J. Braz. Chem. Soc., Vol. 23, No. 7, S1-S17, 2012.
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0103 - 5053 $6.00+0.00

Supplementary Information

The Effect of Neutral Oximes on the Reactivation of Human Acetylcholinesterase Inhibited with Paraoxon

Tatiana S. Ribeiro,[a] Arthur Prates,[b] Sérgio R. Alves,[b] Jefferson J. Oliveira-Silva,[b] Carlos A. S. Riehl[c] and J. Daniel Figueroa-Villar[*,a]*

[a]*Departamento de Química, Instituto Militar de Engenharia, Praça General Tibúrcio, 80, Praia Vermelha, 22290-270 Rio de Janeiro-RJ, Brazil*

[b]*Centro de Estudos da Saúde do Trabalhador e Ecologia Humana (CESTEH), ENSP, Fiocruz, Rua Leopoldo Bulhões, 1480, Manguinhos, 21041-210 Rio de Janeiro-RJ, Brazil*

[c]*Instituto de Química, Universidade Federal do Rio de Janeiro, Ilha do Fundão, Rio de Janeiro-RJ, Brazil*

NMR and IR Data of the Oximes Previously Reported in the Literature

2-Methylbenzaldehyde oxime (**16**)

mp 51-53 ºC (52-54 ºC); ^{1}H NMR (ppm, DMSO-d_6) δ 11.26 (s, 1H), 8.32 (s, 1H), 7.62 (m, 1H), 7.22 (m, 3H), 2.36 (s, 3H); ^{13}C NMR (ppm, DMSO-d_6) δ 147.0, 135.9, 131.1, 130.7, 128.9, 126.1, 126.0, 19.5; IR (KBr) ν_{max}/cm^{-1} 3189, 3069, 2991, 2870, 1624, 1599, 1453, 750.

4-N,N-dimethylaminobenzaldehyde oxime (**20**)

mp 151-153 ºC; ^{1}H NMR (ppm, $CDCl_3$) δ 7.98 (s, 1H), 7.42 (d, 2H, ^3J 8.8 Hz), 6.70 (d, 2H, ^3J 8.8 Hz), 2.94 (s, 6H); ^{13}C NMR (ppm, $CDCl_3$) δ 151.7, 149.0, 128.2, 121.5, 112.4, 40.0; IR (KBr) ν_{max}/cm^{-1} 3243, 3138, 2985, 2913, 1609, 1556, 1445, 1361.

4-Methoxybenzaldehyde oxime (**21**)

mp 131-133 °C; ^{1}H NMR (ppm, DMSO-d_6) δ 8.13 (s, 1H), 7.75 (d, 2H, ^3J 8.6 Hz), 6.91 (d, 2H, ^3J 8.6 Hz), 3.85 (s, 3H); ^{13}C NMR (ppm, DMSO-d_6) δ 160.1, 147.6, 127.8, 125.6; 114.2, 55.2; IR (KBr) ν_{max}/cm^{-1} 3307, 3006, 2966, 2838, 1608, 1574,1466, 1252.

Pyridine-2-carboxylaldehyde oxime(**22**)

mp 110-112 °C; ^{1}H NMR (ppm, $CDCl_3$) δ 8.64 (m, 1H), 8.34 (s, 1H), 7.80 (m, 1H), 7.73 (m, 1H), 7.30 (m, 1H); ^{13}C NMR (ppm, $CDCl_3$) δ 151.8, 150.2, 149.3, 136.8, 124.0, 121.0; IR (KBr) ν_{max}/cm^{-1} 3285, 3187-3005, 1653, 1593-1472, 1322, 737.

Furane-2-carboxyaldehyde oxime (**23**)

mp 71-73 °C; ^{1}H NMR (ppm, $CDCl_3$) δ 7.54 (s, 1H), 7.47 (dd, 1H, ^3J 1.7, ^4J 0.6 Hz), 7.35 (dd, 1H, ^3J 3.5, ^4J 0 Hz), 6.53 (dd, 1H, ^3J 3.5, ^3J 1.7 Hz); ^{13}C NMR (ppm, $CDCl_3$) δ 145.1, 143.4, 137.0, 118.2, 112.3; IR (KBr) ν_{max}/cm^{-1} 3165, 3080-3042, 1645, 1567-1477, 1449, 750.

Thiophene-2-carboxylaldehyde oxime (**24**)

mp 135-137 °C; ^{1}H NMR (ppm, DMSO-d_6) δ 11.86 (s, 1H), 7.84 (s, 1H), 7.73 (d, 1H, ^3J 3.9 Hz), 7.47 (d, 1H, ^3J 3.9 Hz), 7.12 (t, 1H); ^{13}C NMR (ppm, DMSO-d_6) δ 139.8, 131.1, 131.0, 131.0, 126.2; IR (KBr) ν_{max}/cm^{-1} 3121, 3017, 1632, 1507-1435.

Pyrrol-2-carboxyaldehyde oxime (**25**)

mp 183-185 °C; ^{1}H-NMR (ppm, DMSO-d_6) δ 11.14 (s, 1H), 7.26 (s, 1H), 6.88 (d, 1H, ^3J 3.2 Hz), 6.55 (d, 1H, ^3J 3.2 Hz), 6.10 (t, 1H), 3.37 (s, 1H); ^{13}C NMR (ppm, DMSO-d_6) δ 137.1, 129.4, 120.8, 113.8, 108.3; IR (KBr) ν_{max}/cm^{-1} 3426, 3419, 3033, 1646, 1586, 1461, 1429, 1304, 834, 745.

1-Methylimidazole-2-carboxyaldehyde oxime (**26**)

mp 169-171°C; ^{1}H NMR (ppm, DMSO-d_6) δ 11.59 (s, 1H), 8.06 (s, 1H), 7.24 (d, 1H, ^3J 3.0 Hz), 6.98 (d, 1H, ^3J 3.0 Hz), 3.80 (s, 3H); ^{13}C NMR (ppm, DMSO-d_6) δ 141.4, 140.2, 128.5, 124.6, 34.8; IR (KBr) ν_{max}/cm^{-1} 3413, 3118-3078, 2994-2917, 1628, 1556-1523-1477, 1357.

*e-mail: figueroa@ime.eb.br

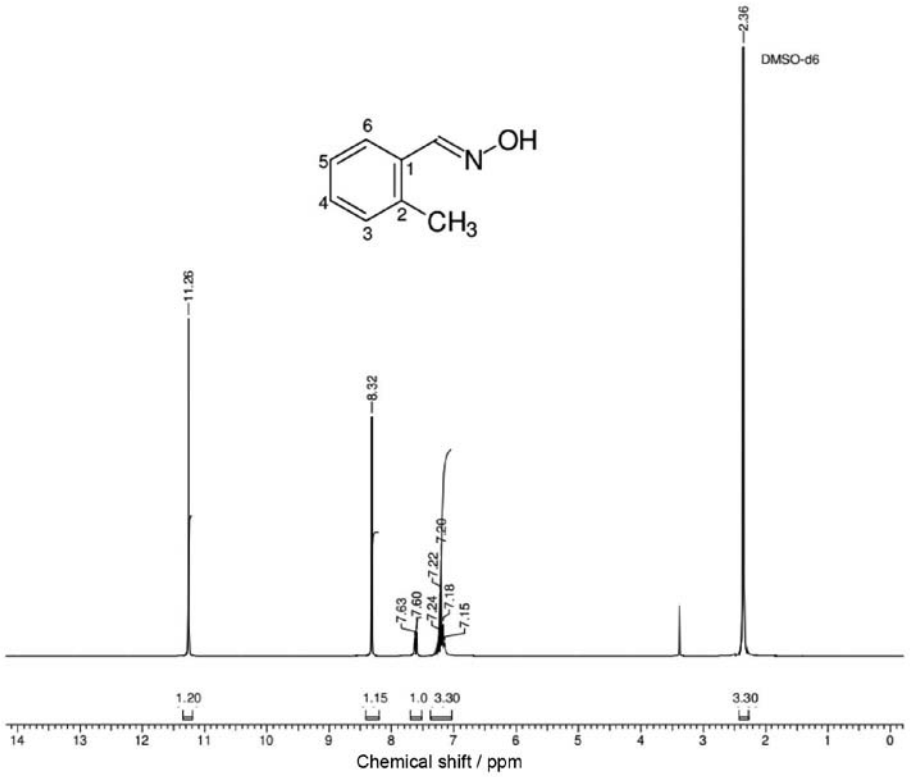

Figure S1. [1]H NMR (300 MHz, DMSO-d_6) of 2-methylbenzaldehyde oxime (**16**).

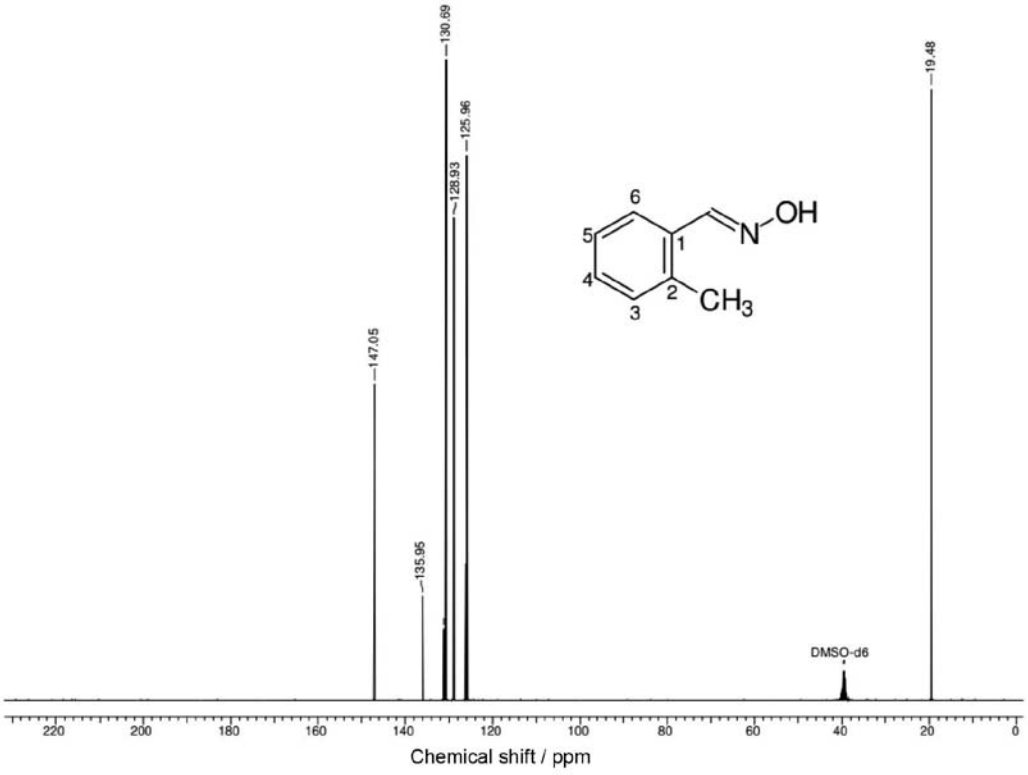

Figure S2. [13]C NMR (75 MHz, DMSO-d_6) of 2-methylbenzaldehyde oxime (**16**).

