

Supporting Information for

Gold-catalyzed domino cycloisomerization/Pictet-Spengler reaction of 2-(4-aminobut-1-yn-1-yl)anilines with aldehydes: Synthesis of tetrahydropyrido[4,3-*b*]indole scaffolds

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1. X Ray Crystallography data

X-ray data for the compounds were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoK α radiation ($\lambda=0.71073\text{\AA}$) with ω -scan method [1]. Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 7382 reflections in the range of $2.44 < \theta < 26.79^\circ$ for AN72.

Integration and scaling of intensity data were accomplished using SAINT program.^[1] The structure was solved by direct methods using SHELXS97^[2] and refinement was carried out by full-matrix least-squares technique using SHELXL97.^[2] Anisotropic displacement parameters were included for all non-hydrogen atoms. The hydrogen atoms attached to nitrogen atoms were located in a difference density map and refined isotropically. All other H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H or $1.2U_{\text{eq}}(\text{C})$ for other H atoms]. The methyl groups were allowed to rotate but not to tip.

Crystal data for AN72: $\text{C}_{24}\text{H}_{21}\text{FN}_2\text{O}_2\text{S}$, $M = 420.49$, colorless block, $0.18 \times 0.16 \times 0.13 \text{ mm}^3$, monoclinic, space group $P2_1/n$ (No. 14), $a = 15.906(4)$, $b = 14.318(3)$, $c = 18.234(4) \text{ \AA}$, $\beta = 97.792(4)^\circ$, $V = 4114.1(16) \text{ \AA}^3$, $Z = 8$, $D_c = 1.358 \text{ g/cm}^3$, $F_{000} = 1760$, CCD Area Detector, MoK α radiation, $\lambda = 0.71073 \text{ \AA}$, $T = 294(2)\text{K}$, $2\theta_{\text{max}} = 50.0^\circ$, 38686 reflections collected, 7245 unique ($R_{\text{int}} = 0.0313$). Final $\text{Goof} = 1.063$, $R1 = 0.0395$, $wR2 = 0.1003$, R indices based on 5440 reflections with $I > 2\sigma(I)$ (refinement on F^2), 550 parameters, 0 restraints, $\mu = 0.190 \text{ mm}^{-1}$.

CCDC 900791 contains supplementary Crystallographic data for the structure **3g**.

Figure Caption: A view of AN72, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

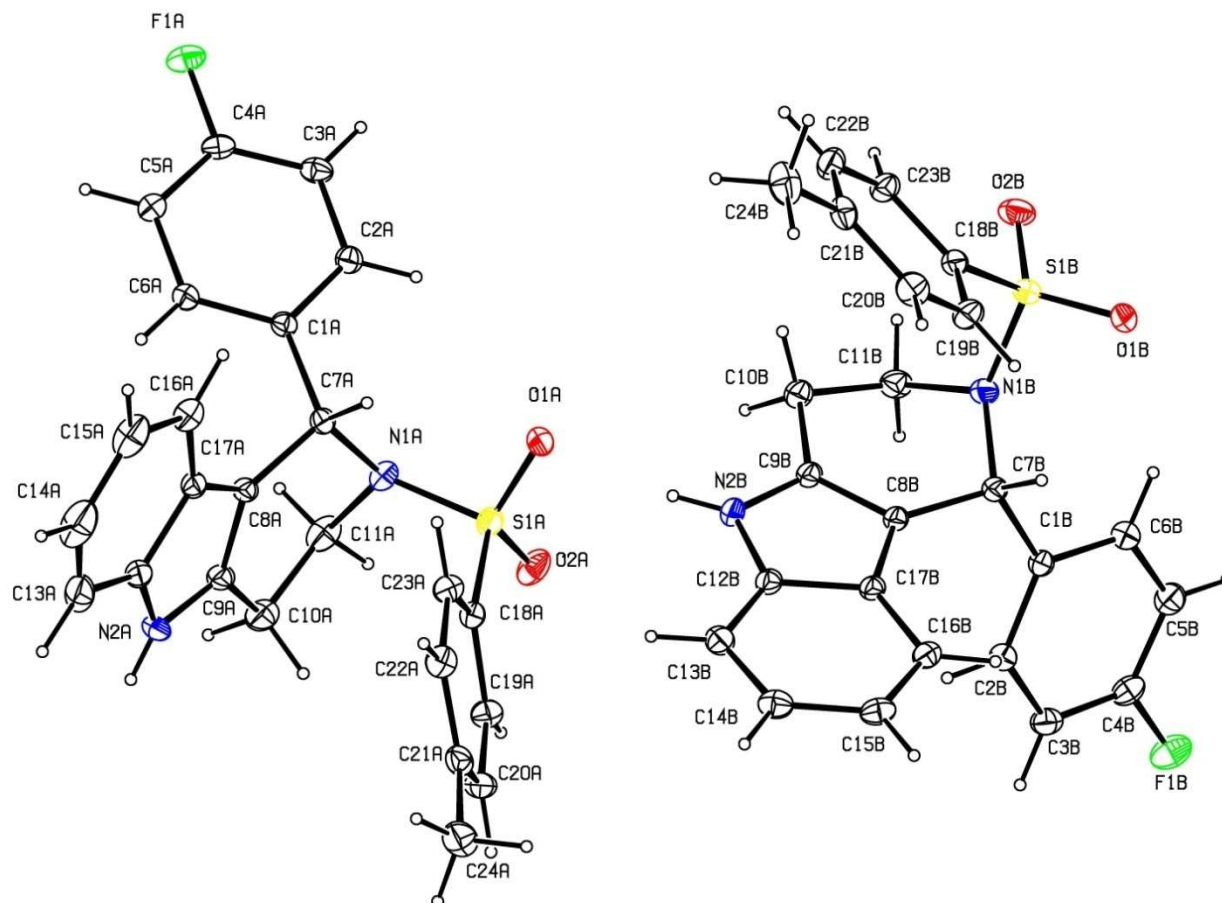


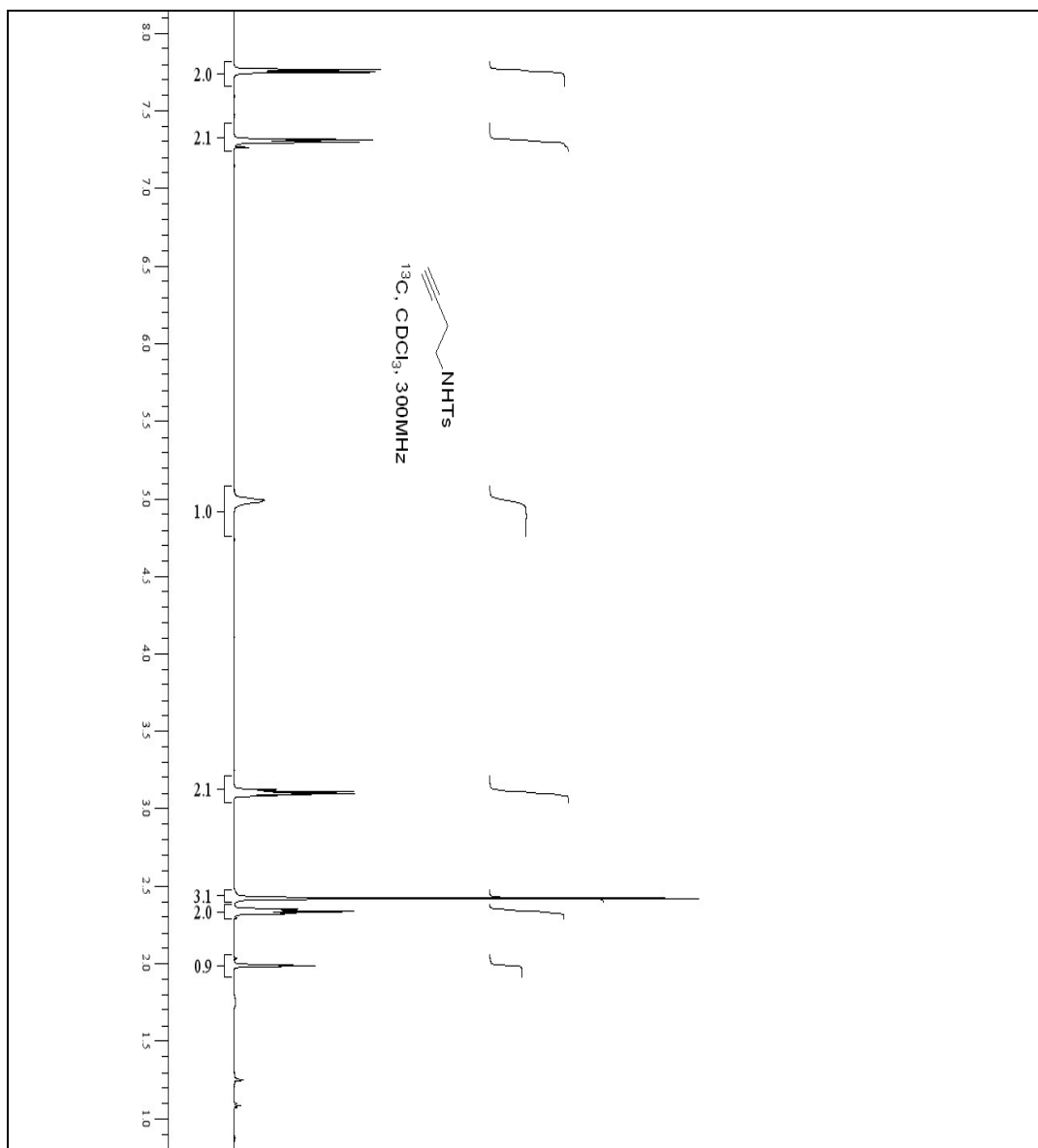
Figure 1: ORTEP diagram of product **3g** (Table 2, Entry **g**)

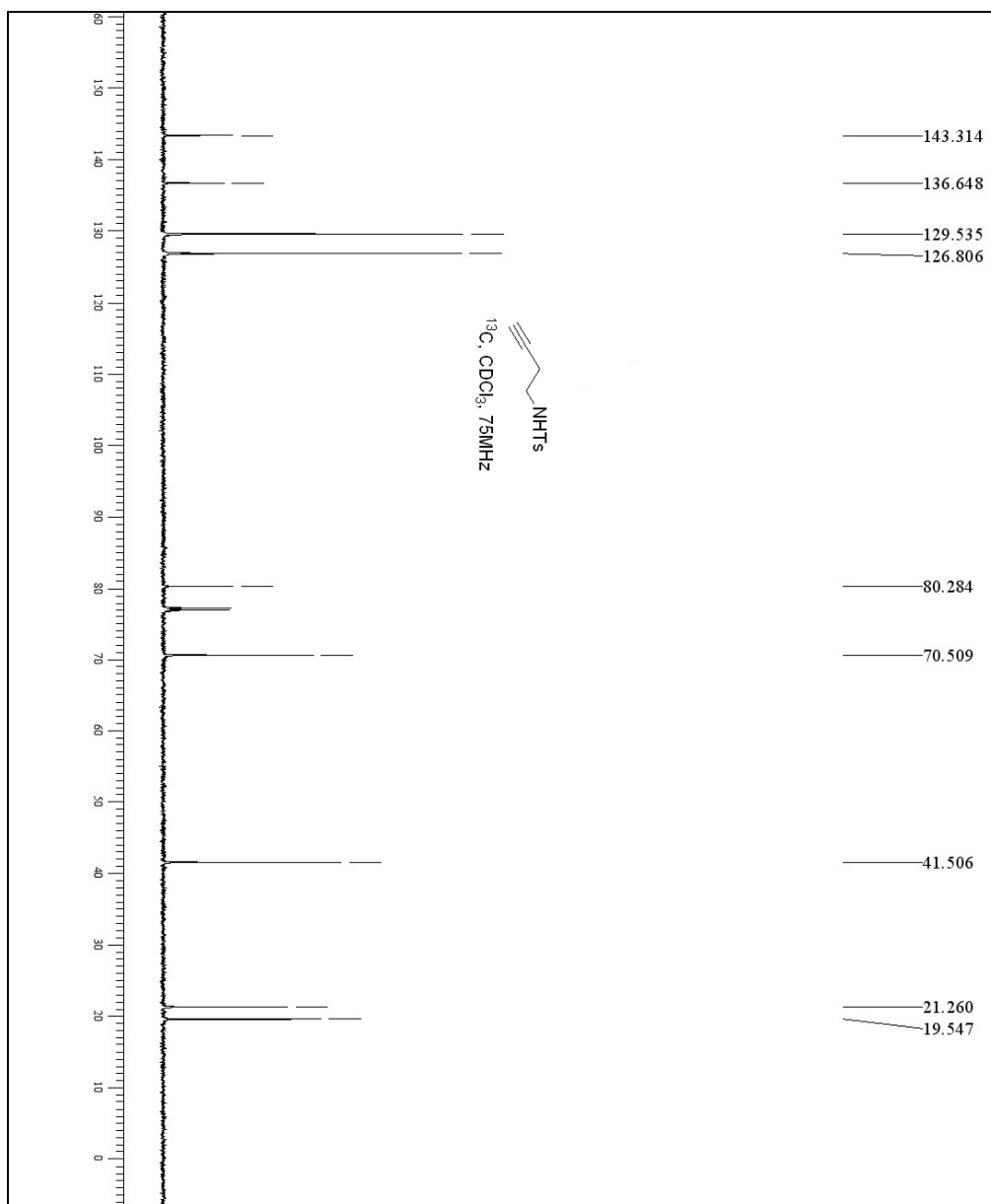
References:

1. Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick, G. M. *Acta Crystallogr* **2008**, *A64*, 112-122.

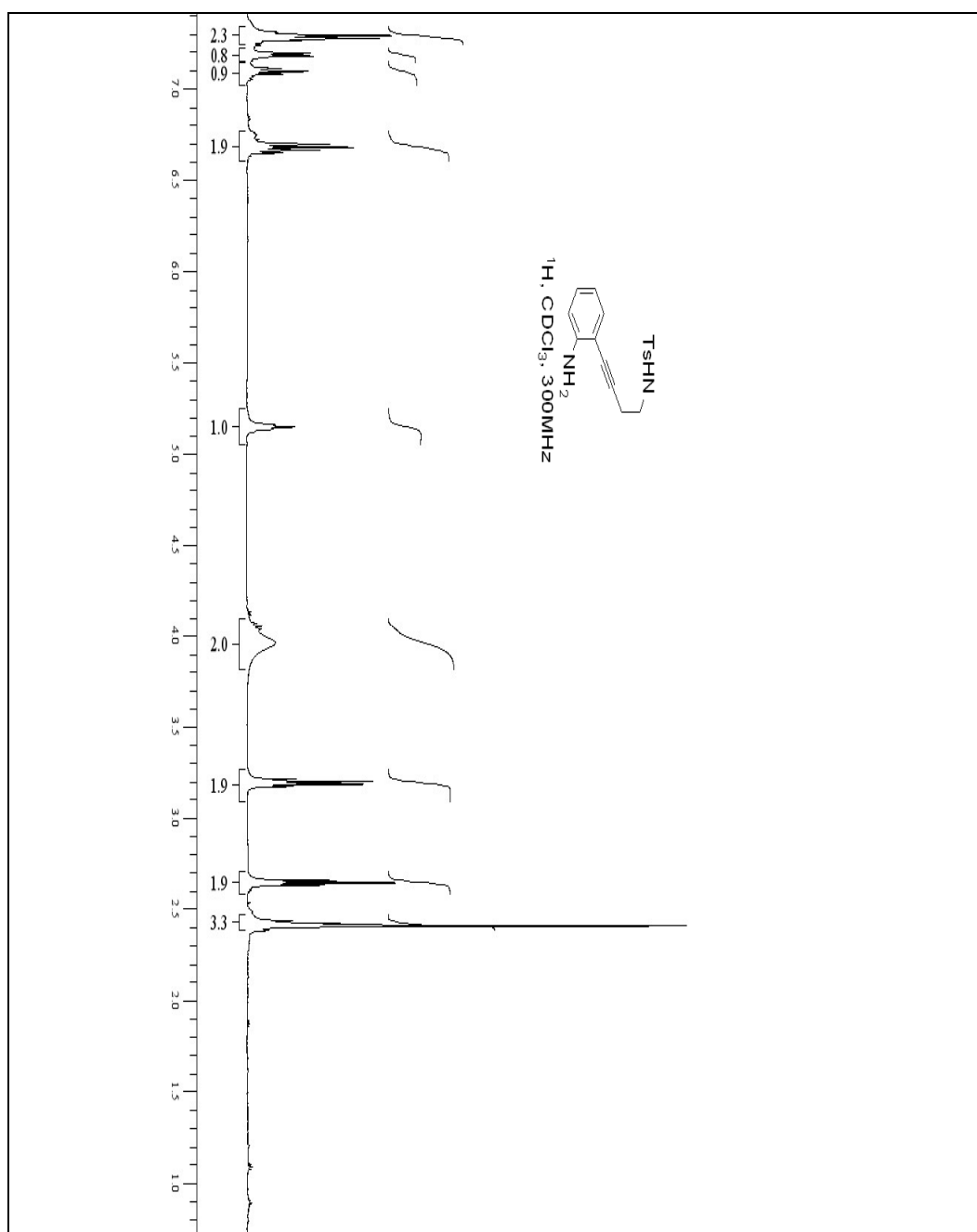
3. Copies of ^1H and ^{13}C NMR spectra of starting materials:

