[Supplementary Materials]

Chiral resolution, absolute configuration assignment, and genotoxicity evaluation of racemic 3,4-dihydroquinazoline as a novel anti-cancer agent

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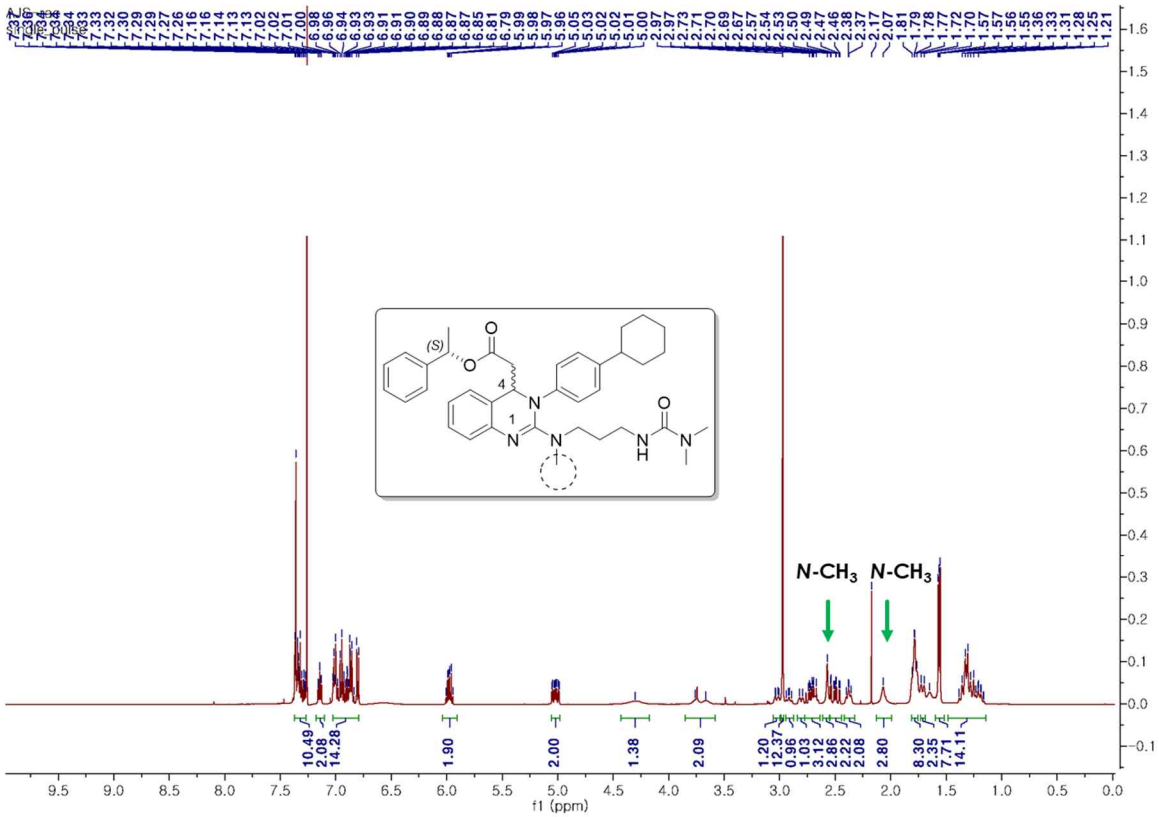


