

Supporting Information

Cu-Mediated Sulfonyl Radical-Enabled 5-*exo-trig* Cyclization of Alkenyl Aldehydes: Access to Sulfonylmethyl 1*H*-Indenes

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1. X-ray structure of compound 3l

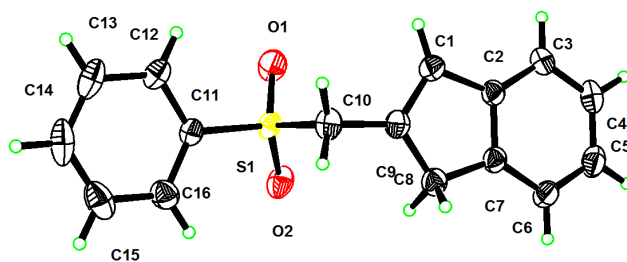


Figure S1. ORTEP drawing of 3l showing thermal ellipsoids at the 50% probability level

Table S1. Crystal data and structure refinement for 3l

CCDC No.	1829188
Empirical formula	C ₁₆ H ₁₄ O ₂ S
Formula weight	270.33
Temperature/K	296.15
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	8.299(3)
b/Å	10.924(4)
c/Å	14.783(5)
α /°	90
β /°	98.016(8)
γ /°	90
Volume/Å ³	1327.1(8)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.353
μ/mm^{-1}	0.238
F(000)	568.0
Crystal size/mm ³	0.28 × 0.15 × 0.12
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection/°	4.652 to 53.038

Index ranges	$-10 \leq h \leq 10, -13 \leq k \leq 12, -18 \leq l \leq 18$
Reflections collected	9223
Independent reflections	2656 [$R_{\text{int}} = 0.0332, R_{\text{sigma}} = 0.0352$]
Data/restraints/parameters	2656/0/172
Goodness-of-fit on F^2	1.071
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0466, wR_2 = 0.1361$
Final R indexes [all data]	$R_1 = 0.0562, wR_2 = 0.1457$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.34/-0.37

2. Copies of NMR Spectra Data

2-(Tosylmethyl)-1*H*-indene (3a)

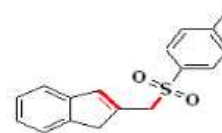
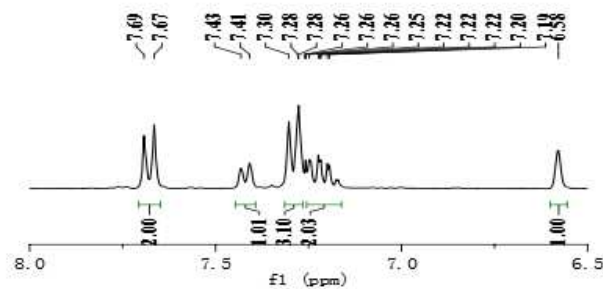
7.69 7.67 7.43 7.41 7.30 7.28 7.26 7.26 7.26 7.25 7.22 7.22 7.22 7.20 7.19 7.18 7.17 6.58

4.25

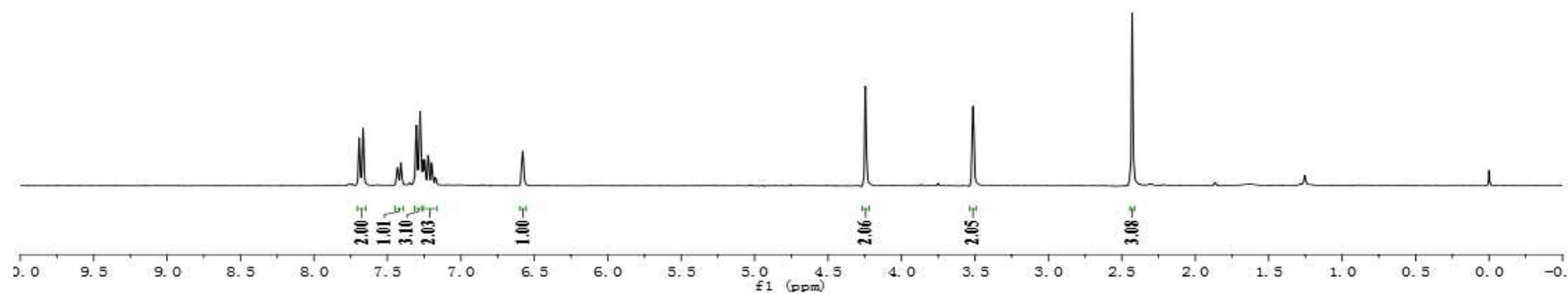
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2.43

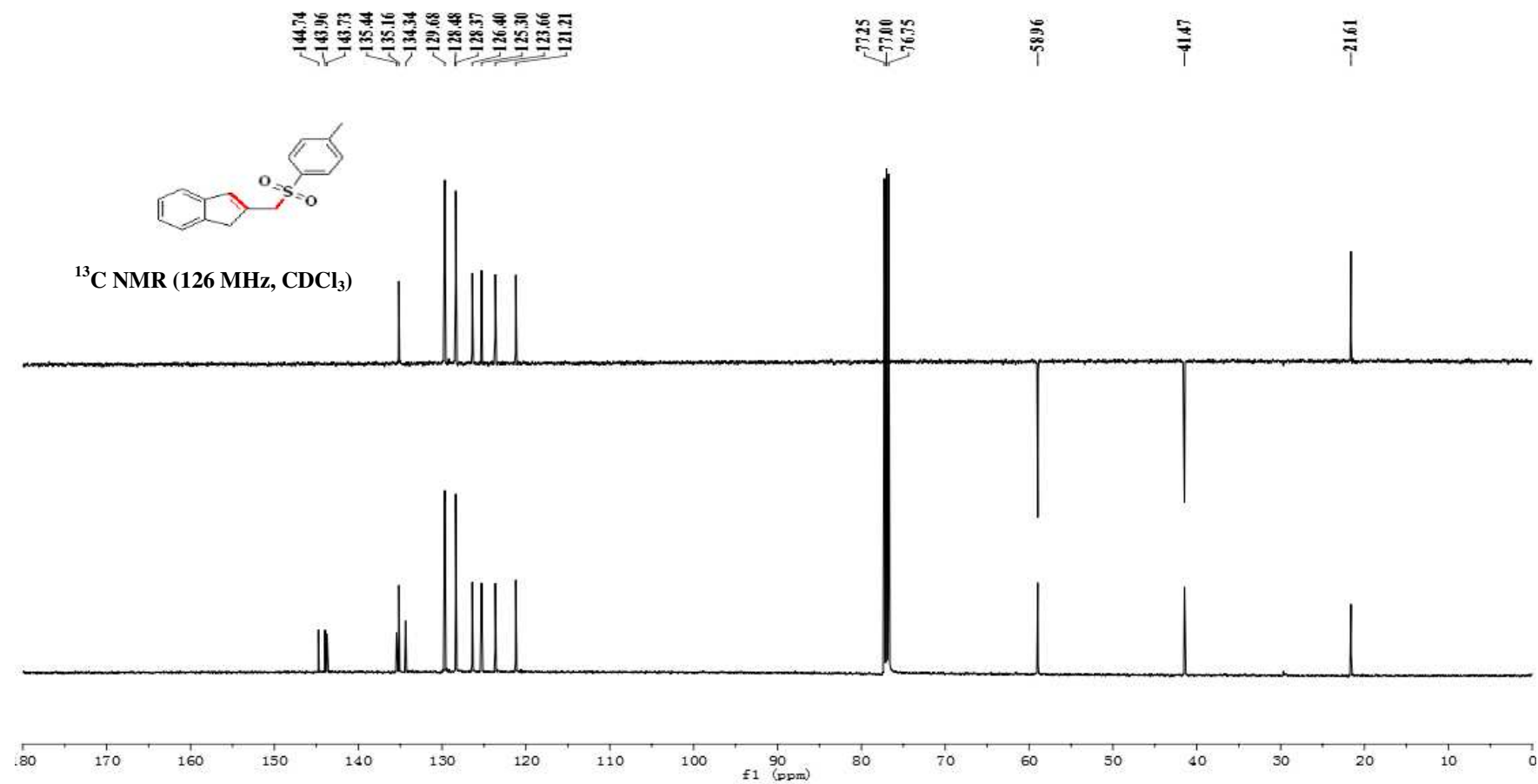
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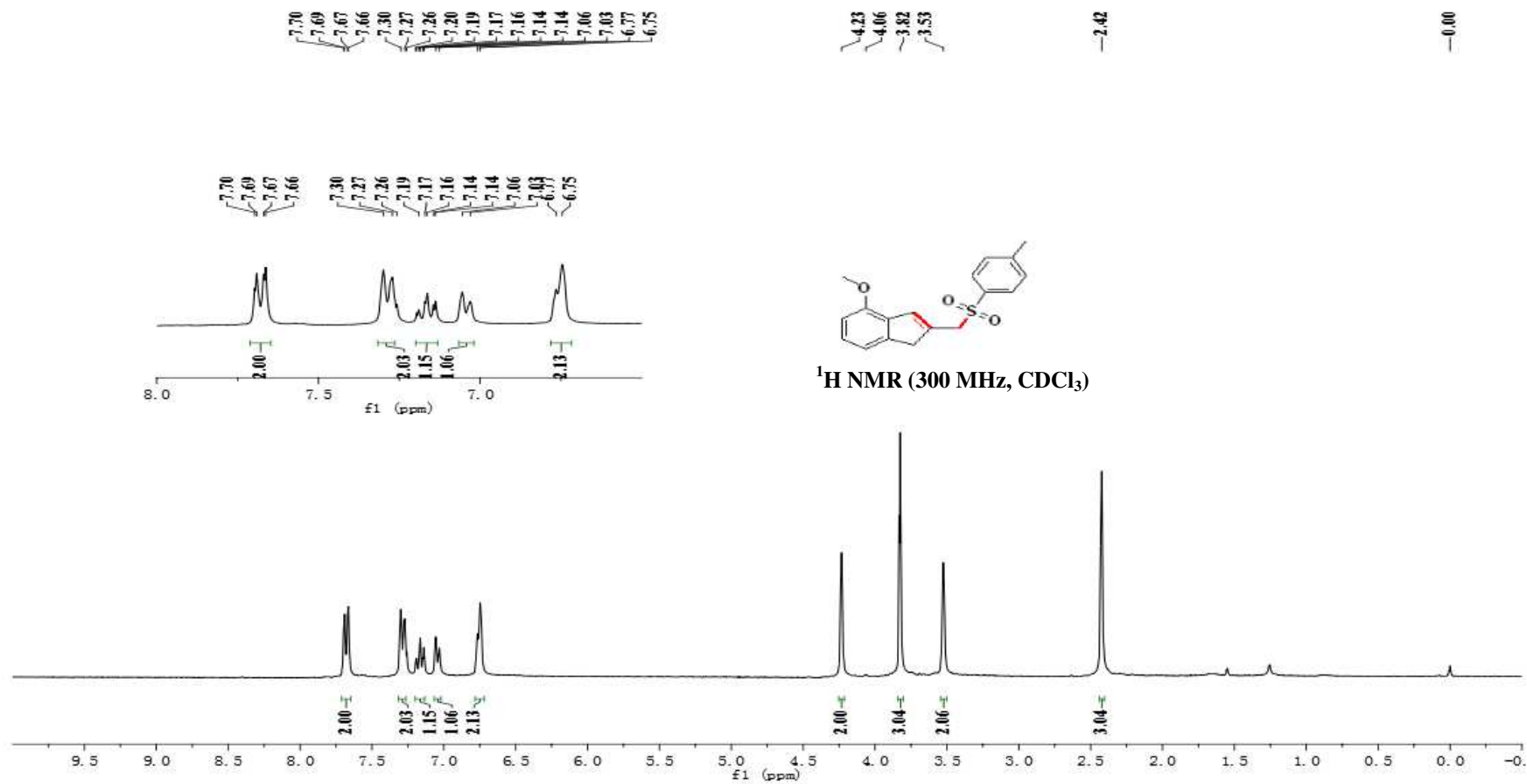
¹H NMR (300 MHz, CDCl₃)



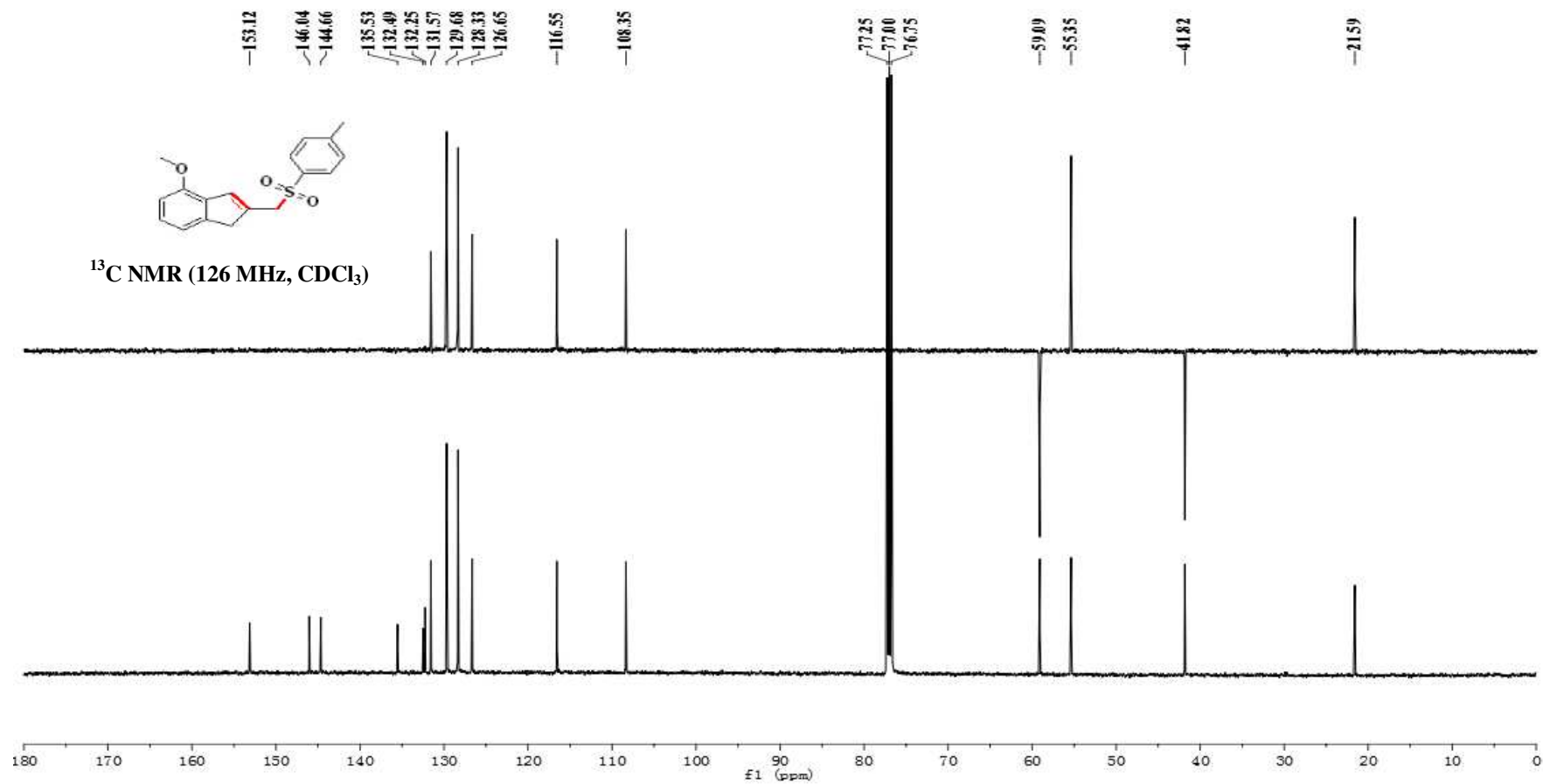
2-(Tosylmethyl)-1*H*-indene (3a)



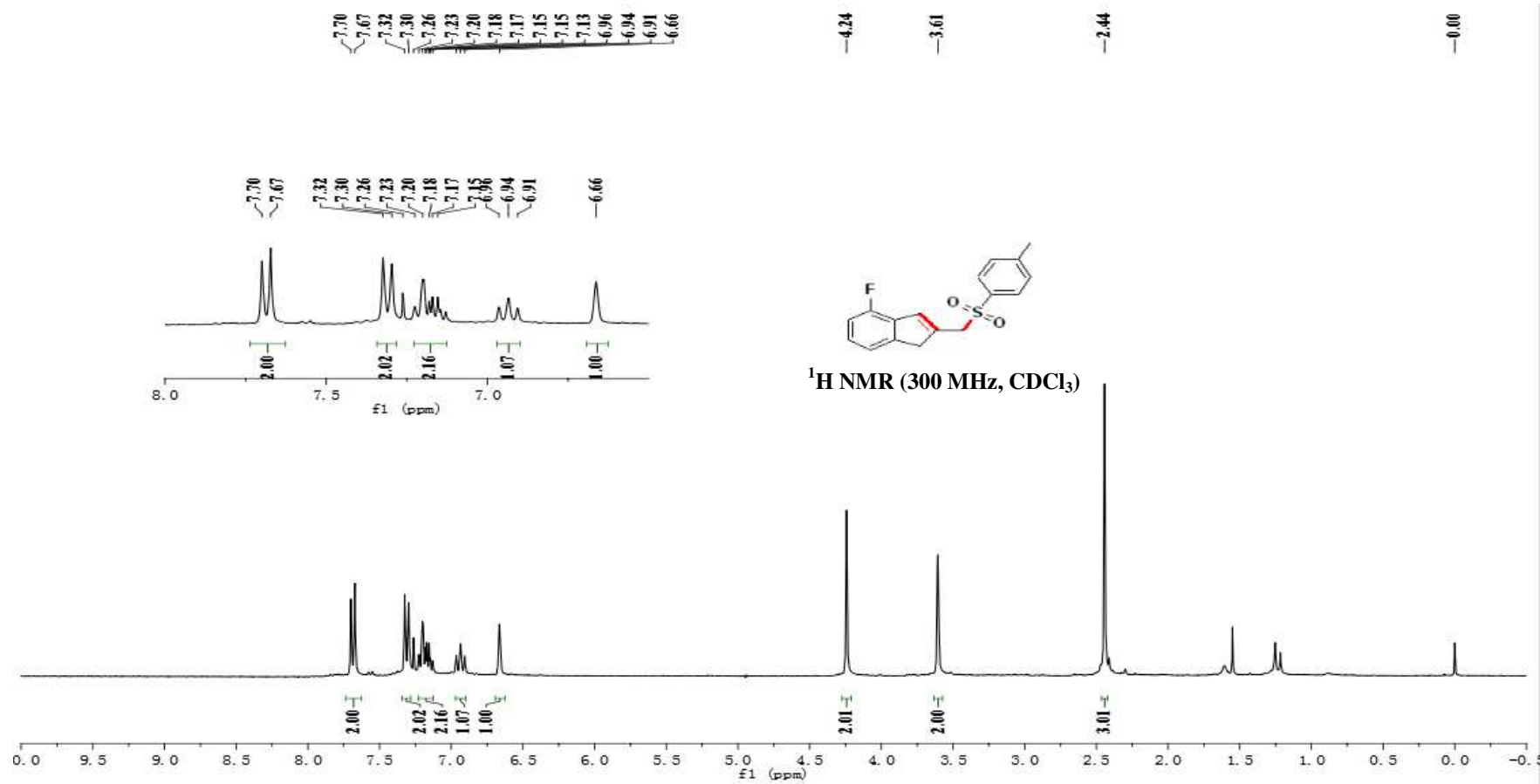
4-Methoxy-2-(tosylmethyl)-1H-indene (3b)



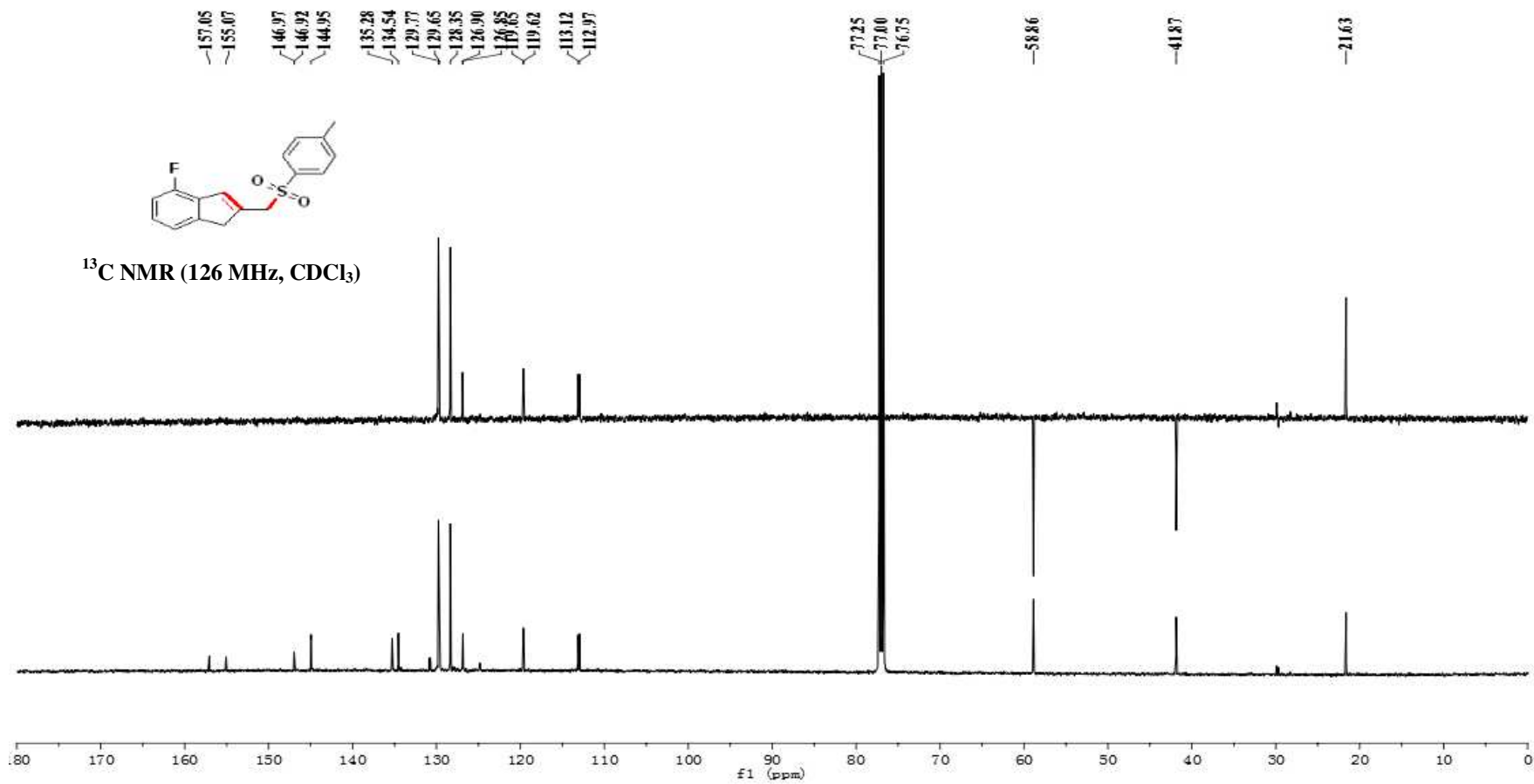
4-Methoxy-2-(tosylmethyl)-1*H*-indene (3b)



