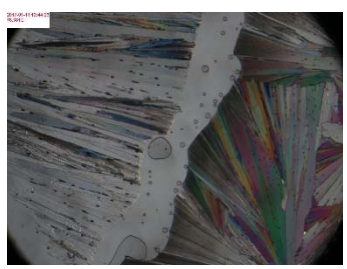

110.2°


119.8°


122.4°

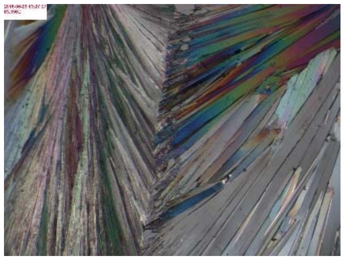
(*S*)-OMe
(*S*)-Cl

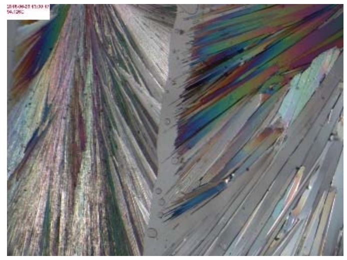

63.3°

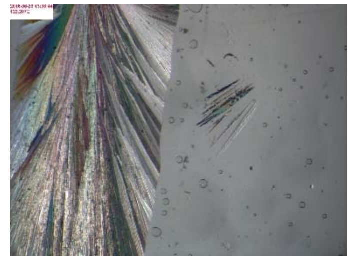

78.4°


78.0°

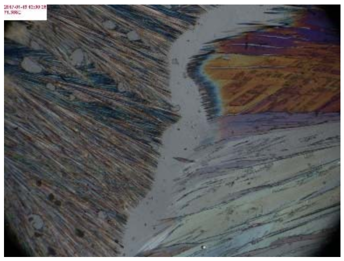
(*R*)-I
(*R*)-Cl

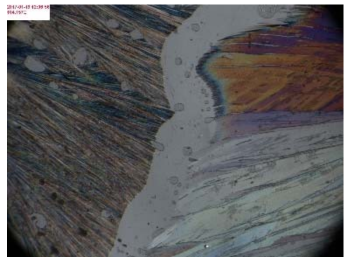

63.4°

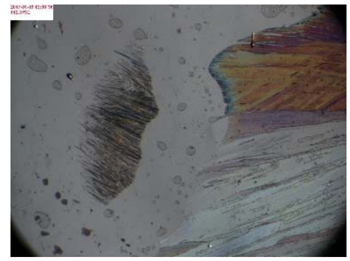

94.1°


122.2°

(*R*)-Phenyl
(*R*)-Cl


71.4°


104.2°


112.4°

Cyano

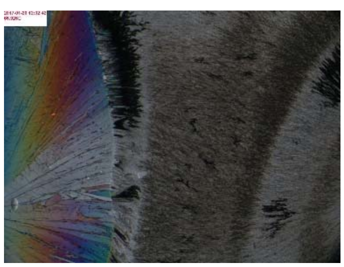
(*R*)-Me
(*R*)-CN


86.2°

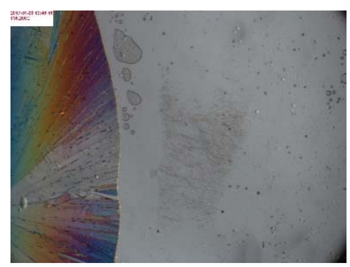

109.1°


111.3°

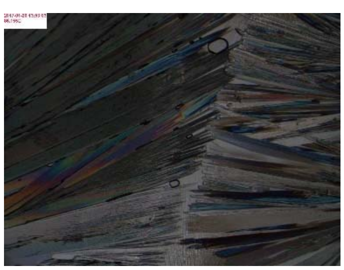
(*R*)-NO_2
(*R*)-CN

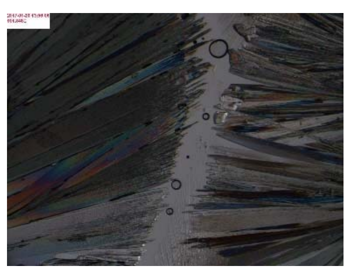

66.9°


126.1°


136.2°

(*R*)-Br
(*R*)-CN


86.2°


101.8°


122.2°

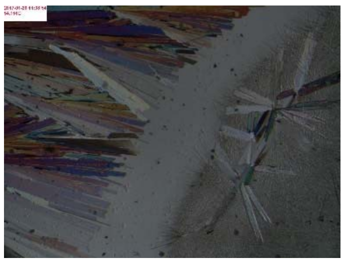
(*R*)-CF_3
(*R*)-CN

106.5°

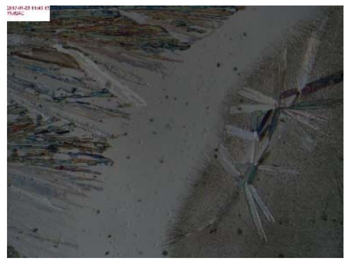
126.2°

134.9°

(*R*)-OMe
(*R*)-CN



54.2°



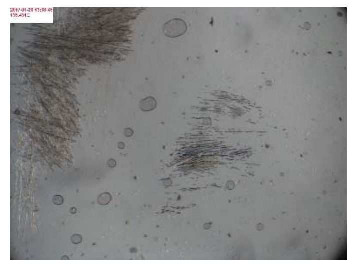
75.6°

78.1°

(*R*)-CN
(*R*)-I

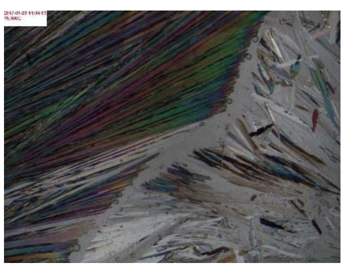
84.0°

121.4°

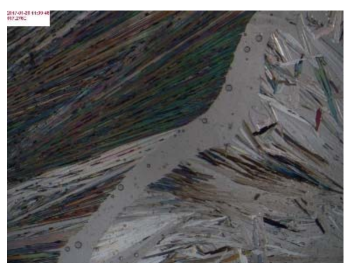


135.4°

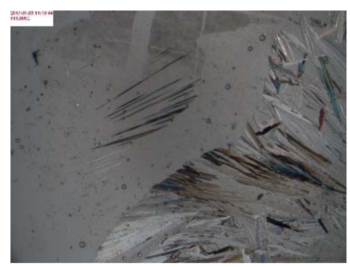
(*R*)-Phenyl
(*R*)-CN



78.6°



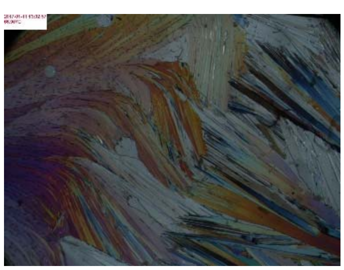
107.3°



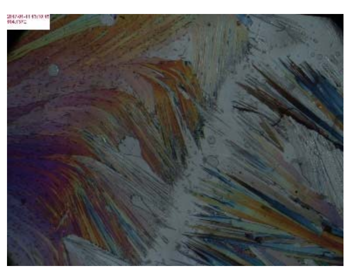
111.8°

