

Supplementary Material

Efficient synthesis of functionalized spiro[imidazolidine-2-thione-oxindoles] via catalyst-free domino Mannich cyclization

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Jinhua 321004, P. R. China

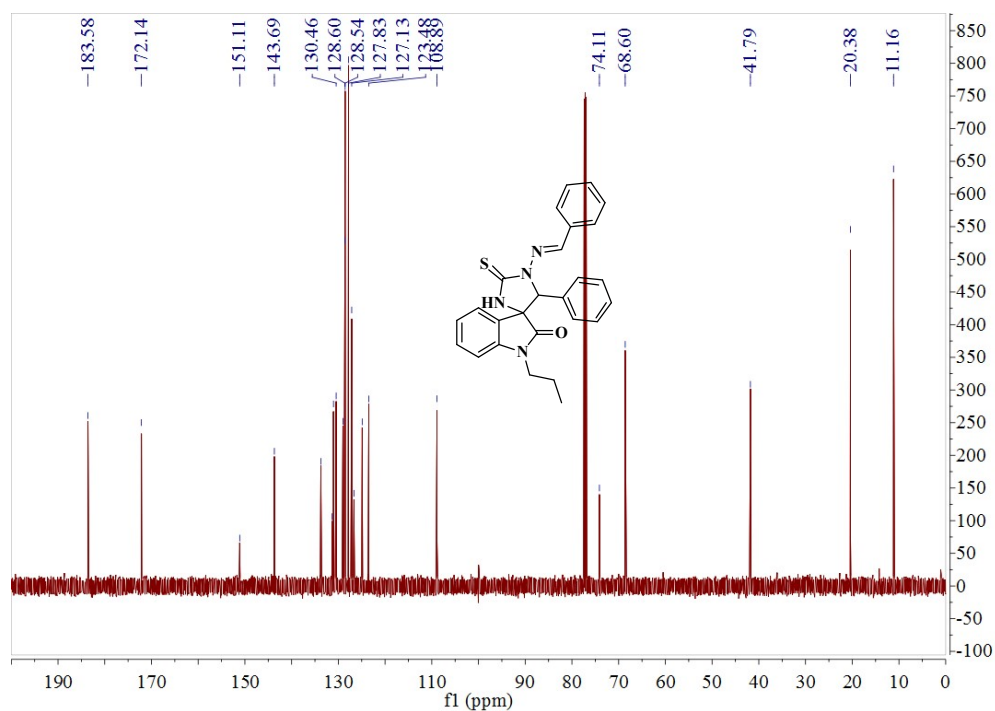
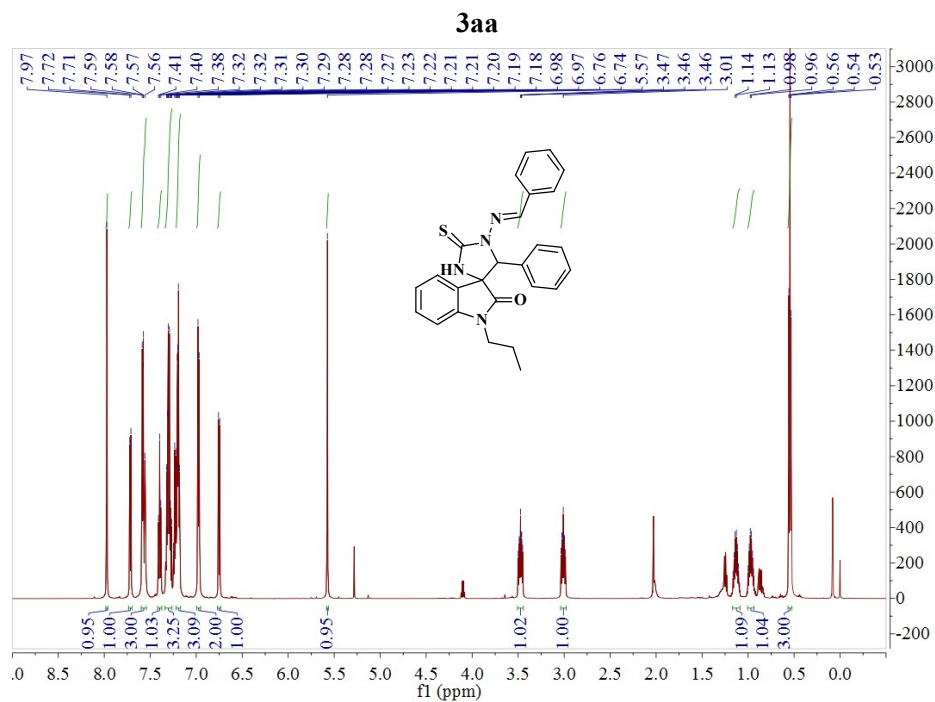
^b Zhejiang Pharmaceutical College, Ningbo 315100, P. R. China

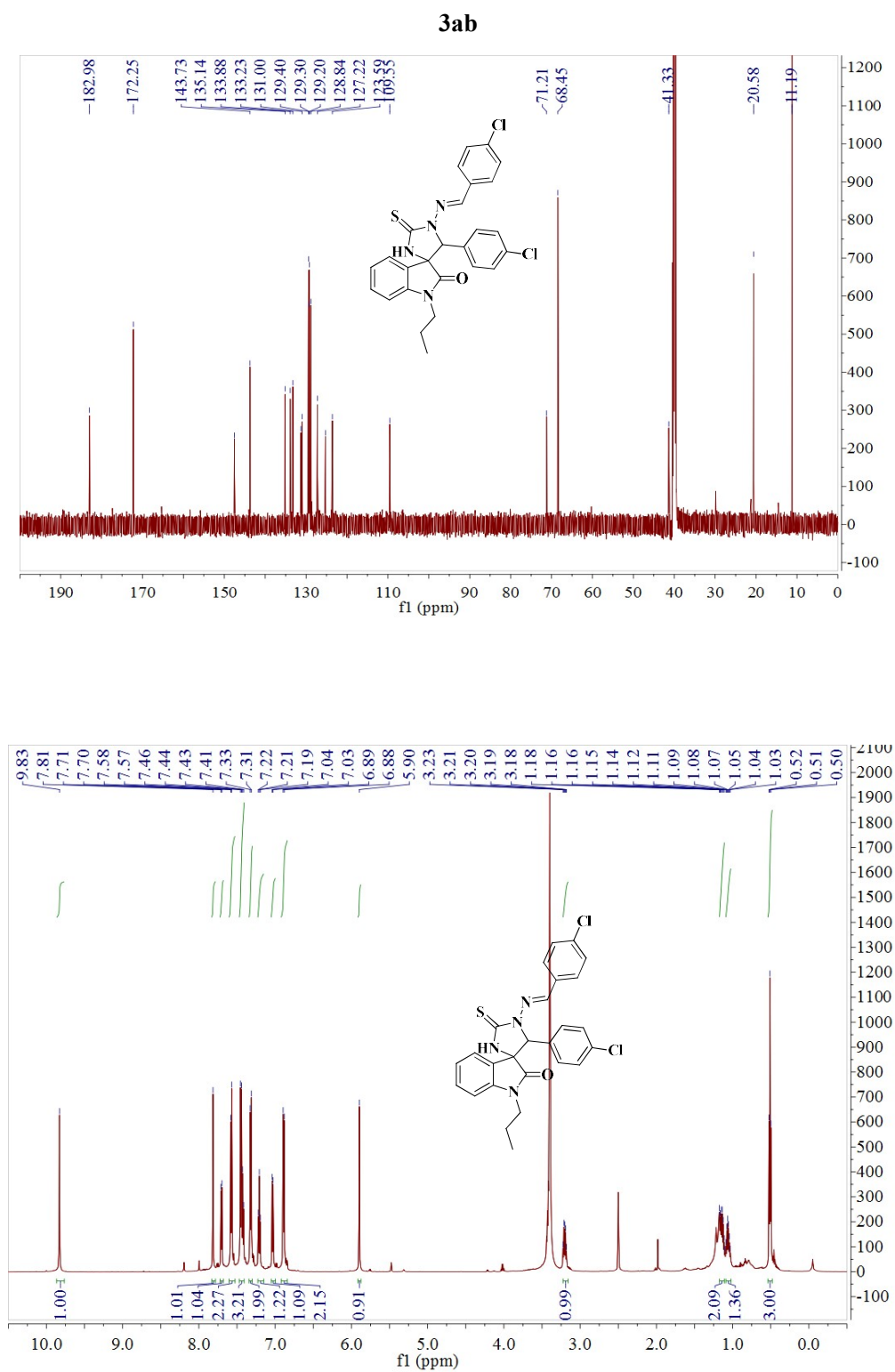
^c Ningbo No. 2 Hospital, Ningbo 315010, P. R. China

