

Synthesis of functional 2-substituted 1,3-dinitroimidazolidines. A new synthetic approach to high-energy compounds

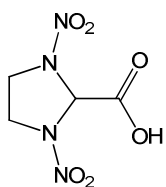
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Supporting Information

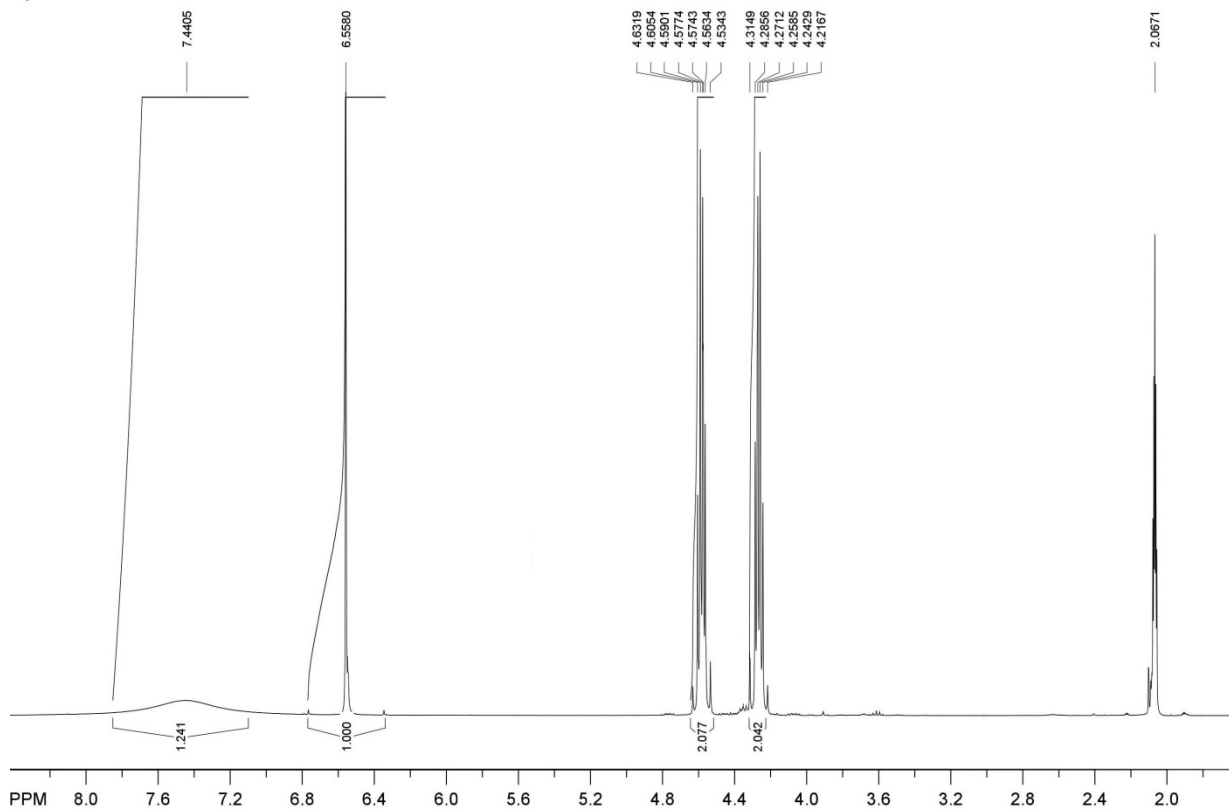
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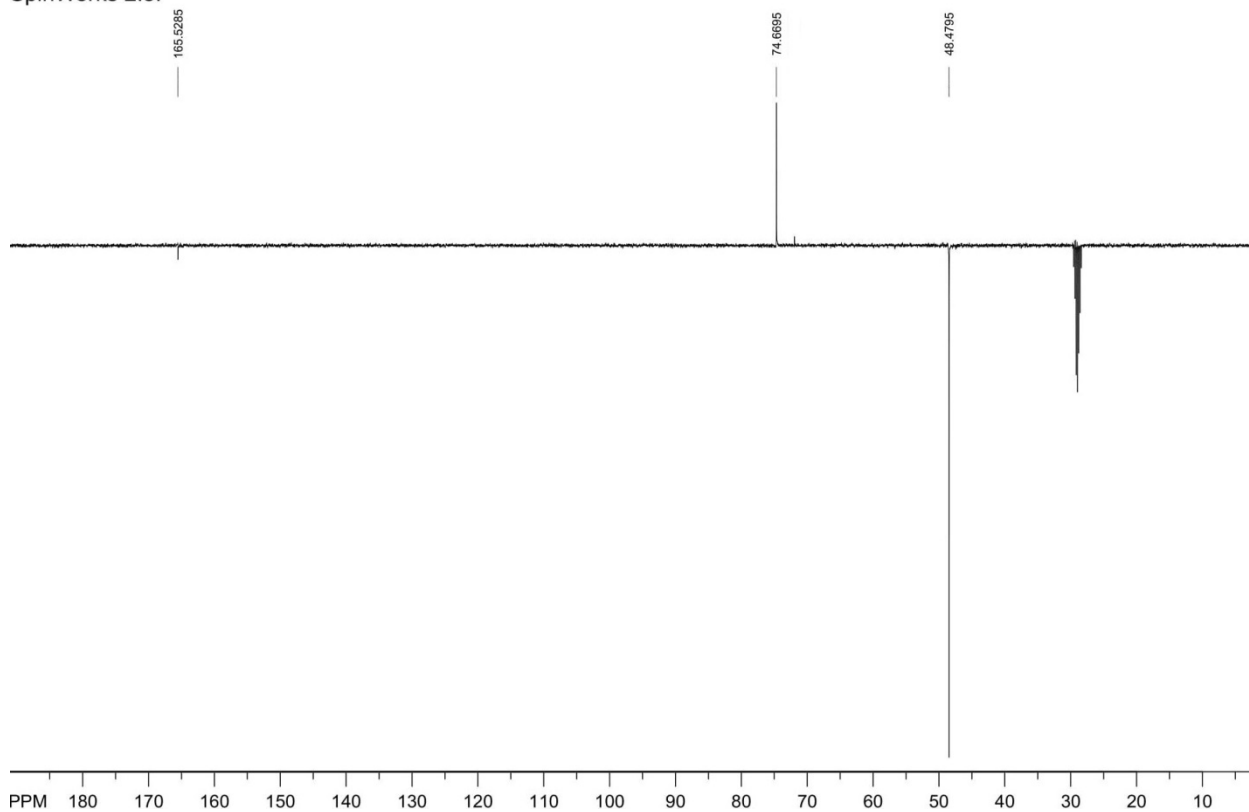