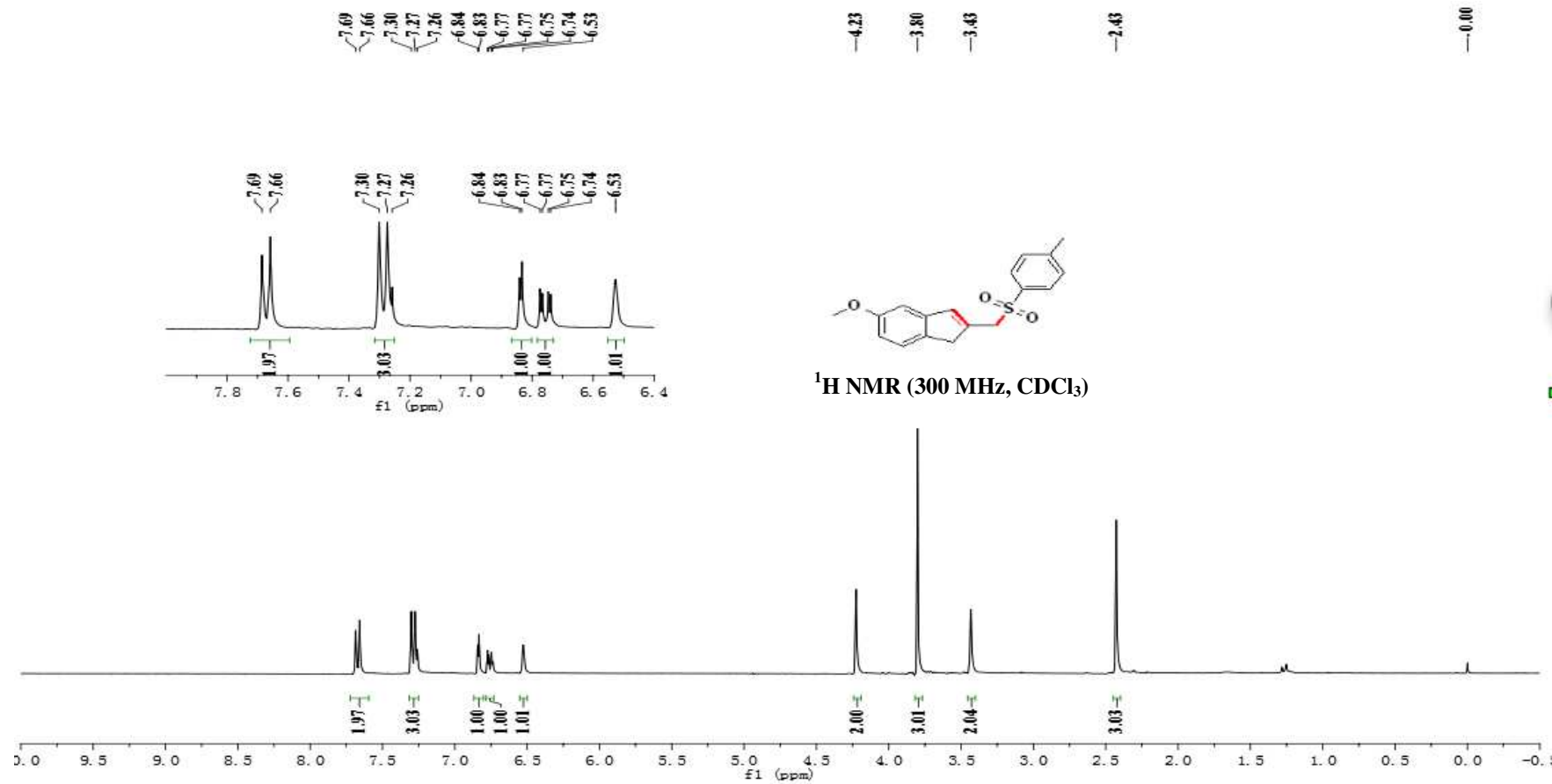
4-Fluoro-2-(tosylmethyl)-1*H*-indene (3c)



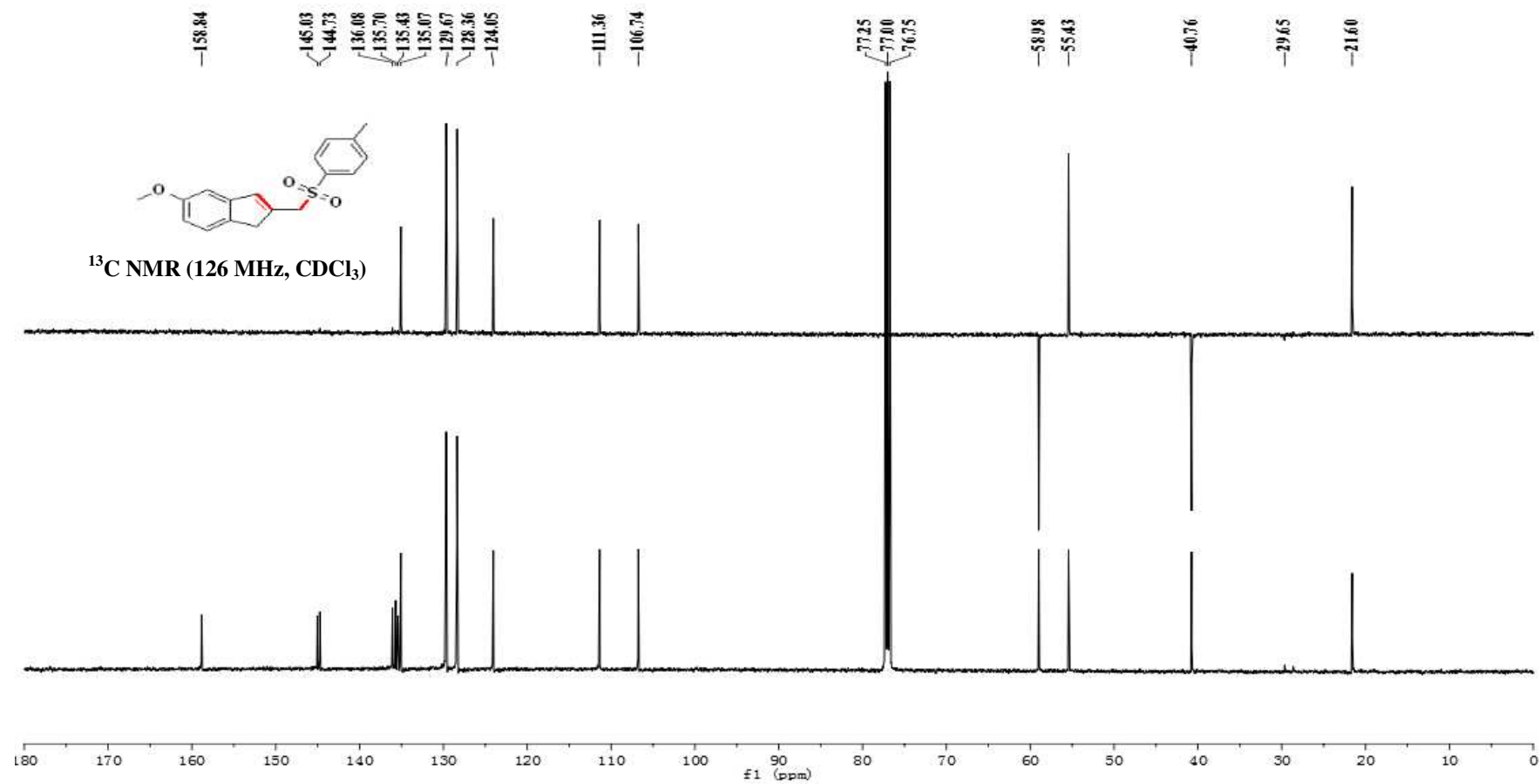
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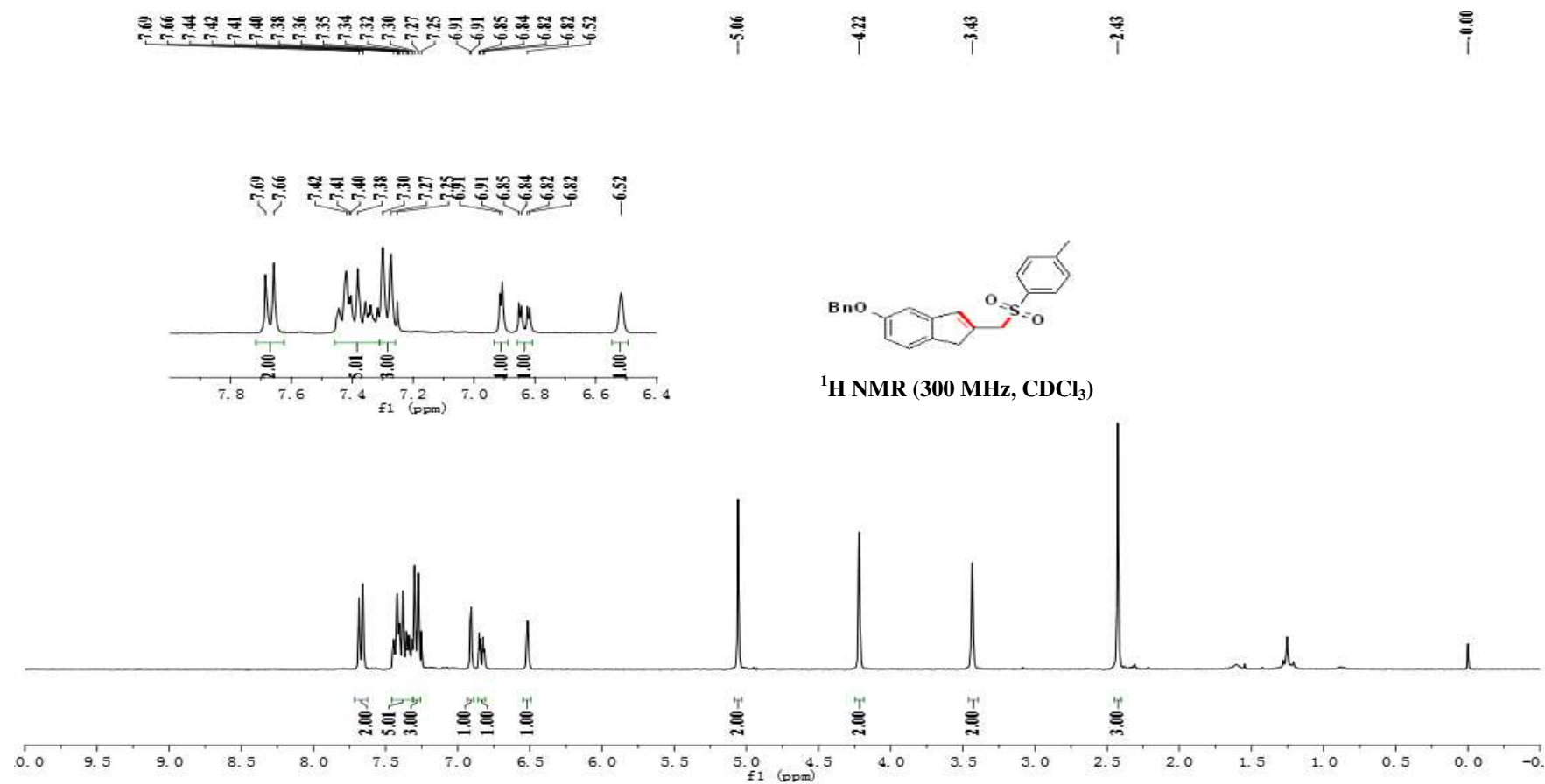
5-Methoxy-2-(tosylmethyl)-1*H*-indene (3d)



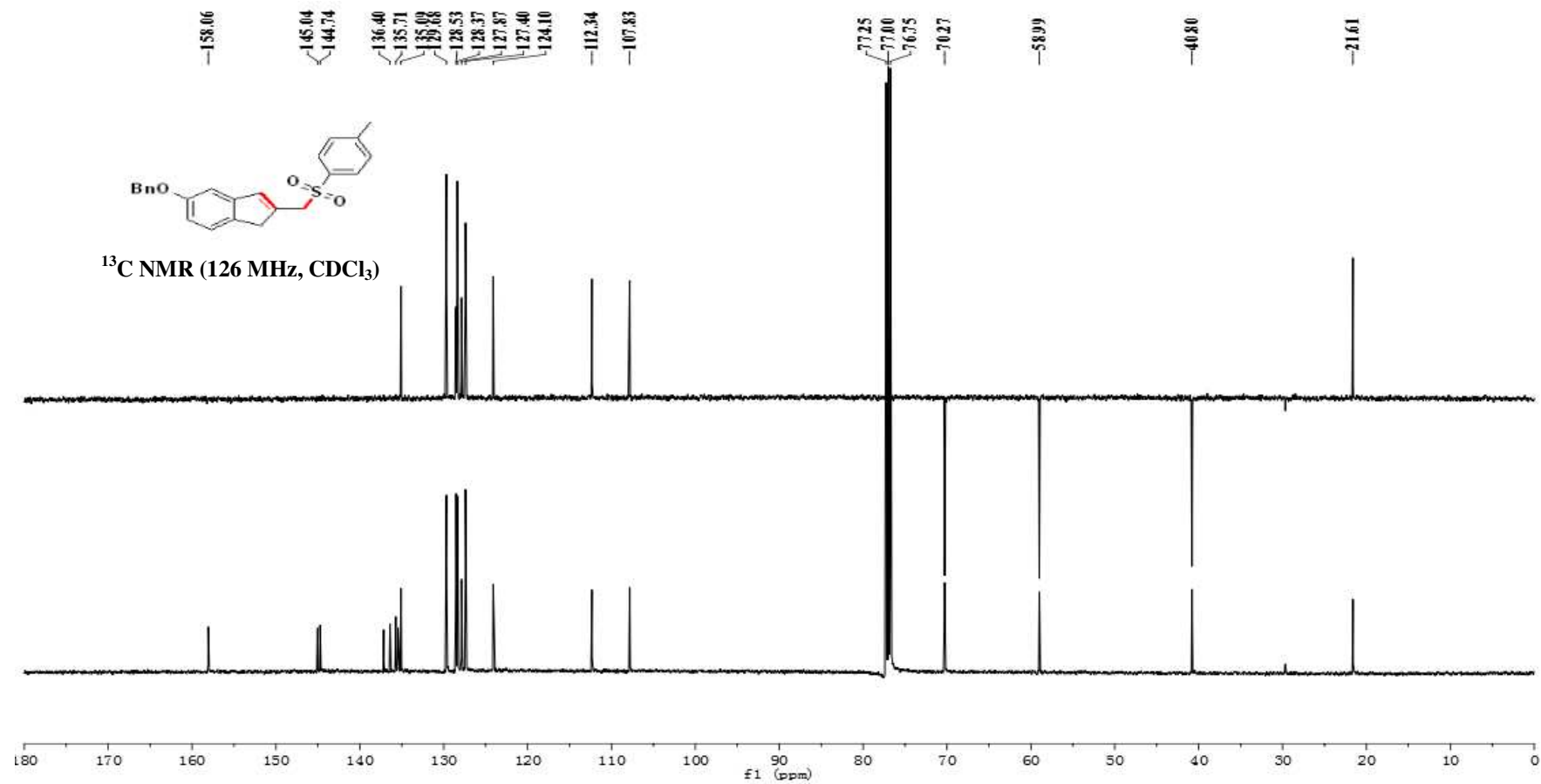
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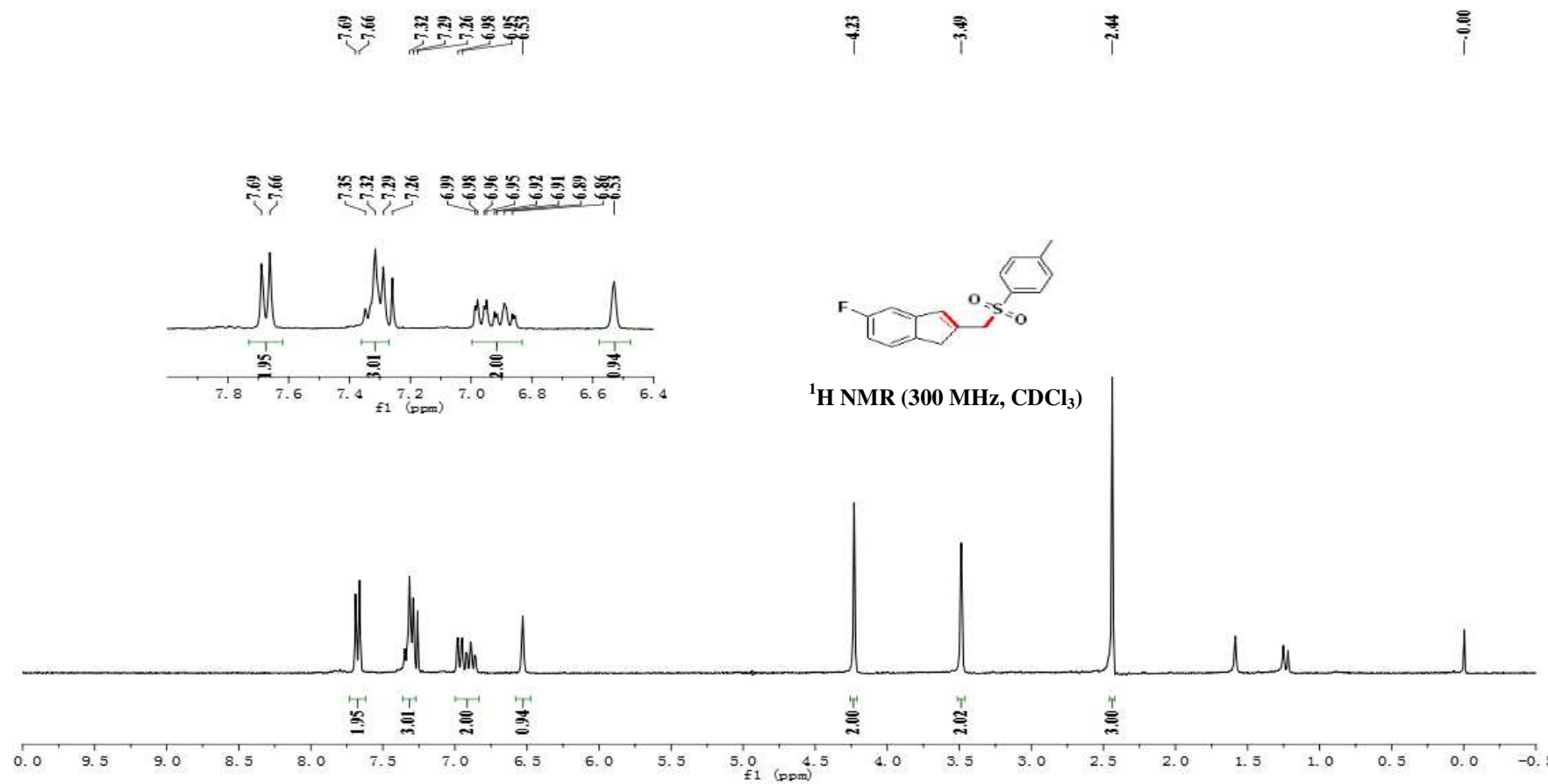
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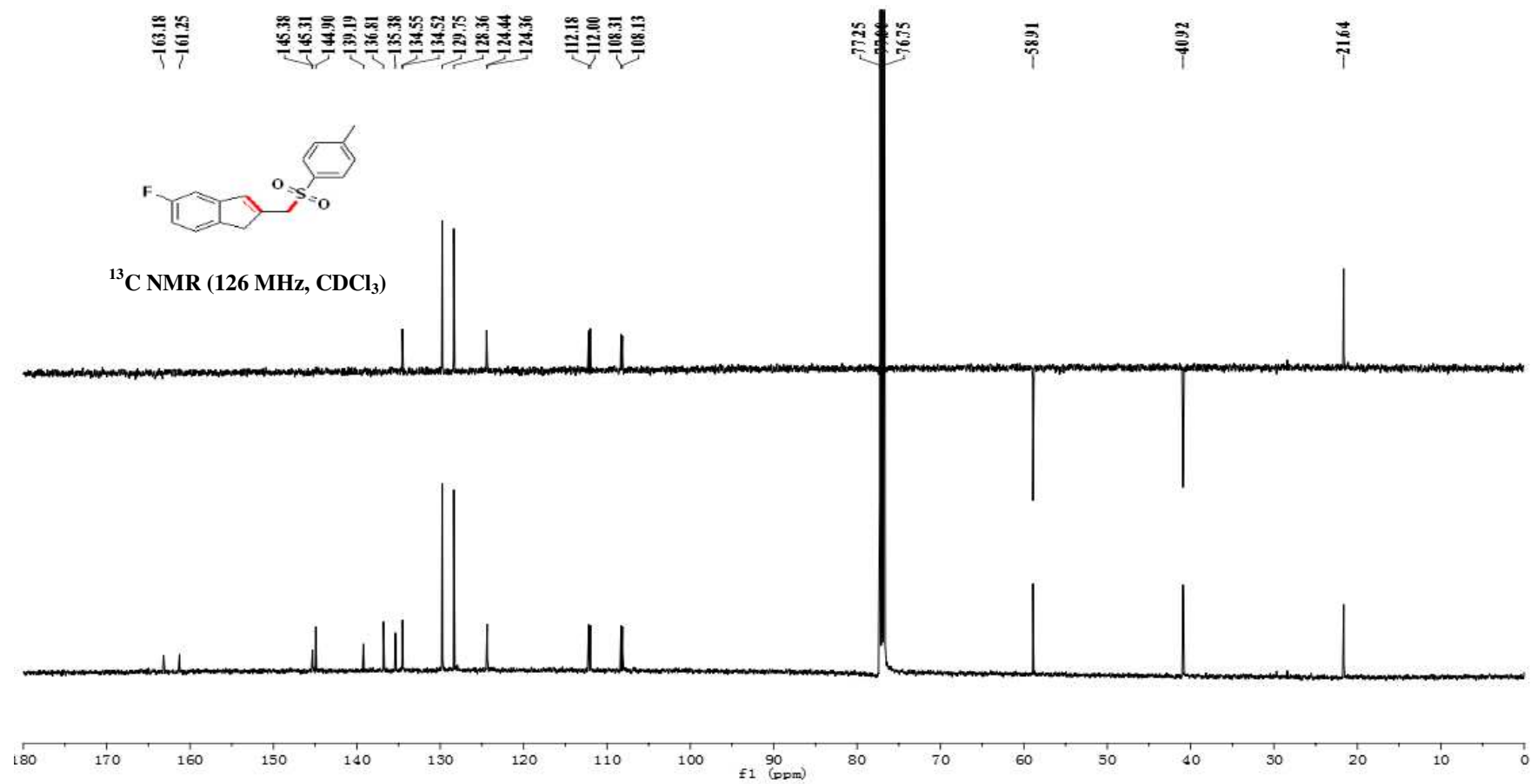
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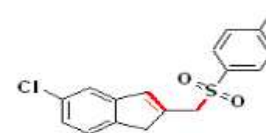
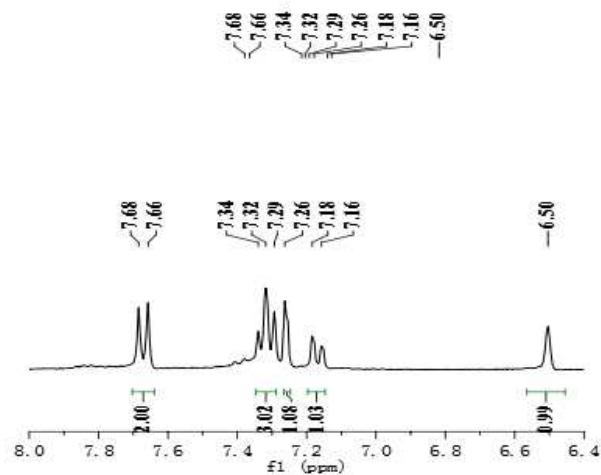
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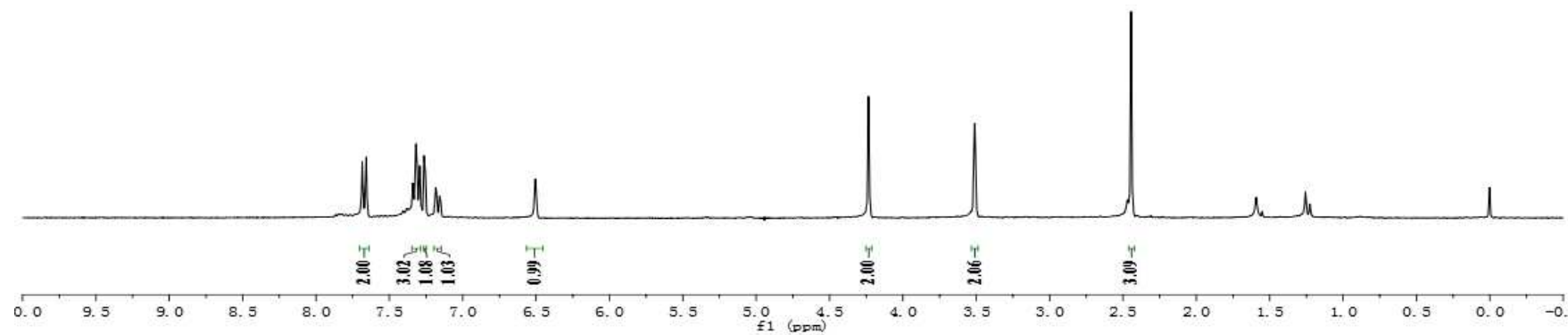
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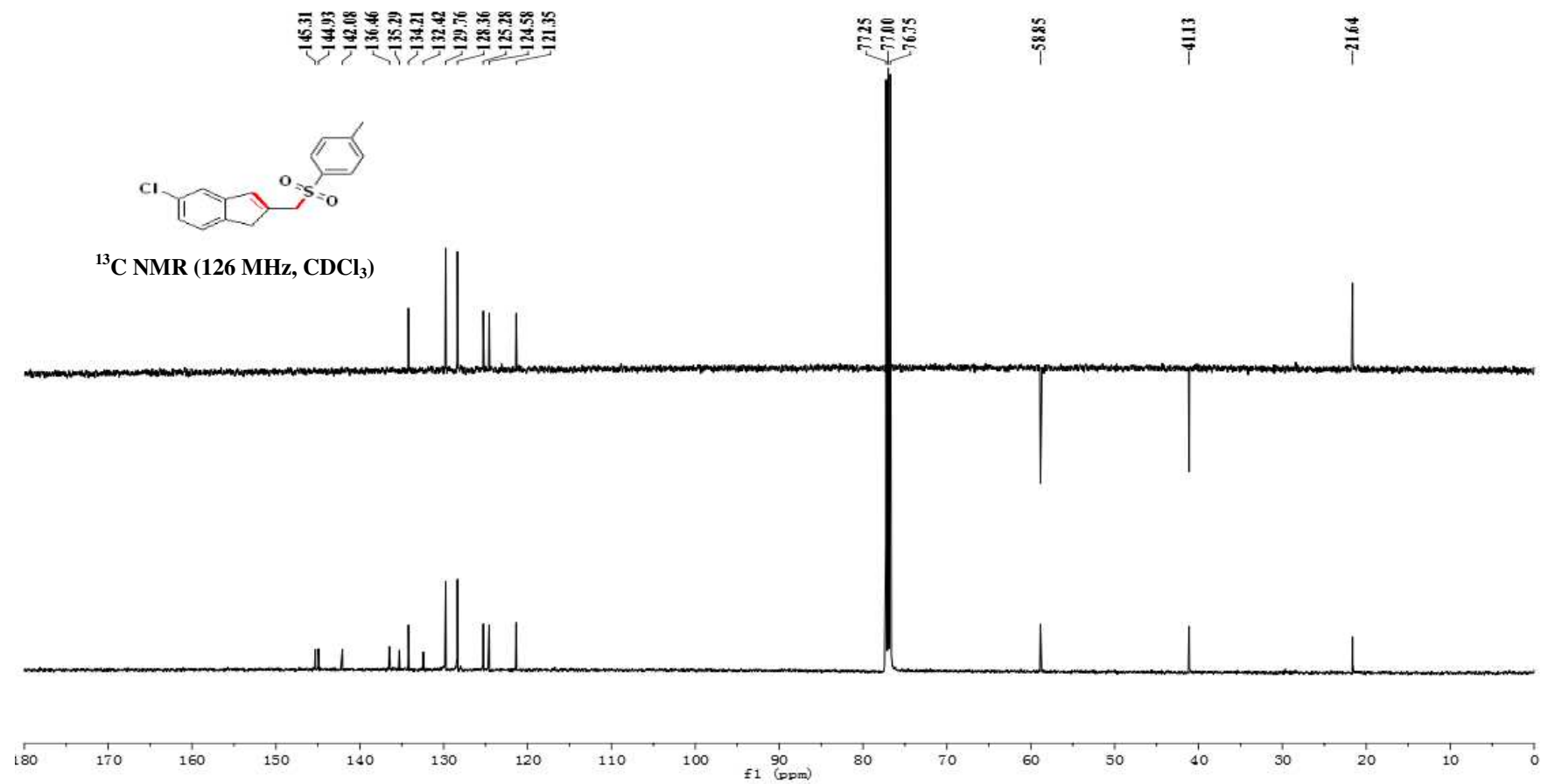
5-Chloro-2-(tosylmethyl)-1*H*-indene (3g)



