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Solvent-free chemoselective oxidation of thioethers and thiophenes by mechanical milling

Giancarlo Cravotto,[a]* Davide Garella,[a] Diego Carnaroglio,[a] Emanuela Calcio Gaudino[a] and Ornelio Rosati.[b]

[a]*Dipartimento di Scienza e Tecnologia del Farmaco, University of Turin, Via P. Giuria 9, I-10125 Turin, Italy*
[b]*Dipartimento di Chimica e Tecnologia del Farmaco. Via del liceo 1, I-06123 Perugia, Italy*
***** *To whom correspondence should be addressed. E-mail: giancarlo.cravotto@unito.it*

SUPPLEMENTARY INFORMATION

Materials

Commercially available reagents and solvents were purchased from Sigma Aldrich, and used without further purification.

Characterization

IR spectra were recorded with a Shimadzu FT-IR 8001 spectrophotometer. Nuclear magnetic resonance spectra (^{1}H and ^{13}C NMR) were recorded on a Bruker Avance 300 spectrometer respectively at 300 MHz and 75 MHz (25°C). Chemical shifts were calibrated to the $CDCl_3$ (for ^{1}H NMR, 7.27 and for ^{13}C NMR, 77.16). Gaschromatography-mass spectrometry (GC-MS) analyses were performed in a gaschromatograph Agilent 6890 (Agilent Technologies - USA) fitted with a mass detector Agilent Network 5973. Total sulphur amount was measurement with elemental analyzer multi EA® 5000.

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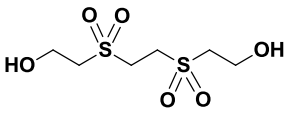
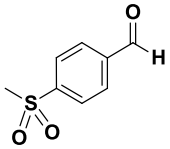
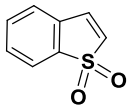
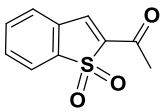
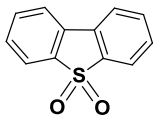
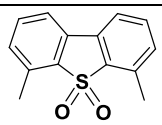
Substrate	Analytical data	
		V. Tak *et. al*, *Rapid. Commun. Mass Spectrom.* 2006, **20**, *2387-2394*
	**MS:** **^{1}H NMR, ^{13}C NMR:** **IR:**	184 [$M^{\cdot+}$], 169 [M – CH_3^+], 122, 105 [M – CH_3SO_2]$^+$ (100%), 77, 51 A. Ulman *et al*, *J. Org. Chem.* 1989, **54**, 4691-4692 2924, 1702, 1293 (*asymm. stretch.* SO_2), 1149 (*symm. stretch.* SO_2), 1084, 963, 766, 695, 564, 529
		Commercially available reagent. CAS N. 825-44-5
	**MS:** **^{1}H NMR:** **^{13}C NMR:** **IR:**	208 [$M]^{\cdot+}$, 193 [M – CH_3]$^+$ (100%), 137, 109, 75, 43 [CH_3CO]$^+$ 7.86 (s, 1H, H3), 7.79 (d, 1H, H7, J = 6.0 Hz), 7.64 (m, 2H, H5-H6), 7.57 (d, 1H, H4, J = 6.0 Hz), 2.60 (s, 3H, Me) 188.2 (-CO-), 140.6 (C8), 137.7 (C2), 137.4 (C3), 133.8 (C5), 133.2 (C6), 128.1 (C9), 127.4 (C4), 121.7 (C7), 26.2 (CH_3CO-) 3058, 2924, 1670 (CO), 1568, 1302 (*asymm. stretch.* SO_2), 1279, 1195, 1153 (*symm. stretch.* SO_2), 764, 541, 529
		Commercially available reagent. CAS N. 825-44-5
		K. Sato *et.al*, *Tetrahedron* 2001, **57,** 2469-2476

