

Supplementary Material

One-pot highly diastereoselective five-component synthesis of polysubstituted 2-hydroxy-2-trifluoromethylpiperidines with four and five stereogenic centers

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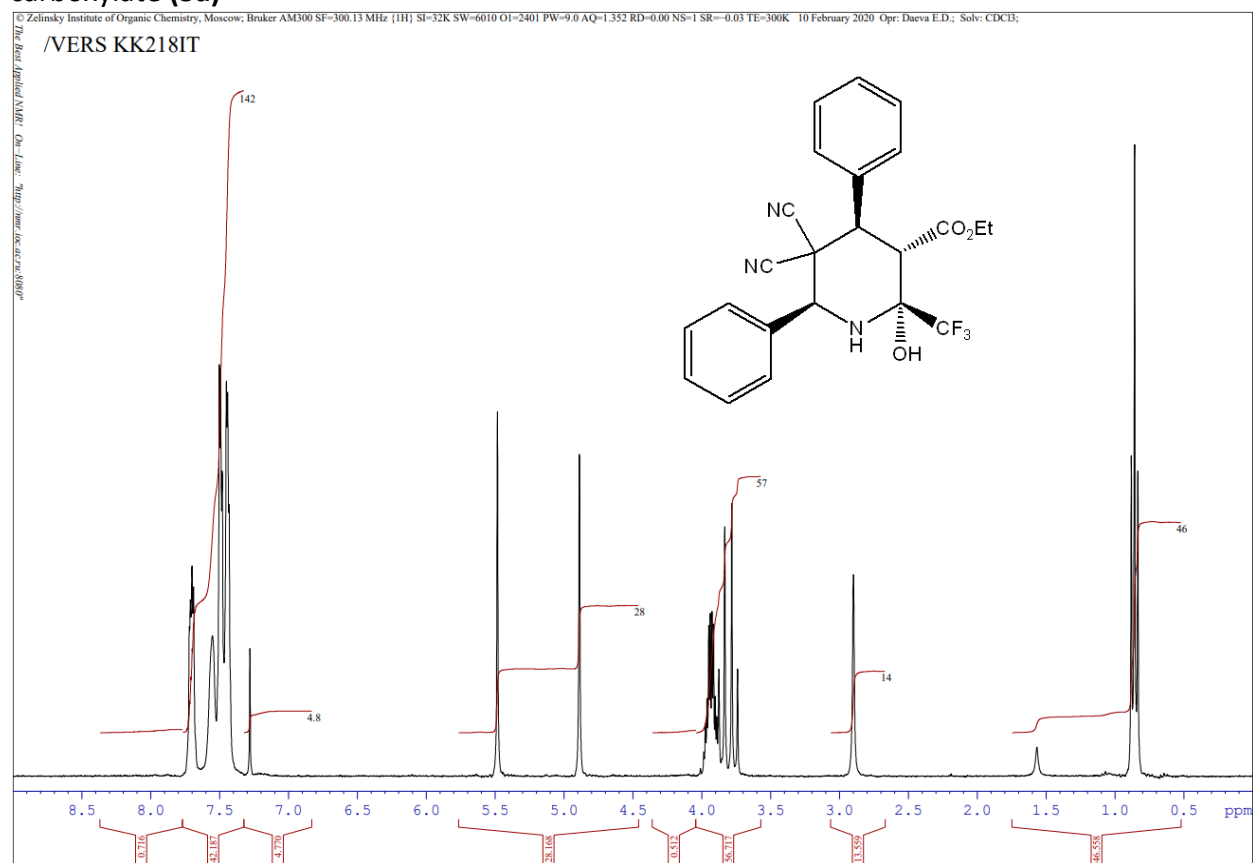
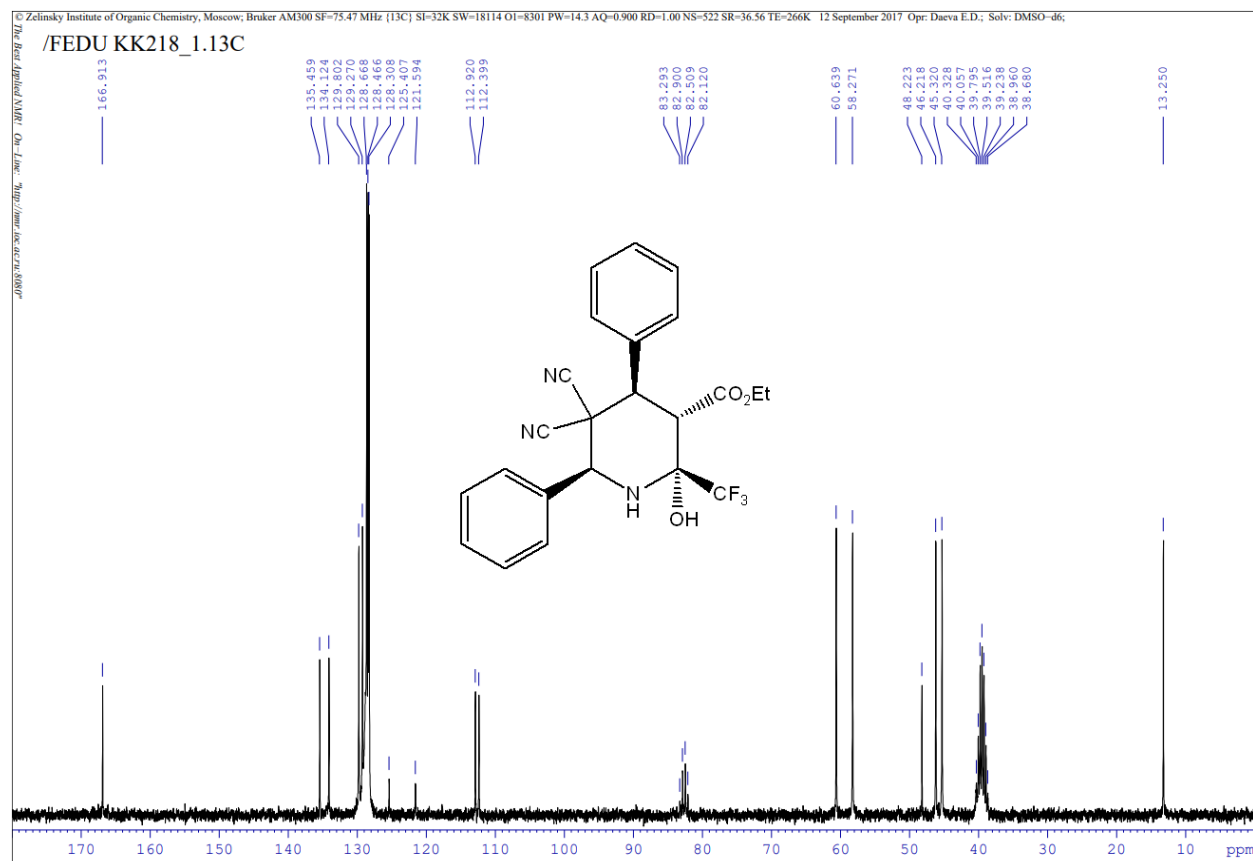
^a *N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 119991 Moscow, Russian Federation*

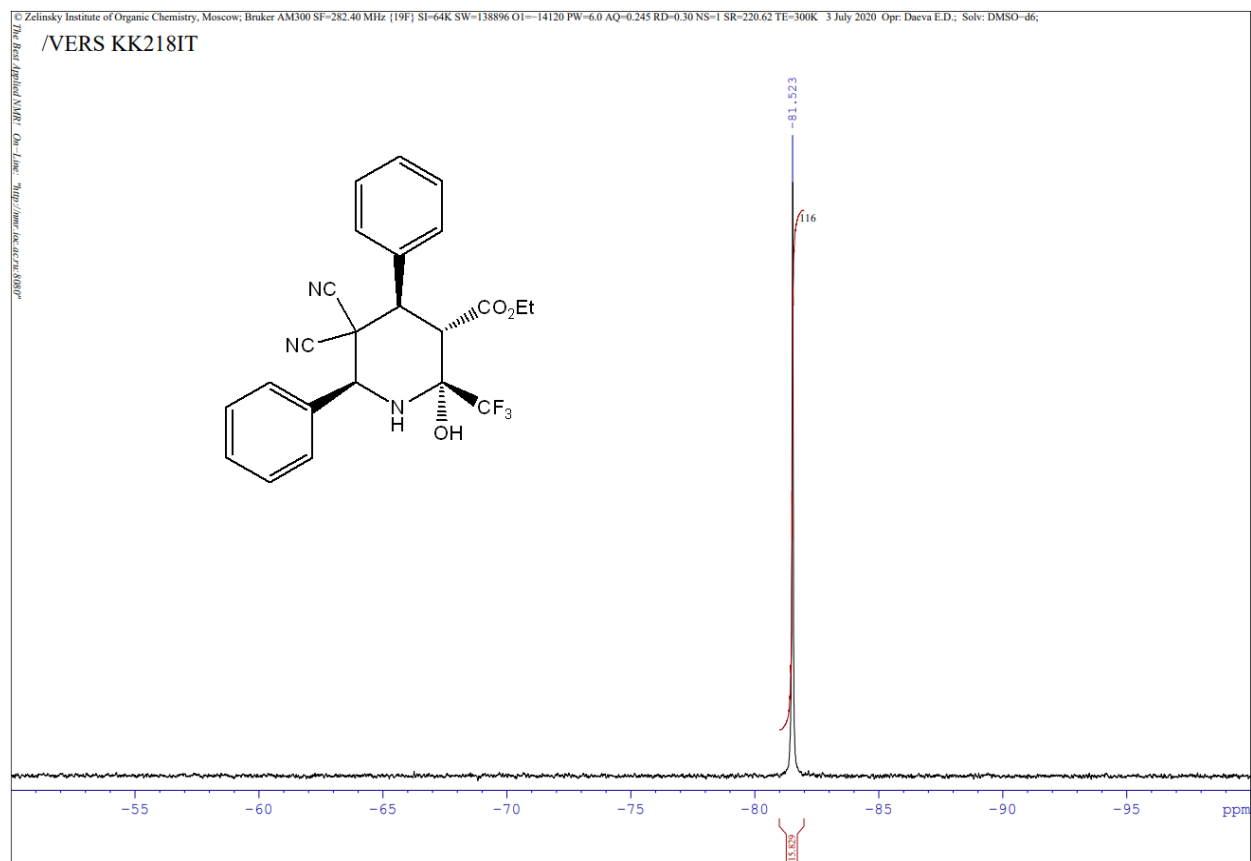
^b *Mendeleev University of Chemical Technology of Russia, 125047, Miusskaya square 9, Moscow, Russian Federation*

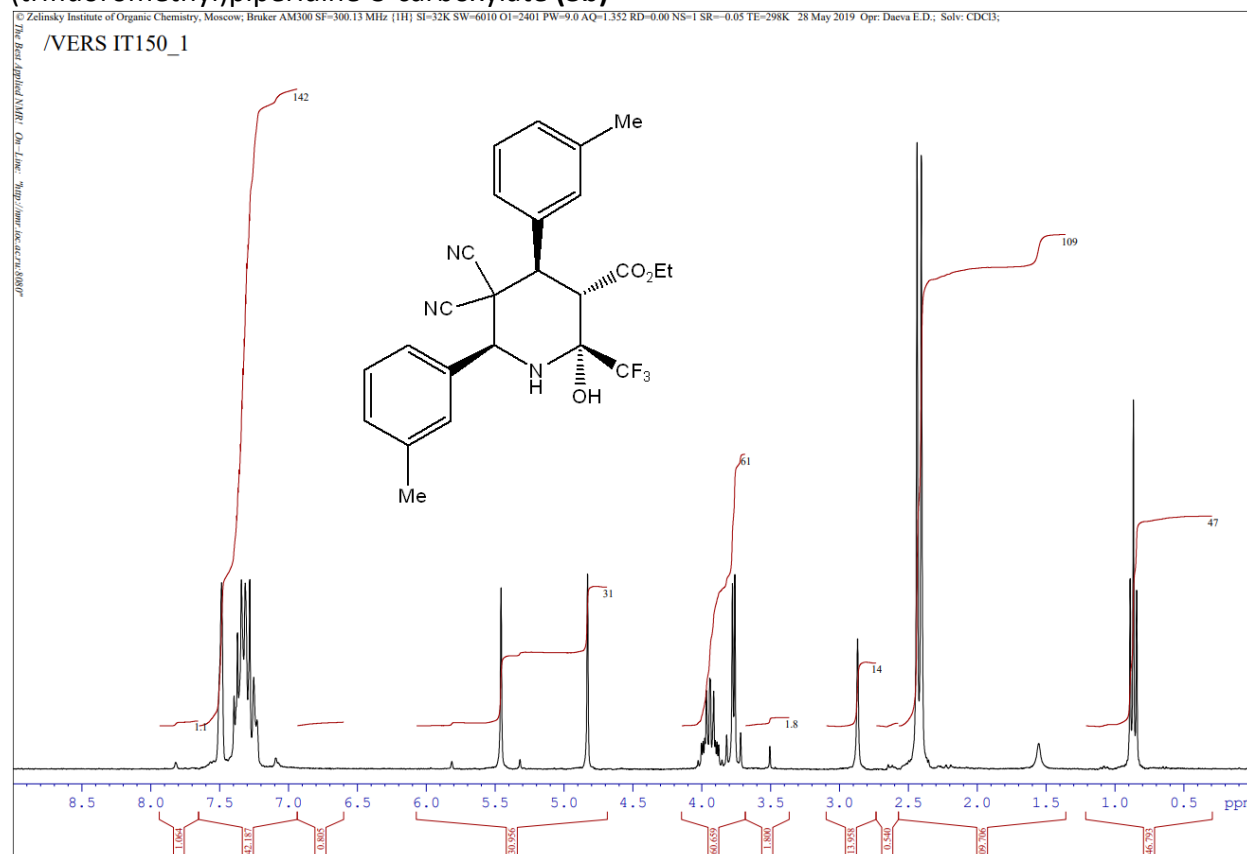
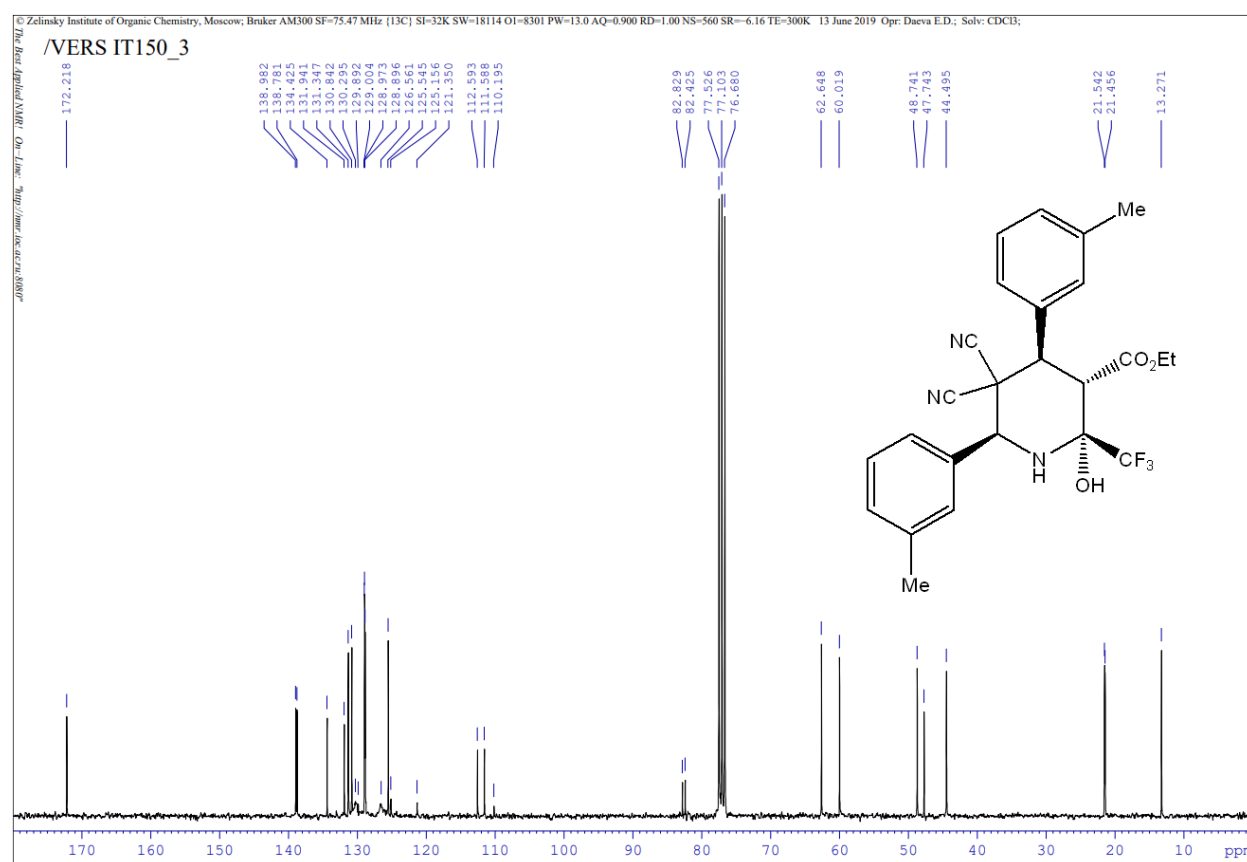
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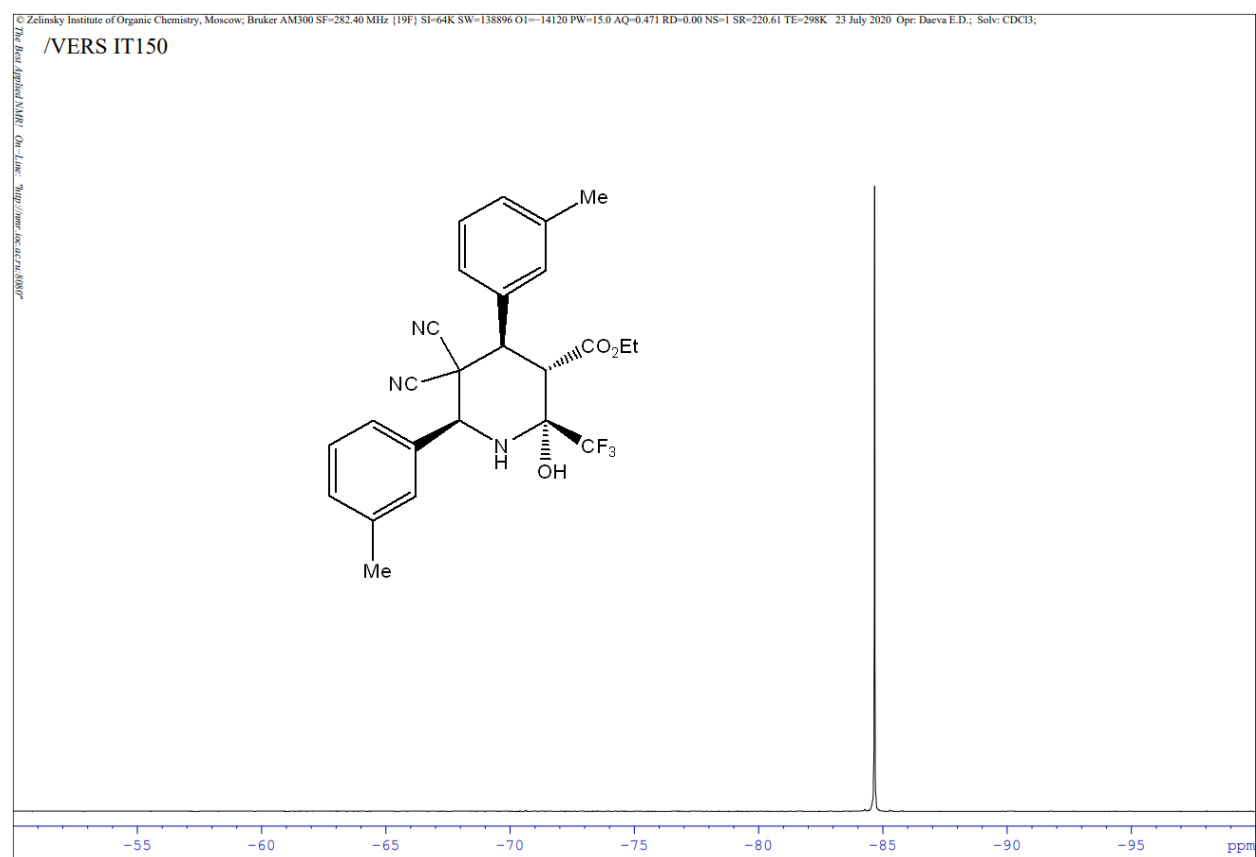
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¹ H, ¹³ C and ¹⁹ F NMR spectra of compounds 3a-o	S2
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¹H NMR of ethyl (2*RS*,3*SR*,4*RS*,6*SR*)-5,5-dicyano-2-hydroxy-4,6-diphenyl-2-(trifluoromethyl)piperidine-3-carboxylate (3a**)****¹³C NMR of **3a****

