

Sorafenib analogue and its rearranged compound: design, synthesis, their in vitro anticancer activity and crystal structure of the rearranged compound dichloromethane solvate

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Supporting Information

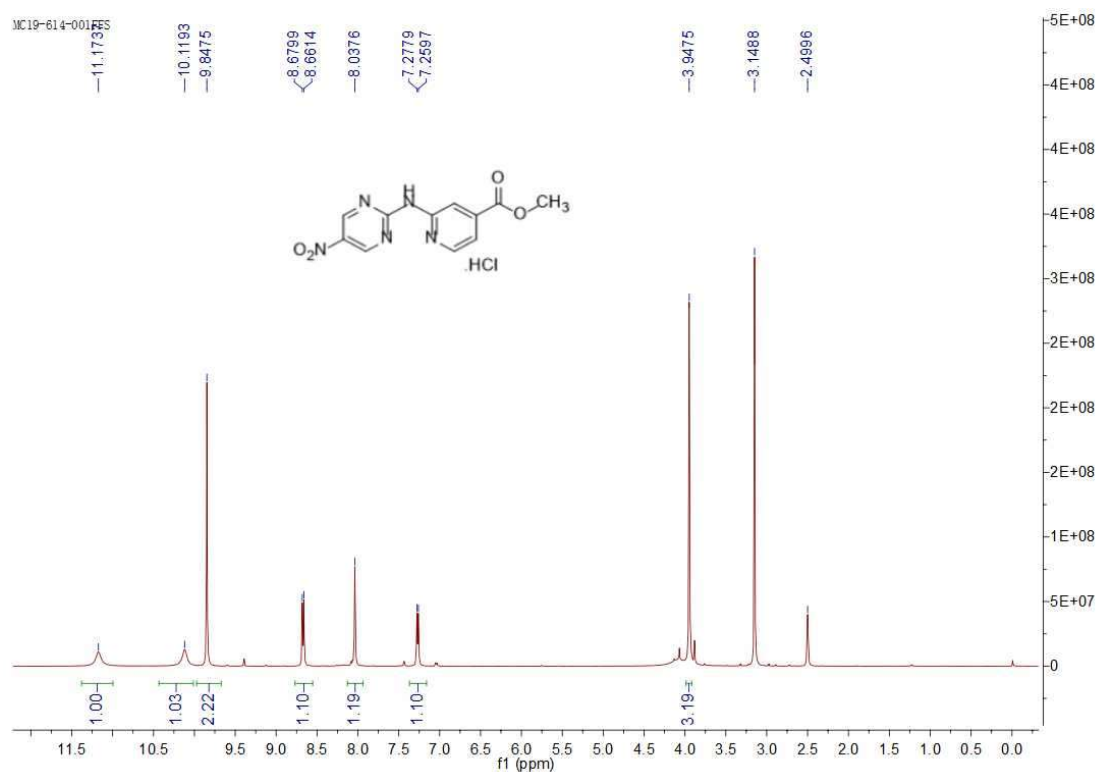
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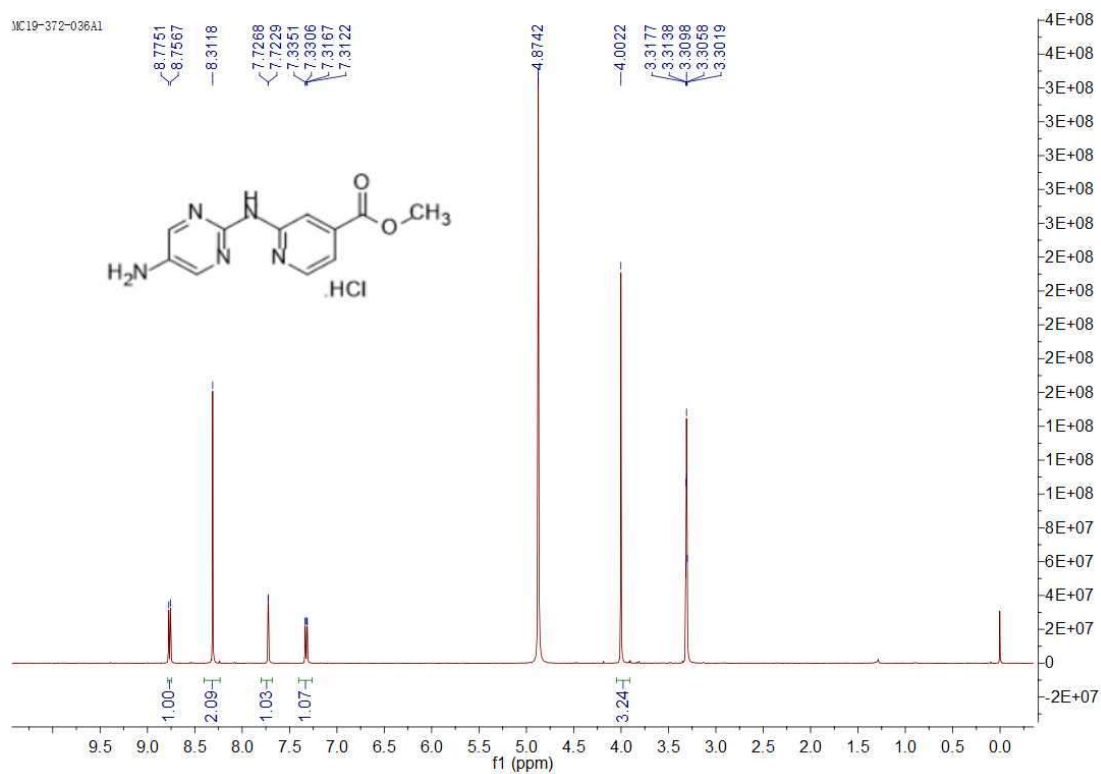
General Information