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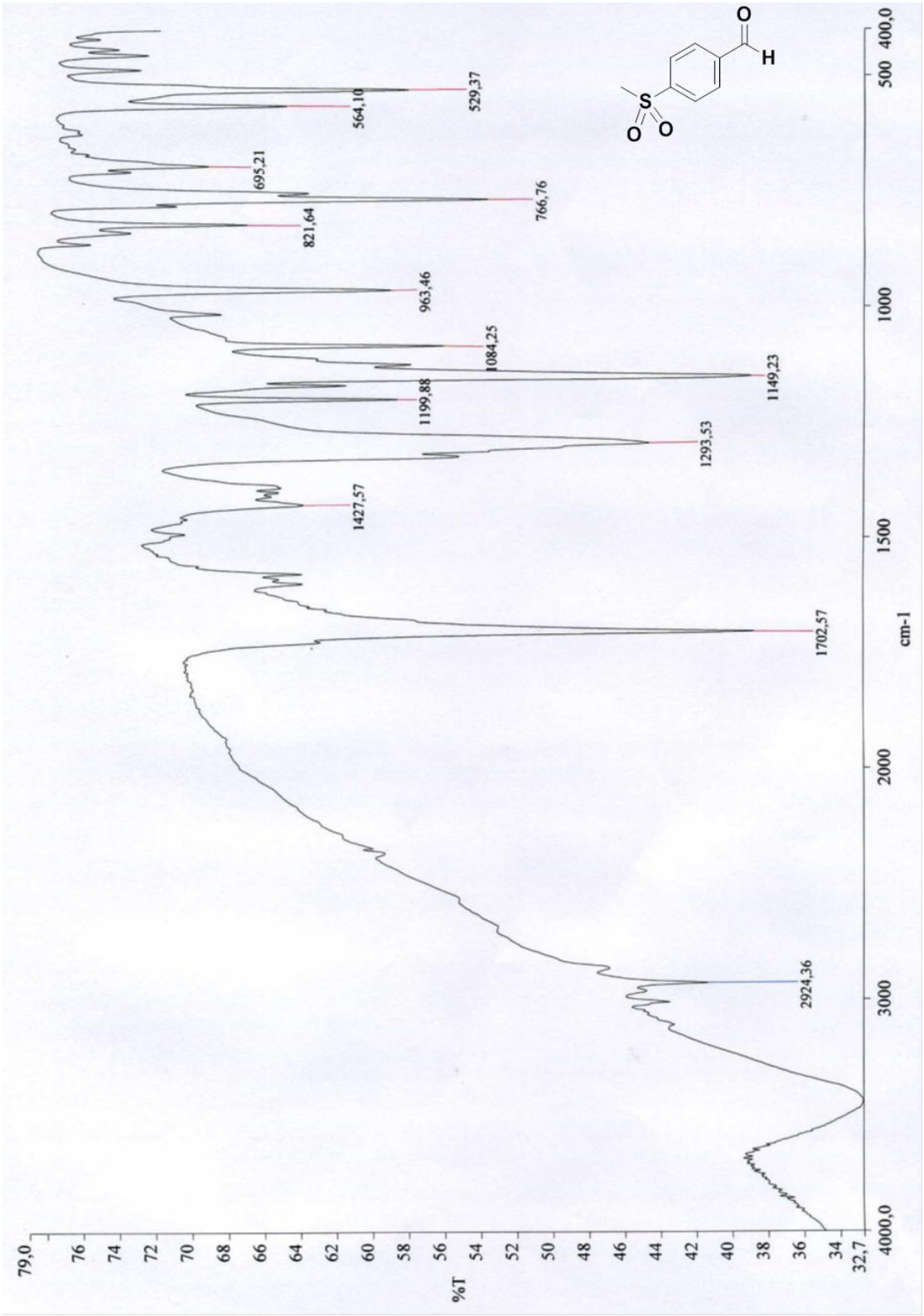

Fig. 1. FT-IR spectra.

