

Supporting Information

Bacterial dioxygenase- and monooxygenase-catalysed sulfoxidation of benzo[*b*]thiophenes

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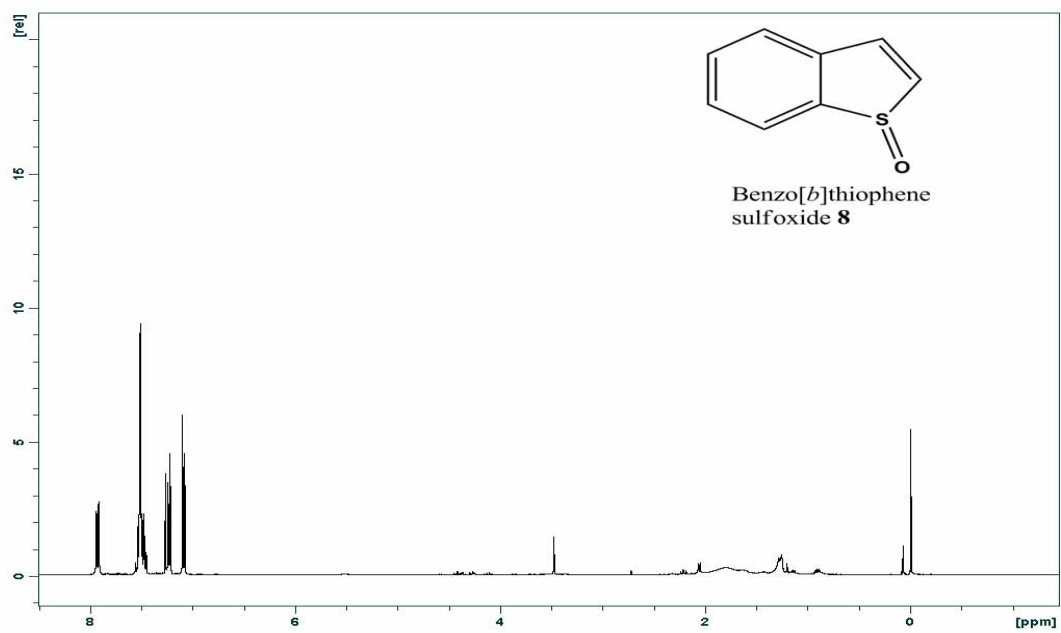
