Supporting Information

On Water: Iodine-Mediated Direct Construction of 1, 3-Benzothiazines from ortho-Alkynylanilines by Regioselective 6-Exo-dig Cyclization

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X-Ray Crystallographic Studies

**Figure I.** ORTEP structure of compound 4h.

The crystal of 4h of suitable quality was obtained from MeOH/CHCl3. The compound 4h crystallized in Orthorhombic crystal system with space group $P_{ccn}$. The single-crystal X-ray data were collected on an Oxford X Calibur CCD diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structures was solved using SIR-92 and refined by full matrix least square technique on $F^2$ using the SHELXL-97 program within the WinGX v 1.80.05 software package. In 4h hydrogens are mixed and all non-hydrogen atoms were refined anisotropically. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compound 4h have been deposited at the Cambridge Crystallographic Data Centre. CCDC deposit number for 4h is 1872209.
Table I. Crystallographic data and structure refinement for compounds 4h

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<td>Largest diff. peak and hole</td>
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</table>

\(^aR = \sum(\| Fo \| - \| Fe \|)/\sum \| Fo \|; ^b wR = \{\sum[w(F_o{^2} - F_c{^2})^2]/\sum[w(F_o{^2})^2]\}^{1/2}\)
References:


General Experimental

General Information and Method. All the reactions were performed in an oven-dried Schlenk flask under an argon atmosphere. Column chromatography was performed using silica gel (mesh 100-200). TLC analysis was performed on commercially prepared 60 F_{254} silica gel plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. ^1H NMR (400 MHz) and ^13C NMR (100 MHz) spectra were recorded in CDCl_3 and (CD_3)_2SO. Chemical shifts for carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, br s = broad singlet), coupling constants in Hertz, and integration. High-resolution mass spectra were recorded with q−TOF electrospray mass spectrometer. All purchased chemicals were used as received. All melting points are uncorrected.

General Procedure for the Synthesis of Starting Substrate 1a-o: To a solution of substituted 2-iodoaniline (0.5 mmol) in MeCN (2 mL), 3 mol% of Pd(PPh_3)_2Cl_2 was added. The reaction vial was then sealed and flushed with nitrogen. Then, 1.5 equiv of Et_3N and 0.51 mmol of alkyne were added to the reaction mixture. The reaction was then stirred at 70 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H_2O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100–200 mesh size silica gels (hexane: ethyl acetate) to afford the corresponding product. The structure and purity of known starting materials 1a-o were confirmed by comparison of their physical and NMR-spectral data (^1H NMR and ^13C NMR) with those reported in the literature.^{17-20}
General Procedure for the Synthesis of Starting Substrate 1p-u: To a solution of substituted 2-iodoaniline (0.5 mmol) in Et₃N (3 mL), 3 mol% of Pd(PPh₃)₂Cl₂ and 1 mol% of CuI were added. The reaction vial was then sealed and flushed with nitrogen. Then 0.51 mmol of alkyne was added to the reaction mixture. The reaction was then stirred at 25 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H₂O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na₂SO₄, concentrated under vacuum, and purified by column chromatography using 100–200 mesh size silica gels (hexane: ethyl acetate) to afford the corresponding product. The structure and purity of known starting materials 1p, 1q, 1t, 1u were confirmed by comparison of their physical and NMR-spectral data (¹H NMR and ¹³C NMR) with those reported in the literature.¹⁷-²⁰

2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r). The product was obtained as a colourless oil, (110.9 mg, 92%); ¹H NMR (400 MHz, CDCl₃) δ 7.49 (s, 1H), 7.28 (d, J = 8.8 Hz, 1H), 6.67 (d, J = 8.8 Hz, 1H), 4.44 (s, 2H), 1.35 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 150.1, 129.3 (q, J_C-F = 3.9 Hz), 125.7 (q, J_C-F = 3.9 Hz), 124.4 (q, J_C-F = 270.3 Hz), 119.7 (q, J_C-F = 32.8 Hz), 113.4, 108.5, 105.4, 74.3, 31.2, 28.4. HRMS (ESI) [M+H]⁺ Calcd for [C₁₃H₁₄F₃N] 242.1157, found 242.1159.

2-(Cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s). The product was obtained as a colourless oil, (101.2 mg, 90%); ¹H NMR (400 MHz, CDCl₃) δ 7.47 (s, 1H), 7.26 (dd, J = 8.5 and 1.9 Hz, 1H), 6.65 (d, J = 8.5 Hz, 1H), 4.46 (br s, 2H), 1.52–1.46 (m, 1H), 0.93–0.88 (m, 2H), 0.83–0.79 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 150.5, 129.6 (q,
$J_{C,F} = 3.9$ Hz), 125.8 (q, $J_{C,F} = 3.9$ Hz), 124.6 (q, $J_{C,F} = 270.3$ Hz), 119.6 (q, $J_{C,F} = 32.7$ Hz), 113.5, 108.4, 100.2, 70.9, 9.0, 0.3. HRMS (ESI) [M+H]$^+$ Calcd for $[C_{12}H_{10}F_{3}N]$ 226.0844, found 226.0837.

**General Procedure for the Synthesis of Starting Substrate 6a-b:** To a solution of substituted 2-iodoaniline (0.5 mmol) in MeCN (2 mL), 5 mol% of Pd(PPh$_3$)$_2$Cl$_2$ was added. The reaction vial was then sealed and flushed with nitrogen. Then, 3 equiv of Et$_3$N and 0.26 mmol of terminal alkyne were added to the reaction mixture. The reaction was then stirred at 70 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H$_2$O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na$_2$SO$_4$, concentrated under vacuum, and purified by column chromatography using 100–200 mesh size silica gels (hexane:ethyl acetate) to afford the corresponding product.

![Diagram](attachment:image.png)

2,2’-(1,3-Phenylenebis(ethyne-2,1-diyl))dianiline (6a). The product was obtained as a yellow needles, mp: 127–129 °C (135.5 mg, 88%); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.68 (s, 1H), 7.47–7.45 (m, 2H), 7.37–7.29 (m, 3H), 7.16–7.12 (m, 2H), 6.73–6.70 (m, 4H), 4.19 (br s, 4H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 148.0, 134.3, 132.3, 131.1, 130.1, 128.7, 123.8, 118.1, 114.5, 107.7, 94.0, 86.8. HRMS (ESI) [M+H]$^+$ Calcd for $[C_{22}H_{16}N_2]$ 309.1392, found 309.1389.

![Diagram](attachment:image.png)

2,2’-(1,3-Phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b). The product was obtained as a yellow needles, mp: 121–123 °C (146.2mg, 85%); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.67 (s, 1H), 7.48–7.46 (m, 2H), 7.36–7.31 (m, 1H), 7.07 (d, $J =$
2.9 Hz, 1H), 7.05 (d, J = 3.0 Hz, 1H), 6.88 (td, J = 8.6 and 2.9 Hz, 2H), 6.65 (dd, J = 8.9 and 4.7 Hz, 2H), 4.15 (br s, 4H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 155.3 (d, \(J_{C,F} = 237.0\) Hz), 144.4, 135.3, 134.4, 132.4 (d, \(J_{C,F} = 16.4\) Hz), 131.5, 130.3, 128.8, 127.8, 123.4, 117.9 (d, \(J_{C,F} = 23.1\) Hz), 117.3 (d, \(J_{C,F} = 23.1\) Hz), 115.5 (d, \(J_{C,F} = 8.7\) Hz), 108.3 (d, \(J_{C,F} = 9.6\) Hz), 94.4, 85.9. HRMS (ESI) [M+H]\(^+\) Calcd for [C\(_{22}\)H\(_{14}\)F\(_2\)N\(_2\)] 345.1203, found 345.1198.