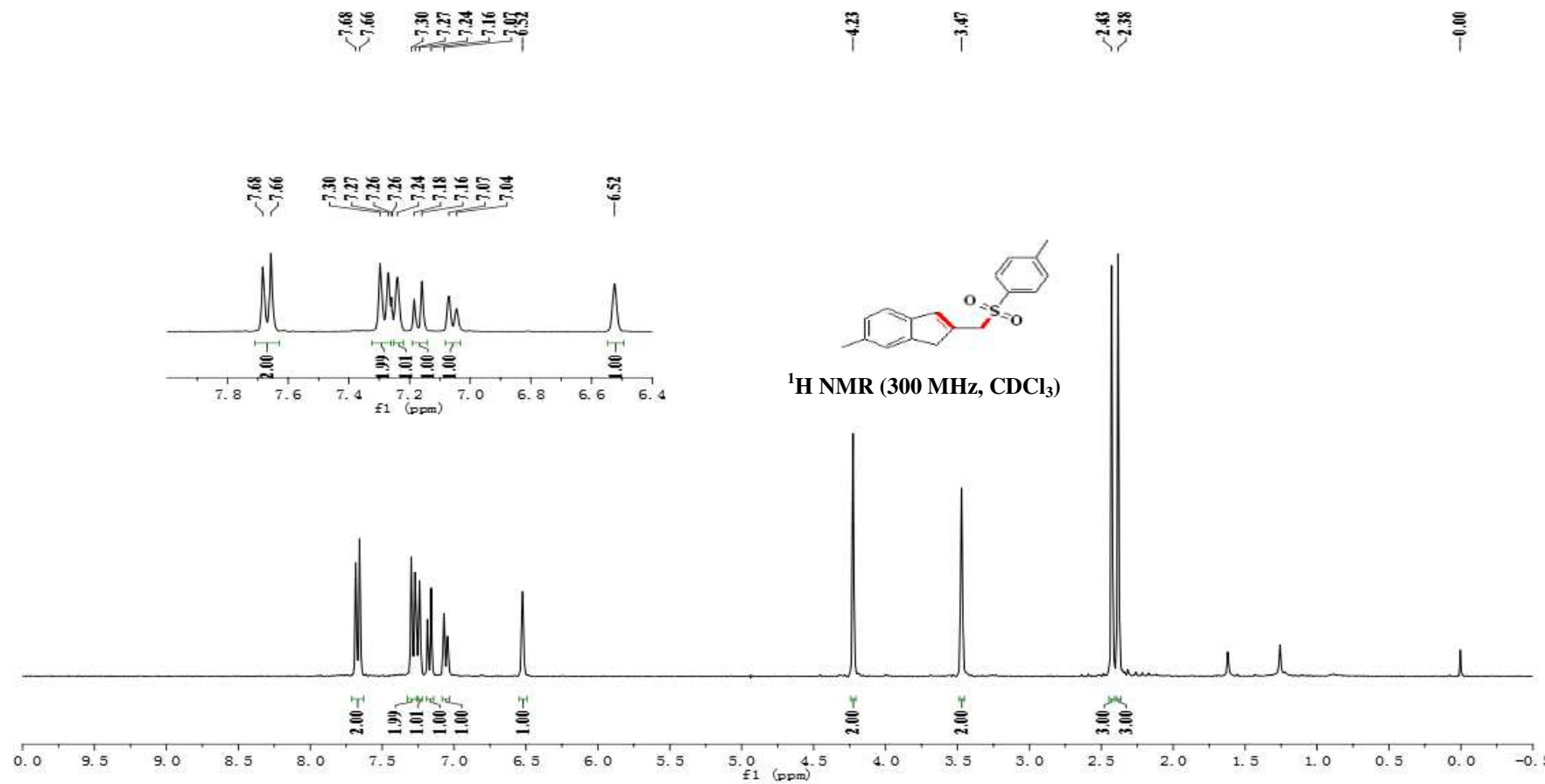
¹H NMR (300 MHz, CDCl₃)



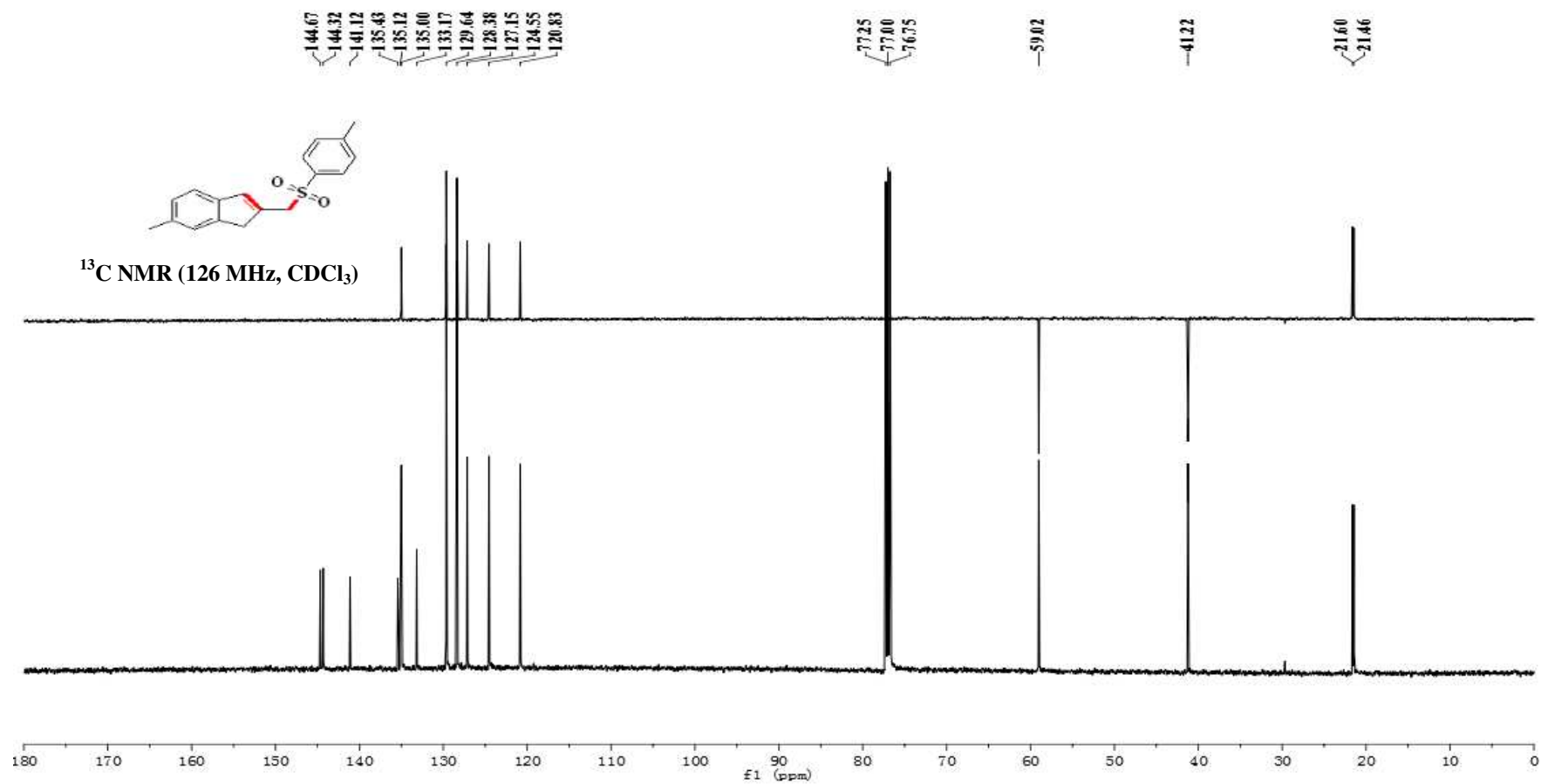
5-Chloro-2-(tosylmethyl)-1*H*-indene (3g)



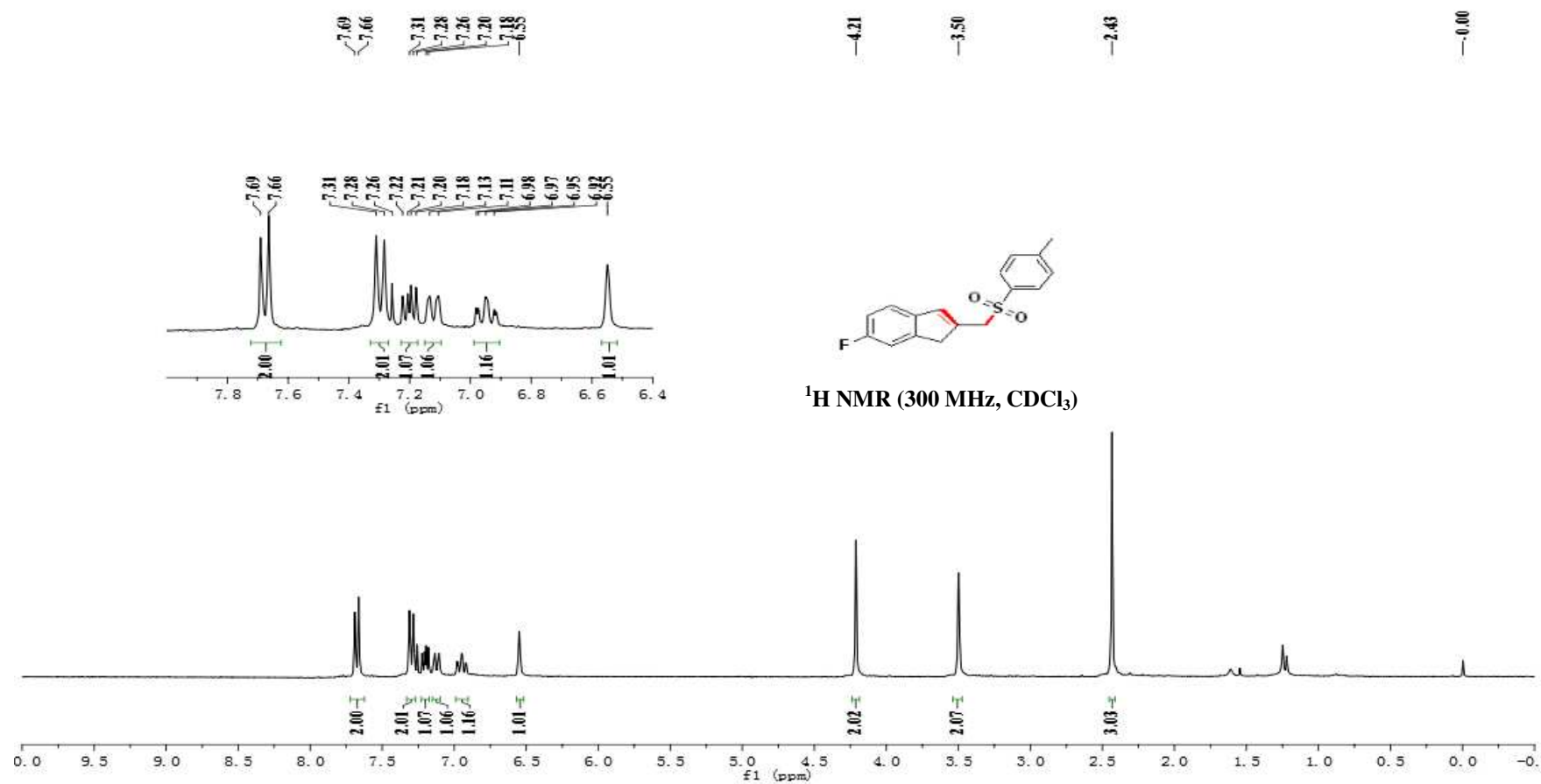
6-Methyl-2-(tosylmethyl)-1*H*-indene (3h)



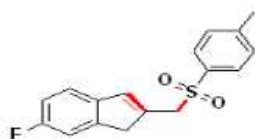
6-Methyl-2-(tosylmethyl)-1*H*-indene (3h)



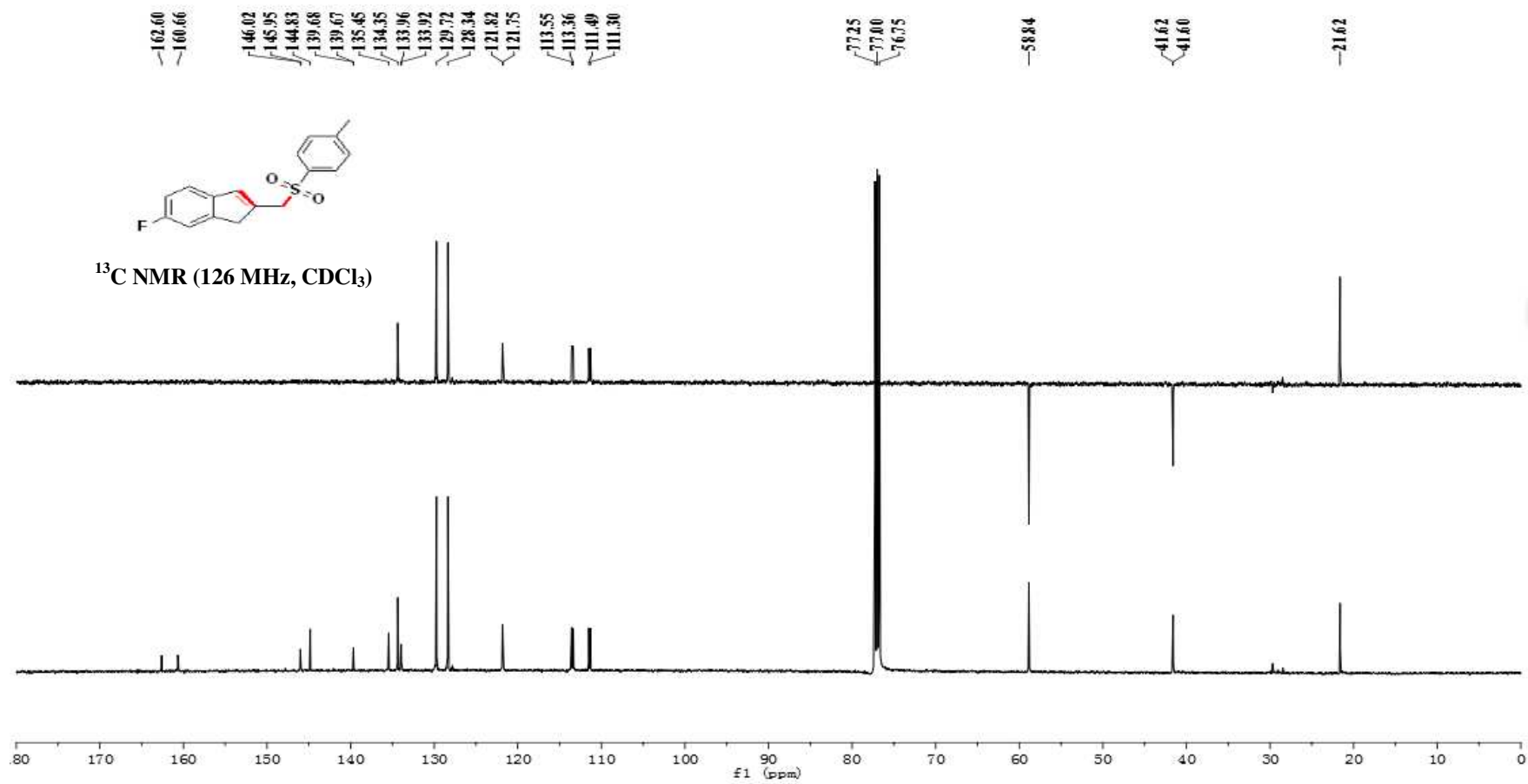
6-Fluoro-2-(tosylmethyl)-1*H*-indene (3i)



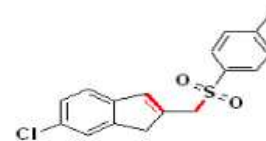
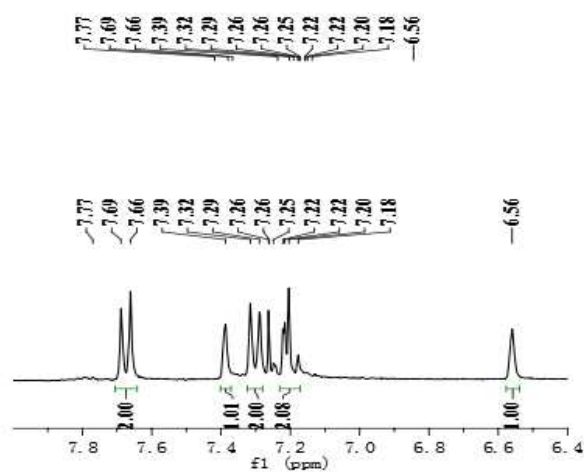
6-Fluoro-2-(tosylmethyl)-1*H*-indene (3i)



