

# Ladder Coordination Polymer based on $\text{Ca}^{2+}$ and (4,5-dicyano-1,2-phenylene)bis(phosphonic acid)

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## Electronic Supporting Information

May30-2016  
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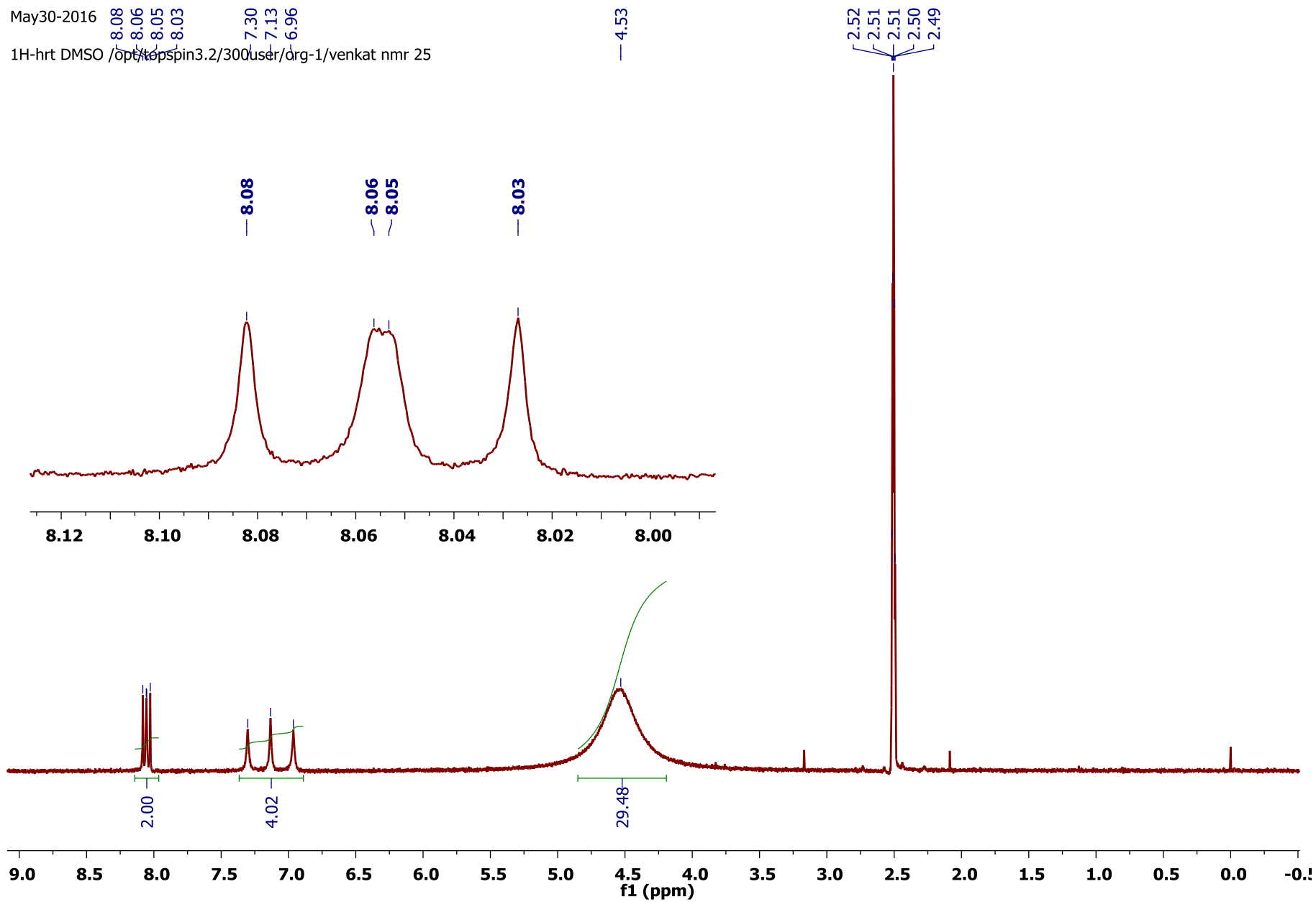
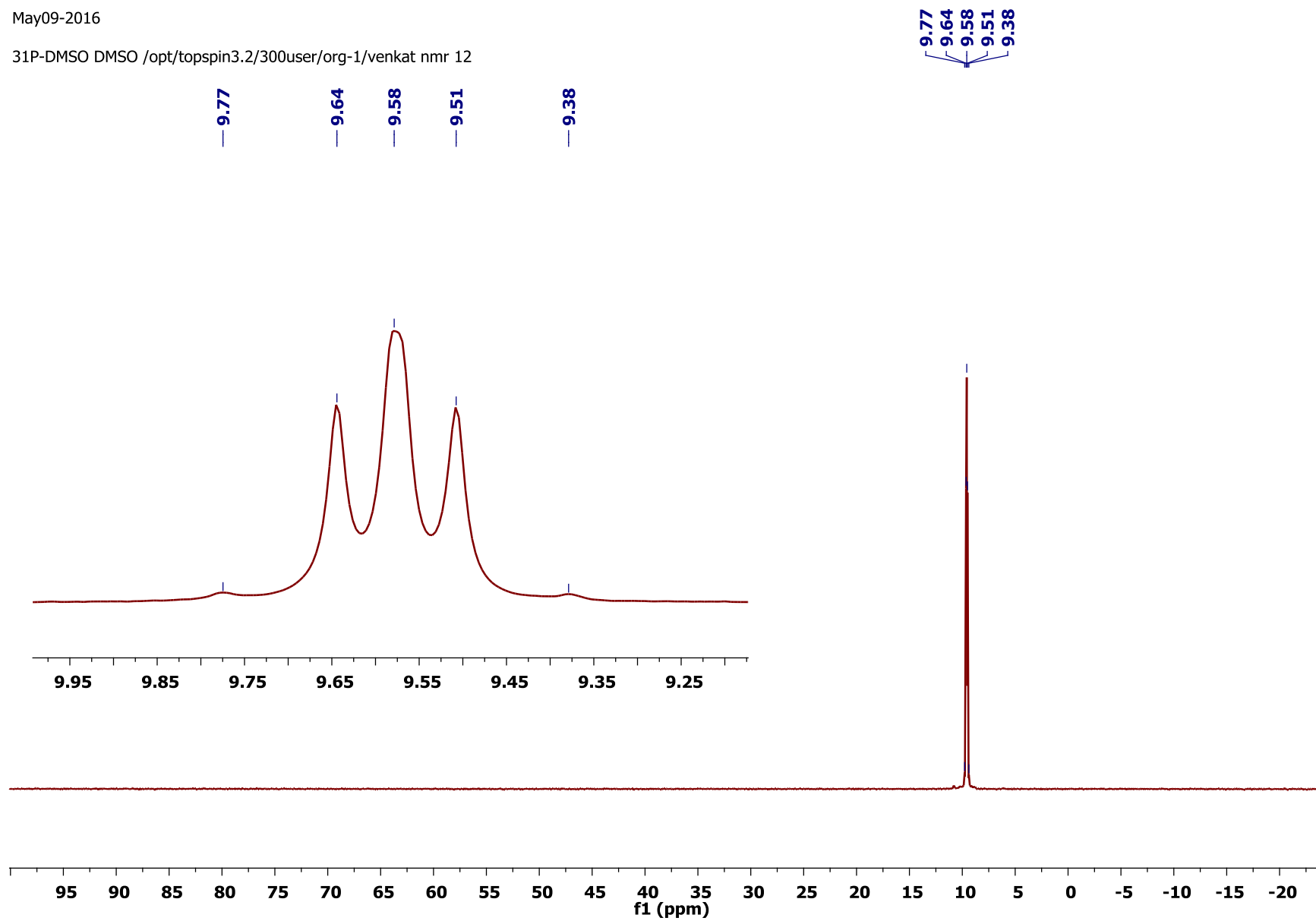


Figure S1 - <sup>1</sup>H NMR (300.13 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) in DMSO-*d*<sub>6</sub>.

