

Supporting information

5-Nitrofurant-Tagged Oxazolyl Pyrazolopiperidines: Synthesis and Activity against ESKAPE Pathogens

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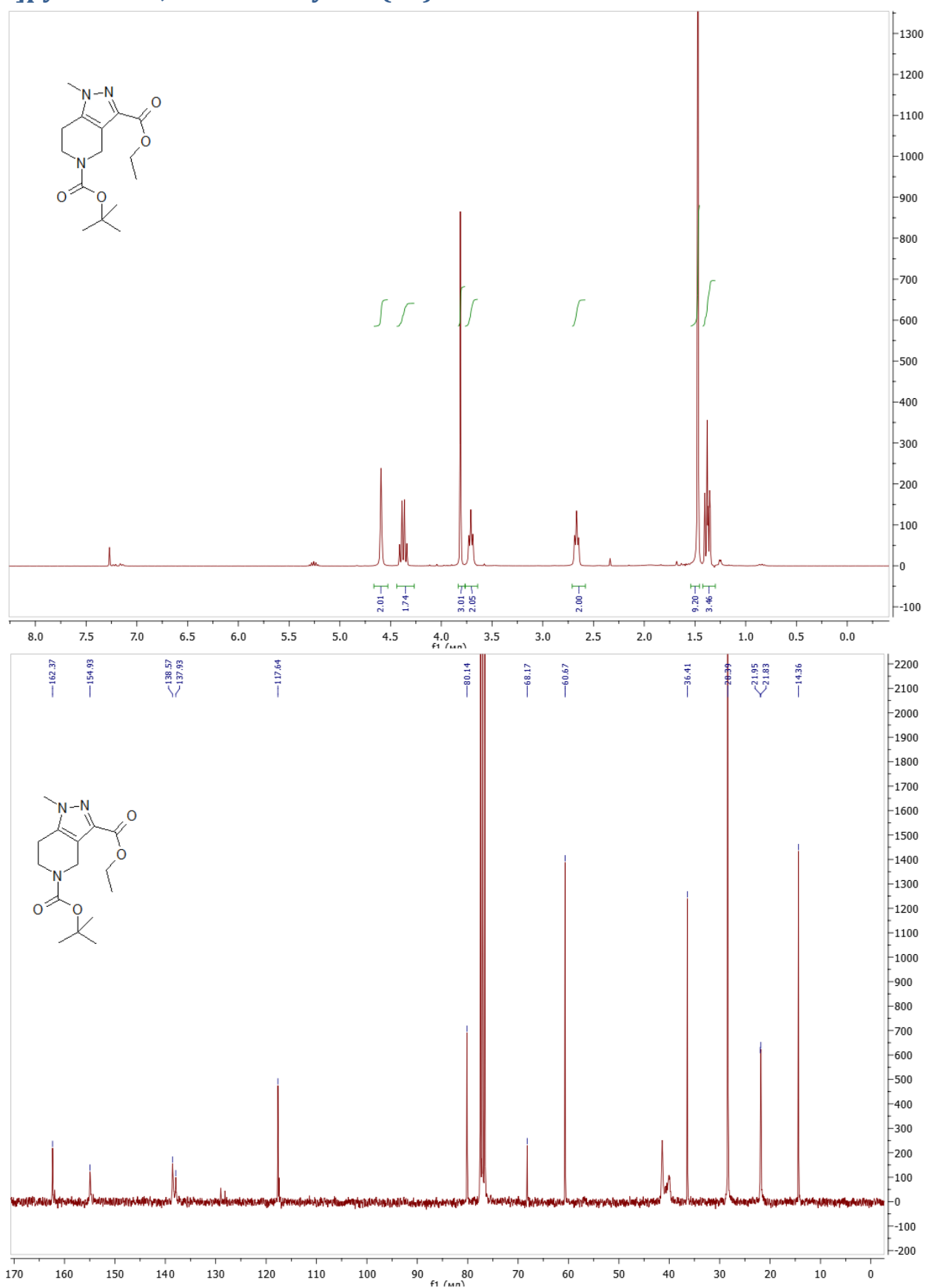
* Correspondence: chudinov@mirea.ru

NMR spectra of synthesized compounds

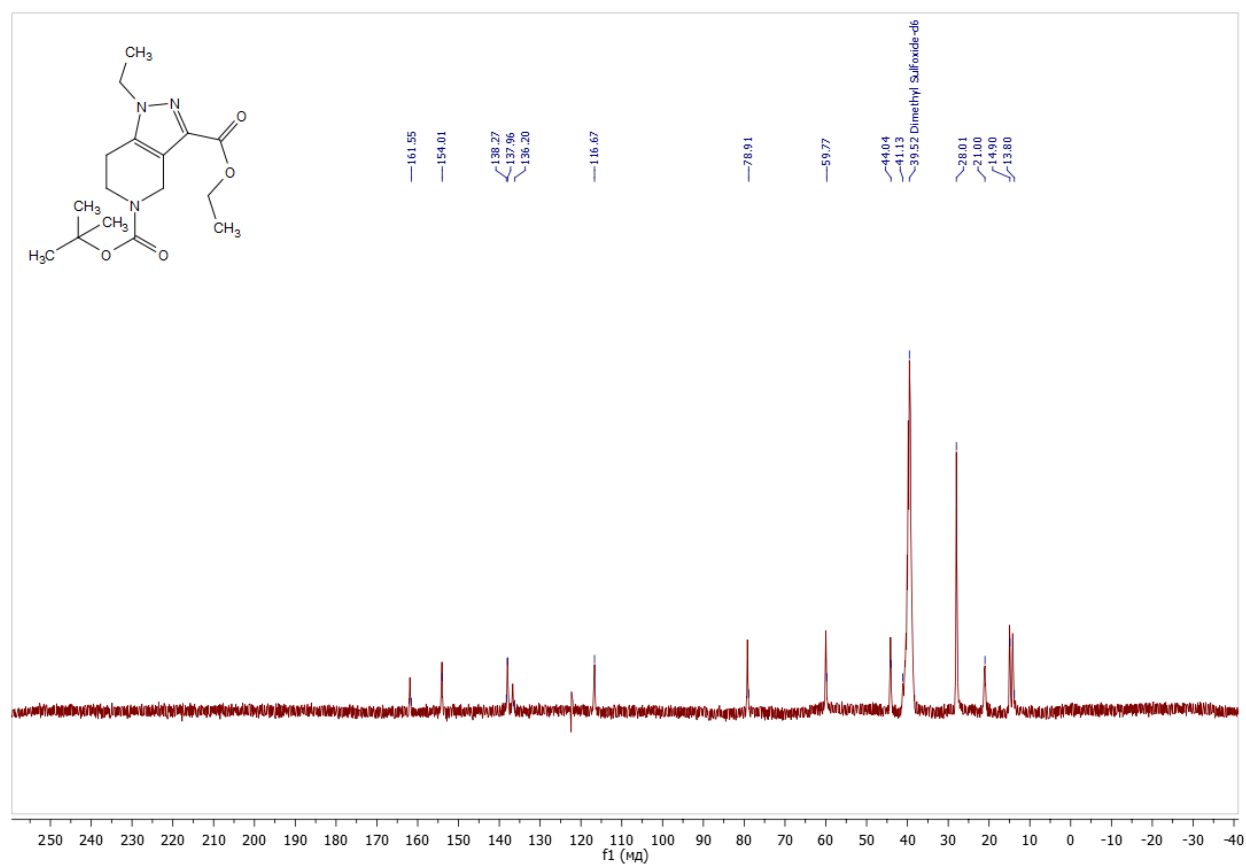
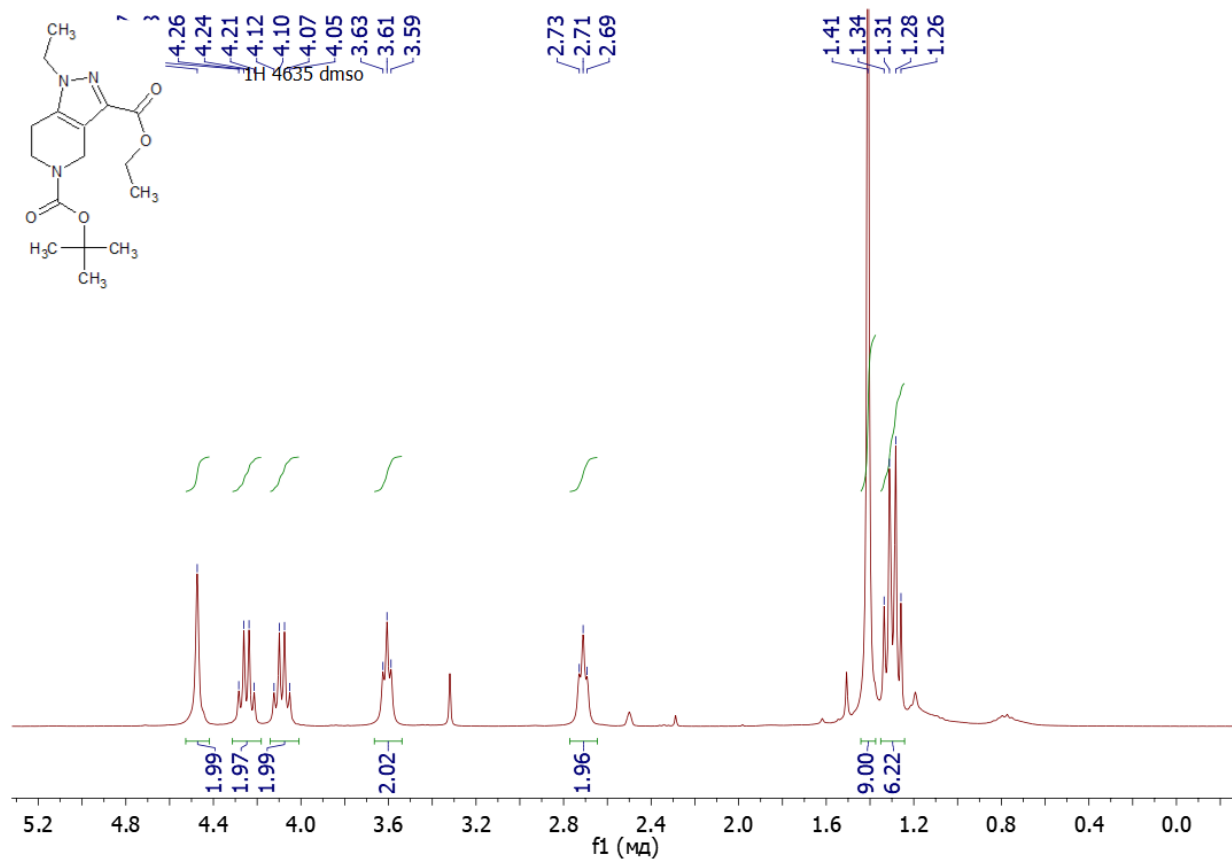
5-tert-butyl 3-ethyl 1-methyl-1,4,6,7-tetrahydro-5H-pyrazolo[4,3-c]pyridine-3,5- dicarboxylate (6a)	3
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1-(2-methoxyethyl)-5-(5-nitro-2-furoyl)-3-(1,3-oxazol-5-yl)-4,5,6,7-tetrahydro-1H-pyrazolo [4,3-c]pyridine, LK01509 (13g)	29
1-(3-methoxypropyl)-5-(5-nitro-2-furoyl)-3-(1,3-oxazol-5-yl)-4,5,6,7-tetrahydro-1H-pyrazolo [4,3-c]pyridine, LK01514 (13h)	30

