New Journal of Chemistry

Highly efficient and stable peracid for rapid and selective oxidation of aliphatic amine to oxime

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Supporting Information

Table of content

DSC analysis of dodecanebis(peroxoic acid)

1.	**Instrument**	DSC Q100 V9.9 Build 303 (Universal V4.5A TA Instrument)	
2.	**Operation conditions**	**Ramp**	: 10.00 °C/min to 300.00 °C
		Gas	: Nitrogen
		Flow rate	: 50.0 ml/min
		Sample weight	: 2.30 mg

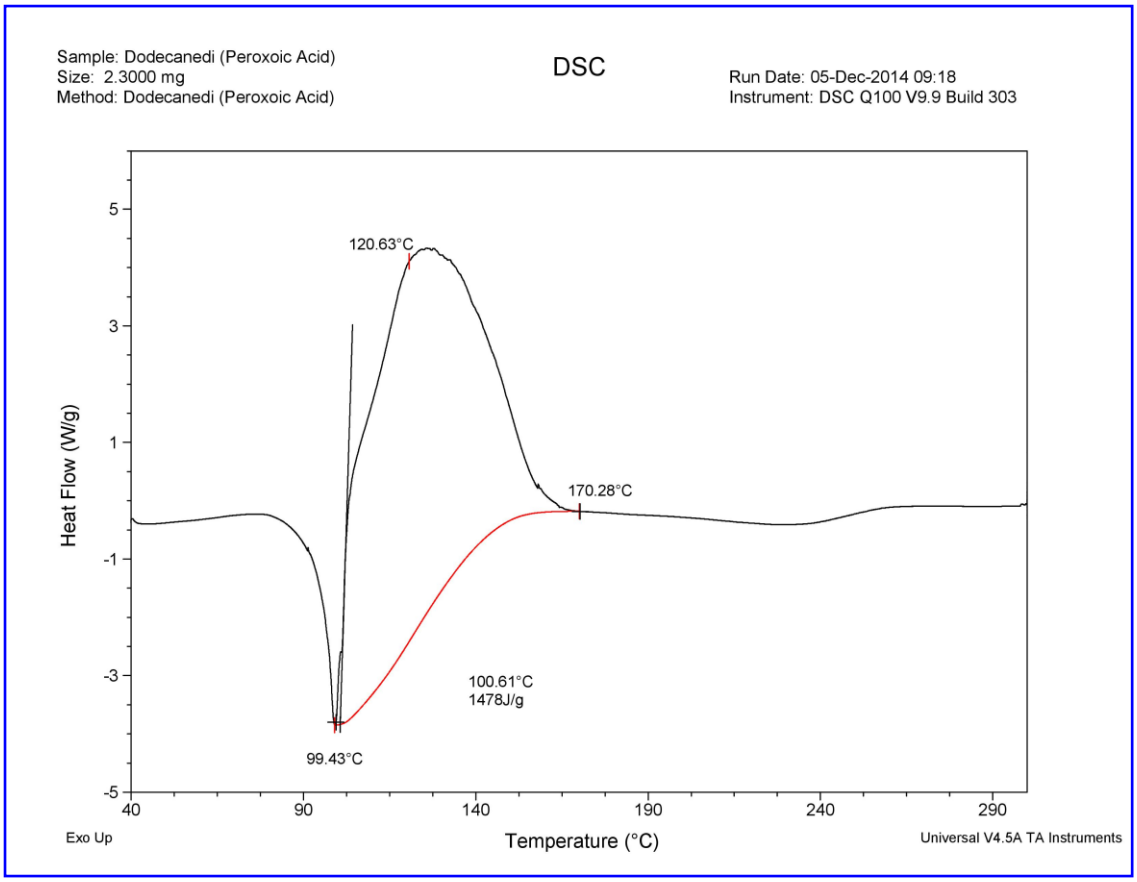


Fig. 1. DSC analysis of dodecanebis(peroxoic acid)

- **Yoshida's correlation equations**[1]**:**

1. Shock Sensitivity (SS) $= [\log (Q_{dsc}) - 0.72] [\log (T_{dsc} - 25) - 0.98]$

2. Explosion Propagation (EP) = [log (Q_{dsc}) - 0.38] [log (T_{dsc} – 25) – 1.67]

Q_{dsc} = Energy of the exotherm in calories/g = 1478 J/g = 0.0003530 calories/g

T_{dsc} = The onset temperature of the exotherm in °C = 100.61 °C

- **Calculations**:

1. **Shock Sensitivity (SS)**

SS = [log (Q_{dsc}) - 0.72] [log (T_{dsc} – 25) – 0.98]

= [log (0.0003530) - 0.72] [log (100.61 – 25) – 0.98]

= [-4.1722] [0.8985]

= **-3.7490**

2. **Explosion Propagation (EP)**

EP = [log (Q_{dsc}) - 0.38] [log (T_{dsc} – 25) – 1.67]

= [log (0.0003530) - 0.38] [log (100.61 – 25) – 1.67]

= [-3.8322] [0.2085]

= **-0.7993**

- **Conclusion**:

"*According to this equation, if the value for Shock sensitivity **(SS)** or Explosion Propagation **(EP)** is ≥ **0.00**, then the material is predicated to be shock sensitive or demonstrate explosive propagating properties, respectively*."