Figure S1. ^{1}H NMR of a mixture of diastereomeric esters **8a** and **8b.**

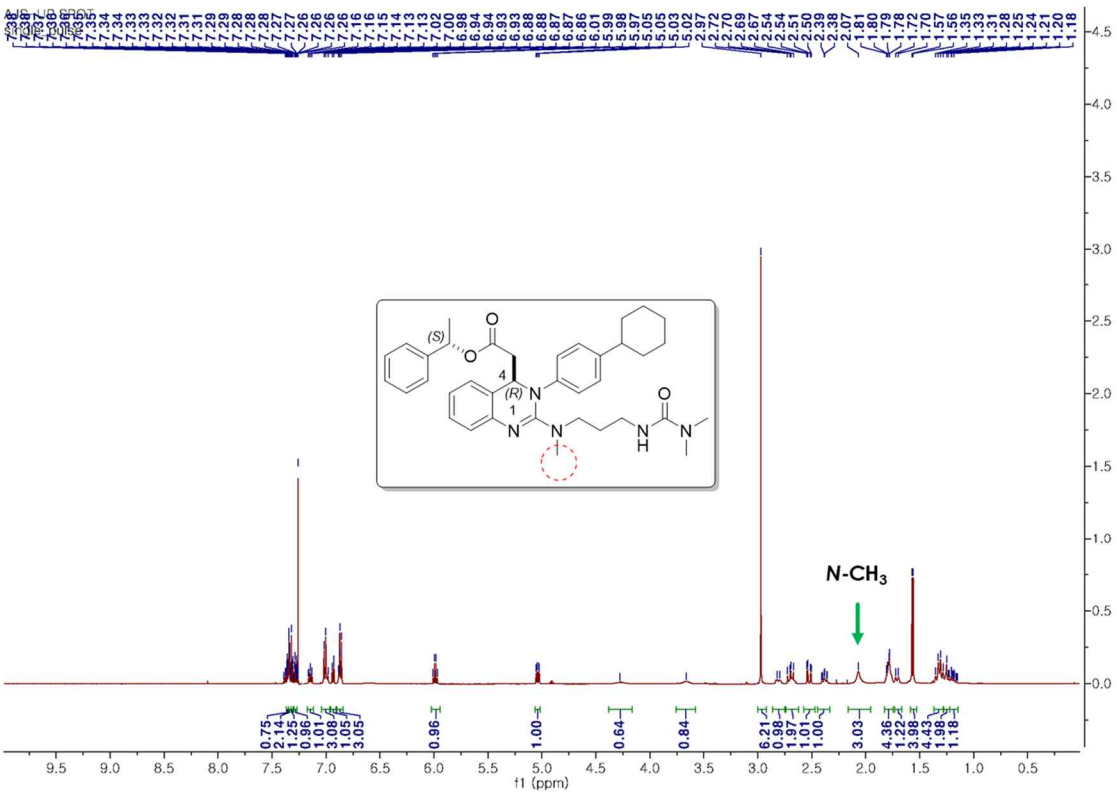


