

Supplementary Materials: Safe Synthesis of Alkylhydroxy and Alkylamino Nitramines

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1. Spectral Data for Selected Compounds

3-Nitrooxazolidin-2-one (8)

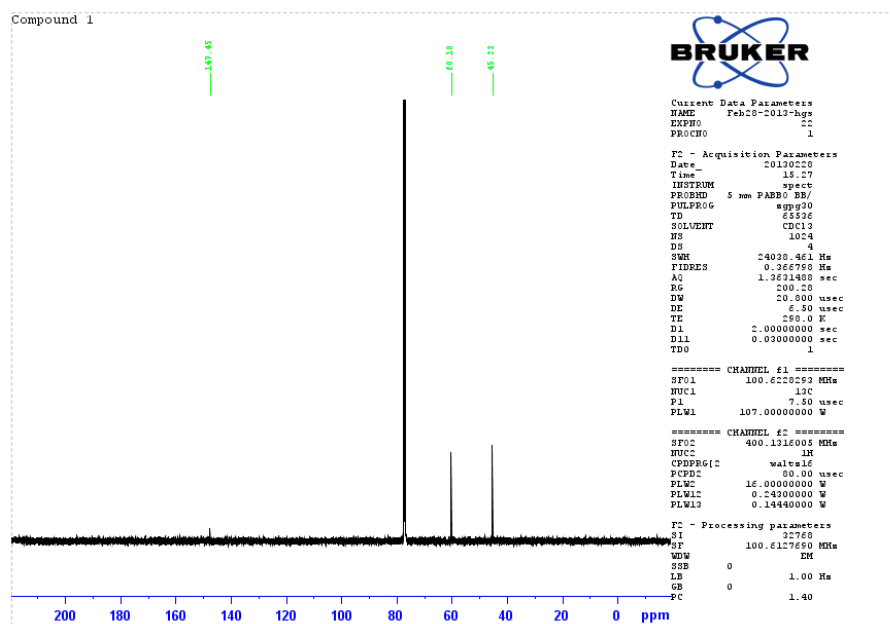


Figure S1. ¹³C-NMR spectrum of 3-nitrooxazolidin-2-one (8).

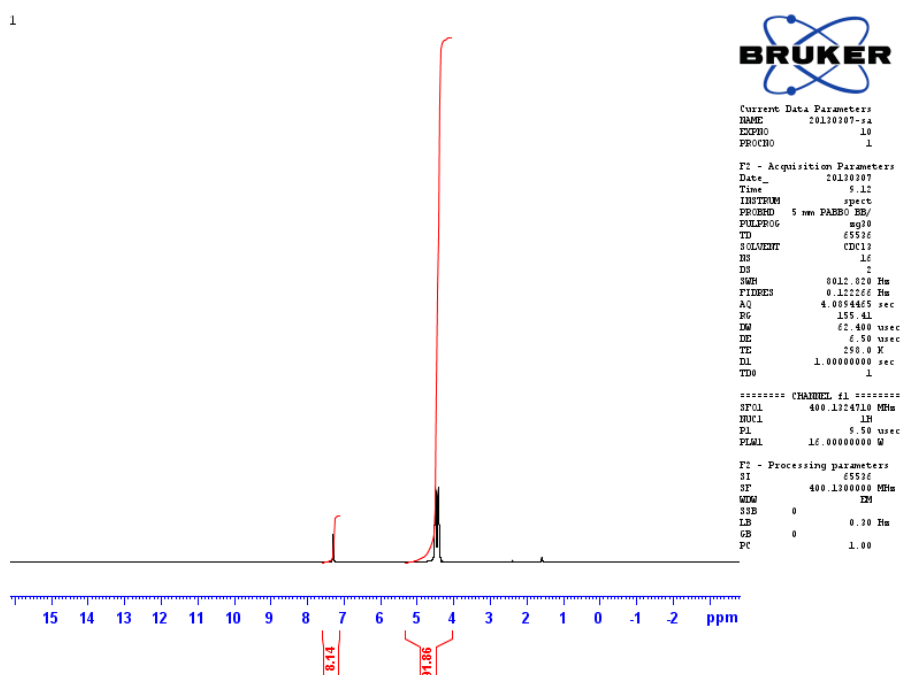


Figure S2. ¹H-NMR spectrum of 3-nitrooxazolidin-2-one (8).

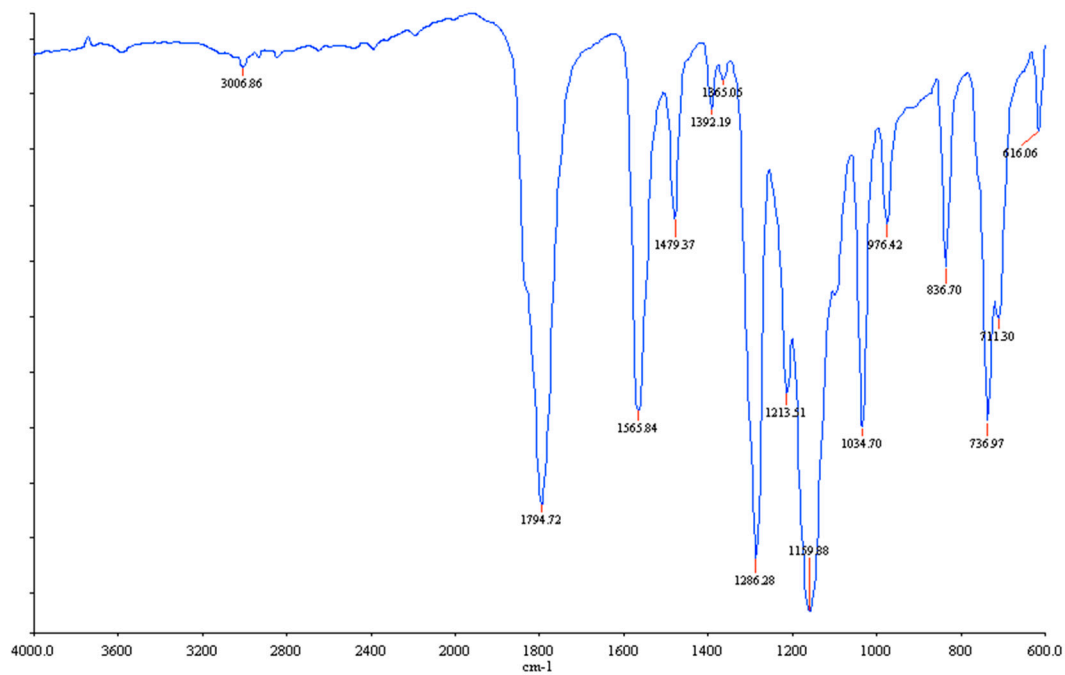
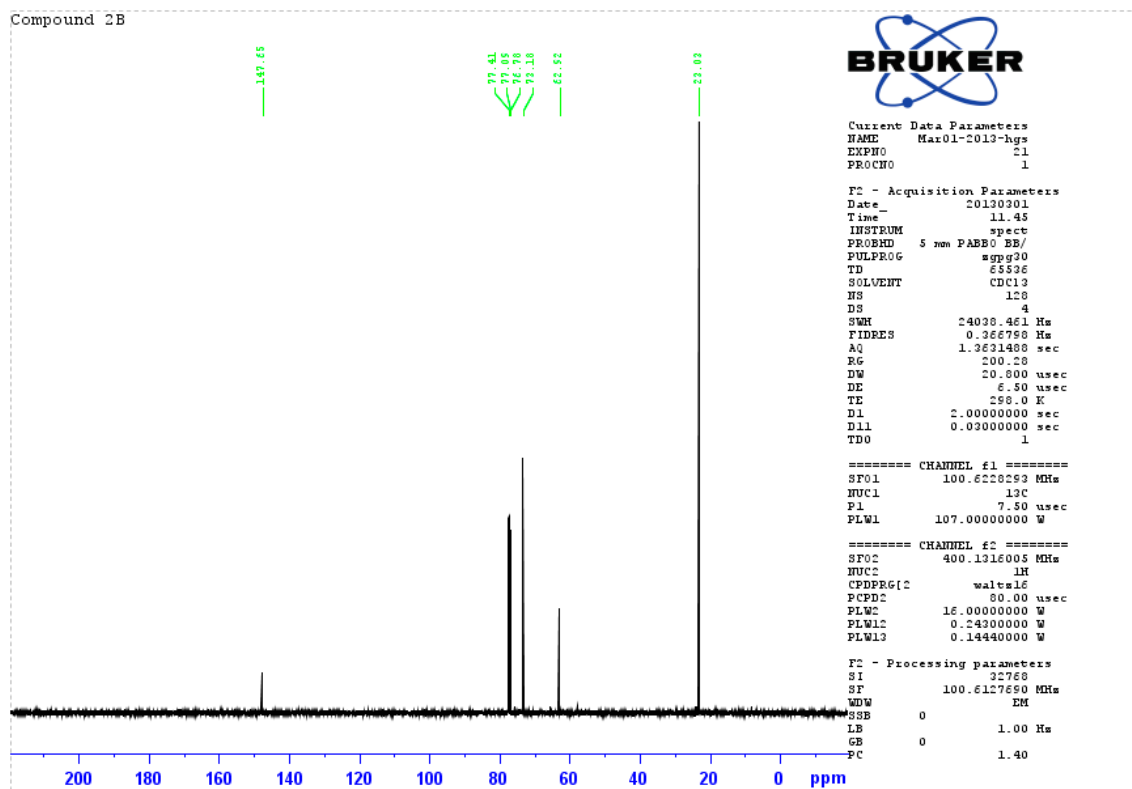