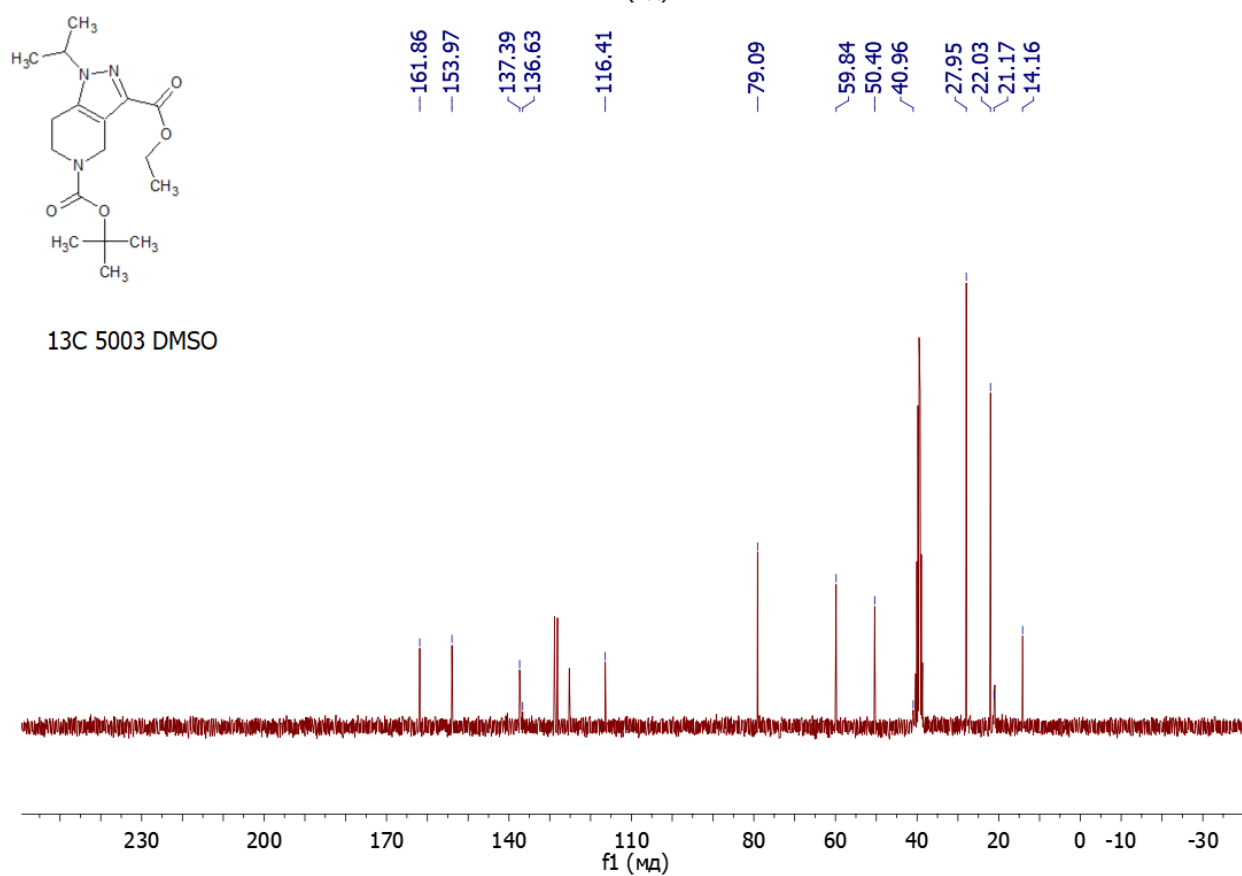
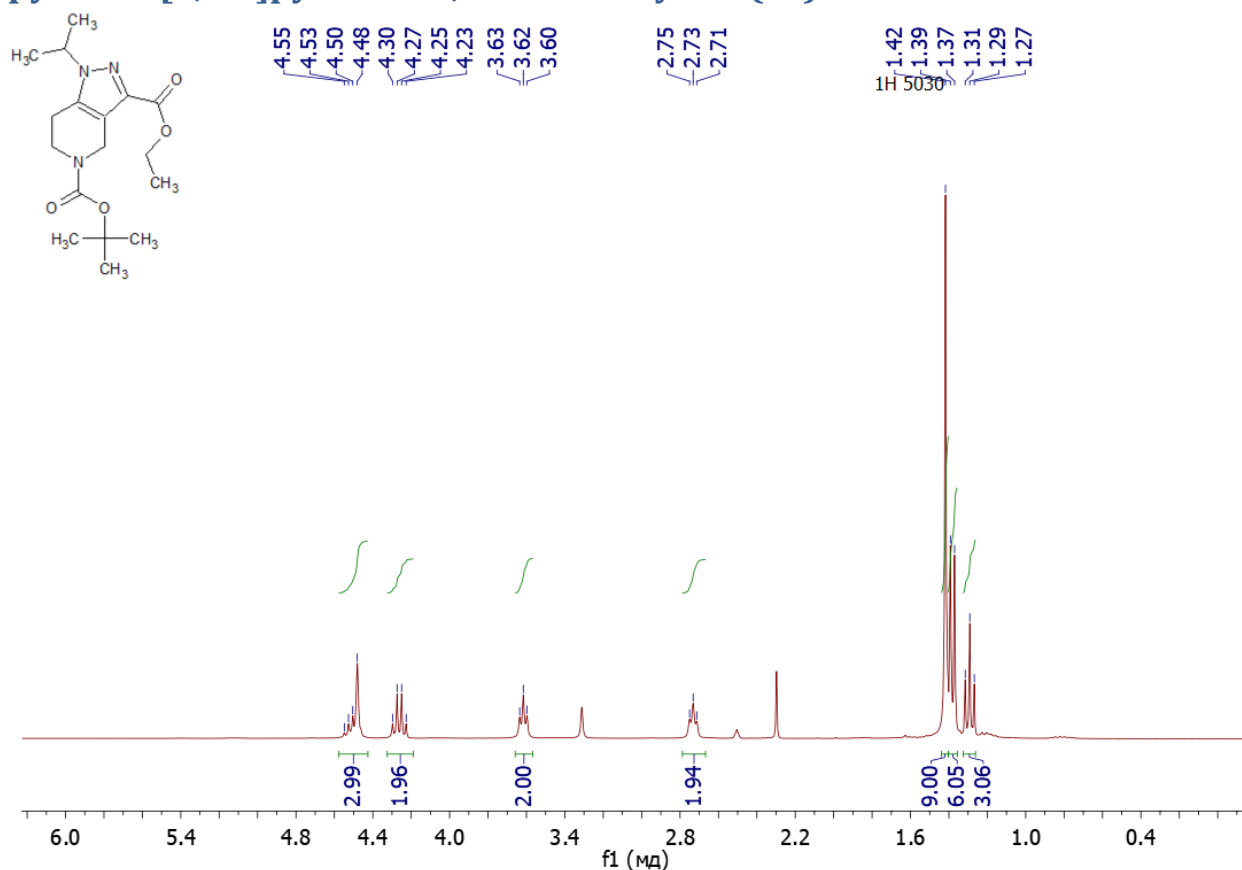
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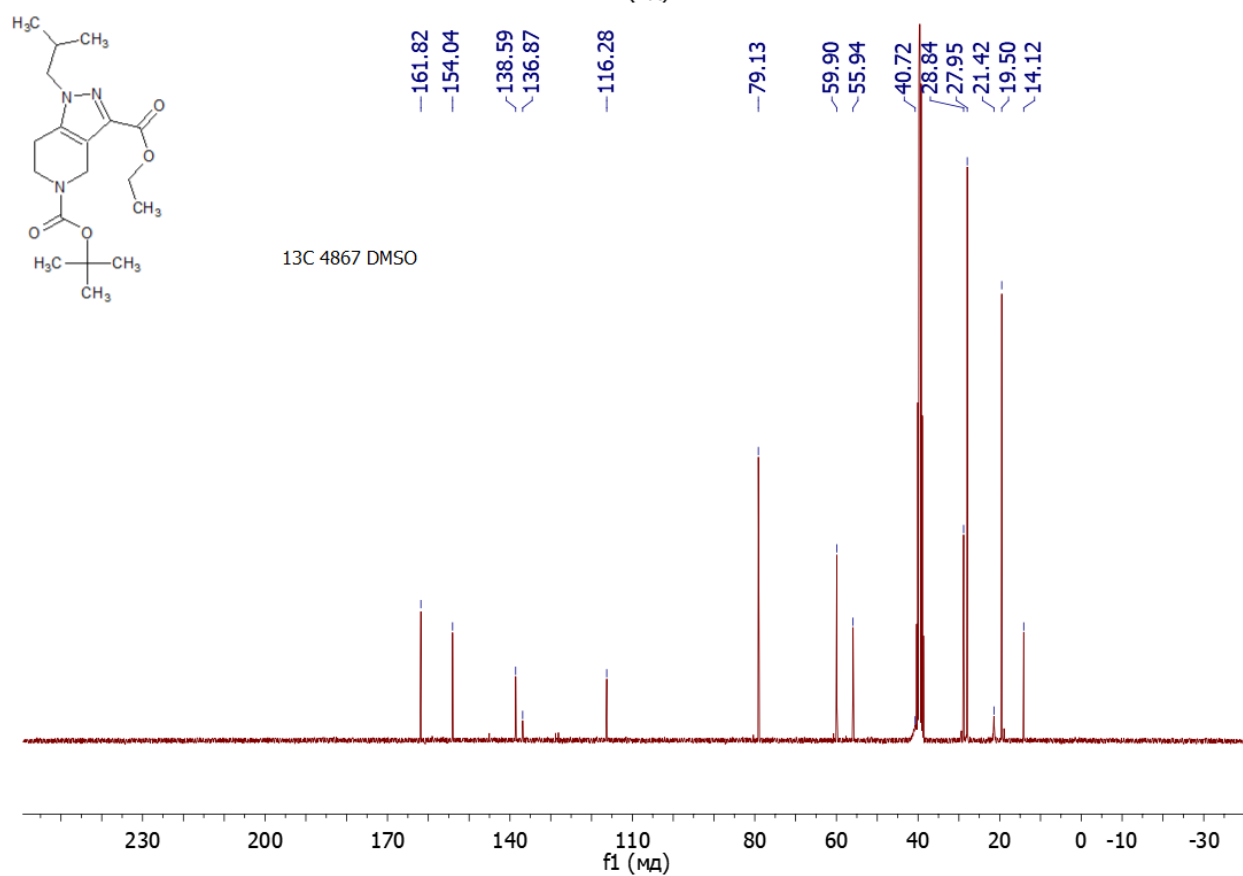
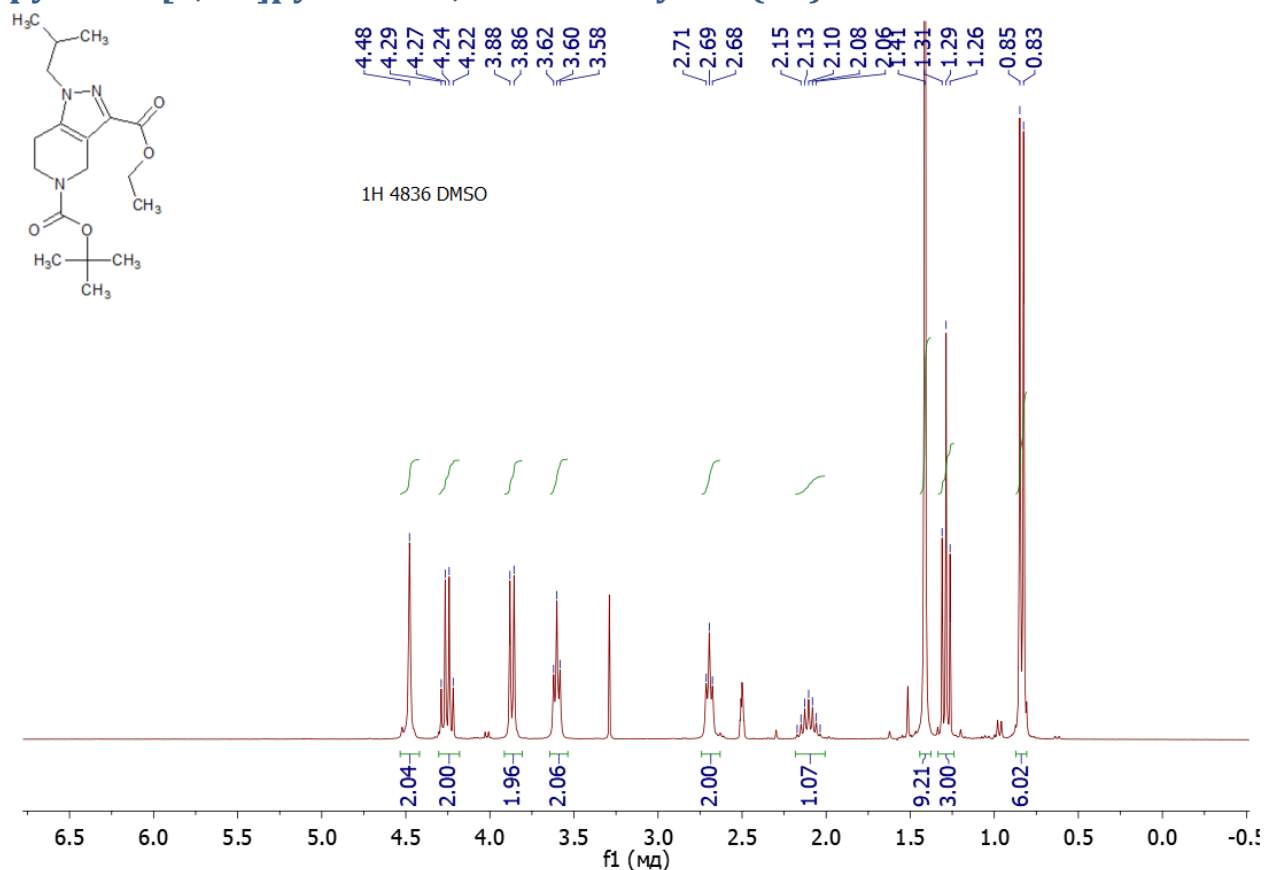
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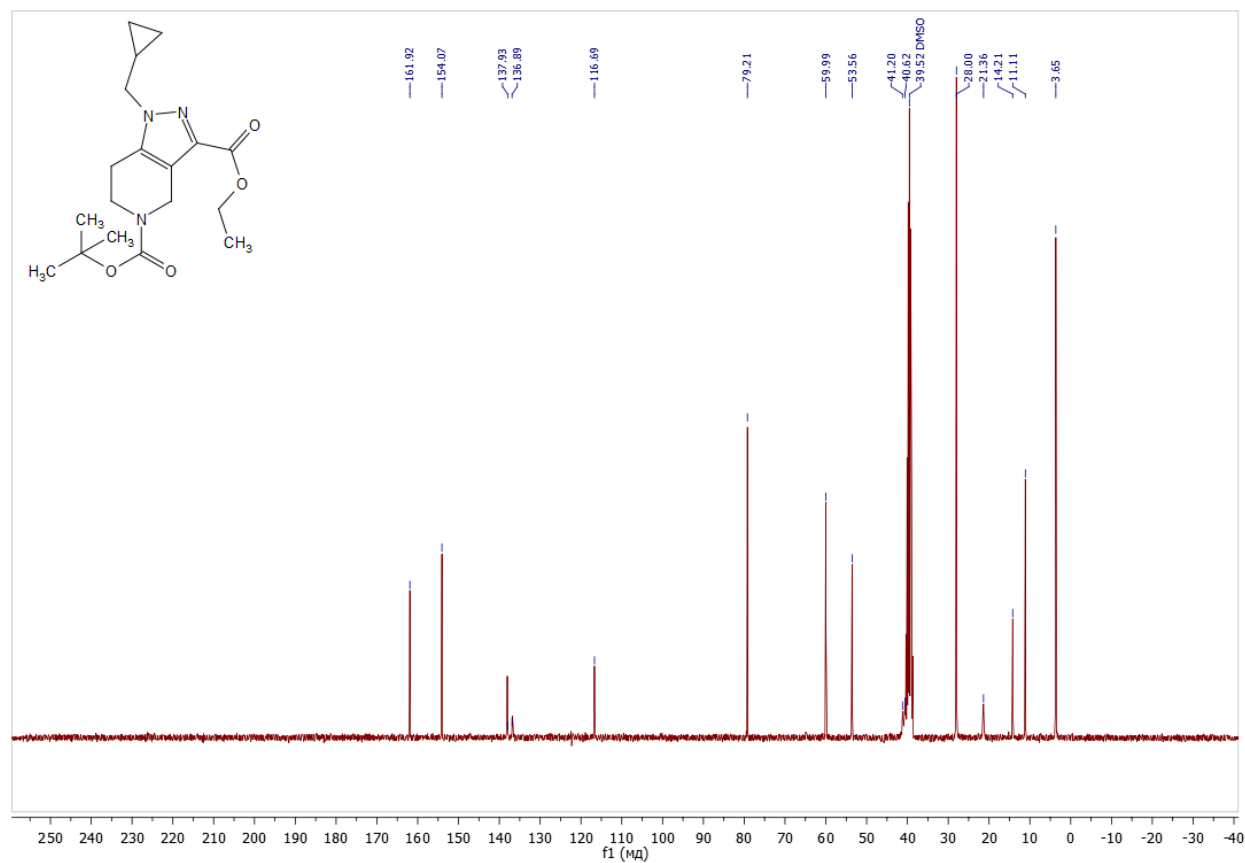
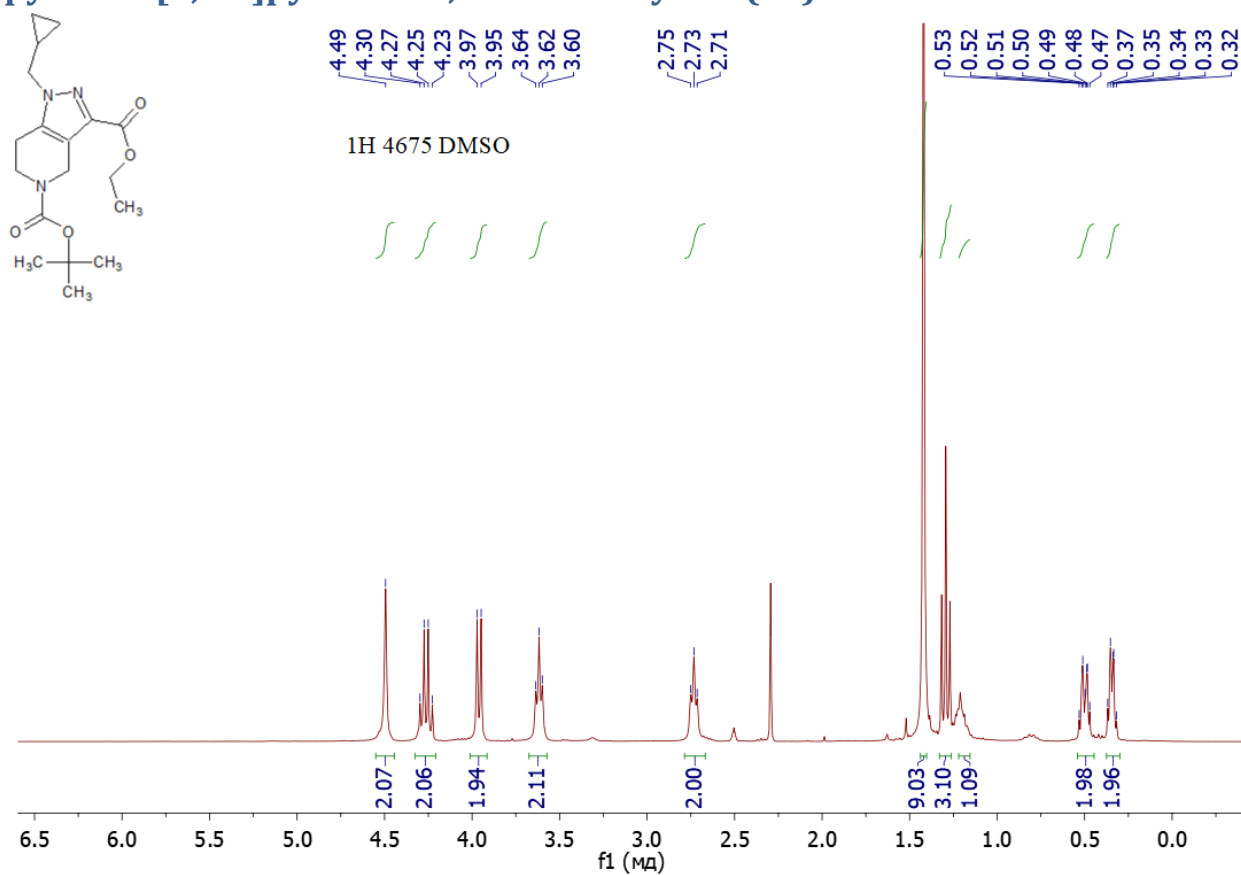
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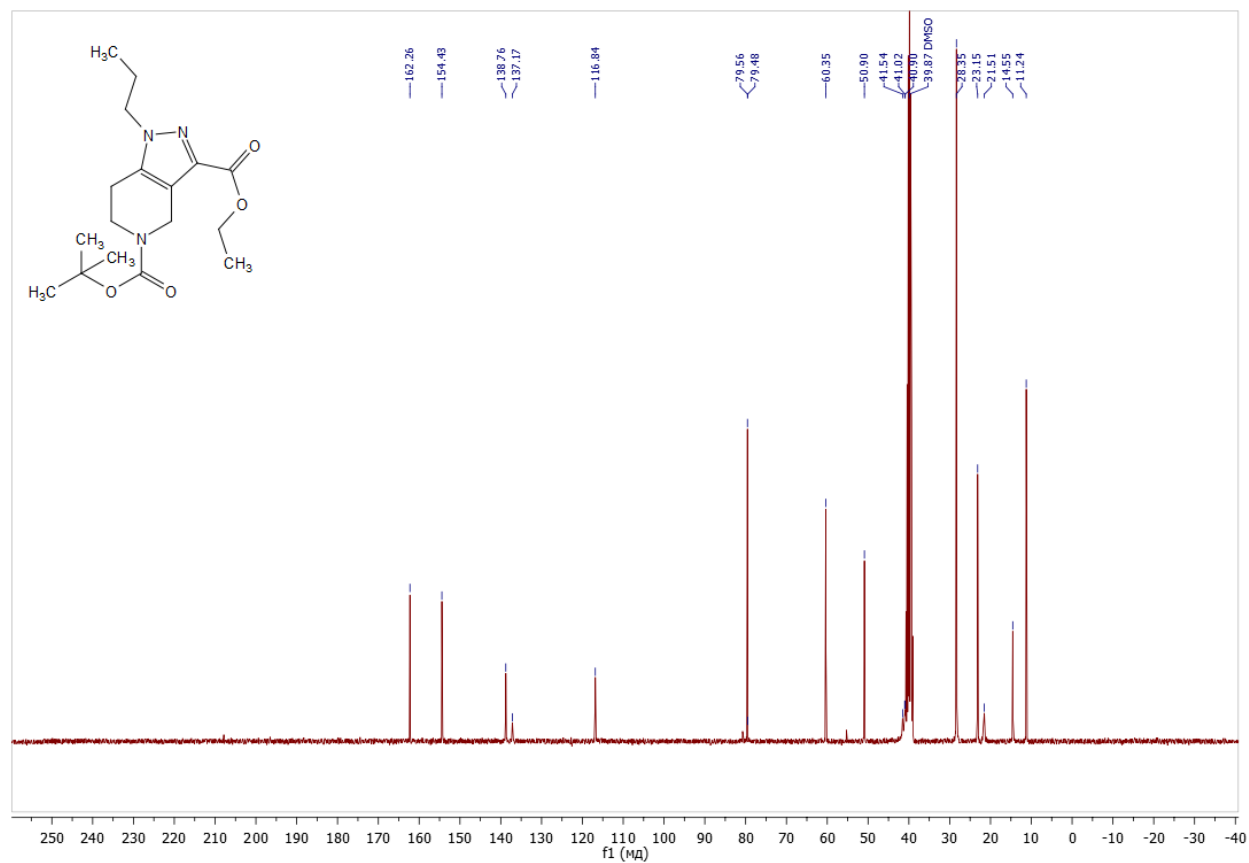
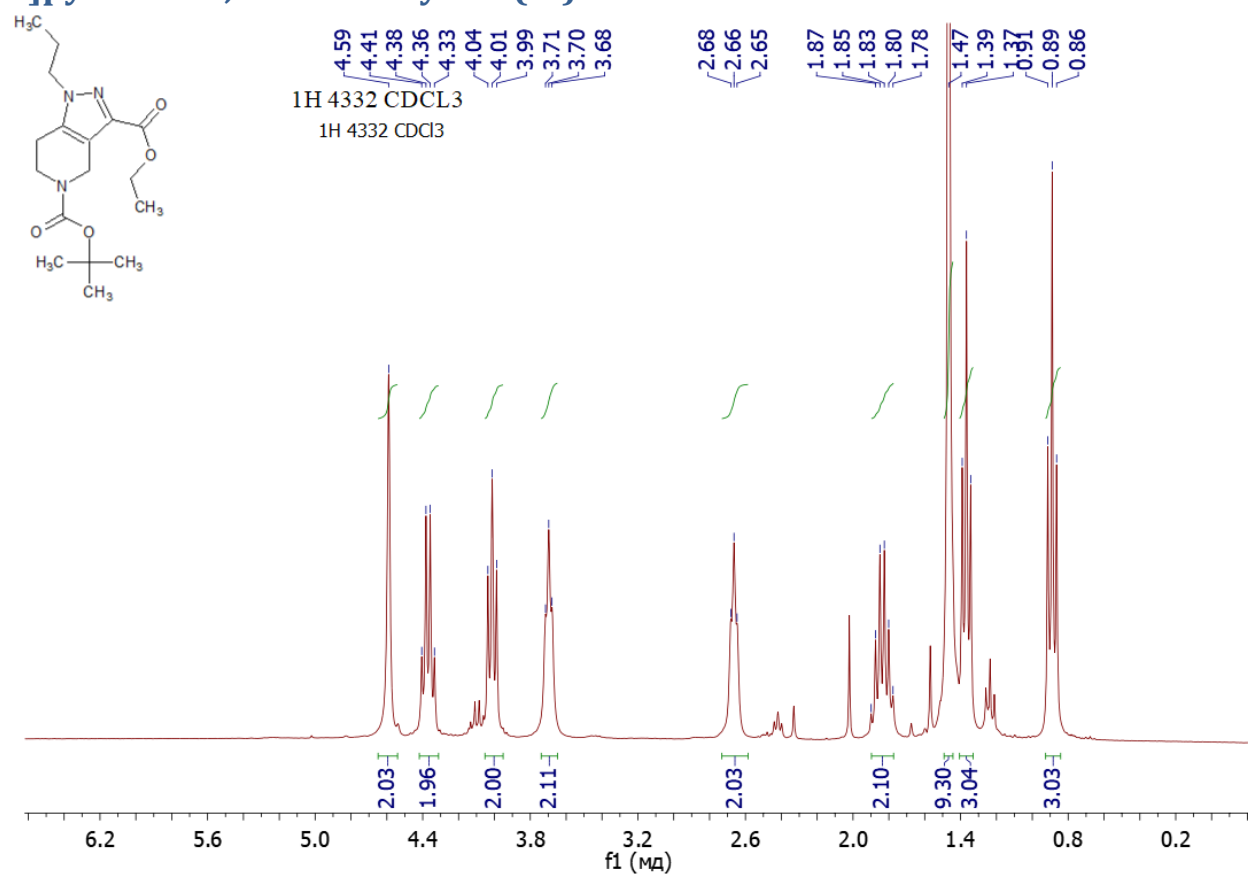
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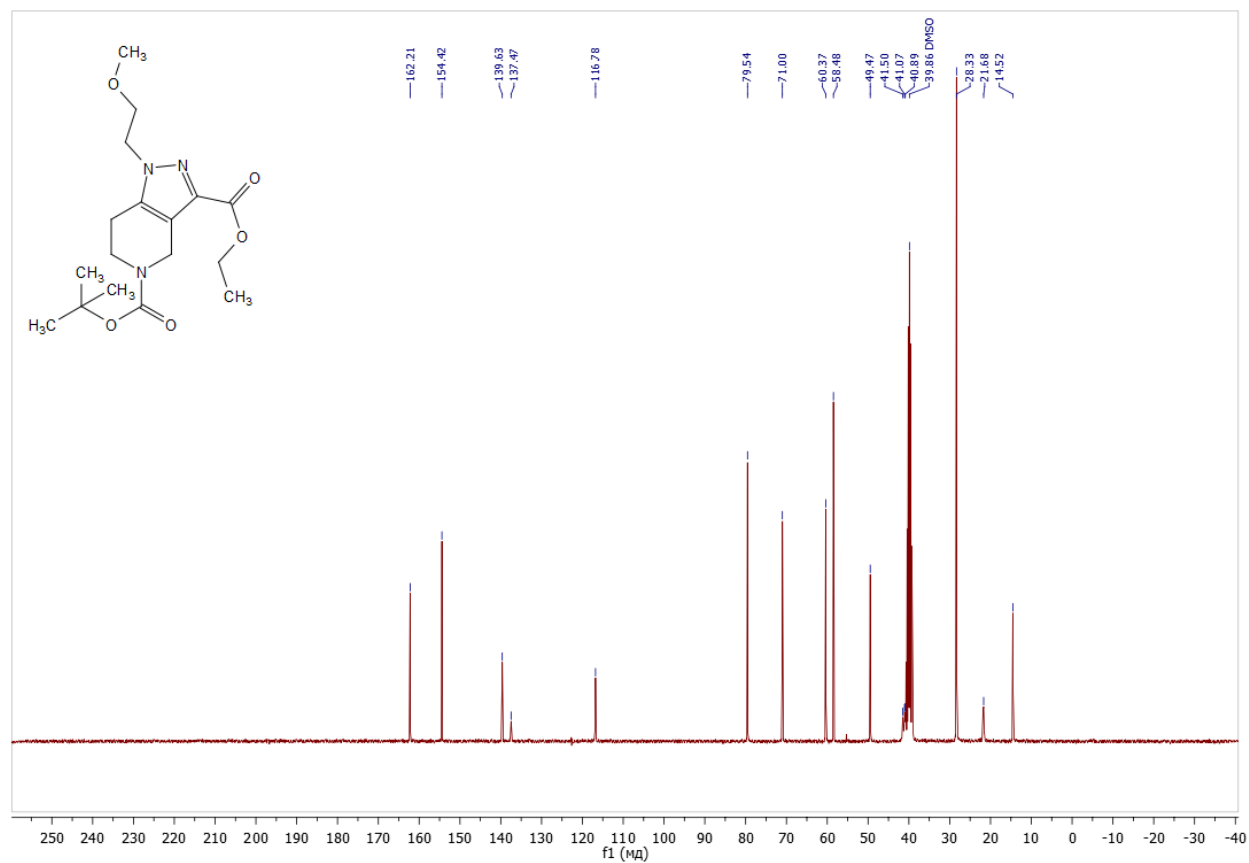
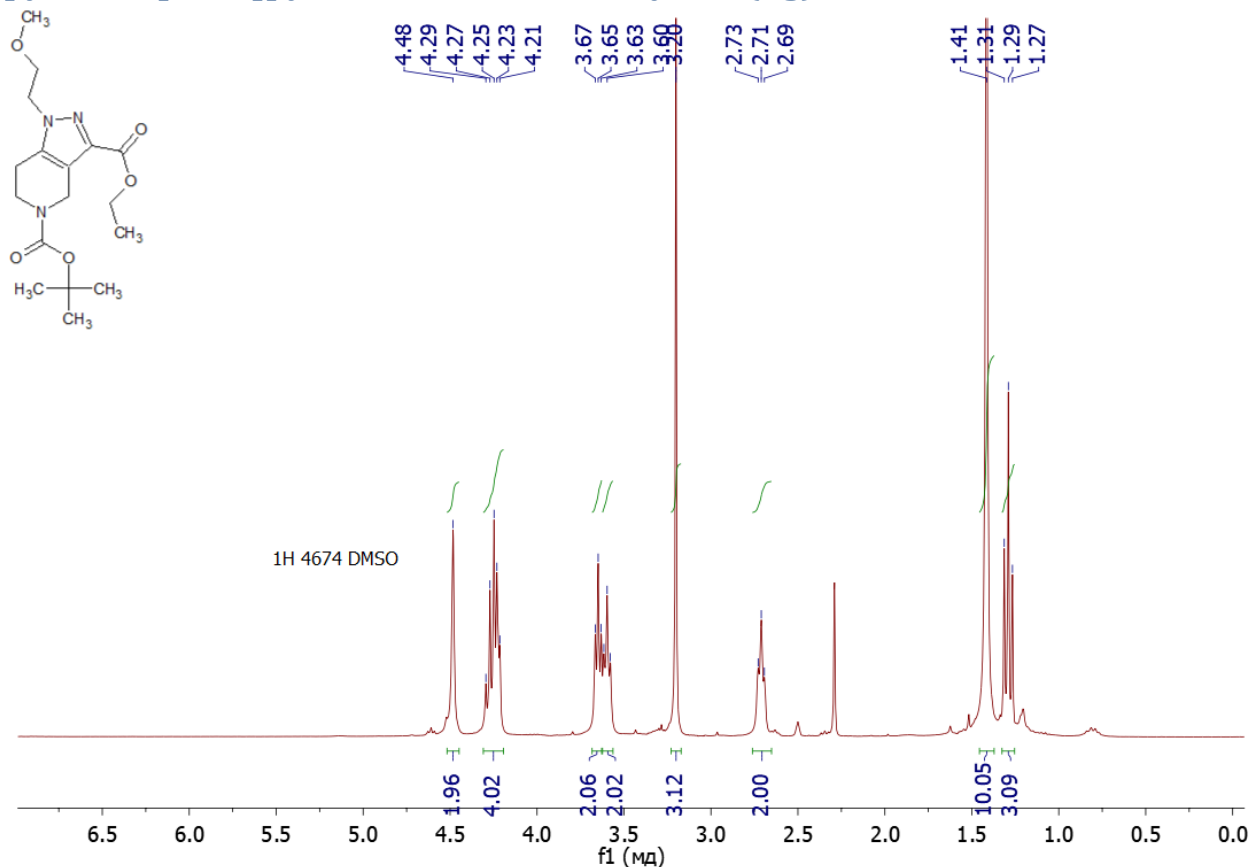
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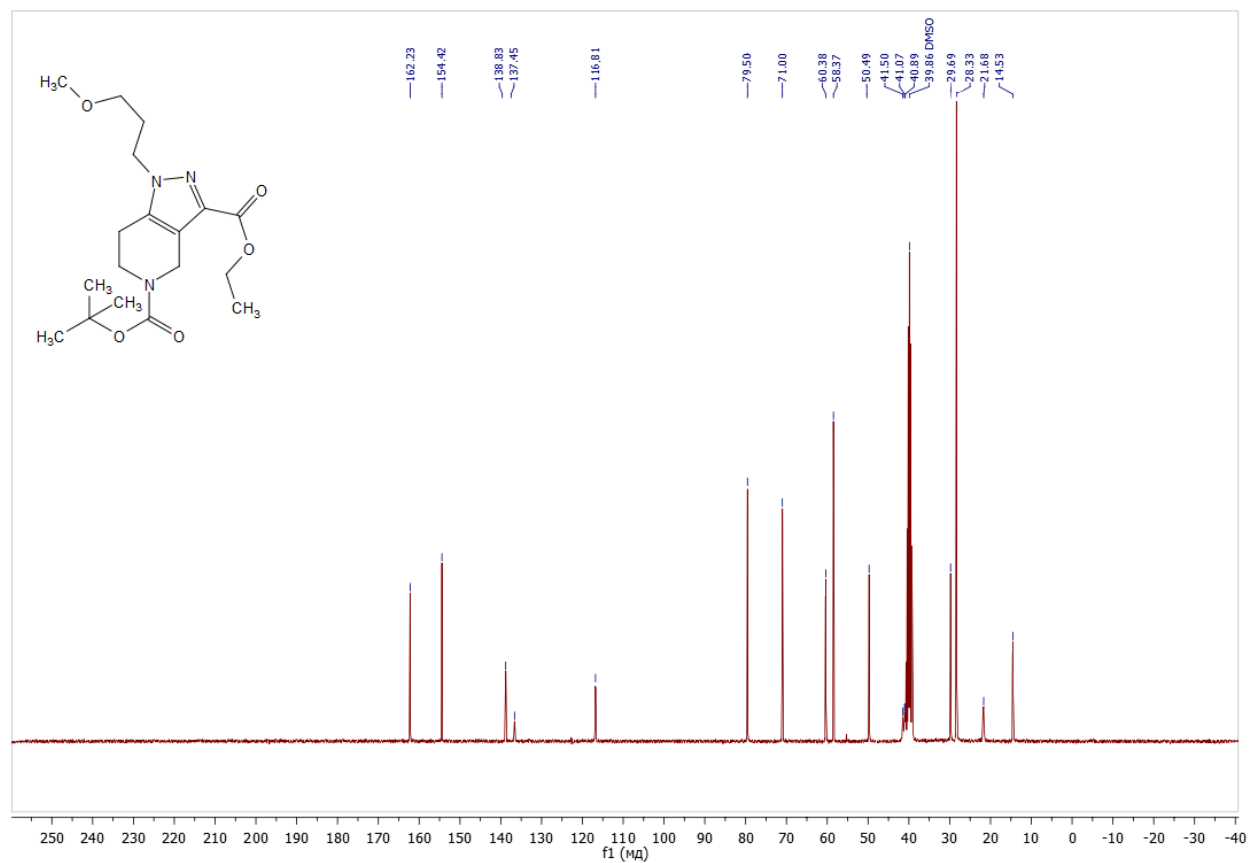
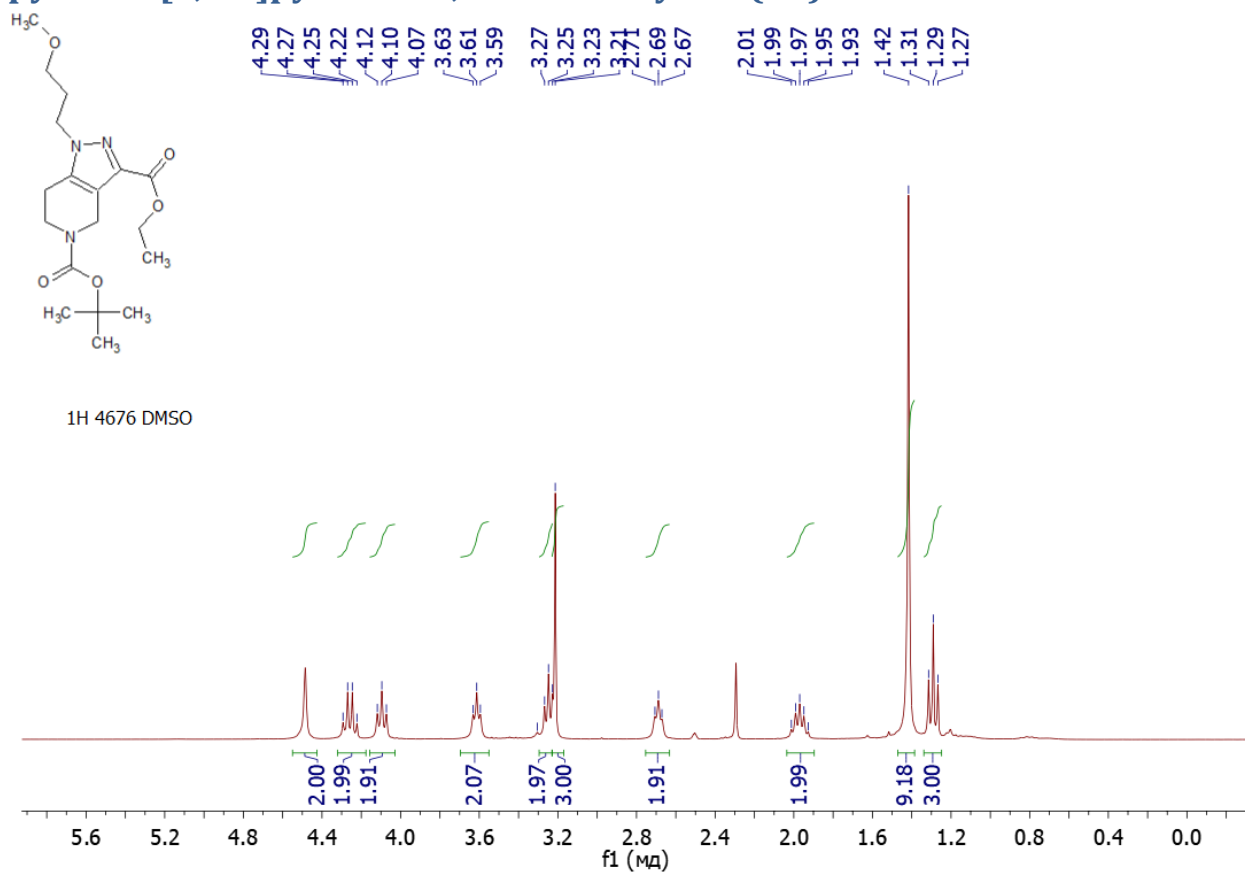
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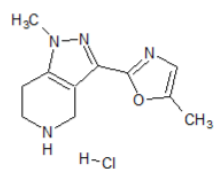
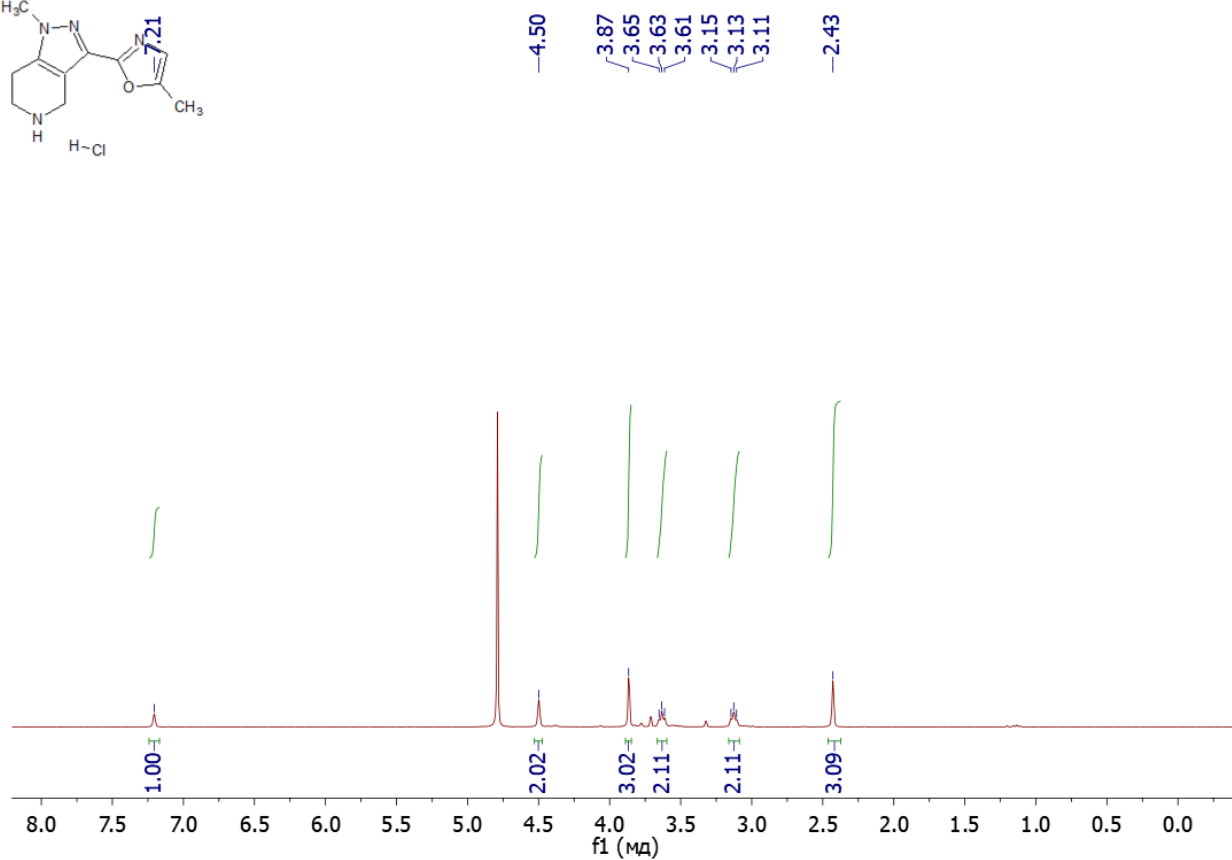
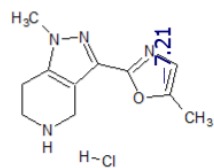
5-tert-butyl-3-ethyl-1-(2-methoxyethyl)-1,4,6,7-tetrahydro-5H-pyrazolo[4,3-c]pyridine-3,5- dicarboxylate (6g)