¹⁹F NMR of **3a**

¹H NMR of ethyl (2*RS*,3*SR*,4*RS*,6*SR*)-5,5-dicyano-2-hydroxy-4,6-bis(3-methylphenyl)-2-(trifluoromethyl)piperidine-3-carboxylate (**3b**)¹³C NMR of **3b**

^{19}F NMR of **3b**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz [1H] SI=32K SW=6010 OI=240I PW=9.0 AO=1.352 RD=0.00 NS=1 SR=0.00 TE=300K 11 March 2021 Opr: Daeva E.D.; Solv: CDCl3.

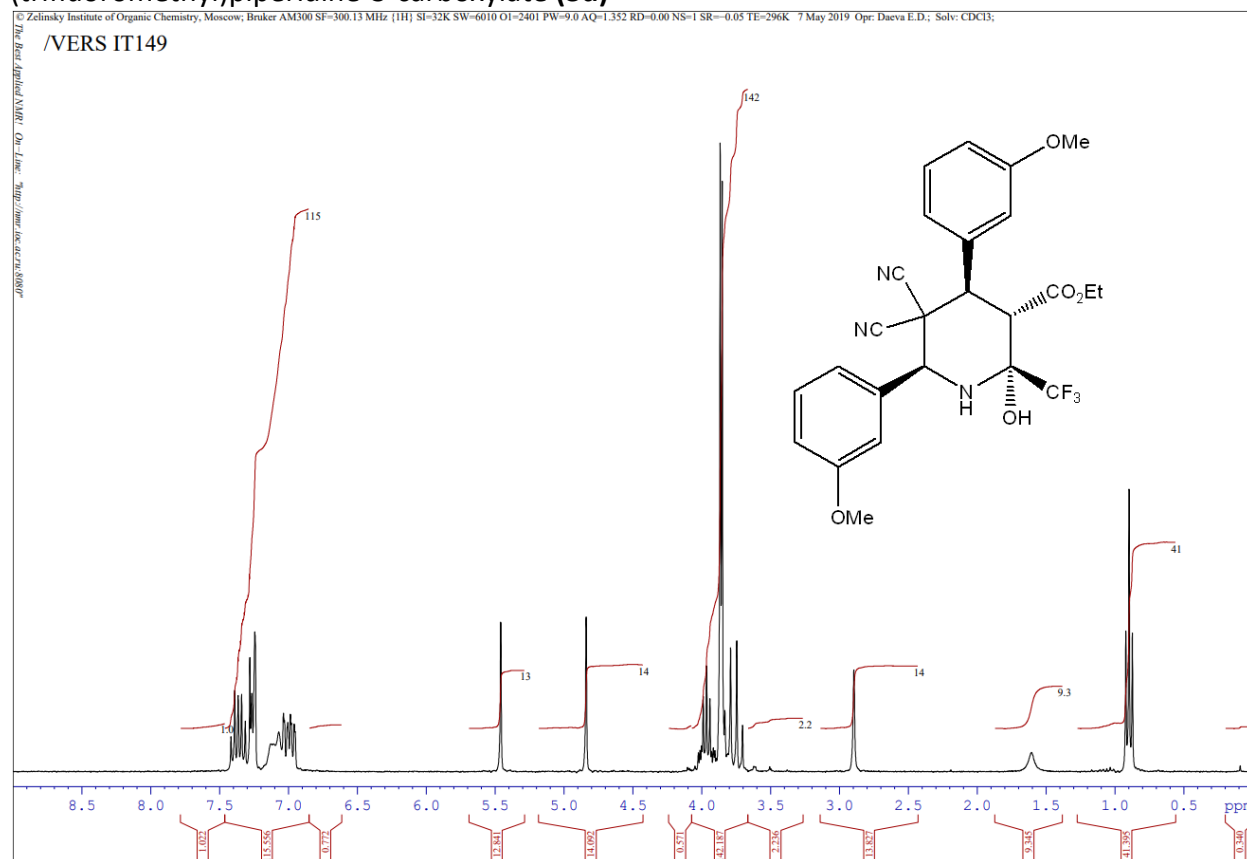


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=282.40 MHz [19F] SI=64K SW=138896 O1=-14120 PW=6.0 AQ=0.245 RD=0.30 NS=1 SR=220.62 TE=300K 15 March 2021 Opr: Dueva E.D.; Solv: CDCl3;
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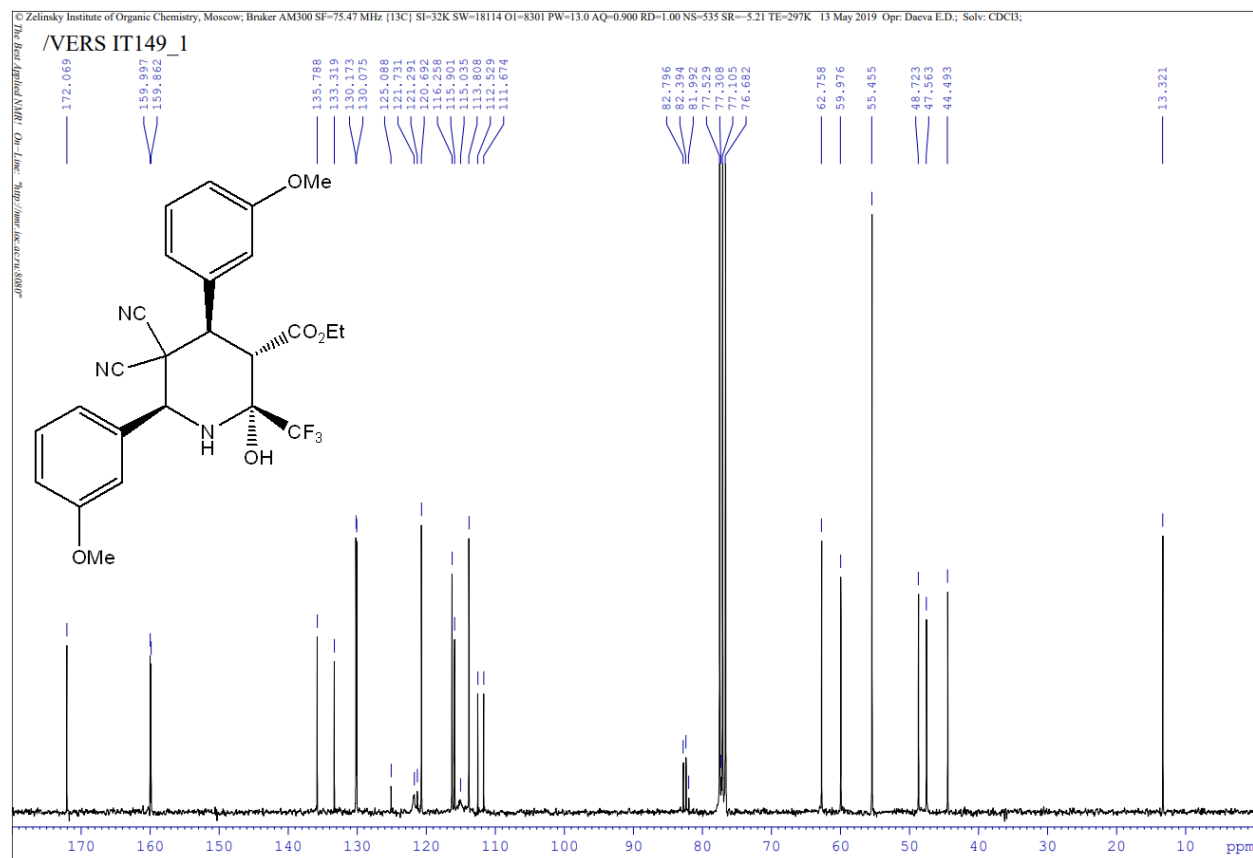
Chemical structure of the compound: CCOC(=O)[C@H]1[C@@H](C(F)(F)F)[C@@H](c2ccc(C)cc2)[C@H](c3ccc(C)cc3)[C@@H]1C#N

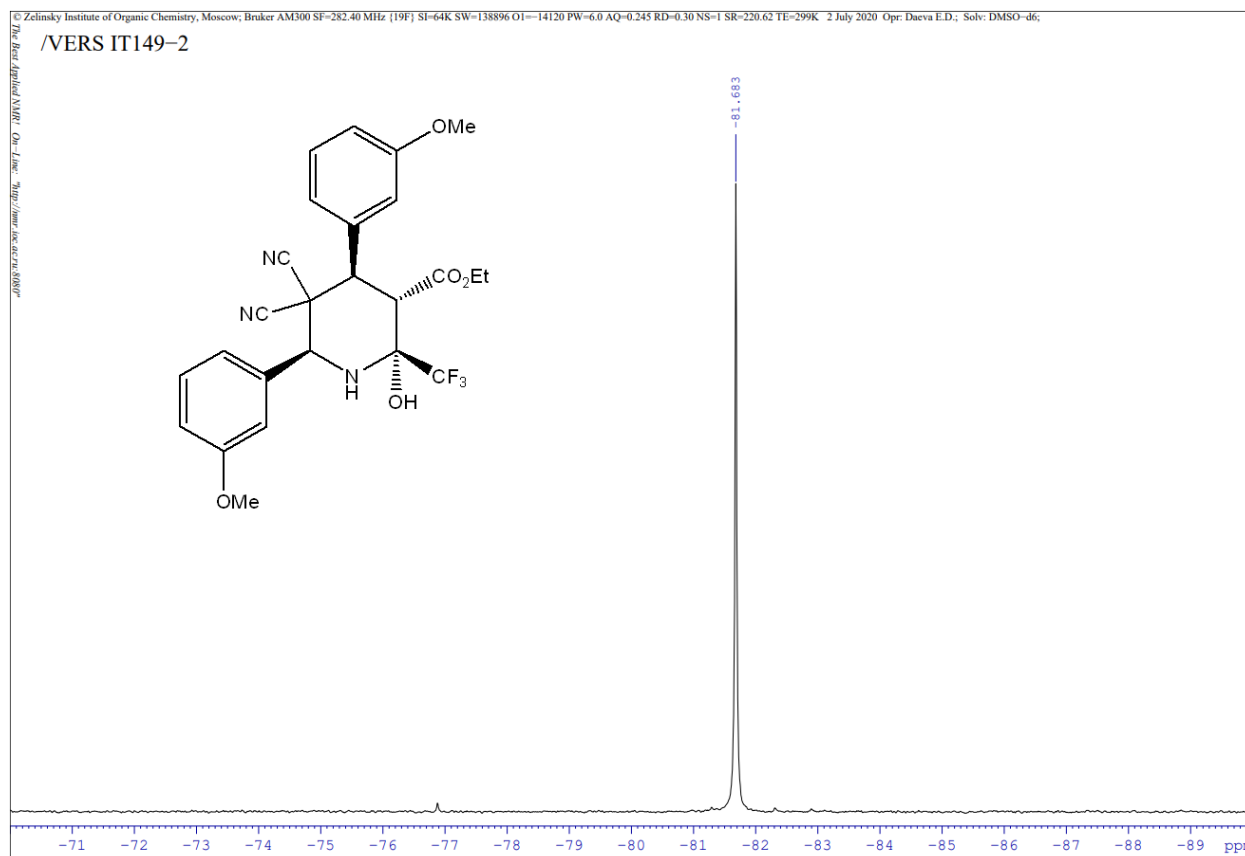
¹⁹F NMR spectrum (CDCl₃) showing chemical shifts (ppm) on the x-axis (ranging from -150 to -300) and intensity on the y-axis. The spectrum displays several peaks, with the most prominent ones labeled with their chemical shifts: -64.581, -65.021, -70.680, -74.051, -74.051, -77.448, and -84.692.