Figure S3. IR spectrum of 3-nitrooxazolidin-2-one (8).

4,4-Dimethyl-3-nitrooxazolidin-2-one (9)

Figure S4. ¹³C-NMR spectrum of 4,4-dimethyl-3-nitrooxazolidin-2-one (9).

Compound 2B

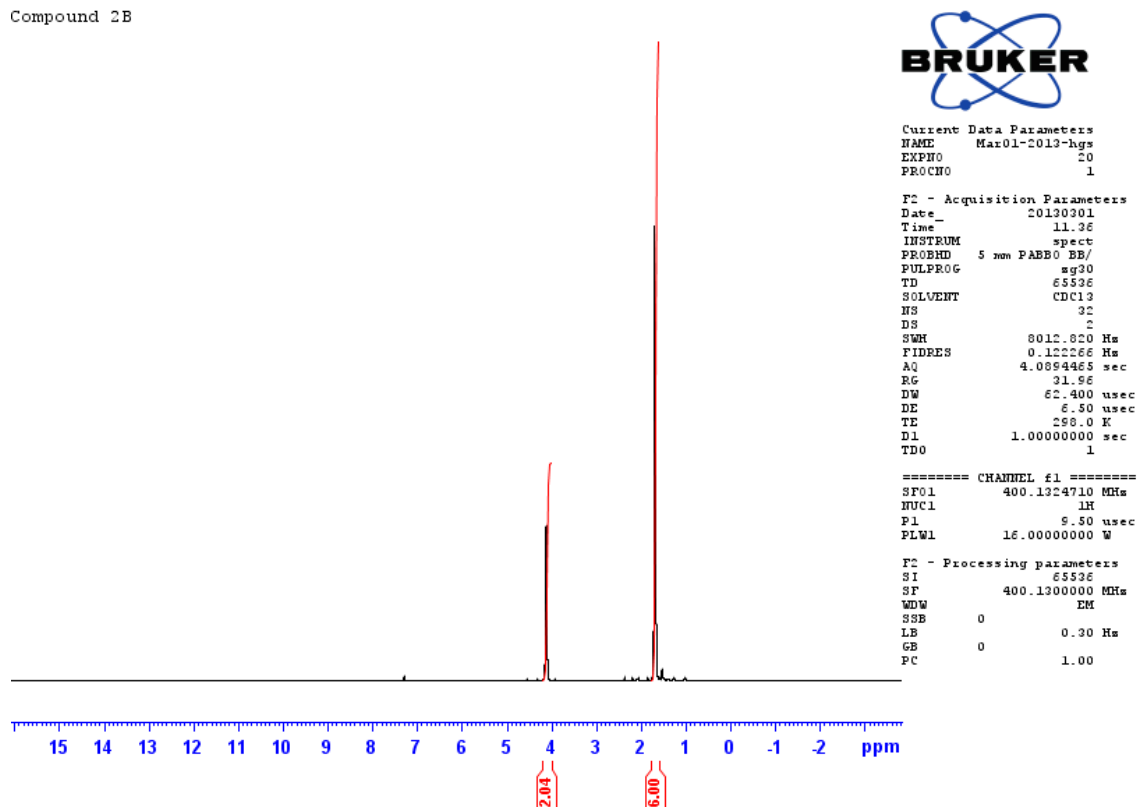
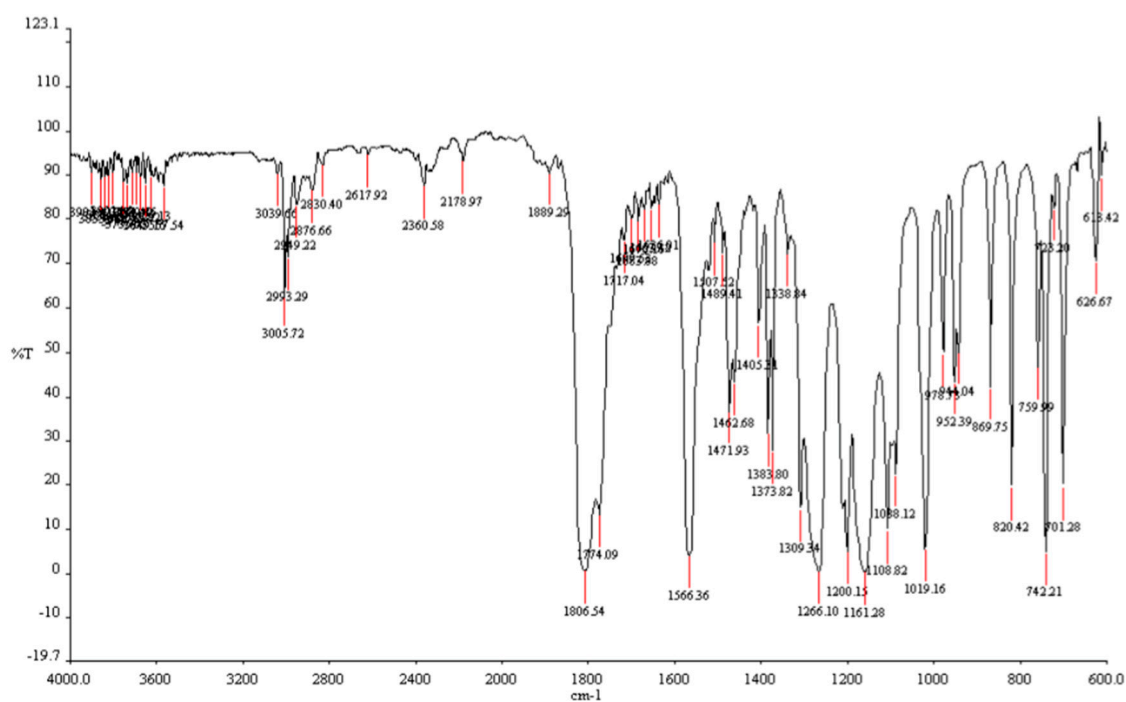
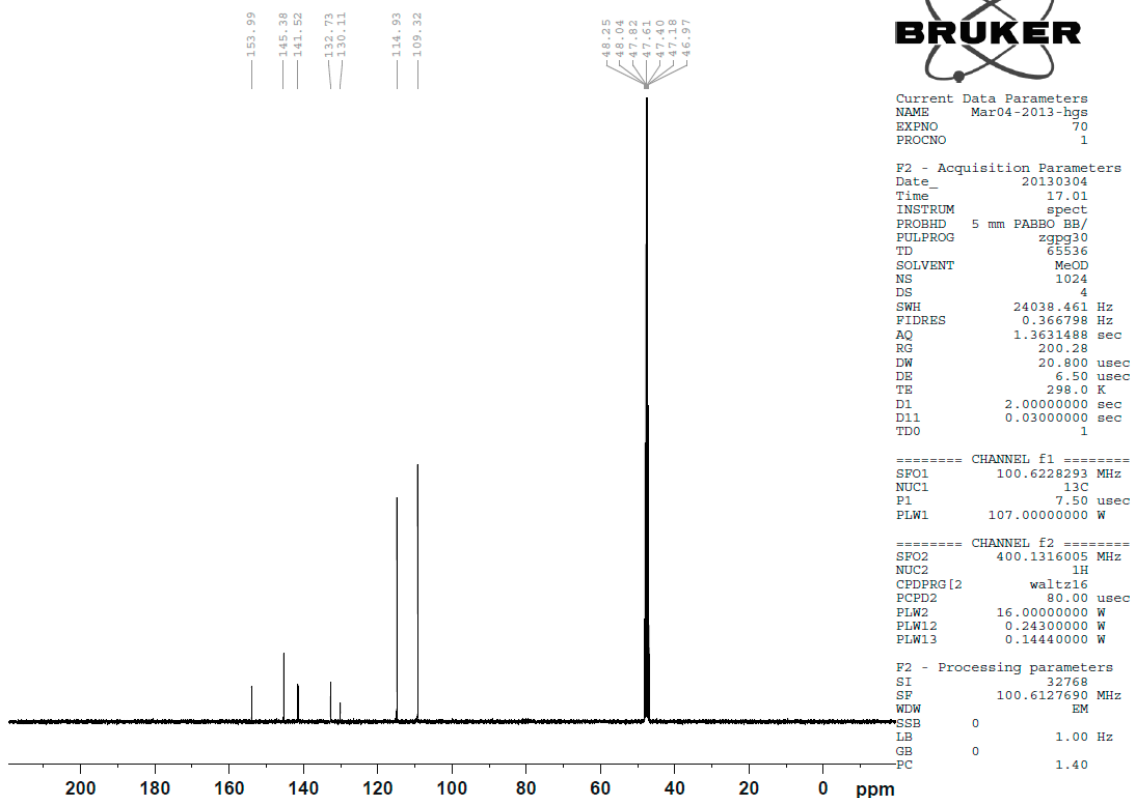
Figure S5. ¹H-NMR spectrum of 4,4-dimethyl-3-nitrooxazolidin-2-one (9).