5-tert-butyl-3-ethyl-1-(2-methoxypropyl)-1,4,6,7-tetrahydro-5H-pyrazolo[4,3-c]pyridine-3,5-dicarboxylate (6h)



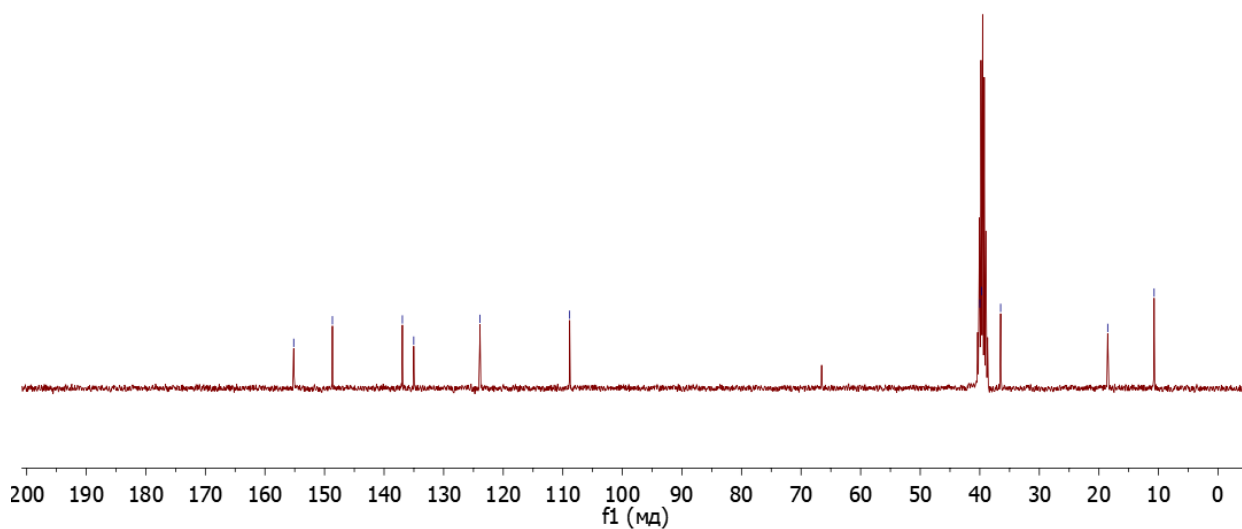
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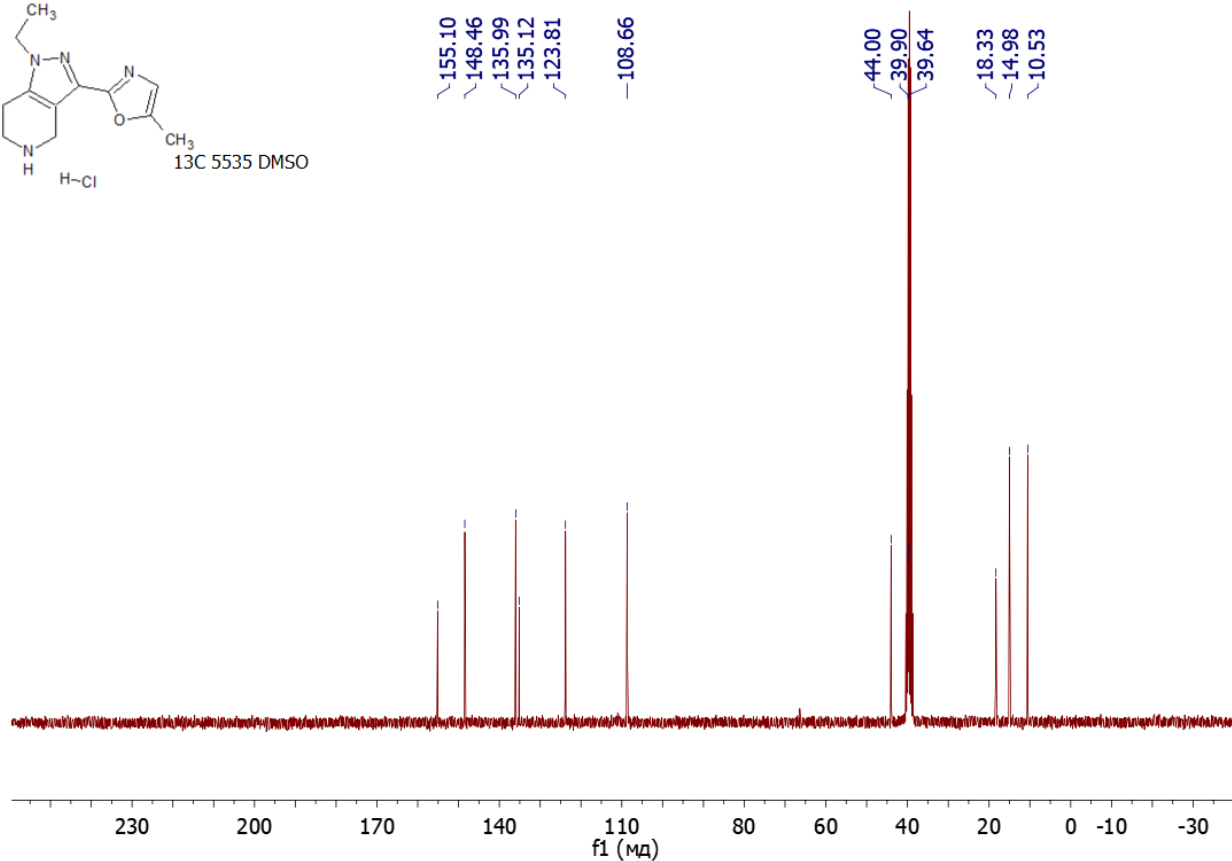
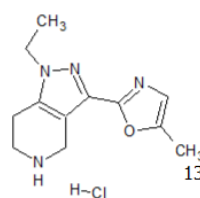
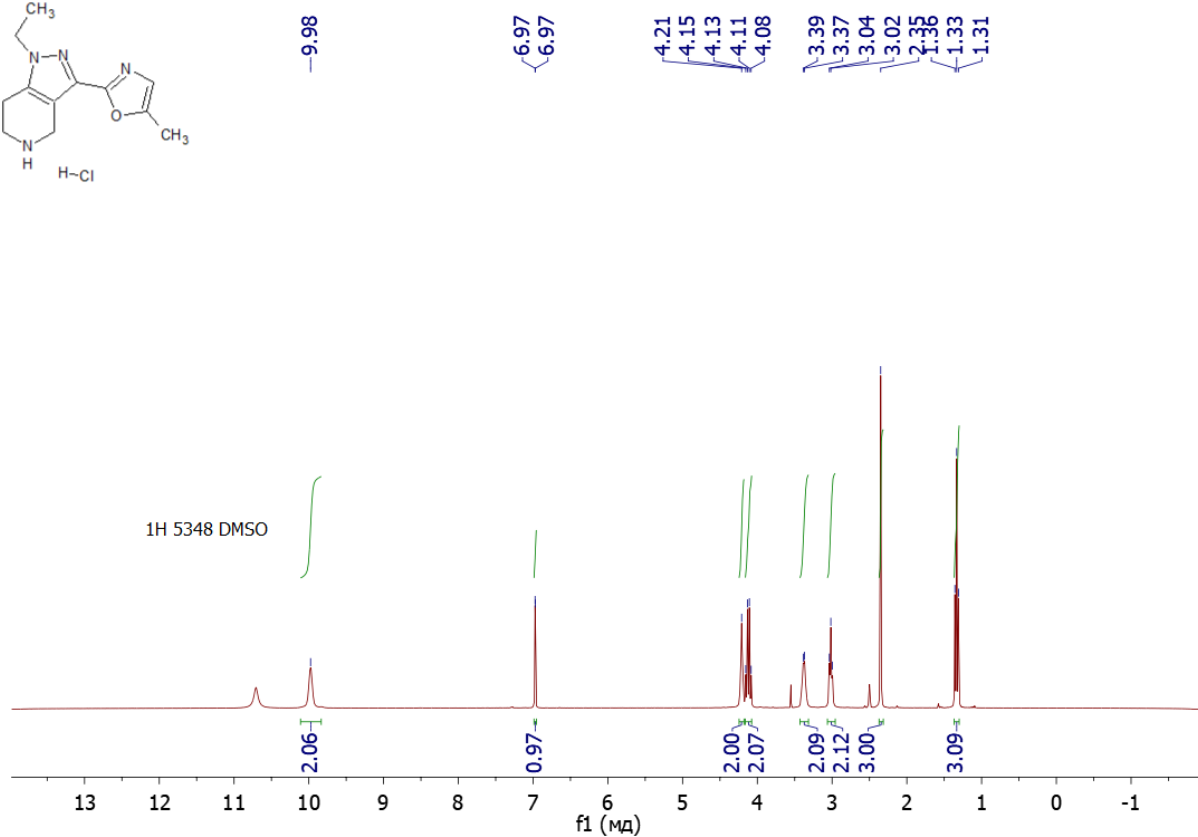
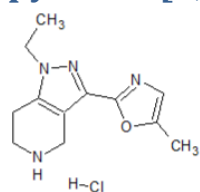
¹³C NMR spectrum (DMSO-d₆) of compound 9a. The x-axis is chemical shift in ppm (f1) from 0.0 to 200.0. The spectrum shows several peaks with chemical shift values.