May09-2016

31P-DMSO DMSO /opt/topspin3.2/300user/org-1/venkat nmr 12



**Figure S2** -  $^{31}\text{P}$  NMR (121.49 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) in  $\text{DMSO-}d_6$ .

Feb14-2014

13C-hrt DMSO /opt/.../user/org-1/ver...

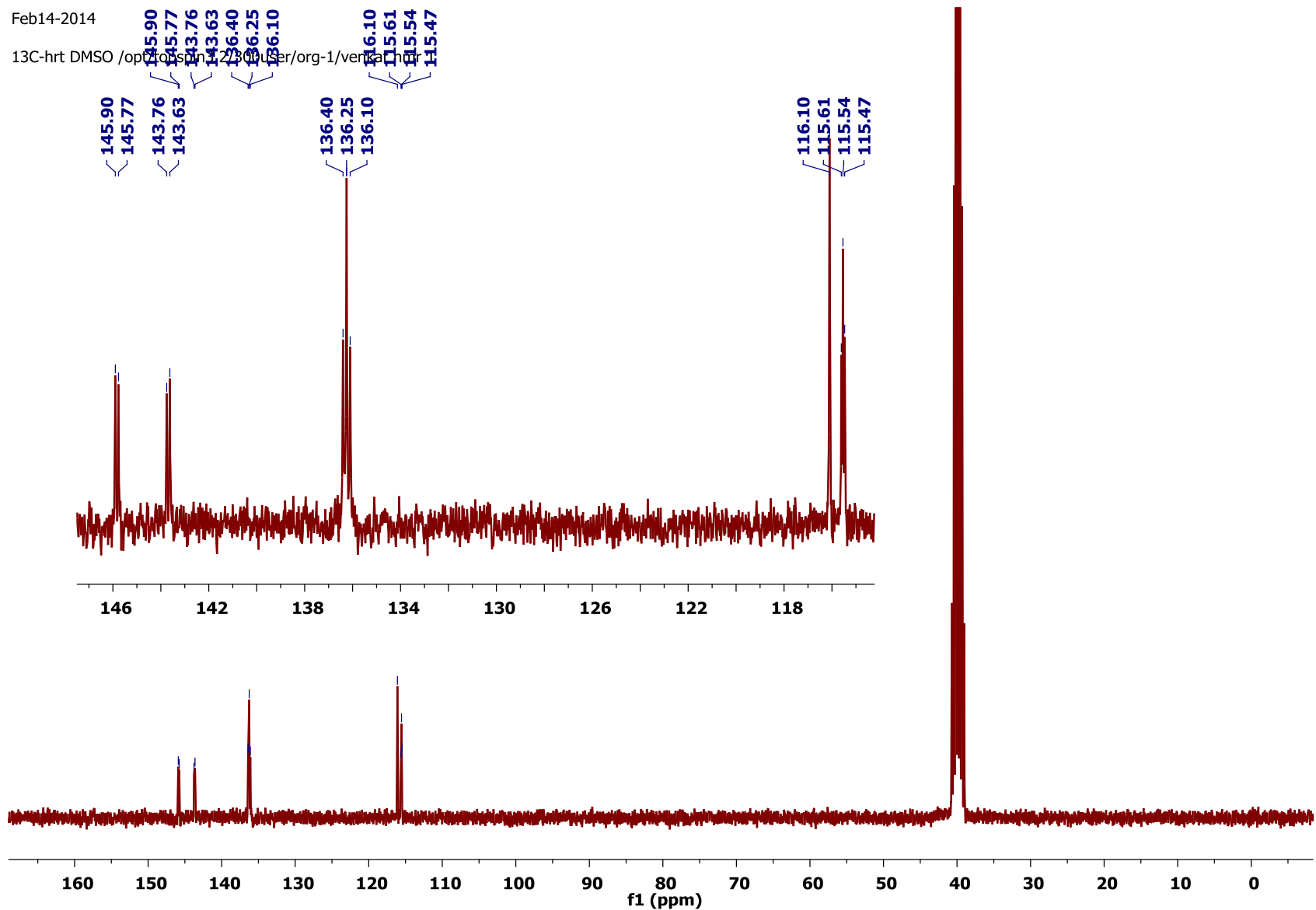
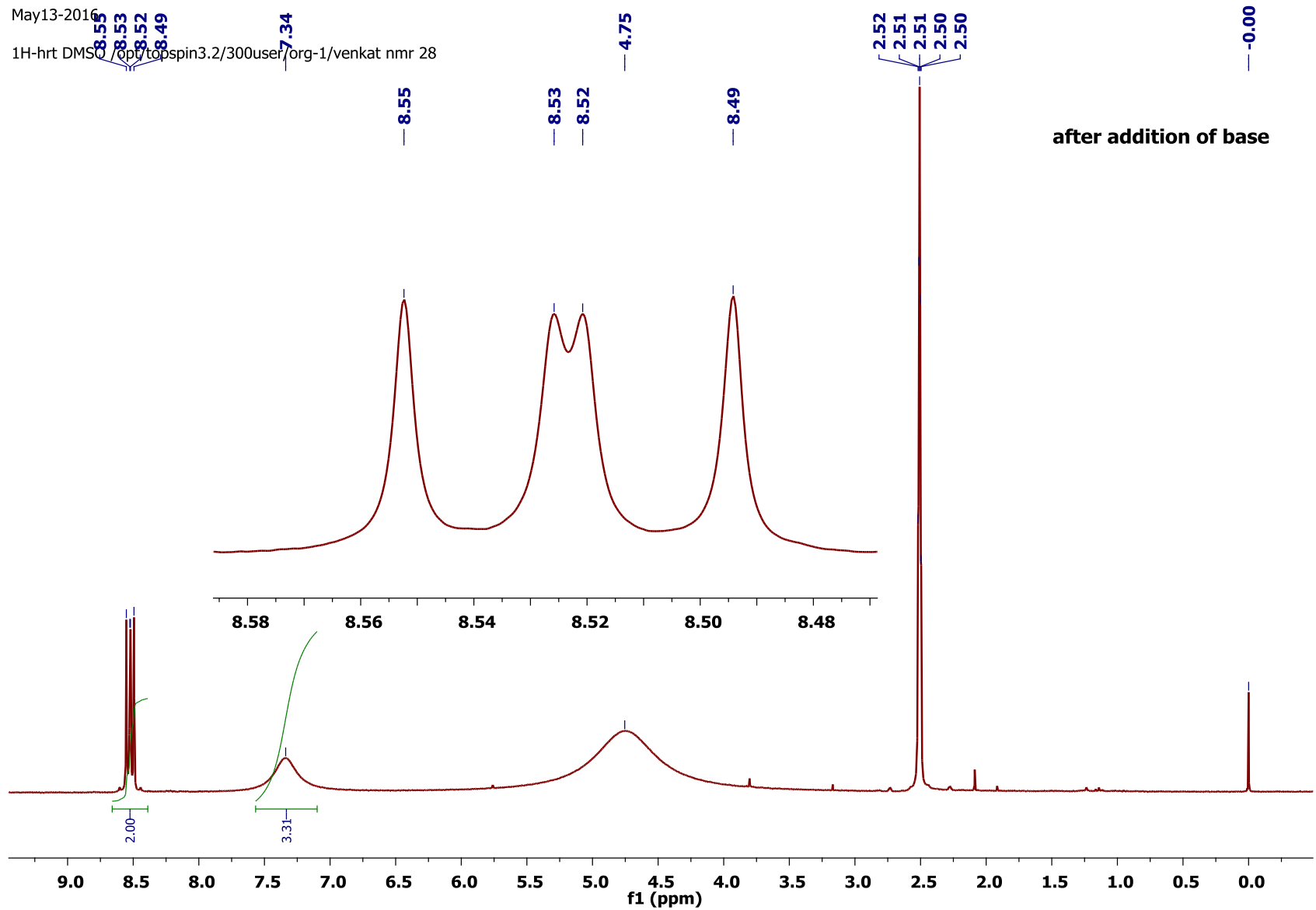


Figure S3 -  $^{13}\text{C}$  NMR (75.47 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) in  $\text{DMSO-}d_6$ .

