Synthesis of \(\alpha\)-Sulfoximino Tetrazoles via Azido-Ugi Four-Component Reaction

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**Abstract** The sulfoximine-based tetrazoles have been synthesized via azido-Ugi four-component reactions of sulfoximines, isocyanides, aldehydes, and TMS-azide in MeOH at 70 °C in the presence of InCl\(_3\). Replacement of sulfoximines with sulfonimidamides (SIA) has delivered the corresponding SIA-based tetrazole. Interestingly, SIA also acts as a surrogate amine to furnish the corresponding aminotetrazole as a by-product.

**Key words** sulfoximines, sulfonimidamides, Ugi reaction, tetrazoles, isocyanides

**Figure 1** Representative tetrazole-bearing derivatives used in various fields

Tetrazoles are of great importance due to their distinctive chemical and biological properties.\(^1\) This moiety has found applications in fields such as medicine,\(^2\) biochemistry,\(^3\) pharmacology,\(^4\) materials,\(^5\) coordination chemistry,\(^6\) and organocatalysis\(^7\) (Figure 1), as well as in synthetic chemistry.\(^8\) Importantly, tetrazoles are well-established bioisosteres of carboxylic acids.\(^9\)

Sulfoximines have recently received very good attention in synthetic, medicinal, and agrochemical areas.\(^10\) Sulfoximine-containing bioactive molecules include Atuveciclib, BAY 1251152, and AZD6738.\(^11\) Additionally, sulfoximines have been used as chiral auxiliaries and ligands in asymmetric synthesis, and as directing groups in ortho-C–H functionalization.\(^12\) Considering the importance of tetrazoles, together with our recent interest in sulfoximines\(^13\) and related chemistry,\(^14\) we herein report that sulfoximine-based tetrazoles, i.e., \(\alpha\)-sulfoximino tetrazoles, have been prepared via four-component reaction of sulfoximines, isocyanides, aldehydes, and TMS-N\(_3\).

The classical four-component Ugi reaction utilizes carboxylic acids as one of the nucleophiles to synthesize the bis-amide.\(^15\) Replacement of the carboxylic acid with an azide delivers the corresponding tetrazole in the Azido-Ugi tetrazole reaction (UT-4CR) (Scheme 1a). UT-4CRs have been widely employed to construct diverse tetrazole-based systems by altering the substituents in the substrate.\(^16\) However, most of the previous reports on UT-4CRs employ sp\(^3\)-hybridized primary or secondary amines as amine component. Hence, despite being a very well-established field, the reaction behavior with sp\(^2\) hybridized imine nucleophiles remains to be studied. In this context, we employed sulfoximines, which contain the sp\(^2\)-hybridized imino group, as nucleophile in the UT-4CR to synthesize \(\alpha\)-sulfoximino tetrazoles (Scheme 1b).

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**Scheme 1a** Synthesis of \(\alpha\)-Sulfoximino Tetrazoles via Azido-Ugi Four-Component Reaction

**Scheme 1b** Preparation of \(\alpha\)-Sulfoximino Tetrazoles via Azido-Ugi Four-Component Reaction
Previously, Bolm et al. prepared N-(1H)-tetrazole sulfoximines via a ZnBr₂-catalyzed cycloaddition reaction (Scheme 2a).17 Recently, the same research group prepared 2-sulfoximido acetic acids via Petasis reaction (Scheme 2b).18 Our α-sulfoximido tetrozoles can be considered as tetrozole isosteres of 2-sulfoximido acetic acid (Scheme 2b).

