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Electronic Supplementary Information (ESI)

Rh(III)-catalyzed direct ortho-C-H diarylation of arylsulfoximines

with arylsilanes

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1. General Information

Analytical methods

Proton nuclear magnetic resonance (¹H NMR) and carbon nuclear magnetic resonance (¹³C NMR) spectroscopy were performed on a Bruker Advance 300, 400 and 500 NMR spectrometers. Chemical shifts ¹H NMR spectra are reported as in units of parts per million (ppm) downfield from SiMe₄ (0.0) and relative to the signal of chloroform-d (J = 7.264, singlet). Multiplicities were given as: s (singlet); d (doublet); t (triplet); q (quartet); dd (doublet of doublets); ddd (doublet of doublets of doublets) of doublets of doublets); dt (doublet of triplets); m (multiplets) and etc. The number of protons (n) for a given resonance is indicated by nH. Coupling constants are reported as a J value in Hz. Carbon nuclear magnetic resonance spectra (¹³C NMR) are reported as d in units of parts per million (ppm) downfield from SiMe₄ (0.0) and relative to the signal of chloroform-d (J = 77.03, triplet). High resolution mass spectral analysis (HRMS) was performed on LCMS Q-TOF (SHIMADZU Corporation) ESI spectrometer. Infrared spectra were recorded on a Nicolet IS50 Fourier transform spectrometer (FT-IR) and are reported in wave numbers (cm⁻¹).

Materials

Unless otherwise noted, all reagents were purchased energy chemistry and tansoole, and used without further purification.



2. Selected molecules featuring sulfoximine scaffold

Fig. S1

3. Optimization of reaction conditions

Table S1 Optimization of Reaction Conditions^{a,b}

O S≲NI 1a	H ₃ H + S 2a	i(OEt) ₃ [Cp*RhC F ⁻ sourc oxidant solvent,	Cl₂]₂ (2 mol%) e (3.0 equiv) (3.0 equiv) 70 ºC, 24 h	O U S NH 3a
Entry	Oxidant	F ⁻ source	Solvent	Yield (%)
1	Ag ₂ O	KF	DMA	n.d.
2	Ag ₂ O	TBAF	DMA	n.d.
3	Ag ₂ O	CsF	DMA	n.d.
4	CuF_2 (3.0) equiv)	DMA	31
5	AgF (3.0	equiv)	DMA	54
6	AgF (3.0	equiv)	THF	51
7	AgF (3.0	equiv)	DMSO	31
8	AgF (3.0	equiv)	DMF	17
9	AgF (3.0	equiv)	dioxane	61
10	AgF (3.0	equiv)	PhCl	79
11	AgF (3.0	equiv)	MeCN	17
12	AgF (3.0	equiv)	acetone	38
13 ^c	AgF (3.0	equiv)	PhCl	77
14^d	AgF (3.0	equiv)	PhCl	62
15^{e}	AgF (3.0	equiv)	PhCl	83
16 ^{<i>f</i>}	AgF (3.0	equiv)	DMA	n.d.
17 ^g	AgF (3.0	equiv)	DMA	28%

^{*a*}Reaction conditions: **1a** (0.2 mmol), **2a** (3.0 equiv), Rh catalyst (2.0 mol%), F⁻ resource (3.0 equiv), Solvent (1.0 mL), at 70 °C for 24 h. ^{*b*}Isolated yield, n.d. (no desired product) was determined by TLC. ^{*c*}T = 60 °C. ^{*e*}T= 80 °C. ^{*e*}1.0 equiv HOAc. ^{*f*}[(*p*-cymene)RuCl₂]₂(5 mol%) instead of [Cp*RhCl₂]₂. ^{*s*}1.0 mmol PhSi(OEt)₃ was used.

4. General procedure

4.1 General procedure for the synthesis of the sulfoximines^[1]



To a 100 mL round bottom flask equipped with a magnetic bar, added phenyl methyl sulphide (5 mmol, 1.0 equiv) and $(NH_4)_2CO_3$ (1.5 equiv) in MeOH (50 mL), the mixture was allowed stirred in room temperature for 10 minutes. After that, PhI(OAc)₂ (2.3 equiv) was added and the solution was stirred overnight. After the reaction was complete monitored by TLC, the solvent was removed under reduced pressure and the crude product was purified with silica gel chromatography (petroleum ether/ethyl acetate) to provide pure product.

4.2 General procedure for the synthesis of the arylsilanes^[2]



(a) Unless otherwise indicated, all reactions were performed on a 30 mmol scale. A 250 mL three-neck, pear-shaped flask was fitted with an addition funnel, a reflux condenser, a rubber septum, and a stir bar. The flask was then charged with freshly washed magnesium turnings (0.792 g, 33.0 mmol), iodine pellets (1 pellet about 10 mg), and back-filled with nitrogen. Then THF (30 mL) was added via syringe. The addition funnel was charged with the aryl halide (30 mmol) in 10 mL THF. The reaction was initiated by addition of 5-10 drops of the aryl halide solution to the flask with stirring, followed by gentle heating. The rest of the aryl halide solution was then added and the THF maintained a moderate reflux.