Figure S2. ^{1}H NMR of diastereomer (*S*, 4*R*)-**8a**.

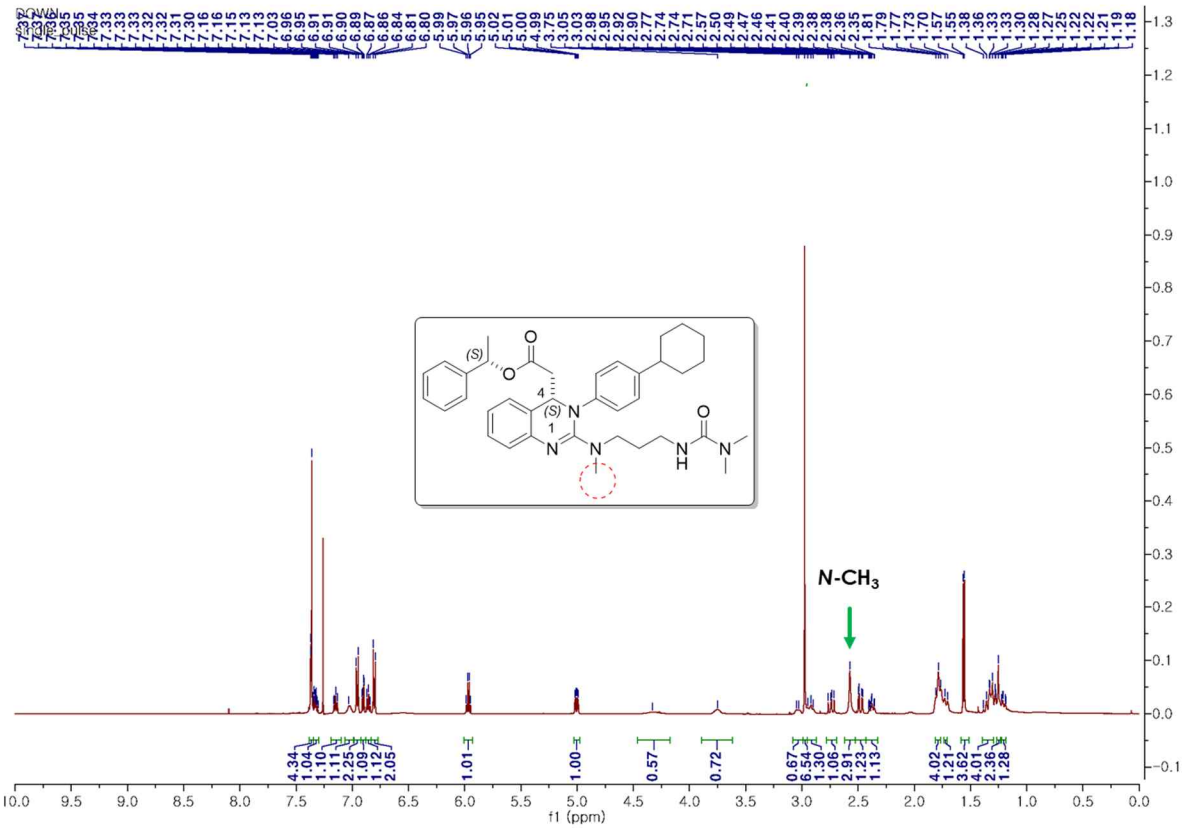
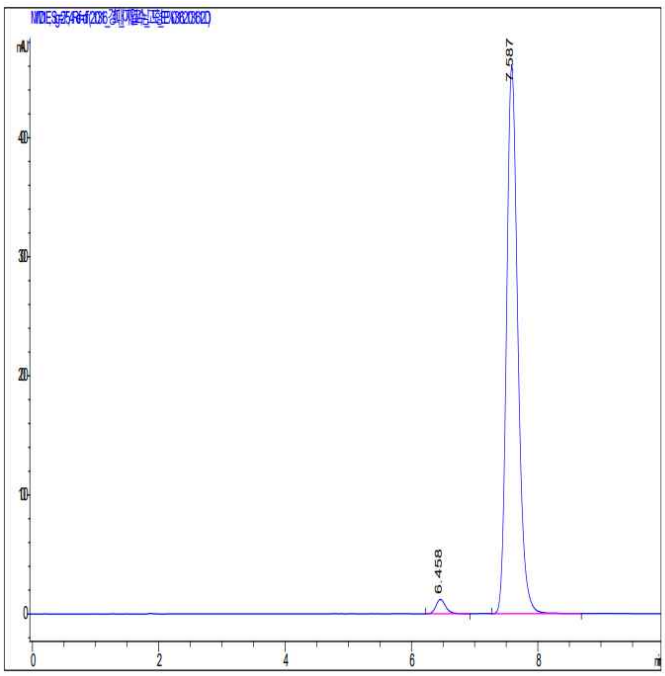