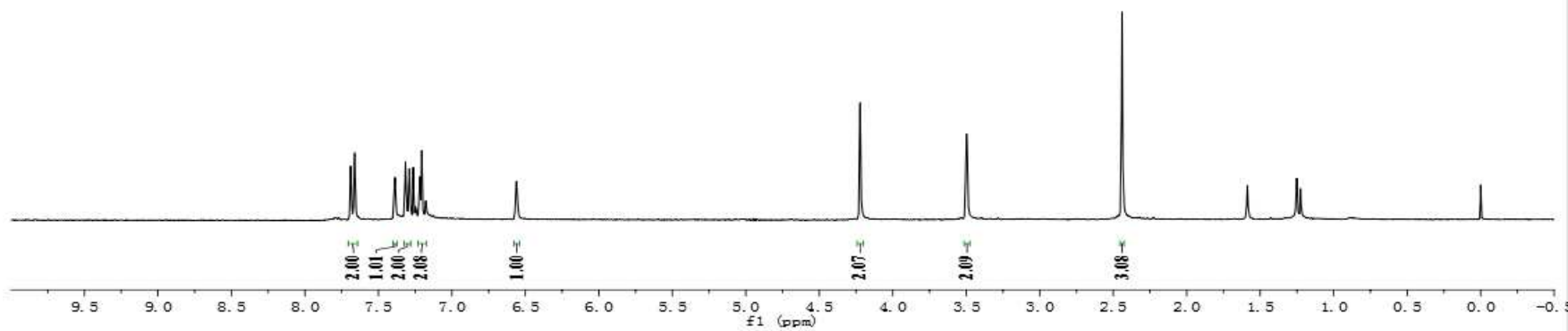
^{13}C NMR (126 MHz, CDCl_3)



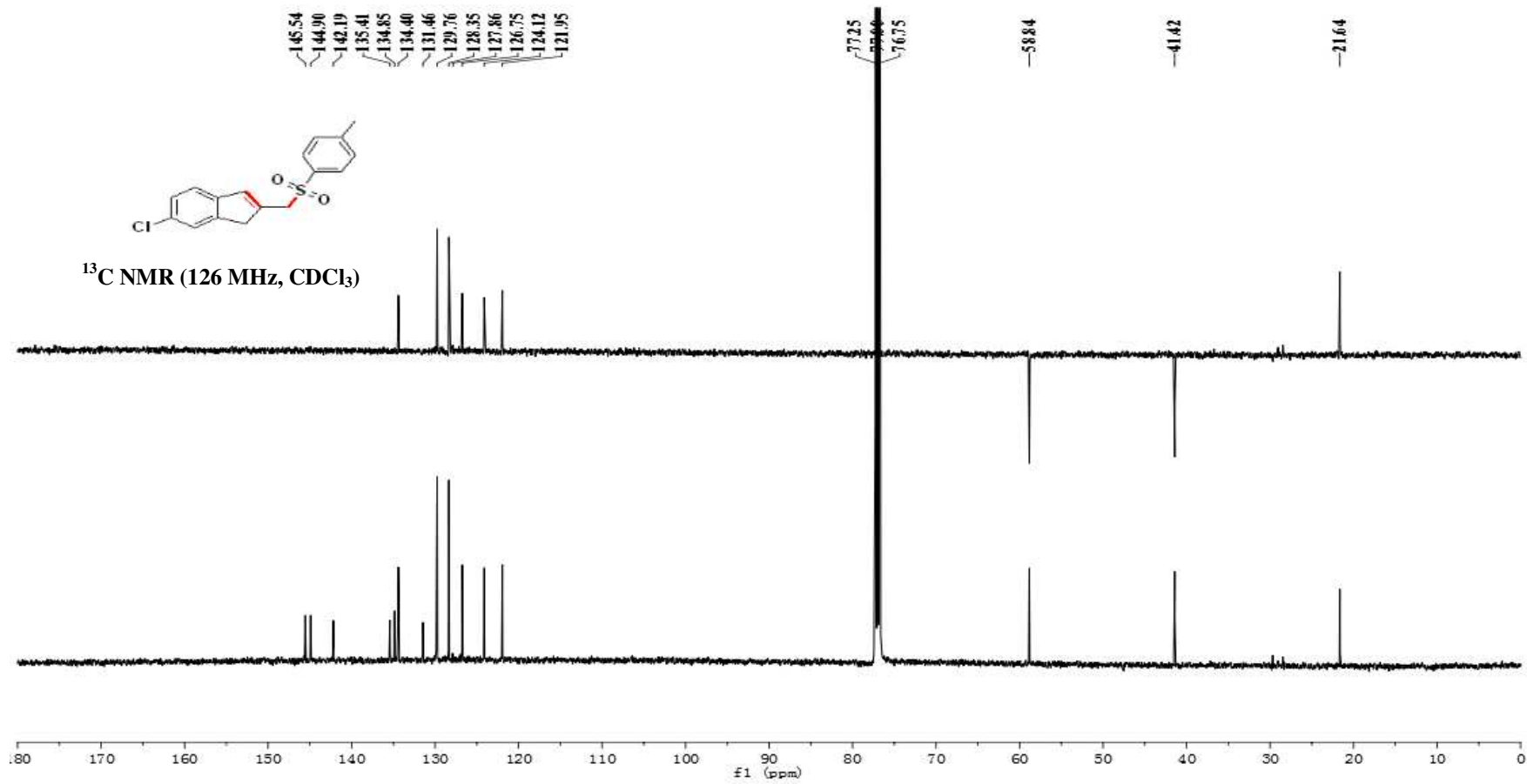
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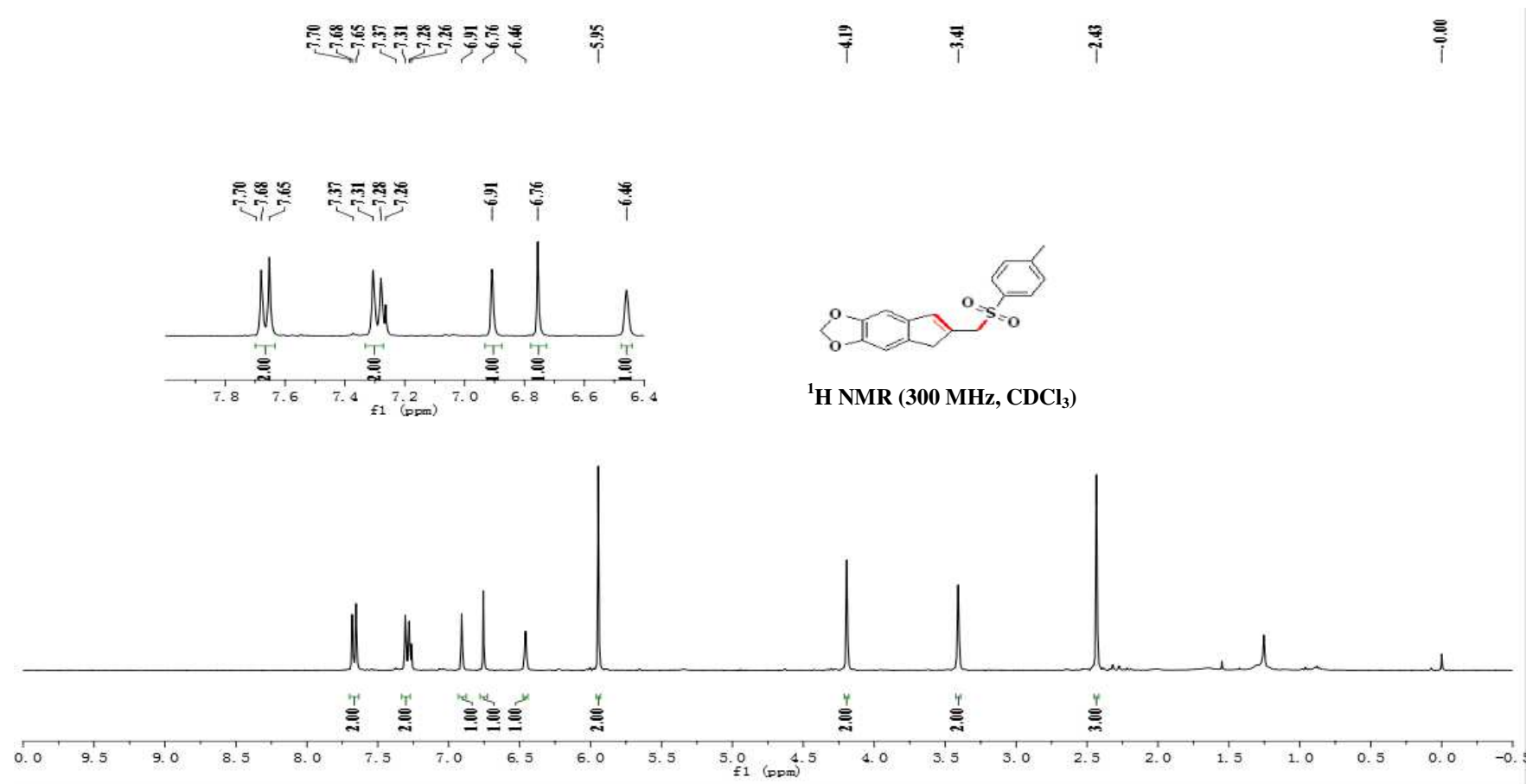
^1H NMR (300 MHz, CDCl_3)



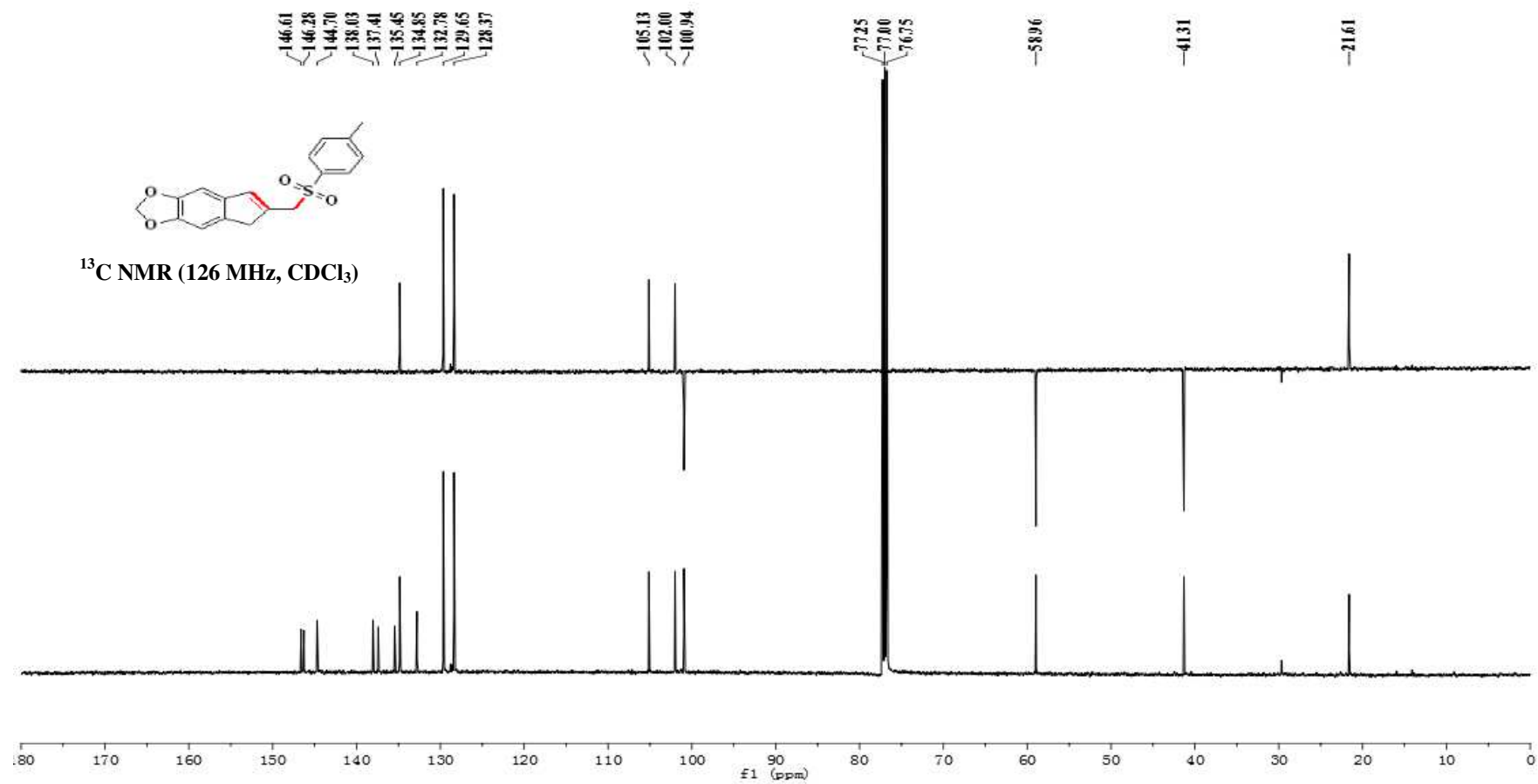
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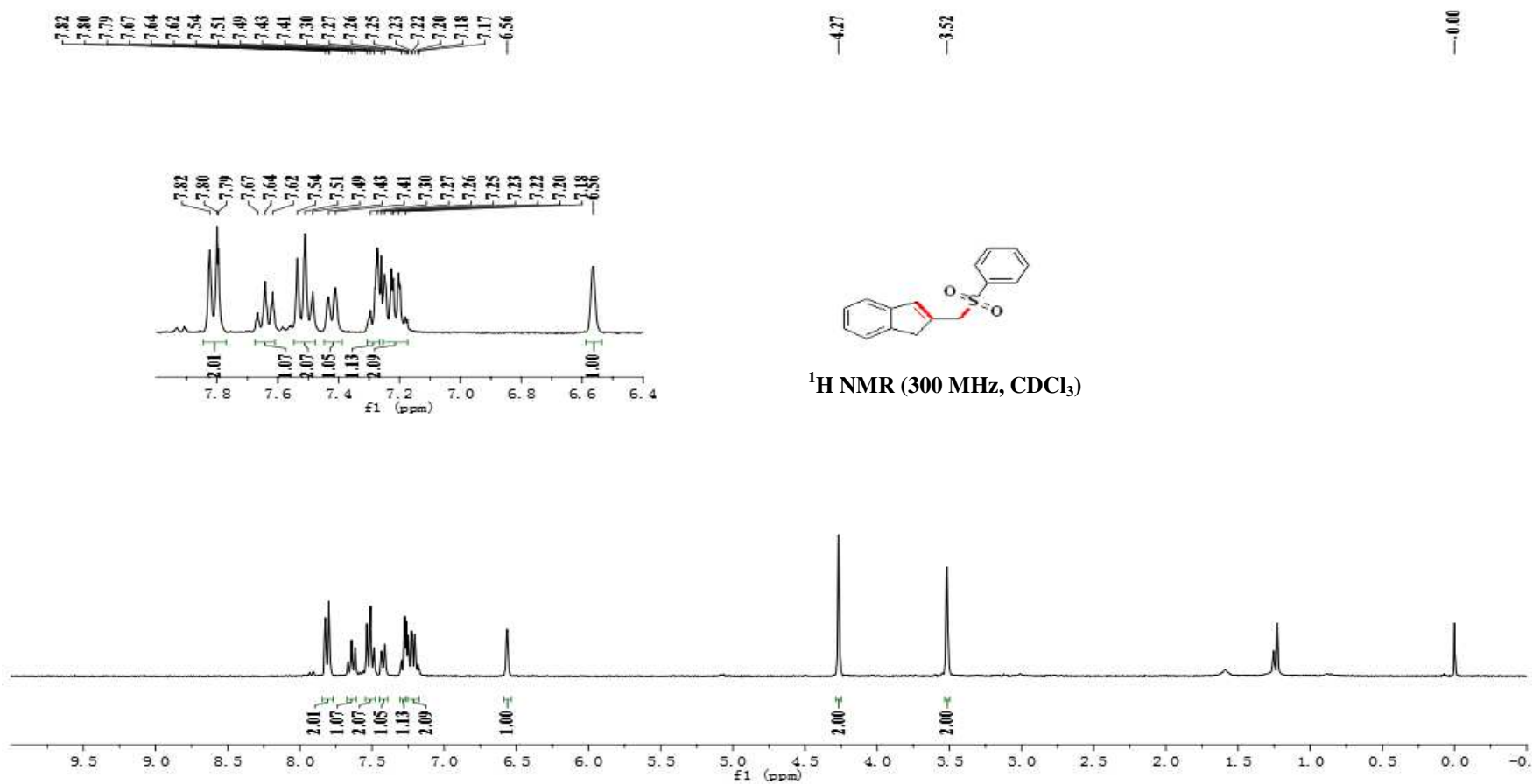
6-(Tosylmethyl)-5*H*-indeno[5,6-*d*][1,3]dioxole (3k)



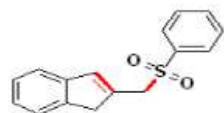
6-(Tosylmethyl)-5*H*-indeno[5,6-*d*][1,3]dioxole (3k)



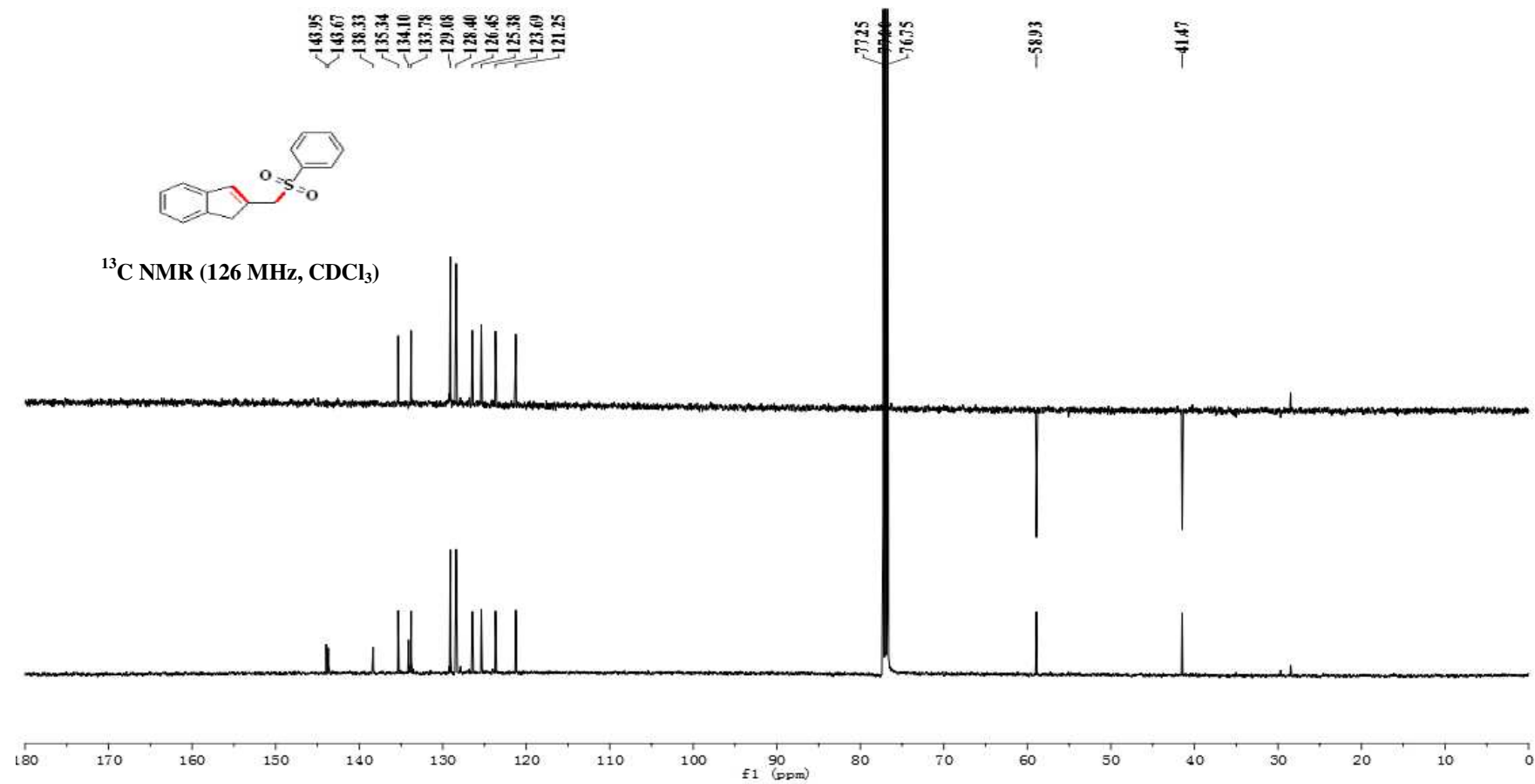
2-((Phenylsulfonyl)methyl)-1*H*-indene (3l)



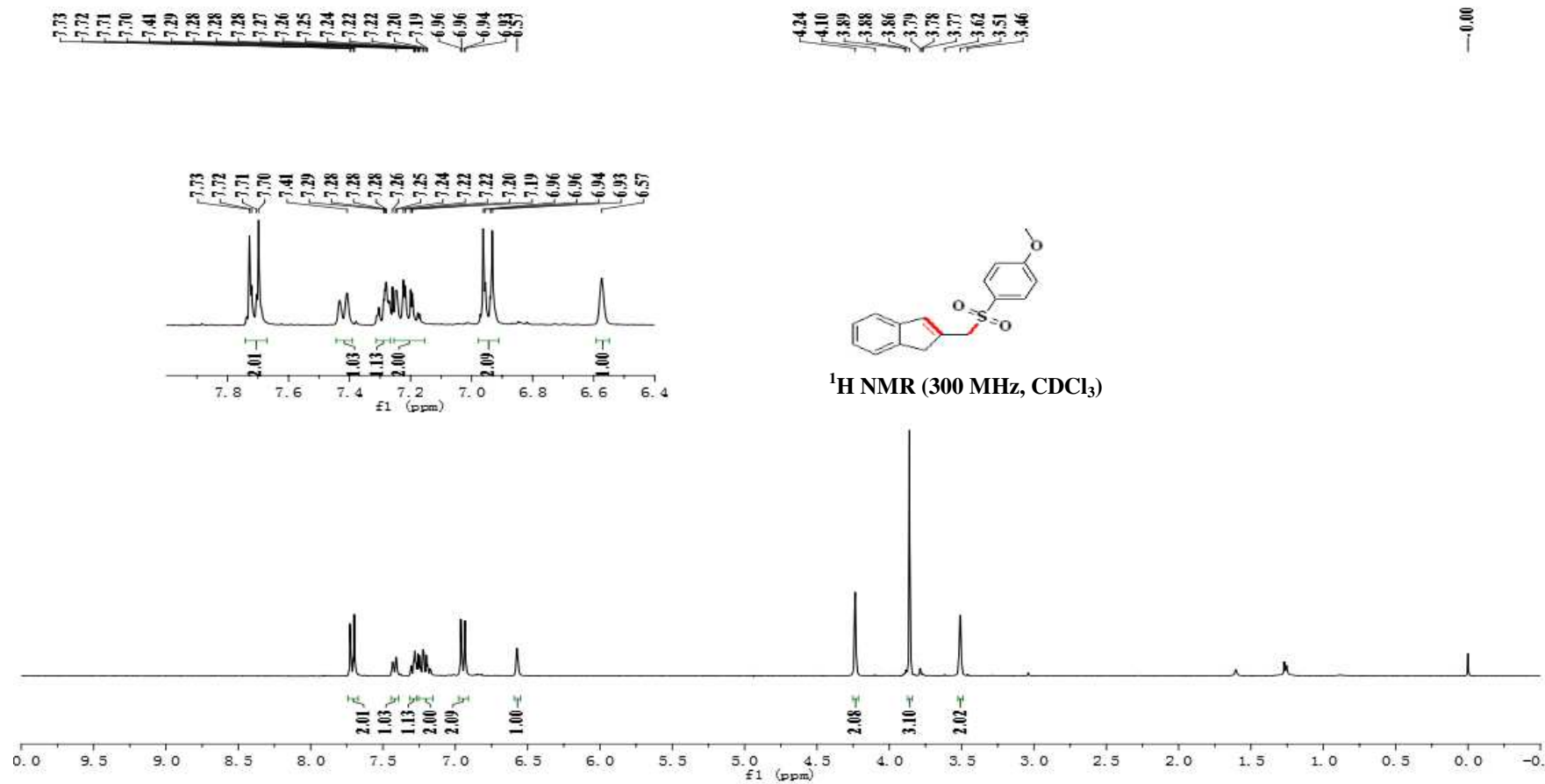
2-((Phenylsulfonyl)methyl)-1*H*-indene (3l)