Chemical Shift (ppm)
155.17
148.68
136.93
135.02
123.92
108.85
39.99
39.70
36.50
18.52
10.73

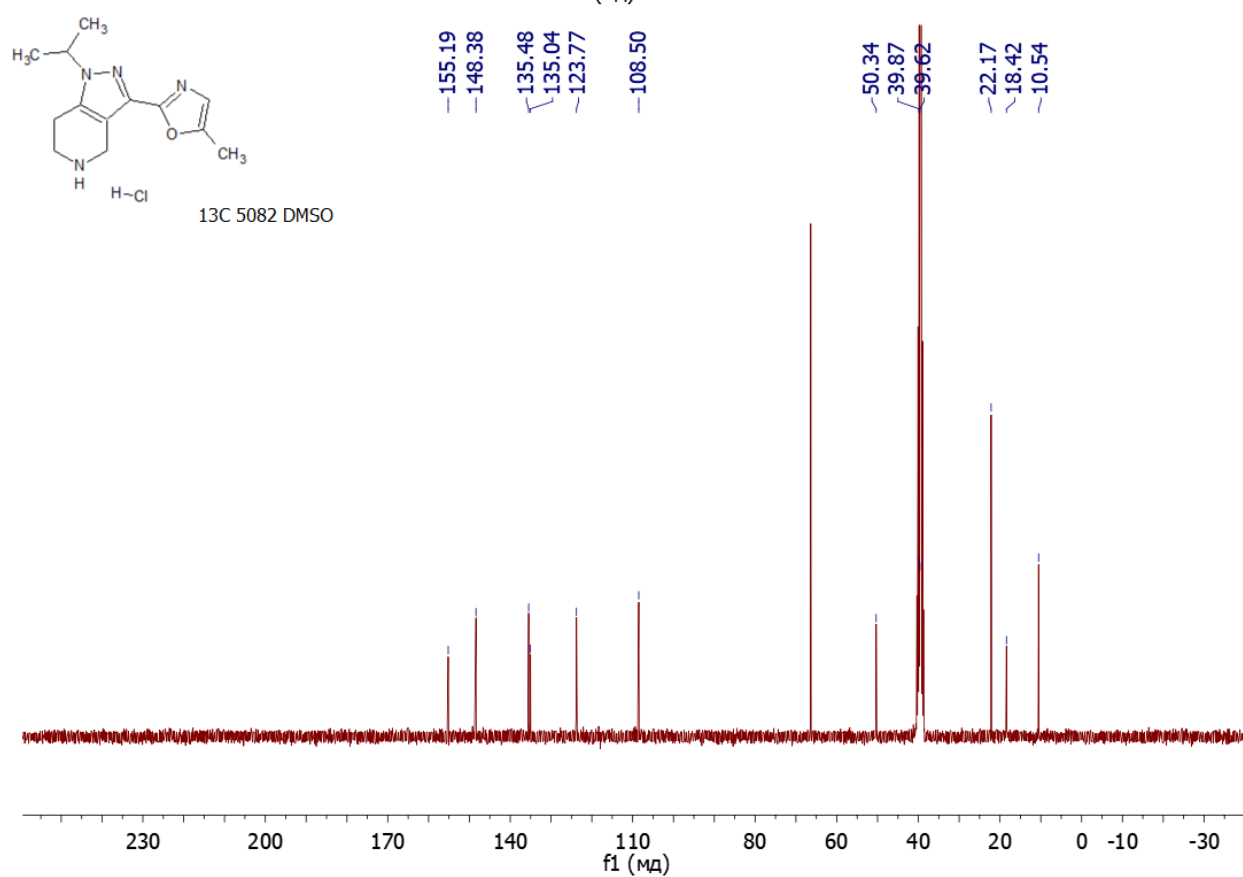
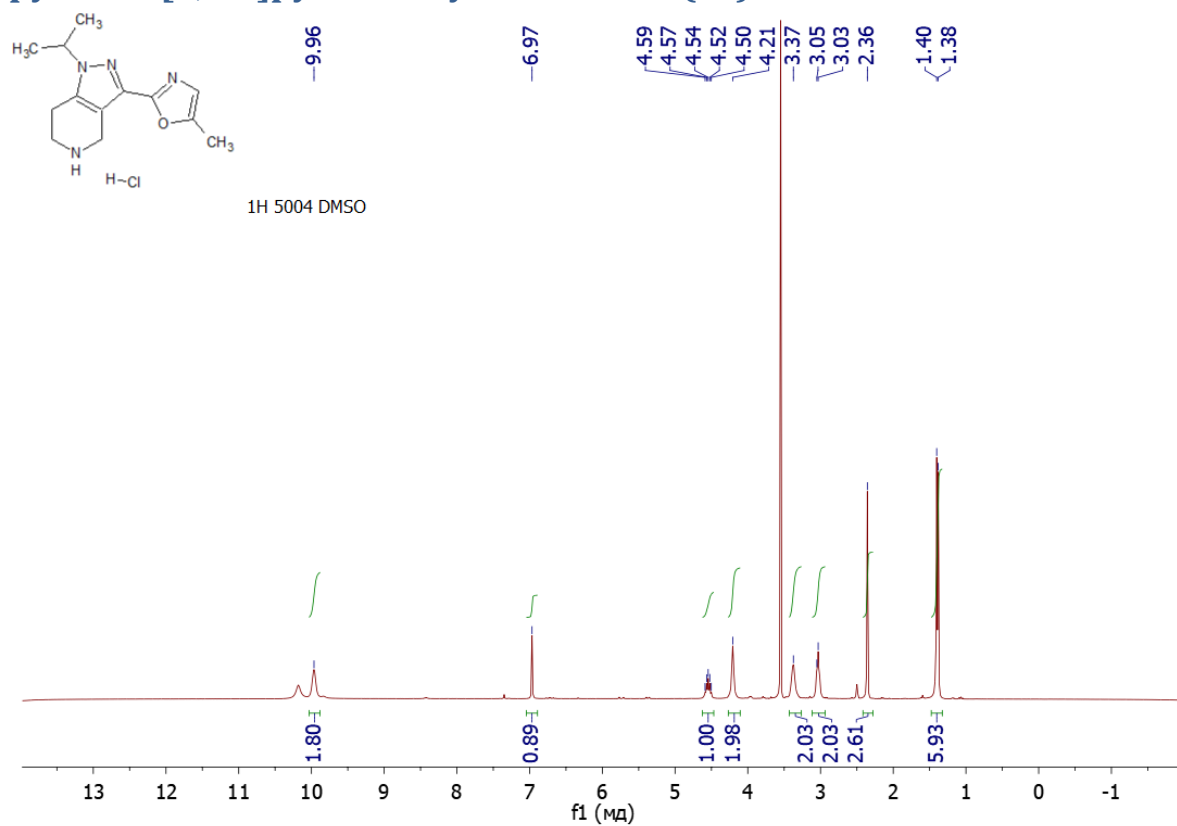
¹³C 5927 DMSO



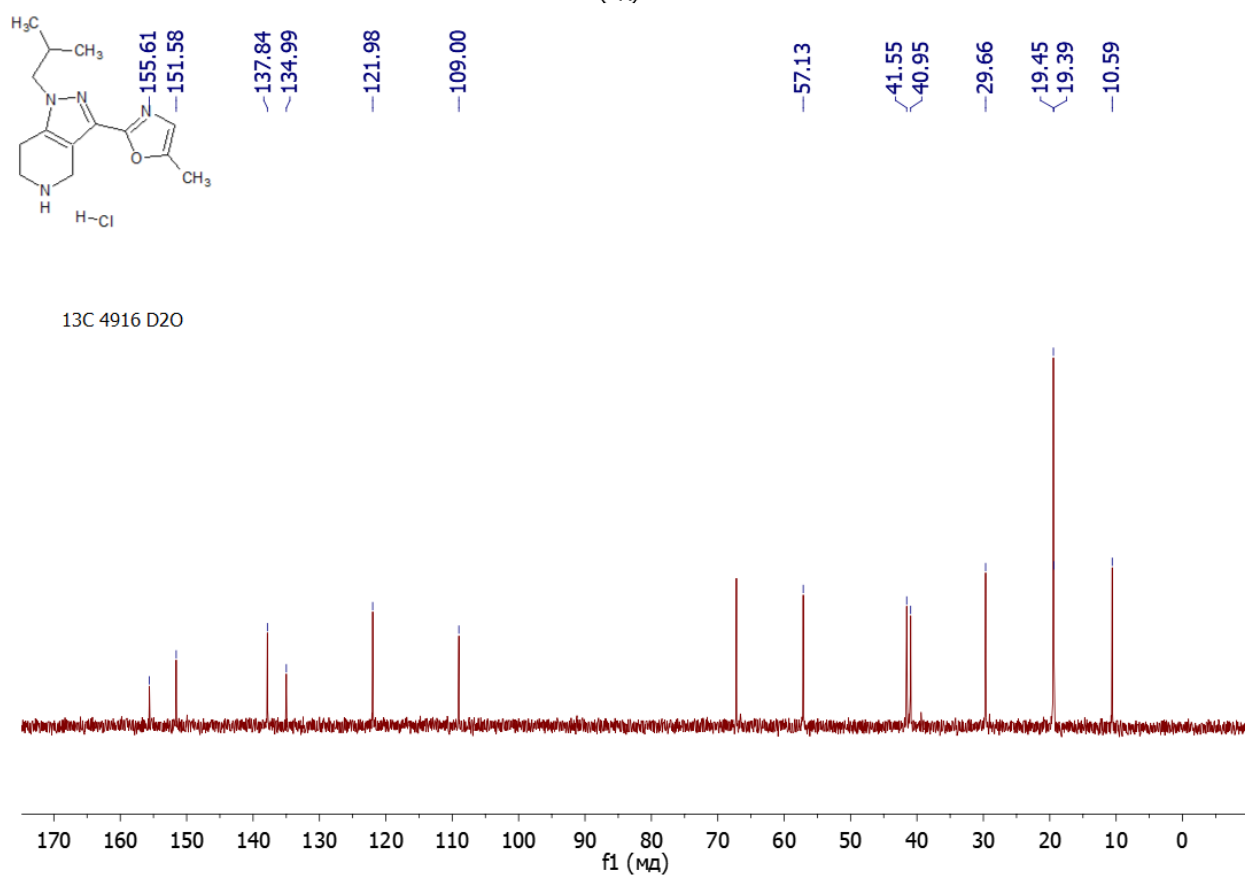
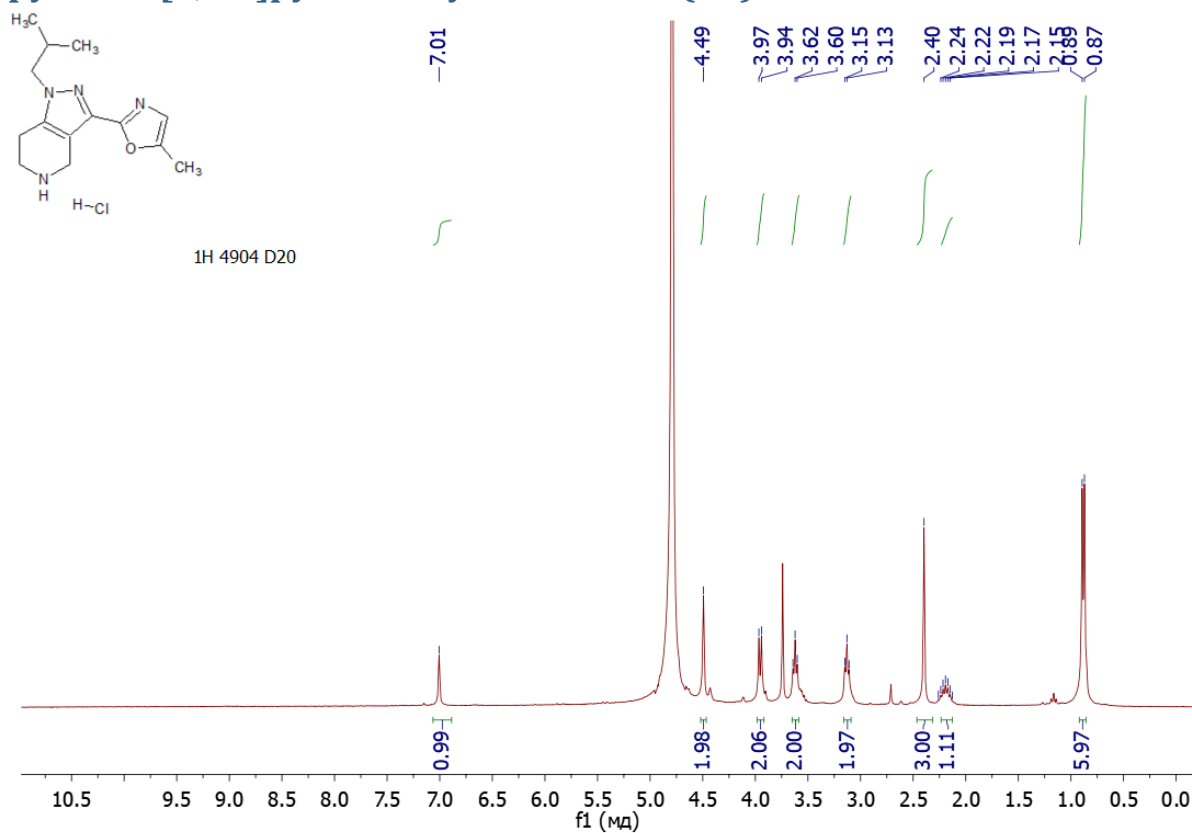
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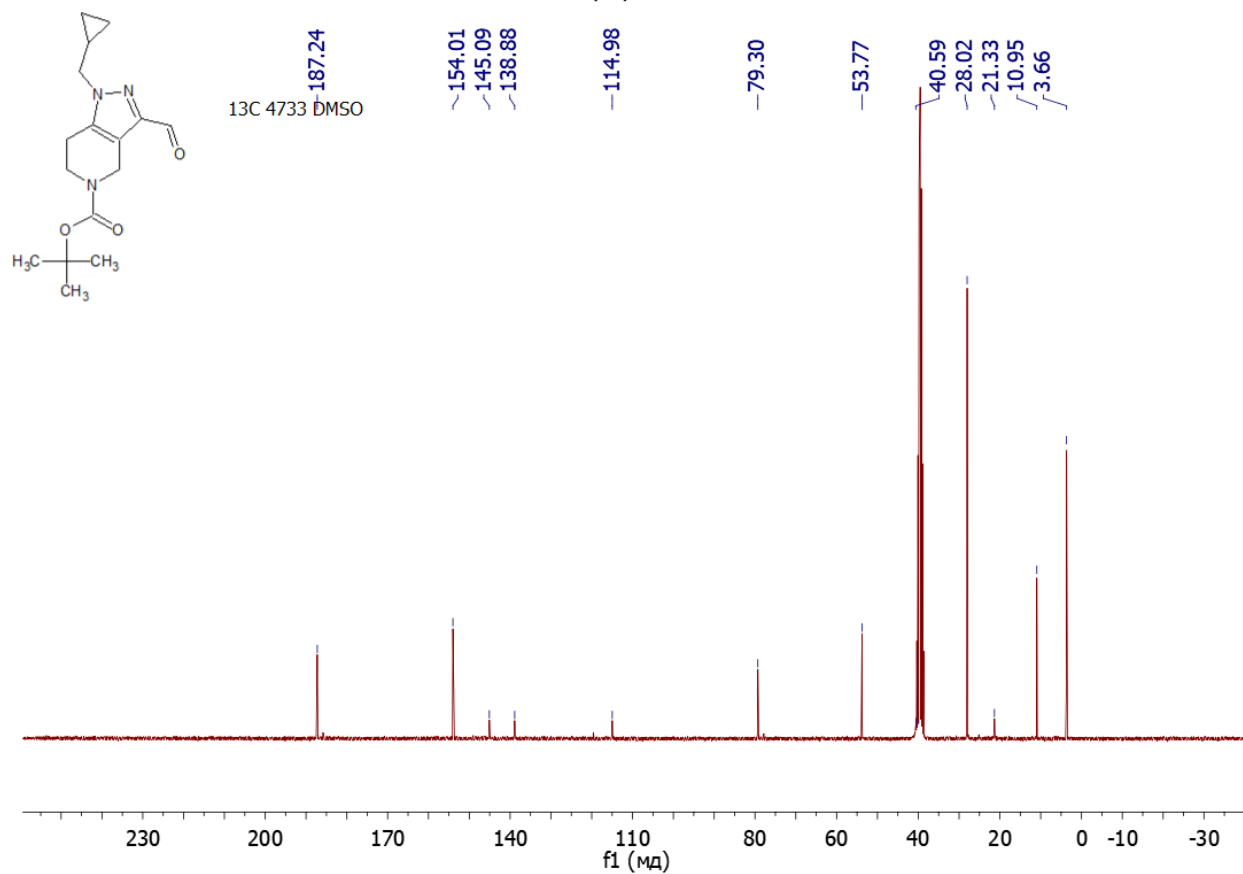
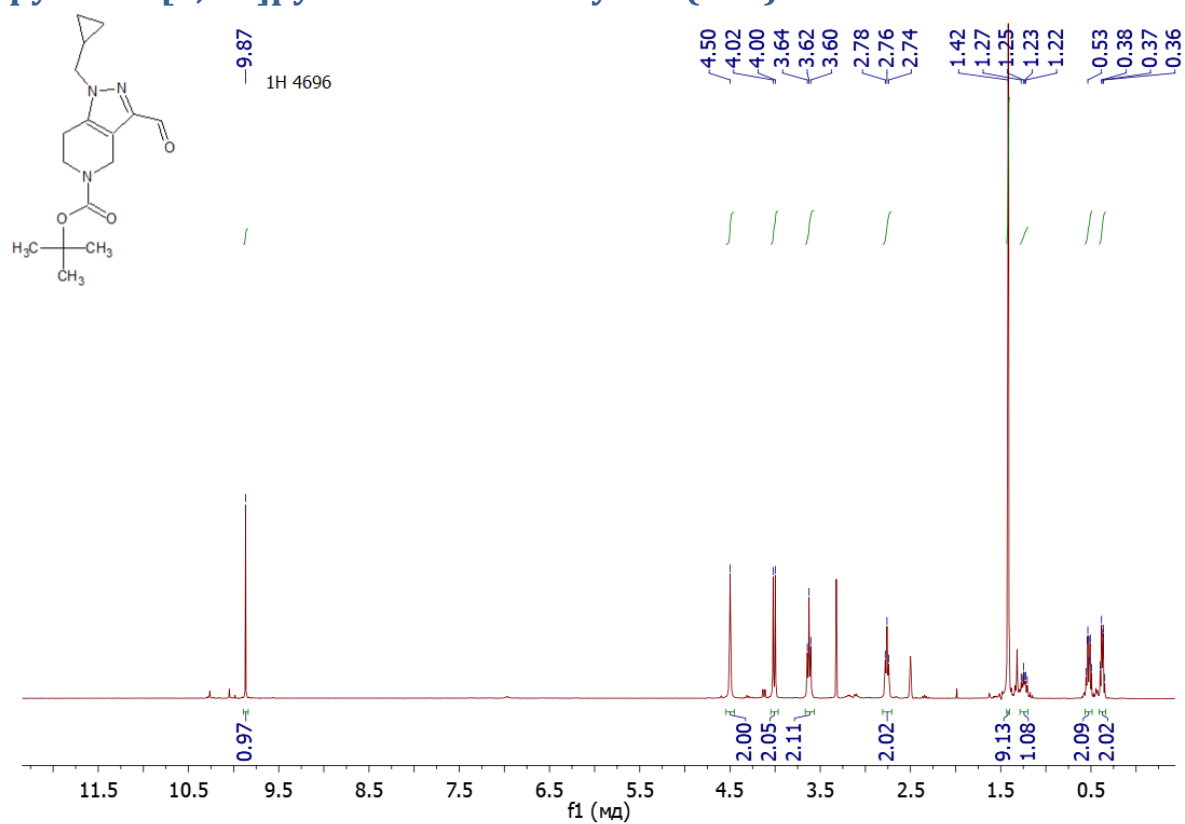
3-(5-methyl-1,3-oxazol-2-yl)-1-(propan-2-yl)-4,5,6,7-tetrahydro-1H-pyrazolo[4,3-c]pyridine hydrochloride (9c)