Room temperature was to be 20-25°C. All reagents obtained from commercial sources were used without further purification. ^1H and ^{13}C spectra were recorded on Bruker DRX-400 instrument with TMS as internal standard. Chemical shifts (δ ppm) are calibrated against the deuterated solvent DMSO (δ 2.50 for ^1H NMR and 39.52 for ^{13}C NMR); CDCl_3 (δ 7.26 for ^1H NMR and 77.16 for ^{13}C NMR). Flash column chromatography was performed with various combinations of dichloromethane and methanol as eluent. ESI-MS analysis was determined on API QSTAR Pulsari spectrometer. Infrared spectra were recorded on a FT-IR spectrometer with KBr pellets. Yields refer to purified, dried and spectroscopically (^1H NMR) homogeneous material. Multiplicities are reported as the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad.

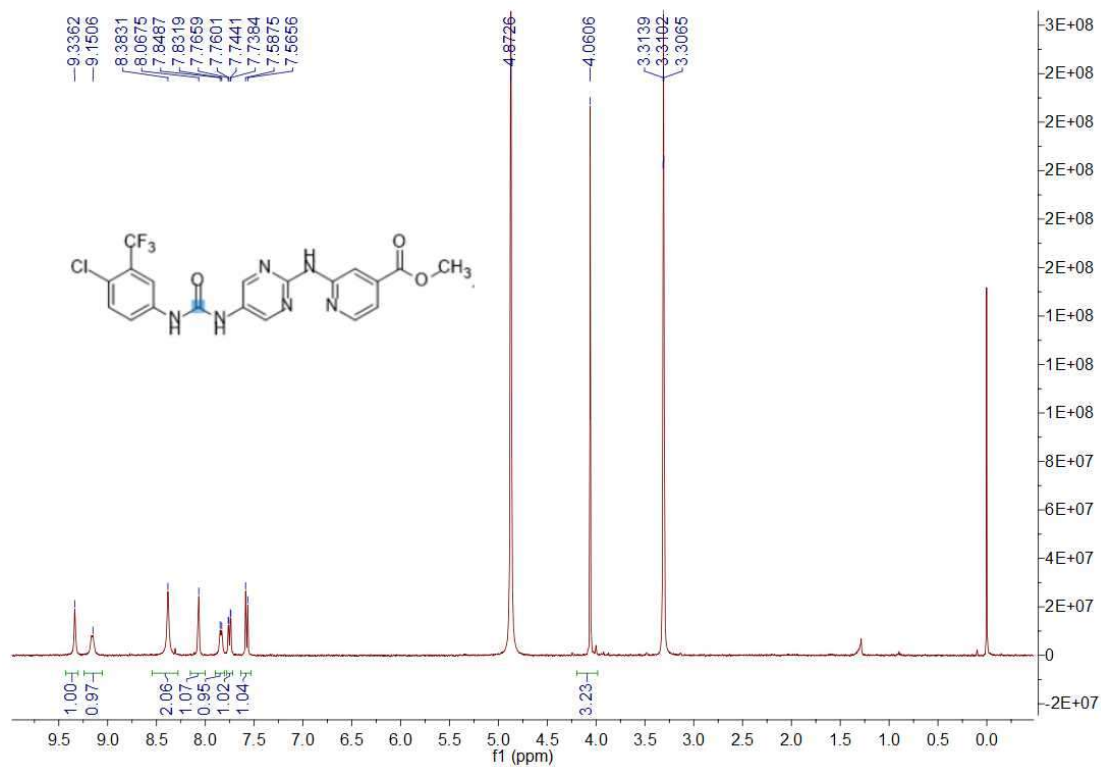
^1H NMR spectrum (400 MHz) of compound 2 in $\text{DMSO}-d_6$



