Electronic Supplementary Information (ESI)

The Use of the Mitsunobu Reagent for the Formation of Heterocycles: a Simple Method for the Preparation of 3-Alkyl-5-aryl-1,3,4-oxadiazol-2(3*H*)-ones from Carboxylic Acids

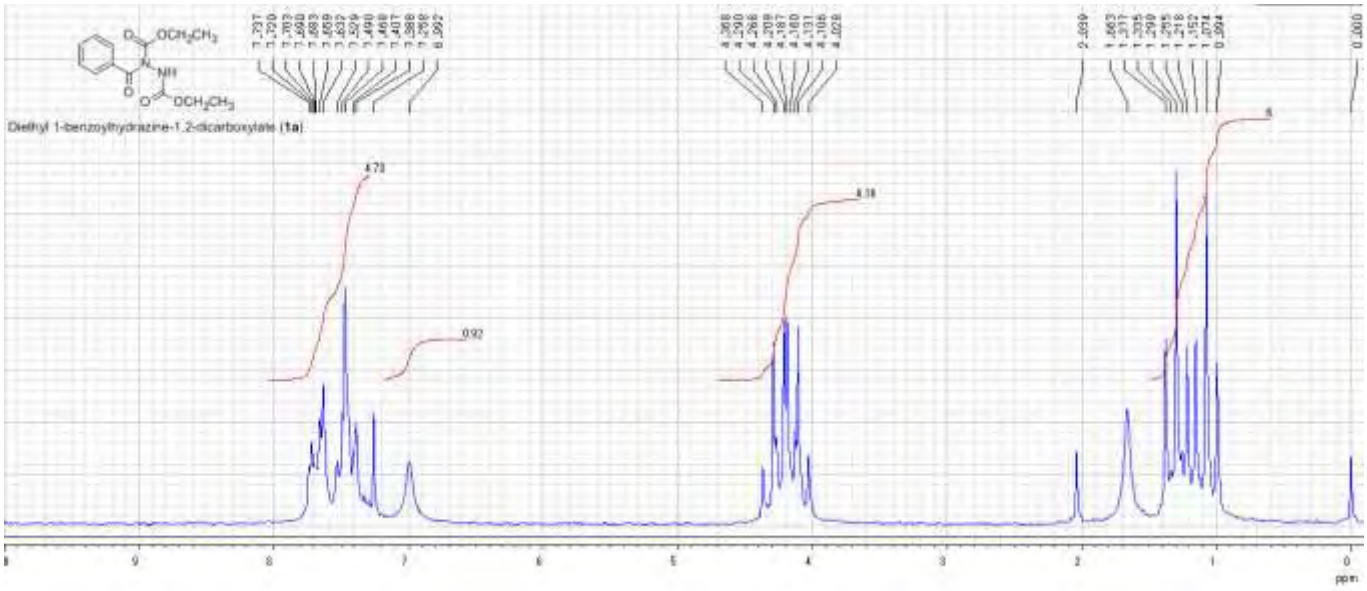
Osamu Sugimoto,* Tomoyo Arakaki, Hiroka Kamio, and Ken-ichi Tanji*

Laboratory of Organic Chemistry, School of Food and Nutritional Sciences, University of Shizuoka, 52-1 Yada, Suruga-ku, Shizuoka 422-8526, Japan.
Fax: +81 54 264 5542
Tel: +81 54 264 5545
E-mail: osamu@u-shizuoka-ken.ac.jp

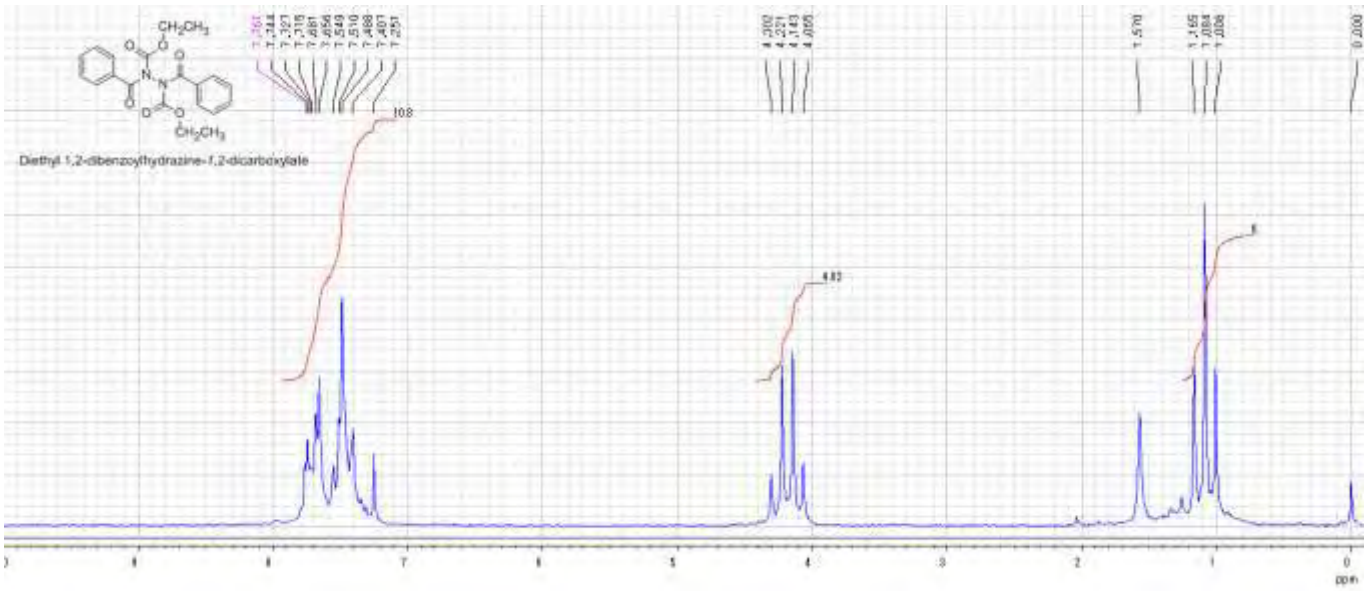
All melting points were not corrected. ^{1}H-NMR and ^{13}C-NMR spectra were measured with HITACHI R-90H spectrometer except ^{13}C-NMR spectra of 3-isopropyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one and 5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one, which were measured with BRUKER ULTRASHIELD 400 PLUS.

Preparation of 3-alkyl 5-aryl-1,3,4-oxadiazol-2(3*H*)-ones (general procedure): In a recovery flask equipped with a magnetic stirrer bar, a toluene solution of diethyl azodicarboxylate was added dropwise to a suspension of carboxylic acid and triphenylphosphine in dichloromethane, and the mixture was heated to reflux. After dichloromethane was removed under atmospheric pressure, the residue was heated. The reaction mixture was treated with silica gel column chromatography to give the desired product.

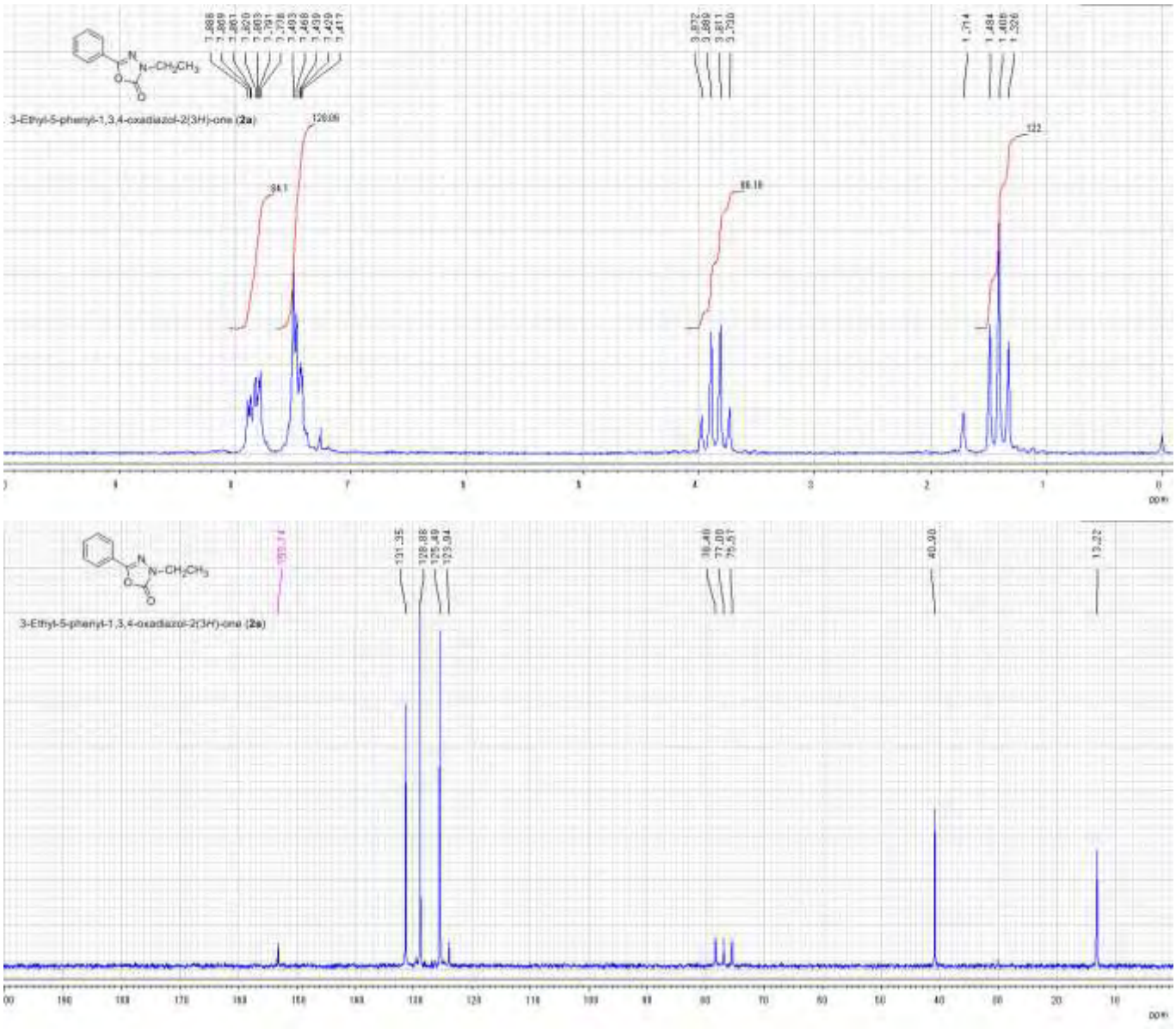
Diethyl 1-benzoylhydrazine-1,2-dicarboxylate (**1a**). Colorless oil. ^{1}H-NMR ($CDCl_3$) δ : 1.07 (3H, *t*, J=7.1 Hz, CH_3), 1.30 (3H, *t*, J=7.2 Hz, CH_3), 4.15 (2H, *q*, J=7.2 Hz, CH_2), 4.25 (2H, *q*, J=7.1 Hz, CH_2), 6.99 (1H, *brs*, NH), 7.30-7.57 (3H, *m*, phenyl-H), 7.57-7.80 (2H, *m*, phenyl-H).



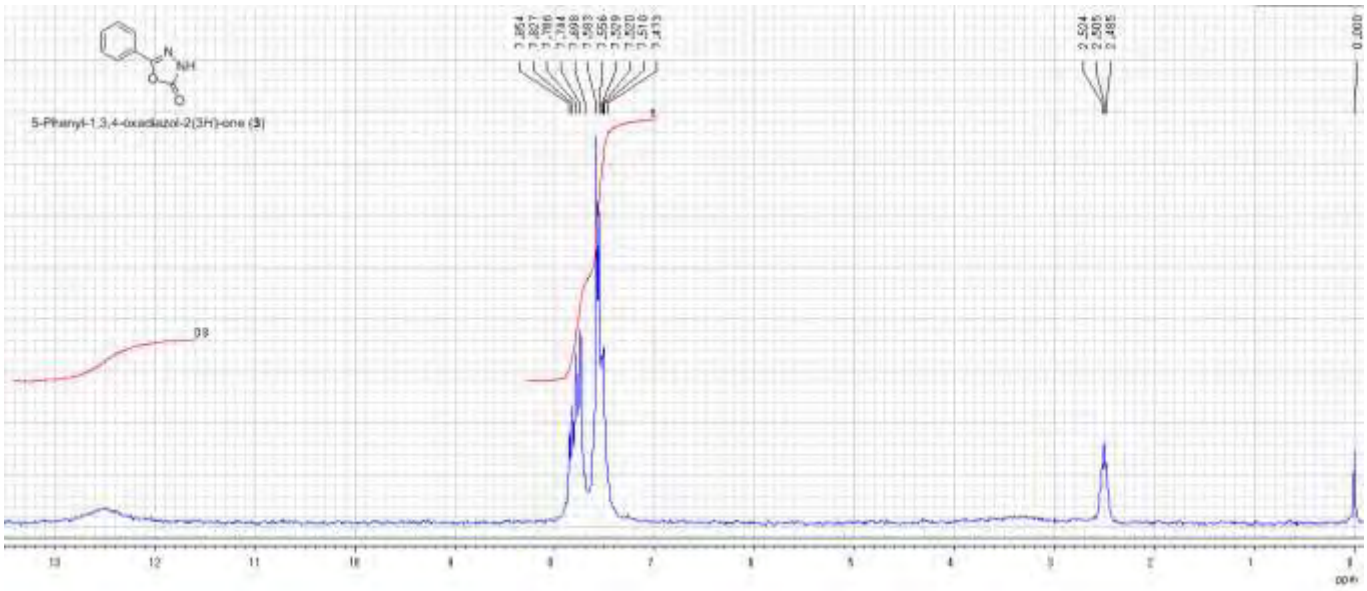
Diethyl 1,2-dibenzoylhydrazine-1,2-dicarboxylate. White solids. Mp 78.7-79.4 °C (lit.[1] 82-83 °C). ^{1}H-NMR ($CDCl_3$) δ : 1.08 (6H, *t*, J=7.1 Hz, CH_3×2), 4.18 (4H, *q*, J=7.1 Hz, CH_2×2), 7.29-7.60 (6H, *m*, phenyl-H), 7.60-7.84 (4H, *m*, phenyl-H).

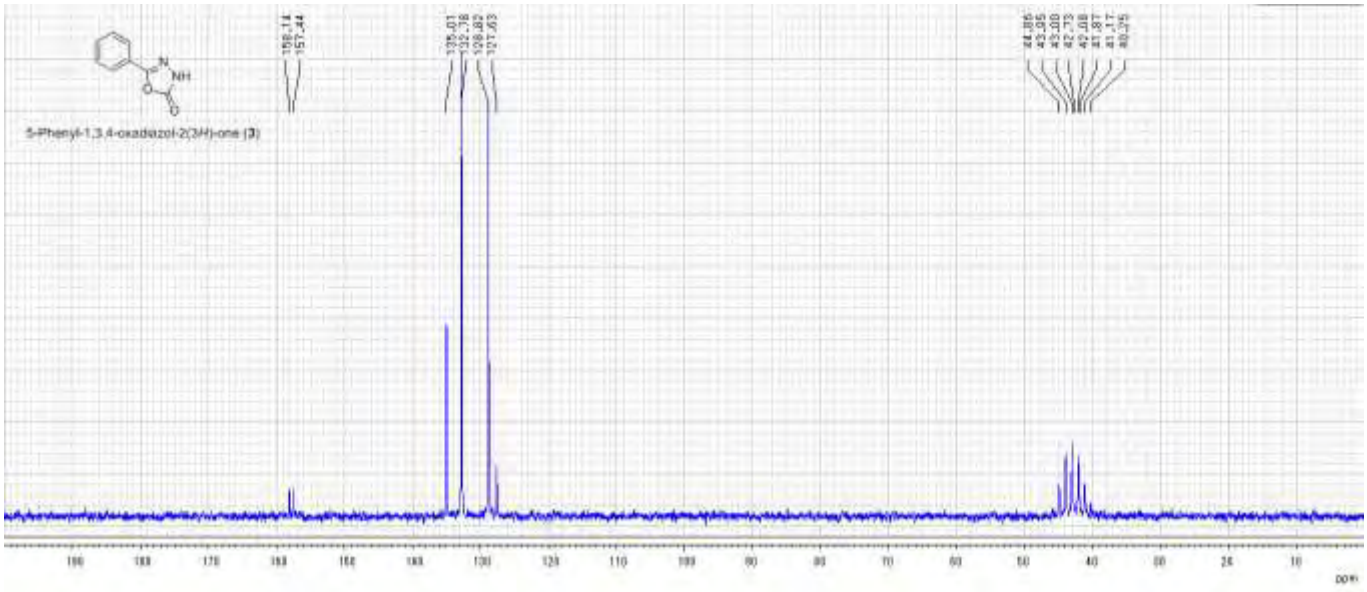


3-Ethyl-5-phenyl-1,3,4-oxadiazol-2(3*H*)-one (**2a**). White solids. Mp 45-46 °C (lit.[2] 49-50 °C). Bp 152 °C / 14 mmHg. ^{1}H-NMR ($CDCl_3$) δ : 1.41 (3H, *t*, J=7.2 Hz, CH_3), 3.85 (2H, *q*, J=7.2 Hz, CH_2), 7.31-7.60 (3H, *m*, phenyl-H), 7.68-7.94 (2H, *m*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.2, 40.9, 123.9, 125.5, 128.9, 131.4, 153.1. *Anal*. Calcd for $C_{10}H_{10}N_2O_2$: C, 63.15; H, 5.30; N, 14.73. Found : C, 62.99; H, 5.25; N, 14.61.

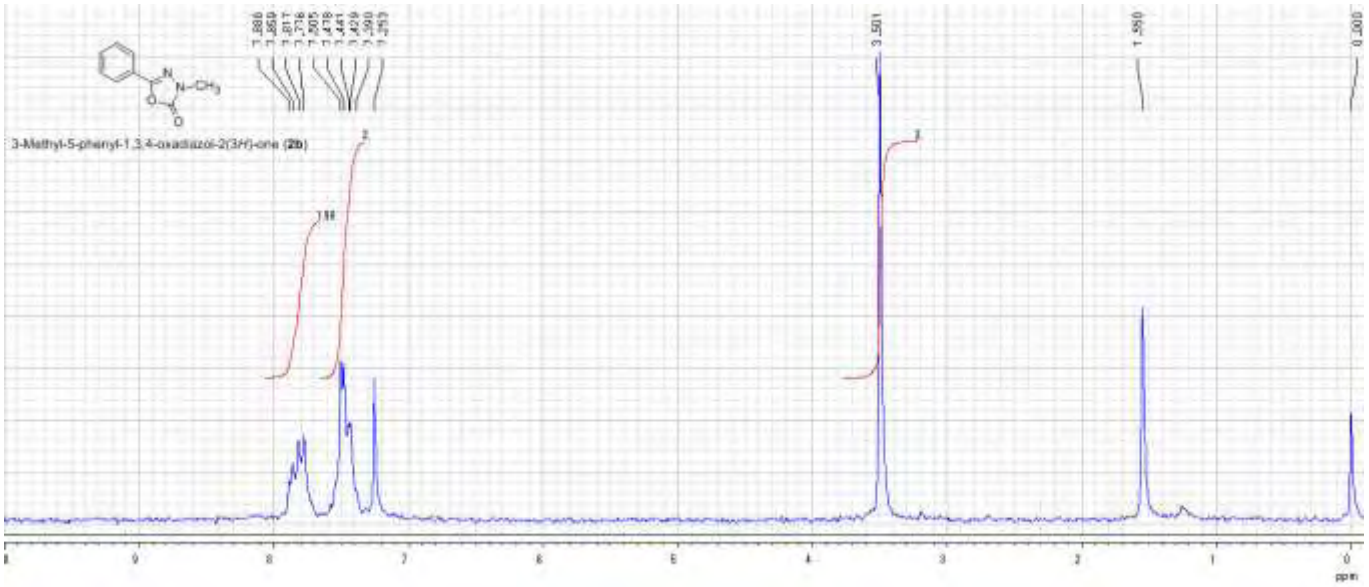


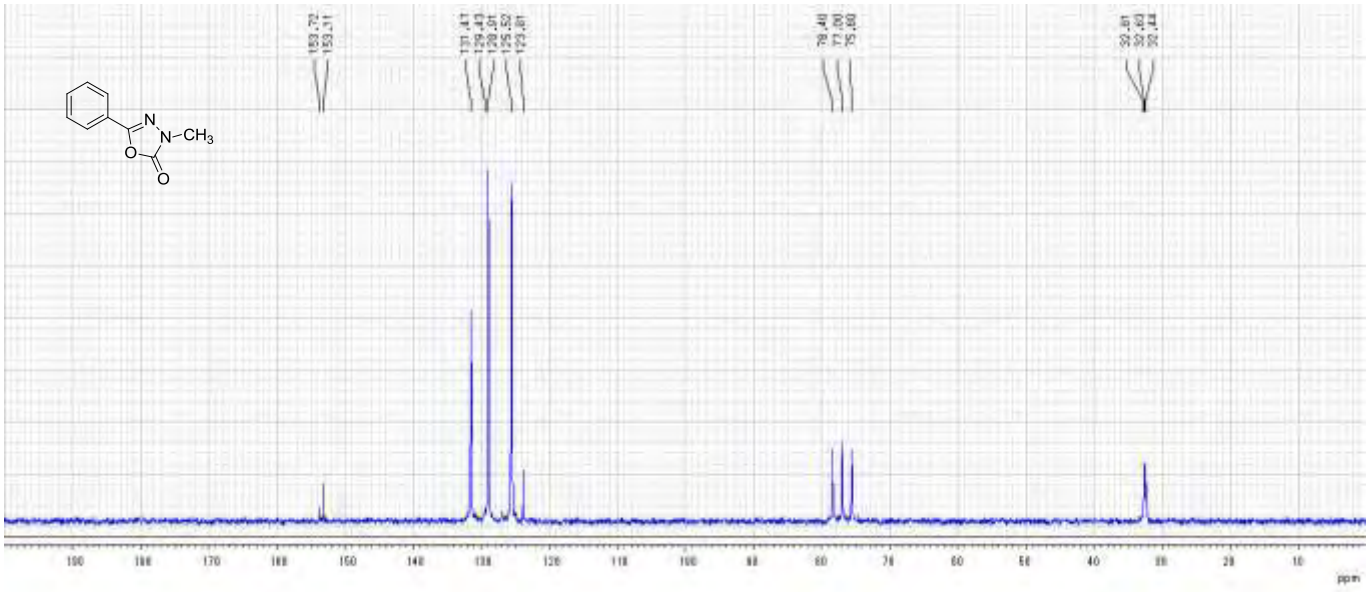
5-Phenyl-1,3,4-oxadiazol-2(3*H*)-one (**3**). White needles (recryst. from hexane – ethyl acetate). Mp 129-130 °C (lit.[3] 135-136 °C). ^{1}H-NMR (lit.[6], DMSO-d_6) δ : 7.38-7.66 (3H, *m*, phenyl-H), 7.66-7.95 (2H, *m*, phenyl-H), 12.50 (1H, *brs*, NH). ^{13}C-NMR (lit.[6], DMSO-d_6) δ : 127.6, 128.8, 132.8, 135.0, 157.4, 158.1. *Anal*. Calcd for $C_8H_6N_2O_2$: C, 59.26; H, 3.73; N, 17.28. Found : C, 59.20; H, 3.80; N, 17.18.



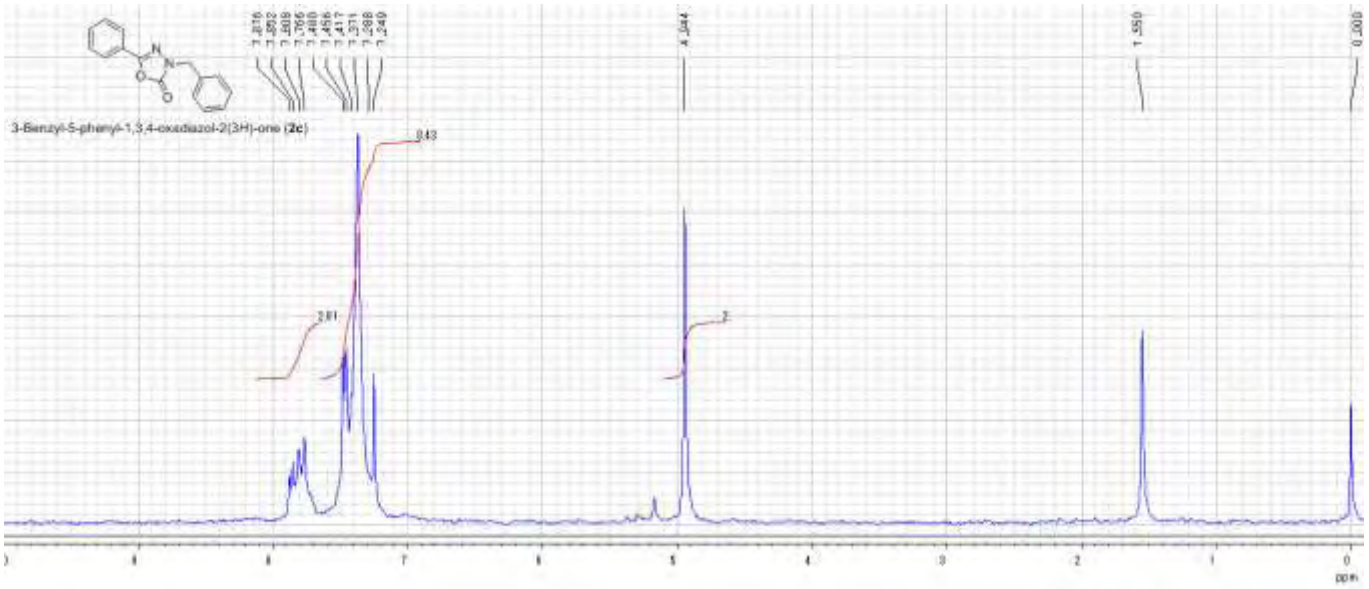


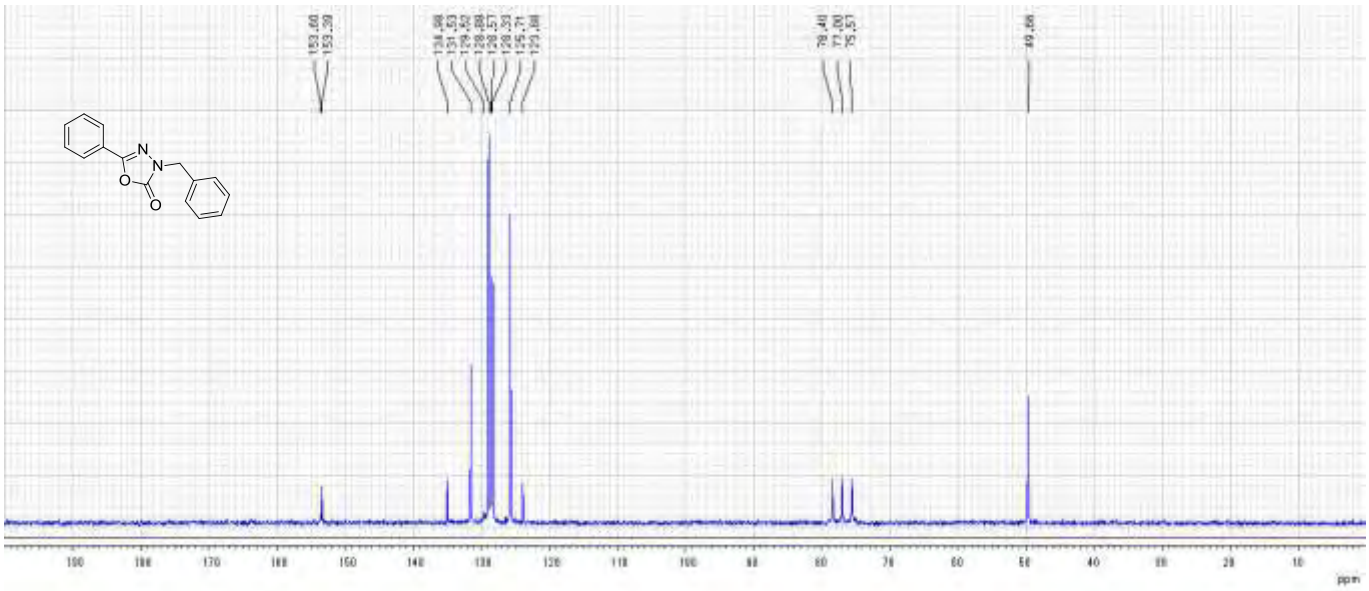
3-Methyl-5-phenyl-1,3,4-oxadiazol-2(3*H*)-one (**2b**). White solids. Mp 98.2-99.8 °C (lit.[2] 100-101 °C). ^{1}H-NMR ($CDCl_3$) δ : 3.50 (3H, *s*, CH_3), 7.32-7.61 (3H, *m*, phenyl-H), 7.67-7.95 (2H, *m*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 32.6, 123.8, 125.5, 128.9, 131.5, 153.1, 153.7.