Figure S3. ^{1}H NMR of diastereomer (*S*, 4*S*)-**8b**.



NO	AREA		% EE
	6.5 min	7.6 min	
1	129	5679.1	95.56
2	133.4	5891.3	95.57
3	134.2	5883.4	95.54
4	131.1	5795.9	95.58
5	133.3	5848.7	95.54
6	134.6	5947.7	95.57
7	133.9	5945.9	95.60
8	134.9	5959	95.57
Averager	133.05	5868.88	95.57
STDEV	2.01	94.66	0.02
%RSD	1.51	1.61	0.02

Figure S4. Chiral HPLC spectrum and enantiomeric excess (% *ee*) of (*R*)-(–)-**KCP-10043F** (**OZ001**): Column: Chiralcel IE-3 (4.6 x 150), mobile phase: diethylamine/hexane/EtOH = 0.1/ 80 / 20.

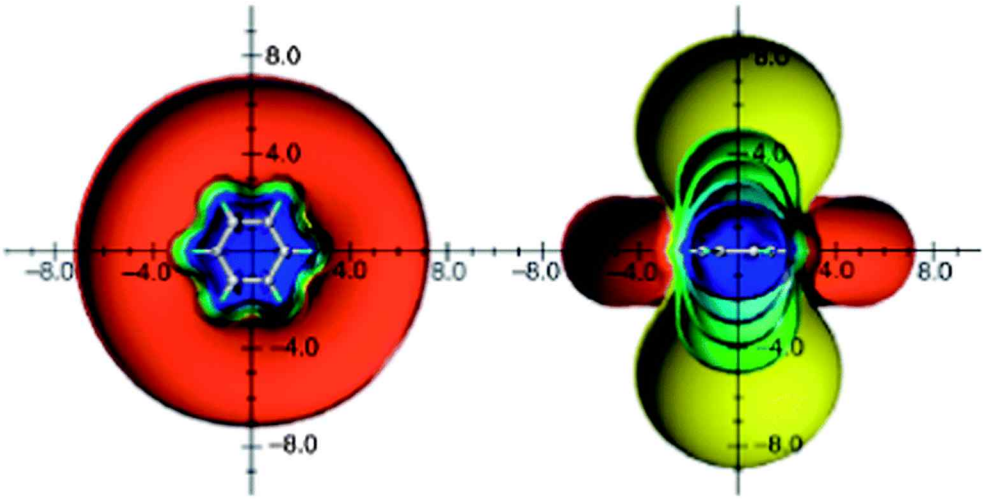


Figure S5. Calculated anisotropic effect of benzene (shielding surfaces at 0.1 ppm in yellow, at 0.5 ppm in green, at 1 ppm in green-blue, at 2 ppm in cyan, and 5 ppm in blue, respectively; deshielding surface at 0.1 ppm in red). View from perpendicular to the molecule and in the plane of the molecule. Reproduced from Klod, S.; Kleinpeter, E. *J. Chem. Soc. Perkin Trans.*, **2001**, *2,*1893.

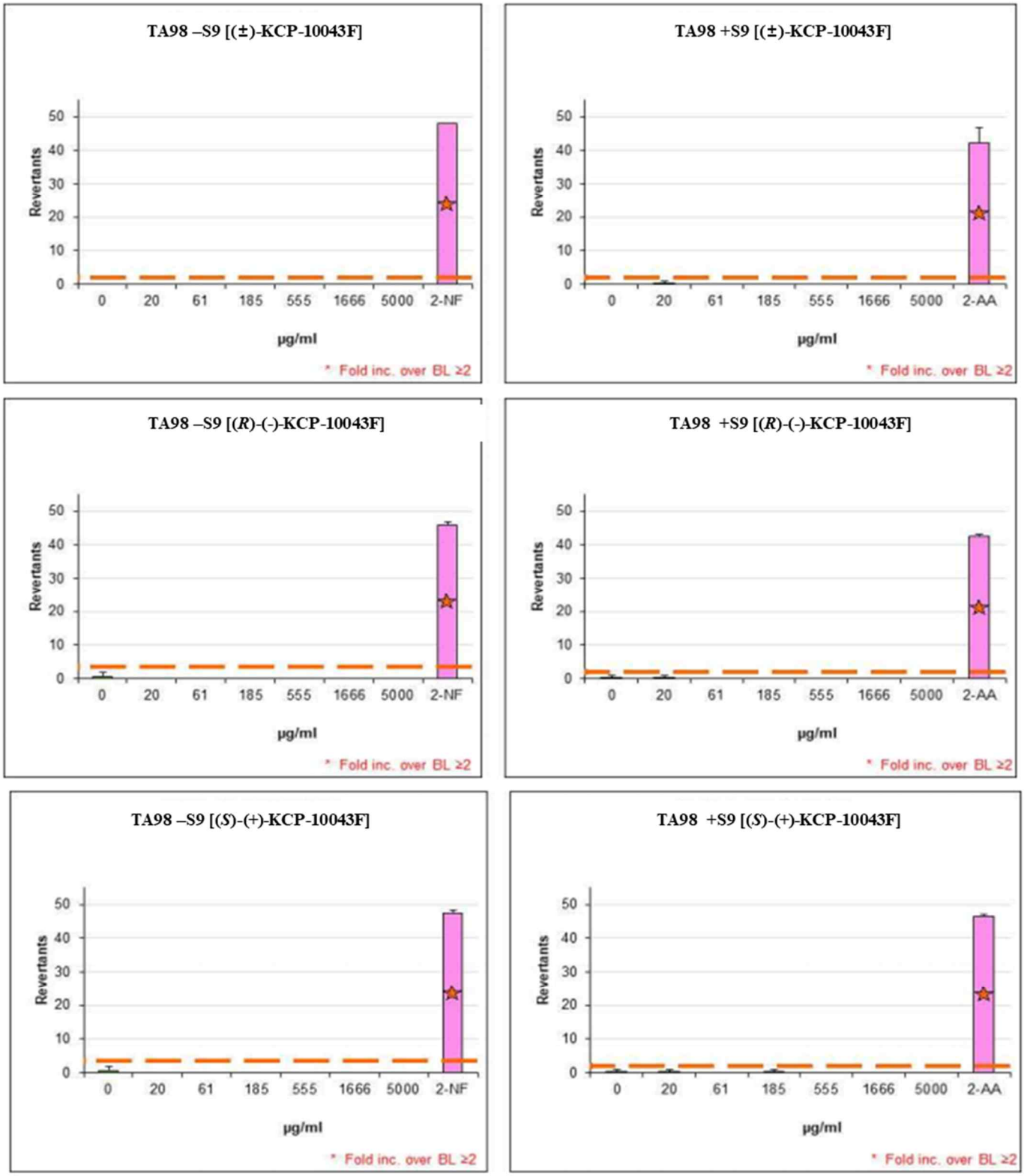


Figure S6. Ames MPF test results of racemate (±)-**KCP10043F (OZ-001)** and its two enantiomers against *Salmonella typhimurium* TA98 with/without rat liver S9 fraction. 2-Nitrofluorene (2-NF, 2 µg/mL) and 2-aminoacridine (2-AA; 0.5 µg/mL) were used as positive controls (mutagens) and DMSO (solvent) was used as a negative control.