Methyl

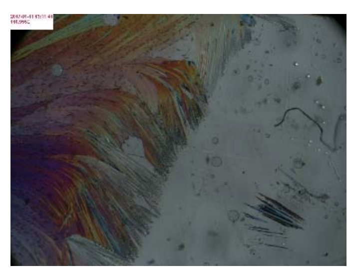
(*S*)-NO_2
(*S*)-Me



66.9°

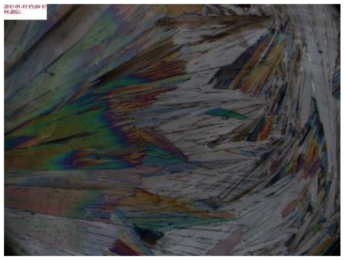


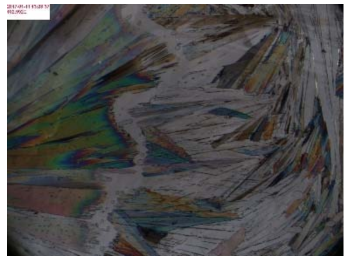
104.1°

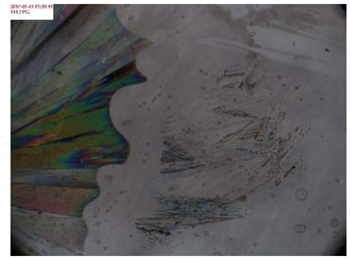


111.0°

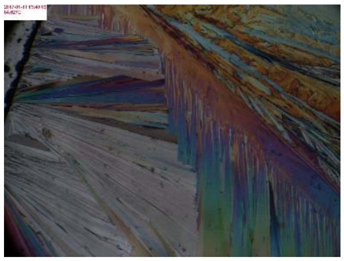
(*S*)-Br
(*S*)-Me


81.3°

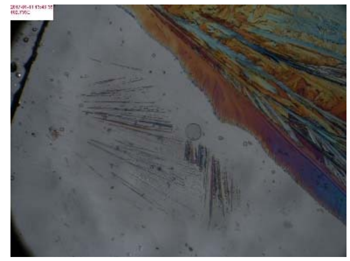

103.0°


111.1°

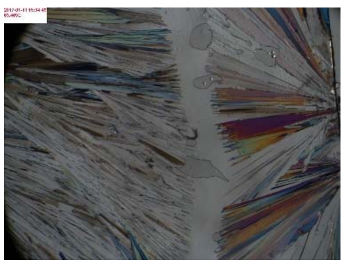
(*R*)-CF_3
(*R*)-Me

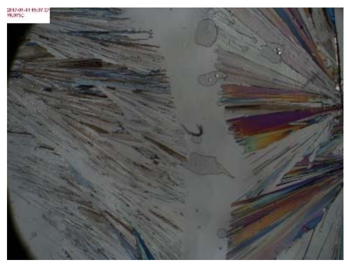

84.6°

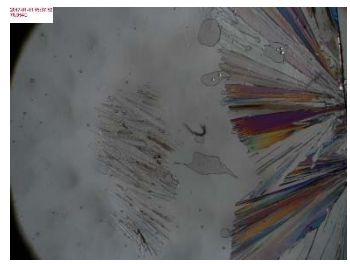

100.9°


102.7°

(*S*)-OMe
(*S*)-Methyl


63.5°

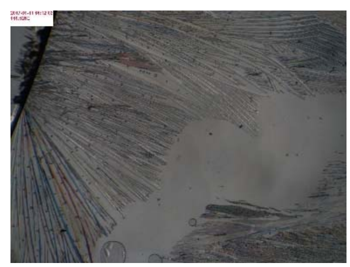

77.0°


79.0°

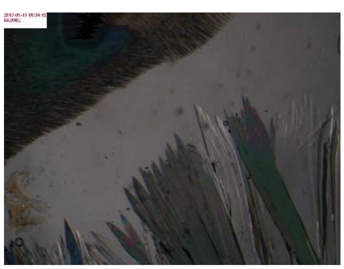
(*R*)-I
(*R*)-Me

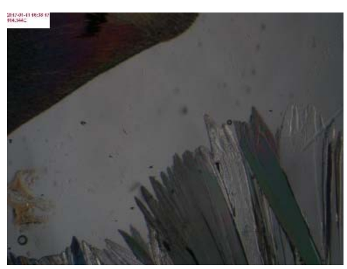

60.2°


101.3°


110.5°

(*R*)-Phenyl
(*R*)-Me

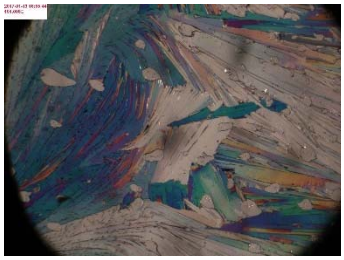

84.1°


104.3°

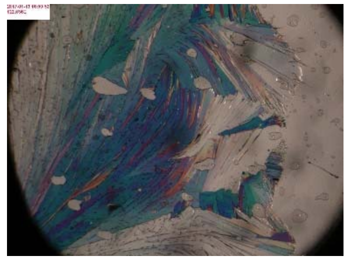

110.7°

Nitro

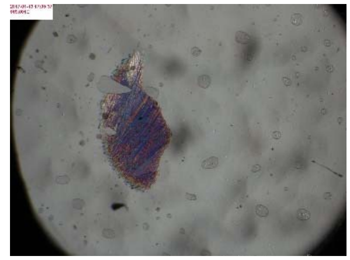
(*S*)-NO_2
(*S*)-Br



101.0°

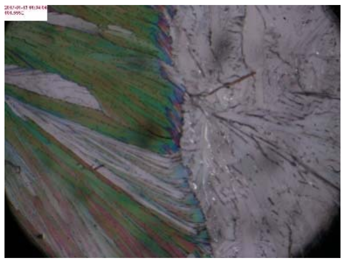


122.0°



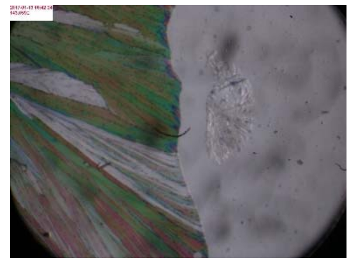
169.0°

(*S*)-NO_2
(*S*)-CF_3



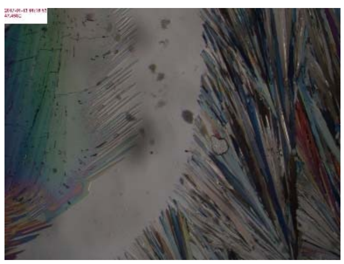
101.6°

140.3°

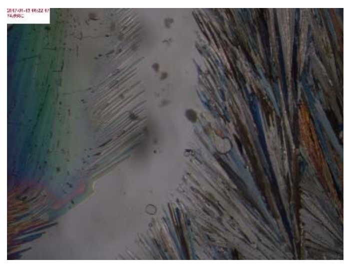


143.1°

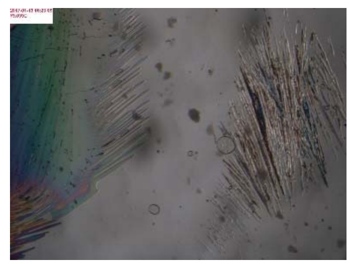
(*S*)-NO_2
(*S*)-OMe



47.5°



74.7°