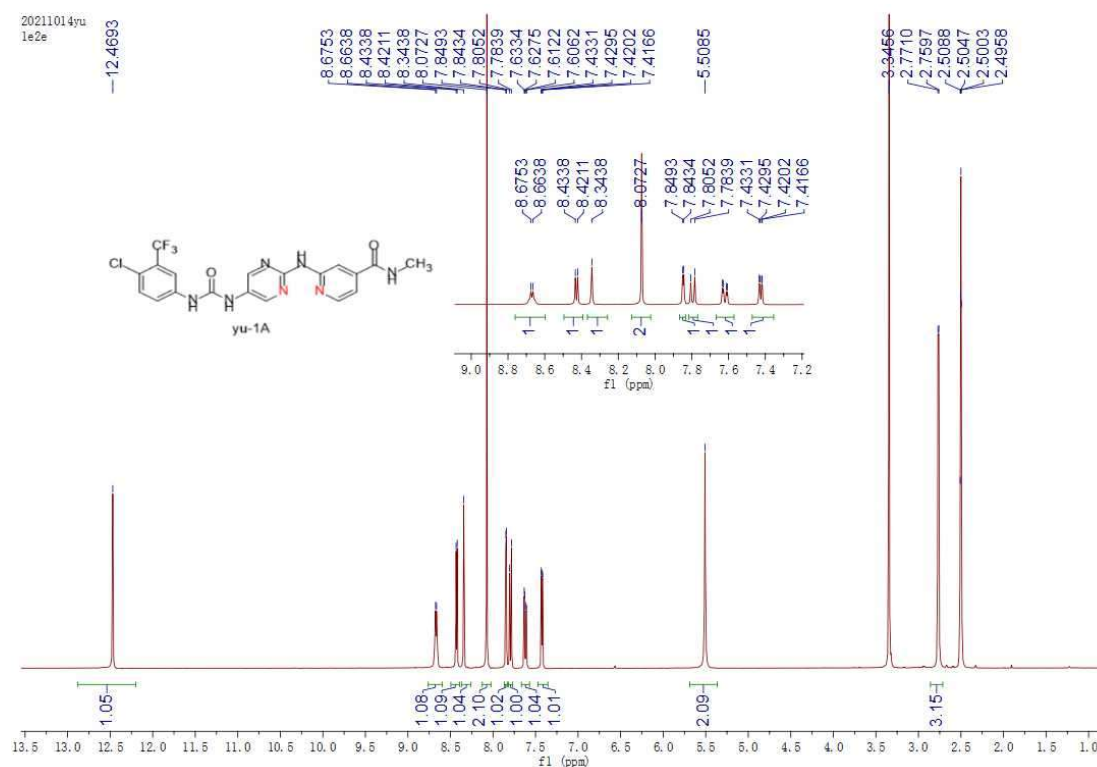
¹H NMR spectrum (400 MHz) of compound 3 in CD₃OD