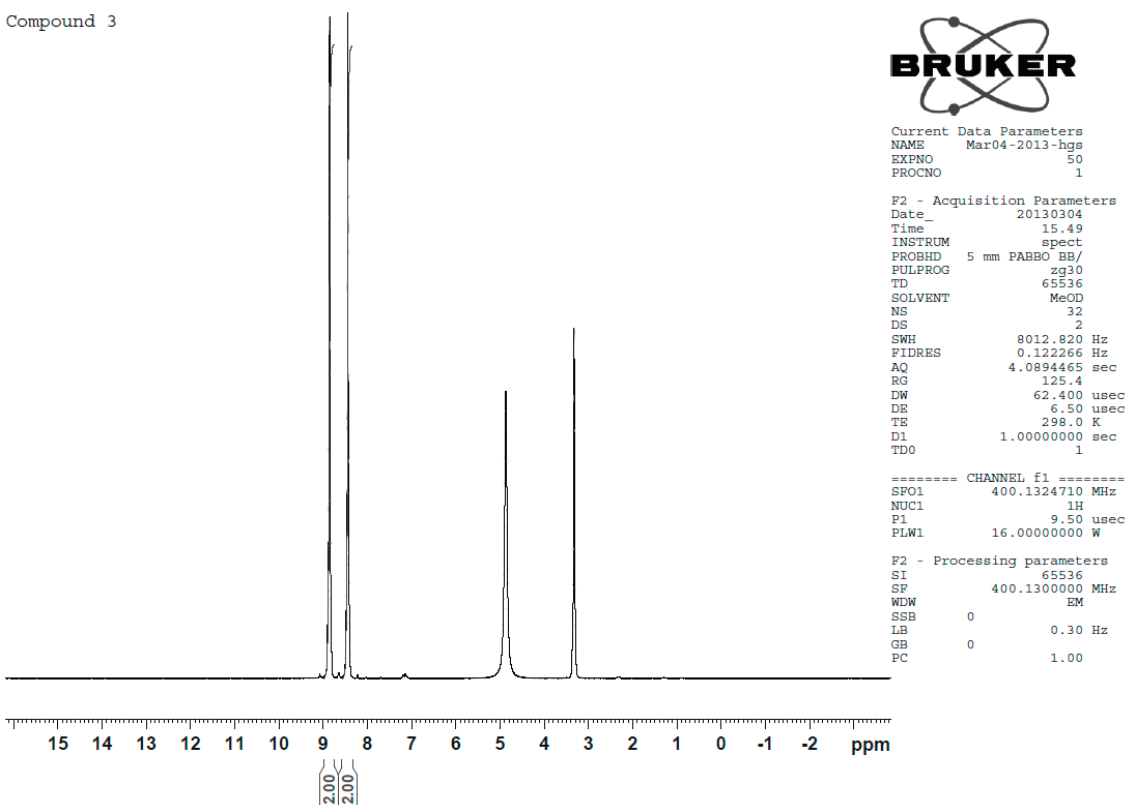
Figure S6. IR spectrum of 4,4-dimethyl-3-nitrooxazolidin-2-one (9).