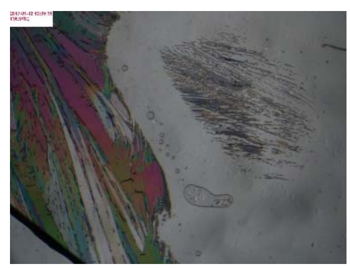


79.0°

(*S*)-NO_2
(*S*)-I

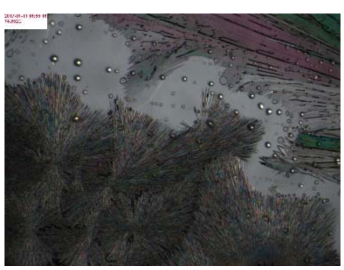
86.2°

120.8°

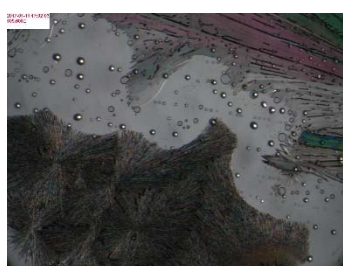


137.0°

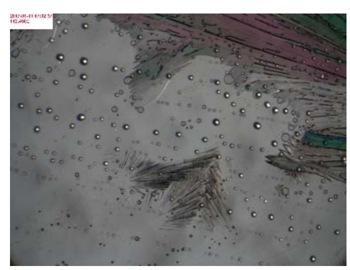
(*R*)-NO_2
(*R*)-Phenyl



74.9°



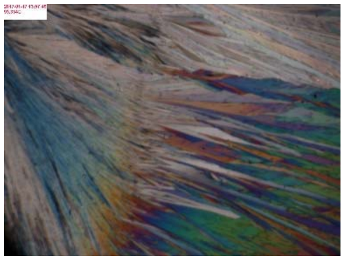
109.7°

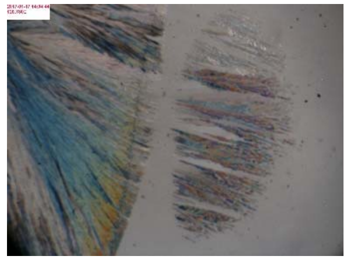


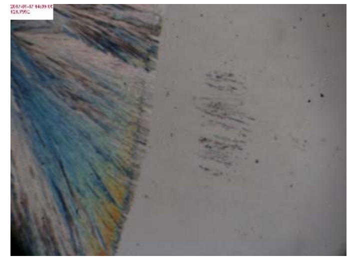
112.5°

Bromide

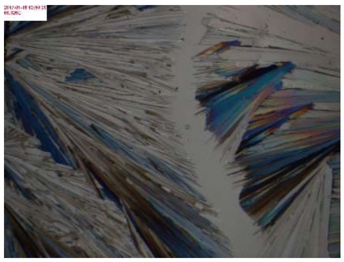
(*R*)-CF_3
(*R*)-Br

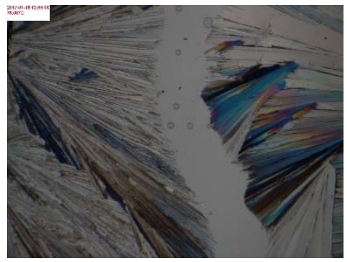

93.3°


120.8°


121.8°

(*S*)-OMe
(*S*)-Br


61.3°


76.1°


78.7°

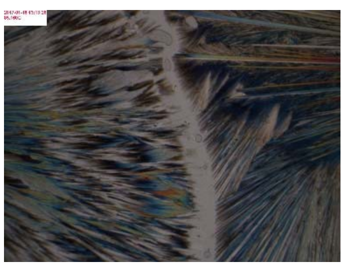
(*S*)-I
(*S*)-Br


96.2°

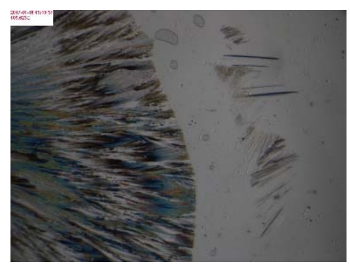

113.5°


121.4°

(*S*)-Br
(*S*)-Phenyl

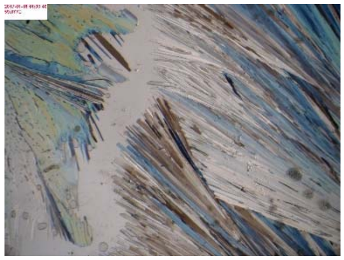

85.2°

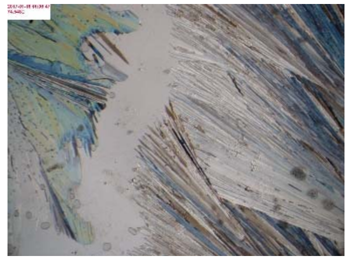

106.6°

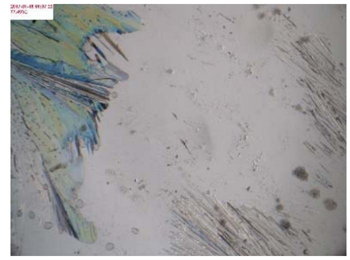

109.6°

Trifluoromethyl

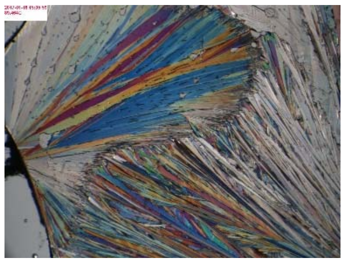
(S)-CF_3
(S)-OMe

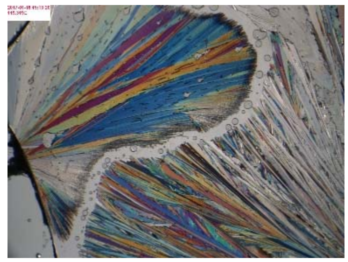

59.1°

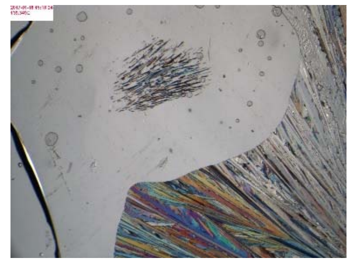

74.5°


77.5°

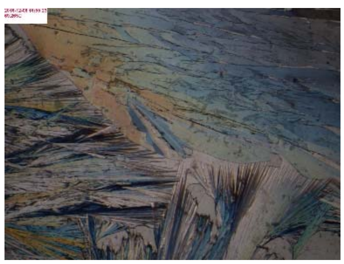
(S)-I
(S)-CF_3

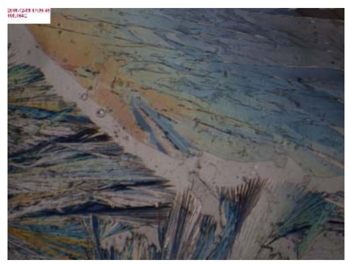

89.5°

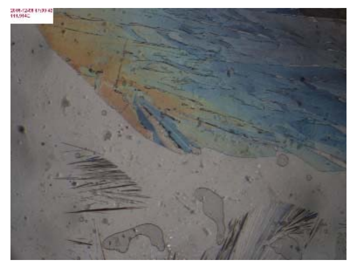

119.3°


139.3°

(R)-CF_3
(R)-Phenyl

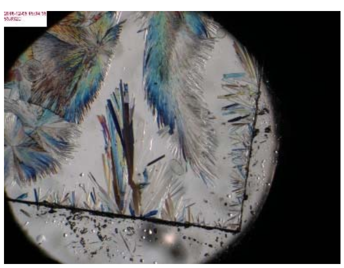

