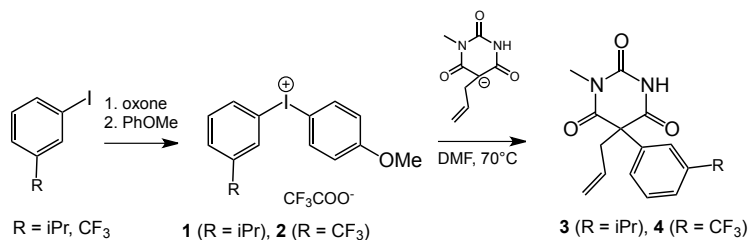


Supporting Information

(1) Synthesis of R-miP-MPAB and R-mCF₃-MPAB



SCHEME 1:

Synthesis of m-iPr-MPAB (5-Allyl-5-(3-isopropylphenyl)-1-methyl-pyrimidine-2,4,6-trione, **3**.) and m-CF₃-MPAB (5-allyl-1-methyl-5-(3-trifluoromethylphenyl)-pyrimidine-2,4,6-trione, **4**.). Compounds **3** and **4** were synthesized as racemates by addition of phenyliodonium salts **1** and **2**, respectively, to 5-allyl-1-methyl-5-pyrimidine-2,4,6-trione, and the racemic mixtures were separated by chiral chromatography as described previously (Savechenkov et al., 2012). Compounds **1** and **2** were also obtained analogously as described earlier (Savechenkov et al., 2012).

1: ¹H NMR (CDCl₃): δ 7.87 (d, *J* = 8.9 Hz, 2H), 7.78 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.28 (m, 1H), 6.90 (d, *J* = 8.9 Hz, 2H), 3.81 (s, 3H), 2.89 (sept, *J* = 6.8 Hz, 1H), 1.21 (d, *J* = 6.8 Hz, 6H).

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¹³C NMR (CDCl₃) δ 162.4, 161.5 (q), 153.1, 136.9, 132.3, 131.5, 131.4, 129.8, 116.7, 104.5, 55.6, 41.1, 23.5 ppm

¹⁹F NMR (CDCl₃) δ -75.2 ppm.

2: ¹H NMR (CDCl₃): δ 8.12 (m, 2H), 7.90 (d, *J* = 9.0 Hz, 2H), 7.77 (d, *J* = 6.8 Hz, 1H), 7.52 (tr, *J* = 7.9 Hz, 1H), 6.93 (d, *J* = 9.0 Hz, 2H), 3.83 (s, 3H).

¹³C NMR (CDCl₃) δ 162.6, 161.5 (q, *J* = 36 Hz), 137.4, 137.2, 133.5 (q, *J* = 33.7 Hz), 131.7, 130.8 (q, *J* = 3.7 Hz), 128.2 (q, *J* = 3.4 Hz), 117.1, 117.7, 105.1, 55.6.

¹⁹F NMR (CDCl₃) δ -62.9, -75.4 ppm.

3: ¹H NMR (CDCl₃): δ 8.42 (brs, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.22 (d, *J* = 7.7 Hz, 1H), 7.18 (brs, 1H), 7.12 (brd, *J* = 7.1 Hz, 1H), 5.70 (m, 1H), 5.27 (d, *J* = 17.1 Hz, 1H), 5.18 (d, *J* = 10.1 Hz, 1H), 3.19 (m, 2H), 2.91 (sept, *J* = 6.8 Hz, 1H), 1.24 (d, *J* = 6.8 Hz, 1H).

¹³C NMR (CDCl₃) δ 170.4, 169.2, 150.1, 149.6, 136.8, 131.5, 129.2, 126.7, 124.4, 123.5, 121.2, 61.2, 40.6, 34.3, 28.2, 23.9, 23.8 ppm.

4: ¹H NMR (CDCl₃): δ 8.71 (brs, 1H), 7.62 (m, 2H), 7.53 (m, 2H), 5.68 (m, 1H), 5.28 (d, *J* = 17.0 Hz, 1H), 5.21 (d, *J* = 10.2 Hz, 1H), 3.35 (s, 3H), 3.21 (m, 2H).

¹⁹F NMR (CDCl₃) δ -62.6 ppm.

Reference

Savechenkov PY, Zhang X, Chiara DC, Stewart DS, Ge R, Zhou X, *et al.* (2012). Allyl m-trifluoromethyldiazirine mephobarbital: an unusually potent enantioselective and photoreactive barbiturate general anesthetic. *J Med Chem* 55: 6554-6565.