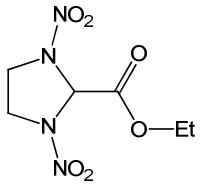
1,3-Dinitro-1,3-diazacyclopentane-2-carboxylic acid (1)

SpinWorks 2.5:



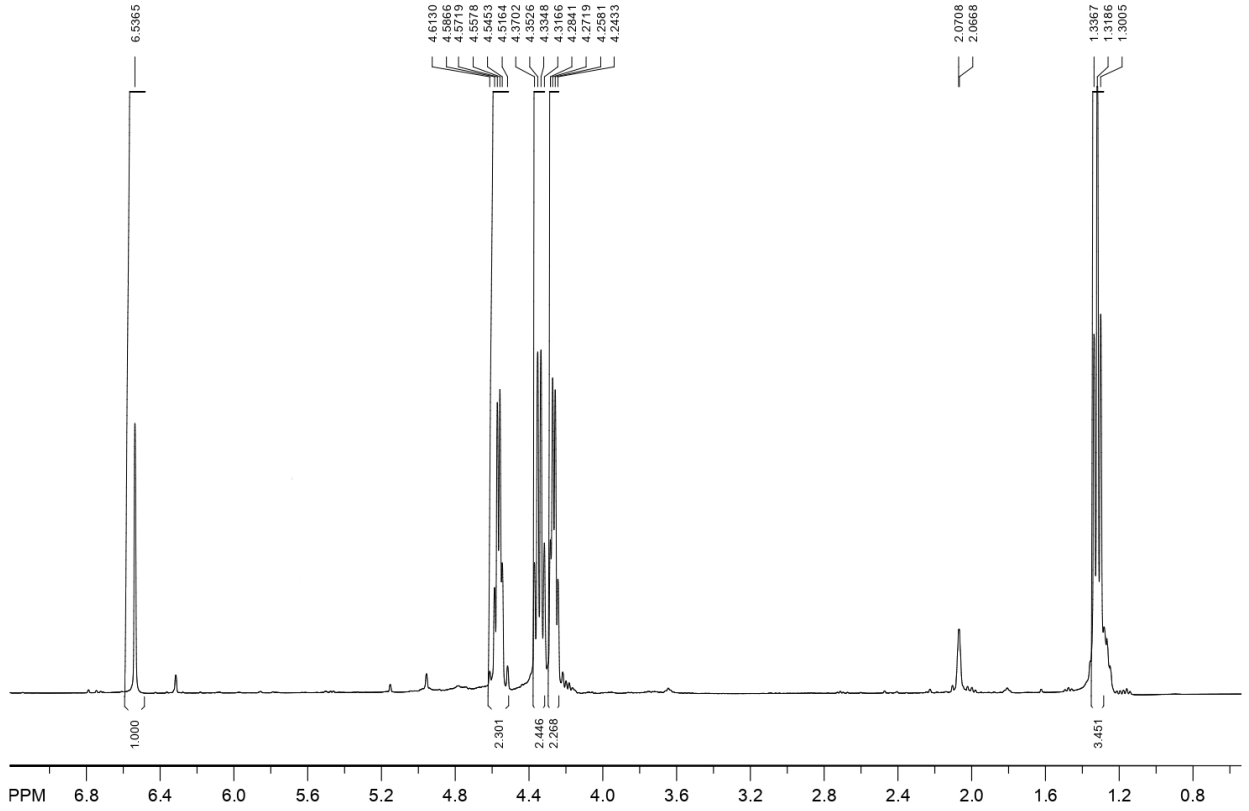
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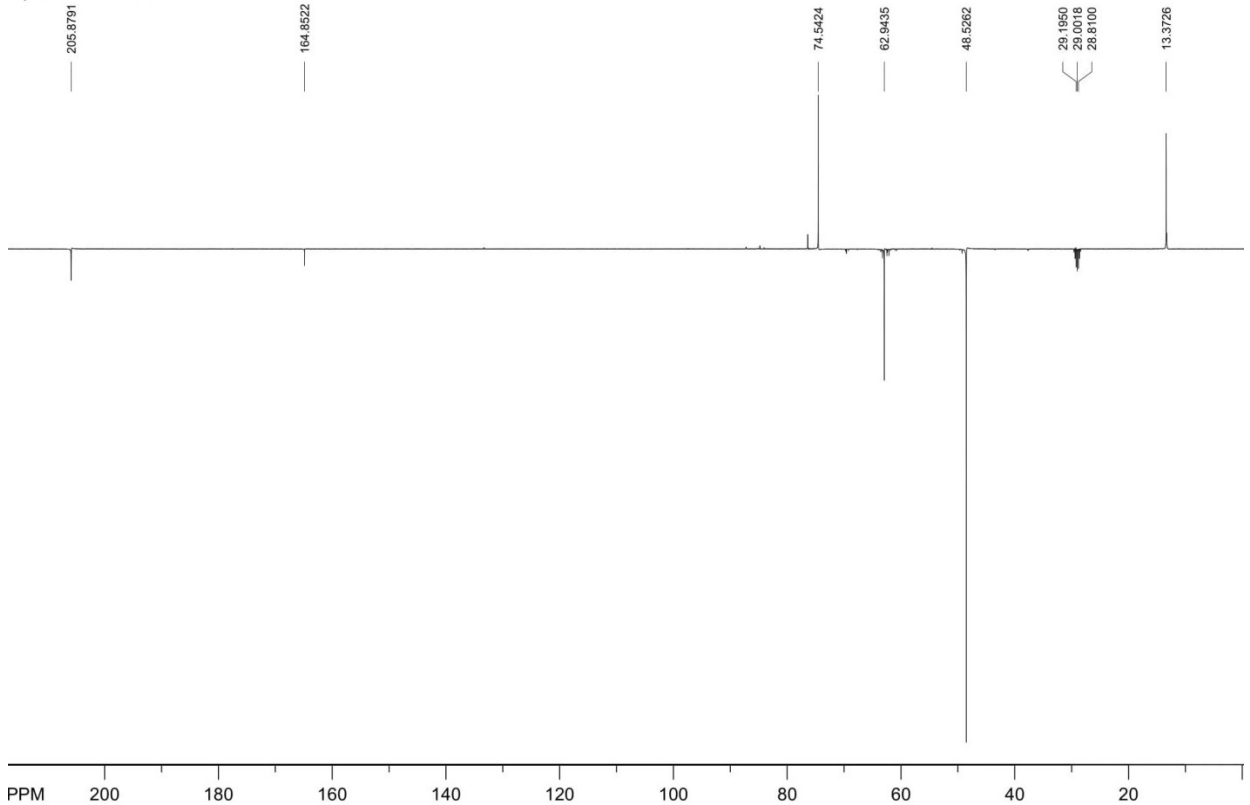