(b) A round-bottom flask, which was fitted tetraethyl orthosilicate (90 mmol) in 30 mL of THF. The silane solution was cooled to -30 °C, and then the arylmagnesiumhalide solution was added dropwise (one drop per second). The solution was allowed to stir at -30 °C for 1 h and then at room temperature for 12 h. After the reaction finished, the mixture was then poured into 50 mL of hexane, and stirred for some time. Then the solution was washed with 3×25 mL of water, dried over Na₂SO₄, and concentrated in vacuo. Purification of the residue by micro-pressure distillation could obtain pure aryltriethoxysilane. All the silicon reagent are known compounds.

4.3 General procedure for Rh(III)-catalyzed direct *ortho*-C-H diarylation of arylsulfoximines with arylsilanes



To a 15 mL of seal tube equipped with a magnetic bar were added sulfoximine **1** (0.2 mmol, 1.0 equiv), arylsilane **2** (0.6 mmol, 3.0 equiv), $[Cp*RhCl_2]_2$ (0.004 mmol, 2.0 mol%), AgF (0.6 mmol, 3.0 equiv), HOAc (0.2 mmol, 1.0 equiv) and PhCl (1 mL) was added subsequently. The reaction mixture was allowed to stir at 70 °C(oil bath) for 24 h. After completed, the reaction was cooled to room temperature, then diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to provide pure product **3**.

5. Procedure for the synthesis of 3a on gram scale

To a 50 mL of seal tube equipped with a magnetic bar were added sulfoximine 1 (5.0 mmol, 1.0 equiv), arylsilane 2 (15.0 mmol, 3.0 equiv), $[Cp*RhCl_2]_2$ (0.1 mmol, 2.0 mol%), AgF (15.0 mmol, 3.0 equiv), HOAc (5.0 mmol, 1.0 equiv) and PhCl (20 mL) was added subsequently. The reaction mixture was allowed to stir at 70 °C(oil bath) for 24 h. After completed, the reaction was cooled to room temperature, then diluted with 20 mL water and extracted with EtOAc (3*30 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to provide pure product **3a** (1.11 g, 72% yield).

6. Synthetic application of 3a

6.1 N-H arylation



To a 15 mL of seal tube equipped with a magnetic bar, added 2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl **3a** (0.2 mmol), phenyltriethoxysilane acid (0.4 mmol, 2.0 equiv), CuSO₄·H₂O (0.2 equiv), CuF₂ (2.0 equiv), DMF (1 mL) was added subsequently. The reaction mixture was allowed to stir at rt for 13 h. After completed, the mixture was diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na2SO4, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to give the desired product **5a** in 72%.

6.2 N-H trifluoromethylation



To a 15 mL of seal tube equipped with a magnetic bar, added 2'-(S-methyl -sulfonimidoyl)-1,1':3',1"-terphenyl **3a** (0.1 mmol), TMSCF₃ (0.5 mmol), Ag₂CO₃ (0.2 equiv), 1,10-phen (0.4 equiv), dioxane (2 mL) was added subsequently. The reaction mixture was allowed to stir at 60 °C for 10 h under O₂. After completed, the mixture was diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to give the desired product **5b** in 60%.^[3]

6.3 Intramolecular cyclization



To a 15 mL of seal tube equipped with a magnetic bar, added 2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl **3a** (0.2 mmol), $Pd(OAc)_2$ (10 mol%), $PhI(OAc)_2$ (2.0 equiv), toluene (1 mL) was added subsequently. The reaction mixture was allowed to stir at 120 °C for 10 h. After completed, the mixture was diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to give the desired product **5c** in 71%.^[4]

7. Preliminary mechanistic studies

7.1 Intermolecular competitive reactions

(a) Competitive experiment between 1e and 1k



To a 15 mL of seal tube equipped with a magnetic bar were added **1e** (0.2 mmol, 1.0 equiv) and **1k** (0.2 mmol, 1.0 equiv), phenyltriethoxysilane **2a** (0.6 mmol, 3.0 equiv), $[Cp*RhCl_2]_2$ (0.004 mmol, 2.0 mol%), AgF (0.6 mmol, 3.0 equiv), HOAc (0.2 mmol, 1.0 equiv) and PhCl (1 mL) was added subsequently. The reaction mixture was allowed to stir at 70 °C(oil bath) for 120 min. After completed, the reaction was cooled to room temperature, then diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to provide pure product **3e** and **3k**, the ratio of the two products was determined by ¹H NMR is 1.86.

(b) Competitive experiment between 2b and 2i



To a 15 mL of seal tube equipped with a magnetic bar were added sulfoximine **1a** (0.2 mmol, 1.0 equiv), arylsilane **2b** and **2i** (0.4mmol ecach, 3.0 equiv), $[Cp*RhCl_2]_2$ (0.004 mmol, 2.0 mol%), AgF (0.6 mmol, 3.0 equiv), HOAc (0.2 mmol, 1.0 equiv) and PhCl (1 mL) was added subsequently. The reaction mixture was allowed to stir at 70 °C(oil bath) for 120 min. After completed, the reaction was cooled to room temperature, then diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to provide pure product **4b** and **4i**, the ratio of the two products was determined by ¹H NMR is 1.57.