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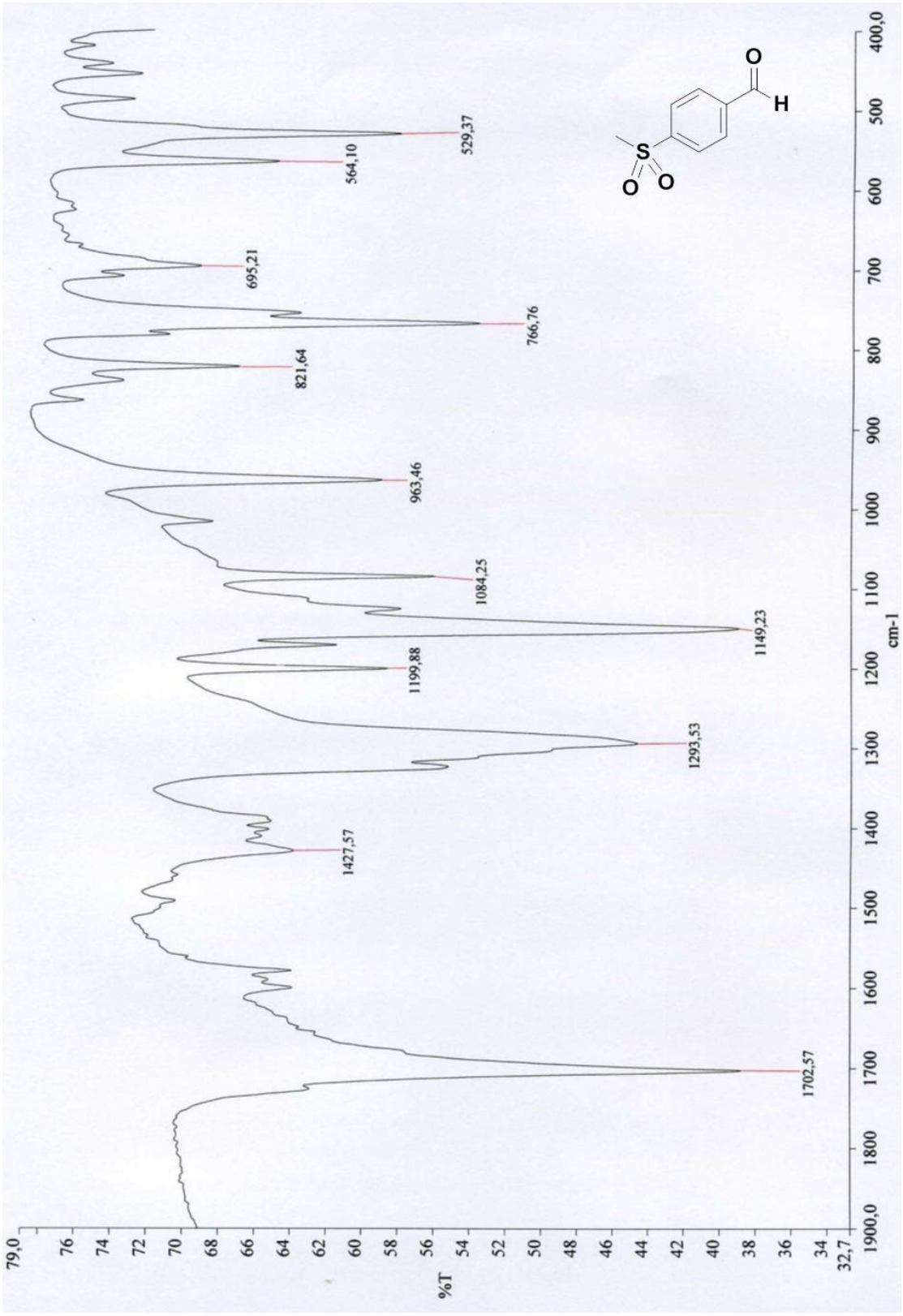

Fig. 2. FT-IR spectra.