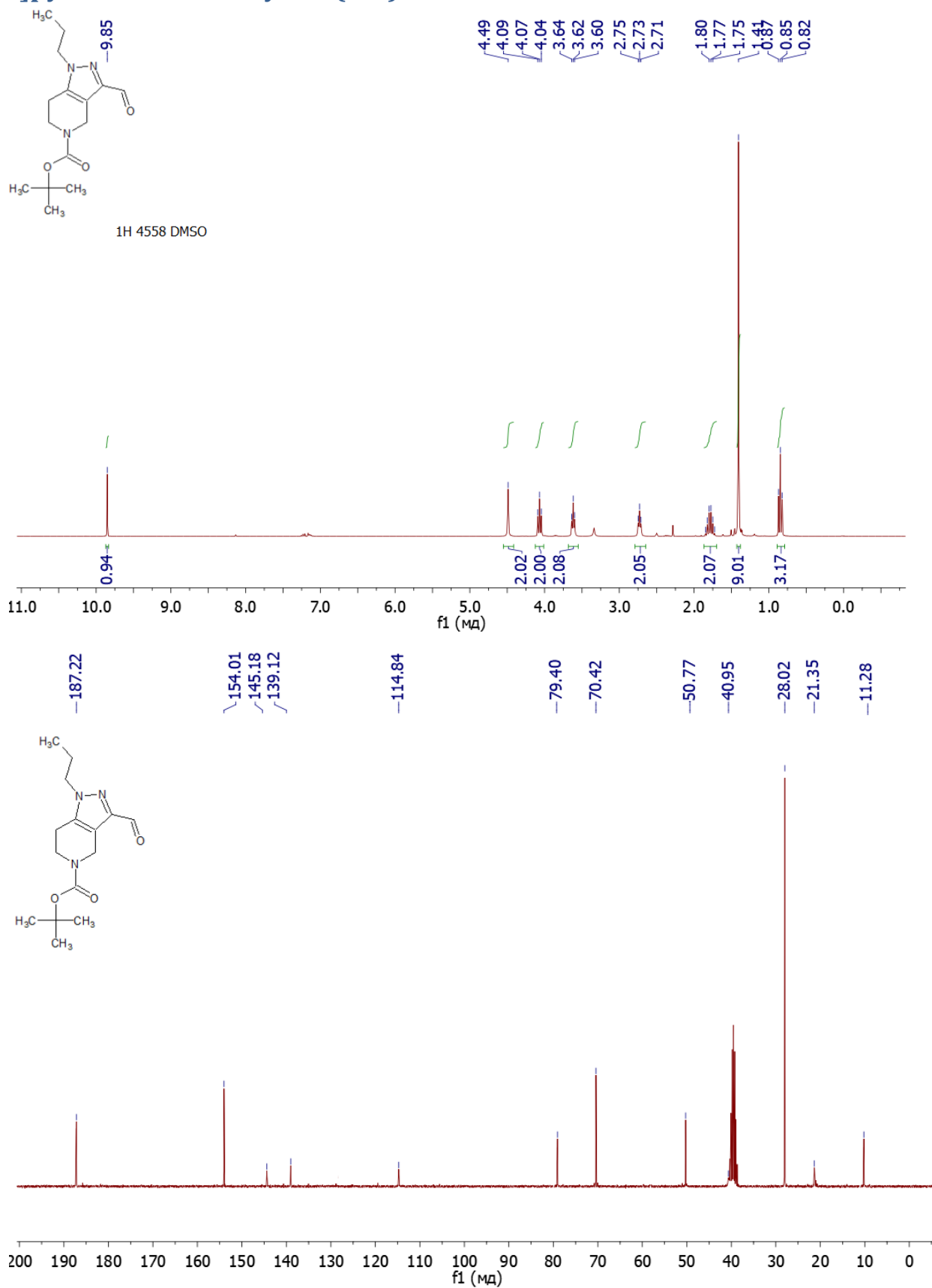
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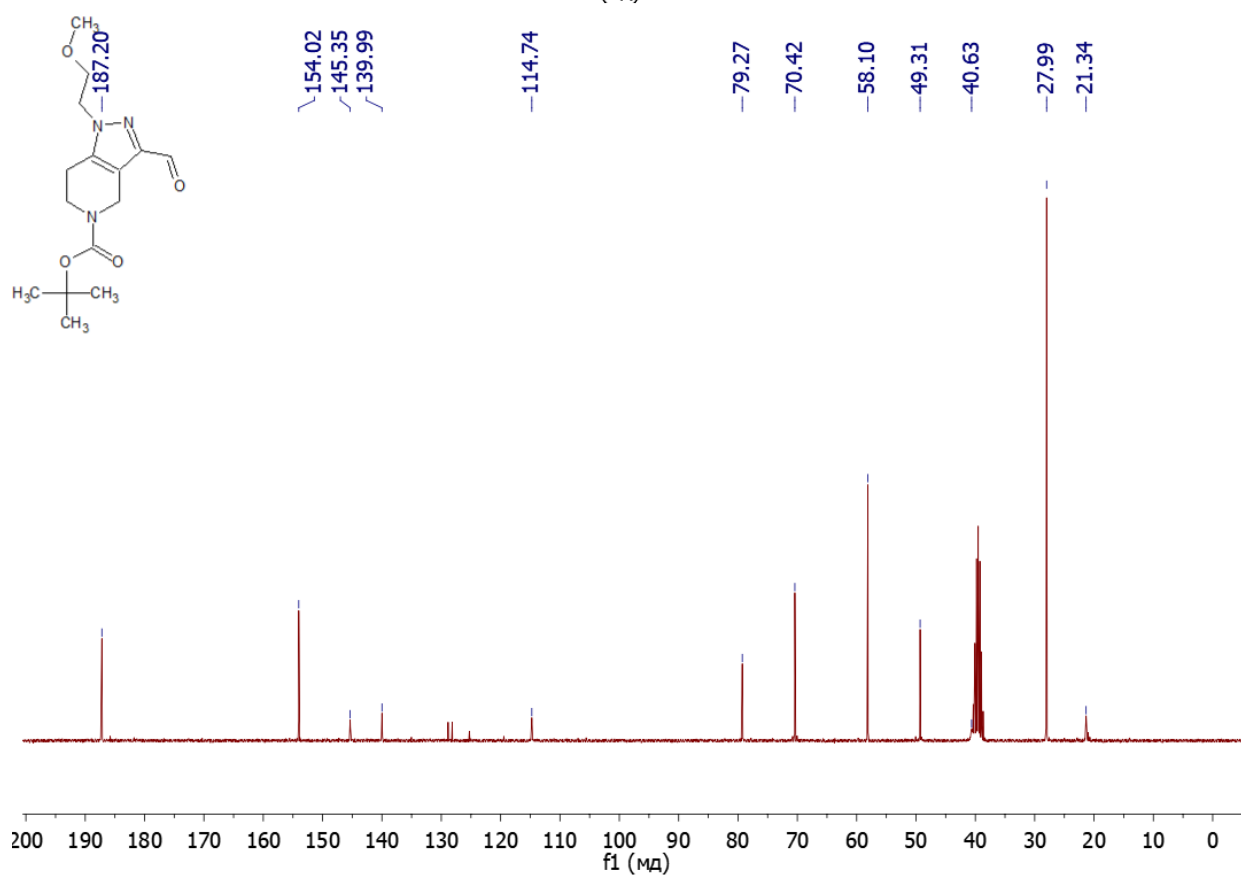
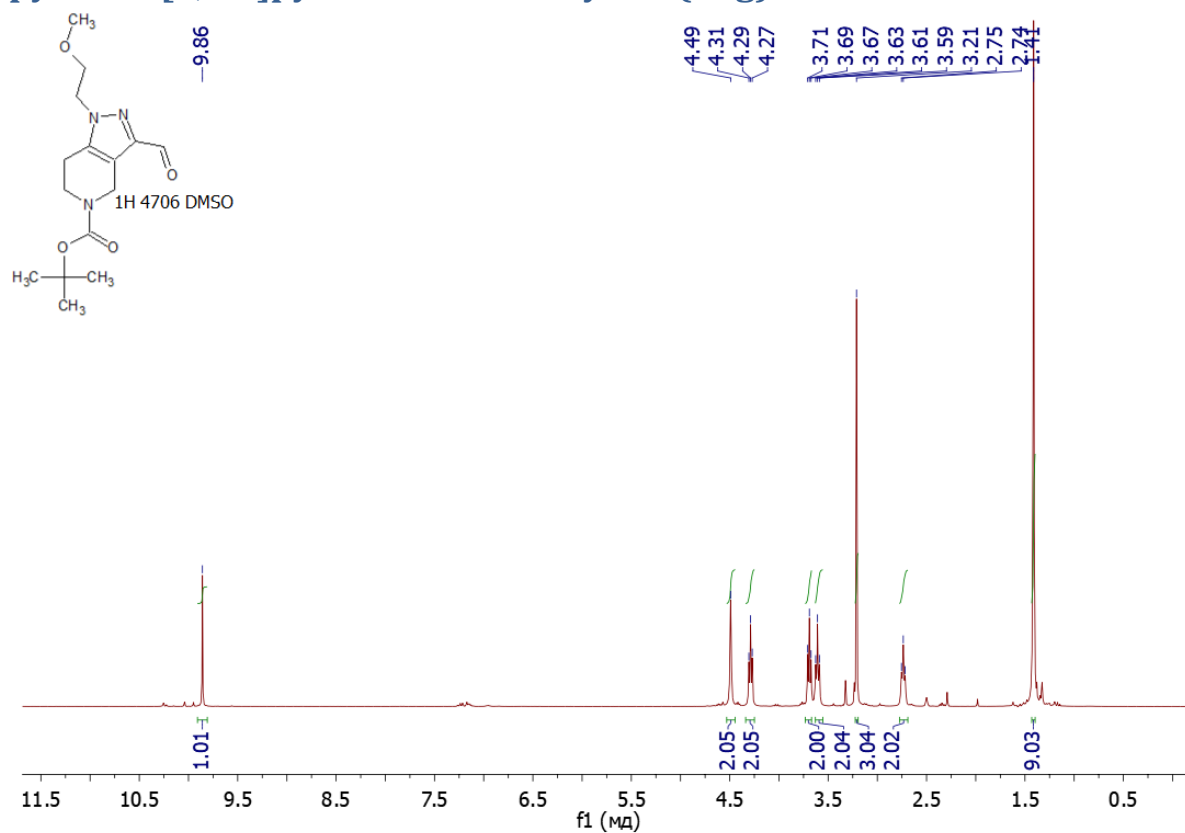
tert-butyl 1-(cyclopropylmethyl)-3-formyl-1,4,6,7-tetrahydro-5H-pyrazolo[4,3-c]pyridine-5- carboxylate (11e)



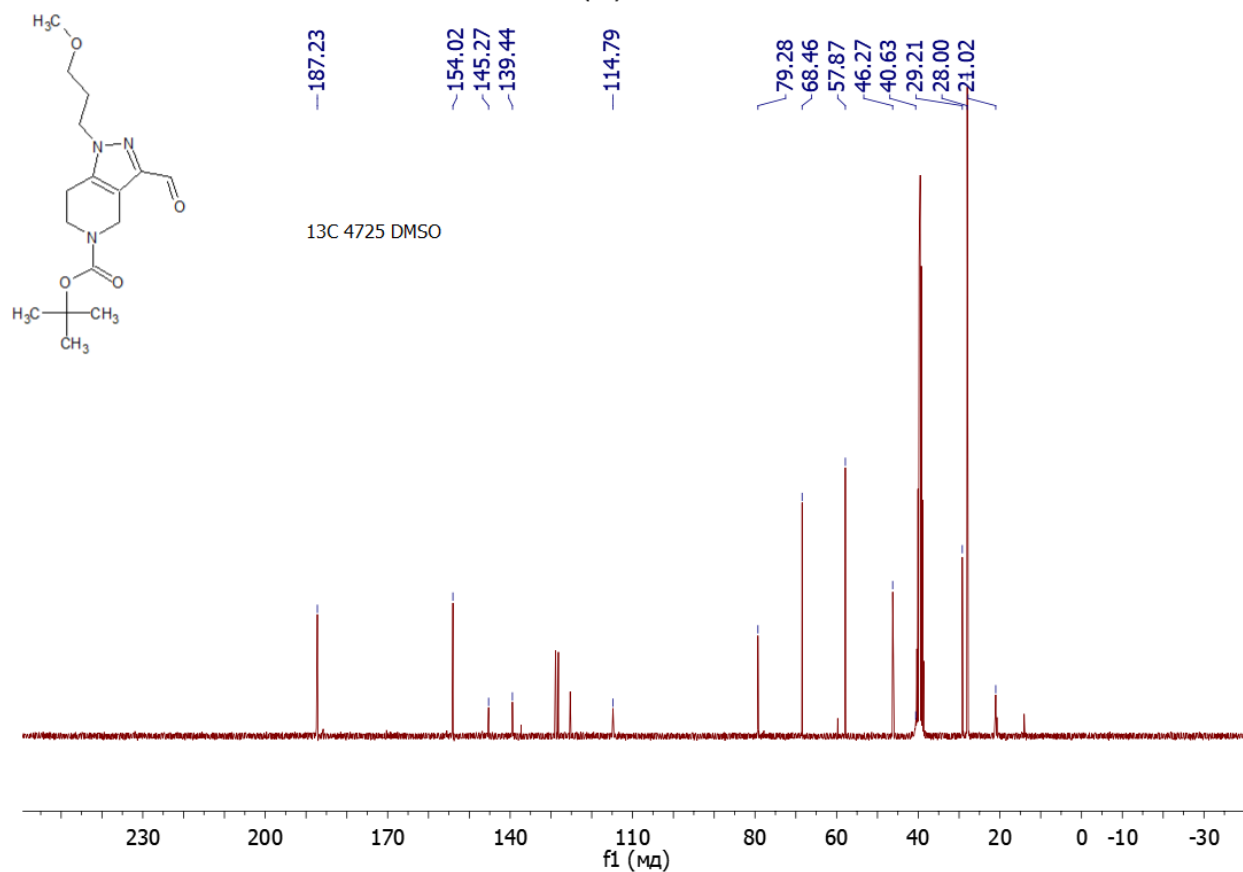
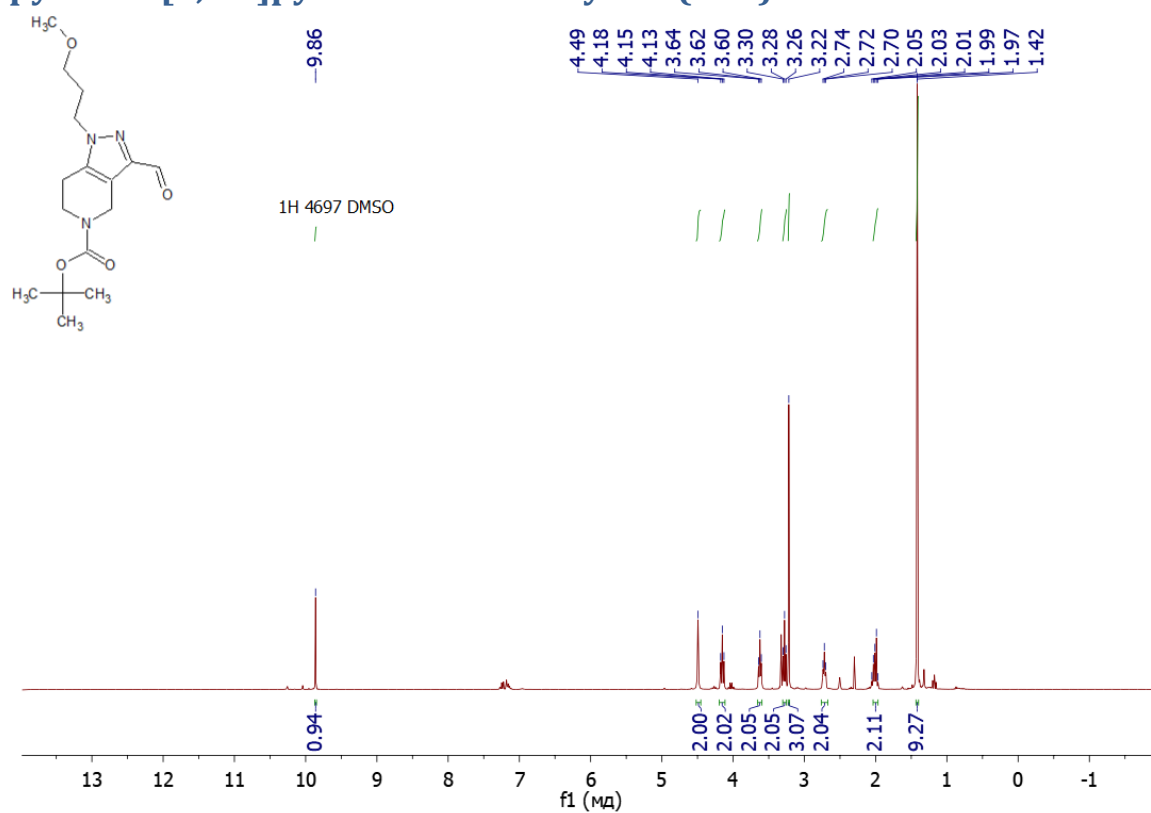
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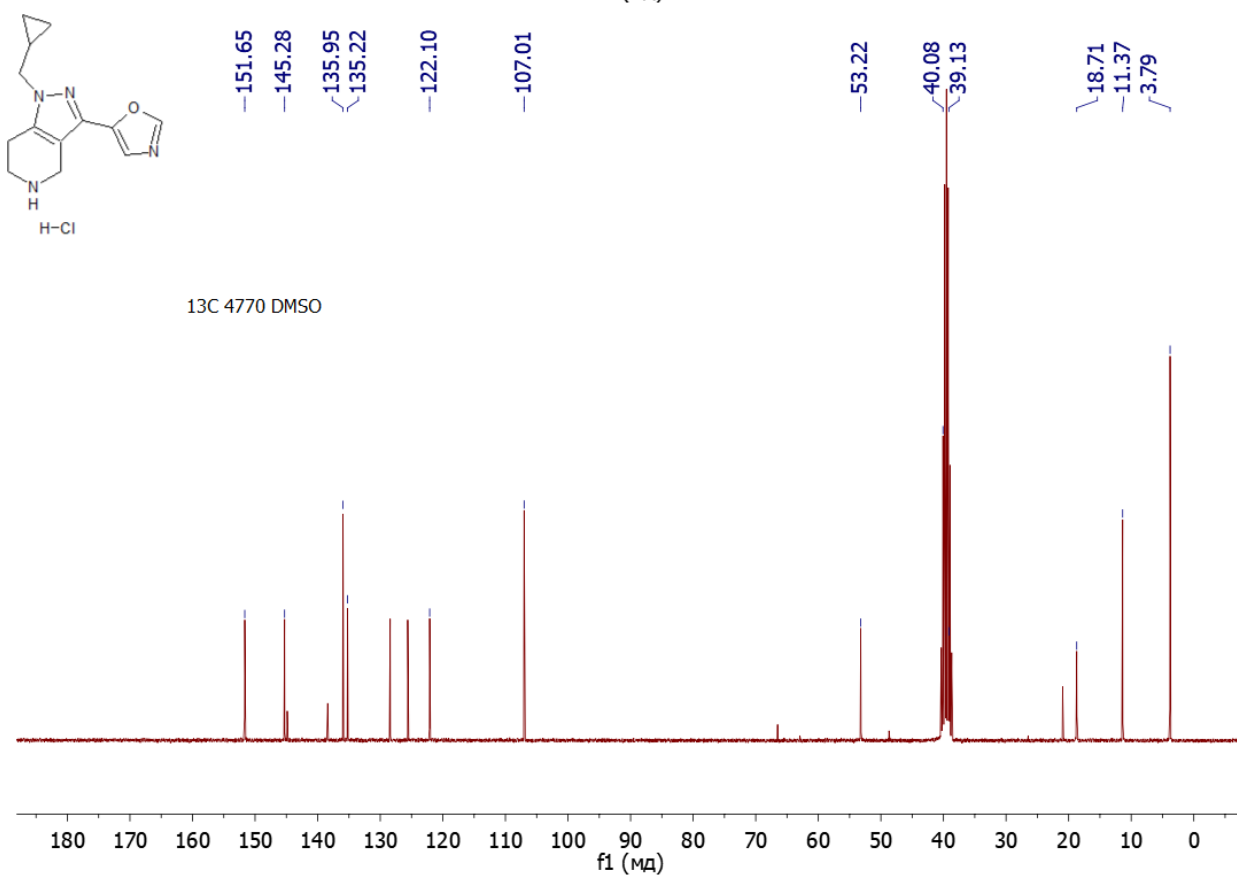
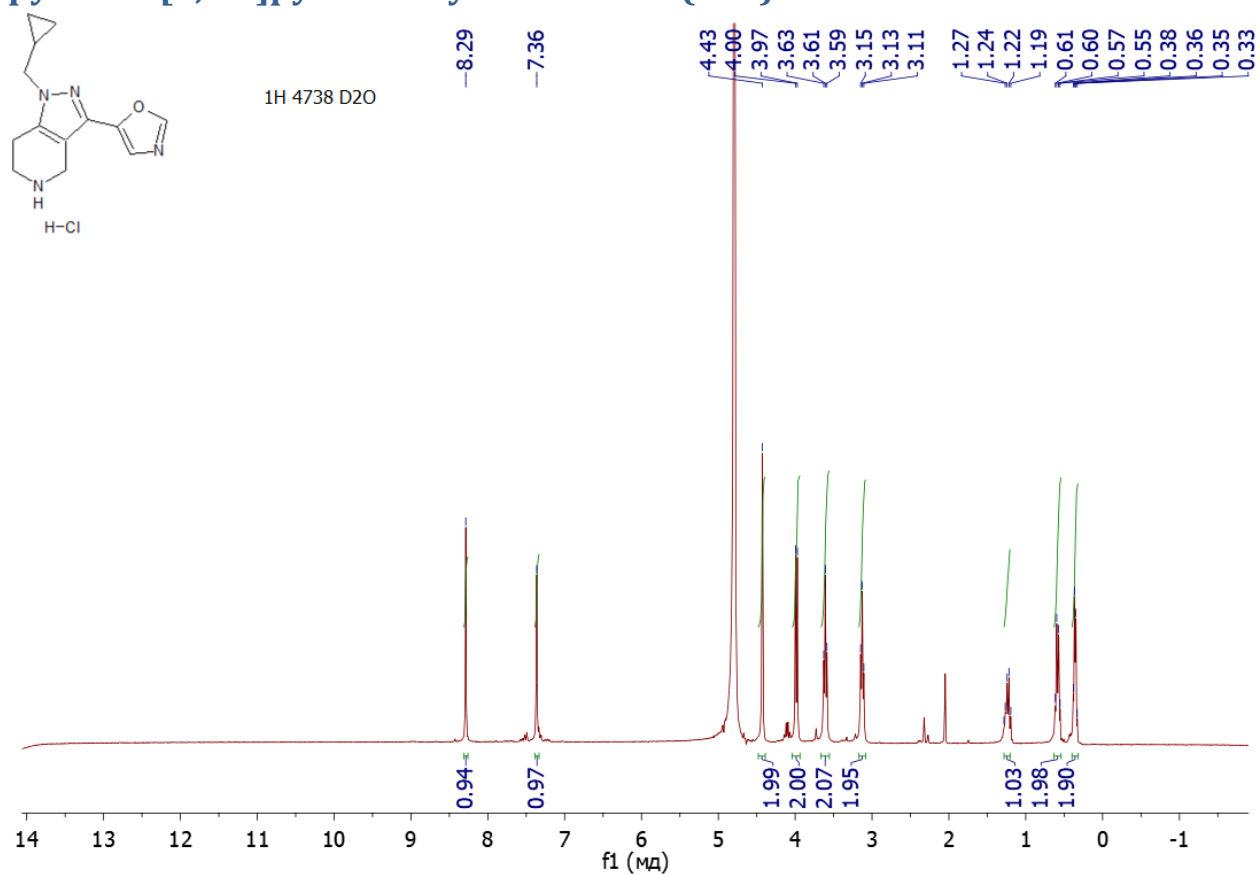
tert-butyl 3-formyl-1-(2-methoxyethyl)-1,4,6,7-tetrahydro-5H-pyrazolo[4,3-c]pyridine-5-carboxylate (11g)



