

Supplementary Data

A novel palladium-catalyzed cyclization of indole phytoalexin brassinin and its 1-substituted derivatives

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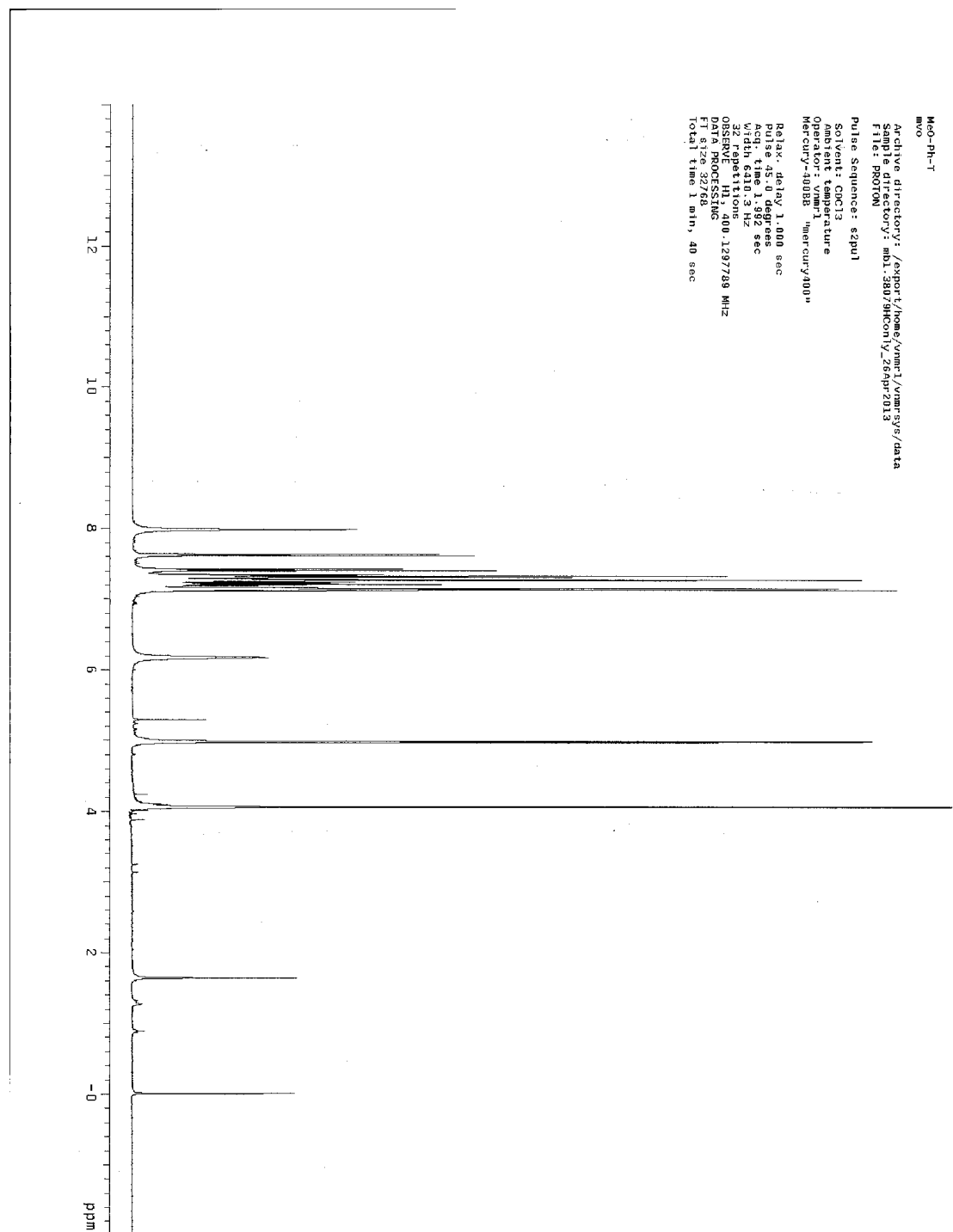
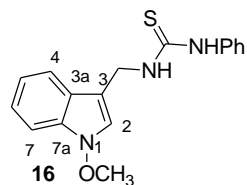
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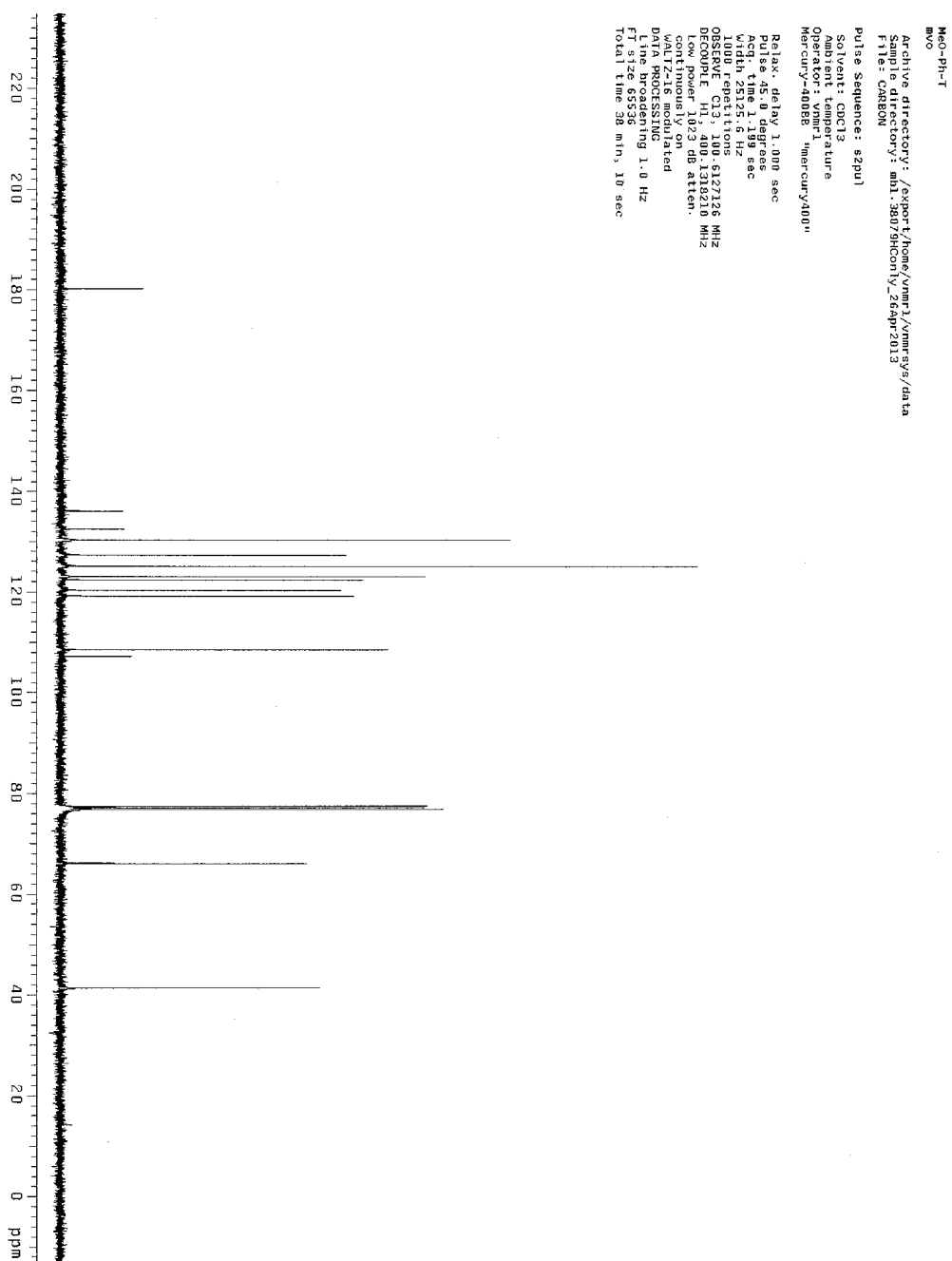
1. Experimental section

¹H NMR (400 MHz) and ¹³C NMR (100 MHz) spectra were measured on a Varian Mercury Plus spectrometer.