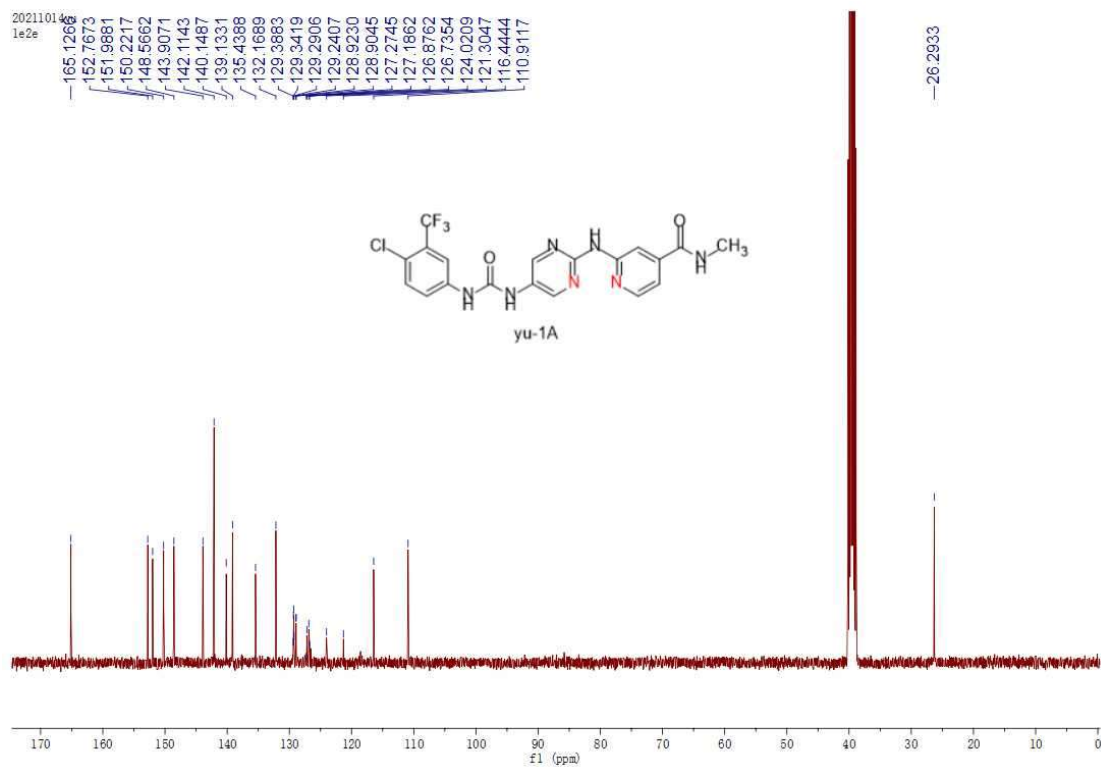
¹H NMR spectrum (400 MHz) of compound 4 in CD₃OD



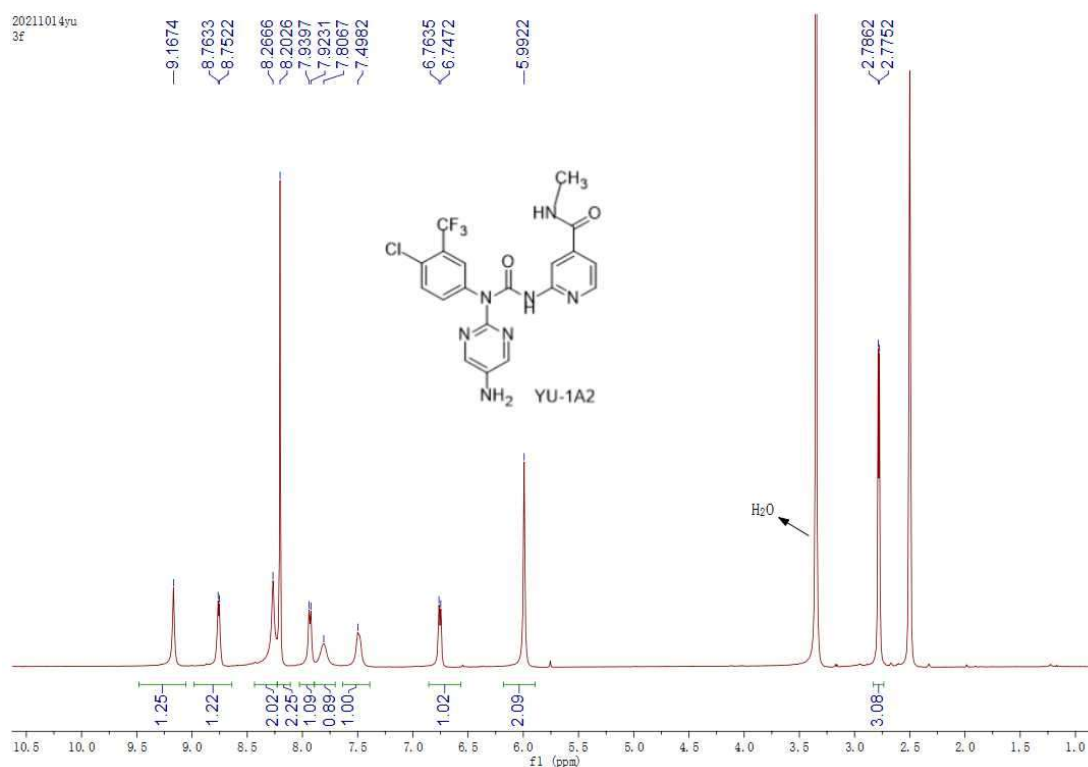
¹H NMR spectrum (400 MHz) of compound 1A in DMSO-*d*₆