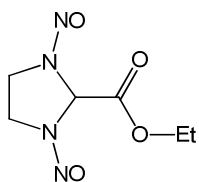
Ethyl 1,3-dinitro-1,3-diazacyclopentane-2-carboxylate (5)

SpinWorks 2.5:



SpinWorks 2.5:

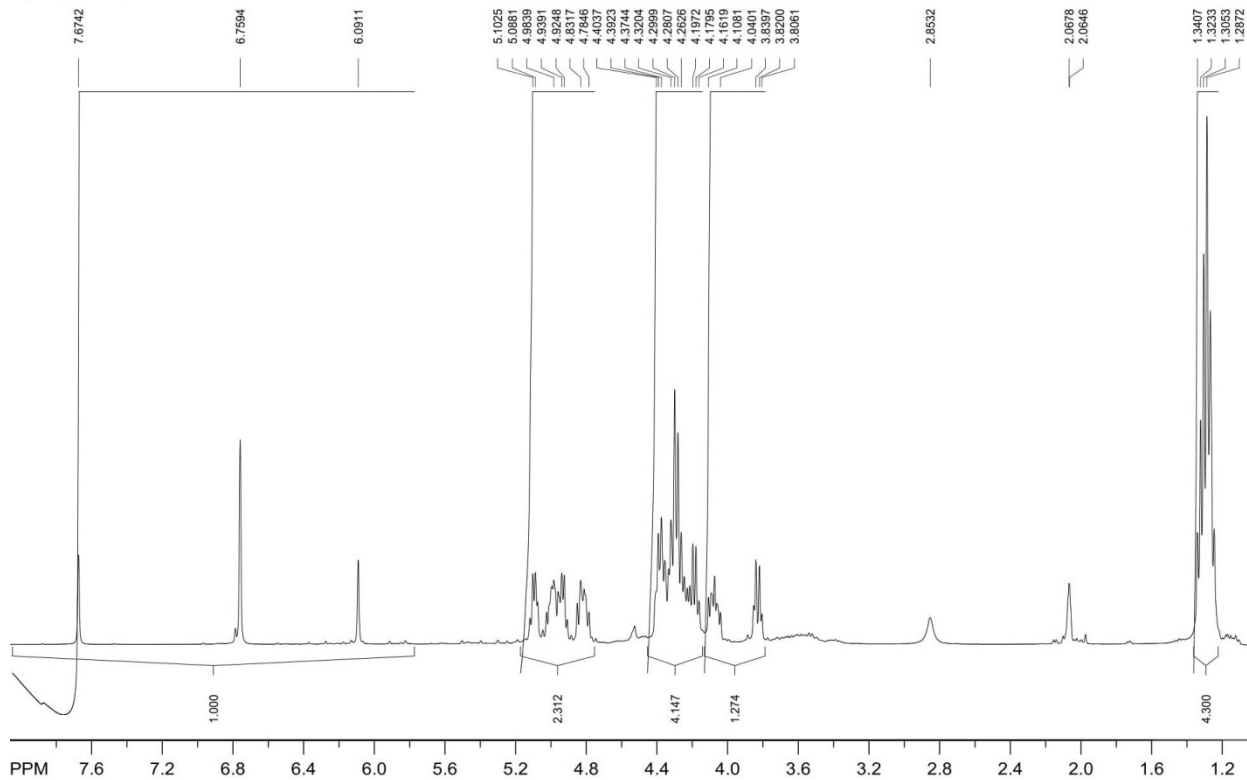




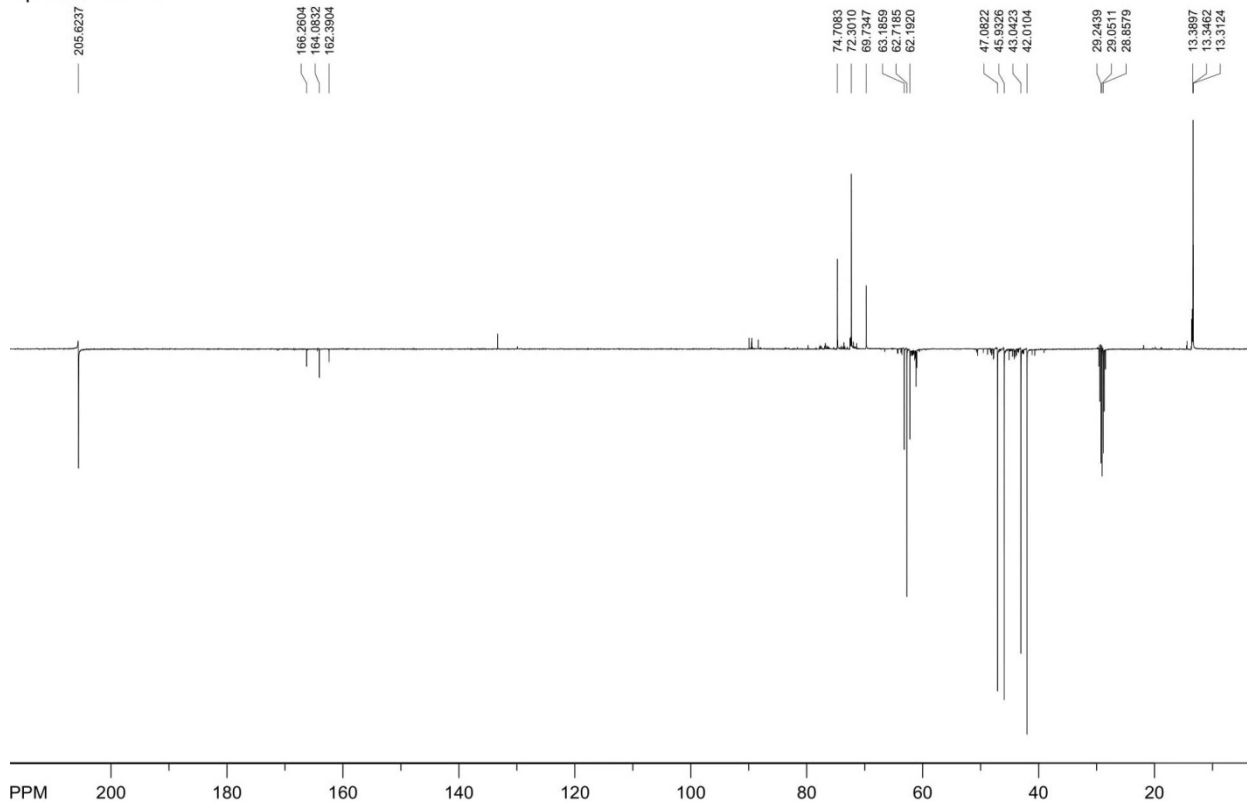
Ethyl 1,3-dinitroso-1,3-diazacyclopentane-2-carboxylate (8). The compound

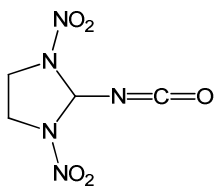
decomposes during analysis, giving probably resonance structures.