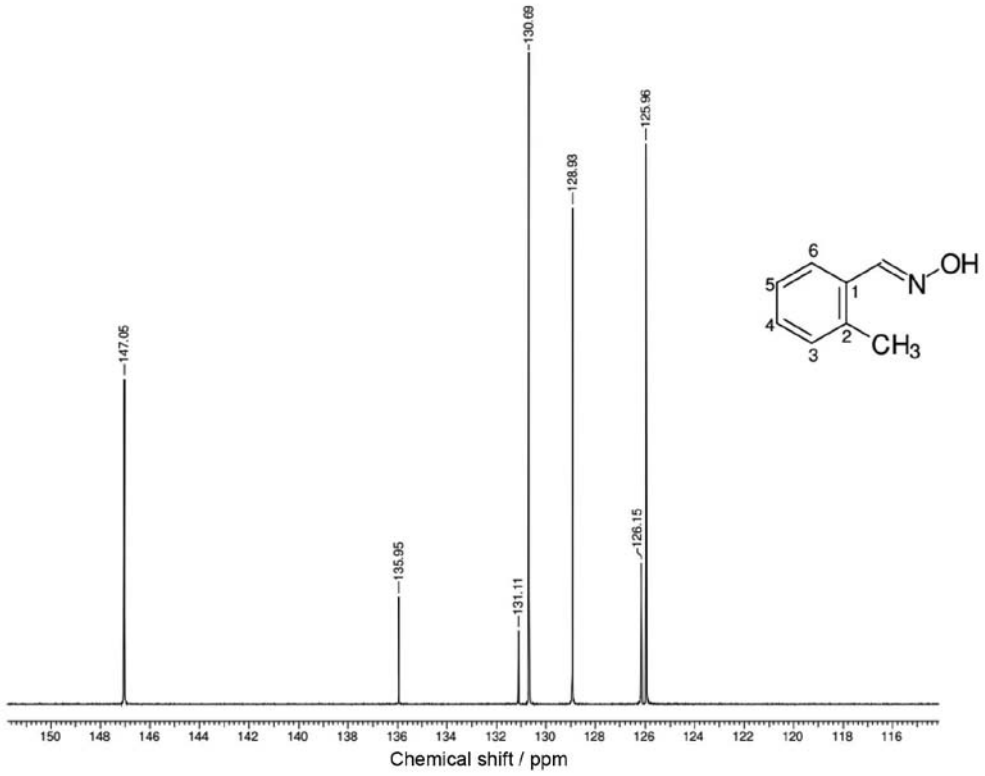

Figure S3. Expansion of ^{13}C NMR (75 MHz, DMSO-d_6) of 2-methylbenzaldehyde oxime (**16**).

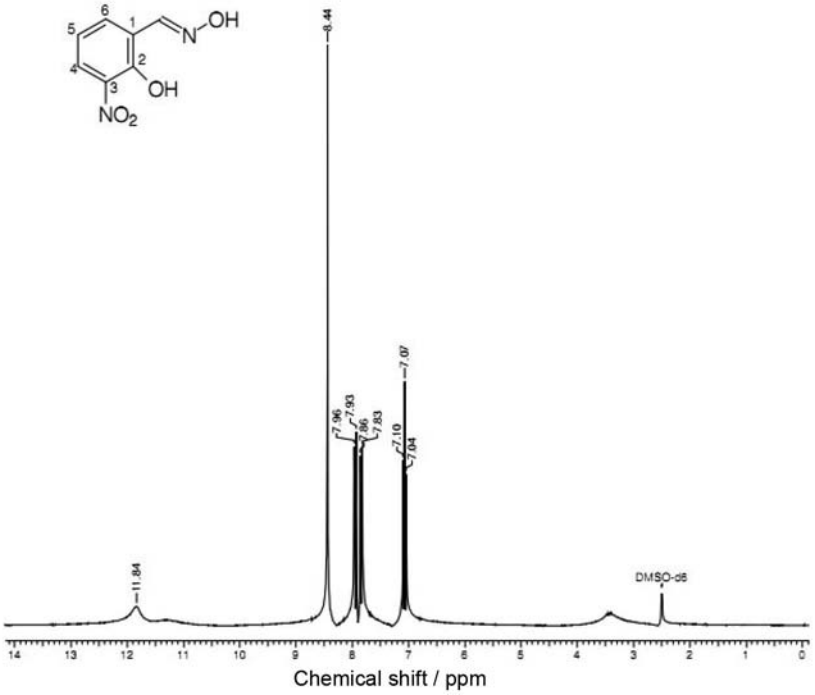

Figure S4. ^{1}H NMR (300 MHz, DMSO-d_6) of 3-nitrosalicylaldehyde oxime (**17**).

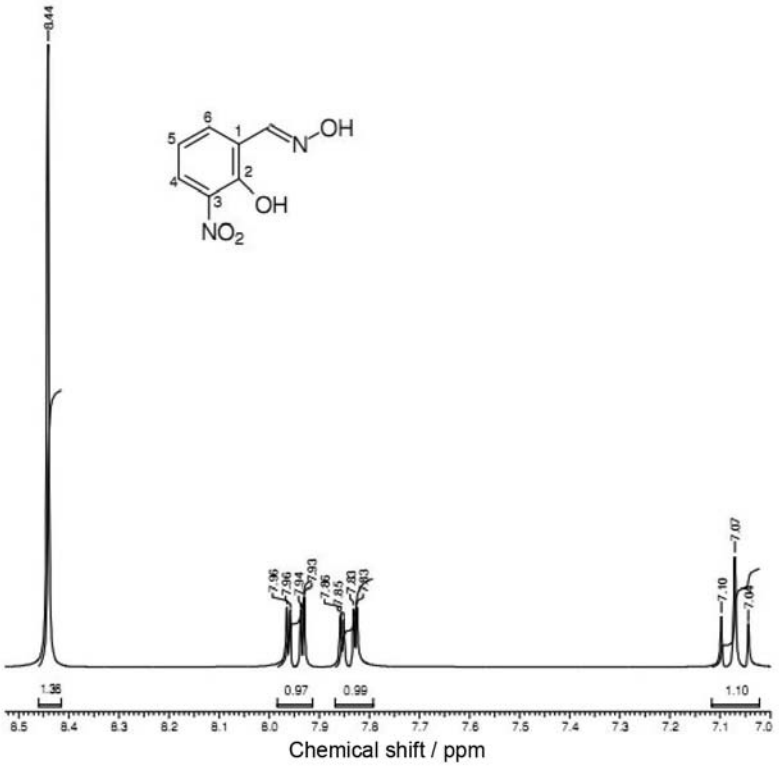

Figure S5. Expansion of ^{1}H NMR (300 MHz, DMSO-d_6) of 3-nitrosalicylaldehyde oxime (**17**).

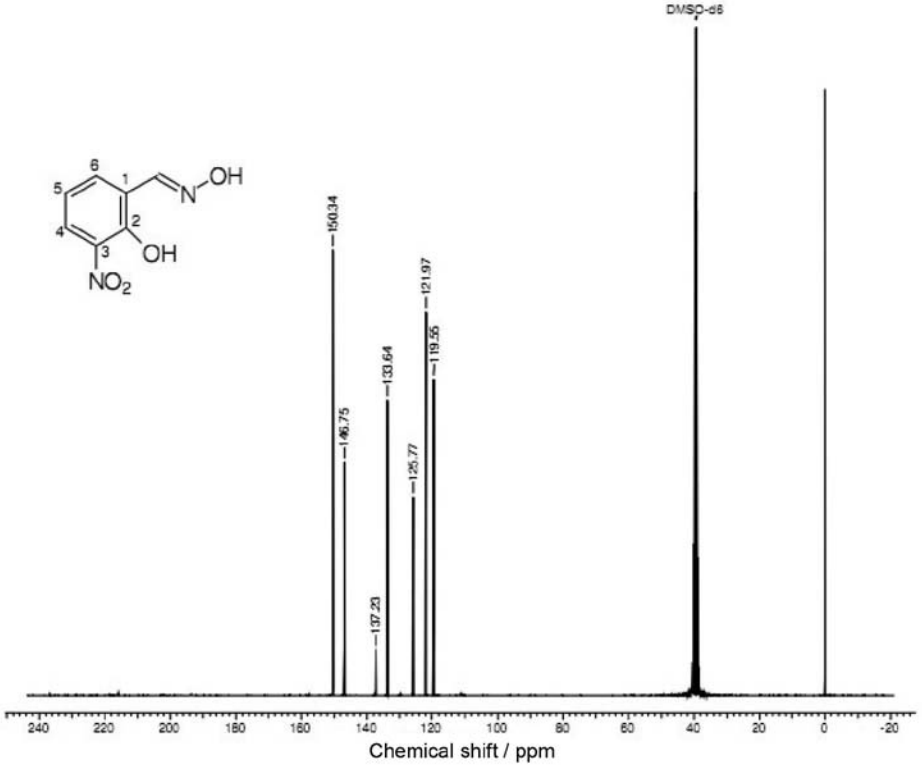

Figure S6. ^{13}C NMR (75 MHz, DMSO-d_6) of 3-nitrosalicylaldehyde oxime (**17**).