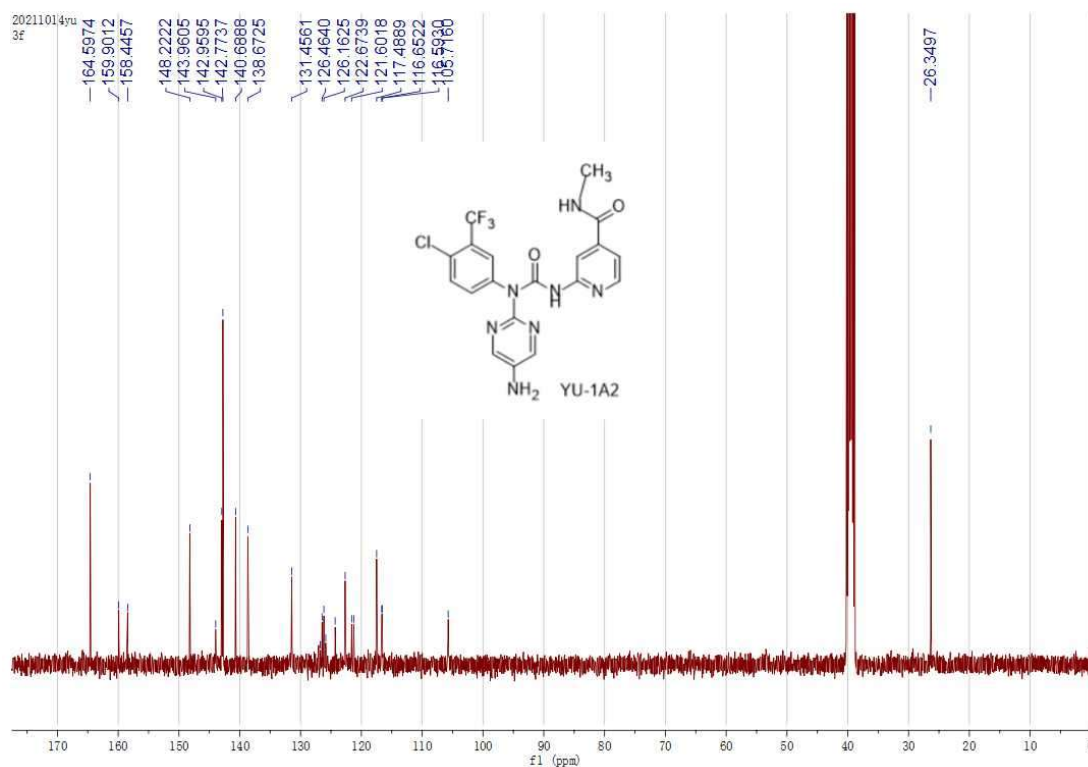
¹³C NMR spectrum (400 MHz) of compound 1A in DMSO-*d*₆



