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Synthesis of 5-substituted-3H-[1, 3, 4]-oxadiazol-2-one derivatives: A carbon dioxide route (CDR)

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Supporting Information:

Spectral Data for compounds 3a-j

Benzhydrazide (3a).[1]HNMR (400 MHz, DMSO-d6) δ 10.00 (brs, 1H,CONH), 6.8-7.2 (m,5H,ArH),4.6 (brs, 2H, NH2). [13]CNMR (100 MHz, DMSO-d_6) 164.70,134.63,134.30133.00,132.80,131.95,131.80.

4-fluorobenzohydrazide (3b).[1]HNMR 9.90 (brs, 1H, J = 8.0, CONH), 7.6 (dd, 2H, ArH),7.2 (dd, 2H, ArH), 4.62 (brs, 2H, NH2). [13]CNMR (100 MHz, DMSO-d_6) δ 161.50,160.00,135.00,134.40,134.00,119.50.

4-Methoxybenzohydrazide(3c).[1]HNMR (400 MHz, DMSO-d6) δ 10.10 (brs, 1H, J = 8.4, CONH), 7.10 (dd, 2H, ArH),7.45 (dd, 2H, ArH), 4.20 (brs, 2H, NH2).3.75(s,3H,OCH_3). [13]CNMR (100 MHz, DMSO-d_6) 166.00,159.91,134.50,134.00,130.10,120.00.

4-nitrobenzohydrazide (3d). [1]HNMR (400 MHz, DMSO-d6) δ 10.35 (brs, 1H, CONH), 7.25 (m, 4H, ArH), 4.73(s,2H, NH2). [13]CNMR (100 MHz, DMSO-d_6) 160.00,151.00,140.00,130.04,129.05,120.50,120.00.

4-methylbenzohydrazide(3e). [1]HNMR (400 MHz, DMSO-d6) δ 10.05 (brs, 1H, J = 8.10, CONH), 7.24 (dd, 2H, ArH),7.44 (dd, 2H, ArH), 4.21 (brs, 2H, NH2).2.60 (s,3H,CH_3). [13]CNMR (100 MHz, DMSO-d_6) 160.00,140.44,126.00,125.80,125.30,125.00,124.77, 20.11.

2-chlorobenzohydrazide (3f). [1]HNMR (400 MHz, DMSO-d6) δ 10.40 (brs, 1H, CONH), 7.45 (m, 4H, ArH), 4.19 (brs, 2H, NH2). [13]CNMR (100 MHz, DMSO-d_6) 155.13,132.60,130.50,130.00,129.50,126.00,120.50.

4-(N,N-dimethyl)-benzohydrazide(3g). [1]HNMR (400 MHz, DMSO-d6) δ (brs, 1H, J = 8.0, CONH), 7.20 (dd, 2H, ArH),7.25 (dd, 2H, ArH), 4.23 (brs, 2H, NH2).3.25(s,6H, 2xNCH_3). [13]CNMR (100 MHz, DMSO-d_6) 160.50,154.00,130.33,130.00124.50,119.99, 119.00, 40.00,39.99.

3,5-(dimethoxy)-benzohydrazide(3h).[1]HNMR (400 MHz, DMSO-d6) δ 10.26 (brs, 1H, J = 7.9, CONH), 7.20 (dd, 2H, ArH),7.40 (dd, 2H, ArH), 4.65 (brs, 2H, NH2).3.95(s,6H,2xOCH_3). [13]CNMR (100 MHz,DMSO-d_6) 161.00,154.87,154.00,135.03,109.00,106.40, 106.01,45.05,45.00.

3-(chloro), 4-(methyl)-benzohydrazide(3i) [1]HNMR (400 MHz, DMSO-d6) δ 10.40 (brs, 1H, CONH), 7.25-7.40(m,2H,ArH),4.00(brs,2H,NH2).2.450(s,3H,CH_3).[13]CNMR(100MHz,DMSO-d_6) 158.78, 138.00, 126.00, 122.00,121.60,117.00,24.50.

Butyrohydrazide(3j). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.40 (brs, 1H, J=8.4, CONH), 4.65 (brs, 2H, NH2).1.98 (m,2H,CH_2), 1.45 (m,5H,CH_2-CH_3). ^{13}CNMR (100 MHz, DMSO-d_6) 168.00,40.00,20.03,14.99.

Spectral Data for compounds 4a-j.

5-(Phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4a). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.190 (brs, 1H,OCONH), 6.8-7.0-7.50 (m,5H,ArH). ^{13}CNMR (100 MHz, DMSO-d_6) 154.60, 154.00, 134.00, 126.00, 125.91, 125.86, 125.69, 117.80.

5-(4-fluoro phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4b). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.20 (brs, 1H, J=7.60, OCONH), 6.90 (dd,2H,ArH) 7.0 (d,2H,ArH). ^{13}CNMR (100 MHz, DMSO-d_6) 164.11, 155.00, 154.30, 135.50, 135.00, 120.01, 115.60.

5-(4-methoxy phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4c). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.25 (brs, 1H, CONH), 6.65 (dd, 2H, ArH) 7.0 (d,2H,ArH), 3.80 (s, 3H, OCH_3). ^{13}CNMR (100 MHz, DMSO-d_6) 150.36, 150.00,140.05,128.00,123.38,120.00,72.70,71.80,71.60,71.38,55.20.

5-(4-nitro phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4d). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.10 (brs, 1H, CONH), 7.00 (m,4H,ArH). ^{13}CNMR (100 MHz, DMSO-d_6) 164.66,164.13,130.00, 124.34,124.11,120.50, 120.00.

5-(4-methyl phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4e). ^{1}HNMR (400 MHz, DMSO-d6) δ R 10.00 (brs, 1H, CONH), 7.00 (m,4H,ArH),2.48 (s,3H,CH_3). ^{13}CNMR (100 MHz, DMSO-d_6) 150.30, 150.10,140.00, 128.00, 127.98,127.90,127.87,120.00,21.50.

5-(2-chloro phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4f). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.50 (brs, 1H, CONH), 7.2 (m,4H,ArH). ^{13}CNMR (100 MHz, DMSO-d_6) 156.80,154.30,134.50,133.10, 133.09, 132.00, 129.50,124.00

5-[4-(N, N-dimethyl)-phenyl]-3H-[1, 3, 4]-oxadiazol-2-one (4g). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.10 (brs, 1H,CONH), 7.20 (m,4H,ArH),3.20 (s,6H,NCH_3). ^{13}CNMR (100 MHz, DMSO-d_6) 160.60, 160.00,159.50, 124.77,124.43,114.80,114.40,114.10,40.10,40.03.

5-(3,5-dimethoxy phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4h). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.20 (brs, 1H, J=7.6, CONH), 7.40 (s, 1H, ArH), 7.20 (dd,2H,ArH), 3.80 (s,6H,OCH_3) ^{13}CNMR (100 MHz,DMSO-d_6) 164.00, 163.88,154.00,150.80,130.00,102.00,101.38,101.00,54.41,50.00

5-(3-chloro,4-methyl-phenyl)-3H-[1, 3, 4]-oxadiazol-2-one (4i). ^{1}HNMR (400 MHz, DMSO-d6) δ 10.20 (brs, 1H,CONH), 7.62 (s,1H,ArH),7.40 (d,1H,ArH),7.17 (d,1H,ArH). ^{13}CNMR (100 MHz, DMSO-d_6) 160.00, 158.30, 140.00,125.90,125.20,125.11,121.00,21.50.

5-propyl-3H-[1, 3, 4]-oxadiazol-2-one (4j). ^{1}HNMR (400 MHz,DMSO-d6) δ 10.18 (brs, 1H,CONH), 2.00 (t,2H,CH_2),1.60 (m,2H,CH_2), 1.00 (d,3H,CH_3).^{13}CNMR (100 MHz, DMSO-d_6) 160.30, 157.00, 30.00, 17.80, 17.20.

