

# Supplementary Materials: Safe Synthesis of Alkylhydroxy and Alkylamino Nitramines

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## 1. Spectral Data for Selected Compounds

### 3-Nitrooxazolidin-2-one (8)

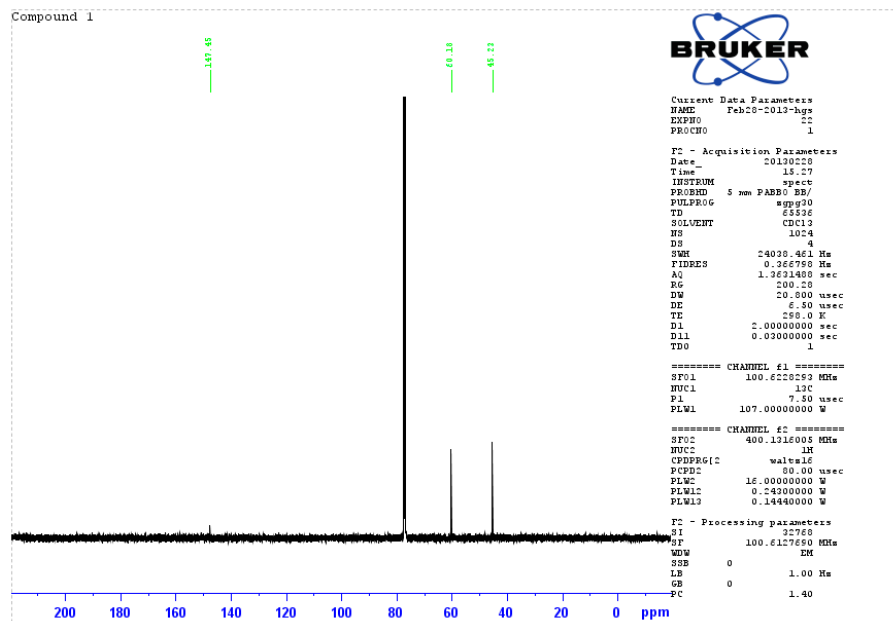


Figure S1. <sup>13</sup>C-NMR spectrum of 3-nitrooxazolidin-2-one (8).

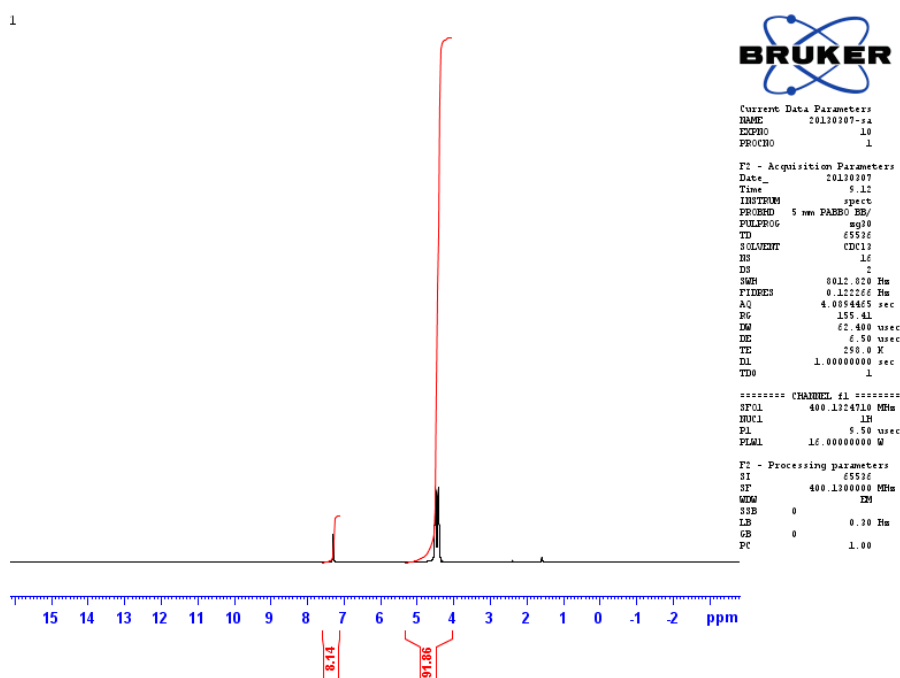


Figure S2. <sup>1</sup>H-NMR spectrum of 3-nitrooxazolidin-2-one (8).

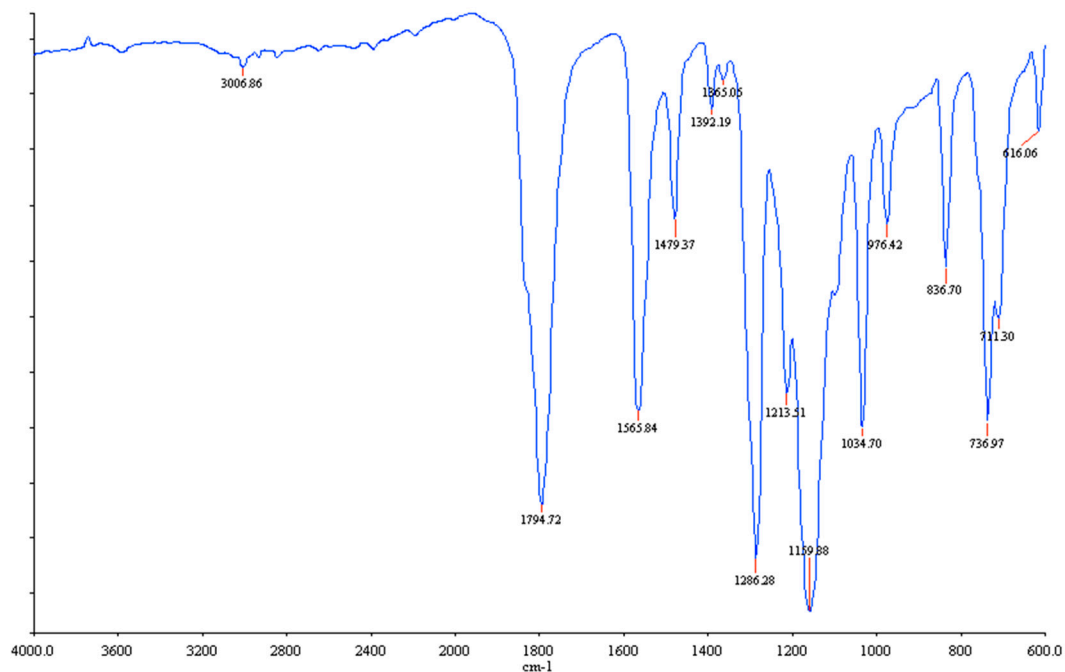
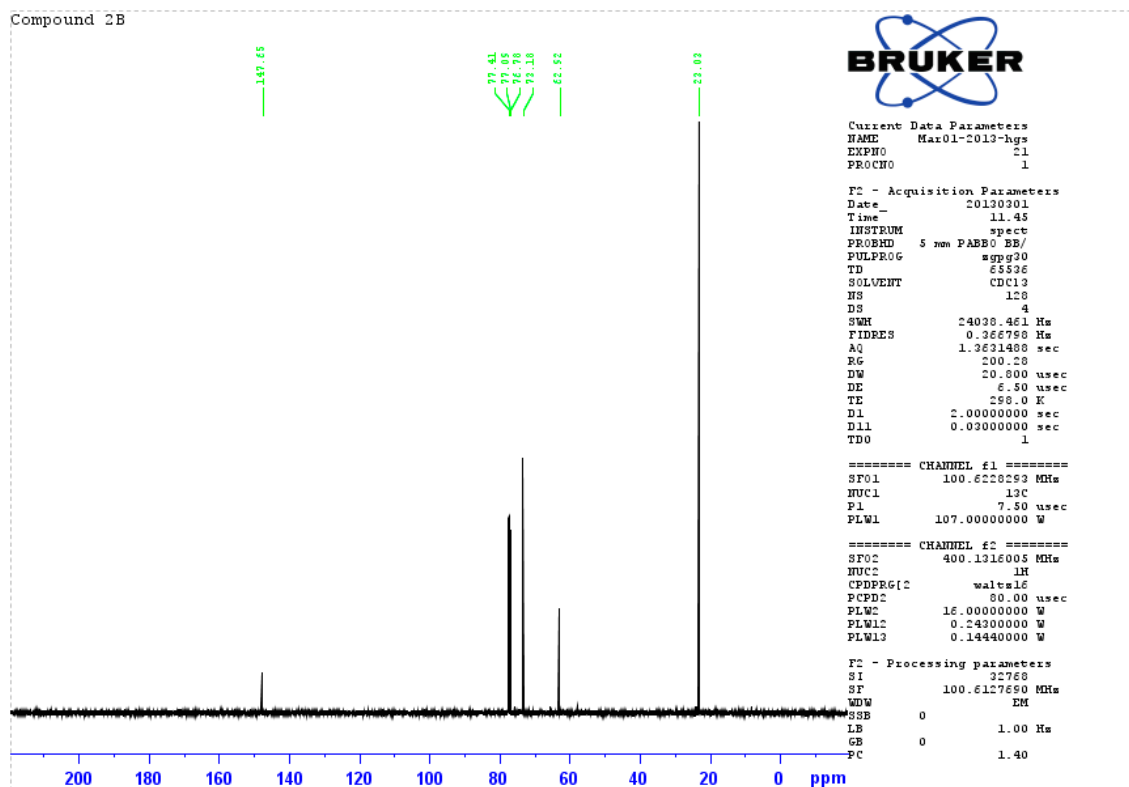