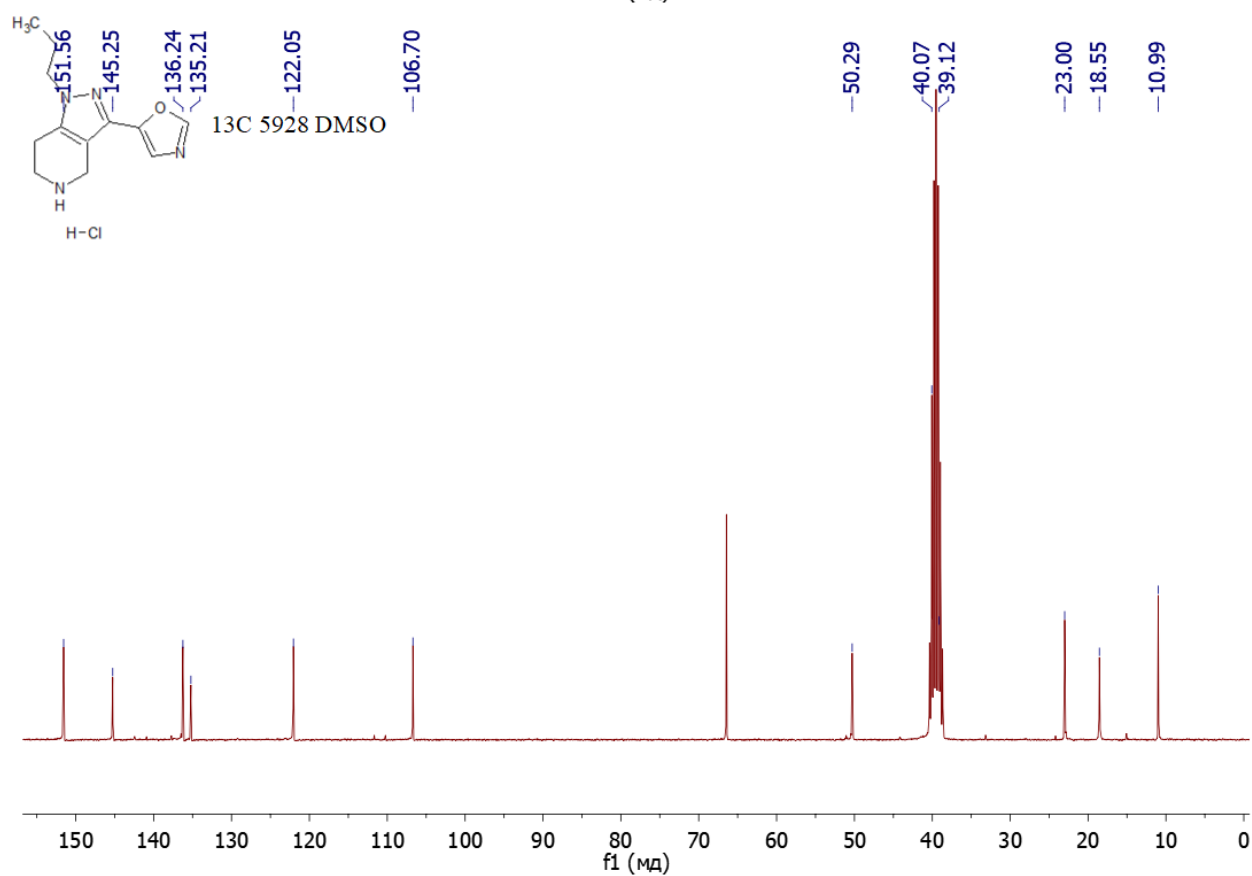
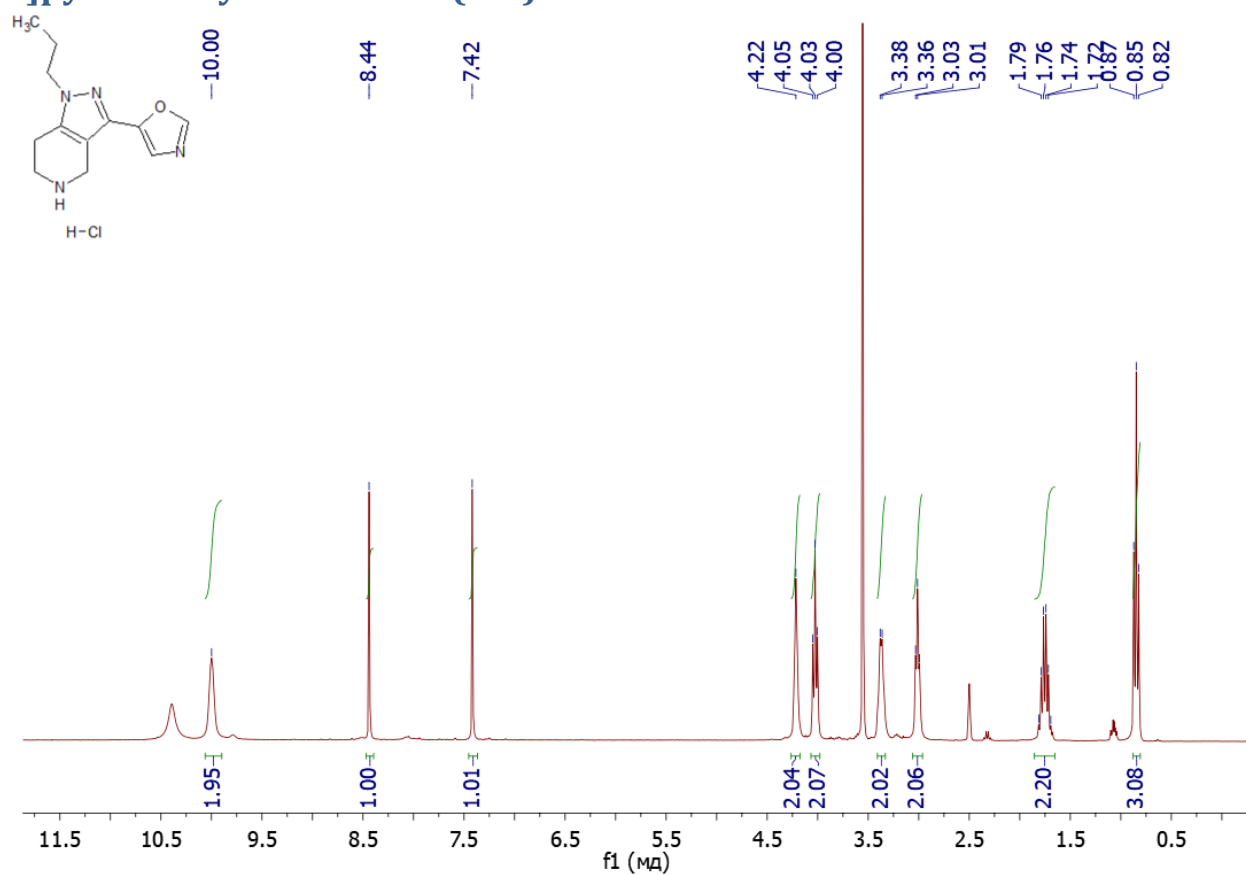
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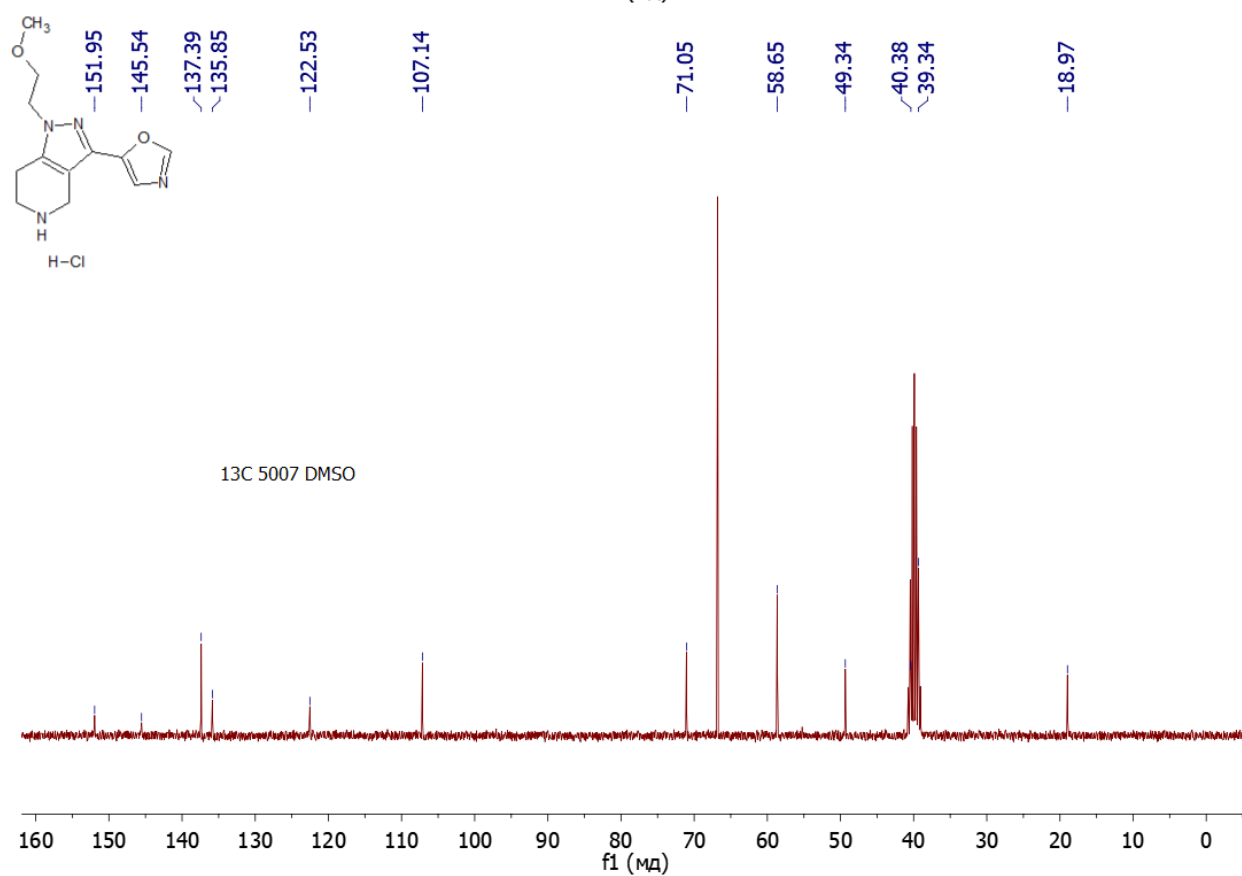
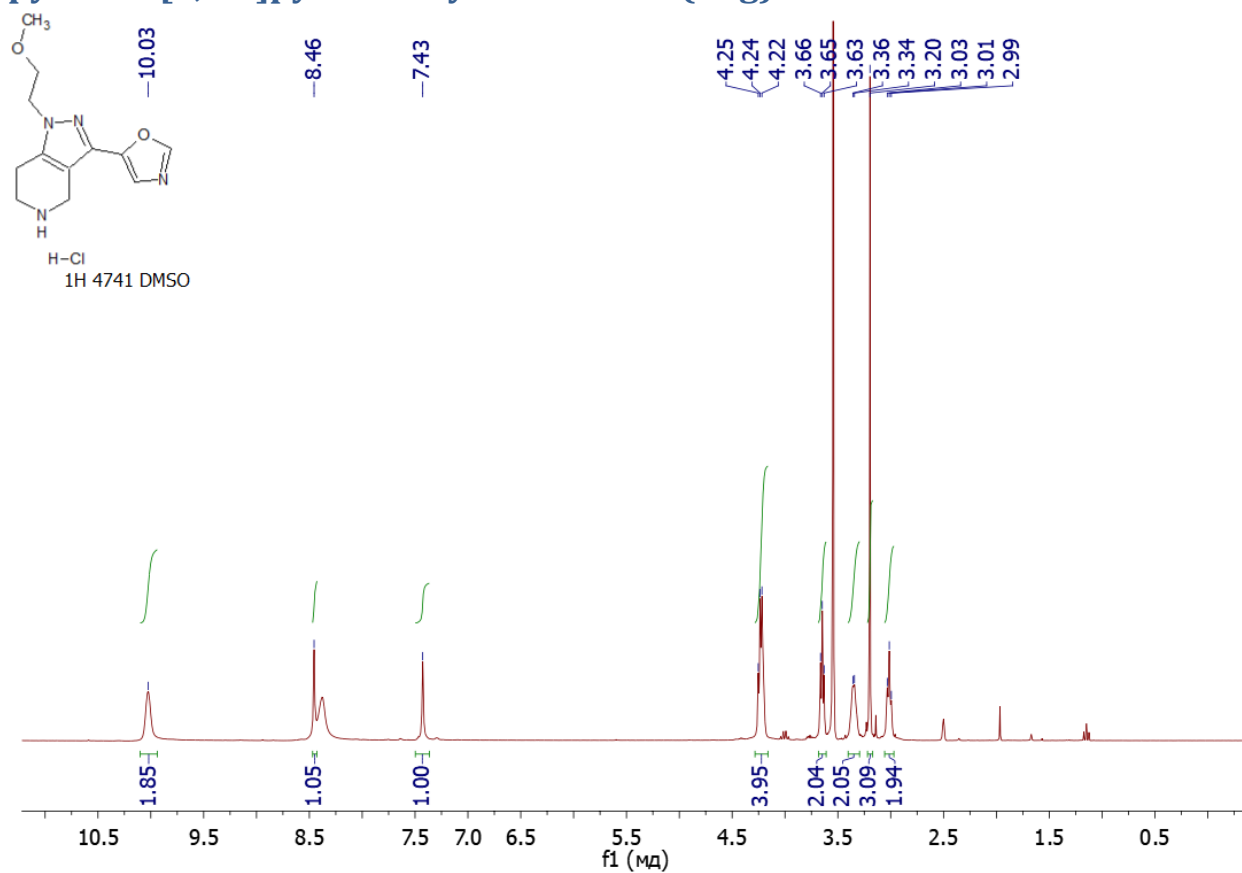
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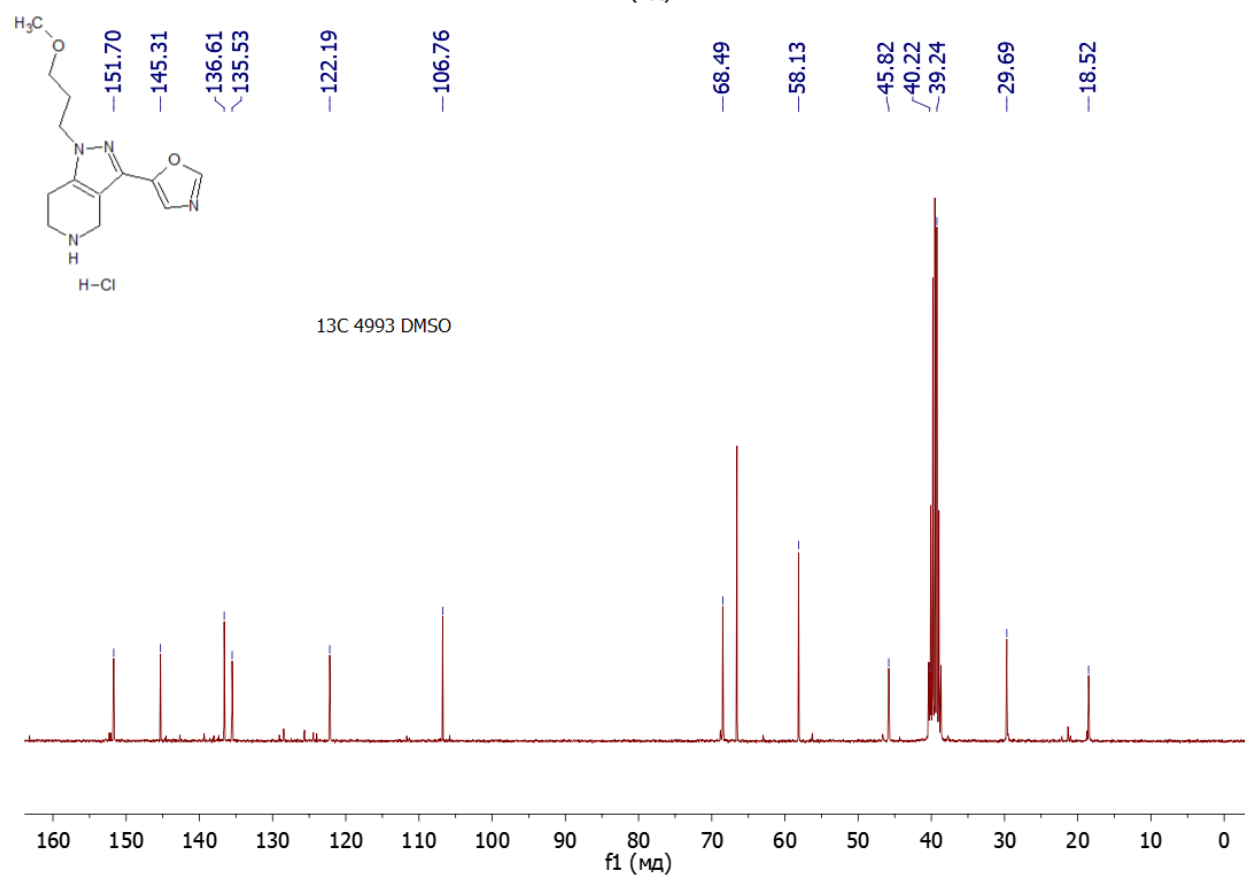
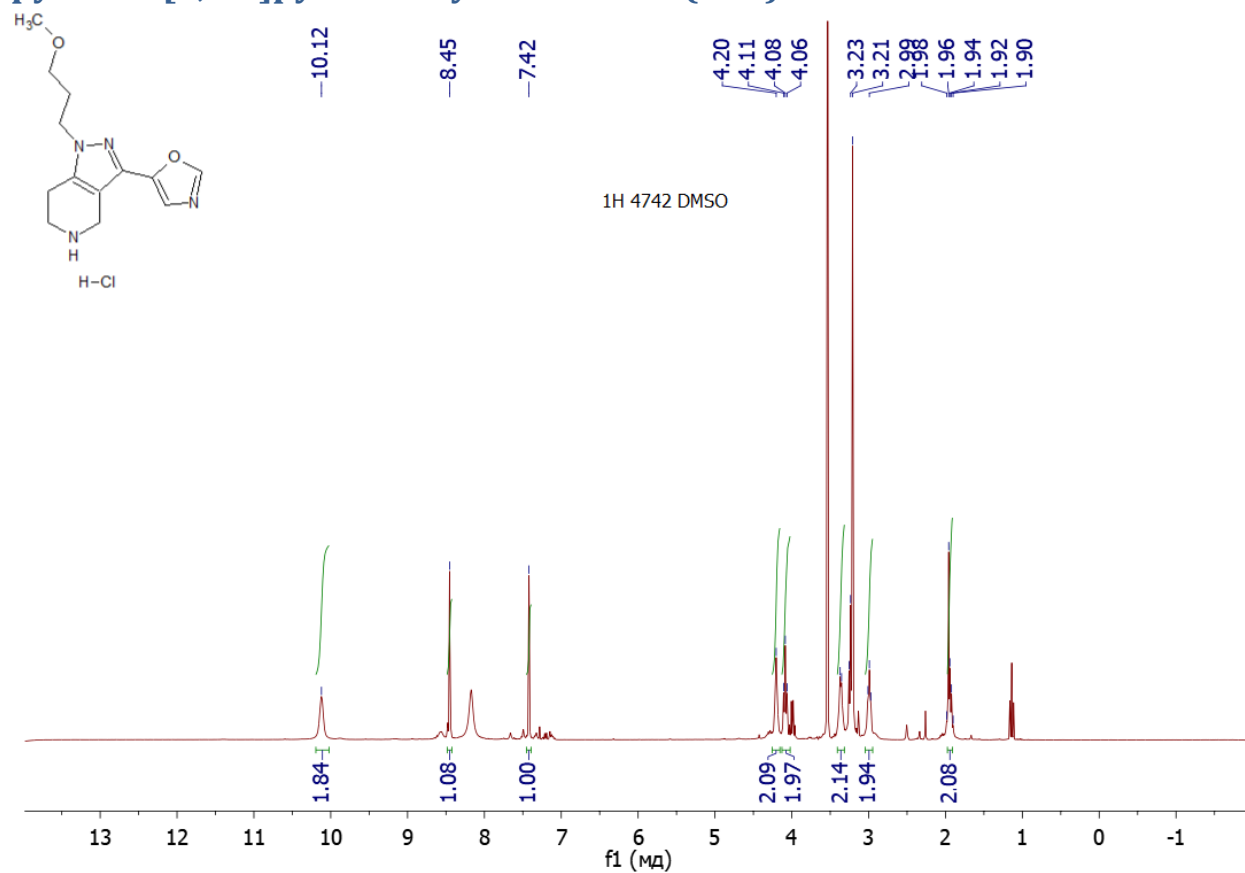
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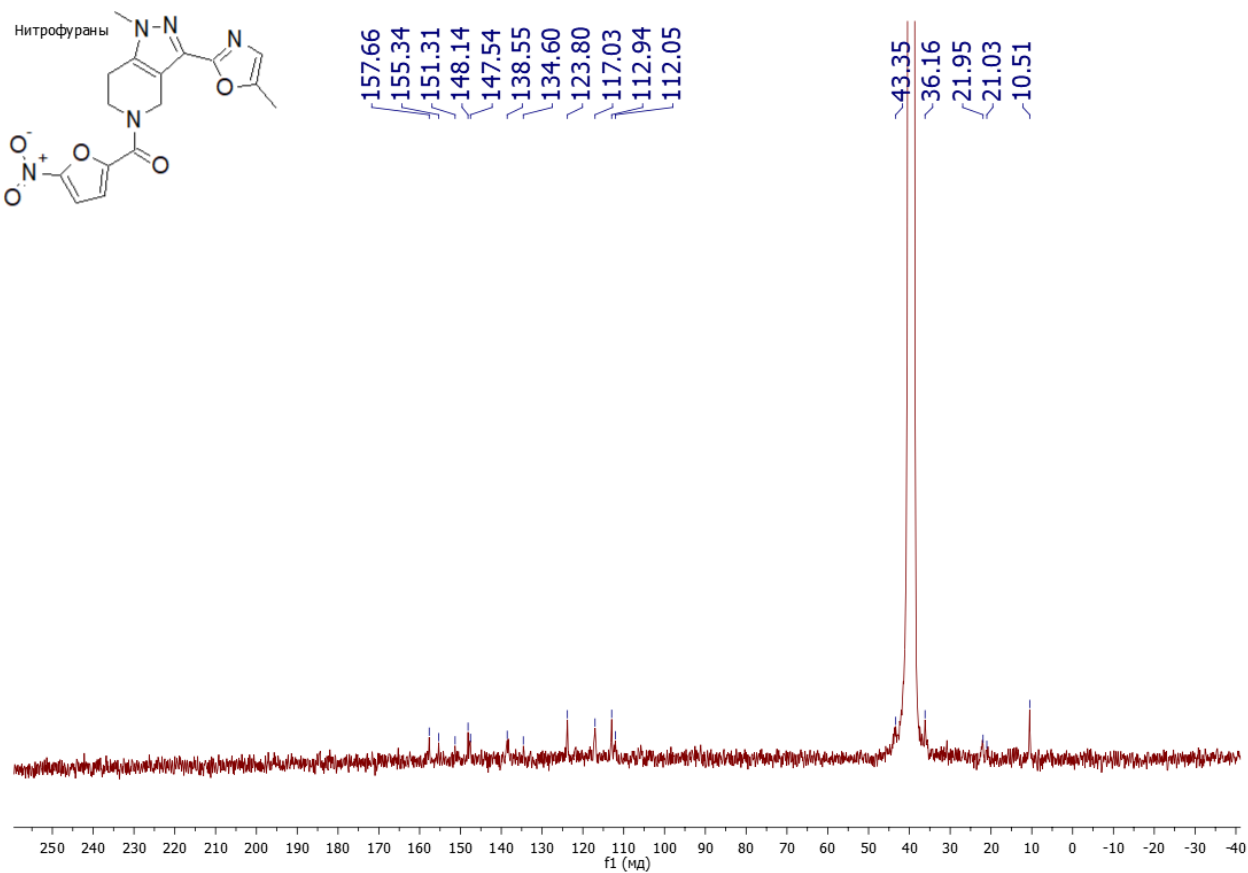
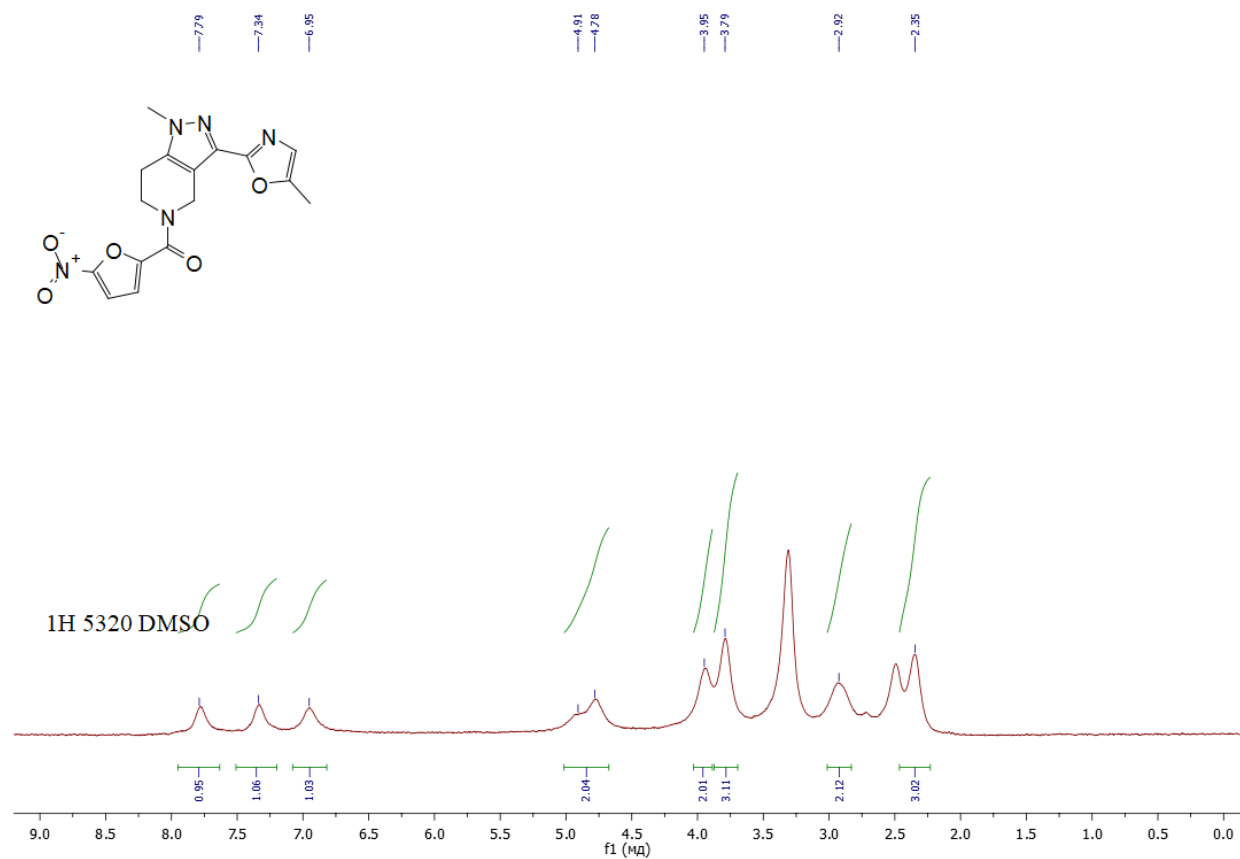
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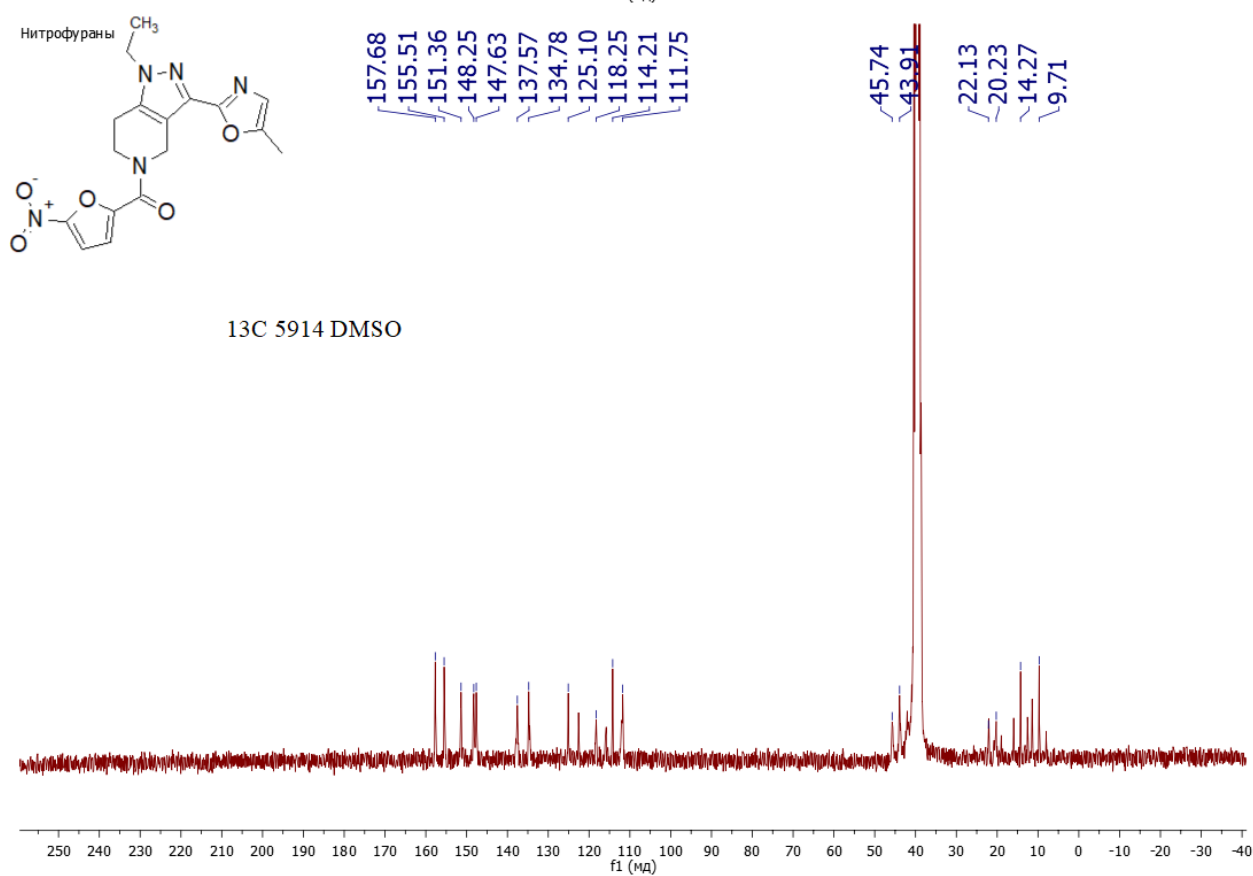
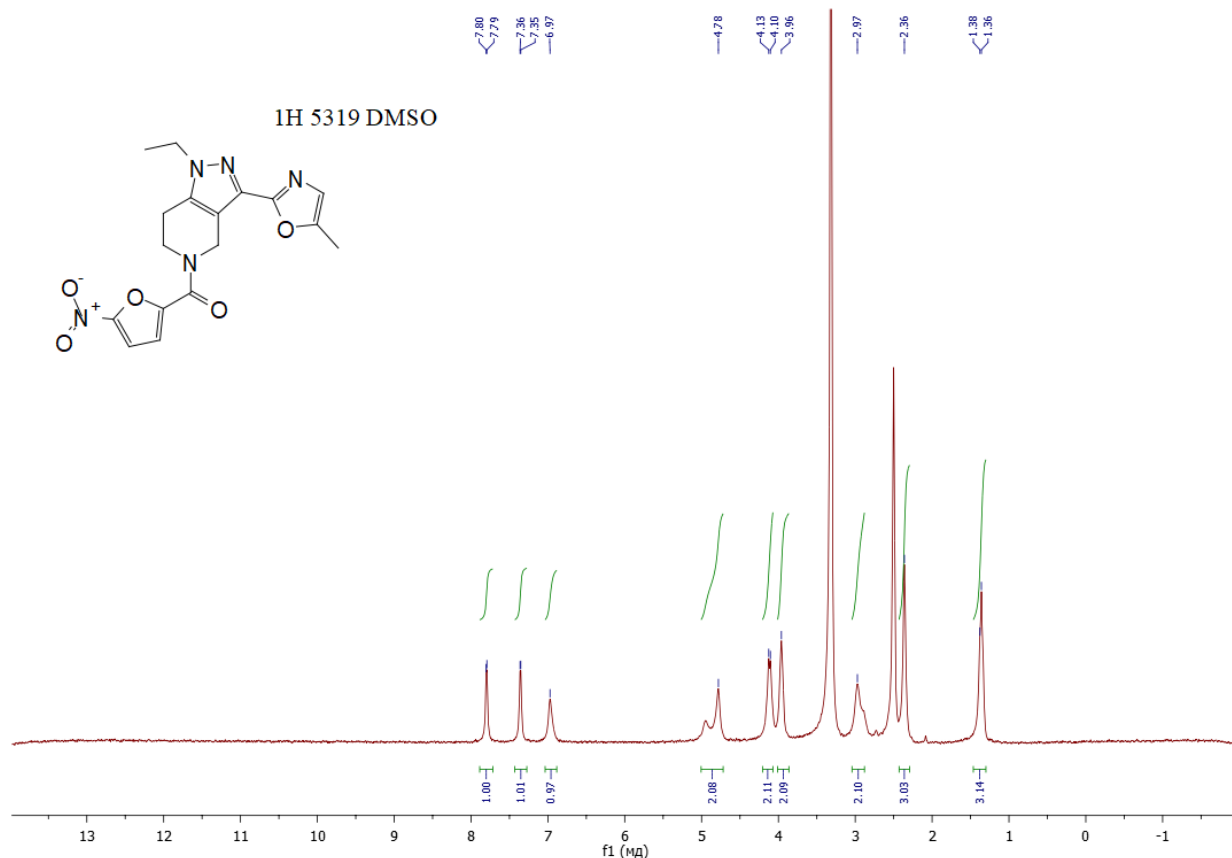
1-(3-methoxypropyl)-3-(1,3-oxazol-5-yl)-4,5,6,7-tetrahydro-1H-pyrazolo[4,3-c]pyridine hydrochloride (12h)