7.2 Deuterium-labelling experiments



To a 15 mL of seal tube equipped with a magnetic bar were added **1a** (0.2 mmol, 1.0 equiv), $[Cp*RhCl_2]_2$ (0.004 mmol, 2.0 mol%), AgF (0.6 mmol, 3.0 equiv), CD₃COOD (0.5 mL) and PhCl (1.0 mL) was added subsequently. The reaction mixture was allowed to stir at 70 °C(oil bath) for 24 h. After completed, the reaction was cooled to room temperature, then diluted with 10 mL water and extracted with EtOAc (3*10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, evaporated under vacuum. The residue was purified with silica gel chromatography (petroleum ether/ethyl acetate) to provide pure product **dueterio-1a**. The deuterium rate (51%) was obtained from ¹H NMR. Deuterium was observed at

both *ortho*-positions, which indicated the possibility of the reaction pathway via *ortho* C-H activation.



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8. Characterization data for the products

2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3a).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3a** was obtained as a pale yellow solid (51.0 mg, 83% yield); mp = 131-133 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.4 (m, 8H), 7.3 (d, *J* = 7.6 Hz, 2H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 143.3, 140.9, 140.5, 132.0, 129.9, 129.7, 128.5, 128.4, 46.5. This compound is known^[4].

2'-(S-ethylsulfonimidoyl)-1,1':3',1''-terphenyl (3b).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3b** was obtained as a yellow solid (49.5 mg, 77% yield); mp = 139-141 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.4 (m, 7H), 7.3 (d, *J* = 7.6 Hz, 2H), 2.6 – 2.5 (m, 1H), 2.4 (dq, *J* = 14.2, 7.2 Hz, 1H), 0.9 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 141.9, 140.6, 140.3, 132.2, 129.9, 129.6, 128.3, 128.3, 50.5, 8.4. This compound is known^[4].

2'-(S-phenylsulfonimidoyl)-1,1':3',1''-terphenyl (3c).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3c** was obtained as a white solid (62.7 mg, 85% yield); mp = 149-151 $^{\circ}$ C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 2H), 7.5 (t, *J* = 7.6 Hz, 2H), 7.4 (s, 1H), 7.3 – 7.3 (m, 3H), 7.2 (dd, *J* = 13.1, 7.5 Hz, 5H), 7.2 – 7.1 (m, 3H), 7.0 (dd, *J* = 8.4, 7.3 Hz, 2H), 2.8 (s, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 142.8, 142.3, 142.0, 140.0, 131.7, 130.8, 129.9, 129.6, 129.4, 127.9, 127.6, 126.7.

IR (KBr) v (cm⁻¹) 3681, 3343, 3052, 2924, 2339, 1970, 1759, 1596, 1451, 1156, 1038, 946.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₄H₂₀NOS 370.1260; found 370.1267.

2'-(S-benzylsulfonimidoyl)-1,1':3',1''-terphenyl (3d).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3d** was obtained as a colorless oil (44.5 mg, 58% yield): ¹H NMR (400 MHz, CDCl₃) δ 7.6 – 7.6 (m, 4H), 7.6 – 7.5 (m, 1H), 7.5 – 7.4 (m, 6H), 7.4 (d, *J* = 7.6 Hz, 2H), 7.3 – 7.2 (m, 3H), 6.9 – 6.9 (m, 2H), 4.0 – 3.8 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 142.5, 141.0, 140.9, 132.5, 131.5, 130.3, 129.9, 128.3, 128.1, 128.0, 61.6.

IR (KBr) v (cm⁻¹) 3364, 3058, 2930, 2606, 2340, 1956, 1735, 1598, 1494, 1156, 1074, 971.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₅H₂₂NOS 384.1417; found 384.1427.

5'-Methyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3e).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3e** was obtained as a white solid (57.2 mg, 89% yield); mp = 136-138 $^{\circ}$ C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.4 (m, 6H), 7.1 (s, 2H), 2.4 (s, 3H), 2.4 (d, J = 0.7 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 141.0, 140.7, 140.6, 140.2, 132.7, 129.7, 128.4, 128.3, 46.6, 20.8. This compound is known^[5].

5'-tert-butyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3f).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3f** was obtained as a white solid (58.1 mg, 80% yield); mp = 168-170 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.4 (m, 7H), 7.3 (s, 2H), 2.4 (s, 3H), 1.4 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 153.3, 141.1, 140.7, 140.6, 129.8, 129.2, 128.5, 128.3, 46.6, 34.8, 31.0.

IR (KBr) v (cm⁻¹) 3361, 3081, 2962, 1950, 1584, 1492, 1362, 1231, 1151, 1062, 1026, 957.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₂₆NOS 364.1730; found 364.1734.