3-Nitrobenzo[d]oxazol-2(3H)-one (16)

Compound 3

Figure S7. ¹³C-NMR spectrum of 3-nitrobenzo[d]oxazol-2(3H)-one (16).

Compound 3

Figure S8. ¹H-NMR spectrum of 3-nitrobenzo[d]oxazol-2(3H)-one (16).

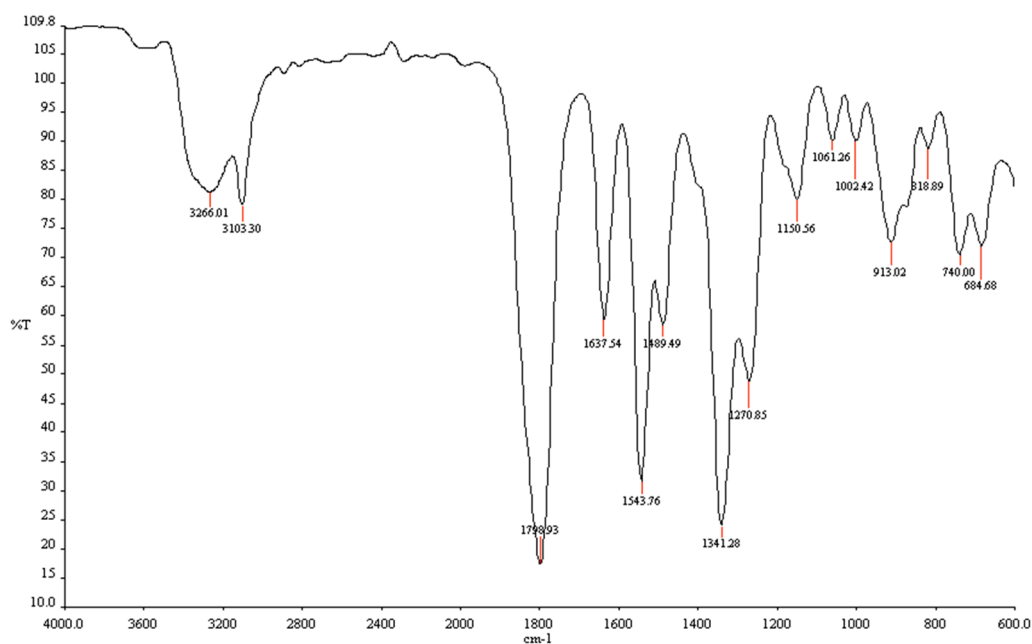


Figure S9. IR spectrum of 3-nitrobenzo[d]oxazol-2(3H)-one (16).

5-(Chloromethyl)-3-nitrooxazolidin-2-one (17)

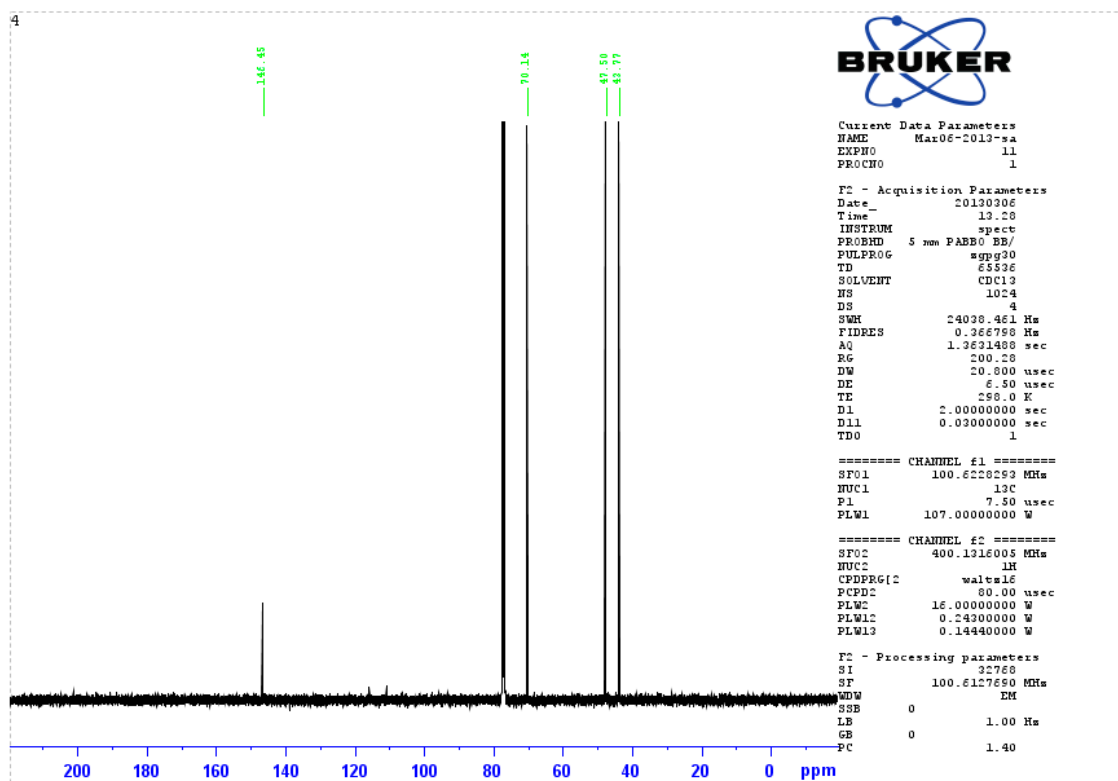


Figure S10. ¹³C-NMR spectrum of 5-(chloromethyl)-3-nitrooxazolidin-2-one (17).