Figure S3. IR spectrum of 3-nitrooxazolidin-2-one (8).

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

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

Compound 2B

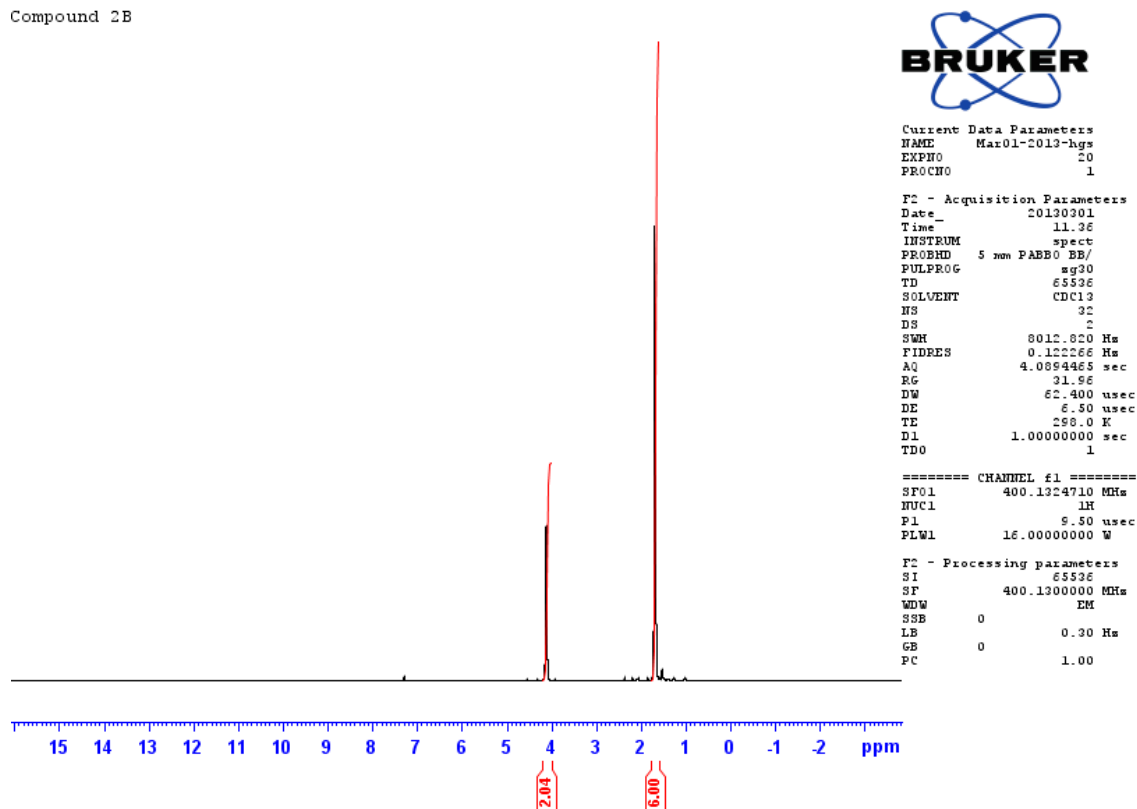
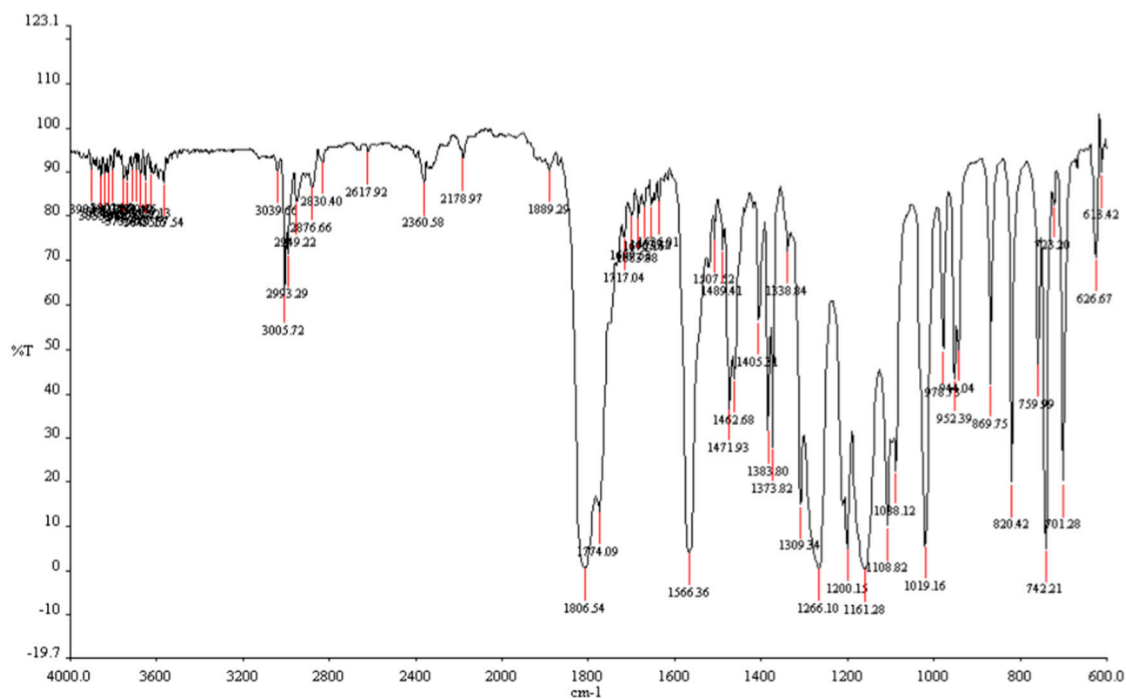