SpinWorks 2.5:



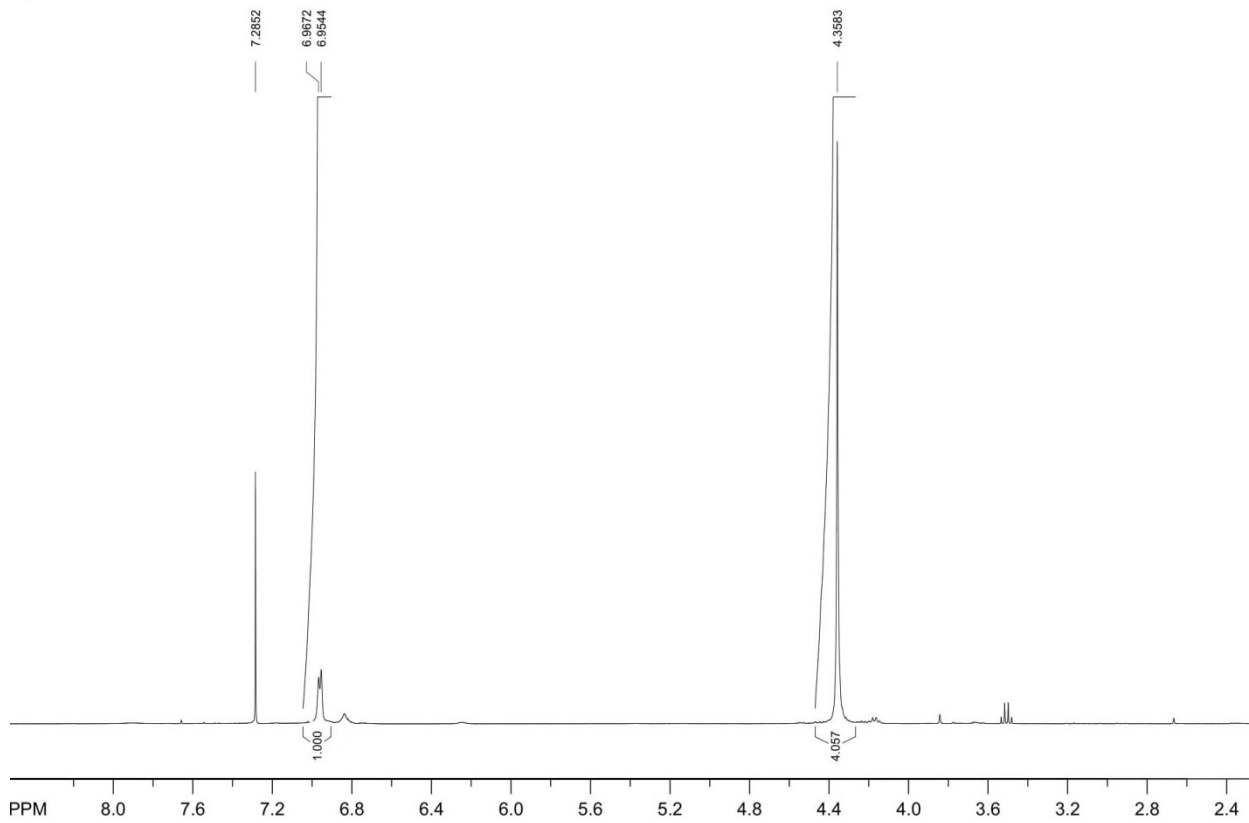
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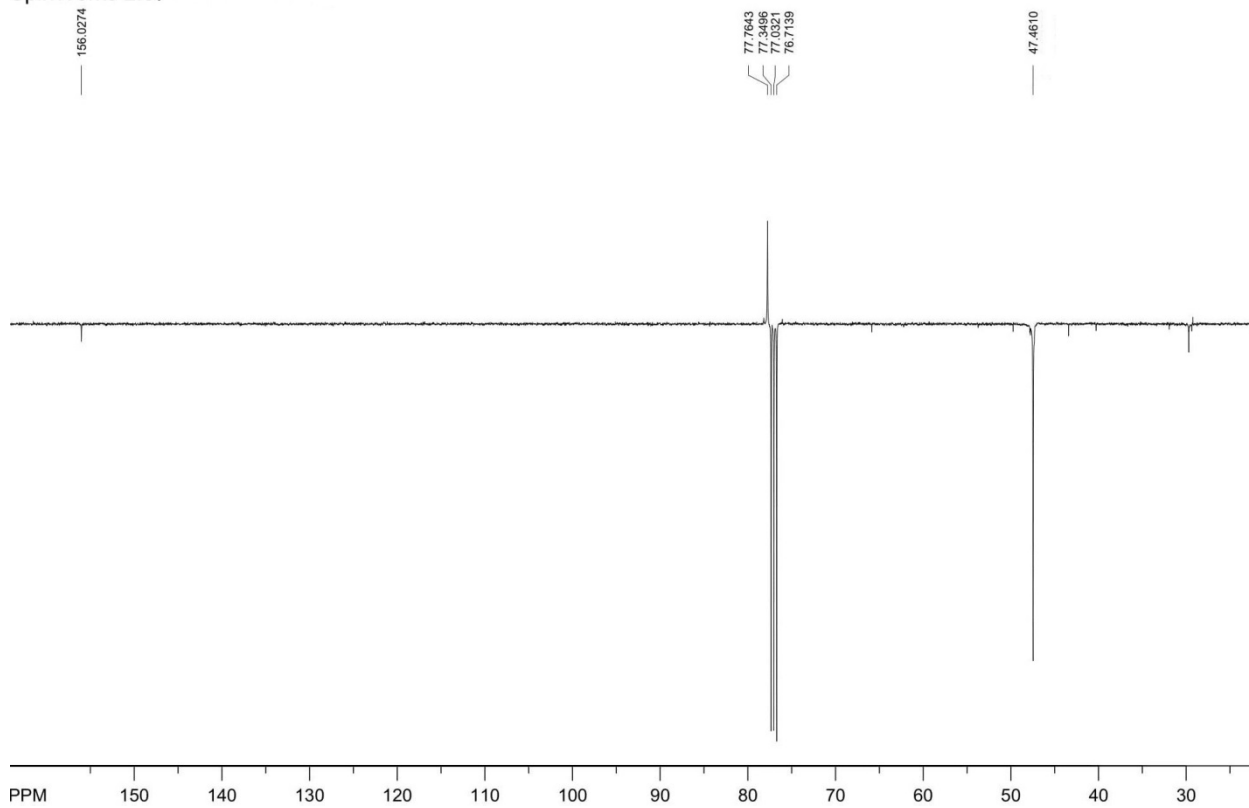