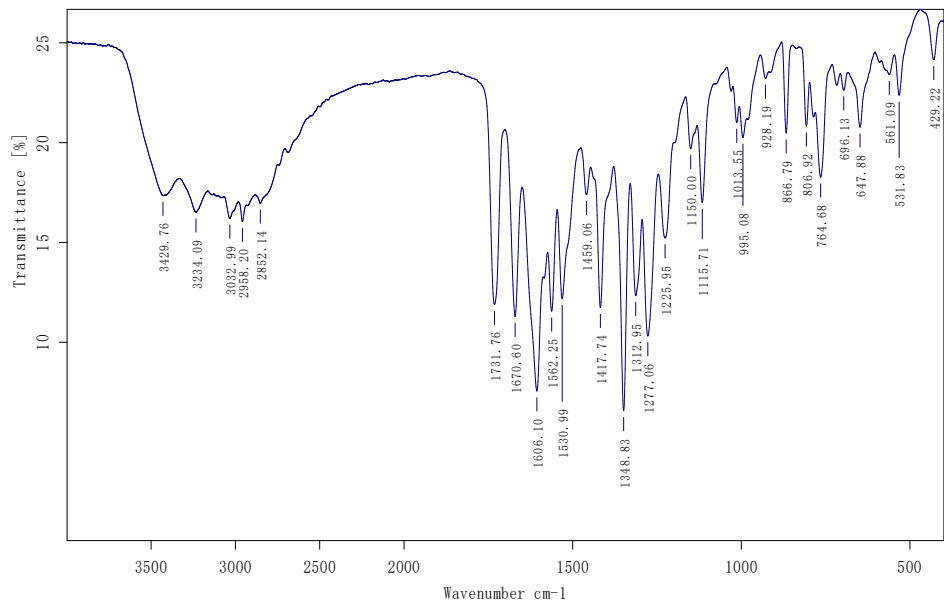
¹H NMR spectrum (400 MHz) of compound 1A2 in DMSO-*d*₆