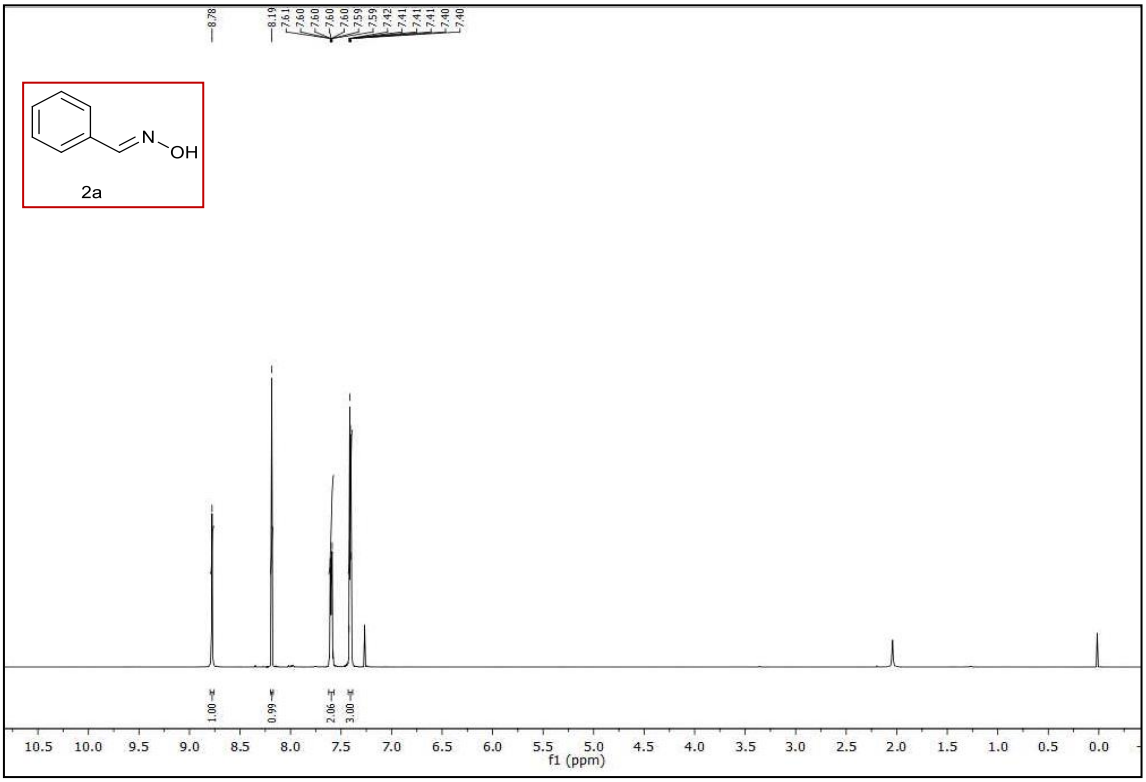
As per the above assumption, it is clear that, dodecanbis(peroxoic acid) is non-shock sensitive as well as it does not exhibit explosive propagation properties.

Reference

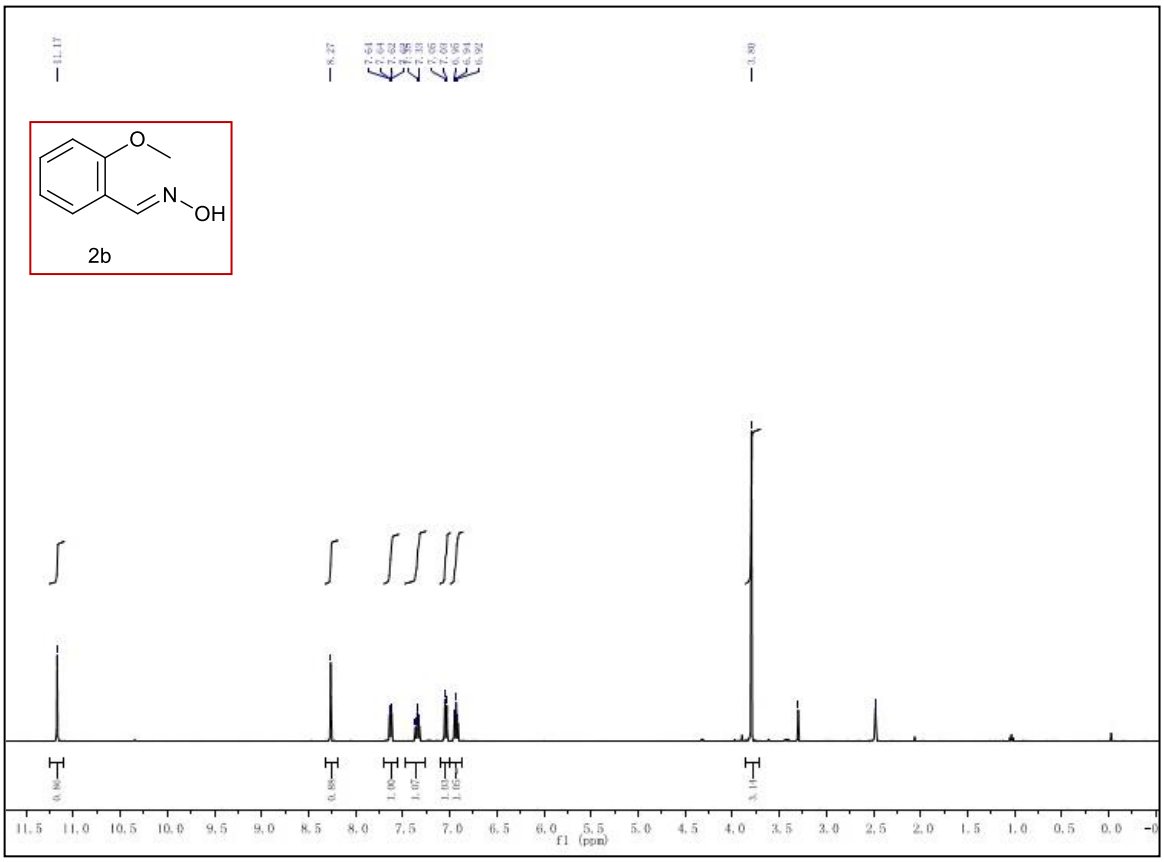
1 R. Kwasny, *Process Saf. News*, 2010, **17**, 4–5.