N-(1-Methoxyindol-3-yl)methyl-N'-phenylthiourea (16)
¹H NMR spectrum of 16

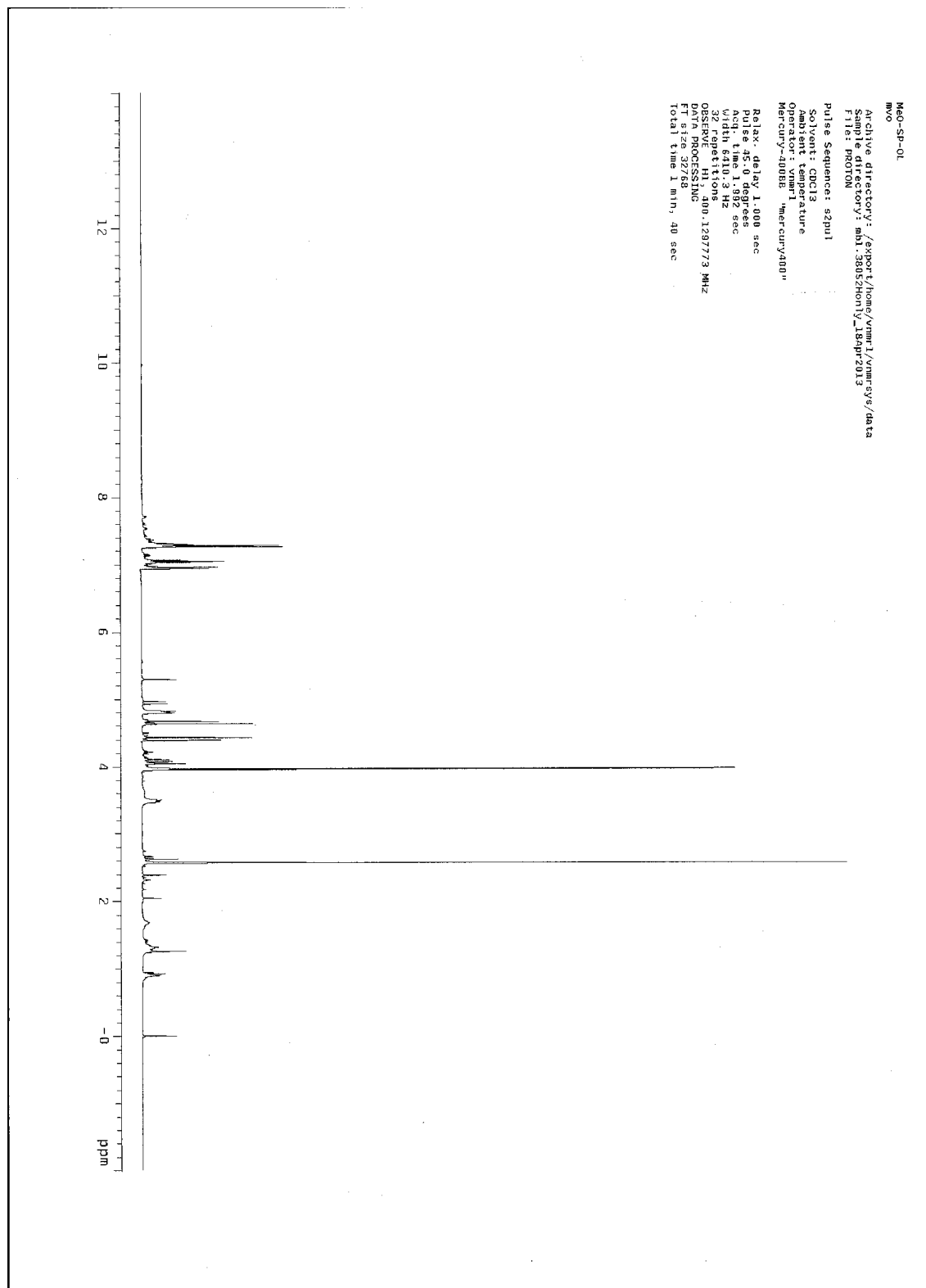
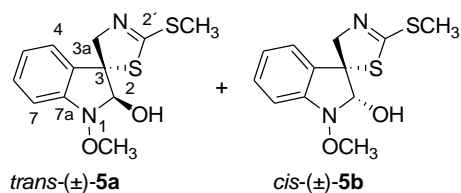


¹³C NMR spectrum of 16



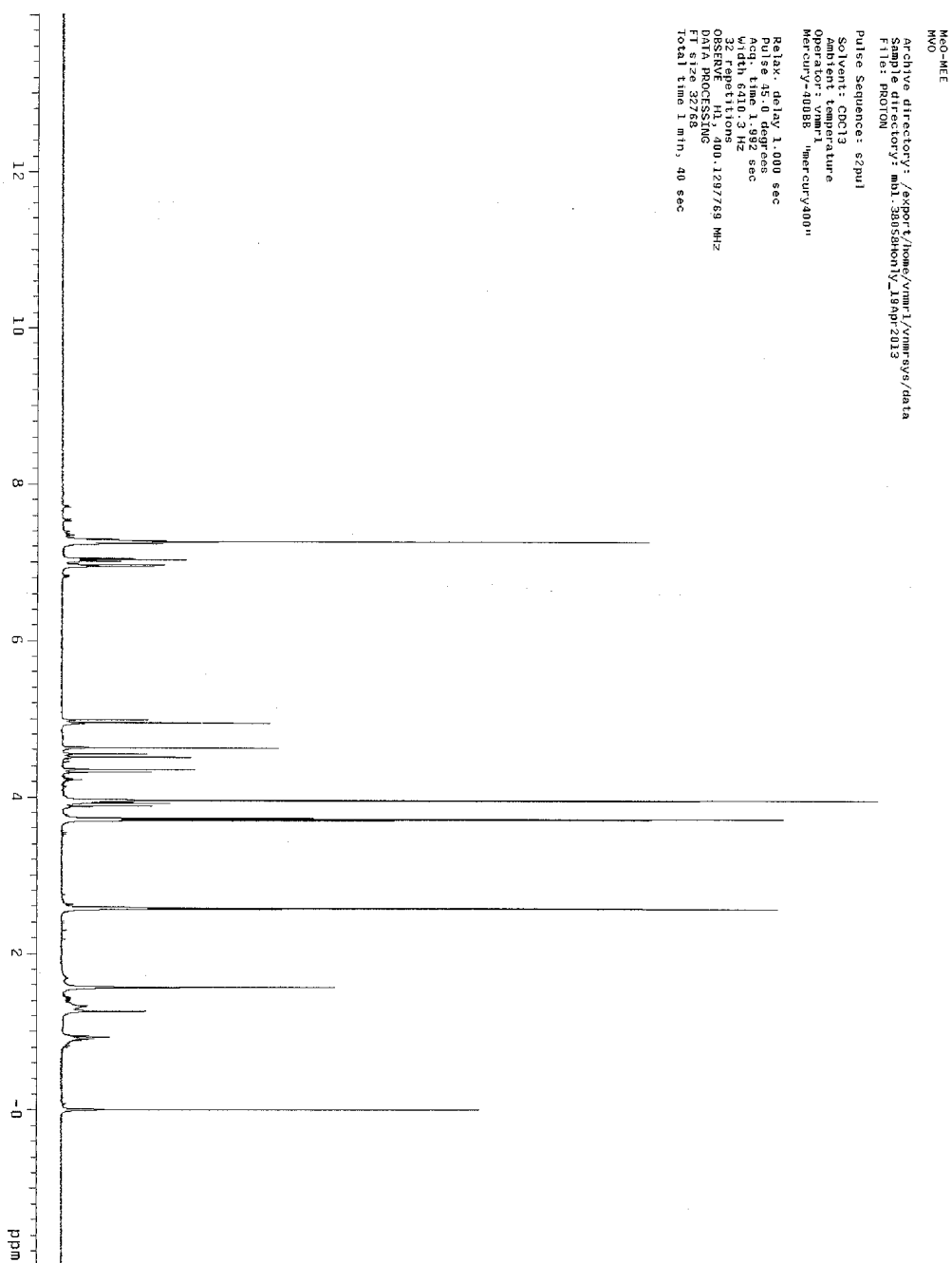
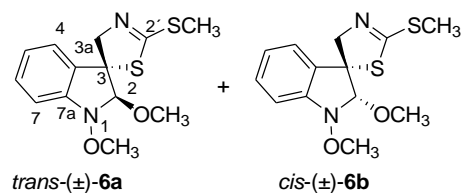
***trans* and *cis*-(±)-1-Methoxyspirobrassinol [(±)-5a and (±)-5b]**