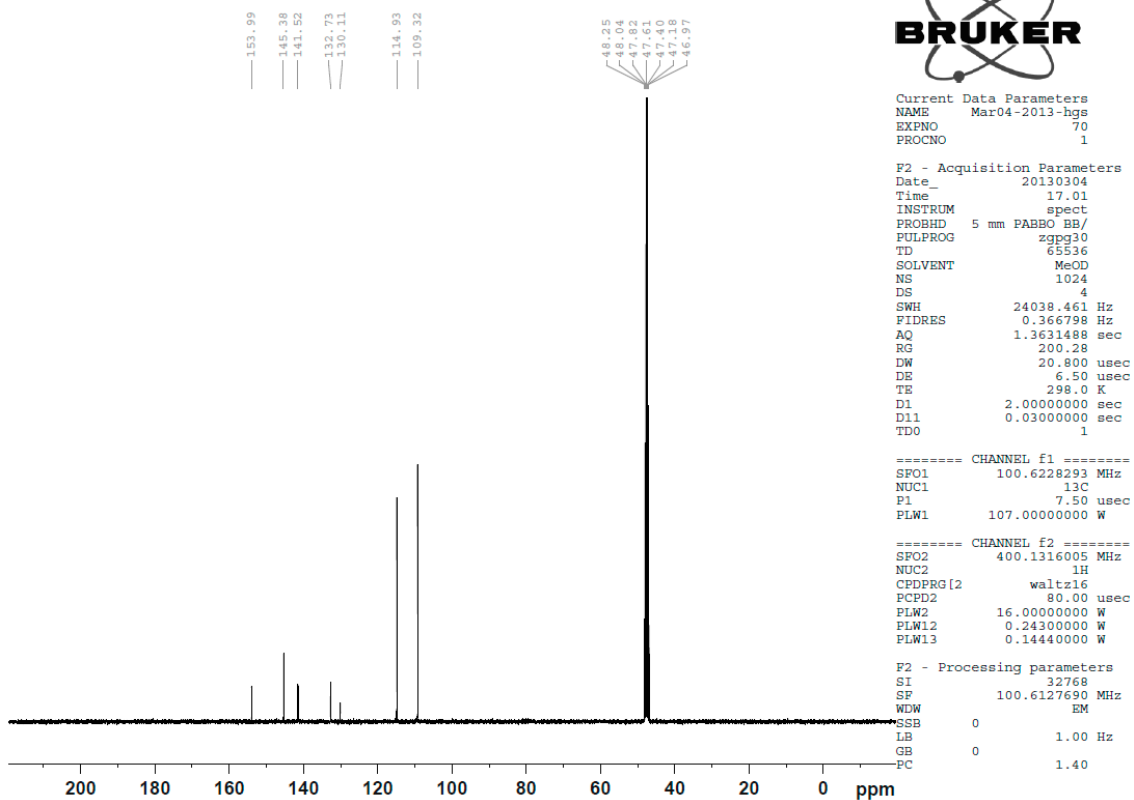
Figure S5. <sup>1</sup>H-NMR spectrum of 4,4-dimethyl-3-nitroazolidin-2-one (9).

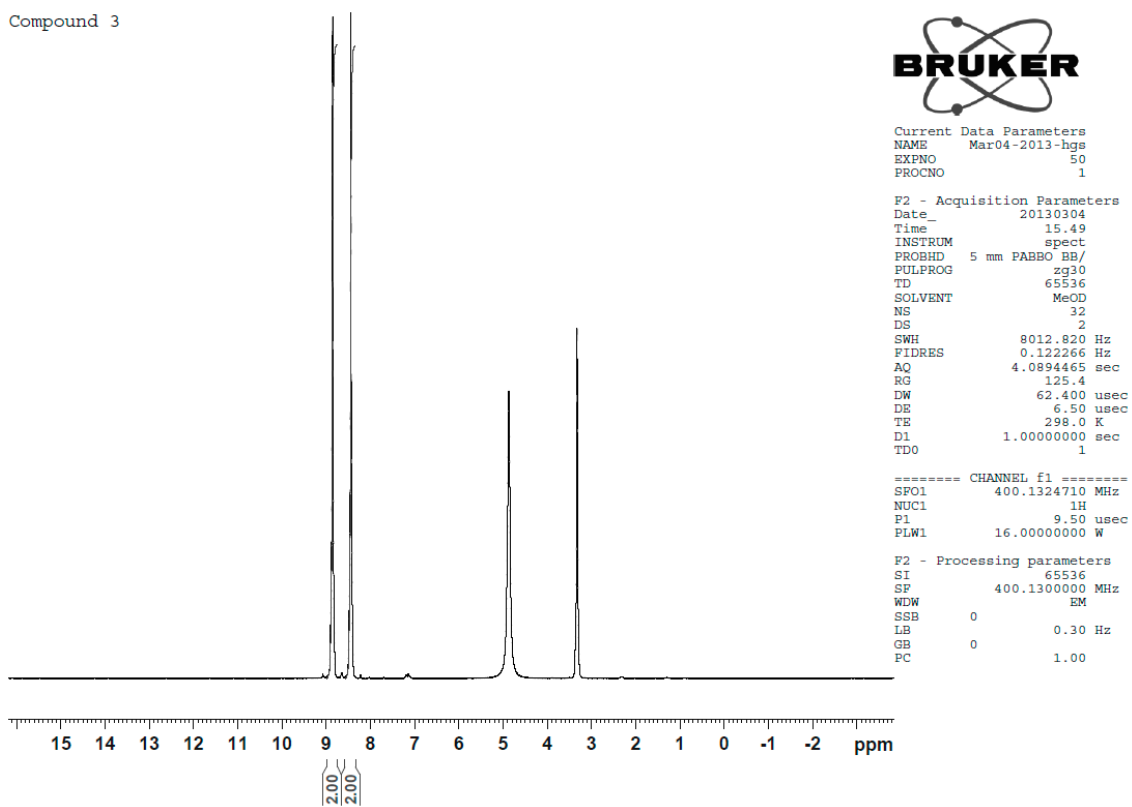
Figure S6. IR spectrum of 4,4-dimethyl-3-nitroazolidin-2-one (9).