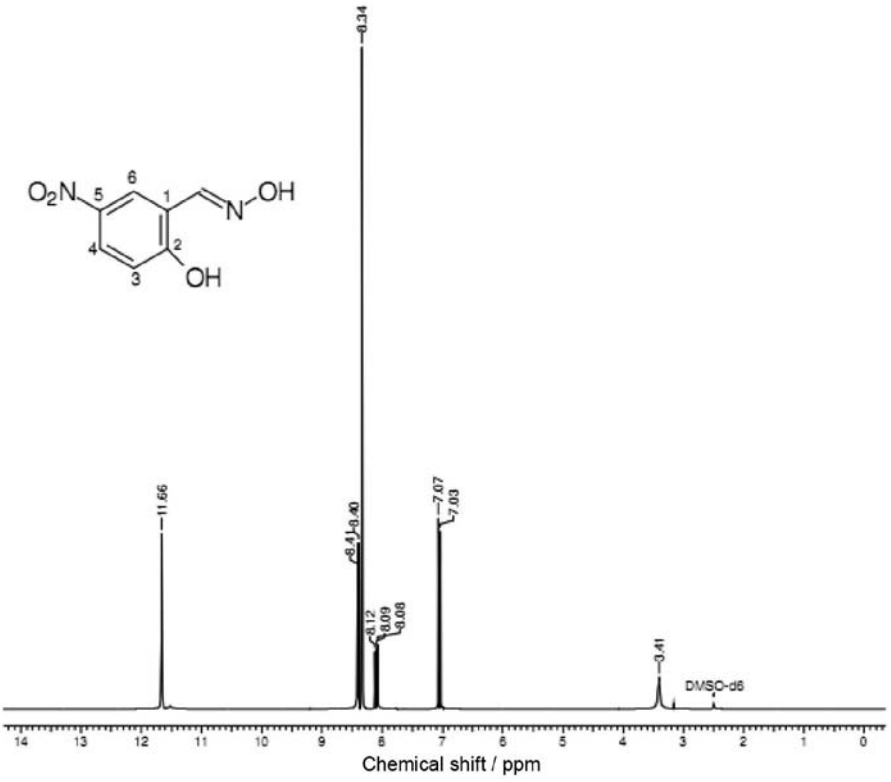

Figure S7. [1]H NMR (300 MHz, DMSO-d_6) of 5-nitrosalicylaldehyde oxime (**18**).

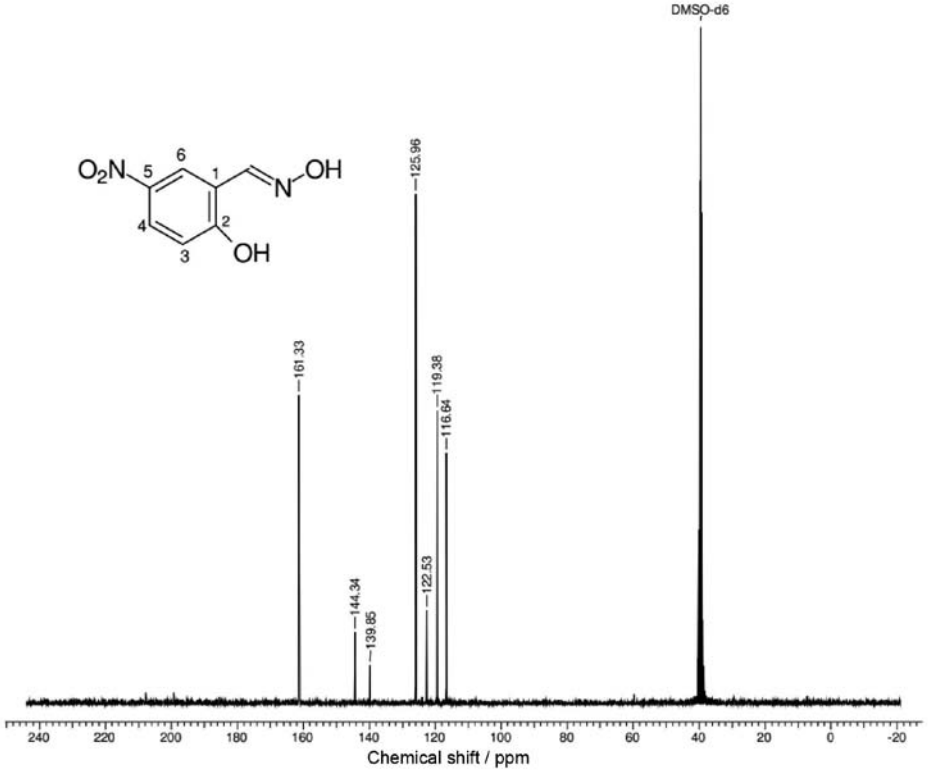

Figure S8. [13]C NMR (75 MHz, DMSO-d_6) of 5-nitrosalicylaldehyde oxime (**18**).

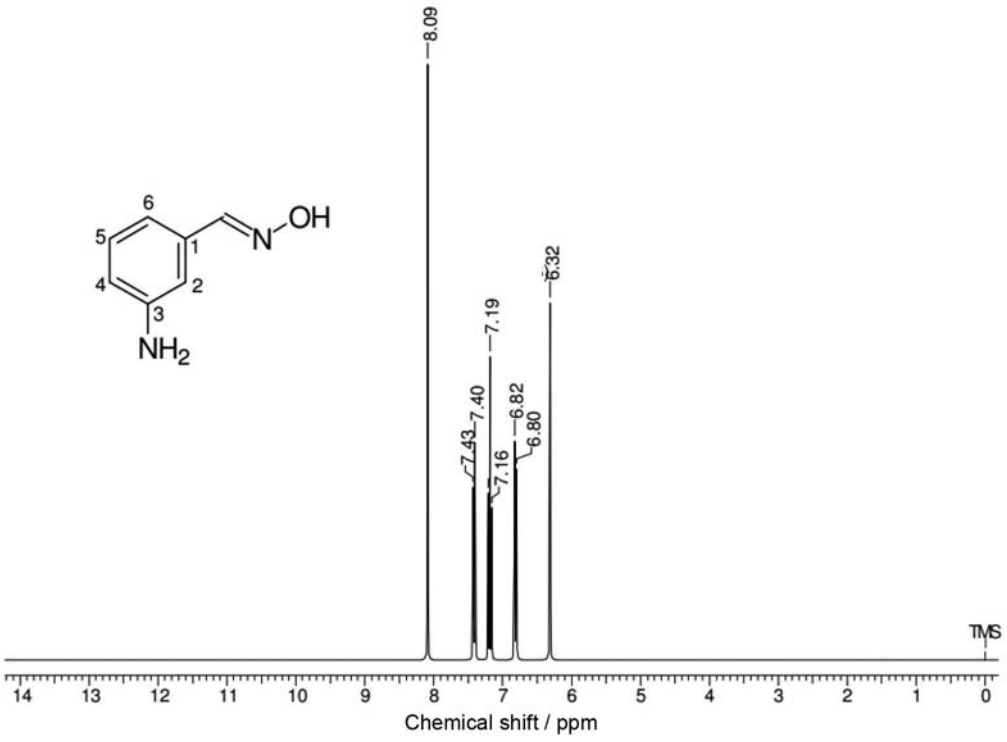

Figure S9. ^{1}H NMR (300 MHz, $CDCl_3$) of 3-aminobenzaldehyde oxime (**19**).

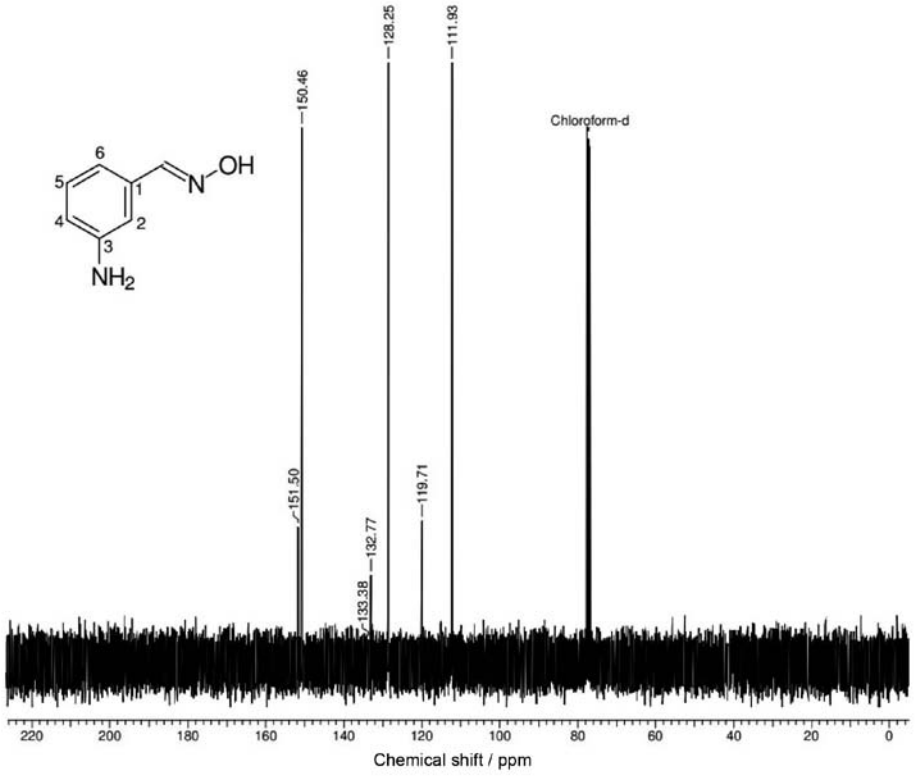

Figure S10. ^{13}C NMR (75 MHz, $CDCl_3$) of 3-aminobenzaldehyde oxime (**19**).