The starting NH-sulfoximines were prepared by following the reported protocol.19a We initiated the investigations with a four-component reaction of sulfoximine 1a, p-tolualdehyde (2a), t-butyl isocyanide (3a), and TMS-N₃ (4) under conditions that are summarized in Table 1. Initially, the reaction mixture was stirred in methanol at room temperature for 24 h, but the desired tetrozole 5a was obtained only in 10% yield, along with unreacted sulfoximine and aldehyde (entry 1). To obtain a better outcome, the Lewis acid ZnCl₂ was added as mediator and a 40% yield of 5a was isolated (entry 2). Increased temperature gave a better yield of 5a (entries 3 and 4), and replacement of ZnCl₂ with InCl₃ resulted in a further improved yield at 70 °C (entry 6). Other Lewis acids such as Cu(OTf)₂, CuBr, and Zn(OTf)₂ were not as effective as InCl₃ at 70 °C (entries 6–9). Other solvents, including EtOH, CH₃CN, DCE, toluene, and DCM were investigated (entries 10–14), but MeOH was found to be the best solvent for the transformation. When we replaced the TMS-N₃ in the reaction with NaN₃ we could isolate only 41% of 5a (entry 15). It should be noted that the Lewis acids were needed in 50 mol%; the use of lesser amounts (5/10/20/30/40 mol%) InCl₃ led to diminished product formation along with isolation of unreacted starting sulfoximine and aldehyde. A higher amount of InCl₃ (60%) did not give a better outcome.

| Entry | Solvent | Lewis acid | Temp (°C) | Time (h) | Yield (%) |
|-------|---------|------------|-----------|----------|-----------|
| 1a    | MeOH    | –          | r.t.      | 24       | 10        |
| 1b    | MeOH    | ZnCl₂      | r.t.      | 15       | 40        |
| 1c    | MeOH    | InCl₃      | 45        | 12       | 55        |
| 1d    | MeOH    | Cu(OTf)₂   | 45        | 12       | 61        |
| 2a    | MeOH    | CuBr       | 70        | 12       | NR        |
| 2b    | MeOH    | Zn(OTf)₂   | 70        | 12       | 54        |
| 3a    | EtOH    | InCl₃      | 70        | 12       | 36        |
| 3b    | CH₃CN   | InCl₃      | 70        | 12       | 21        |
| 4a    | DCE     | InCl₃      | 70        | 12       | NR        |
| 4b    | Toluene | InCl₃      | 70        | 12       | 12        |
| 5a    | DCM     | InCl₃      | 70        | 12       | 26        |
| 5b    | MeOH    | InCl₃      | 45        | 12       | 41        |

With the optimal reaction condition in hand, next we explored the scope and limitations of the method for the synthesis of sulfoximine based tetrozoles 5. Differently substituted sulfoximines, aldehydes, and isocyanides were utilized, and the results are shown in Scheme 3. Various aromatic aldehydes with electron-poor and electron-rich substitution patterns underwent successful reaction. It was noted that electron-deficient aryl aldehydes provided better outcomes than their electron-rich counterparts. Bulky triphenylamine aldehyde and heteroaromatic benzothiophene aldehyde also delivered 5n–p in good yields. Several cyclic and acyclic isocyanides such as cyclohexyl,adamantyl, and t-butyl isocyanide furnished the desire products in moderate to good yields. Unfortunately, the primary alkyl isocyanide (p-toluenesulfonylmethyl isocyanide) and aro-

### Notes

- General conditions for the one-pot four-component reaction: 1a (1.2 equiv), 2a (1.2 equiv), 3a (1.0 equiv), 4 (1.0 equiv), Lewis acid (0.5 equiv) in 1 mL solvent unless otherwise stated.
- Isolated yield.
- 1:1:1:1 ratio of all substrates.
- NaN₃ was used instead of TMSN₃.
matic isocyanide (4-methoxyphenyl isocyanide) both failed to produce the desired products 5s and 5t. The modifications of the S-aryl group (phenyl to substituted phenyl) and S-alkyl group (methyl to ethyl) of the NH-sulfoximines were well tolerated in the conversion.

In addition to S-aryl S-alkyl sulfoximines, diaryl/dialkyl symmetrical sulfoximines underwent reaction smoothly to produce the corresponding products 5q–r. The electronic effects induced by S-aryl substituents appeared to have only a minor influence on product formation.