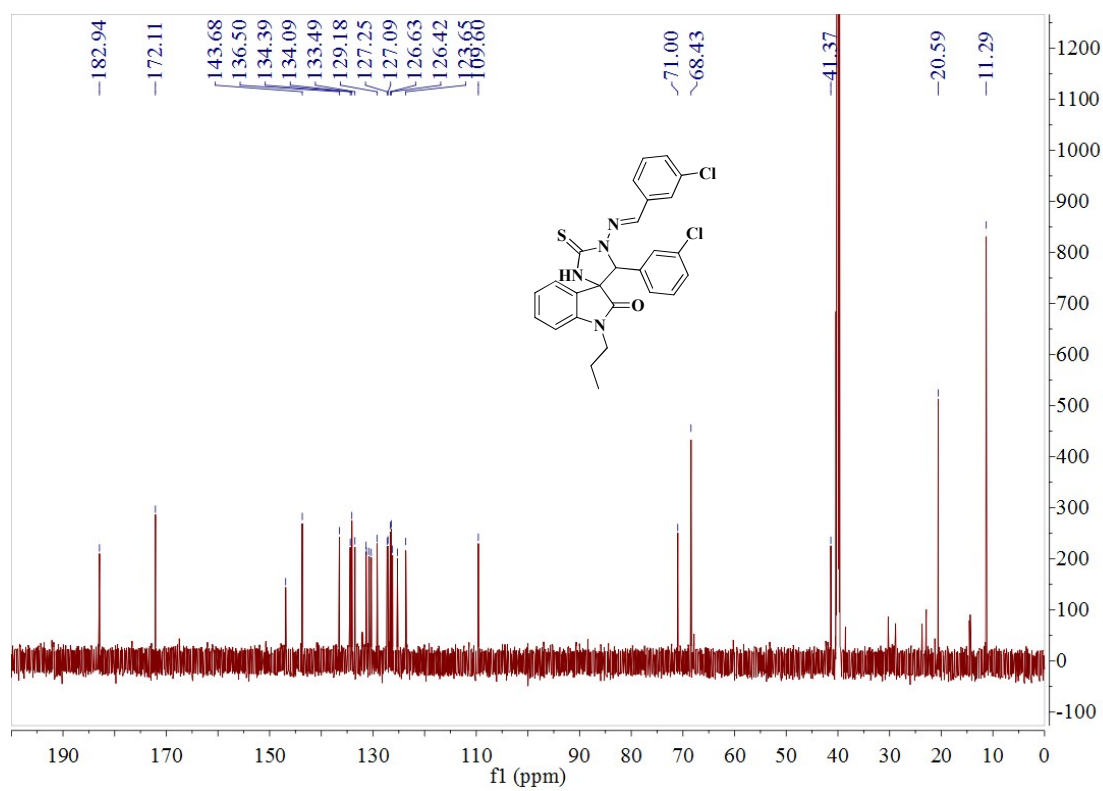
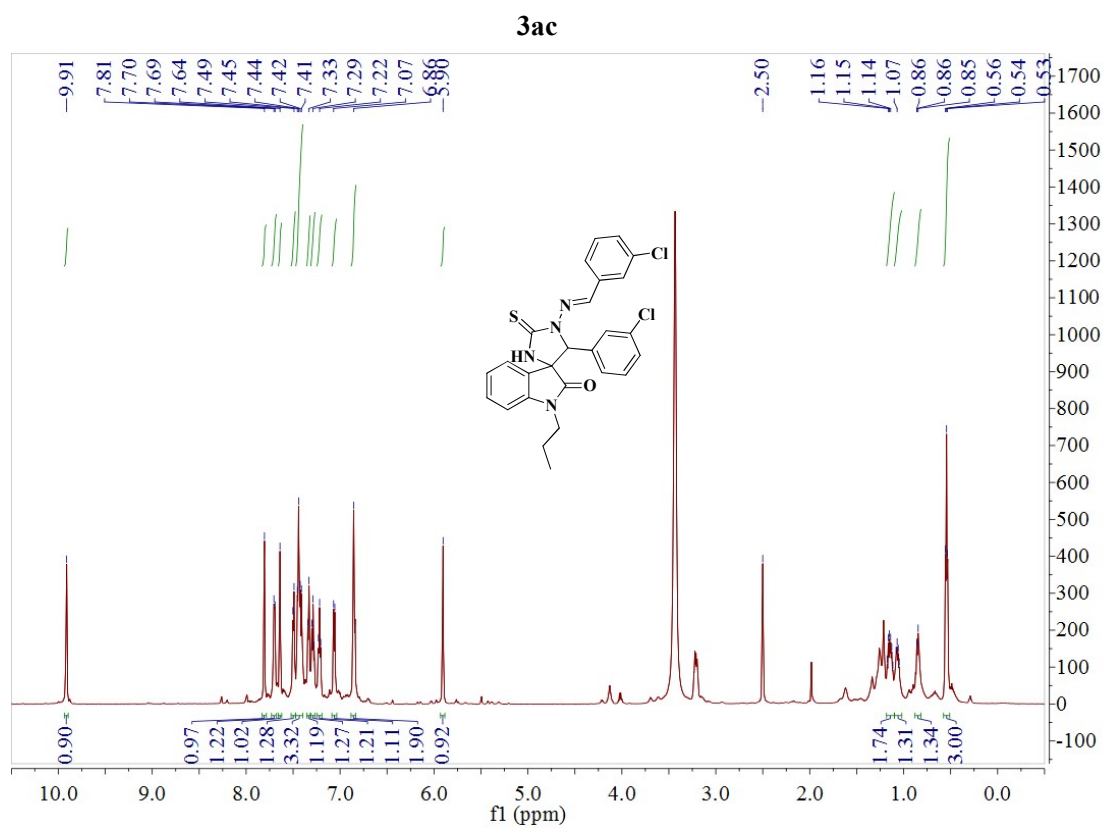
E-mail: xiejw@zjnu.cn