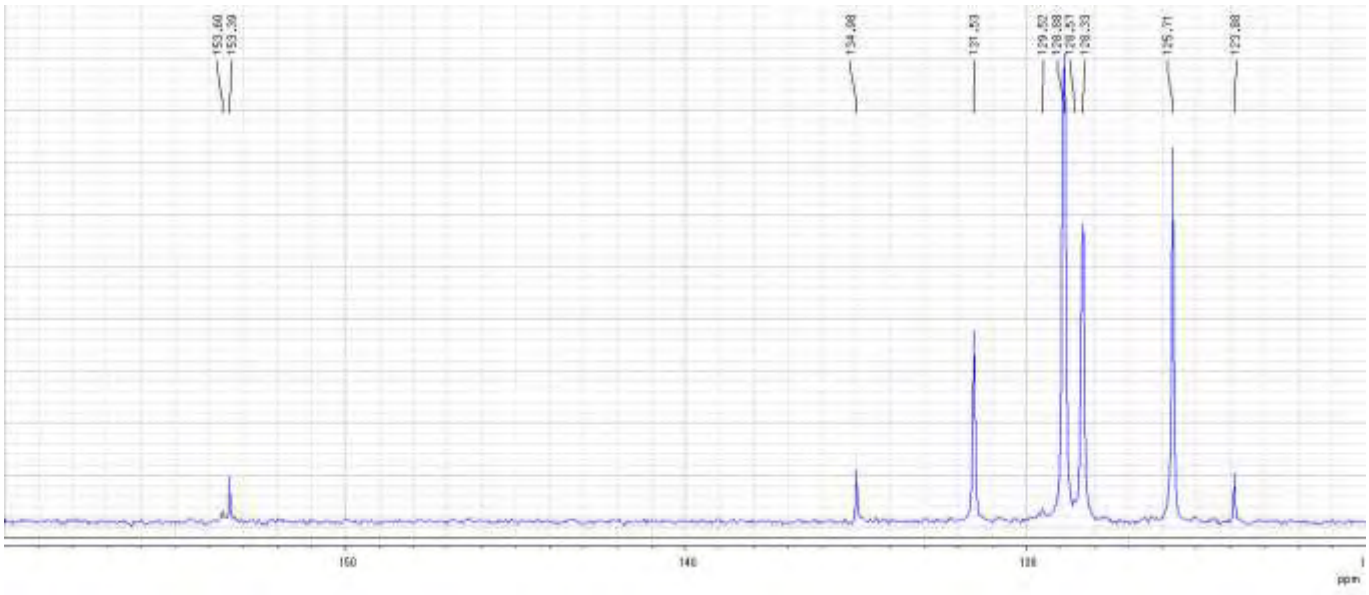




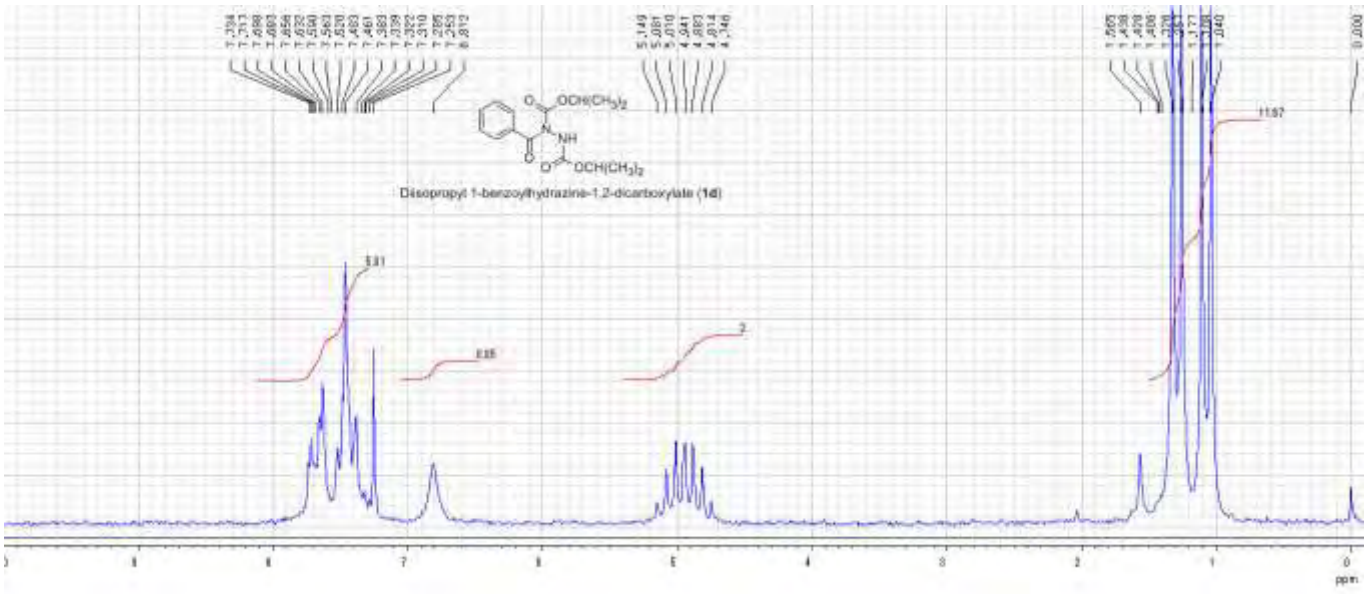
3-Benzyl-5-phenyl-1,3,4-oxadiazol-2(3*H*)-one (**2c**). White solids. Mp 112-114 °C (lit.[4] 115-119 °C). ^{1}H-NMR ($CDCl_3$) δ : 4.94 (2H, *s*, CH_2), 7.23-7.58 (8H, *m*, phenyl-H), 7.68-7.92 (2H, *m*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 49.7, 123.9, 125.7, 128.3, 128.9, 131.5, 135.0, 153.4, 153.6.



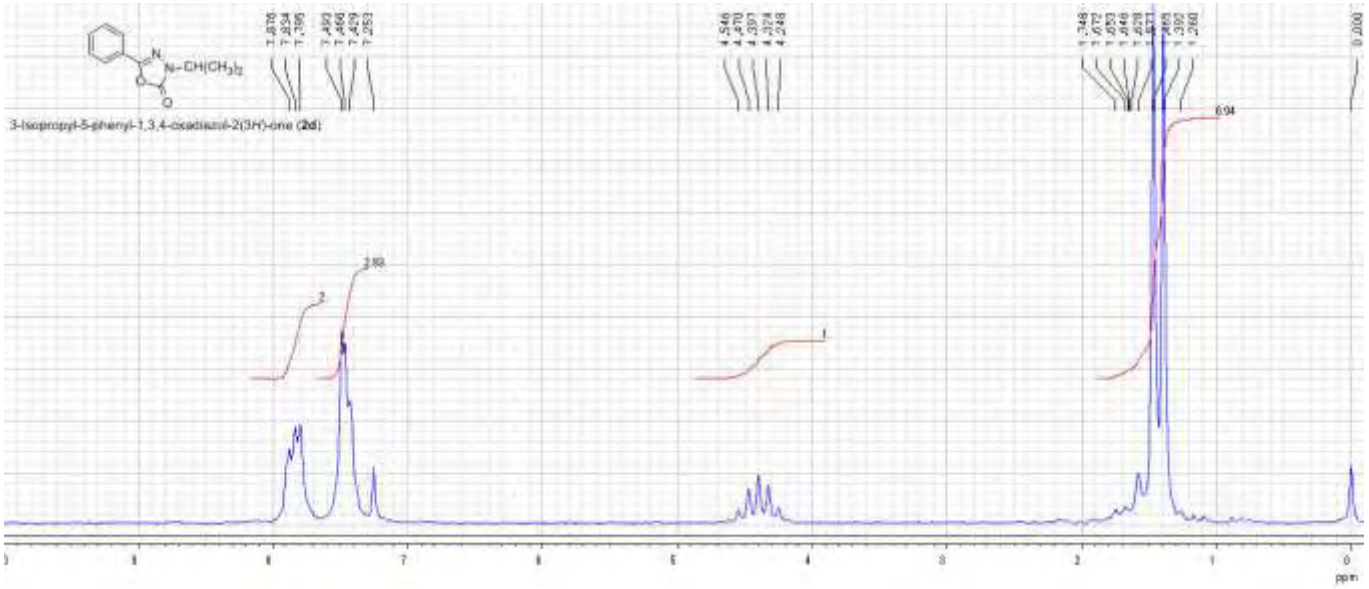


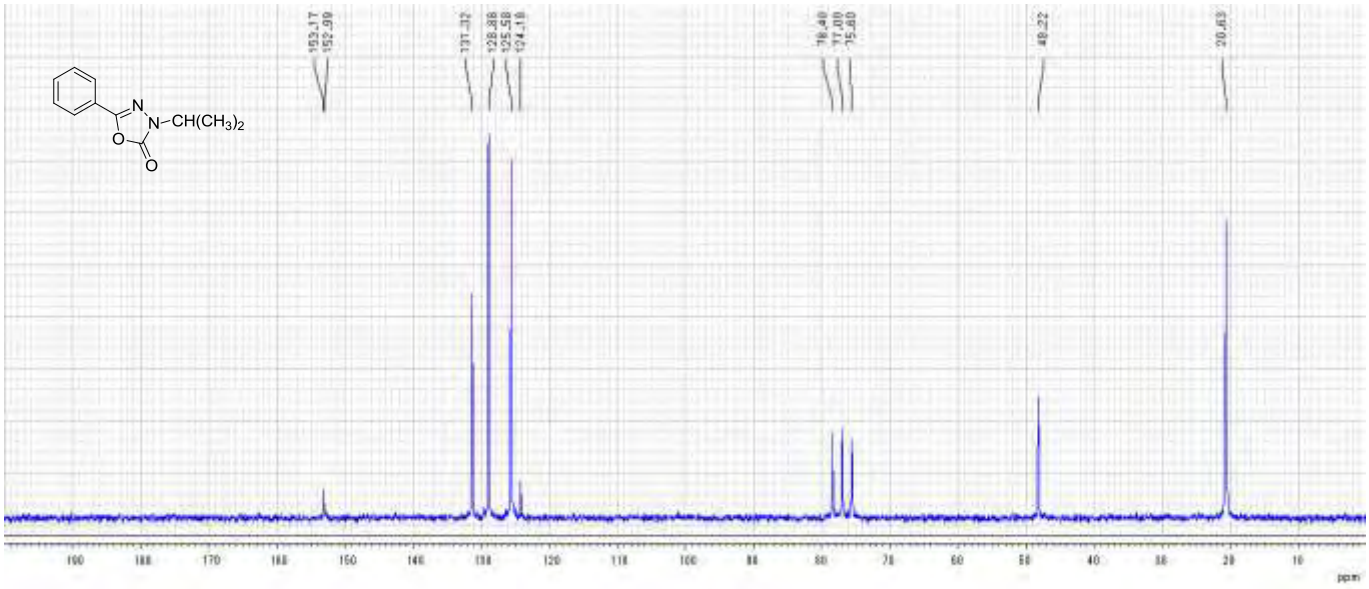


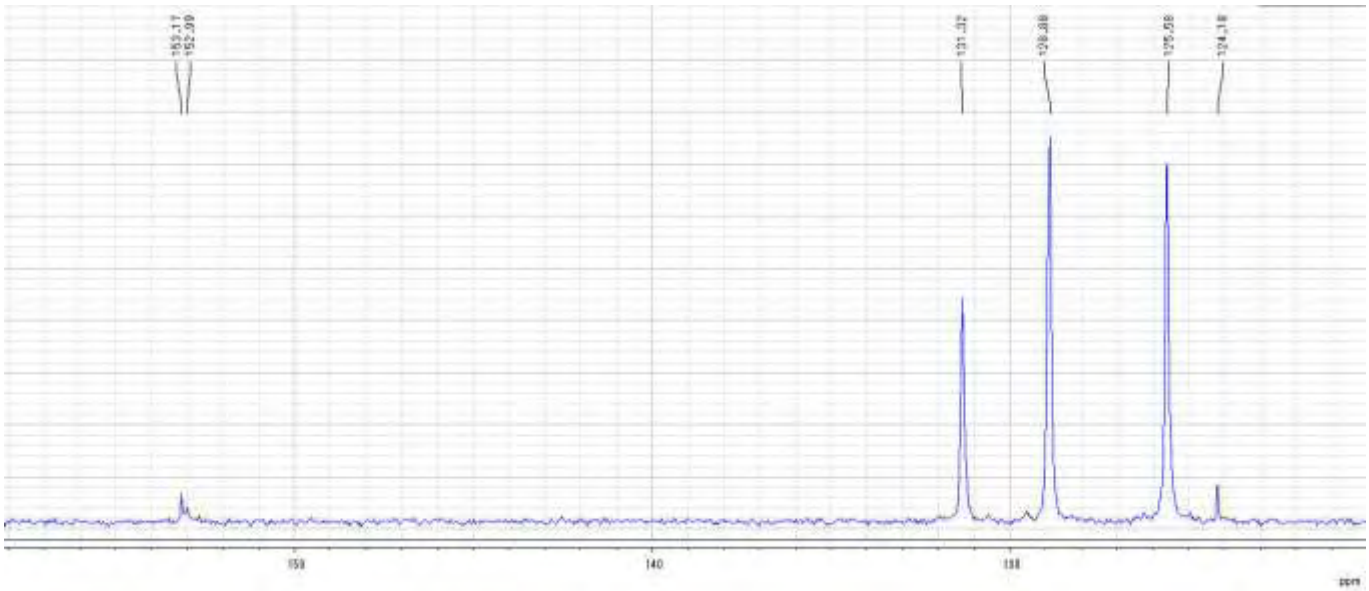
Diisopropyl 1-benzoylhydrazine-1,2-dicarboxylate. White solids. Mp 120-122 °C (lit.[5] 120-121 °C). ^{1}H-NMR ($CDCl_3$) δ : 1.07 (6H, *d*, J=6.2 Hz, CH_3), 1.29 (6H, *d*, J=6.2 Hz, CH_3), 4.88 (1H, *septet*, J=6.2 Hz, CH), 5.01 (1H, *septet*, J=6.2 Hz, CH), 6.81 (1H, *brs*, NH), 7.30-7.57 (3H, *m*, phenyl-H), 7.57-7.80 (2H, *m*, phenyl-H).



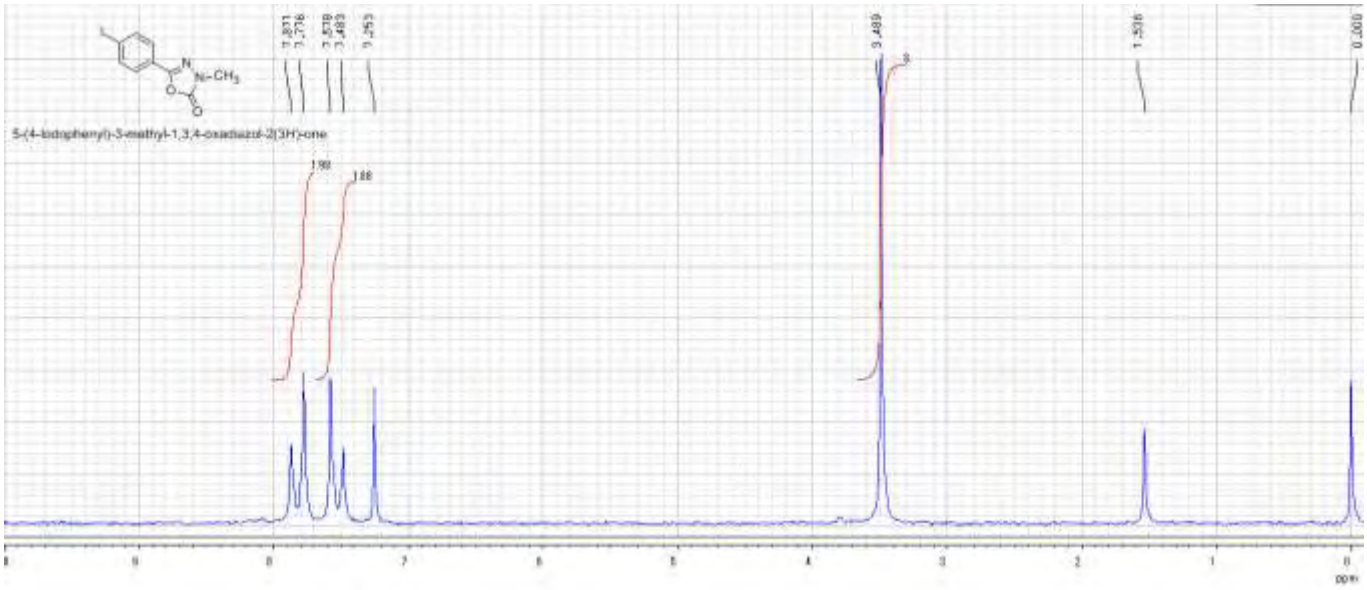
3-Isopyopyl-5-phenyl-1,3,4-oxadiazol-2(3*H*)-one (**2d**). White solids. Mp 61-62 °C (lit.[2] 62.5-63.5 °C). ^{1}H-NMR ($CDCl_3$) δ : 1.43 (6H, *d*, J=6.6 Hz, CH_3×2), 4.40 (1H, *septet*, J=6.6 Hz, CH), 7.27-7.62 (3H, *m*, phenyl-H), 7.63-7.98 (2H, *m*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 20.6, 48.2, 124.2, 125.6, 128.9, 131.3, 153.0, 153.2.

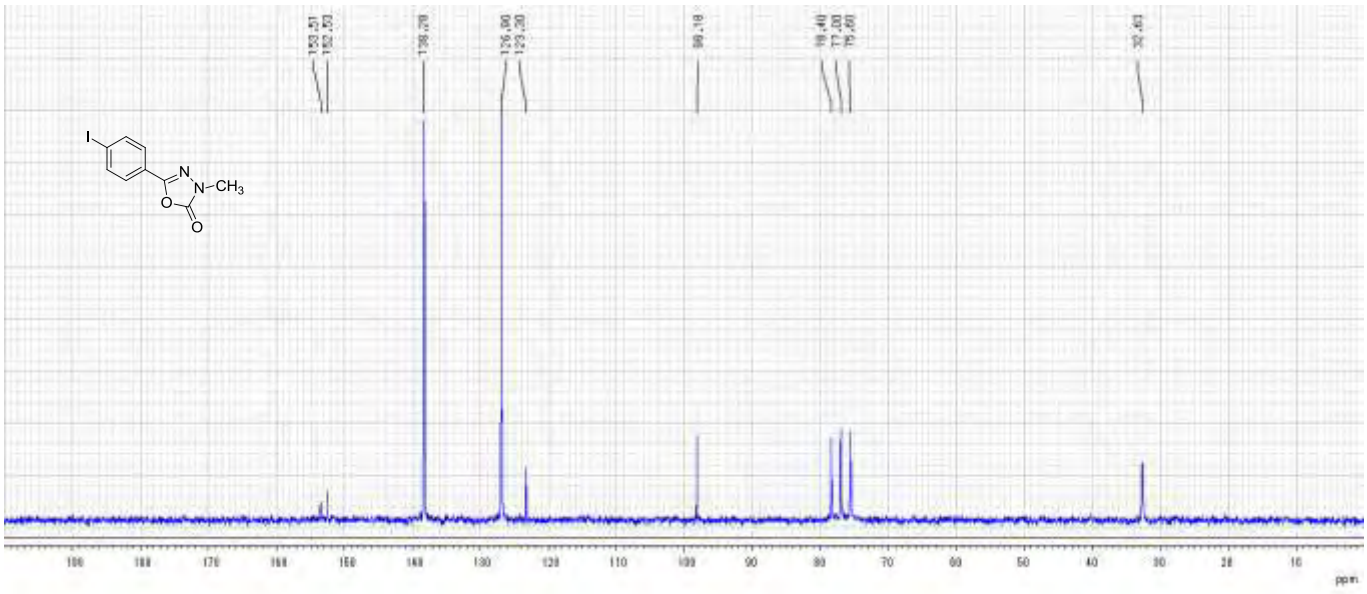




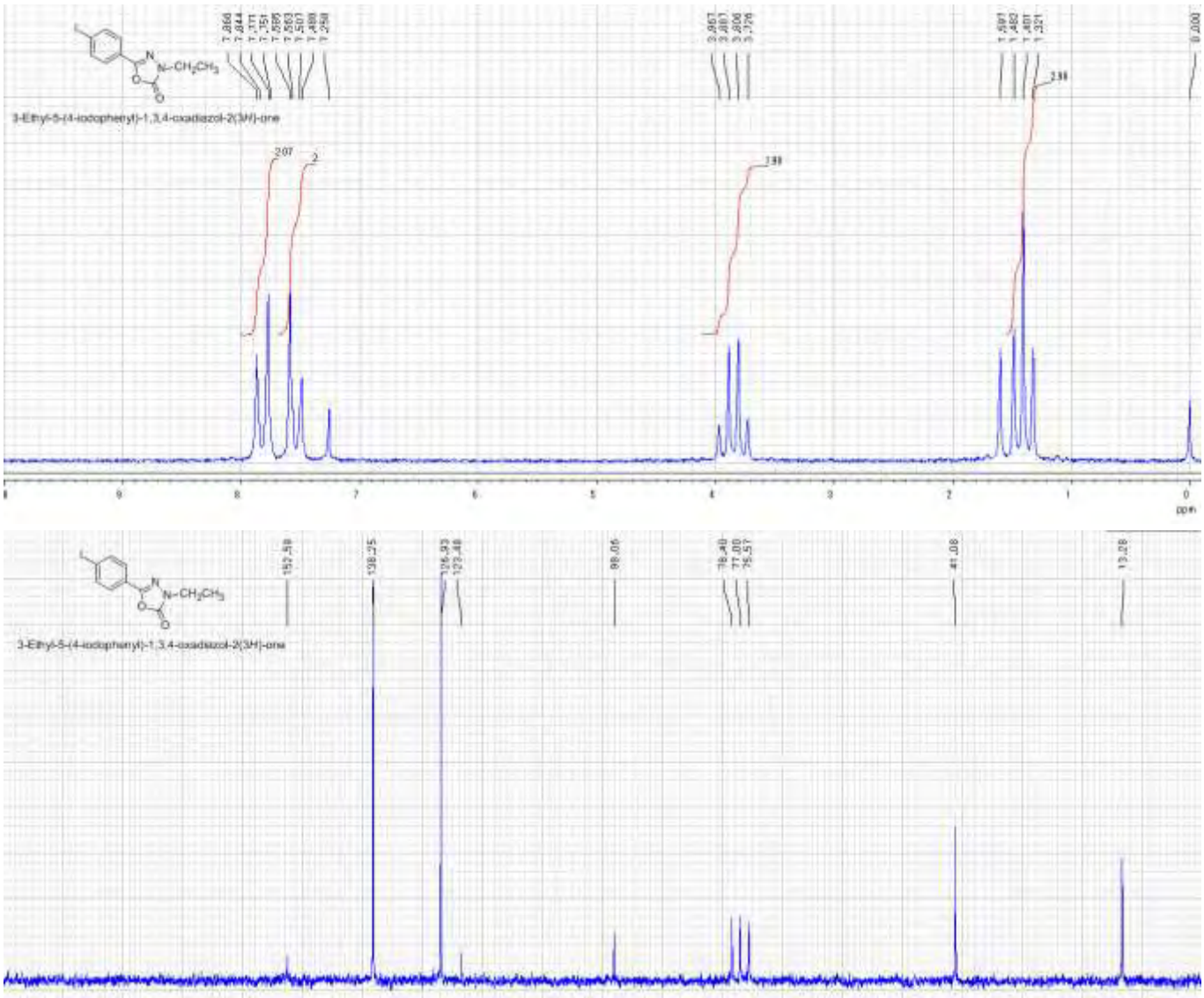


3-Methyl-5-(4-iodophenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 167.1-173.5 °C. ^{1}H-NMR ($CDCl_3$) δ : 3.49 (3H, *s*, CH_3), 7.53 (2H, *d*, J=8.7 Hz, phenyl-H), 7.82 (2H, *d*, J=8.7 Hz, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 32.6, 98.2, 123.3, 126.9, 138.3, 152.5, 153.5. *Anal*. Calcd for $C_9H_7IN_2O_2$: C, 35.79; H, 2.34; N, 9.27. Found : C, 35.88; H, 2.36; N, 9.11.

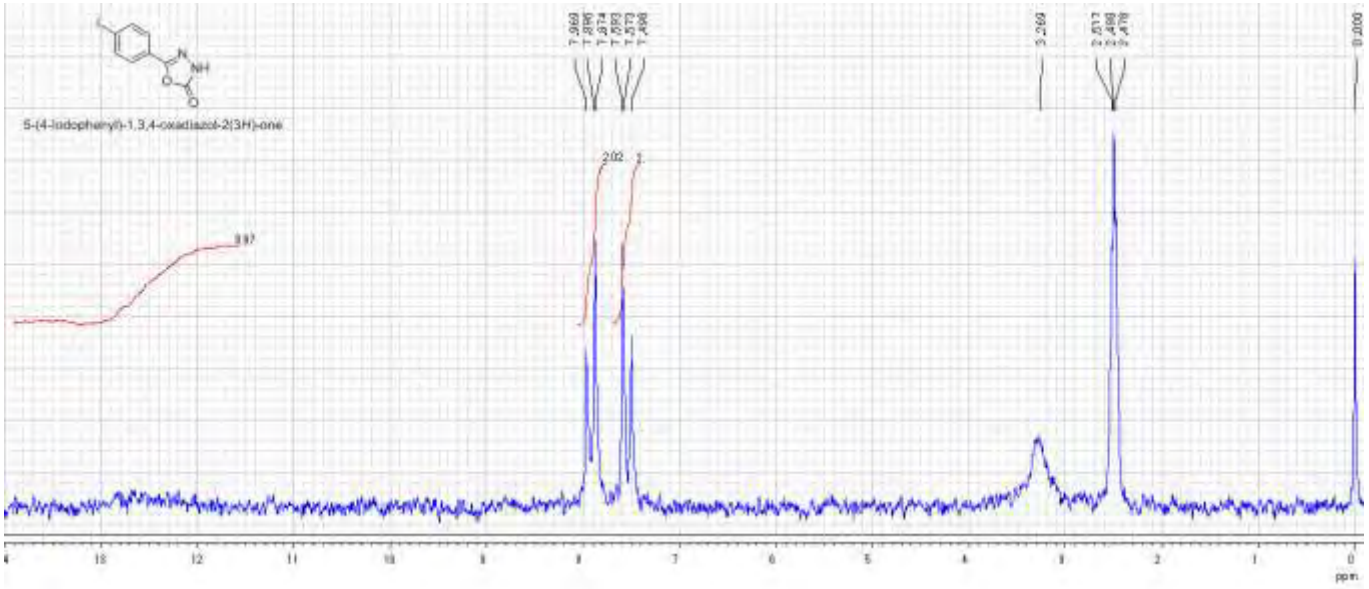


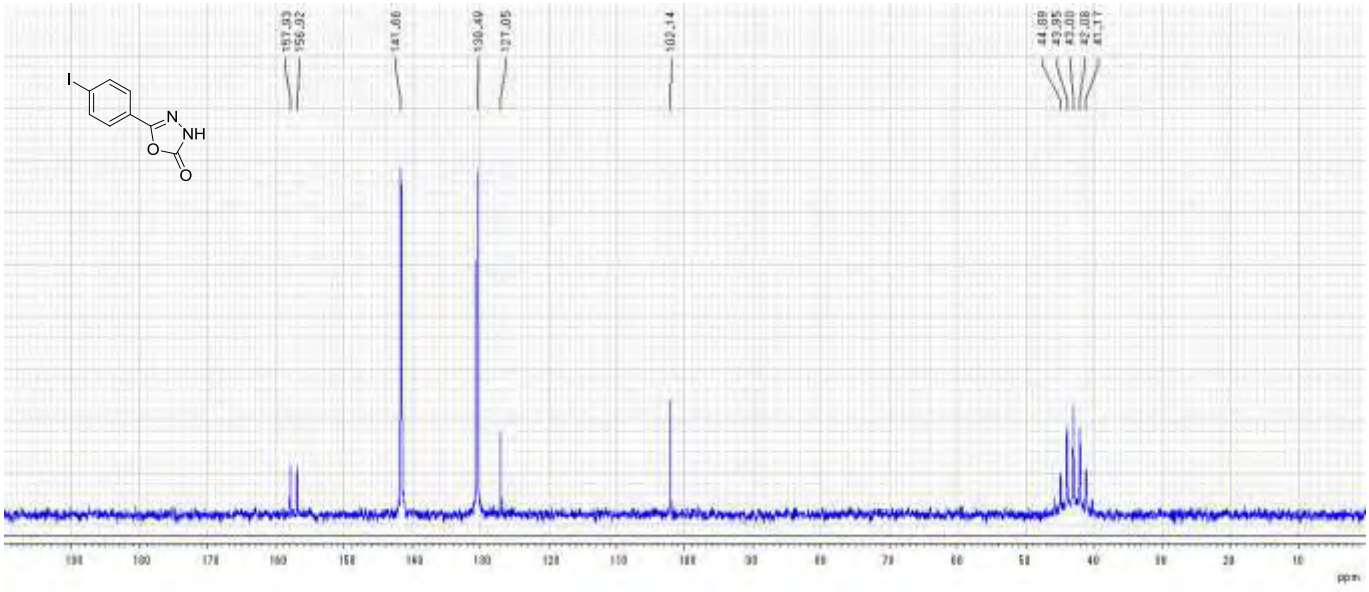


3-Ethyl-5-(4-iodophenyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane-ethyl acetate). Mp 107-108 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.40 (3H, *t*, J=7.2 Hz, CH_3), 3.85 (2H, *q*, J=7.2 Hz, CH_2), 7.54 (2H, *d*, J=8.6 Hz, phenyl-H), 7.82 (2H, *d*, J=8.6 Hz, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.3, 41.1, 98.1, 123.5, 126.9, 138.3, 152.6. *Anal*. Calcd for $C_{10}H_9IN_2O_2$: C, 38.00; H, 2.87; N, 8.86. Found : C, 37.81; H, 2.86; N, 8.82.