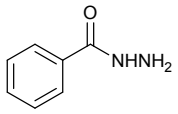
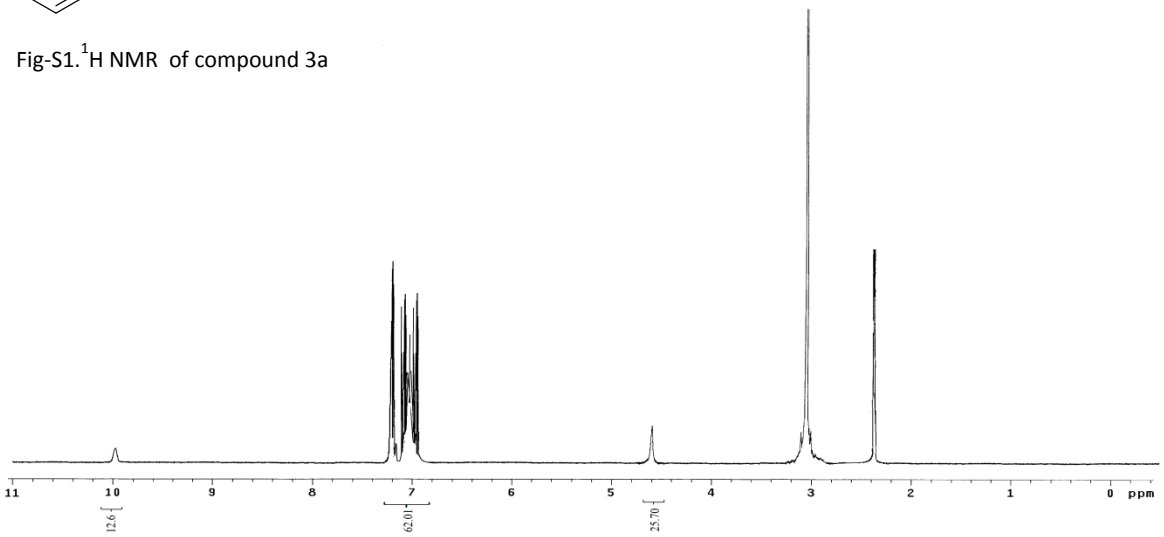


Fig-S1.[1]H NMR of compound 3a



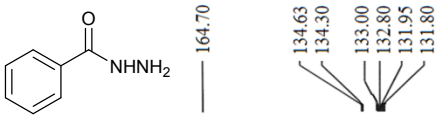
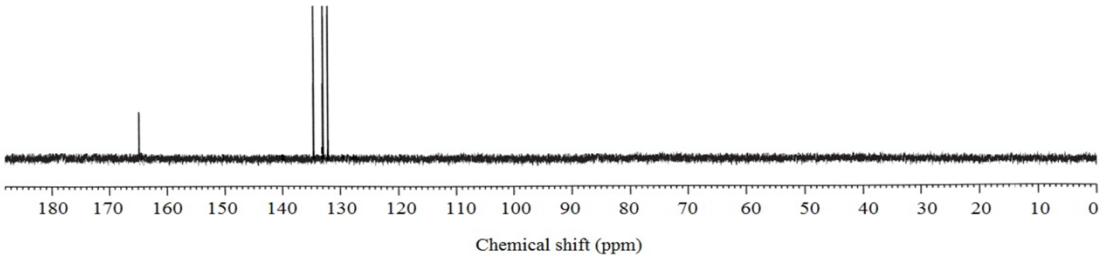


Fig-S2.[13] CNMR of compound 3a



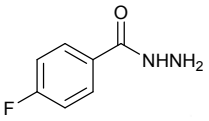
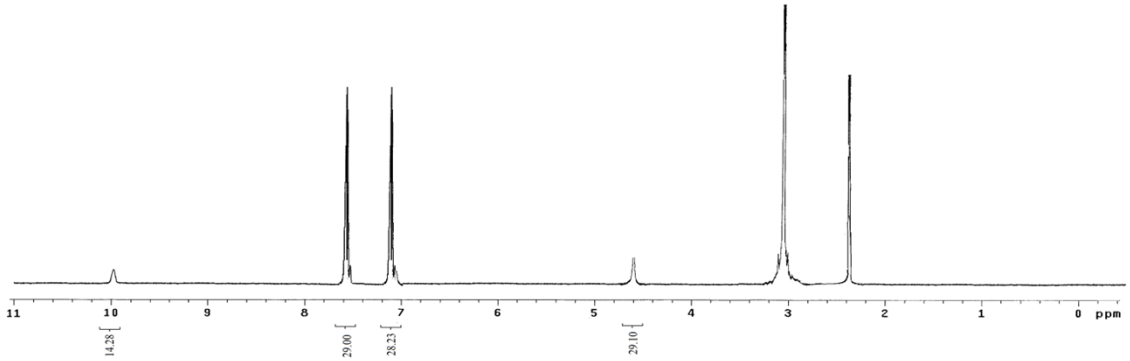


Fig-S3.[1] HNMR of compound 3b



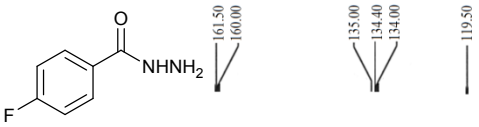
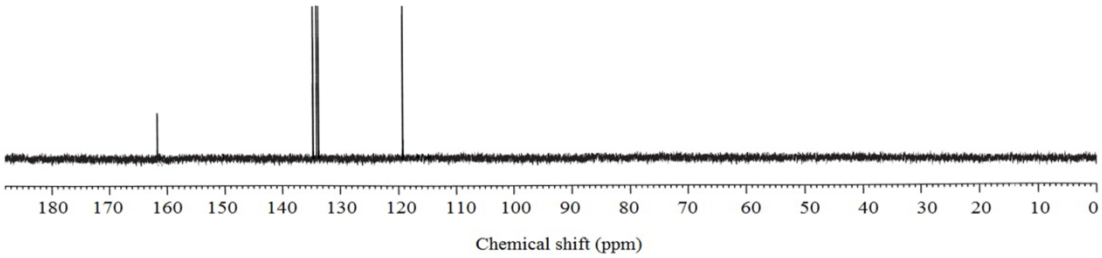


Fig-S4.[13] CNMR of Compound 3b



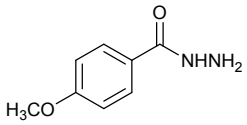
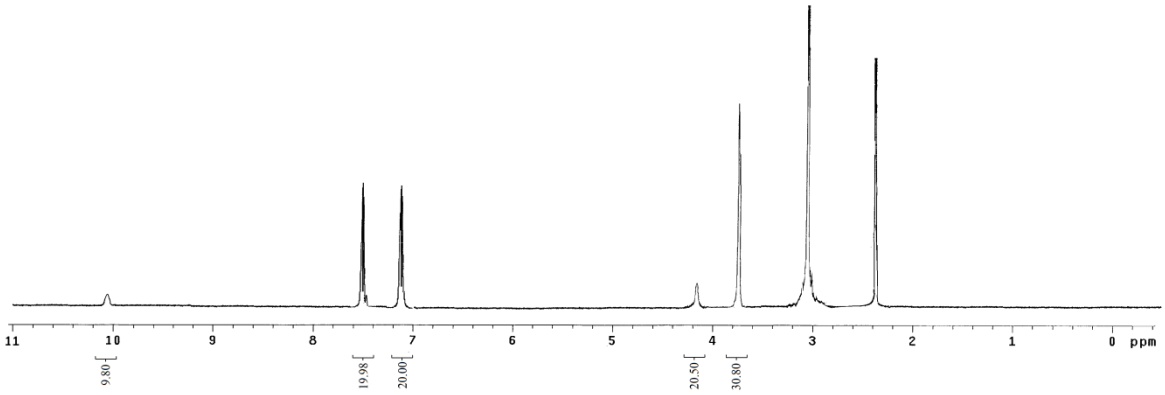


Fig-S5.[1]H NMR of compound 3c



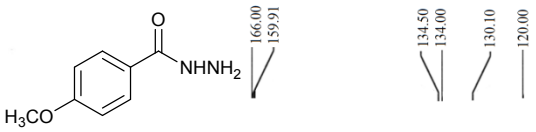
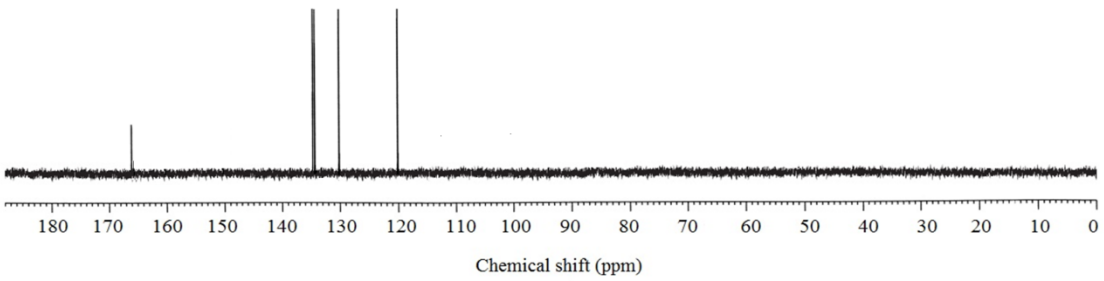


Fig-S6. [13] CNMR of compound 3c



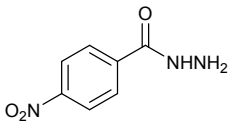
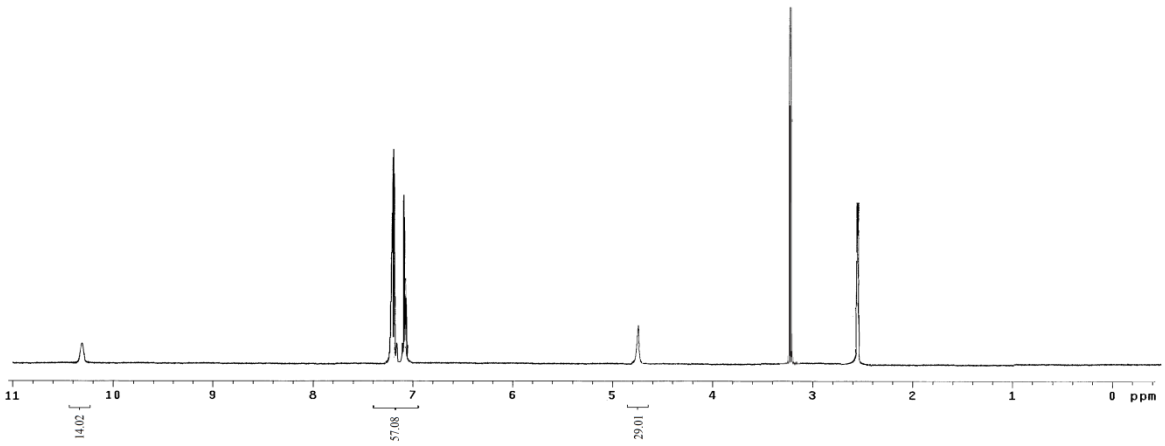