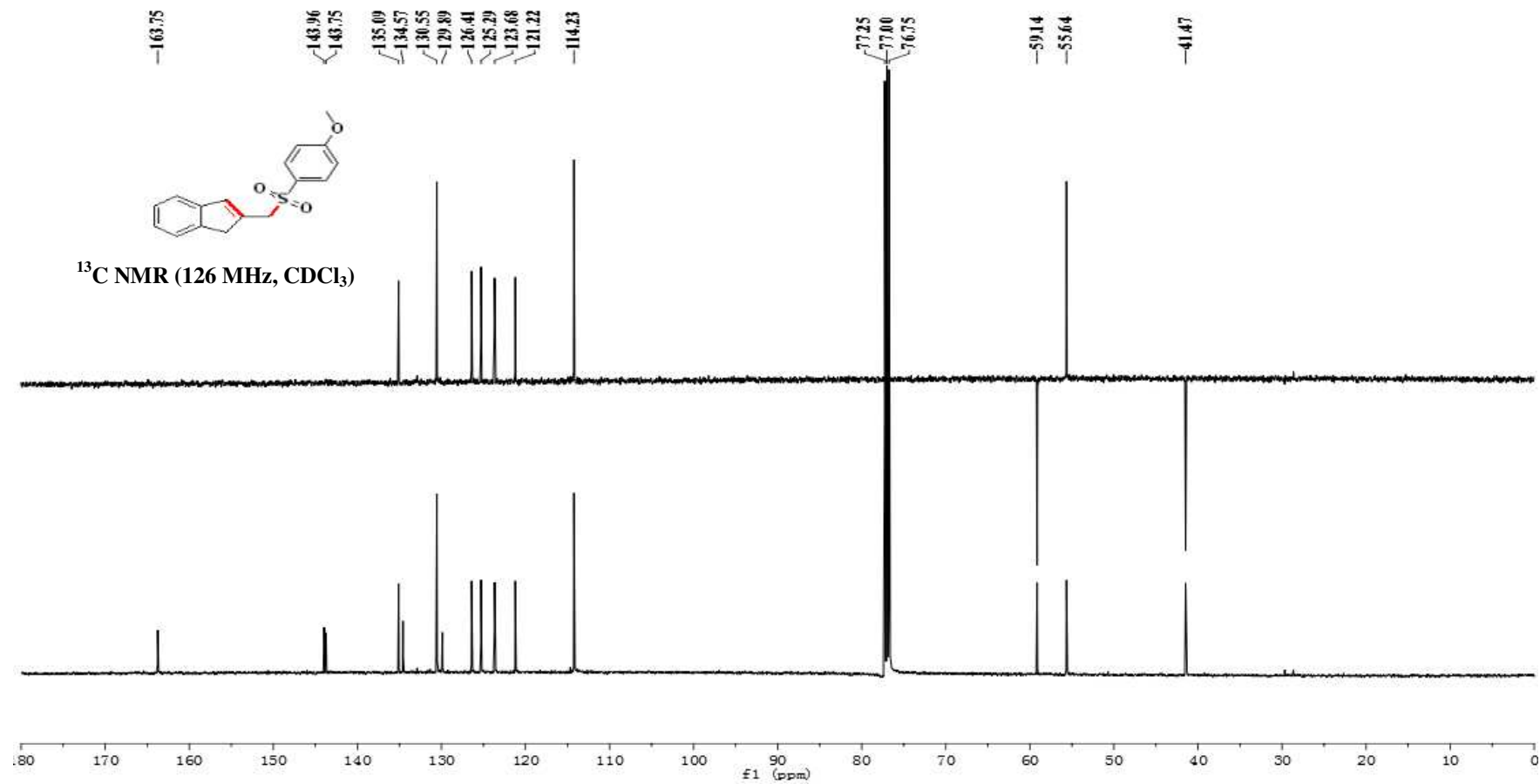
^{13}C NMR (126 MHz, CDCl_3)



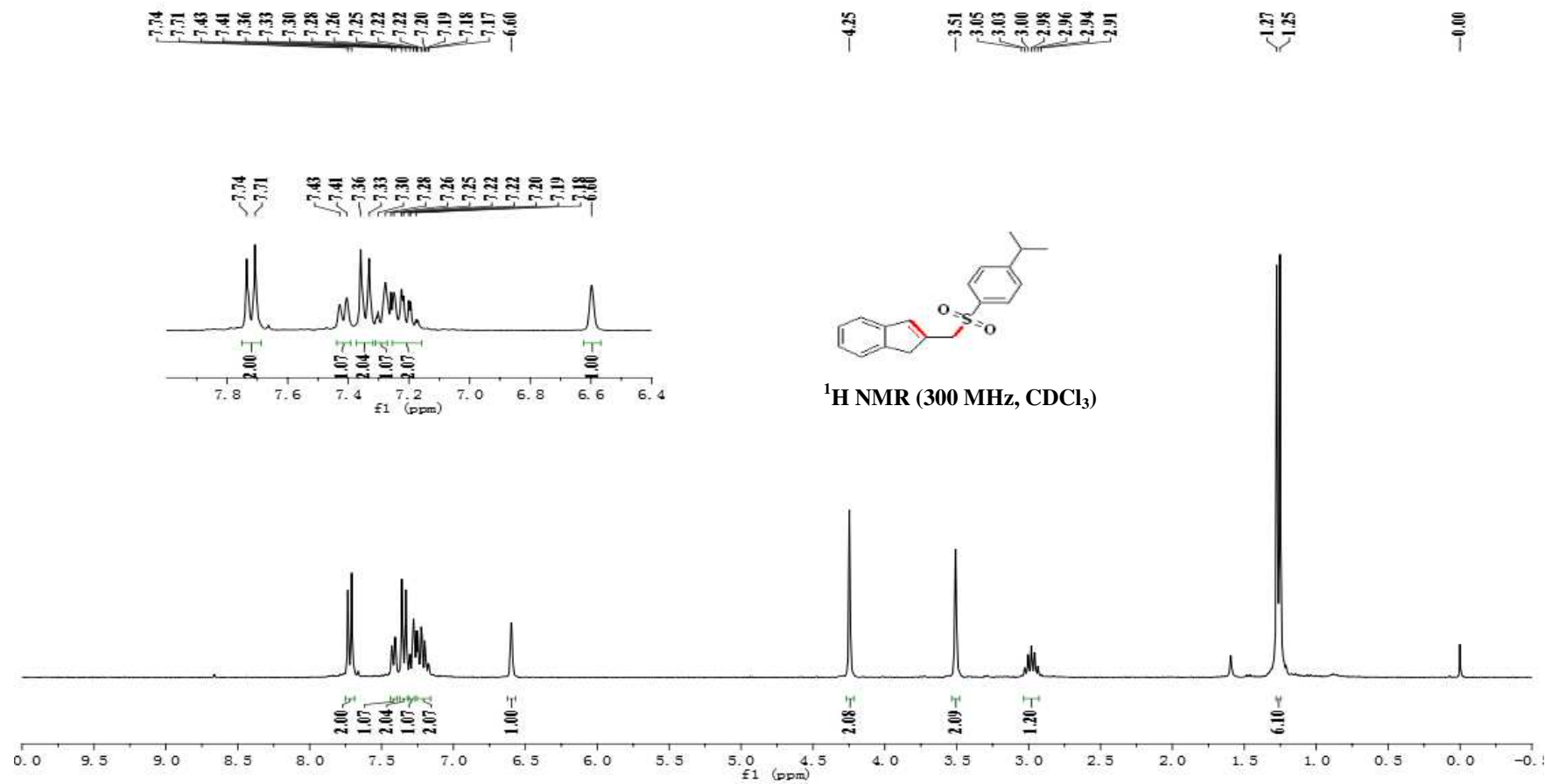
2-(((4-Methoxyphenyl)sulfonyl)methyl)-1*H*-indene (3m)



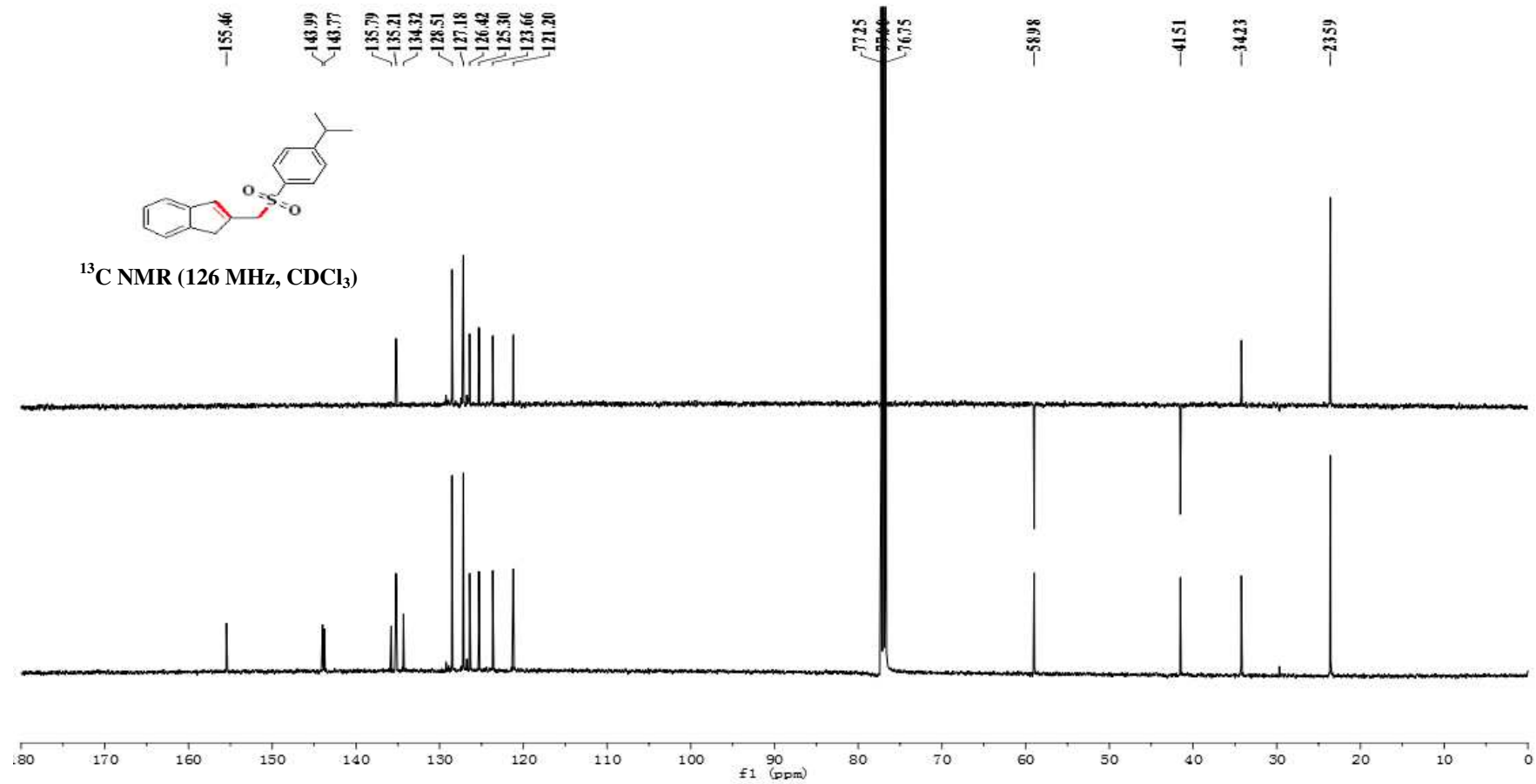
2-(((4-Methoxyphenyl)sulfonyl)methyl)-1*H*-indene (3m)



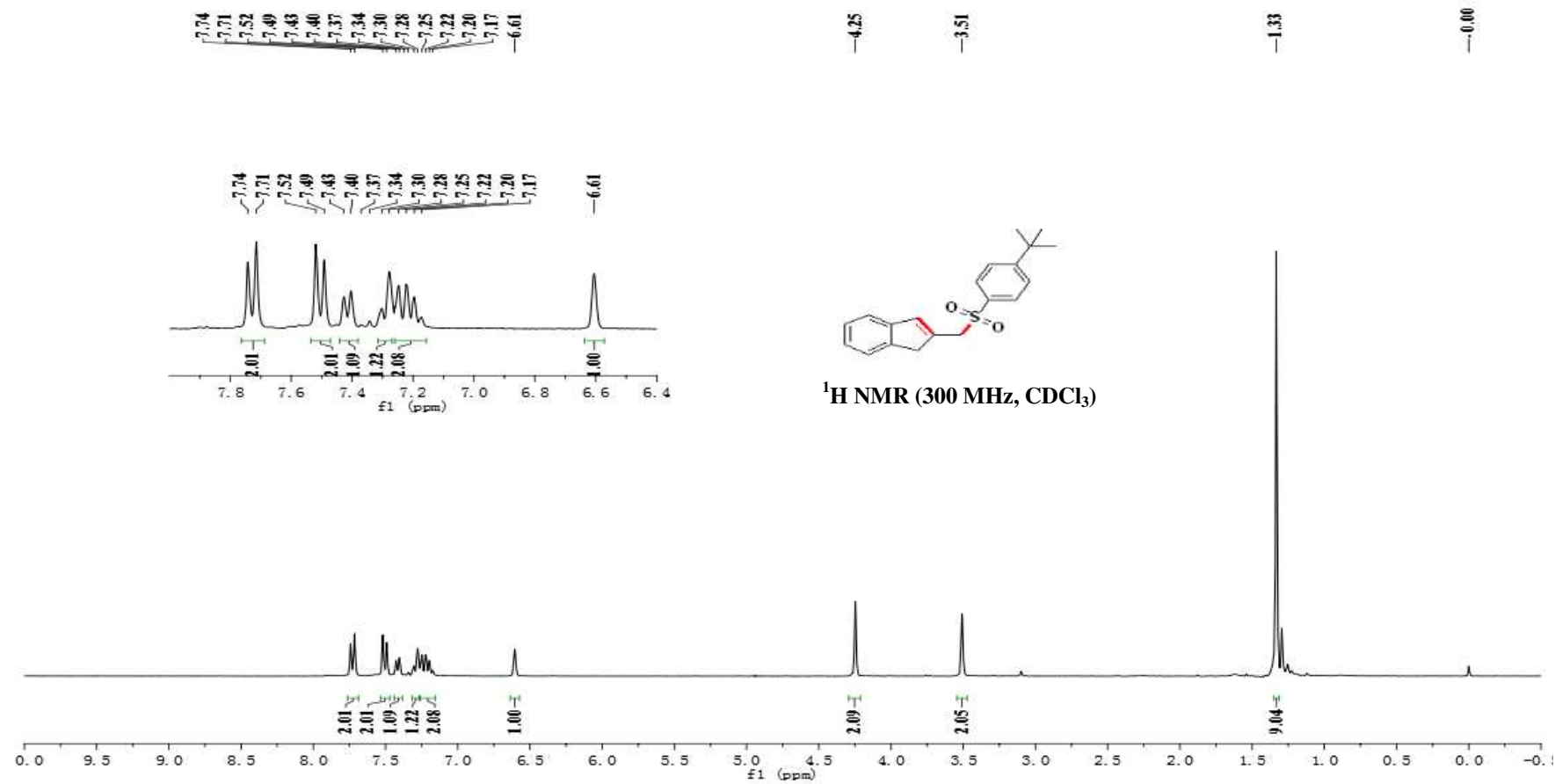
2-(((4-Isopropylphenyl)sulfonyl)methyl)-1H-indene (3n)



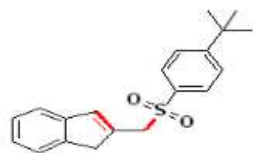
2-(((4-Isopropylphenyl)sulfonyl)methyl)-1H-indene (3n)



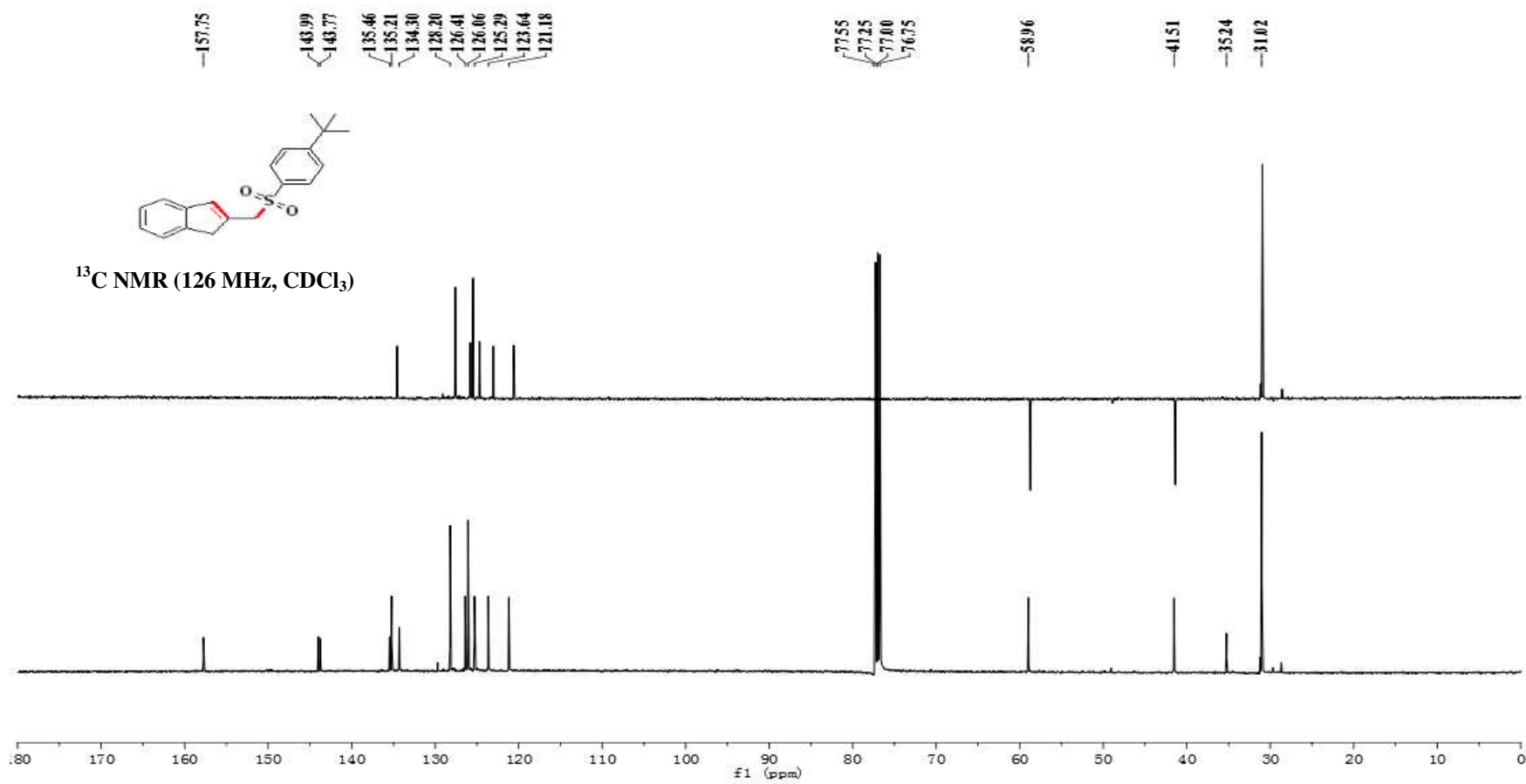
2-(((4-(*tert*-Butyl)phenyl)sulfonyl)methyl)-1*H*-indene (3o)



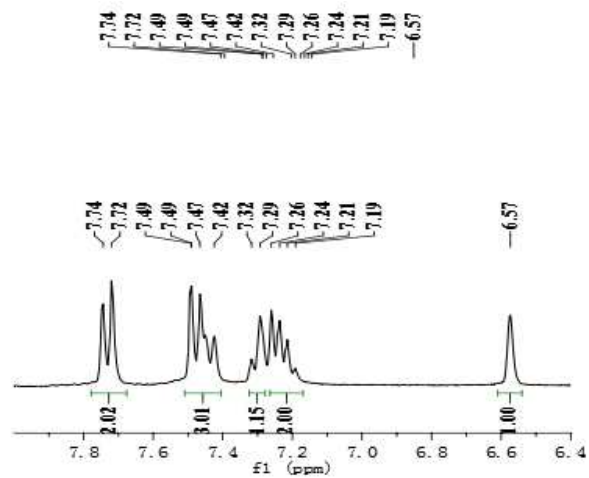
2-(((4-(*tert*-Butyl)phenyl)sulfonyl)methyl)-1*H*-indene (3o)



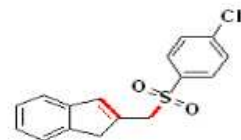
^{13}C NMR (126 MHz, CDCl_3)