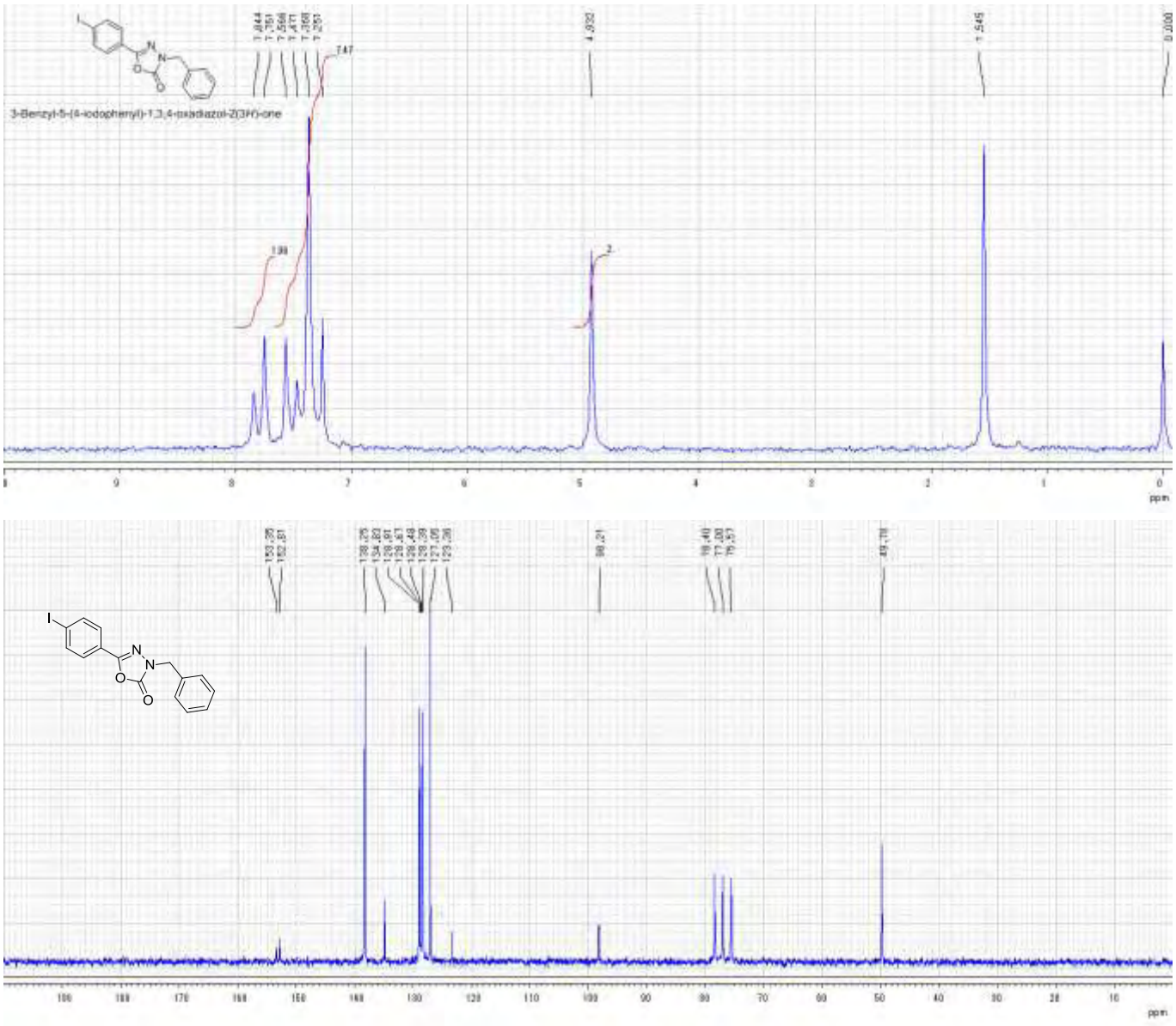


5-(4-Iodophenyl)-1,3,4-oxadiazol-2(3*H*)-one. White powder (recryst. from hexane – ethyl acetate). Mp 194.1-196.0 °C. ^{1}H-NMR (DMSO-d_6) δ : 7.55 (2H, *d*, J=8.6 Hz, phenyl-H), 7.92 (2H, *d*, J=8.6 Hz, phenyl-H), 11.70-13.20 (1H, *br*, NH). ^{13}C-NMR (DMSO-d_6) δ : 102.1, 127.1, 130.5, 141.7, 156.9, 157.9. *Anal*. Calcd for $C_8H_5IN_2O_2$: C, 33.24; H, 1.74; N, 9.69. Found : C, 33.20; H, 1.75; N, 9.67.

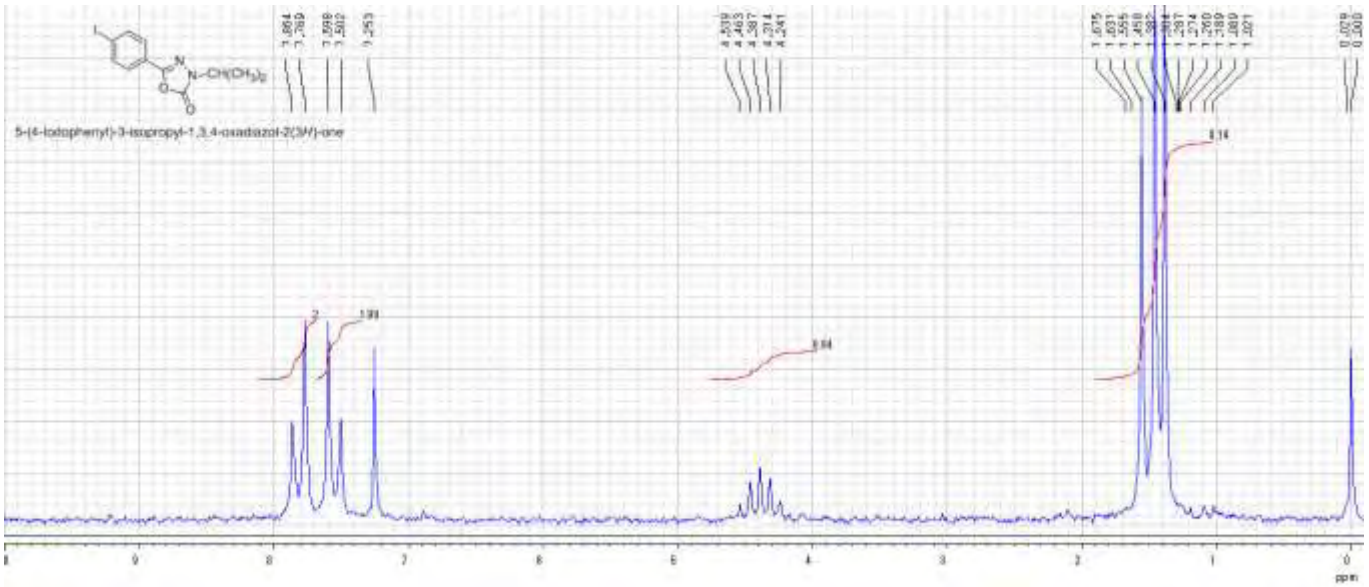


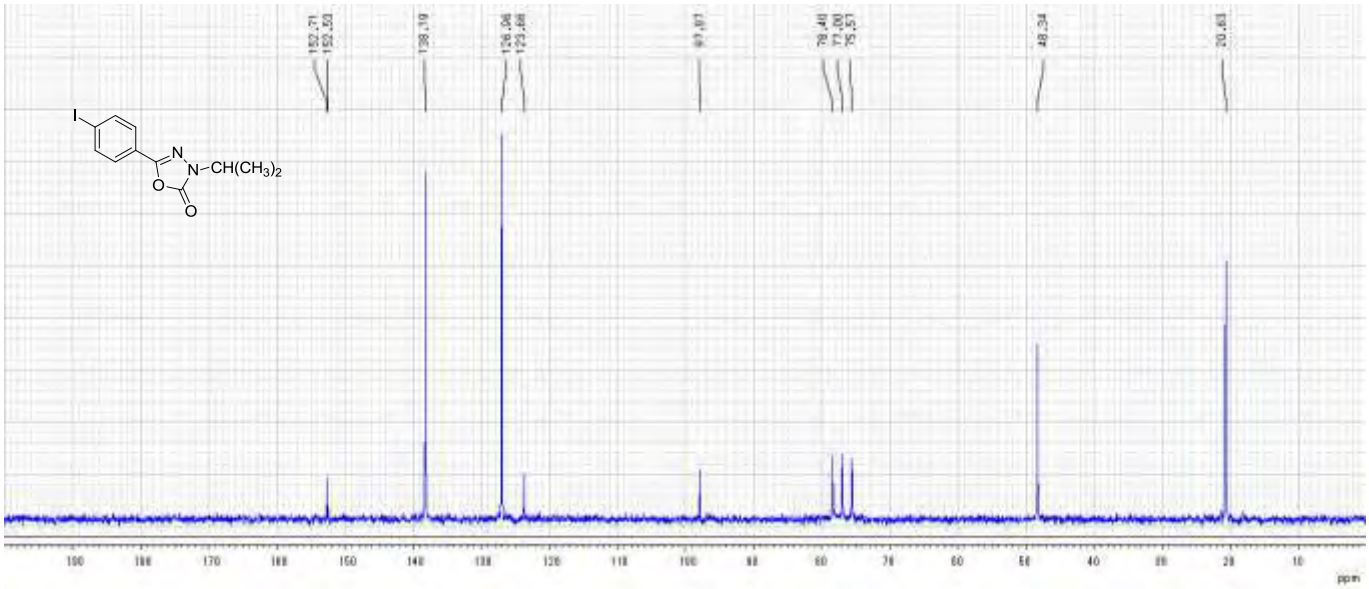


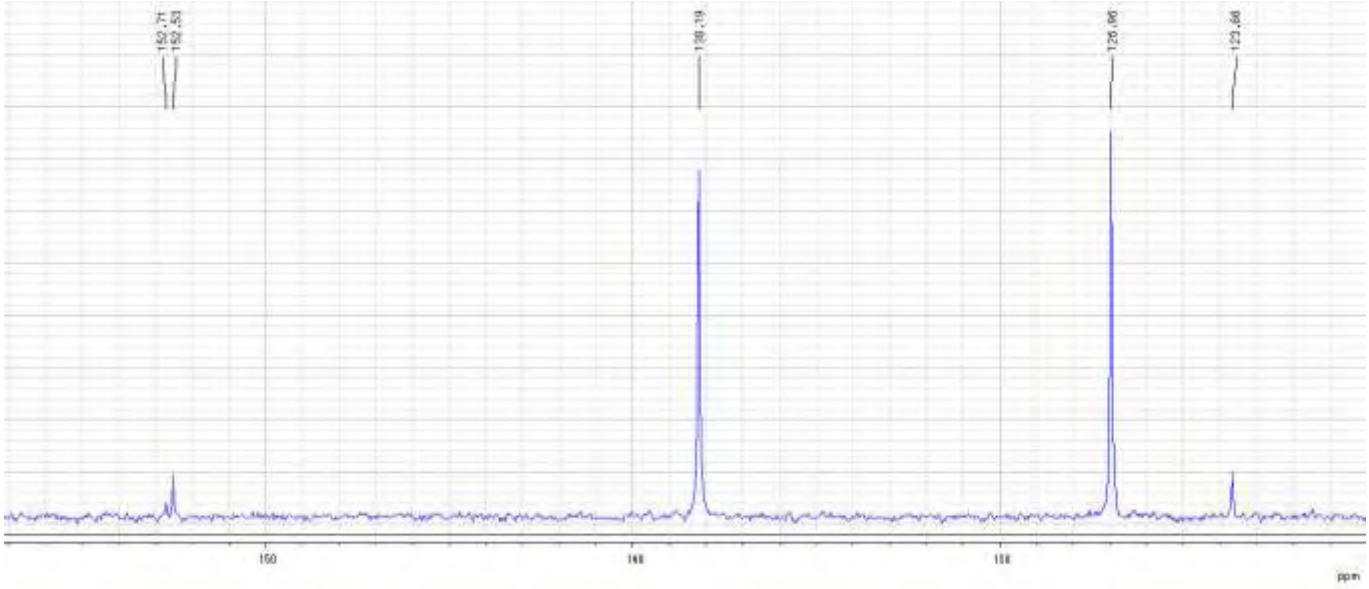
3-Benzyl-5-(4-iodophenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 123.6-124.0 °C. ^{1}H-NMR ($CDCl_3$) δ : 4.93 (2H, *s*, CH_2), 7.37 (5H, *s*, phenyl-H), 7.52 (2H, *d*, J=8.5 Hz, iodophenyl-H), 7.80 (2H, *d*, J=8.5 Hz, iodophenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 49.8, 98.2, 123.4, 127.1, 128.4, 128.5, 128.9, 134.8, 138.3, 152.8, 153.4. *Anal*. Calcd for $C_{15}H_{11}IN_2O_2$: C, 47.64; H, 2.93; N, 7.41. Found : C, 47.63; H, 2.93; N, 7.35.



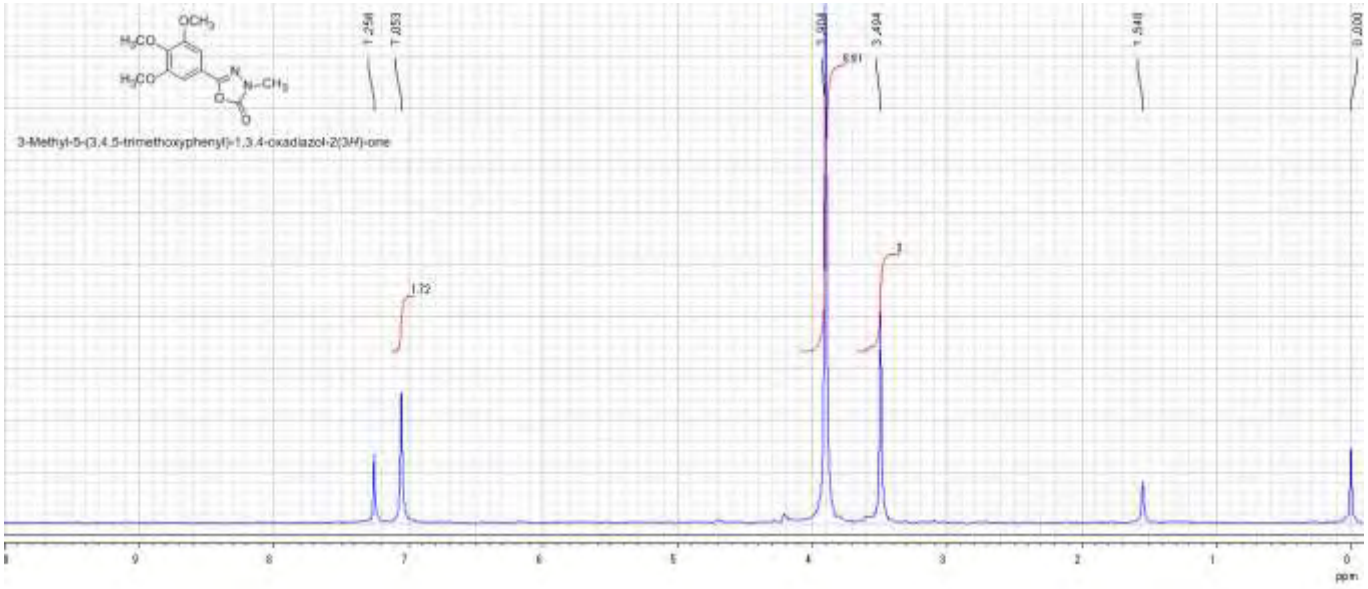
5-(4-Iodophenyl)-3-isopropyl-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 104.0-105.7 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.42 (6H, *d*, J=6.8 Hz, CH_3×2), 4.39 (1H, *septet*, J=6.8 Hz, CH), 7.55 (2H, *d*, J=8.6 Hz, phenyl-H), 7.82 (2H, *d*, J=8.6 Hz, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 20.6, 48.3, 97.9, 123.7, 127.0, 138.2, 152.5, 152.7. *Anal*. Calcd for $C_{11}H_{11}IN_2O_2$: C, 40.02; H, 3.36; N, 8.49. Found : C, 40.29; H, 3.43; N, 8.35.

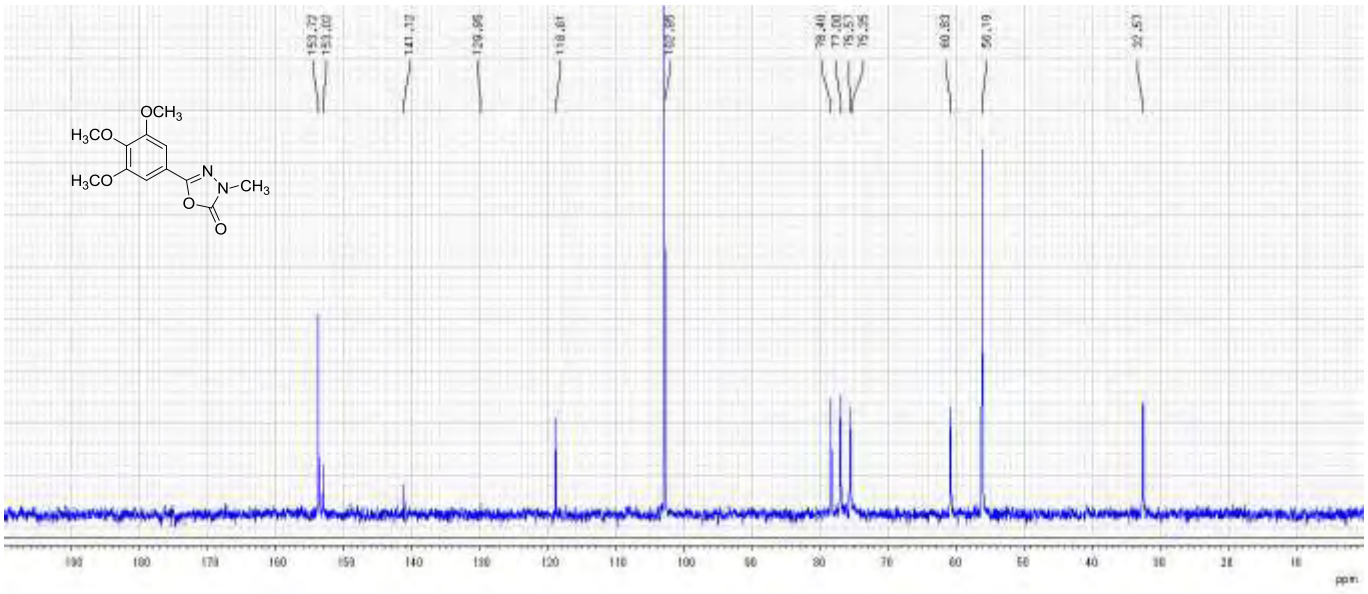




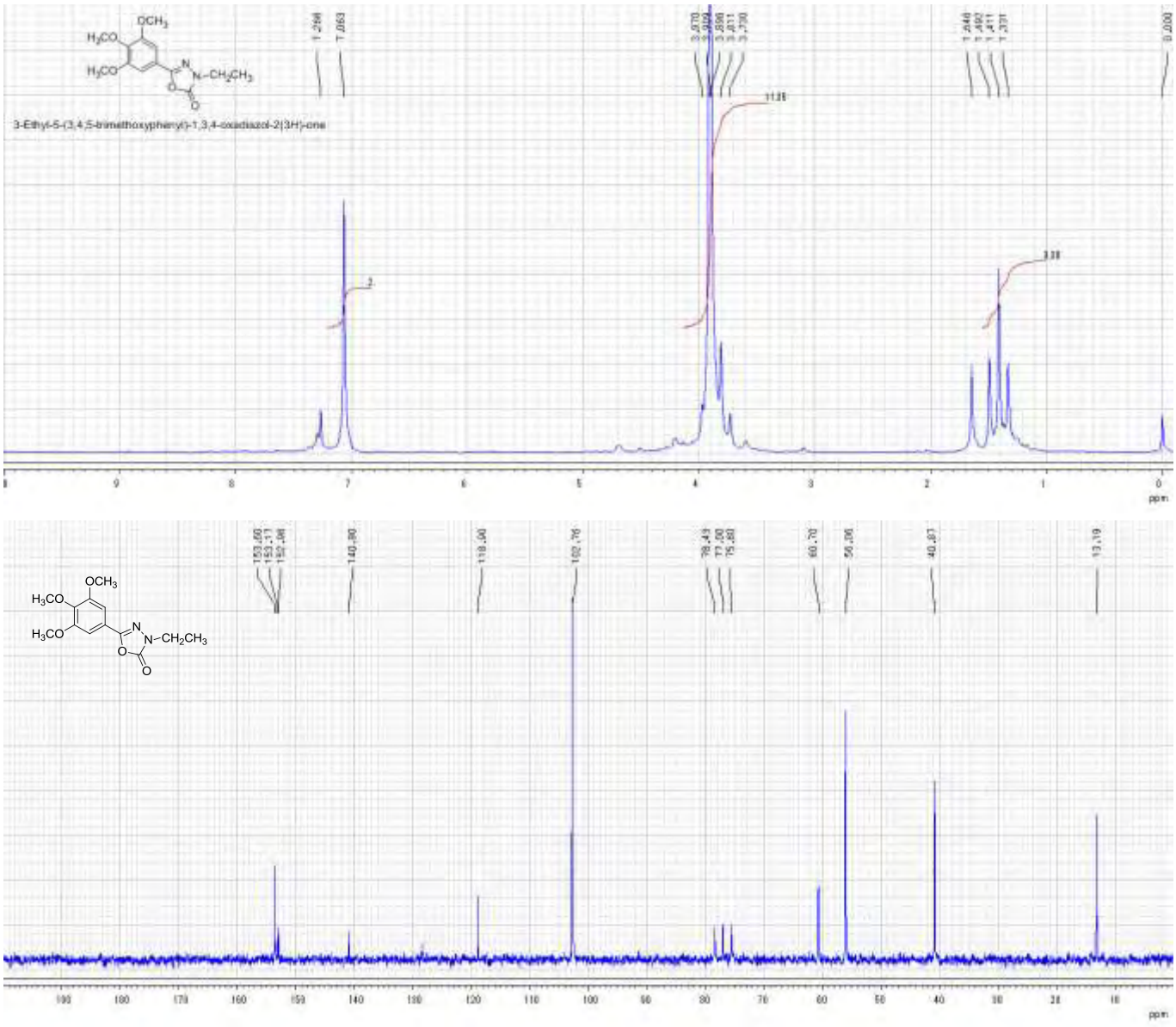


3-Methyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 136.9-138.0 °C. ^{1}H-NMR ($CDCl_3$) δ : 3.49 (3H, *s*, NCH_3), 3.90 (9H, *s*, OCH_3×3), 7.05 (2H, *s*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 32.6, 56.2, 60.8, 102.9, 118.8, 141.1, 153.0, 153.7. *Anal*. Calcd for $C_{12}H_{14}N_2O_5$: C, 54.13; H, 5.30; N, 10.52. Found : C, 54.37; H, 5.38; N, 10.52.

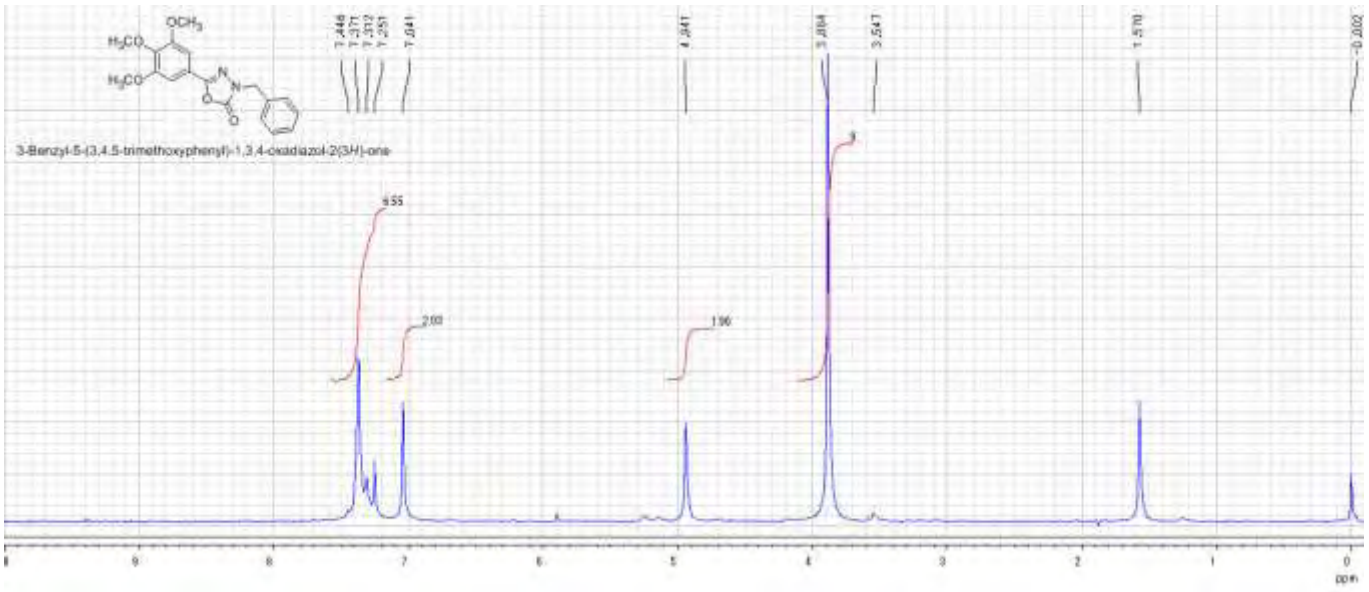


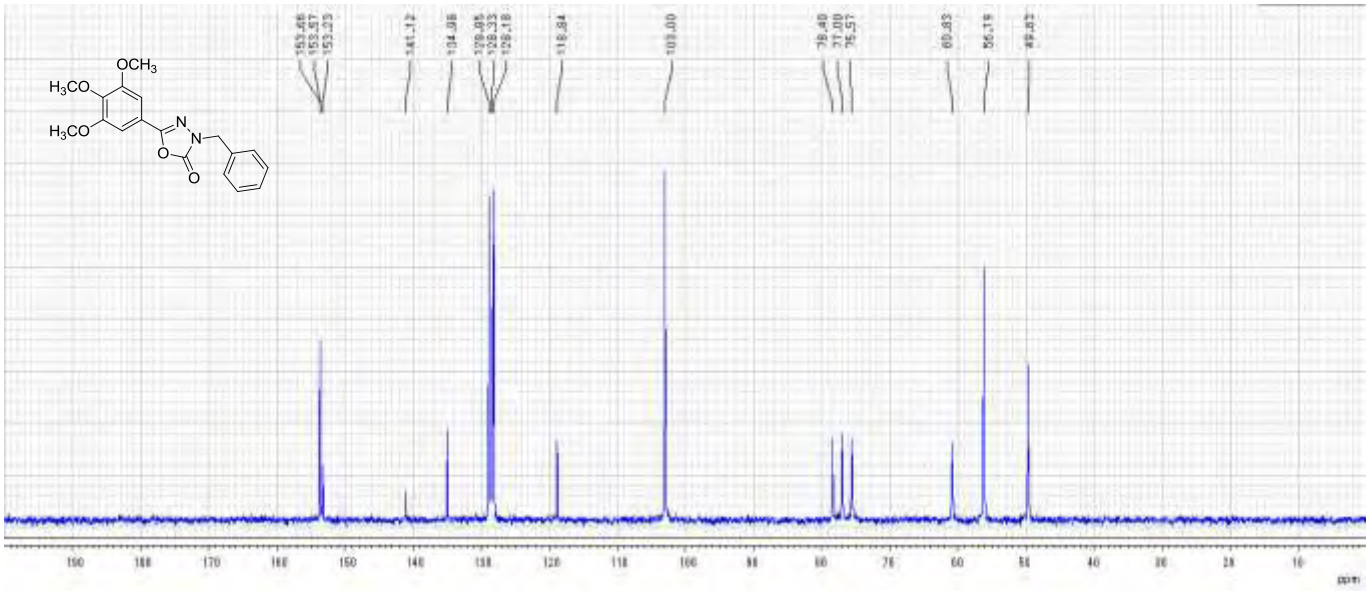


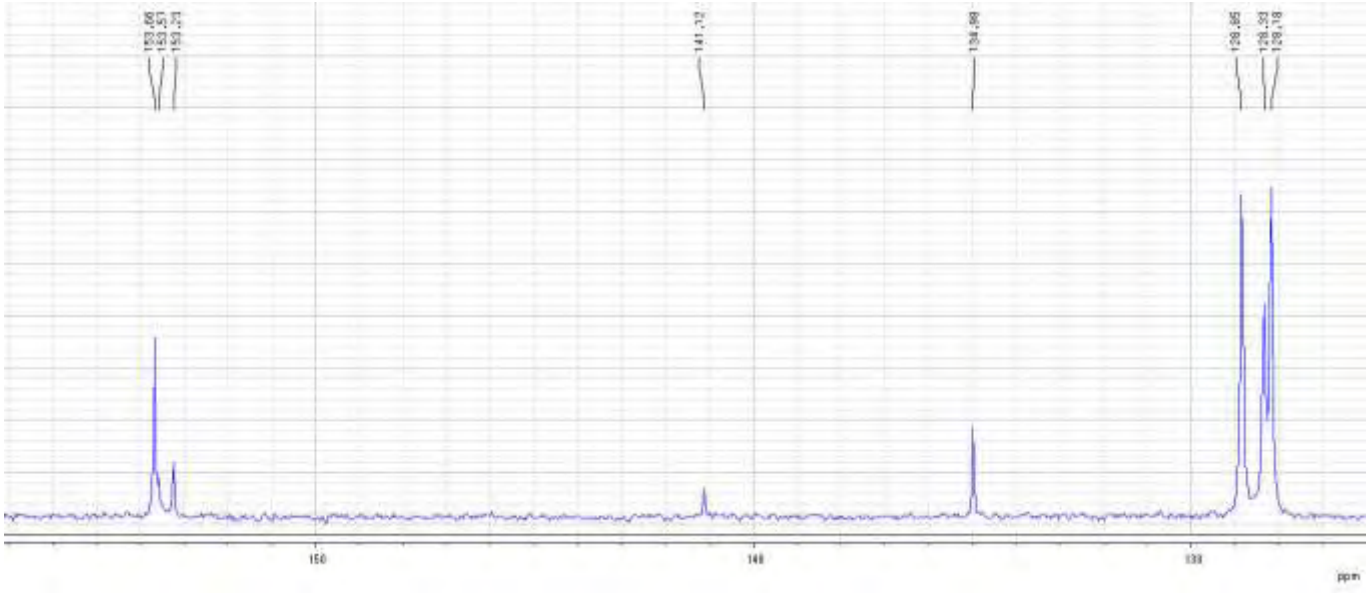
3-Ethyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane-ethyl acetate). Mp 115-116 °C (lit.[6] 112-113 °C). MS 280 (M^+). ^{1}H-NMR ($CDCl_3$) δ : 1.41 (3H, *t*, J=7.2 Hz, $CH_2C\underline{H}_3$), 3.85 (2H, q, J=7.2 Hz, CH_2), 3.90 (9H, *s*, OCH_3×3), 7.06 (2H, *s*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.2, 40.9, 56.1, 60.7, 102.8, 118.9, 140.9, 153.0, 153.2, 153.6. *Anal*. Calcd for $C_{13}H_{16}N_2O_5$: C, 55.71; H, 5.75; N, 9.99. Found : C, 55.99; H, 5.78; N, 10.04.