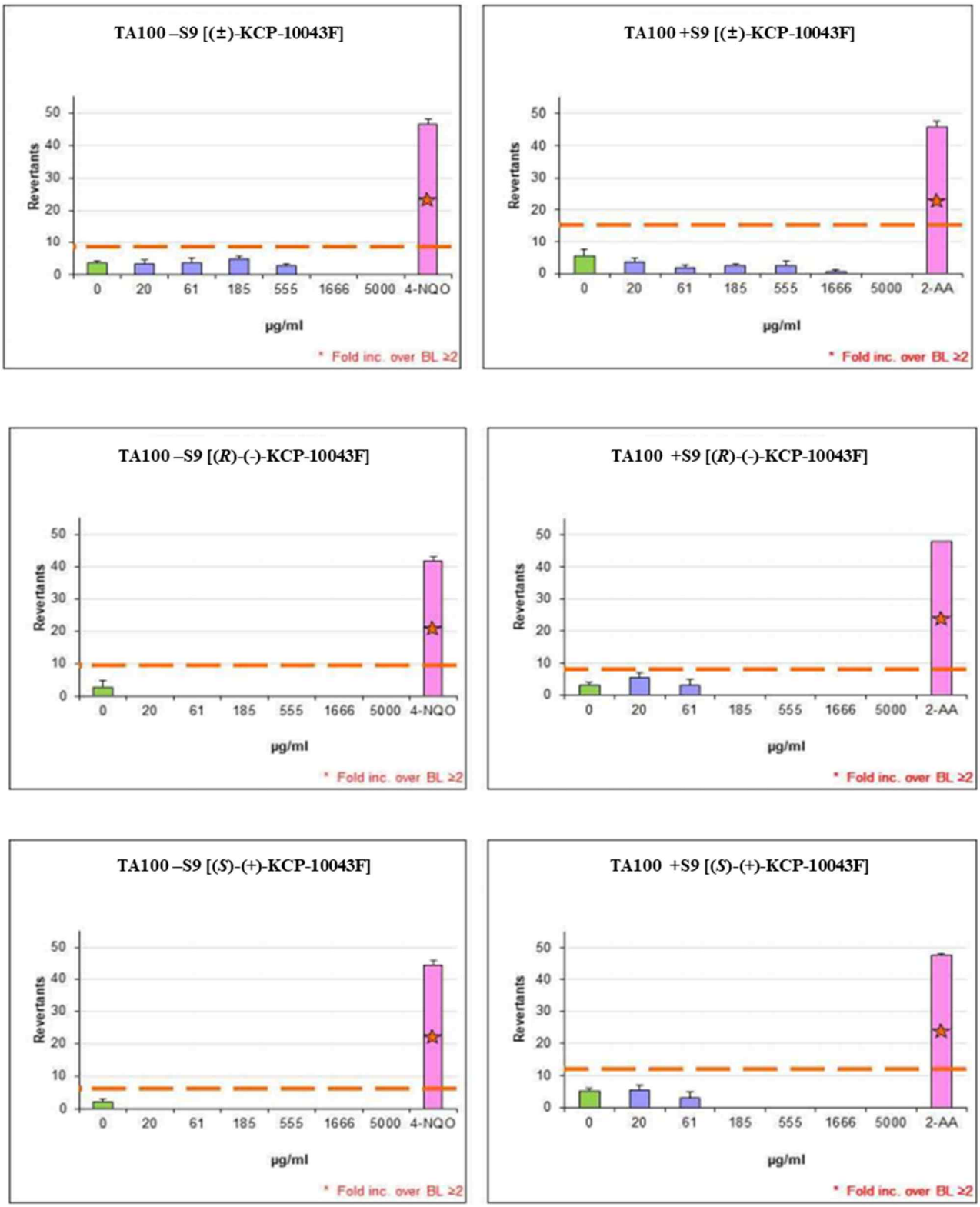


Figure S7. Ames MPF test results of racemic (±)-**KCP10043F (OZ-001)** and its two enantiomers against *Salmonella typhimurium* TA100 with/without rat liver S9 fraction. 4-Nitroquinoline-*N*-oxide (4-NQO, 0.1 µg/mL) and 2-aminoacridine (2-AA, 1.25 µg/mL) were used as positive controls (mutagens) and DMSO (solvent) was used as a negative control.