Fig-S7. ^{1}H NMR of Compound 3d



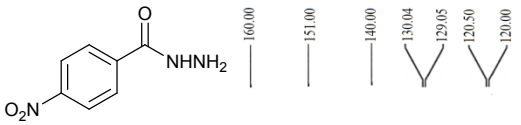
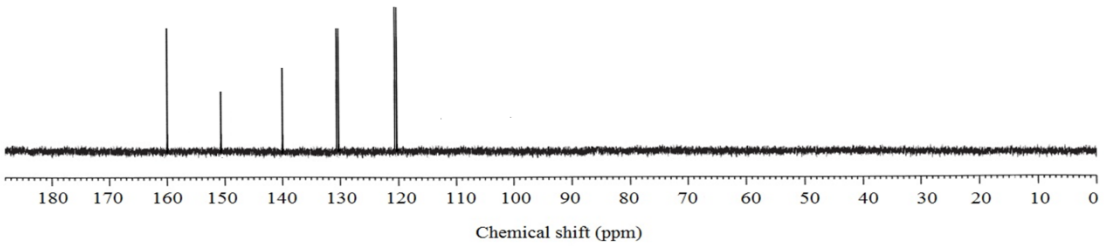


Fig-S8. ^{13} CNMR of Compound 3d



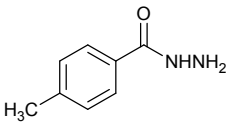
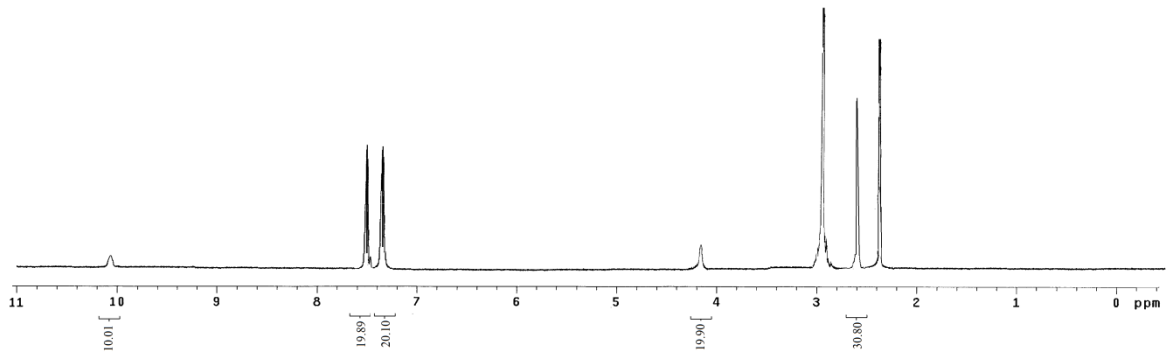


Fig-S9. ^{1}HNMR of Compound 3e



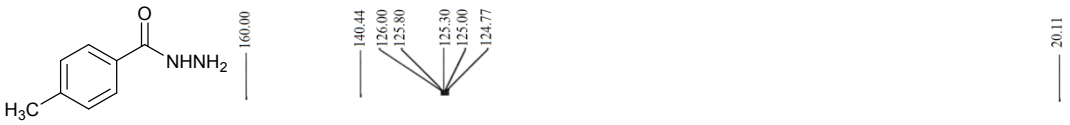
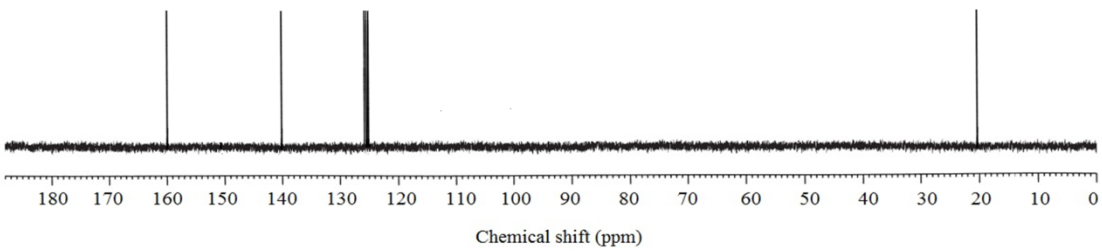


Fig-S10. ^{13}CNMR of Compound 3e



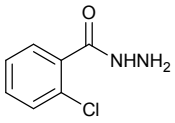


Fig-S11.[1]H NMR of compound 3f

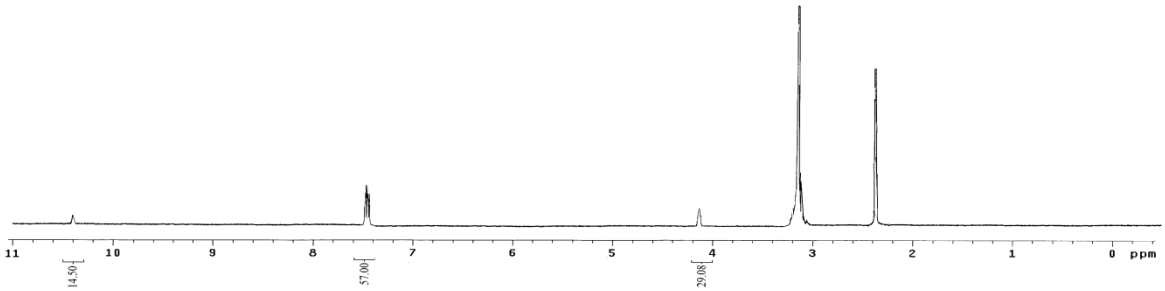
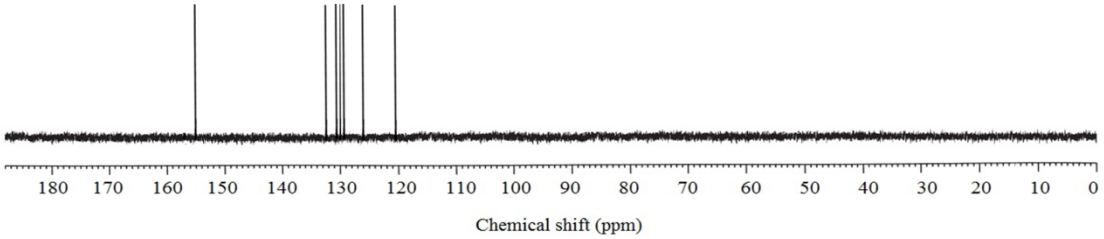


Fig-S12.[13] CNMR compound 3f



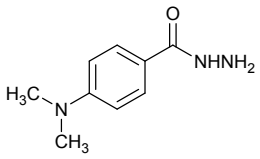
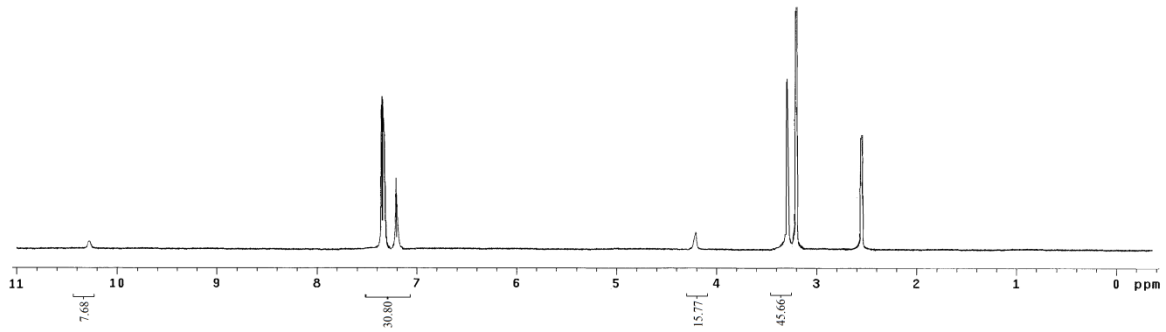


Fig-S13. ^{1}HNMR of compound 3g



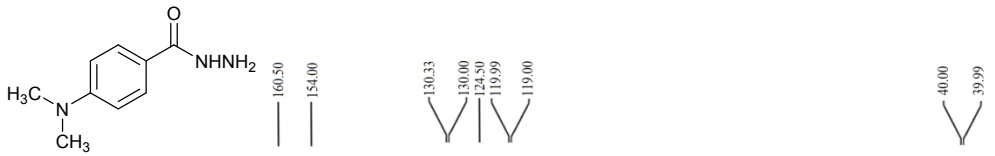
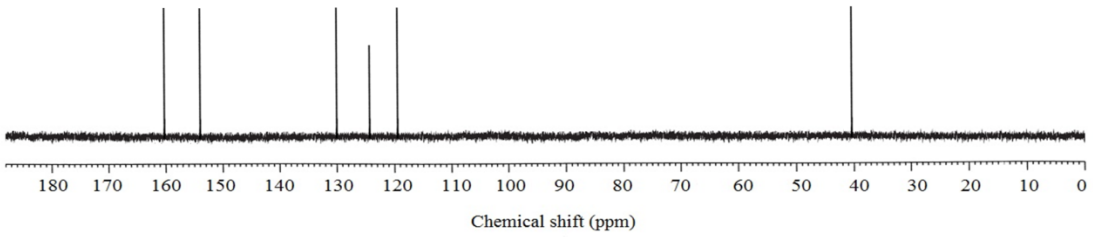