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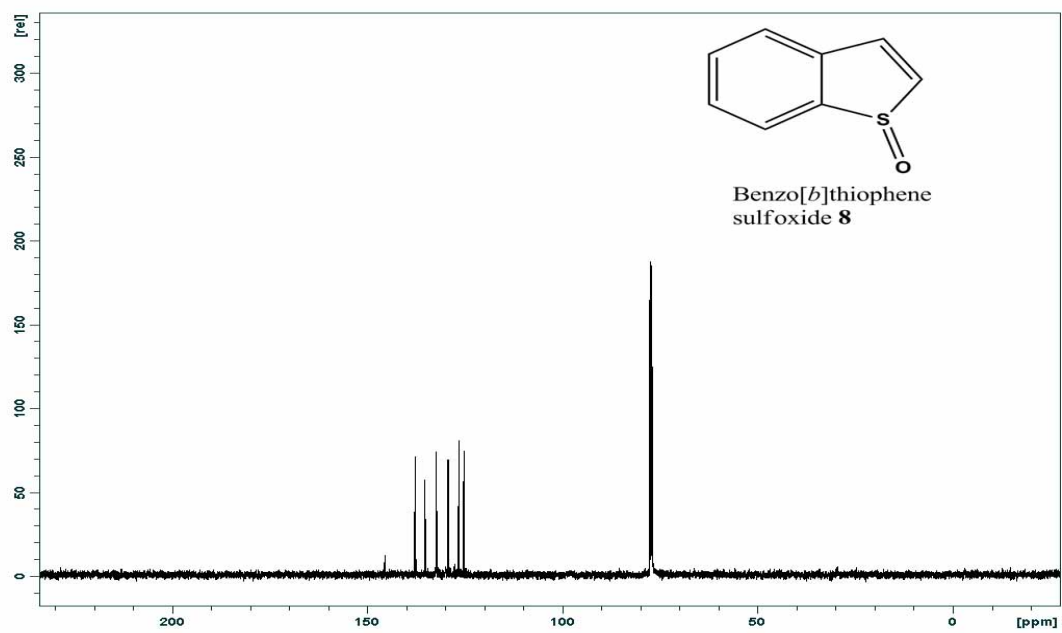
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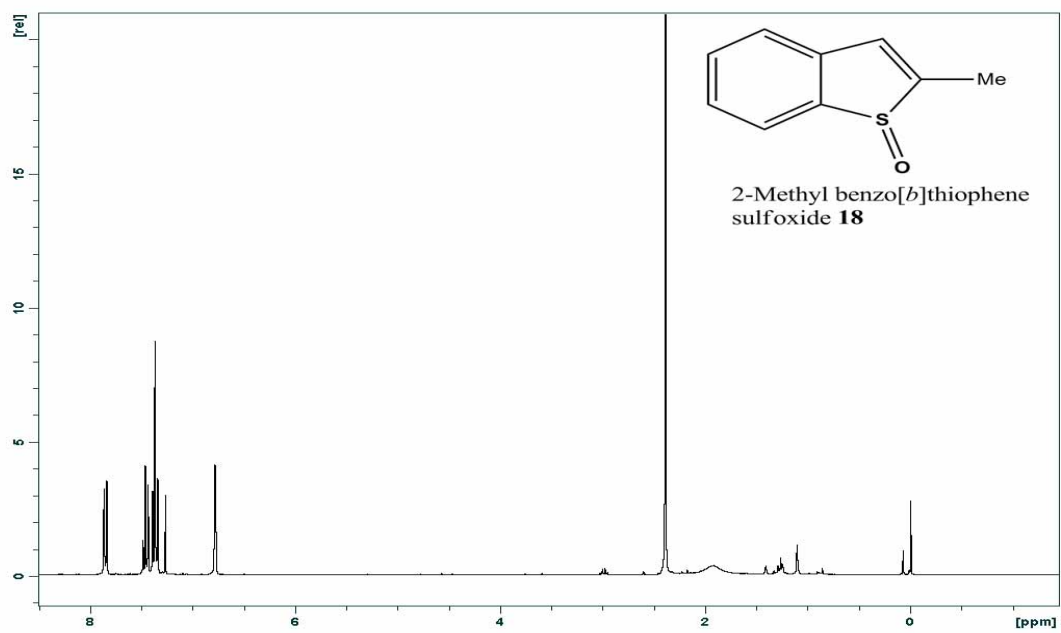
NMR: 1