^{1}H-NMR-Spectra of Selected Compounds

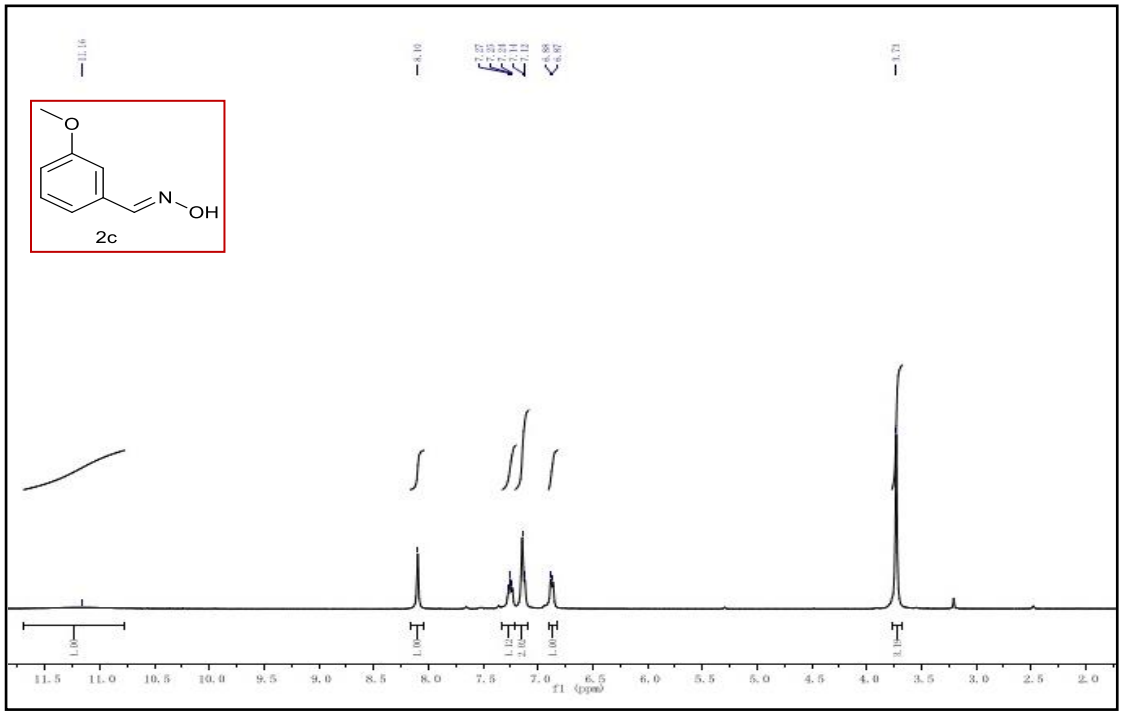
1. Benzaldehyde oxime (*2a*)