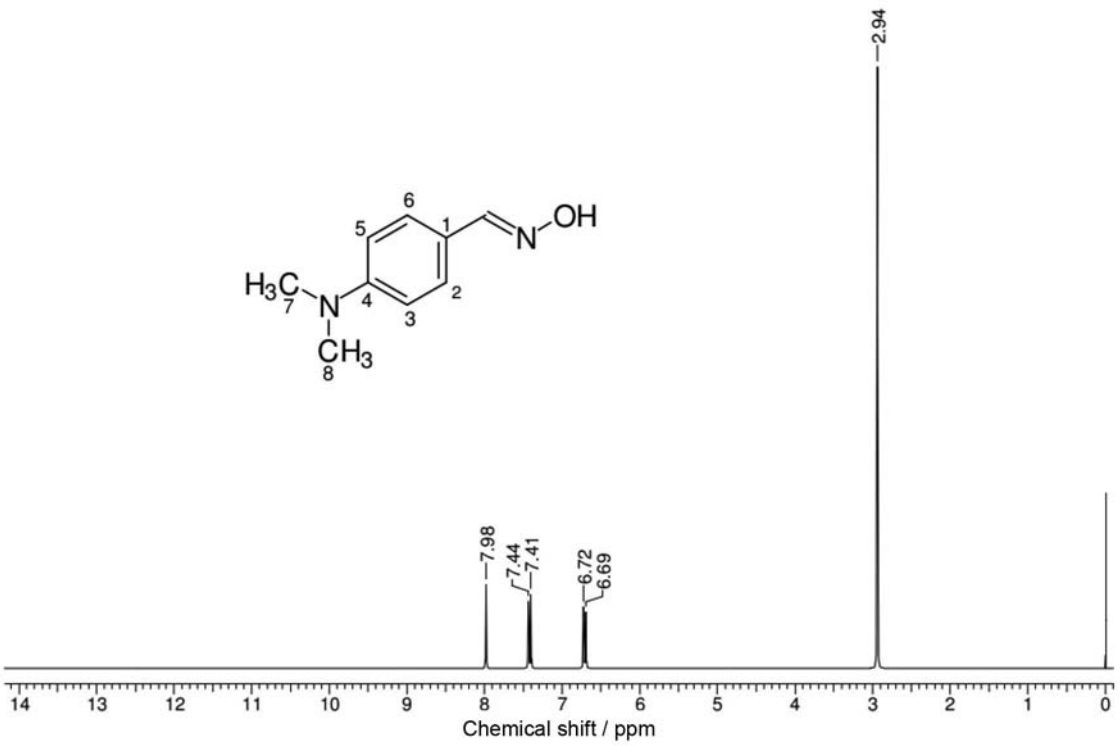

Figure S11. ^{1}H NMR (300 MHz, $CDCl_3$) of 4-*N,N*-dimethylaminobenzaldehyde oxime (**20**).

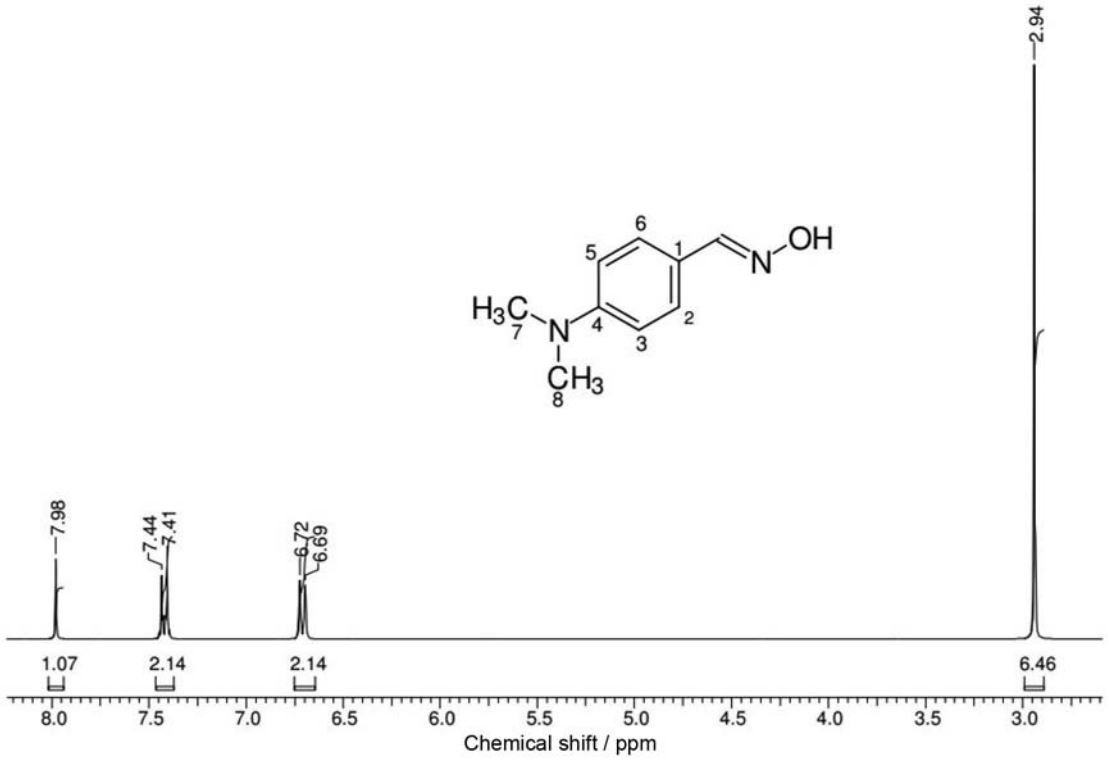

Figure S12. Expansion of ^{1}H NMR (300 MHz, $CDCl_3$) of 4-*N,N*-dimethylaminobenzaldehyde oxime (**20**).

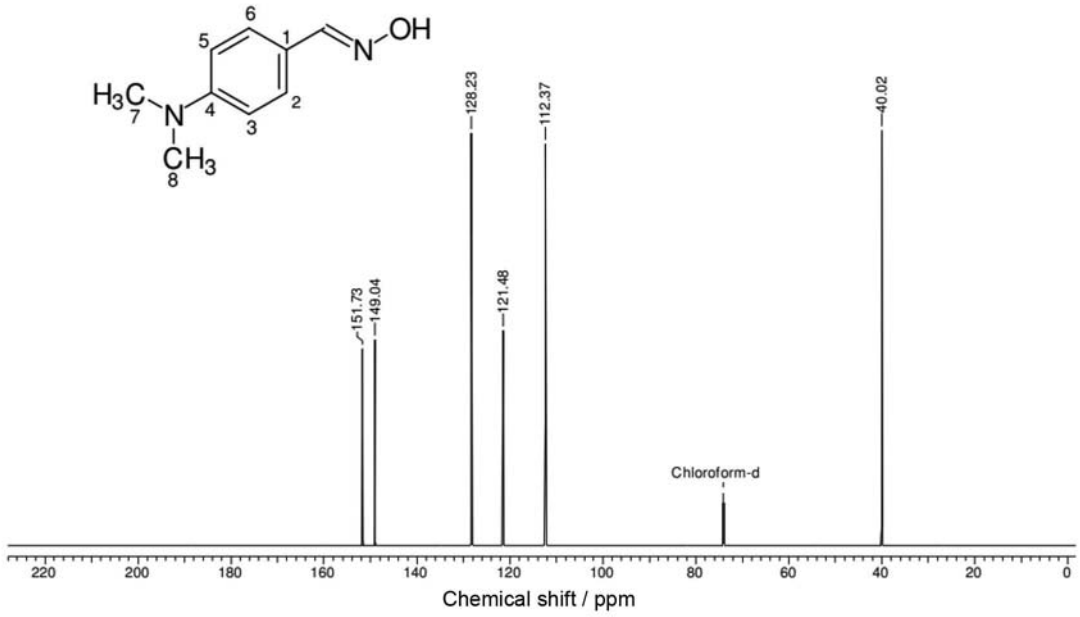

Figure S13. ^{13}C NMR (75 MHz, $CDCl_3$) of 4-*N,N*-dimethylaminobenzaldehyde oxime (**20**).

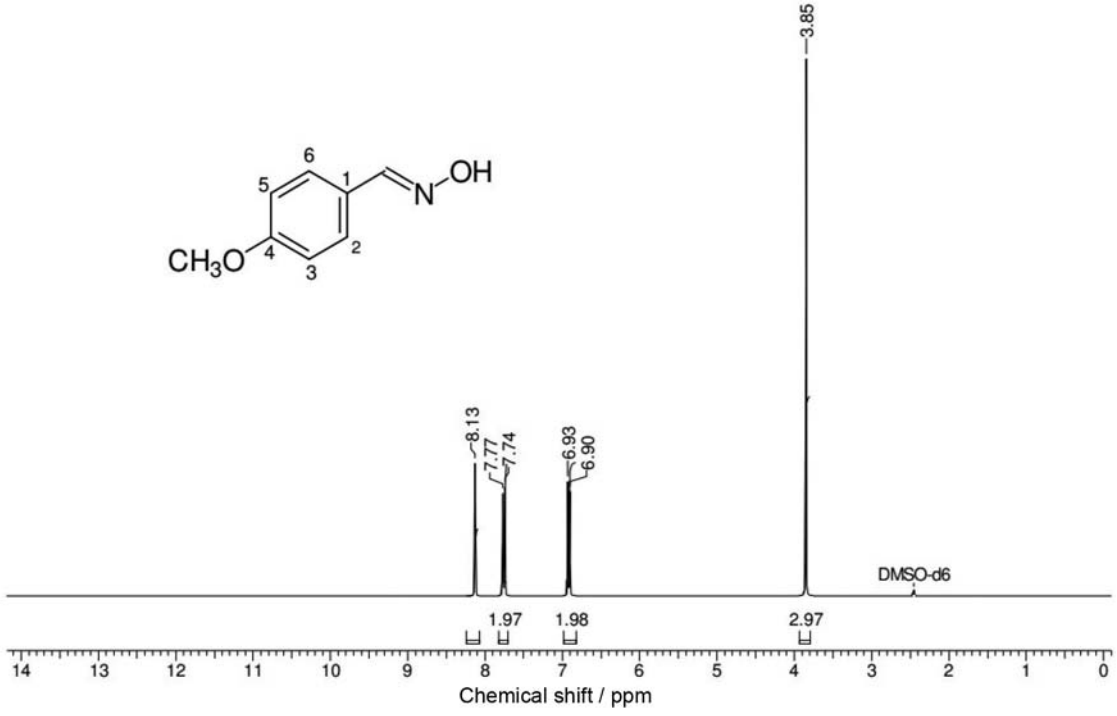

Figure S14. ^{1}H NMR (300 MHz, DMSO-d_6) of 4-methoxybenzaldehyde oxime (**21**).