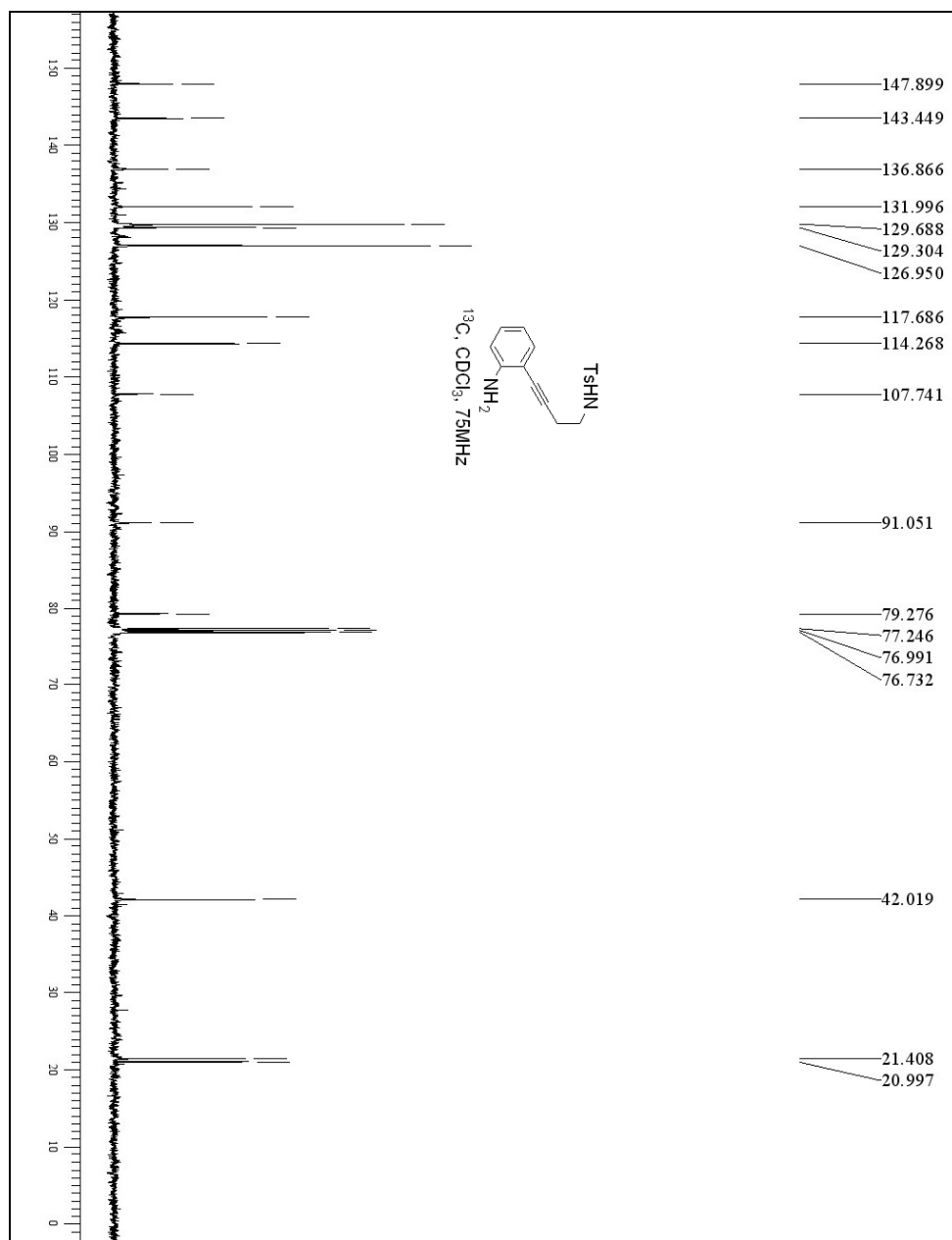
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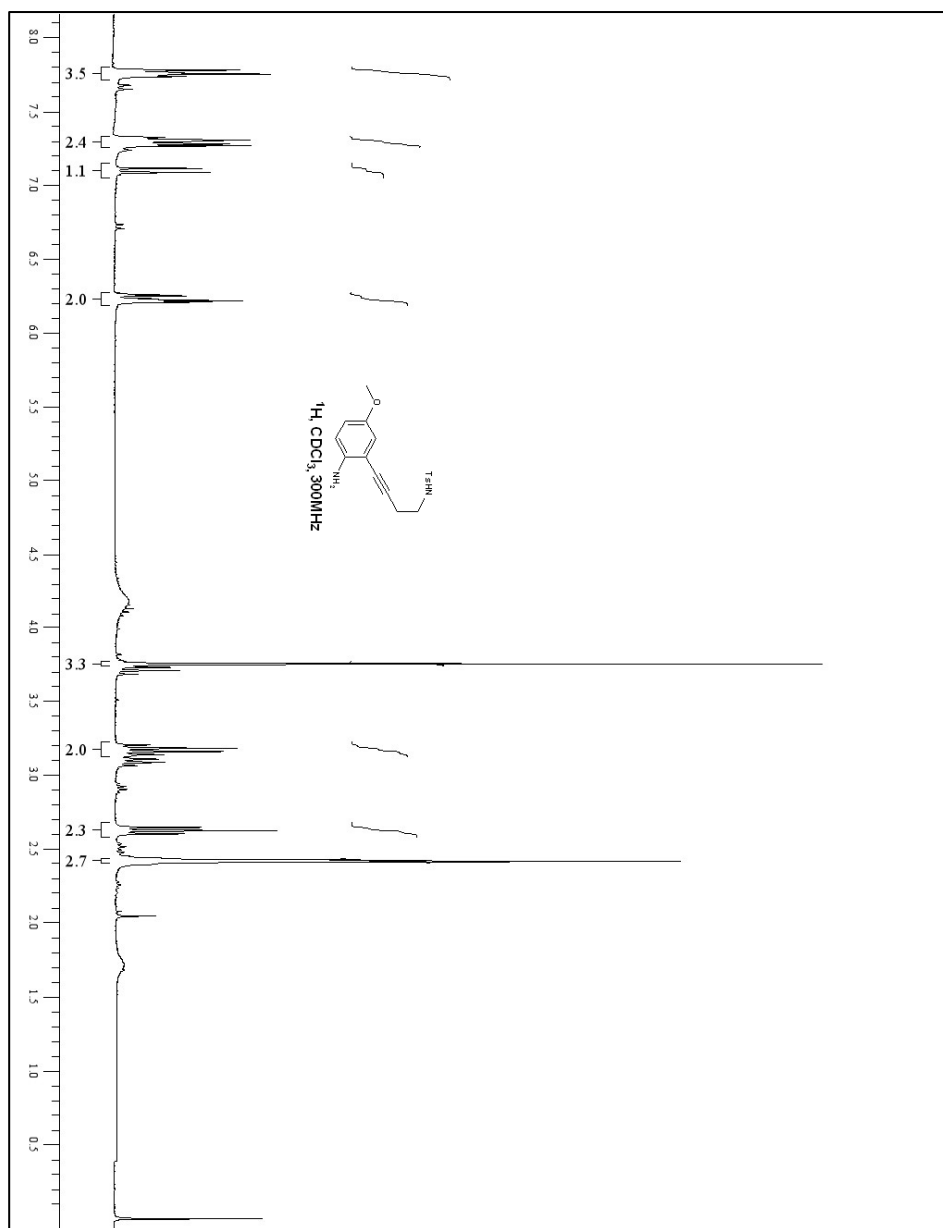


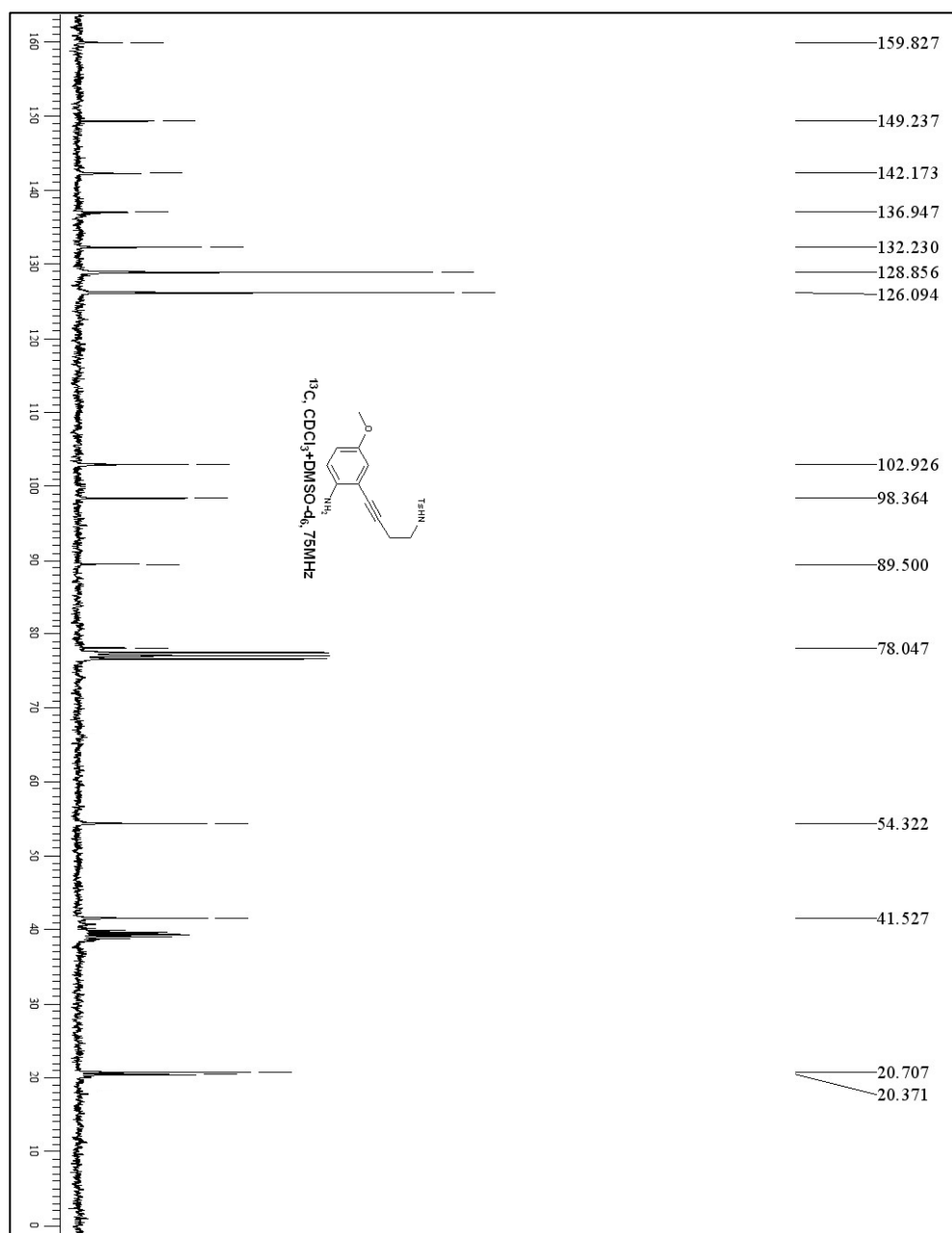
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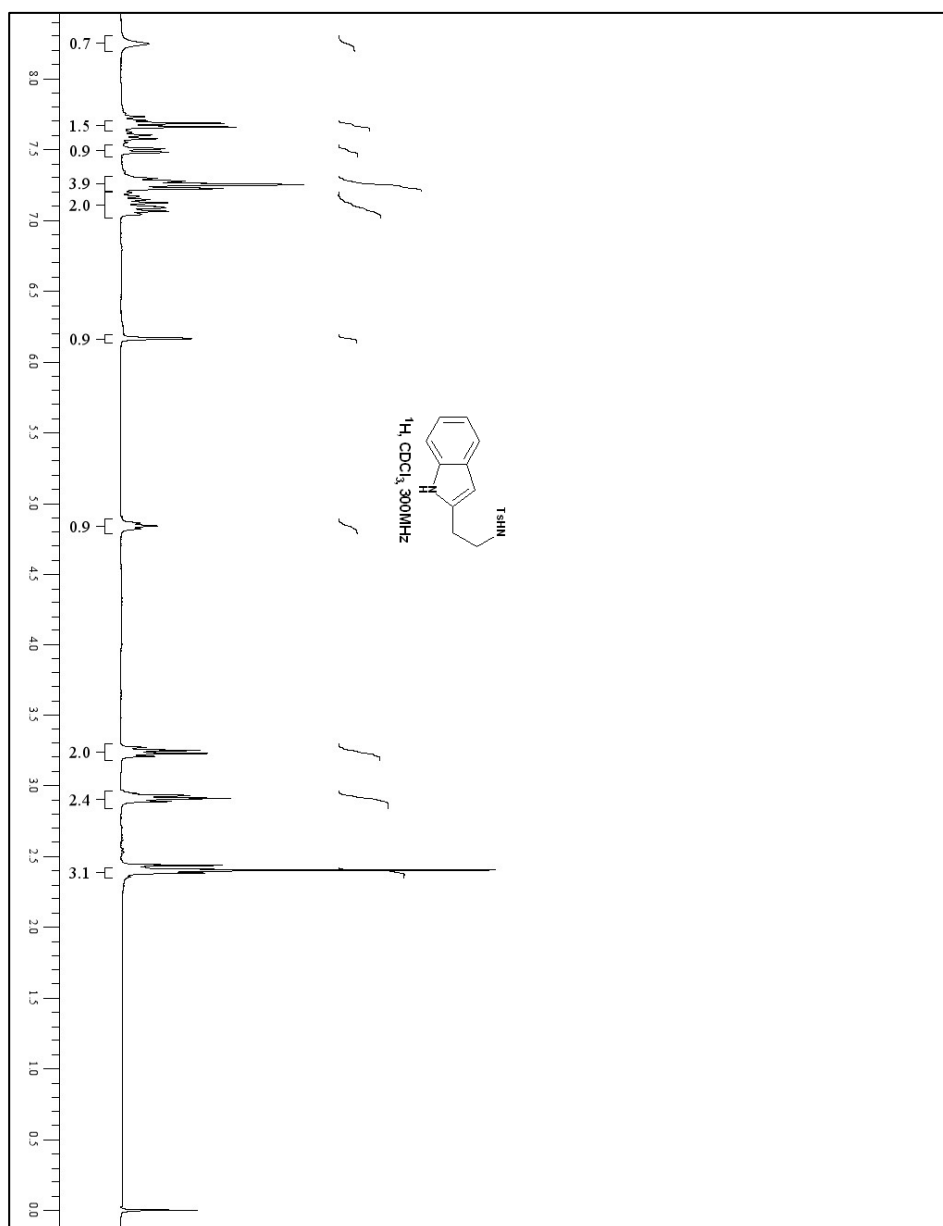


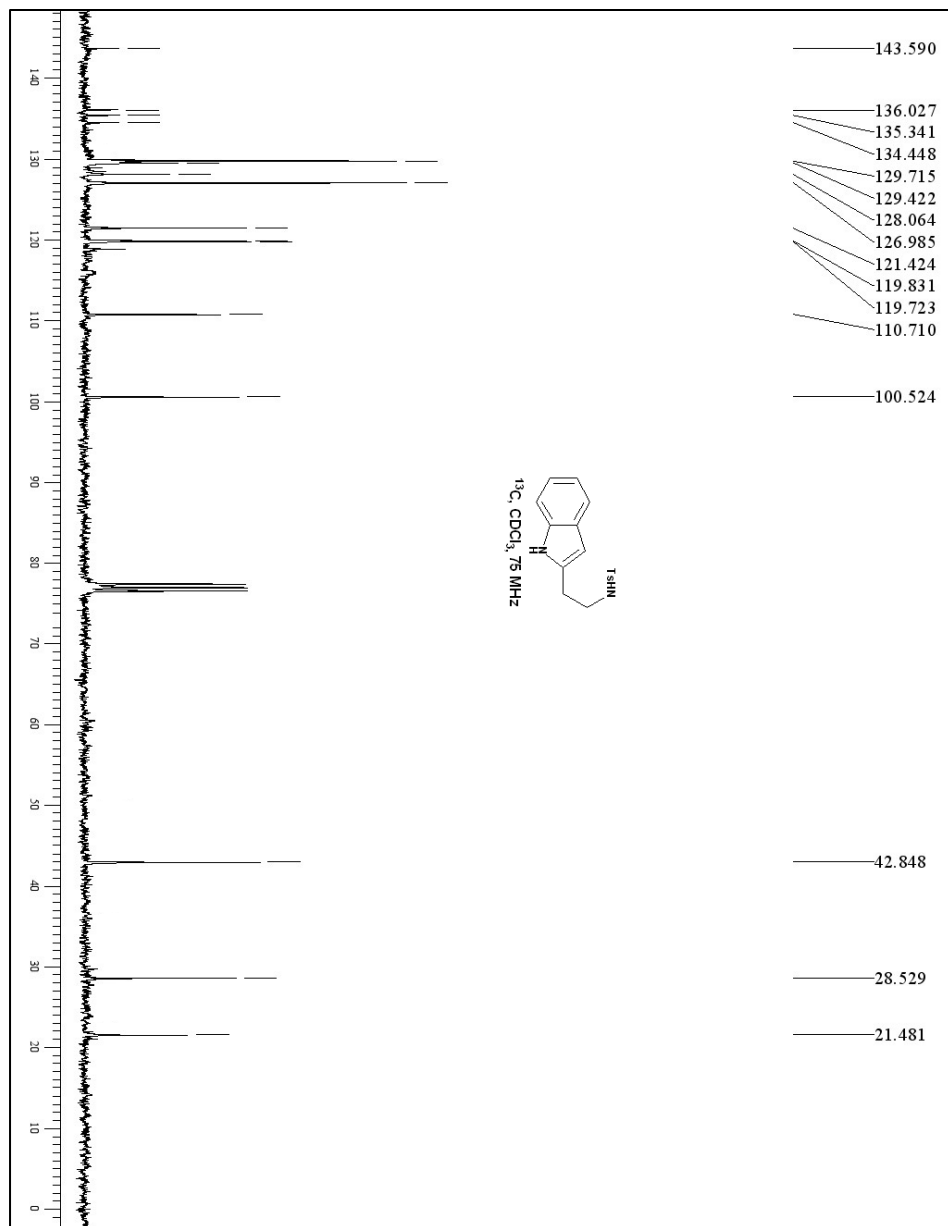
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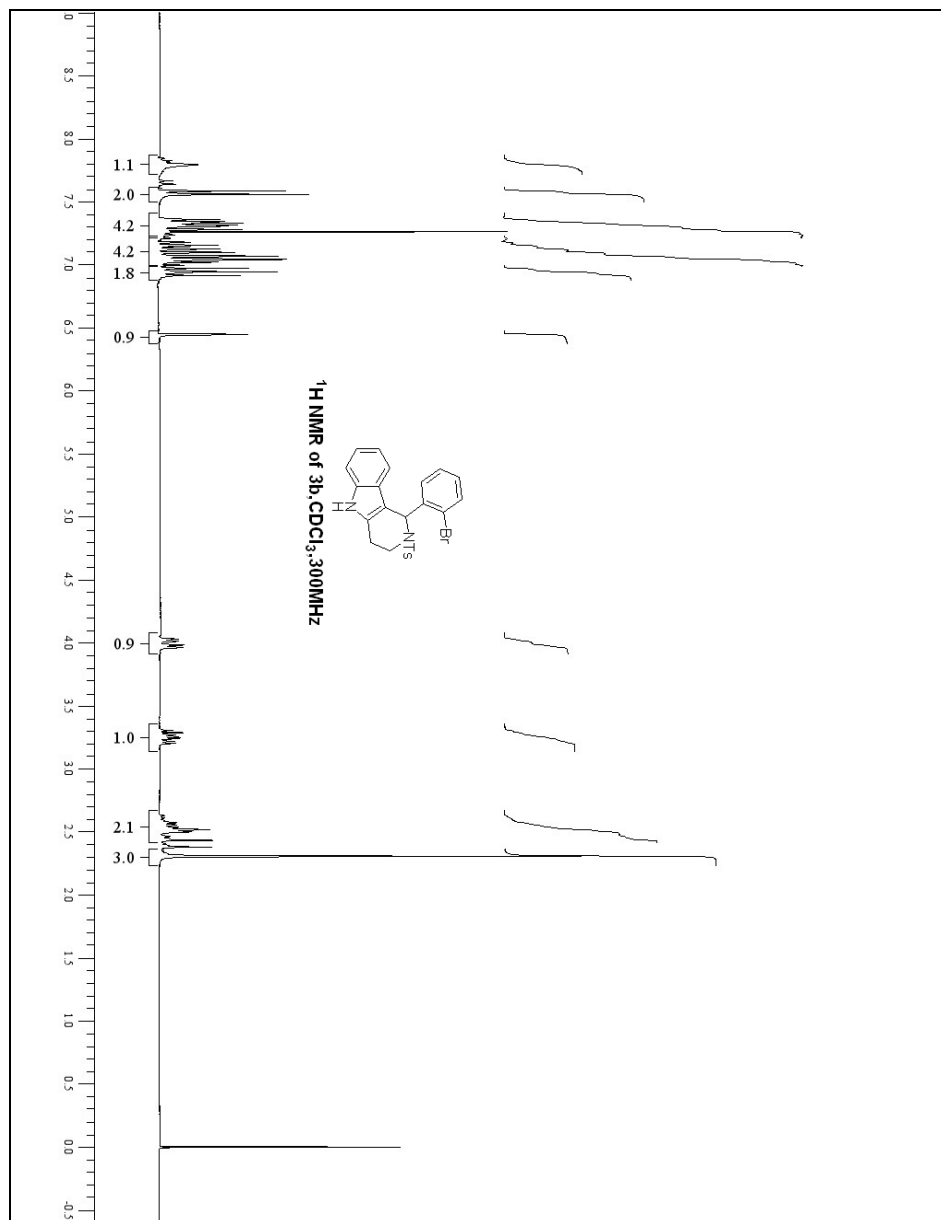