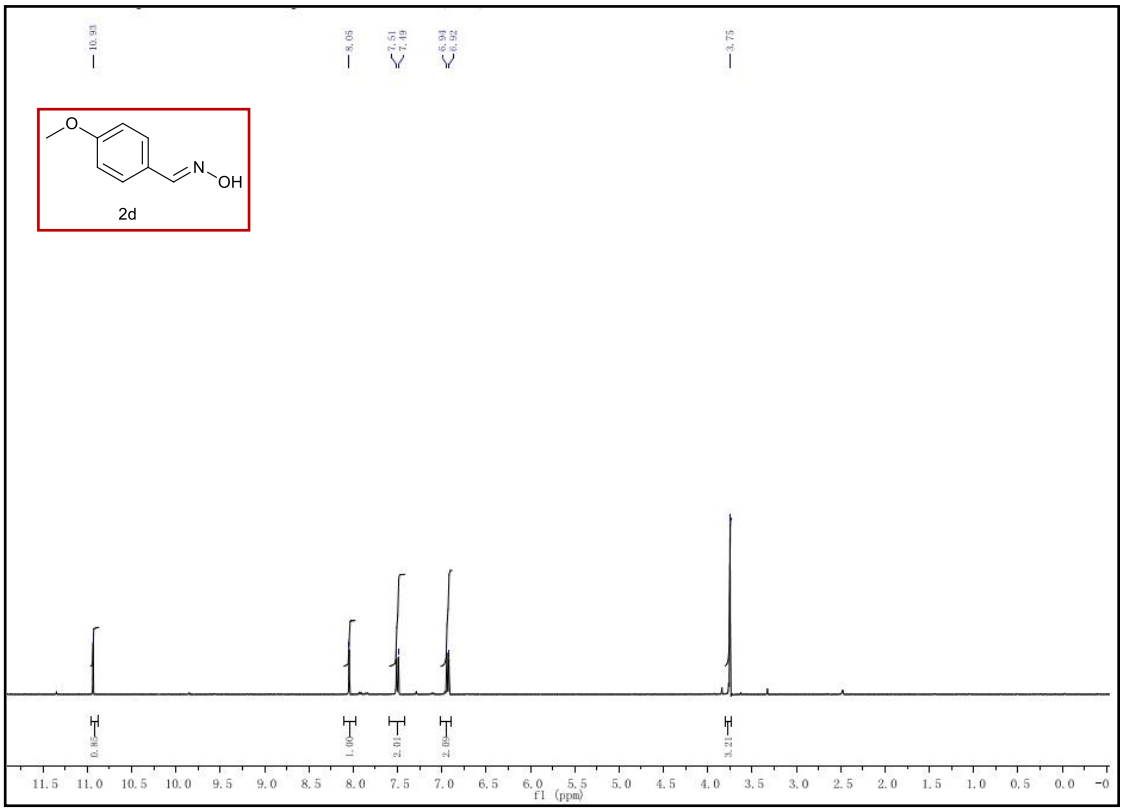
2. 2-methoxybenzaldehyde oxime (2b)



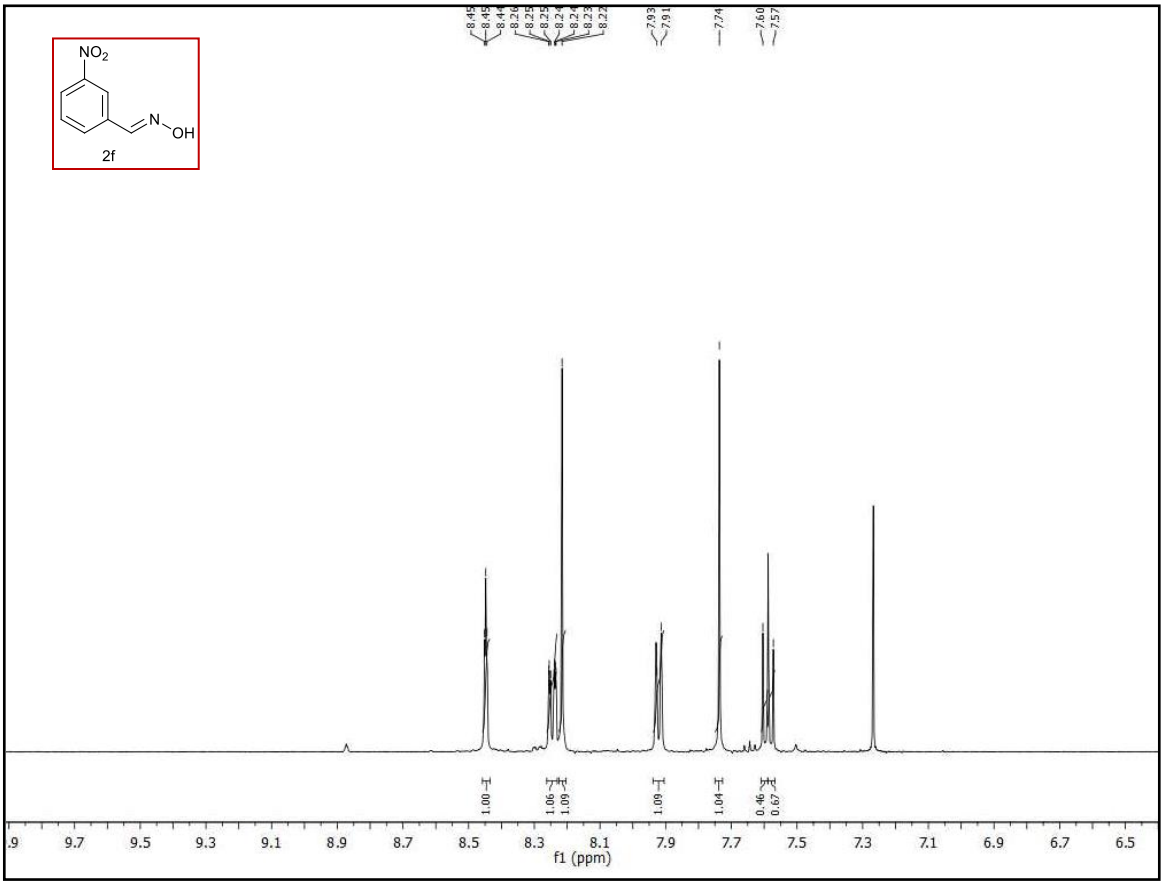
3. 3-methoxybenzaldehyde oxime (2c)