5'-methoxy-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3g).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3g** was obtained as a yellow solid (51.9 mg, 77% yield); mp = 103-105 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.4 (m, 6H), 6.8 (s, 2H), 3.9 (s, 3H), 2.4 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 159.4, 143.4, 140.7, 135.9, 129.6, 128.4, 127.4, 117.1, 55.6, 46.8.

IR (KBr) v (cm⁻¹) 3584, 3356, 2922, 2235, 1949, 1879, 1635, 1588, 1492, 1342, 1147, 1076.

HRMS (**ESI**) **m/z:** [M+H]⁺ Calcd for C₂₀H₂₀NO₂S 338.1209; found 338.1218.

5'-acetyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3h).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3h** was obtained as a white solid (18.6 mg, 27% yield); mp = 179-181 $^{\circ}$ C; ¹H NMR (400 MHz, CDCl₃) δ 7.9 (s, 2H), 7.6 (s, 4H), 7.5 – 7.5 (m, 6H), 2.6 (s, 3H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 196.6, 147.1, 141.5, 139.8, 137.1, 131.5, 129.7, 128.9, 128.8, 46.3, 26.8.

IR (KBr) v (cm⁻¹) 3360, 3055, 2924, 2355, 1672, 1561, 1407, 1228, 1151, 1075, 1042, 1029.

HRMS (**ESI**) **m/z:** [M+H]⁺ Calcd for C₂₁H₂₀NO₂S 350.1209; found 350.1219.

5'-carboxylate-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3i).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3i** was obtained as a yellow solid (45.7 mg, 63% yield); mp = 172-174 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.0 (s, 2H), 7.6 (s, 4H), 7.5 (dt, J = 8.5, 6.0 Hz, 6H), 3.9 (s, 3H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.3, 147.0, 141.2, 139.7, 132.7, 130.8, 129.7, 128.8, 128.7, 52.5, 46.3.

IR (KBr) v (cm⁻¹) 3890, 3419, 3352, 3057, 2952, 2852, 1952, 1715, 1564, 1406, 1211, 997.

HRMS (**ESI**) **m/z:** [M+H]⁺ Calcd for C₂₁H₂₀NO₃S 366.1158; found 366.1166.

5'-nitro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3j).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3j** was obtained as a yellow solid (31.7 mg, 45% yield); mp = 192-194 °C;¹H NMR (400 MHz, CDCl₃) δ 8.2 (s, 2H), 7.7 (s, 4H), 7.6 – 7.5 (m, 6H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 148.9, 146.9, 142.9, 138.7, 129.6, 129.6, 129.1, 126.2, 46.2. This compound is known^[4].

5'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3k).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3k** was obtained as a yellow oil (57.2 mg, 88% yield): ¹**H** NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.4 (m, 6H), 7.1 (d, *J* = 8.6 Hz, 2H), 2.4 (s, 3H). ¹³**C** NMR (101 MHz, CDCl₃) δ 162.8, 160.2, 144.1, 144.1, 139.8, 139.7, 139.6, 139.6, 129.5, 128.9, 128.6, 118.7, 118.5, 46.6. ¹⁹**F** NMR (377 MHz, CDCl₃) δ -109.26. **IR (KBr) v (cm⁻¹)** 3364, 3058, 2929, 2342, 1735, 1586, 1447, 1336, 1220, 1142, 1043, 1029.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₉H₁₇FNOS 326.1009; found 326.1017.





Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **31** was obtained as a white solid (47.2 mg, 69% yield); mp = 100-102 $^{\circ}$ C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 (d, *J* = 6.5 Hz, 6H), 7.3 (s, 2H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 142.8, 142.0, 139.4, 135.6, 131.6, 129.6, 128.9, 128.7, 46.5.

IR (KBr) v (cm⁻¹) 3363, 3056, 2929, 2250, 1892, 1735, 1600, 1493, 1397, 1219, 1146, 1059.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₉H₁₇ClNOS 342.0714; found 342.0724.

5'-bromo-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3m).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3m** was obtained as a white solid (53.9 mg, 70% yield); mp = 140-142 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 – 7.5 (m, 8H), 2.4 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 142.8, 142.6, 139.3, 134.5, 129.6, 129.0, 128.7, 124.0, 46.5. This compound is known^[4].

5'-iodo-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3n).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3n** was obtained as a white solid (65.0 mg, 75% yield); mp = 189-191 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.7 (s, 2H), 7.6 (bs, 4H), 7.5 (dt, *J* = 8.0, 2.8 Hz, 6H), 2.4 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 143.3, 142.3, 140.3, 139.0, 129.6, 128.8, 128.6, 96.5, 46.4.

IR (KBr) v (cm⁻¹) 3357, 3054, 2930, 1547, 1489, 1445, 1384, 1310, 1075, 1047, 558, 524.

HRMS (**ESI**) **m/z:** [M+H]⁺ Calcd for C₁₉H₁₇INOS 434.0070; found 434.0081.