**General experimental procedure for green one-pot synthesis of benzo[1,3]thiazin-2-yl]benzimidic acid 3-5:** To a solution of ortho-alkynlanilines \(1\) (0.5 mmol), aroyl isothiocyanates \(2\) (0.52 mmol) and 2.0 equiv of I\(_2\) was added in water (2.0 mL). The reaction was then stirred at room temperature until TLC revealed a complete conversion of the starting material. After the completion of the reaction, the reaction mixture was quenched with saturated aq sodium thiosulfate solution and extracted with EtOAc (3X10 mL). The combined organic layers were dried over Na\(_2\)SO\(_4\), concentrated under vacuum, and purified by column chromatography using 100–200 mesh size silica gels (EtOAc: hexane) to afford the corresponding product.

\[
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3a).
\]

The product was obtained as a pale yellow needles, mp: 155–157 \(^\circ\)C (216.9 mg, 90%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3429, 2922, 1597, 1554, 1411, 1310, 1285, 1079, 762, 748, 708; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.55 (s, 1H), 8.12 (d, \(J = 7.8\) Hz, 1H), 7.96 (d, \(J = 7.8\) Hz, 2H), 7.48–7.27 (m, 10H), 7.09 (d, \(J = 7.8\) Hz, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 143.1, 138.6, 134.3, 132.8, 130.6, 129.9, 129.5, 129.3, 129.0, 128.9, 128.7, 128.6, 128.5, 126.3, 125.4, 124.4, 121.3, 114.2, 98.1. HRMS (ESI) [M+H]\(^+\) Calcd for [C\(_{22}\)H\(_{14}\)F\(_2\)N\(_2\)OS] 483.0028, found 483.0022.
(Z)-N-((E)-4-(Iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3b). The product was obtained as a yellow needles, mp: 154–156 °C (207.9 mg, 84%); FTIR (Zn–Se ATR, cm⁻¹) 3495, 2988, 1611, 1584, 1501, 1399, 1310, 1089, 712, 698, 658; ¹H NMR (400 MHz, CDCl₃) δ 11.64 (br s, 1H), 8.22 (d, J = 7.8 Hz, 1H), 7.99 (d, J = 6.8 Hz, 2H), 7.50–7.46 (m, 1H), 7.42–7.36 (m, 3H), 7.32–7.28 (m, 1H), 7.26–7.17 (m, 4H), 7.07 (d, J = 7.8 Hz, 1H), 2.28 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 146.7, 143.2, 139.0, 137.0, 135.3, 134.9, 133.6, 133.3, 132.7, 131.2, 131.1, 129.5, 127.5, 125.5, 100.0, 23.7.

HRMS (ESI) [M+H]⁺ Calcd for [C₂₃H₁₇I₂N₂O] 497.0185, found 497.0172.

(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c). The product was obtained as a yellow needles, mp: 86–88 °C (215.7 mg, 87%); FTIR (Zn–Se ATR, cm⁻¹) 3299, 2838, 1610, 1588, 1420, 1338, 1198, 1038, 1001, 848, 708, 690; ¹H NMR (400 MHz, CDCl₃) δ 11.79 (br s, 1H), 8.10 (d, J = 7.8 Hz, 1H), 8.00 (d, J = 7.8 Hz, 2H), 7.49–7.46 (m, 1H), 7.42–7.35 (m, 3H), 7.30–7.25 (m, 2H), 7.16–7.14 (m, 3H), 7.07 (d, J = 8.8 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) 142.1, 137.6, 133.9, 131.6, 129.5, 129.4, 128.7, 128.1, 127.7, 127.4, 125.3, 124.2, 123.4, 119.8, 97.0, 20.5. HRMS (ESI) [M+H]⁺ Calcd for [C₂₃H₁₇I₂N₂O] 497.0185, found 497.0186.

(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3d). The product was obtained as a yellow needles, mp: 146–148 °C

[9]
(230.6 mg, 93%); FTIR (Zn–Se ATR, cm$^{-1}$) 3313, 1691, 1446, 1388, 1232, 1074, 748, 702, 617; $^1$H NMR (400 MHz, CDCl$_3$) δ 10.24 (br s, 1H), 8.09 (dd, $J = 7.8$ and 1.4 Hz, 1H), 7.97 (d, $J = 7.3$ Hz, 2H), 7.47–7.43 (m, 1H), 7.39–7.32 (m, 3H), 7.29–7.24 (m, 3H), 7.18 (d, $J = 8.2$ Hz, 2H), 7.09 (dd, $J = 7.8$ and 0.9 Hz, 1H), 2.35 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 140.2, 139.7, 138.5, 134.3, 132.8, 129.8, 129.5, 129.3, 129.0, 128.7, 128.5, 125.7, 125.4, 124.5, 121.2, 98.7, 21.6. HRMS (ESI) [M+H]$^+$ Calcd for [C$_{23}$H$_{17}$IN$_2$OS] 497.0185, found 497.0196.

(Z)-N-((E)-4-((4-Butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3e). The product was obtained as a yellow needles, mp: 161–163 °C (236.7 mg, 88%); FTIR (Zn–Se ATR, cm$^{-1}$) 3310, 2968, 1605, 1585, 1433, 1355, 1275, 1040, 862, 748, 690; $^1$H NMR (400 MHz, CDCl$_3$) δ 11.83 (s, 1H), 8.08 (d, $J = 7.8$ Hz, 1H), 7.95 (d, $J = 6.8$ Hz, 2H), 7.46–7.42 (m, 1H), 7.38–7.24 (m, 6H), 7.19 (d, $J = 8.8$ Hz, 2H), 7.03 (d, $J = 7.8$ Hz, 1H), 2.61 (t, $J = 7.8$ Hz, 2H), 1.66–1.58 (m, 2H), 1.43–1.36 (m, 2H), 0.94 (t, $J = 7.3$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 144.6, 140.4, 134.9, 132.6, 130.5, 129.4, 129.1, 129.06, 128.8, 128.4, 125.8, 125.2, 124.7, 121.0, 98.6, 35.6, 33.4, 22.6, 14.1. HRMS (ESI) [M+H]$^+$ Calcd for [C$_{26}$H$_{23}$IN$_2$OS] 539.0654, found 539.0667.

(Z)-N-((E)-4-((4-tert-Butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3f). The product was obtained as a pale yellow needles, mp: 184–186 °C (231.3 mg, 86%); FTIR (Zn–Se ATR, cm$^{-1}$) 3267, 2958, 1653, 1577, 1562, 1465, 1257, 1186, 914, 754, 661; $^1$H NMR (400 MHz, CDCl$_3$) δ 11.78 (br s, 1H), 8.01
(d, $J = 8.8$ Hz, 1H), 7.88 (d, $J = 6.8$ Hz, 2H), 7.38–7.31 (m, 3H), 7.29–7.24 (m, 5H), 7.20–7.16 (m, 1H), 6.96 (d, $J = 8.8$ Hz, 1H), 1.26 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 151.6, 138.9, 137.4, 133.8, 129.4, 128.6, 128.2, 128.1, 128.0, 127.8, 127.5, 127.3, 124.7, 124.4, 124.1, 123.6, 119.9, 97.7, 33.9, 30.3. HRMS (ESI) [M+H]$^+$ Calcd for [C$_{26}$H$_{23}$IN$_2$OS] 539.0654, found 539.0646.