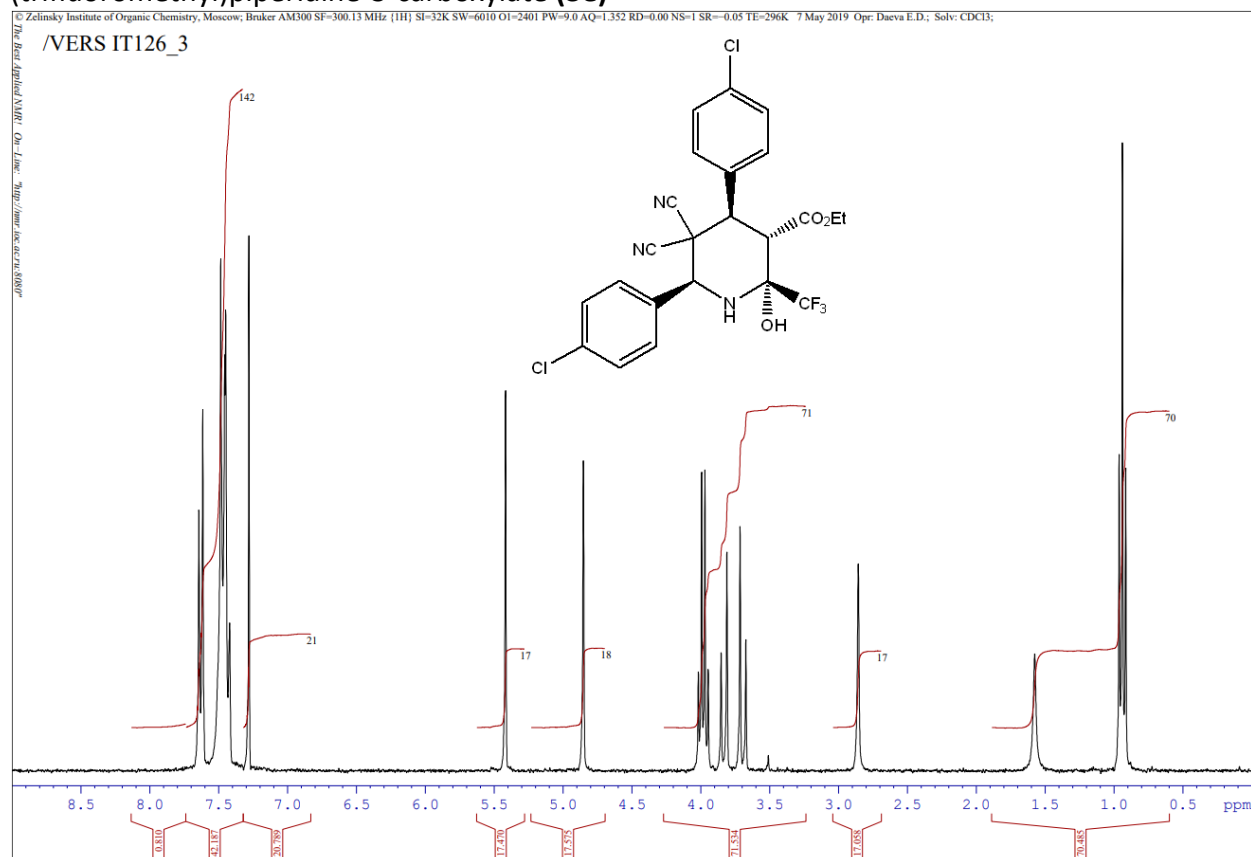
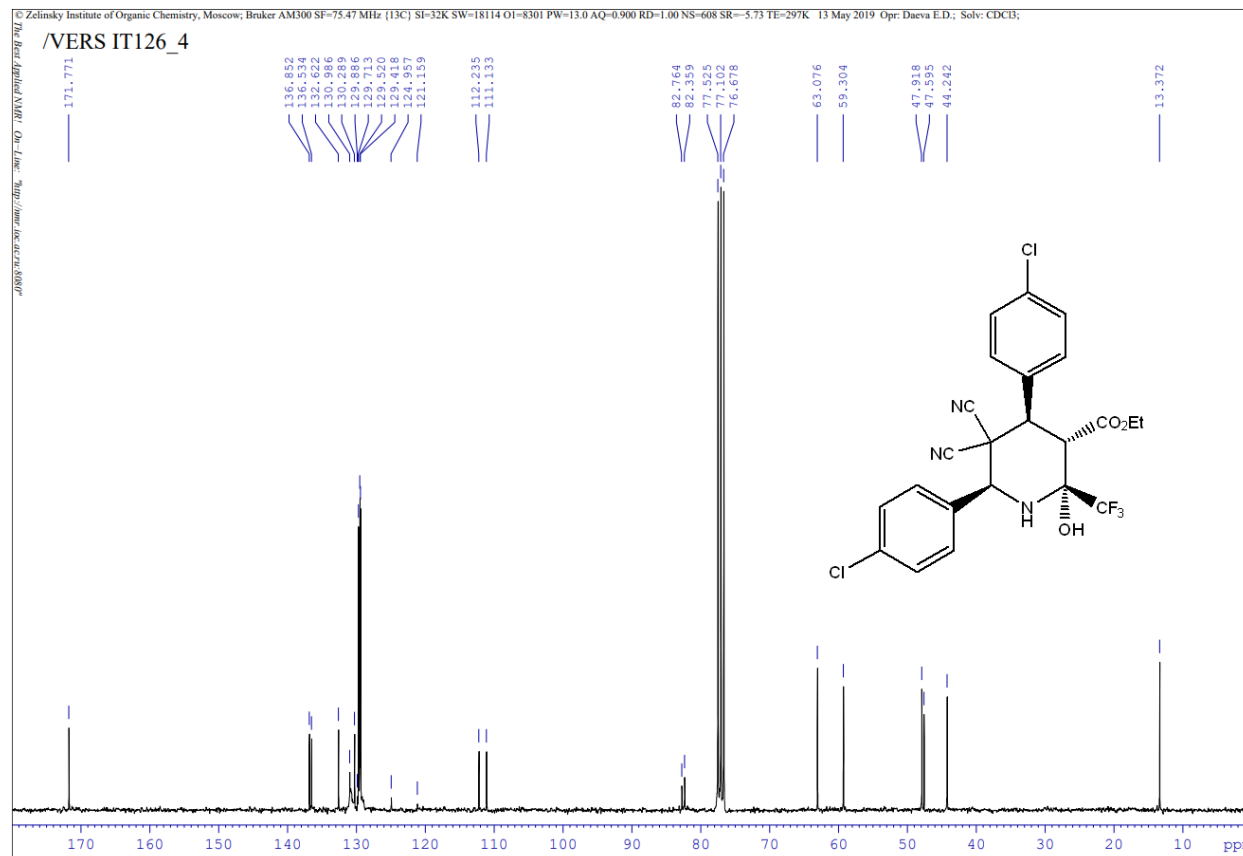
¹H NMR of ethyl (2*RS*,3*SR*,4*RS*,6*SR*)-5,5-dicyano-2-hydroxy-4,6-bis(3-methoxyphenyl)-2-(trifluoromethyl)piperidine-3-carboxylate (**3d**)

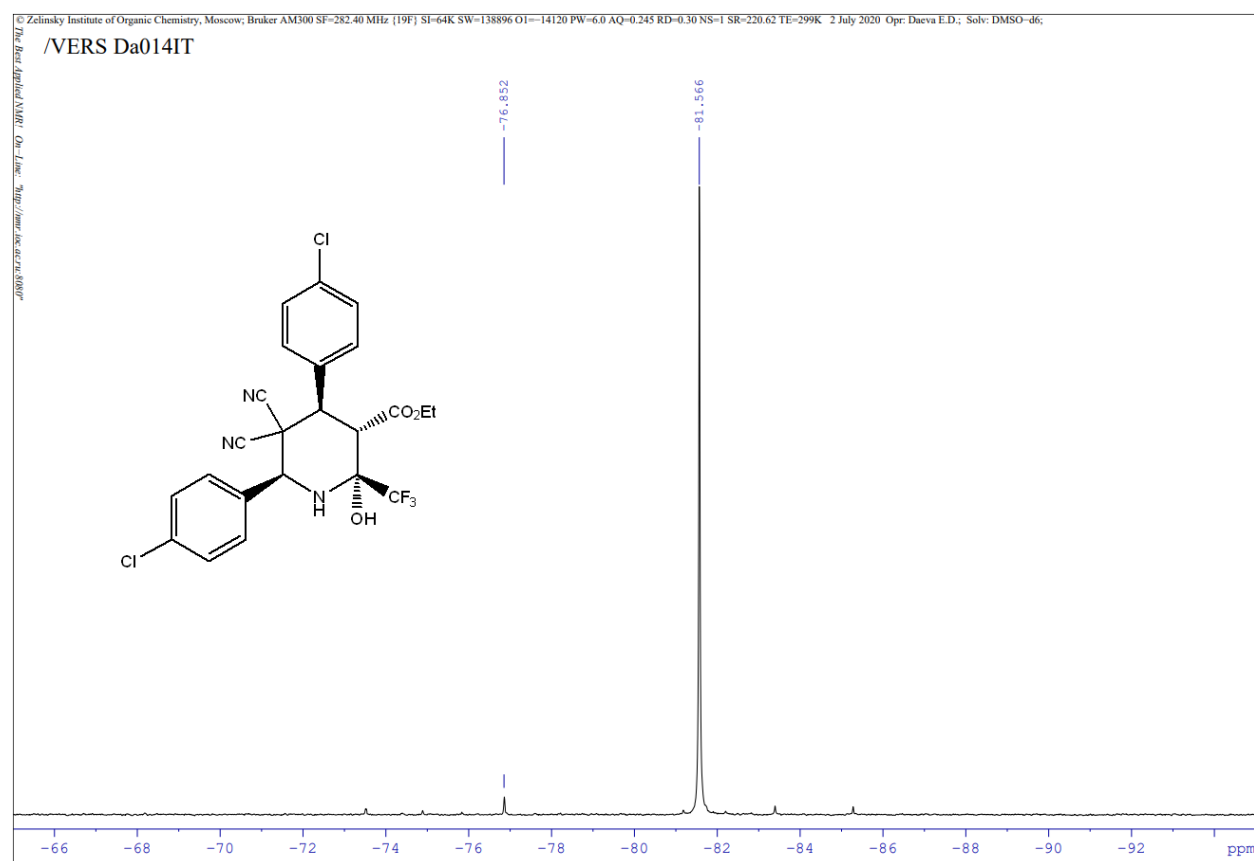


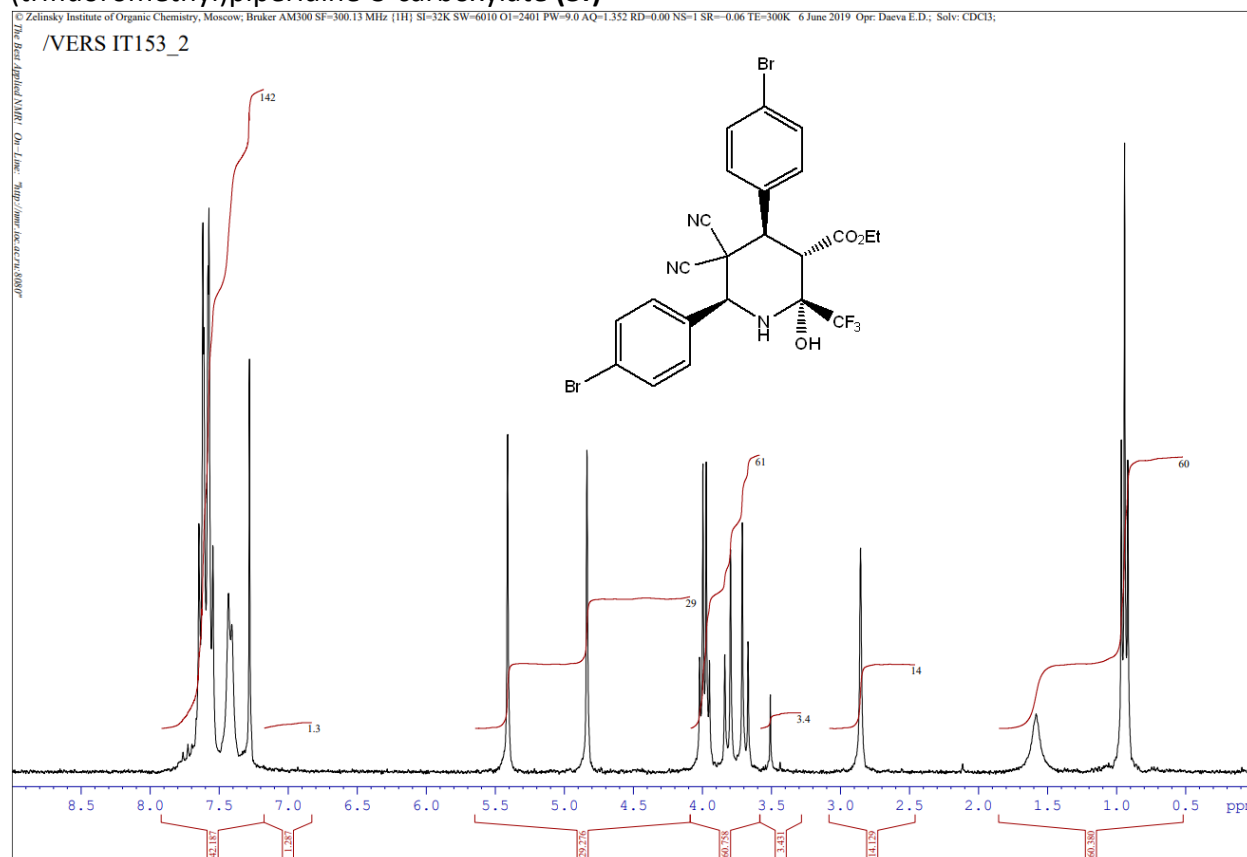
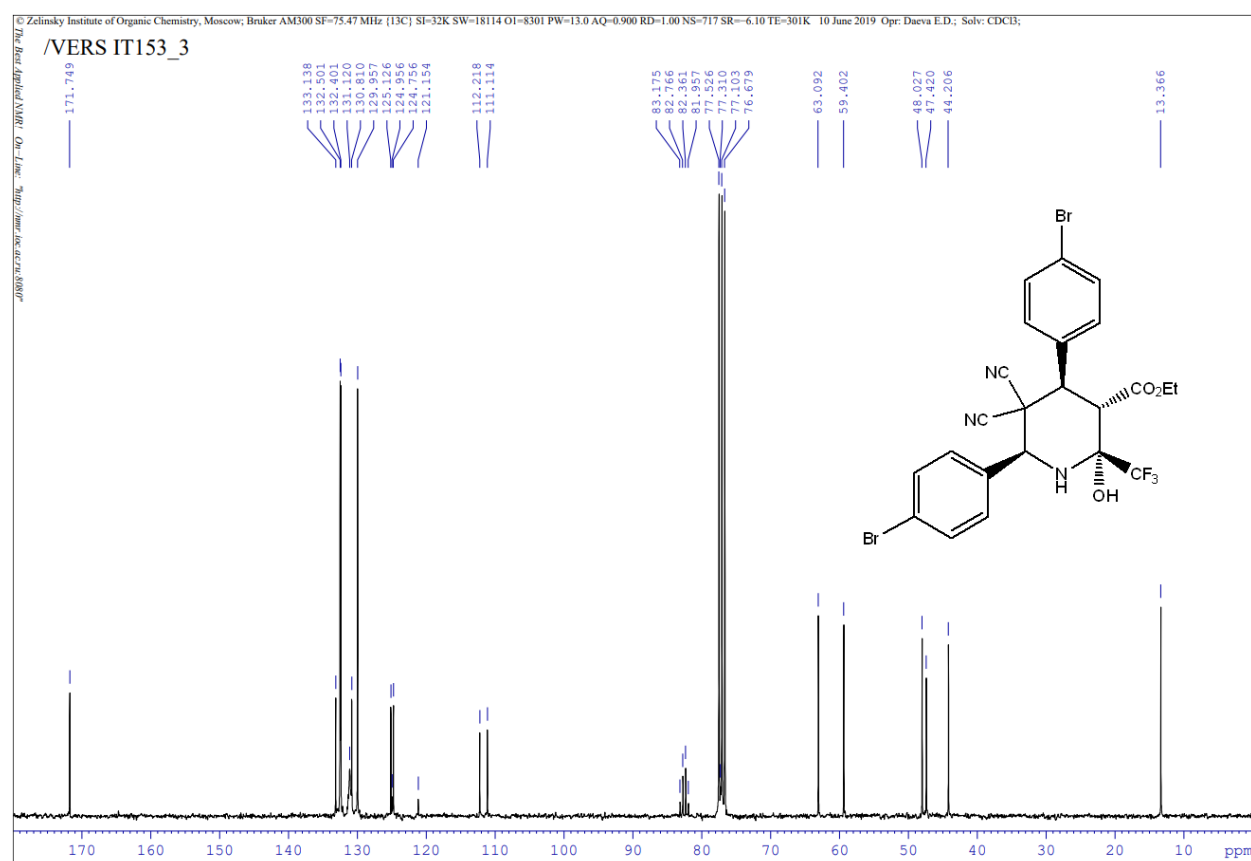
¹³C NMR of **3d**