¹³C NMR spectrum (400 MHz) of compound 1A2 in DMSO-*d*₆

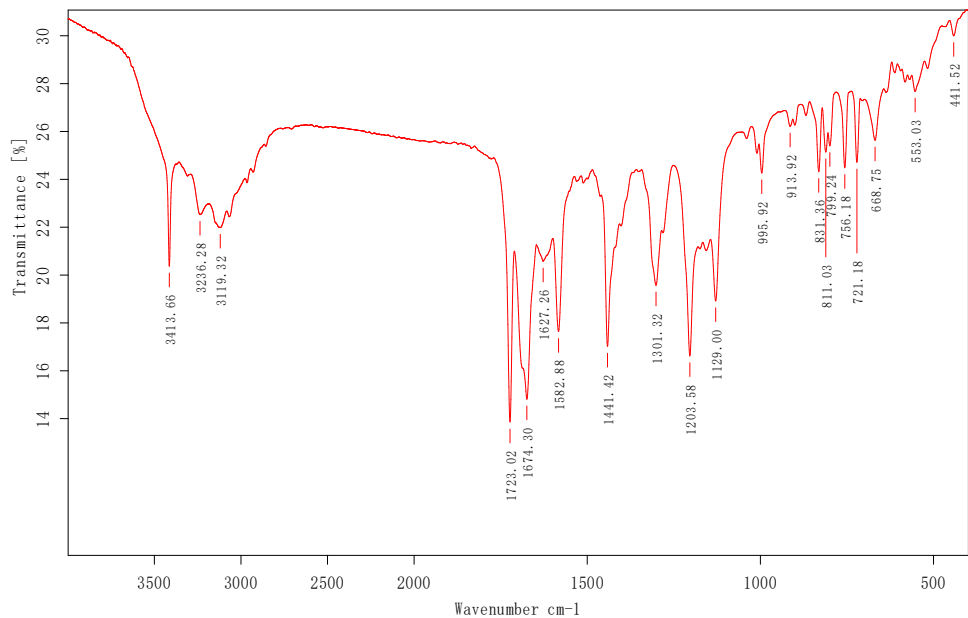


IR spectrum of 2



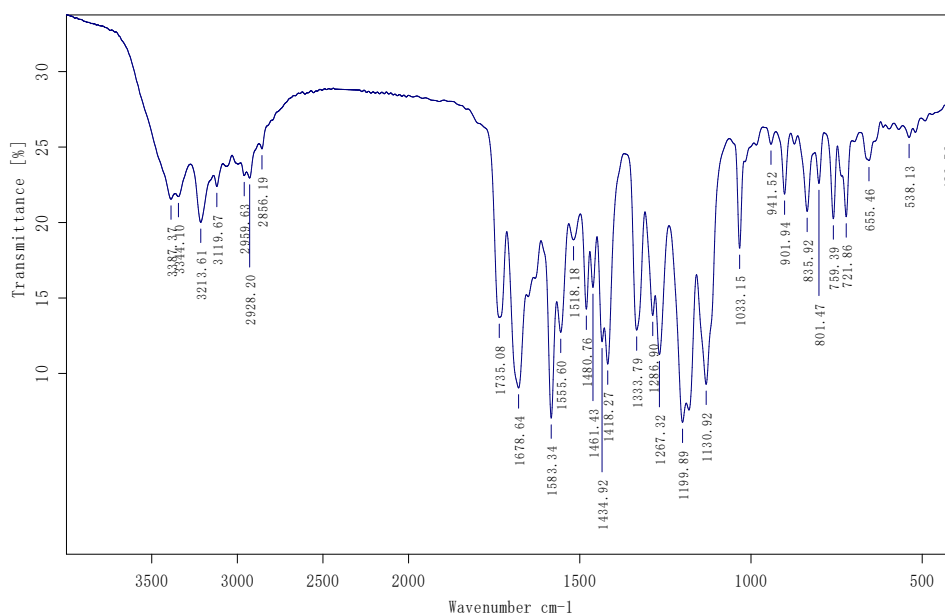
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IR spectrum of 3



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IR spectrum of 4



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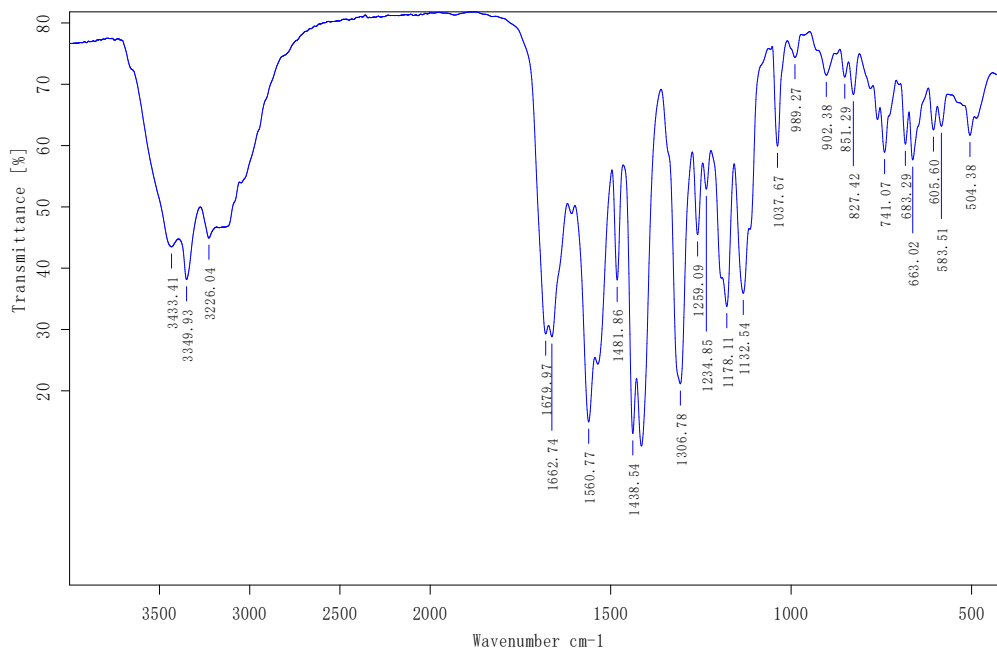
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IR spectrum of 1A2