(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g). The product was obtained as a brown needles, mp: 135–137 ºC (212.4 mg, 85%); FTIR (Zn–Se ATR, cm$^{-1}$) 3237, 2920, 1893, 1696, 1502, 1466, 1259, 1232, 1156, 1026, 836, 750, 702; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.46 (br s, 1H), 8.07 (d, $J = 7.8$ Hz, 1H), 7.97 (d, $J = 7.8$ Hz, 1H), 7.56–7.24 (m, 7H), 7.20–7.04 (m, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 162.9 (d, $J = 250.5$ Hz, 1C), 139.1 (d, $J = 2.9$ Hz, 1C), 138.5, 133.8, 133.0, 131.3 (d, $J = 8.7$ Hz, 1C), 130.7, 129.0, 128.8, 128.6, 126.7, 125.7, 124.2, 121.5, 116.0 (d, $J = 22.2$ Hz, 1C), 96.7. HRMS (ESI) [M+H]$^+$ Calcd for [C$_{22}$H$_{14}$FIN$_2$OS] 500.9934, found 500.9932.

(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h). The product was obtained as a pale yellow needles, mp: 226–228 ºC (199.8 mg, 80%); FTIR (Zn–Se ATR, cm$^{-1}$) 3228, 3068, 1693, 1583, 1543, 1446, 1269, 1217, 744, 698, 677; $^1$H NMR (400 MHz, DMSO-d$_6$) $\delta$ 11.97 (br s, 1H), 8.07 (d, $J = 7.8$ Hz, 1H), 7.96 (d, $J = 5.9$ Hz, 2H), 7.55–7.33 (m, 8H), 7.26–7.19 (m, 2H); $^{13}$C NMR (100 MHz, DMSO-d$_6$) $\delta$ 157.9 (d, $J = 246.6$ Hz, 1C), 133.1, 131.8 (d, $J = 8.7$ Hz, 1C),

[11]
131.5, 131.4, 131.2, 130.3, 129.4, 128.9, 128.1, 125.5, 123.7, 116.6 (d, \( J = 21.2 \) Hz, 1C), 89.6.

HRMS (ESI) [M+H]^+ Calcd for \([C_{22}H_{14}FIN_2OS]\) 500.9934, found 500.9936.

\[
\text{(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[\text{d}][1,3]thiazin-2-yl)benzimidic acid (3i).} \]

The product was obtained as a yellow needles, mp: 126–128 °C (200.1 mg, 82%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3210, 3020, 1697, 1534, 1424, 1316, 1280, 1235, 979, 752, 728, 688; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 11.14 (br s, 1H), 8.04 (d, \( J = 7.8 \) Hz, 1H), 7.94 (d, \( J = 7.8 \) Hz, 2H), 7.47–7.42 (m, 2H), 7.40–7.33 (m, 4H), 7.27–7.24 (m, 1H), 7.18 (d, \( J = 3.9 \) Hz, 1H), 7.05 (d, \( J = 7.8 \), 1H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 141.7, 137.8, 133.3, 131.6, 129.4, 128.1, 127.8, 127.6, 127.4, 126.6, 126.3, 125.4, 124.9, 124.1, 123.4, 120.4, 90.0. HRMS (ESI) [M+H]^+ Calcd for \([C_{20}H_{13}IN_2OS]\) 488.9592, found 488.9592.

\[
\text{(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[\text{d}][1,3]thiazin-2-yl)benzimidic acid (3j).} \]

The product was obtained as a yellow needles, mp: 146–148 °C (213.2 mg, 86%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3320, 2822, 1589, 1554, 1429, 1318, 1293, 1179, 832, 762, 718, 688; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 9.70 (s, 1H), 8.09 (d, \( J = 7.8 \) Hz, 1H), 7.83 (d, \( J = 7.8 \) Hz, 2H), 7.39–7.21 (m, 7H), 7.13 (d, \( J = 8.8 \) Hz, 2H), 7.07 (d, \( J = 7.8 \) Hz, 1H), 2.32 (s, 3H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 143.6, 143.1, 139.0, 131.3, 130.5, 129.9, 129.7, 129.5, 129.3, 129.26, 129.0, 128.8, 128.79, 128.6, 126.5, 125.4, 124.4, 121.6, 97.9, 21.8. HRMS (ESI) [M+H]^+ Calcd for \([C_{23}H_{17}IN_2OS]\) 497.0185, found 497.0169.
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k). The product was obtained as a pale yellow needles, mp: 144–146 °C (224.4 mg, 88%); FTIR (Zn–Se ATR, cm⁻¹) 3626, 3280, 2917, 1721, 1592, 1555, 1406, 1303, 1286, 1186, 1018, 954, 817, 793, 749; ¹H NMR (400 MHz, CDCl₃) δ 10.97 (br s, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.83 (d, J = 7.8 Hz, 2H), 7.36–7.32 (m, 1H), 7.25–7.24 (m, 3H), 7.17–7.12 (m, 4H), 7.05 (d, J = 7.8 Hz, 1H), 2.33 (s, 3H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 143.6, 140.2, 139.7, 138.9, 131.5, 130.4, 129.9, 129.5, 129.3, 129.27, 129.0, 128.9, 125.9, 125.4, 124.5, 121.5, 98.5, 21.8, 21.6. HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₁₉N₂O₅S] 511.0341, found 511.0319.

(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l). The product was obtained as a yellow needles, mp: 161–163 °C (221.8 mg, 87%); FTIR (Zn–Se ATR, cm⁻¹) 3301, 2920, 2852, 1683, 1604, 1546, 1467, 1442, 1259, 1211, 1111, 1039, 920, 790, 738, 719; ¹H NMR (400 MHz, CDCl₃) δ 11.39 (br s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.86 (d, J = 7.8 Hz, 2H), 7.39–7.35 (m, 1H), 7.28–7.24 (m, 2H), 7.16–7.12 (m, 5H), 7.07 (d, J = 7.8 Hz, 1H), 2.35 (s, 3H), 2.33 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 142.30, 141.9, 137.4, 129.3, 129.2, 128.6, 128.2, 128.0, 127.9, 127.7, 127.5, 125.2, 125.0, 124.1, 123.2, 120.2, 96.8, 20.5, 20.4. HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₁₉N₂O₅S] 511.0341, found 511.0328.
(Z)-N-(((E)-4-(4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m). The product was obtained as a yellow needles, mp: 147–149 °C (248.4 mg, 90%); FTIR (Zn–Se ATR, cm⁻¹) 3216, 2812, 1610, 1552, 1472, 1343, 1285, 1179, 1099, 755, 688; ¹H NMR (400 MHz, CDCl₃) δ 11.86 (br s, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.85 (d, J = 7.8 Hz, 2H), 7.38–7.33 (m, 3H), 7.30–7.22 (m, 3H), 7.14 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 7.8 Hz, 1H), 2.32 (s, 3H), 1.31 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 151.5, 142.2, 138.9, 129.3, 128.2, 128.1, 124.6, 124.0, 123.6, 119.9, 97.4, 33.8, 30.2, 20.6. HRMS (ESI) [M+H]⁺ Calcd for [C₂₇H₂₅IN₂OS] 553.0811, found 553.0808.

(Z)-N-(((E)-4-(4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n). The product was obtained as a pale yellow needles, mp: 193–195 °C (210.7 mg, 82%); FTIR (Zn–Se ATR, cm⁻¹) 3360, 3062, 2922, 1664, 1604, 1558, 1462, 1436, 1259, 1226, 1151, 1085, 1041, 958, 827, 738, 650, 586; ¹H NMR (400 MHz, CDCl₃) δ 9.29 (br s, 1H), 8.07 (dd, J = 7.8 and 1.4 Hz, 1H), 7.83 (d, J = 7.8 Hz, 2H), 7.38–7.32 (m, 3H), 7.28–7.24 (m, 1H), 7.15 (d, J = 8.2 Hz, 2H), 7.08–7.04 (m, 3H), 2.33 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 162.9 (d, J = 250.5 Hz, 1C), 143.7, 139.2 (d, J = 2.9 Hz, 1C), 131.3 (d, J = 8.7 Hz, 1C), 130.6, 129.5, 129.3, 129.0, 128.7, 127.2, 125.4, 124.2, 121.8, 115.9 (d, J = 22.2 Hz, 1C), 114.2, 96.0, 21.7. HRMS (ESI) [M+H]⁺ Calcd for [C₂₃H₁₆FIN₂OS] 515.0090, found 515.0085.