All the synthesized compounds were characterized by ¹H and ¹³C NMR spectroscopy, and HRMS, and structures were unambiguously confirmed by single-crystal XRD analysis of two representative compounds (5c and 5e; see the Supporting Information).

The successful utilization of NH-sulfoximines as nucleophiles in the UT-4CR, inspired us to apply sulfonimidamide (SIA) (6) (Scheme 4) to construct SIA derived tetrazoles via UT-4CR. SIAs, the mono-aza analogues of sulfonamides, with a stereogenic tetrahedral sulfur atom and sp² hybrid-
ized imino group (free -NH), are considered an important emerging scaffold due to their applications in asymmetric synthesis and the medicinal and agrochemical industries.\textsuperscript{20}

Initially, SIA (6a) was treated with aldehyde 2a, isocyanide 3a, and TMS-N\textsubscript{3} (4) under the previously optimized reaction conditions (Table 1, entry 6), but the desired product 7a was formed in only minor amounts, accompanied by the side-product, cyclic amine-based tetrazole 8a as the major product. SIA 6 would appear to be acting as surrogate amine to yield 8. A previous report from our group had already described the surrogate nature of SIA under specific conditions.\textsuperscript{14a} Considering that the elevated reaction temperatures may result in S–N bond cleavage, the reaction was performed at lower temperature (Table 2, entry 3) and 7a was obtained as the major product (52%) at 45 °C, along with 18% of by-product 8a. Screening of other Lewis acids, such as ZnCl\textsubscript{2} and Zn(OTf)\textsubscript{2} showed that they were not as effective as InCl\textsubscript{3} (entries 4 and 5).

Hence, by following the optimized condition (Table 2, entry 3), we scrutinized the scope and generality of the reaction with SIA (Scheme 5). Reaction of SIAs with various S-aryl (-Ph, 4-MePh, 4-OMePh) and S-cyclic amines (pyrroli-
The starting sulfoximines/sulfonimidamides were synthesized by following reported methods. The aldehydes, isocyanides, TMSN₃, InCl₃, and MeOH were purchased from various suppliers and used as received. ¹H and ¹³C NMR spectra were recorded with a Bruker spectrometer operating at 500 and 125 MHz, respectively, in CDCl₃ or CD₆CO as solvents. Mass spectra were recorded with an Agilent QTOF G6545 XT spectrometer at 50,000 resolutions using ESI mode. Melting points are uncorrected.

**Sulfoximine Synthesis; General Procedure**

To a stirred solution of diaryl (or alkylaryl) sulfide (1 mmol) in MeOH (5 mL), NH₄CO₂NH₂ (1.5 equiv) and Ph(ΟAc)₂ (2.3 equiv) were added, and the solution was stirred at r.t. for 3–4 h. After the disappearance of the sulfide (checked by TLC), the solvent was removed under reduced pressure. The crude product was purified by flash column chromatography (25–40% EtOAc/hexane).

For the gram-scale reaction, sulfide (20 mmol) and MeOH (100 mL) were used.
One-Pot Tandem Synthesis of Tetrazole Based Sulfoximine/Sulfonimidamide (57); General Procedure

Precautions: We have not experienced any problems with the use of TMSI under the reaction conditions employed and working on small scale. However, essential precautions should be taken on scaling up this chemistry.

A solution of sulfoximine (30 mg 1.2 equiv), aldehyde (1.2 equiv), isocyanide (1.0 equiv), and InCl3 (0.5 equiv) in MeOH (1 ml) in a 20 mL sealed tube was stirred at 70 °C under argon atmosphere. After 15 min, TMS-azole (1.0 equiv) was added to the reaction mixture and the reaction was stirred for the stipulated period. Upon completion of reaction (confirmed by TLC), the reaction mixture was poured in water and extracted with EtOAc (2 × 10 mL). The organic layers were washed with sat. aq. NaHCO3, water, brine and dried over anhydrous Na2SO4. After filtration, the solvent was evaporated under reduced pressure, and the resulting crude product was purified by silica gel column chromatography with 20–30% of EtOAc in hexane as the eluent.