¹H NMR spectrum of mixture (±)-5a and (±)-5b



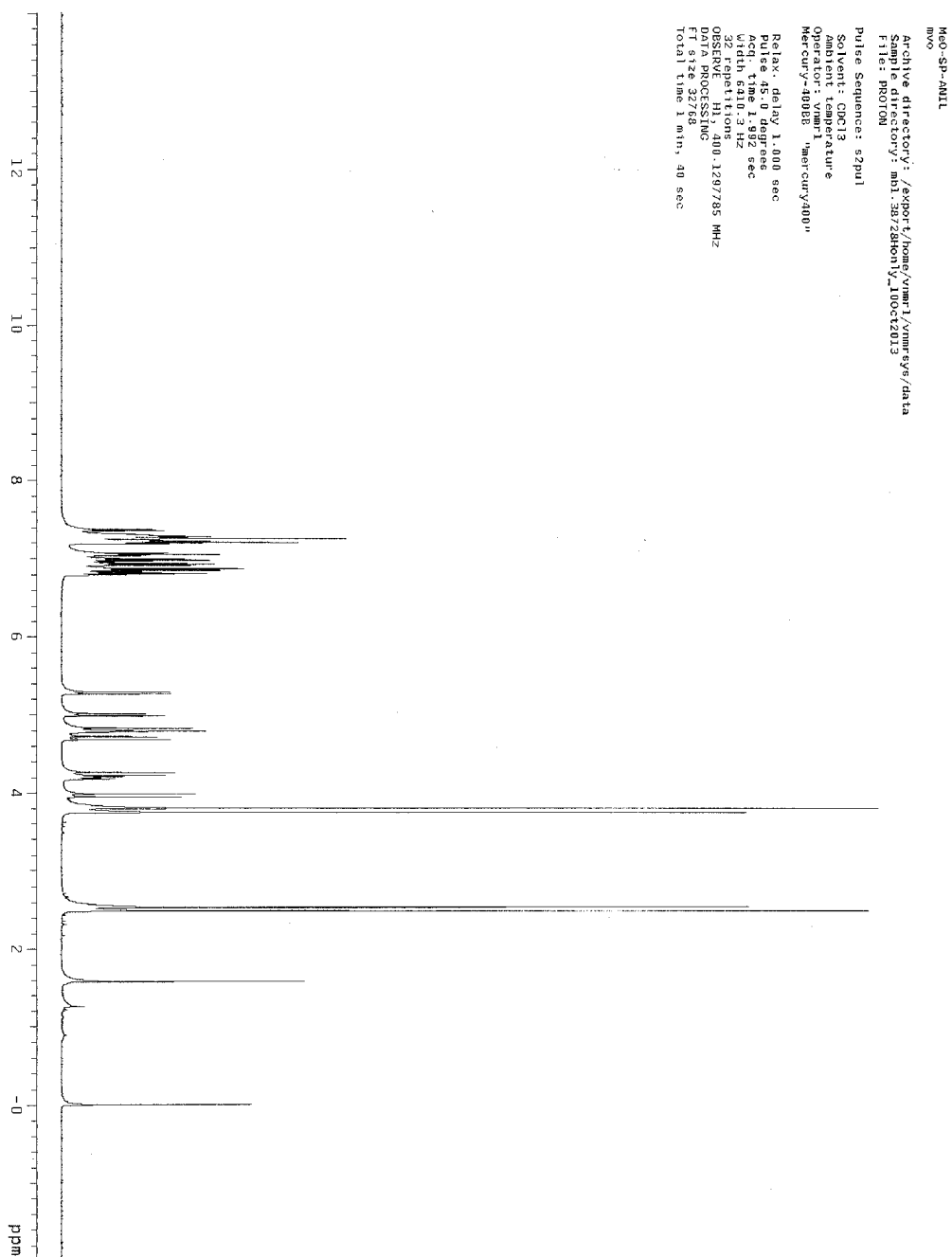
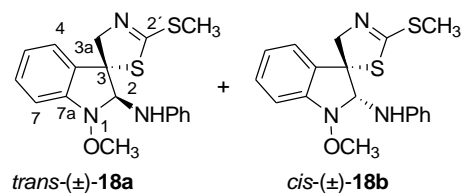
***trans* and *cis*-(±)-1-Methoxyspirobrassinol methyl ether [(±)-6a and (±)-6b]**

¹H NMR spectrum of mixture (±)-6a and (±)-6b

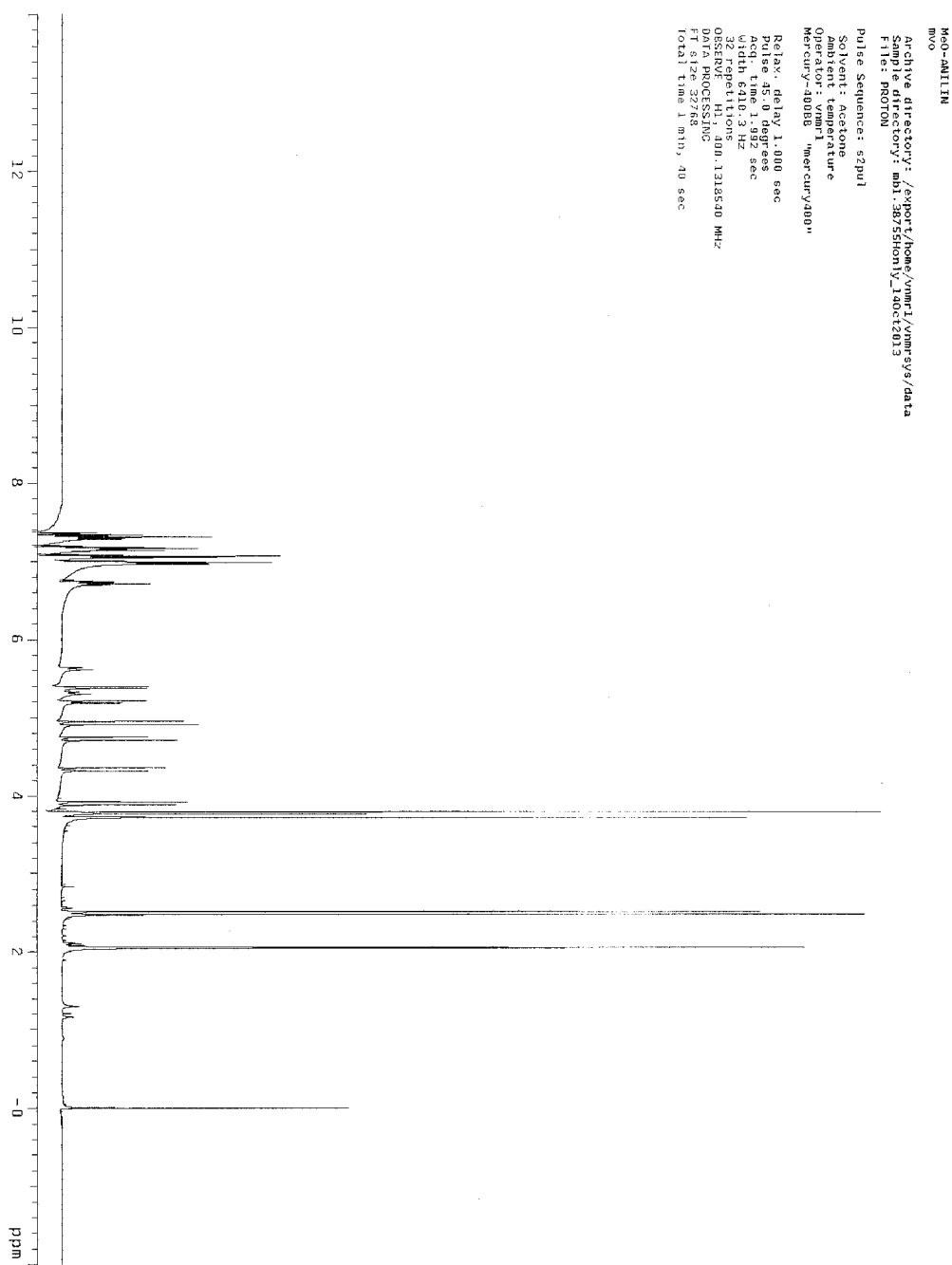


trans and *cis*-(±)-1-Methoxy-2-phenylamino-2'-(methylsulfonyl)spiro[indoline-3,5'-
[4',5']-dihydrothiazol] [(±)-18a and (±)-18b]