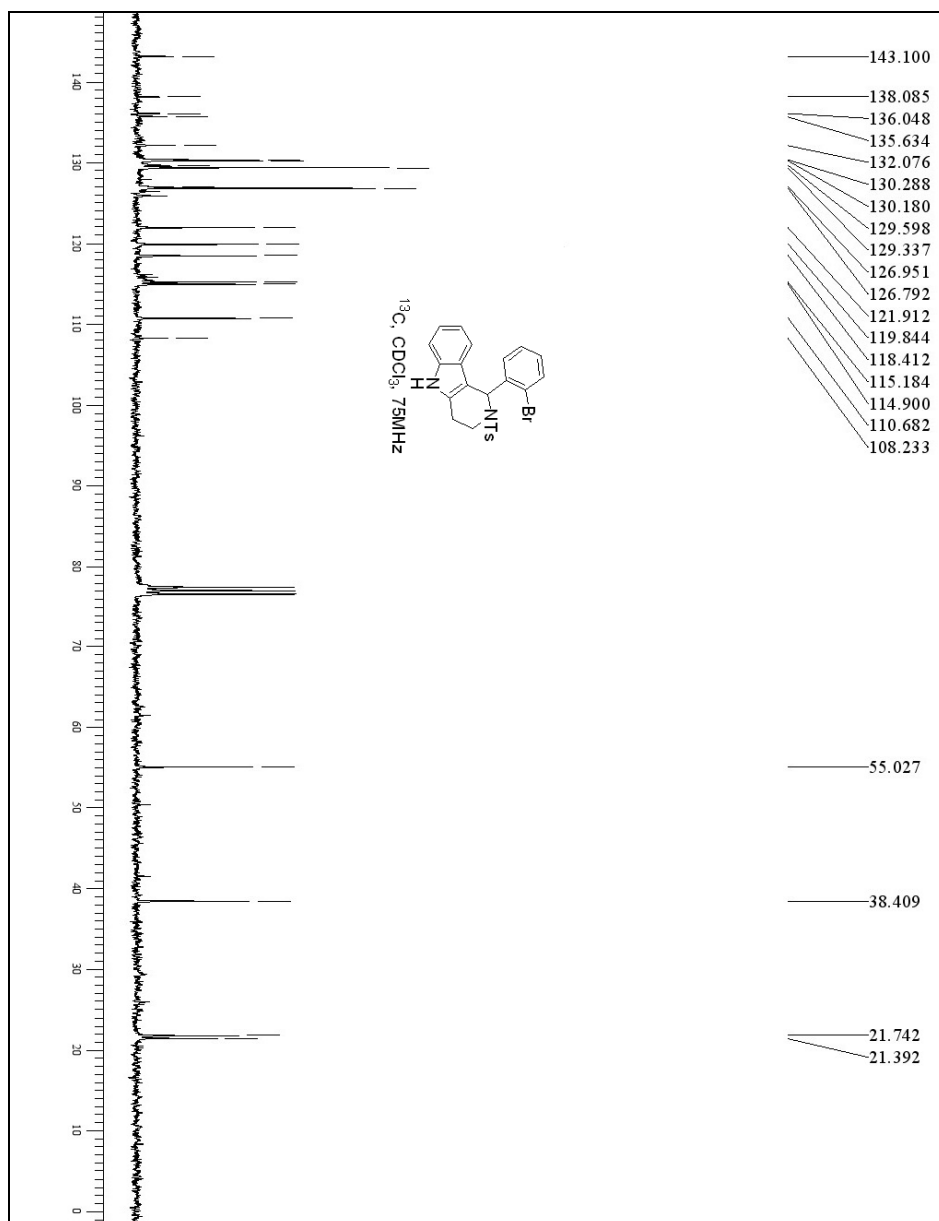
***N*-(2-(1H-indol-2-yl)ethyl)-4-methylbenzenesulfonamide (1c):**



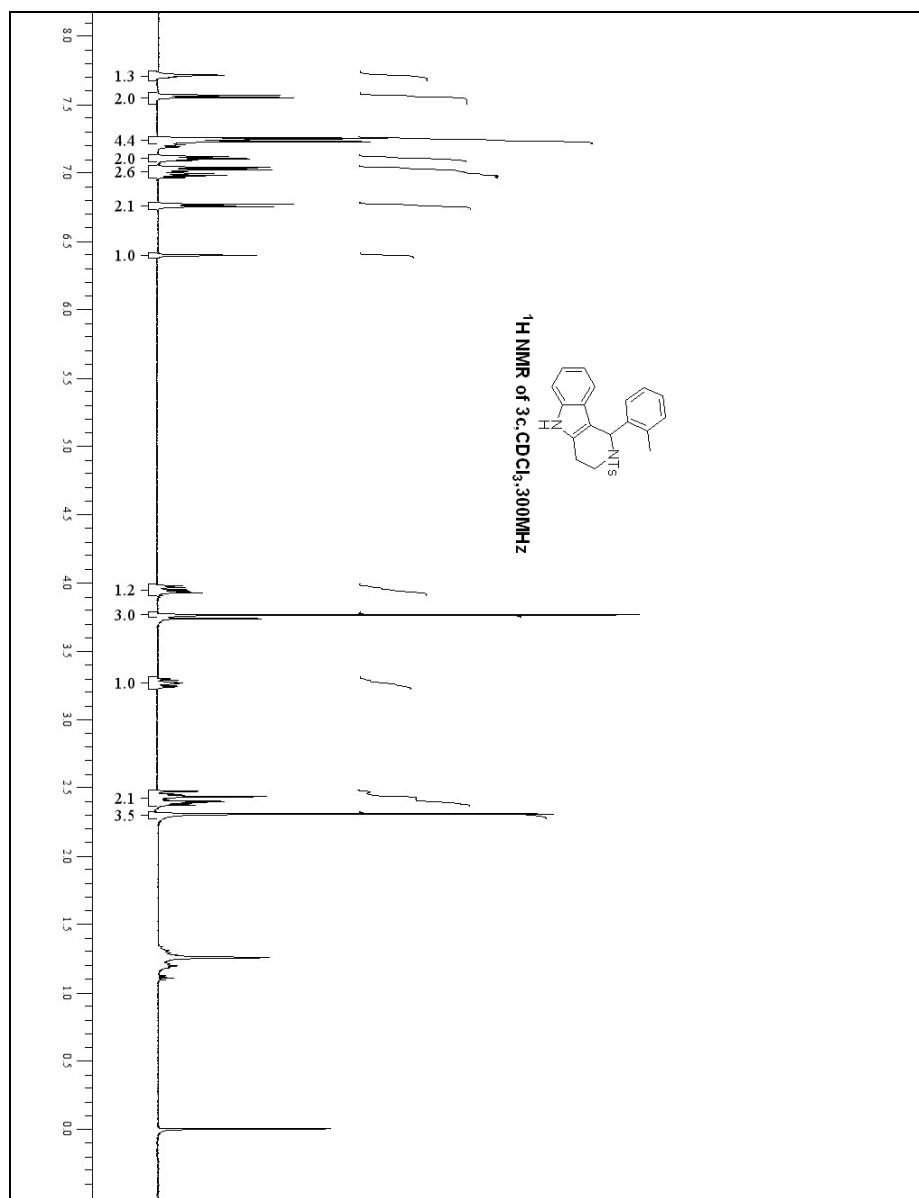


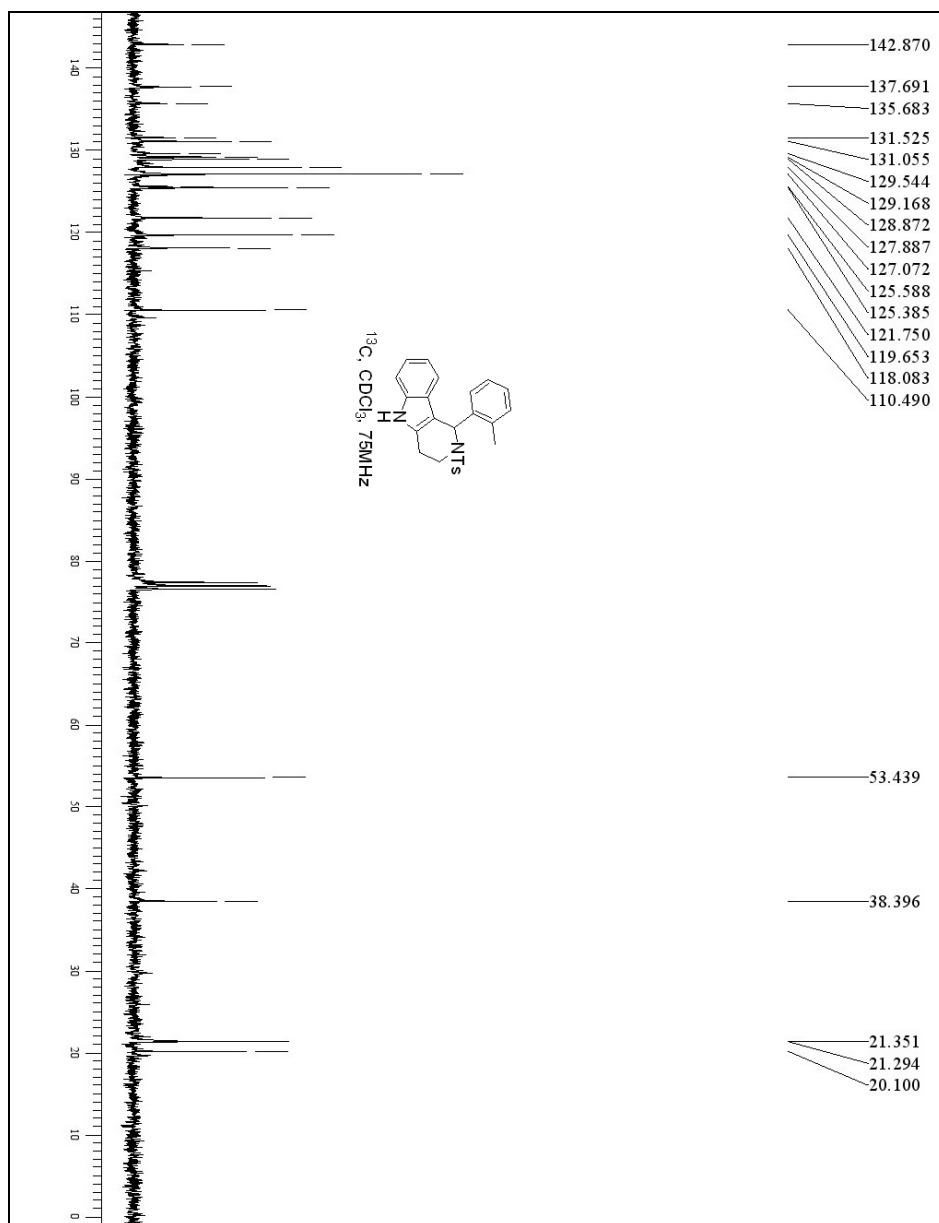
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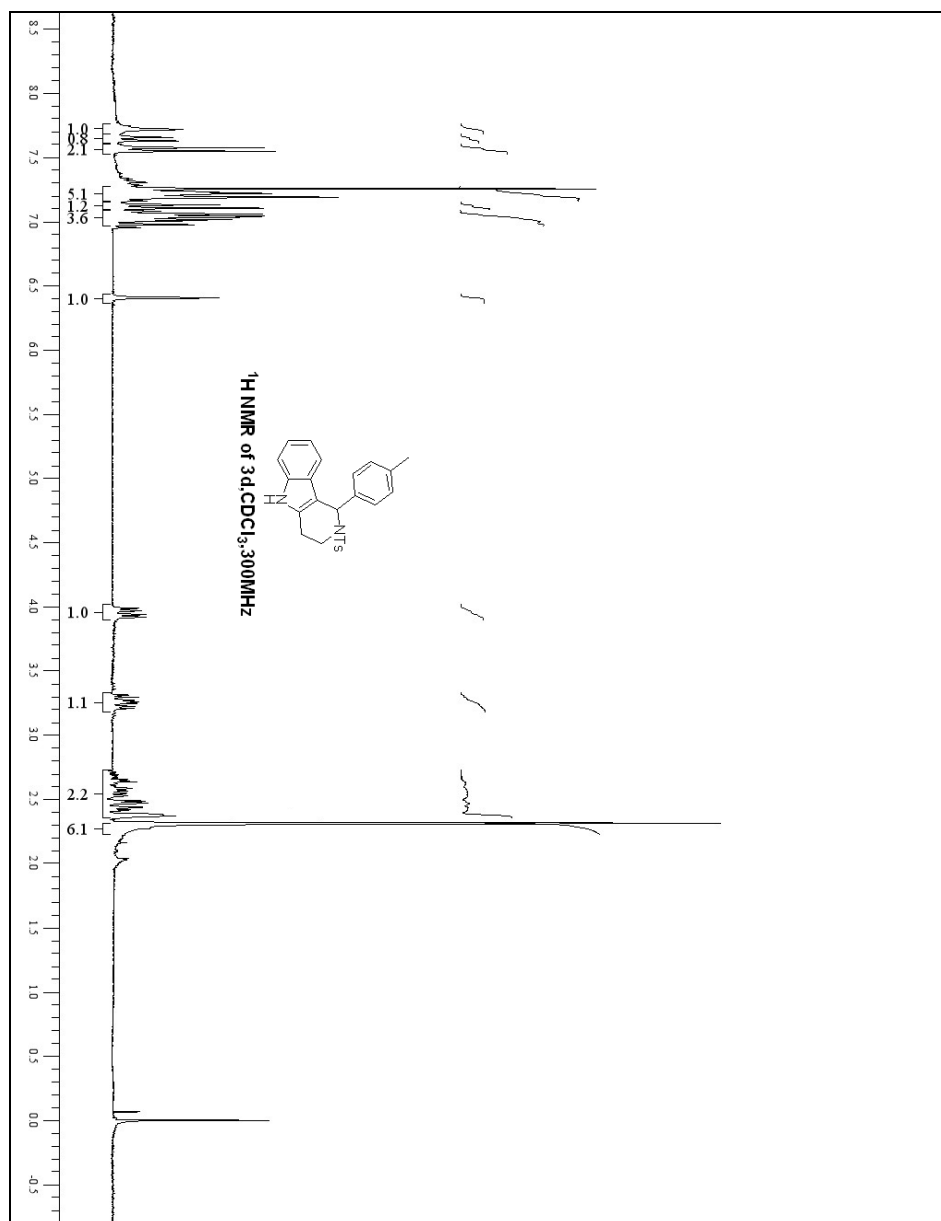


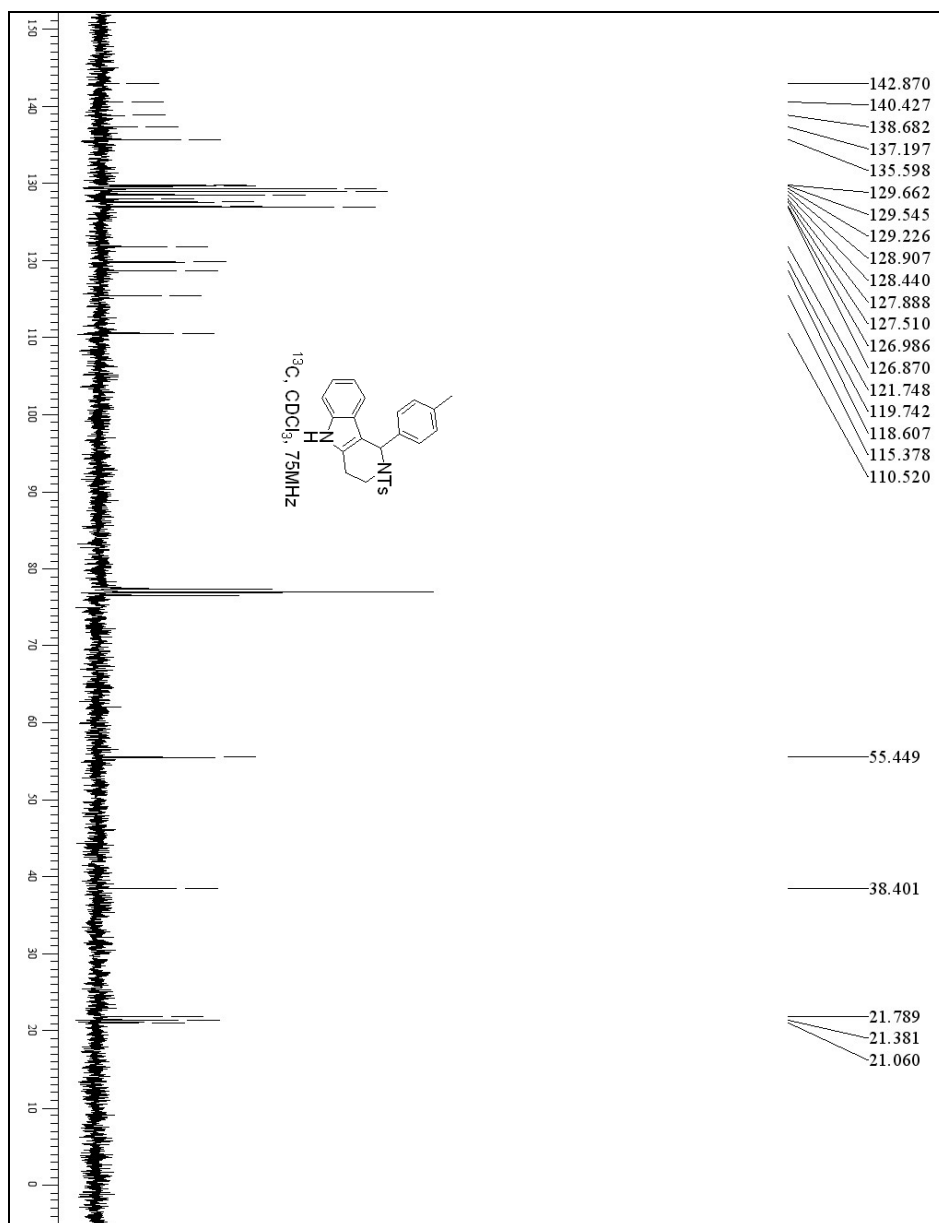
1-(*o*-Tolyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3c; Table 2; Entry c)