For sulfonimidamides, the reaction was stirred at 45 °C.

All the synthesized compounds (except 5q/5r) have more than one (generally two) stereogenic centers. Hence, mixtures of diastereomers could be expected to form. However, we isolated only single diastereomer for 5a-m, 5p, 5q, and 7. Another diastereomer was formed in trace amounts for 5a-m, 5p, 5q, and 7. For compounds 5n–o, two diastereomers were isolated in almost equal amounts.

N-((1-(tert-Butyl)-1H-tetrazol-5-yl)(p-tolyl)methyl) S-Methyl S-4-Bromophenyl Sulfoximine (5a)

Colorless viscous liquid; 61% yield. TLC (SiO2): Rf 0.25 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.63 (d, J = 8.5 Hz, 2 H), 7.57 (d, J = 8.5 Hz, 2 H), 7.23 (d, J = 8.0 Hz, 2 H), 7.10 (d, J = 8.0 Hz, 2 H), 6.01 (s, 1 H), 3.08 (s, 3 H), 2.29 (s, 3 H), 1.41 (s, 9 H).

13C NMR (125 MHz, CDCl3): δ = 156.2, 139.9, 138.9, 137.7, 137.4, 132.7, 130.2, 129.4, 127.5, 61.7, 52.3, 45.6, 29.9, 21.1.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C20H26N5OS: 384.1853; found: 384.1857.

N-((1-(tert-Butyl)-1H-tetrazol-5-yl)(phenyl)methyl) S-Methyl S-4-Tolyl Sulfoximine (5b)

Yellowish viscous liquid; 60% yield. TLC (SiO2): Rf 0.26 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.65 (d, J = 7.0 Hz, 1 H), 7.57 (d, J = 8.5 Hz, 2 H), 7.32 (d, J = 7.5 Hz, 1 H), 7.27–7.24 (m, 2 H), 7.19 (d, J = 8.0 Hz, 2 H), 7.05 (t, J = 8.0 Hz, 1 H), 6.01 (s, 1 H), 3.06 (s, 3 H), 2.34 (s, 3 H), 1.36 (s, 9 H).

13C NMR (125 MHz, CDCl3): δ = 156.3, 144.5, 140.8, 137.5, 136.5, 130.1, 128.7, 127.5, 123.6, 61.7, 52.6, 45.6, 29.9, 21.6.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C19H22BrClN5OS: 348.1855; found: 348.1857.

N-((1-(tert-Butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl) S-Methyl S-4-Chlorophenyl Sulfoximine (5c)

White solid; mp 117–118 °C; 68% yield. TLC (SiO2): Rf 0.21 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.67 (d, J = 8.5 Hz, 2 H), 7.57 (d, J = 8.5 Hz, 2 H), 7.38 (d, J = 8.0 Hz, 2 H), 7.29 (d, J = 8.5 Hz, 2 H), 5.91 (s, 1 H), 4.51–4.46 (m, 1 H), 3.18 (s, 3 H), 2.25–2.24 (m, 2 H), 1.96–1.93 (m, 2 H), 1.81–1.76 (m, 2 H), 1.49–1.46 (m, 2 H), 1.32–1.30 (m, 2 H).

13C NMR (125 MHz, CDCl3): δ = 155.2, 140.6, 138.1, 137.2, 133.9, 133.1, 130.1, 128.8, 128.0, 58.3, 51.5, 45.5, 33.2, 25.5, 24.9.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C21H27ClN5O2S: 448.1568; found: 448.1567.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)(4-chlorophenyl)methyl) S-Methyl S-4-Bromophenyl Sulfoximine (5e)

White solid; mp 120–122 °C; 62% yield. TLC (SiO2): Rf 0.25 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.67 (d, J = 8.0, 1.0 Hz, 2 H), 7.56 (t, J = 7.5 Hz, 1 H), 7.44 (t, J = 8.0 Hz, 2 H), 7.29–7.26 (m, 4 H), 6.06 (s, 1 H), 3.34–3.19 (m, 2 H), 1.41 (s, 9 H), 1.26 (t, J = 8.0 Hz, 3 H).