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

Compound 3

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

Compound 3

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

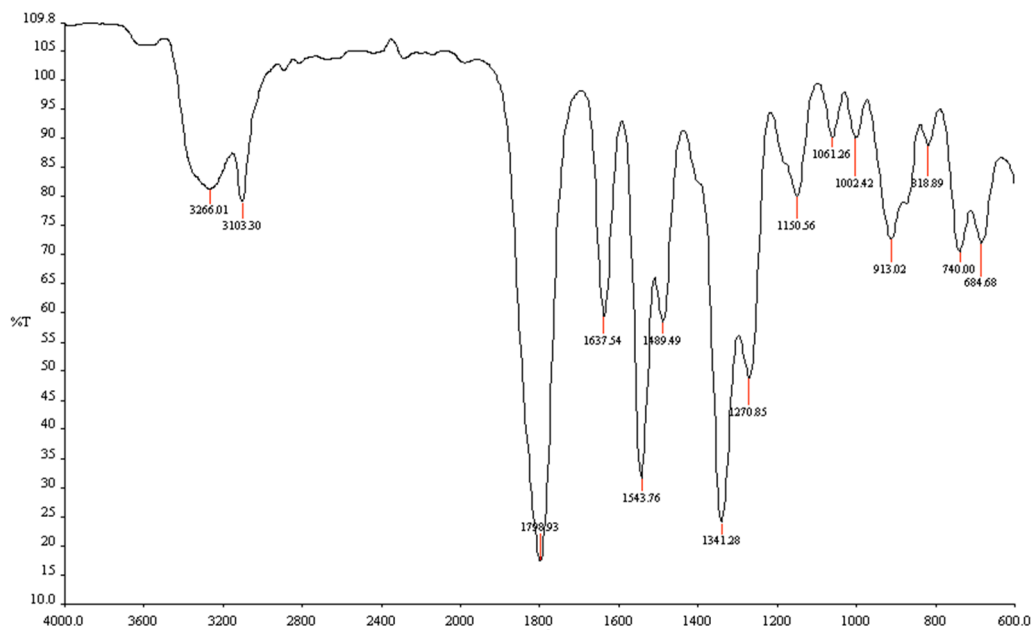


Figure S9. IR spectrum of 3-nitrobenzo[d]oxazol-2(3H)-one (16).

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

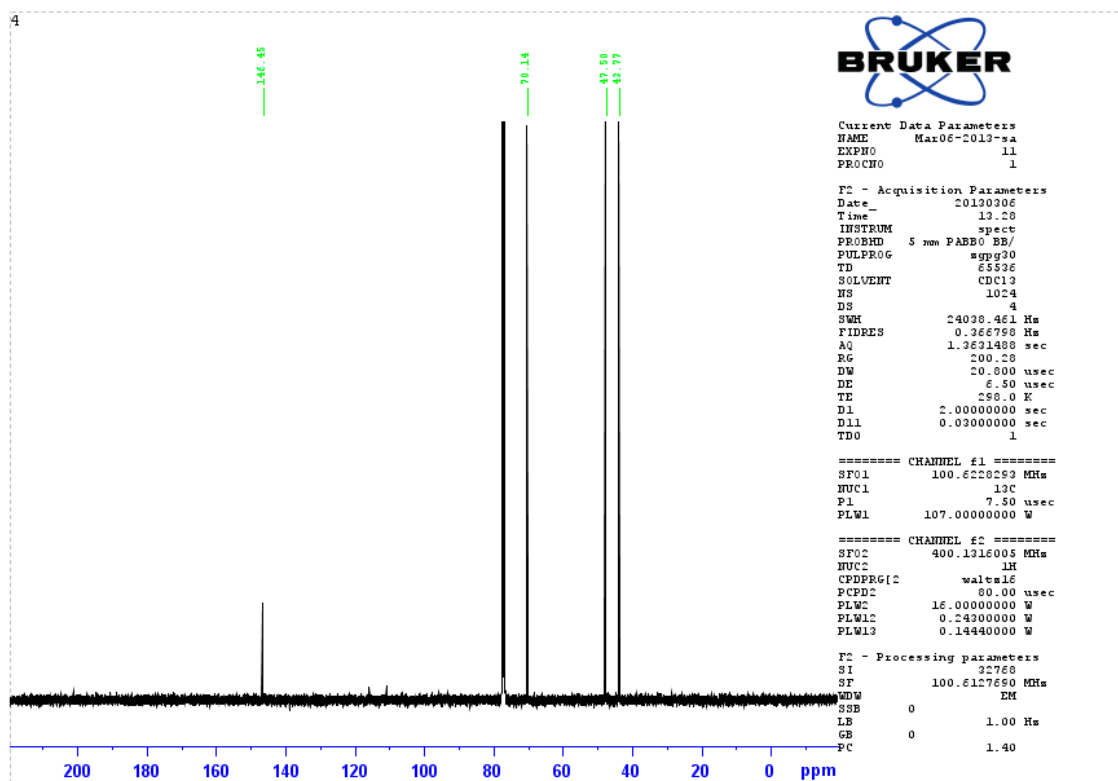


Figure S10.  $^{13}\text{C}$ -NMR spectrum of 5-(chloromethyl)-3-nitrooxazolidin-2-one (17).