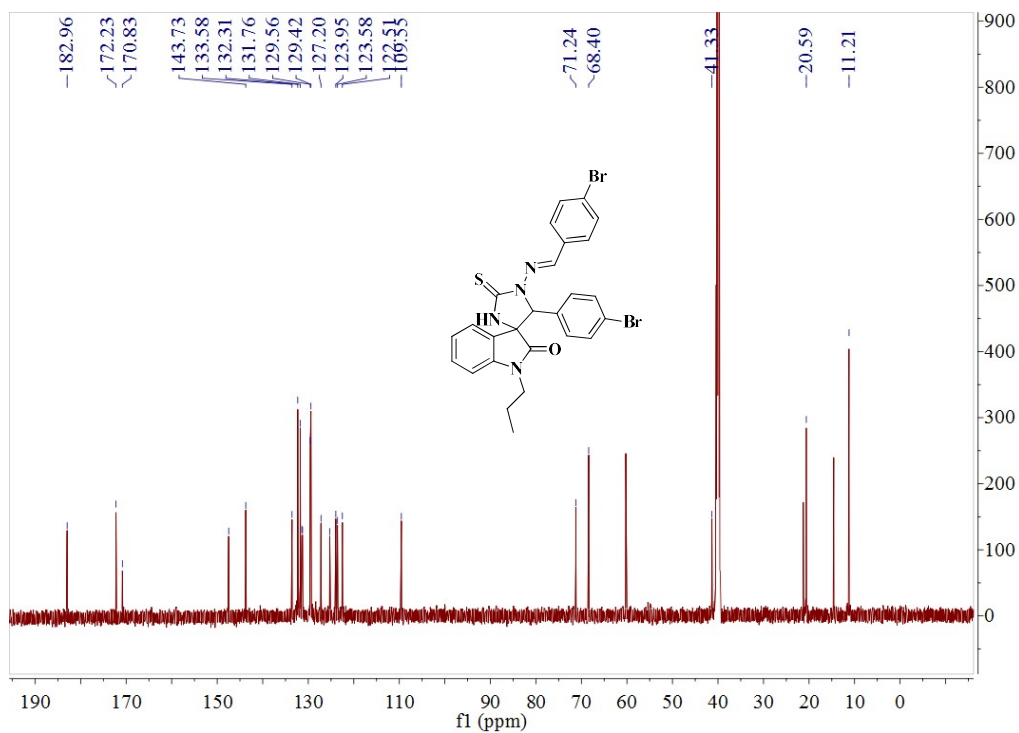
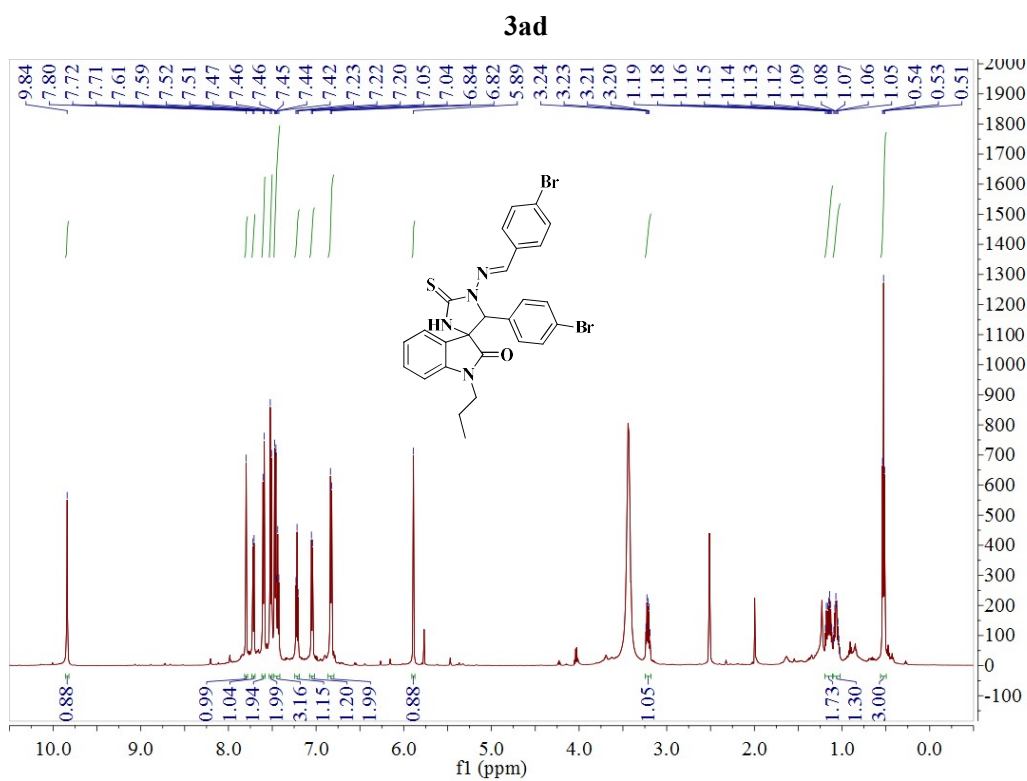
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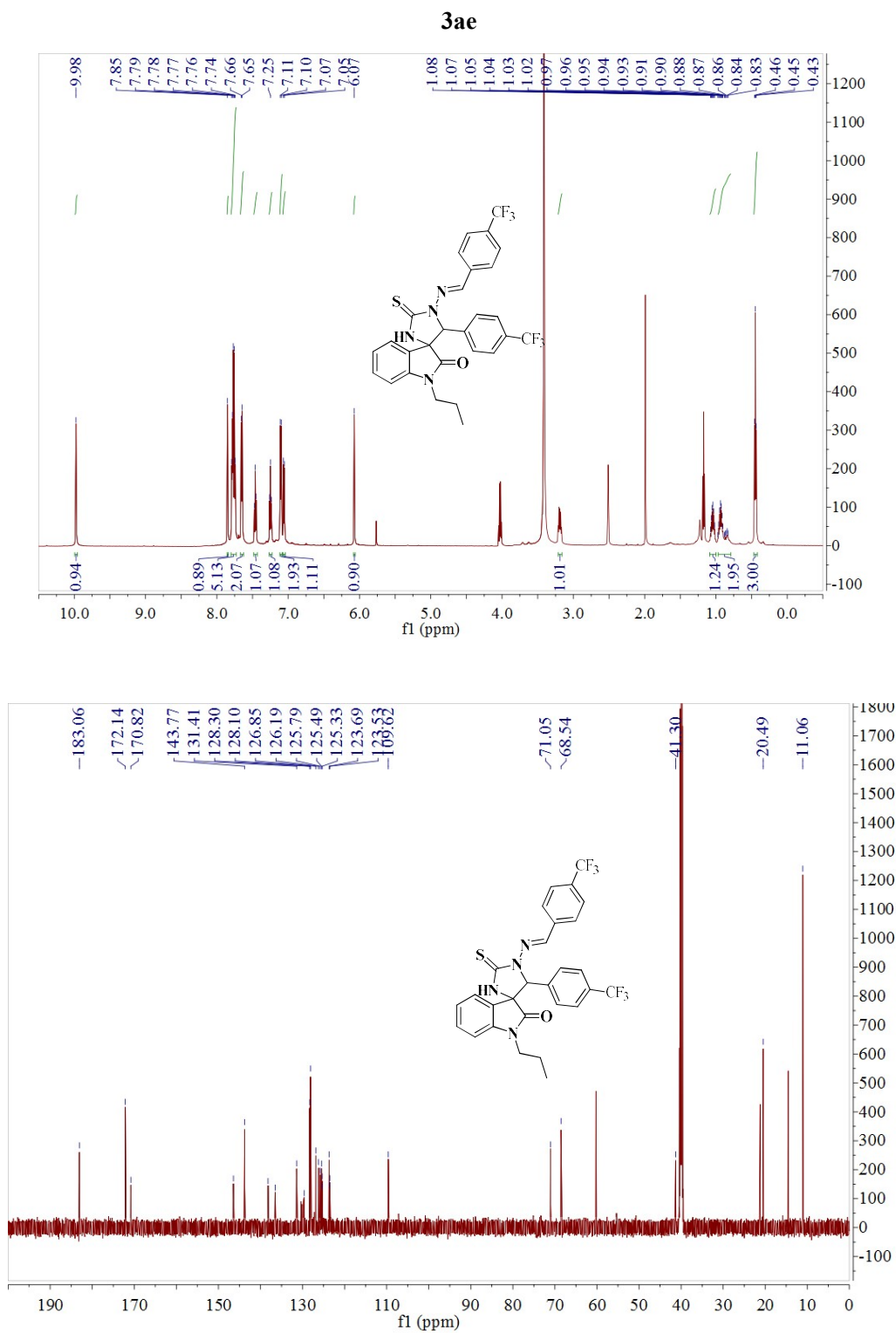
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1. Crystal data	S15-S23