Fig-S14. ^{13} CNMR of compound 3g



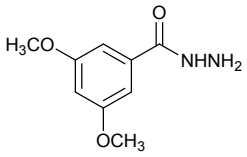
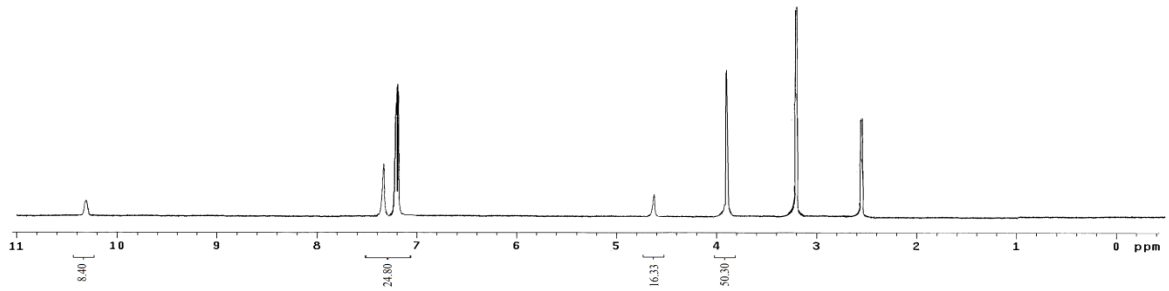


Fig-S15. ^{1}H NMR of compound 3h



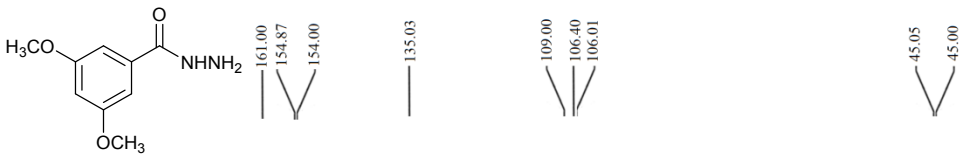
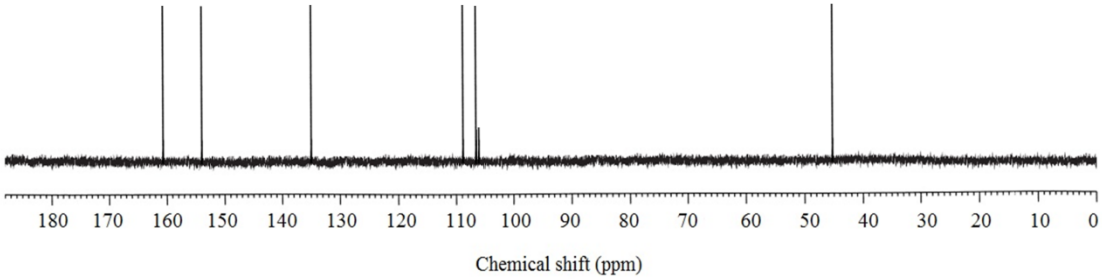


Fig-S16. ^{13}CNMR of compound 3h



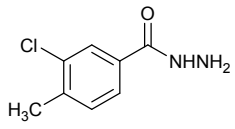


Fig-S17. ^{1}H NMR of Compound 3i

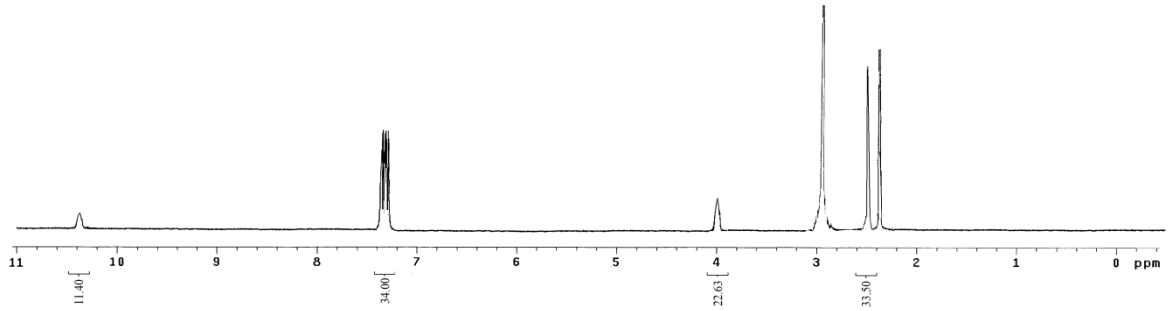
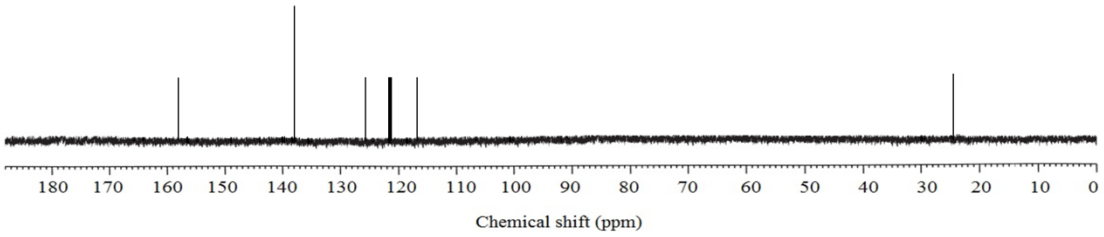


Fig-S18. ^{13}CNMR of compound 3i



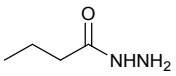


Fig-S19.[1]H NMR of compound 3j

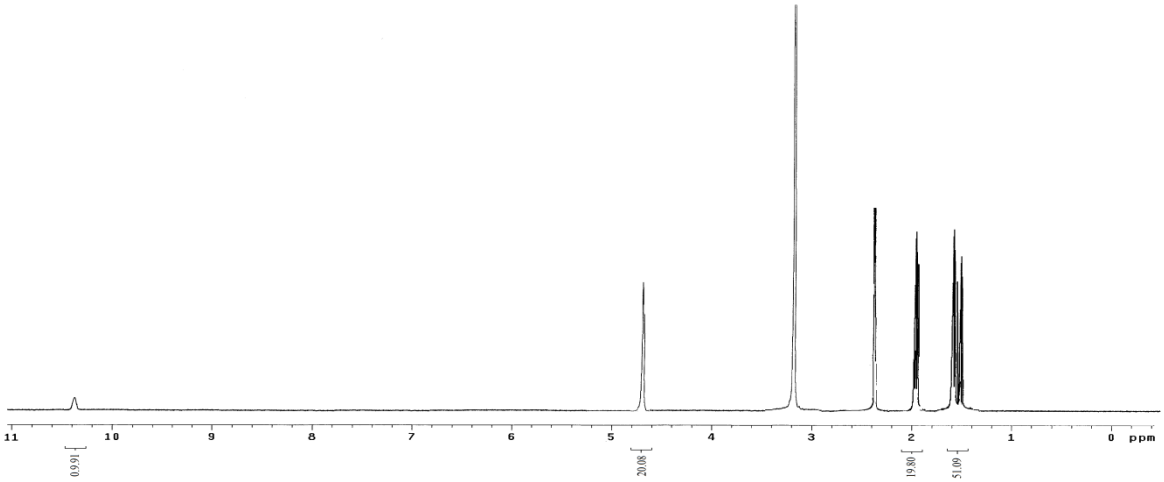
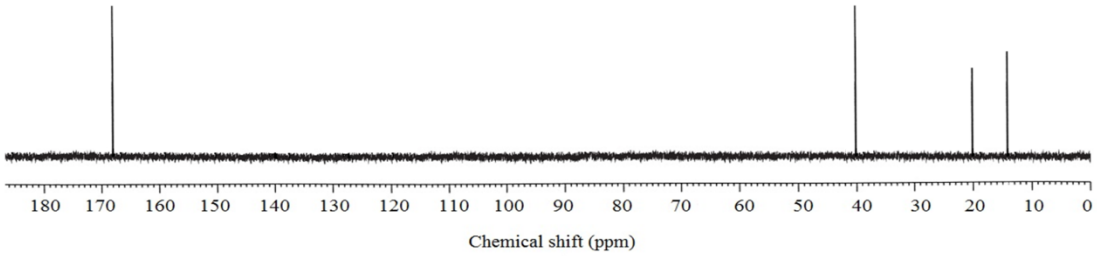