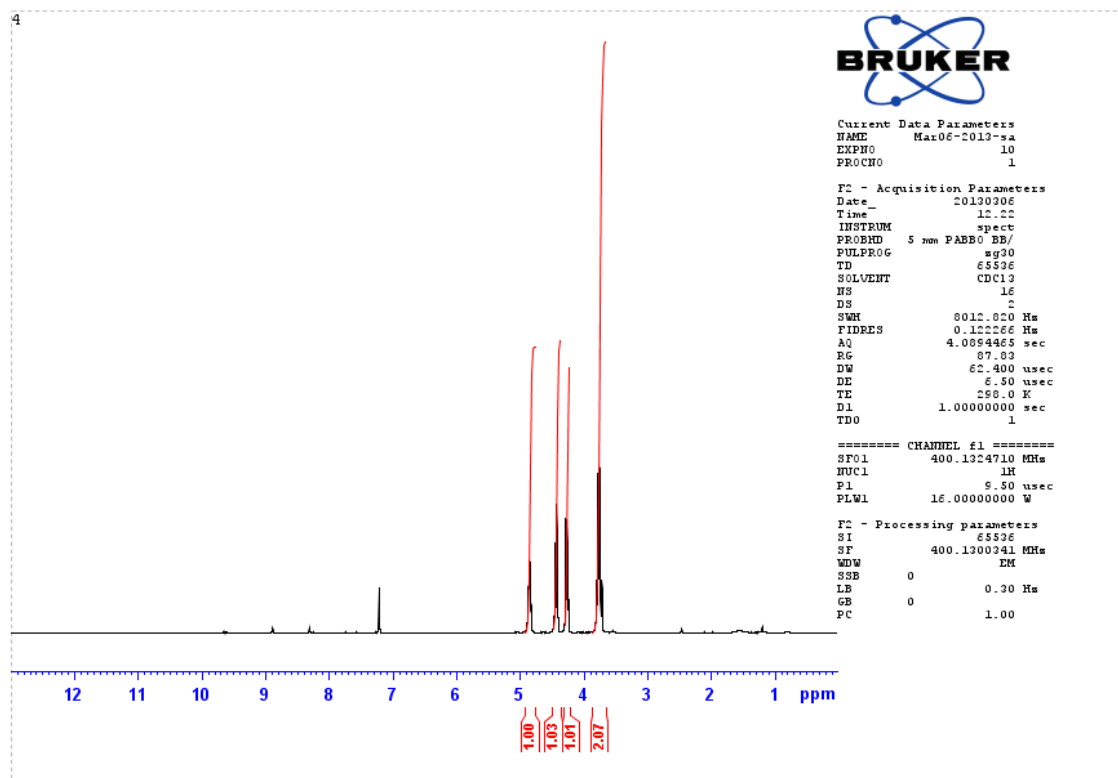


Figure S11. <sup>1</sup>H-NMR spectrum of 5-(chloromethyl)-3-nitrooxazolidin-2-one (17).

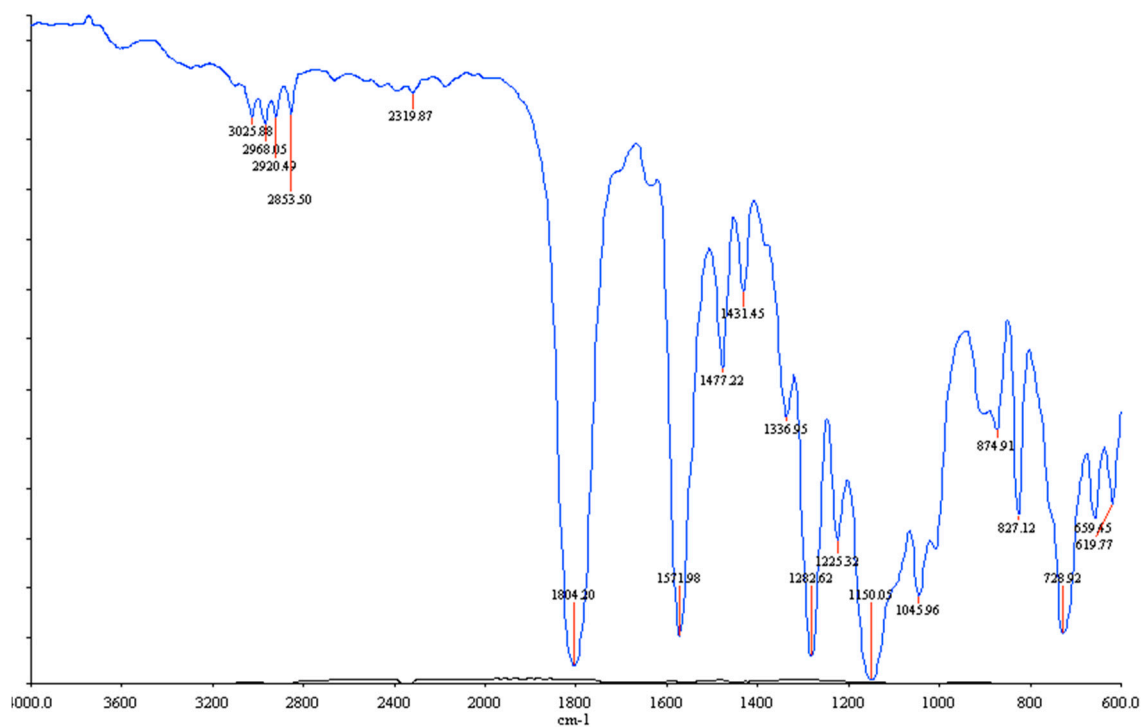
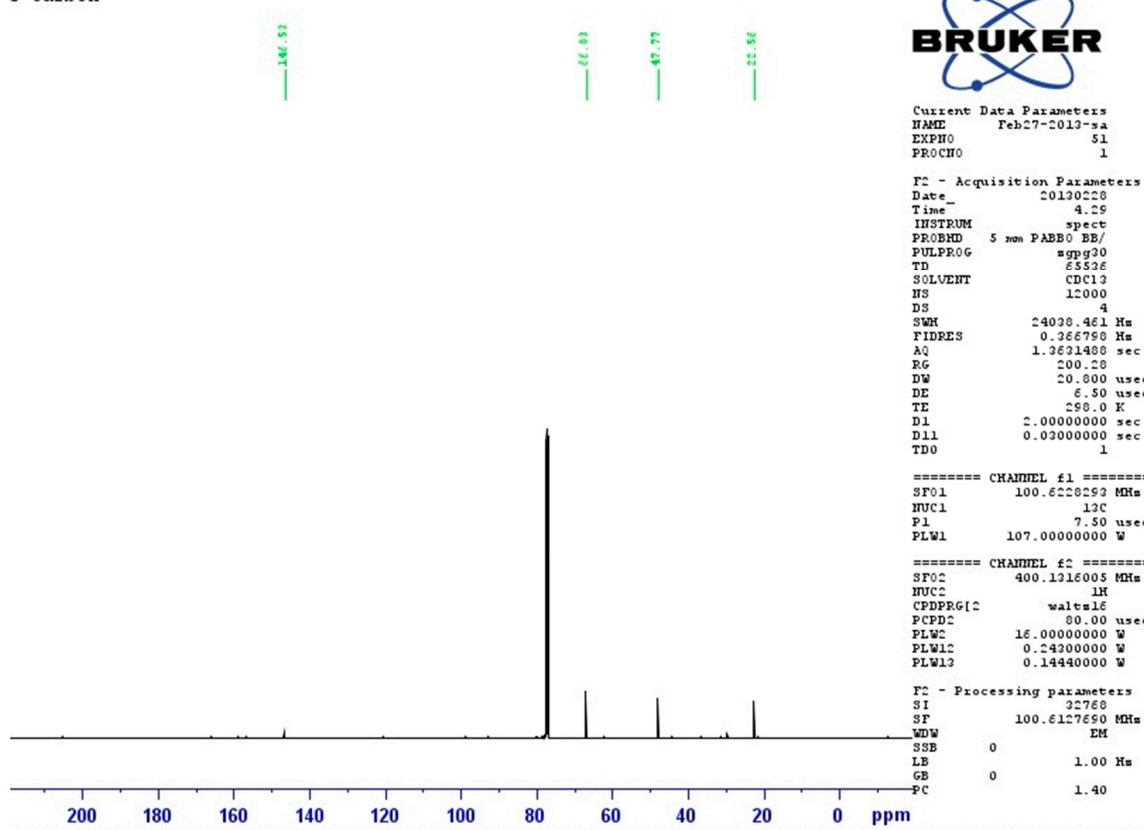
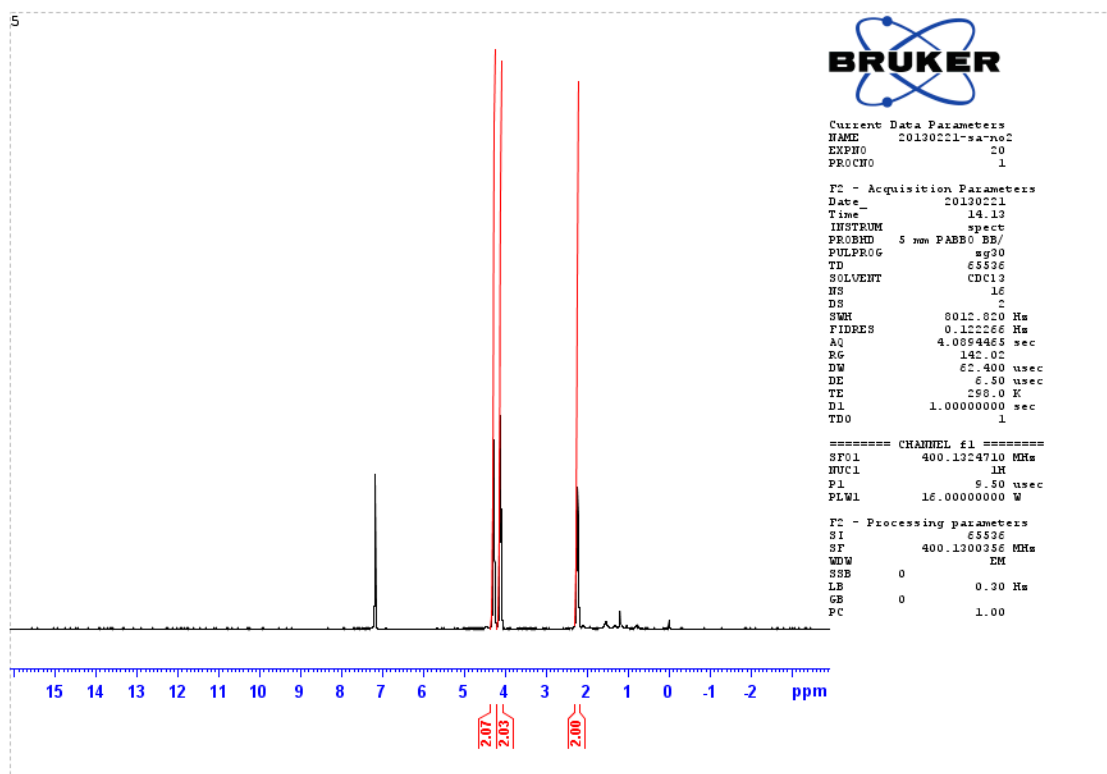