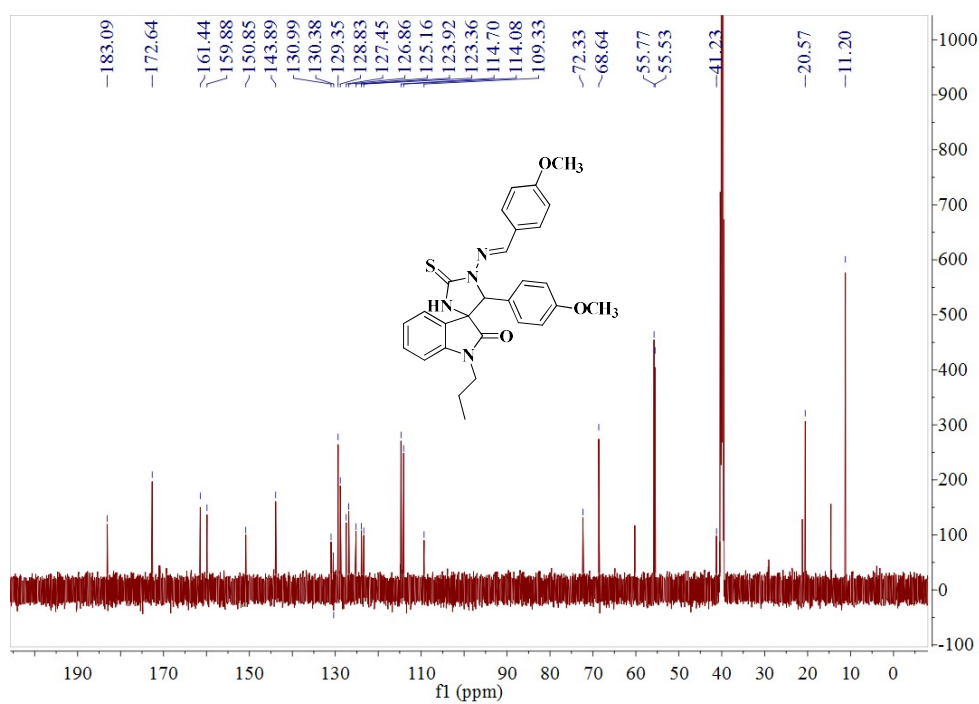
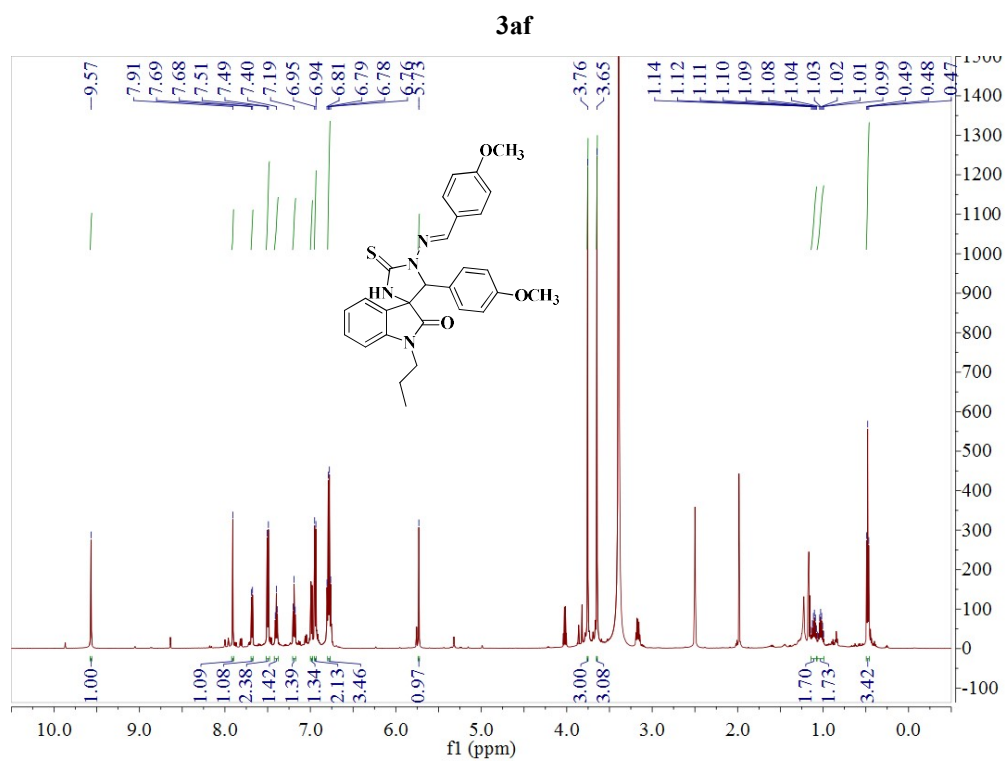
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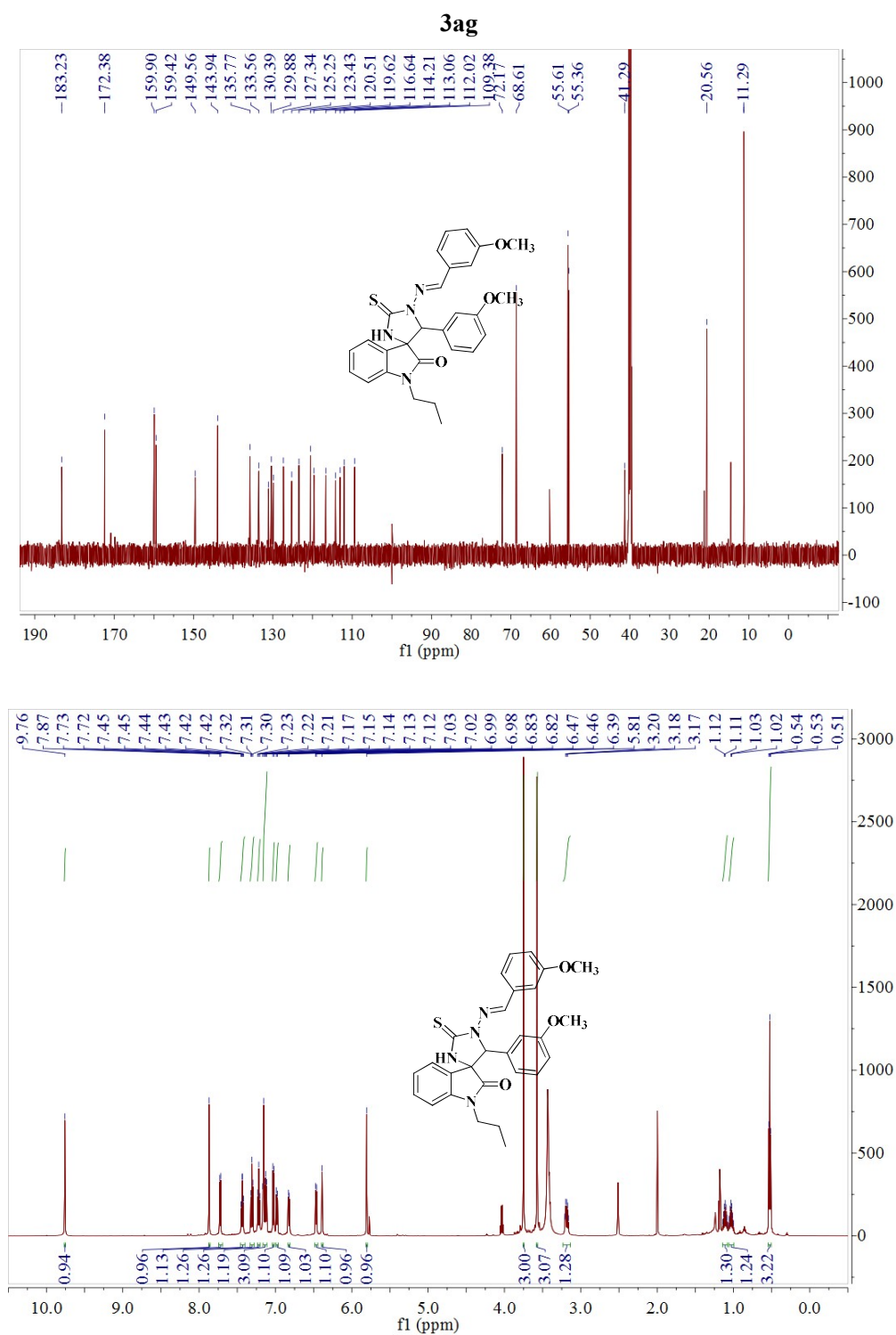