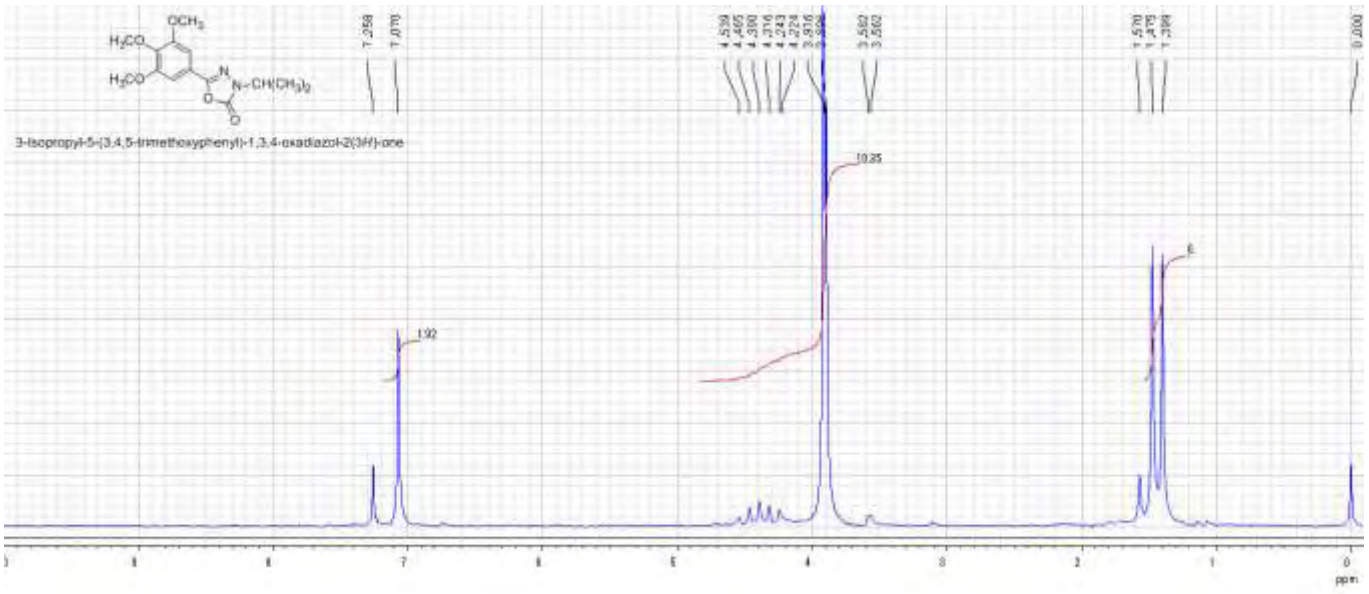
3-Benzyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane-ethyl acetate). Mp 107.8-110.0 °C. ^{1}H-NMR ($CDCl_3$) δ : 3.88 (9H, *s*, OCH_3×3), 4.94 (2H, s, CH_2), 7.04 (2H, *s*, C_6H_2-H), 7.45 (5H, *s*, C_6H_5-H). ^{13}C-NMR ($CDCl_3$) δ : 49.6, 56.2, 60.8, 103.0, 118.8, 128.2, 128.3, 128.9, 141.1, 153.2, 153.6, 153.7. *Anal*. Calcd for $C_{18}H_{18}N_2O_5$: C, 63.15; H, 5.30; N, 8.18. Found : C, 63.28; H, 5.35; N, 8.30.

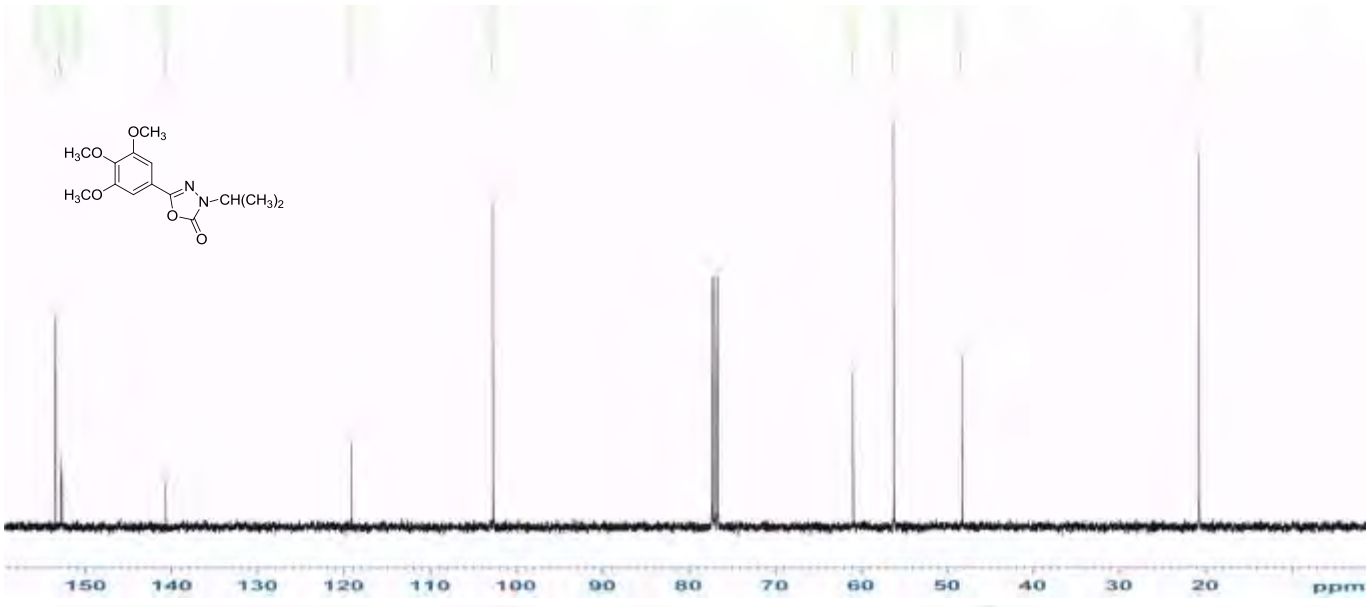


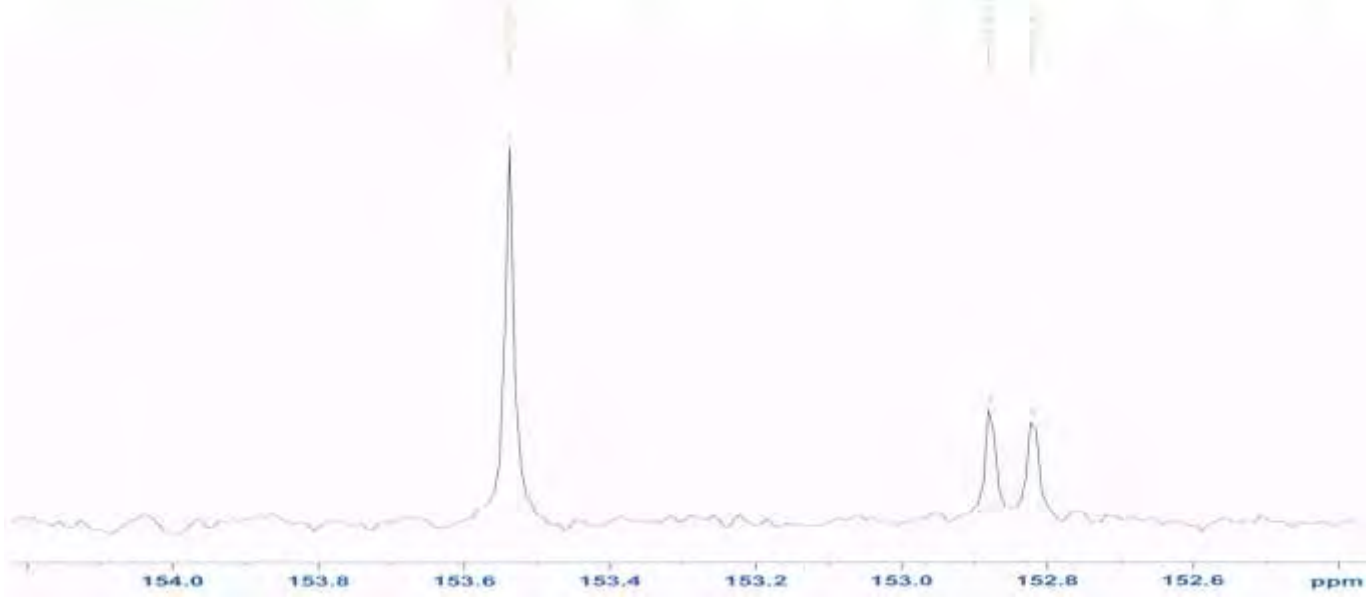




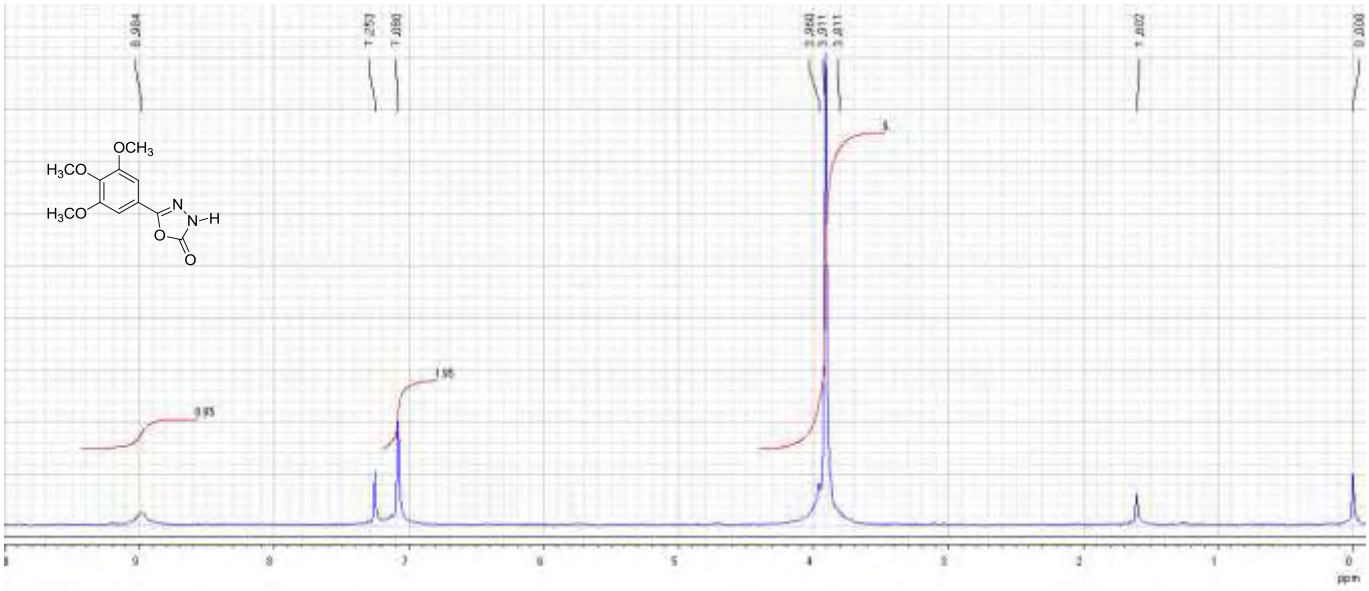
3-Isopropyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one. Colorless solids (recryst. from hexane-ethyl acetate). Mp 86.1-86.9 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.44 (6H, *d*, J=6.8 Hz, CH_3×2), 3.90 (3H, *s*, OCH_3), 3.92 (6H, *s*, OCH_3×3), 4.39 (1H, *septet*, J=6.8 Hz, CH), 7.07 (2H, *s*, C_6H_2-H). ^{13}C-NMR ($CDCl_3$) δ : 20.7, 48.3, 56.2, 60.9, 102.8, 119.2, 140.7, 152.8, 152.9, 153.5. *Anal*. Calcd for $C_{14}H_{18}N_2O_5$: C, 57.13; H, 6.16; N, 9.52. Found : C, 57.24; H, 6.19; N, 9.68.

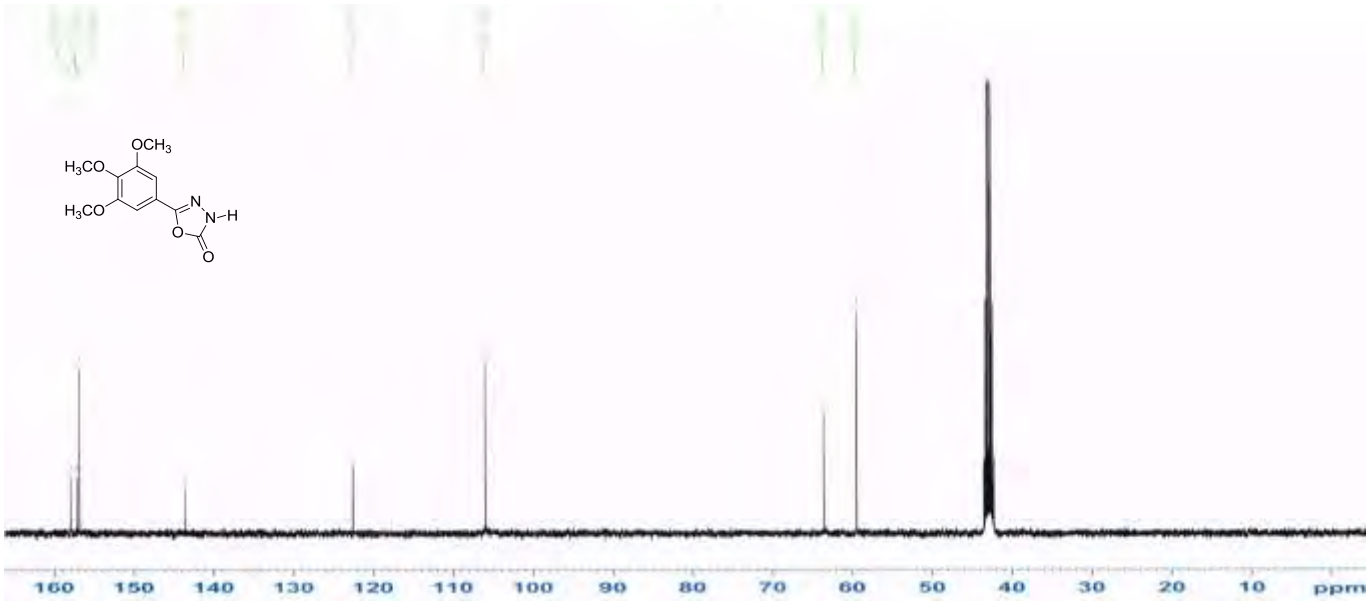




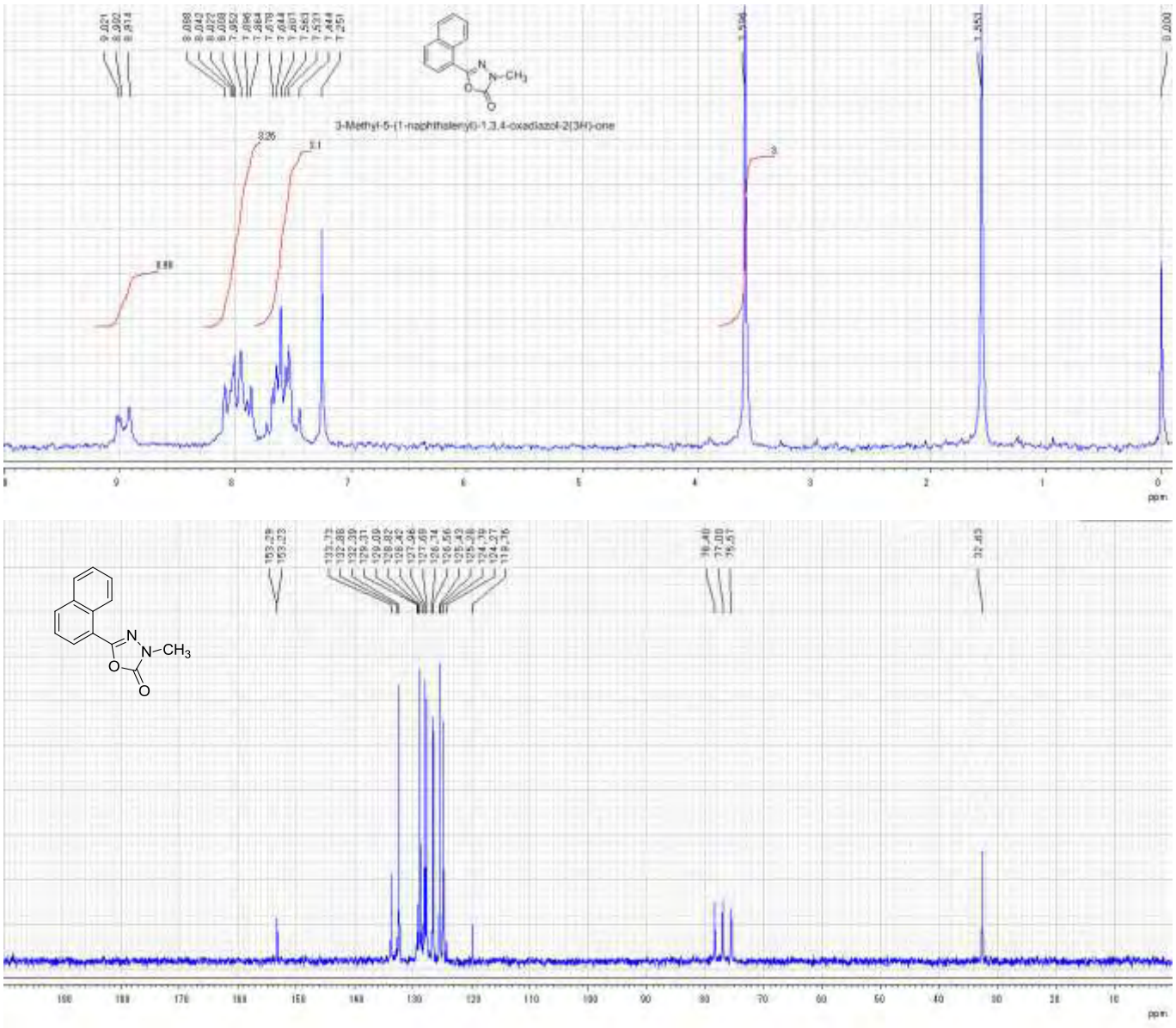


5-(3,4,5-Trimethoxyphenyl)-1,3,4-oxadiazol-2(3*H*)-one. White scales (recryst. from ethyl acetate). Mp 192 °C (lit.[7] 189-190 °C). ^{1}H-NMR ($CDCl_3$) δ : 3.91 (9H, *s*, CH_3×3), 1.95 (2H, *s*, phenyl-H), 8.98 (1H, *brs*, NH). ^{13}C-NMR (DMSO-d_6) δ : 59.6, 63.7, 106.1, 122.7, 143.6, 156.8, 157.1, 158.0. *Anal*. Calcd for $C_{11}H_{12}N_2O_5$: C, 52.38; H, 4.80; N, 11.11. Found: C, 52.43; H, 5.00; N, 11.09.

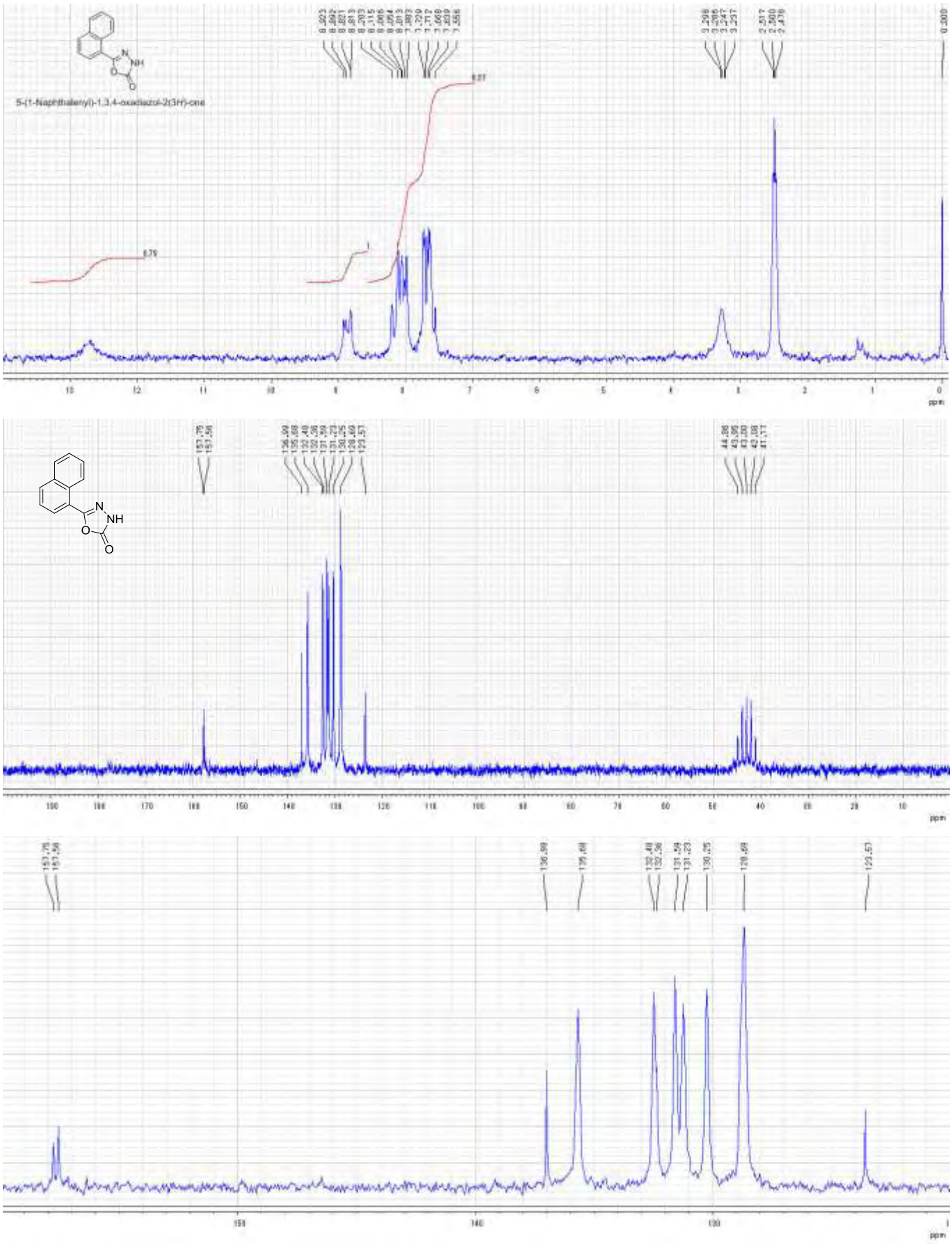




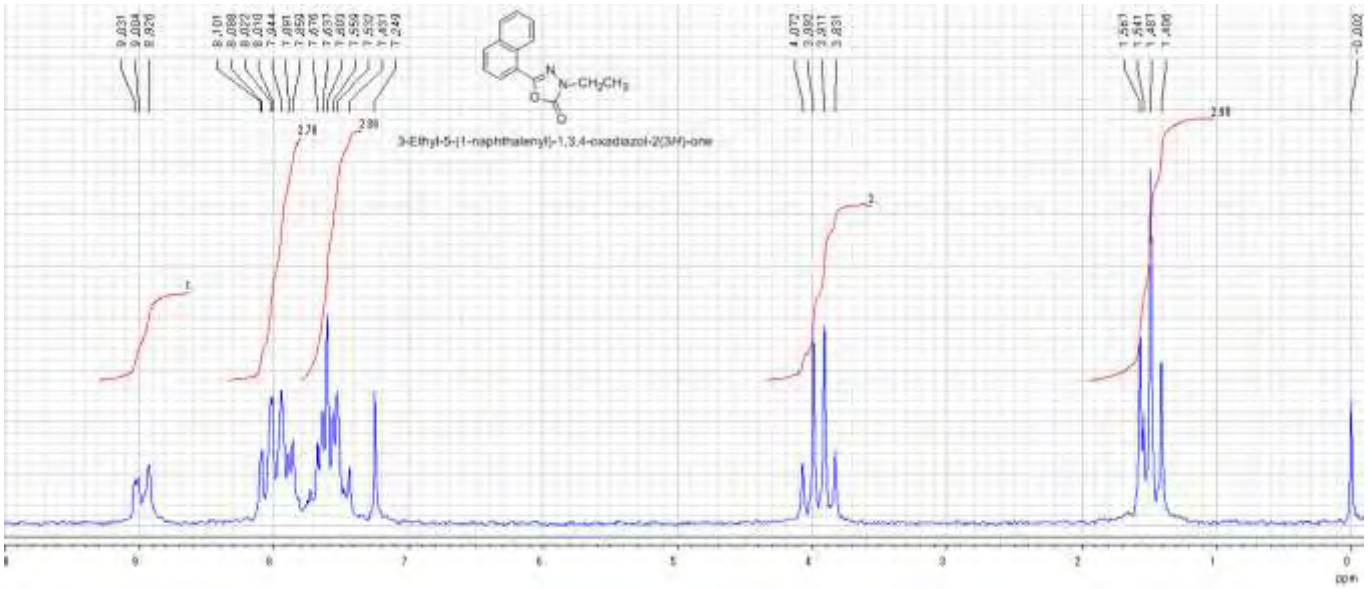
3-Methyl-5-(1-naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 112.8-115.0 °C. ^{1}H-NMR ($CDCl_3$) δ : 3.60 (3H, *s*, CH_3), 7.35-7.78 (3H, *m*, naphthalenyl-H), 7.78-8.22 (3H, *m*, naphthalenyl-H). 8.82-9.10 (1H, *m*, naphthalenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 32.6, 119.8, 124.8, 125.4, 126.6, 127.7, 128.0, 128.8, 129.3, 132.4, 133.7, 153.2, 153.3. *Anal*. Calcd for $C_{13}H_{10}N_2O_2$: C, 69.02; H, 4.46; N, 12.38. Found : C, 69.26; H, 4.31; N, 12.41.