Figure S12. IR spectrum of 5-(chloromethyl)-3-nitrooxazolidin-2-one (17).

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

5 Carbon

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

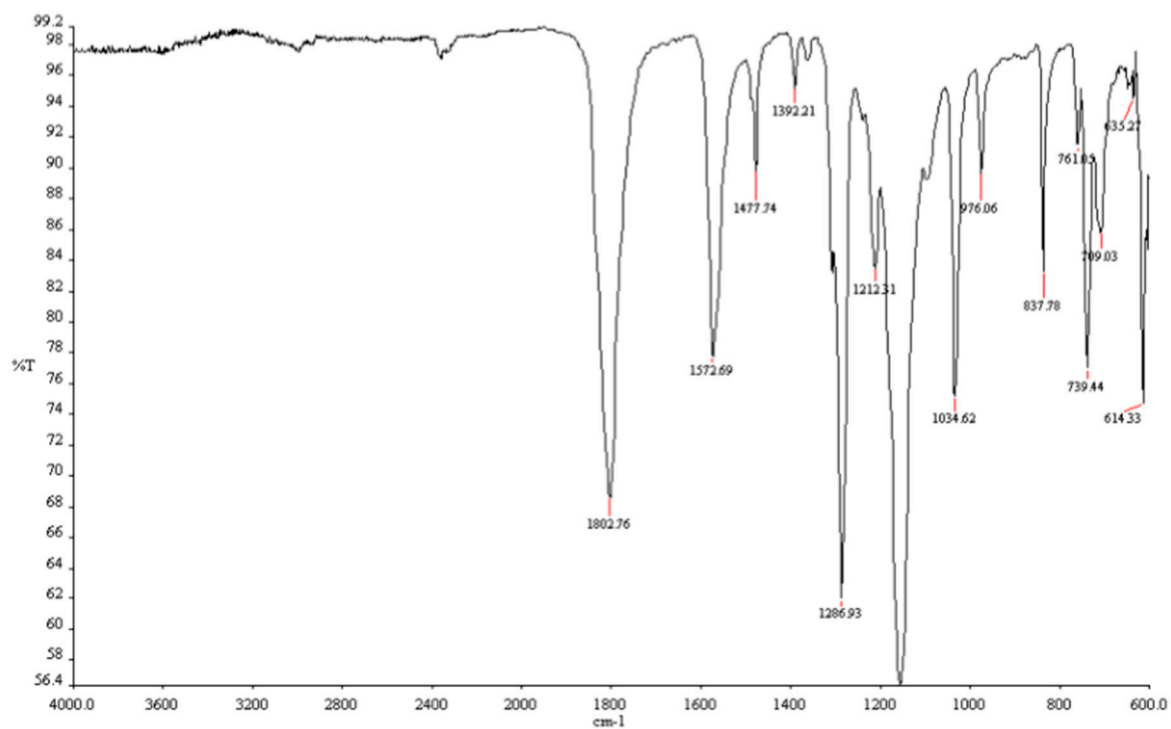


Figure S15. IR spectrum of <sup>13</sup>C-NMR spectrum of 3-nitro-1,3-oxazinan-2-one (18).