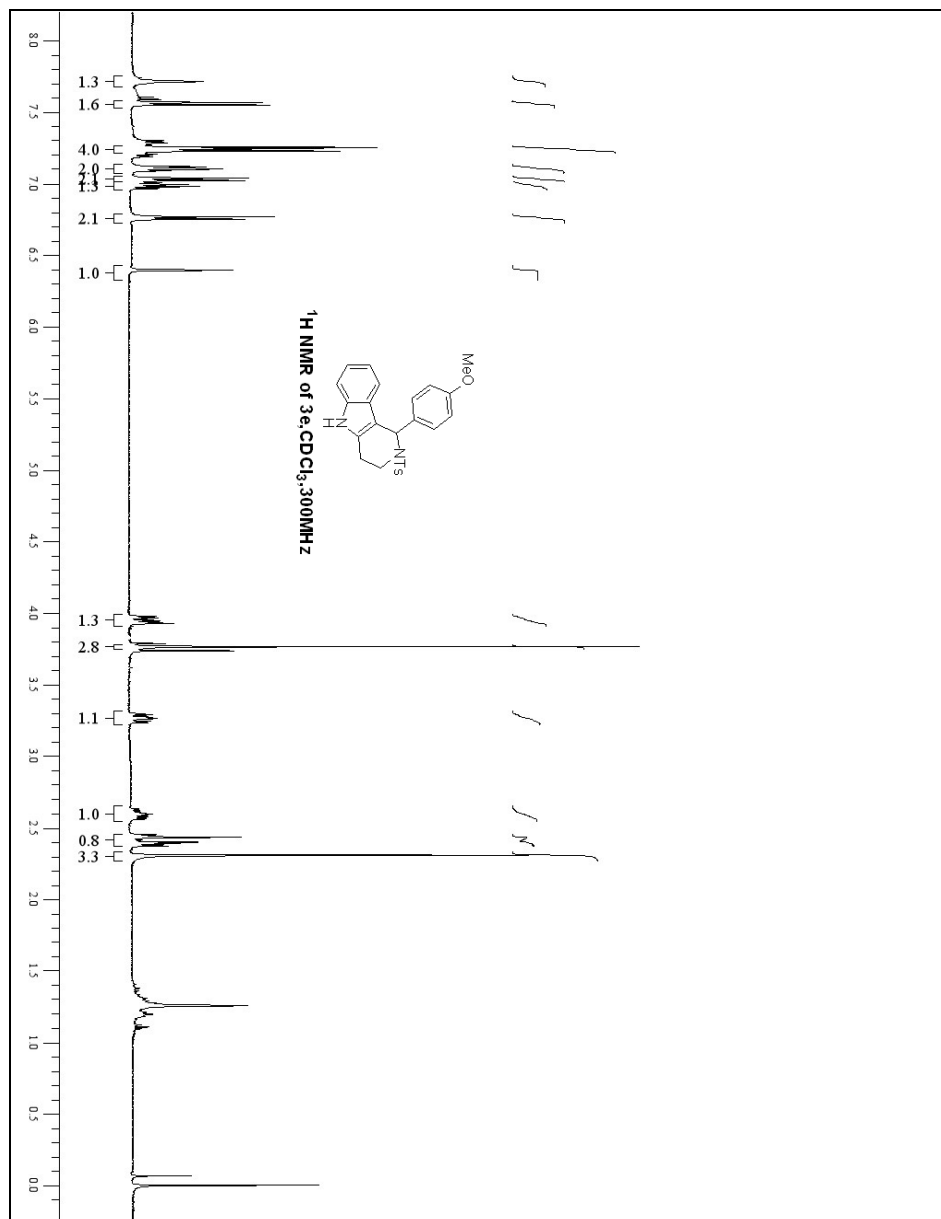


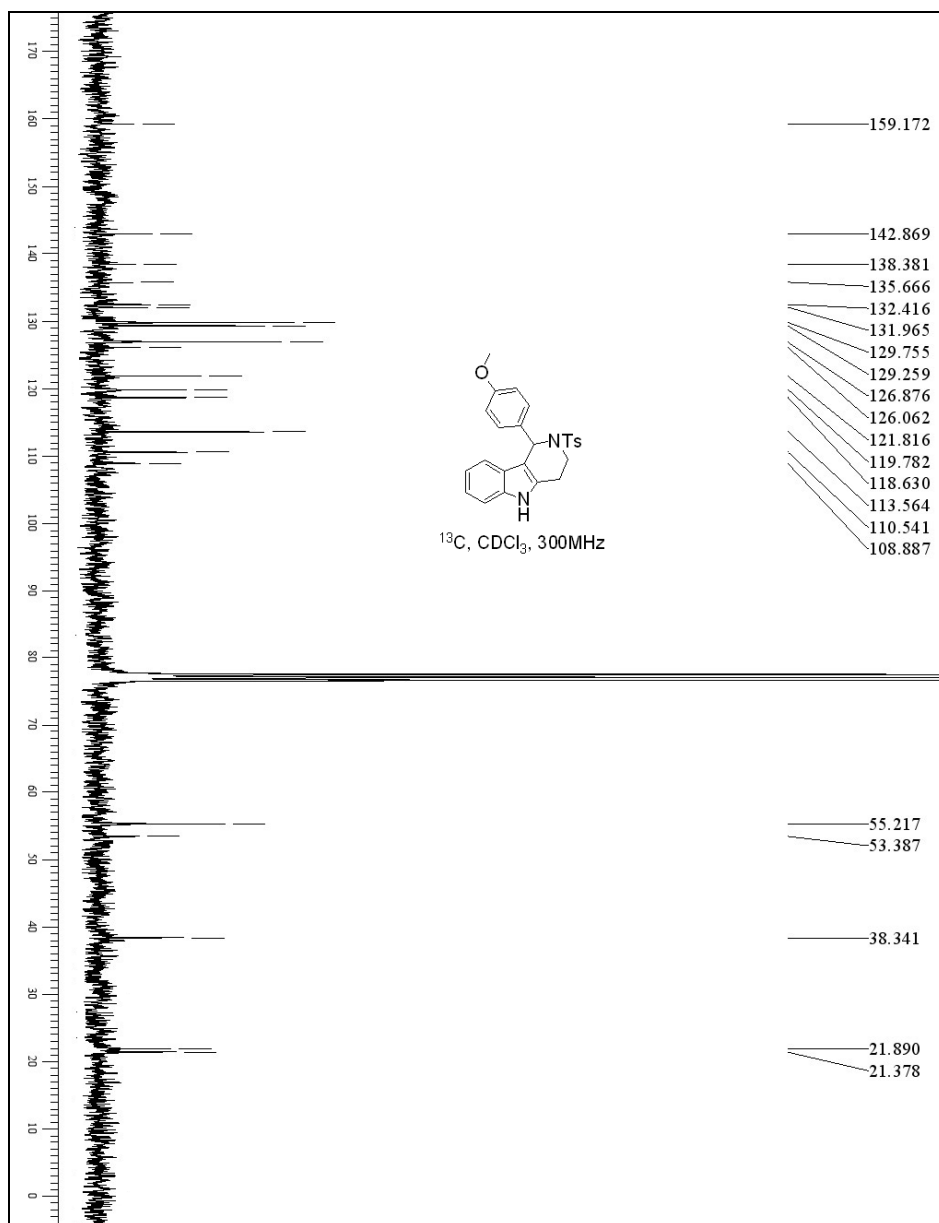
1-(*p*-Tolyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3d; Table 2; Entry d)



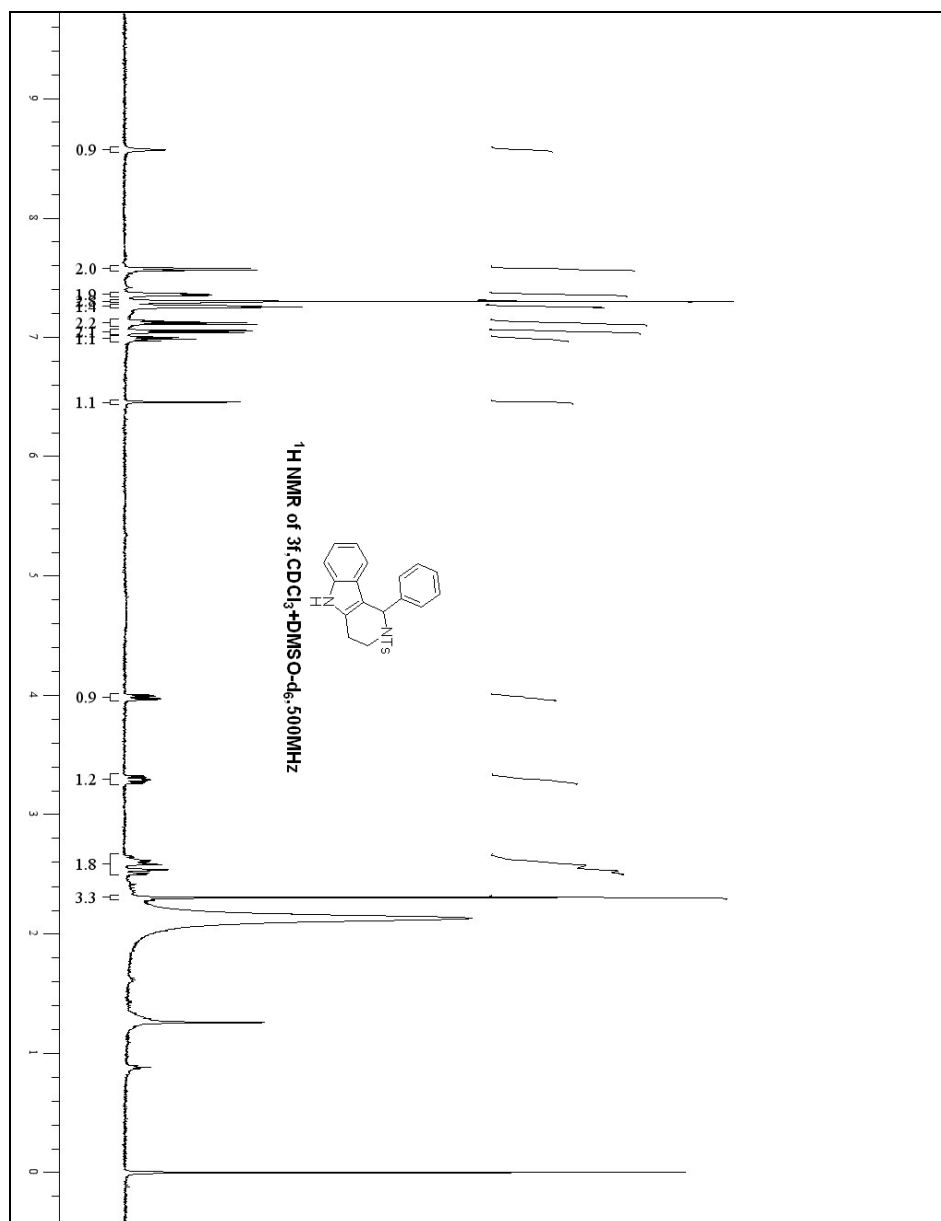


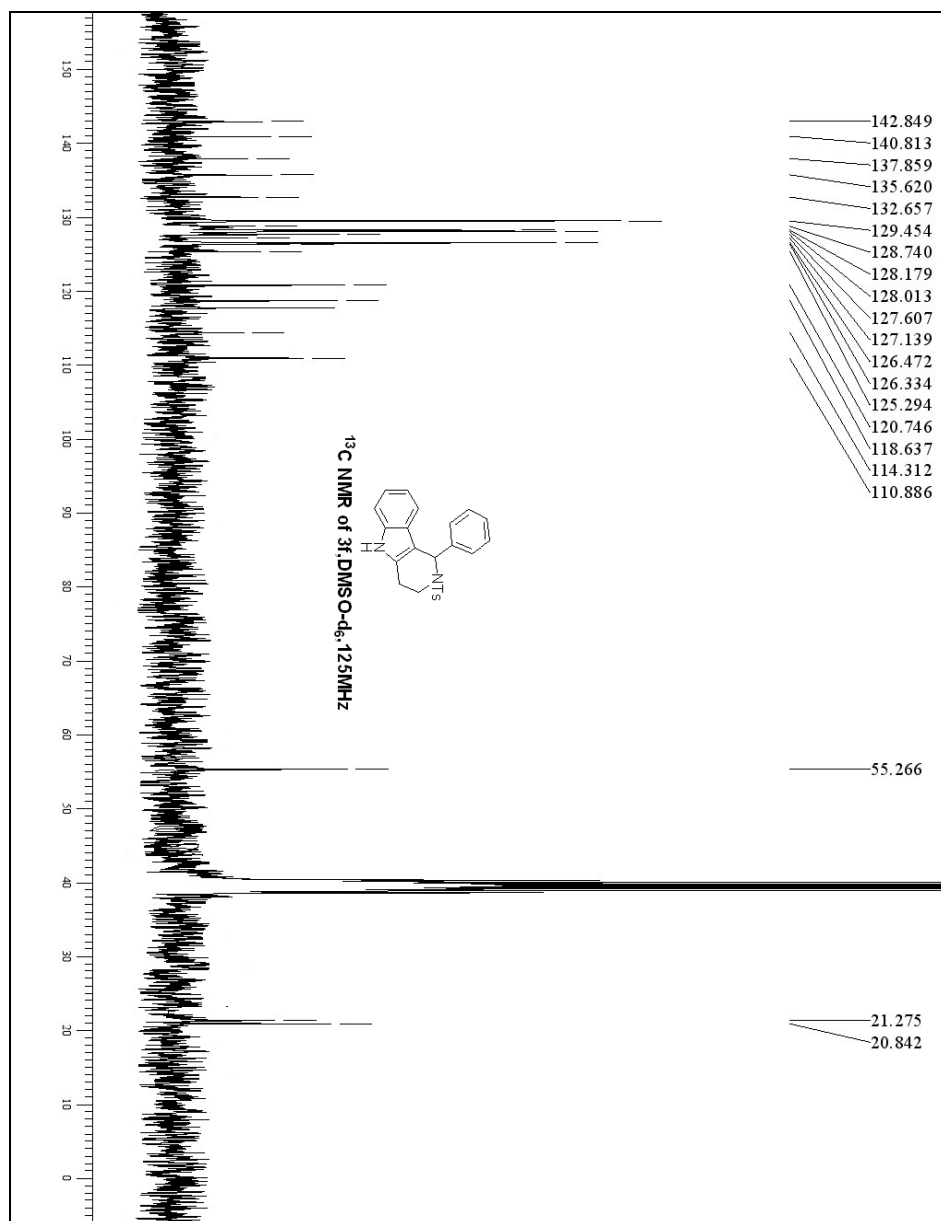
1-(4-Methoxyphenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3e; Table 2; Entry e)



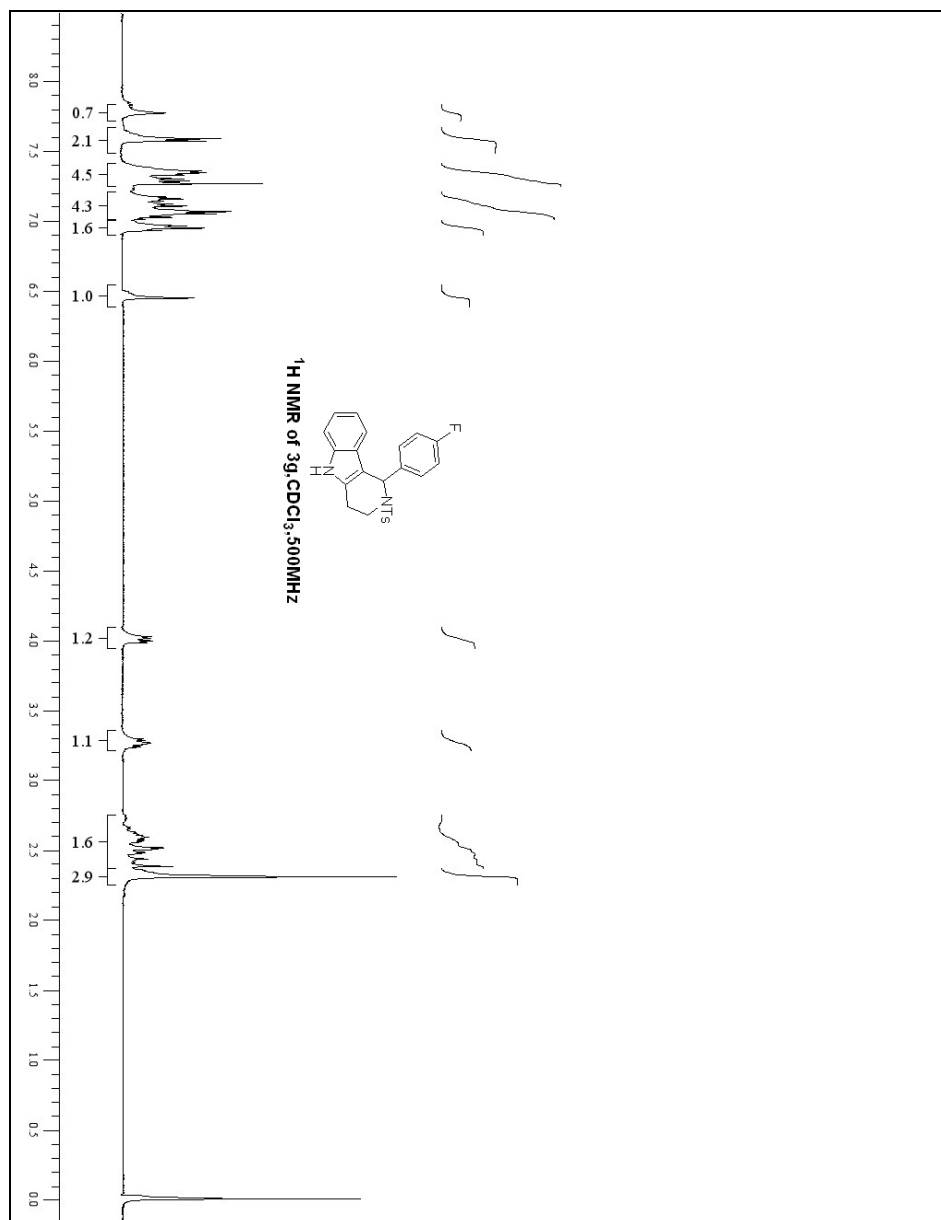


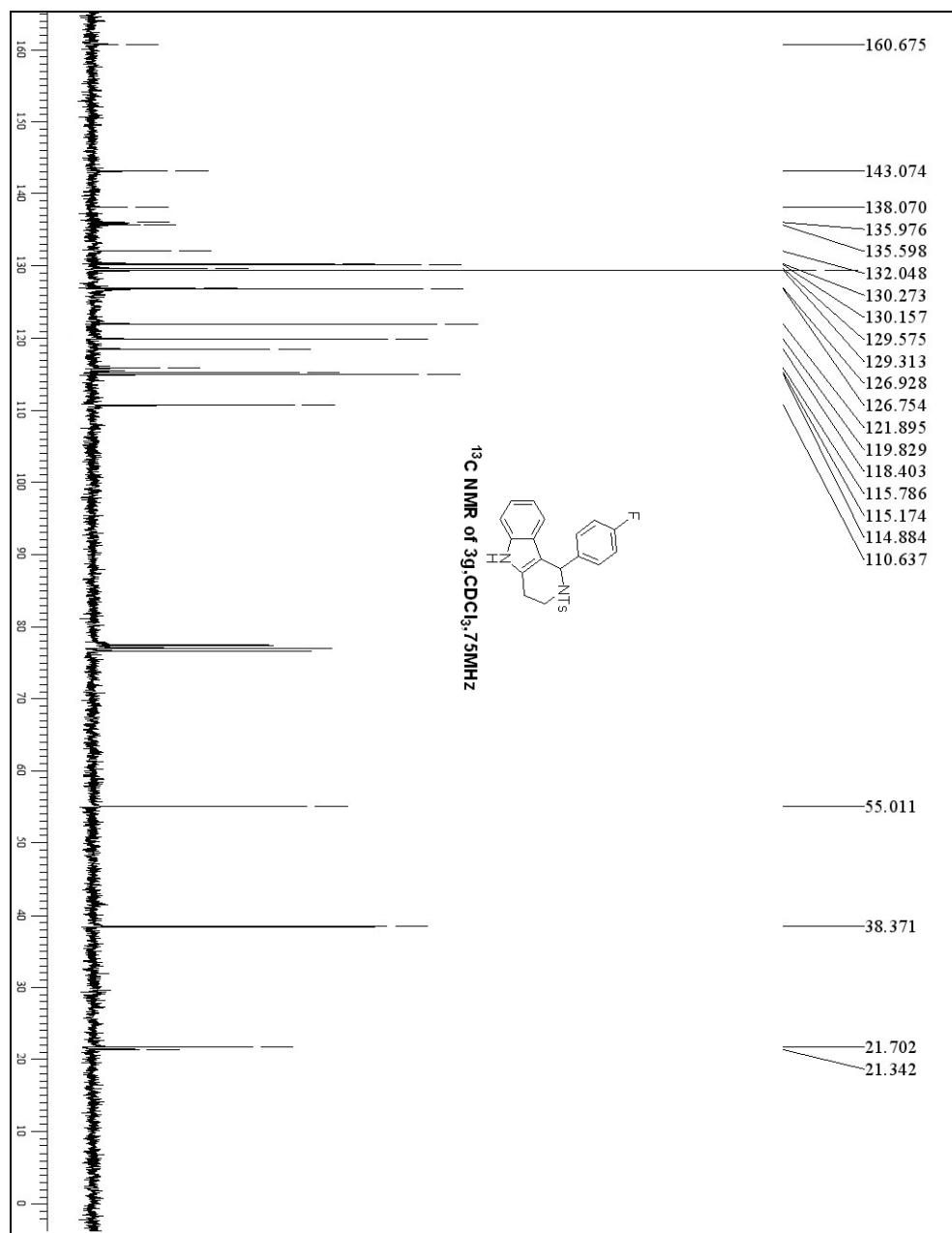
1-Phenyl-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3f; Table 2; Entry f)