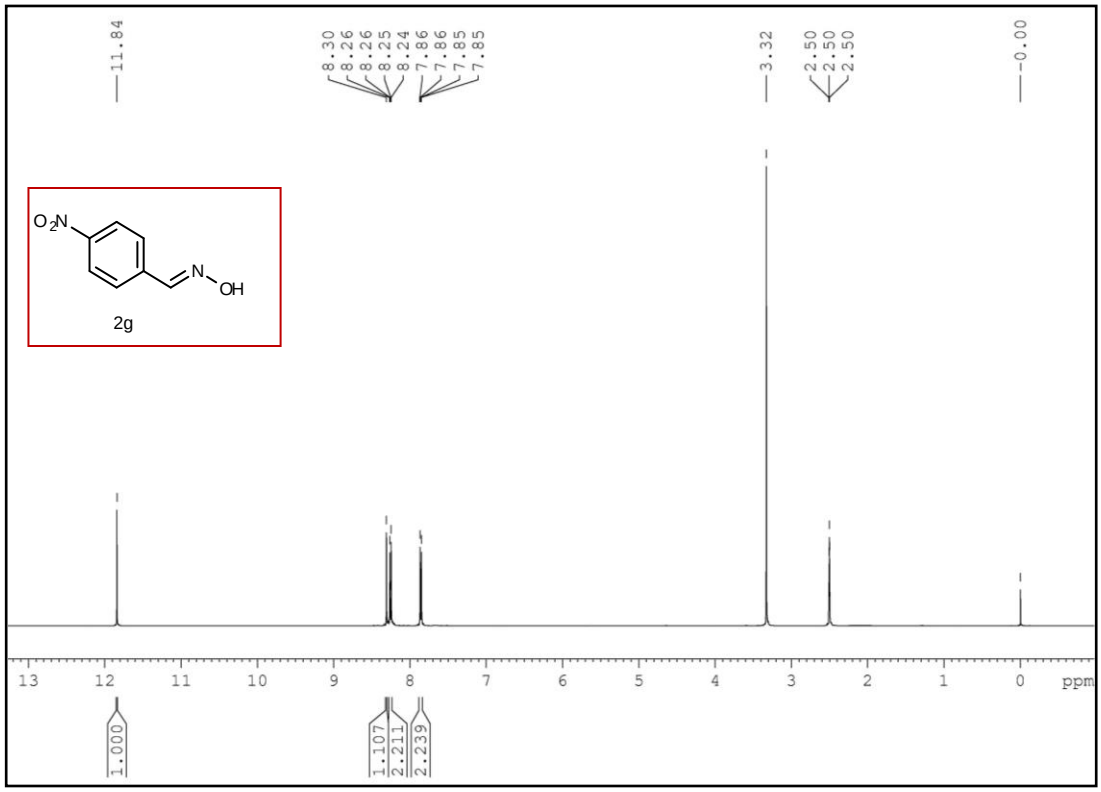
4. 4-methoxybenzaldehyde oxime (2d)