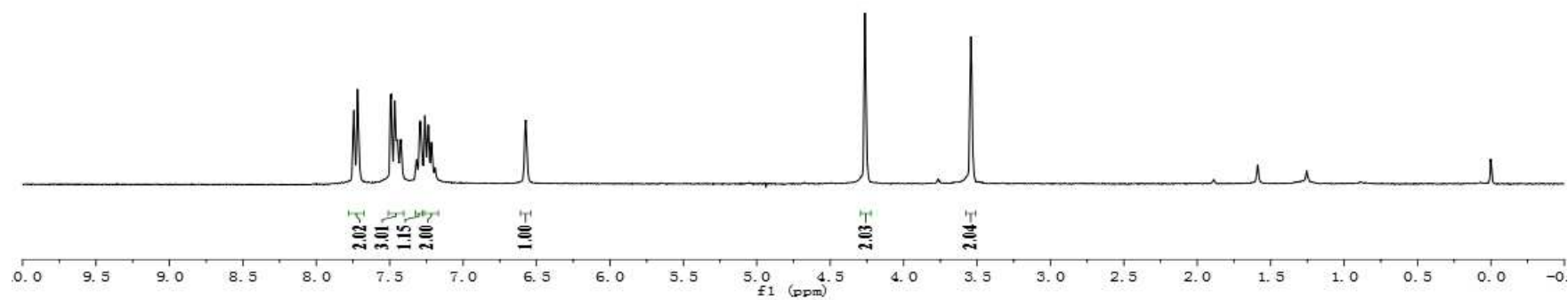
2-(((4-Chlorophenyl)sulfonyl)methyl)-1H-indene (3p)



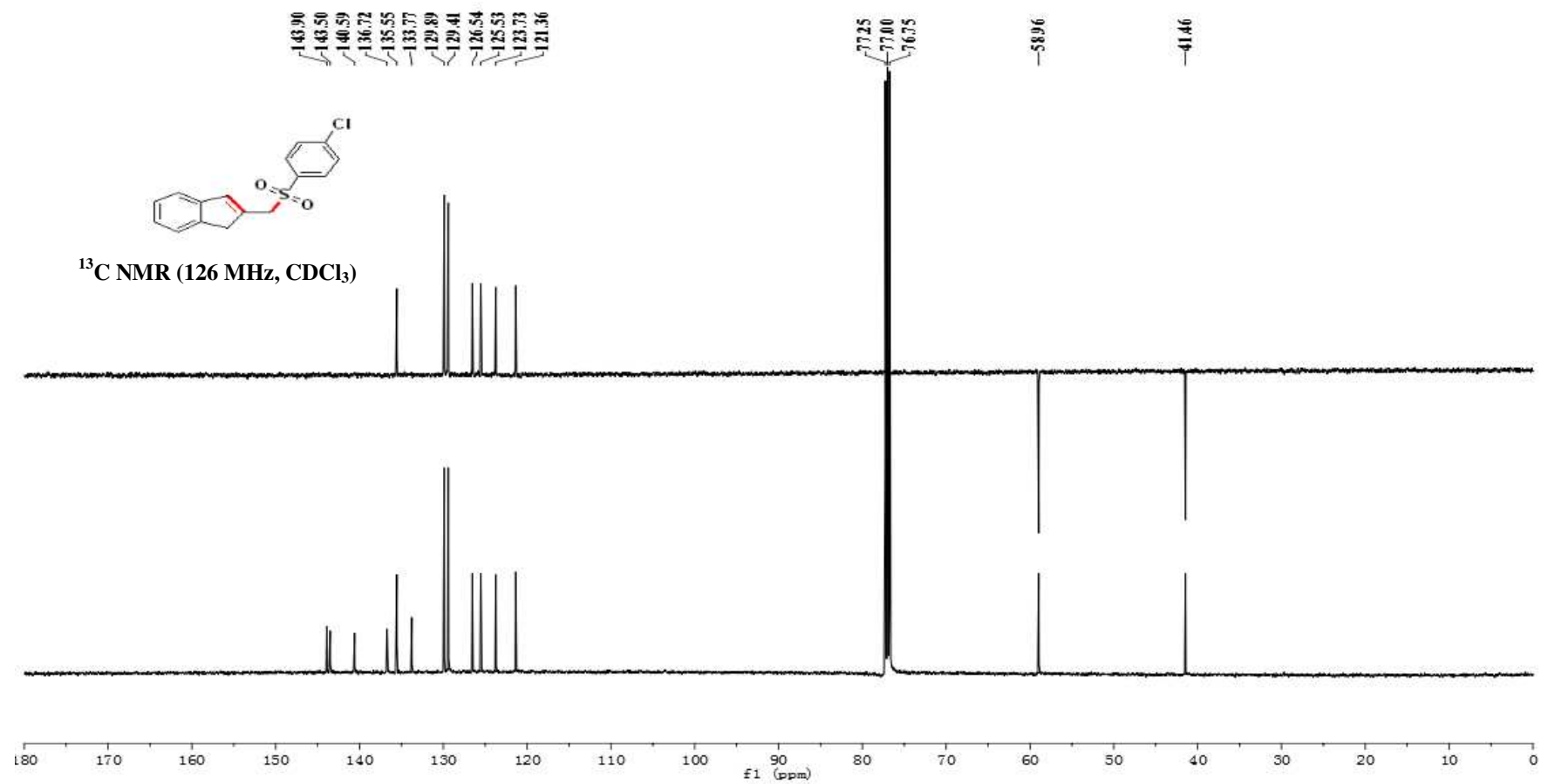
4.26
3.76
3.54
1.89
1.59
1.25
0.00



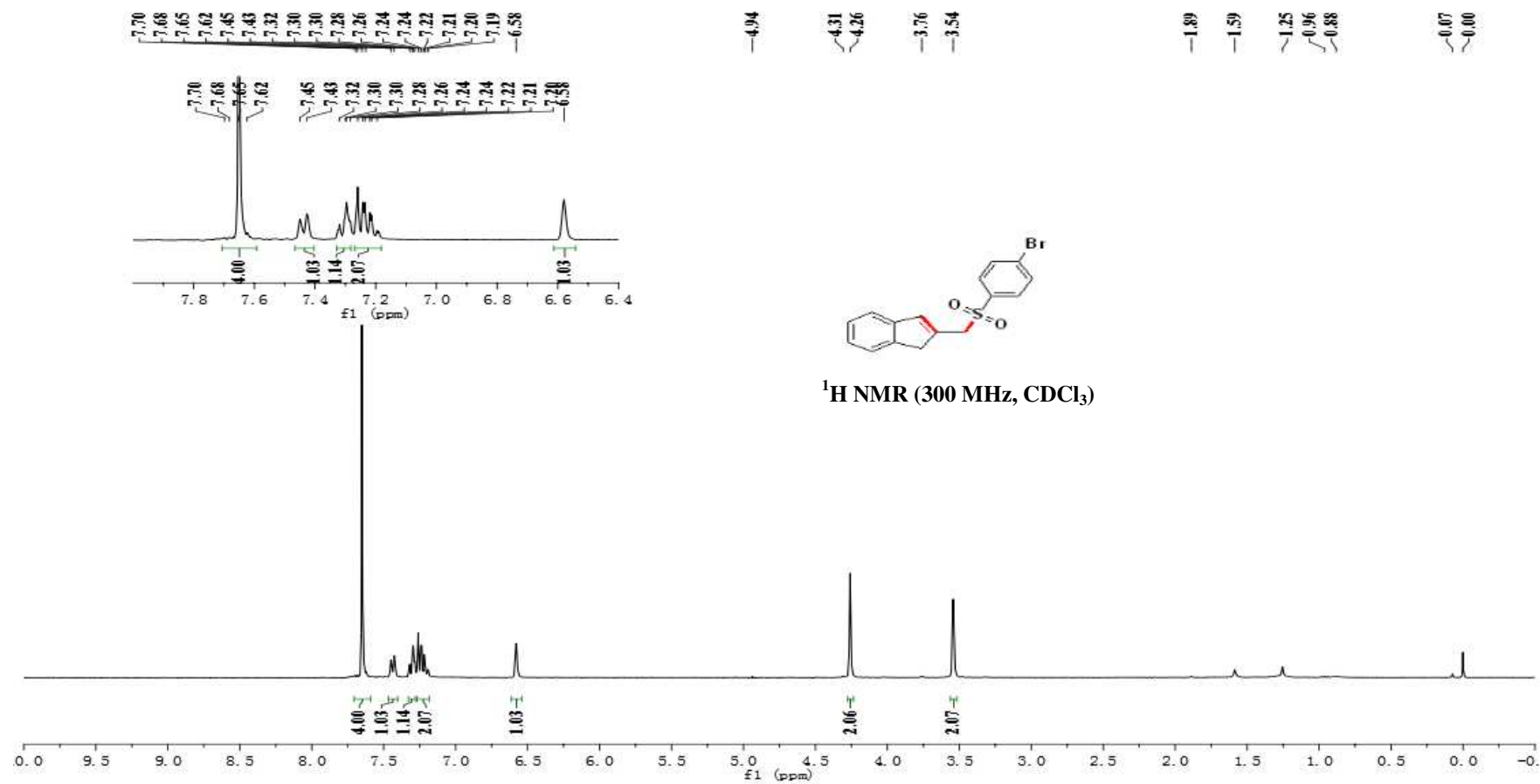
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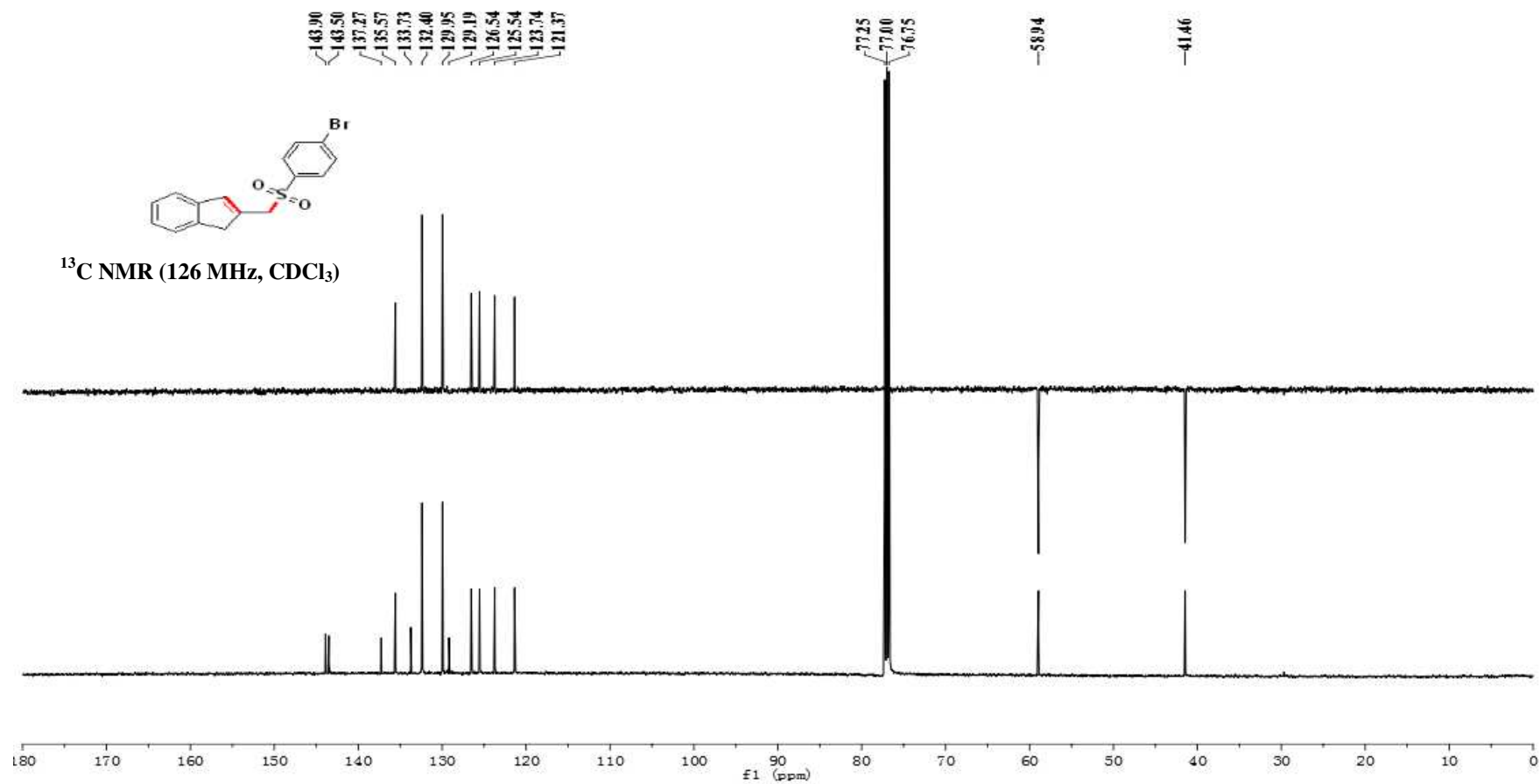
2-(((4-Chlorophenyl)sulfonyl)methyl)-1H-indene (3p)



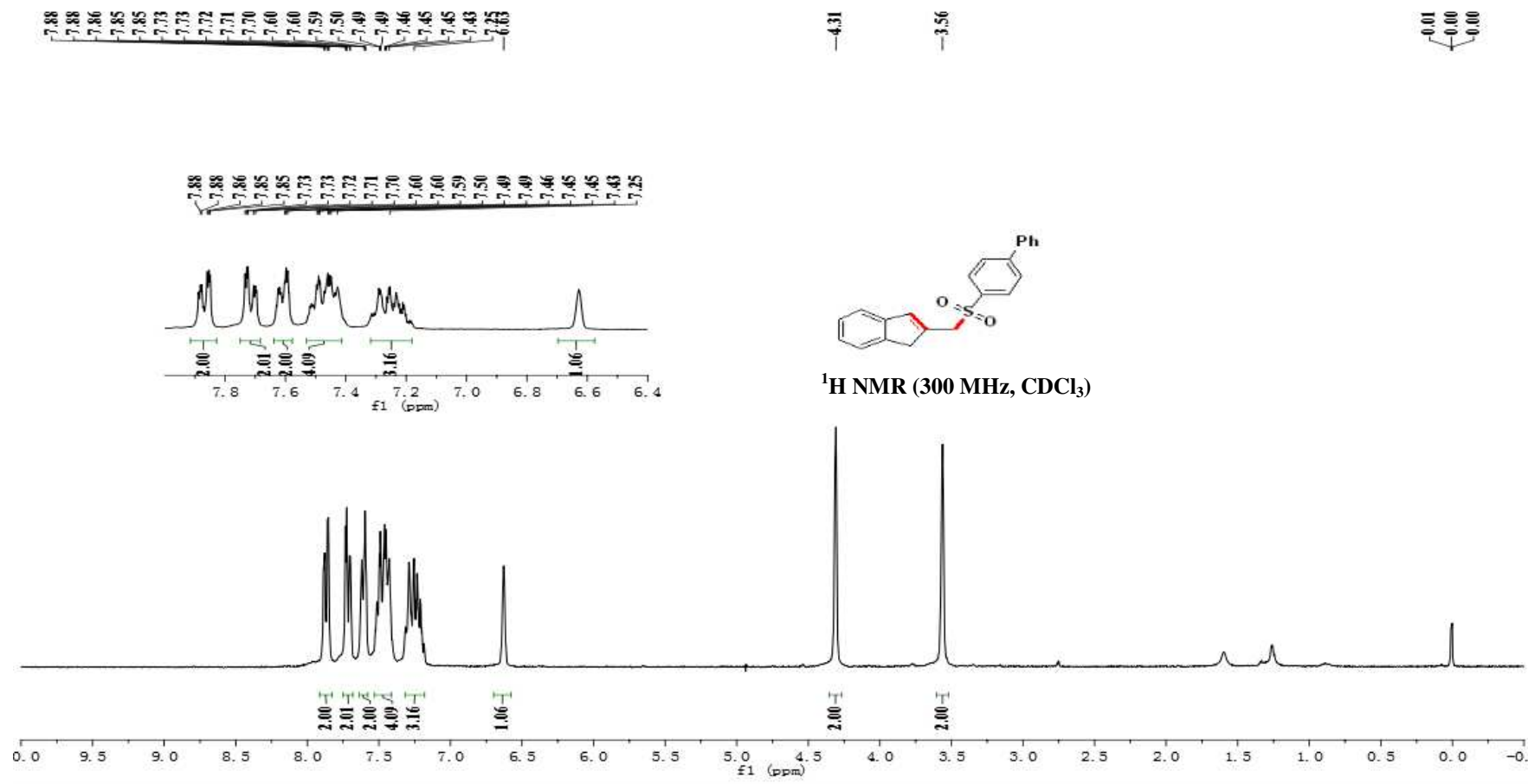
2-(((4-Bromophenyl)sulfonyl)methyl)-1H-indene (3q)



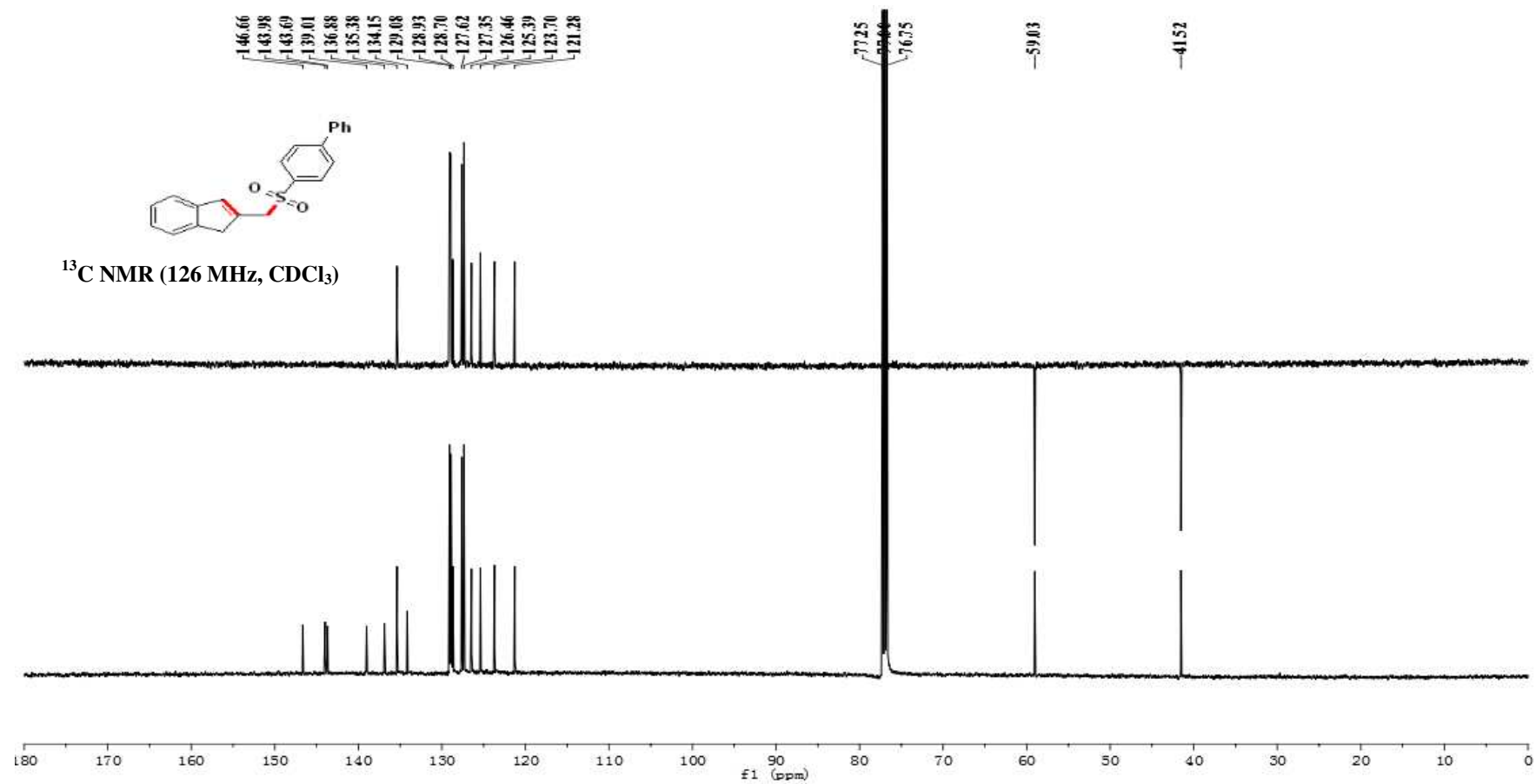
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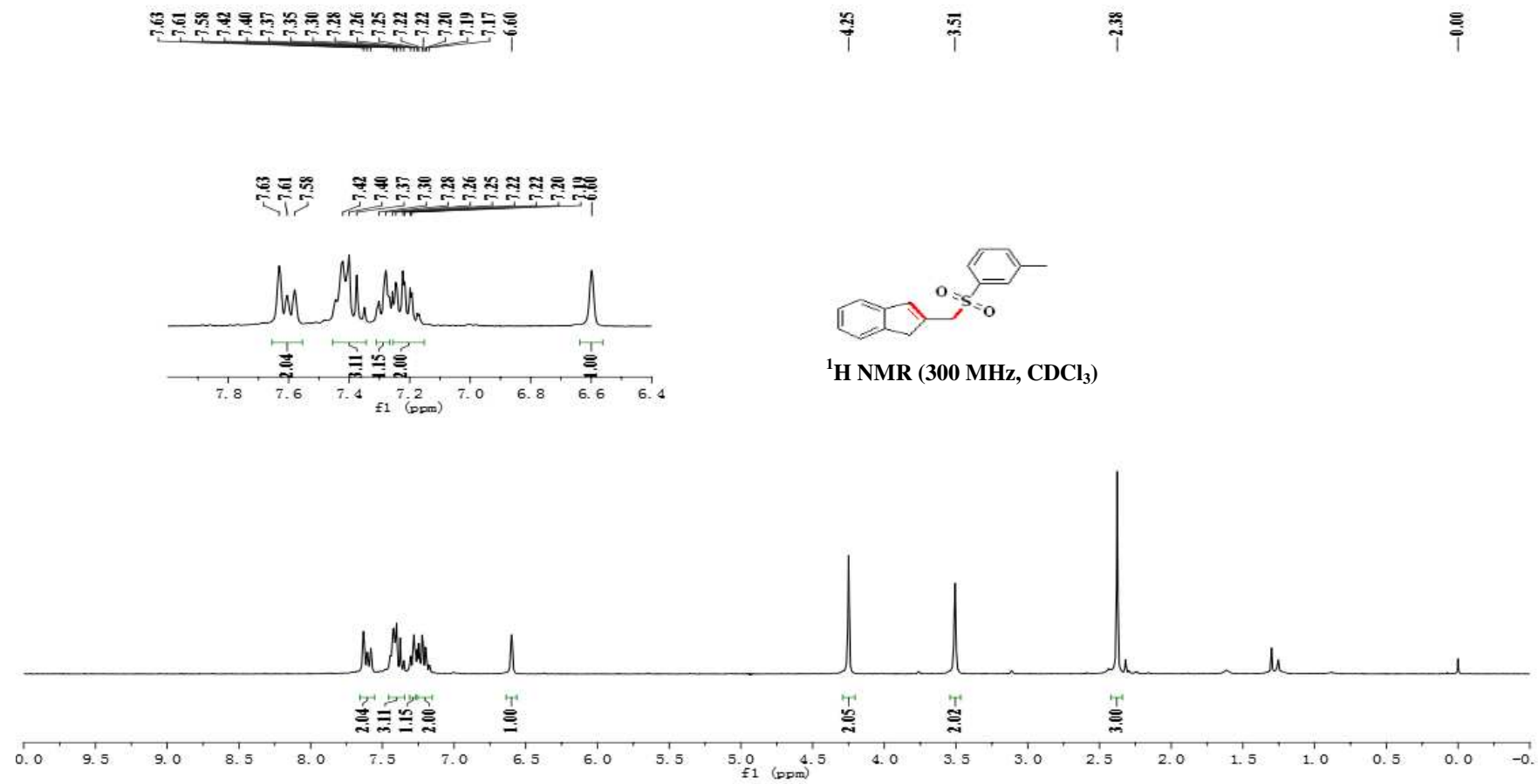
2-((1,1'-biphenyl)-4-ylsulfonyl)methyl)-1*H*-indene (3r)