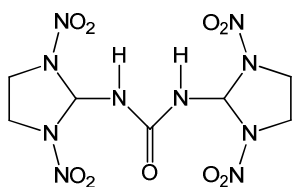
2-Isocyanato-1,3-dinitroimidazolidine (17)

SpinWorks 2.5:



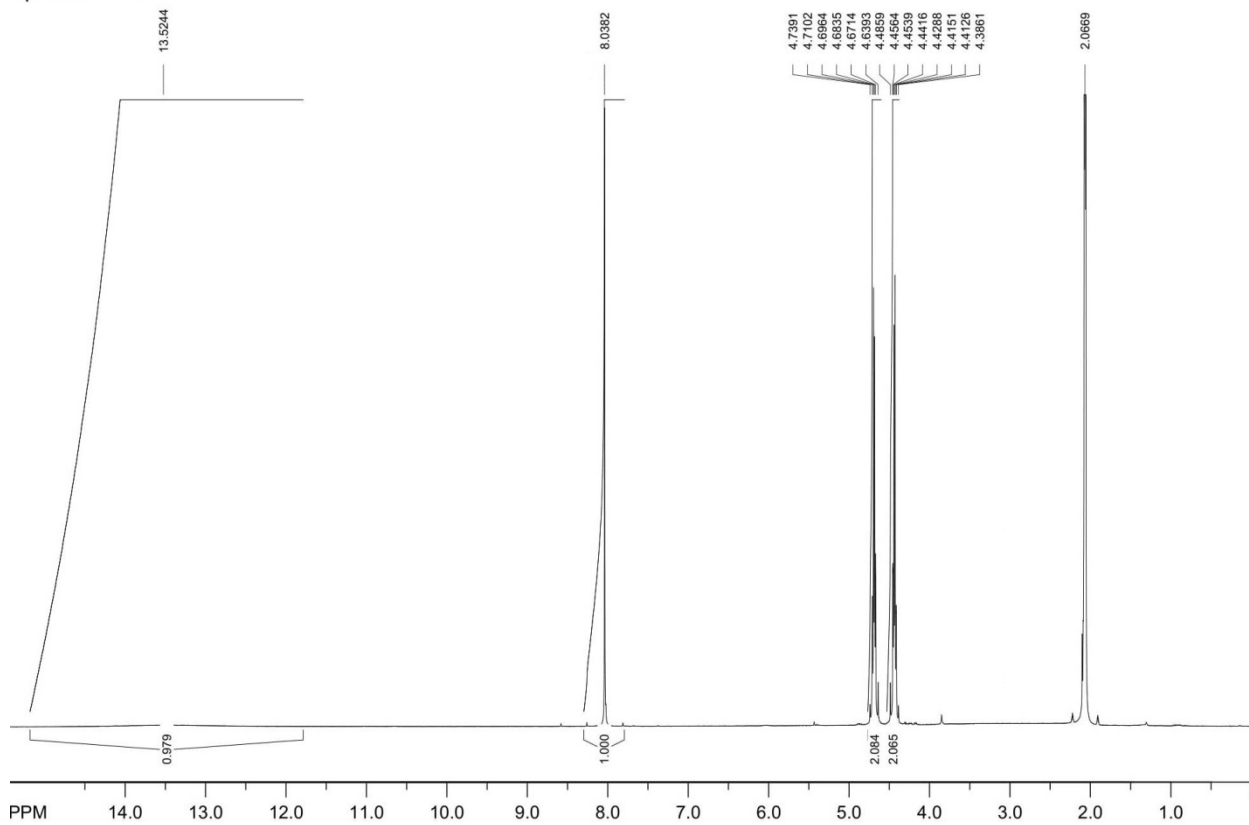
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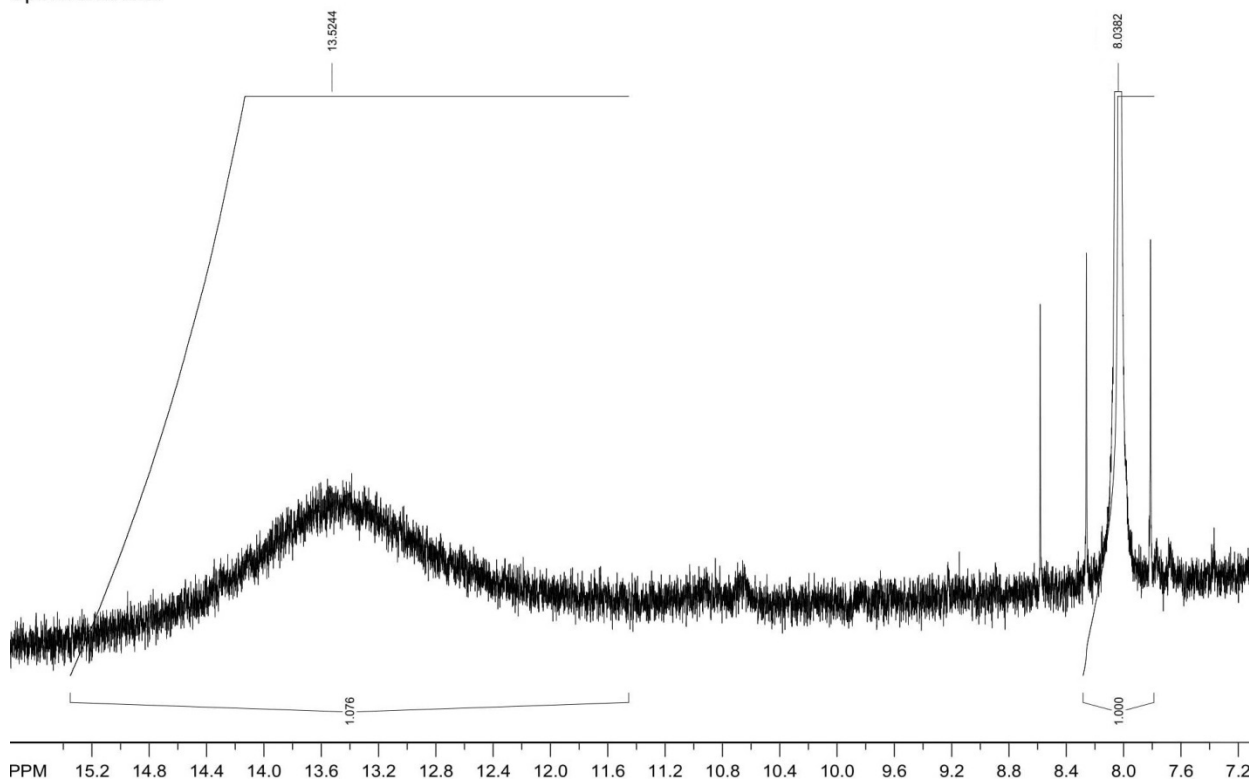