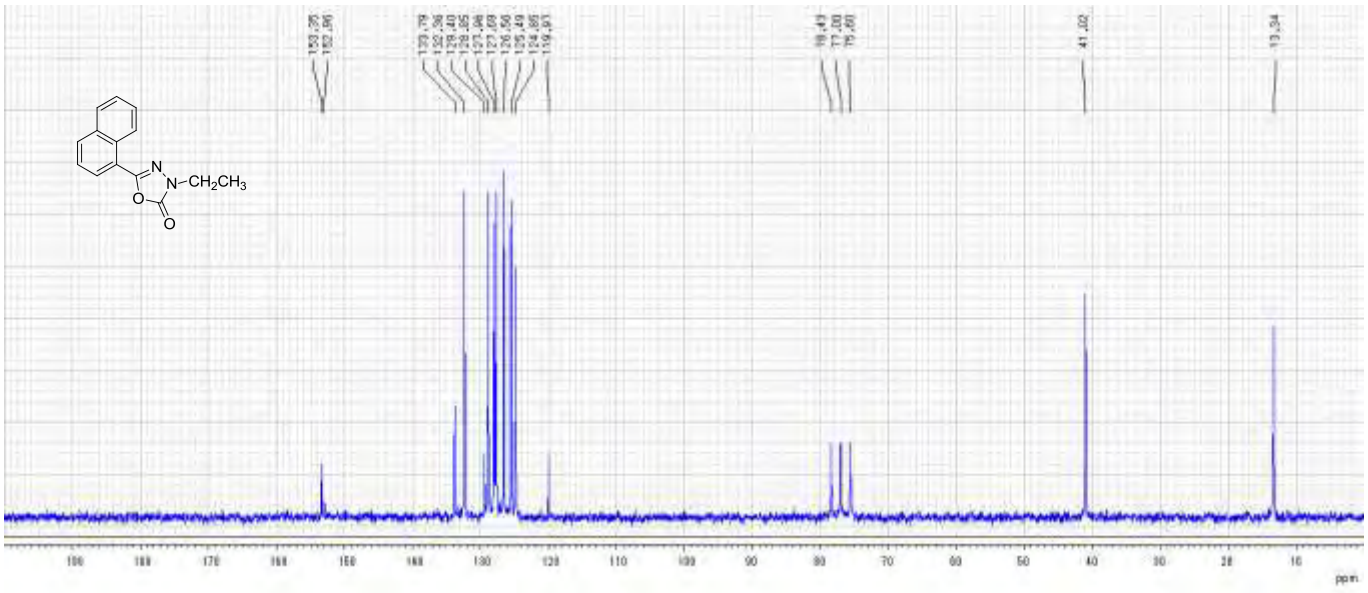


5-(1-Naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids. Mp 179-180 °C (lit.[8] 190.5-191.1 °C). ^{1}H-NMR (lit.[6], DMSO-d_6) δ : 7.45-7.85 (3H, *m*, naphthalenyl-H), 7.85-8.35 (3H, *m*, naphthalenyl-H), 8.70-9.05 (1H, *m*, naphthalenyl-H). 12.70 (1H, *brs*, NH). ^{13}C-NMR (DMSO-d_6) δ : 123.6, 128.7, 130.3, 131.2, 131.6, 132.5, 135.7, 137.0, 157.6, 157.8.

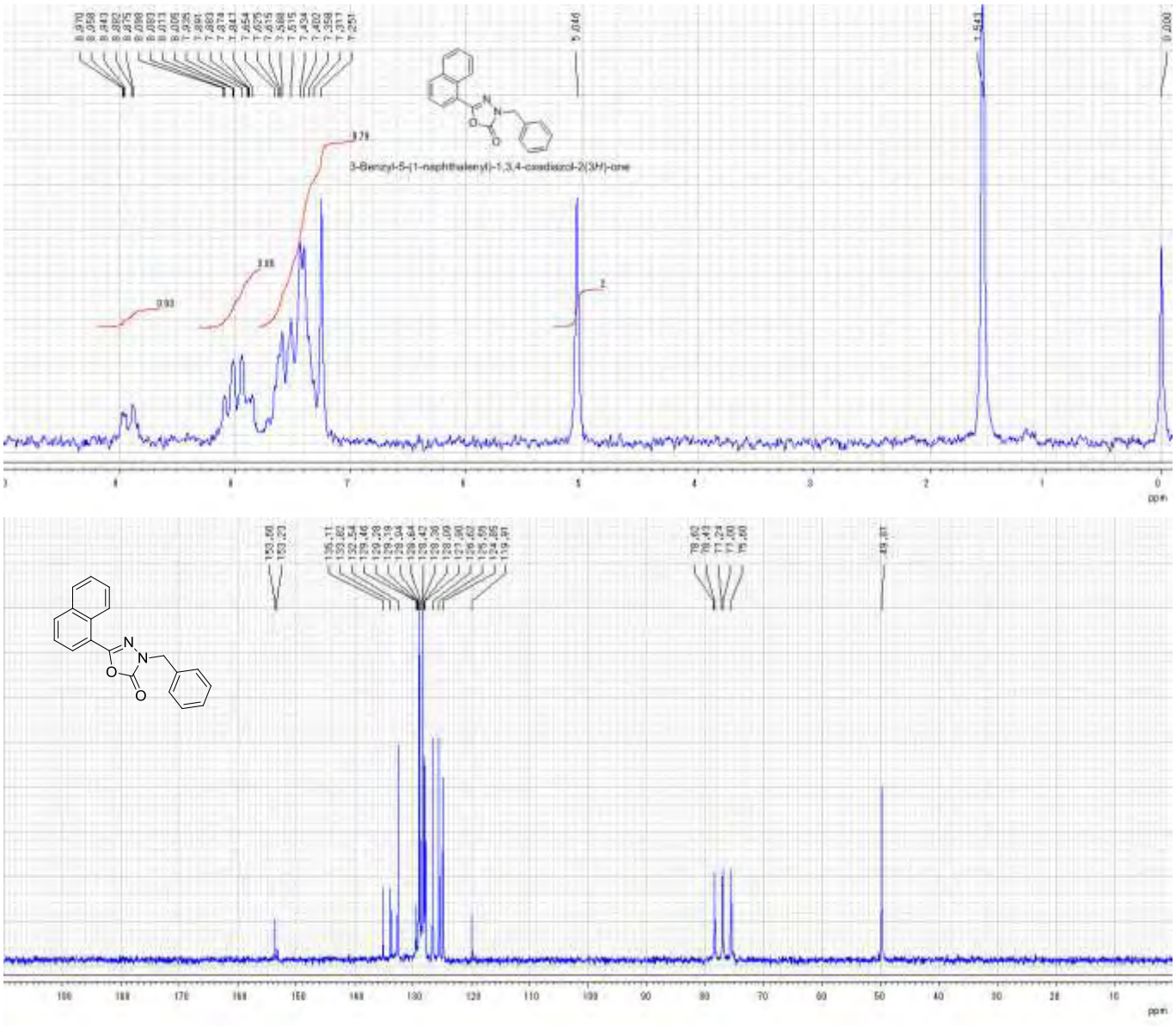


3-Ethyl-5-(1-naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane). Mp 85.0-85.8 °C. MS 240 (M^+). ^{1}H-NMR ($CDCl_3$) δ : 1.49 (3H, *t*, J=7.2 Hz, CH_3), 3.95 (2H, *q*, J=7.2 Hz, CH_2), 7.39-7.78 (3H, *m*, naphthalenyl-H), 7.78-8.16 (3H, *m*, naphthalenyl-H), 8.80-9.15 (1H, *m*, naphthalenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.3, 41.0, 120.0, 124.9, 125.5, 126.6, 127.7, 128.0, 128.9, 129.4, 132.4, 133.8, 153.0, 153.4. *Anal*. Calcd for $C_{14}H_{12}N_2O_2$: C, 69.99; H, 5.03; N, 11.66. Found : C, 70.00; H, 5.10; N, 11.83.

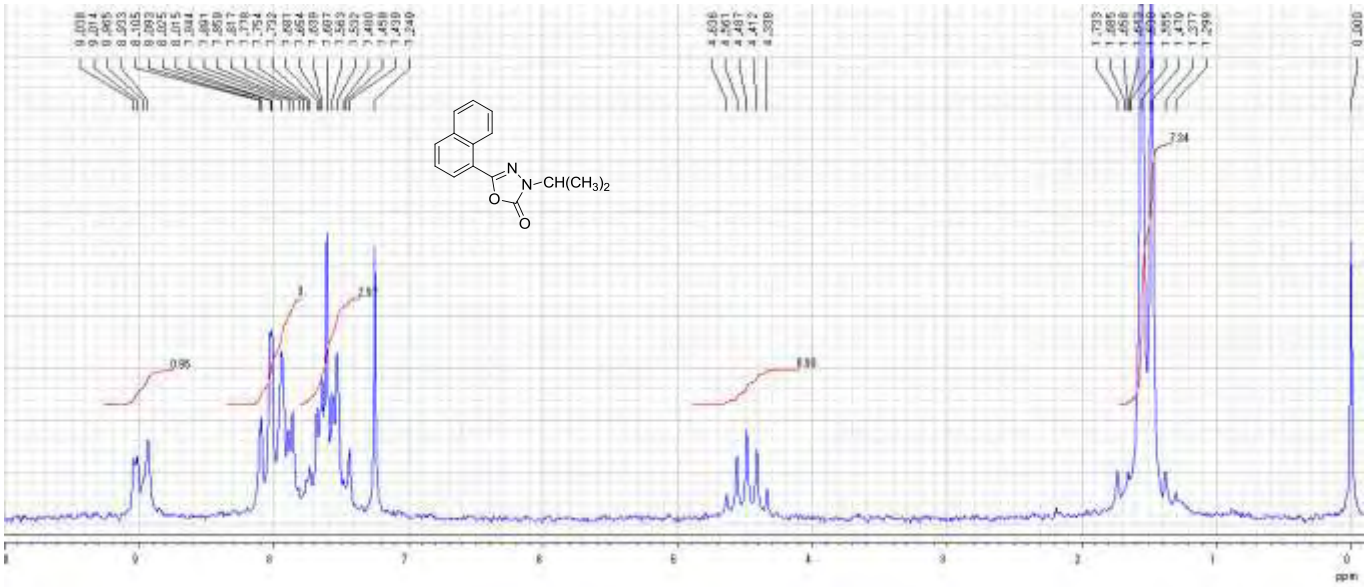


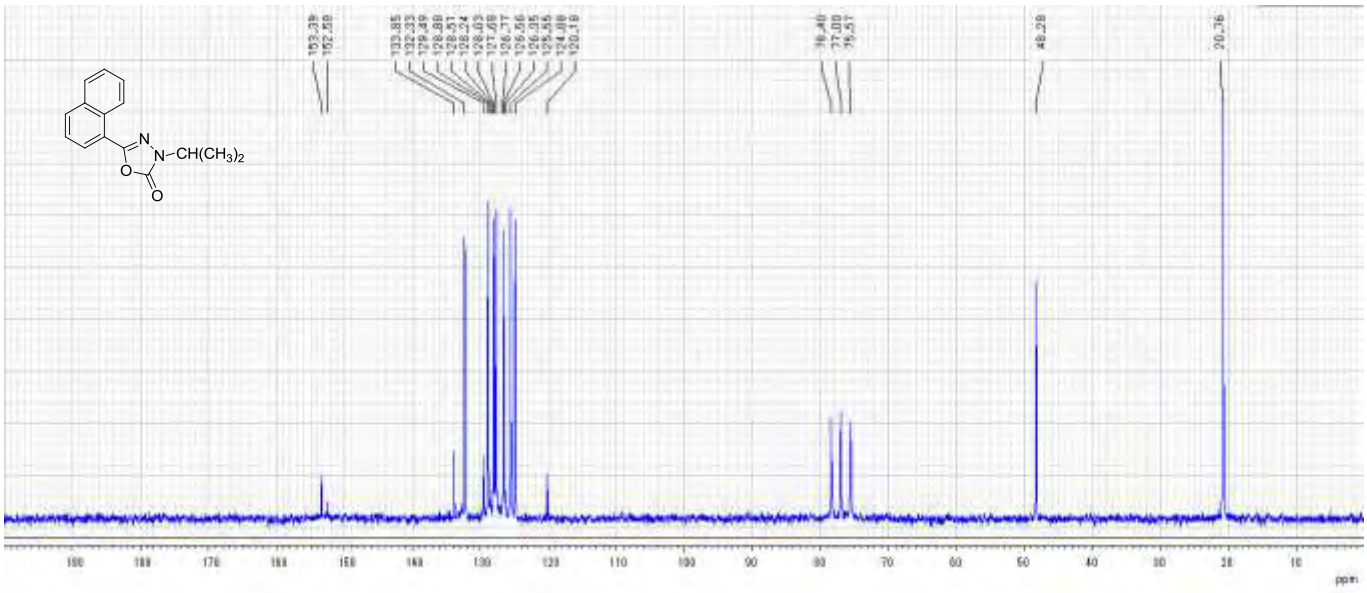


3-Benzyl-5-(1-naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 119-120 °C. ^{1}H-NMR ($CDCl_3$) δ : 5.04 (2H, *s*, CH_2), 7.22-7.75 (8H, *m*, naphthalenyl and phenyl-H), 7.75-8.19 (3H, *m*, naphthalenyl-H), 8.78-9.02 (1H, *m*, naphthalenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 49.8, 119.9, 124.9, 125.6, 126.6, 127.9, 128.1, 128.36, 128.42, 128.9, 129.5, 132.5, 133.8, 135.1, 153.2, 153.6. *Anal*. Calcd for $C_{19}H_{14}N_2O_2$: C, 75.48; H, 4.67; N, 9.27. Found : C, 75.58; H, 4.75; N, 9.39.

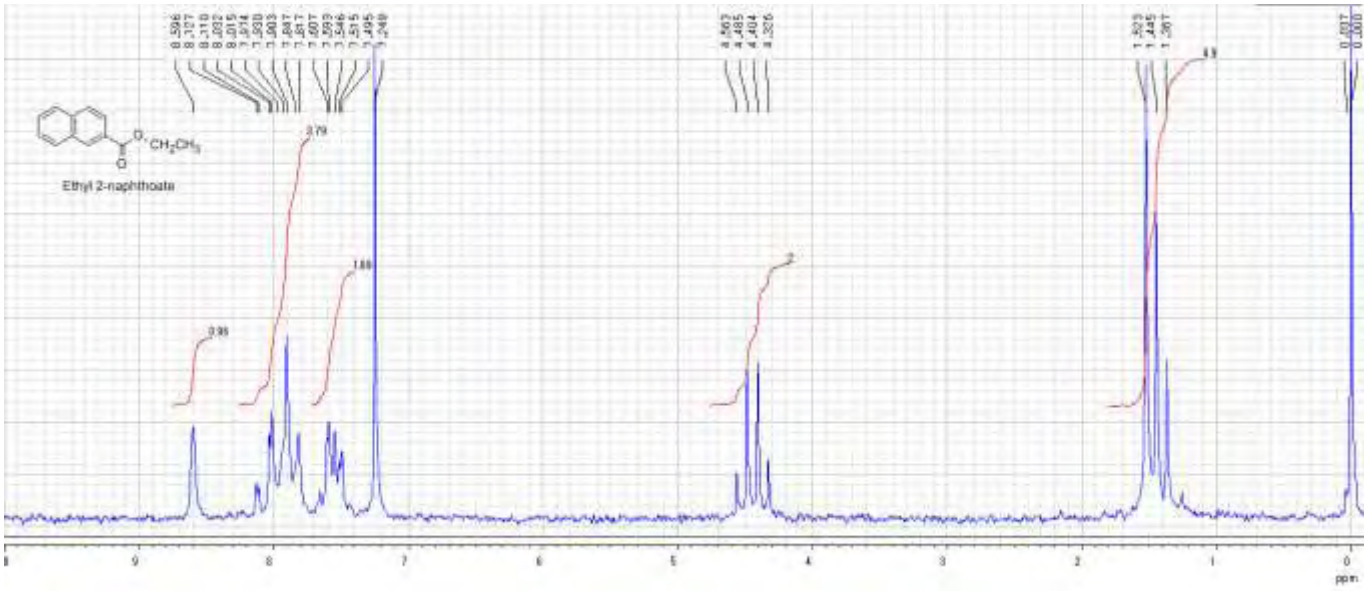


3-Isopropyl-5-(1-naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane). Mp 106-107 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.52 (6H, *d*, J=6.8 Hz, CH_3×2), 4.49 (1H, *septet*, J=6.8 Hz, CH), 7.35-7.80 (3H, *m*, naphthalenyl-H), 7.80-8.20 (3H, *m*, naphthalenyl-H), 8.99 (1H, *dd*, J=6.9 Hz, 2.1 Hz, naphthalenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 20.8, 48.3, 120.2, 124.9, 125.6, 126.6, 127.7, 128.0, 128.9, 129.5, 132.3, 133.9, 152.6, 153.4. *Anal*. Calcd for $C_{15}H_{14}N_2O_2$: C, 70.85; H, 5.55; N, 11.02. Found : C, 70.85; H, 5.55; N, 10.97.

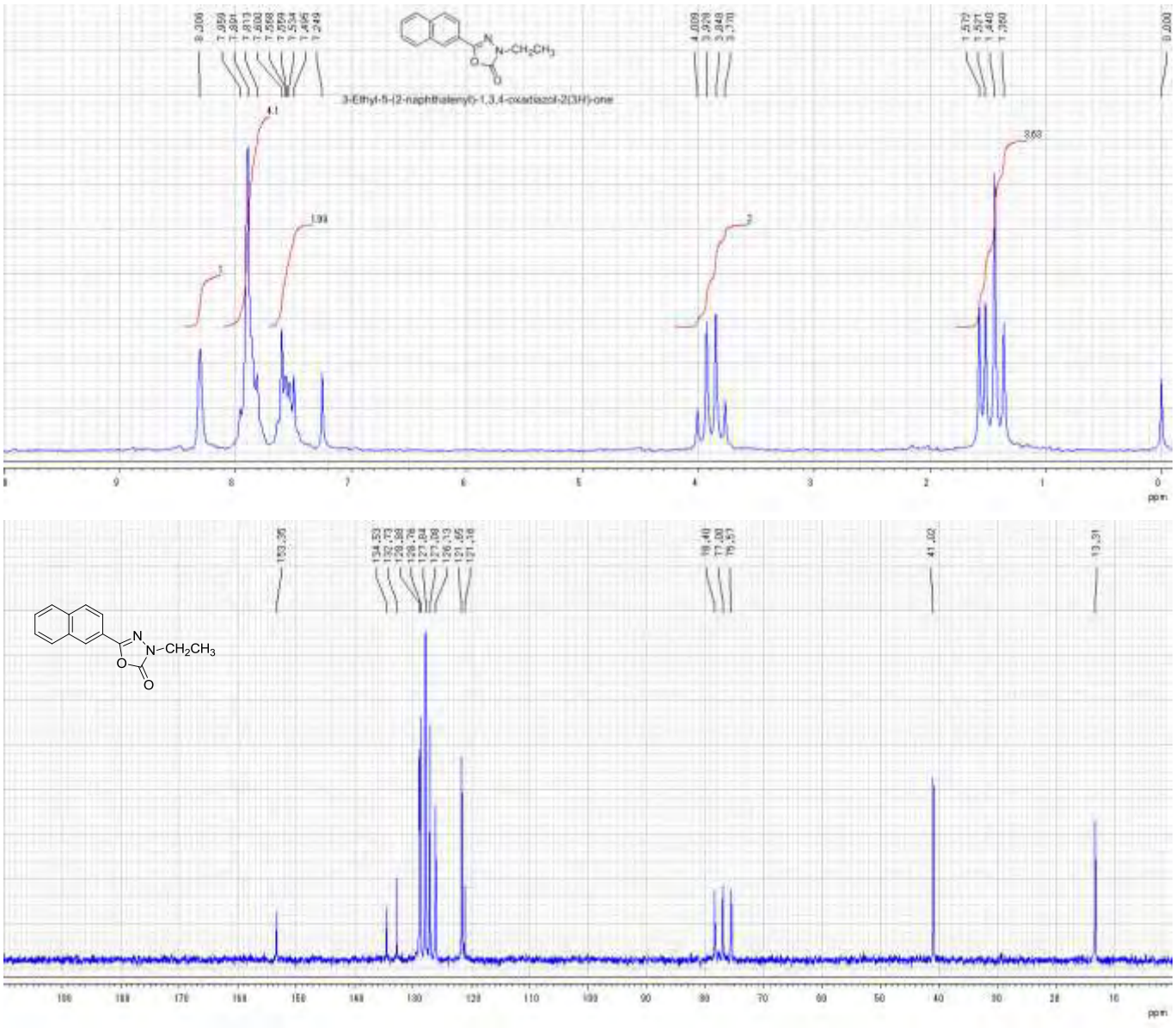




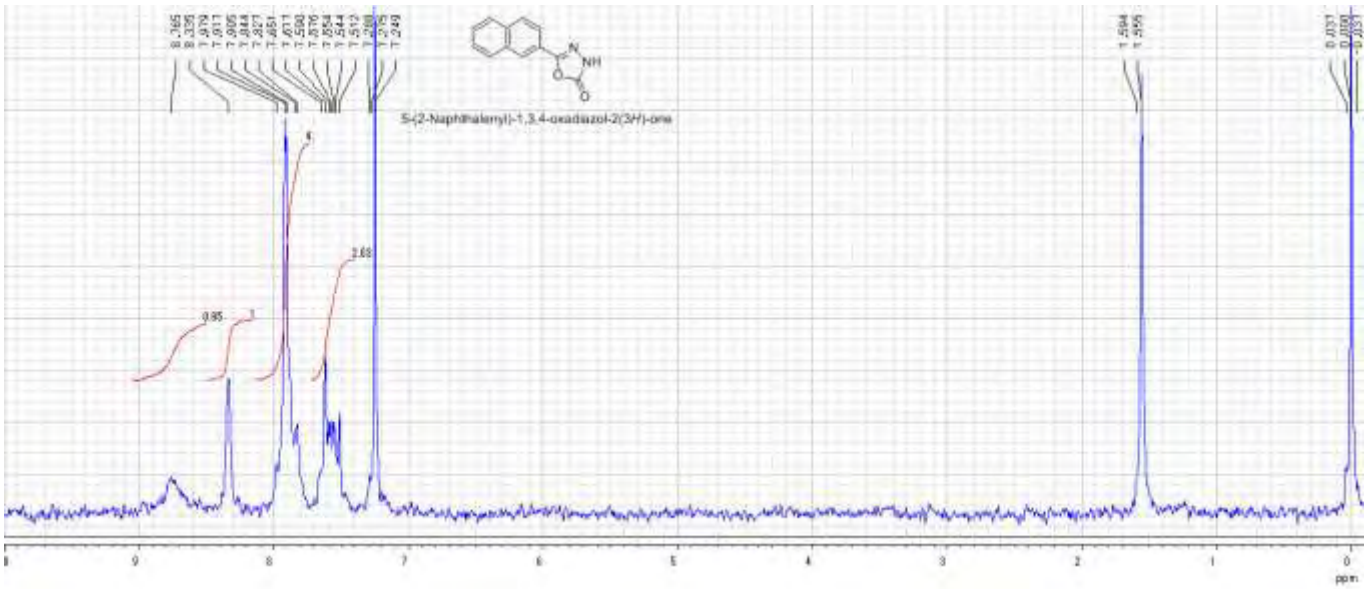
Ethyl 2-naphthoate. Slight yellow oil. Bp 185 °C / 11 mmHg (lit.[9] 146-147 °C / 1-2 mmHg). ^{1}H-NMR ($CDCl_3$) δ : 1.45 (3H, *t*, J=7.0 Hz, CH_3), 4.44 (2H, *q*, J=7.0 Hz, CH_2), 7.39-7.72 (2H, *m*, naphthalenyl-H), 7.72-8.19 (4H, *m*, naphthalenyl-H), 8.60 (1H, *s*, naphthalenyl-H).

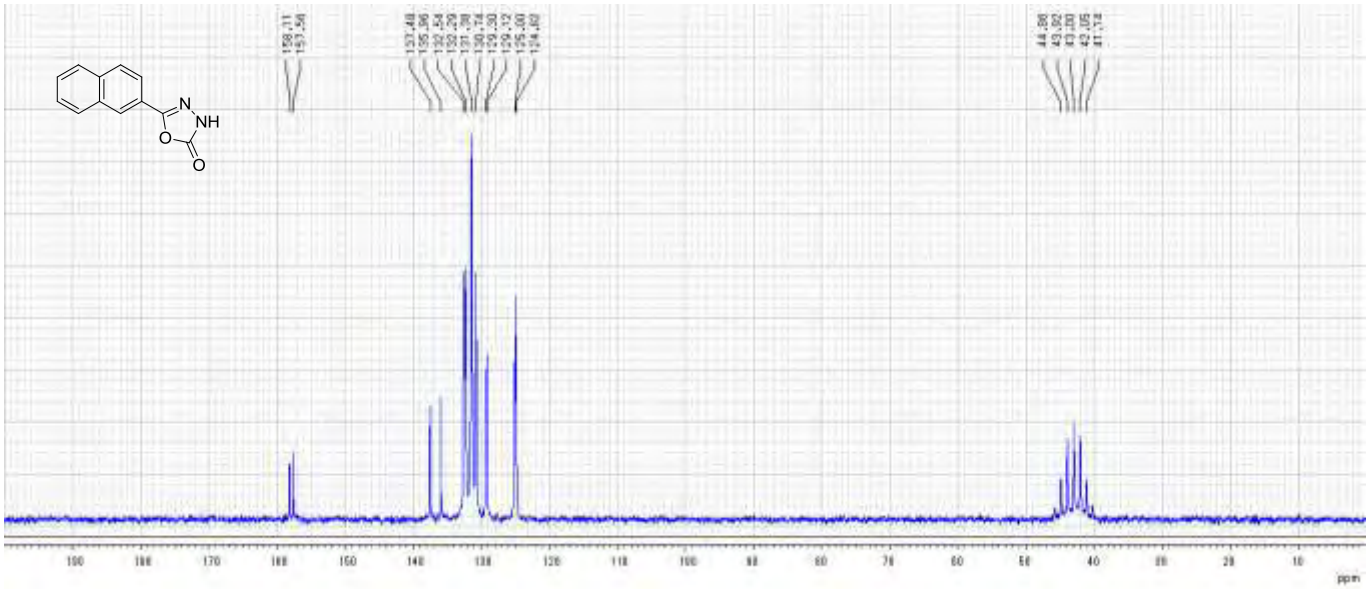


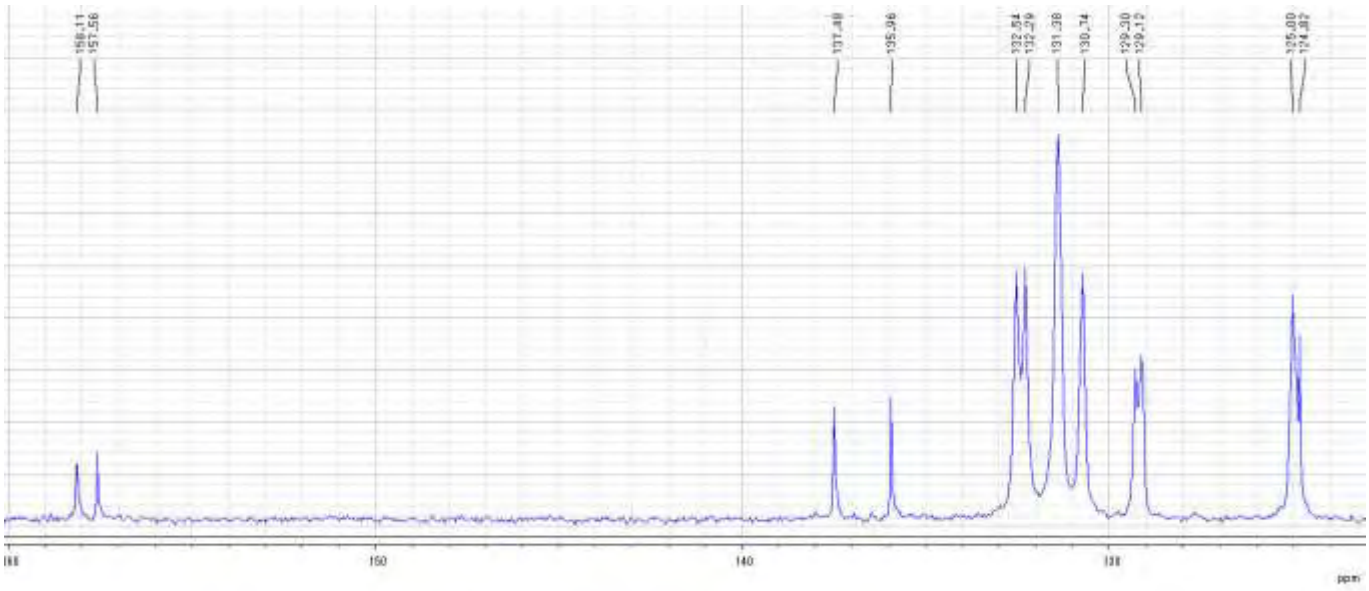
3-Ethyl-5-(2-naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White plates (recryst. from hexane). Mp 115-117 °C. MS 240 (M^+). ^{1}H-NMR ($CDCl_3$) δ : 1.44 (3H, *t*, J=7.2 Hz, CH_3), 3.89 (2H, *q*, J=7.2 Hz, CH_2), 7.35-7.70 (2H, *m*, naphthalenyl-H), 7.70-8.07 (4H, *m*, naphthalenyl-H), 8.31 (1H, *s*, naphthalenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.3, 41.0, 121.2, 121.7, 126.1, 127.1, 127.8, 128.8, 128.9, 132.7, 134.5, 153.4. *Anal*. Calcd for $C_{14}H_{12}N_2O_2$: C, 69.99; H, 5.03; N, 11.66. Found : C, 70.14; H, 5.06; N, 11.63.