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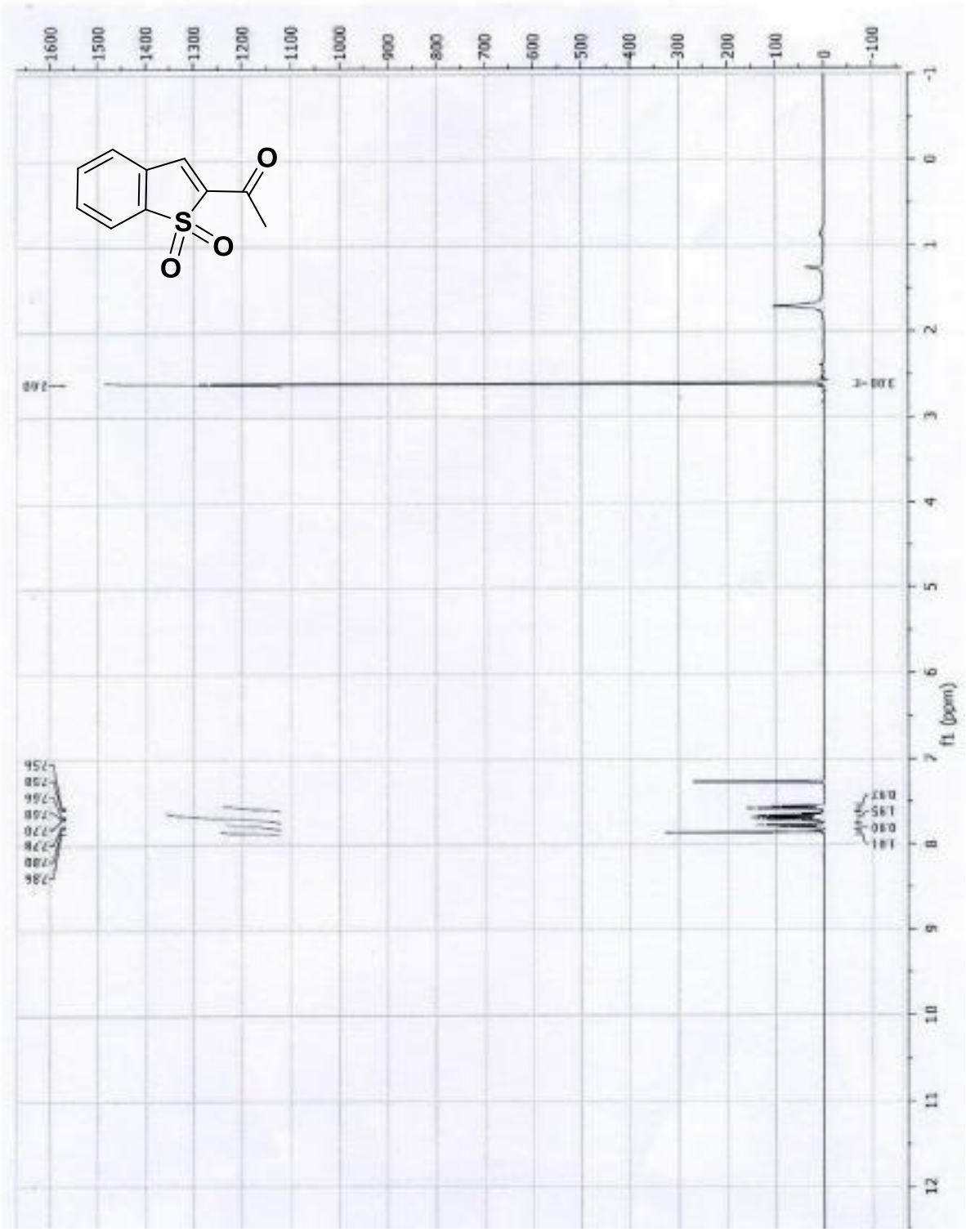

Fig. 3. ^{1}H NMR.