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(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o). The product was obtained as a pale yellow needles, mp: 140–142 °C (213.2 mg, 86%); FTIR (Zn–Se ATR, cm⁻¹) 3220, 2918, 1681, 1595, 1537, 1446, 1352, 1282, 1192, 1072, 999, 866, 760, 738, 698, 677; ¹H NMR (400 MHz, CDCl₃) δ 11.14 (br s, 1H), 8.11 (d, J = 7.8 Hz, 1H), 7.74–7.72 (m, 2H), 7.41–7.22 (m, 9H), 7.07 (d, J = 7.83, 1H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 143.2, 139.3, 138.3, 134.4, 133.5, 130.5, 129.5, 129.3, 128.8, 128.4, 126.7, 126.0, 125.3, 124.4, 121.7, 115.6, 97.5. HRMS (ESI) [M+H]⁺ Calcd for [C₂₃H₁₇IN₂OS] 497.0185, found 497.0201.

(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p). The product was obtained as a yellow needles, mp: 129–131 °C (216.6 mg, 84%); FTIR (Zn–Se ATR, cm⁻¹) 3066, 2922, 1687, 1546, 1357, 1284, 1251, 1072, 788, 713, 678; ¹H NMR (400 MHz, CDCl₃) δ 12.05 (br s, 1H), 8.13 (d, J = 7.8 Hz, 1H), 8.03 (s, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.43–7.34 (m, 7H), 7.32–7.24 (m, 2H), 7.05 (d, J = 7.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 143.1, 137.3, 134.5, 132.5, 130.7, 129.6, 129.55, 129.2, 129.1, 128.9, 127.4, 125.9, 125.3, 124.3, 120.1, 98.5. HRMS (ESI) [M+H]⁺ Calcd for [C₂₂H₁₄ClIN₂OS] 516.9638, found 516.9627.

(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a). The product was obtained as a yellow needles,
mp: 167–169 °C (232.1 mg, 91%); FTIR (Zn–Se ATR, cm⁻¹) 3230, 2918, 1693, 1570, 1541, 1467, 1267, 1024, 977, 815, 754, 694; ¹H NMR (400 MHz, DMSO-d₆) δ 7.93 (d, J = 8.3 Hz, 2H), 7.86 (d, J = 8.3 Hz, 1H), 7.50 (d, J = 7.3 Hz, 1H), 7.42–7.38 (m, 2H), 7.19–7.09 (m, 4H), 7.06–7.03 (m, 2H), 2.32 (s, 3H), 2.25 (s, 3H); ¹³C NMR (100 MHz, DMSO-d₆) δ 140.8, 140.6, 139.1, 134.3, 133.0, 130.0, 129.7, 129.6, 129.4, 129.0, 128.9, 128.6, 127.2, 126.2, 122.2, 98.7, 21.5, 21.4. HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₁₉IN₂OS] 511.0341, found 511.0343.

(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b). The product was obtained as a yellow needles, mp: 170–172 °C (234.05 mg, 83%); FTIR (Zn–Se ATR, cm⁻¹) 3275, 2924, 1699, 1546, 1489, 1319, 1284, 1114, 1064, 1016, 786, 711; ¹H NMR (400 MHz, CDCl₃) δ 11.31 (br s, 1H), 8.01 (d, J = 7.8 Hz, 3H), 7.66 (d, J = 7.8 Hz, 2H), 7.50–7.45 (m, 3H), 7.40–7.36 (m, 2H), 7.13 (d, J = 7.8 Hz, 1H), 6.94 (s, 1H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 146.6, 141.6, 133.0, 130.8 (q, J C-F = 32.7 Hz), 129.6, 129.0, 128.6, 128.3, 126.6 126.2 (q, J C-F = 272.3 Hz), 125.9 (q, J C-F = 3.5 Hz), 121.6, 120.9, 94.1, 21.4. HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₁₆F₃IN₂OS] 565.0058, found 565.0041.

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4c). The product was obtained as a yellow needles, mp: 152–154 °C (221.8 mg, 87%); FTIR (Zn–Se ATR, cm⁻¹) 3226, 2918, 1691, 1544, 1467, 1265, 1213, 1024, 977, 815, 754, 694; ¹H NMR (400 MHz, DMSO-d₆) δ 10.52 (br s, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.85 (d, J = 8.8 Hz, 2H), 7.41–7.37 (m, 2H),
7.32–7.28 (m, 3H), 7.24 (d, J = 7.8 Hz, 2H), 7.14 (d, J = 8.8 Hz, 1H), 7.09 (s, 1H), 2.36 (s, 3H), 2.32 (s, 3H); 13C NMR (100 MHz, DMSO-d6) δ 143.8, 143.3, 140.7, 130.0, 129.5, 129.46, 129.4, 129.2, 129.1, 128.4, 127.8, 126.2, 122.0, 98.1, 21.6, 21.5. HRMS (ESI) [M+H]⁺ Calcd for [C_{24}H_{19}IN_2OS] 511.0341, found 511.0346.

(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d). The product was obtained as a dark yellow needles, mp: 135–137 °C (235.8 mg, 90%); FTIR (Zn–Se ATR, cm⁻¹) 3288, 2890, 1695, 1580, 1482, 1301, 1225, 1201, 1024, 997, 801, 754, 680; 1H NMR (400 MHz, CDCl₃) δ 11.53 (br s, 1H), 7.99 (d, J = 8.8 Hz, 1H), 7.93 (d, J = 8.8 Hz, 2H), 7.26 (d, J = 7.8 Hz, 2H), 7.20–7.17 (m, 4H), 7.11 (d, J = 8.8 Hz, 1H), 6.97 (s, 1H), 2.39 (s, 3H), 2.37 (s, 3H), 2.36 (s, 3H); 13C NMR (100 MHz, CDCl₃) δ 143.8, 141.2, 140.2, 139.7, 137.6, 131.8, 129.9, 129.6, 129.3, 129.2, 128.8, 127.7, 126.6, 125.1, 121.6, 121.2, 114.2, 98.0, 21.8, 21.5, 21.4. HRMS (ESI) [M+H]⁺ Calcd for [C_{25}H_{21}IN_2OS] 525.0498, found 525.0495.

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e). The product was obtained as a yellow needles, mp: 151–153 °C (221.8 mg, 87%); FTIR (Zn–Se ATR, cm⁻¹) 3494, 3024, 1587, 1535, 1419, 1344, 1282, 1190, 858, 808, 777, 736, 653; 1H NMR (400 MHz, CDCl₃) δ 11.17 (br s, 1H), 8.01 (d, J = 8.2 Hz, 1H), 7.78–7.76 (m, 2H), 7.41–7.31 (m, 5H), 7.28–7.22 (m, 2H), 7.11–7.08 (m, 1H), 6.88 (s, 1H), 2.37 (s, 3H), 2.32 (s, 3H); 13C NMR (100 MHz, CDCl₃) δ 143.3, 141.1, 138.2, 134.7, 133.5, 129.6, 129.3, 128.8, 128.6, 128.4, 126.6,
126.2, 121.6, 96.4, 21.5, 21.4. HRMS (ESI) [M+H]^+ Calcd for [C_{24}H_{19}IN_{2}OS] 511.0341, found 511.0329.