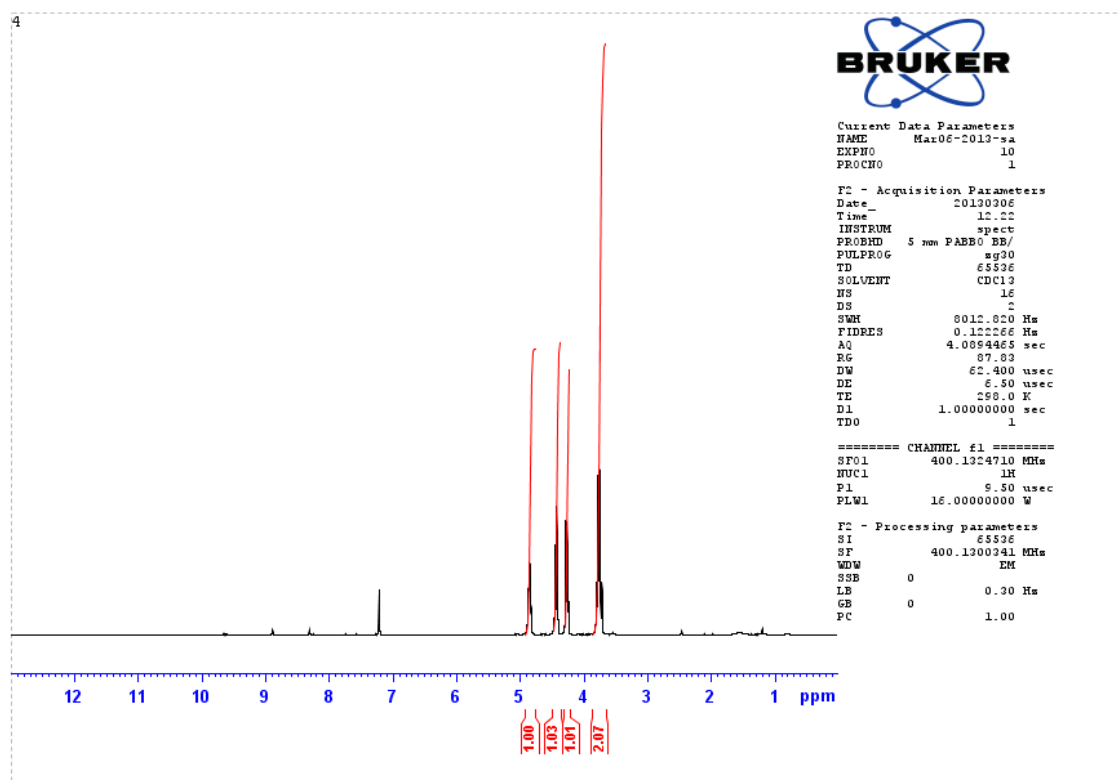


Figure S11. ¹H-NMR spectrum of 5-(chloromethyl)-3-nitrooxazolidin-2-one (17).

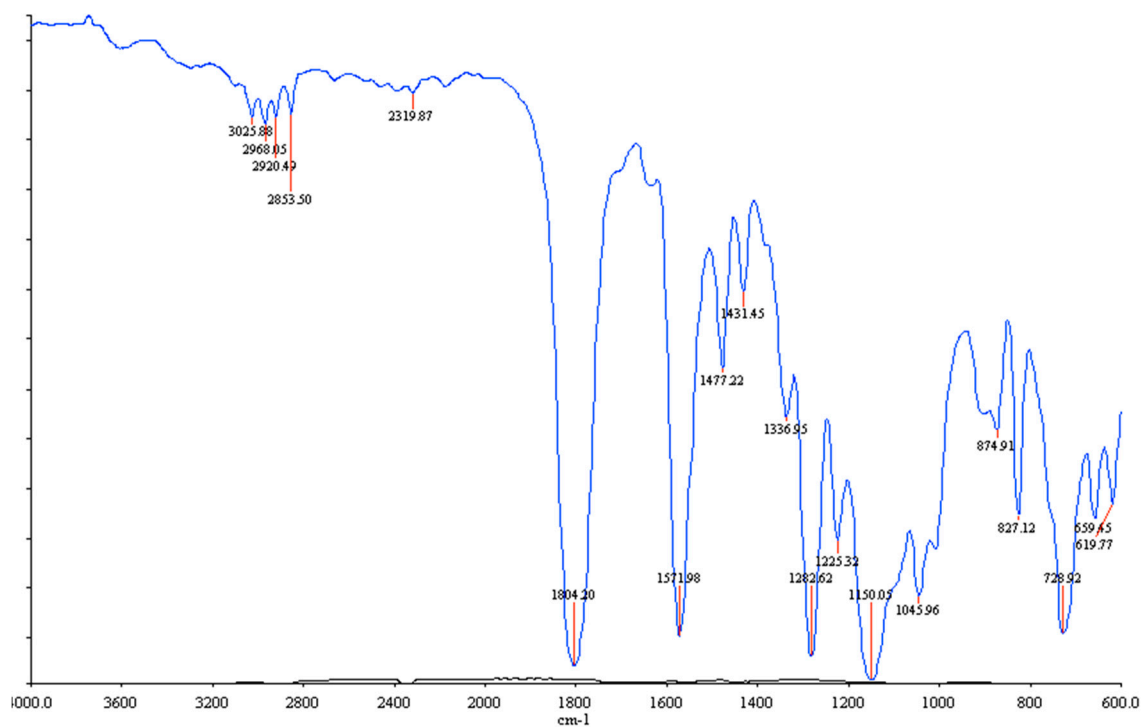
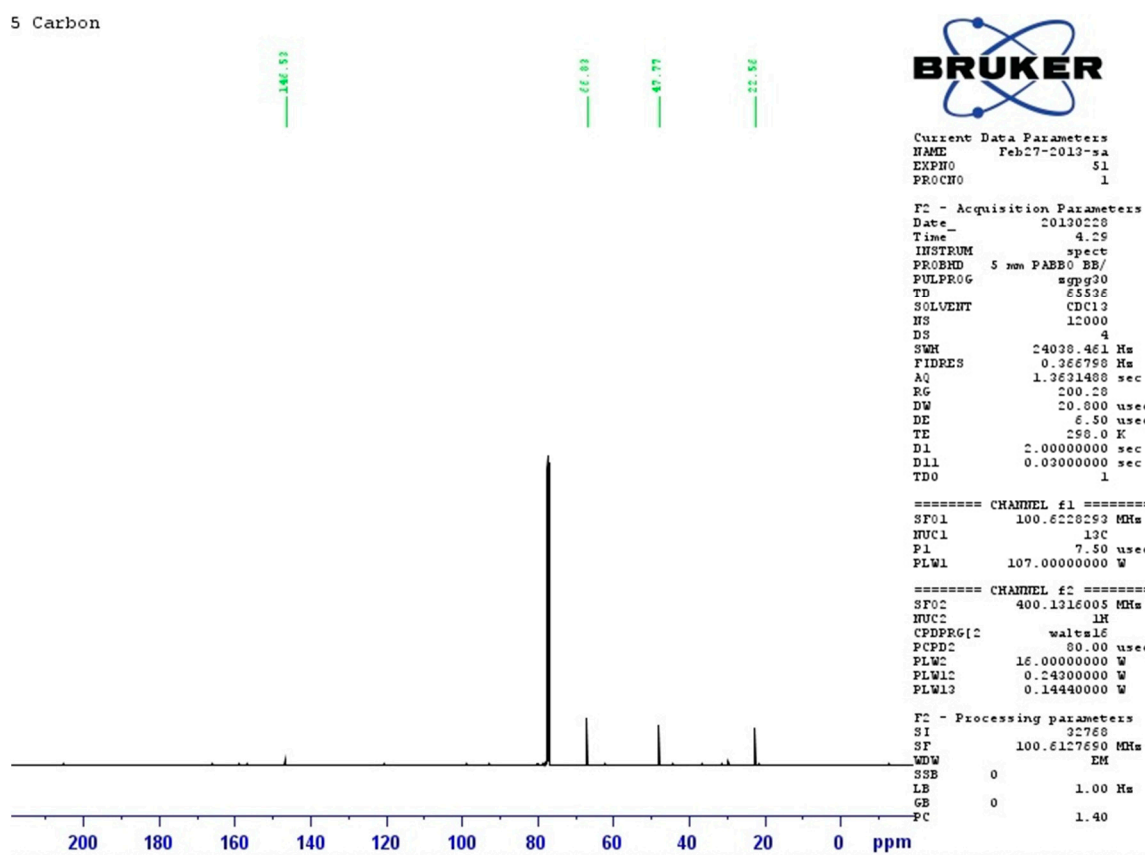
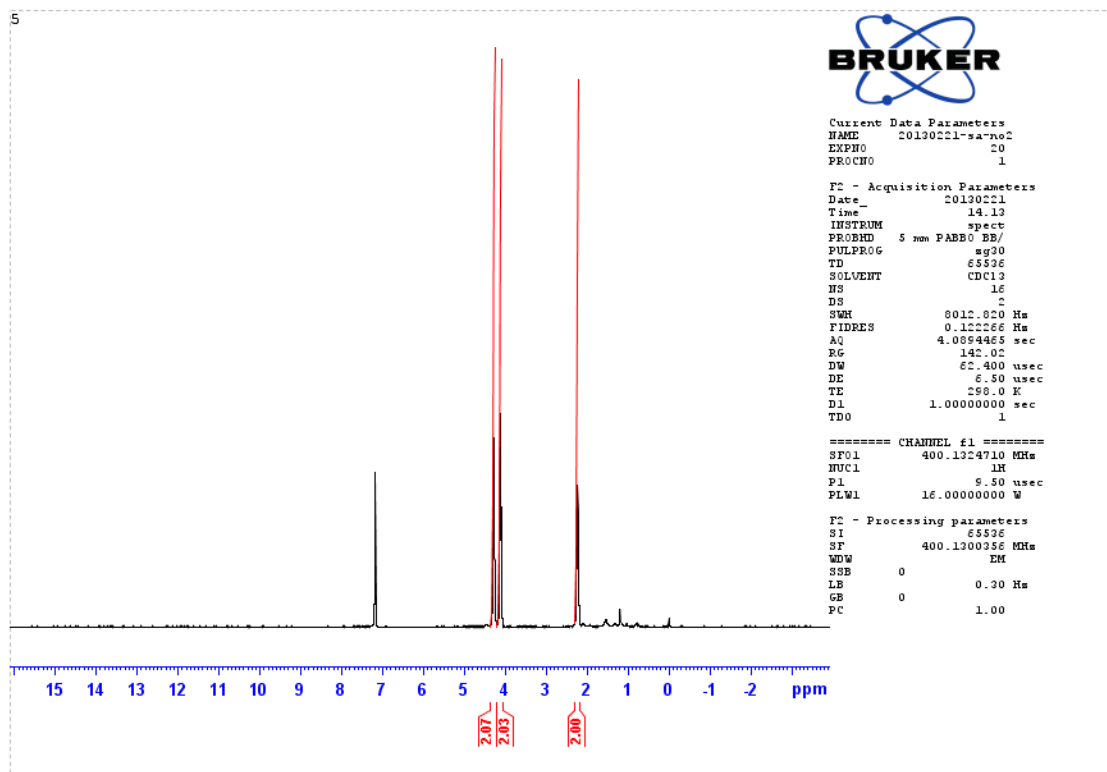