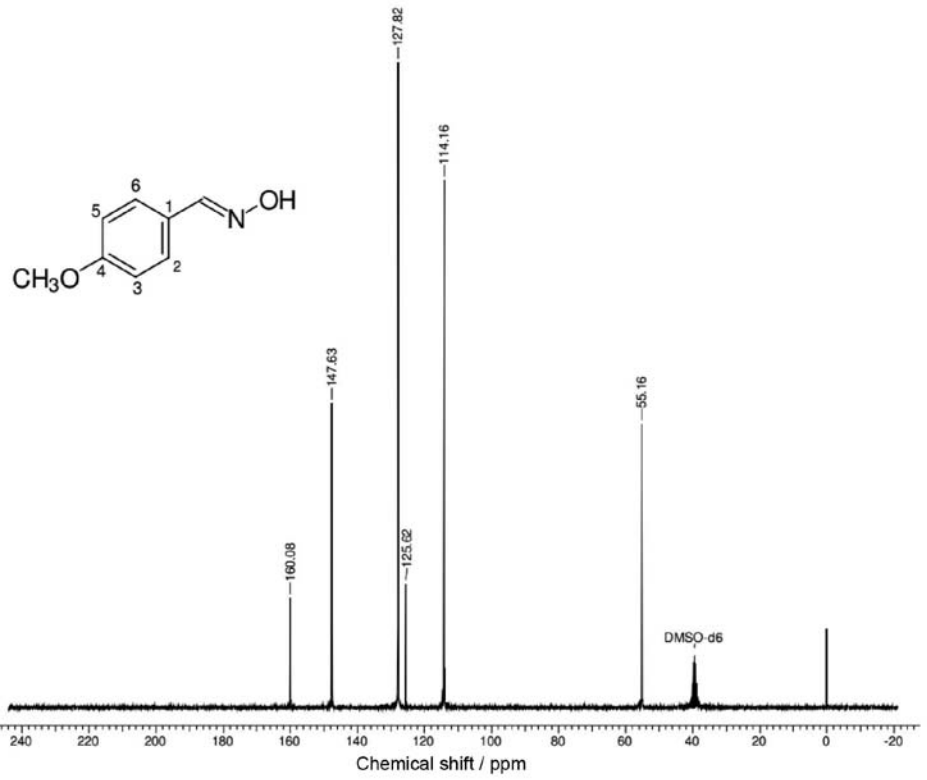

Figure S15. ^{13}C NMR (75 MHz, DMSO-d_6) of 4-methoxybenzaldehyde oxime (**21**).

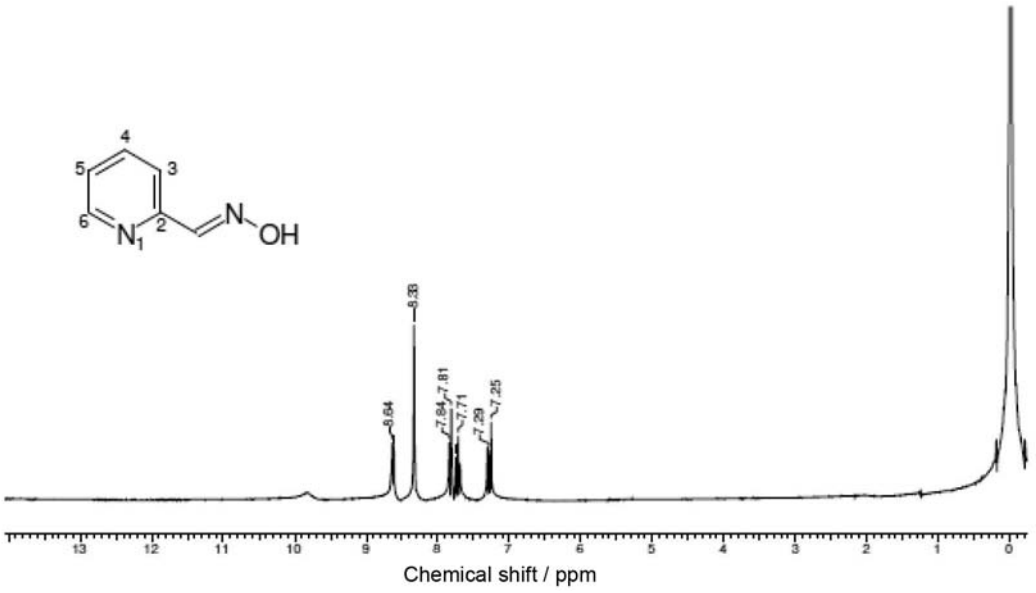

Figure S16. ^{1}H NMR (300 MHz, $CDCl_3$) of pyridine-2-carboxyladehyde oxime (**22**).

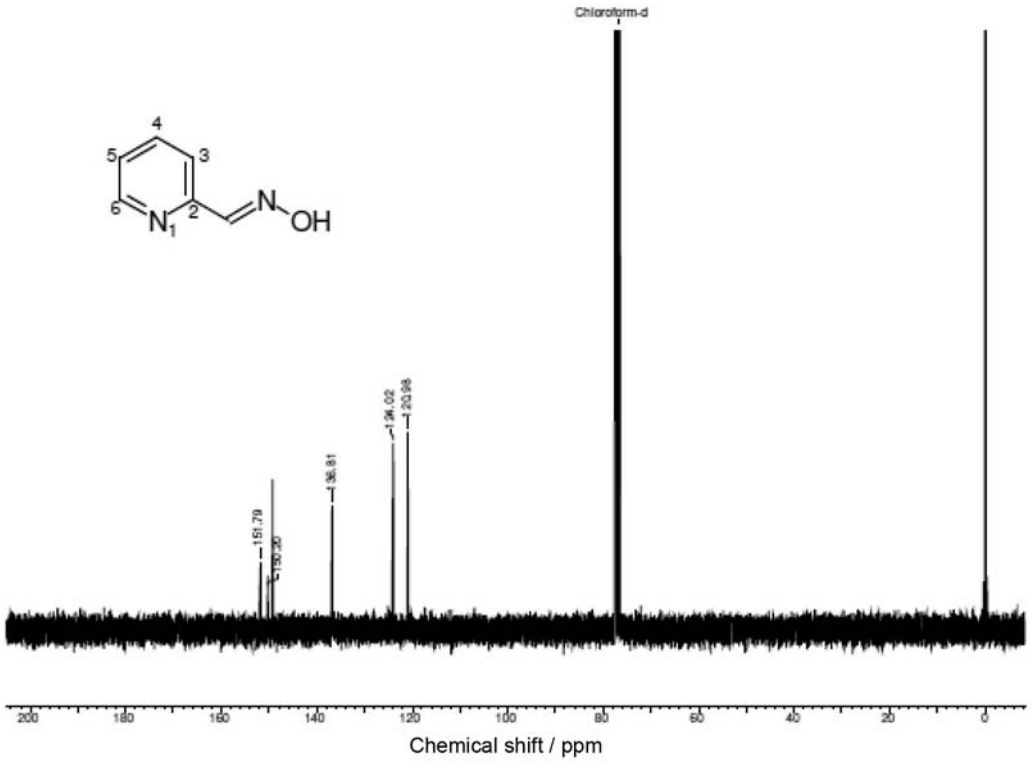

Figure S17. ^{13}C NMR (75 MHz, $CDCl_3$) of pyridine-2-carboxyladehyde oxime (**22**).

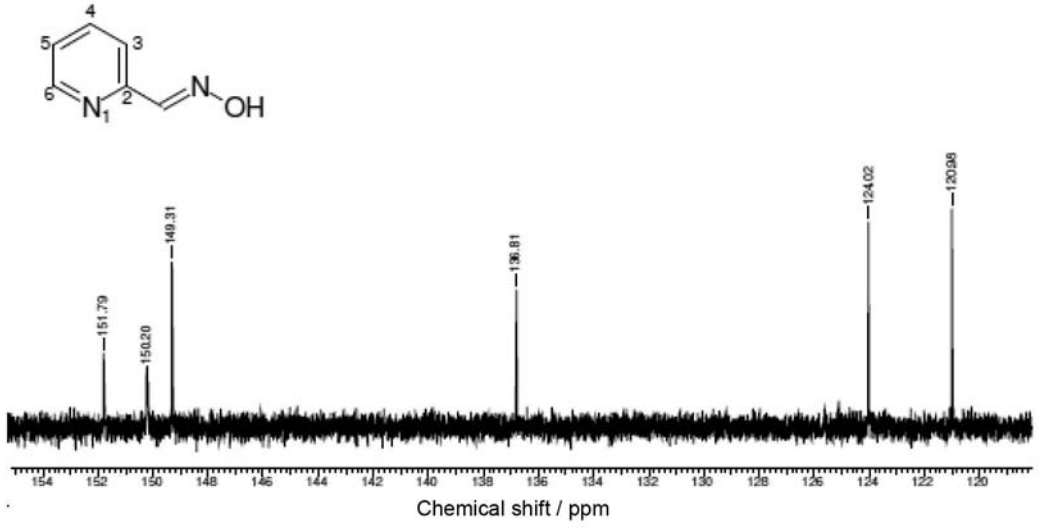

Figure S18. Expansion of ^{13}C NMR (75 MHz, $CDCl_3$) of pyridine-2-carboxyladehyde oxime (**22**).