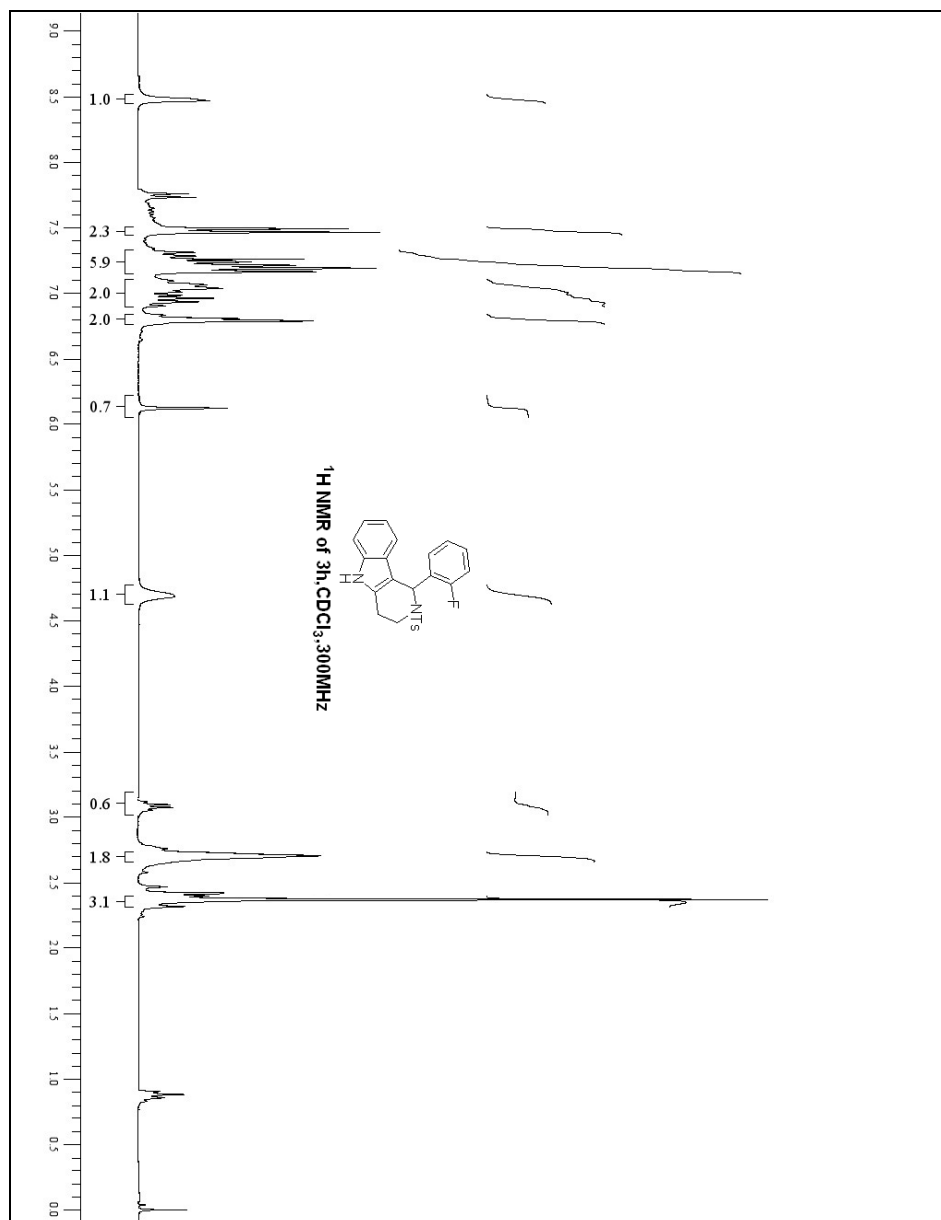


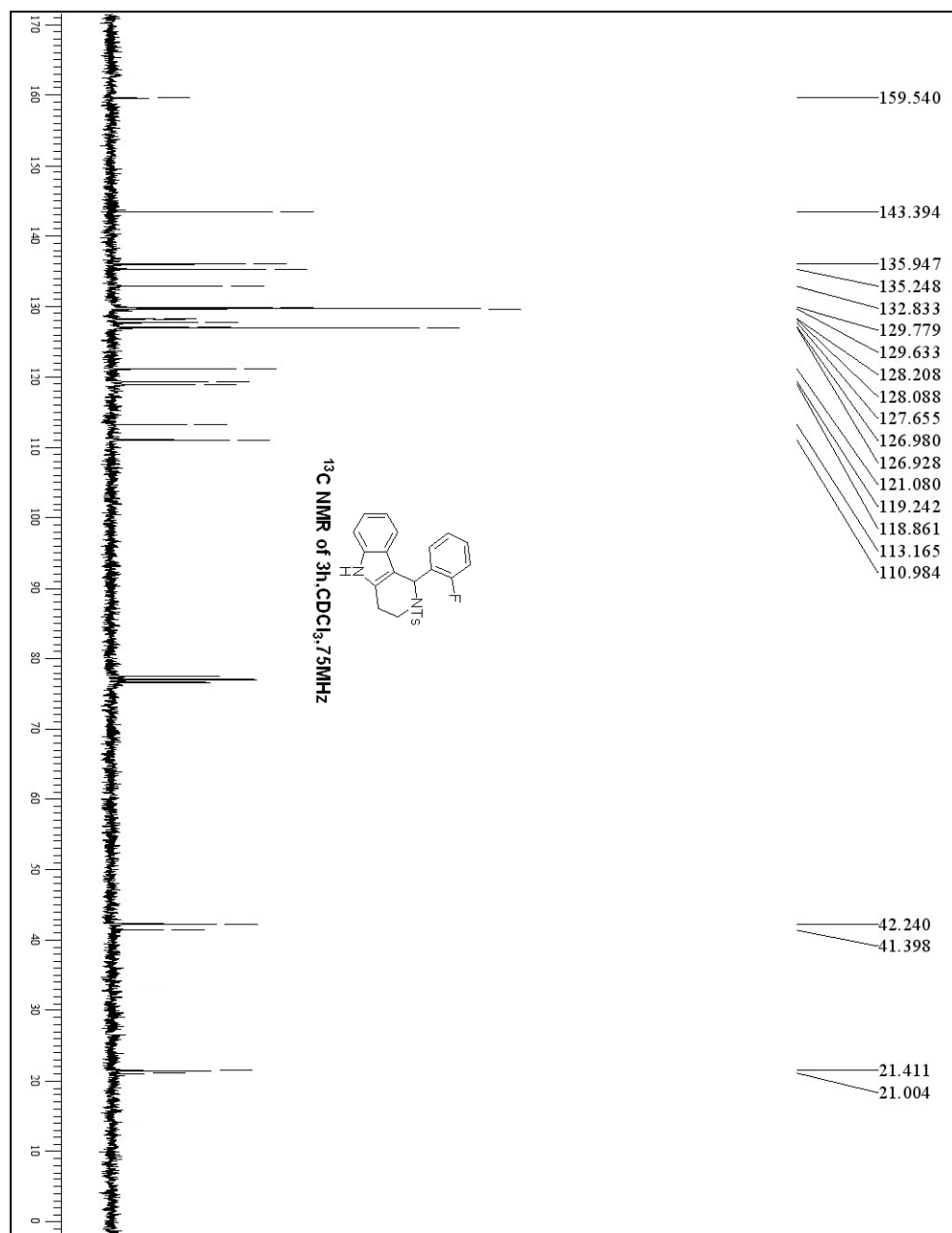
1-(4-Fluorophenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3g; Table 2; Entry g)



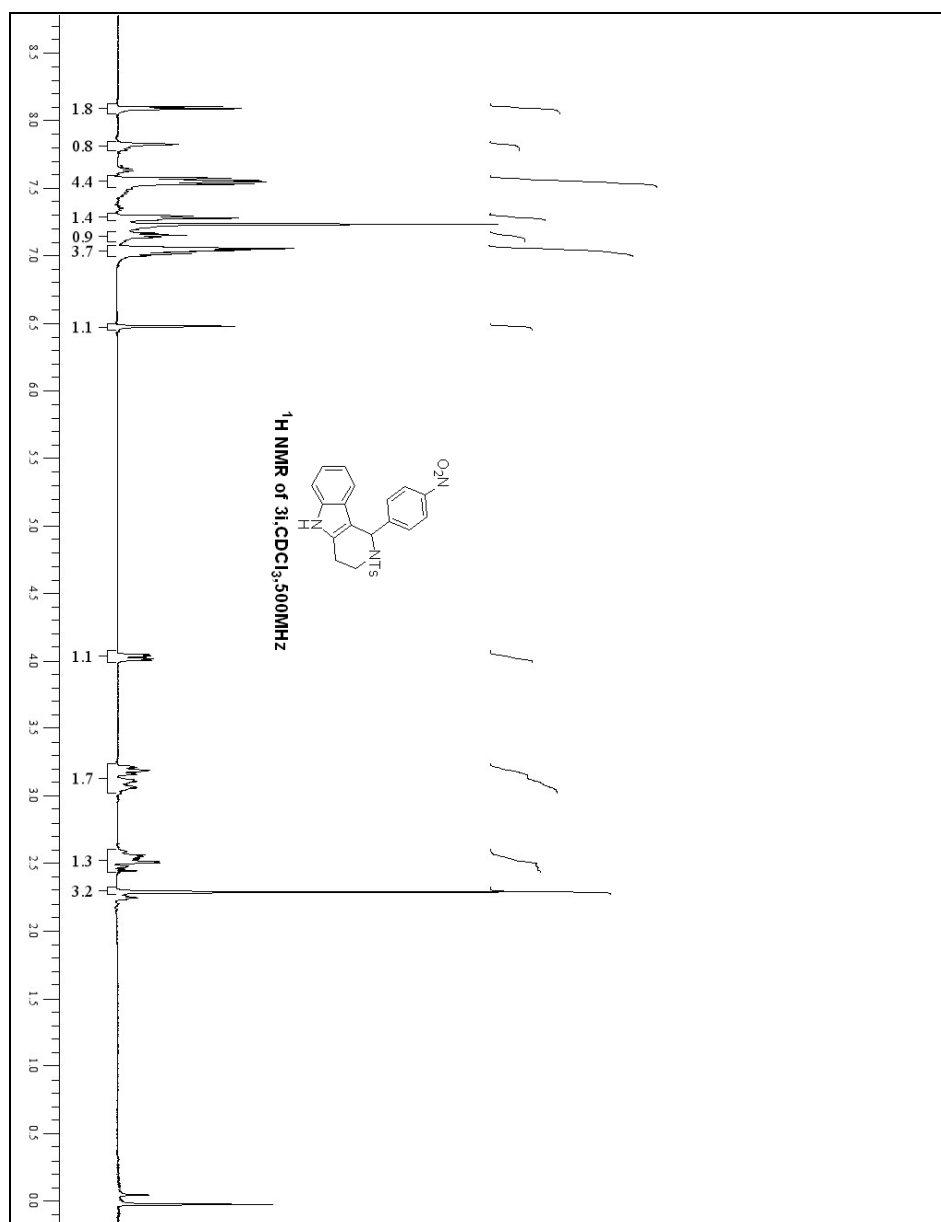


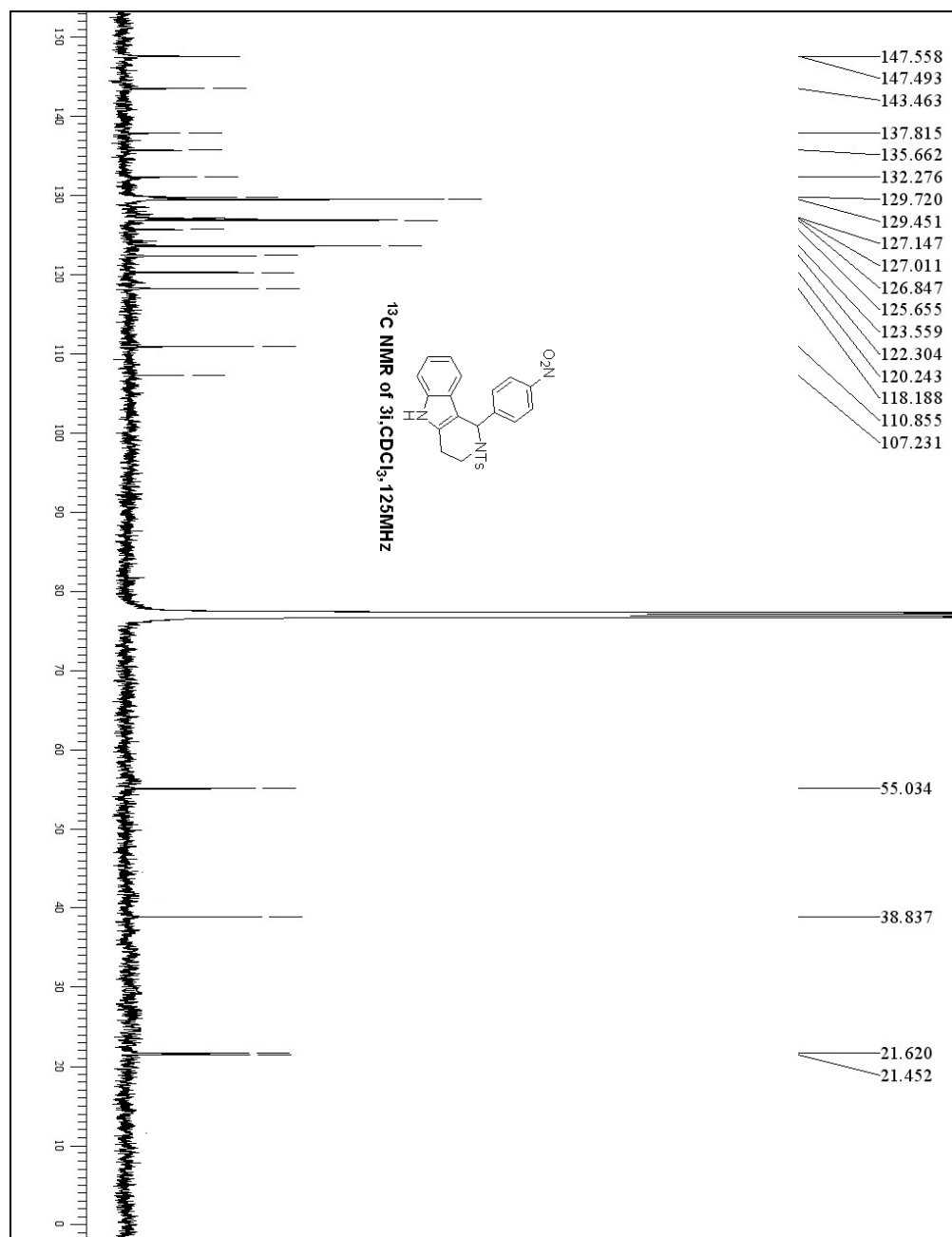
1-(2-Fluorophenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3h; Table 2; Entry h)



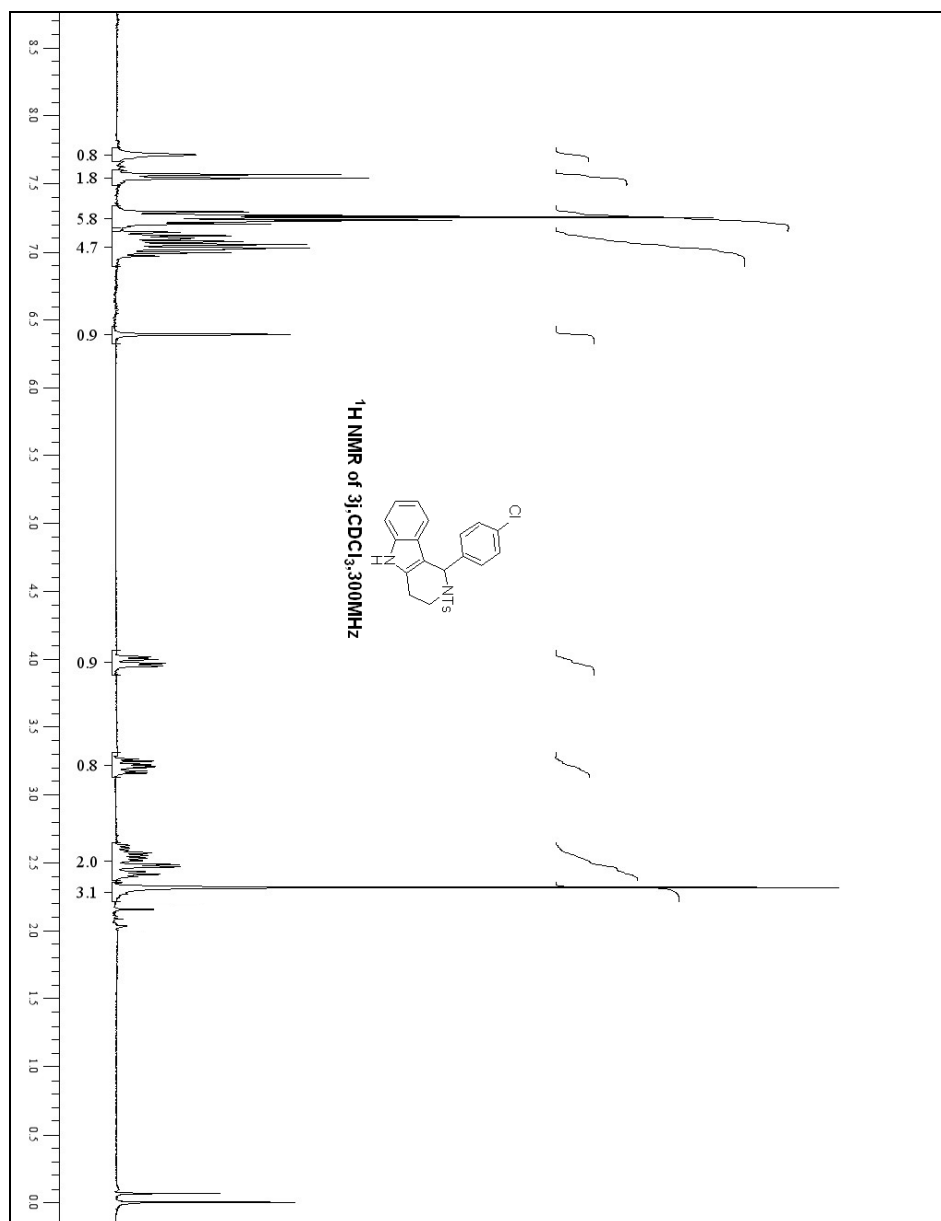


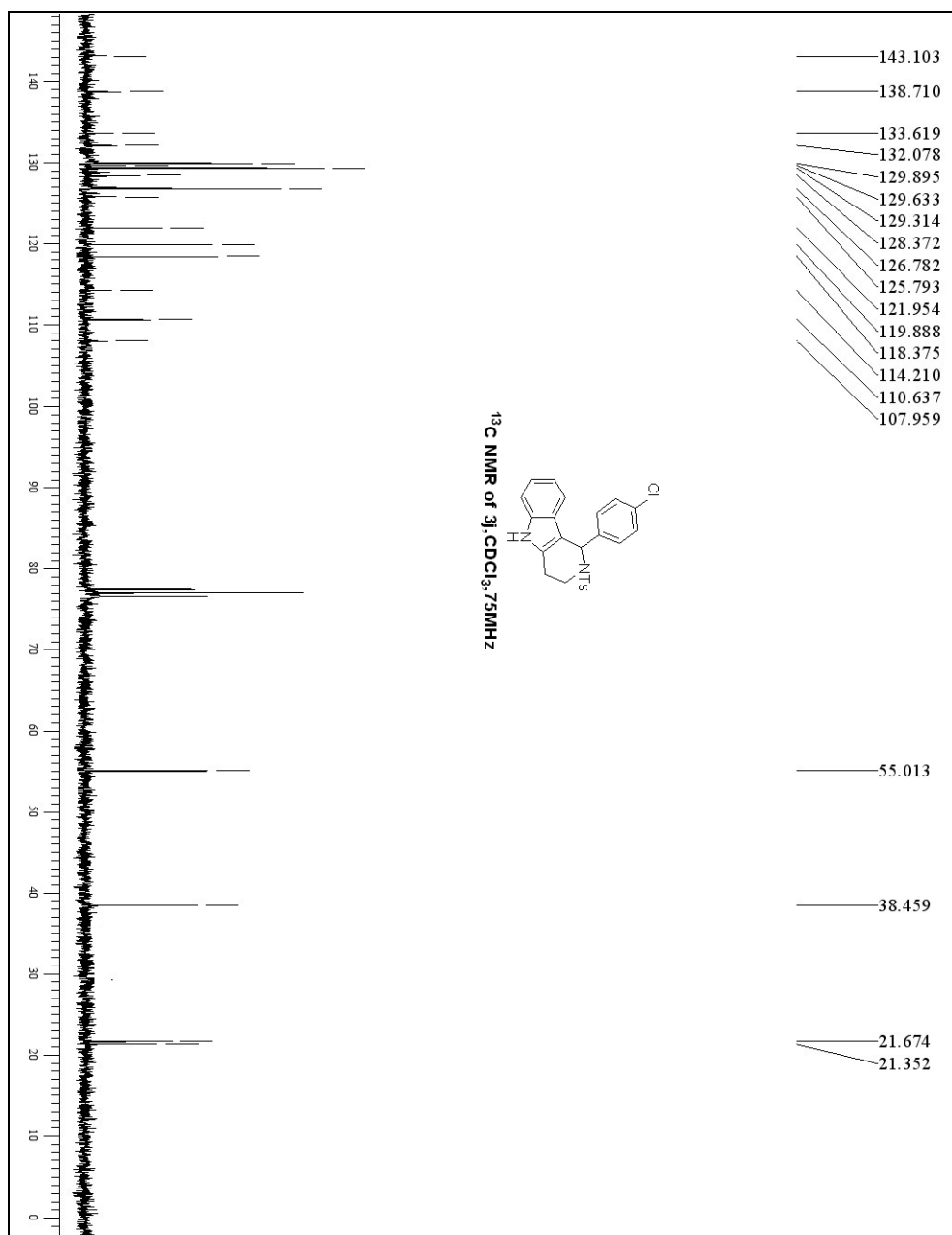
1-(4-Nitrophenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3i; Table 2; Entry i).