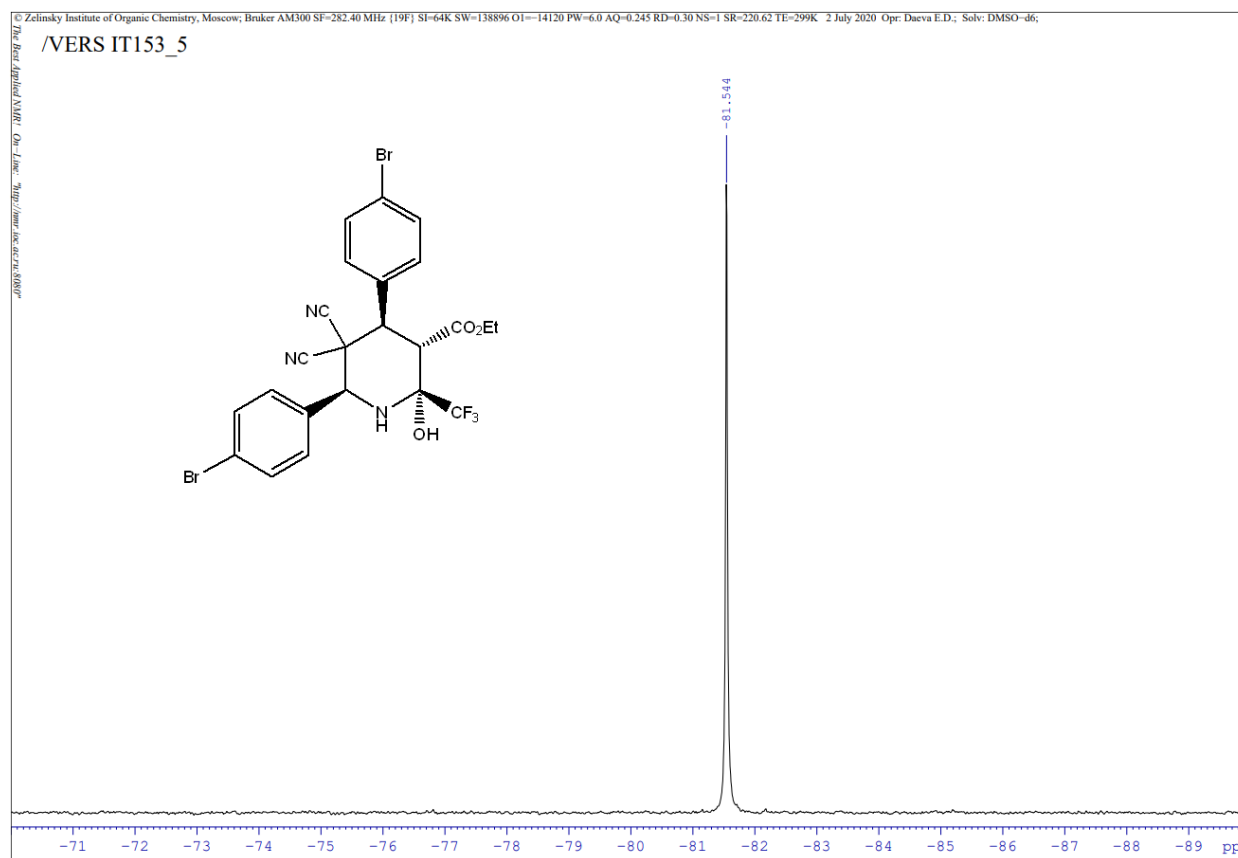


¹⁹F NMR of **3d**

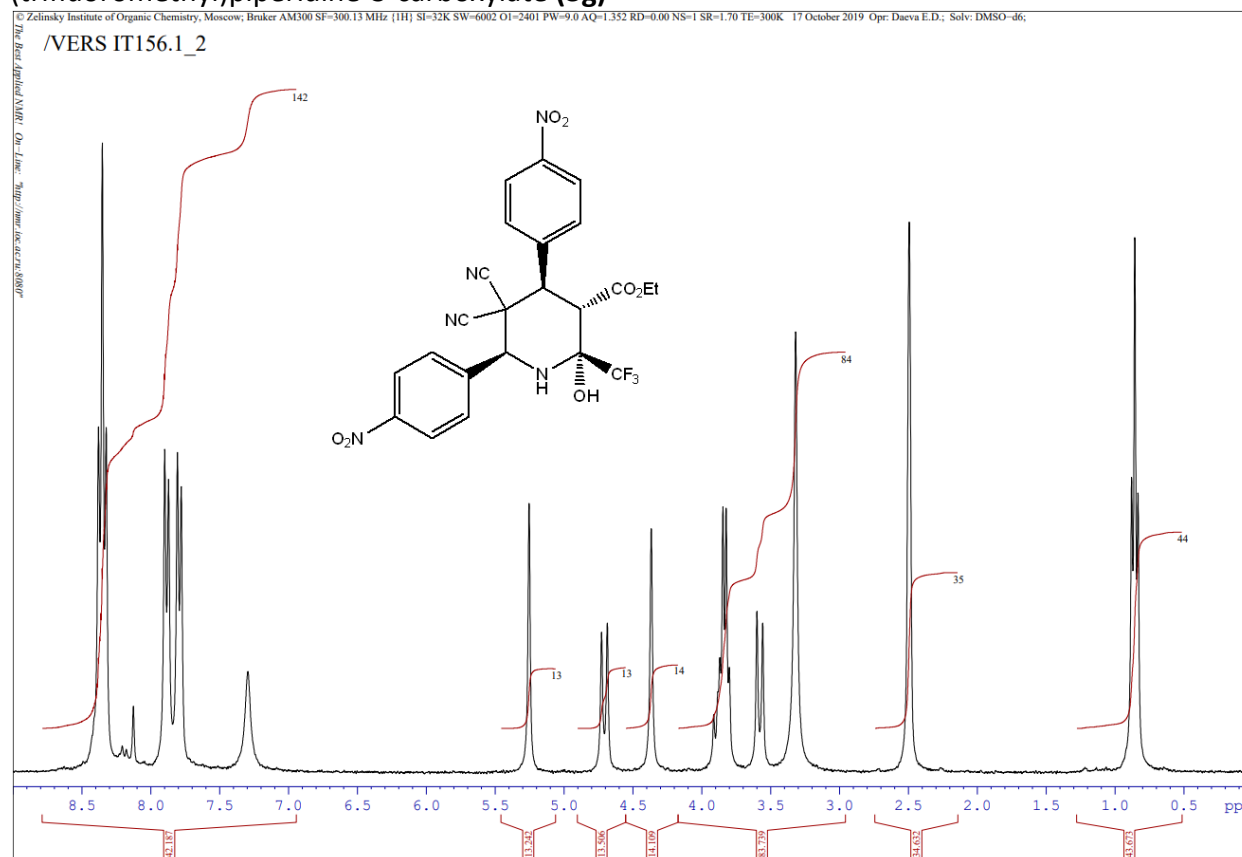
^1H NMR of ethyl (2*RS*,3*SR*,4*RS*,6*SR*)-5,5-dicyano-2-hydroxy-4,6-bis(4-chlorophenyl)-2-(trifluoromethyl)piperidine-3-carboxylate (3e**)** **^{13}C NMR of **3e****

¹⁹F NMR of **3e**

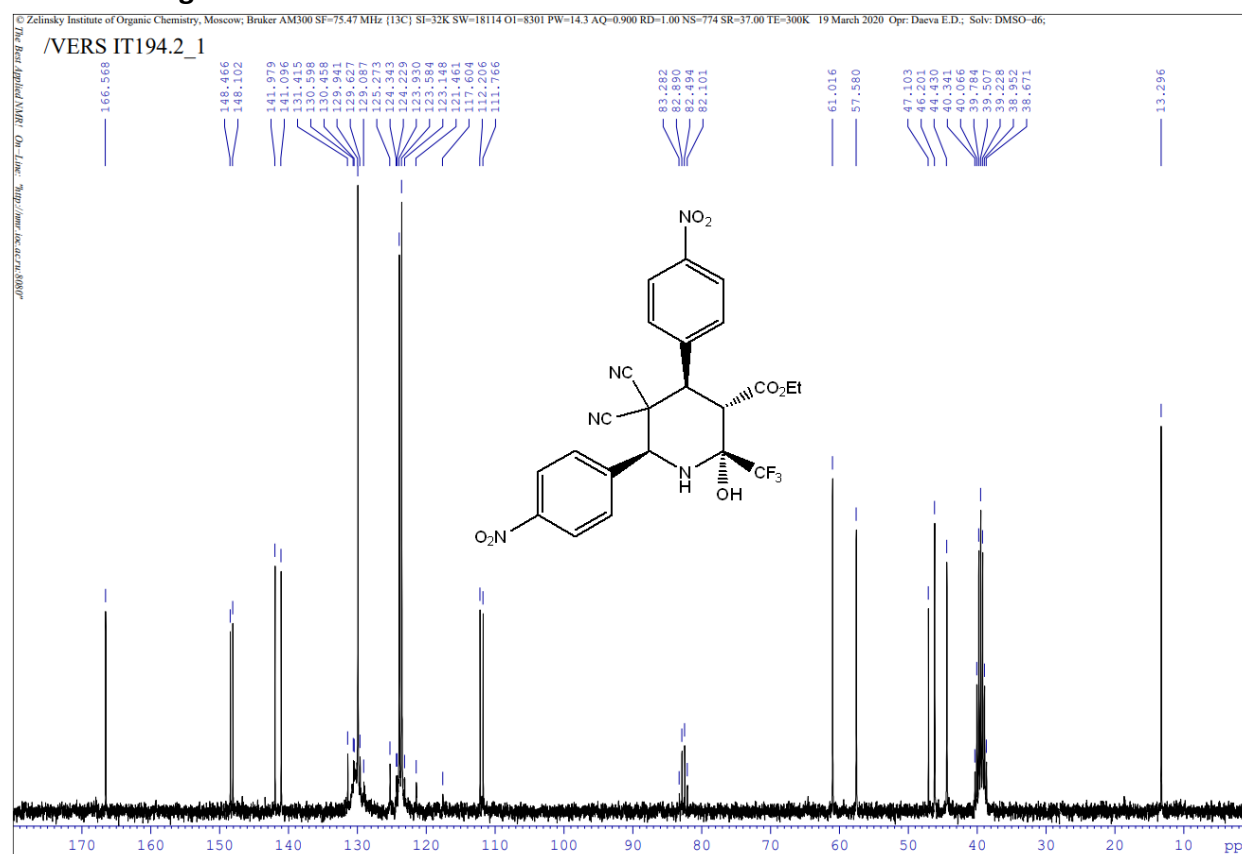
¹H NMR of ethyl (2*RS*,3*SR*,4*RS*,6*SR*)-5,5-dicyano-2-hydroxy-4,6-bis(4-bromophenyl)-2-(trifluoromethyl)piperidine-3-carboxylate (**3f**)¹³C NMR of **3f**

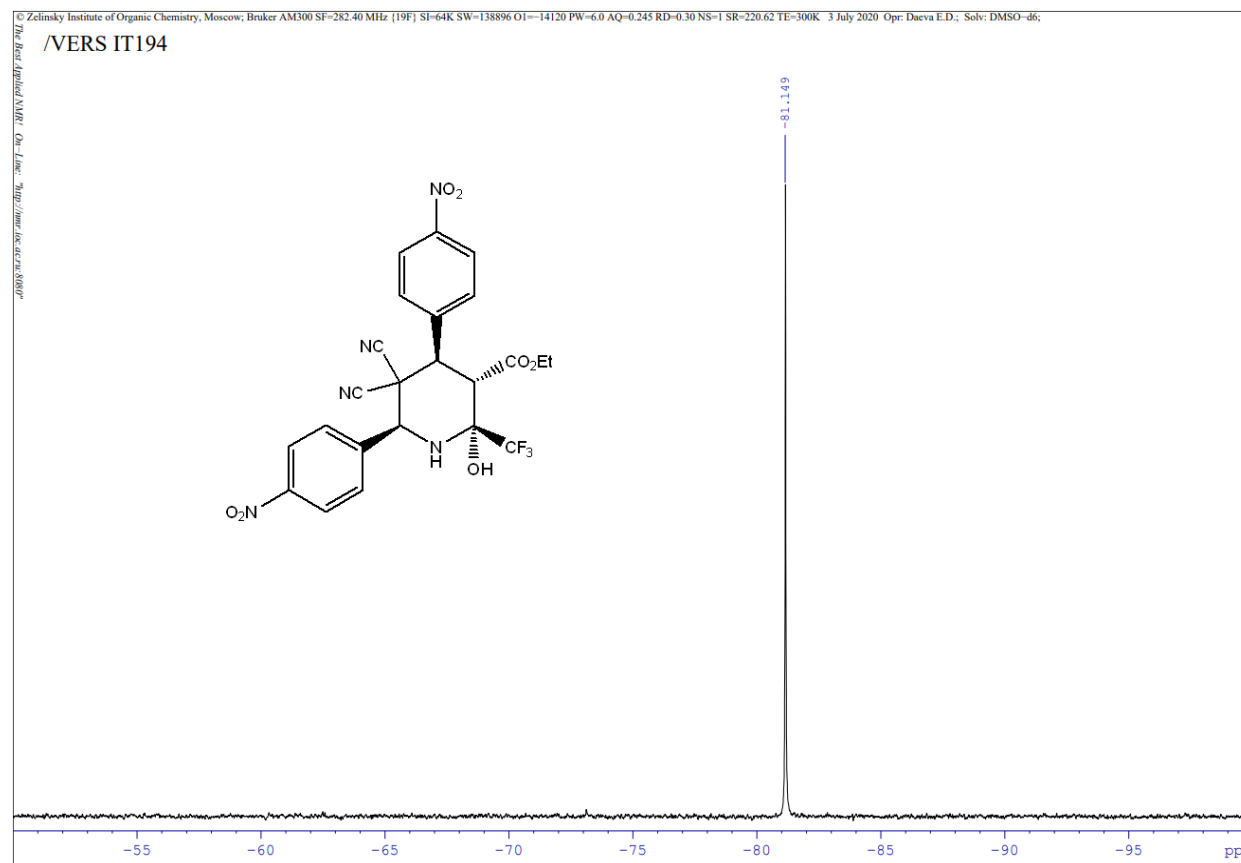
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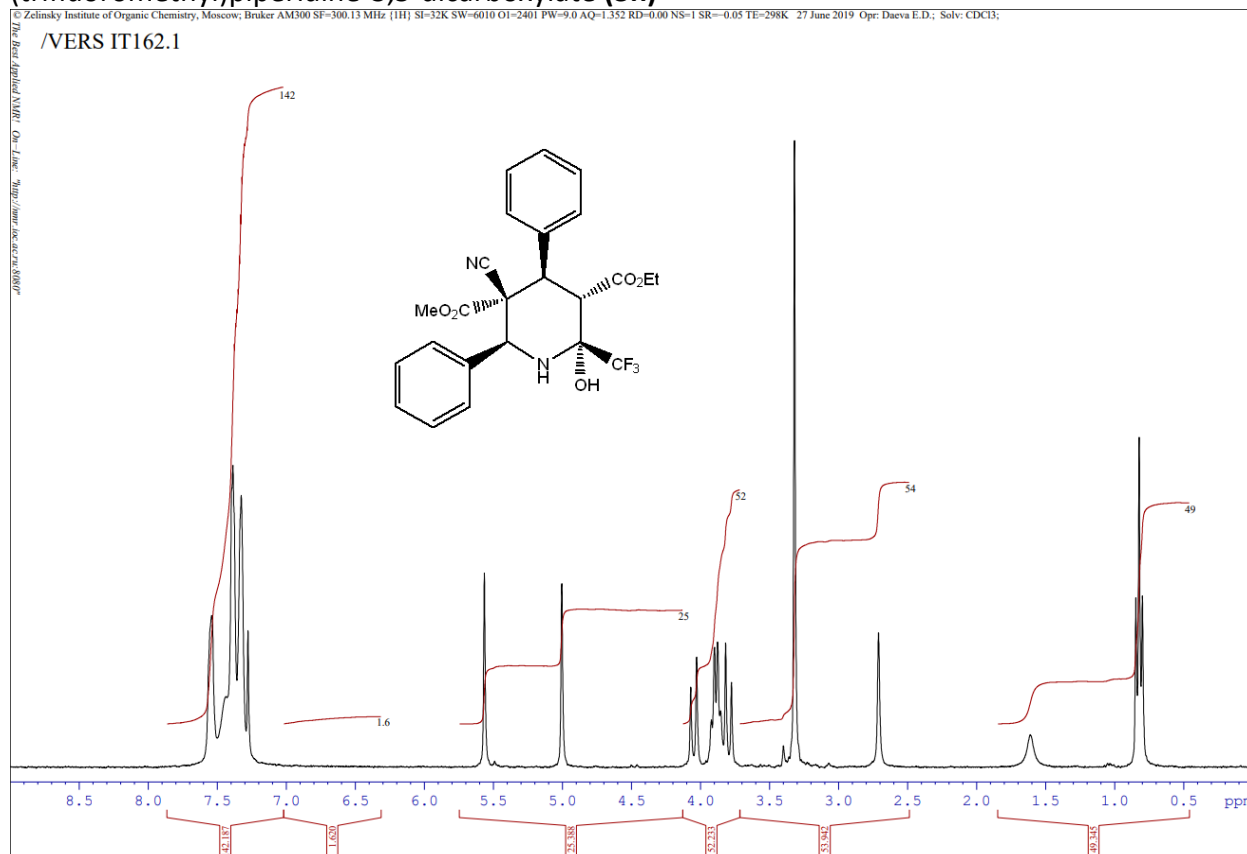
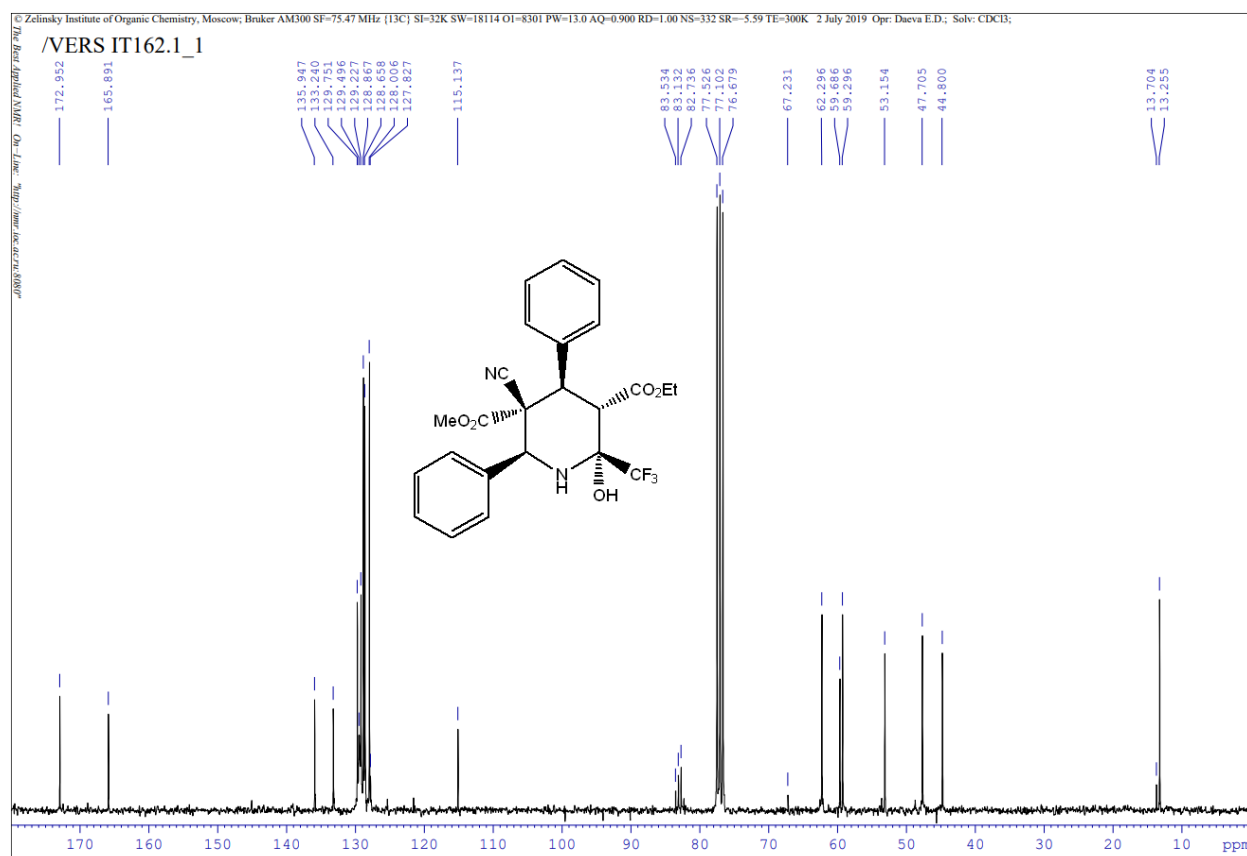
¹H NMR of ethyl (2*RS*,3*SR*,4*RS*,6*SR*)-5,5-dicyano-2-hydroxy-4,6-bis(4-nitrophenyl)-2-(trifluoromethyl)piperidine-3-carboxylate (**3g**)