69.3°

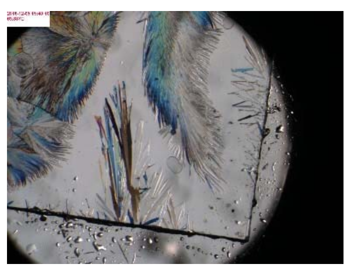

100.2°


111.9°

Methoxy

(S)-I
(S)-OMe


53.8°


69.9°


77.6°

(R)-OMe
(R)-Phenyl

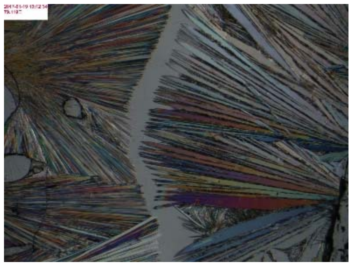

46.1°


73.1°

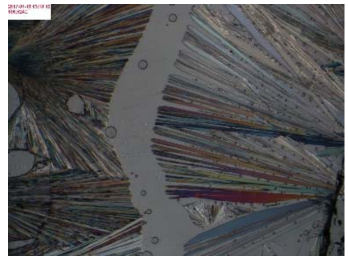

78.0°

Iodide

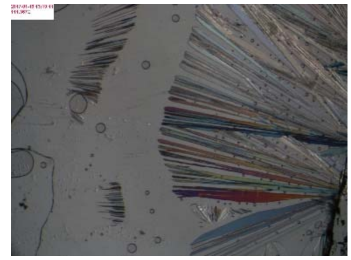
(*R*)-Phenyl
(*R*)-I



79.1°



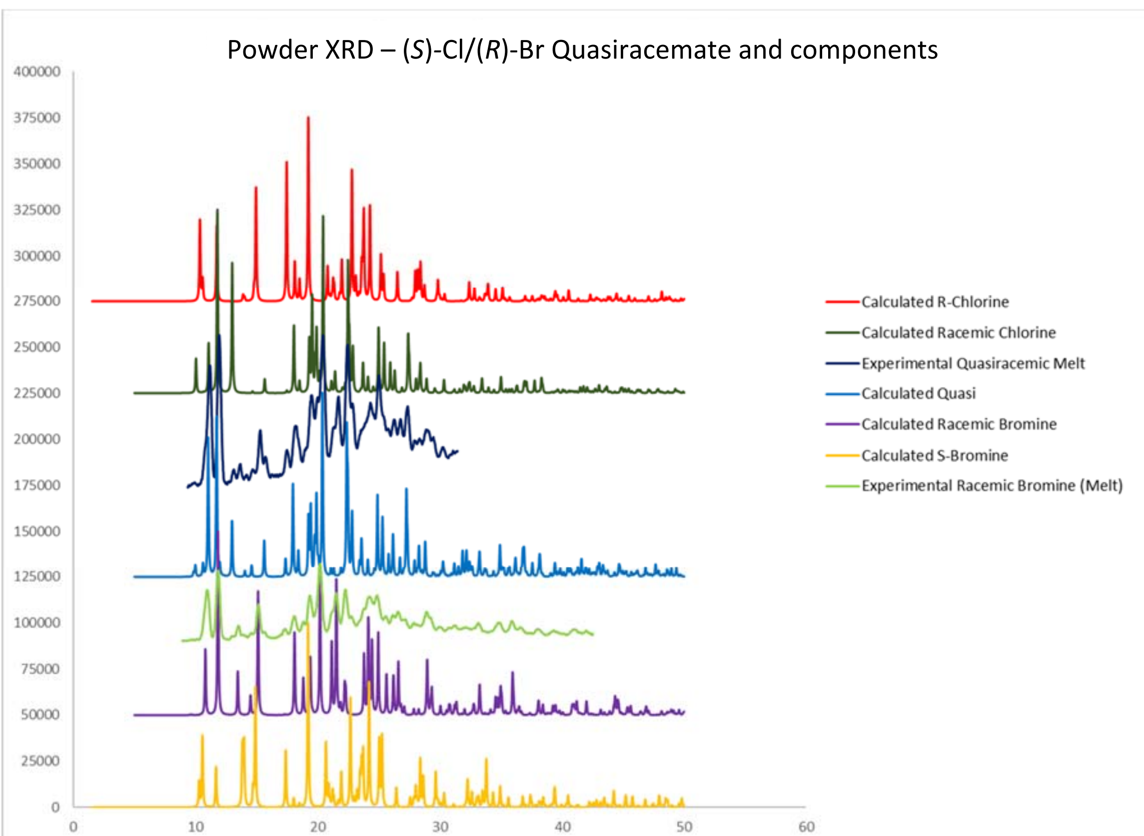
106.5°

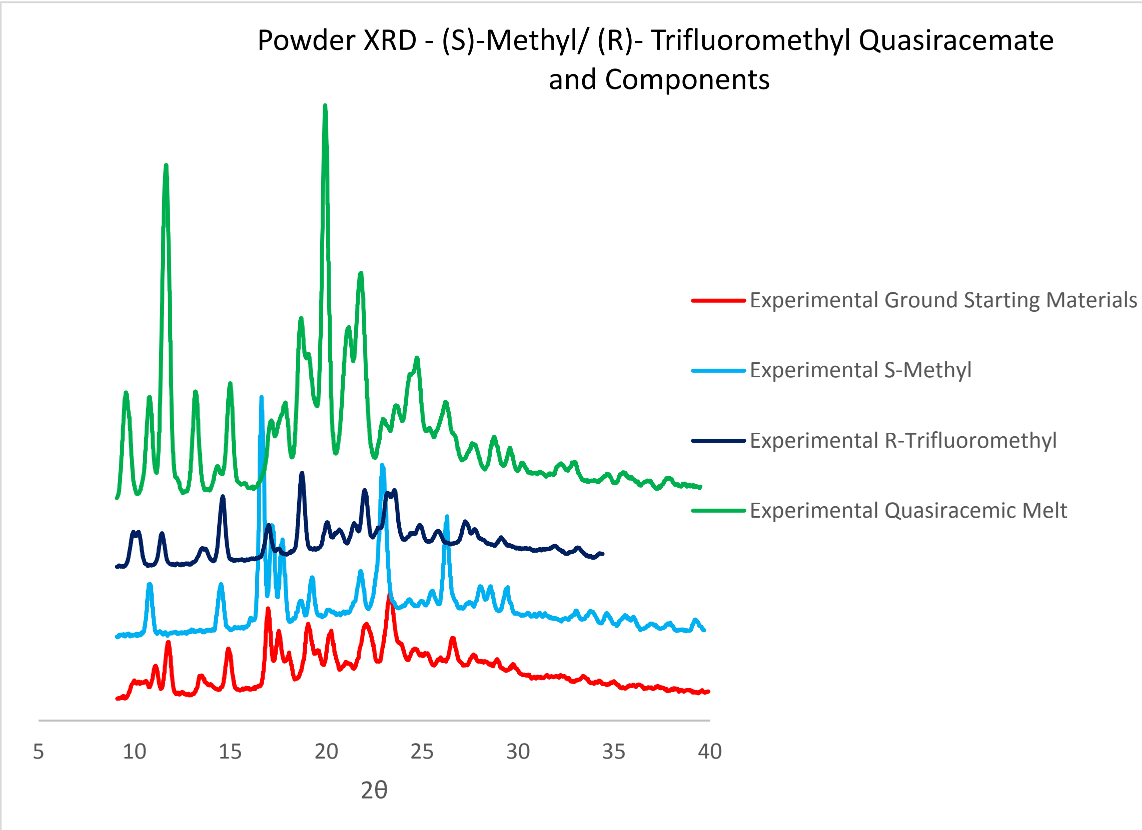


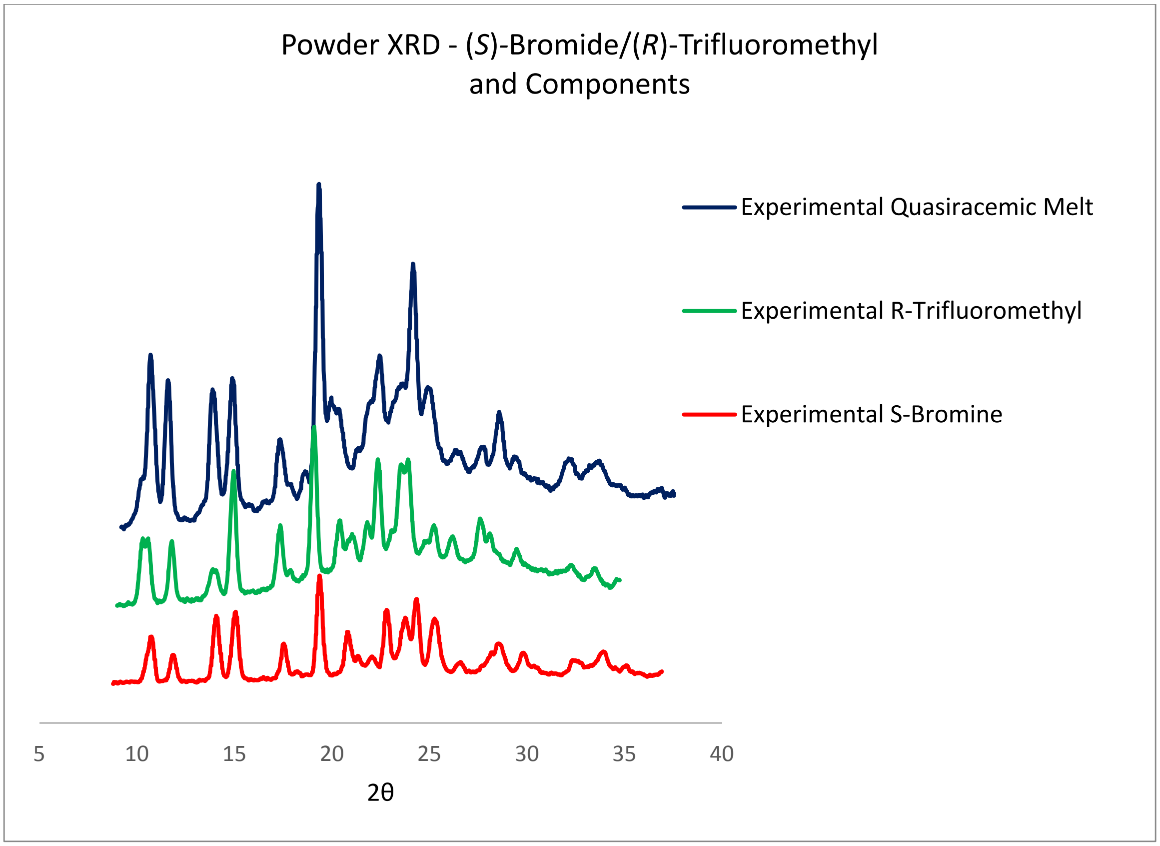
111.4°

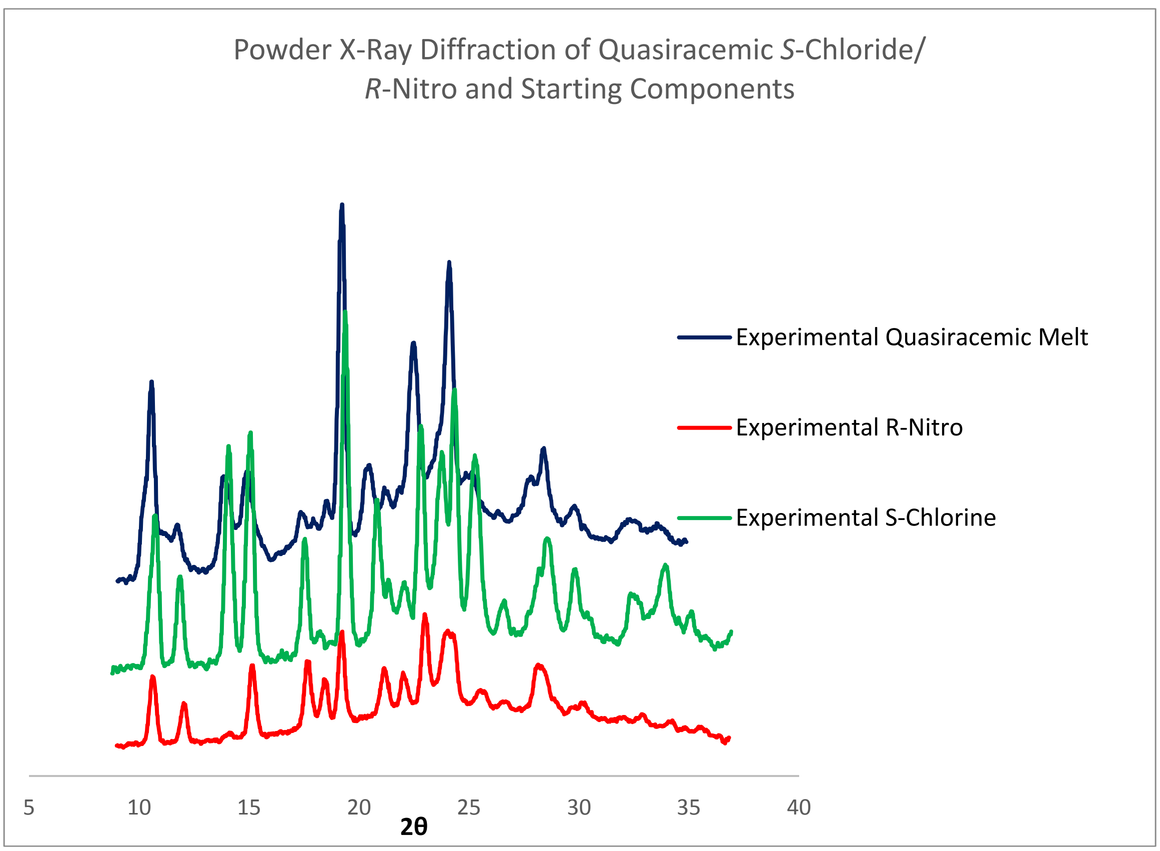
S3. X-ray Crystallography - Powder Diffraction

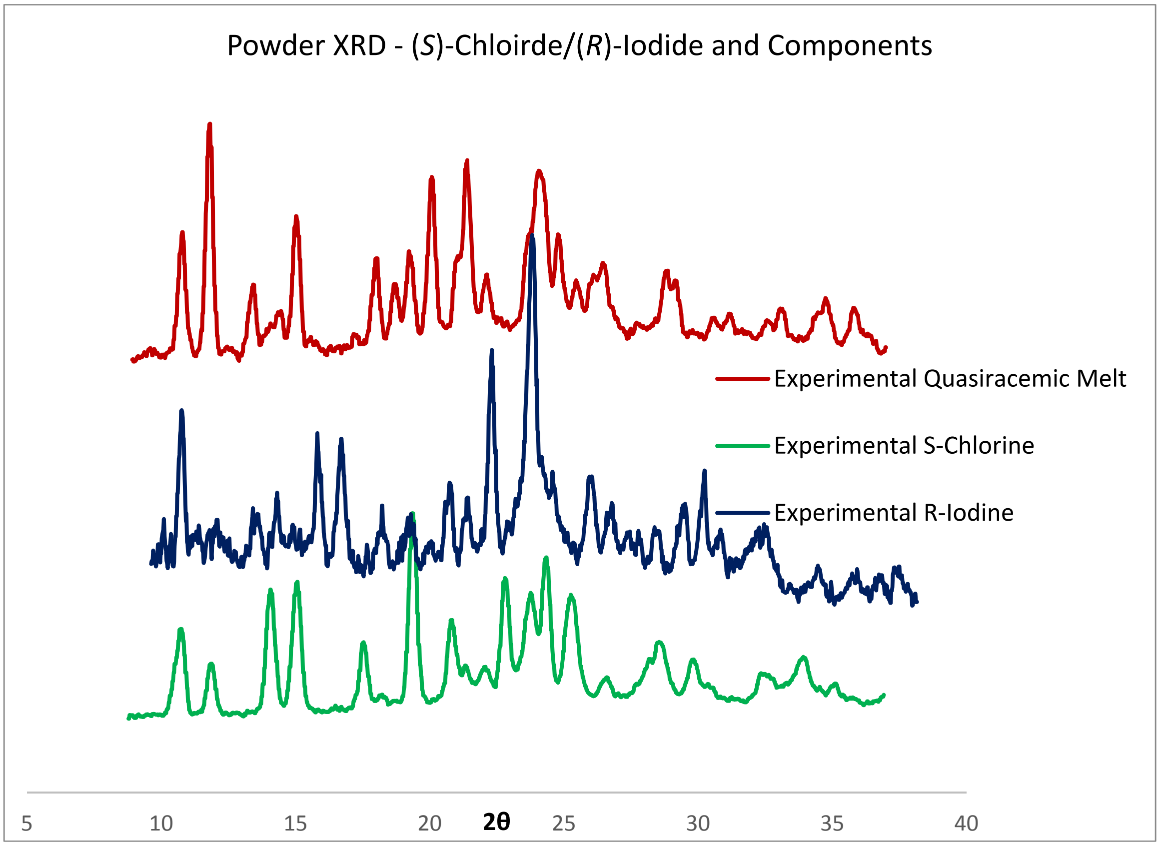
Powder X-ray diffraction data were collected on a Bruker APEX II CCD diffractometer using phi and omega scans with graphite monochromatic Cu Mo $K\alpha$ (λ = 1.54178 Å) radiation. Data sets were collected at a detector distance of 15 cm using 4 Phi scans with 10° increments in 2θ (-20° → -50°) and omega (170° → 140°). The images were integrated using the APEX II XRD^2 plugin.




Powder XRD - (S)-Methyl/ (R)- Trifluoromethyl Quasiracemate and Components
Experimental Ground Starting Materials
Experimental S-Methyl
Experimental R-Trifluoromethyl
Experimental Quasiracemic Melt
5
10
15
20
25
30
35
40
2θ


Powder XRD - (S)-Bromide/(R)-Trifluoromethyl and Components