¹H NMR spectrum of mixture (±)-18a and (±)-18b in CDCl₃

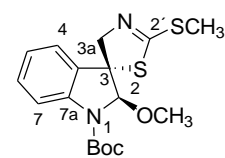


^1H NMR spectrum of mixture (\pm)-**18a** and (\pm)-**18b** in $(\text{CD}_3)_2\text{CO}$

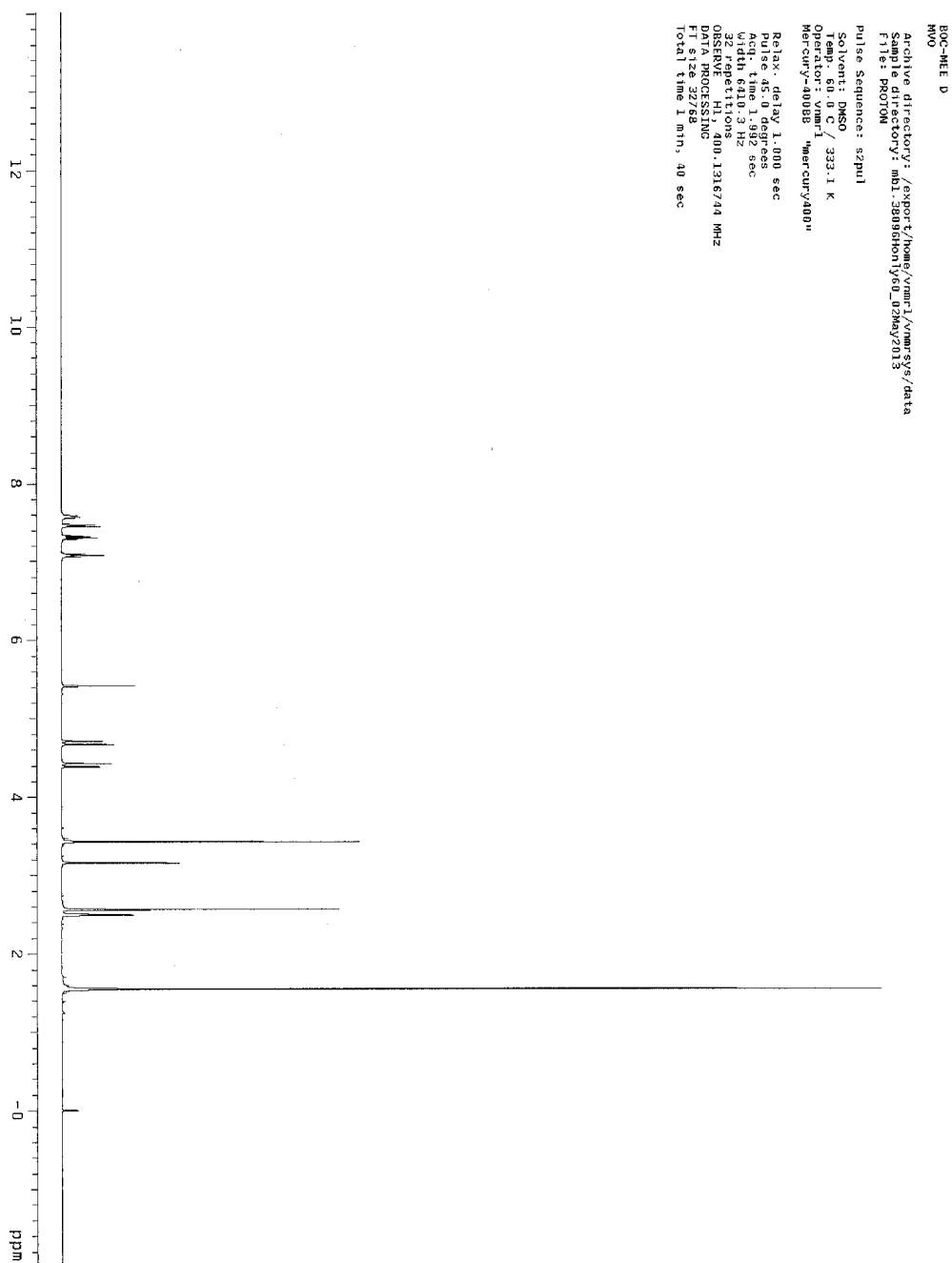


***trans* and *cis*-(±)-1-(*tert*-Butoxycarbonyl)spirobrassinol methyl