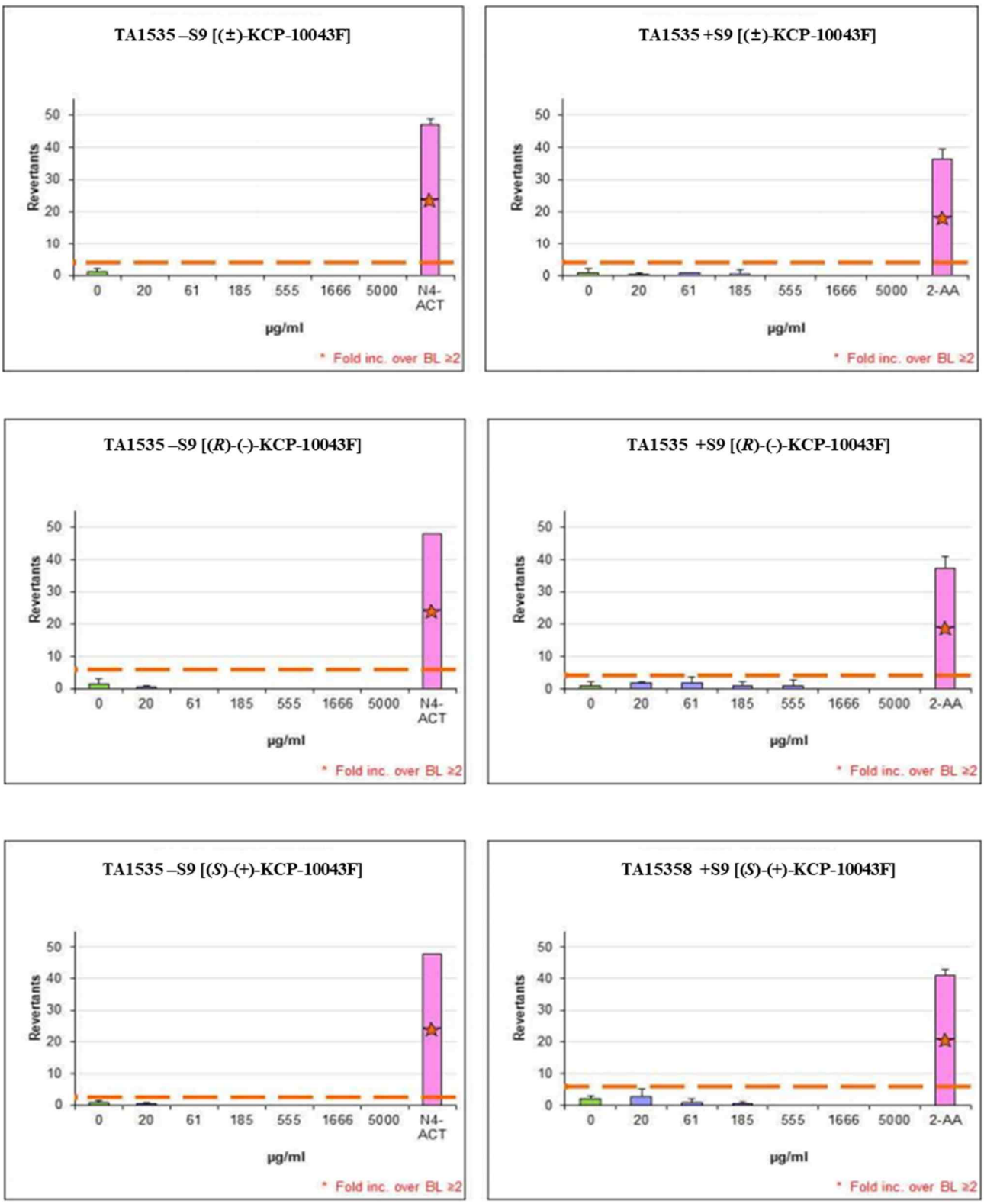


Figure S8. Ames MPF test results of racemic (±)-**KCP10043F (OZ-001)** and its two enantiomers against *Salmonella typhimurium* TA1535 with/without rat liver S9 fraction. N4-Aminocytidine (N4-ACT, 100 µg/mL) and 2-aminoacridine (2-AA, 2.5 µg/mL) were used as positive controls (mutagens) and DMSO (solvent) was used as a negative control.