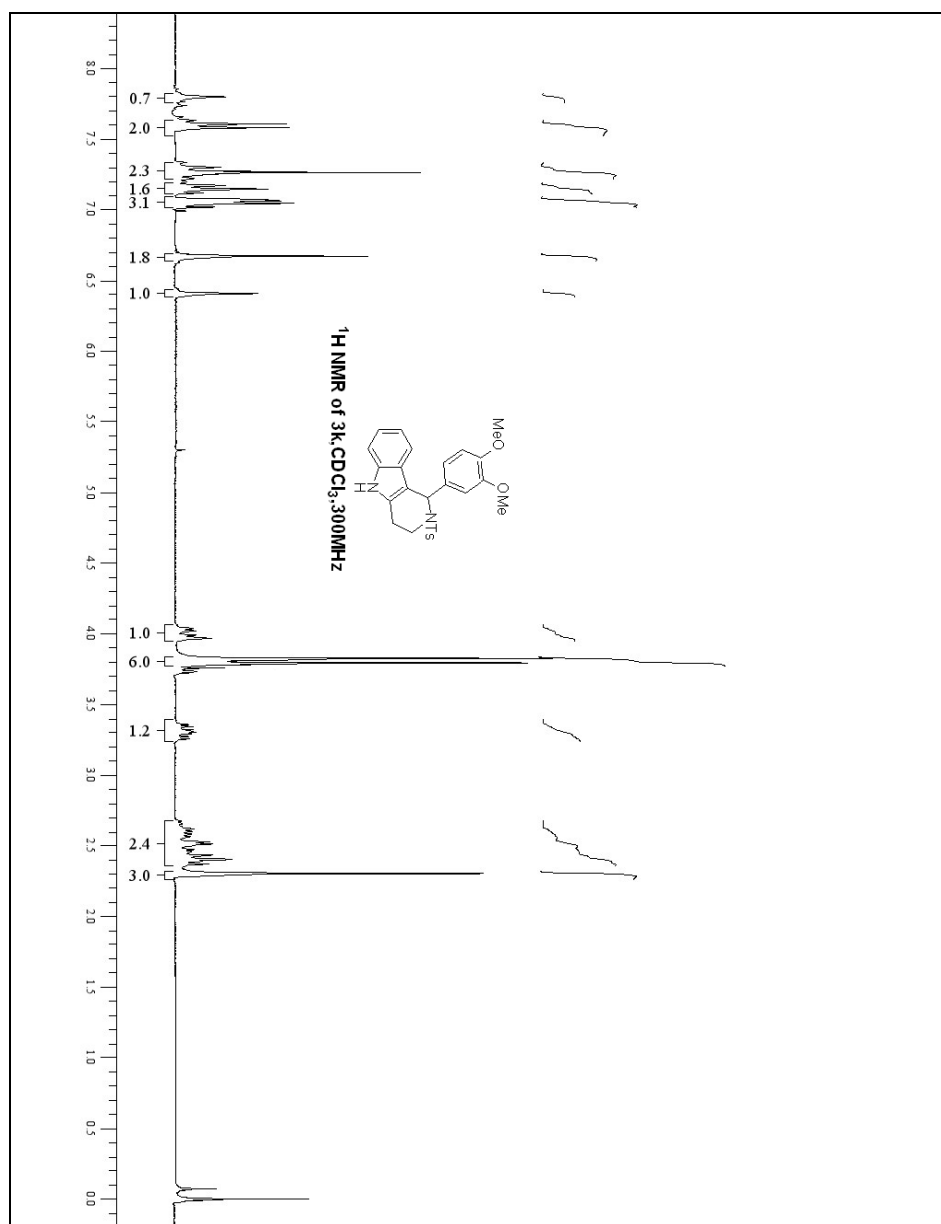


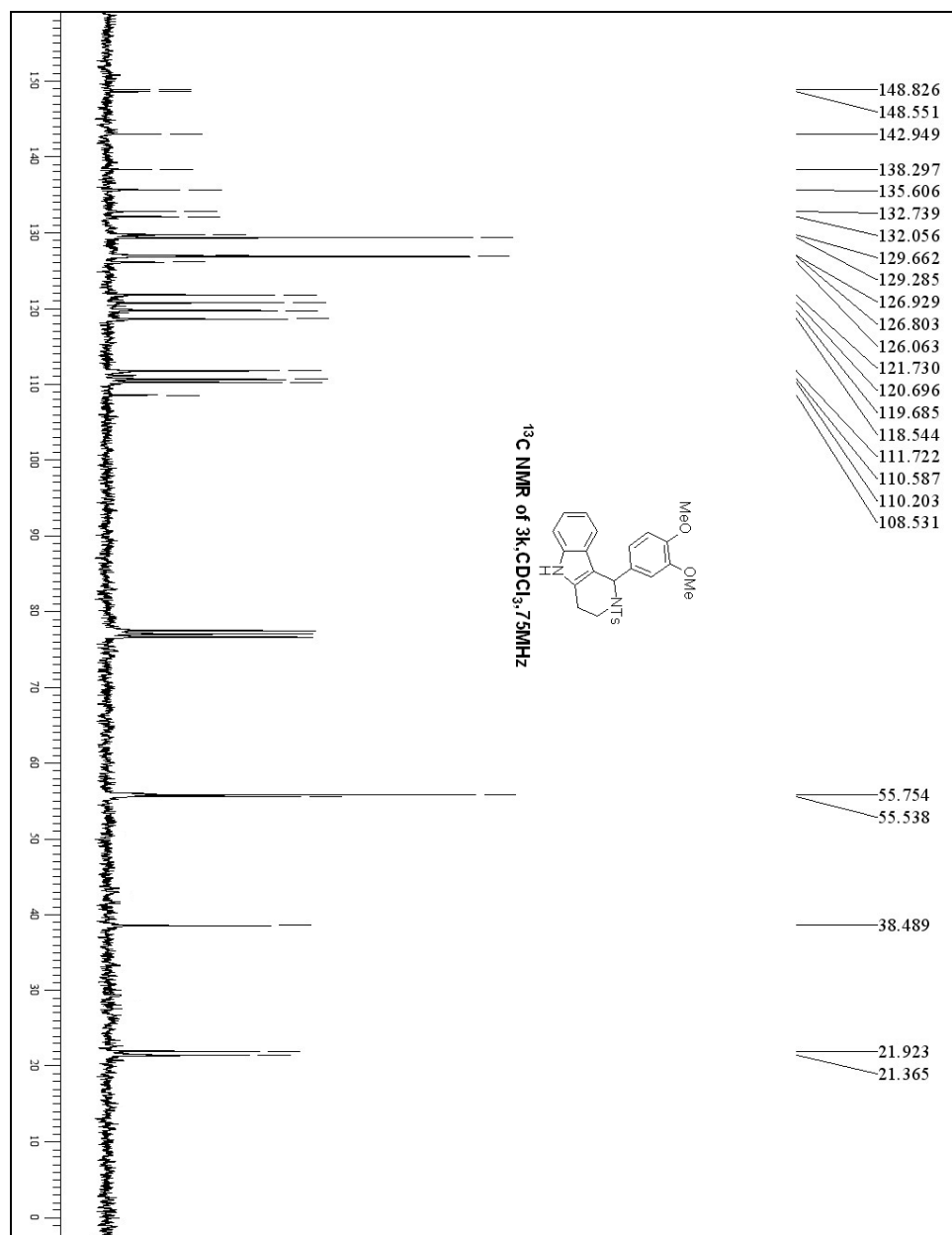
1-(4-Chlorophenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3j; Table 2; Entry j)





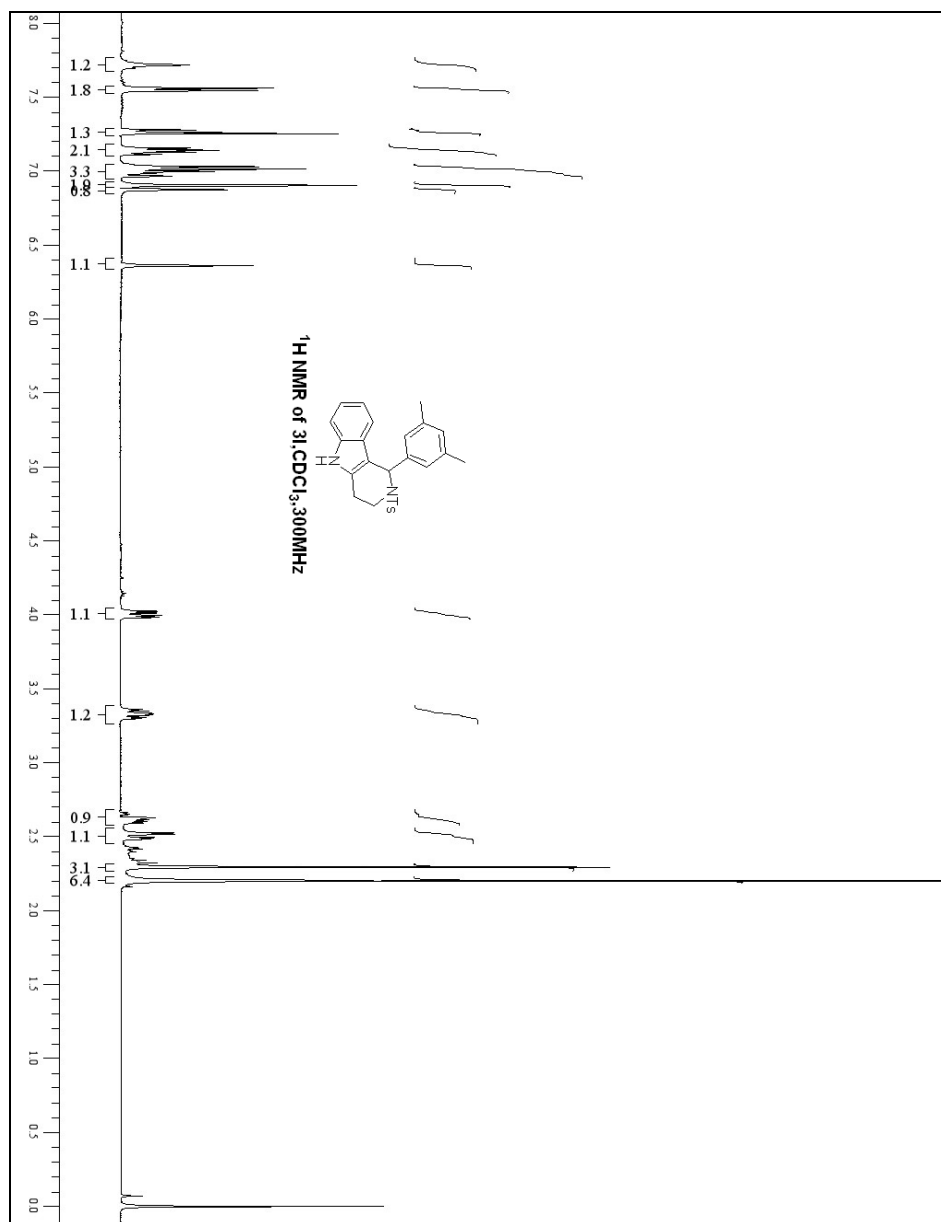
**1-(3,4-Dimethoxyphenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3k; Table 2;
Entry k)**

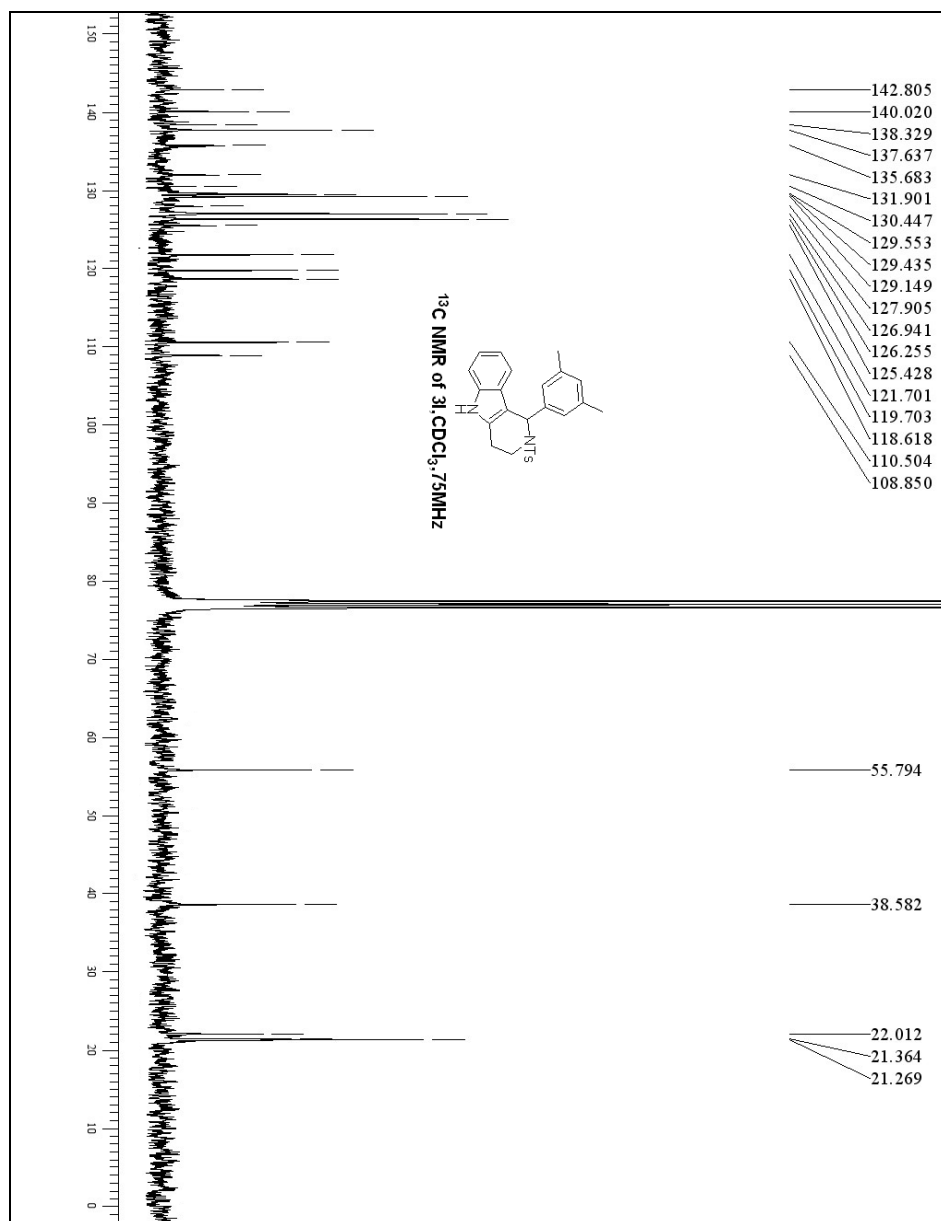




1-(3,5-Dimethylphenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3l; Table 2;

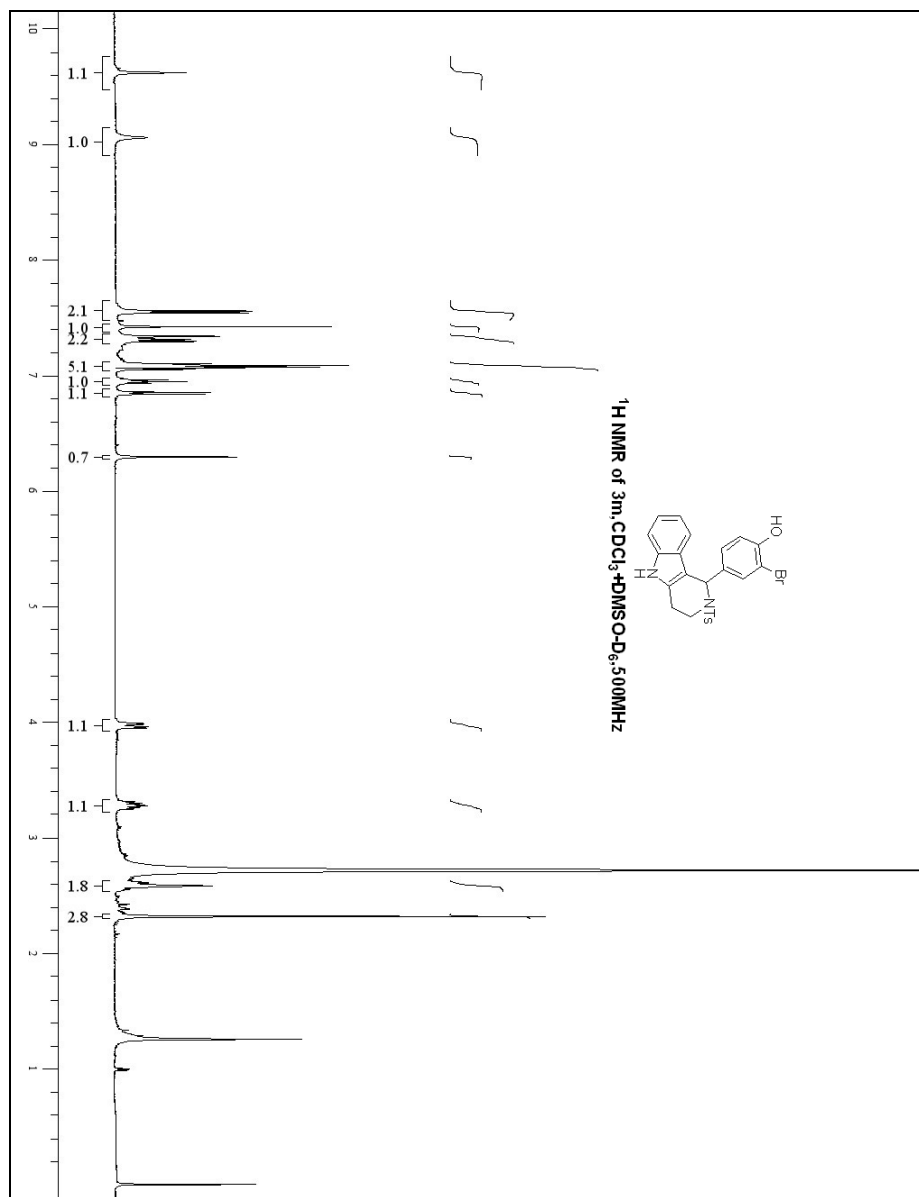
Entry I)