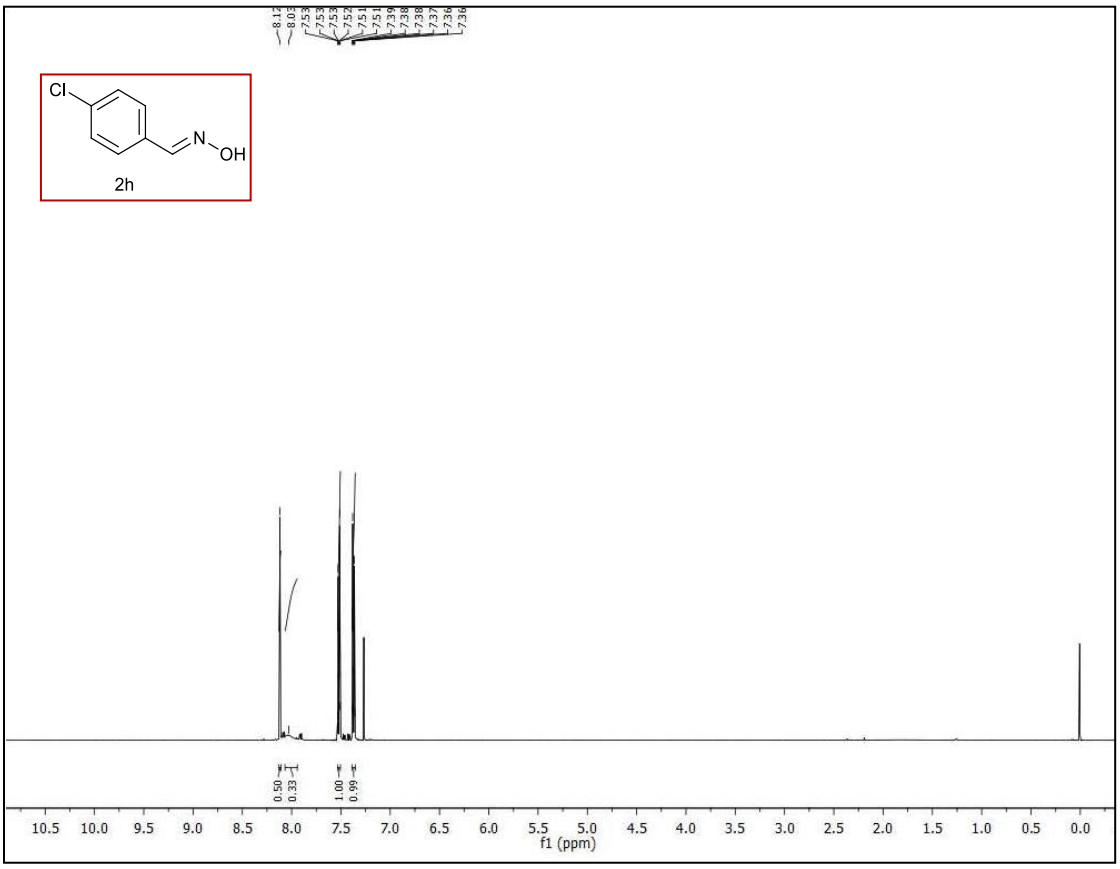
5. 3-nitrobenzaldehyde oxime (*2f*)



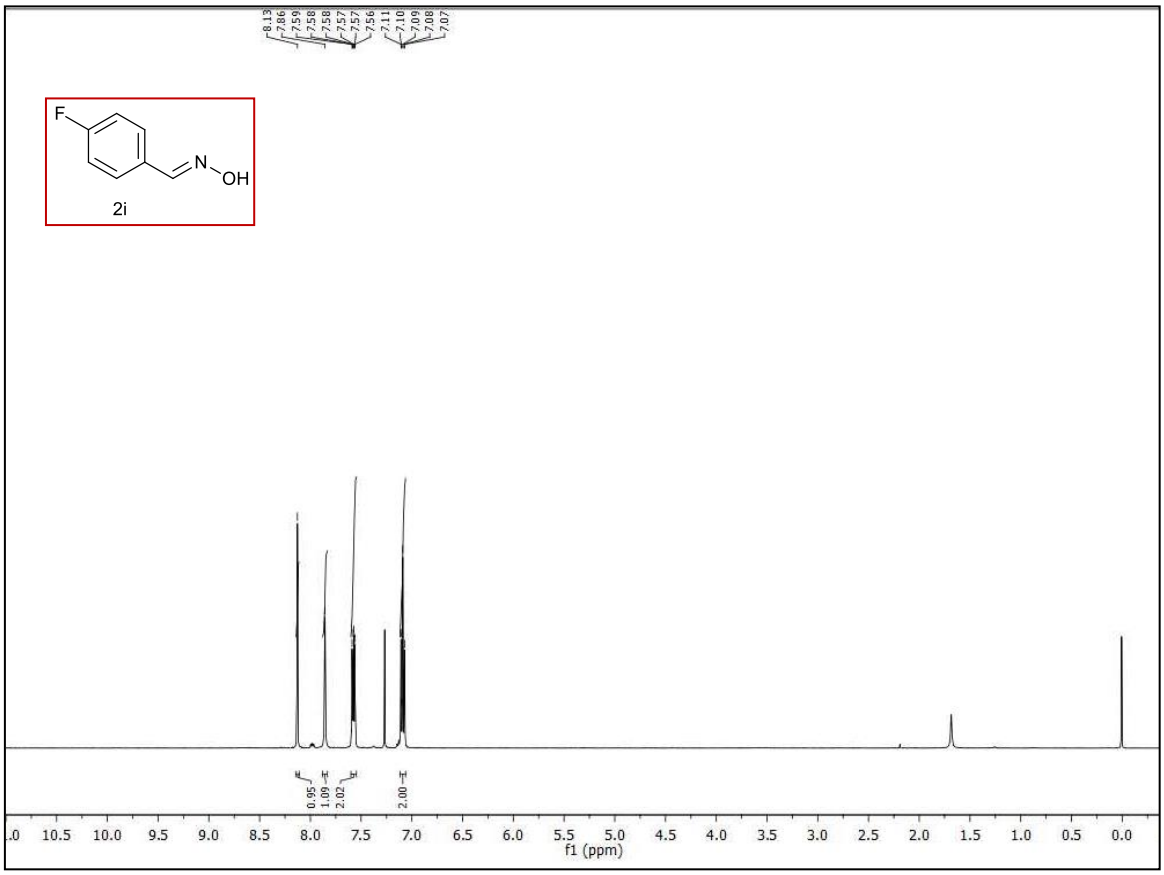
6. 4-nitrobenzaldehyde oxime (*2g*)