Figure S12. IR spectrum of 5-(chloromethyl)-3-nitrooxazolidin-2-one (17).

3-Nitro-1,3-oxazinan-2-one (18)

5 Carbon

Figure S13. ¹³C-NMR spectrum of 3-nitro-1,3-oxazinan-2-one (18).Figure S14. ¹H-NMR spectrum of ¹³C-NMR spectrum of 3-nitro-1,3-oxazinan-2-one (18).

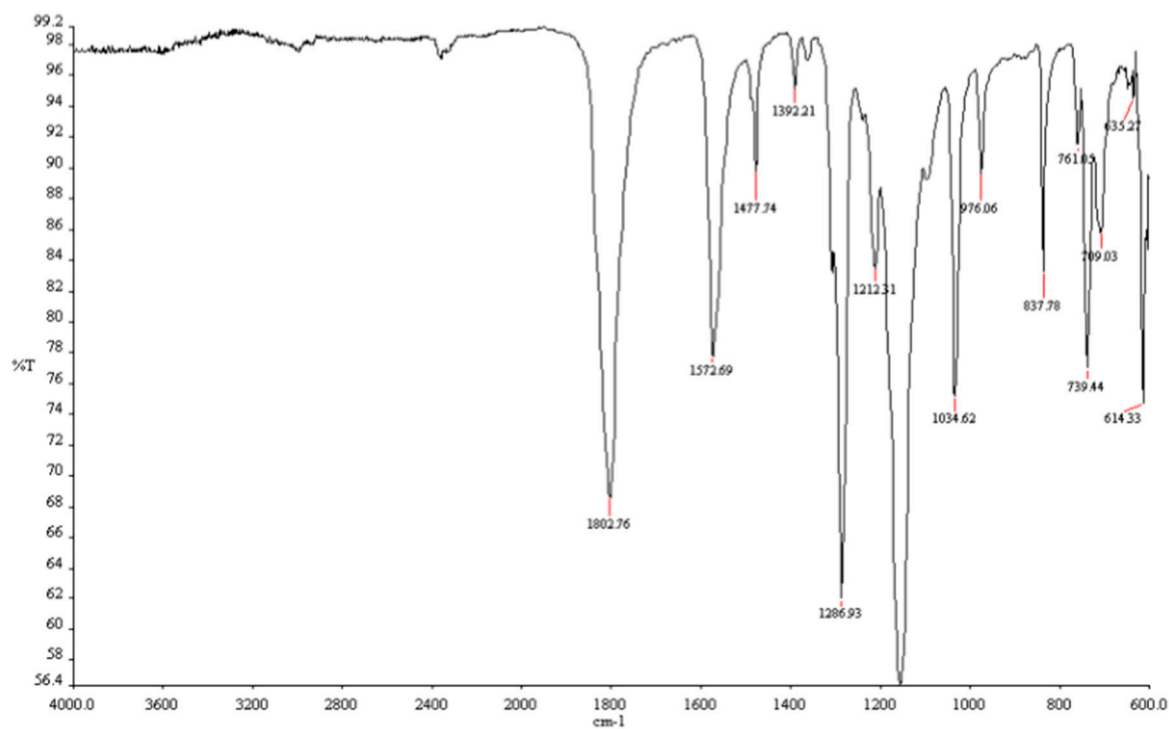


Figure S15. IR spectrum of ¹³C-NMR spectrum of 3-nitro-1,3-oxazinan-2-one (18).