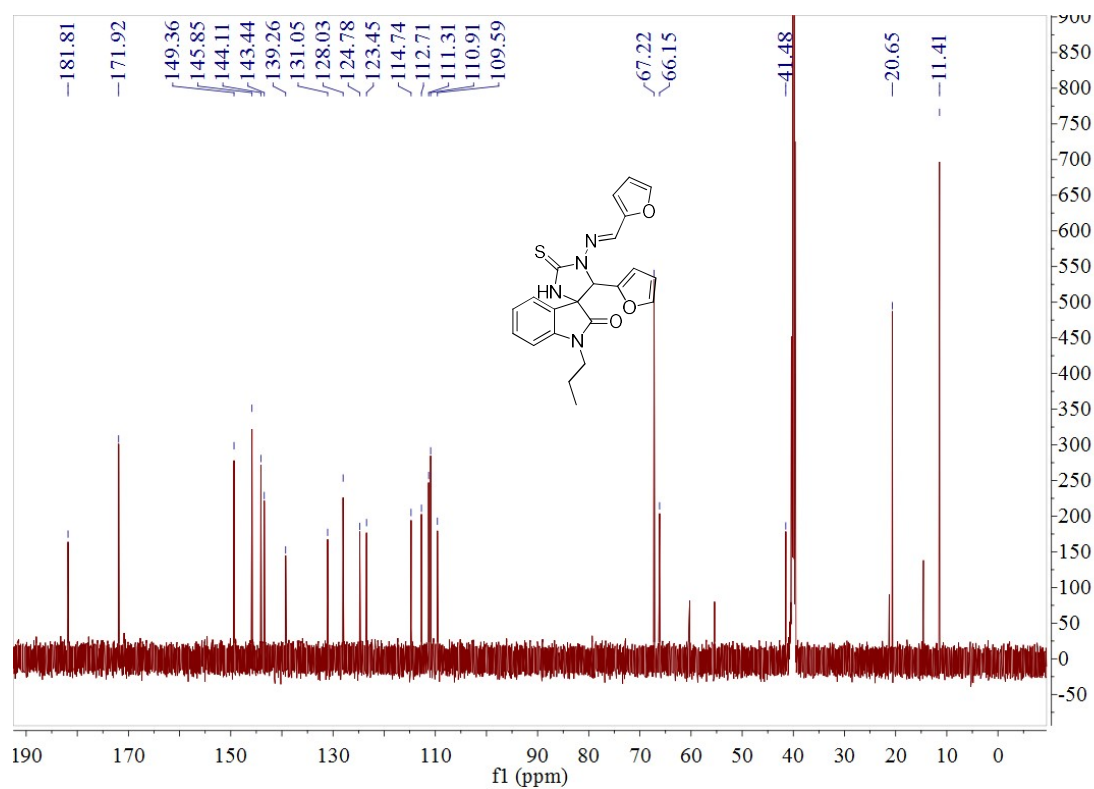
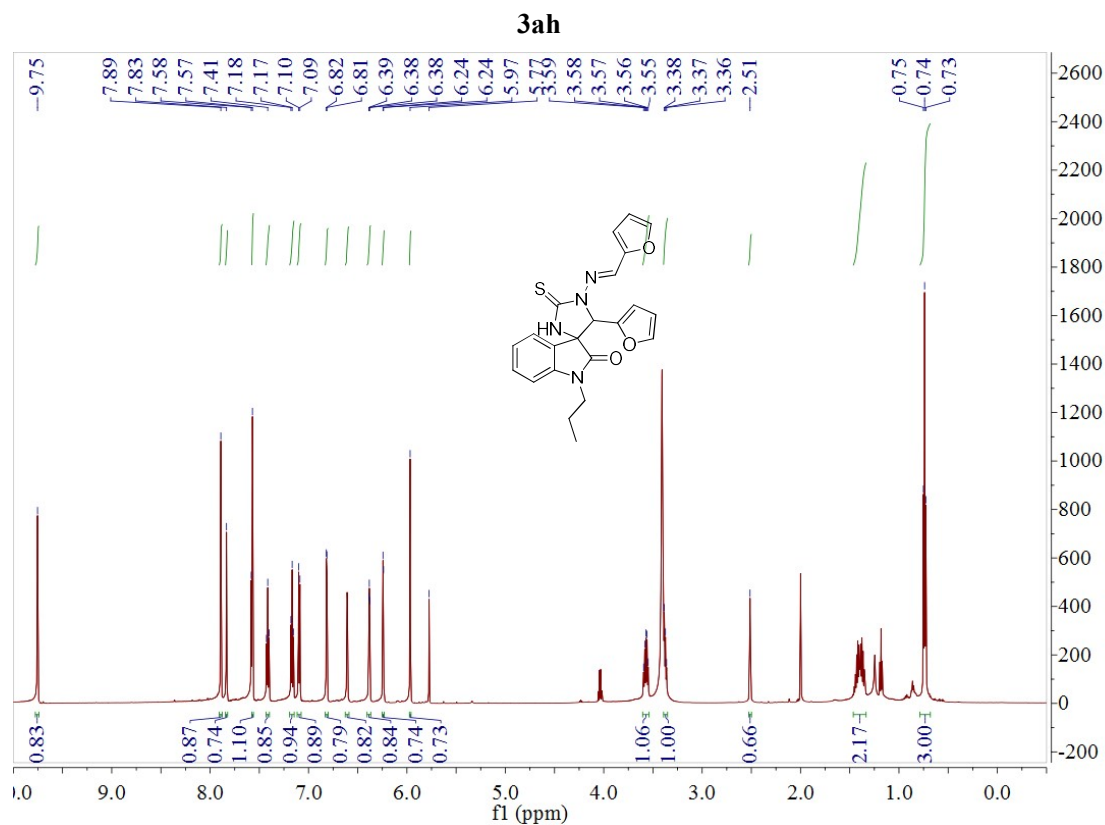


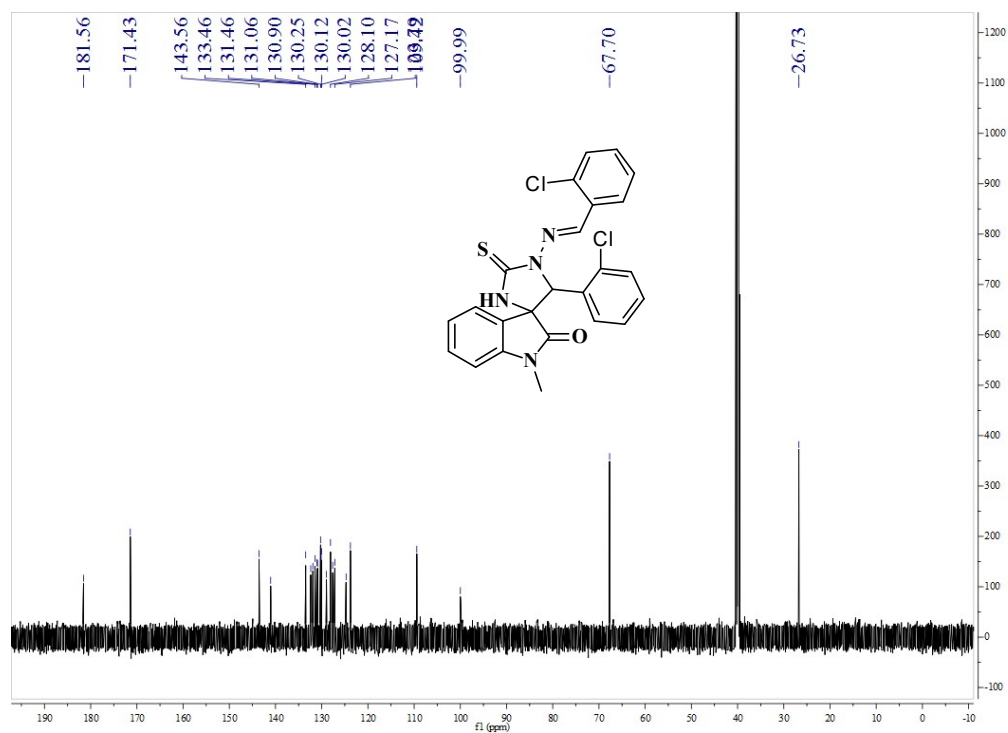
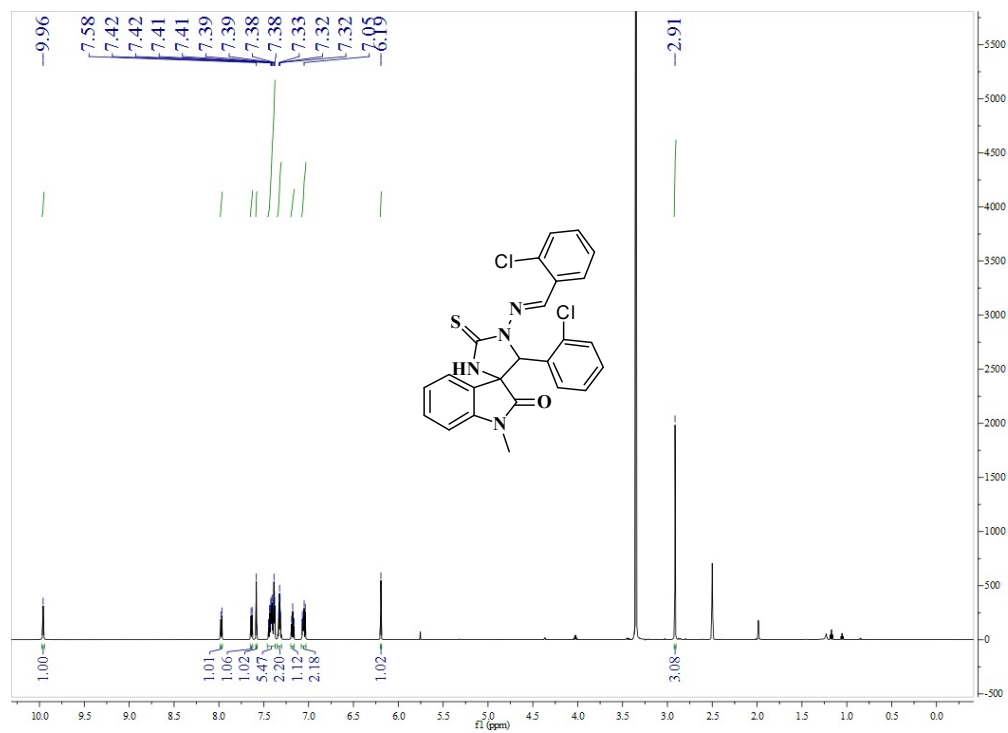