13C NMR (125 MHz, CDCl3): δ = 156.1, 139.9, 139.7, 137.7, 133.5, 129.5, 129.4, 128.9, 128.7, 61.8, 51.8, 51.4, 30.0, 7.1.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C13H23N5O2S: 418.1463; found: 418.1473.

N-((1-(tert-Butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl) S-Ethyl S-Phenyl Sulfoximine (5f)

White solid; mp 129–130 °C; 67% yield. TLC (SiO2): Rf 0.21 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.56 (d, J = 9.0 Hz, 2 H), 7.31–7.25 (m, 4 H), 6.90 (d, J = 9.0 Hz, 2 H), 6.09 (s, 1 H), 3.84 (s, 3 H), 3.29–3.17 (m, 2 H), 1.45 (s, 9 H), 1.25 (t, J = 7.5 Hz, 3 H).

13C NMR (125 MHz, CDCl3): δ = 163.6, 156.1, 139.8, 133.3, 131.4, 128.7, 128.3, 114.6, 61.8, 55.6, 51.7, 51.6, 29.8, 7.1.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C13H23N5O2S: 448.1568; found: 448.1578.
N-((1-Adamantyl-1H-tetrazol-5-yl)-(4-chlorophenyl)methyl) S-Ethyl S-Phenyl Sulfoximine (5h)

White solid; mp 132–134 °C; 66% yield. TLC (SiO2): Rf 0.25 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.66 (d, J = 8.5 Hz, 2 H), 7.55 (t, J = 7.5 Hz, 1 H), 7.44 (t, J = 7.5 Hz, 2 H), 7.31–7.26 (m, 4 H), 6.08 (s, 1 H), 3.33–3.21 (m, 2 H), 2.07–2.01 (m, 6 H), 1.94–1.92 (m, 3 H), 1.67–1.64 (m, 3 H), 1.60–1.57 (m, 3 H), 1.27 (t, J = 7.5 Hz, 3 H).

13C NMR (125 MHz, CDCl3): δ = 156.1, 154.0, 137.9, 133.5, 133.4, 129.4, 129.3, 128.9, 128.7, 62.9, 51.9, 51.4, 42.1, 35.6, 29.6, 7.1.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C26H31ClN5OS: 496.1932; found: 496.1935.

N-((1-Adamantyl-1H-tetrazol-5-yl)-(4-bromophenyl)methyl) S-Methyl S-4-Methoxyphenyl Sulfoximine (5j)

White solid; mp 179–181 °C; 70% yield. TLC (SiO2): Rf 0.24 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.63 (d, J = 9.0 Hz, 2 H), 7.29 (q, J = 8.5 Hz, 4 H), 6.91 (d, J = 9.0 Hz, 2 H), 6.04 (s, 1 H), 3.84 (s, 3 H), 3.14 (s, 3 H), 2.08–2.04 (m, 6 H), 1.98–1.96 (m, 3 H), 1.68–1.65 (m, 3 H), 1.61–1.59 (m, 3 H).

13C NMR (125 MHz, CDCl3): δ = 167.3, 156.1, 139.8, 133.5, 130.8, 130.5, 128.9, 128.7, 63.0, 55.8, 52.2, 46.0, 42.0, 35.6, 29.6.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C23H29BrN5O2S: 518.1220; found: 518.1229.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)-(4-bromophenyl)methyl) S-Ethyl S-2-Thiophenyl Sulfoximine (5m)

Brownish viscous liquid; 67% yield. TLC (SiO2): Rf 0.30 (30% EtOAc in hexane).