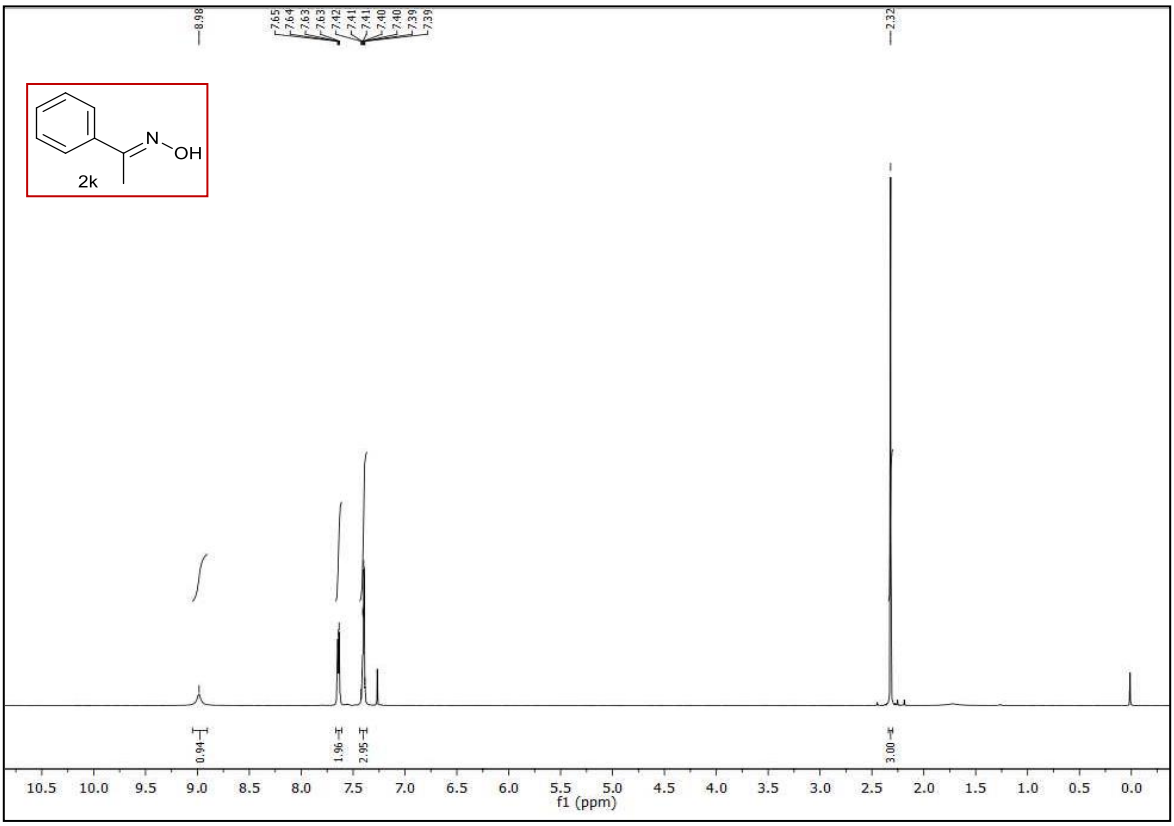
7. 4-chlorobenzaldehyde oxime (*2h*)