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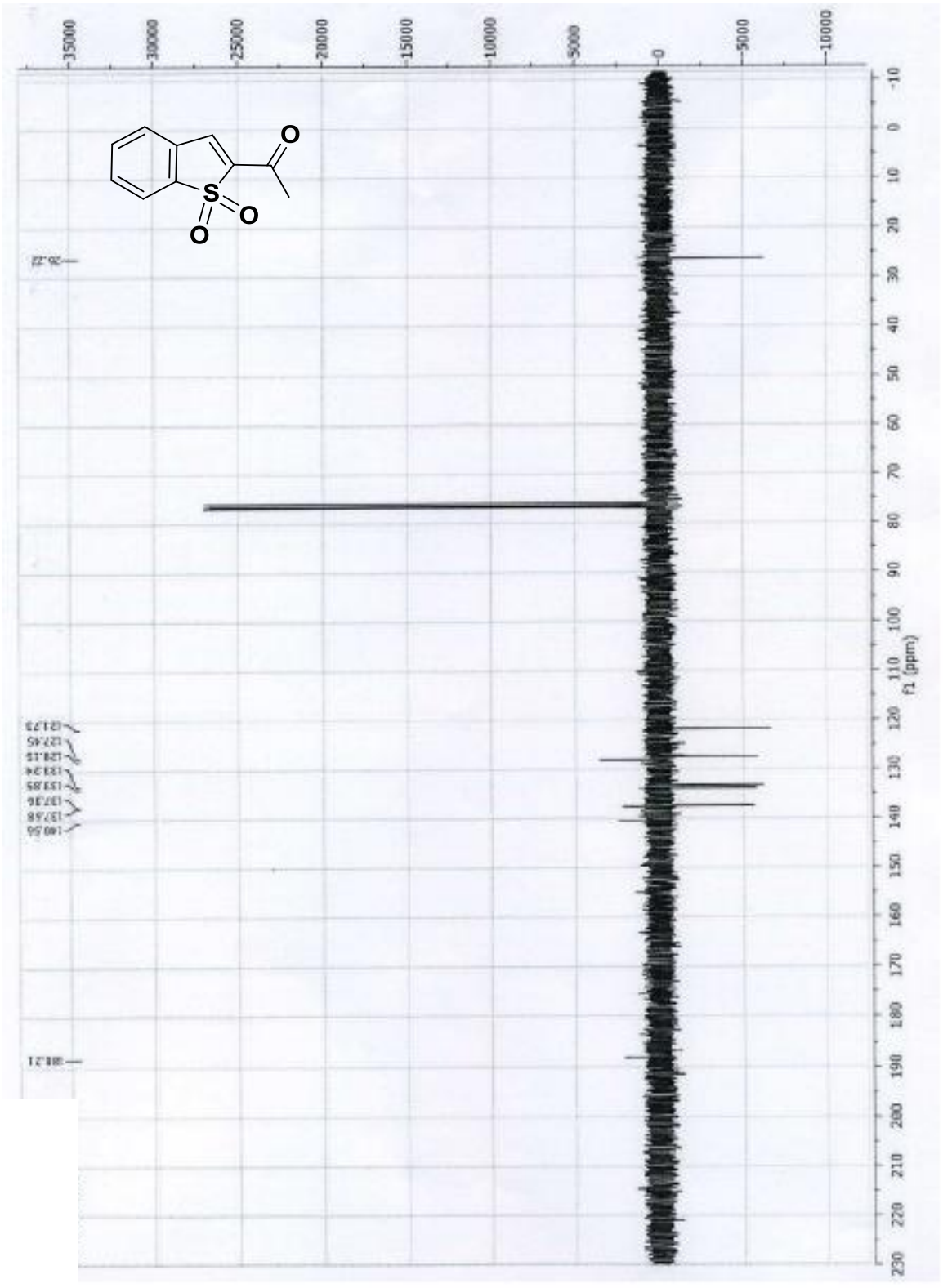

Fig. 4. ^{13}C [^{1}H] APT NMR.