4'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (30).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **30** was obtained as a yellow solid (46.1 mg, 71% yield); mp = 130-132 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 – 7.6 (m, 2H), 7.6 – 7.4 (m, 8H), 7.4 – 7.3 (m, 2H), 2.4 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.1, 157.7, 144.9, 139.8, 136.7, 136.7, 133.5, 133.4, 132.3, 130.8, 130.7, 129.7, 129.1, 128.6, 128.5, 128.4, 128.2, 128.0, 117.7, 117.5, 46.5. ¹⁹F NMR (377 MHz, CDCl₃) δ -111.73.

IR (KBr) v (cm⁻¹) 3850, 3360, 3059, 2937, 2354, 1974, 1827, 1598, 1454, 1224, 1141, 1029.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₉H₁₇FNOS 326.1009; found 326.1017.

3-Methyl-2-(S-methylsulfonimidoyl)-1,1'-biphenyl (3p).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3p** was obtained as a yellow solid (36.8 mg, 75% yield); mp = 92-94 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.4 – 7.4 (m, 5H), 7.3 (dt, *J* = 7.9, 2.7 Hz, 2H), 7.1 (d, *J* = 5.7 Hz, 1H), 2.9 (s, 3H), 2.8 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 141.8, 141.1, 138.2, 132.8, 131.0, 130.6, 129.1, 128.6, 128.2, 127.7, 46.7, 22.9. This compound is known^[4].

4-Methyl-2-(S-methylsulfonimidoyl)-1,1'-biphenyl (3q).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **3q** was obtained as a pale yellow oil (45.1 mg, 92% yield): ¹H NMR (400 MHz, CDCl₃) δ 8.0 (dd, J = 1.7, 0.8 Hz, 1H), 7.4 – 7.4 (m, 6H), 7.2 (d, J = 7.7 Hz, 1H), 2.8 (s, 3H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 141.8, 139.1, 138.1, 132.8, 132.7, 129.9, 128.3, 127.9, 127.7, 44.6, 21.0. This compound is known^[4].





Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4b** was obtained as a white solid (44.9 mg, 67% yield); mp = 90-192 $^{\circ}$ C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 – 7.4 (m, 5H), 7.3 (dd, *J* = 7.8, 4.3 Hz, 6H), 2.5 (s, 3H), 2.4 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 143.4, 140.9, 138.4, 137.6, 131.8, 129.8, 129.6, 129.3, 46.5, 21.2.

IR (KBr) v (cm⁻¹) 3616, 3460, 336, 3045, 2372, 2206, 1950, 1821, 1671, 1563, 1115, 1046.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₂₂NOS 336.1417; found 336.1424.

3,3"-Dimethyl-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4c).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4c** was obtained as a colorless oil (41.6 mg, 62% yield): ¹H NMR (400 MHz, CDCl₃) δ 7.5 – 7.3 (m, 7H), 7.3 (d, *J* = 7.6 Hz, 2H), 7.3 – 7.2 (m, 2H), 2.5 (s, 3H), 2.4 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 143.3, 141.0, 140.5, 138.3, 131.8, 130.4, 129.7, 129.2, 128.4, 126.9, 46.4, 21.3.

IR (KBr) v (cm⁻¹) 3361, 3050, 2922, 2862, 2733, 2248, 1948, 1603, 1487, 1171, 1102, 1044.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₂₂NOS 336.1417; found 336.1429.

3,3'',5,5''-tetramethyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (4d).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4d** was obtained as a white solid (21.8 mg, 30% yield); mp = 174-176 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.5 (dd, J = 8.0, 7.1 Hz, 1H), 7.3 – 7.2 (m, 6H), 7.1 (d, J = 2.1 Hz, 2H), 2.5 (s, 3H), 2.4 (s, 12H). ¹³C NMR (101 MHz, CDCl₃) δ 143.3, 141.0, 140.5, 138.2, 131.7, 130.1, 129.6, 127.6, 46.5, 21.3.

IR (KBr) v (cm⁻¹) 3858, 3626, 3360, 3003, 2733, 2424, 2056, 1887, 1736, 1570, 1173, 1004.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₂₆NOS 364.1730; found 364.1736.



4,4''-di-tertbutyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (4e).

Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4e** was obtained as a white solid (54.5 mg, 65% yield); mp = 212-214 $^{\circ}$ C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (d, *J* = 7.4 Hz, 4H), 7.5 – 7.5 (m, 4H), 7.5 – 7.4 (m, 1H), 7.3 (d, *J* = 7.6 Hz, 2H), 2.4 (s, 3H), 1.4 (s, 18H). ¹³C NMR (101 MHz, CDCl₃) δ 151.6, 143.5, 140.8, 137.5, 131.8, 129.7, 129.4, 125.5, 46.4, 34.6, 31.3. **IR (KBr) v (cm⁻¹)** 3898, 3356, 2955, 2867, 1914, 1609, 1573, 1450, 1269, 1212, 1119, 1045.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₇H₃₄NOS 420.2356; found 420.2360.





Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4f** was obtained as a pale yellow solid (38.2 mg, 52% yield); mp = 132-134 °C; ¹**H NMR** (400 MHz, CDCl₃) δ 7.6 – 7.5 (m, 4H), 7.5 (dd, *J* = 8.0, 7.2 Hz, 1H), 7.3 (d, *J* = 7.6 Hz, 2H), 7.0 – 7.0 (m, 4H), 3.9 (s, 6H), 2.5 (s, 3H). ¹³C NMR

(101 MHz, CDCl₃) δ 159.8, 143.5, 140.6, 132.7, 131.8, 131.0, 129.8, 114.1, 55.3, 46.5. This compound is known^[4].



3,3"-dimethoxy-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4g).

Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4g** was obtained as a yellow oil (64.6 mg, 88% yield): ¹**H** NMR (400 MHz, CDCl₃) δ 7.5 (dd, J = 8.0, 7.1 Hz, 1H), 7.4 (dd, J = 10.6, 7.7 Hz, 4H), 7.2 (s, 4H), 7.0 (ddd, J = 8.3, 2.6, 1.0 Hz, 2H), 3.9 (s, 6H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 159.5, 143.4, 141.8, 140.7, 131.9, 129.8, 129.6, 122.1, 115.2, 114.4, 55.3, 46.4.

IR (KBr) v (cm⁻¹) 3358, 3052, 2836, 2248, 1941, 1735, 1599, 1458, 1210, 1171, 1041, 997.

HRMS (**ESI**) **m/z:** [M+H]⁺ Calcd for C₂₁H₂₂NO₃S 368.1315; found 368.1326.





Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4h** was obtained as a yellow solid (47.4 mg, 60% yield); mp = 171-173 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.5 (dd, J = 8.0, 7.2 Hz, 1H), 7.3 (d, J = 7.6 Hz, 2H), 7.1 (s, 4H), 6.9 (d, J = 8.0 Hz, 2H), 6.0 (s, 4H), 2.6 (s, 3H). ¹³C NMR

(101 MHz, CDCl₃) δ 147.9, 147.7, 143.4, 140.5, 134.0, 131.9, 129.8, 123.6, 110.2, 108.3, 101.4, 46.5. This compound is known^[4].





Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4i** was obtained as a yellow solid (46.7 mg, 68% yield); mp = 177-179 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.6 (s, 4H), 7.5 (dd, J = 8.0, 7.2 Hz, 1H), 7.3 (d, J = 7.5 Hz, 2H), 7.2 – 7.1 (m, 4H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 164.0, 161.5, 143.3, 140.1, 136.4, 136.4, 132.3, 131.5, 131.4, 130.1, 115.7, 115.5, 46.7. ¹⁹F NMR (377 MHz, CDCl₃) δ -112.65. This compound is known^[4].

4,4"-Dichloro-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4j).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4j** was obtained as a yellow solid (54.2 mg, 72% yield); mp = 124-126 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.5 (dt, *J* = 7.6, 3.7 Hz, 5H), 7.5 – 7.4 (m, 4H), 7.3 (d, *J* = 7.6 Hz, 2H), 2.5 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 142.9, 140.1, 138.8, 134.6, 132.3, 130.9, 130.2, 128.7, 46.7. This compound is known^[4].

4,4''-Bis(trifluoromethyl)-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (4k).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **4k** was obtained as a yellow solid (49.8 mg, 45% yield); mp = 152-154 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.7 (q, *J* = 8.1 Hz, 8H), 7.6 (t, *J* = 7.6 Hz, 1H), 7.4 (d, *J* = 7.6 Hz, 2H), 2.6 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 144.2, 142.6, 140.3, 132.7, 130.6, 130.5 (d, *J* = 33.2 Hz), 130.0, 125.3, 122.5, 46.9. ¹⁹F NMR (377 MHz, CDCl₃) -62.70.

IR (KBr) v (cm⁻¹) 3343, 3282, 3055, 2926, 2302, 1708, 1616, 1451, 1412, 1326, 1065, 849.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₆F₆NOS 444.0851; found 444.0856.

rac-N-Phenyl-S-triphenyl-S-methylsulfoximine (5a).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 2/1), the desired product **5a** was obtained as a yellow oil (55.2 mg, 72% yield): ¹**H** NMR (400 MHz, CDCl₃) δ 7.6 – 7.5 (m, 5H), 7.4 (dd, J = 5.2, 2.0 Hz, 6H), 7.3 (d, J = 7.6 Hz, 2H), 7.2 – 7.1 (m, 2H), 7.0 – 6.9 (m, 1H), 6.8 (dd, J = 8.4, 1.2 Hz, 2H), 2.7 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 144.8, 143.2, 141.1, 138.2, 132.7, 130.9, 129.5, 128.8, 127.7, 127.7, 123.6, 121.8, 45.1.

IR (KBr) v (cm⁻¹) 3368, 3054, 2925, 2054, 1732, 1592, 1487, 1446, 1265, 1207, 1055, 758.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₅H₂₂NOS 384.1417; found 384.1427.