1H NMR (500 MHz, CDCl3): δ = 7.69 (d, J = 6.5 Hz, 1 H), 7.42 (d, J = 8.5 Hz, 2 H), 7.32 (d, J = 3.5 Hz, 1 H), 7.29 (d, J = 8.5 Hz, 2 H), 7.12–7.10 (m, 1 H), 6.11 (s, 1 H), 4.50–4.47 (m, 1 H), 3.38–3.36 (m, 2 H), 2.26–2.23 (m, 2 H), 1.95–1.92 (m, 3 H), 1.81–1.76 (m, 2 H), 1.73–1.71 (m, 1 H), 1.48–1.45 (m, 2 H), 1.37 (t, J = 7.0 Hz, 3 H).

13C NMR (125 MHz, CDCl3): δ = 155.2, 140.7, 138.9, 135.7, 135.3, 131.6, 128.5, 128.3, 121.8, 58.9, 53.3, 51.1, 33.2, 25.5, 24.9, 7.9.

HRMS (ESI-TOF): m/z [M + H]+ calcd for C23H29BrN5O2S: 518.1229.

S-((1-Butyl)-1H-tetrazol-5-yl)-(N,N-diphenylaniline)methyl) S-Methyl S-4-Methoxyphenyl Sulfoximine (5n)

Obtained as a diastereomeric mixture. Total yield 72%.

Diastereomer 1

White solid; mp 170–172 °C. TLC (SiO2): Rf 0.24 (40% EtOAc in hexane).

IR (KBr): 3059, 3038, 2935, 2825, 1735, 1575, 1508, 1478, 1405, 1375, 1317, 1295, 1215, 1154, 1078, 1025, 981, 800, 697 cm⁻¹.

1H NMR (500 MHz, CDCl3): δ = 7.79 (d, J = 6.0 Hz, 6 H), 7.04 (dd, J = 7.5 Hz, 4 H), 7.00–6.98 (m, 4 H), 6.89 (d, J = 9.0 Hz, 2 H), 6.02 (s, 1 H), 3.83 (s, 3 H), 3.12 (s, 3 H), 1.46 (s, 9 H).

13C NMR (125 MHz, CDCl3): δ = 163.5, 156.5, 147.6, 147.1, 134.6, 130.8, 130.7, 129.2, 128.4, 124.3, 123.5, 122.9, 114.5, 61.6, 55.7, 51.9, 45.9, 29.9.

HRMS (ESI-TOF): m/z [M + Na]+ calcd for C25H34N4NaS: 589.2356; found: 589.2356.

Diastereomer 2

White solid; mp 172–173 °C.

1H NMR (500 MHz, CDCl3): δ = 7.71 (d, J = 9.0 Hz, 2 H), 7.23–7.17 (m, 6 H), 7.01–6.99 (m, 2 H), 6.97–6.95 (m, 4 H), 6.92 (d, J = 9.0 Hz, 2 H), 6.83 (d, J = 8.5 Hz, 2 H), 6.02 (s, 1 H), 3.87 (s, 3 H), 3.10 (s, 3 H), 1.68 (s, 9 H).

13C NMR (125 MHz, CDCl3): δ = 163.1, 157.0, 147.5, 147.1, 133.2, 130.3, 129.2, 128.9, 125.4, 124.3, 123.1, 122.9, 114.3, 61.5, 55.6, 52.5, 46.3, 30.1.

HRMS (ESI-TOF): m/z [M + Na]+ calcd for C25H34N4NaS: 589.2356; found: 589.2357.
**N-((1-,(tert-Butyl)-1H-tetrazol-5-yl)(N,N-diphenylaniline)methyl)-S-Methyl S-Phenyl Sulfoximine (5o)**

Obtained as a diastereomeric mixture. Total yield 70%.

**Diastereomer 1**

White solid; mp 169–170 °C. TLC (SiO2): Rf 0.26 (40% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7a) | 0.26 | 52 | EtOAc in hexane |

**Diastereomer 2**

White solid; mp 167–168 °C.