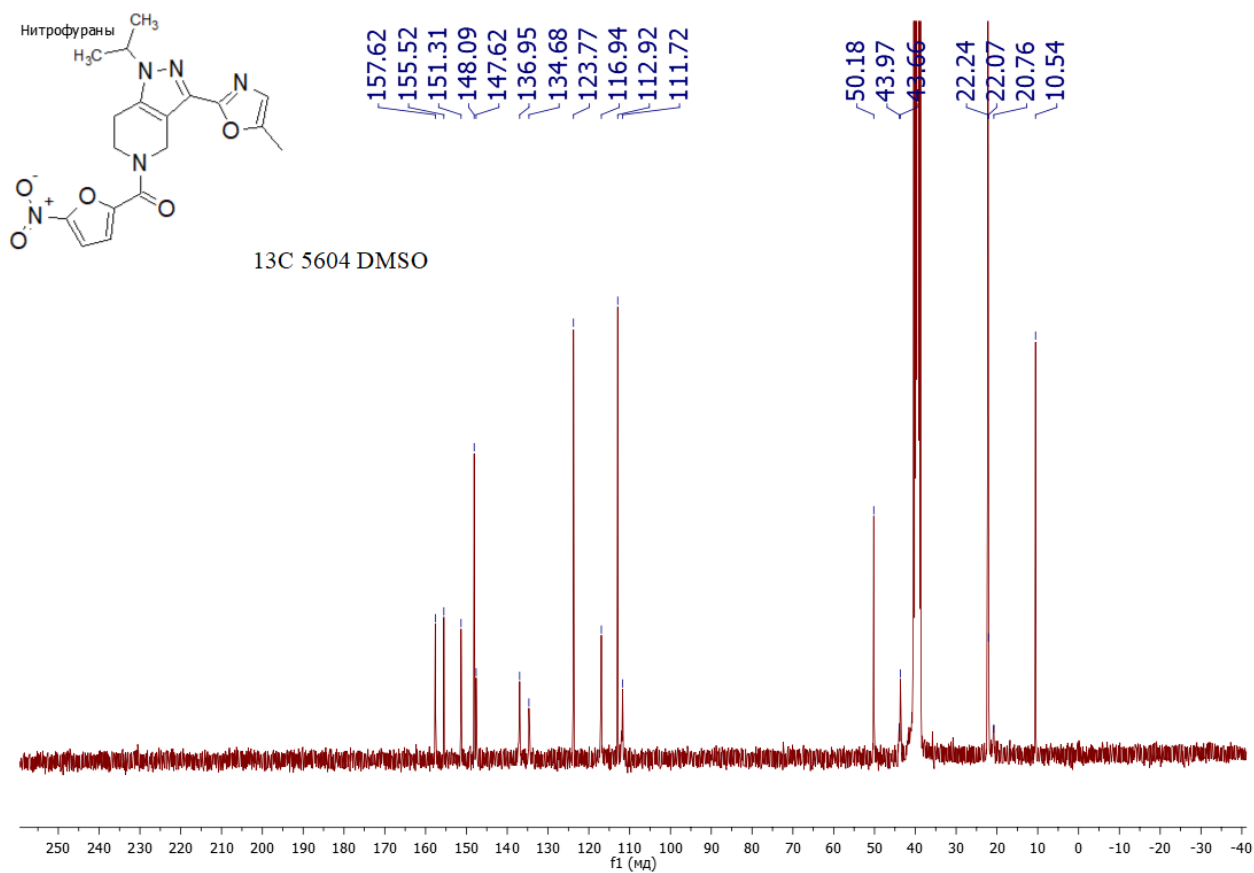
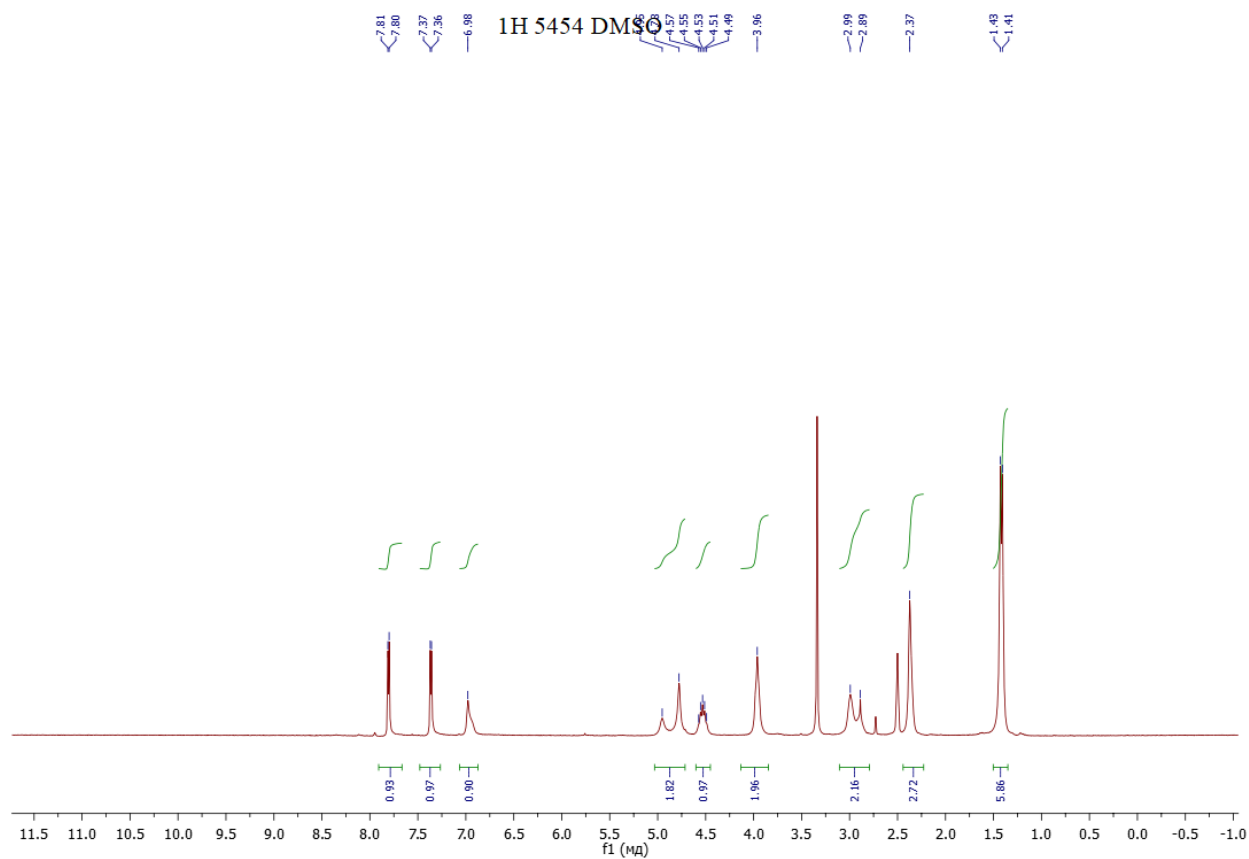
1-methyl-3-(5-methyl-1,3-oxazol-2-yl)-5-(5-nitro-2-furoyl)-4,5,6,7-tetrahydro-1H-pyrazolo [4,3-c]pyridine, LK01510 (10a)