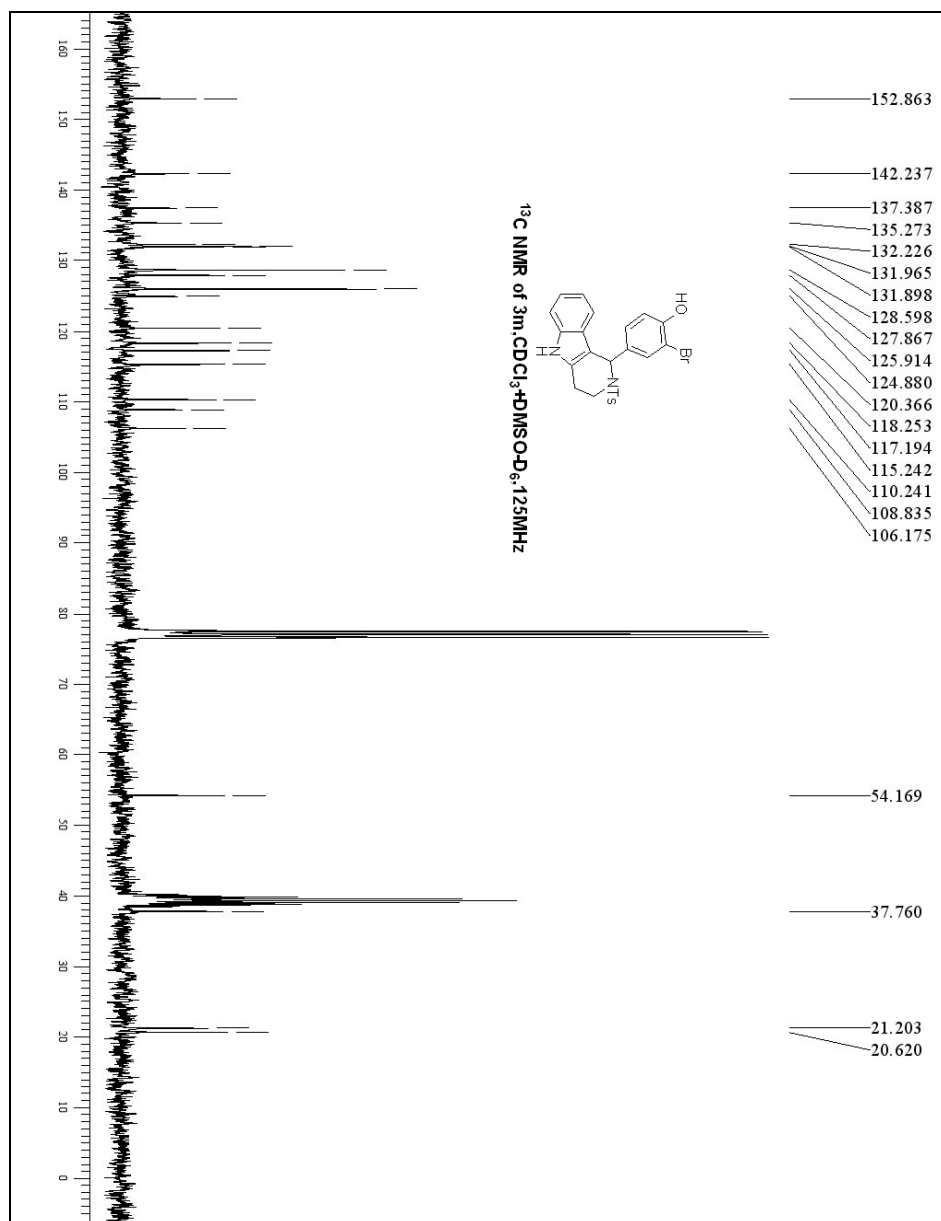




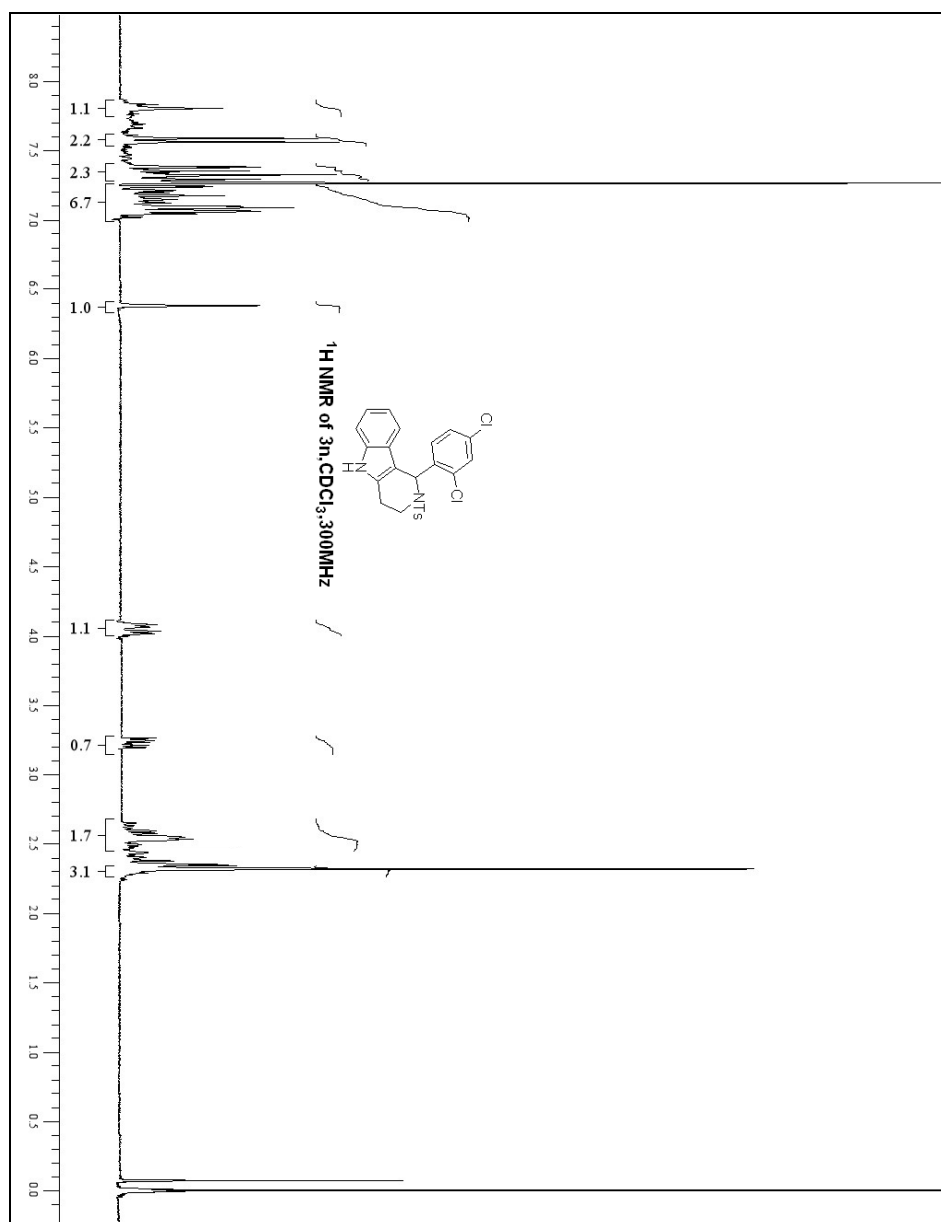
2-Bromo-4-(2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indol-1-yl)phenol (3m; Table 2;

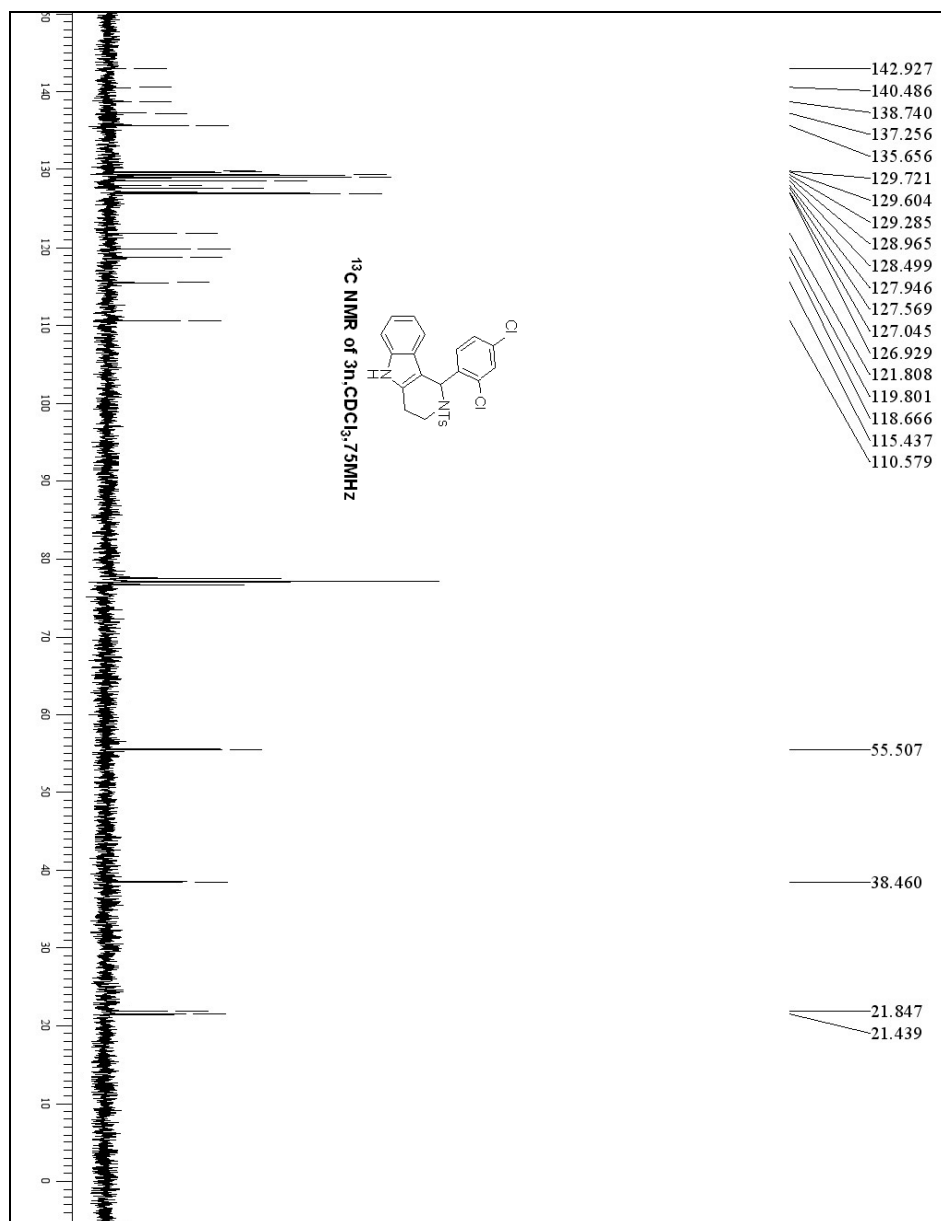
Entry m)



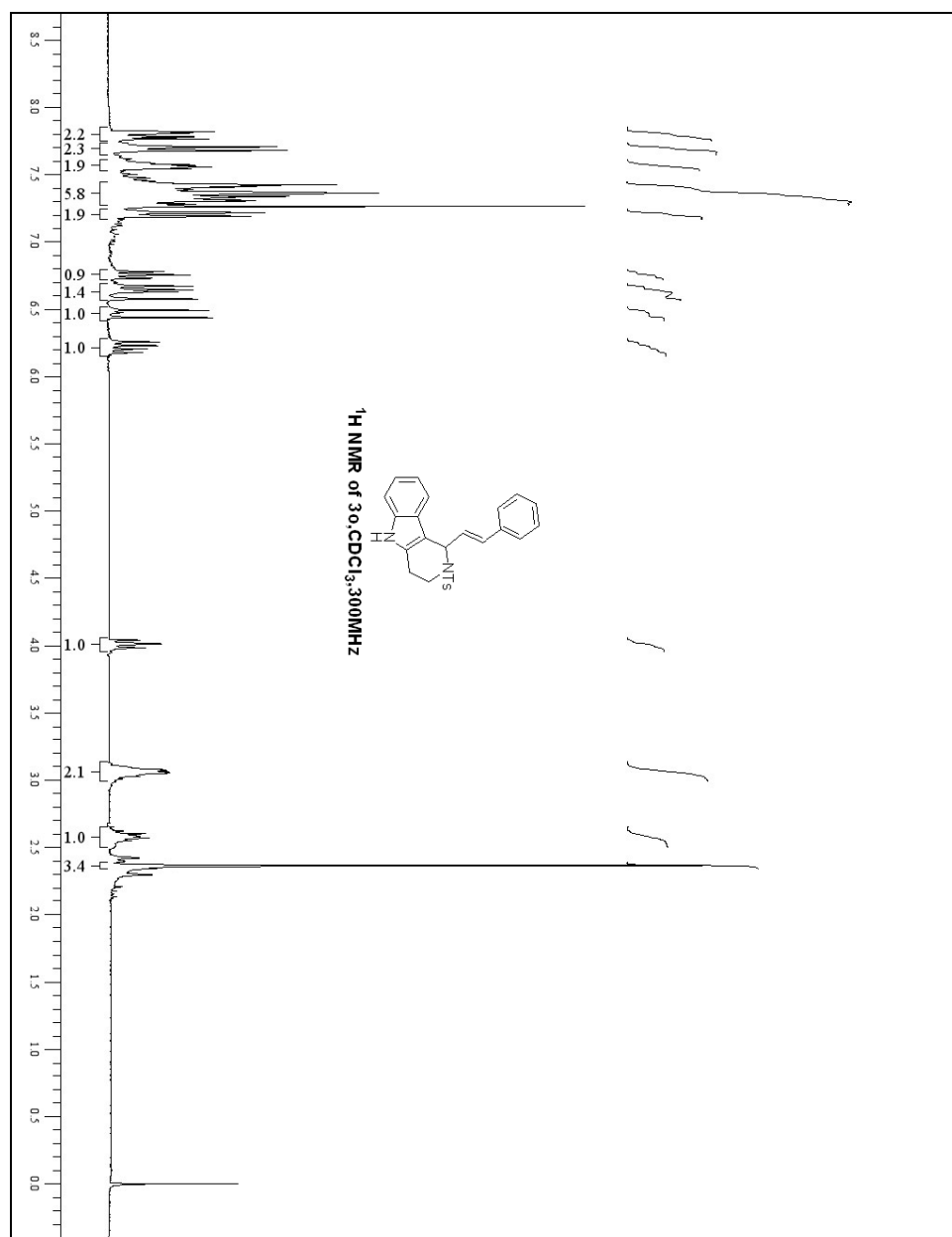


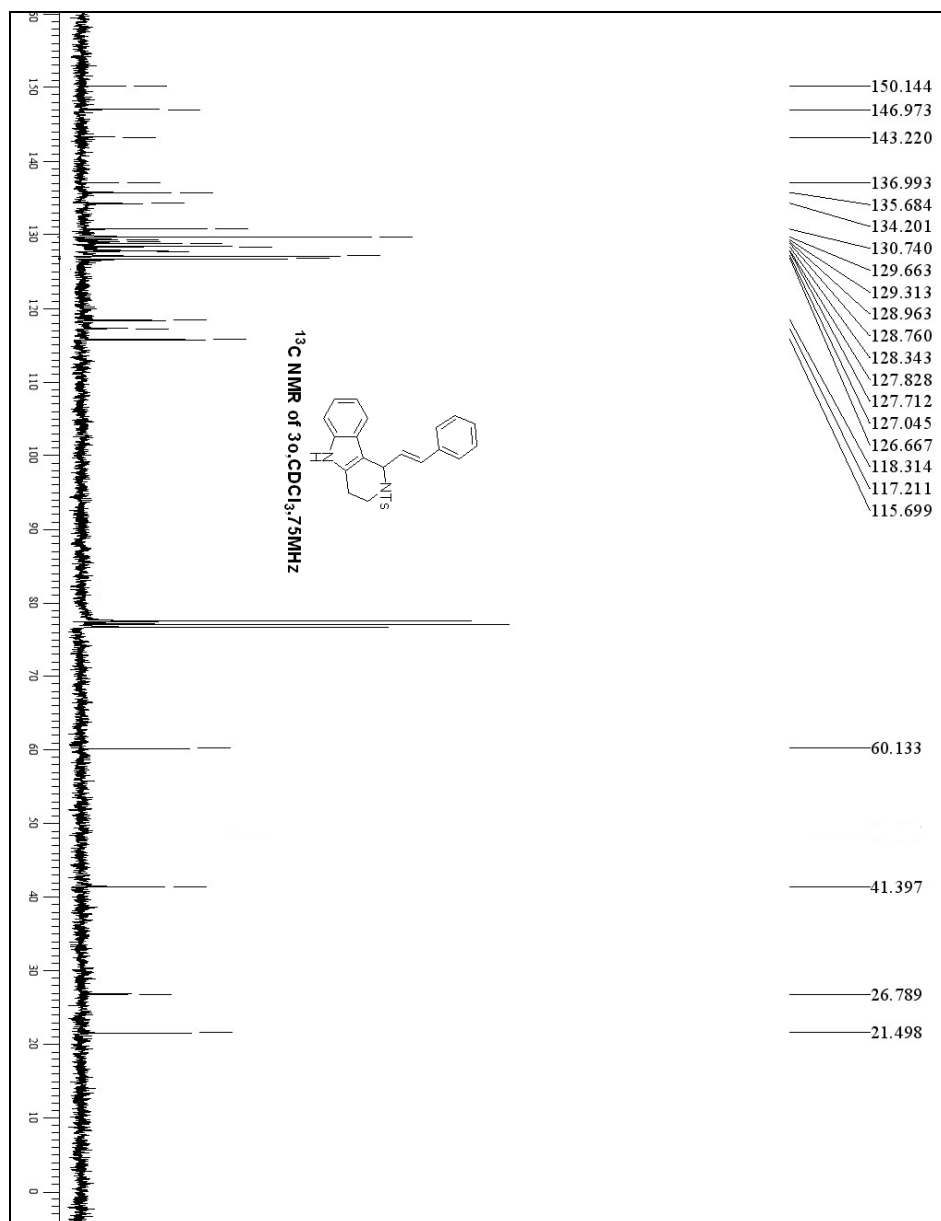
1-(2,4-Dichlorophenyl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3n; Table 2; Entry n)