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

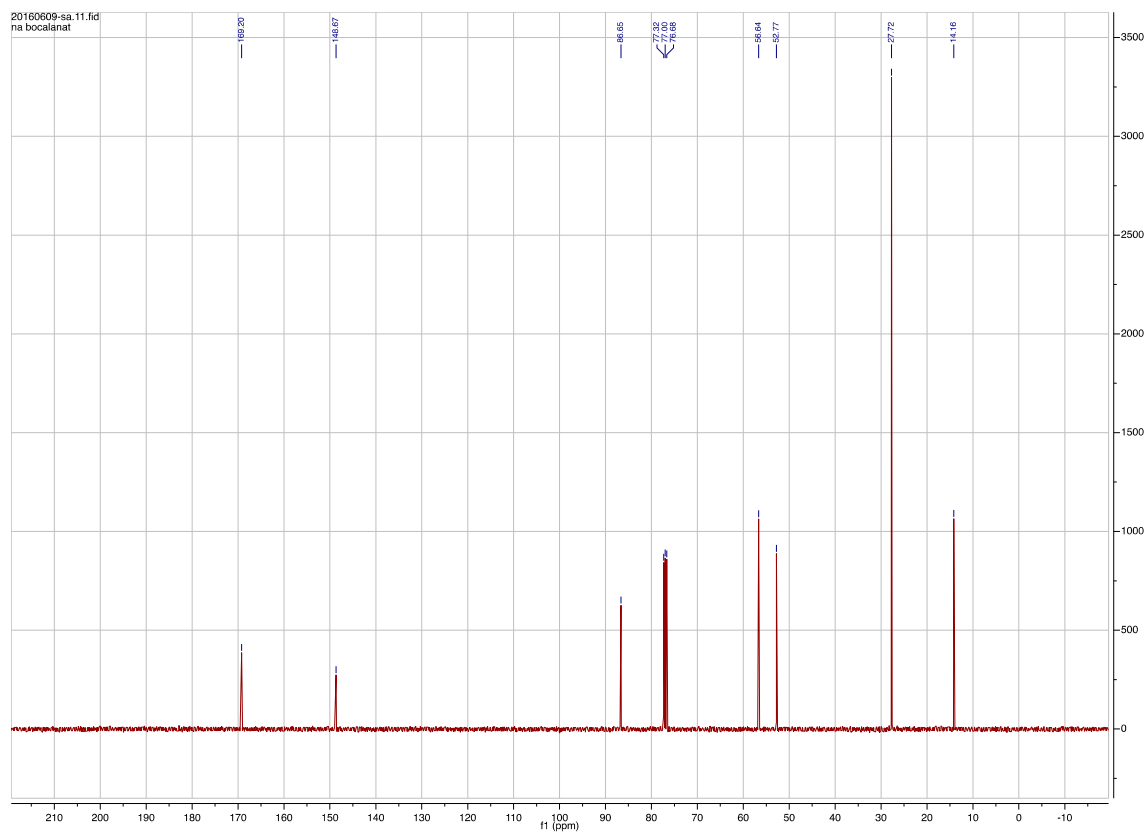


Figure S16. <sup>13</sup>C-NMR spectrum of Methyl *N*-(tert-butoxycarbonyl)-*N*-nitro-alaninate (19).



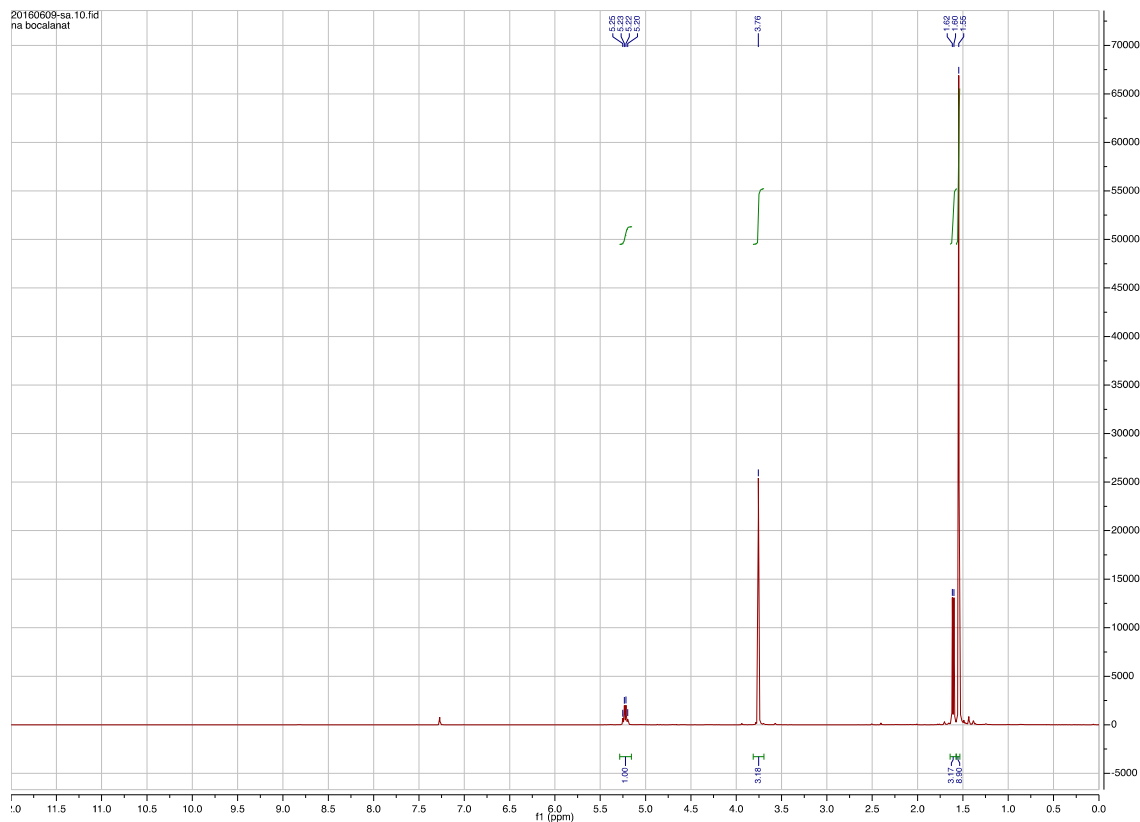


Figure S17.  $^1\text{H}$ -NMR spectrum of Methyl *N*-(tert-butoxycarbonyl)-*N*-nitro-alaninate (19).