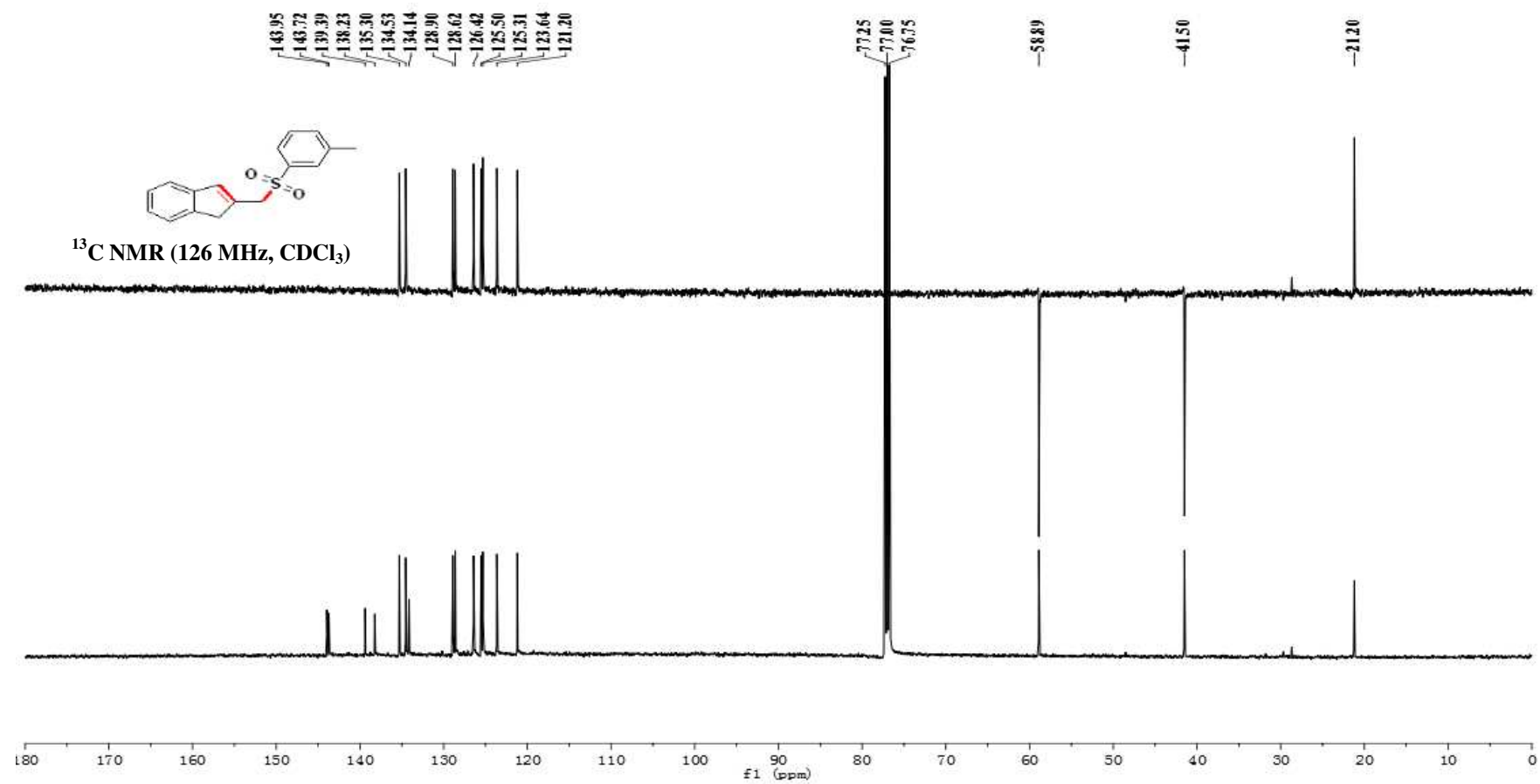
2-([1,1'-biphenyl]-4-ylsulfonylmethyl)-1*H*-indene (3r)



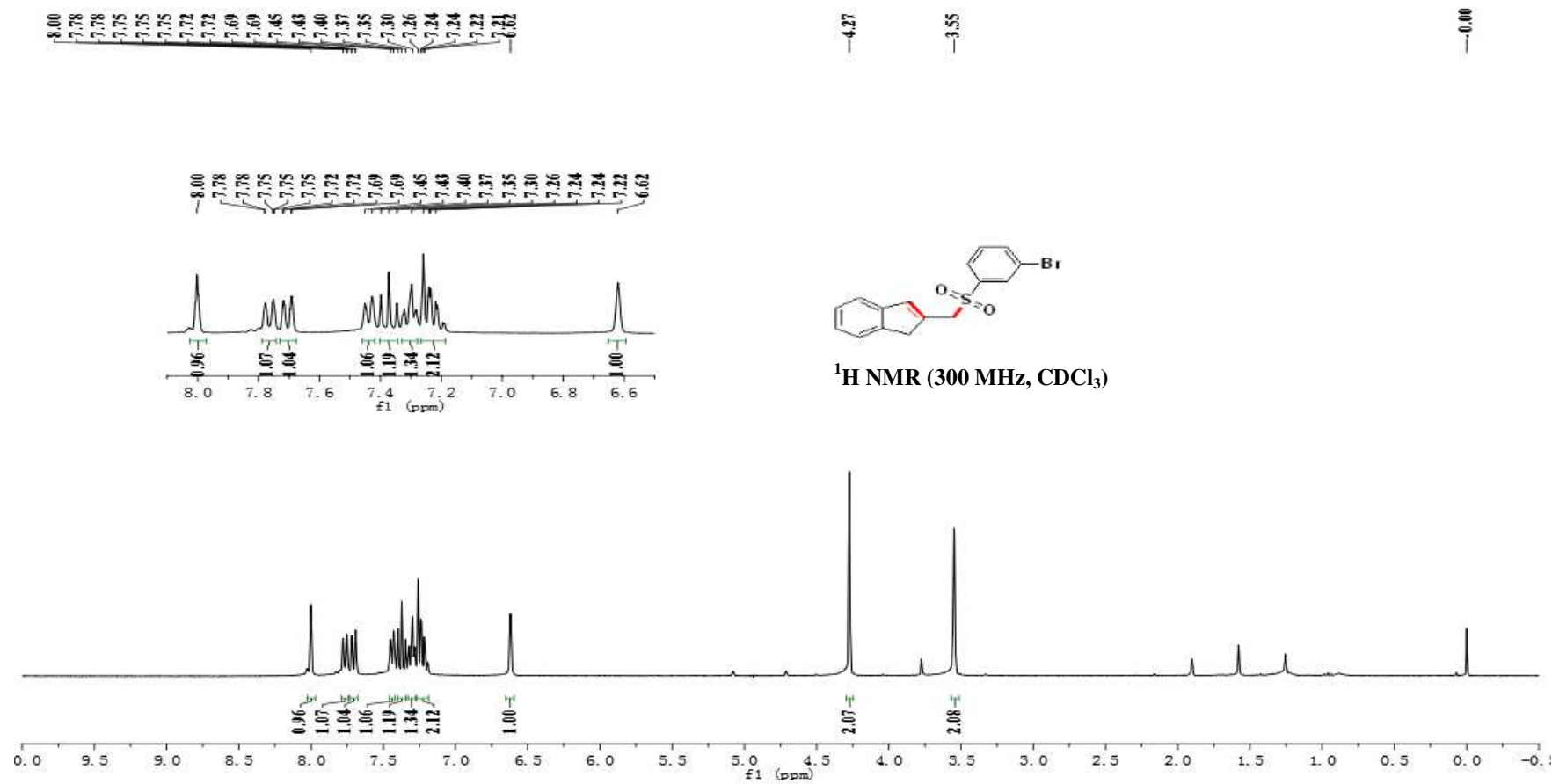
2-((*m*-Tolylsulfonyl)methyl)-1*H*-indene (3s)



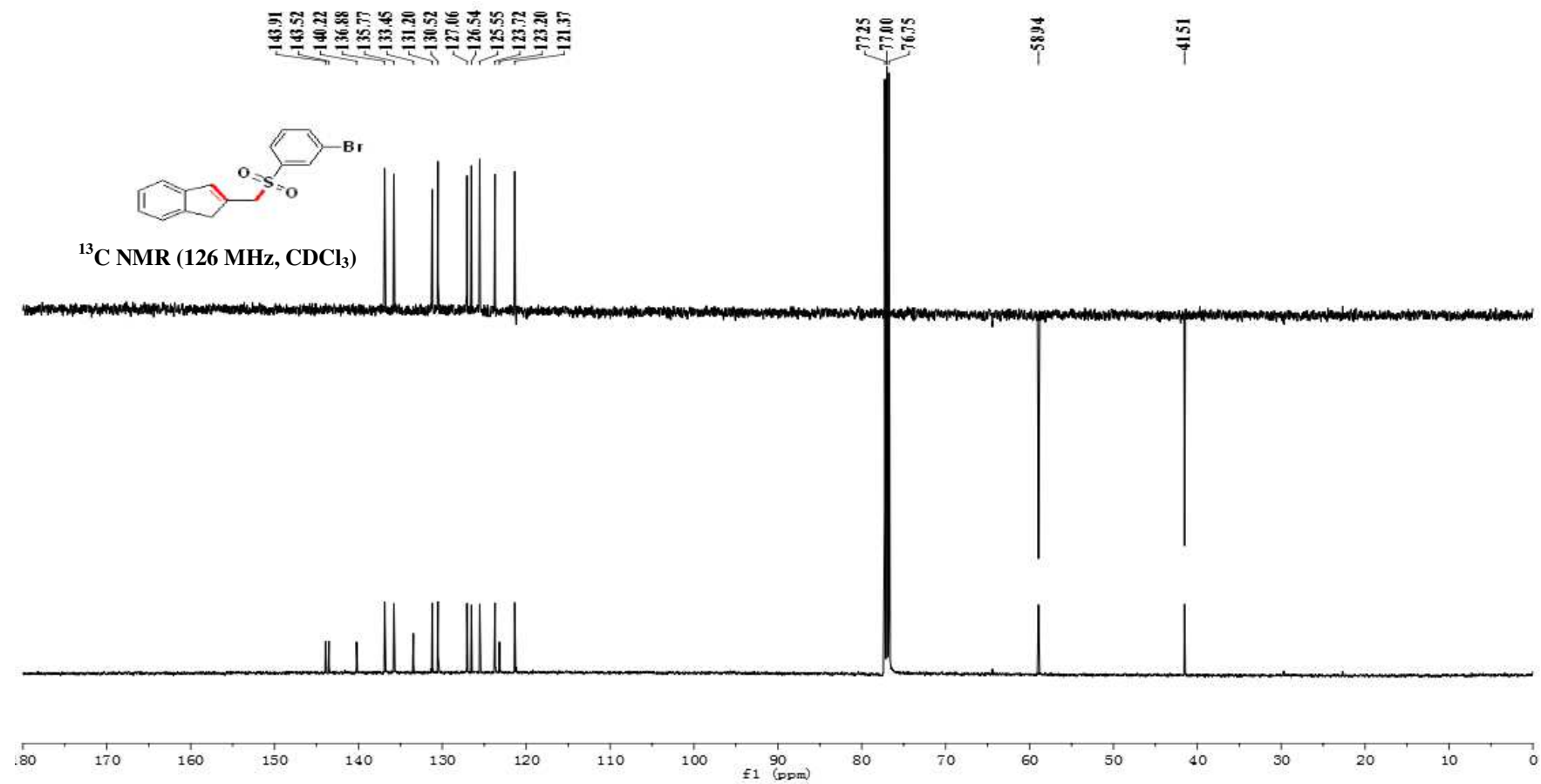
2-((*m*-Tolylsulfonyl)methyl)-1*H*-indene (3s)



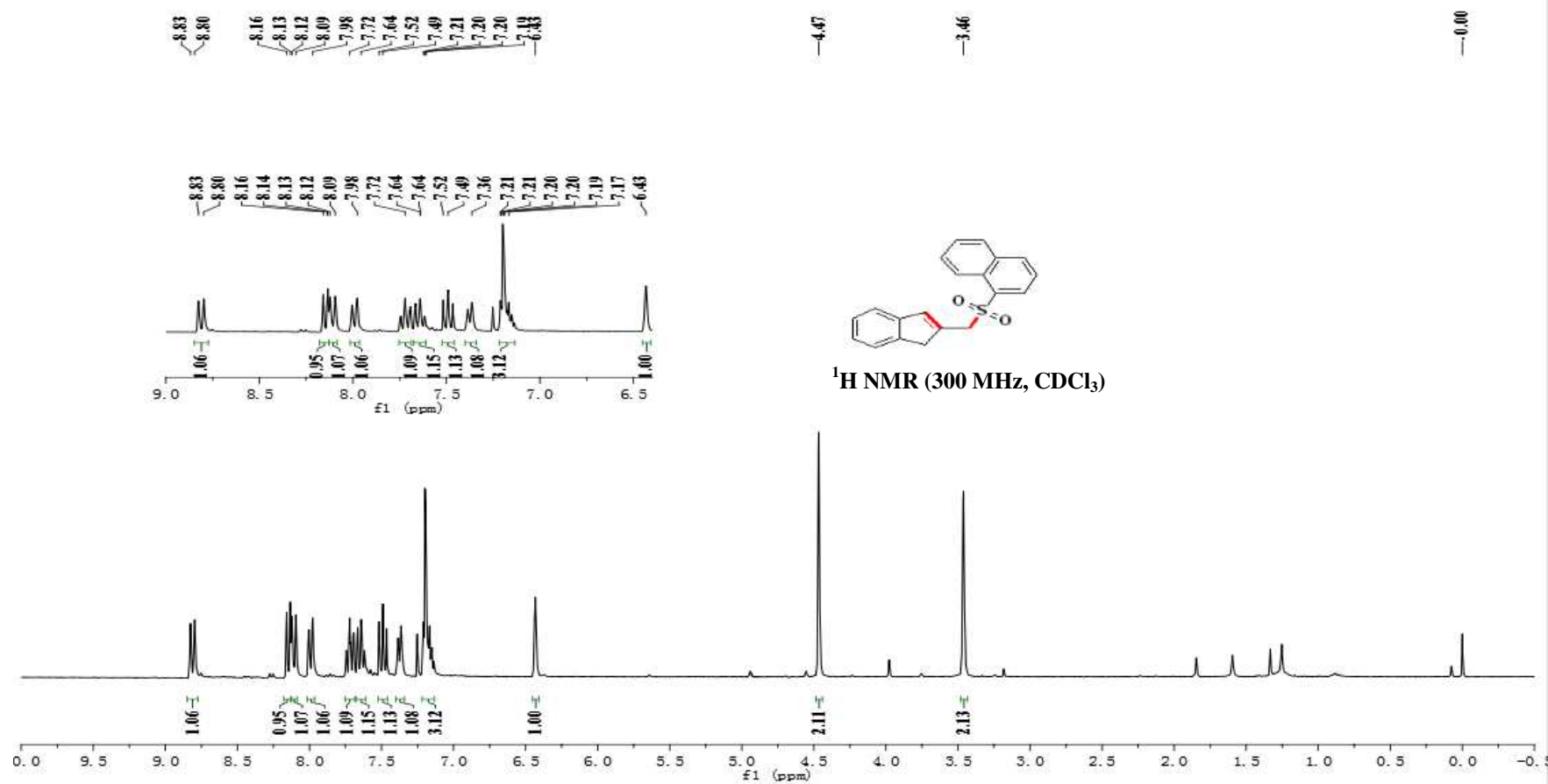
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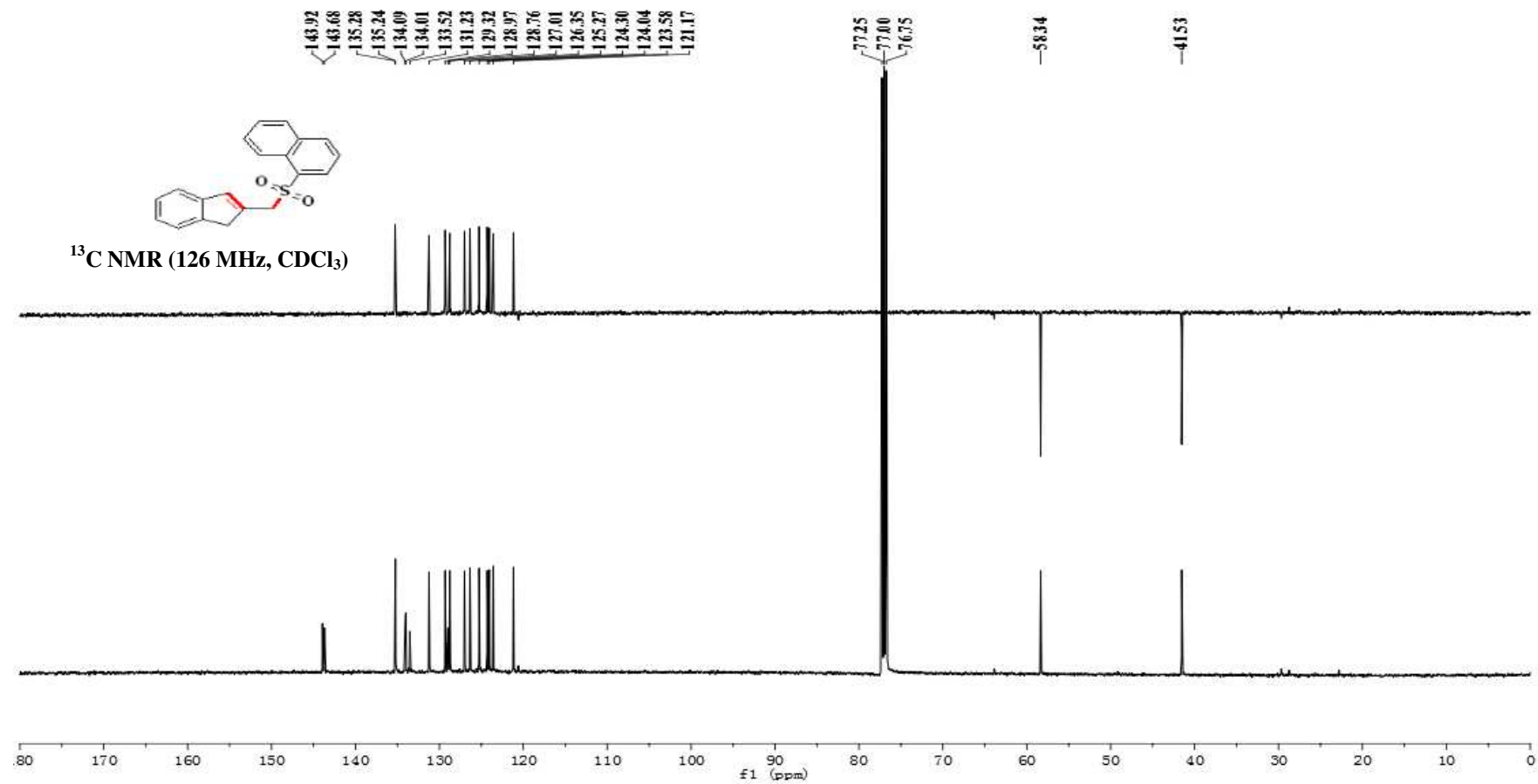
2-(((3-Bromophenyl)sulfonyl)methyl)-1H-indene (3t)



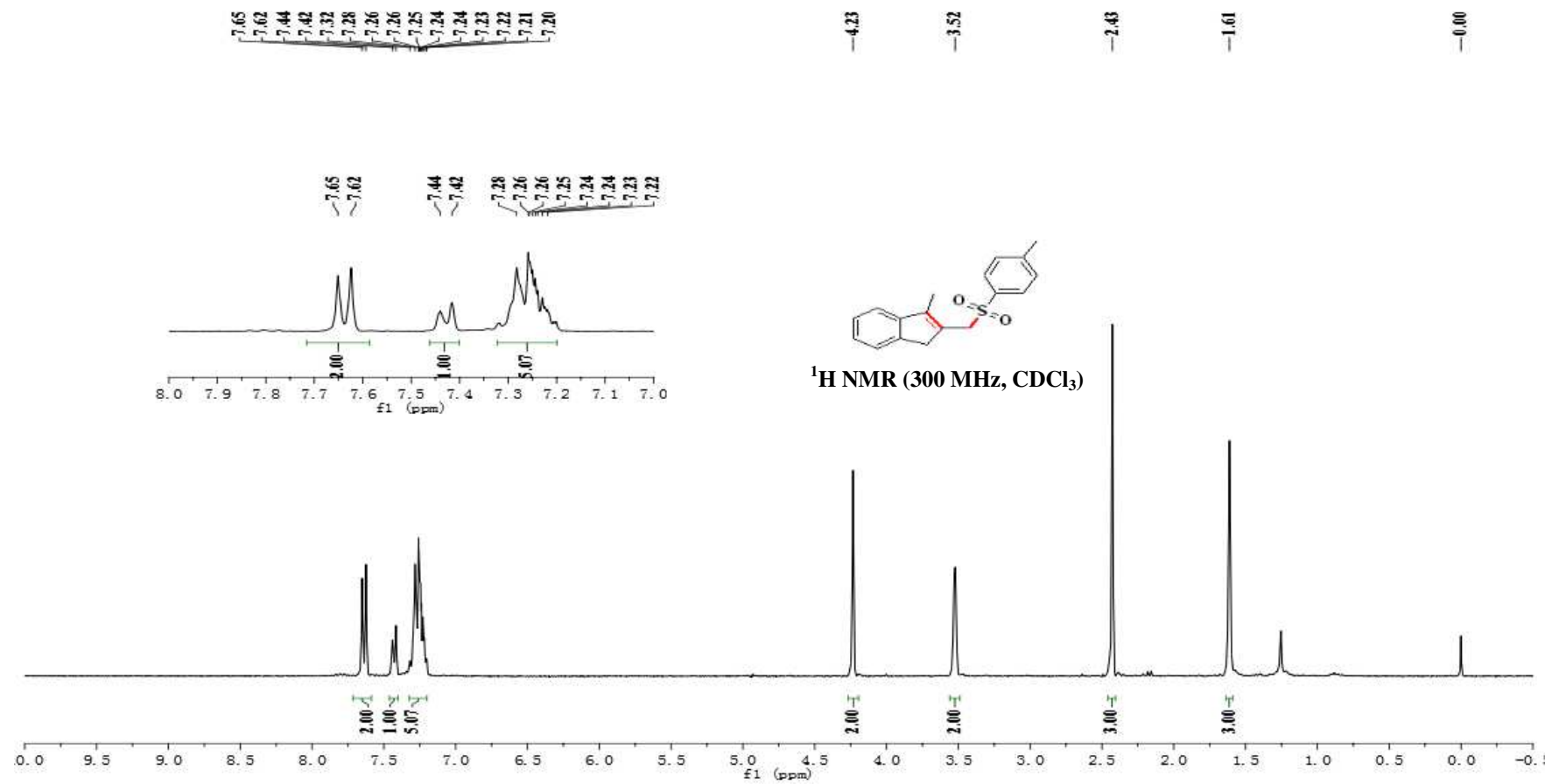
1-(((1*H*-Inden-2-yl)methyl)sulfonyl)naphthalene (3u)