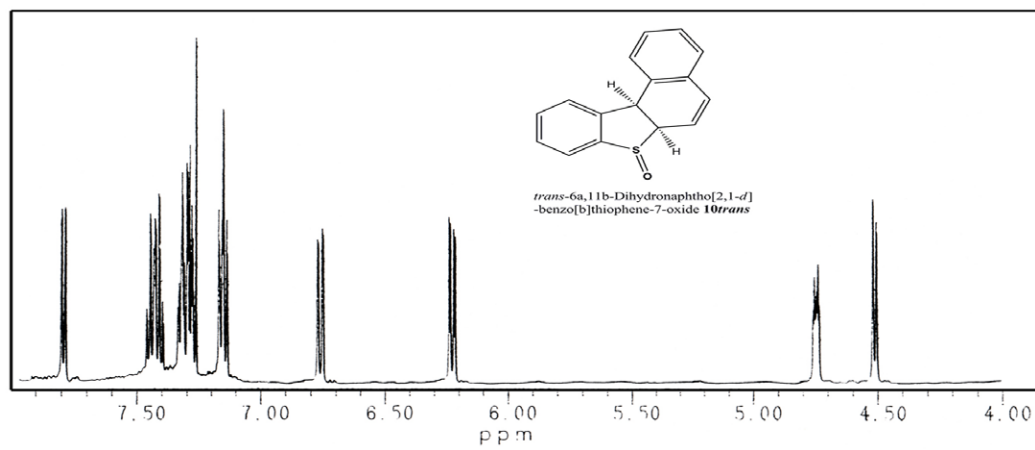
NMR: 2



NMR: 3



NMR 4



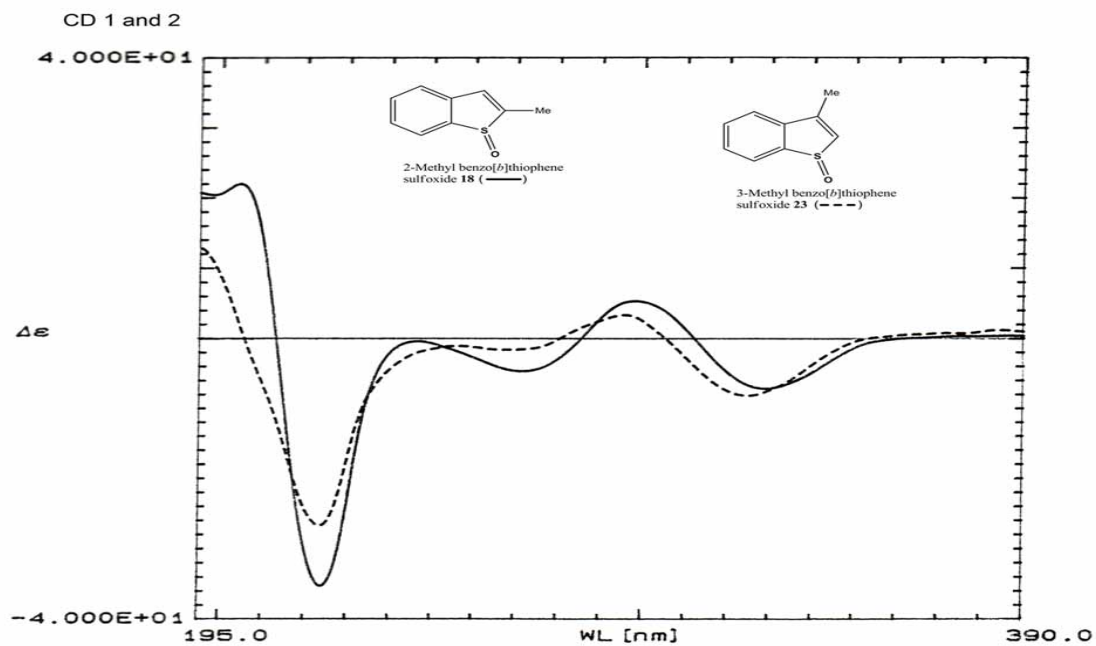


Table 2 (part a) Measurement of optical rotation $[\alpha]_D$ with time (t) (c. 0.41 in CHCl_3) at 25°C for metabolite (-)-**18**.
Table 2 (part b) Measurement of optical rotation $[\alpha]_D$ with time (t) (c. 0.2 in CHCl_3) at 50°C for metabolite (-)-**18**.

time t/min	rotation α	$\log_{10}\alpha$	time t/min	rotation α	$\log_{10}\alpha \times 10^{-1}$
4	-1.951	0.290	1.5	-0.816	-0.883
144	-1.912	0.281	41.5	-0.684	-1.649
284	-1.871	0.272	81.5	-0.573	-2.422
424	-1.832	0.263	121.6	-0.483	-3.160
564	-1.794	0.254	161.6	-0.405	-3.925
705	-1.757	0.245	201.7	-0.340	-4.685
845	-1.721	0.236	241.7	-0.288	-5.410
985	-1.686	0.227	281.8	-0.243	-6.144
1125	-1.652	0.218	321.8	-0.205	-6.882
1265	-1.618	0.209	361.8	-0.174	-7.544
-	-	-	401.9	-0.145	-8.386
-	-	-	441.9	-0.126	-9.014
-	-	-	81.0	-0.107	-9.706

Results at T= 25°C:

$$\text{Gradient} = 6.393 \times 10^{-5} \text{ min}^{-1}$$

$$= 1.066 \times 10^{-6} \text{ s}^{-1}$$

$$k = 2.454 \times 10^{-6} \text{ s}^{-1}$$

$$\therefore \Delta G^\ddagger = 25.06 \text{ kcal mol}^{-1}$$

Results at T= 50°C:

$$\text{Gradient} = 1.852 \times 10^{-3} \text{ min}^{-1}$$

$$= 3.086 \times 10^{-5} \text{ s}^{-1}$$

$$k = 7.108 \times 10^{-5} \text{ s}^{-1}$$

$$\therefore \Delta G^\ddagger = 25.06 \text{ kcal mol}^{-1}$$