ether [(±)-20a and (±)-20b]**

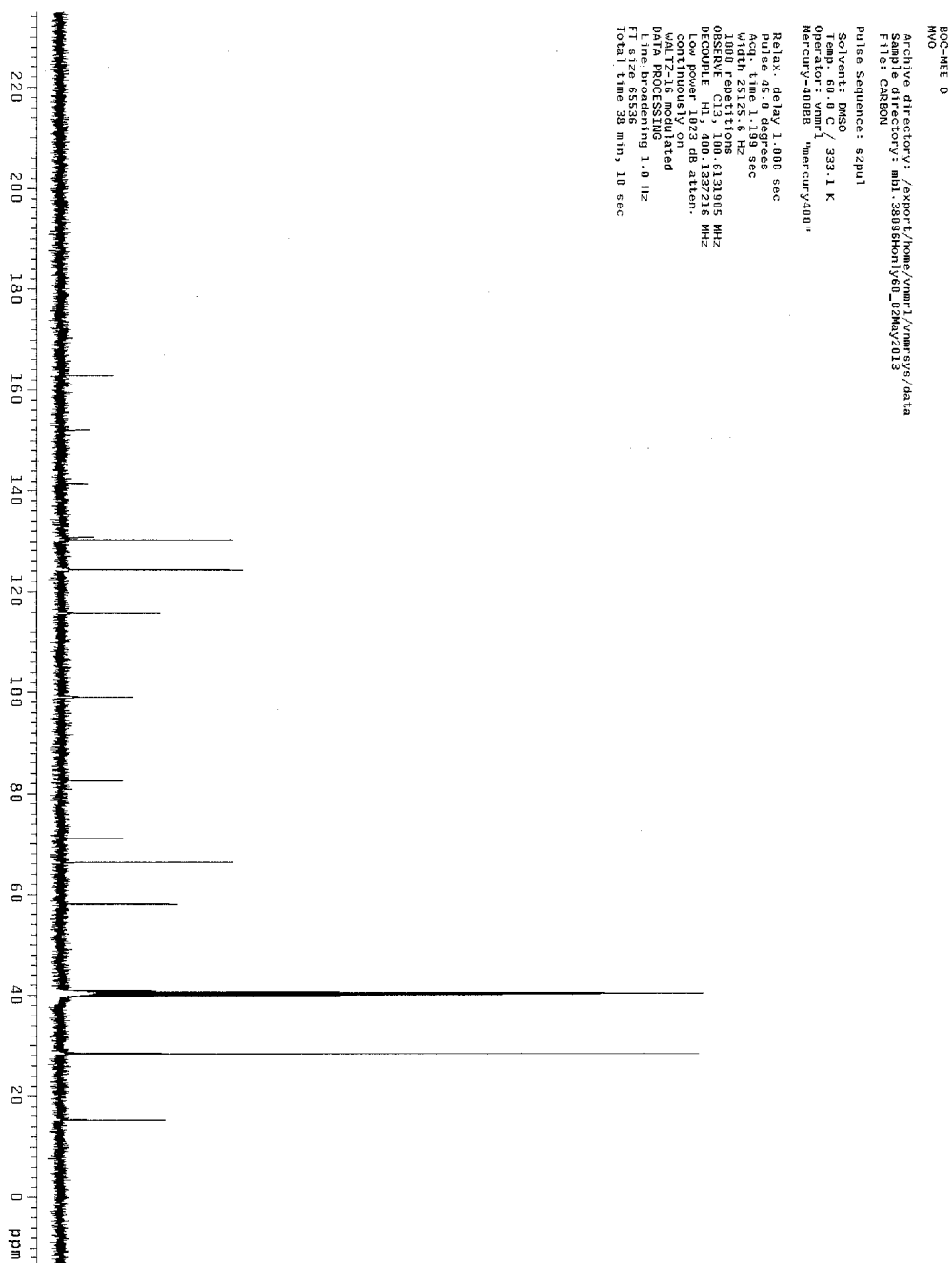
¹H NMR spectrum of (±)-20a



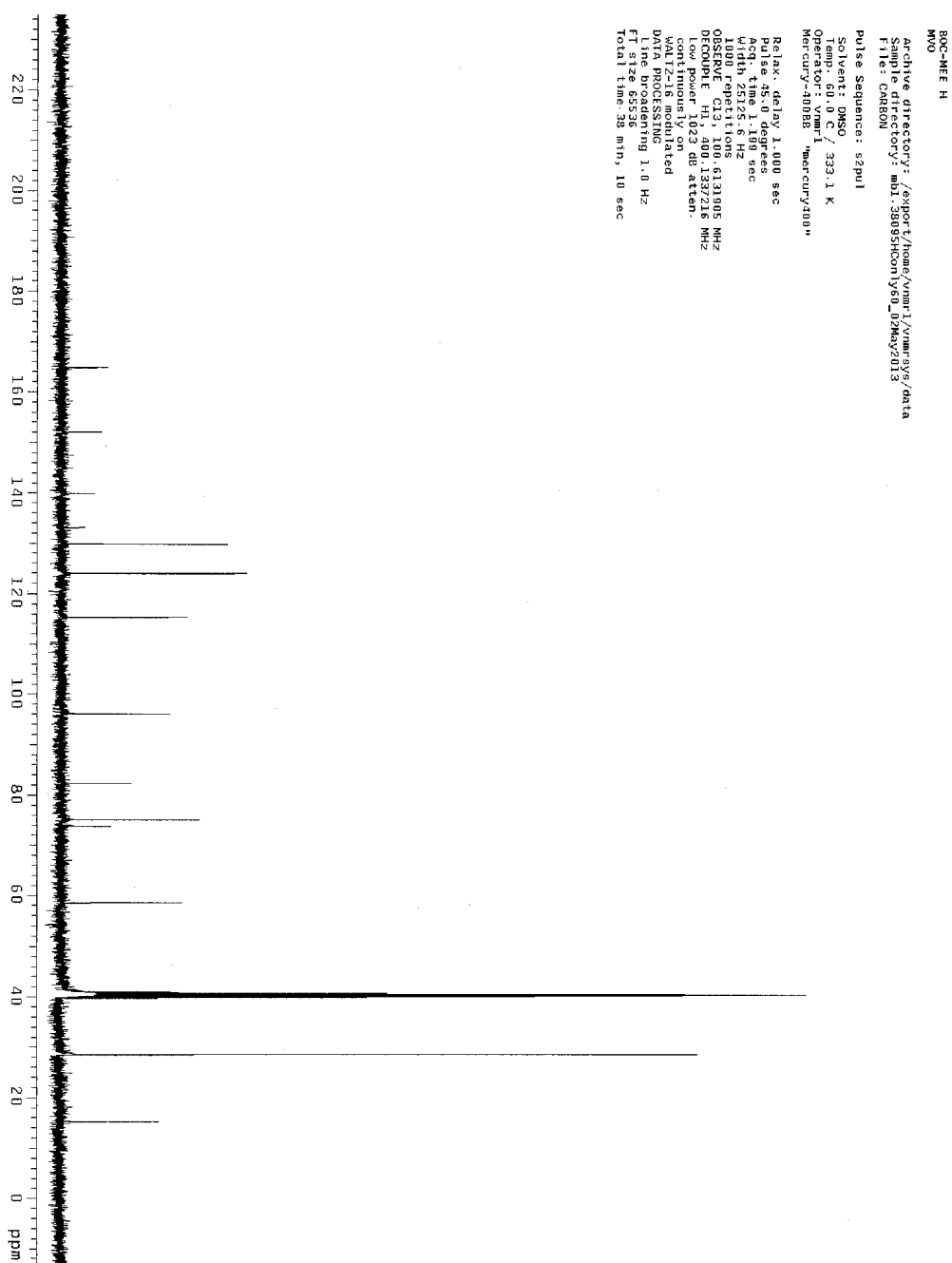
***trans*-(±)-20a**



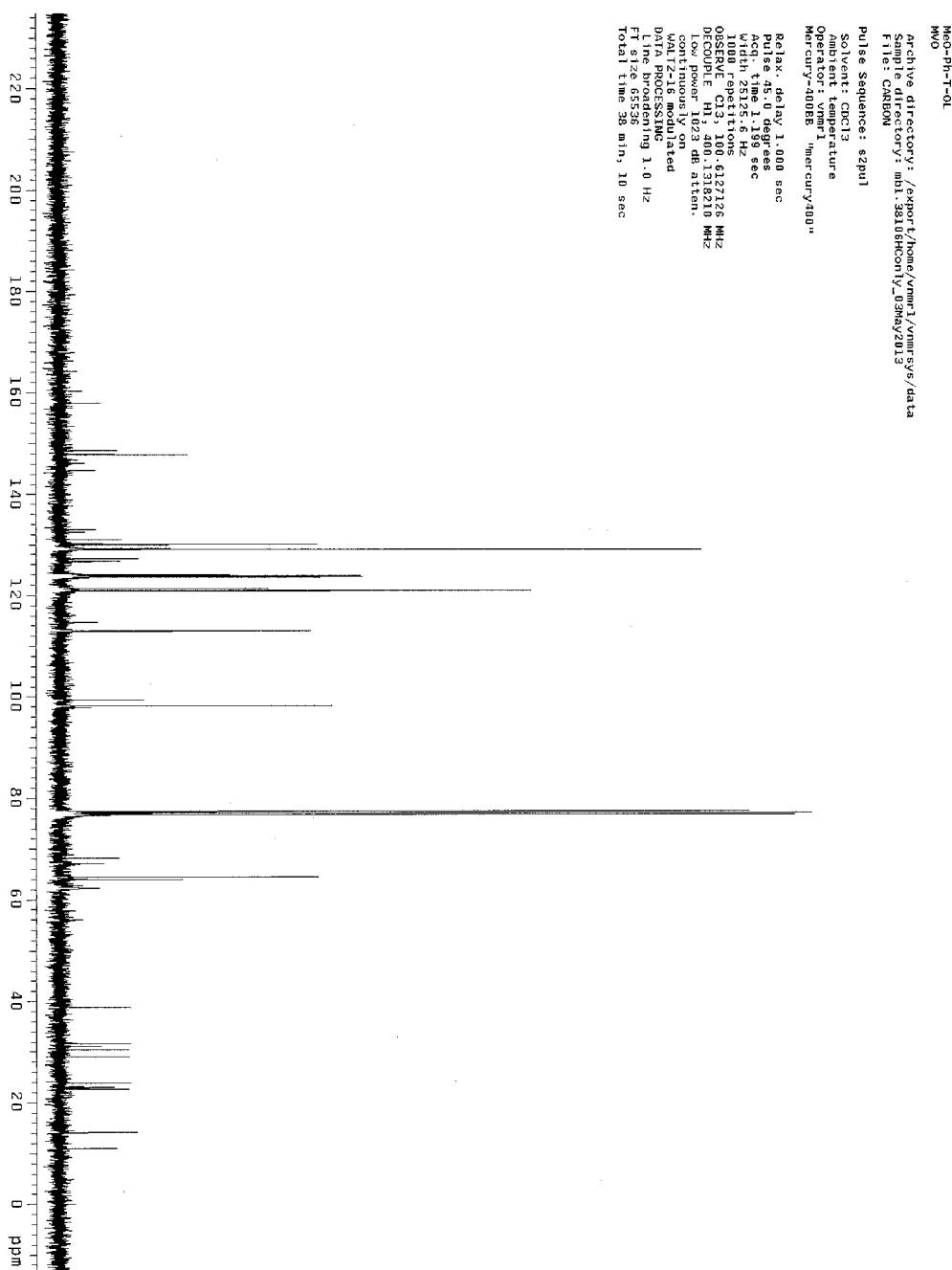
^{13}C NMR spectrum of (\pm)-20a



^{13}C NMR spectrum of (\pm)-**20b**