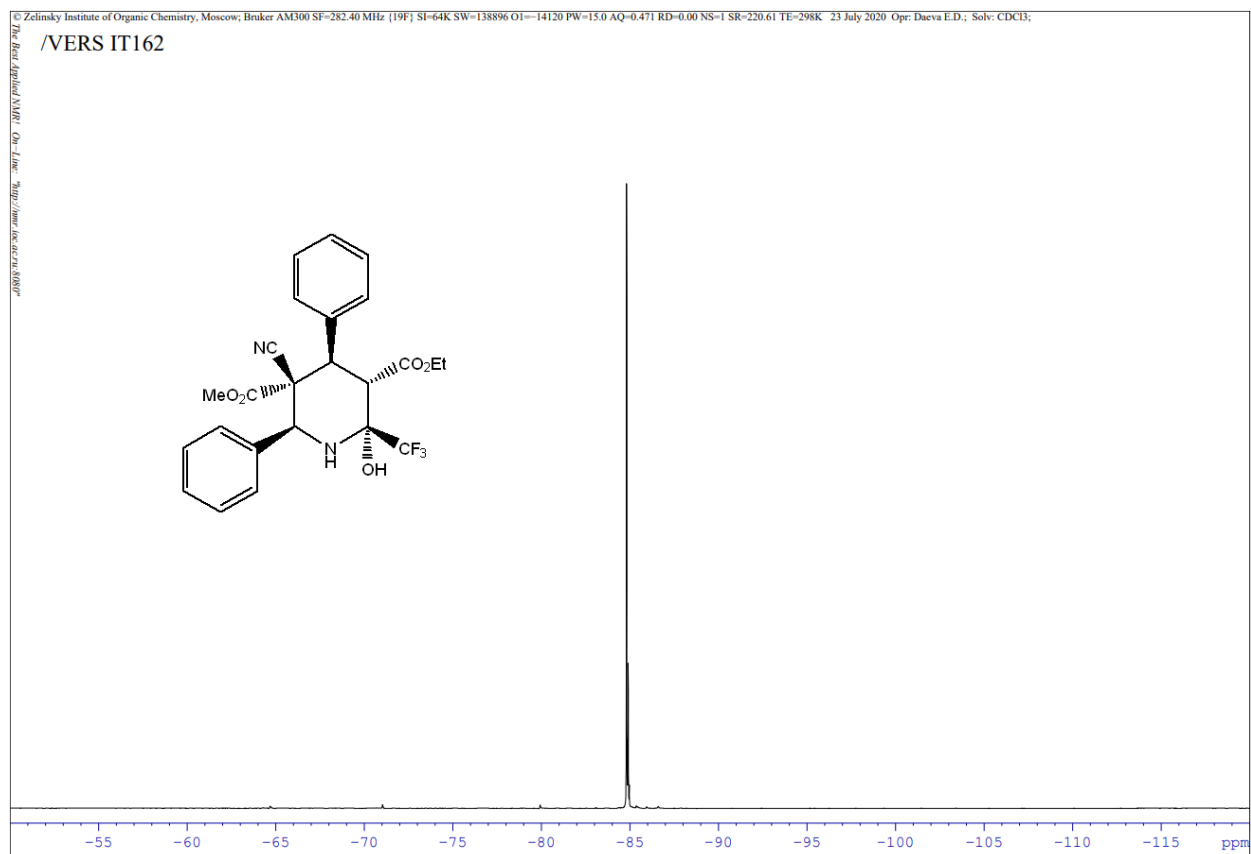


¹³C NMR of **3g**

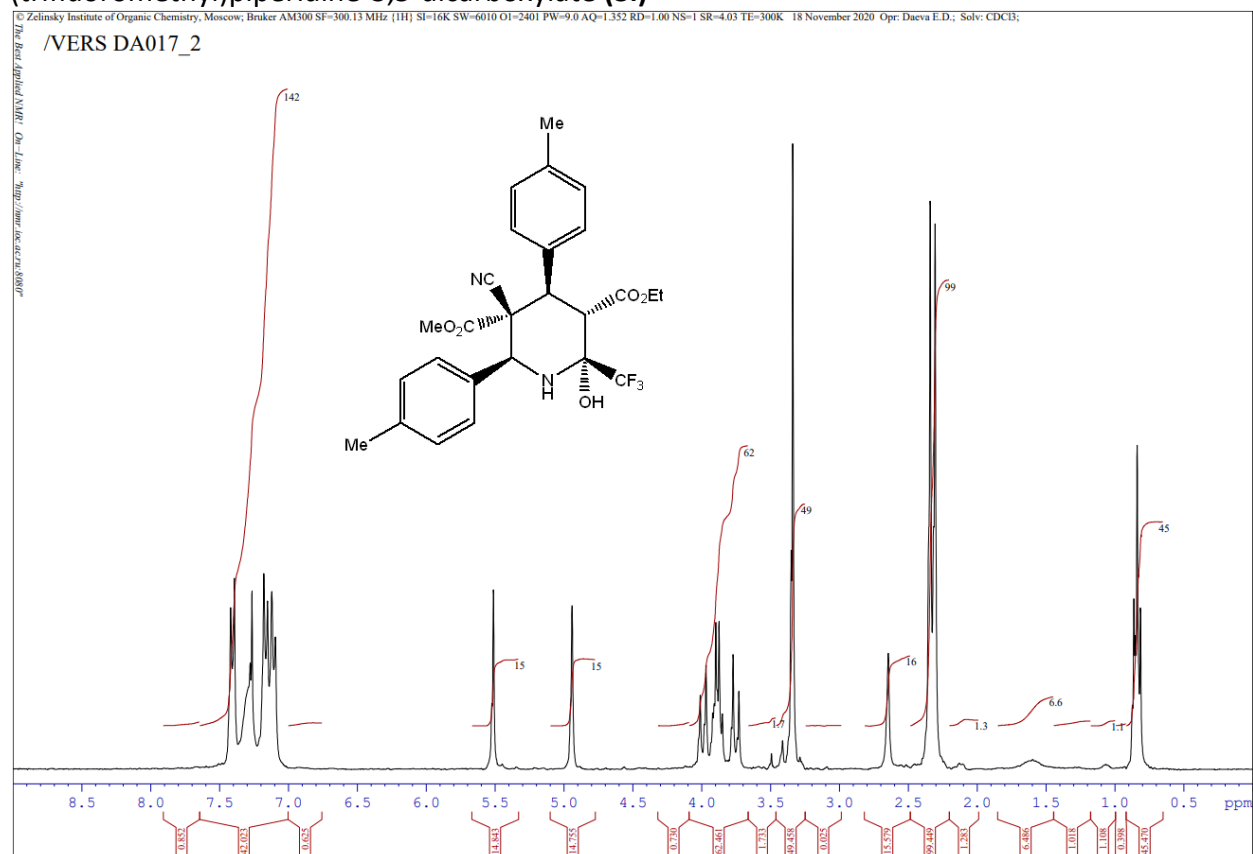


^{19}F NMR of **3g**

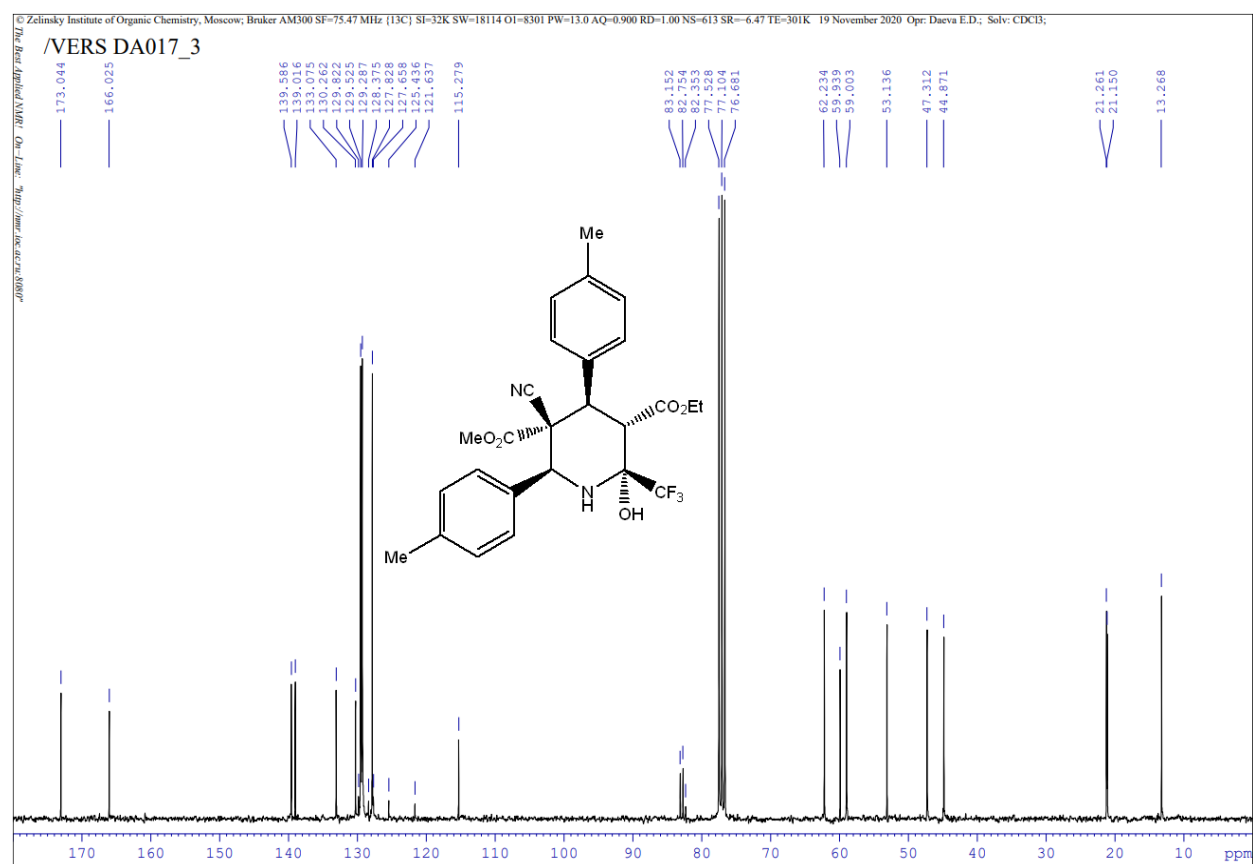
¹H NMR of 3-ethyl 5-methyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-5-cyano-2-hydroxy-4,6-diphenyl-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (3h**)****¹³C NMR of **3h****

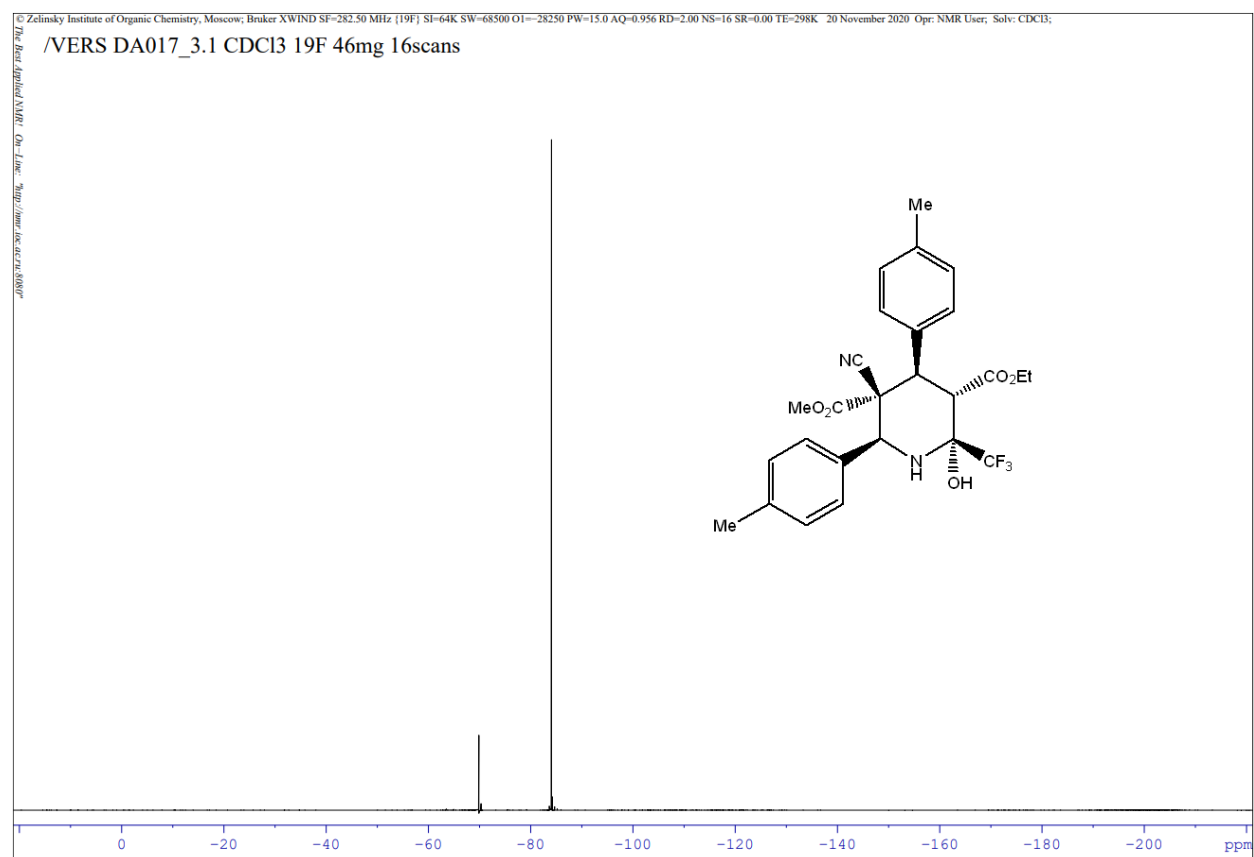
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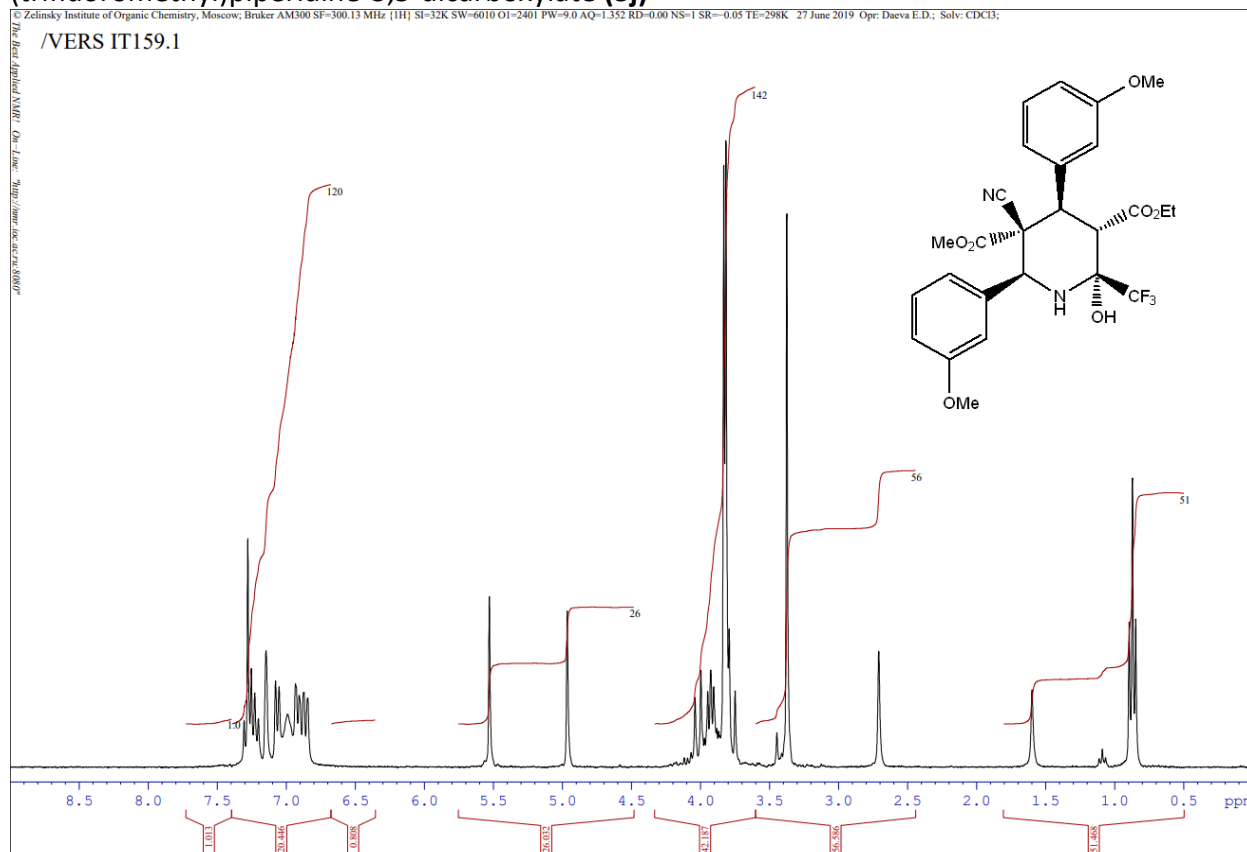
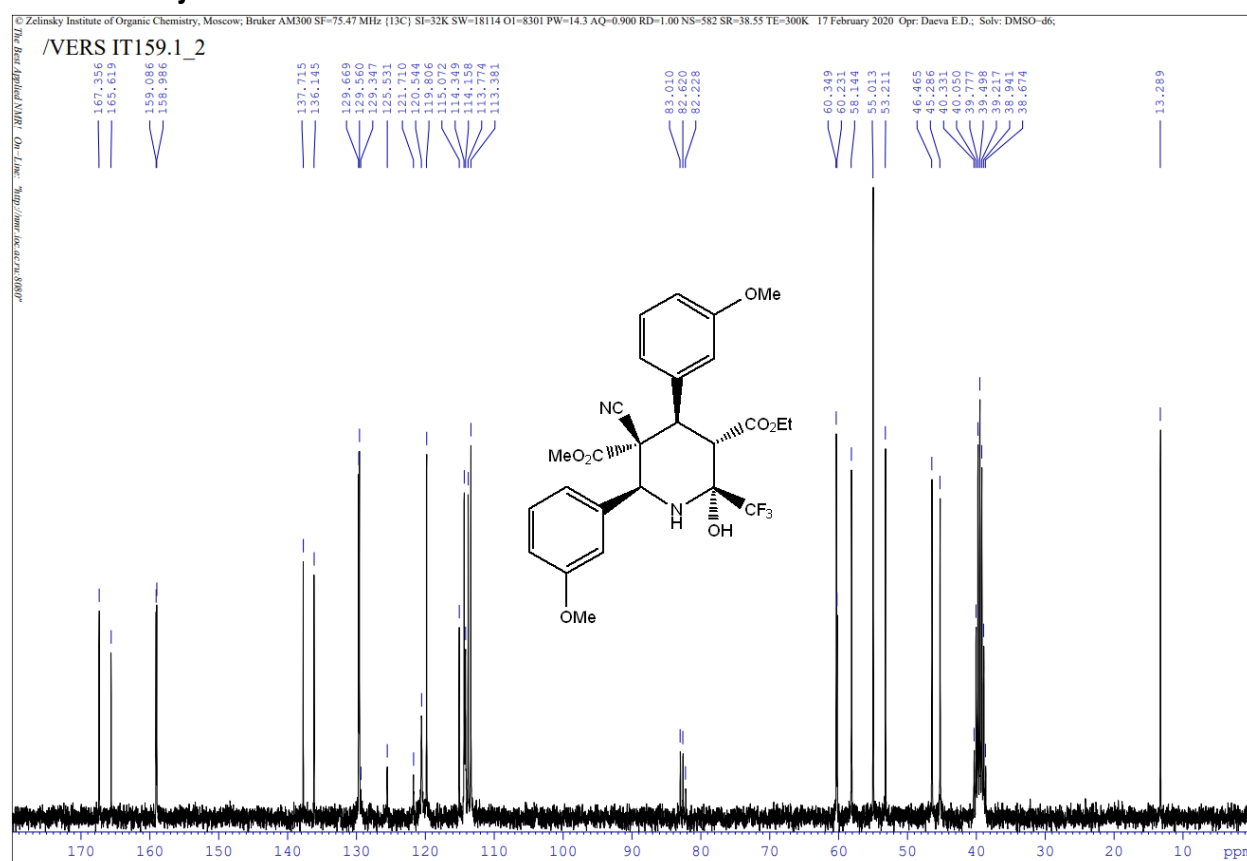
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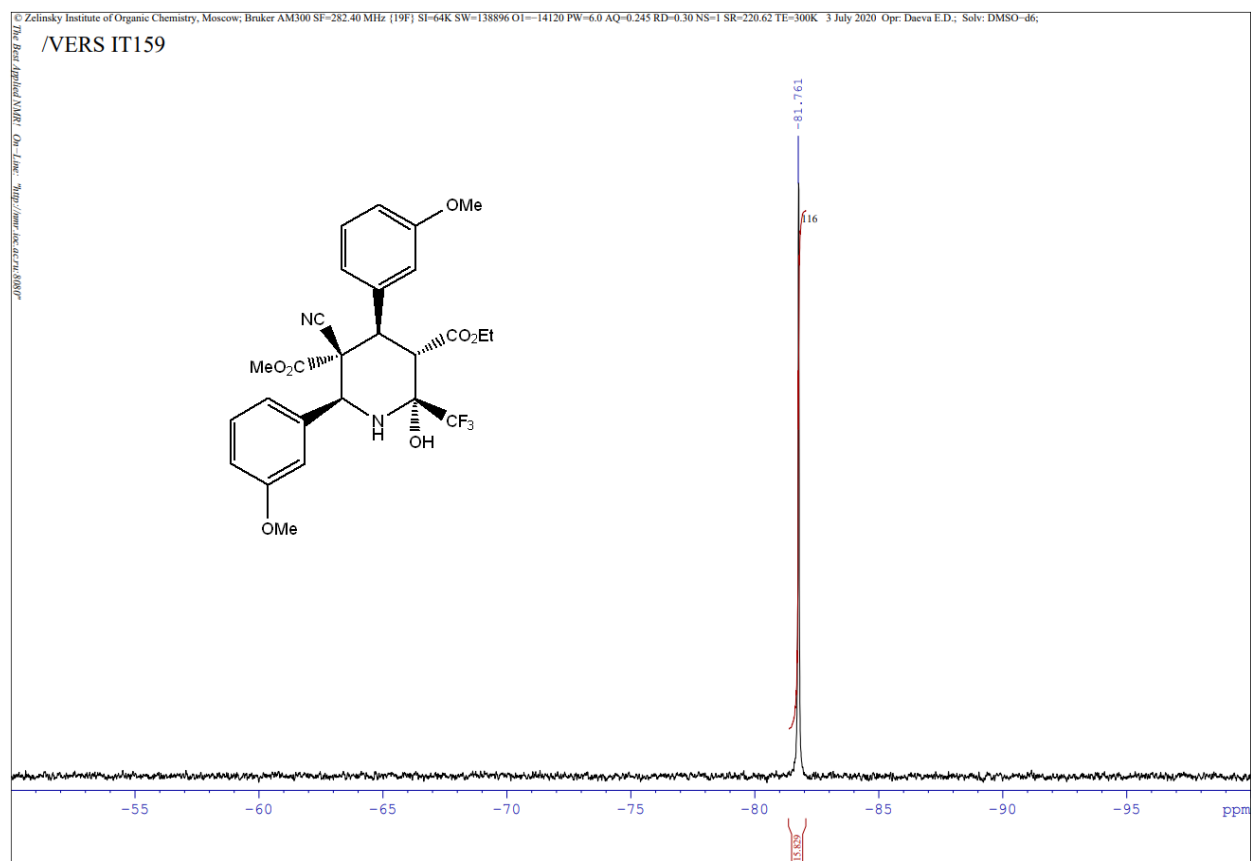