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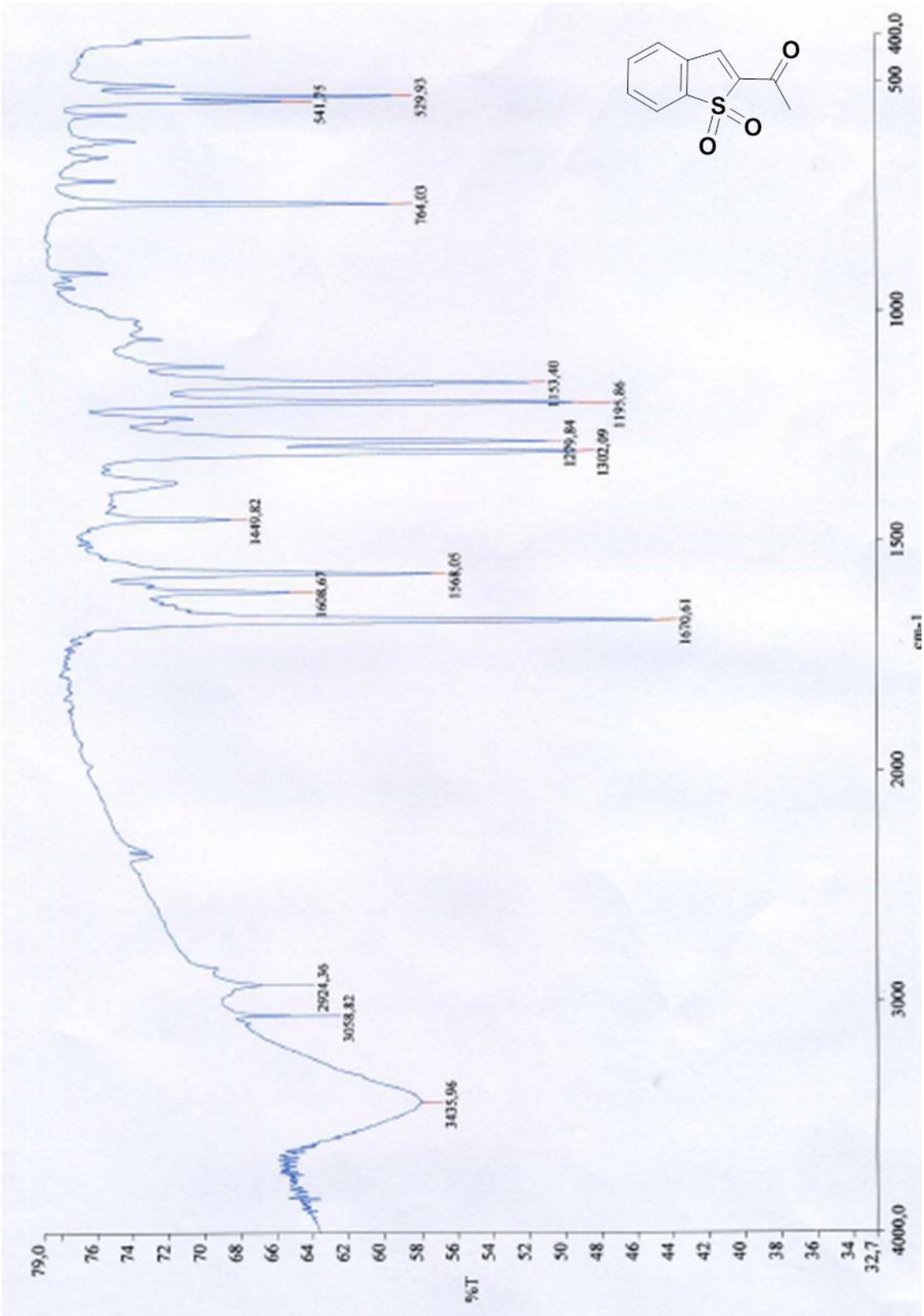

Fig. 5. FT-IR spectra.