(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4f). The product was obtained as a yellow needles, mp: 175–177 °C (227.8 mg, 86%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3515, 2918, 1585, 1533, 1429, 1419, 1344, 1284, 1155, 1068, 777, 690; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 12.65 (br s, 1H), 8.06 (s, 1H), 8.02 (d, \(J\) = 7.8 Hz, 1H), 7.94 (d, \(J\) = 7.8 Hz, 1H), 7.43–7.34 (m, 6H), 7.31–7.27 (m, 1H), 7.24 (d, \(J\) = 6.8 Hz, 1H), 7.11 (d, \(J\) = 7.8 Hz, 1H), 6.86 (s, 1H), 2.40 (s, 3H); \(^1\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 143.2, 141.4, 137.7, 136.8, 134.4, 132.4, 129.8, 129.6, 129.55, 129.2, 128.9, 128.9, 128.6, 127.5, 126.2, 125.9, 121.5, 120.1, 97.1, 21.5. HRMS (ESI) [M+H]^+ Calcd for [C_{23}H_{16}ClIN_{2}OS] 530.9795, found 530.9783.

(Z)-N-((E)-6-Fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g). The product was obtained as a yellow needles, mp: 165–167 °C (222.5 mg, 84%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3311, 2910, 1688, 1539, 1467, 1400, 1218, 1155, 1085, 1024, 977, 815, 710; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.32 (br s, 1H), 7.85–7.83 (m, 2H), 7.82 (d, \(J\) = 2.7 Hz, 1H), 7.47–7.43 (m, 1H), 7.36–7.32 (m, 2H), 7.29–7.25 (m, 1H), 7.07–6.98 (m, 2H), 6.92–6.90 (m, 1H), 6.86–6.84 (m, 2H), 3.78 (s, 3H); \(^1\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 160.1 (d, \(J\) = 245.6 Hz, 1C), 159.6, 144.1, 133.5, 132.9, 129.9, 128.6, 128.5, 126.2, 125.7 (d, \(J\) = 7.7 Hz, 1C), 124.4, 121.6, 117.4 (d, \(J\) = 2.3 Hz, 1C), 115.3, 115.1, 115.1. 

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114.6, 93.0, 55.5. HRMS (ESI) [M+H]⁺ Calcd for [C\textsubscript{23}H\textsubscript{16}FIN\textsubscript{2}O\textsubscript{2}S] = 531.0039, found 531.0028.

(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h). The product was obtained as a pale yellow needles, mp: 154–156 °C (211.5 mg, 82%); FTIR (Zn–Se ATR, cm\textsuperscript{-1}) 3257, 2851, 1654, 1571, 1548, 1506, 1458, 1396, 1263, 1199, 1178, 1080, 1026, 966, 817, 709, 684; \textsuperscript{1}H NMR (400 MHz, DMSO-d\textsubscript{6}) \(\delta\) 11.81 (br s, 1H), 8.02 (d, \(J = 1.8\) Hz, 1H), 7.91 (d, \(J = 7.3\) Hz, 2H), 7.53–7.48 (m, 2H), 7.42–7.34 (m, 4H), 7.31–7.25 (m, 4H); \textsuperscript{13}C NMR (100 MHz, DMSO-d\textsubscript{6}) \(\delta\) 143.4, 133.2, 130.4, 129.6, 129.5, 129.3, 129.2, 128.9, 128.3, 126.4, 126.2, 101.2. HRMS (ESI) [M+H]⁺ Calcd for [C\textsubscript{22}H\textsubscript{14}ClIN\textsubscript{2}OS] = 516.9638, found 516.9636.

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4i). The product was obtained as a pale yellow needles, mp: 139–141 °C (219.9 mg, 80%); FTIR (Zn–Se ATR, cm\textsuperscript{-1}) 3429, 2855, 1720, 1627, 1555, 1441, 1328, 1277, 1157, 1122, 1073, 1025, 968, 832, 710; \textsuperscript{1}H NMR (400 MHz, DMSO-d\textsubscript{6}) \(\delta\) 12.46 (br s, 1H), 8.35 (s, 1H), 7.96 (d, \(J = 7.8\) Hz, 2H), 7.81 (d, \(J = 7.8\) Hz, 1H), 7.58–7.51 (m, 1H), 7.48–7.28 (m, 8H); \textsuperscript{13}C NMR (100 MHz, DMSO-d\textsubscript{6}) \(\delta\) 143.3, 133.3, 129.7, 129.5, 129.4, 129.2, 129.0, 127.3, 127.26, 126.4, 126.35, 126.0, 125.95, 125.0, 123.3, 102.3. HRMS (ESI) [M+H]⁺ Calcd for [C\textsubscript{23}H\textsubscript{14}F\textsubscript{3}IN\textsubscript{2}OS] = 550.9902, found 550.9897.
(Z)-N-((E)-4-(1-Iodopentylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5a). The product was obtained as a yellow needles, mp: 129–131 °C (182.4 mg, 79%); FTIR (Zn–Se ATR, cm⁻¹) 3365, 2980, 2855, 1685, 1556, 1504, 1437, 1305, 1210, 1039, 955, 815, 754, 684; ¹H NMR (400 MHz, CDCl₃) δ 11.47 (br s, 1H), 7.99 (d, J = 7.8 Hz, 2H), 7.84 (d, J = 7.8 Hz, 1H), 7.48–7.45 (m, 1H), 7.38–7.34 (m, 2H), 7.30–7.25 (m, 1H), 7.21–7.17 (m, 1H), 6.97 (d, J = 7.8 Hz, 1H), 3.07 (t, J = 7.3 Hz, 2H), 1.65–1.58 (m, 2H), 1.44–1.35 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 138.8, 134.5, 132.7, 129.8, 129.0, 128.9, 128.6, 125.4, 125.0, 123.1, 121.1, 107.8, 44.0, 31.6, 21.7, 14.1. HRMS (ESI) [M+H]+ Calcd for [C₂₀H₁₉IN₂OS] 463.0341, found 463.0340.

(Z)-N-((E)-4-(4-Chloro-1-iodobutylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5b). The product was obtained as a yellow needles, mp: 135–137 °C (192.7 mg, 80%); FTIR (Zn–Se ATR, cm⁻¹) 3231, 2985, 1665, 1574, 1477, 1385, 1301, 1287, 1153, 1101, 1029, 932, 732, 704; ¹H NMR (400 MHz, CDCl₃) δ 11.23 (br s, 1H), 8.03 (d, J = 6.8 Hz, 2H), 7.85 (d, J = 7.8 Hz, 1H), 7.54–7.50 (m, 1H), 7.44–7.40 (m, 2H), 7.36–7.32 (m, 1H), 7.25–7.21 (m, 1H), 7.03 (d, J = 7.8 Hz, 1H), 3.61 (t, J = 6.4 Hz, 2H), 3.25 (t, J = 7.3 Hz, 2H), 2.17–2.10 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 139.1, 134.3, 132.9, 130.0, 129.0, 128.8, 128.6, 125.2, 125.1, 124.8, 121.4, 104.8, 43.3, 41.3, 32.0. HRMS (ESI) [M+H]+ Calcd for [C₁₉H₁₆ClIN₂OS] 482.9795, found 482.9800.
(Z)-N-((E)-4-(1-Iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c). The product was obtained as a pale yellow needles, mp: 121–123 °C (204.1 mg, 77%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3205, 2972, 1660, 1554, 1469, 1327, 1257, 1153, 1114, 1070, 904, 732, 704, 671; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 11.02 (br s, 1H), 7.96–7.94 (m, 3H), 7.51–7.43 (m, 2H), 7.40–7.34 (m, 2H), 7.04–7.01 (m, 1H), 1.56 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 142.8, 133.5, 133.1, 129.5, 128.8, 128.2, 127.4 (q, \(J_{C-F} = 32.7\) Hz), 125.9, 125.4, 122.7, 122.2, 121.8, 42.4, 33.2. HRMS (ESI) [M+H]\(^+\) Calcd for [C\(_{21}\)H\(_{18}\)F\(_3\)IN\(_2\)OS] 531.0215, found 531.0222.