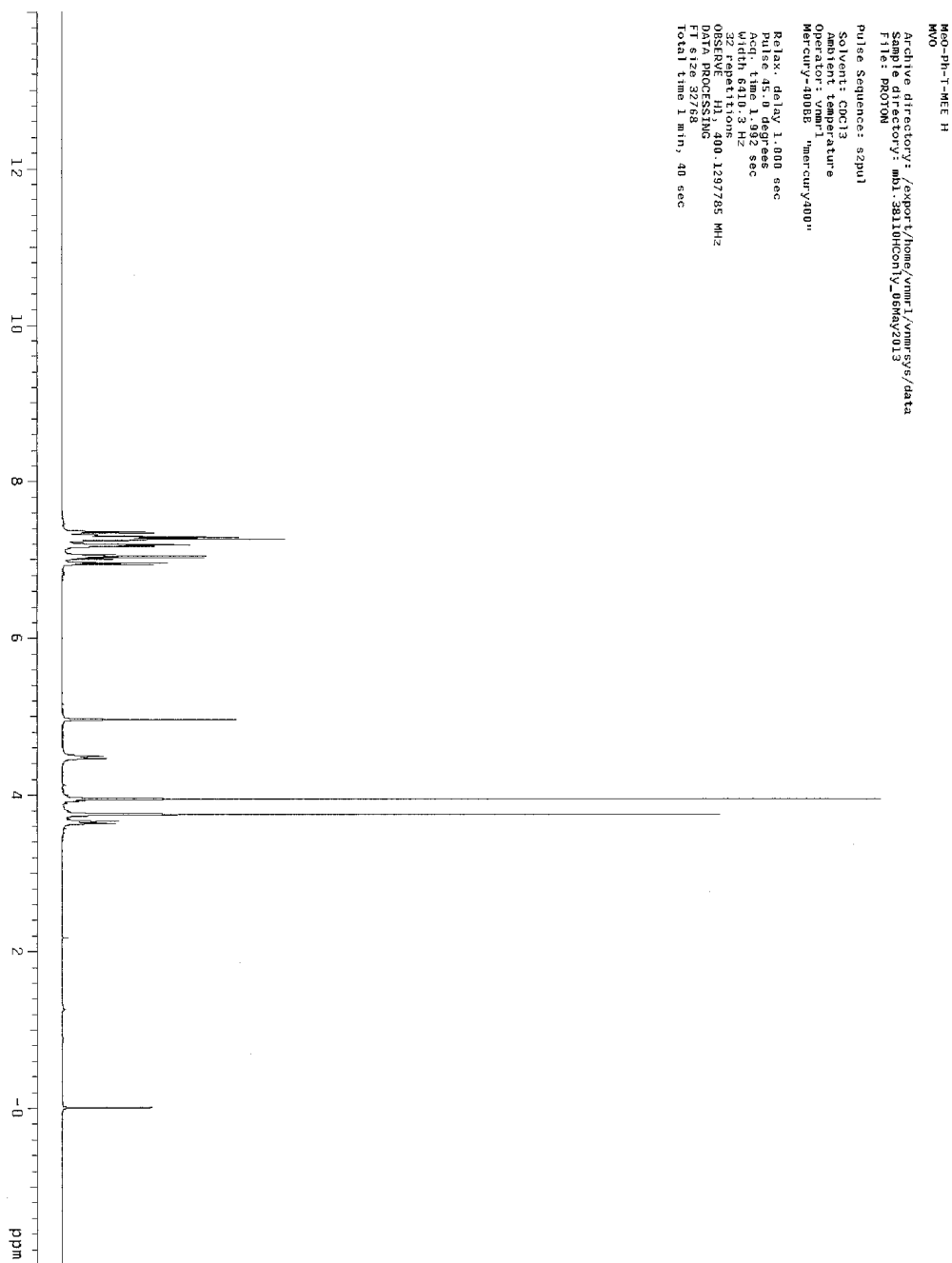
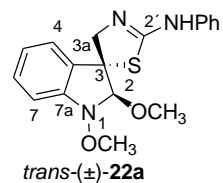


^{13}C NMR spectrum of mixture (\pm)-**21a** and (\pm)-**21b**

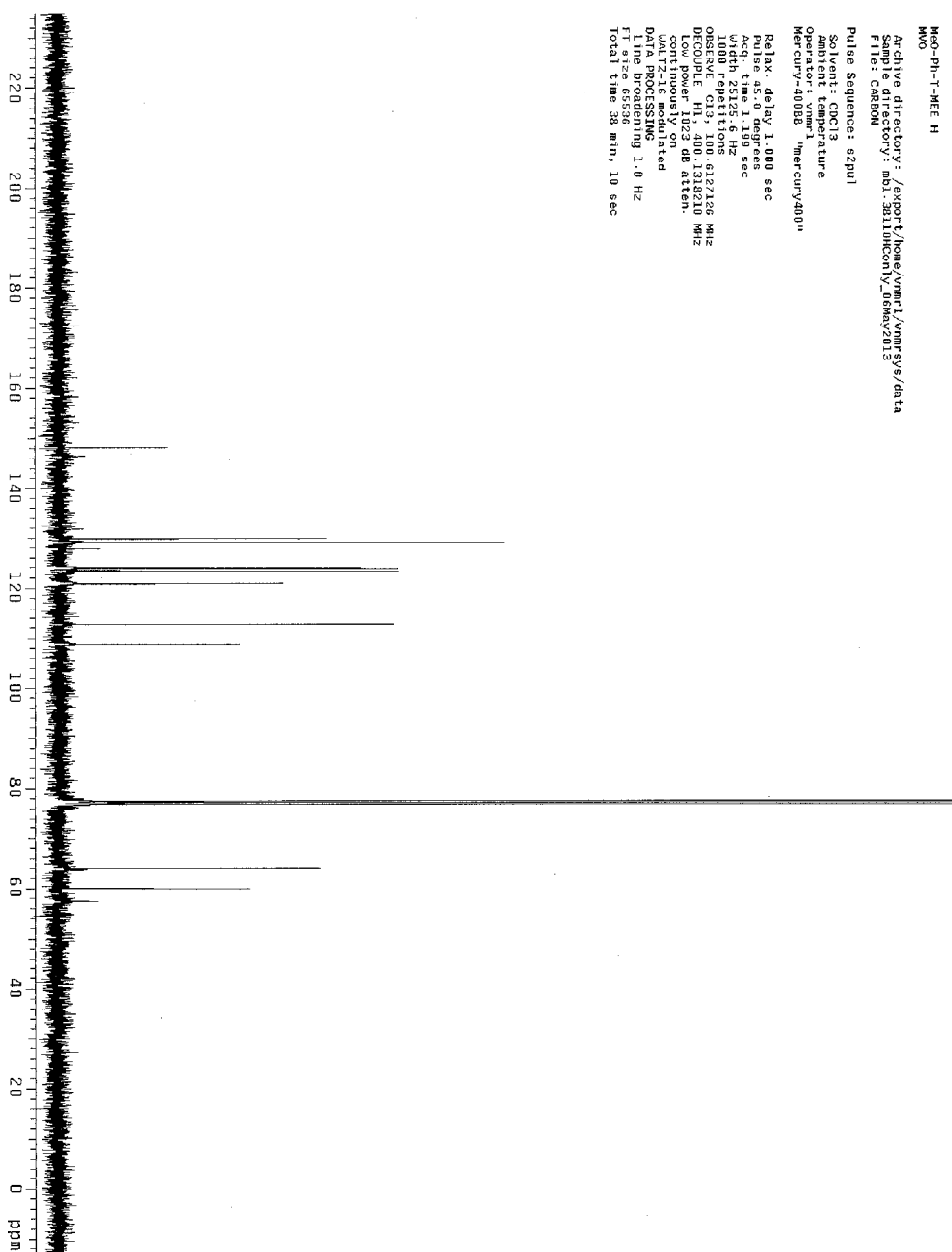


***trans* and *cis*-(±)-1-Methoxy-2-methoxy-2'-(phenylamino)spiro{indoline-3,5'-[4',5']-dihydrothiazol} [(±)-22a and (±)-22b].**