Experimental Quasiracemic Melt
Experimental R-Trifluoromethyl
Experimental S-Bromine
5
10
15
20
25
30
35
40
2θ


Powder X-Ray Diffraction of Quasiracemic S-Chloride/ R-Nitro and Starting Components
Experimental Quasiracemic Melt
Experimental R-Nitro
Experimental S-Chlorine
5
10
15
20
25
30
35
40
2θ



S4. X-ray Crystallography – Single Crystal Diffraction

Crystallographic details for each diarylamide quasiracemate are summarized in Table S1. X-ray data were collected on a Bruker APEX II CCD diffractometer using phi and omega scans with graphite monochromatic Cu Mo $K\alpha$ (λ = 1.54178 Å) radiation. Data sets were corrected for Lorentz and polarization effects as well as absorption. The criterion for observed reflections is $I > 2\sigma(I)$. Lattice parameters were determined from least-squares analysis and reflection data. Empirical absorption corrections were applied using SADABS.[2] Structures were solved by direct methods and refined by full-matrix least-squares analysis on F^2 using X-SEED[3] equipped with SHELXS[4]. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using the SHELXL[4] program. H atoms (for OH and NH) were located in difference Fourier synthesis and refined isotropically with independent O/N-H distances or restrained to 0.85(2) Å.