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7b) | 0.26 | 52 | EtOAc in hexane |

**N-((1-,(tert-Butyl)-1H-tetrazol-5-yl)(benzo[b]thiophen-3-yl)methyl)-S-Ethyl S-4-Methoxybenzyl Sulfoximine (5q)**

Brown viscous liquid; 58% yield. TLC (SiO2): Rf 0.18 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7c) | 0.18 | 52 | EtOAc in hexane |

**N-((1-,(tert-Butyl)-1H-tetrazol-5-yl)(4-bromophenyl)methyl) S-Diisopropyl Sulfoximine (5s)**

Off-white solid; mp 87–88 °C; 44% yield. TLC (SiO2): Rf 0.20 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7d) | 0.20 | 52 | EtOAc in hexane |

**N-((1-Cyclohexyl-1H-tetrazol-5-yl)(4-chlorophenyl)methyl) Di-S-4-methoxybenzyl Sulfoximine (5r)**

Yellowish viscous liquid; 47% yield. TLC (SiO2): Rf 0.28 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7e) | 0.28 | 52 | EtOAc in hexane |

**N-((1-,(tert-Butyl)-1H-tetrazol-5-yl)(p-toly)methyl) S-Pyrrolylid S-Phenyl Sulfinimidamide (7a)**

Yellowish solid; mp 110–112 °C; 52% yield. TLC (SiO2): Rf 0.45 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7f) | 0.45 | 52 | EtOAc in hexane |

**N-((1-,(tert-Butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl) S-Pyrrolylid S-Phenyl Sulfinimidamide (7b)**

Off-white solid; mp 107–108 °C; 56% yield. TLC (SiO2): Rf 0.45 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7g) | 0.45 | 52 | EtOAc in hexane |

**N-((1-,(tert-Butyl)-1H-tetrazol-5-yl)(4-bromophenyl)methyl) S-Pyrrolylid S-p-Tolyl Sulfinimidamide (7c)**

White solid; mp 89–91 °C; 59% yield. TLC (SiO2): Rf 0.44 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7h) | 0.44 | 52 | EtOAc in hexane |

**N-((1-Adamantyl-1H-tetrazol-5-yl)(4-chlorophenyl)methyl) S-Pyrrolylid S-4-Methoxybenzyl Sulfinimidamide (7d)**

White solid; mp 83–95 °C; 61% yield. TLC (SiO2): Rf 0.42 (30% EtOAc in hexane).

| Compound | Rf Value | Yield (%) | TLC Conditions |
|----------|----------|-----------|----------------|
| Phenyl Sulfonimidamide (7i) | 0.42 | 52 | EtOAc in hexane |
IR (KBr): 3357, 3259, 2960, 2839, 2157, 1988, 1727, 1590, 1494, 1390, 1325, 1261, 1154, 1098, 1059, 917, 892, 833, 753, 677 cm⁻¹.

1H NMR (500 MHz, CDCl₃): δ = 7.84 (d, J = 9.0 Hz, 2 H), 7.69 (d, J = 8.5 Hz, 2 H), 7.39 (d, J = 8.5 Hz, 2 H), 7.09 (d, J = 9.0 Hz, 2 H), 6.45 (s, 1 H), 5.38 (s, 1 H), 2.78–2.77 (m, 4 H), 1.67 (s, 9 H), 1.43–1.39 (m, 4 H), 1.33–1.31 (m, 2 H).

13C NMR (125 MHz, CDCl₃): δ = 163.9, 157.6, 141.6, 133.6, 130.7, 130.2, 129.2, 128.1, 114.9, 62.5, 56.1, 51.3, 48.3, 25.9, 24.2.

HRMS (EI-TOF): m/z [M + H]+ calcd for C₅₀H₄₀ClN₈O₄S: 621.0641; found: 621.0644.

**Conflict of Interest**

The authors declare no conflict of interest.

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**Supporting Information**

Supporting information for this article is available online at https://doi.org/10.1055/a-1981-9151.

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