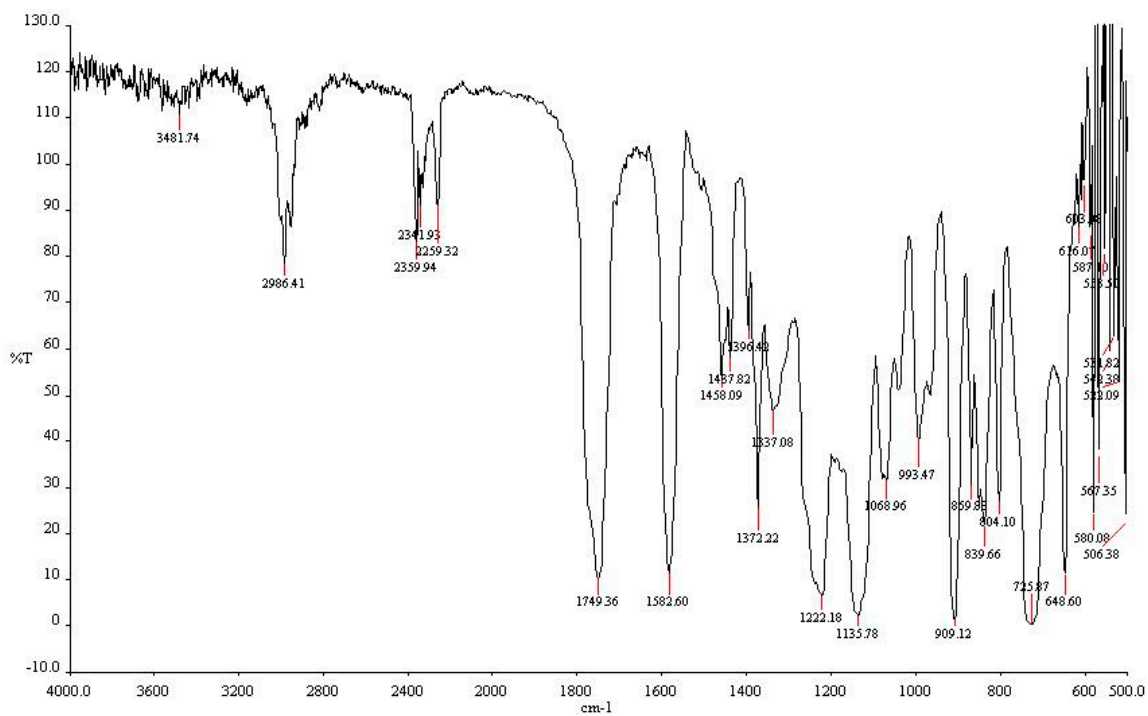
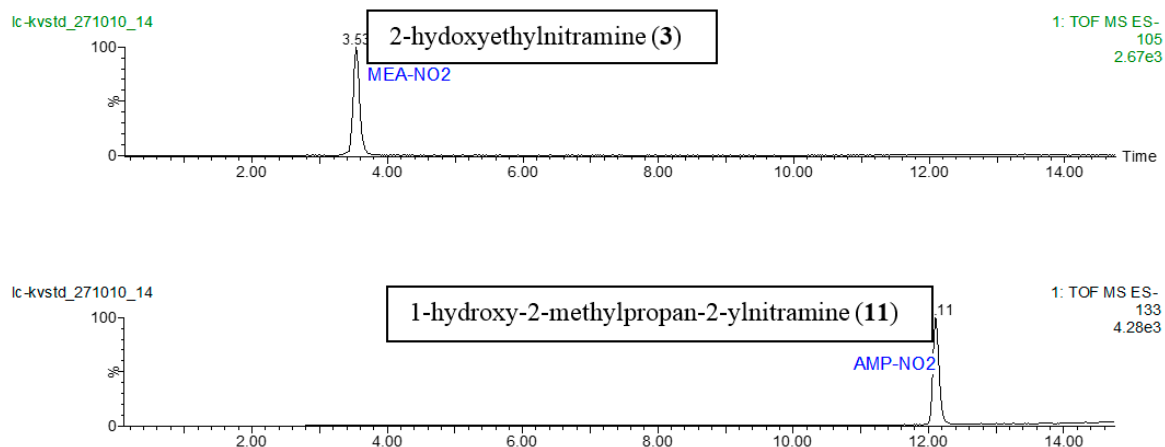
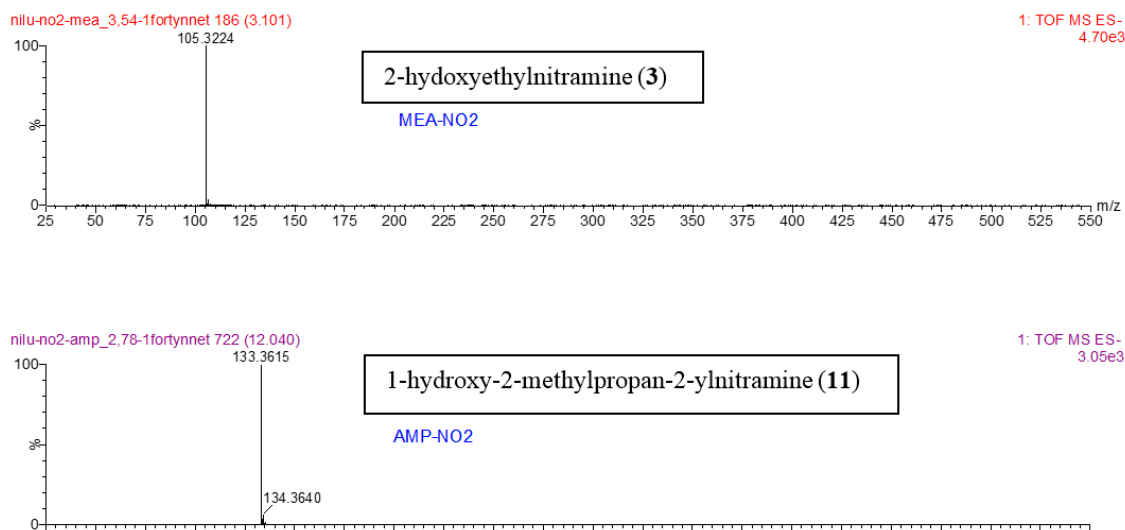


Figure S18. IR spectrum of Methyl *N*-(tert-butoxycarbonyl)-*N*-nitro-alaninate (19).

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

Analyte	Molecular Weight *	Monit. Ion [M – H] <sup>-</sup>	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  $\mu$ m, 2.1  $\times$  150 mm, using a binary water/acetonitrile gradient.**Figure S20.** HRMS spectra of the ions [M – H]<sup>-</sup> of 2-hydroxyethylnitramine and 1-hydroxy-2-methylpropan-2-yl nitramine obtained by HPLC/HRMS.

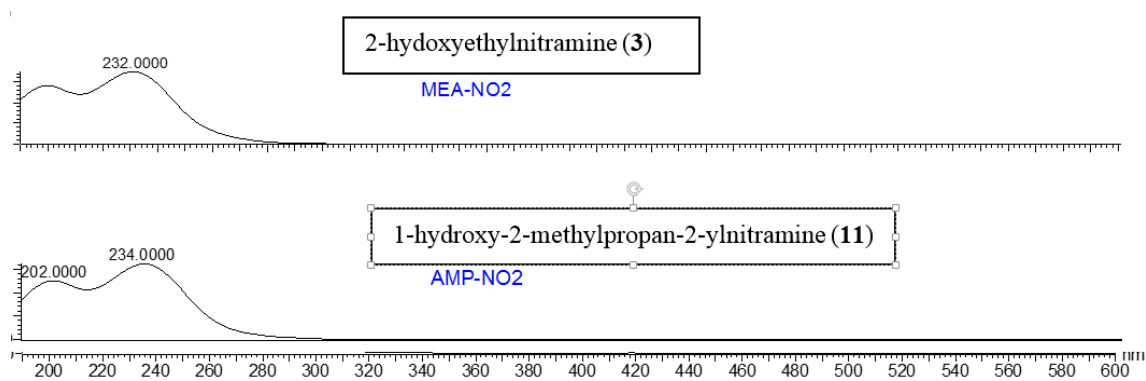


Figure S21. UV-spectra of the nitramines obtained by HPLC/UV.