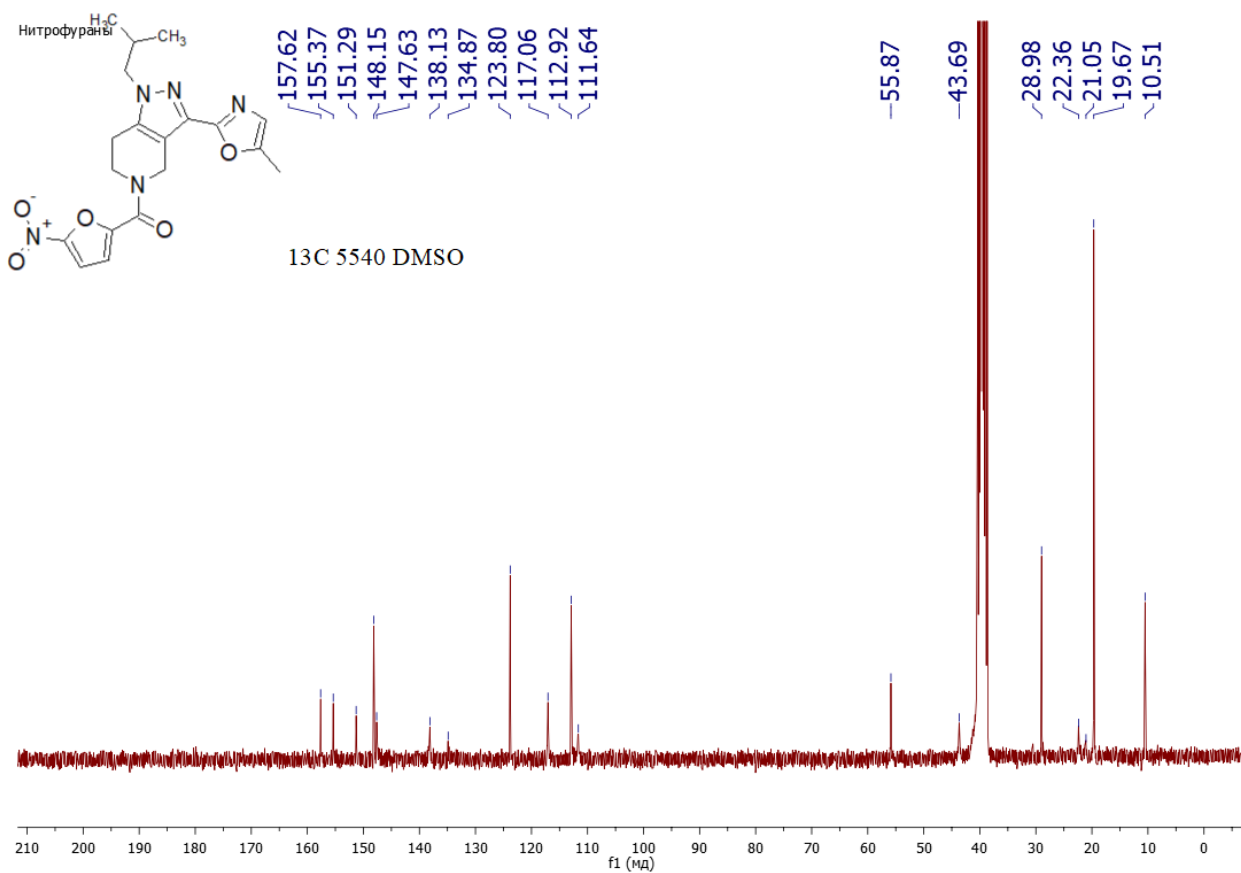
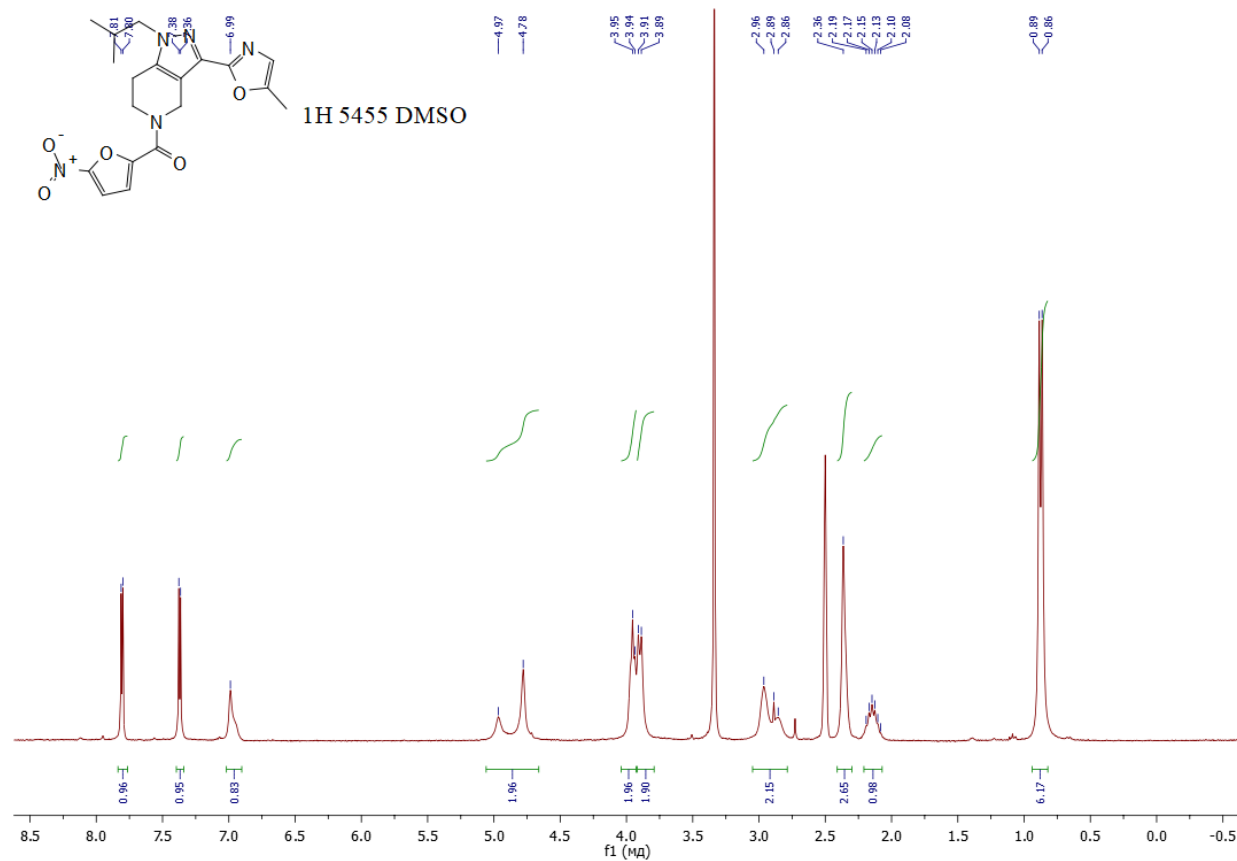
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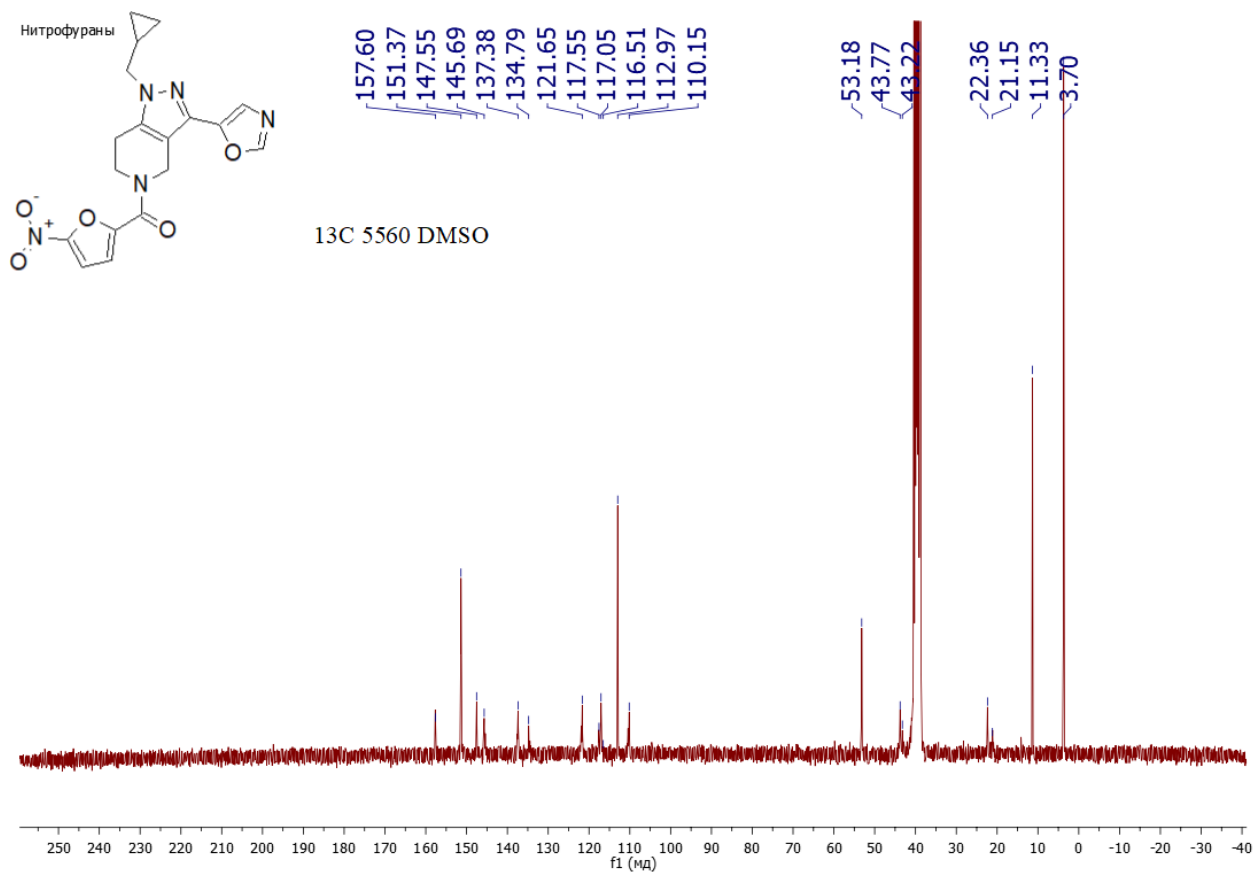
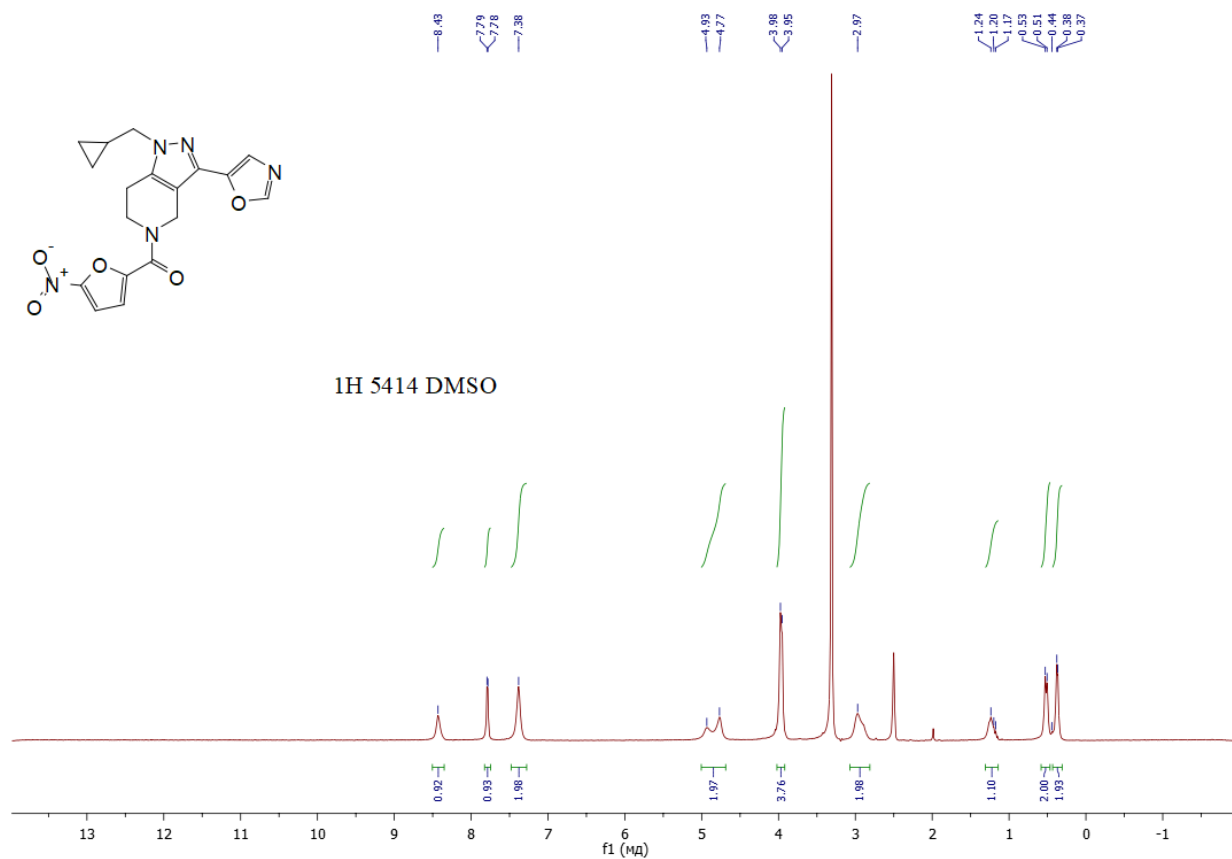
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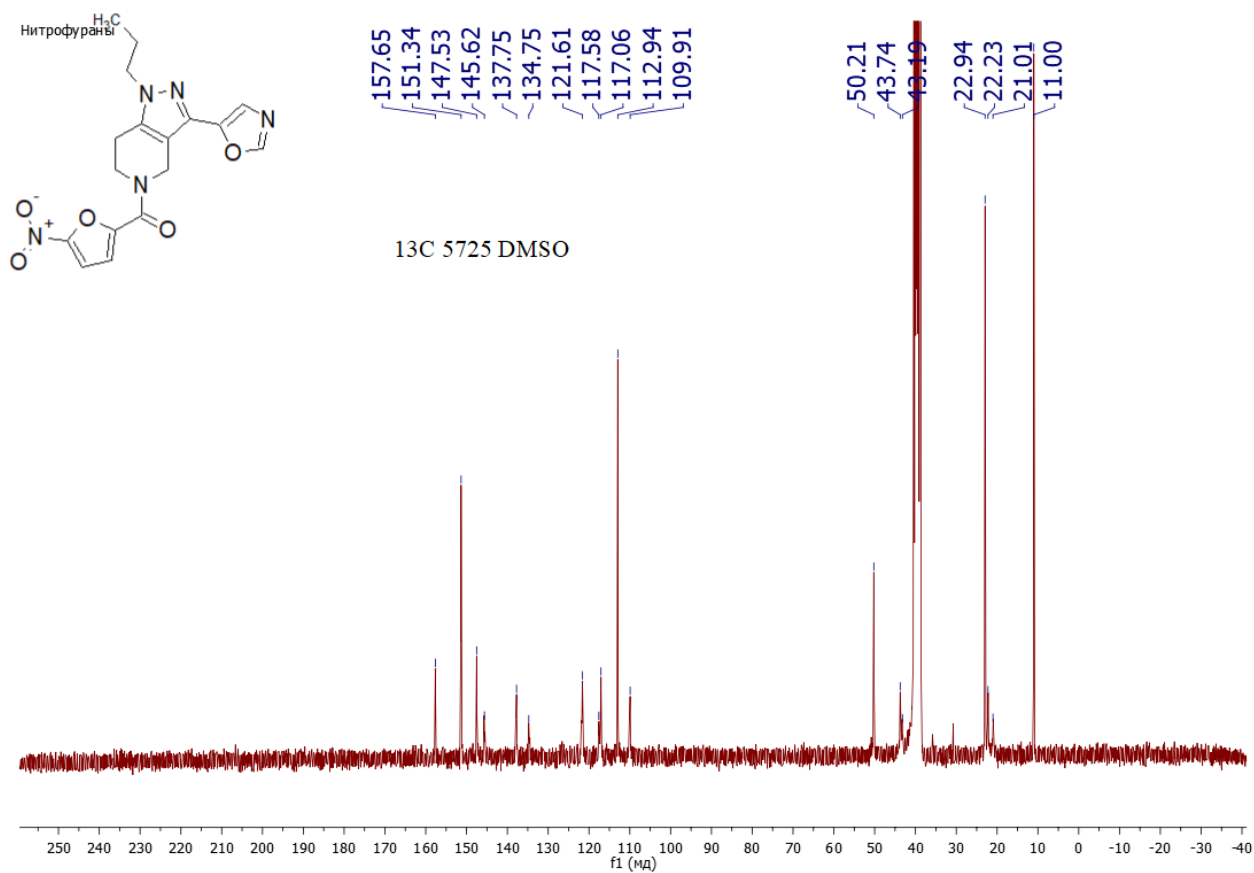
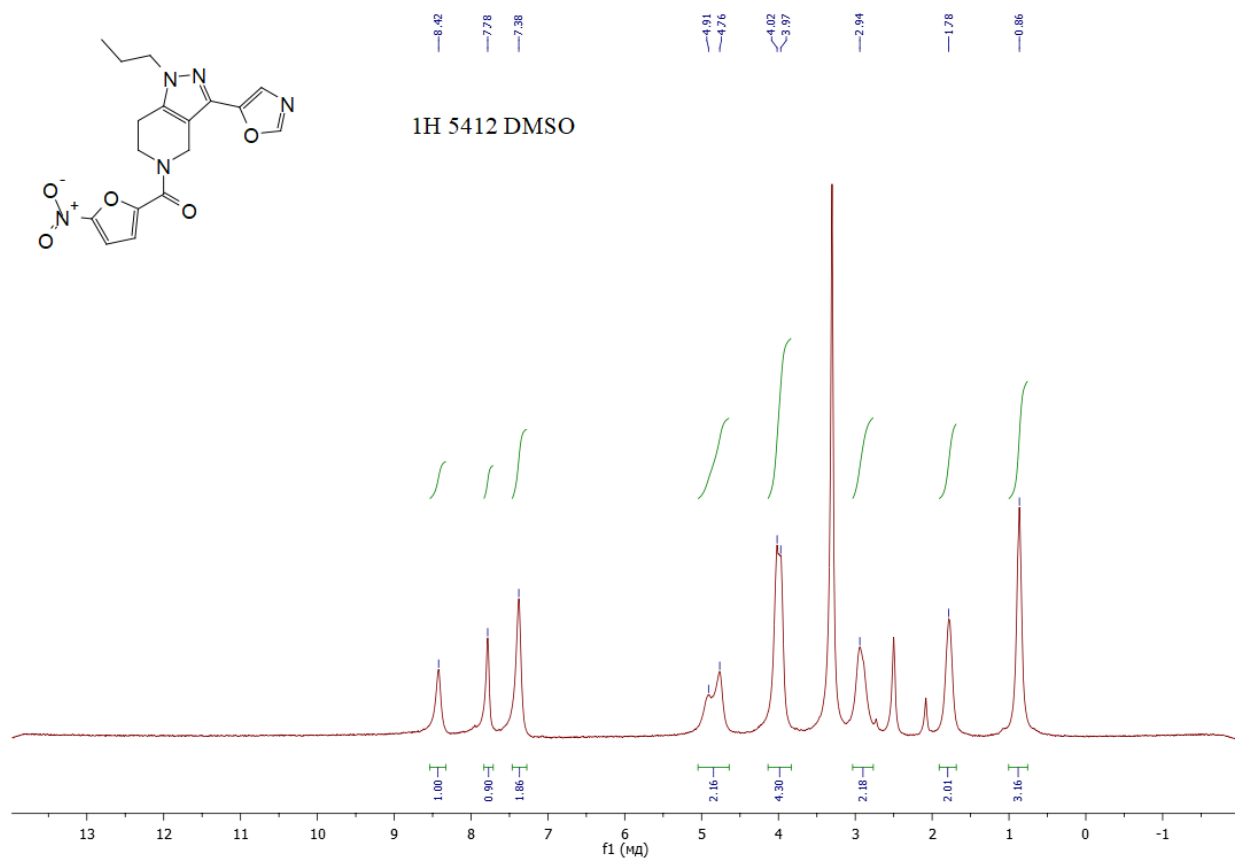
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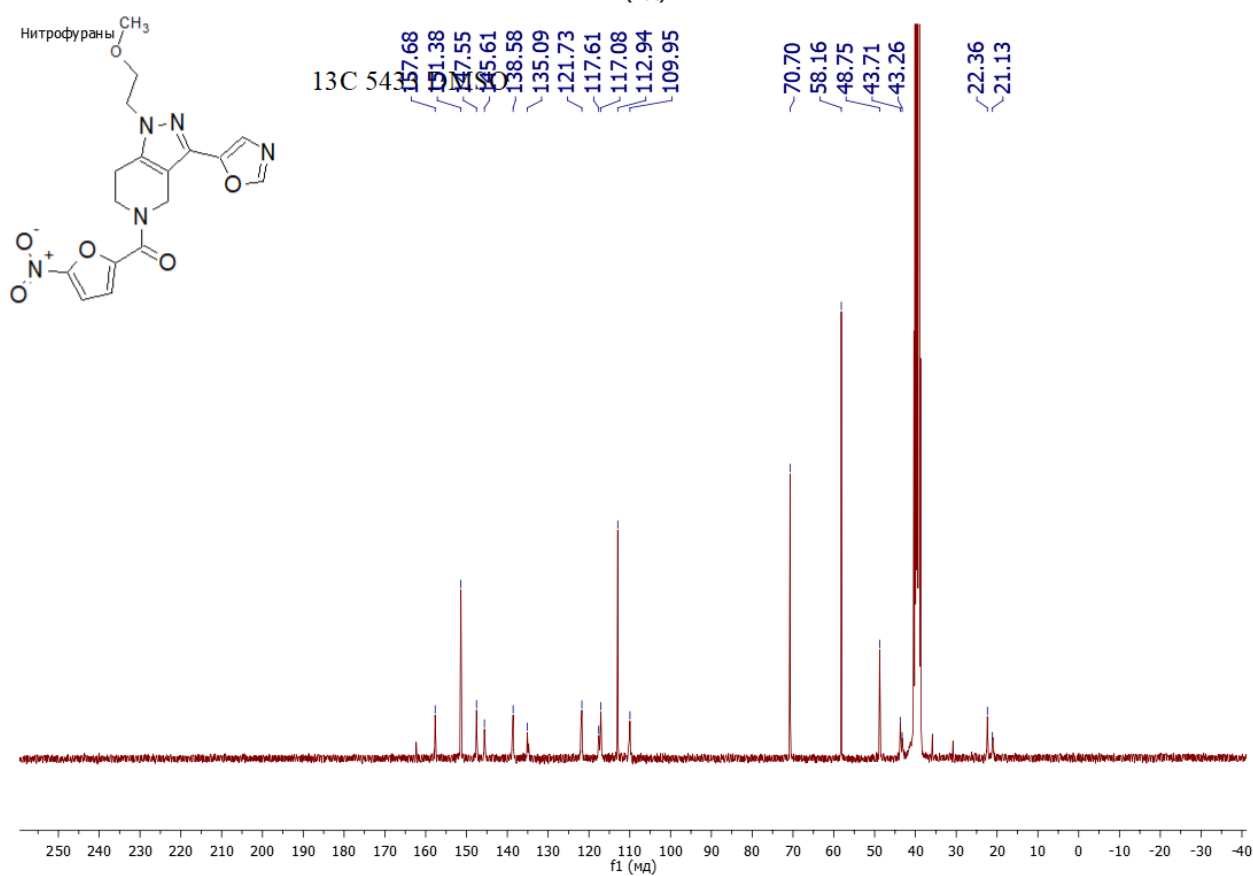
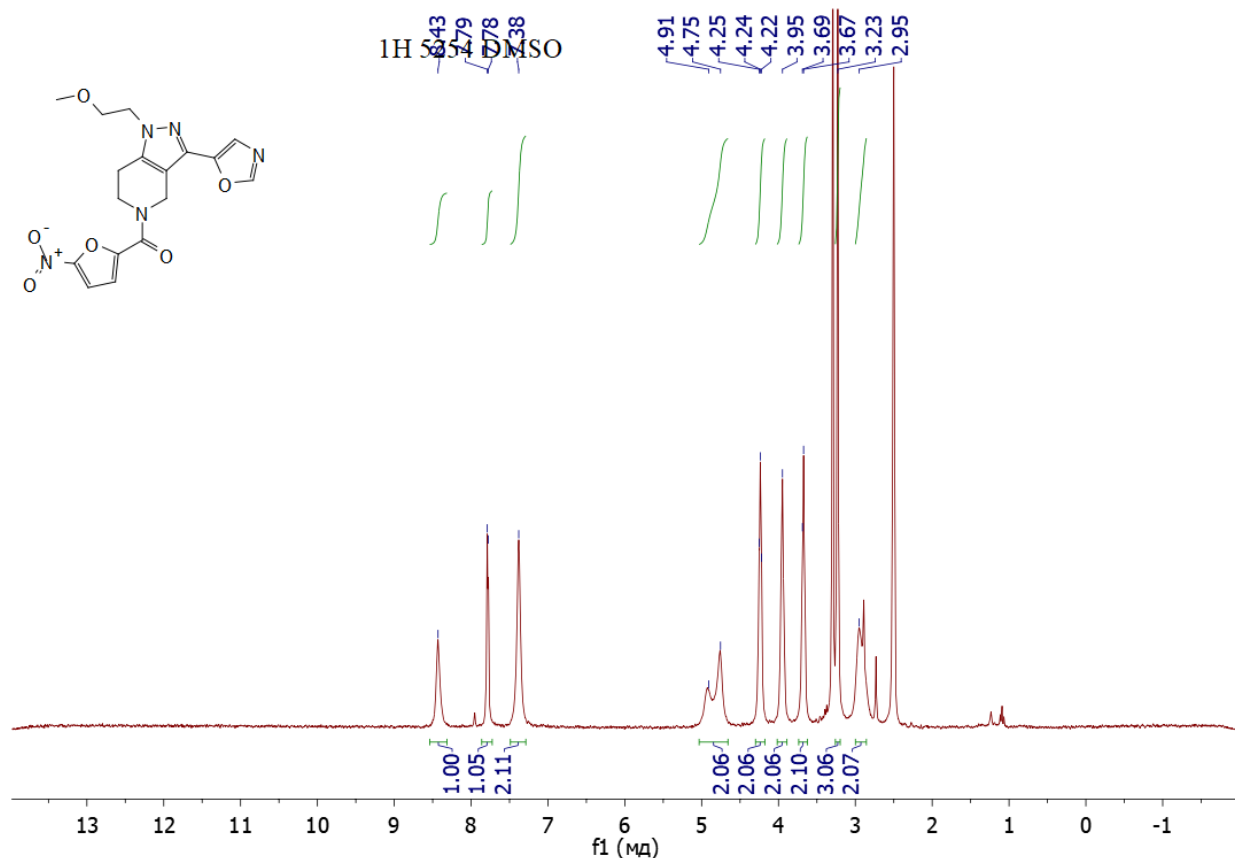
1-(cyclopropylmethyl)-5-(5-nitro-2-furoyl)-3-(1,3-oxazol-5-yl)-4,5,6,7-tetrahydro-1H-pyrazolo [4,3-c]pyridine, LK01512 (13e)



5-(5-nitro-2-furoyl)-3-(1,3-oxazol-5-yl)-1-propyl-4,5,6,7-tetrahydro-1H-pyrazolo[4,3-c]pyridine, LK01513 (13f)



1-(2-methoxyethyl)-5-(5-nitro-2-furoyl)-3-(1,3-oxazol-5-yl)-4,5,6,7-tetrahydro-1H-pyrazolo [4,3-c]pyridine, LK01509 (13g)



1-(3-methoxypropyl)-5-(5-nitro-2-furoyl)-3-(1,3-oxazol-5-yl)-4,5,6,7-tetrahydro-1H-pyrazolo [4,3-c]pyridine, LK01514 (13h)