N-Trifluoromethyl-S-triphenyl-S-methylsulfoximine (5b).



Following the general procedure (eluent: petroleum ether/ethyl acetate = 15/1), the desired product **5b** was obtained as a yellow solid (45.0 mg, 60% yield); mp = 117-119 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.7 – 7.5 (m, 5H), 7.5 – 7.4 (m, 6H), 7.4 (d, *J* = 7.6 Hz, 2H), 2.7 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 142.8, 139.9, 136.9, 132.8, 131.8, 129.6, 128.2, 127.9, 121.4 (d, *J* = 256.0 Hz), 47.1. ¹⁹F NMR (377 MHz, CDCl₃) -42.25.

IR (KBr) v (cm⁻¹) 3361, 3084, 2928, 2514, 2356, 2083, 1959, 1734, 1450, 1396, 1102, 953.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₀H₁₇F₃NOS 376.0977; found 376.0998.





Following the general procedure (eluent: petroleum ether/ethyl acetate = 5/1), the desired product **5c** was obtained as a white Solid (43.3 mg, 71% yield); mp = 171-173 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.2 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.1 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.9 (s, 1H), 7.7 (dd, *J* = 8.2, 7.4 Hz, 1H), 7.5 – 7.5 (m, 3H), 7.5 – 7.4 (m, 3H), 7.3 – 7.3 (m, 1H), 7.1 (ddd, *J* = 8.3, 7.1, 1.4 Hz, 1H), 2.8 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 141.9, 138.8, 138.5, 134.1, 131.4, 130.4, 130.3, 128.7, 126.3, 124.4, 124.1, 123.9, 120.9, 118.6, 45.2. This compound is known^[4].

9. X-ray analysis of 4f



Table S2 Crystal data and structure refinement for 2a-p-OMe.

Identification code	2a-p-OMe
Empirical formula	$C_{21}H_{21}NO_3S$
Formula weight	367.45
Temperature/K	294.67(12)
Crystal system	triclinic
Space group	P-1
a/Å	9.0766(3)
b/Å	9.3193(3)
c/Å	11.4115(4)
α/°	73.245(3)
β/°	83.671(3)
γ/°	84.492(2)
Volume/Å ³	916.57(6)
Z	2
$\rho_{calc}g/cm^3$	1.331
µ/mm⁻¹	1.736
F(000)	388.0
Crystal size/mm ³	$0.16\times0.14\times0.12$
Radiation	Cu Ka ($\lambda = 1.54184$)
2Θ range for data collection/	° 8.122 to 150.782
Index ranges	$\text{-}11 \leq h \leq 10, \text{-}11 \leq k \leq 11, \text{-}14 \leq l \leq 14$



10. ¹H, ¹³C NMR spectra of the products

2'-(*S*-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3a). ¹H NMR (400 MHz, CDCl₃)



2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3a).

¹³ C NMR (101 MHz, CDCl ₃)		
143.31 40.91 132.02 129.85 128.54	77.32 77.00 76.68	-46.48

NH SO C

200 190 180 170 150 140 130 120 110 100 90 f1 (ppm) -10 160 80 70 60 40 10 6 50 30 20



28

100 90 f1 (ppm) 80 70 60 50 40 30 20

10 0 -10

200 190 180 170 160 150 140 130 120 110



140 130

100 90 f1 (ppm)

 -10



142.46 140.96 132.52 133.52 123.52 128.33 128.33 128.12 128.02 128.02	77.32 77.00 76.68	61.65
	\checkmark	





5'-Methyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3e).

140.97 140.68 140.59 132.65 122.65 128.44 128.29	77.32 77.00 76.68	46.56	20.84
		I	I







5'-tert-butyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3f).

¹³C NMR (101 MHz, CDCl₃)

153.27	141.11 140.71 140.60 129.83 129.20 128.51 128.31	77.32 77.00 76.68	46.56	34.82 30.99
	\checkmark	\searrow	1	1 1





5'-methoxy-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3g). ¹³C NMR (101 MHz, CDCl₃)

- 159.41 143.36 140.70 135.86 129.57 127.44 - 117.09	₹77.32 ₹77.00 76.68	- 55.60	- 46.82
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5'-acetyl-2'-(*S*-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3h). ¹³C NMR (101 MHz, CDCl₃)

- 196.58 147.08 137.10 137.10 137.10 137.10 137.10 128.81 128.81	77.32 77.00 76.68	- 46.32	- 26.82
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5'-carboxylate-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3i).

¹H NMR (400 MHz, CDCl₃)



5'-carboxylate-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3i).

- 165.31	146.98 139.66 132.70 132.70 129.65 128.68 128.68	<pre>77.32 77.00 76.68</pre>	52.48 46.27
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¹H NMR (400 MHz, CDCl₃)



5'-nitro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3j).

148.91 146.91 142.93 138.65 129.63 129.09 126.22 126.22	77.32 77.00 76.68	46.24
	\checkmark	i



5'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3k).

¹H NMR (400 MHz, CDCl₃)



5'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3k).