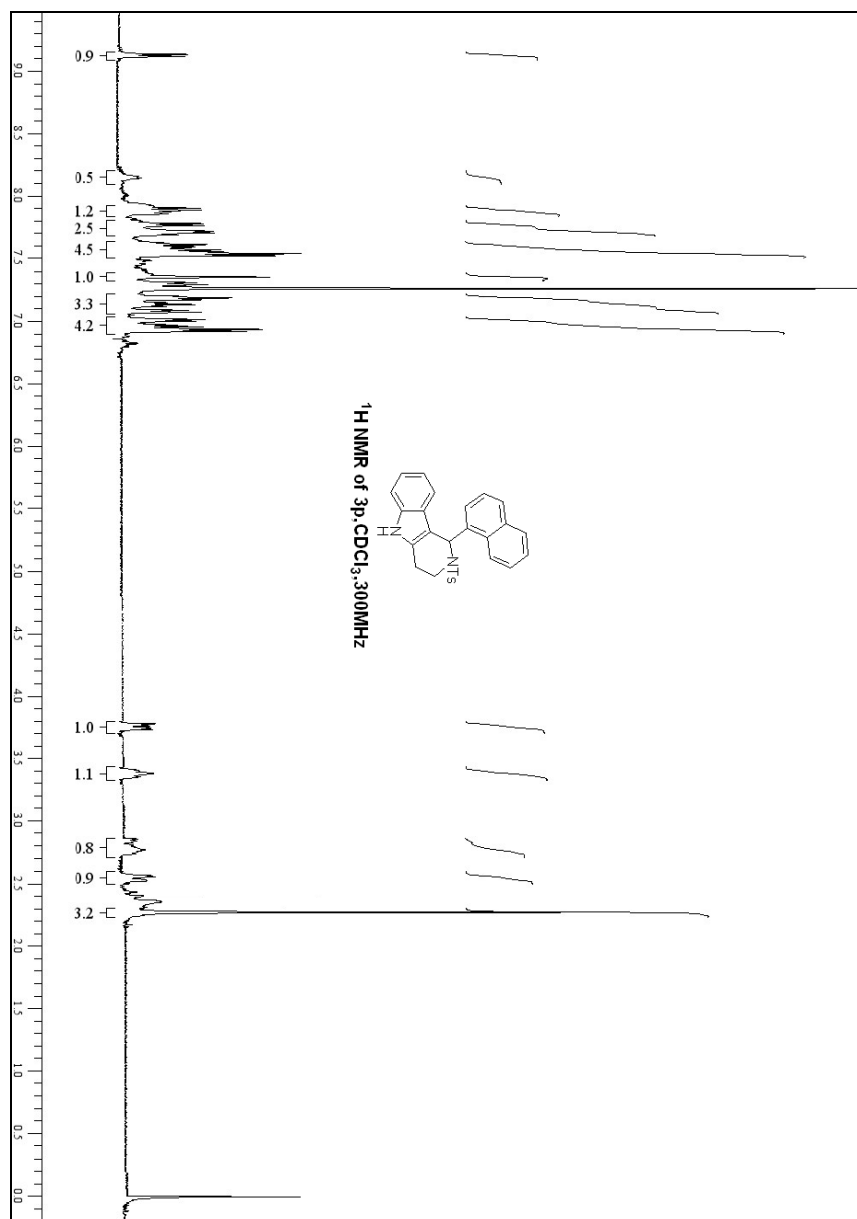


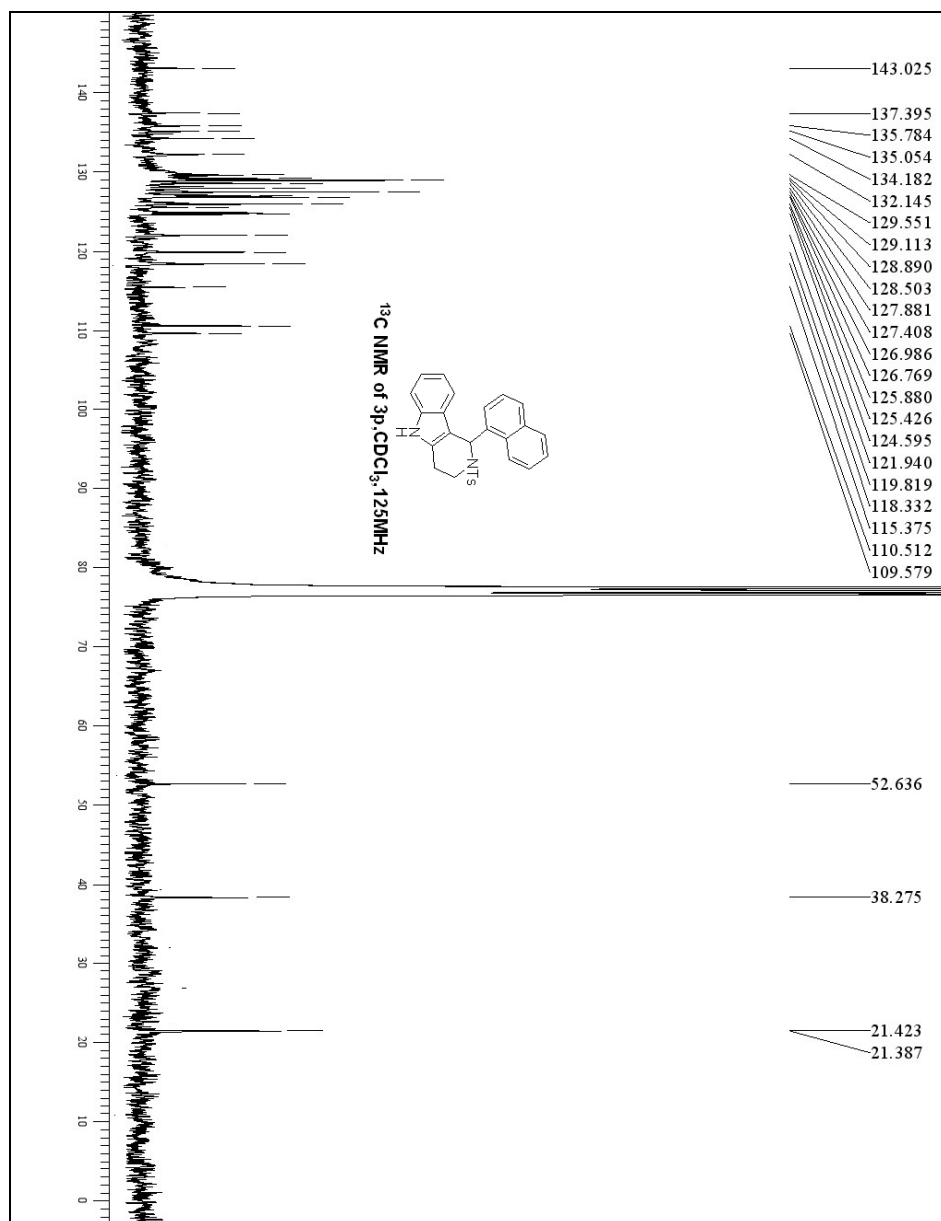
(*E*)-1-Styryl-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3o; Table 2; Entry o):



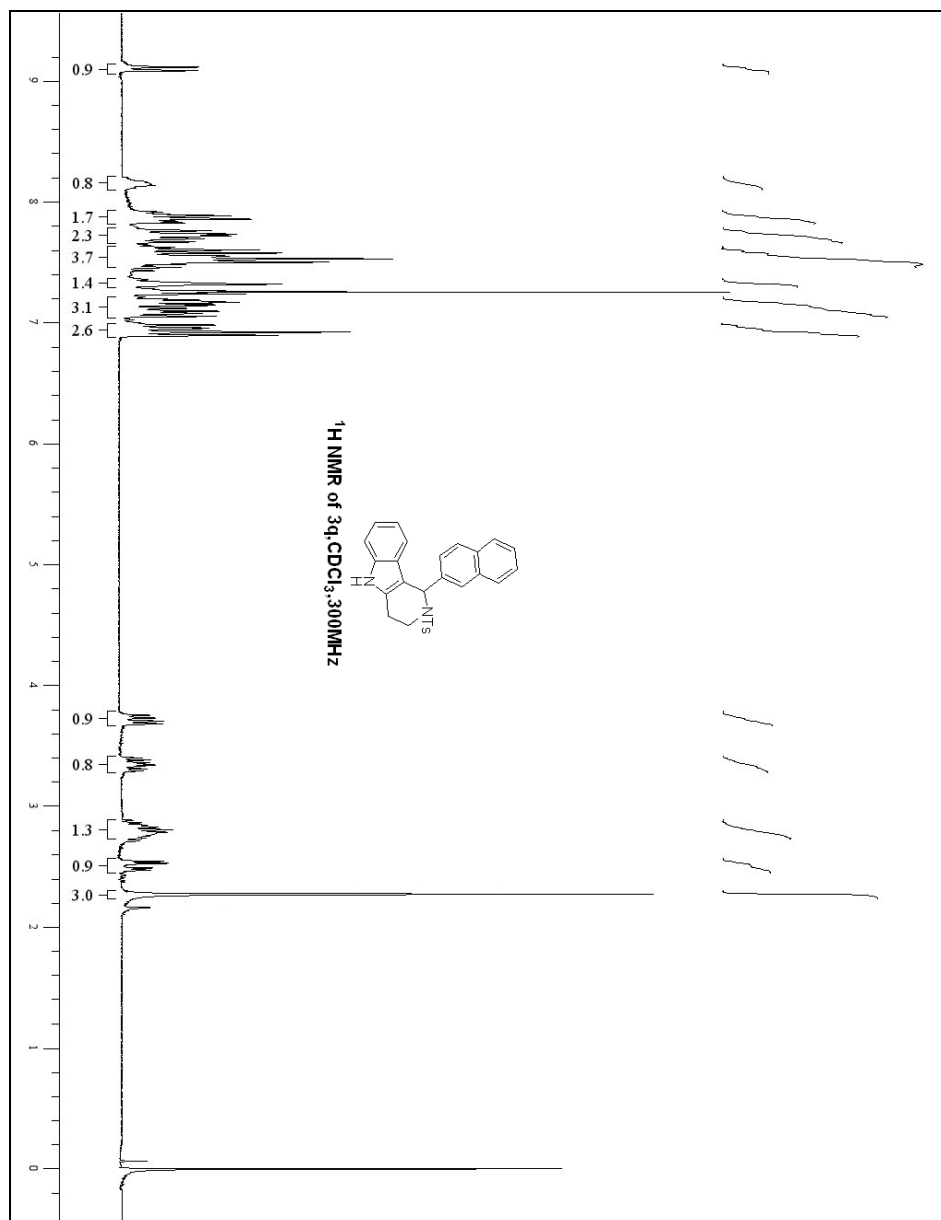


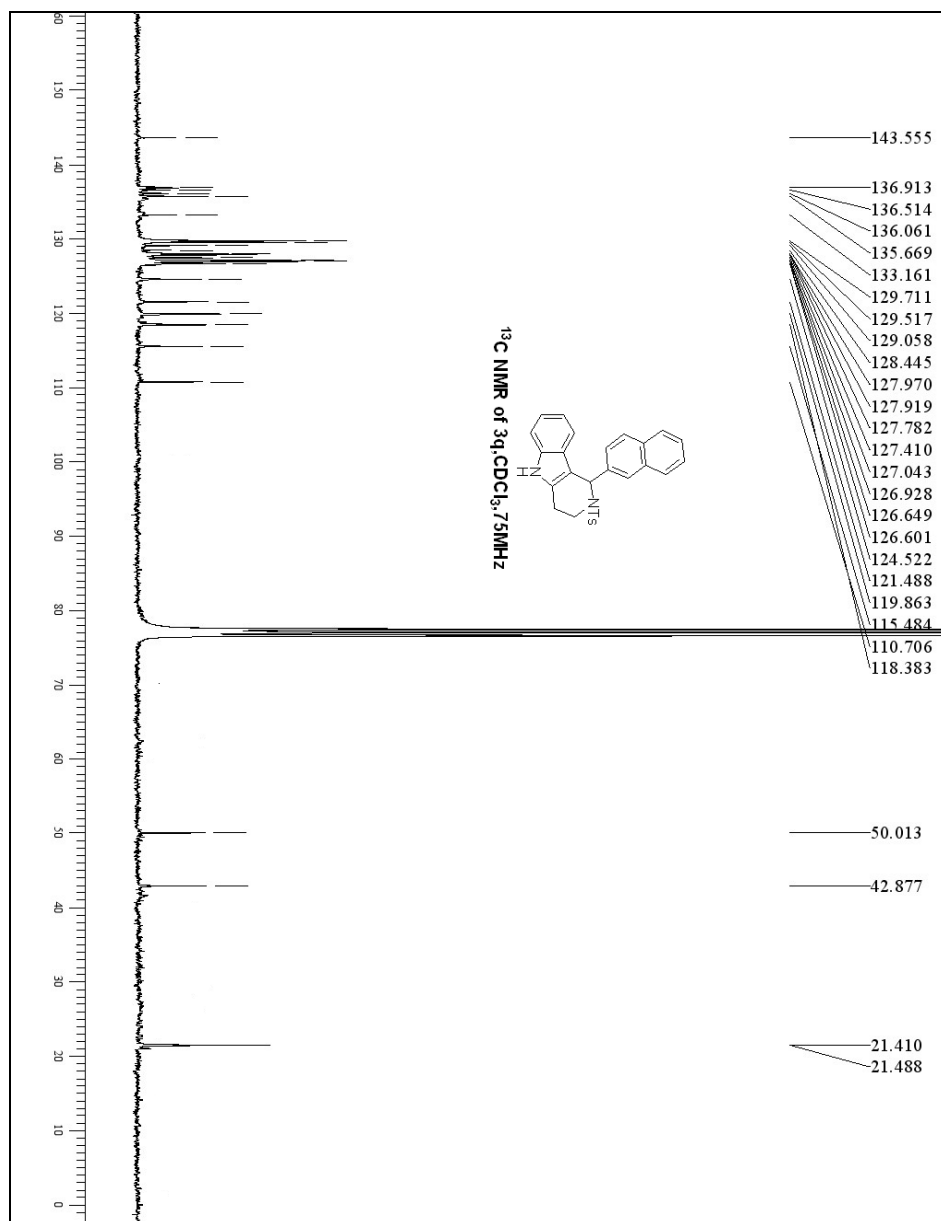
1-(Naphthalen-1-yl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3p; Table 2; Entry p)



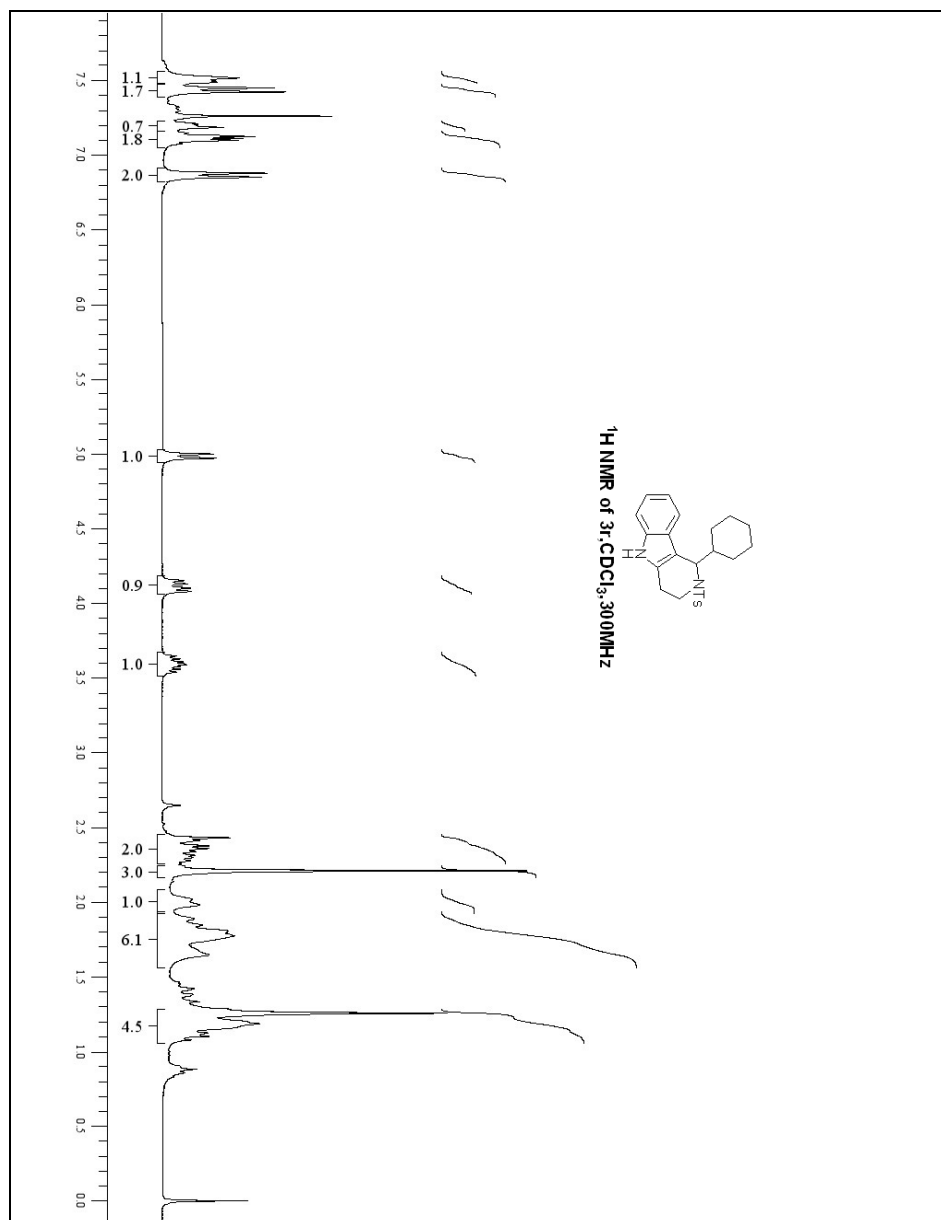


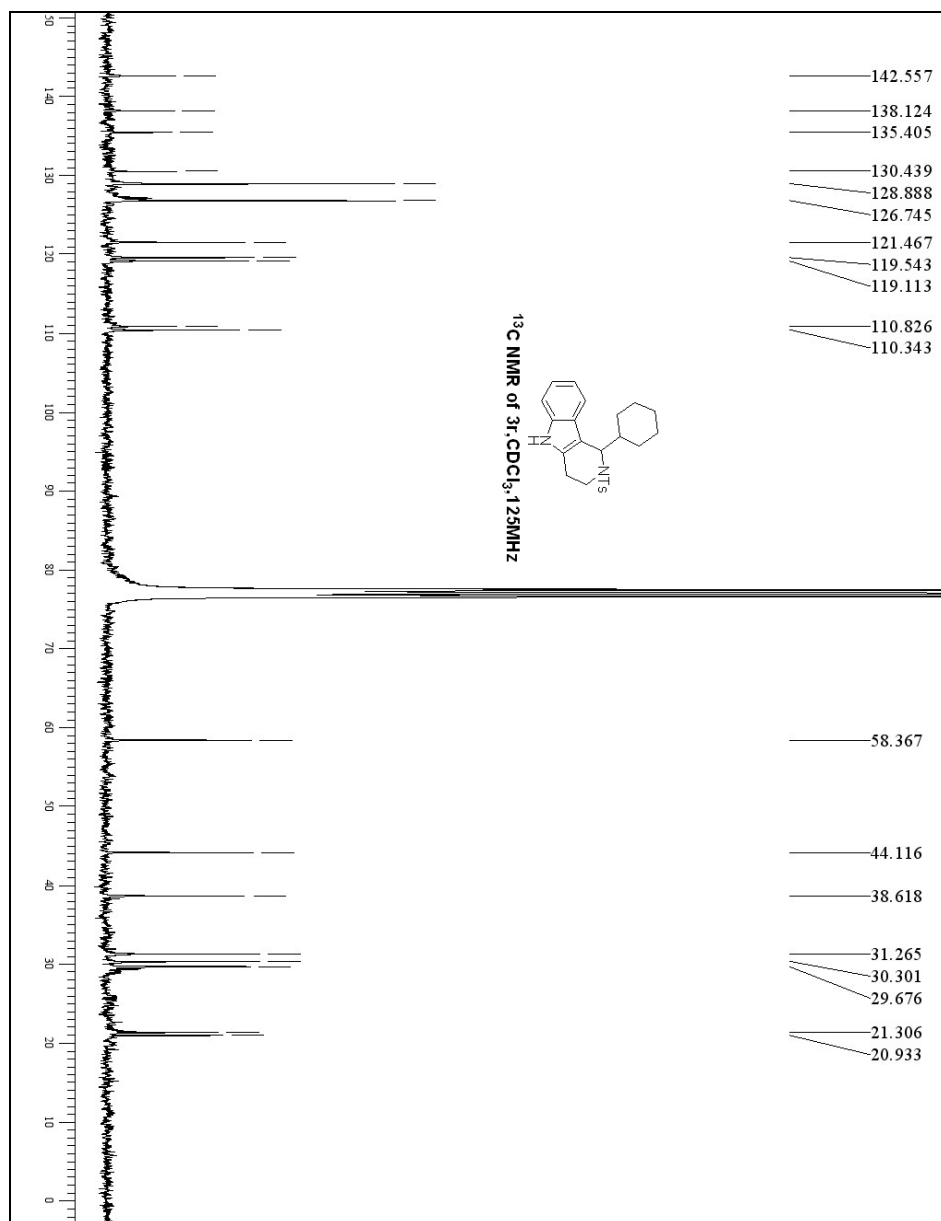
1-(Naphthalen-2-yl)-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3q; Table 2; Entry q)





1-Cyclohexyl-2-tosyl-2,3,4,5-tetrahydro-1*H*-pyrido[4,3-*b*]indole (3r; Table 2; Entry r):





1-(4-chlorophenyl)-8-methoxy-2-tosyl-2,3,4,5-tetrahydro-1H-pyrido[4,3-b]indole (3s)