¹³C NMR of **3i**

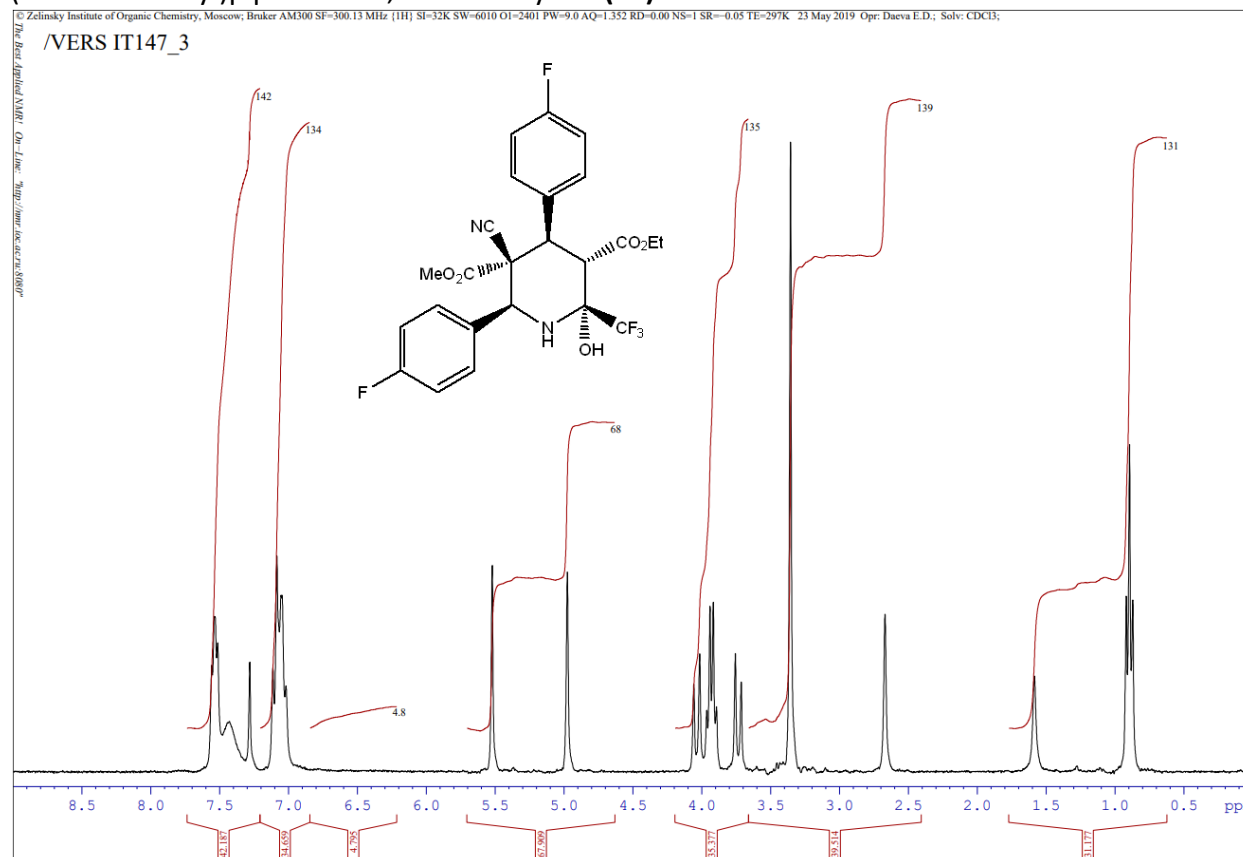


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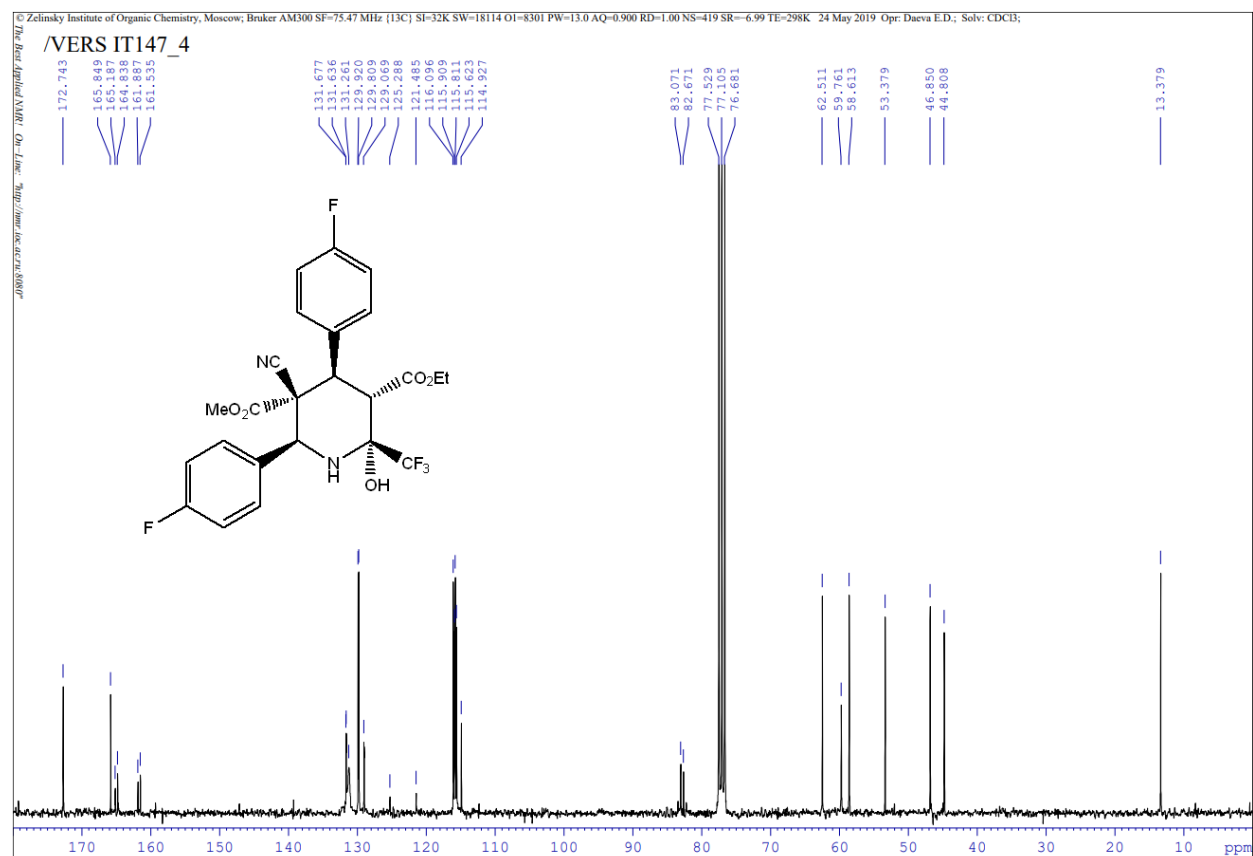
¹H NMR of 3-ethyl 5-methyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-5-cyano-2-hydroxy-4,6-bis(3-methoxyphenyl)-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (3j**)****¹³C NMR of **3j****

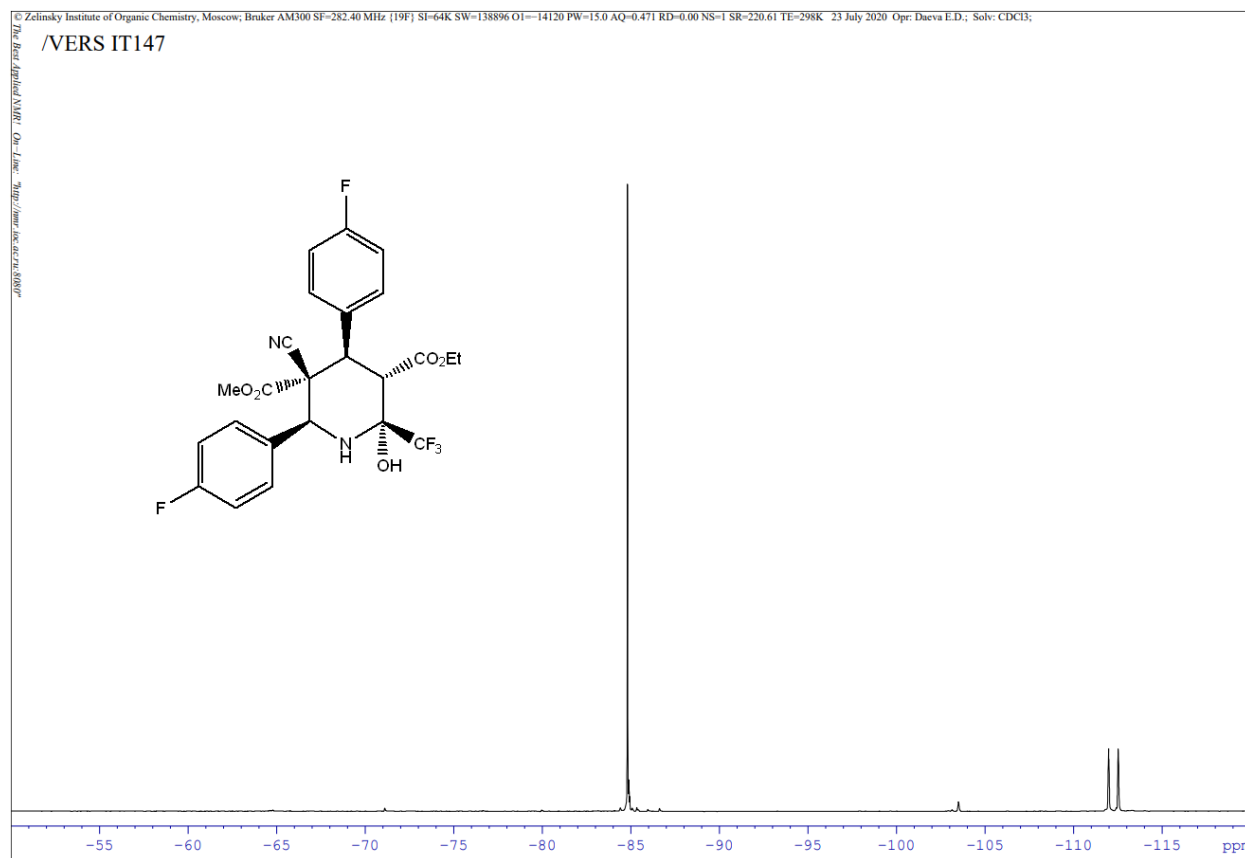
¹⁹F NMR of **3j**

¹H NMR of 3-ethyl 5-methyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-5-cyano-2-hydroxy-4,6-bis(4-fluorophenyl)-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (**3k**)