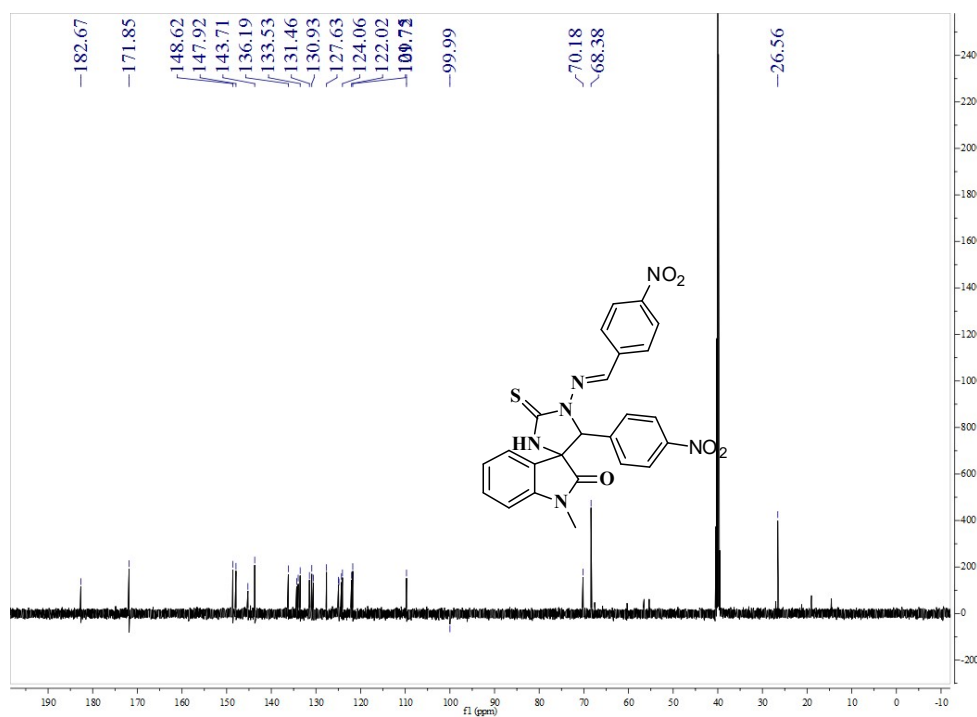
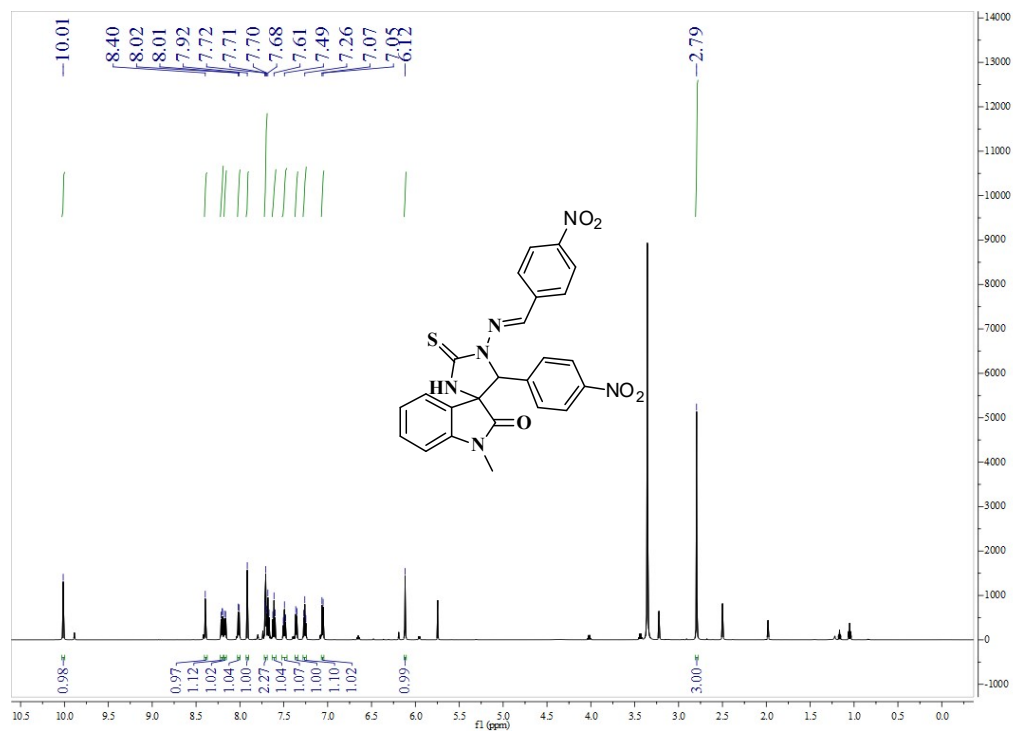


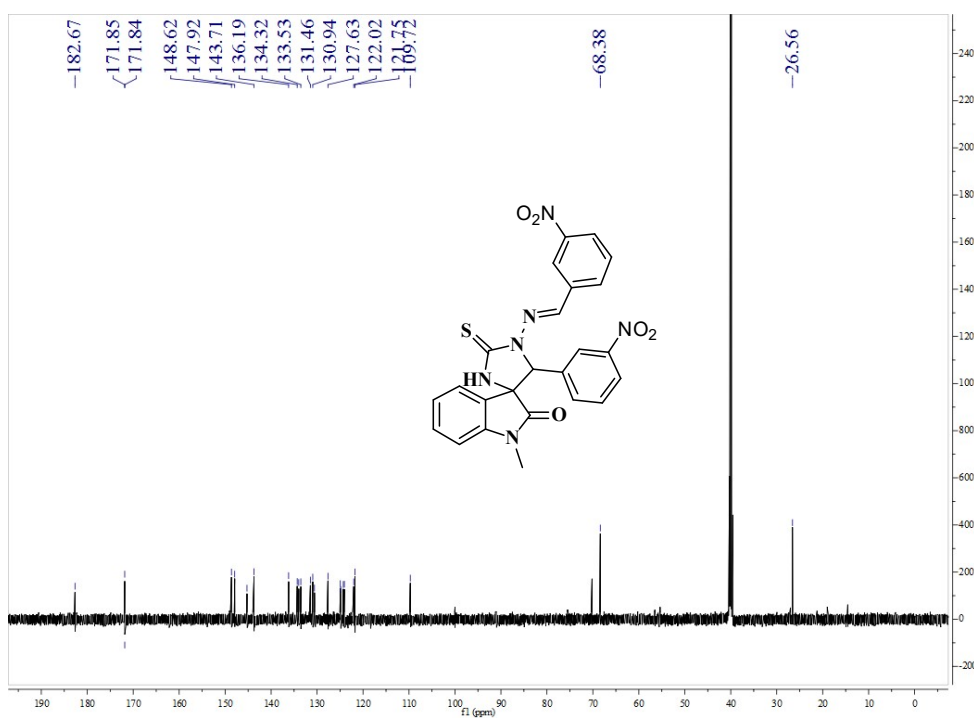
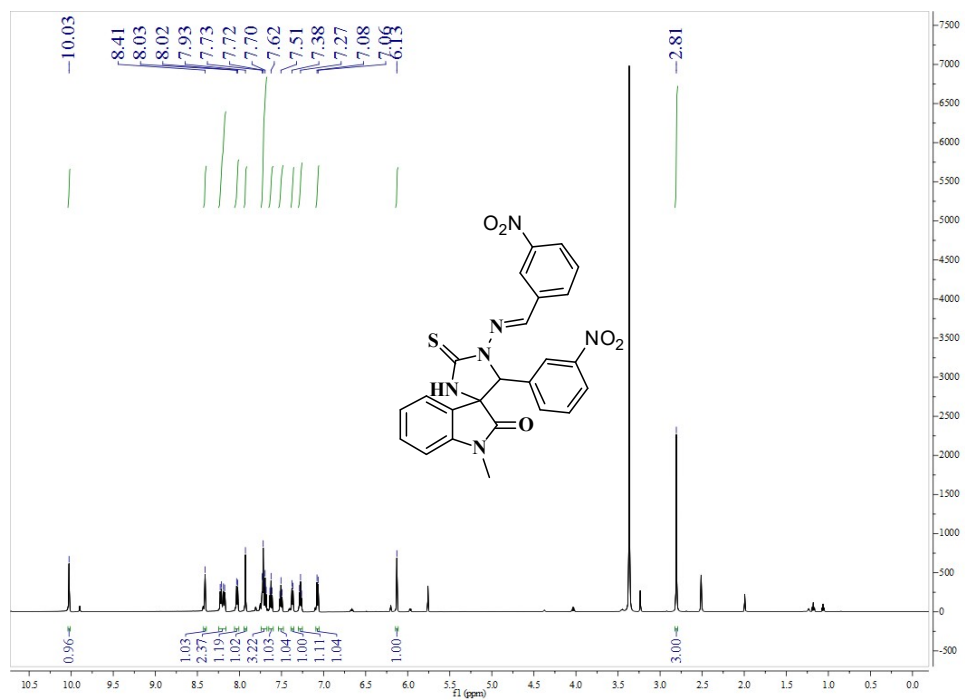