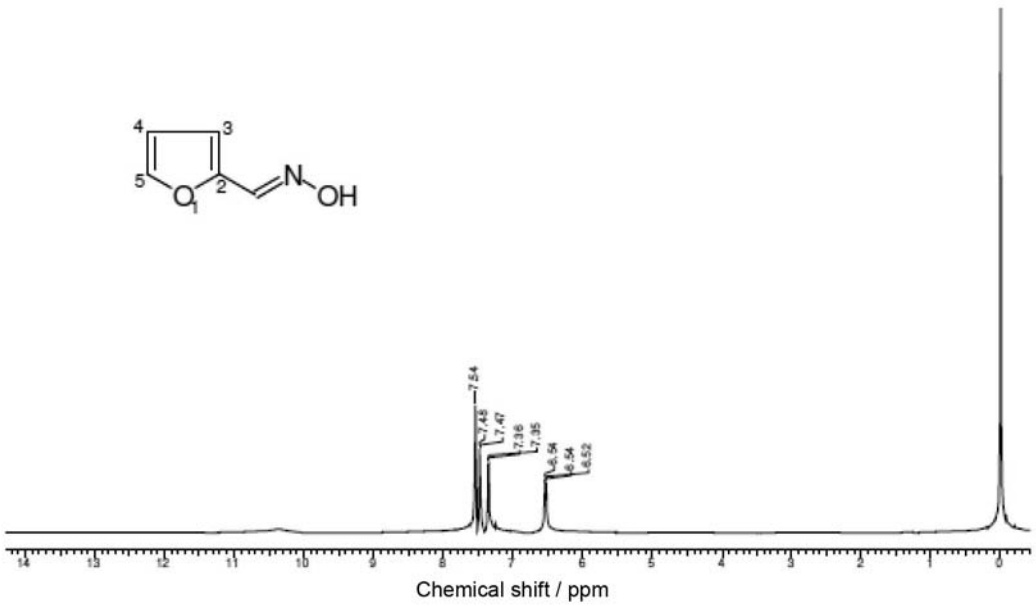

Figure S19. ^{1}H NMR (300 MHz, $CDCl_3$) of furane-2-carboxyaldehyde oxime (**23**).

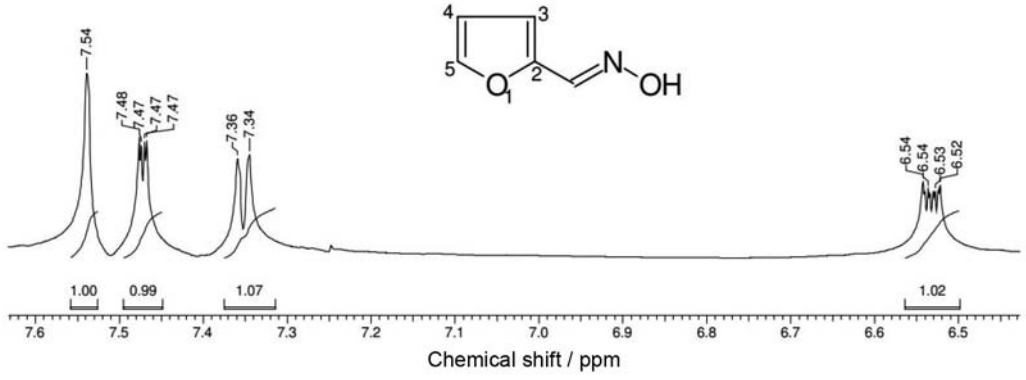

Figure S20. Expansion of ^{1}H NMR (300 MHz, $CDCl_3$) of furane-2-carboxyaldehyde oxime (**23**).

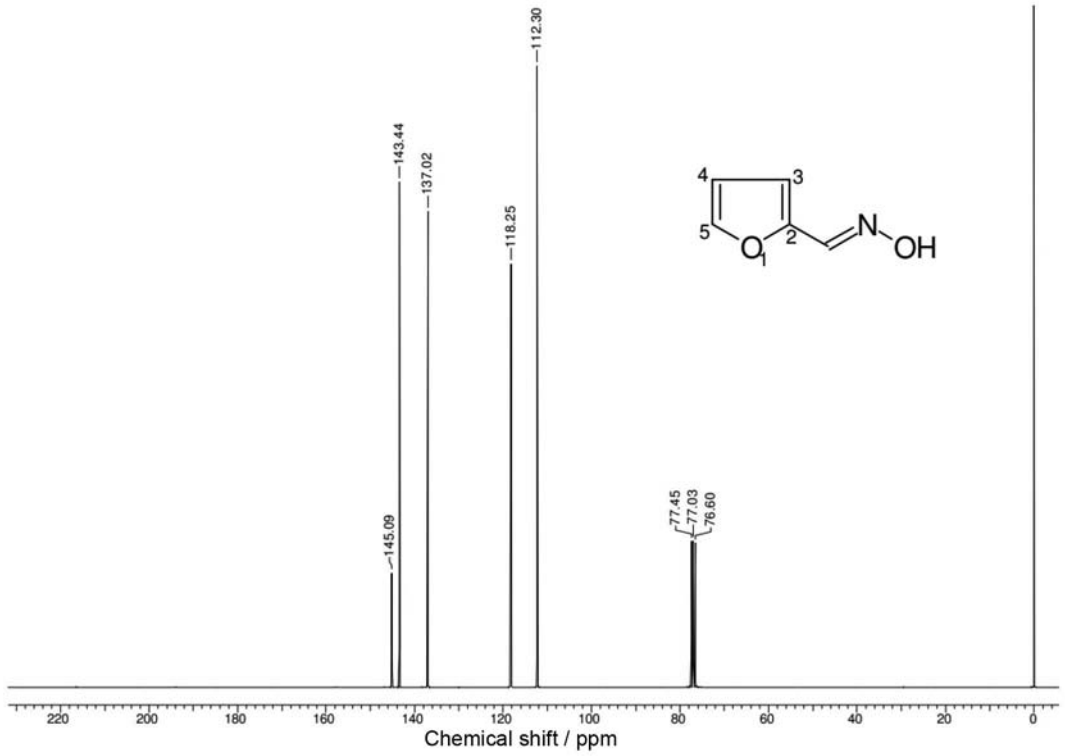

Figure S21. ^{13}C NMR (75 MHz, $CDCl_3$) of furane-2-carboxyaldehyde oxime (**23**).

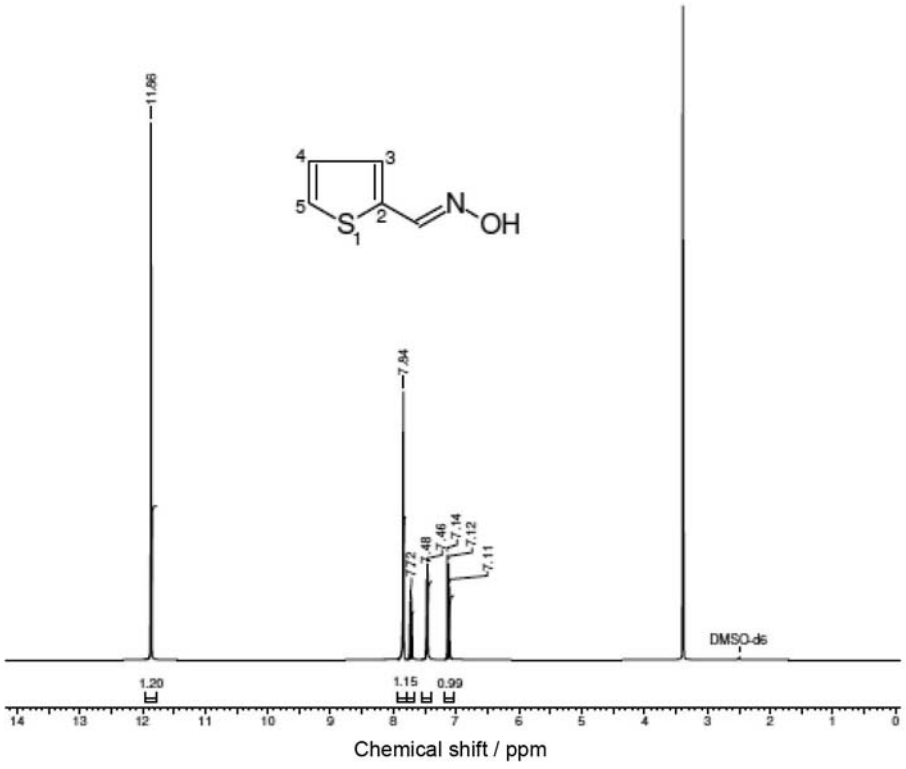

Figure S22. ^{1}H NMR (300 MHz, DMSO-d_6) of thiophene-2-carboxyladehyde oxime (**24**).

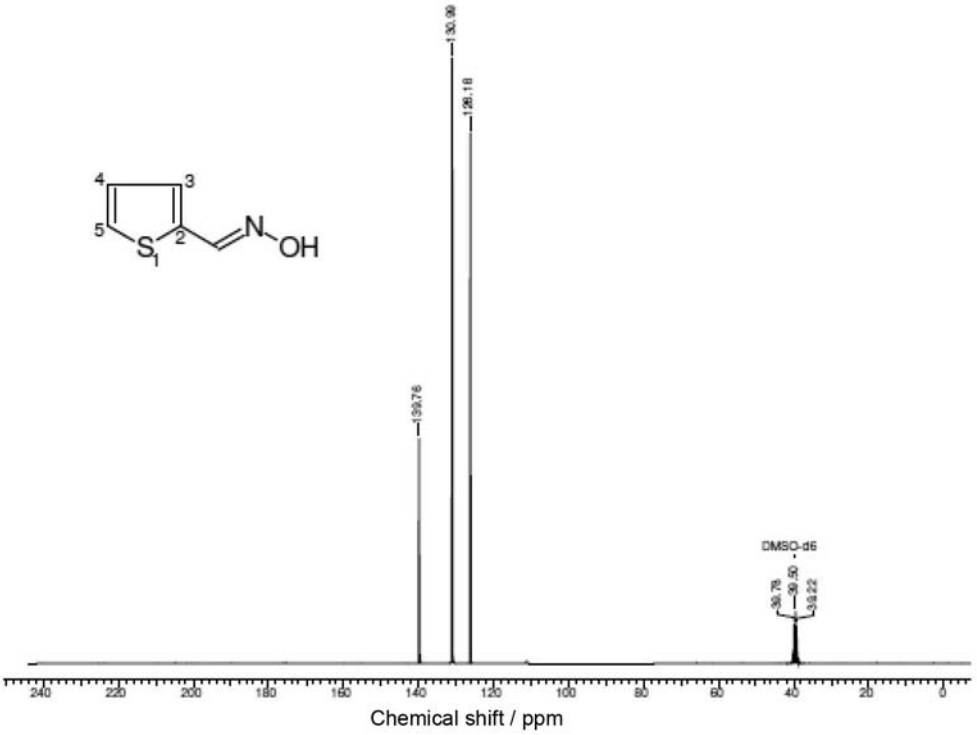

Figure S23. ^{13}C NMR (75 MHz, DMSO-d_6) of thiophene-2-carboxyladehyde oxime (**24**).