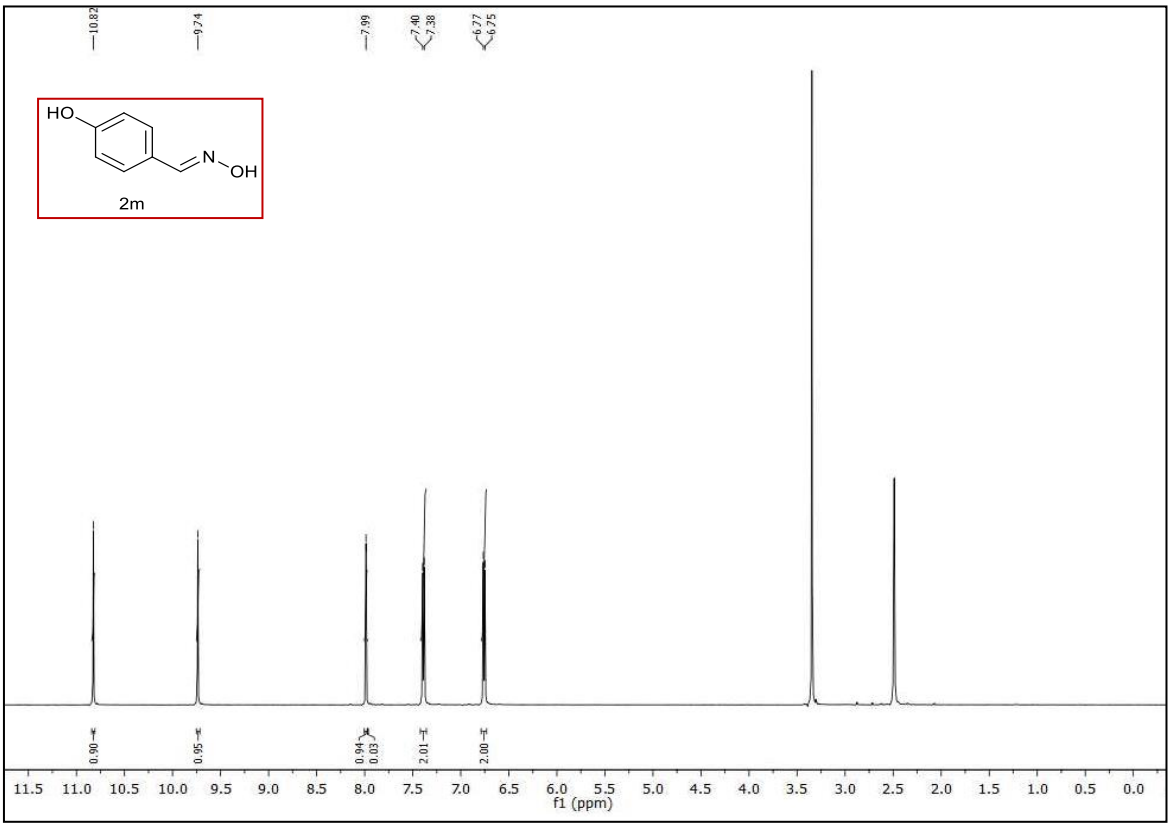
8. 4-fluorobenzaldehyde oxime (*2i*)



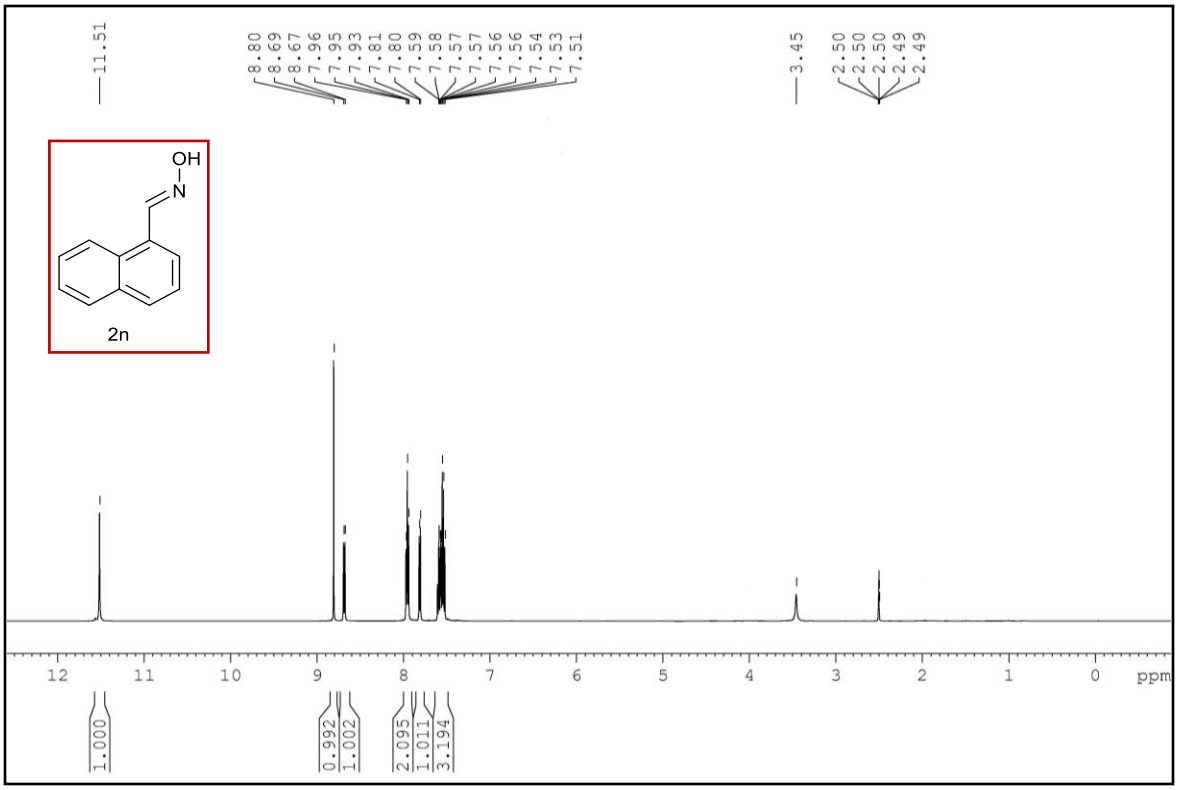
9. Acetophenone oxime (*2k*)



10. 4-hydroxybenzaldehyde oxime (*2m*)



11. 1-naphthaldehyde oxime (*2n*)



12. Cyclohexanone oxime (*2p*)