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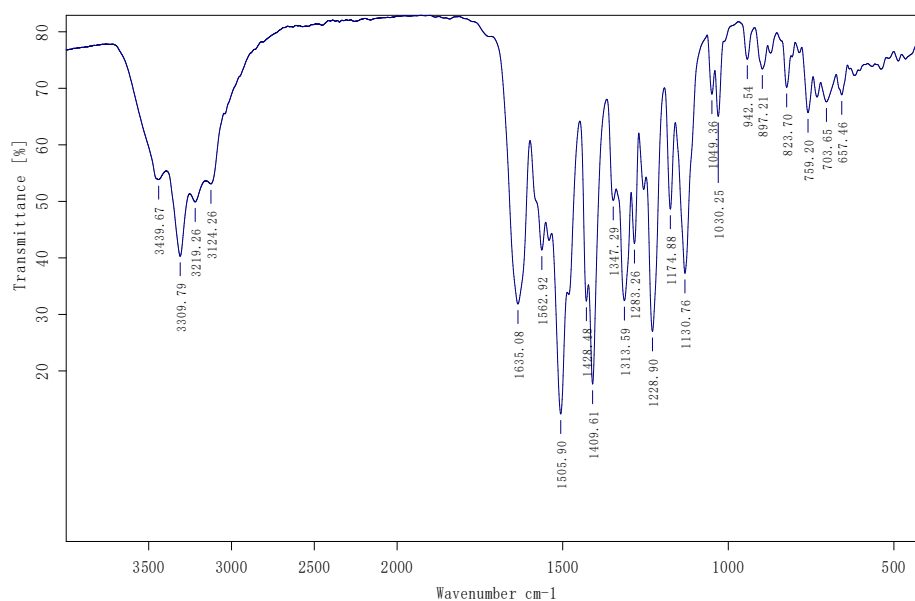
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IR spectrum of 1A



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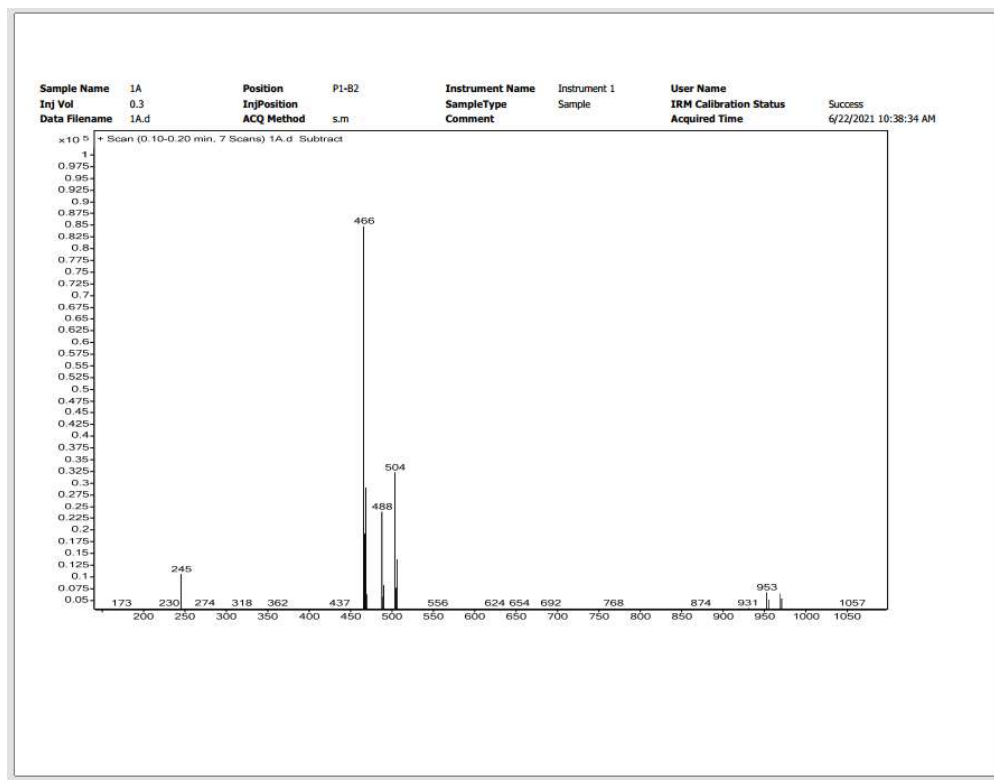
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ESI-MS spectrum of 1A



ESI-MS spectrum of 1A2