Fig-S20. [13] CNMR of compound 3j



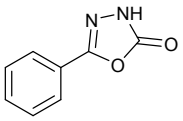
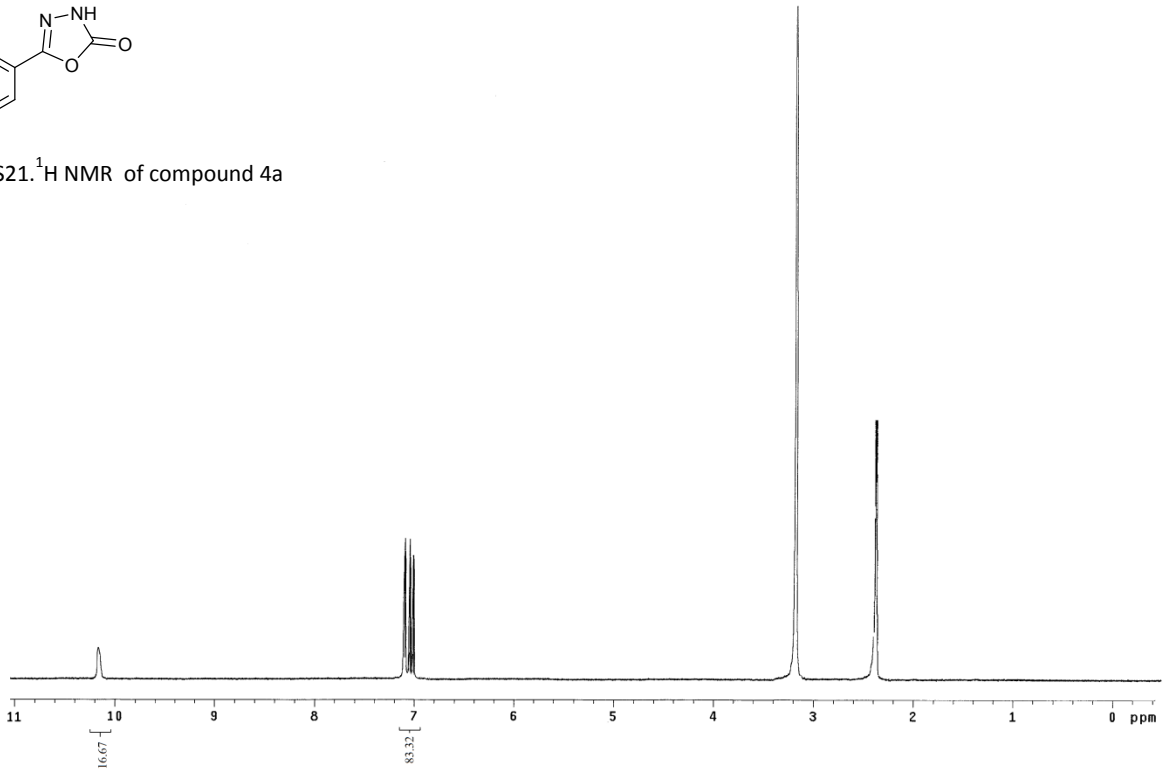


Fig-S21.[1]H NMR of compound 4a



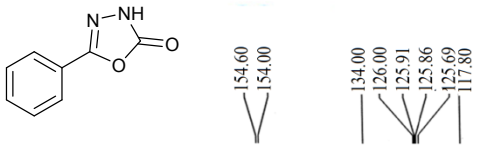
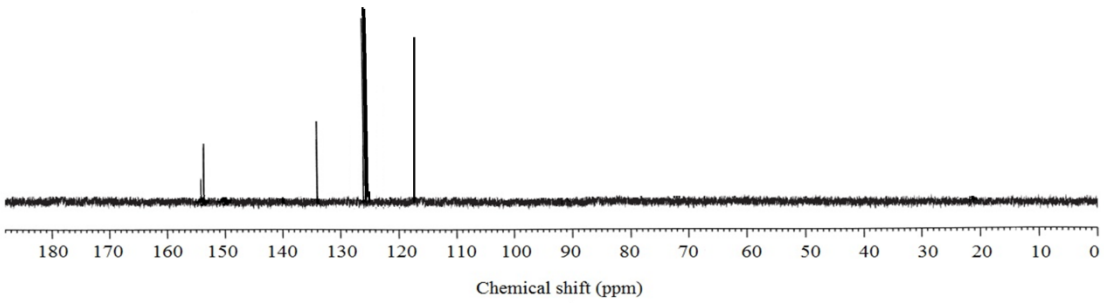


Fig-S22. [13] CNMR of compound 4a



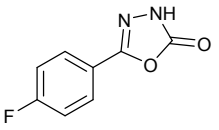
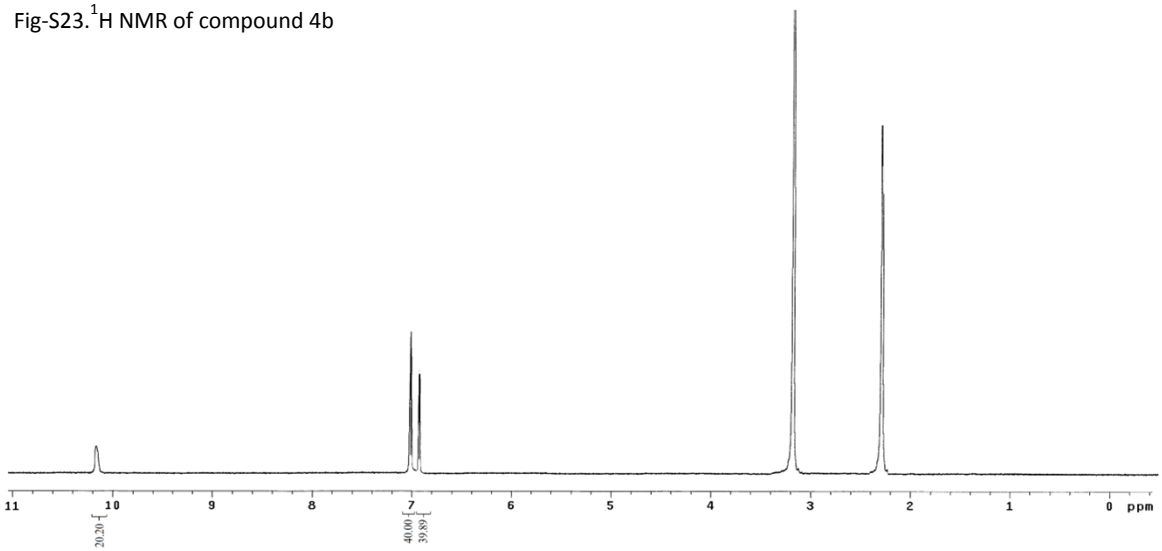


Fig-S23. ^{1}H NMR of compound 4b



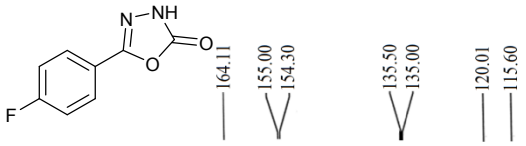


Fig-S24. ^{13}CNMR of compound 4b

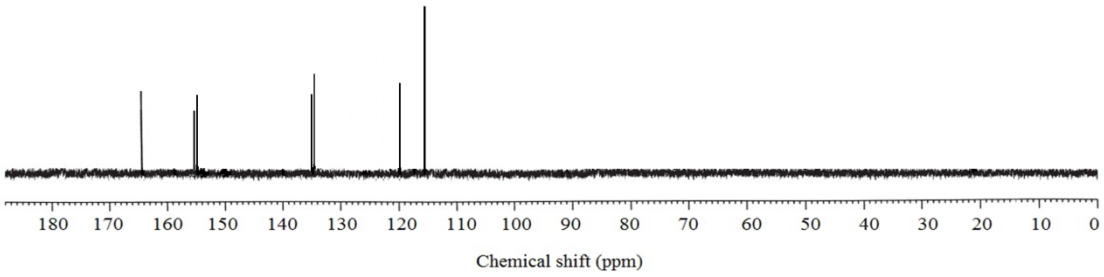
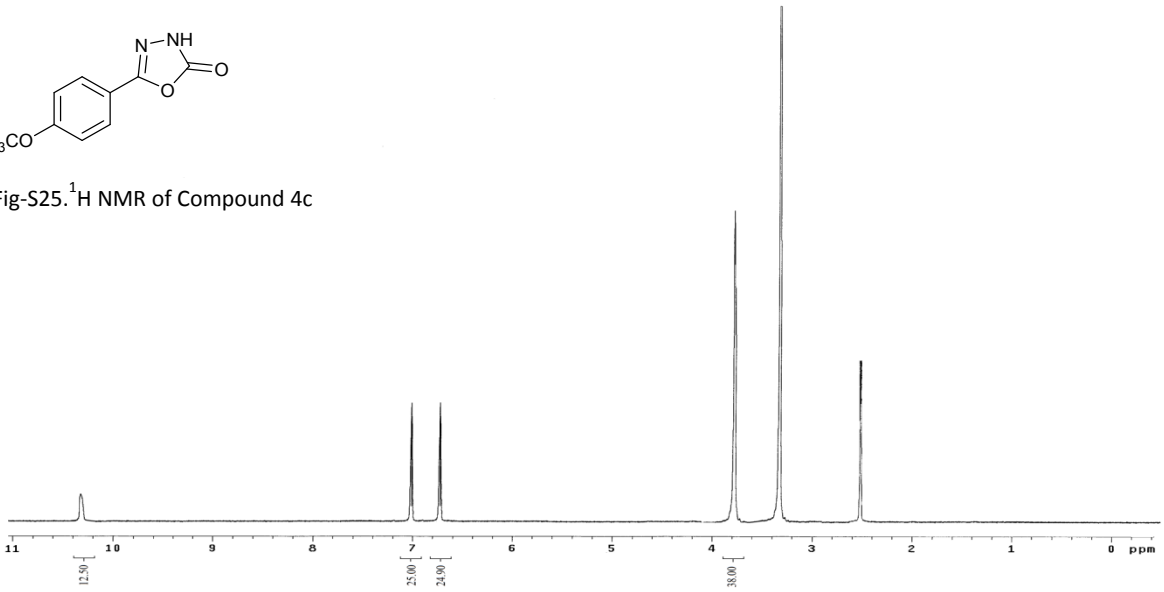