(Z)-N-((E)-4-(Cyclopropyliodomethylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5d). The product was obtained as a pale yellow needles, mp: 117–119 °C (200.4 mg, 78%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3272, 2933, 1640, 1562, 1473, 1390, 1272, 1151, 1112, 1070, 1032, 955, 732, 701; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.82 (br s, 1H), 7.98 (s, 1H), 7.81 (d, \(J = 7.8\) Hz, 2H), 7.38–7.31 (m, 2H), 7.27–7.24 (m, 2H), 6.91 (d, \(J = 7.8\) Hz, 1H), 2.04–1.96 (m, 1H), 0.85–0.83 (m, 4H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 143.1, 133.2, 133.1, 128.7, 128.6, 126.9, 126.6 (br s, C-F), 126.1, 125.9 (br s, C-F), 125.6 (q, \(J_{C-F} = 270.3\) Hz), 122.7 (br s, C-F), 121.8, 115.2, 82.0, 20.9, 11.4. HRMS (ESI) [M+H]\(^+\) Calcd for [C\(_{20}\)H\(_{14}\)F\(_3\)IN\(_2\)OS] 514.9902, found 514.9892.
(Z)-N-((E)-4-(Cyclohexyliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5e). The product was obtained as a yellow needles, mp: 125–127 °C (190.3 mg, 78%); FTIR (Zn–Se ATR, cm⁻¹) 3255, 2853, 1601, 1549, 1337, 1257, 1114, 1070, 904, 855, 732, 702, 688; ¹H NMR (400 MHz, CDCl₃) δ 11.39 (br s, 1H), 8.11 (d, J = 7.8 Hz, 2H), 7.87 (d, J = 7.8 Hz, 1H), 7.55–7.51 (m, 1H), 7.46–7.40 (m, 2H), 7.36–7.30 (m, 1H), 7.28–7.20 (m, 1H), 7.08–7.02 (m, 1H), 2.79–2.73 (m, 1H), 1.91–1.70 (m, 4H), 1.60–1.49 (m, 4H), 1.37–1.20 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) 138.5, 135.0, 132.7, 132.6, 129.9, 129.8, 129.2, 129.1, 128.5, 125.6, 125.4, 124.8, 120.6, 120.2, 113.6, 45.9, 33.5, 25.6, 25.4. HRMS (ESI) [M+H]⁺ Calcd for [C₂₂H₂₈IN₂OS] 489.0498, found 489.0519.

(Z)-N-((E)-4-(Cyclohex-1-en-1-ylidomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f). The product was obtained as a yellow needles, mp: 125–127 °C (157.9 mg, 65%); FTIR (Zn–Se ATR, cm⁻¹) 3198, 2972, 1654, 1567, 1439, 1257, 1201, 1153, 1114, 1070, 910, 832, 732, 671; ¹H NMR (400 MHz, CDCl₃) δ 11.89 (br s, 1H), 8.09–7.99 (m, 2H), 7.55–7.47 (m, 2H), 7.43–7.39 (m, 2H), 7.37–7.31 (m, 1H), 7.27–7.20 (m, 1H), 7.02 (d, J = 7.8 Hz, 1H), 5.91 (t, J = 3.9 Hz, 1H), 2.70–2.56 (m, 2H), 2.15–2.12 (m, 2H), 1.79–1.63 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 140.9, 132.7, 132.6, 130.3, 129.7, 129.2, 128.6, 128.5, 128.2, 124.9, 123.2, 120.7, 103.6, 26.5, 25.9, 22.3, 21.7. HRMS (ESI) [M+H]⁺ Calcd for [C₂₂H₁₉IN₂OS] 487.0341, found 487.0349.

General experimental procedure for green one-pot synthesis of Bisbenzo[1,3]thiazin-2-yl)di benzimidic acid 7: To a solution of ortho-haloanilines 1 (0.5 mmol), aroyl
isothiocyanates 2 (1.04 mmol) and 3.5 equiv of I₂ were added in water (2.0 mL). The reaction was then stirred at room temperature until TLC revealed complete conversion of the starting material. After the completion of the reaction, the reaction mixture was quenched with saturated aq sodium thiosulfate solution and extracted with EtOAc (3X10 mL). The combined organic layers were dried over Na₂SO₄, concentrated under vacuum, and purified by column chromatography using 100–200 mesh size silica gels (EtOAc:hexane) to afford the corresponding product.

\[(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-Phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7a).\]

The product was obtained as a yellow needles, mp: 136–138 °C (314.1 mg, 71%); FTIR (Zn–Se ATR, cm⁻¹) 3310, 2990, 2868, 1616, 1578, 1503, 1210, 926, 743; ¹H NMR (400 MHz, CDCl₃) δ 11.06 (br s, 2H), 8.11–8.06 (m, 4H), 7.95 (d, J = 7.8 Hz, 3H), 7.60–7.56 (m, 1H), 7.47–7.39 (m, 6H), 7.33–7.27 (m, 6H), 7.17 (d, J = 7.8 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 143.2, 139.6, 134.0, 133.5, 132.7, 130.6, 130.5, 130.2, 130.0, 129.3, 129.0, 128.6, 128.5, 128.4, 127.4, 125.6, 124.5, 122.0, 96.3. HRMS (ESI) [M+H]^+ Calcd for [C₃₈H₂₄I₂N₄O₂S₂]  886.9508, found  886.9505.

\[(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-Phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b).\] The product was obtained as a yellow needles, mp: 156–158 °C
(342.2 mg, 75%); FTIR (Zn–Se ATR, cm⁻¹) 3290, 2916, 2848, 1676, 1602, 1541, 1255, 906, 721; ¹H NMR (400 MHz, CDCl₃) δ 11.80 (br s, 2H), 8.06 (d, J = 7.8 Hz, 2H), 7.82 (m, 3H), 7.43–7.37 (m, 4H), 7.33 (d, J = 7.8 Hz, 2H), 7.29–7.24 (m, 3H), 7.11–7.07 (m, 6H), 2.31 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 143.3, 130.6, 130.2, 130.15, 129.3, 129.2, 129.0, 128.7, 127.6, 125.3, 124.3, 95.9, 21.7. HRMS (ESI) [M+H]⁺ Calcd for [C₄₀H₂₈I₂N₄O₂S₂] 914.9798, found 914.9791.

(1Z,1'Z)-N,N'-((4Z,4'E) ((1,3-Phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene)) dibenzimidic acid (7e). The product was obtained as a pale yellow needles, mp: 134–136 °C (322.3 mg, 70%); FTIR (Zn–Se ATR, cm⁻¹) 3197, 2922, 2852, 1674, 1550, 1462, 1259, 1195, 999, 817, 702; ¹H NMR (400 MHz, CDCl₃) δ 10.55 (br s, 2H), 7.85–7.80 (m, 5H), 7.50–7.42 (m, 3H), 7.35–7.26 (m, 8H), 7.13 (d, J = 6.4 Hz, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 160.2 (d, J_C-F = 244.7 Hz), 143.4, 143.2, 133.6, 132.9, 132.8, 130.5 (d, J_C-F = 8.7 Hz), 130.1, 129.7, 129.5, 129.3, 128.9, 128.6, 128.4, 125.5 (d, J_C-F = 7.7 Hz), 117.6 (d, J_C-F = 22.1 Hz), 115.1 (d, J_C-F = 26.0 Hz), 96.5. HRMS (ESI) [M+H]⁺ Calcd for [C₃₈H₂₂F₂I₂N₄O₂S₂] 922.9320, found 922.9295.
ylidene)bisis(4-methylbenzimidic acid) (7d). The product was obtained as a pale yellow needles, mp: 148–150 °C (341.6 mg, 72%); FTIR (Zn–Se ATR, cm⁻¹) 3238, 2965, 2823, 1624, 1543, 1476, 1320, 1211, 1156, 923, 817, 710; ¹H NMR (400 MHz, CDCl₃) δ 11.12 (br s, 2H), 7.98 (d, J = 7.8 Hz, 1H), 7.79 (d, J = 8.8 Hz, 2H), 7.73–7.68 (m, 3H), 7.43–7.40 (m, 1H), 7.35–7.24 (m, 3H), 7.13–7.06 (m, 8H), 2.30 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 160.3 (d, J_C-F = 245.6 Hz), 144.3, 143.6, 143.1, 130.2, 130.17, 130.0, 129.4, 129.3, 128.5, 127.6, 127.2, 125.7 (d, J_C-F = 8.7 Hz), 117.5 (d, J_C-F = 23.1 Hz), 114.9 (d, J_C-F = 25.1 Hz), 96.5, 21.7. HRMS (ESI) [M+H]+ Calcd for [C₄₀H₂₆F₂I₂N₄O₂S₂] 950.9633, found 950.9638.