200 190 180		4/4/1/	140	130	120	110	80		-60 		F knaper 40		Me O	
× ×	162.77 160.24 144.14	144.05 139.76 139.72	139.62	128.86	L 118.71		<u>∫</u> 77.32 77.00	76.68		- 46.60				

5'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3k).

¹⁹F NMR (377 MHz, CDCl₃)



5'-chloro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3l).



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5'-chloro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3l).

¹³C NMR (101 MHz, CDCl₃)



5'-bromo-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3m).



5'-bromo-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3m).



 $\label{eq:stable} 5'\mbox{-iodo-2'-} (S\mbox{-methylsulfonimidoyl})\mbox{-}1,1'\mbox{-}3',1''\mbox{-terphenyl}\ (3n).$



5'-iodo-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (3n).

¹³C NMR (101 MHz, CDCl₃)



4'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (30).





4'-fluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (30).

¹⁹F NMR (377 MHz, CDCl₃)



-10 -20 -90 -100 f1 (ppm) -130 -150 -30 -40 -50 -60 -70 -80 -110 -120 -140-160 -170



4-Methyl-2-(S-methylsulfonimidoyl)-1,1'-biphenyl (3q).



4-Methyl-2-(S-methylsulfonimidoyl)-1,1'-biphenyl (3q).

$\int_{-127.71}^{-141.75} \int_{-138.12}^{-138.12} \int_{-132.65}^{-138.12} \int_{-122.65}^{-132.65} \int_{-127.94}^{-127.94} \int_{-127.71}^{-127.94} \int_{-127.71}^{-127.94$	77.32 77.00 76.68	- 44.61	- 21.04
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4,4"-Dimethyl-2'-(*S*-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4b).

4,4"-Dimethyl-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4b).





¹H NMR (400 MHz, CDCl₃)

3,3'',5,5''-tetramethyl-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (4d).

4,4"-di-tertbutyl-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4e).

¹H NMR (400 MHz, CDCl₃)

4,4"-di-tertbutyl-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4e).

151.65 143.46 140.77 137.53 137.53 131.82 131.82 129.70 129.43 125.50	77.32 77.00 76.68	46.44	34.63 31.26
ノーチンノイ	\checkmark	1	57

¹H NMR (400 MHz, CDCl₃)

4,4"-Dimethoxy-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4f).

¹³C NMR (101 MHz, CDCl₃)

210 200 190 180 170 160 150

140 130 120 110

NMR (101 MHZ, C.	DCI ₃)			
- 159.84	/ 143.51 / 142.63 / 132.73 / 131.77 / 130.99	- 114.09	₹77.32 ₹77.00 76.68	- 55.30 - 46.53
				OMe NH SSO OMe

100 90 f1 (ppm) 60 50 40 30 20 10

70

80

-10

0

3,3"-dimethoxy-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4g).

¹H NMR (400 MHz, CDCl₃)

3,3"-dimethoxy-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4g).

¹³C NMR (101 MHz, CDCl₃)

159.47	143.45 141.77 140.71 131.91 129.83 129.63 122.14 115.19 114.41	77.32 77.00 76.68	55.34	46.39
	SV SV CV	\checkmark	1	1

5,5'-(2-(S-Methylsulfonimidoyl)-1,3-phenylene)bis(benzo[d][1,3]dioxole) (4h).

¹H NMR (400 MHz, CDCl₃)

5,5'-(2-(S-Methylsulfonimidoyl)-1,3-phenylene)bis(benzo[d][1,3]dioxole) (4h).

¹H NMR (400 MHz, CDCl₃)

200 190

180 170

160

150 140

130 120

110

100 90 f1 (ppm) 70 60 50 40

80

20 10 0 -1

30

4,4"-Difluoro-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4i).

¹⁹F NMR (377 MHz, CDCl₃)

4,4"-Dichloro-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4j).

4,4"-Bis(trifluoromethyl)-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4k).

4,4"-Bis(trifluoromethyl)-2'-(S-methylsulfonimidoyl)-1,1':3',1"-terphenyl (4k).

4,4''-Bis(trifluoromethyl)-2'-(S-methylsulfonimidoyl)-1,1':3',1''-terphenyl (4k). ¹⁹F NMR (377 MHz, CDCl₃)

N-Trifluoromethyl-*S*-triphenyl-*S*-methylsulfoximine (5b).

N-Trifluoromethyl-S-triphenyl-S-methylsulfoximine (5b).

N-Trifluoromethyl-*S*-triphenyl-*S*-methylsulfoximine (5b).

¹⁹F NMR (377 MHz, CDCl₃)

5-Methyl-4-phenyldibenzo[c,e][1,2]thiazine 5-oxide (5c).

5-Methyl-4-phenyldibenzo[c,e][1,2]thiazine 5-oxide (5c).

¹³C NMR (101 MHz, CDCl₃)

200

190 180

170

160 150 140

130 120 110

100 90 f1 (ppm) 80 70 60 50 40 30 20

10 0 -1

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