Methyl N-(tert-butoxycarbonyl)-N-nitro-alaninate (19)

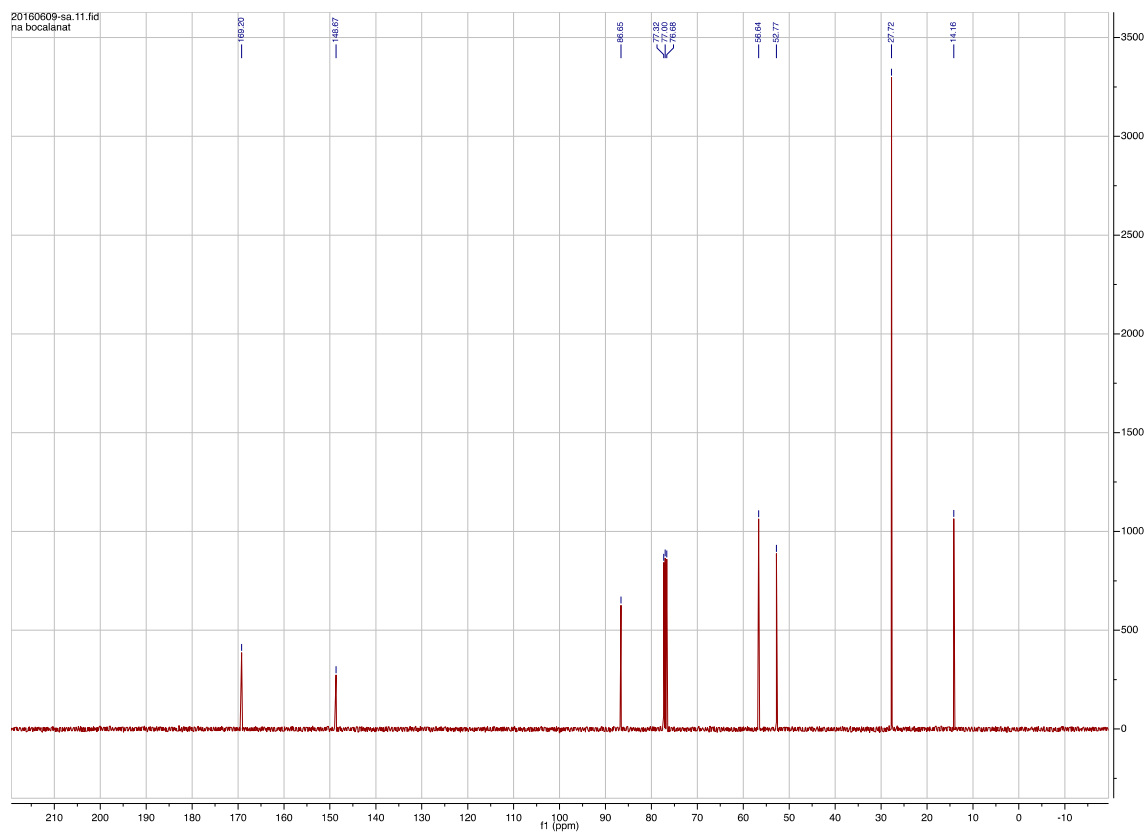


Figure S16. ¹³C-NMR spectrum of Methyl N-(tert-butoxycarbonyl)-N-nitro-alaninate (19).

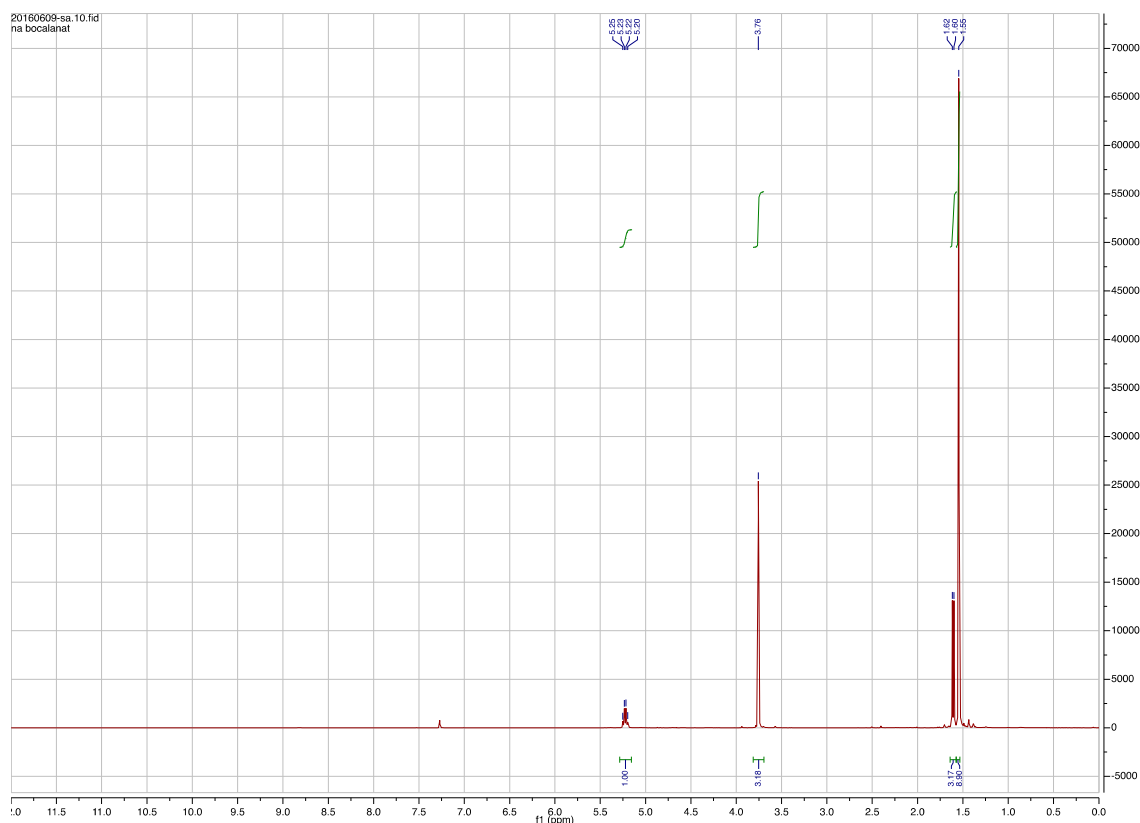


Figure S17. ^1H -NMR spectrum of Methyl *N*-(tert-butoxycarbonyl)-*N*-nitro-alaninate (19).