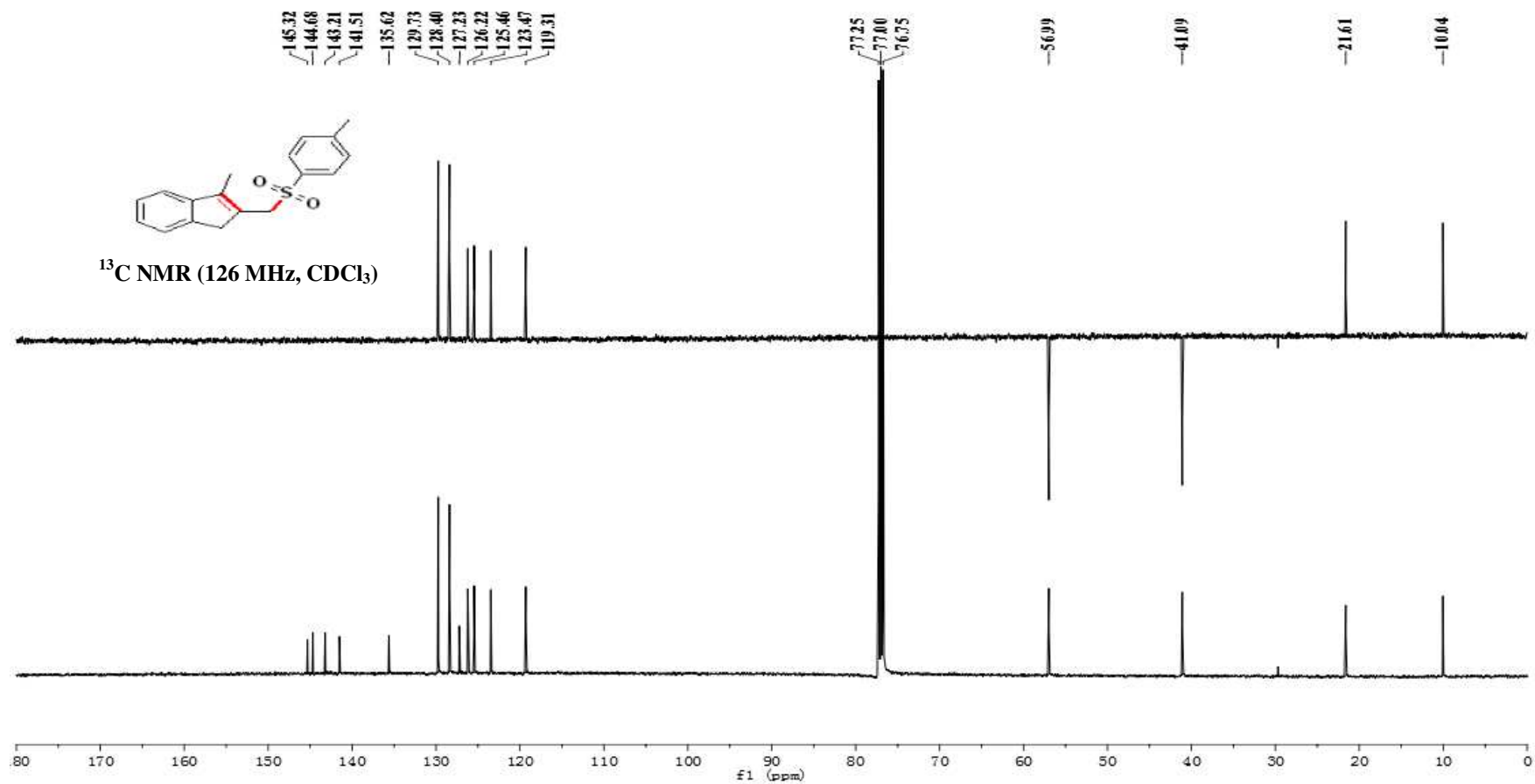
1-(((1*H*-Inden-2-yl)methyl)sulfonyl)naphthalene (3u)



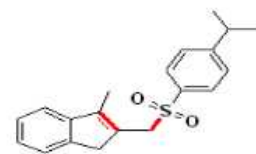
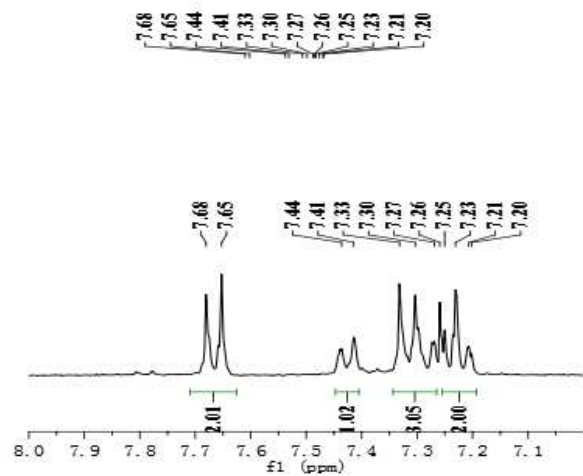
3-Methyl-2-(tosylmethyl)-1*H*-indene (5a)



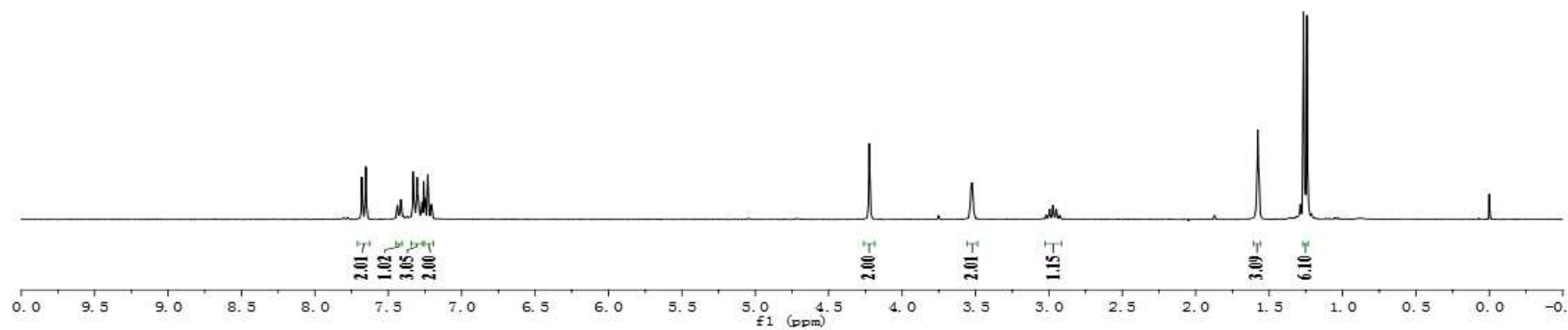
3-Methyl-2-(tosylmethyl)-1*H*-indene (5a)



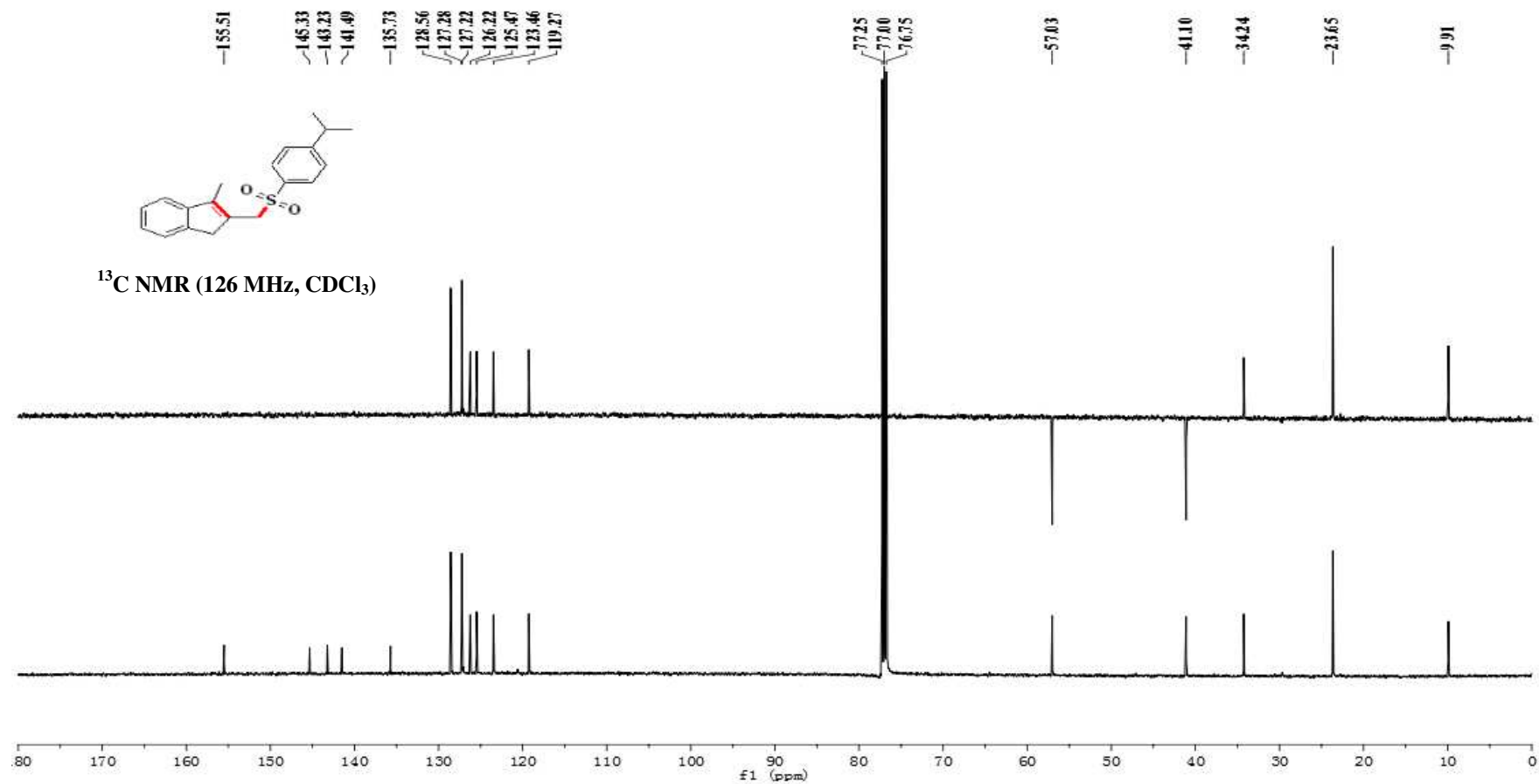
2-(((4-isopropylphenyl)sulfonyl)methyl)-3-methyl-1*H*-indene (5b)



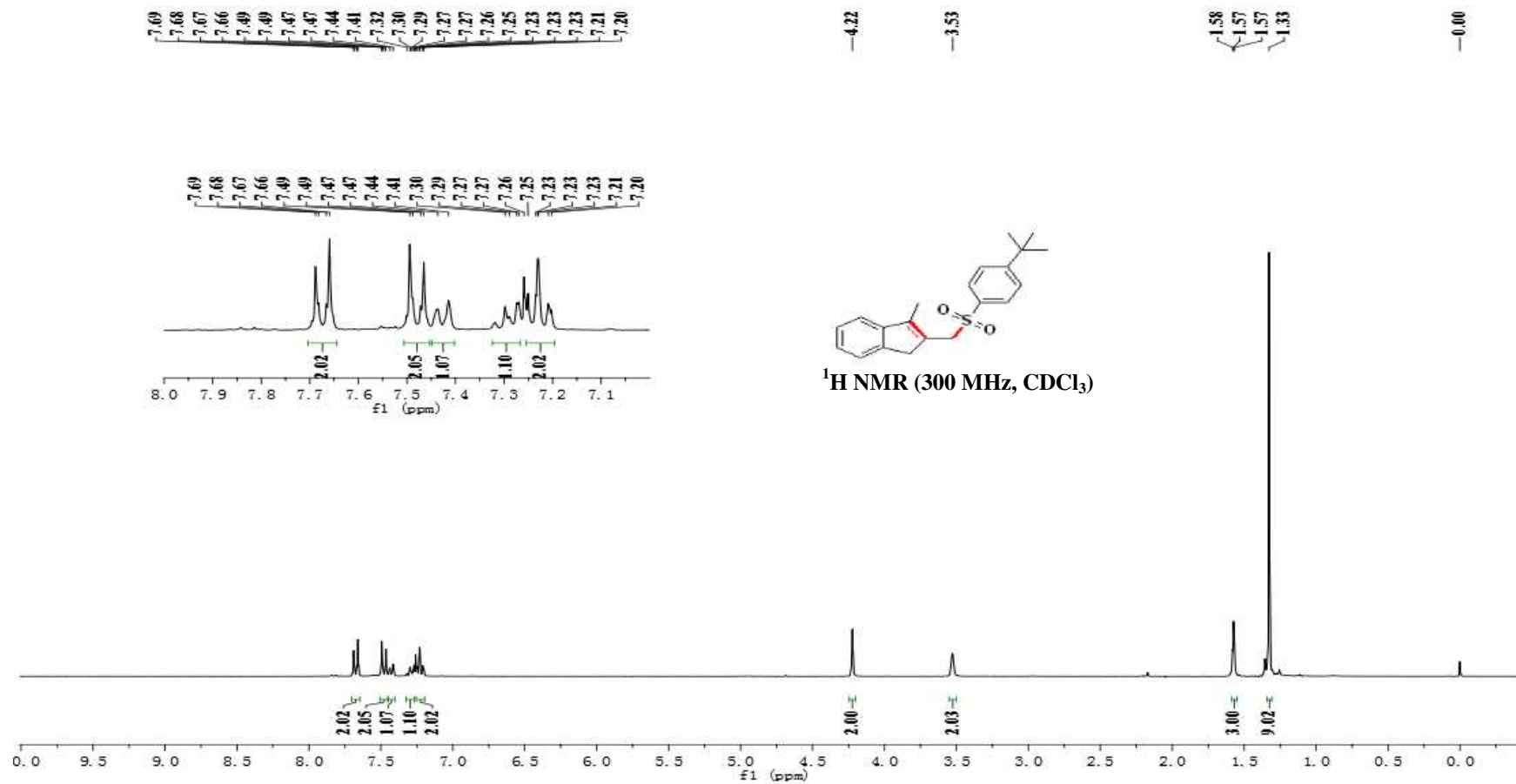
¹H NMR (300 MHz, CDCl₃)



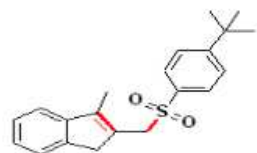
2-(((4-isopropylphenyl)sulfonyl)methyl)-3-methyl-1H-indene (5b)



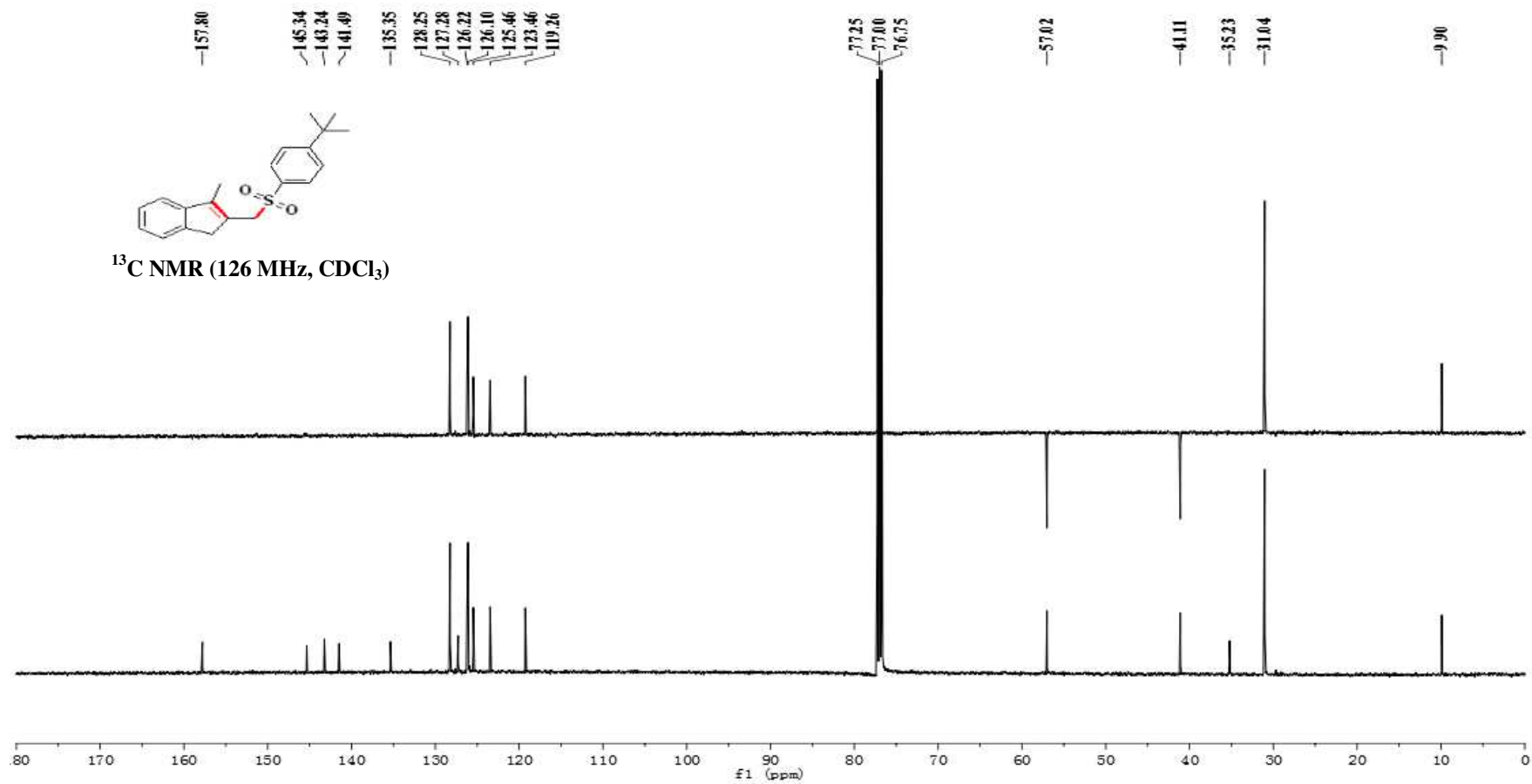
2-(((4-(*tert*-Butyl)phenyl)sulfonyl)methyl)-3-methyl-1*H*-indene (5c)



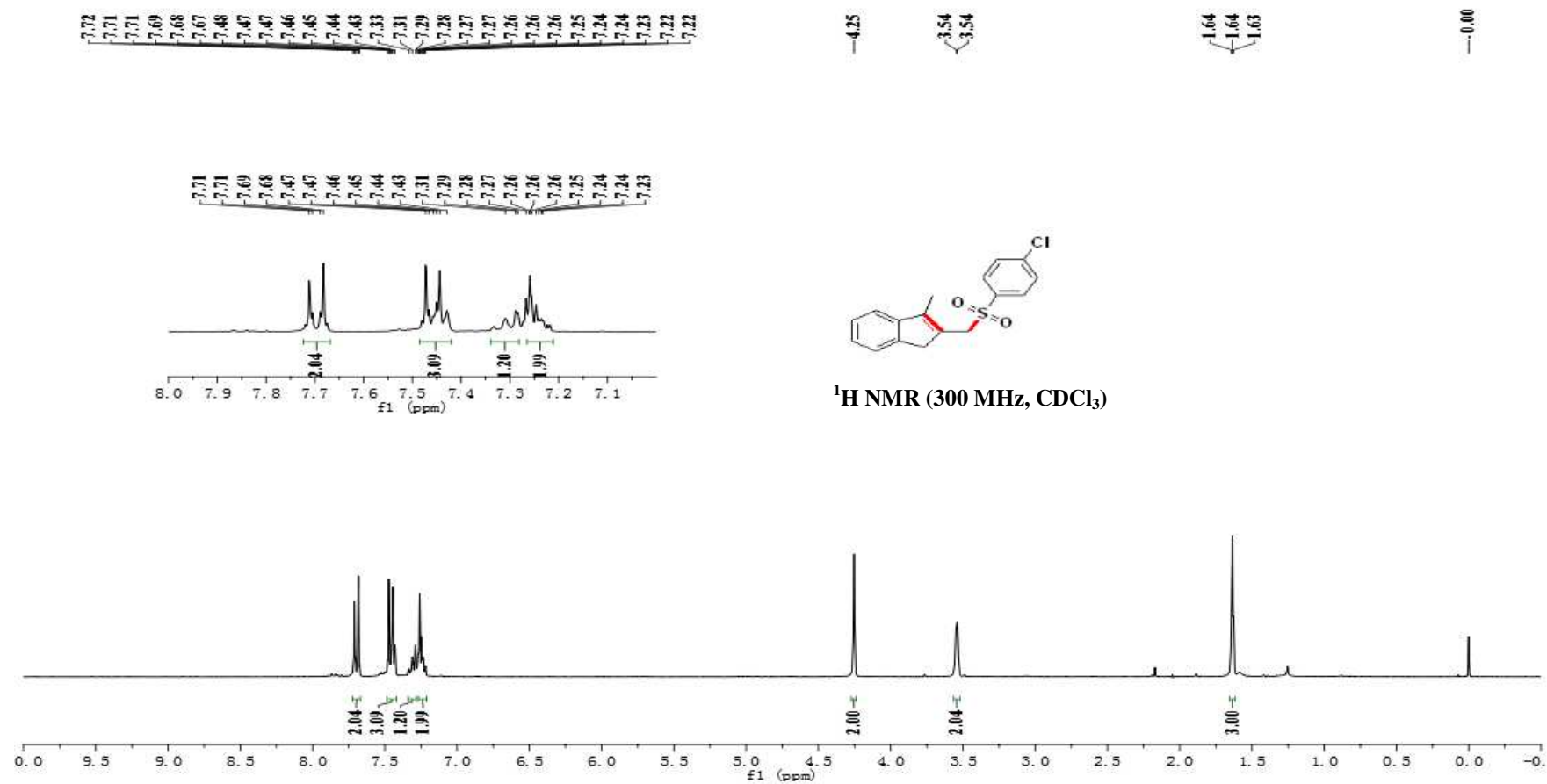
2-(((4-(*tert*-Butyl)phenyl)sulfonyl)methyl)-3-methyl-1*H*-indene (5c)



^{13}C NMR (126 MHz, CDCl_3)



2-(((4-Chlorophenyl)sulfonyl)methyl)-3-methyl-1*H*-indene (5d)



2-(((4-Chlorophenyl)sulfonyl)methyl)-3-methyl-1*H*-indene (5d)