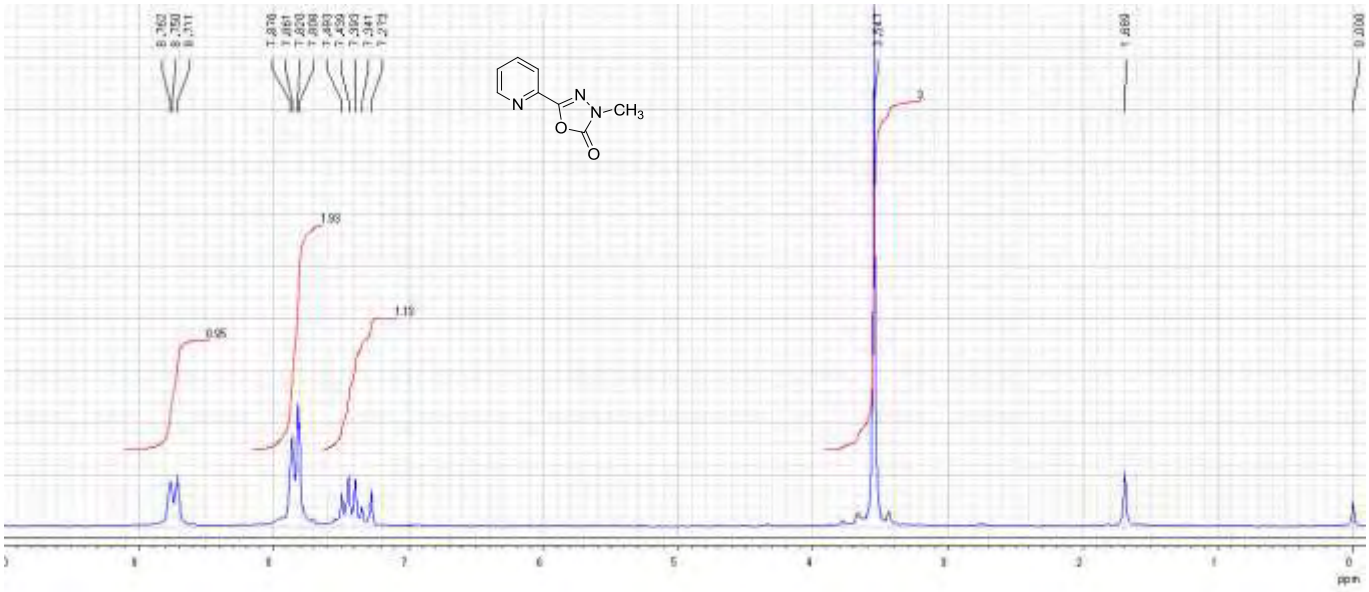
5-(2-Naphthalenyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids. Mp 194-196 °C (lit.[10] 182-184 °C). ^{1}H-NMR ($CDCl_3$) δ : 7.40-7.72 (2H, *m*, naphthalenyl-H), 7.72-8.03 (4H, *m*, naphthalenyl-H), 8.34 (1H, *s*, naphthalenyl-H), 8.77 (1H, *brs*, NH). ^{13}C-NMR (DMSO-d_6) δ : 124.8, 125.0, 129.1, 129.3, 130.7, 131.4, 132.3, 132.5, 136.0, 137.5, 157.6, 158.1.

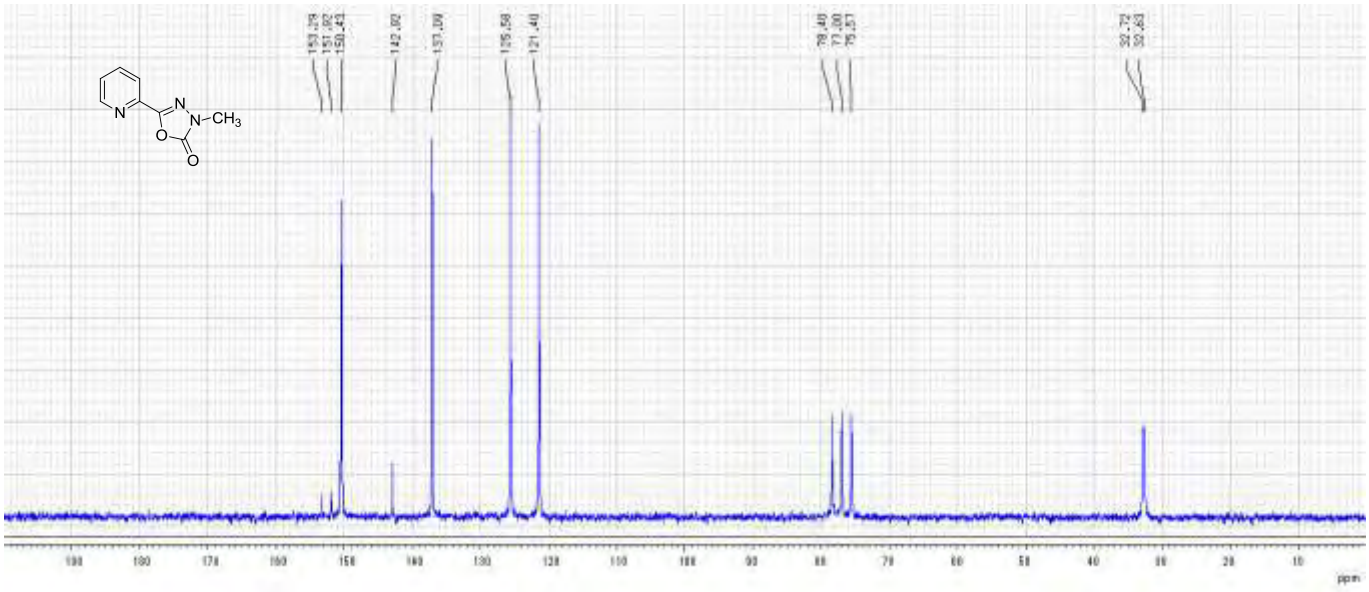




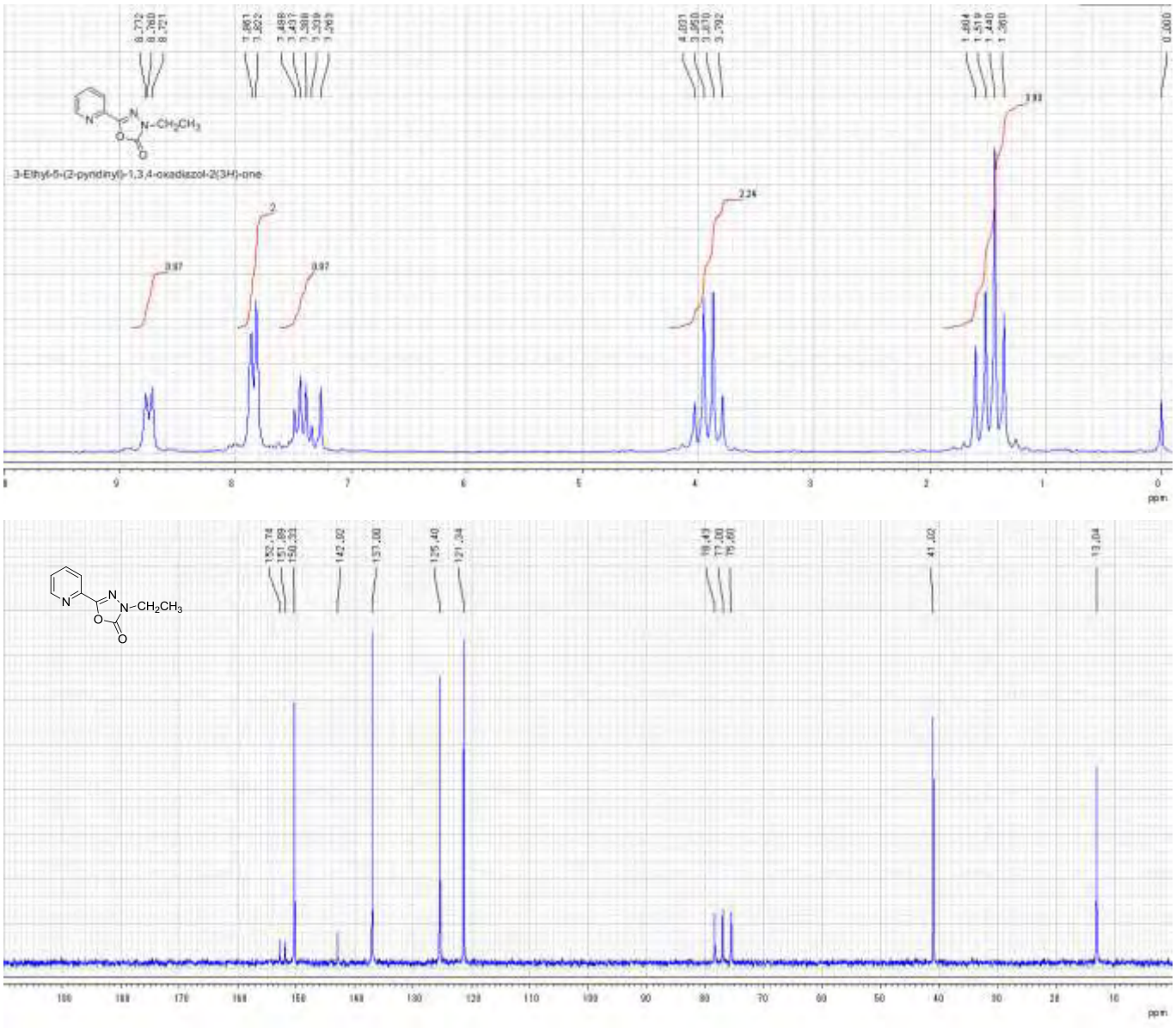


3-Methyl-5-(2-pyridinyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids. Mp 109-110 °C (lit.[11] 75-76 °C). ^{1}H-NMR ($CDCl_3$) δ : 3.55 (3H, *s*, CH_3), 7.30-7.60 (1H, *m*, pyridine-H), 7.70-7.95 (2H, *m*, pyridine-H), 8.74 (1H, *d*, J=4.7 Hz, pyridine-H). ^{13}C-NMR ($CDCl_3$) δ : 32.7, 121.4, 125.6, 137.1, 142.9, 150.4, 151.9, 153.3.

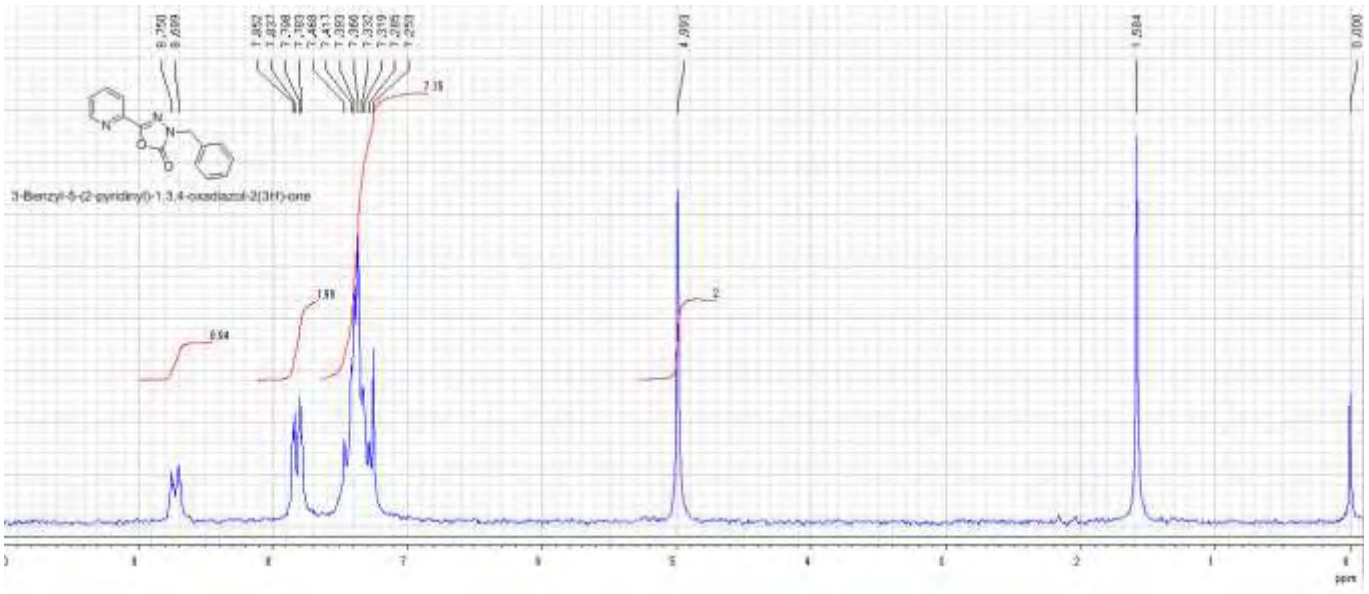


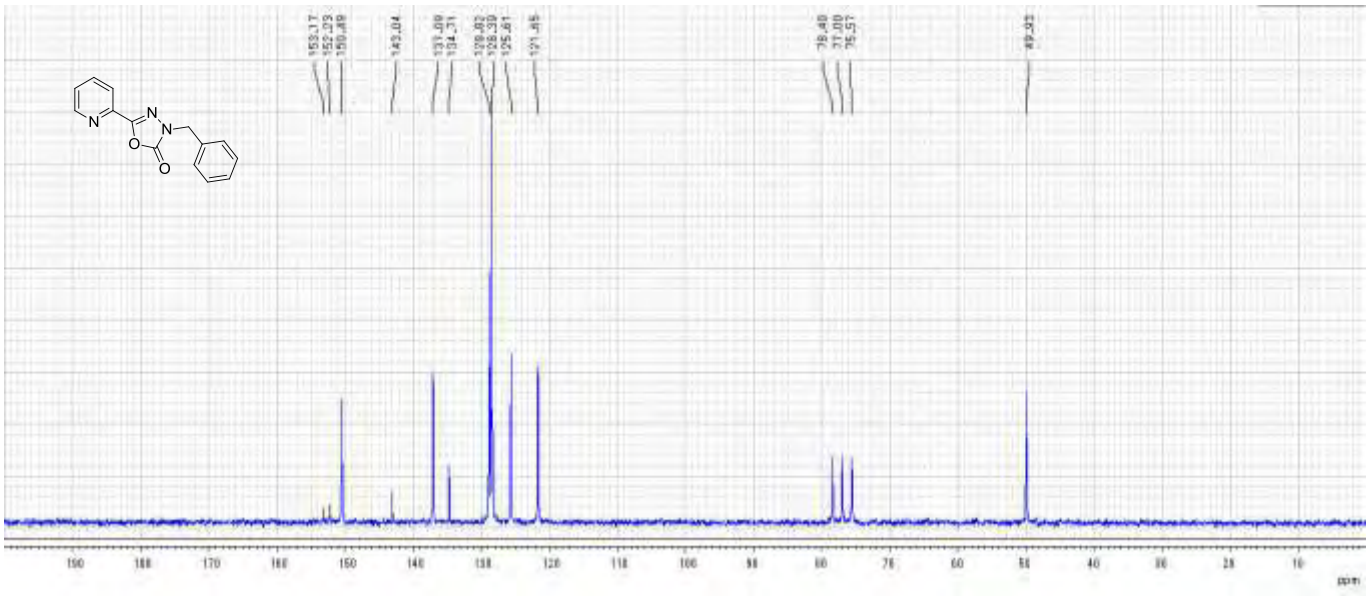


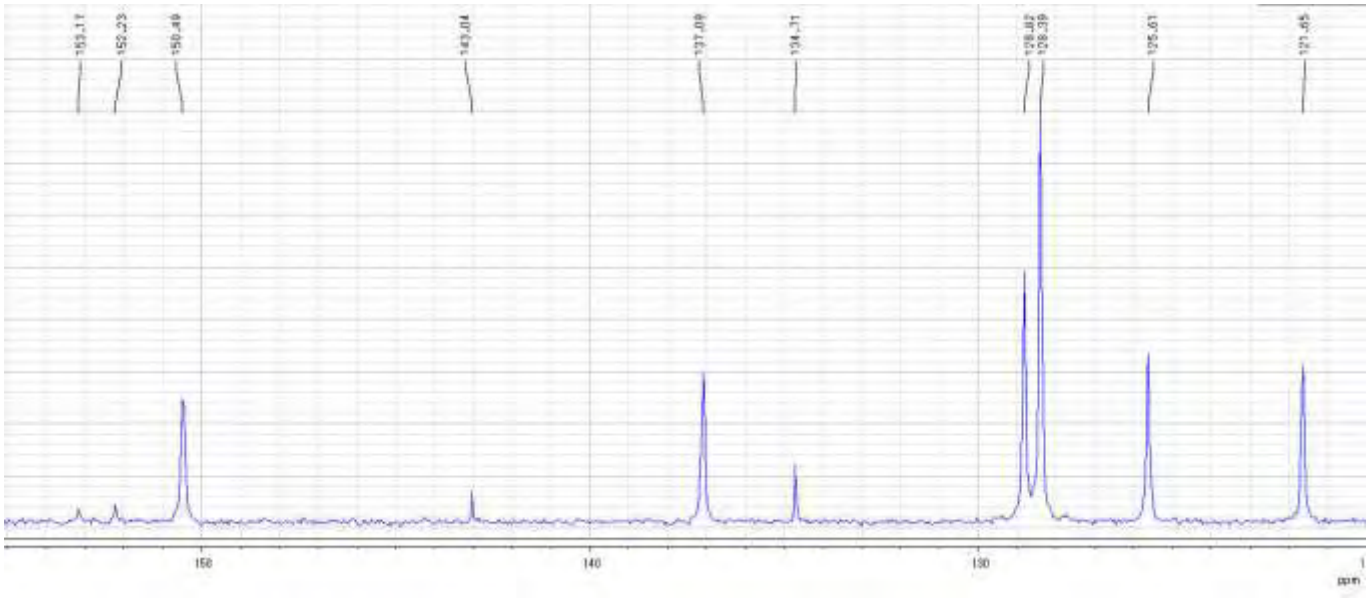
3-Ethyl-5-(2-pyridinyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane-ethyl acetate). Mp 85-86 °C. MS 191 (M^+). ^{1}H-NMR ($CDCl_3$) δ : 1.44 (3H, *t*, J=7.2 Hz, CH_3), 3.91 (2H, *q*, J=7.2 Hz, CH_2), 7.30-7.56 (1H, *m*, pyridinyl-H), 7.72-7.95 (2H, *m*, pyridinyl-H), 8.75 (1H, *d*, J=4.6 Hz, pyridinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.0, 41.0, 121.3, 125.4, 137.0, 142.9, 150.3, 151.9, 152.7. *Anal*. Calcd for $C_9H_9N_3O_2$: C, 56.54; H, 4.74; N, 21.98. Found : C, 56.44; H, 4.67; N, 21.92.



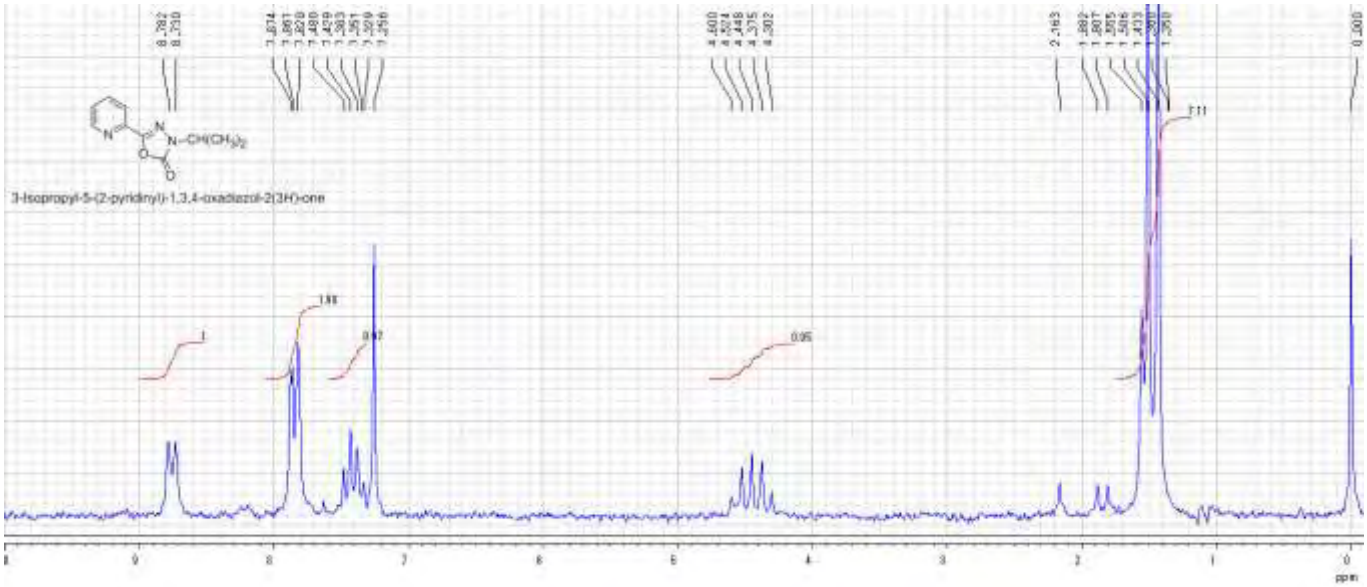
3-Benzyl-5-(2-pyridinyl)-1,3,4-oxadiazol-2(3*H*)-one. Slight yellow solids (recryst. from hexane-ethyl acetate). Mp 98.5-99.0 °C. ^{1}H-NMR ($CDCl_3$) δ : 4.99 (2H, *s*, CH_2), 7.20-7.54 (6H, *m*, pyridinyl and phenyl-H), 7.70-7.90 (2H, *m*, pyridinyl-H), 8.72 (1H, *d*, J=4.6 Hz, pyridinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 49.9, 121.7, 125.6, 128.4, 128.8, 134.7, 137.1, 143.0, 150.5, 152.2, 153.2. *Anal*. Calcd for $C_{14}H_{11}N_3O_2$: C, 66.40; H, 4.38; N, 16.59. Found : C, 66.30; H, 4.42; N, 16.33.

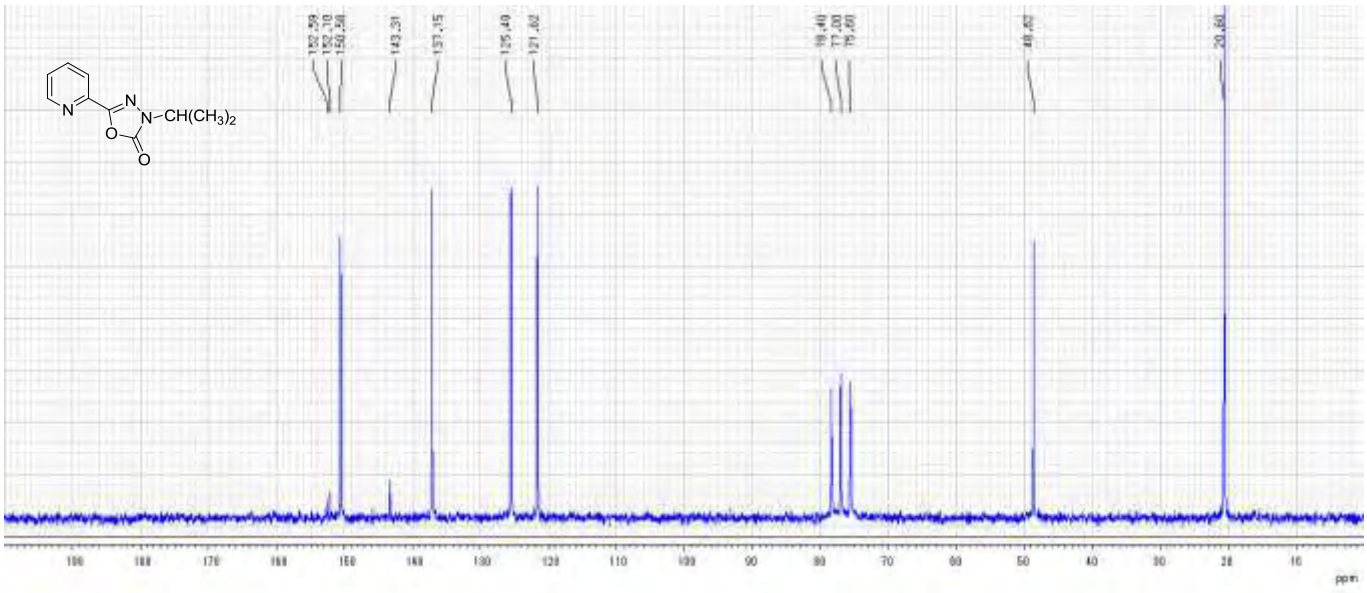




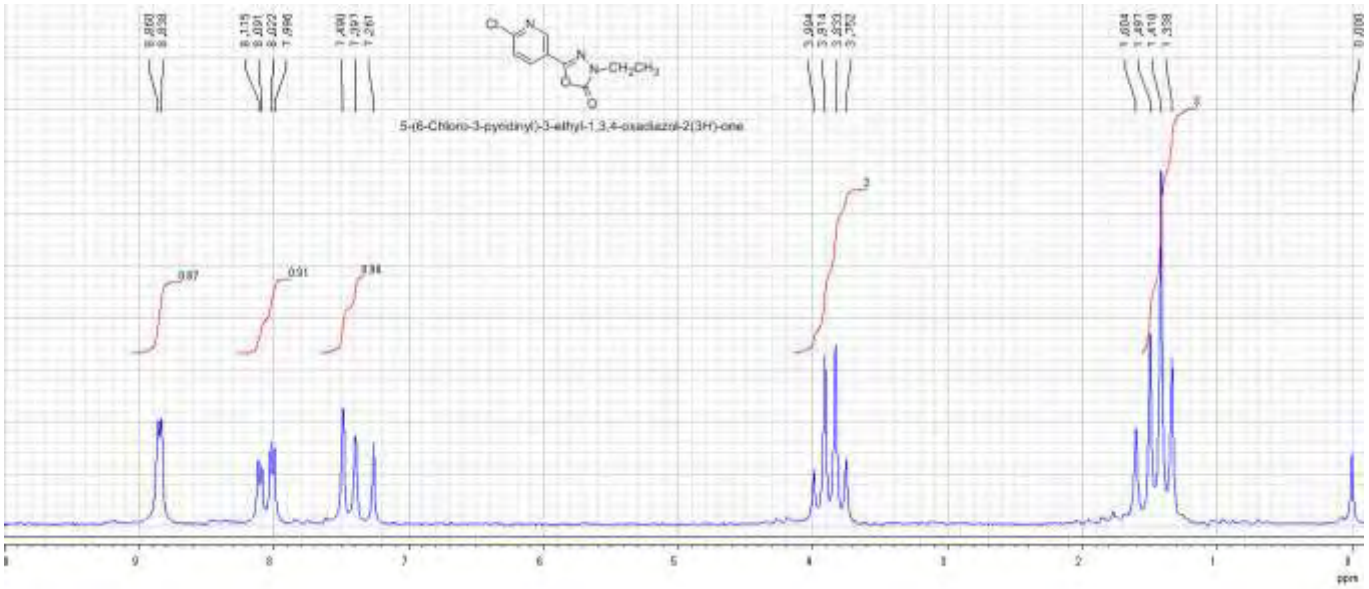


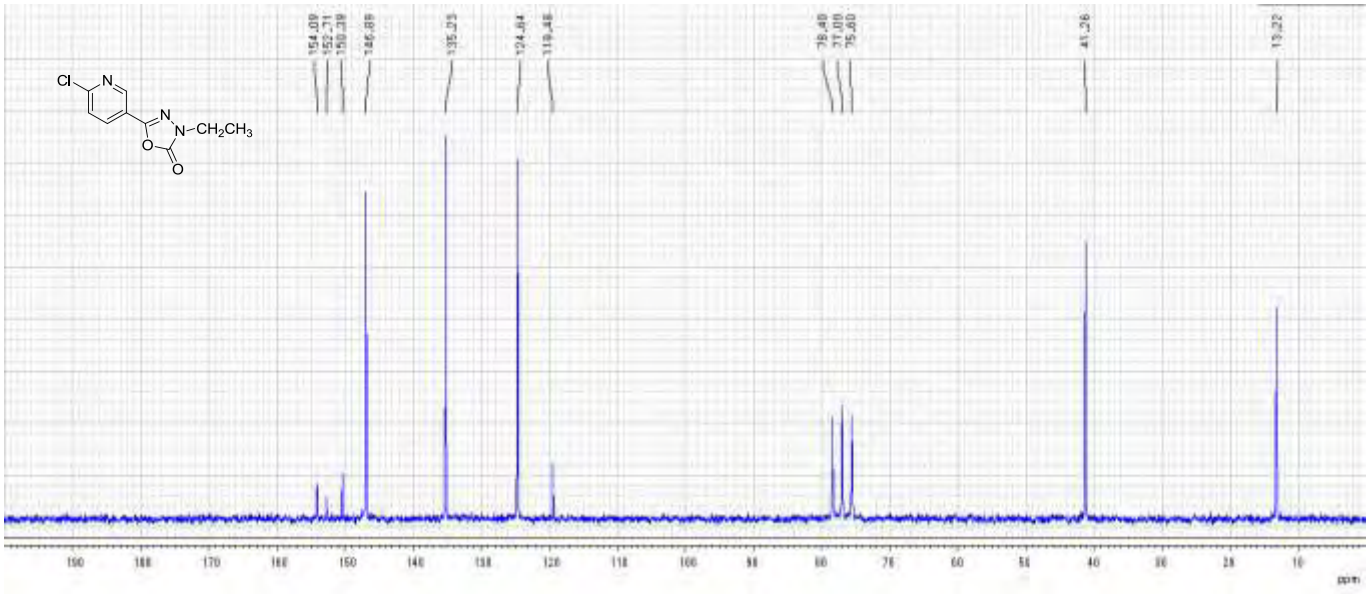
3-Isopropyl-5-(2-pyridinyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane-ethyl acetate). Mp 80-82 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.47 (6H, *d*, J=6.6 Hz, CH_3×2), 4.45 (1H, *septet*, J=6.6 Hz, CH), 7.30-7.55 (1H, *m*, pyridinyl-H), 7.66-8.00 (2H, *m*, pyridinyl-H), 8.76 (1H, *d*, J=4.7 Hz, pyridinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 20.6, 48.6, 121.6, 125.5, 137.2, 143.3, 150.6, 152.1, 152.6. *Anal*. Calcd for $C_{10}H_{11}N_3O_2$: C, 58.53; H, 5.40; N, 20.48. Found : C, 58.55; H, 5.47; N, 20.25.