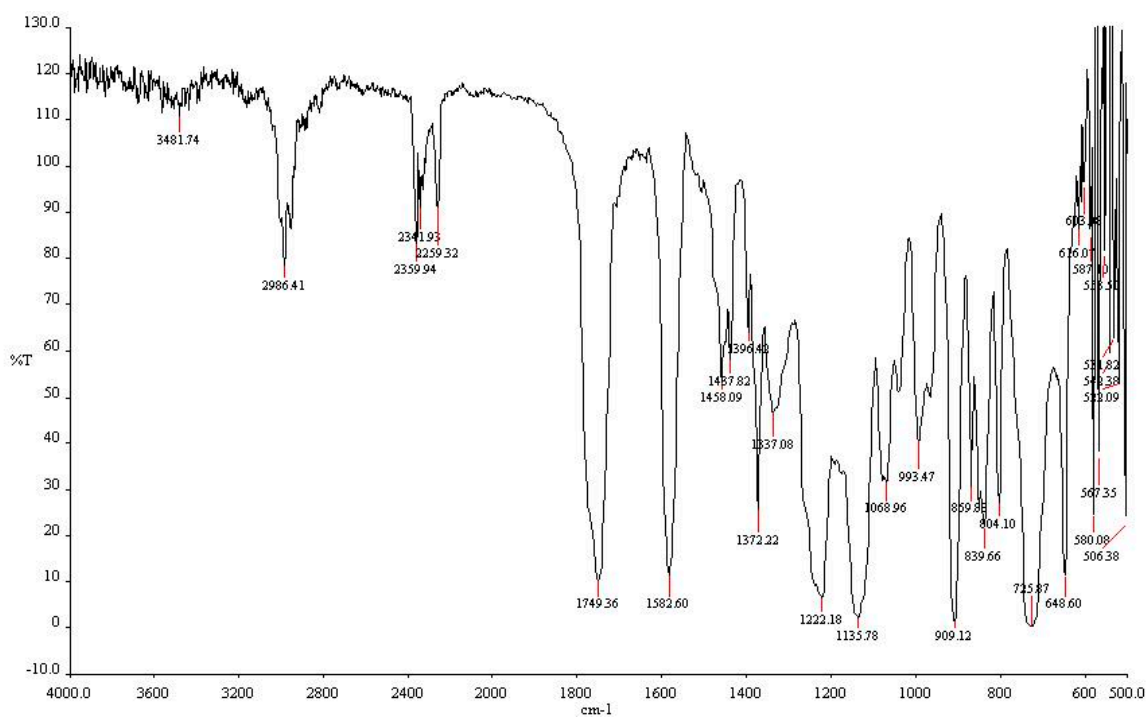
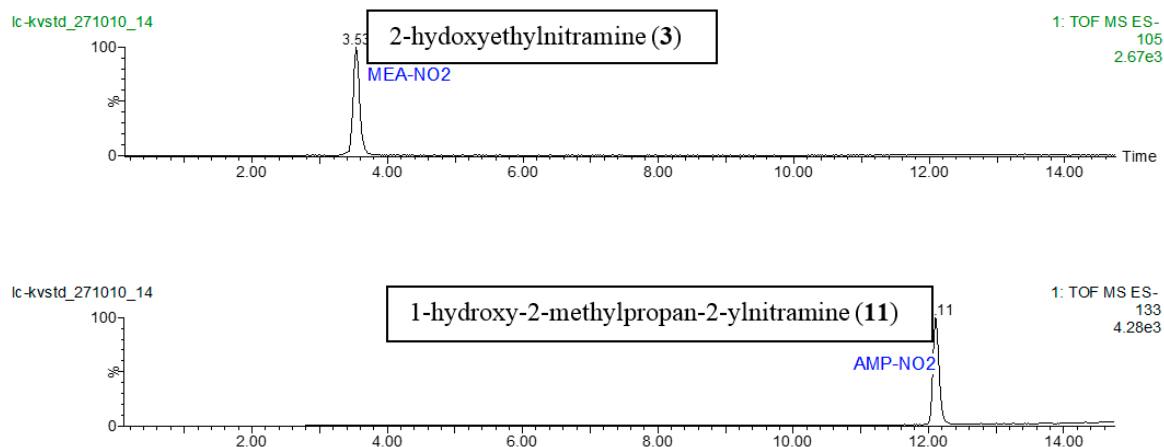
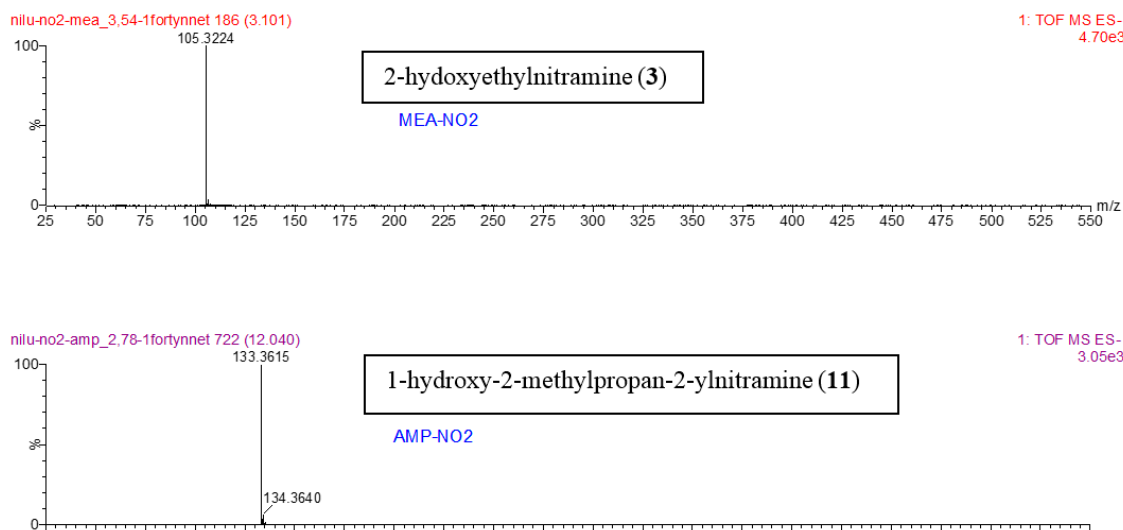


Figure S18. IR spectrum of Methyl *N*-(tert-butoxycarbonyl)-*N*-nitro-alaninate (19).

Table S1. Monitoring parameters for detection of nitramines with HPLC/UV/HRMS.

Analyte	Molecular Weight *	Monit. Ion [M – H] [–]	Ionisation Mode
2-hydroxyethylnitramine	106.0378	105.0300	ES [–]
1-hydroxy-2-methylpropan-2-yl nitramine	134.0691	133.0613	ES [–]

* Monoisotopic.

**Figure S19.** Separation of the nitramines by the HPLC column Waters Atlantis dC18, 3 μ m, 2.1 $\times$ 150 mm, using a binary water/acetonitrile gradient.**Figure S20.** HRMS spectra of the ions [M – H][–] of 2-hydroxyethylnitramine and 1-hydroxy-2-methylpropan-2-yl nitramine obtained by HPLC/HRMS.

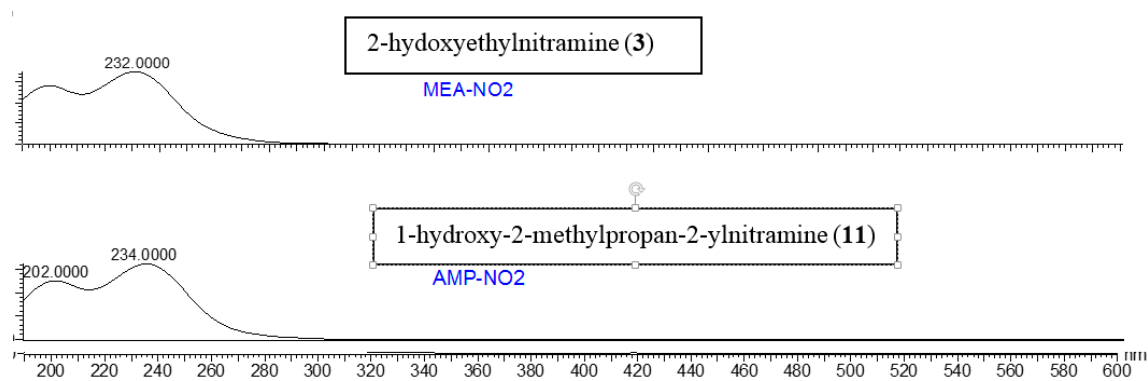


Figure S21. UV-spectra of the nitramines obtained by HPLC/UV.