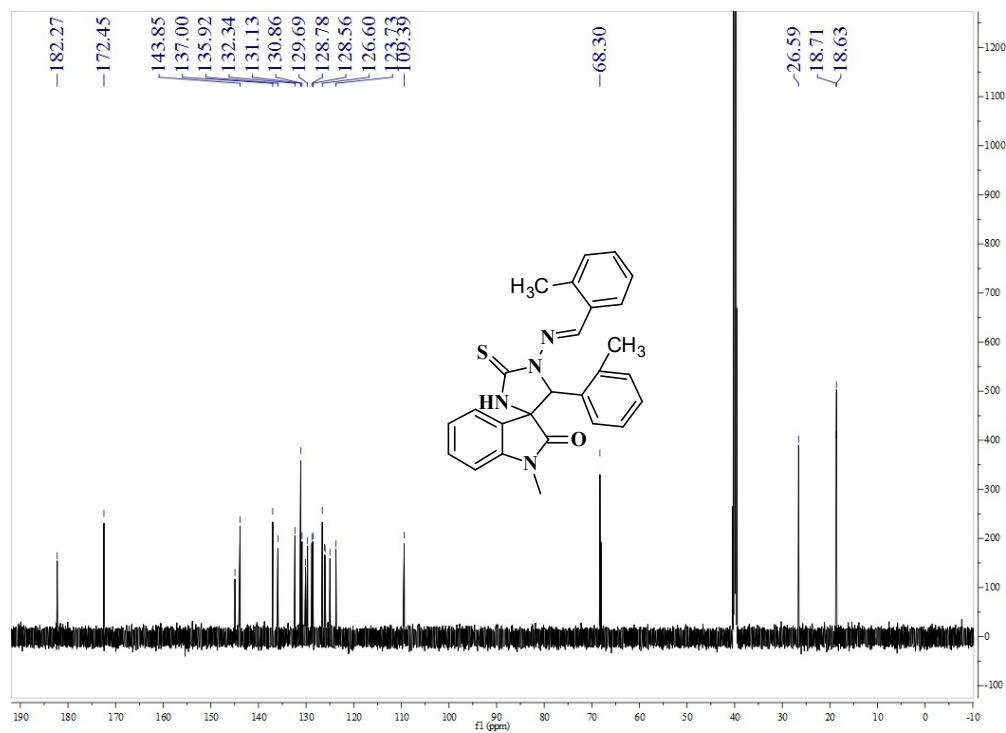
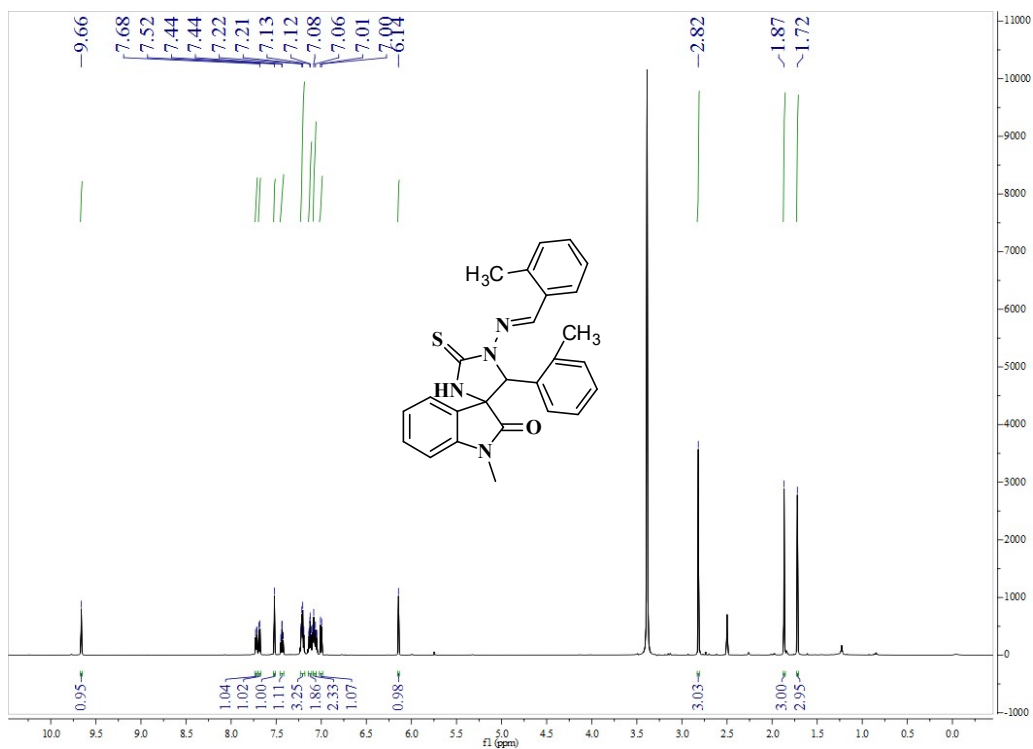


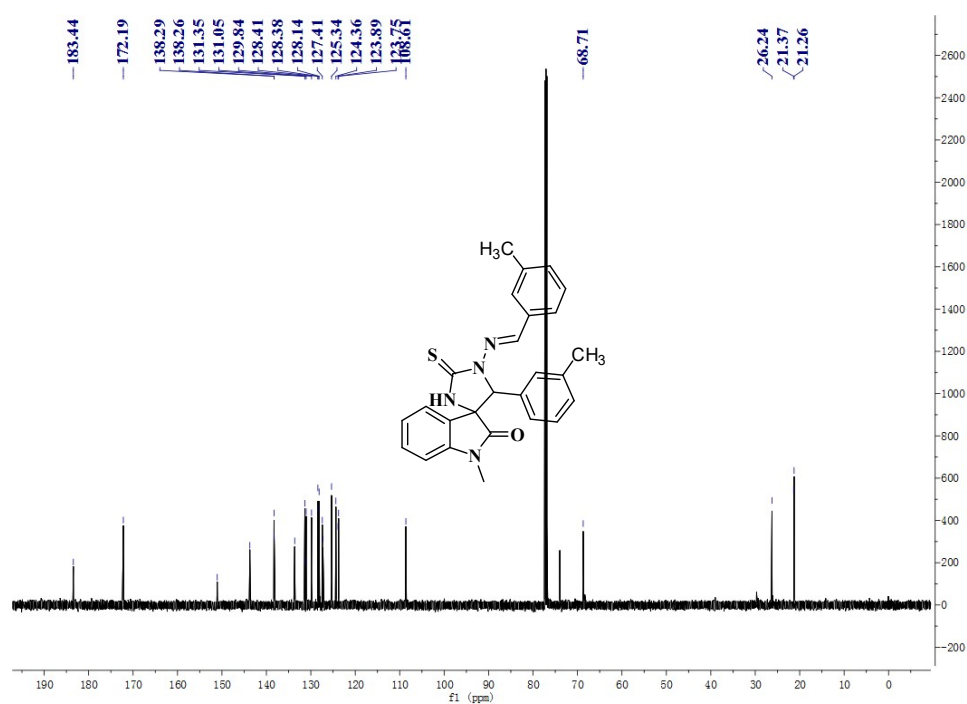
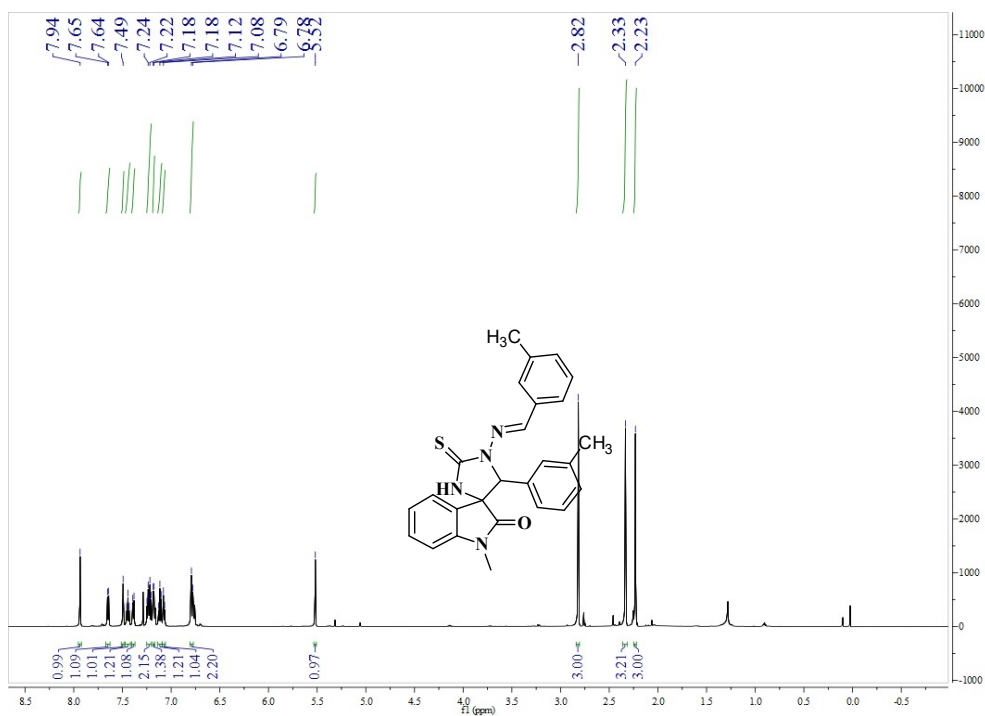


