Supporting information

An Efficient Approach to Construct Benzisothiazol-3(2H)-ones via Coppercatalyzed Consecutive Reaction of 2-Halobenzamides and Carbon disulfide

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Table of Contents

1. A preliminary validation study on the genera	ation of carbon monosulfide 2
2. Copies of NMR spectra of compounds 2a-2v	3-27

1. A preliminary validation study on the generation of carbon monosulfide

We designed a reaction to trap the generating carbon monosulfide (CS) and prove it. First, the generating red CS could be observed during the purification process, which dissolved in a mixture of petroleum ether and ethyl acetate as the eluent. Next, some nucleophilic amines, such as piperazine, aniline and benzylamine, were added into the red mixed solution respectively. The red solution clarified quickly and the light gray floc was obtained simultaneously. We reasoned that CS was trapped by these nucleophilic amines due to its weak eletrophilicity^{1,2}, and gave these possible products **A** (m/z = 173.1, [M - H]⁻), **B** (m/z = 227.2, [M - H]⁻) and **C** (m/z = 255.1, [M - H]⁻), which were confirmed by MS as follows (Figure 1).



Figure 1. MS spectra of products A, B and C.

References

- 1. Moltzen, E. K.; Kramer, M. P.; Senning, A.; Klabunde, K. J. J. Org. Chem. 1987, 52, 1156-1161.
- 2. Moltzen, E. K.; Klabunde, K. J. Chem. Rev. 1988, 88, 391-406.

2. Copies of NMR spectra of compounds 2a-2y

¹H NMR spectra of **2a**



¹³C NMR spectra of **2a**



220 200 180 160 140 120 100 80 60 40 20 0 f1 (ppm)



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<sup>13</sup>C NMR spectra of 2b
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¹³C NMR spectra of **2c**





230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 f1 (ppm)



¹³C NMR spectra of **2e**



¹H NMR spectra of **2f**



¹³C NMR spectra of **2f**



¹H NMR spectra of **2g**









¹³C NMR spectra of **2h**



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm)



¹³C NMR spectra of **2i**





¹³C NMR spectra of **2j**



¹H NMR spectra of **2k**



¹³C NMR spectra of **2k**







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<sup>13</sup>C NMR spectra of 2I
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¹H NMR spectra of **2m**



¹³C NMR spectra of **2m**



15



230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 f1 (ppm)







¹³C NMR spectra of **2p**



¹H NMR spectra of **2q**





220 200 180 160 140 120 100 80 60 40 20 0 fl (ppm)

¹H NMR spectra of **2r**



¹³C NMR spectra of **2r**



¹H NMR spectra of **2s**



¹³C NMR spectra of **2s**











¹H NMR spectra of **2w**



¹³C NMR spectra of **2w**



230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 f1 (ppm)





¹³C NMR spectra of **2x**





¹³C NMR spectra of **2y**