1,3-Di-(1,3-dinitro-1,3-diazacyclopentyl-2)urea (19)

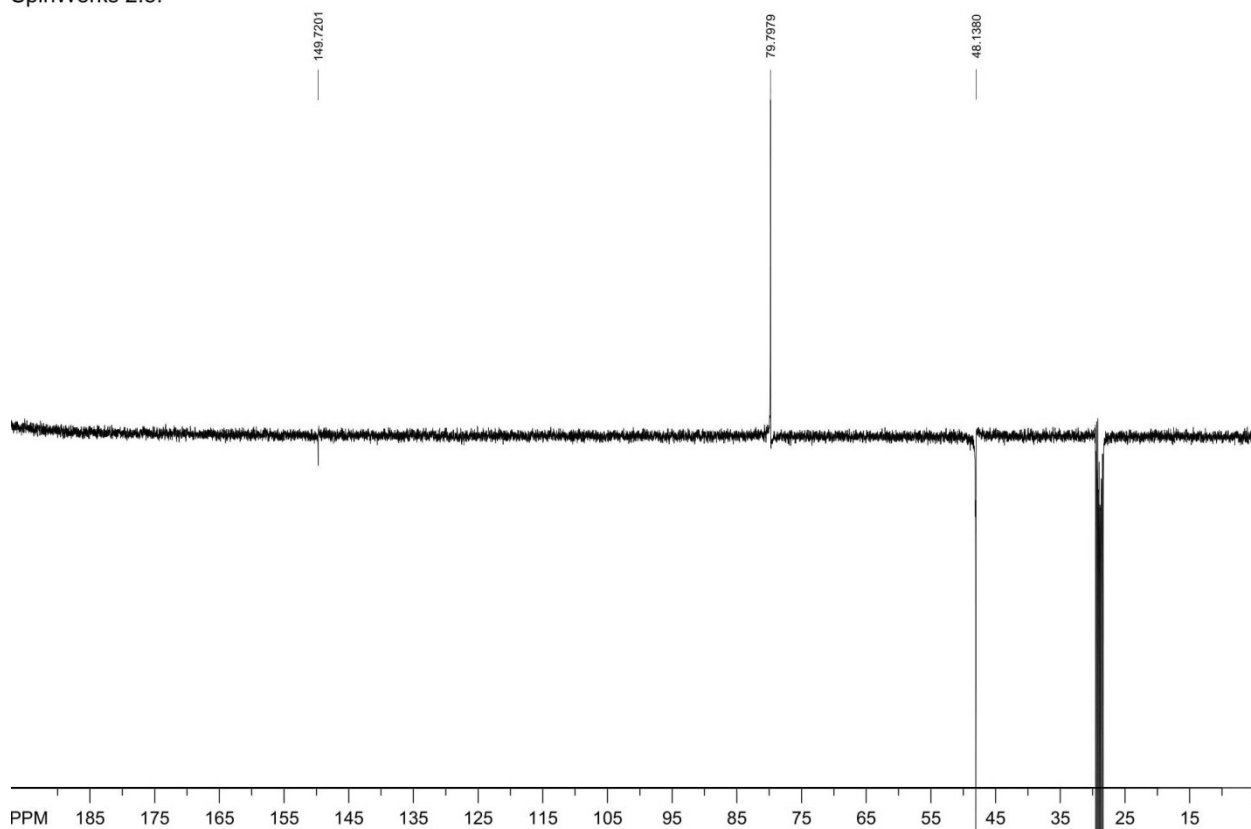
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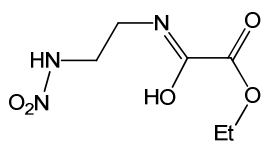
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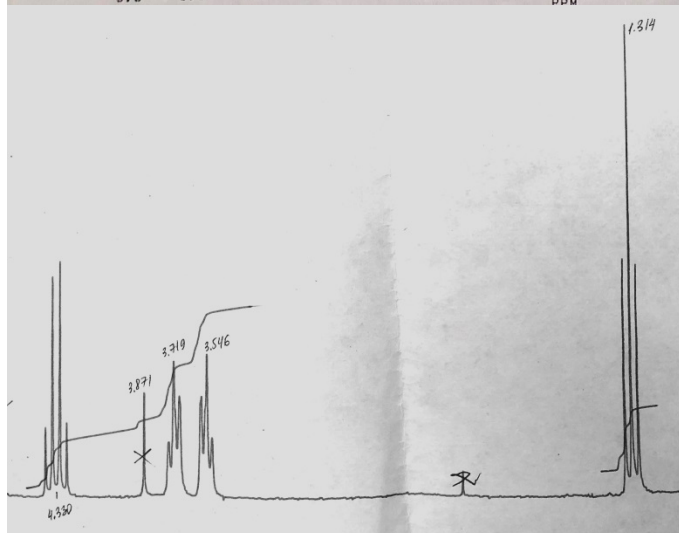
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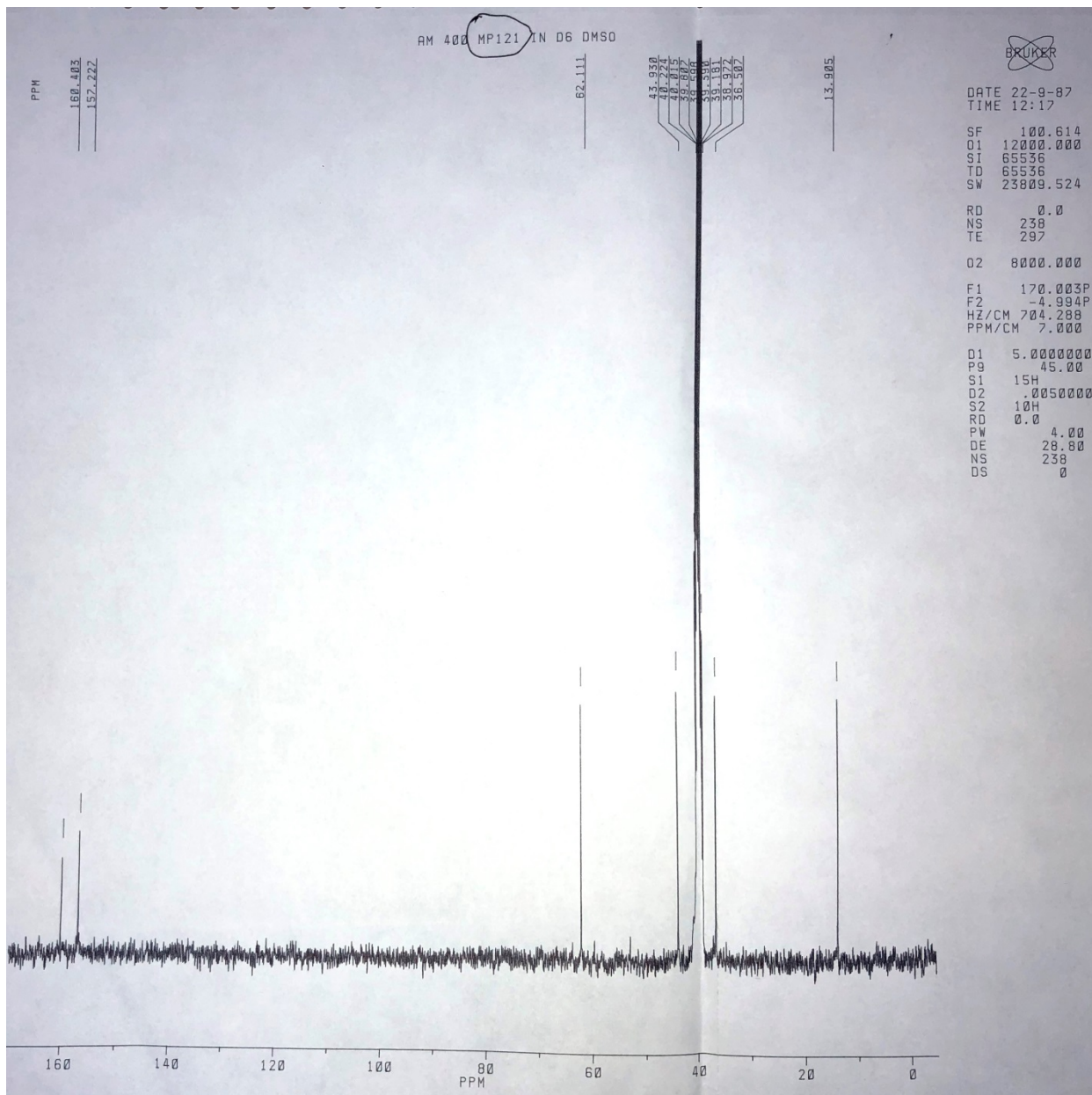