Fig-S25. ^{1}H NMR of Compound 4c



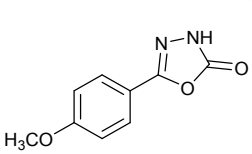


Fig-S26. ^{13} CNMR of compound 4c

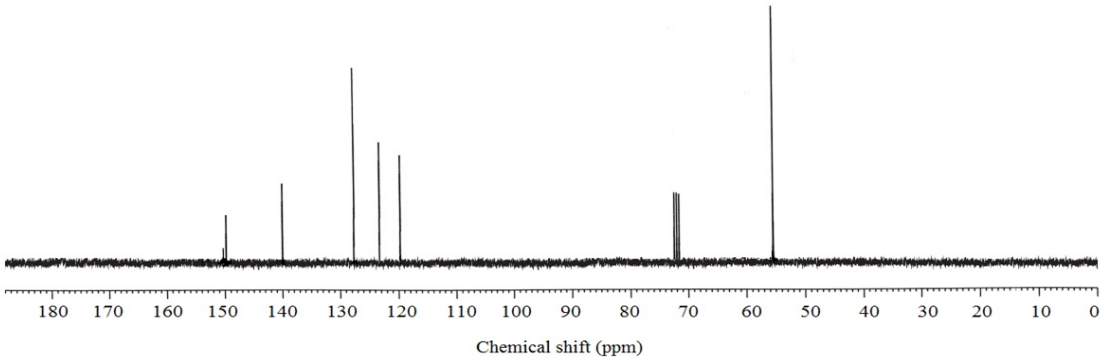
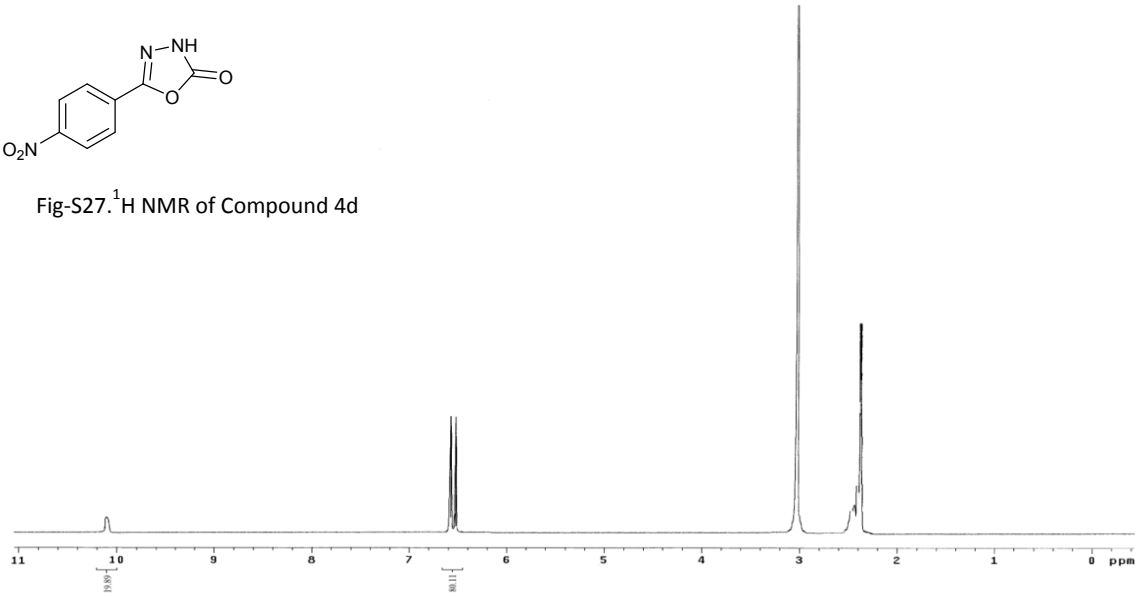


Fig-S27. ^{1}H NMR of Compound 4d



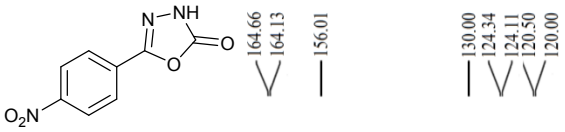
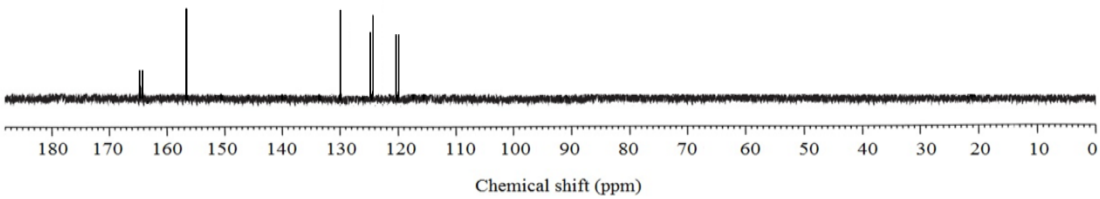


Fig-S28. ^{13} CNMR of compound 4d



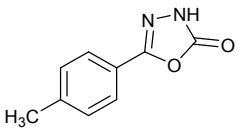


Fig-S29.[1]H NMR of compound 4e

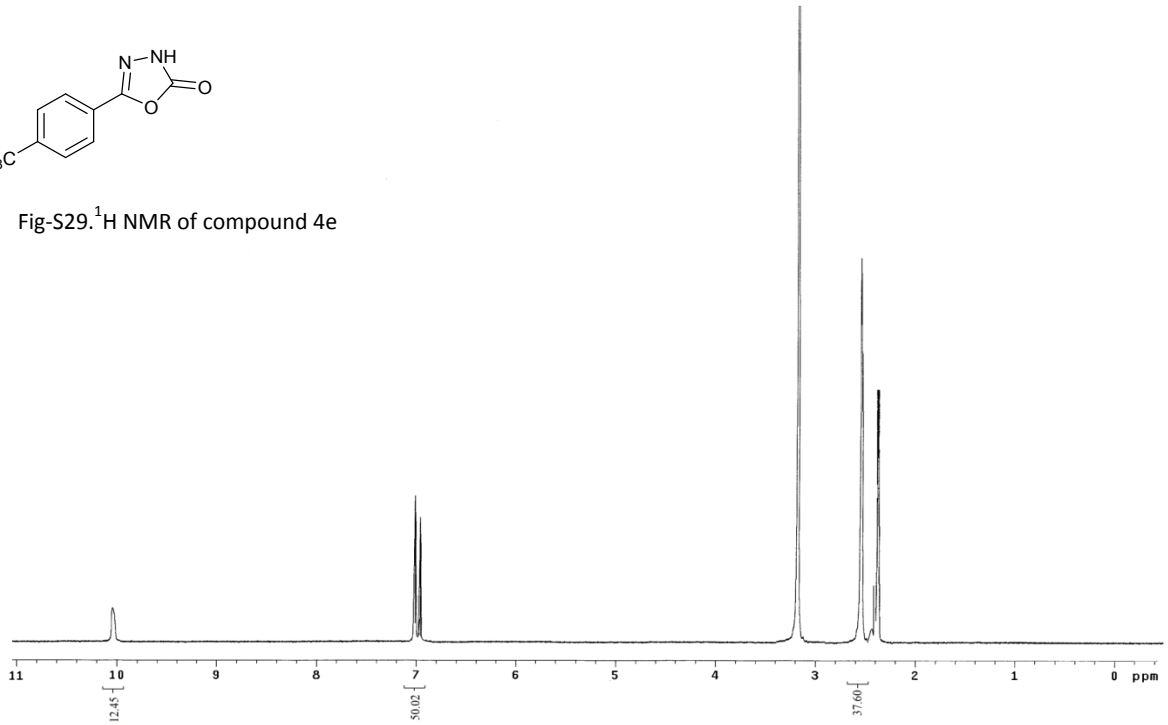
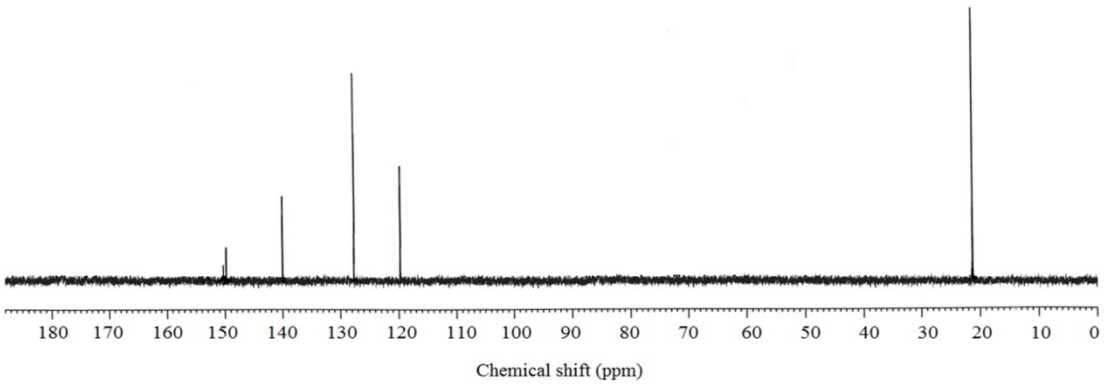