3bi

3bj

3bk

3bl

3bm

2. Crystal data

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Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

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N4 N 0.15026(13) 0.56095(7) 0.5789(2) 0.0412(4) Uani 1 1 d . . .
C4 C 0.12329(16) 0.35362(9) 0.7745(3) 0.0400(4) Uani 1 1 d . . .
C5 C 0.0464(2) 0.26298(13) 0.6520(4) 0.0722(8) Uani 1 1 d . . .
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C6 C 0.1214(3) 0.23082(12) 0.7643(4) 0.0786(9) Uani 1 1 d . . .
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C7 C 0.04714(19) 0.32575(11) 0.6543(3) 0.0550(6) Uani 1 1 d . . .
H7A H -0.0023 0.3478 0.5770 0.066 Uiso 1 1 calc R . .
C8 C 0.1997(2) 0.25878(11) 0.8823(4) 0.0662(7) Uani 1 1 d . . .
H8A H 0.2512 0.2367 0.9561 0.079 Uiso 1 1 calc R . .
C9 C 0.19927(18) 0.32043(9) 0.8869(3) 0.0457(5) Uani 1 1 d . . .
C10 C 0.23949(16) 0.41719(9) 0.9673(2) 0.0410(4) Uani 1 1 d . . .
C11 C 0.3572(2) 0.34092(14) 1.1328(3) 0.0676(7) Uani 1 1 d . . .
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H11B H 0.3685 0.3706 1.2210 0.081 Uiso 1 1 calc R . .
C12 C 0.4587(3) 0.3344(2) 1.0720(5) 0.1214(16) Uani 1 1 d . . .
H12A H 0.4489 0.3026 0.9897 0.146 Uiso 1 1 calc R . .
H12B H 0.4710 0.3713 1.0181 0.146 Uiso 1 1 calc R . .
C13 C 0.5510(4) 0.3209(4) 1.2067(8) 0.209(4) Uani 1 1 d . . .
H13A H 0.6114 0.3168 1.1623 0.314 Uiso 1 1 calc R . .
H13B H 0.5397 0.2842 1.2600 0.314 Uiso 1 1 calc R . .
H13C H 0.5626 0.3529 1.2867 0.314 Uiso 1 1 calc R . .
C14 C 0.29388(15) 0.44685(9) 0.6639(2) 0.0404(4) Uani 1 1 d . . .
C15 C 0.3255(2) 0.39857(12) 0.5831(3) 0.0613(6) Uani 1 1 d . . .
H15A H 0.2757 0.3716 0.5247 0.074 Uiso 1 1 calc R . .
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C20 C 0.18335(15) 0.55063(9) 0.4499(3) 0.0409(4) Uani 1 1 d . . .
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C21 C 0.20518(16) 0.59968(9) 0.3468(3) 0.0427(5) Uani 1 1 d . . .
C22 C 0.20879(19) 0.58800(11) 0.1853(3) 0.0535(5) Uani 1 1 d . . .
H22A H 0.1979 0.5491 0.1440 0.064 Uiso 1 1 calc R . .
C23 C 0.2284(3) 0.63335(16) 0.0841(4) 0.0792(9) Uani 1 1 d . . .
H23A H 0.2303 0.6250 -0.0249 0.095 Uiso 1 1 calc R . .
C24 C 0.2447(4) 0.68950(17) 0.1427(5) 0.1271(18) Uani 1 1 d . . .
H24A H 0.2589 0.7200 0.0749 0.153 Uiso 1 1 calc R . .
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H25A H 0.2508 0.7408 0.3398 0.181 Uiso 1 1 calc R . .
C26 C 0.2211(3) 0.65742(13) 0.4041(4) 0.0886(11) Uani 1 1 d . . .
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C8 0.092(2) 0.0368(12) 0.0744(17) 0.0108(11) 0.0301(15) 0.0061(12)
C9 0.0573(13) 0.0361(10) 0.0488(11) 0.0055(9) 0.0227(10) 0.0037(9)
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C17 0.0453(17) 0.178(4) 0.088(2) 0.031(3) 0.0288(17) 0.034(2)
C18 0.0430(15) 0.126(3) 0.088(2) 0.022(2) 0.0074(14) -0.0174(17)
C19 0.0434(12) 0.0658(16) 0.0666(15) 0.0030(12) 0.0099(11) -0.0067(11)
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C23 0.092(2) 0.094(2) 0.0569(16) 0.0095(15) 0.0277(15) -0.0137(18)
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are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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N1 C9 1.407(3) . ?

N1 C11 1.458(3) . ?

C1 N2 1.454(2) . ?

C1 C4 1.506(3) . ?

C1 C10 1.548(3) . ?

C1 C2 1.564(3) . ?

N2 C3 1.344(2) . ?

C2 N3 1.473(2) . ?

C2 C14 1.509(3) . ?

N3 C3 1.361(2) . ?

N3 N4 1.381(2) . ?

N4 C20 1.273(3) . ?

C4 C7 1.370(3) . ?

C4 C9 1.394(3) . ?

C5 C6 1.375(5) . ?

C5 C7 1.400(4) . ?

C6 C8 1.378(4) . ?

C8 C9 1.376(3) . ?

C11 C12 1.547(5) . ?

C12 C13 1.458(6) . ?

C14 C19 1.379(3) . ?

C14 C15 1.386(3) . ?

C15 C16 1.378(4) . ?

C16 C17 1.361(6) . ?

C17 C18 1.381(5) . ?

C18 C19 1.392(4) . ?

C20 C21 1.460(3) . ?

C21 C26 1.370(3) . ?

C21 C22 1.378(3) . ?

C22 C23 1.379(4) . ?

C23 C24 1.341(5) . ?

C24 C25 1.352(5) . ?

C25 C26 1.374(4) . ?

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C10 N1 C9 111.16(17) . . ?

C10 N1 C11 122.5(2) . . ?

C9 N1 C11 126.3(2) . . ?

N2 C1 C4 117.94(16) . . ?

N2 C1 C10 110.95(15) . . ?

C4 C1 C10 102.35(16) . . ?

N2 C1 C2 101.07(14) . . ?

C4 C1 C2 112.49(15) . . ?

C10 C1 C2 112.45(15) . . ?

C3 N2 C1 112.78(15) . . ?

N3 C2 C14 115.59(16) . . ?

N3 C2 C1 100.62(14) . . ?

C14 C2 C1 114.28(15) . . ?

C3 N3 N4 120.58(16) . . ?

C3 N3 C2 111.97(15) . . ?

N4 N3 C2 125.68(15) . . ?

N2 C3 N3 107.90(16) . . ?

N2 C3 S 125.45(15) . . ?

N3 C3 S 126.61(15) . . ?

C20 N4 N3 117.05(17) . . ?

C7 C4 C9 120.9(2) . . ?

C7 C4 C1 131.0(2) . . ?

C9 C4 C1 107.98(18) . . ?

C6 C5 C7 120.7(3) . . ?

C5 C6 C8 121.6(2) . . ?

C4 C7 C5 117.7(3) . . ?

C9 C8 C6 117.7(3) . . ?

C8 C9 C4 121.3(2) . . ?

C8 C9 N1 128.5(2) . . ?

C4 C9 N1 110.23(18) . . ?

O C10 N1 126.1(2) . . ?

O C10 C1 126.17(19) . . ?
N1 C10 C1 107.78(17) . . ?
N1 C11 C12 111.9(2) . . ?
C13 C12 C11 112.8(4) . . ?
C19 C14 C15 119.7(2) . . ?
C19 C14 C2 122.87(19) . . ?
C15 C14 C2 117.4(2) . . ?
C16 C15 C14 120.3(3) . . ?
C17 C16 C15 120.1(3) . . ?
C16 C17 C18 120.6(3) . . ?
C17 C18 C19 119.7(3) . . ?
C14 C19 C18 119.6(3) . . ?
N4 C20 C21 121.03(19) . . ?
C26 C21 C22 118.4(2) . . ?
C26 C21 C20 122.4(2) . . ?
C22 C21 C20 119.2(2) . . ?
C21 C22 C23 120.7(2) . . ?
C24 C23 C22 120.1(3) . . ?
C23 C24 C25 119.8(3) . . ?
C24 C25 C26 121.4(3) . . ?
C21 C26 C25 119.6(3) . . ?

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