2. G. M. Sheldrick, SADABS and TWINABS—Program for Area Detector Absorption Corrections, University of Göttingen, Göttingen, Germany, 2010.
3. L. J. Barbour, *J. Supramol. Chem*., 2001, **1**, 189.
4. G. M. Sheldrick, *Acta Crystallogr., Sect. A: Fundam. Crystallogr*., 2008, **64**, 112.

The remaining H atoms were included in idealized geometric positions with U_{iso}=1.2U_{eq} of the atom to which they were attached (U_{iso}=1.5U_{eq} for methyl groups). Molecular configurations were compared to both the known chirality of the methylbenzylamine and estimated Flack parameters[5] and where applicable, atomic coordinates were inverted to achieve correct structural configurations. Hydrogen bond parameters are given in Table S2.

Table S1. Crystallographic data for diarylamide quasiracemates.

	(*R*)-Cl/(*S*)Br[1]	(±)-Br[1]	(*S*)-H/(*R*)-F	(*S*)-NO_2/(*R*)-CF_3
Crystal data				
CCDC deposit no.	LUNQIU	LUNQEQ	1534590	1534591
Empirical formula	$C_{30}H_{28}BrClN_2O_2$	$C_{15}H_{14}NOBr$	$C_{30}H_{14}FN_2O_2$	$C_{31}H_{28}F_3N_3O_3$
Crystal System, space group	Monoclinic $P2_1$ (no. 4)	Orthorhombic *Pbca* (no. 61)	Triclinic *P*1 (no. 1)	Monoclinic $P2_1$ (no. 4)
M_r	563.90	304.18	468.55	563.56
a, Å	8.7790(8)	9.4207(7)	5.3540(2)	8.3035(14)
b, Å	17.699(2)	16.361(1)	8.3824(4)	9.6853(13)
c, Å	9.4652(9)	18.348(2)	13.8585(7)	17.333(3)
α, deg	90	90	96.477(3)	90
β, deg	108.391(8)	90	93.829(3)	101.057(9)
γ, deg	90	90	105.841(3)	90
V, (Å^3)	1395.6(2)	2828.0(4)	591.42(5)	1368.0(4)
Z, *Z'*	2, 1	8, 1	1, 1	2, 1
D_{calc} (g cm^{-3})			1.316	1.368
μ (mm^{-1}), rad. type			0.705, Cu $K\alpha$	0.882, Cu $K\alpha$
F_{000}			248	588
temp (K)			100(2)	100(2)
Crystal form, color			plate, colorless	plate, colorless
Crystal size, mm			0.39 x 0.07 x 0.07	0.26 x 0.01 x 0.03
Data collection				
Diffractometer			Bruker Apex II	Bruker Apex II
T_{min}/ T_{max}			0.653/0.753	0.591/0.753
No. of refls. (meas., uniq., and obs.)			13271/3785/2730	20018/4899/3797
R_{int}			0.0760	0.0992
ϑ_{max} (°)			68.25	68.22
Refinement				
R/R^2_{ω} (obs data)			0.0668/0.1661	0.0616/0.1599
R/R^2_{ω} (all data)			0.0946/0.1886	0.0787/0.1708
S			1.045	1.061
No. of refls.			3785	4899
No. of parameters			406	380
$\Delta\rho_{max/min}$ (e·Å^{-3})			0.638/-0.204	0.341/-0.350
flack			-0.1(4)	0.23(15)

[5] H. D. Flack, *Acta Crystallogr.,* 1983, **39**¸ 876-881.

Table S1. Crystallographic data for diarylamide quasiracemates. (Continued)

	(*R*)-CH_3/(*S*)-CF_3	(*R*)-NO_2/(*S*)-Br	(*R*)-CF_3/(*S*)-I	(*S*)-OMe
Crystal data				
CCDC deposit no.	1534592	1534593	1534594	1534589
Empirical formula	$C_{32}H_{31}F_3N_2O_2$	$C_{30}H_{28}BrN_3O_4$	$C_{31}H_{28}F_3IN_2O_2$	$C_{16}H_{17}NO_2$
Crystal System, space group	Monoclinic $P2_1$ (no. 4)	Monoclinic $P2_1$ (no. 4)	Orthorhombic $P2_12_12_1$ (no. 19)	Orthorhombic $P2_12_12_1$ (no. 19)
M_r	532.59	574.46	644.45	255.30
a, Å	8.7183(13)	8.2953(5)	9.4943(2)	5.8757(10)
b, Å	18.007(2)	9.5761(5)	16.1705(4)	14.464(2)
c, Å	9.5051(11)	17.2423(9)	18.3454(5)	15.887(3)
α, deg	90	90	90	90
β, deg	106.811(8)	101.342(3)	90	90
γ, deg	90	90	90	90
V, (Å^3)	1428.4(3)	1342.92(13)	2816.52(12)	1350.2(4)
Z, *Z'*	2, 1	2, 1	4, 1	4, 1
D_{calc} (g cm^{-3})	1.572	1.421	1.520	1.256
μ (mm^{-1}), rad. type	0.748, Cu $K\alpha$	2.420, Cu $K\alpha$	9.367, Cu $K\alpha$	0.661, Cu $K\alpha$
F_{000}	560	592	1296	544
temp (K)	100(2)	100(2)	100(2)	100(2)
Crystal form, color	plate, colorless	plate, colorless	plate, colorless	block, colorless
Crystal size, mm	0.44 x 0.17 x 0.10	0.15 x 0.11 x 0.03	0.15 x 0.15 x 0.10	0.31 x 0.15 x 0.06
Data collection				
Diffractometer	Bruker Apex II	Bruker Apex II	Bruker Apex II	Bruker Apex II
T_{min}/ T_{max}	0.591/0.753	0.587/0.753	0.532/0.753	0.669/0.753
No. of refls. (meas., uniq., and obs.)	20723/5088/3596	20609/4825/3810	43195/5159/4723	5676/2162/1911
R_{int}	0.0734	0.1097	0.0765	0.0381
ϑ_{max} (°)	68.20	68.25	68.23	68.22
Refinement				
R/R^2_ω (obs data)	0.0515/0.1446	0.0737/0.1536	0.0277/0.0582	0.0371/0.0852
R/R^2_ω (all data)	0.0712/0.1662	0.0967/0.1652	0.0328/0.0612	0.0435/0.0893
S	1.073	1.088	1.004	1.060
No. of refls.	5088	4825	5159	2162
No. of parameters	363	351	362	178
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.157/-0.172	1.047/-0.821	0.624/-0.507	0.172/-0.161
flack	0.0(2)	0.10(2)	-0.005(3)	0.0(2)

Table S2. Hydrogen Bond Parameters for Diarylamide Quasiracemate Structures.