Fig-S30. [13] CNMR of compound 4e



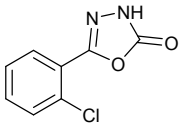
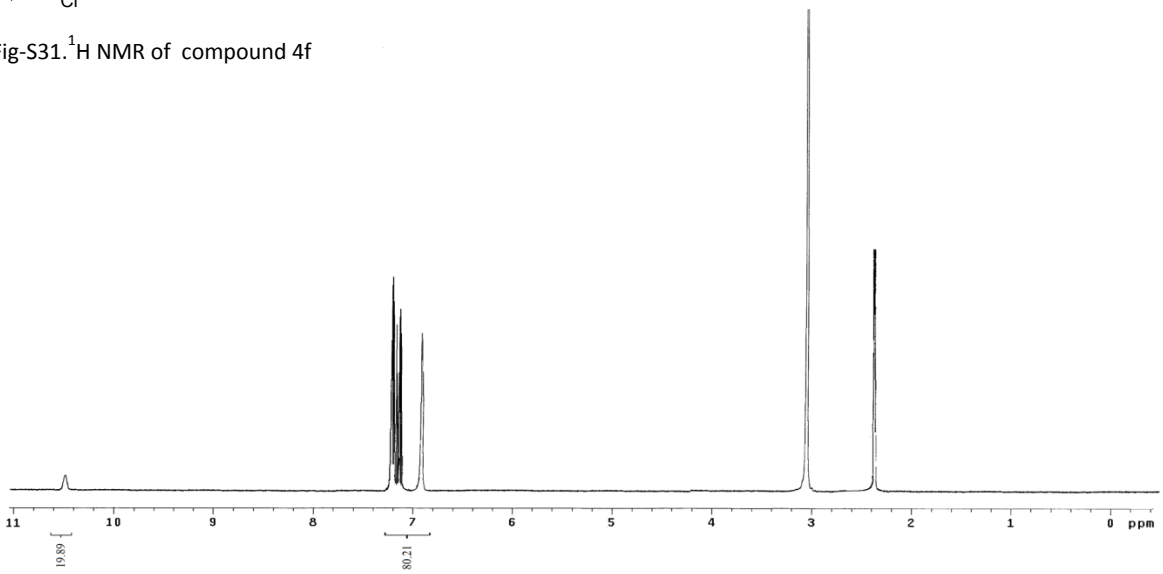


Fig-S31.[1]H NMR of compound 4f



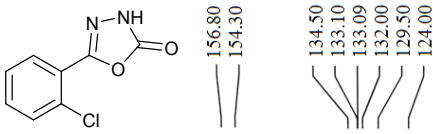


Fig-S32. [13] CNMR of compound 4f

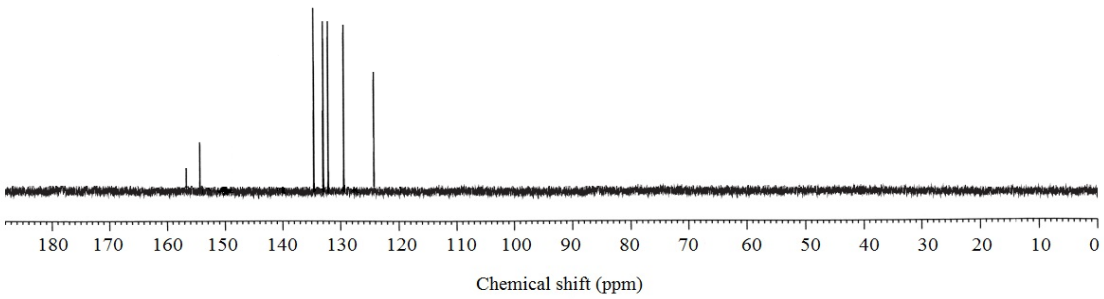
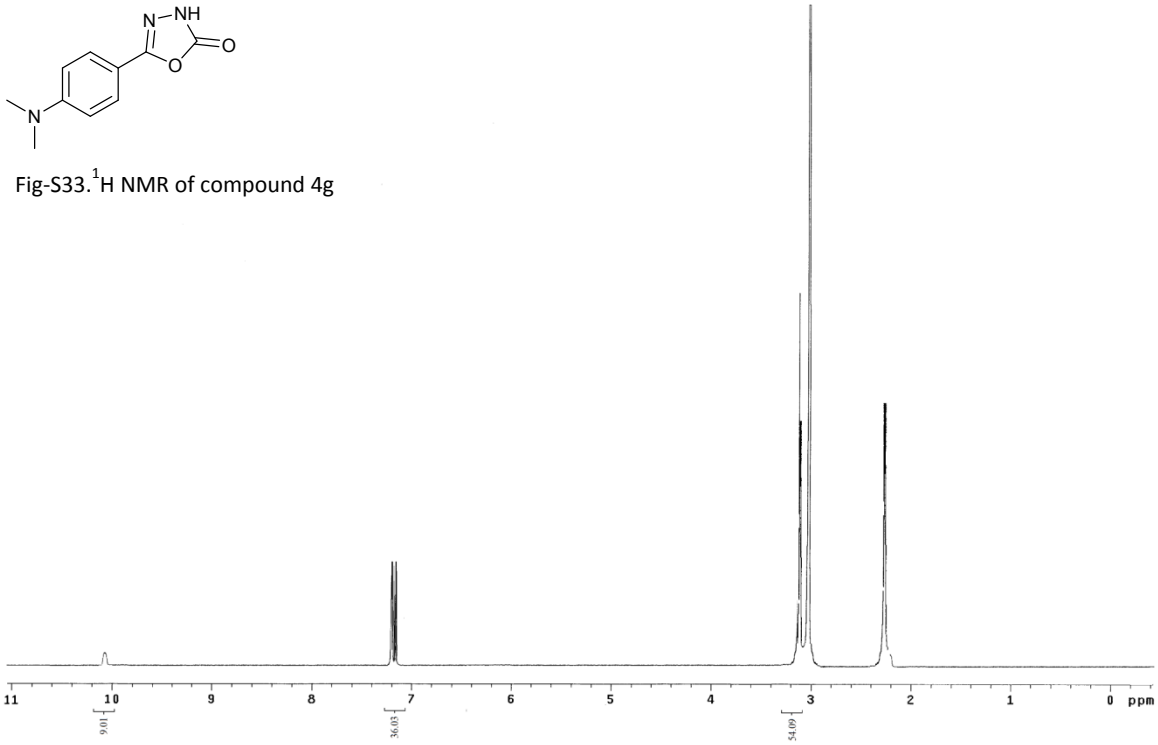


Fig-S33.[1]H NMR of compound 4g



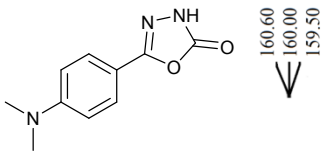
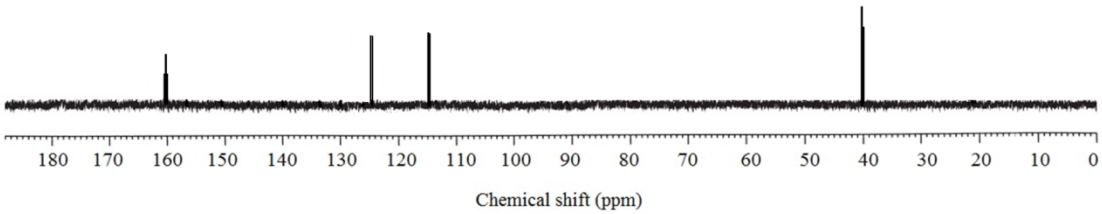