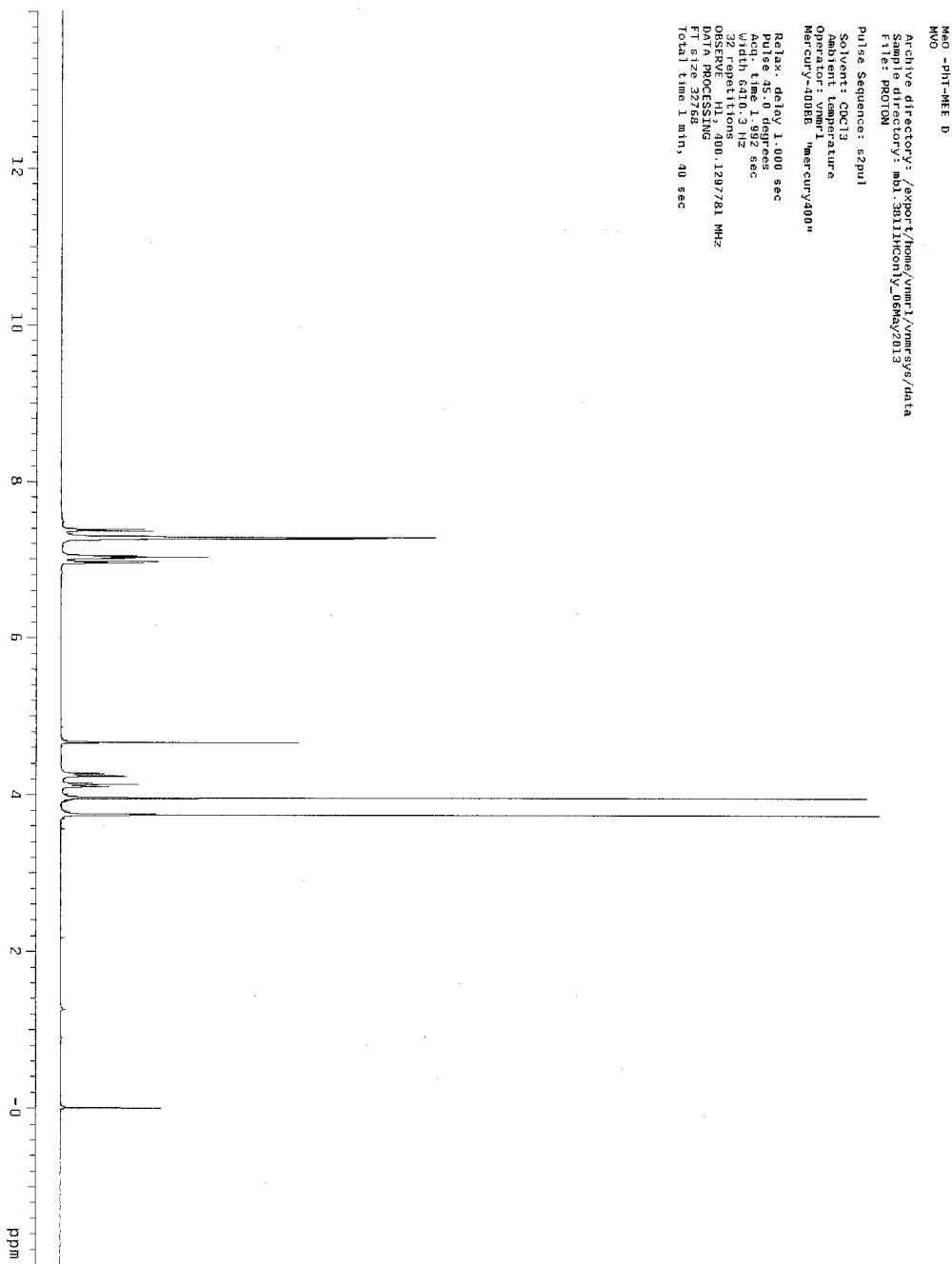
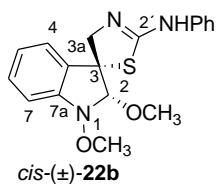
¹H NMR spectrum of (±)-22a