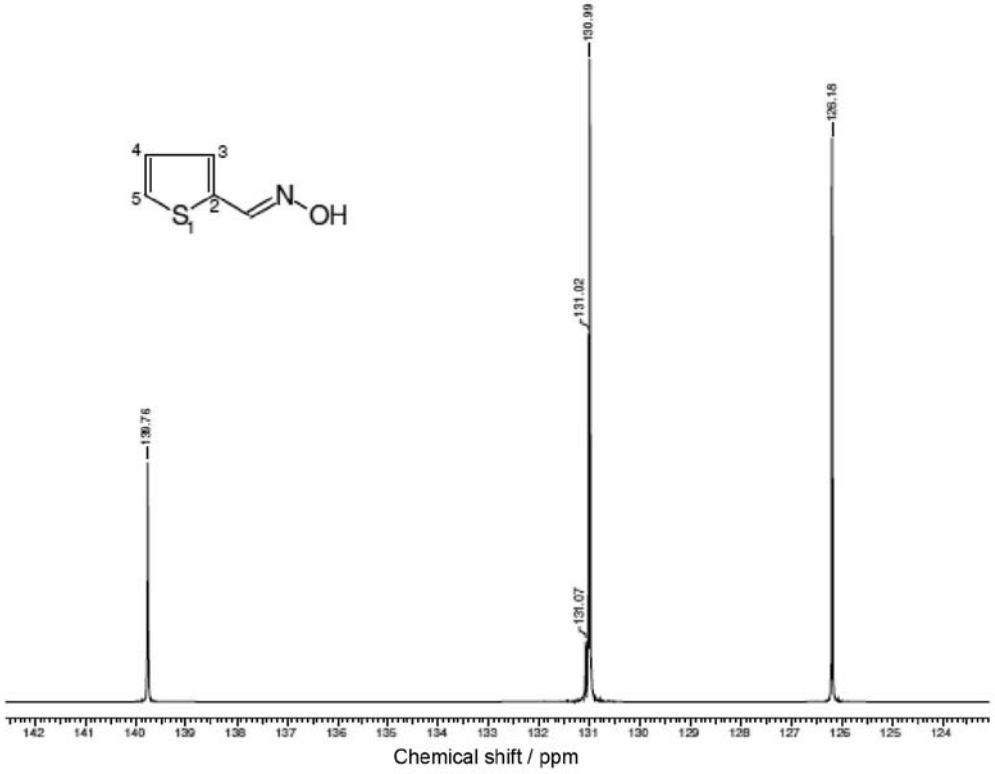

Figure S24. Expansion of ^{13}C NMR (75 MHz, DMSO-d_6) of thiophene-2-carboxyladehyde oxime (**24**).

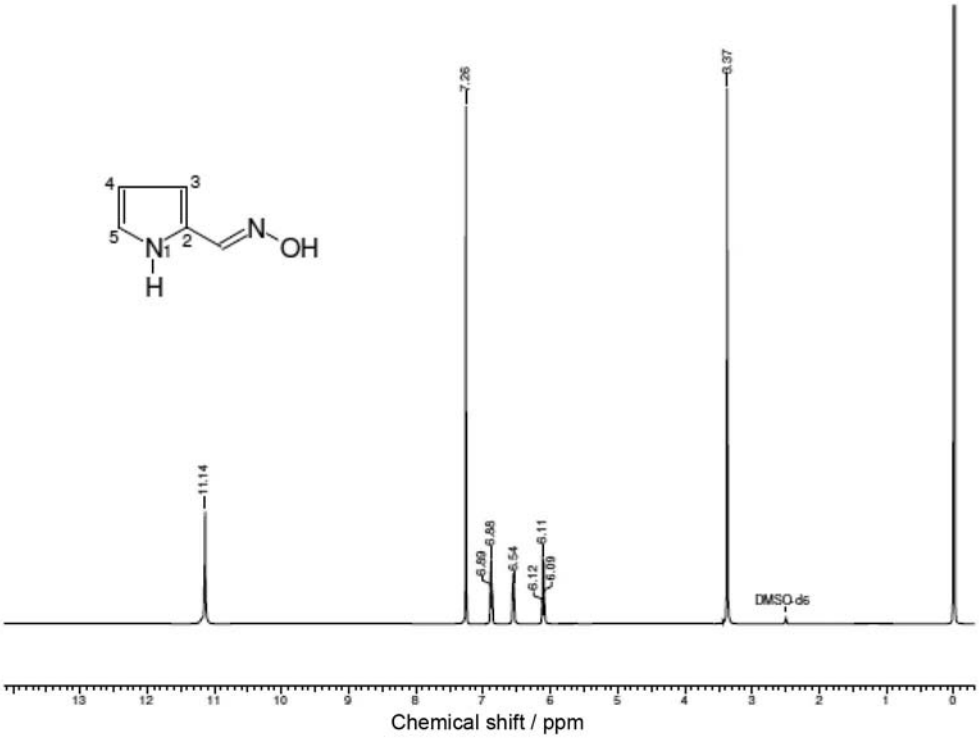

Figure S25. ^{1}H NMR (300 MHz, DMSO-d_6) of pyrrol-2-carboxyladehyde oxime (**25**).

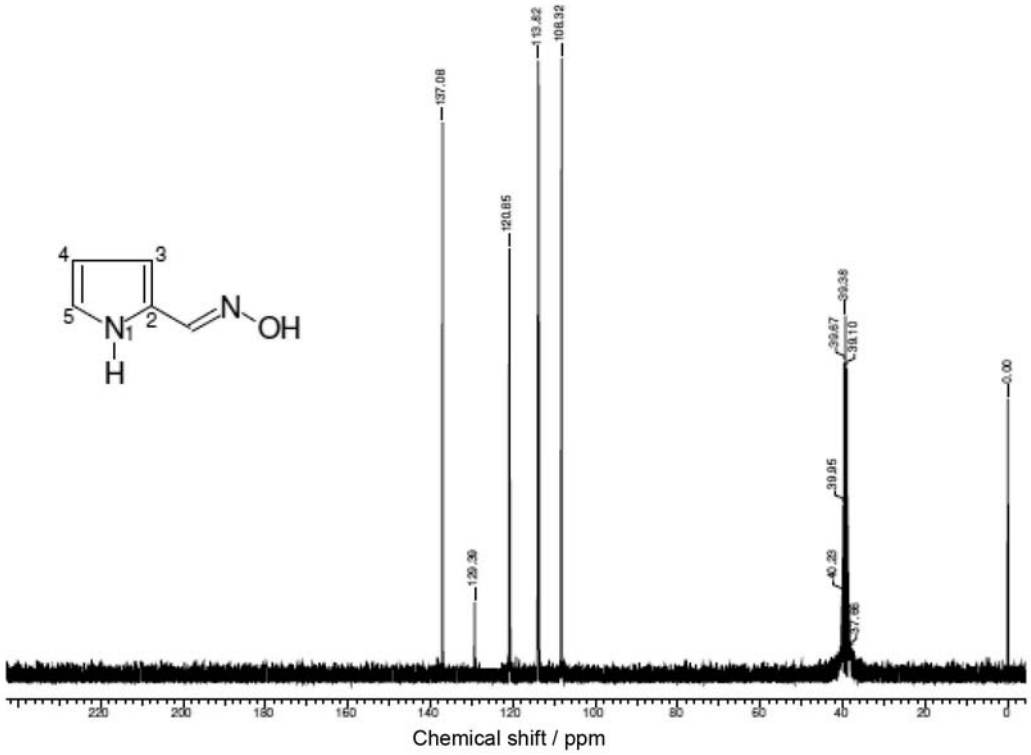

Figure S26. ^{13}C NMR (75 MHz, DMSO-d_6) of pyrrol-2-carboxyladehyde oxime (**25**).

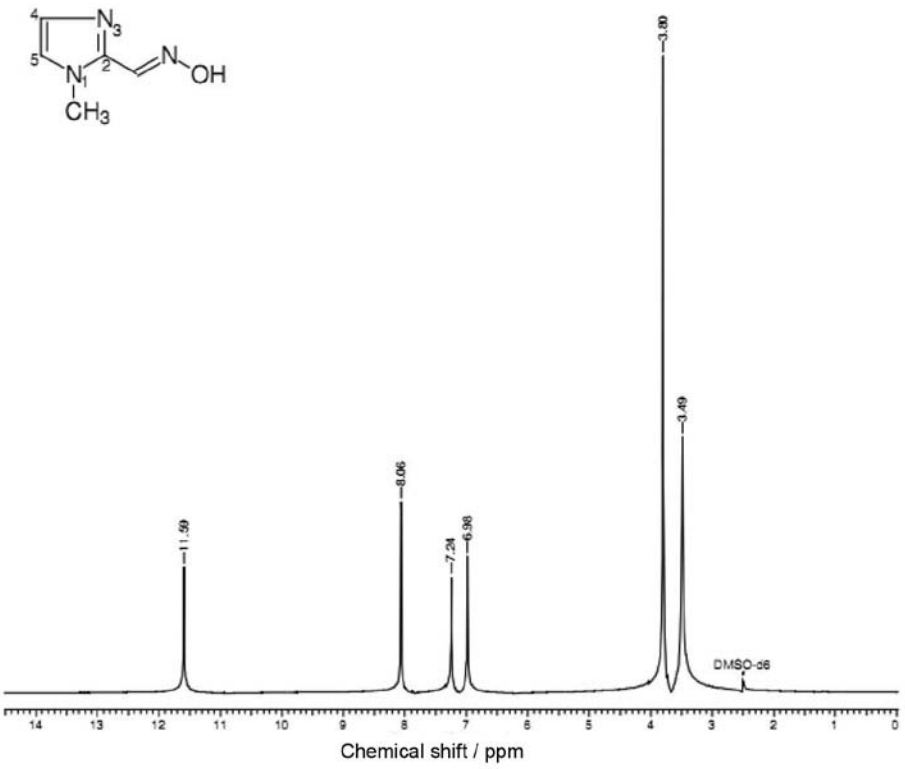

Figure S27. [1]H NMR (300 MHz, DMSO-d_6) of 1-methylimidazol-2-carboxyladehyde oxime (**26**).