(Z)-N-((Z)-4-(3-(4-Methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3] thiazin-2-yl)benzimidic acid (9). The product was obtained as a yellow needles, mp: 205–207 °C (197.5 mg, 79%); FTIR (Zn–Se ATR, cm⁻¹) 3297, 2852, 2176, 1682, 1592, 1552, 1503, 1363, 1249, 1023, 825, 719; ¹H NMR (400 MHz, CDCl₃) δ 12.17 (br s, 1H), 8.72 (d, J = 7.8 Hz, 1H), 8.04 (d, J = 6.8 Hz, 2H), 7.49–7.45 (m, 1H), 7.41–7.35 (m, 3H), 7.32–7.24 (m, 7H), 7.07 (d, J = 7.8 Hz, 1H), 6.81 (d, J = 8.8 Hz, 2H), 3.78 (s, 3H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.7, 137.0, 135.9, 135.0, 133.0, 132.7, 132.2, 130.7, 130.5, 130.4, 129.1, 128.8, 128.6, 128.2, 128.1, 127.6, 126.4, 124.9, 121.1, 120.6, 114.9, 113.9, 96.2, 88.0, 55.1, 19.2. HRMS (ESI) [M+H]+ Calcd for [C₃₂H₂₄N₂O₂S] 501.1637, found 501.1625.

(Z)-N-((E)-4-(4-(tert-Butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3] thiazin-2-yl)-4-methylbenzimidic acid (11). The
The product was obtained as a yellow needles, mp: 96–98 °C (199.5 mg, 75%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3215, 2838, 1644, 1592, 1544, 1501, 1415, 1240, 1123, 1033, 825, 710; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.42 (br s, 1H), 7.97 (d, \(J = 7.8\) Hz, 2H), 7.36 (d, \(J = 7.8\) Hz, 2H), 7.17 (d, \(J = 7.8\) Hz, 3H), 7.08 (d, \(J = 7.8\) Hz, 2H), 6.98 (d, \(J = 7.8\) Hz, 1H), 6.92–6.81 (m, 4H), 6.69 (d, \(J = 8.8\) Hz, 2H), 3.73 (s, 3H), 2.35 (s, 3H), 1.33 (s, 9H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 159.3, 151.9, 145.4, 143.2, 138.0, 133.7, 132.4, 130.3, 129.4, 129.1, 129.0, 125.3, 124.9, 124.0, 120.1, 116.1, 114.9, 113.7, 55.3, 34.9, 31.4, 21.7. HRMS (ESI) [M+H]\(^+\) Calcd for [C\(_{34}\)H\(_{32}\)N\(_2\)O\(_2\)S] 533.2263, found 533.2254.

\[
N\text{---}((2\text{---}(o\text{-Tolylethynyl)}\text{phenyl})\text{carbamothioyl})\text{benzamide} \quad (12a)
\]

The product was obtained as a white needles, mp: 130–132 °C (175.8 mg, 95%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3323, 2923, 2197, 1682, 1602, 1526, 1340, 1147, 1078, 832, 708, 656; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 13.03 (s, 1H), 9.19 (br s, 1H), 8.53 (d, \(J = 7.8\) Hz, 1H), 7.88 (d, \(J = 7.8\) Hz, 2H), 7.68 (d, \(J = 7.8\) Hz, 1H), 7.65–7.60 (m, 2H), 7.54–7.50 (m, 2H), 7.42–7.38 (m, 1H), 7.27–7.14 (m, 4H), 2.50 (s, 3H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 182.6, 170.7, 144.7, 143.2, 138.1, 136.9, 136.8, 136.0, 133.8, 133.6, 133.1, 132.8, 132.0, 130.8, 130.0, 128.6, 127.0, 122.5, 99.9, 92.9, 25.11. HRMS (ESI) [M+H]\(^+\) Calcd for [C\(_{23}\)H\(_{18}\)N\(_2\)OS] 371.1218, found 371.1210.

\[
N\text{---}((2\text{---}(4\text{-Butylphenyl)}\text{ethynyl})\text{phenyl})\text{carbamothioyl})\text{benzamide} \quad (12b)
\]

The product was obtained as a white needles, mp: 113–115 °C (191.6 mg, 93%); FTIR (Zn–Se ATR, cm\(^{-1}\)) 3315, 2897, 2210, 1680, 1612, 1565, 1410, 1147, 1078, 813, 707; \(^1\)H
NMR (400 MHz, CDCl$_3$) $\delta$ 13.17 (s, 1H), 9.17 (s, 1H), 8.74 (d, $J = 8.8$ Hz, 1H), 7.91 (d, $J = 7.8$ Hz, 2H), 7.67–7.59 (m, 4H), 7.57–7.53 (m, 2H), 7.42–7.38 (m, 1H), 7.26–7.22 (m, 1H), 7.18 (d, $J = 8.8$ Hz, 2H), 2.63 (t, $J = 7.8$ Hz, 2H), 1.64–1.57 (m, 2H), 1.39–1.33 (m, 2H), 0.94 (t, $J = 7.3$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 177.7, 166.3, 143.9, 139.1, 133.7, 132.4, 131.9, 131.8, 129.3, 128.5, 128.3, 127.6, 126.1, 123.4, 120.0, 117.5, 97.3, 84.1, 35.7, 33.5, 22.4, 14.0. HRMS (ESI) [M+H]$^+$ Calcd for [C$_{26}$H$_{24}$N$_2$OS] 413.1688, found 413.1699.

$N$-((2-(Hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (12c). The product was obtained as a white needles, mp: 140–142 °C (159.6 mg, 95%); FTIR (Zn–Se ATR, cm$^{-1}$) 3110, 2995, 2190, 1570, 1323, 1147, 1078, 1000, 921, 832, 701; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 12.96 (s, 1H), 9.10 (s, 1H), 8.70 (d, $J = 8.2$ Hz, 1H), 7.90–7.88 (m, 2H), 7.65–7.61 (m, 1H), 7.54–7.51 (m, 2H), 7.45 (dd, $J = 7.7$, 1.4 Hz, 1H), 7.34–7.30 (m, 1H), 7.16 (td, $J = 7.6$, 1.0 Hz, 1H), 2.54 (t, $J = 7.1$ Hz, 2H), 1.68–1.60 (m, 2H), 1.51–1.44 (m, 2H), 0.91 (t, $J = 7.4$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 177.5, 166.1, 139.5, 133.7, 132.1, 131.9, 129.3, 127.7, 127.9, 126.0, 123.0, 117.9, 99.1, 75.8, 30.6, 22.2, 19.6, 13.8. HRMS (ESI) [M+H]$^+$ Calcd for [C$_{20}$H$_{20}$N$_2$OS] 337.1375, found 337.1375.