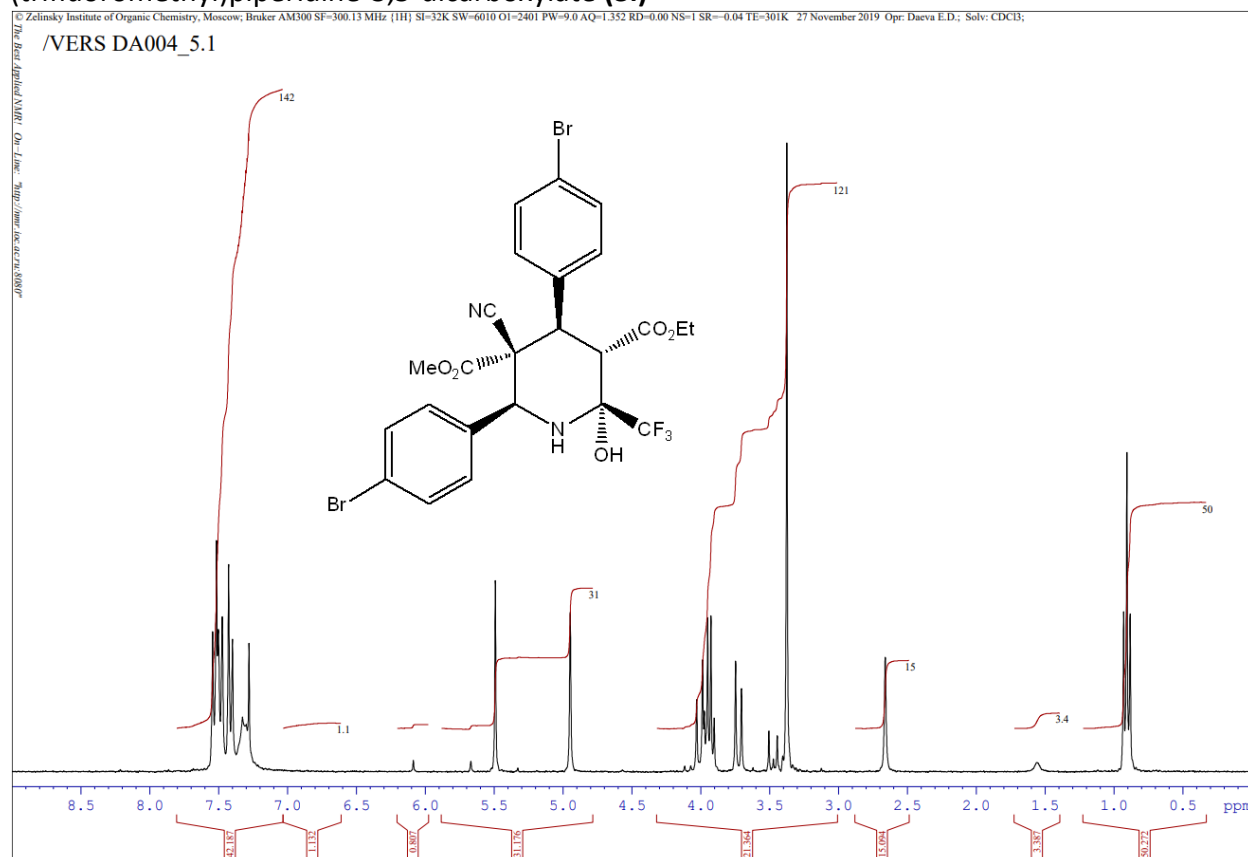


¹³C NMR of **3k**

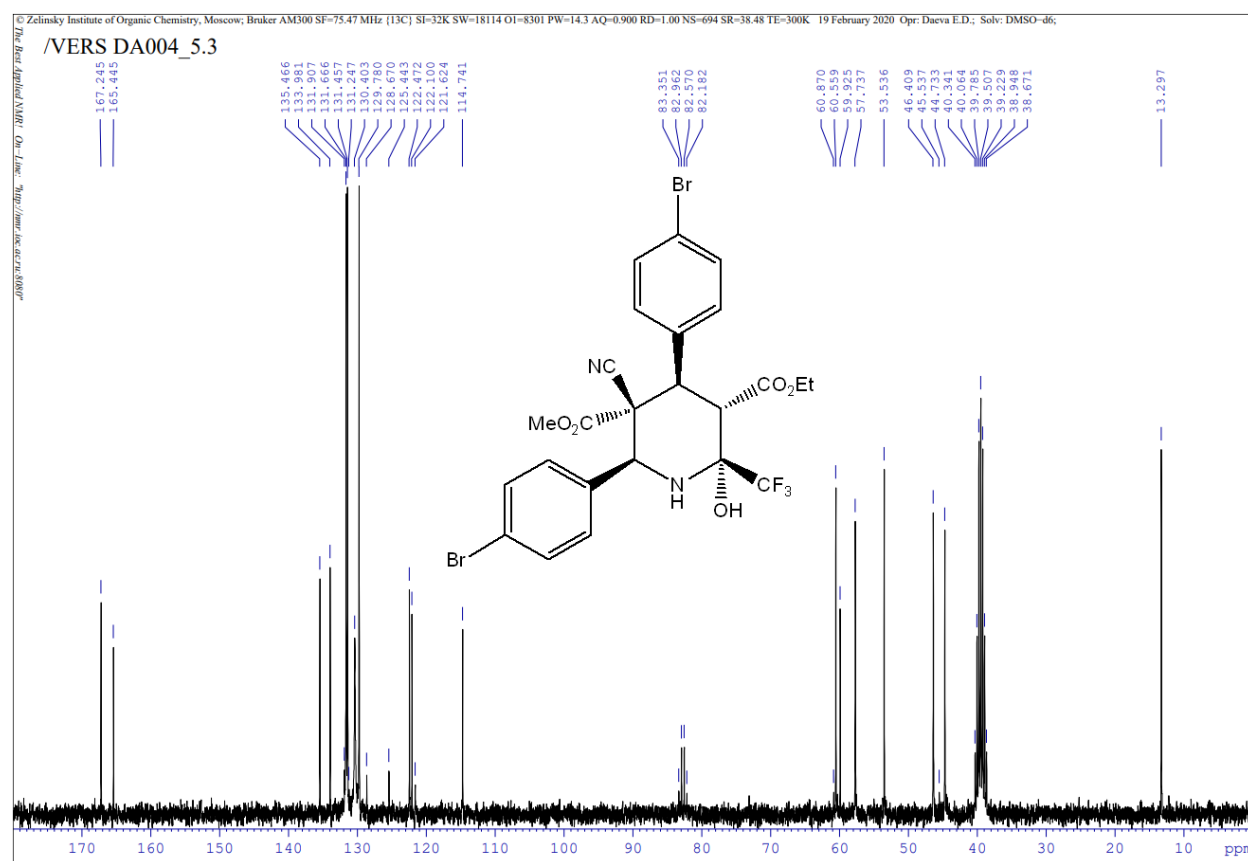


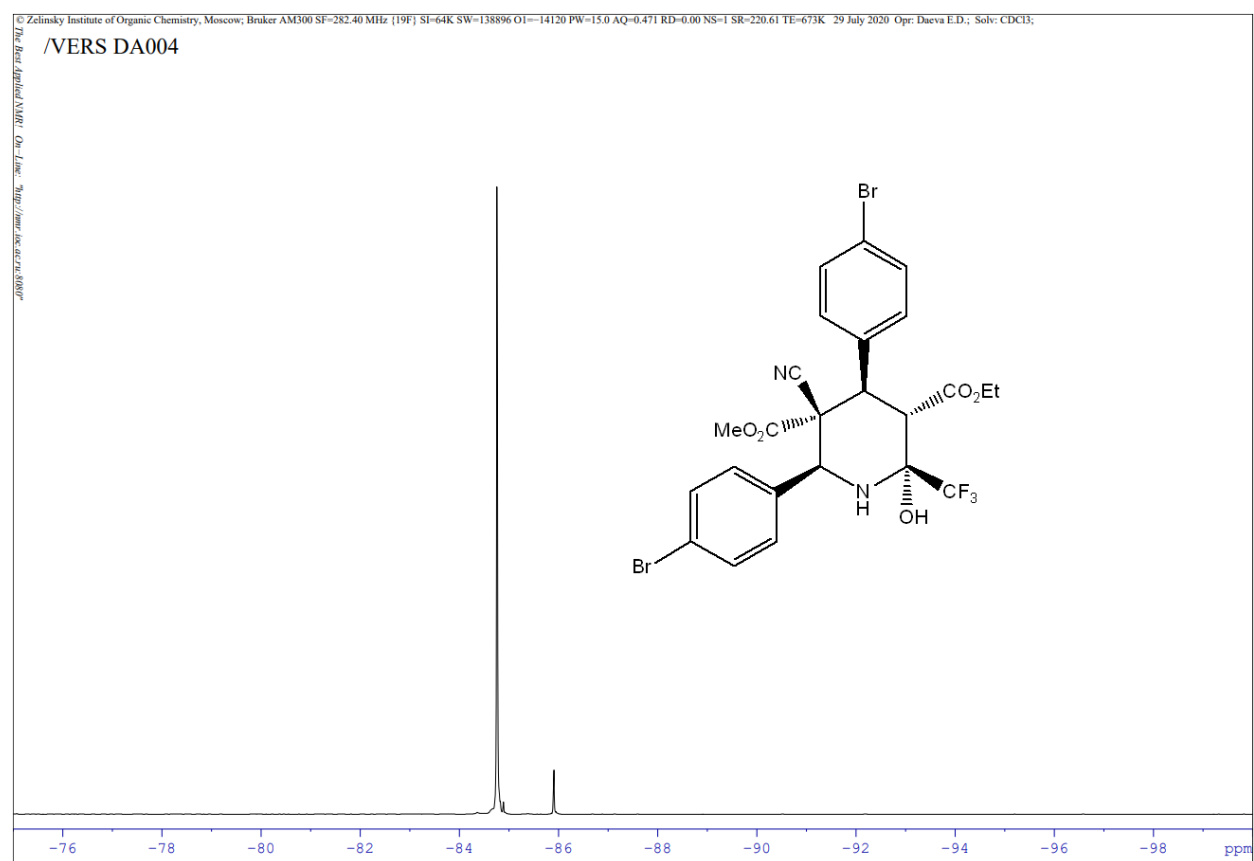
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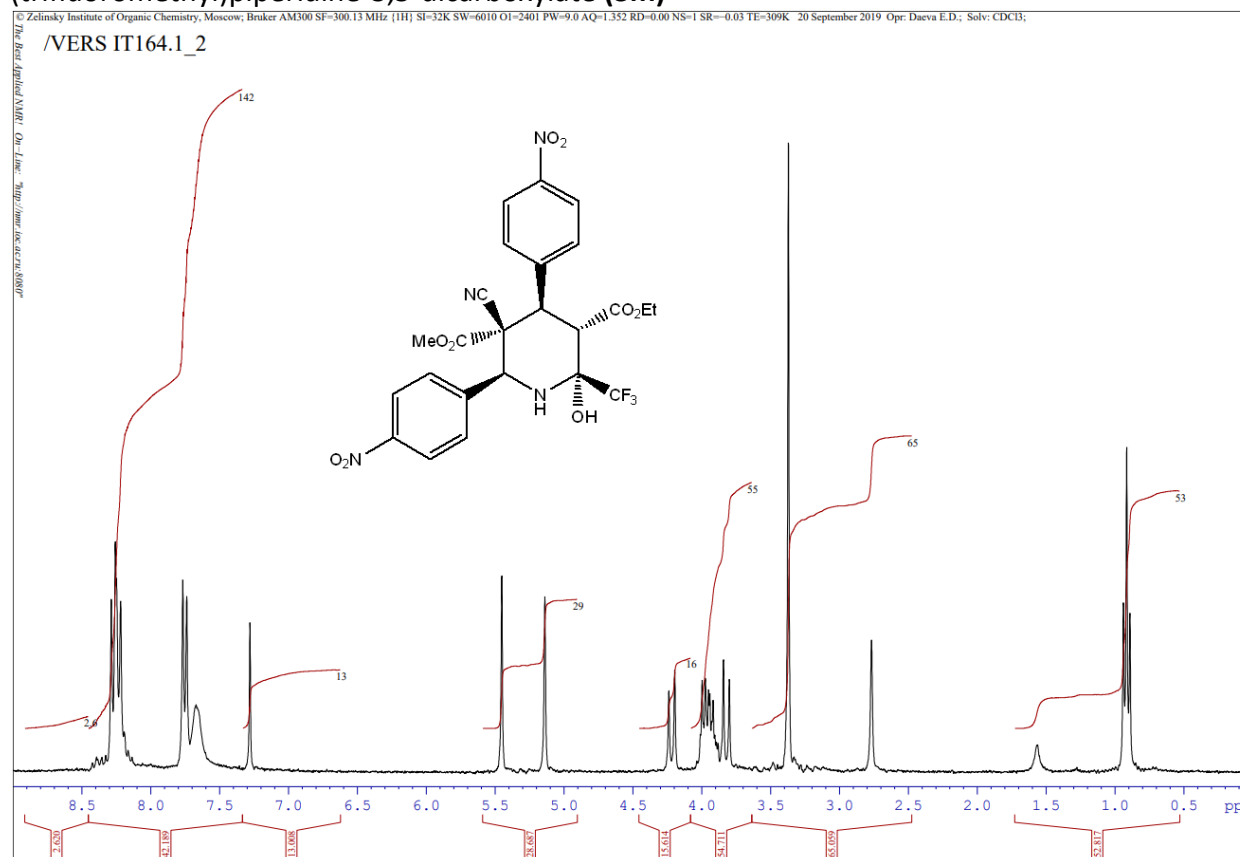
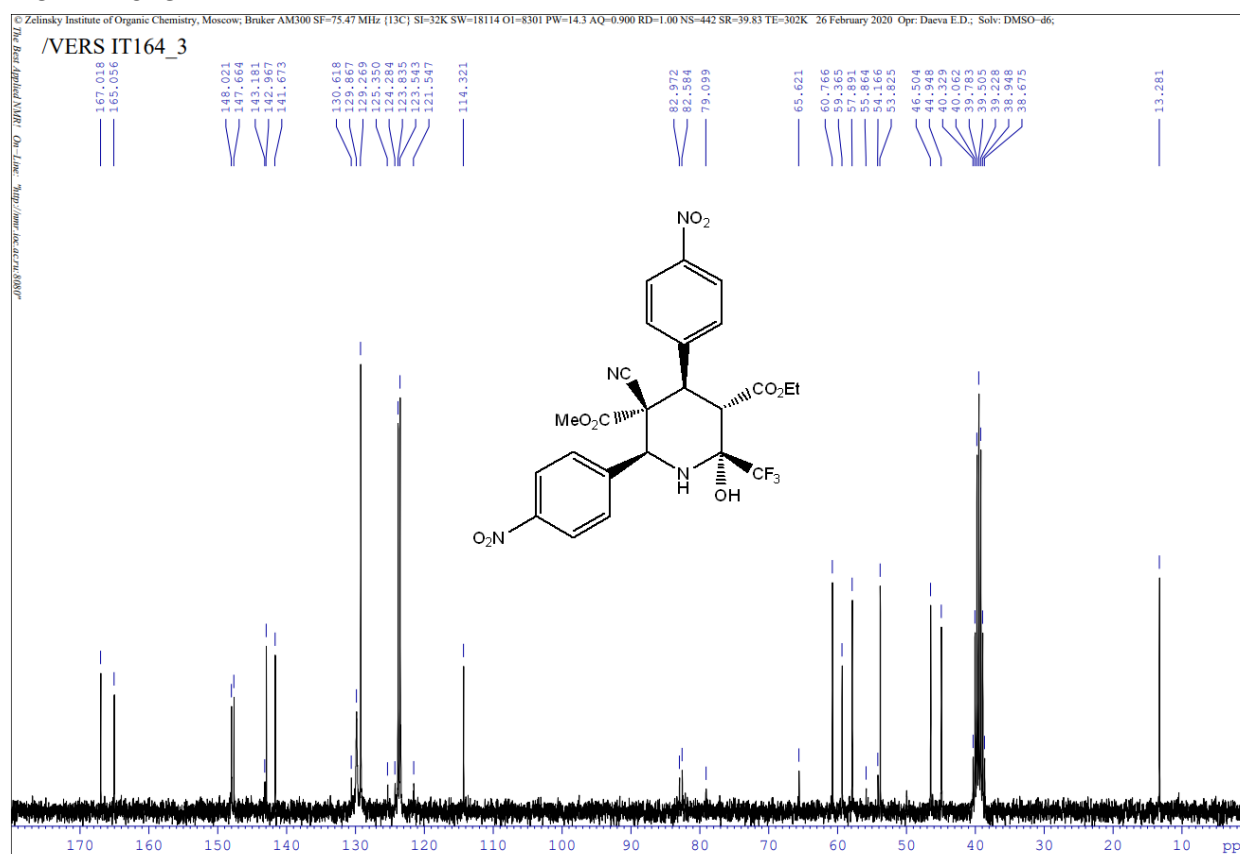
¹H NMR of 3-ethyl 5-methyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-4,6-bis(4-bromophenyl)-5-cyano-2-hydroxy-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (**3I**)