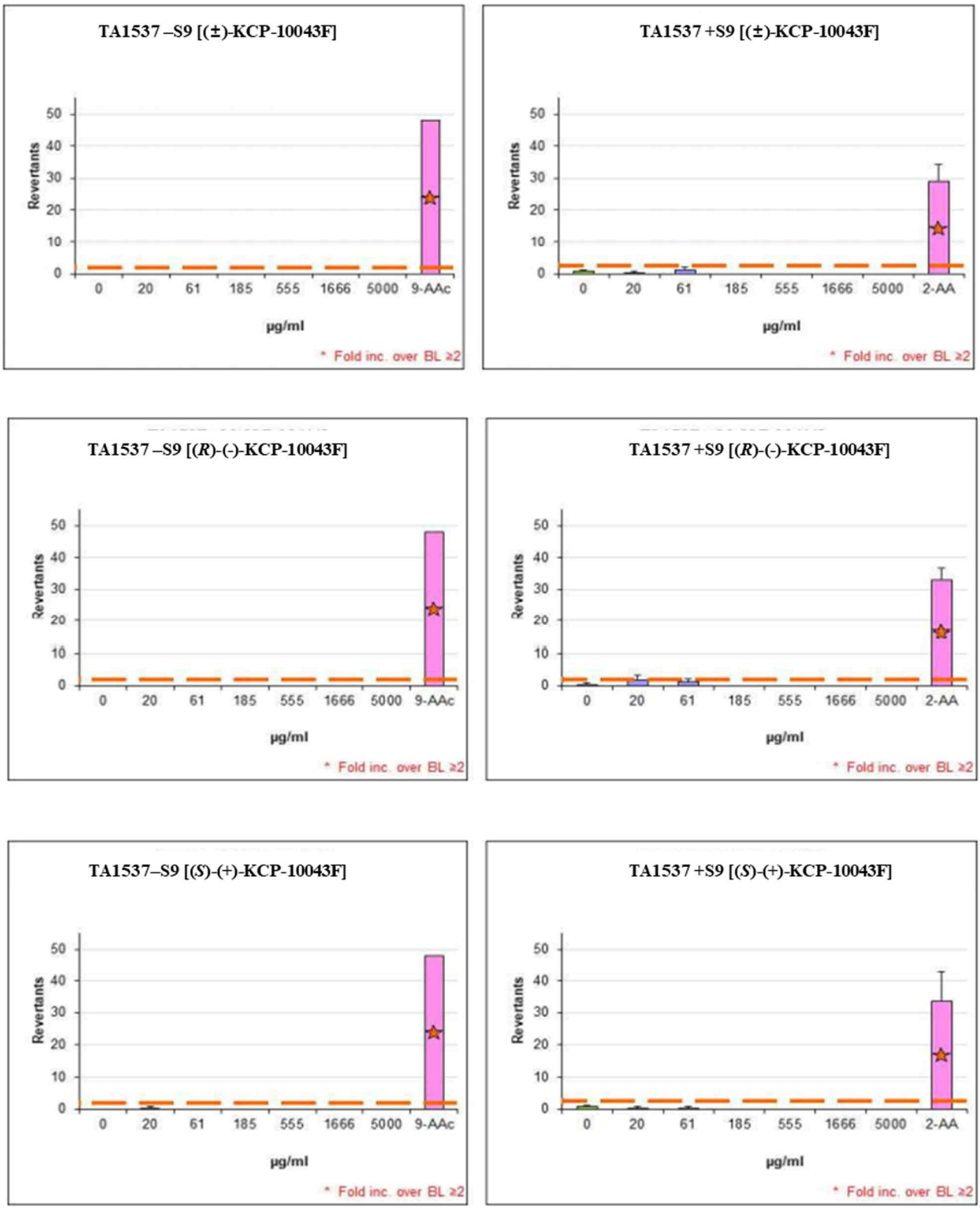


Figure S9. Ames MPF test results of racemic (±)-**KCP10043F (OZ-001)** and its two enantiomers against *Salmonella typhimurium* TA1537 with/without rat liver S9 fraction. 9-Aminoacridine (9-AAC, 15 µg/mL) and 2-aminoacridine (2-AA, 2.5 µg/mL) were used as positive controls (mutagens) and DMSO (solvent) was used as a negative control.