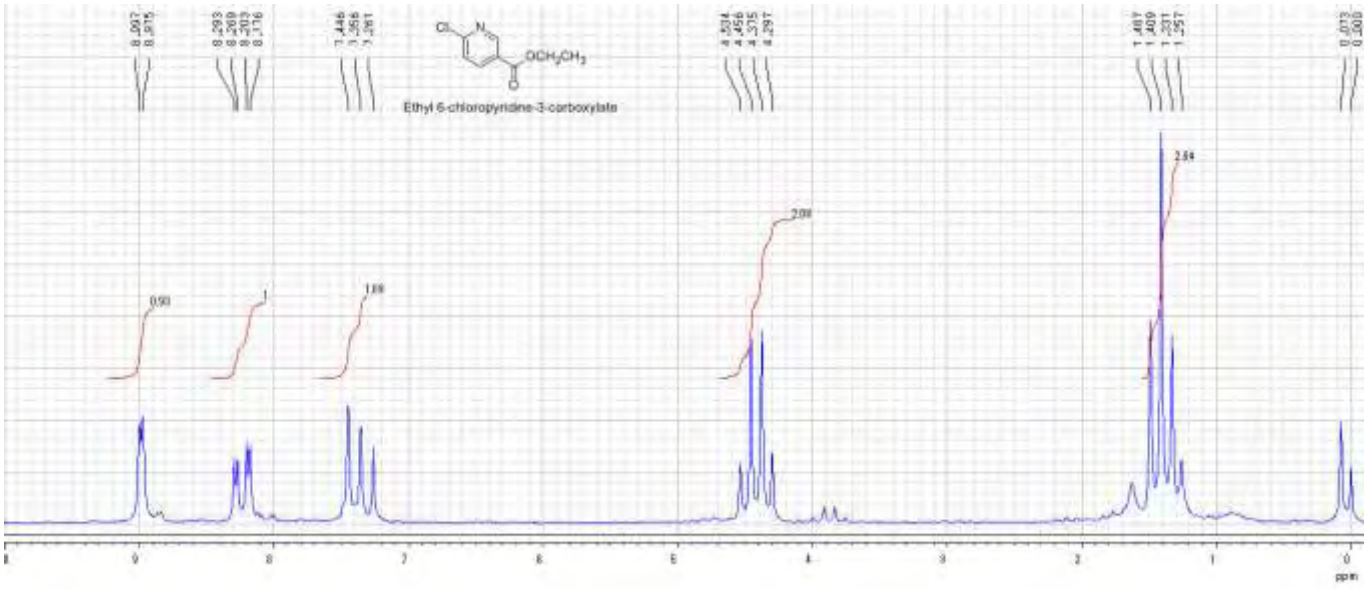


3-Ethyl-5-(6-chloro-3-pyridinyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane). Mp 96-97 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.42 (3H, *t*, J=7.2 Hz, CH_3), 3.87 (2H, *q*, J=7.2 Hz, CH_2), 7.44 (1H, *d*, J=8.3 Hz, pyridine-H), 8.06 (1H, *dd*, J=8.3 Hz, 2.2 Hz, pyridine-H), 8.85 (1H, *d*, J=2.2 Hz, pyridine-H). ^{13}C-NMR ($CDCl_3$) δ : 13.2, 41.3, 119.5, 124.6, 135.2, 146.9, 150.4, 152.7, 154.1. *Anal*. Calcd for $C_9H_8ClN_3O_2$: C, 47.91; H, 3.57; N, 18.62. Found : C, 47.80; H, 3.52; N, 18.70.

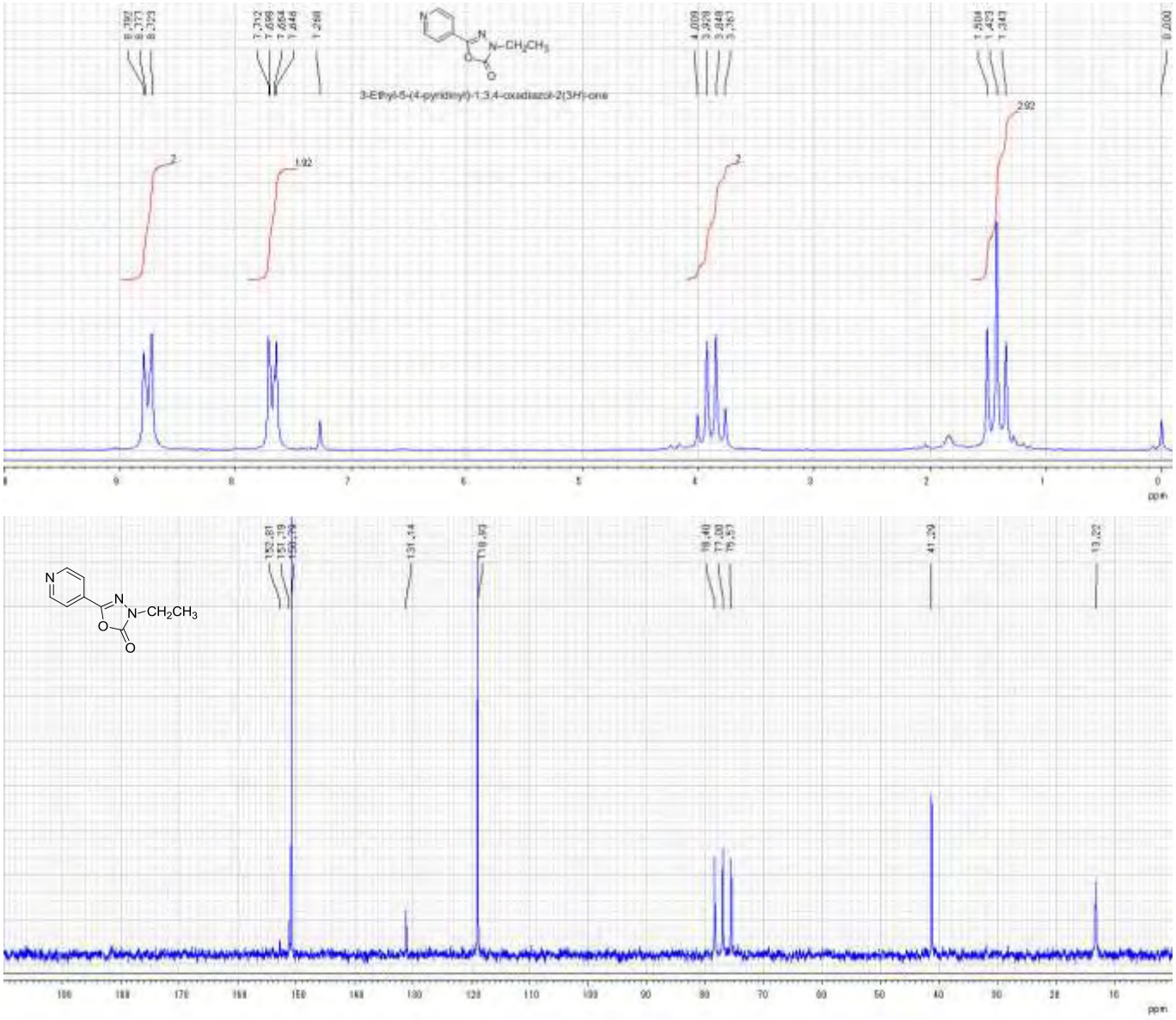




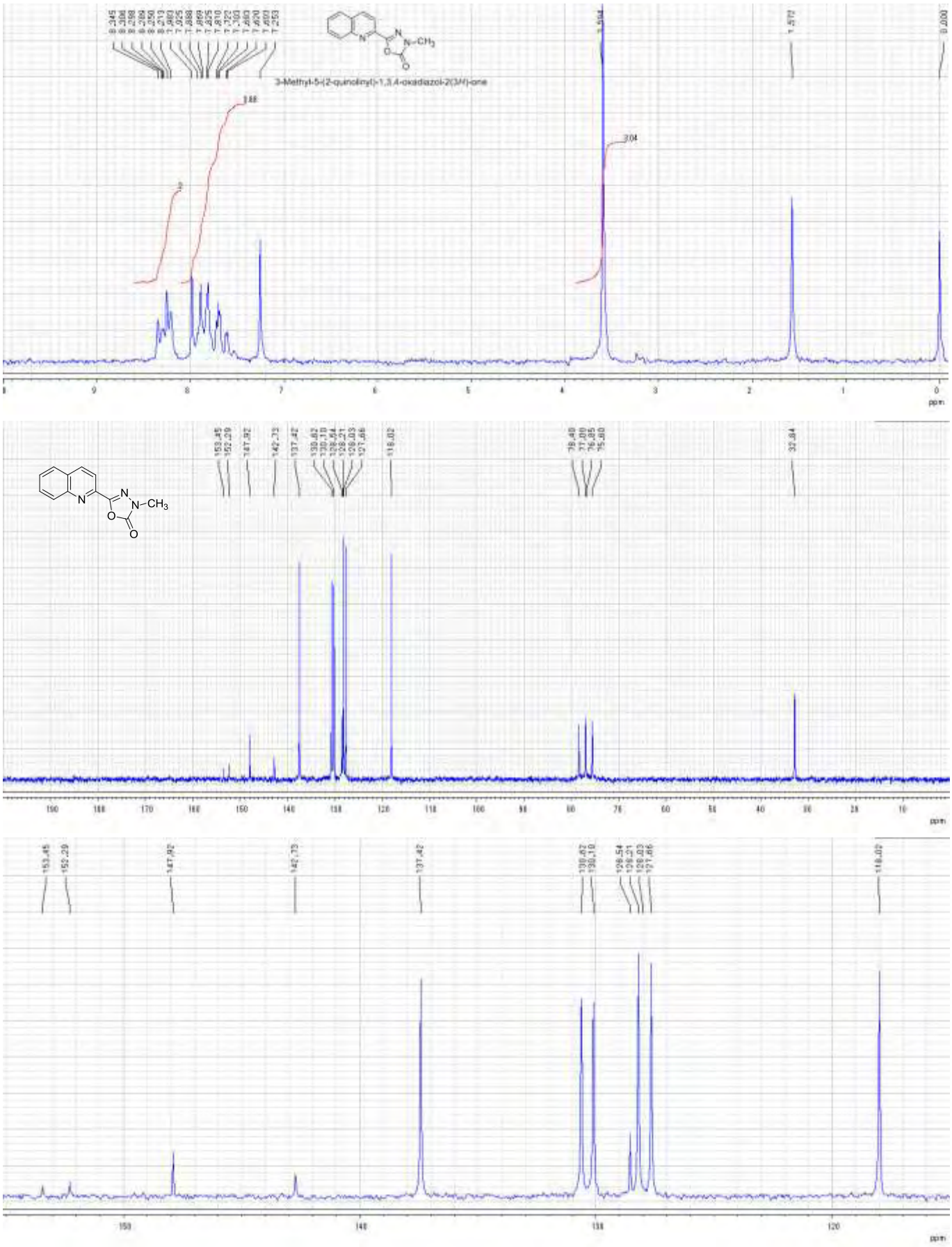
Ethyl 6-chloropyridine-3-carboxylate.[12] Colorless oil. ^{1}H-NMR ($CDCl_3$) δ : 1.41 (3H, *t*, J=7.0 Hz, CH_3), 4.42 (2H, *q*, J=7.0 Hz, CH_2), 7.40 (2H, *d*, J=8.1 Hz, pyridine-H), 8.24 (1H, *dd*, J=8.1 Hz, 2.2 Hz, pyridine-H), 8.99 (1H, *d*, J=2.2 Hz, pyridine-H).



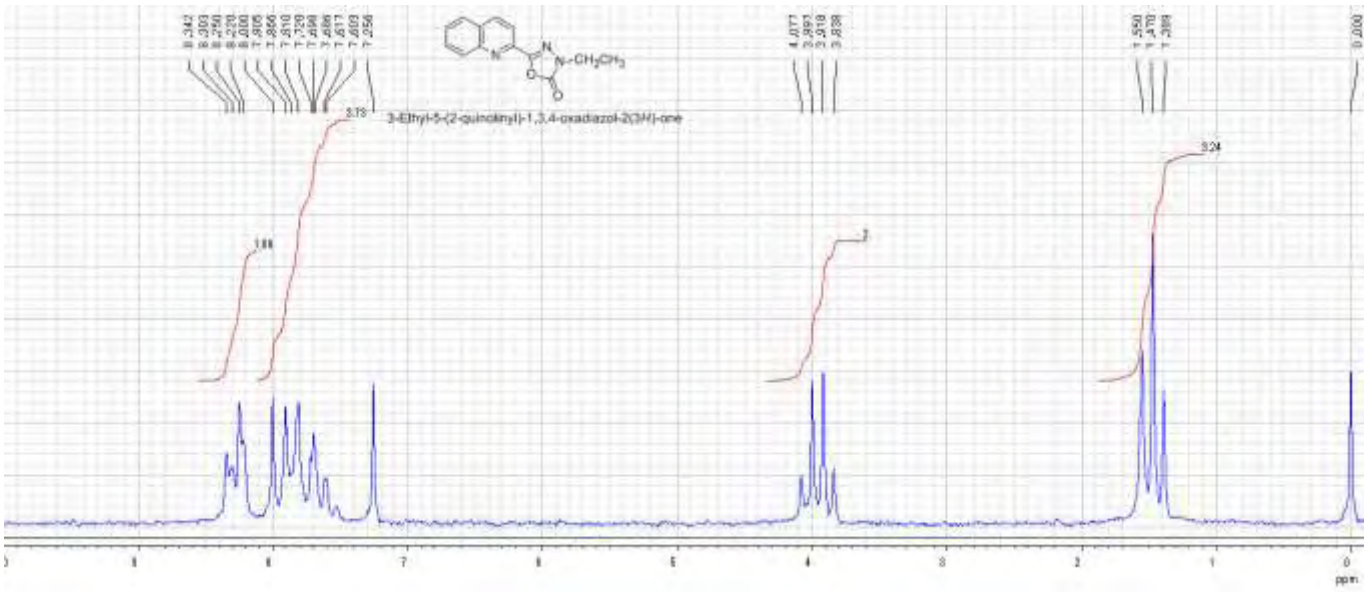
3-Ethyl-5-(4-pyridinyl)-1,3,4-oxadiazol-2(3*H*)-one. Pale yellow solids. Mp 100-101 °C (lit.[13] 104-105 °C). ^{1}H-NMR ($CDCl_3$) δ : 1.42 (3H, *t*, J=7.3 Hz, CH_3), 3.89 (2H, *q*, J=7.3 Hz, CH_2), 7.68 (2H, *d*, J=6.1 Hz, pyridine-H), 8.76 (2H, *d*, J=6.1 Hz, pyridine-H). ^{13}C-NMR ($CDCl_3$) δ : 13.2, 41.3, 118.9, 131.1, 150.8, 151.2, 152.8.

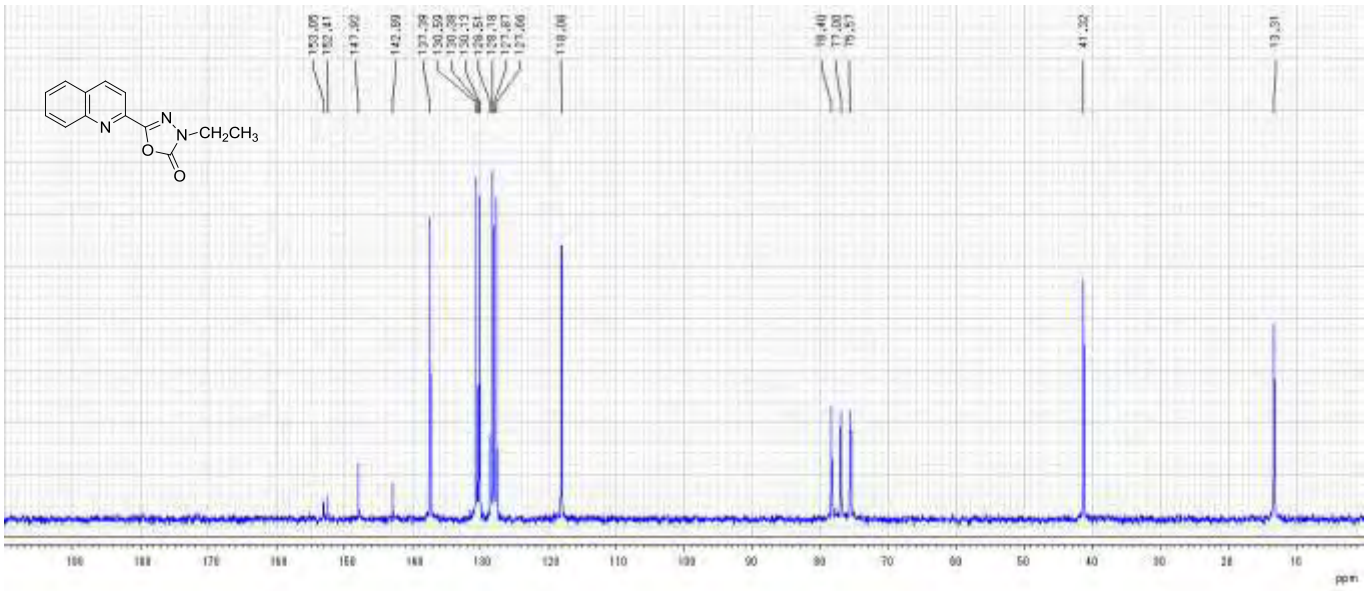


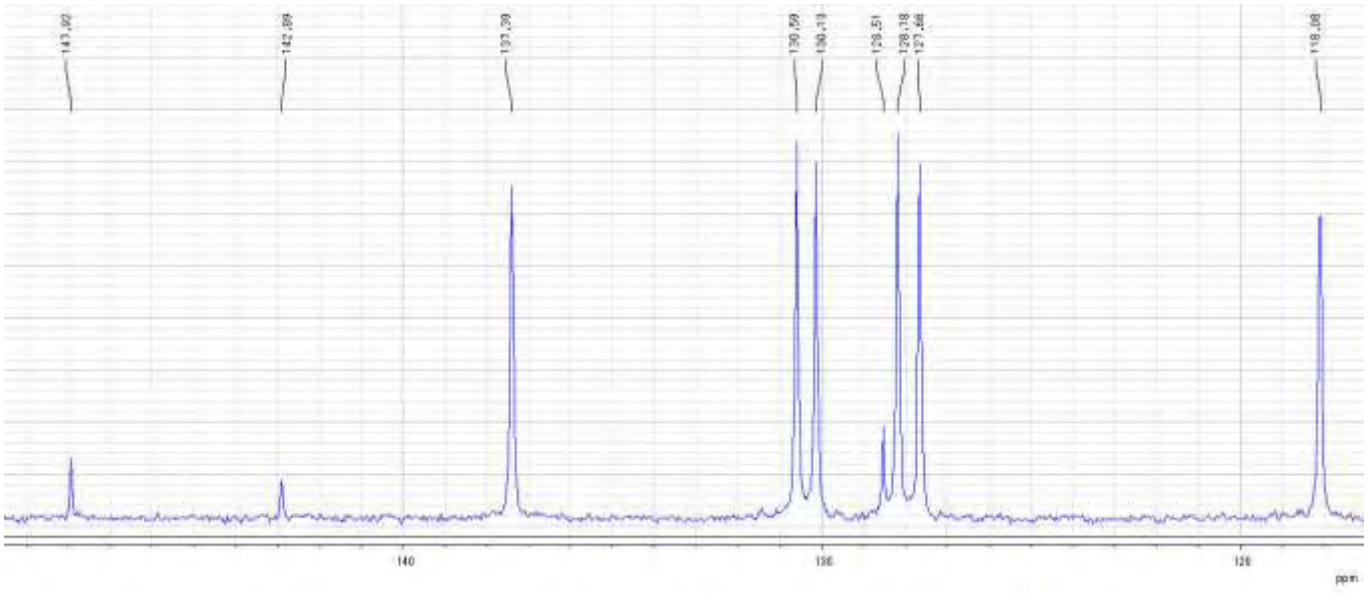
3-Methyl-5-(2-quinolinyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 189-192 °C. ^{1}H-NMR ($CDCl_3$) δ : 3.59 (3H, *s*, CH_3), 7.48-8.03 (4H, *m*, quinolinyl-H), 8.10-8.41 (2H, *m*, quinolinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 32.8, 118.0, 127.7, 128.2, 128.5, 130.1, 130.6, 137.4, 142.7, 147.9, 152.3, 153.5. *Anal*. Calcd for $C_{12}H_9N_3O_2$: C, 63.43; H, 3.99; N, 18.49. Found : C, 63.61; H, 4.13; N, 18.45.



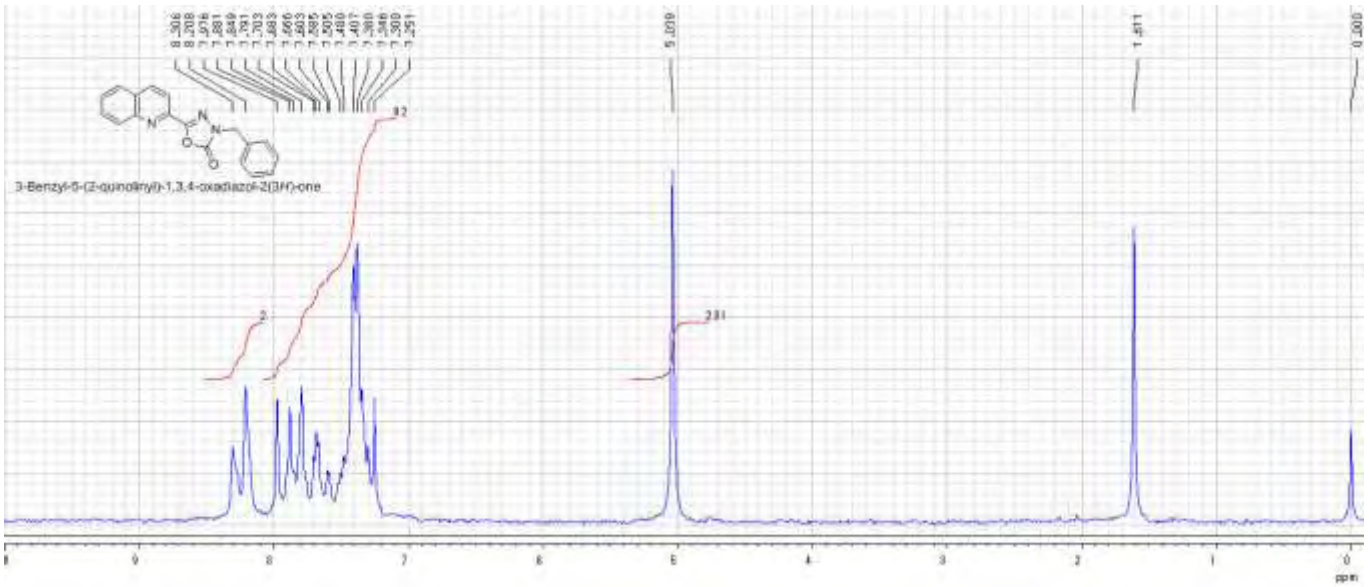
3-Ethyl-5-(2-quinolinyl)-1,3,4-oxadiazol-2(3*H*)-one. White needles (recryst. from hexane-ethyl acetate). Mp 161 °C. MS 241 (M^+). ^{1}H-NMR ($CDCl_3$) δ : 1.47 (3H, *t*, J=7.2 Hz, CH_3), 3.96 (2H, *q*, J=7.2 Hz, CH_2), 7.45-8.10 (4H, *m*, quinolinyl-H), 8.10-8.45 (2H, *m*, quinolinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.3, 41.3, 118.1, 127.7, 128.2, 128.5, 130.1, 130.6, 137.4, 142.9, 147.9, 152.4, 153.1. *Anal*. Calcd for $C_{13}H_{11}N_3O_2$: C, 64.72; H, 4.60; N, 17.42. Found : C, 64.57; H, 4.54; N, 17.35.

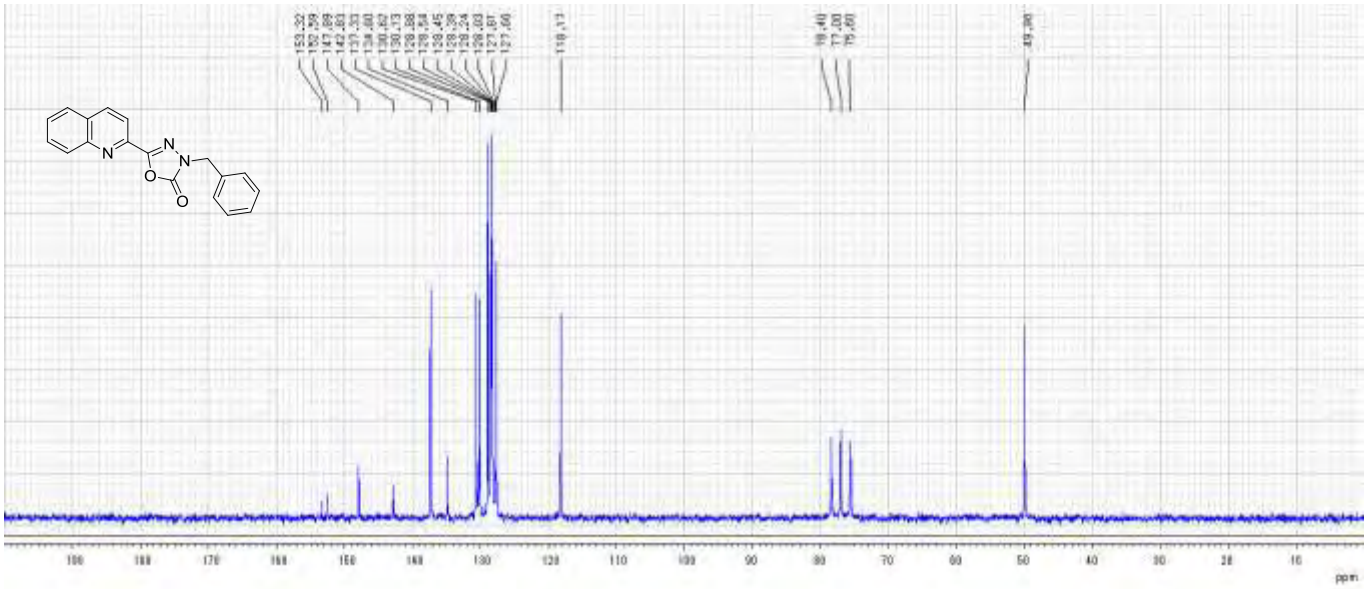


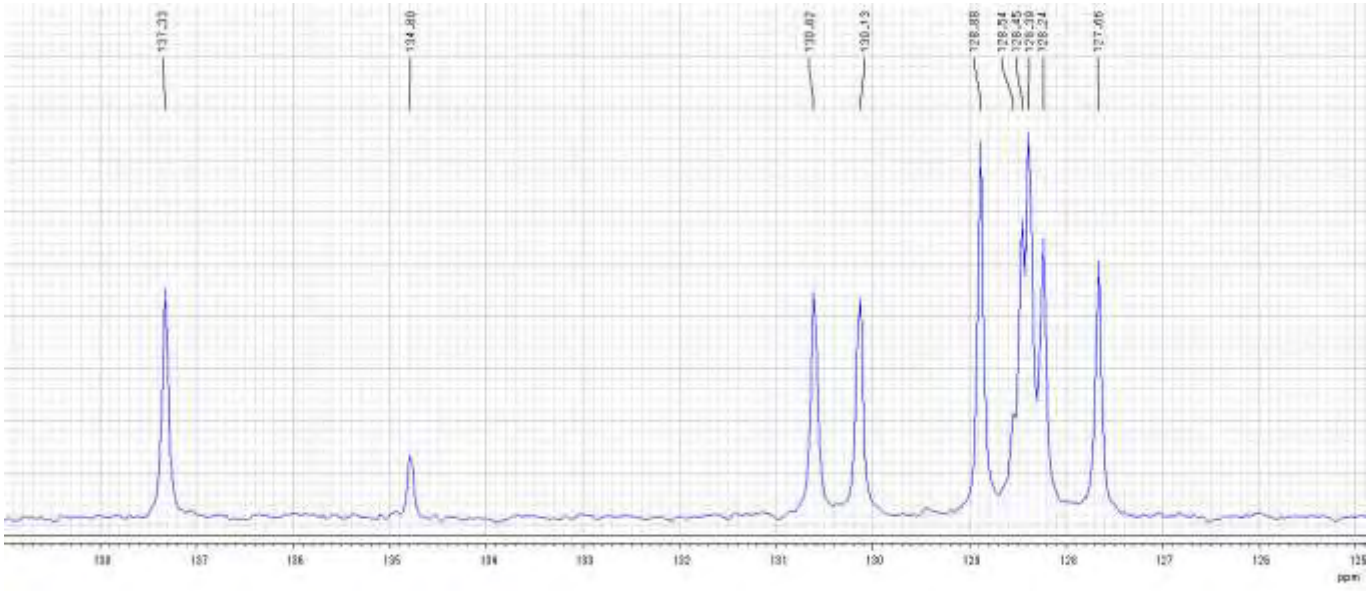




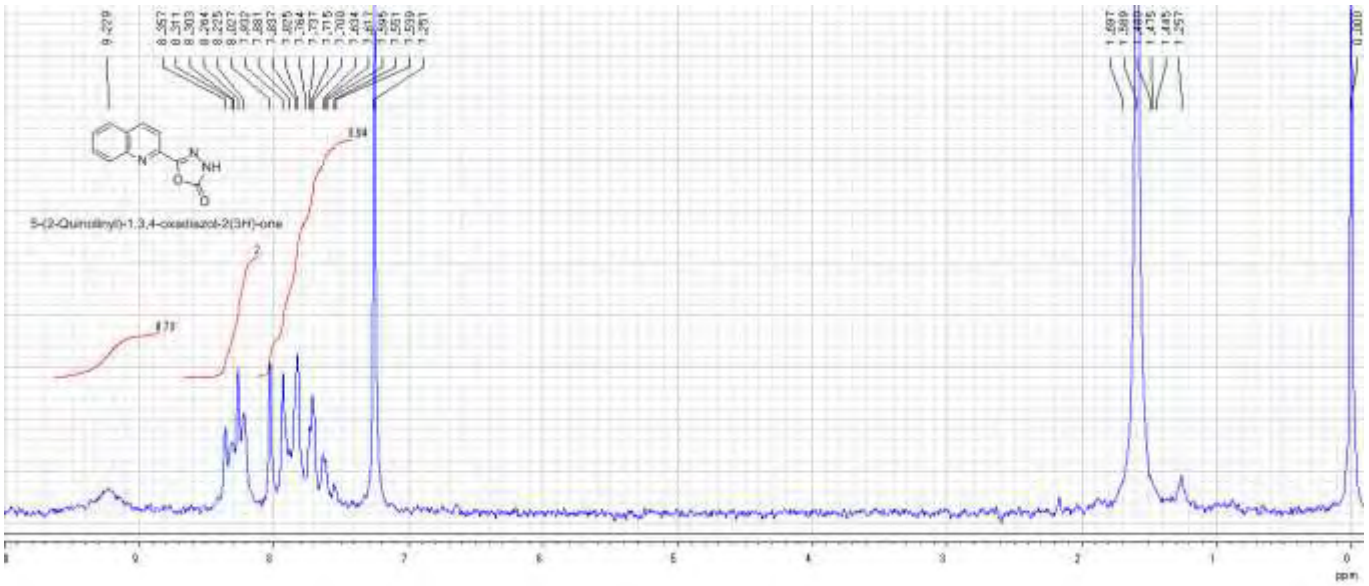
3-Benzyl-5-(2-quinolinyl)-1,3,4-oxadiazol-2(3*H*)-one. White solids (recryst. from hexane-ethyl acetate). Mp 171 °C. ^{1}H-NMR ($CDCl_3$) δ : 5.04 (2H, *s*, CH_2), 7.22-7.56 (5H, *m*, phenyl-H), 7.56-8.03 (4H, *m*, quinolinyl-H), 8.10-8.40 (2H, *m*, quinolinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 50.0, 118.2, 127.7, 128.2, 128.39, 128.45, 128.54, 128.9, 130.1, 130.6, 134.8, 137.3, 142.8, 147.9, 152.6, 153.3. *Anal*. Calcd for $C_{18}H_{13}N_3O_2$: C, 71.28; H, 4.32; N, 13.85. Found : C, 71.16; H, 4.39; N, 13.71.