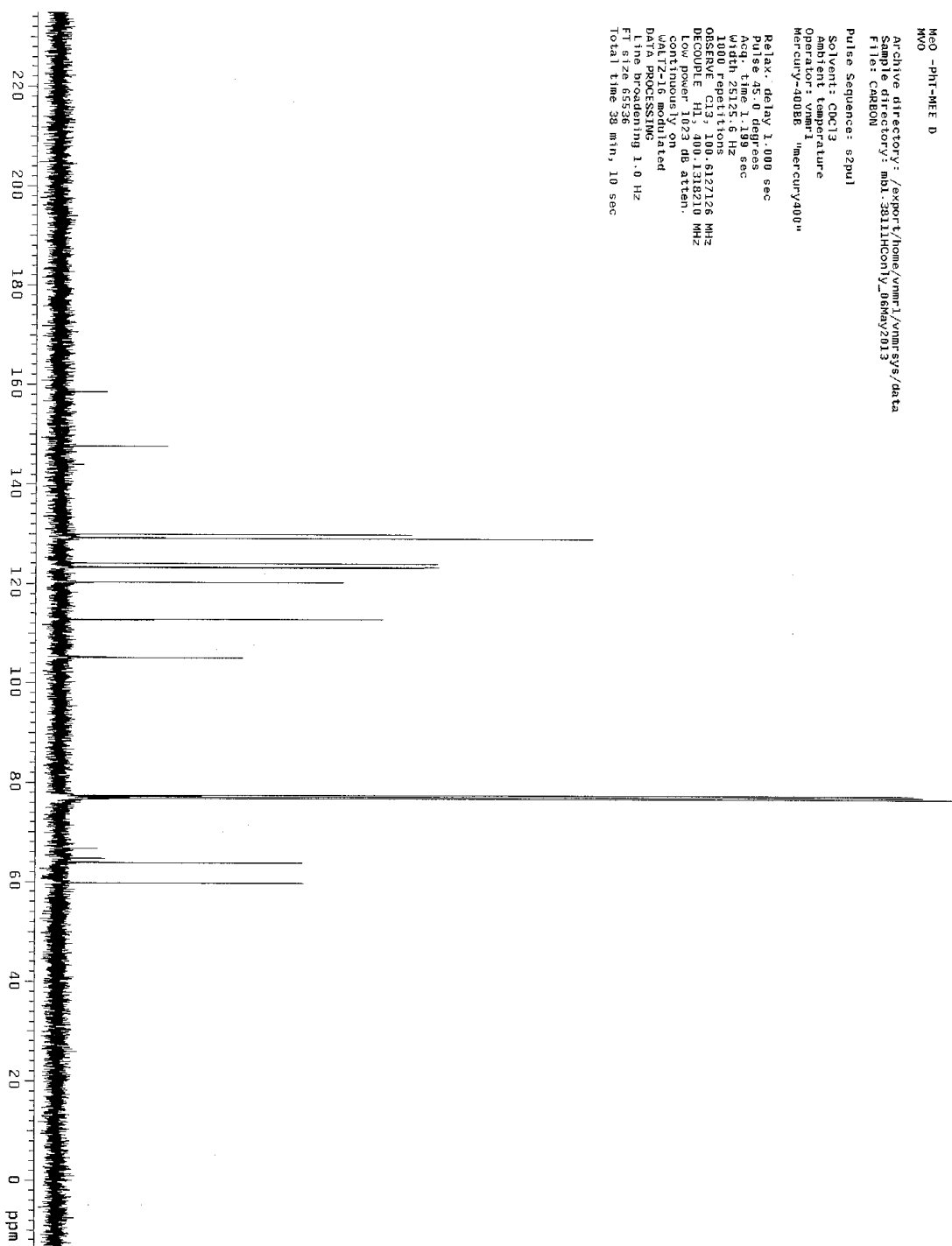
^{13}C NMR spectrum of (+)-**22a**



^1H NMR spectrum of (\pm)-**22b**

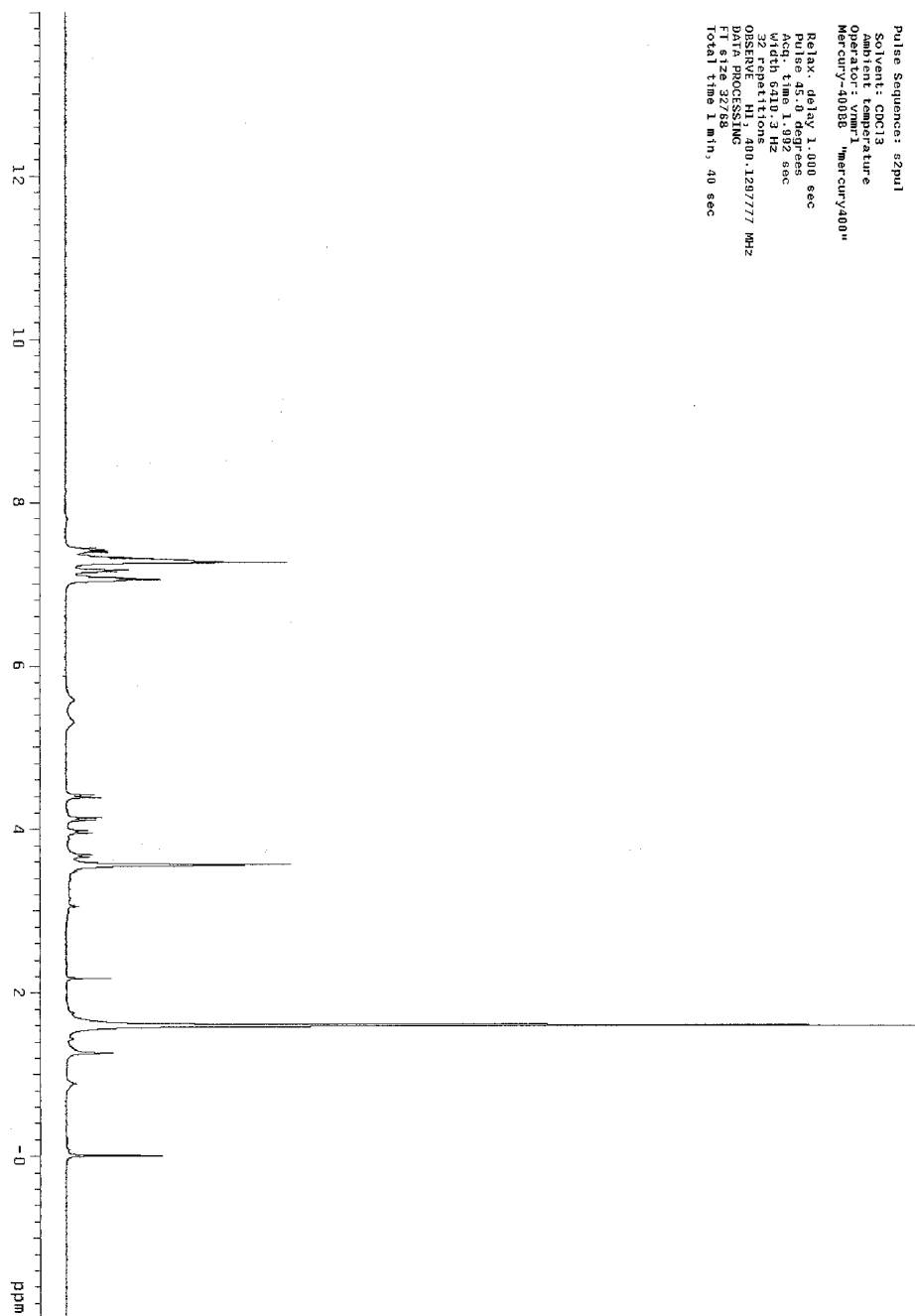
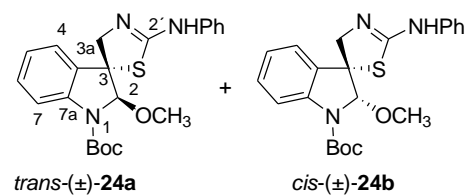


^{13}C NMR spectrum of (\pm)-22b



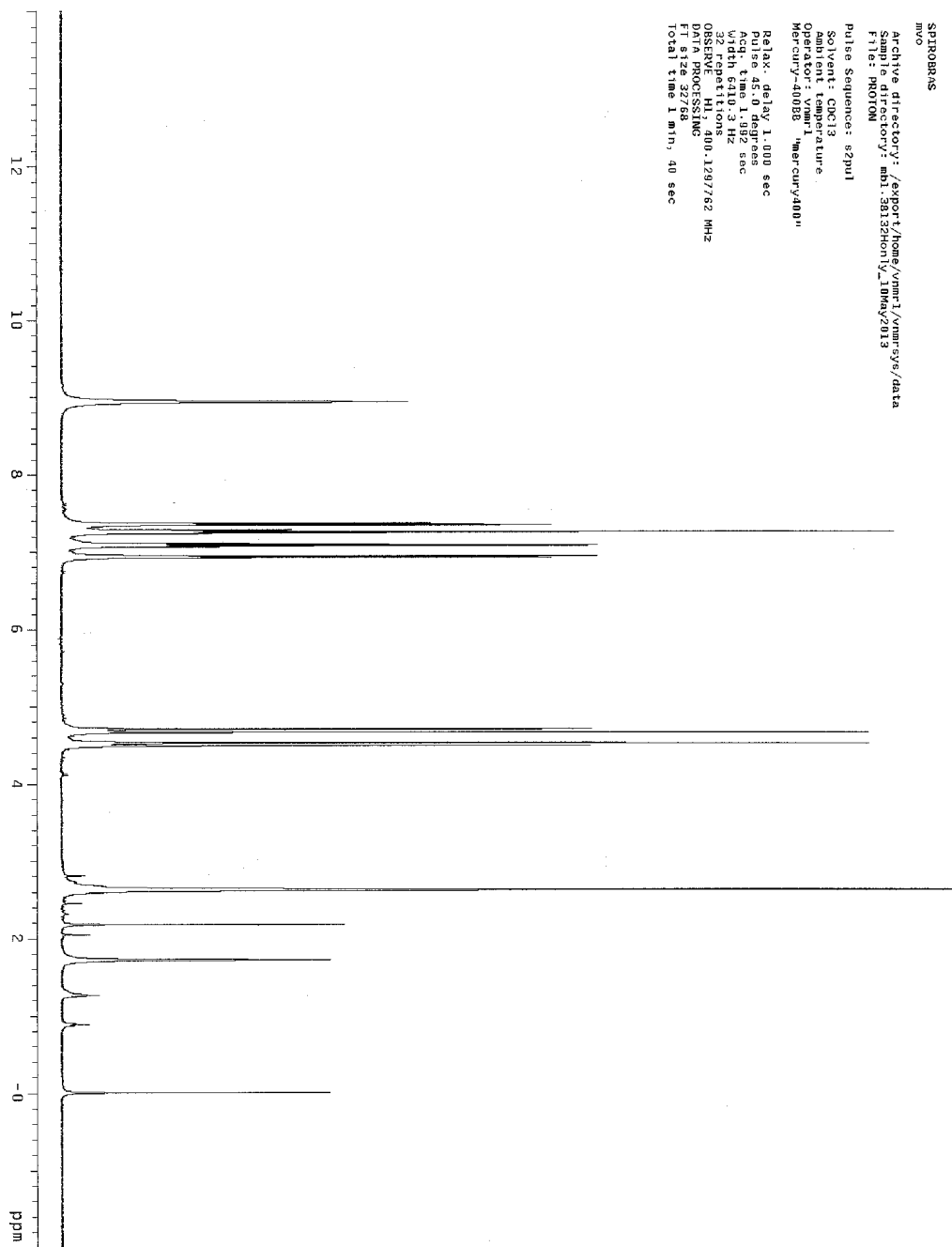
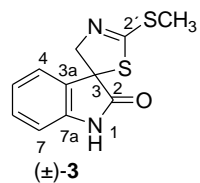
trans and *cis*-(±)-1-(*tert*-Butoxycarbonyl)-2-methoxy-2'-(phenylamino)spiro[indoline-3,5'-[4',5']-dihydrothiazol] [(±)-24a and (±)-24b].

¹H NMR spectrum of mixture (±)-24a and (±)-24b



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Ambient temperature
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(±)-Spirobrassinin [(±)-3]
¹H NMR spectrum of (±)-3



(±)-1-Methylspirobrassinin [(±)-25]
¹H NMR spectrum of (±)-25