Fig-S34. [13] CNMR of compound 4g



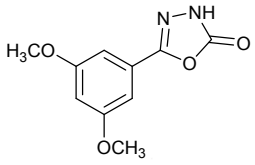


Fig-S35. ^{1}H NMR of compound 4h

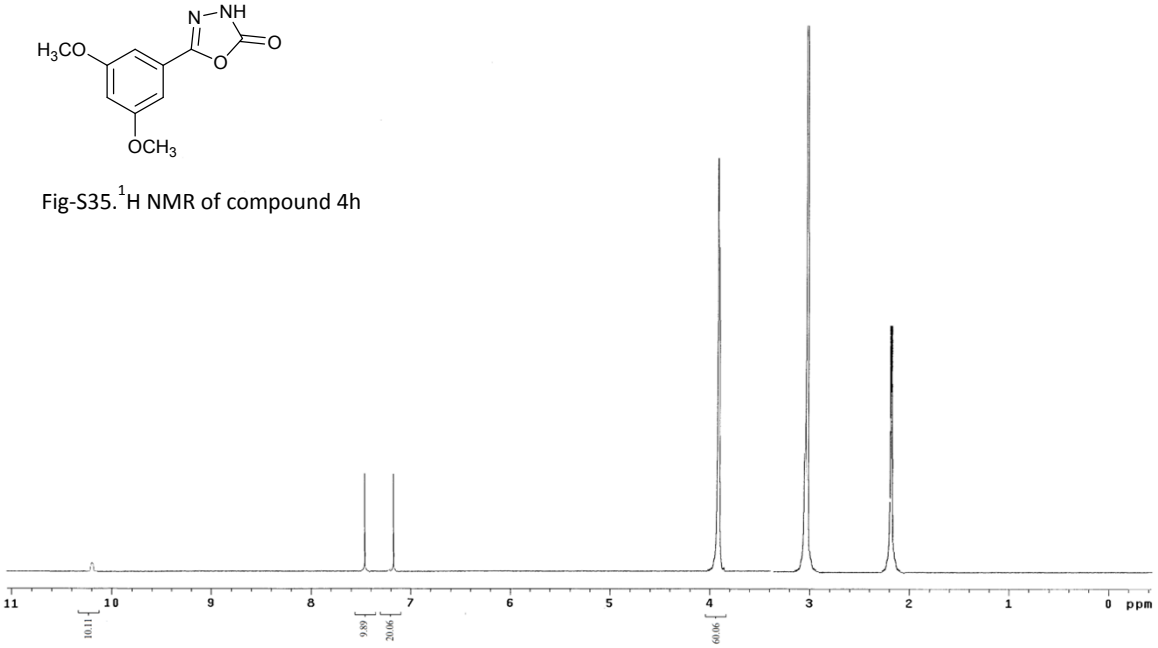
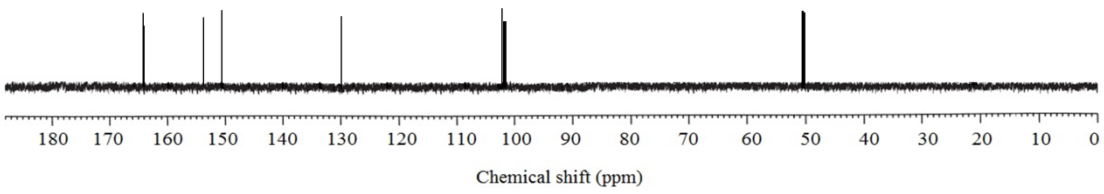


Fig-S36. ^{13} CNMR of compound 4h



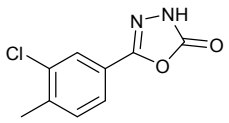
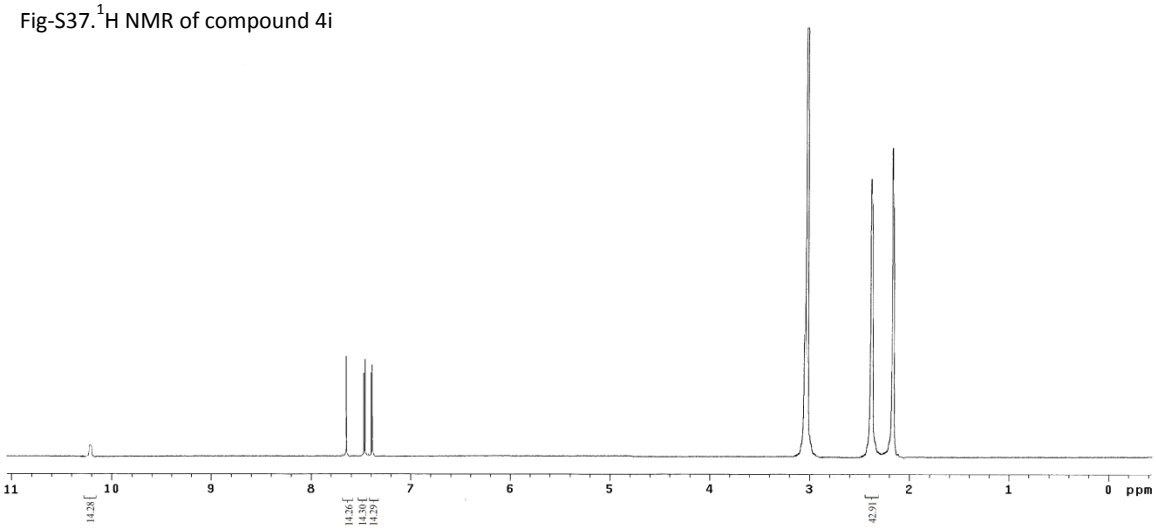


Fig-S37. ^{1}H NMR of compound 4i



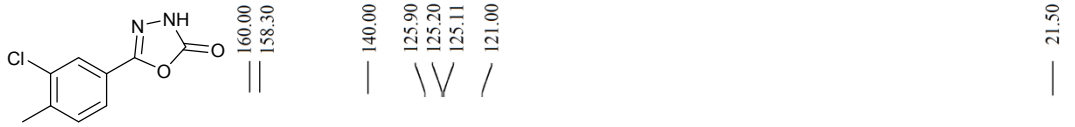
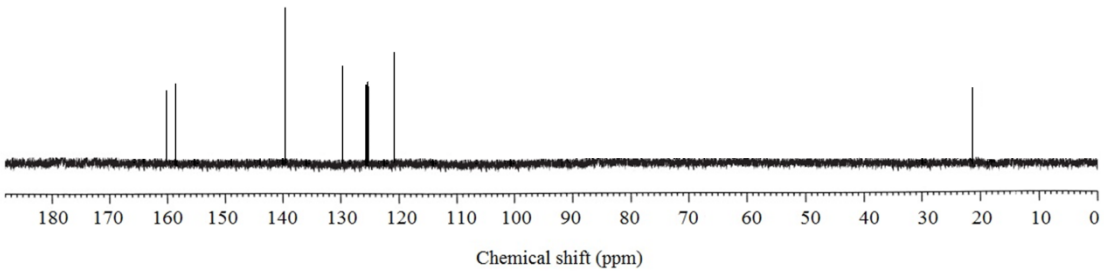


Fig-S38. ^{13}CNMR of compound 4i



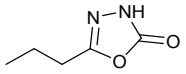
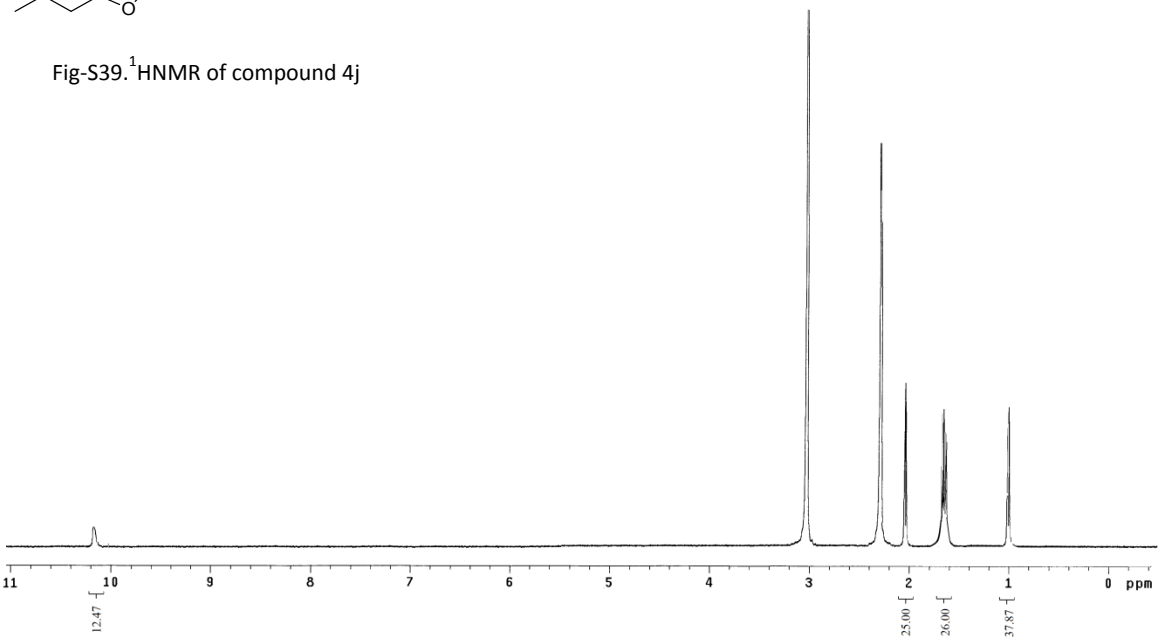


Fig-S39. ^{1}HNMR of compound 4j



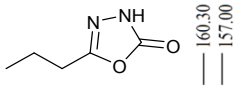


Fig-S40. ^{13} CNMR of compound 4j