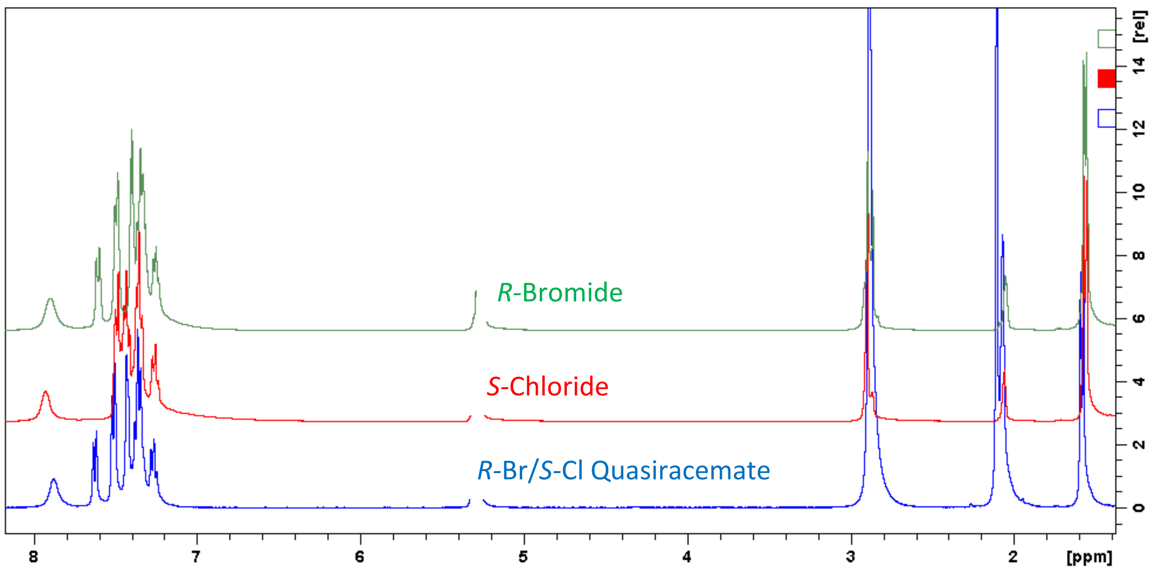
Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
(*S*)-H/(*R*)-H	N1A–H1A···O1A^{i}	0.87(3)	2.33(3)	3.143(6)	156(5)
	N1B–H1B···O1B^{ii}	0.87(3)	2.32(3)	3.122(7)	154(5)
(*S*)-NO_2/(*R*)-CF_3	N1–H1···O1^{iii}	0.86(3)	2.02(3)	2.870(6)	170(9)
	N1A–H1A···O1A^{iv}	0.86(3)	2.02(3)	2.855(6)	164(6)
(*R*)-CH_3/(*S*)-CF_3	N1A–H1A···O1^{v}	0.85(2)	2.08(3)	2.911(5)	164(4)
	N1–H1···O1A^{vi}	0.87(2)	2.11(3)	2.923(5)	156(5)
(*R*)-NO_2/(*S*)-Br	N1–H1···O1^{vii}	0.85(3)	1.97(4)	2.802(11)	166(12)
	N1A–H1A···O1A^{viii}	0.84(2)	2.06(3)	2.871(11)	164(10)
(*R*)-CF_3/(*S*)-I	N1–H1···O1A^{v}	0.82(3)	2.15(3)	2.946(5)	163(5)
	N1A–H1A···O1^{ii}	0.84(2)	2.13(3)	2.948(5)	164(4)
(*S*)-OMe	N1–H1···O2^{v}	0.883(19)	1.94(2)	2.669(3)	139(3)

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

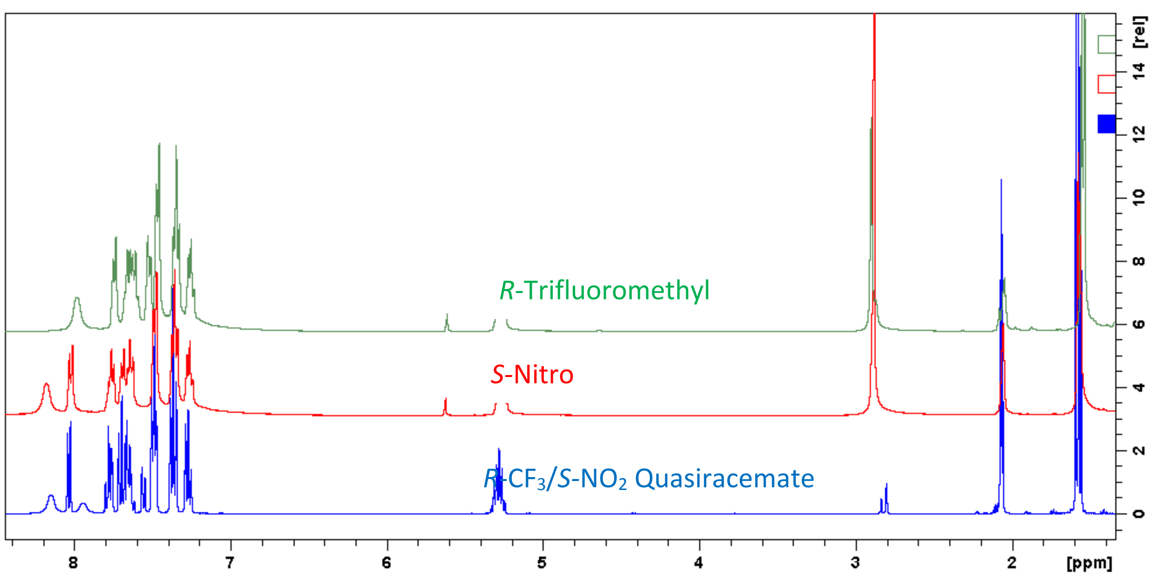
S5. [1]H NMR Overlays

[1]H-NMR (acetone-d_6) spectra collected on quasiracemic samples were retrieved from the melt.