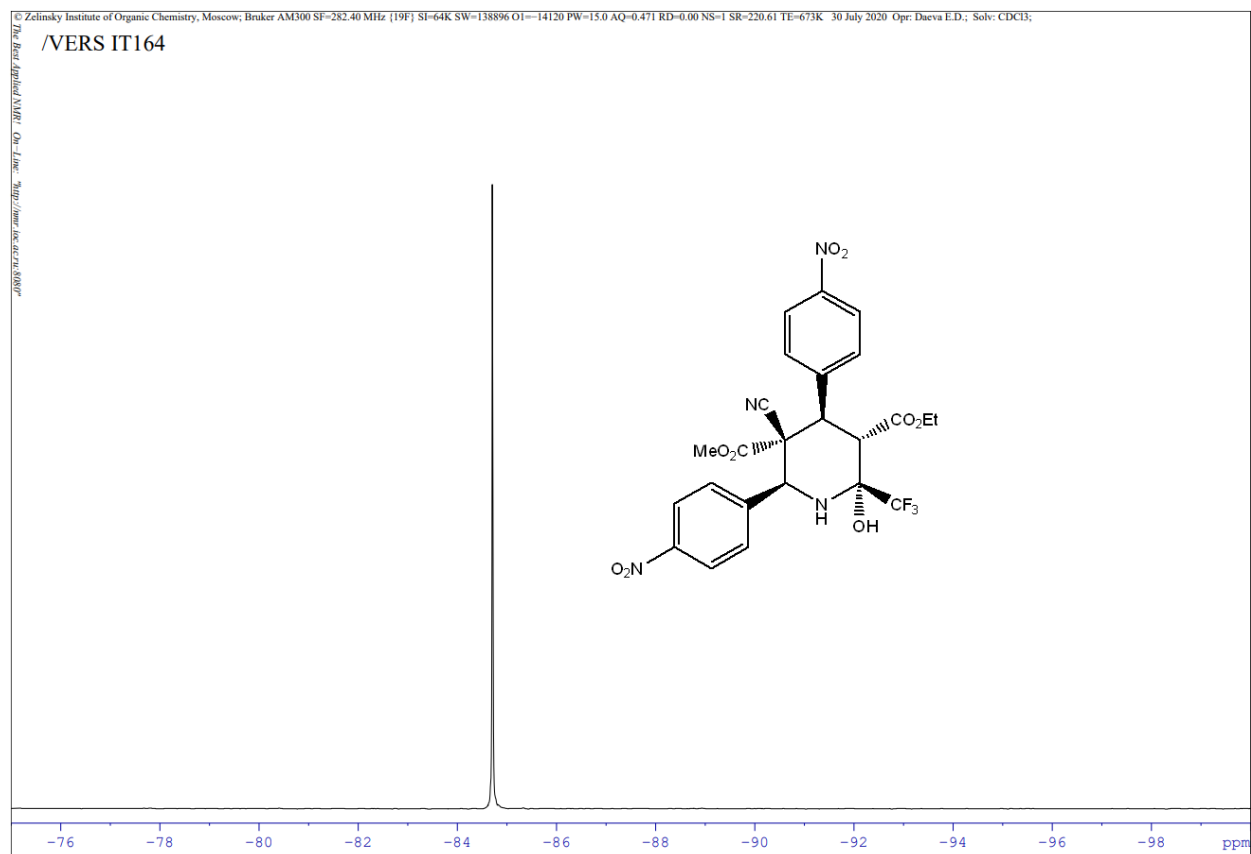


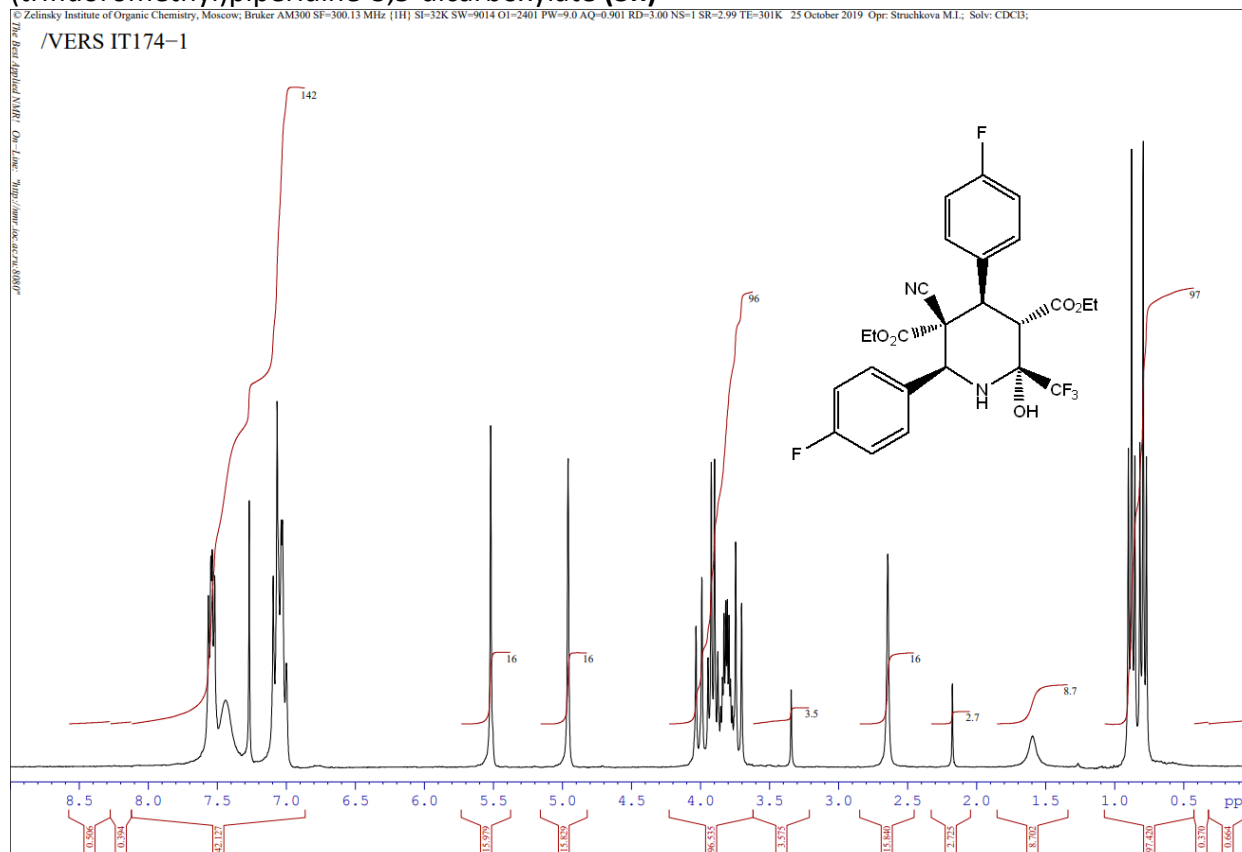
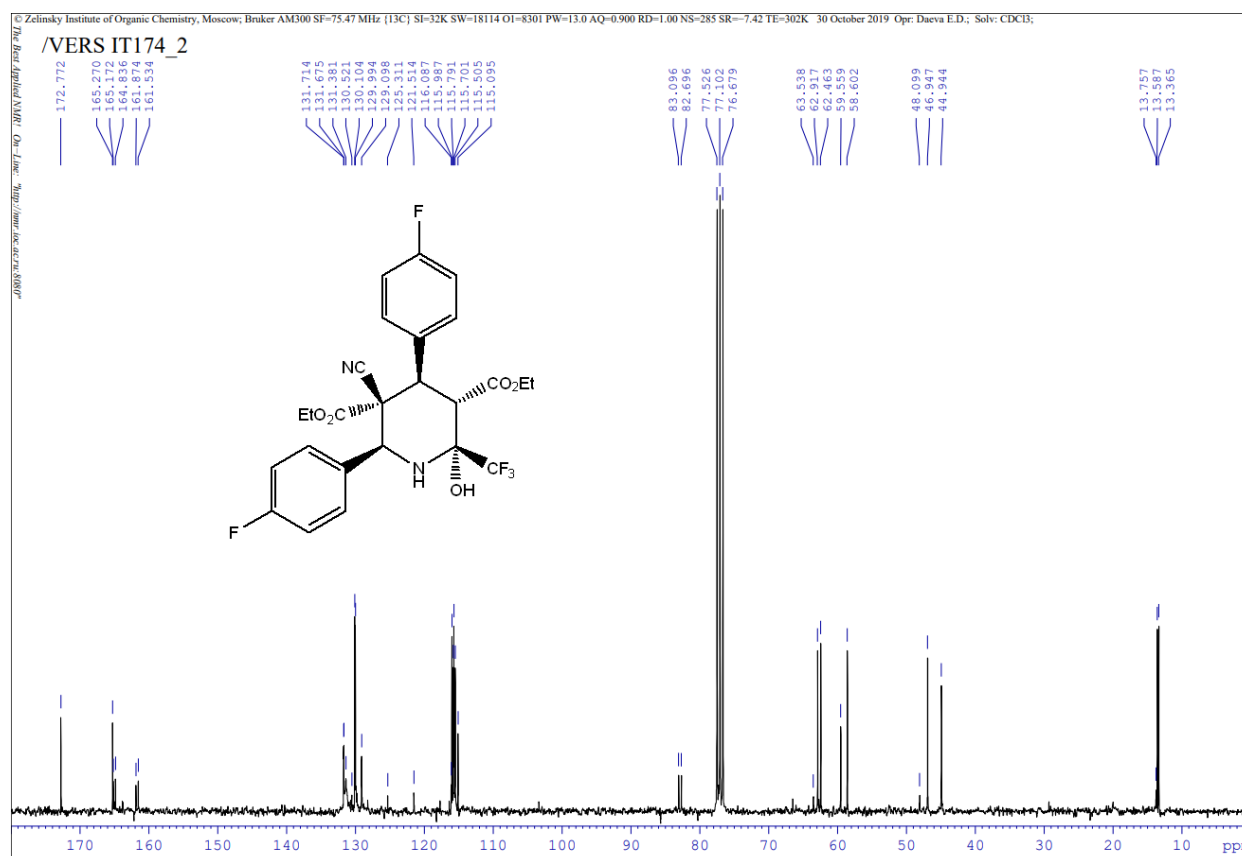
¹³C NMR of **3I**

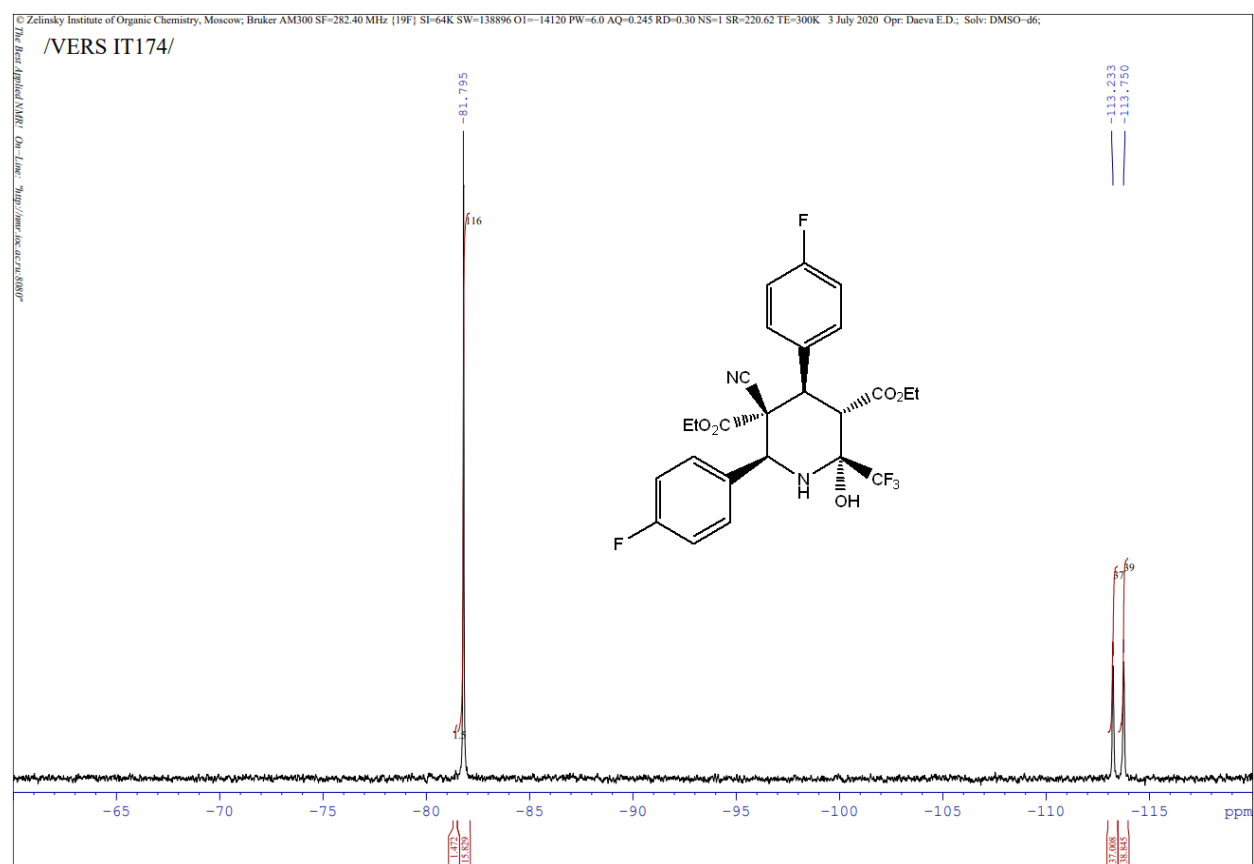


¹⁹F NMR of **3l**

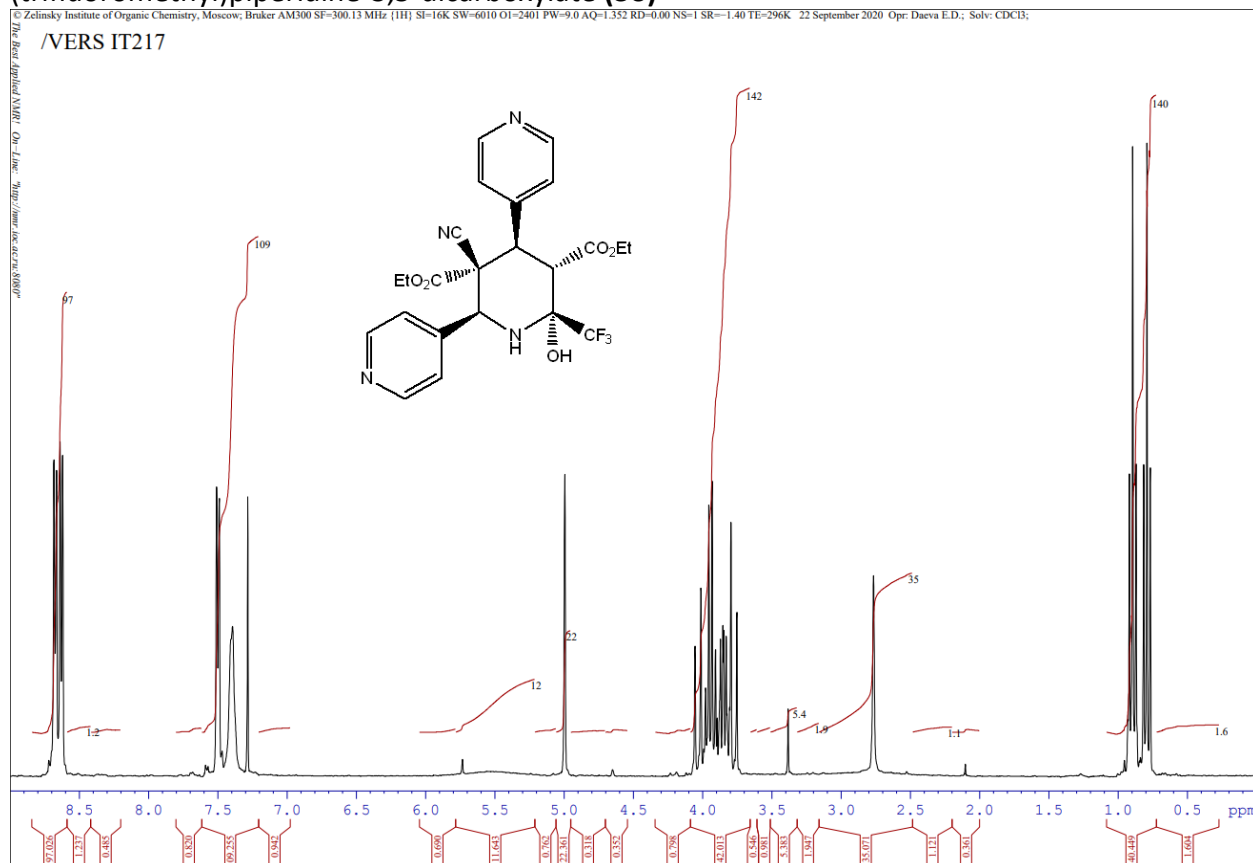
¹H NMR of 3-ethyl 5-methyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-5-cyano-2-hydroxy-4,6-bis(4-nitrophenyl)-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (**3m**)¹³C NMR of **3m**

¹⁹F NMR of **3m**

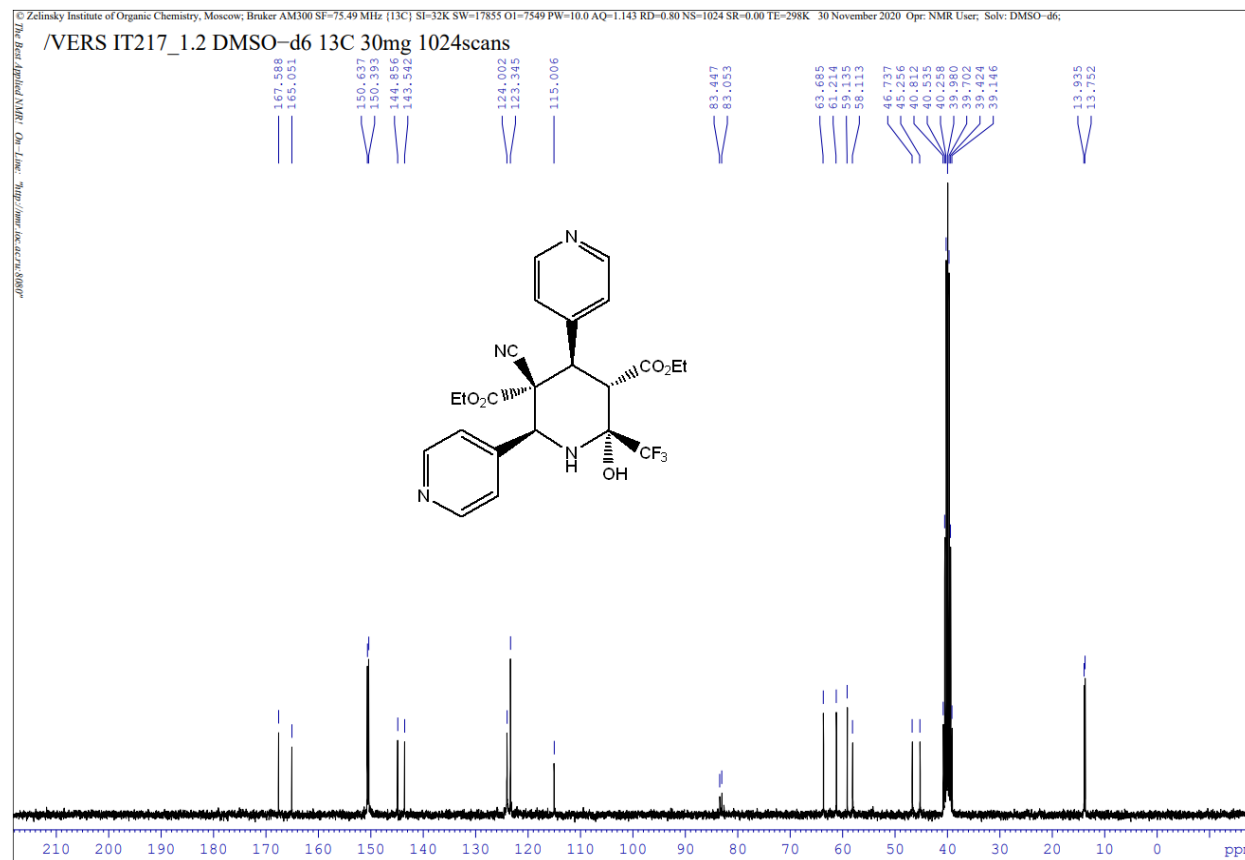
^1H NMR of 3,5-diethyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-4,6-bis(4-fluorophenyl)-5-cyano-2-hydroxy-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (3n**)** **^{13}C NMR of **3n****

^{19}F NMR of **3n**

¹H NMR of 3,5-diethyl (2*RS*,3*SR*,4*RS*,5*RS*,6*SR*)-4,6-bis(pyridin-4-yl)-5-cyano-2-hydroxy-2-(trifluoromethyl)piperidine-3,5-dicarboxylate (**3o**)



¹³C NMR of **3o**



¹⁹F NMR of **3o**