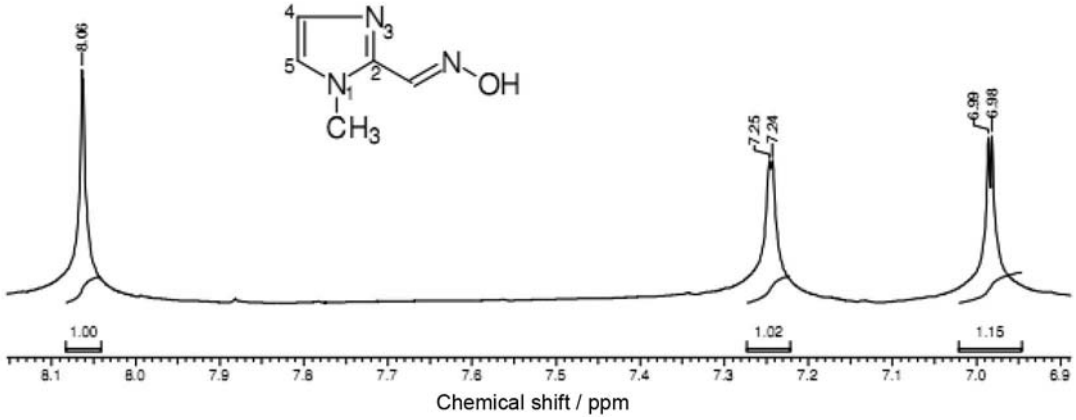

Figure S28. Expansion of [1]H NMR (300 MHz, DMSO-d_6) of 1-methylimidazol-2-carboxyladehyde oxime (**26**).

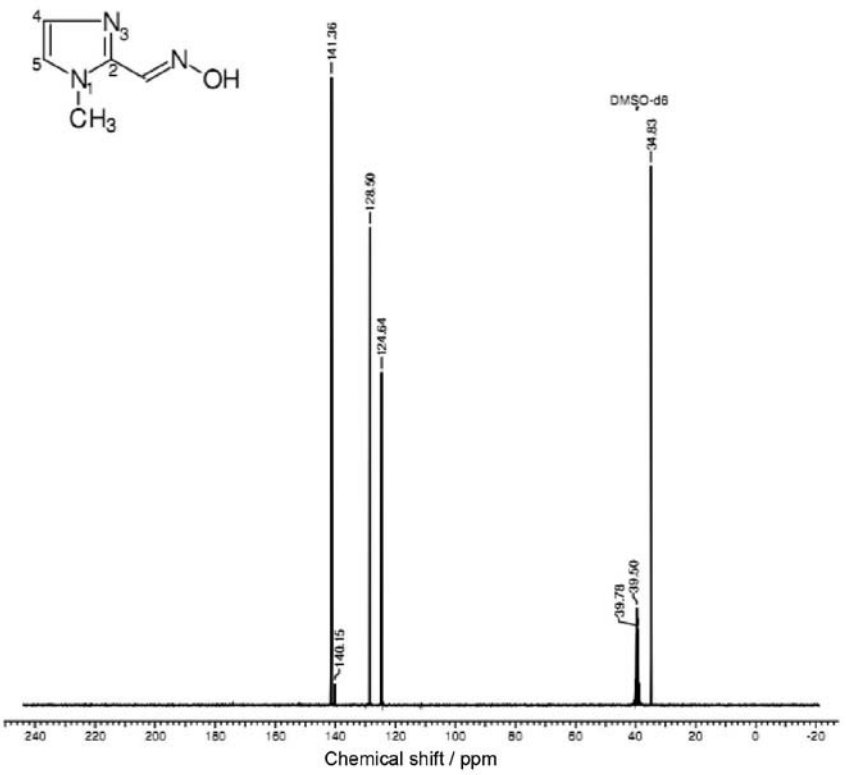

Figure S29. ^{13}C NMR (75 MHz, DMSO-d_6) of 1-methylimidazol-2-carboxyladehyde oxime (**26**).

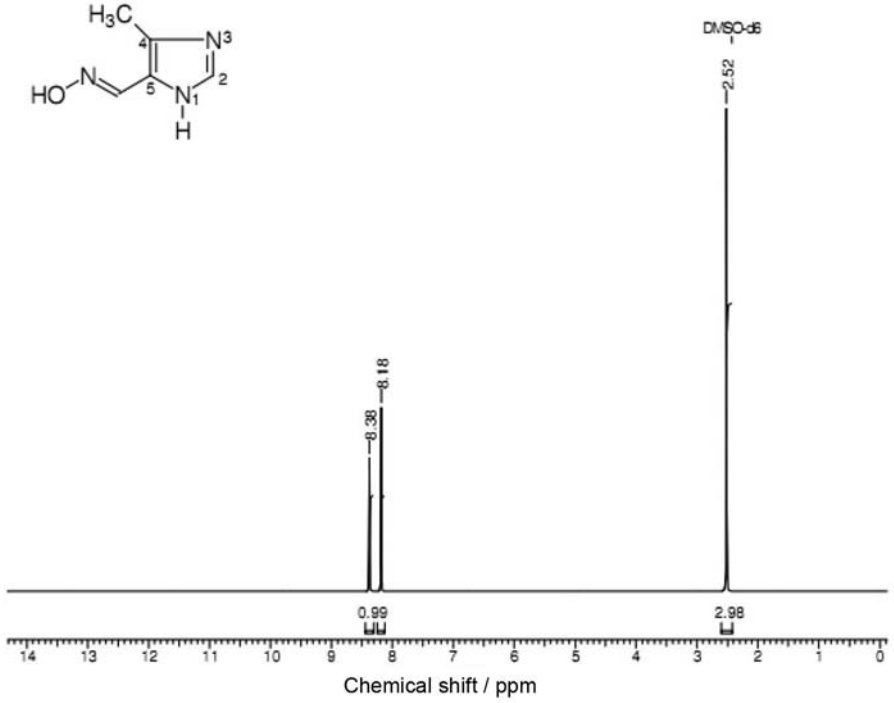

Figure S30. ^{1}H NMR (300 MHz, DMSO-d_6) of 4-methylimidazol-5-carboxyladehyde oxime (**27**).

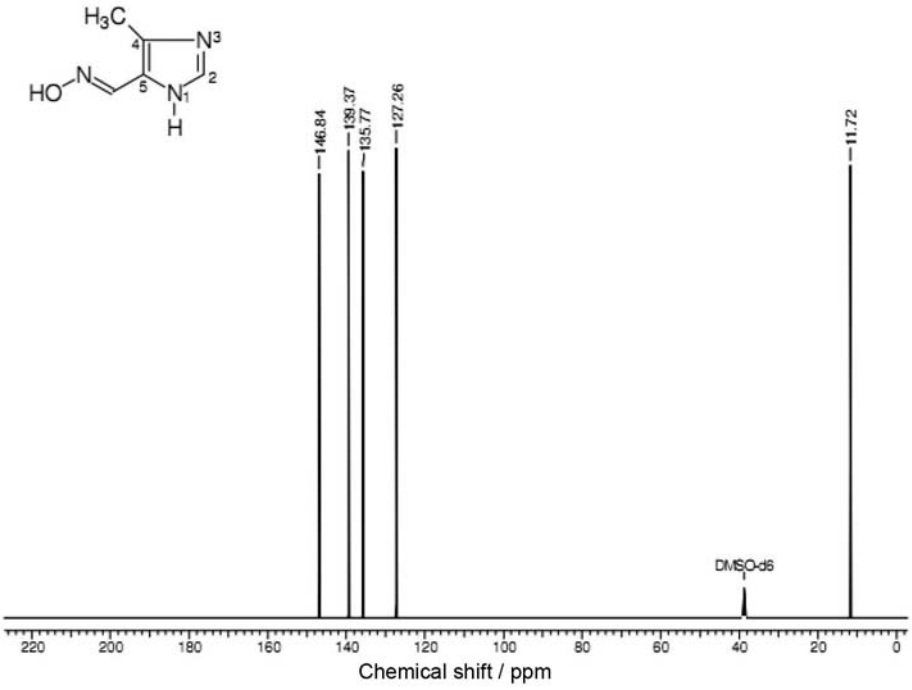

Figure S31. ^{13}C NMR (75 MHz, DMSO-d_6) of 4-methylimidazol-5-carboxyladehyde oxime (**27**).

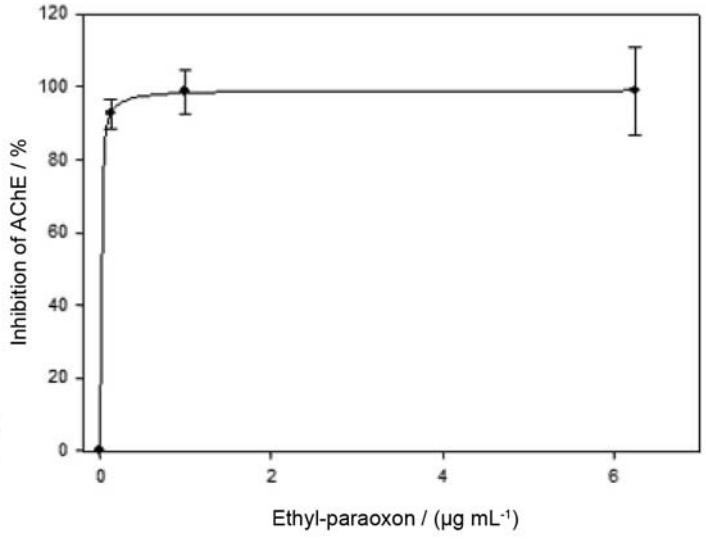

Figure S32. Graphic of ethyl-paraoxon inhibition on human AChE (*in vitro*).