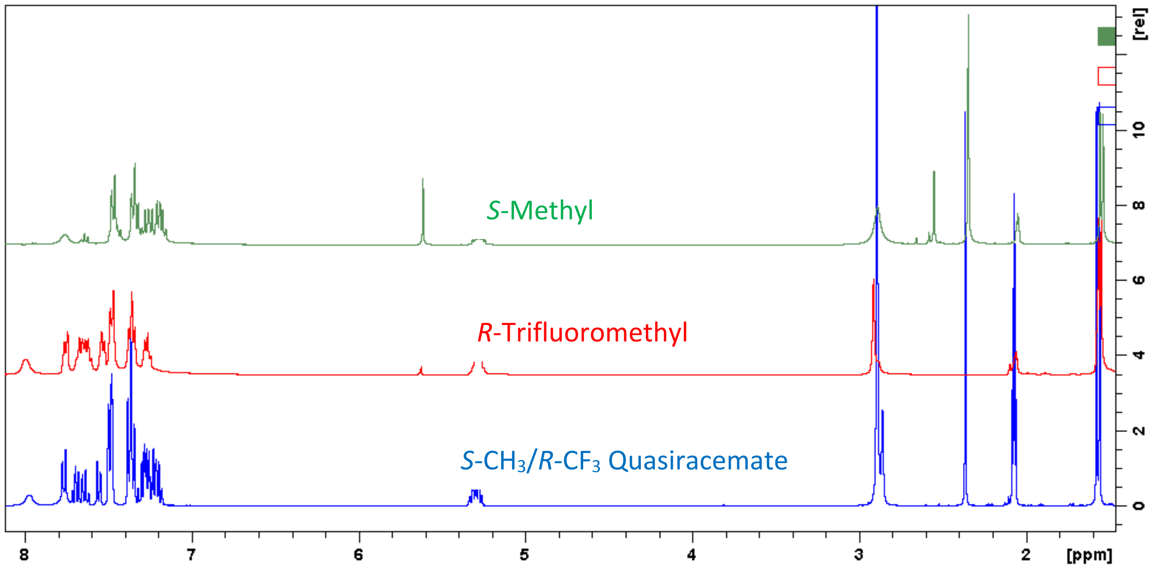
(*S*)-Cl/(*R*)-Br Quasiracemate



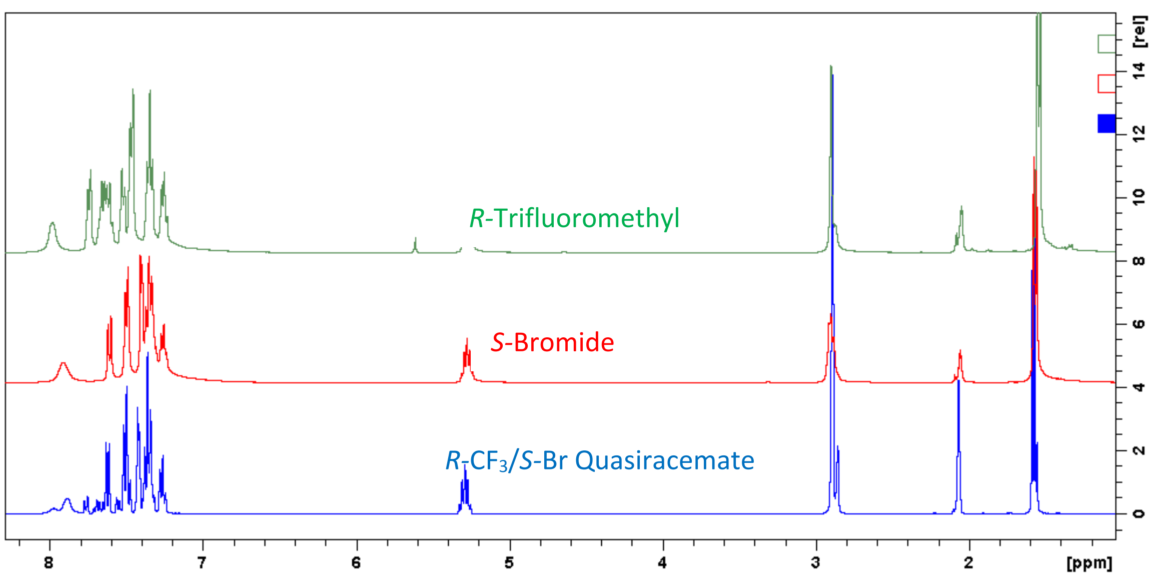
(*S*)-NO_2/(*R*)-CF_3 Quasiracemate



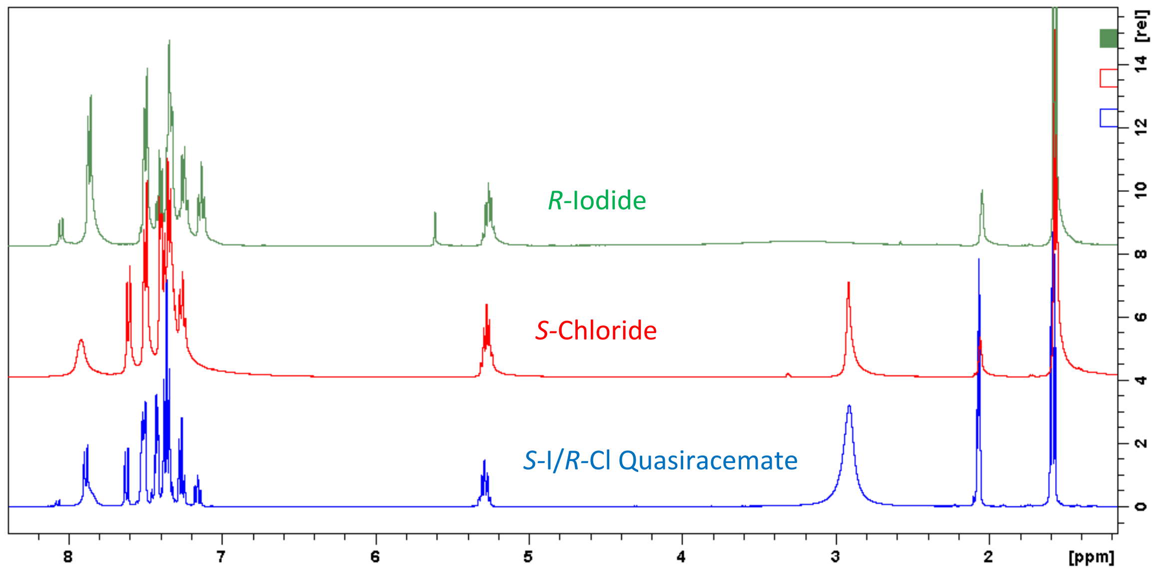
(*S*)-Me/(*R*)-CF_3 Quasiracemate



(*S*)-Br/(*R*)-CF_3 Quasiracemate



(*S*)-Cl/(*R*)-I Quasiracemate



S6 – Functional Group and Chemical Framework Volume and Surface Area Comparisons

Functional group volume and surface area approximations were taken from previously reported values.[6] The following table provides percent increases of the volume and surface areas corresponding to both functional group and the 2-substituted diarylamide molecular frameworks.

Volume Comparisons

Group Volume (Å^3)		H	F	Cl	CN	CH_3	NO_2	Br	CF_3	OCH_3	I	C_6H_5
5.9	H											
7.8	F	32.2										
19.6	Cl	232.2	151.3									
21.0	CN	255.9	169.2	7.1								
22.3	CH_3	278.0	185.9	13.8	6.2							
23.2	NO_2	293.2	197.4	18.4	10.5	4.0						
27.6	Br	367.8	253.8	40.8	31.4	23.8	19.0					
28.9	CF_3	389.8	270.5	47.4	37.6	29.6	24.6	4.7				
32.6	OCH_3	452.5	317.9	66.3	55.2	46.2	40.5	18.1	12.8			
34.6	I	486.4	343.6	76.5	64.8	55.2	49.1	25.4	19.7	6.1		
82.9	C_6H_5	1305.1	962.8	323.0	294.8	271.7	257.3	200.4	186.9	154.3	139.6	

Diarylamide Molecular Volume (Å^3)		H	F	Cl	CN	CH_3	NO_2	Br	CF_3	OCH_3	I	C_6H_5
221.9	H											
223.8	F	0.9										
235.6	Cl	6.2	5.3									
237.0	CN	6.8	5.9	0.6								
238.3	CH_3	7.4	6.5	1.1	0.5							
239.2	NO_2	7.8	6.9	1.5	0.9	0.4						
243.6	Br	9.8	8.8	3.4	2.8	2.2	1.8					
244.9	CF_3	10.4	9.4	3.9	3.3	2.8	2.4	0.5				
248.6	OCH_3	12.0	11.1	5.5	4.9	4.3	3.9	2.1	1.5			
250.6	I	12.9	12.0	6.4	5.7	5.2	4.8	2.9	2.3	0.8		
298.9	C_6H_5	34.7	33.6	26.9	26.1	25.4	25.0	22.7	22.0	20.2	19.3	

6. A. Gavezzotti, *J. Am. Chem. Soc.*, 1985, **107**, 962. A. Gavezzotti, *J. Am. Chem. Soc.*, 1983, **105**, 5220.

Surface Area Comparisons

Group Surface Areas (Å^2)

Group Surface Areas (Å^2)		H	F	Cl	CN	CH_3	NO_2	Br	CF_3	OCH_3	I	C_6H_5
6.8	H											
12.1	F	77.9										
29.0	Cl	326.5	139.7									
32.2	CN	373.5	166.1	11.0								
33.4	CH_3	391.2	176.0	15.2	3.7							
37.0	NO_2	444.1	205.8	27.6	14.9	10.8						
37.1	Br	445.6	206.6	27.9	15.2	11.1	0.3					
37.3	CF_3	448.5	208.3	28.6	15.8	11.7	0.8	0.5				
40.1	OCH_3	489.7	231.4	38.3	24.5	20.1	8.4	8.1	7.5			
45.0	I	561.8	271.9	55.2	39.8	34.7	21.6	21.3	20.6	12.2		
94.9	C_6H_5	1295.6	684.3	227.2	194.7	184.1	156.5	155.8	154.4	136.7	110.9	

Diarylamide Molecular Surface Areas (Å^3)

Diarylamide Molecular Surface Areas (Å^3)		H	F	Cl	CN	CH_3	NO_2	Br	CF_3	OCH_3	I	C_6H_5
302.8	H											
308.1	F	1.8										
325.0	Cl	7.3	5.5									
328.2	CN	8.4	6.5	1.0								
329.4	CH_3	8.8	6.9	1.4	0.4							
333.0	NO_2	10.0	8.1	2.5	1.5	1.1						
333.1	Br	10.0	8.1	2.5	1.5	1.1	0.0					
333.3	$CF3_3$	10.1	8.2	2.6	1.6	1.2	0.1	0.1				
336.1	OCH_3	11.0	9.1	3.4	2.4	2.0	0.9	0.9	0.8			
341.0	I	12.6	10.7	4.9	3.9	3.5	2.4	2.4	2.3	1.5		
390.9	C_6H_5	29.1	26.9	20.3	19.1	18.7	17.4	17.4	17.3	16.3	14.6	