References


Copies of $^1$H and $^{13}$C NMR
$^1$H NMR

2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r)
$^{13}$C NMR

$\text{NH}_2$

F$	ext{Me}$

F$	ext{Me}$

2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r)
HRMS

2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r)
$^1$H NMR

2-(cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s)
$^{13}$C NMR

2-(cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s)
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- Algorithm: Find by Molecular Feature
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**HRMS**

2-(cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s)
$^1$H NMR

2,2'-((1,3-phenylenebis(ethyne-2,1-diyl))dianiline (6a)
$^{13}$C NMR

2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))dianiline (6a)
2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))dianiline (6a)
$^1$H NMR

2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b)
$^{13}$C NMR

$2,2'-(1,3$-phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b)
2,2’-(1,3-phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b)

**Qualitative Compound Report**

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**HRMS**
$^1$H NMR

(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3a)
$^{13}$C NMR

(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3a)
HRMS

(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3a)
\(^1\)H NMR

(Z)-N-((E)-4-(iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3b)
$^{13}$C NMR

(Z)-N-((E)-4-(iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3b)
(Z)-N-((E)-4-(iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3b)
$^1$H NMR

(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4$H$-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c)
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c)
$^1$H NMR

(Z)-N-((E)-4-(Iodo (p-tolyl)methylene)-4H-benzo[\textit{d}][1,3]thiazin-2-yl)benzimidic acid (3d)
\[ ^{13}\text{C NMR} \]

(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3d)
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3d)
\[ ^1H \text{NMR} \]

(Z)-N-((E)-4-((4-butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3e)
$^{13}$C NMR

(Z)-N-((E)-4-(4-butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3e)
(Z)-N-((E)-4-((4-butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3e)
**^1H NMR**

(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3f)
$^{13}$C NMR

(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3f)
HRMS

(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3f)

Qualitative Compound Report

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[59]
$^1$H NMR

(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g)
$^{13}$C NMR

(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g)
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g)
$^1$H NMR

(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h)
$^{13}$C NMR

(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h)
(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h)
$^1$H NMR

(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3i)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3i)
(Z)-N-((E)-4-(Iodo thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl) benzimidic acid (3i)
$^{1}$H NMR

(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3j)
$^{13}$C NMR

(Z)-N-((E)-4-((iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3j)
(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3j)
(Z)-N-((E)-4-(Iodo(p-toly)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k)
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k)
$^1$H NMR

(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)

```
HRMS

![Chemical Structure Image]

(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)

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**MFT MS Spectrum**

**MFT MS Spectrum**

**MS Spectrum Peak List**

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End of Report

[77]
$^1$H NMR

(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m)
$^{13}$C NMR

(Z)-N-((E)-4-((4-( tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m)
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m)
\(^1\)H NMR

(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n)
$^{13}$C NMR

(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n)
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n)
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[\textit{d}][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o)
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o)
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o)
$^1$H NMR

(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p)
(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p)
(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p)
$^1$H NMR

(Z)-N-((E)-4-(iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a)
(Z)-N-((E)-4-(iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a)
(Z)-\text{N-([E]-4-\text{(iodo(p-tolyl)methylene})-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a)}}
(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b)
(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b)
\(^{1}\text{H NMR}\)

\((Z)-N-((E)-4-\text{(Iodo(phenyl)methylene)}-7\text{-methyl-4H-benzo[d][1,3]thiazin-2-yl})-4\text{-methylbenzimidic acid (4c)}\)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4c)
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4c)
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[de][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d)
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d)
$^1$H NMR

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e)
$^{13}$C NMR

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e)
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e)
$^1$H NMR

\[
\text{(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[\text{d}][1,3]\text{thiazin-2-yl})benzimidic acid (4f)}}
\]
(Z)-3-Chloro-N-((E)-4-iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4f)
(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4f)
$^1$H NMR

(Z)-N-((E)-6-fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g)
\[^{13}\text{C} \text{NMR}\]

(Z)-N-((E)-6-fluoro-4-((iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g)
HRMS

(Z)-N-((E)-6-fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g)
$^1$H NMR

(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h)
$^{13}$C NMR

(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h)
(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h)
$^1$H NMR

(Z)-N-((E)-4-(Iodo(phenyl)methylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4i)
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$^1$H NMR

(Z)-N-((E)-4-(1-Iodopentylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5a)
$^{13}$C NMR

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$^{13}$C NMR
(Z)-N-((E)-4-(4-chloro-1-iodobutylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5b)
(Z)-N-((E)-4-(1-iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c)
$^{13}$C NMR

(Z)-N-((E)-4-(1-iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c)
(Z)-N-((E)-4-(1-iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c)
(Z)-N-((E)-4-(cyclopropyldiiodomethylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5d)
\(^{13}\text{C} \text{NMR}\)

\[
(Z)-N-((E)-4-\text{(cyclopropyliodomethylene)}-6-\text{(trifluoromethyl)}-4\text{H-} \text{benzo}[d][1,3]\text{thiazin-2-yl})\text{benzimidic acid (5d)}
\]
(Z)-N-((E)-4-(cyclohexyliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5e)
$^{13}$C NMR

(Z)-N-((E)-4-(cyclohexyliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5e)
HRMS

(Z)-N-((E)-4-(cyclohexyloiodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5e)

[Image of the chemical structure]

Qualitative Compound Report

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PKE MS Spectrum

PKE MS Journal Spectrum

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[131]
$^1$H NMR

(Z)-N-((E)-4-(cyclohex-1-en-1-ylidomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f)
(Z)-N-((E)-4-(cyclohex-1-en-1-yliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f)
(Z)-N-((E)-4-(cyclohex-1-en-1-ylidomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f)
$^1$H NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene)dibenzimidic acid (7a)
$^{13}$C NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene)dibenzimidic acid (7a)
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7a)
$^1$H NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b)
$^{13}$C NMR

(1Z,1′Z)-N,N′-((4Z,4′E)-(1,3-phenylenebis(iodomethylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b)
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b)
$^1$H NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene)dibenzimidic acid (7c)
$^{13}$C NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-((1,3-phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7c)
(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-y1-4-ylidene)dibenzimidic acid (7c)
$^1$H NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7d)
$^{13}$C NMR

(1Z,1'Z)-N,N'-(4Z,4'E)-(1,3-phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7d)
(1Z,1’Z)-N,N’-((4Z,4’E)-(1,3-phenylenebis(iodomethanylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7d)
$^1$H NMR

(Z)-N-((Z)-4-(3-(4-methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (9)
$^{13}$C NMR

\[ \text{(Z)-N-((Z)-4-(3-(4-methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (9)} \]
(Z)-N-((Z)-4-(3-(4-methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (9)
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (11)
$^{13}\text{C NMR}$

(Z)-N-((E)-4-((4-(tert-butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (11)
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (11)
$^1$H NMR

N-((2-(o-tolyethynyl)phenyl)carbamothioyl)benzamide (12a)
\(^{13}\text{C NMR}\)

\[ \text{N-} \left(2\text{-}o\text{-tolylethynyl)}\text{phenyl} \text{carbamothioyl} \right) \text{benzamide (12a)} \]
N-((2-(o-tolylethynyl)phenyl)carbamothioyl)benzamide (12a)
N-((2-((4-Butylphenyl)ethynyl)phenyl)carbamothioyl)benzamide (12b)
N-((2-((4-Butylphenyl)ethyl)phenyl)carbamothioyl)benzamide (12b)
N-((2-((4-Butylphenyl)ethynyl)phenyl)carbamothioyl)benzamide (12b)

HRMS

Qualitative Compound Report

Compound Table

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HRE MS Spectrum

MS Spectrum Peak List

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[158]
$^1$H NMR

N-((2-(hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (12c)
\(^{13}\text{C NMR}\)

\[
\text{N-((2-(hex-1-yn-1-yl)phenyl)carbamoithiyl)benzamide (12c)}
\]
N-((2-(hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (12c)