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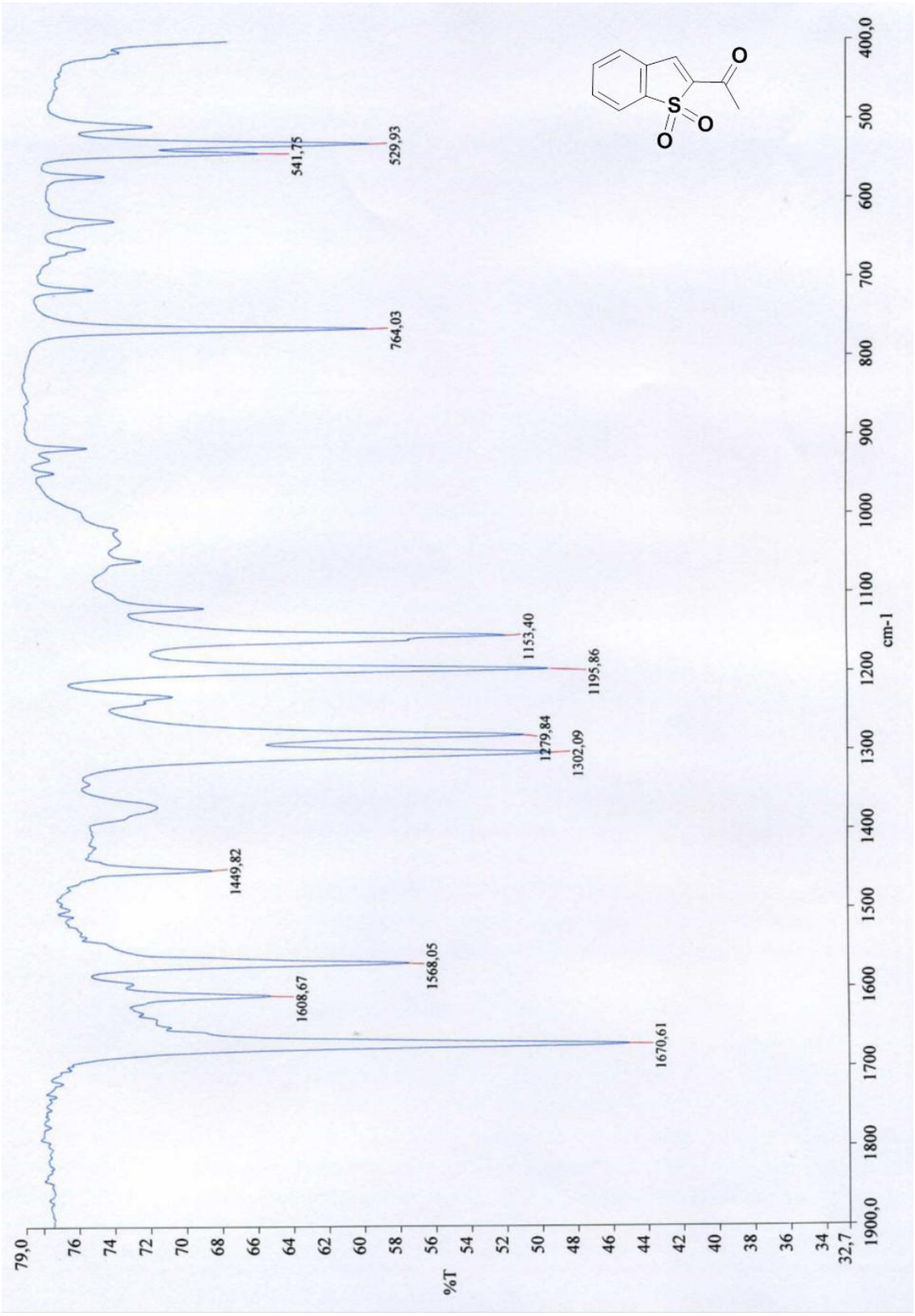

Fig. 6. FT-IR spectra.