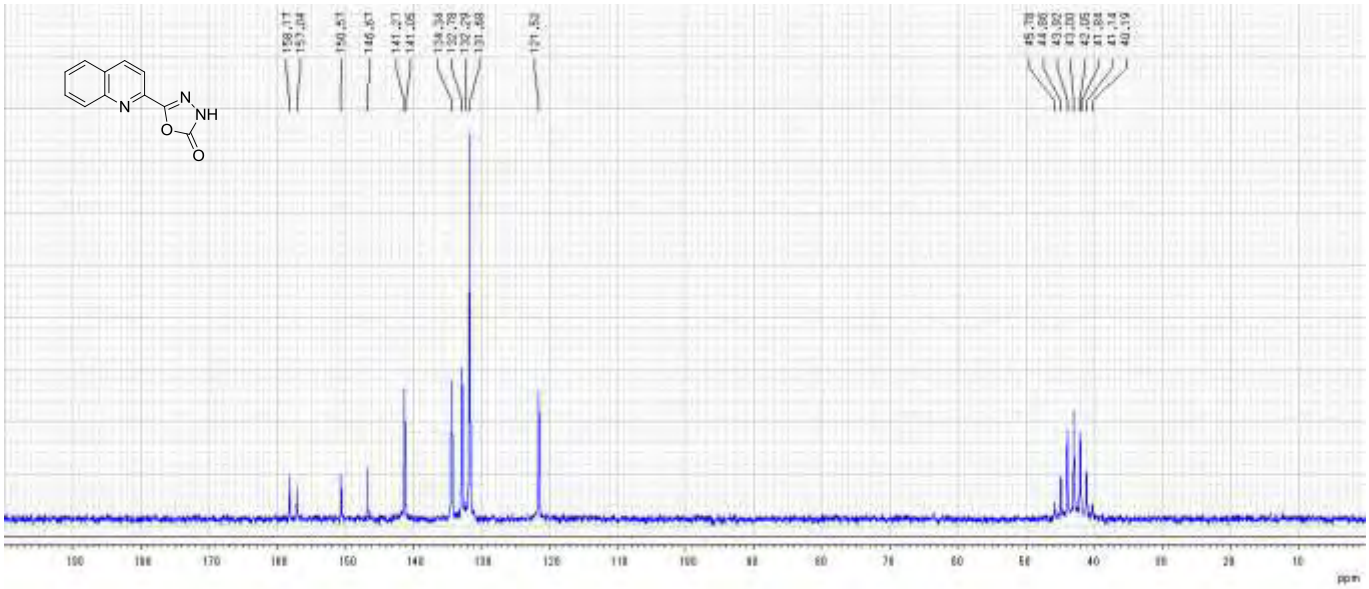


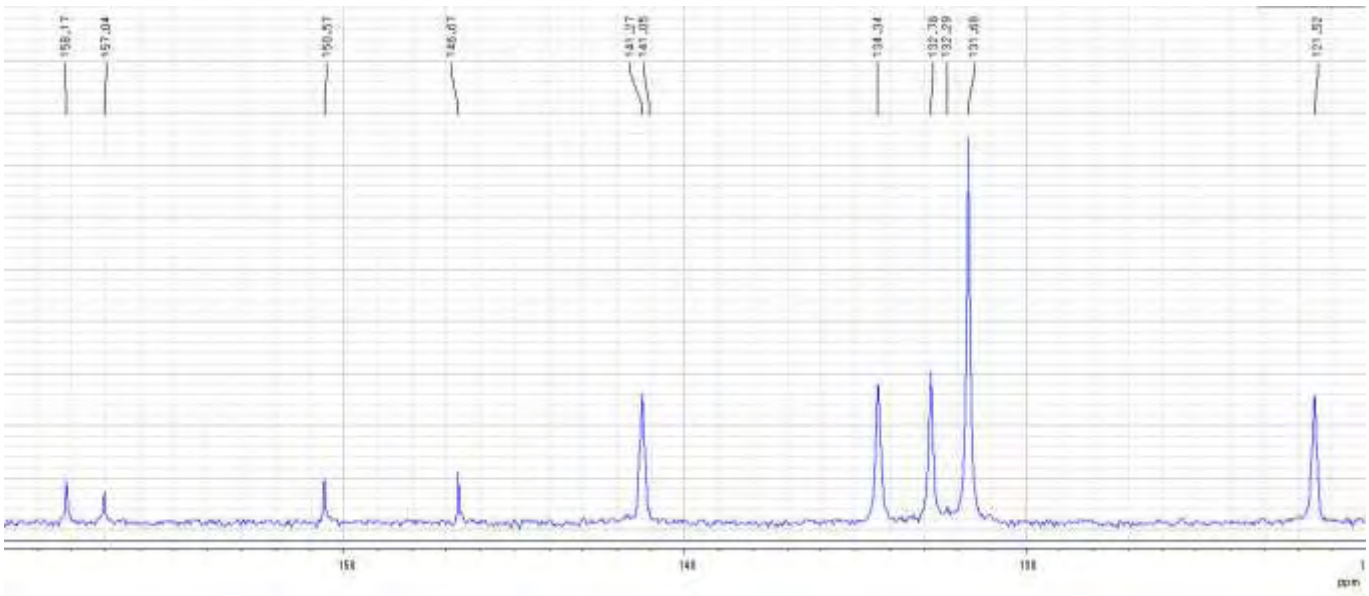




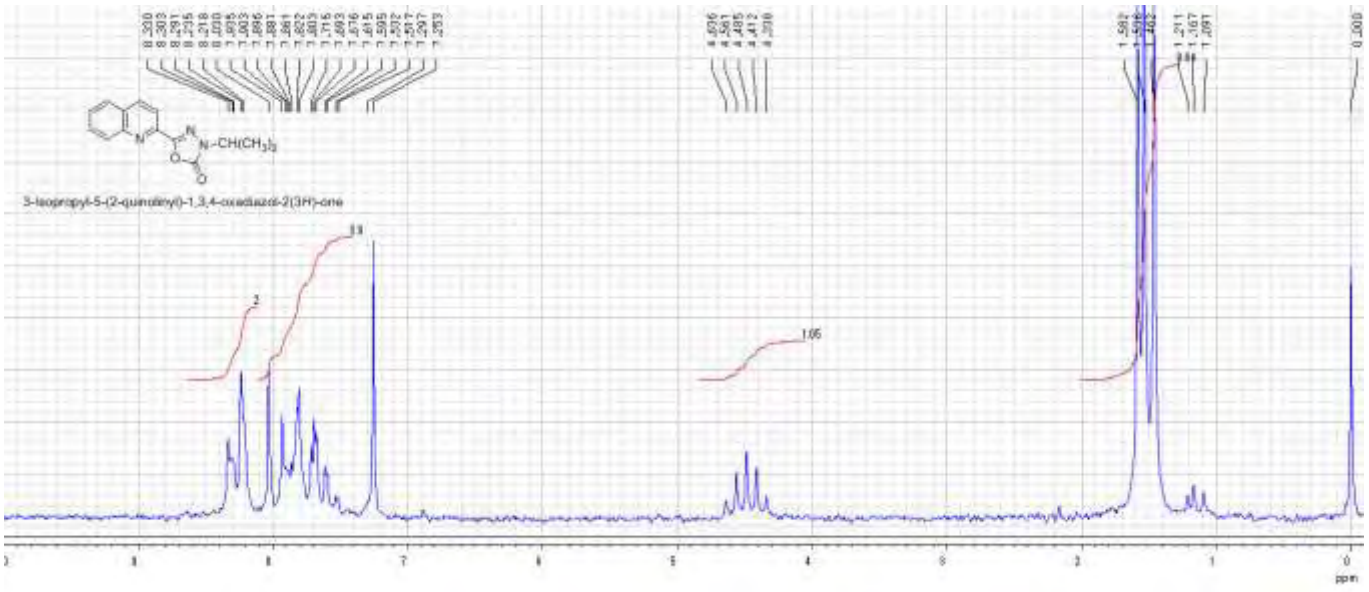
5-(2-Quinolinyl)-1,3,4-oxadiazol-2(3*H*)-one. Pale brown solids (recryst. from hexane-ethyl acetate). Mp 184-186 °C. ^{1}H-NMR ($CDCl_3$) δ : 7.46-8.10 (4H, *m*, quinolinyl-H), 8.10-8.48 (2H, *m*, quinolinyl-H), 9.23 (1H, *brs*, NH). ^{13}C-NMR (DMSO-d_6) δ : 121.5, 131.7, 132.8, 134.3, 141.3, 146.7, 150.6, 157.0, 158.2. *Anal*. Calcd for $C_{11}H_7N_3O_2$: C, 61.97; H, 3.31; N, 19.71. Found : C, 61.86; H, 3.50; N, 19.61.

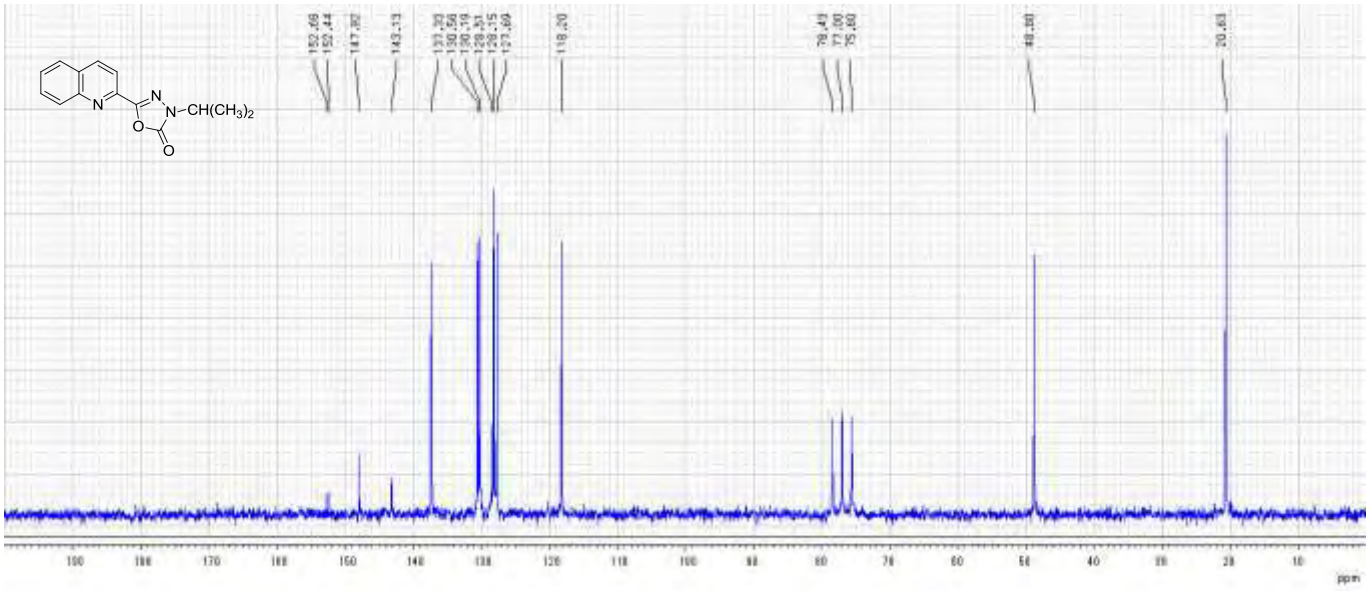


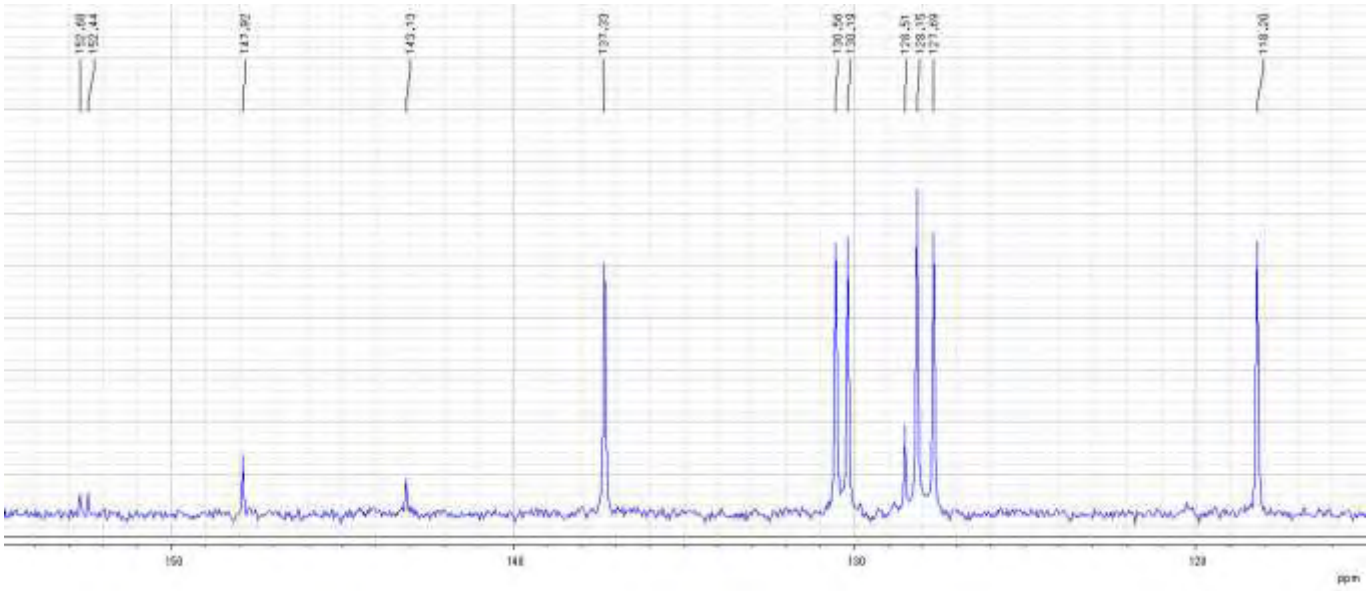




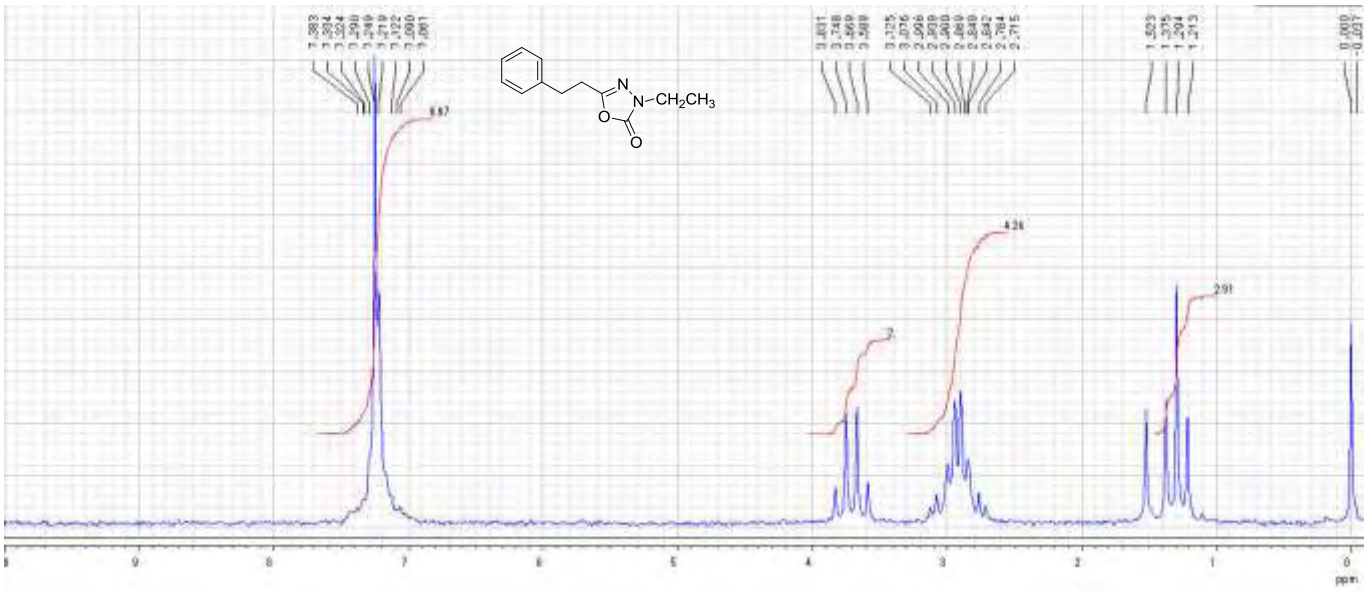
3-Isopropyl-5-(2-quinolinyl)-1,3,4-oxadiazol-2(3*H*)-one. Slight pink solids (recryst. from hexane-ethyl acetate). Mp 122-123 °C. ^{1}H-NMR ($CDCl_3$) δ : 1.50 (6H, *d*, J=6.7 Hz, CH_3×2), 4.49 (1H, *septet*, J=6.7 Hz, CH), 7.40-8.10 (4H, *m*, quinolinyl-H), 8.10-8.40 (2H, *m*, quinolinyl-H). ^{13}C-NMR ($CDCl_3$) δ : 20.6, 48.8, 118.2, 127.7, 128.2, 128.5, 130.2, 130.6, 137.3, 143.1, 147.9, 152.4, 152.7. *Anal*. Calcd for $C_{14}H_{13}N_3O_2$: C, 65.87; H, 5.13; N, 16.46. Found : C, 65.84; H, 5.14; N, 16.30.

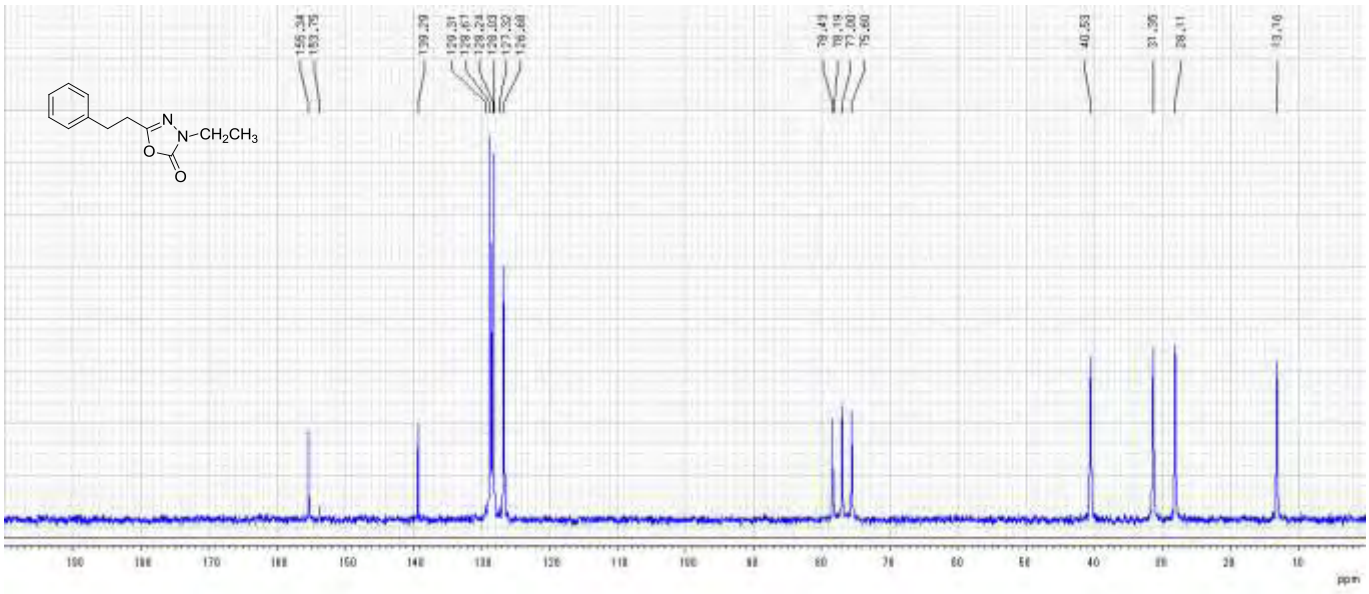


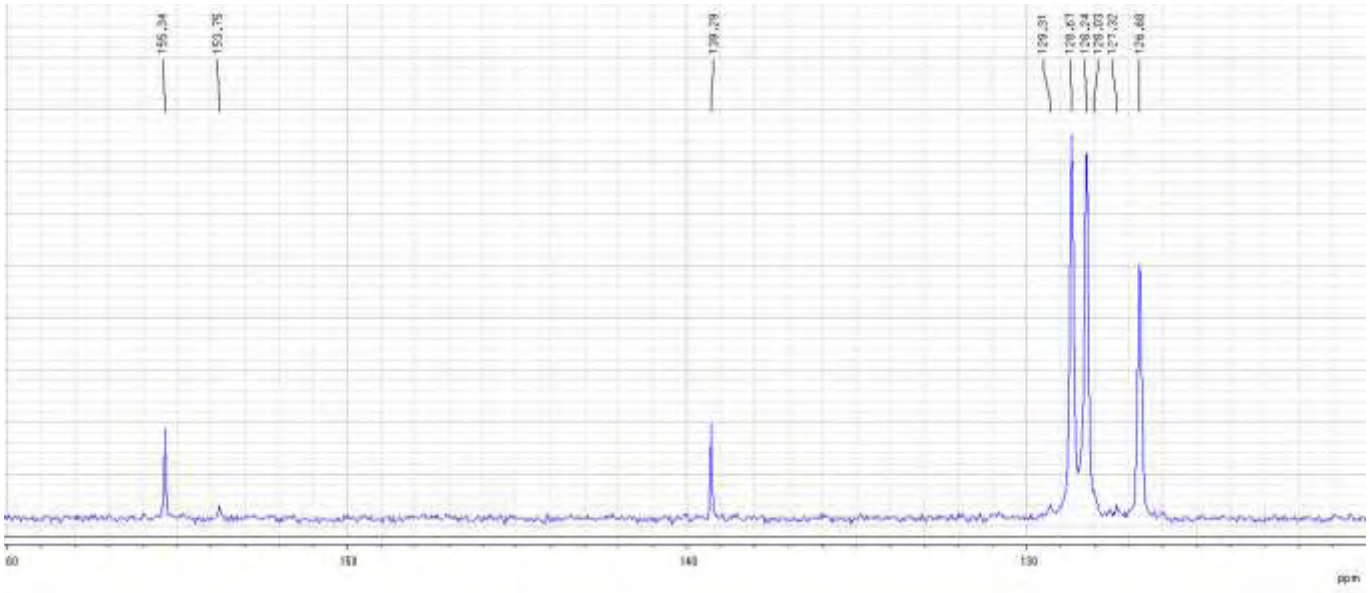




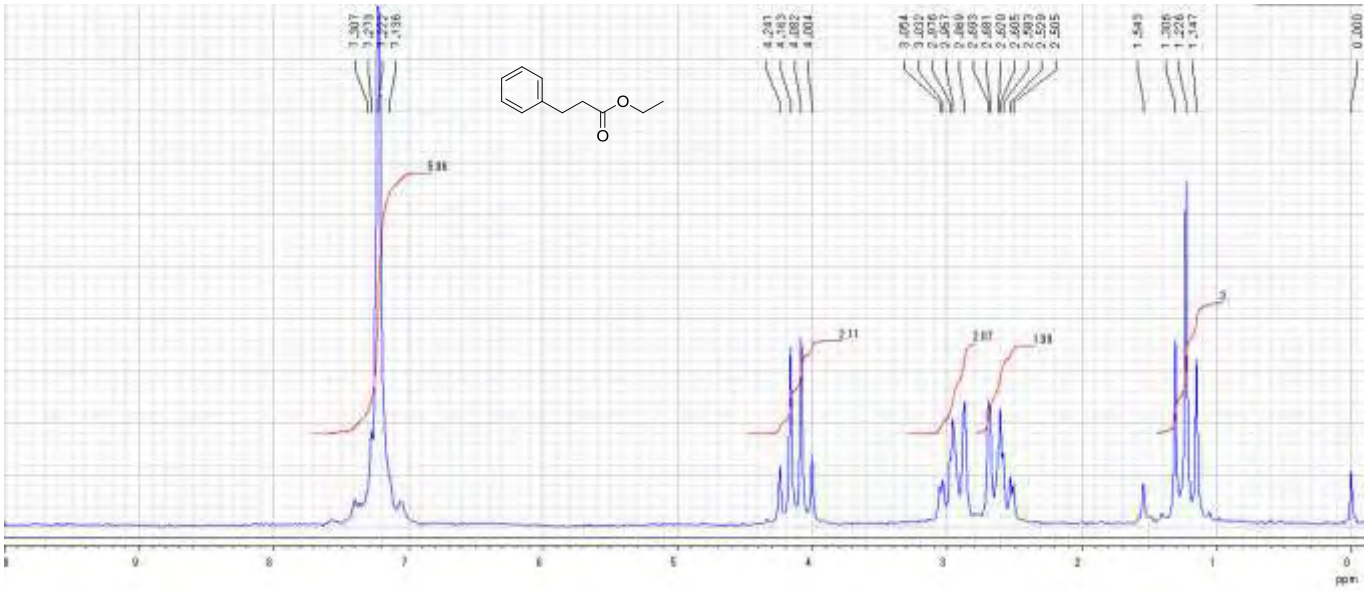
3-Ethyl-5-phenethyl-1,3,4-oxadiazol-2(3*H*)-one. Colorless liquids. Bp 180 °C / 17 mmHg. ^{1}H-NMR ($CDCl_3$) δ : 1.29 (3H, *t*, J=7.3 Hz, CH_3), 2.65-3.20 (4H, *m*, CH_2CH_2), 3.72 (2H, *q*, J=7.3 Hz, CH_2N), 7.25 (5H, *s*, phenyl-H). ^{13}C-NMR ($CDCl_3$) δ : 13.2, 28.1, 31.4, 40.5, 126.7, 128.2, 128.7, 139.3, 153.8, 155.3. *Anal*. Calcd for $C_{12}H_{14}N_2O_2$: C, 66.04; H, 6.47; N, 12.84. Found : C, 66.07; H, 6.51; N, 13.01.







Ethyl 3-phenylpropionate.[14] Pale yellow liquids. ^{1}H-NMR ($CDCl_3$) δ : 1.23 (3H, *t*, J=7.2 Hz, CH_3), 2.45-2.78 (2H, *m*, CH_2), 2.78-3.15 (2H, *m*, CH_2), 4.12 (2H, *q*, J=7.2 Hz, CH_2O), 7.22 (5H, *s*, phenyl-H).



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