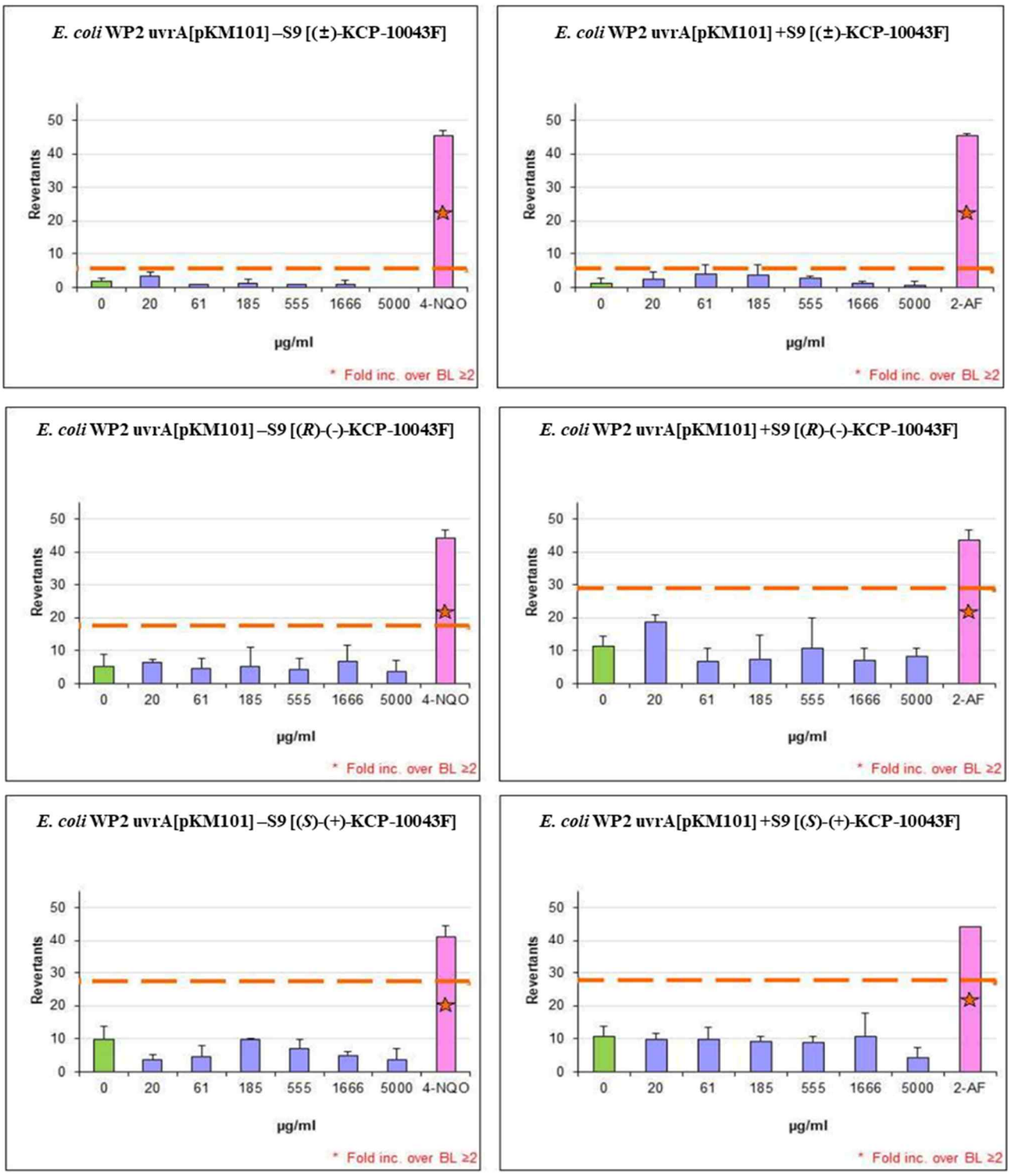


Figure S10. Ames MPF test results of racemic (±)-**KCP10043F (OZ-001)** and its two enantiomers against *E. coli* WP2 uvrA[pKM101 with/without rat liver S9 fraction. 4-Nitroquinoline-*N*-oxide (4-NQO, 2.0 µg/mL) and 2-aminofluorene (2-AF, 400 µg/mL) were used as positive controls (mutagens) and DMSO (solvent) was used as a negative control.

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