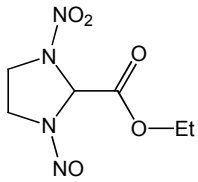
Synthesis and analysis of compounds **9**, **11** and **13** were done as far back as 1987-1990-ies. So, only hard-copies of NMR data for **9** and **13** have survived.



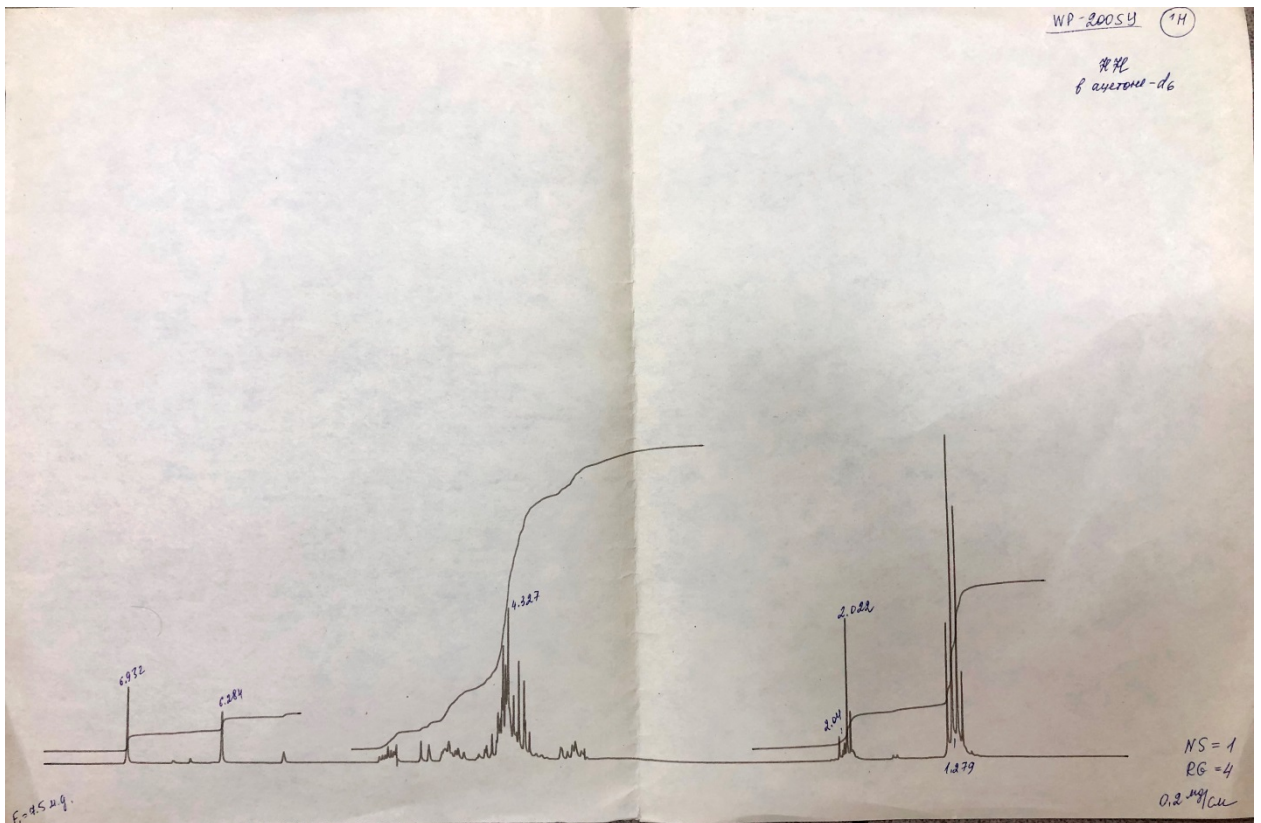
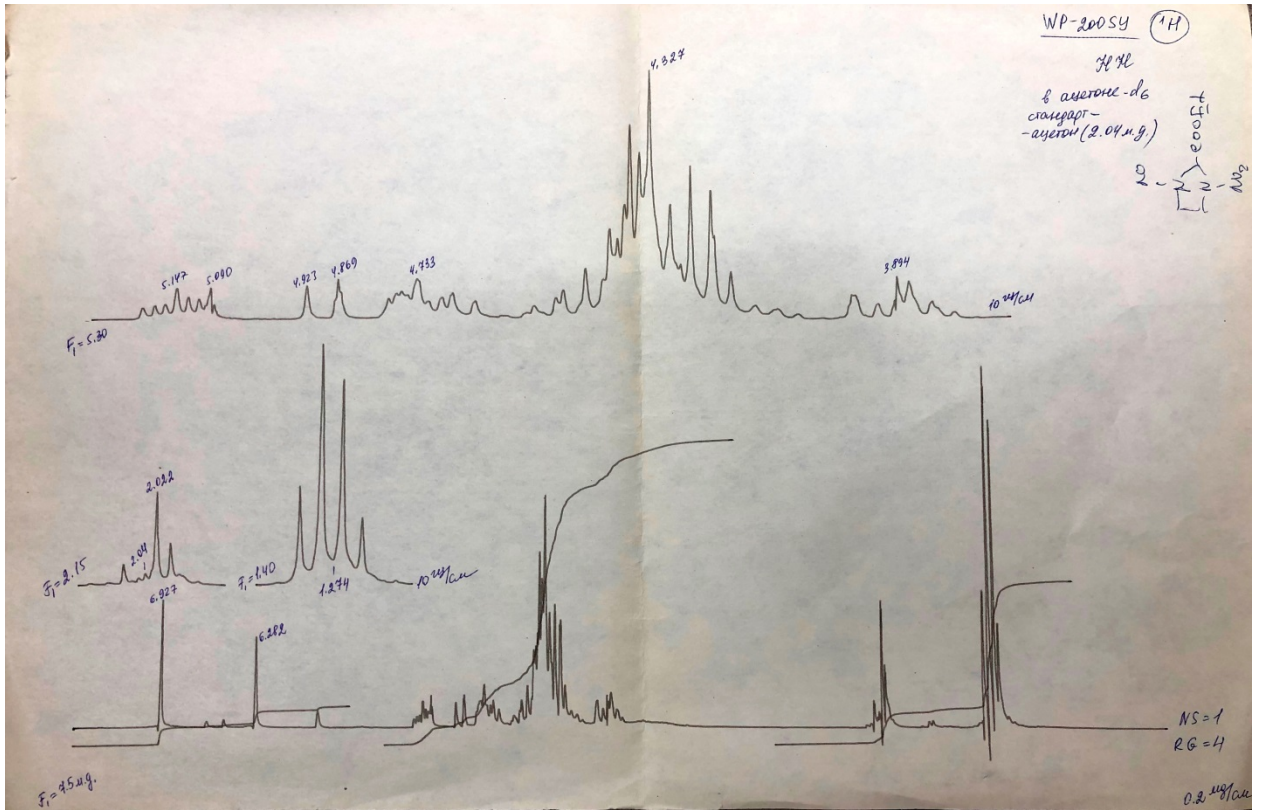
Ethyl 2-ethoxy-N-(2-nitramino)ethyl-2-oxoacetimidic acid (13)



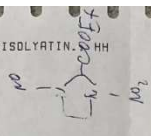




Ethyl 1-nitroso-3-nitro-1,3-diazacyclopentane-2-carboxylate (9)



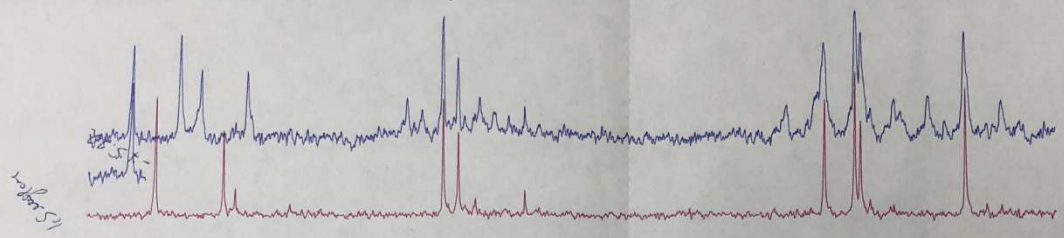
4C-200.. NIOCH SO AN SSSR.. C13.. IN /CD3/2CO.. SISDLYATIN.. HH



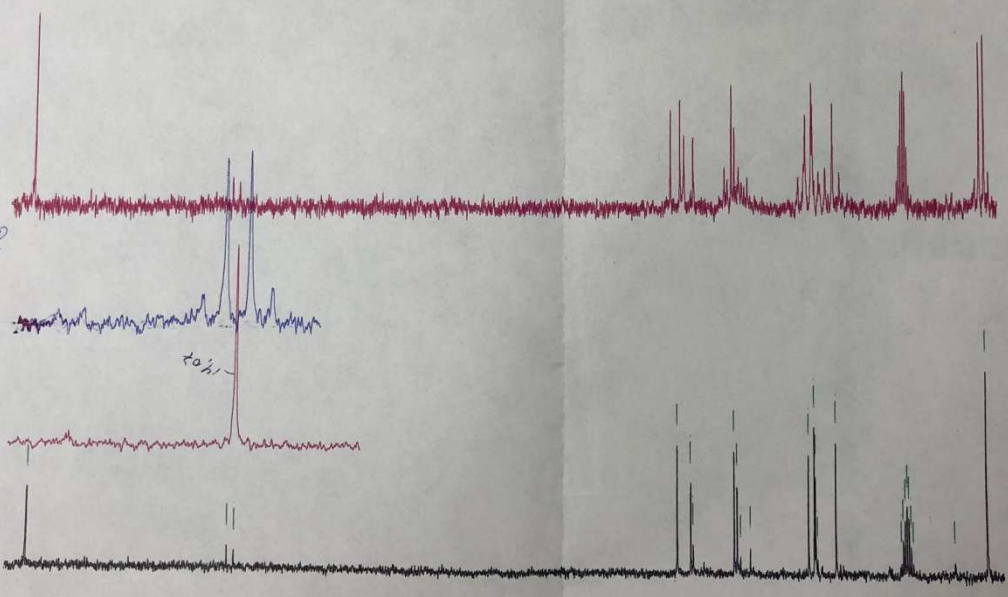
PPM
288.321

166.312
166.302

25.228
22.881
22.871
22.861
19.281
19.271
19.261
19.251
18.040
18.030
18.020
18.010
17.805
17.795
17.785
17.775
14.804



offes
AQ = 2400
WP = 184
RD = 3
WS = 64



BRUKER
VERA.017
SF 50.324
D1 6000.000
S1 32768
TD 32768
SW 12195.122
HZ/PT .744
RD 0.0
AQ 1.543
RC 200
NS 16
D2 4400.000
DP 10H CPD
PPM/CM 8.000

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
PPM