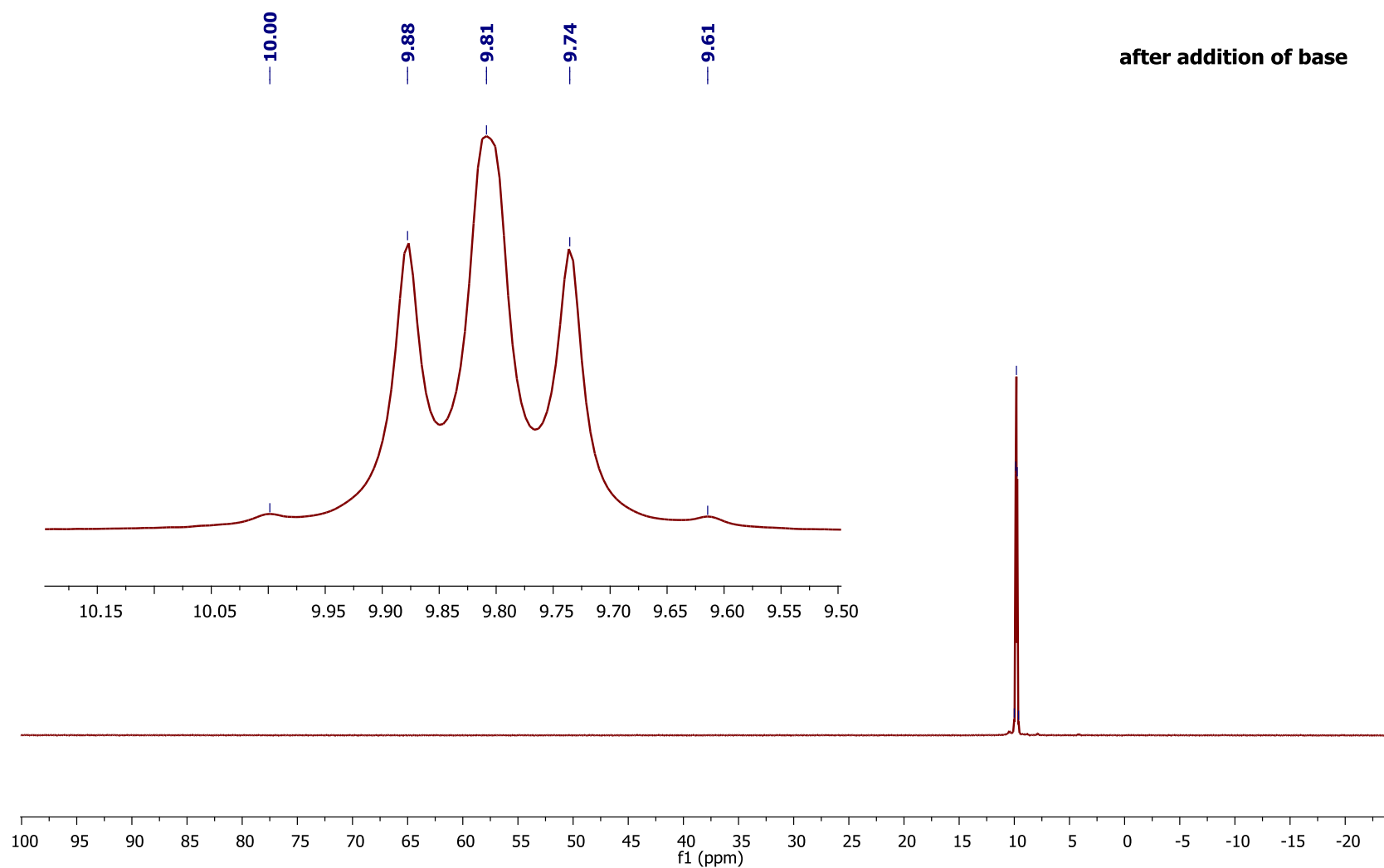


**Figure S4** -  $^1\text{H}$  NMR (300.13 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) upon addition of  $\text{K}_2\text{CO}_3$  in  $\text{DMSO}-d_6$ .

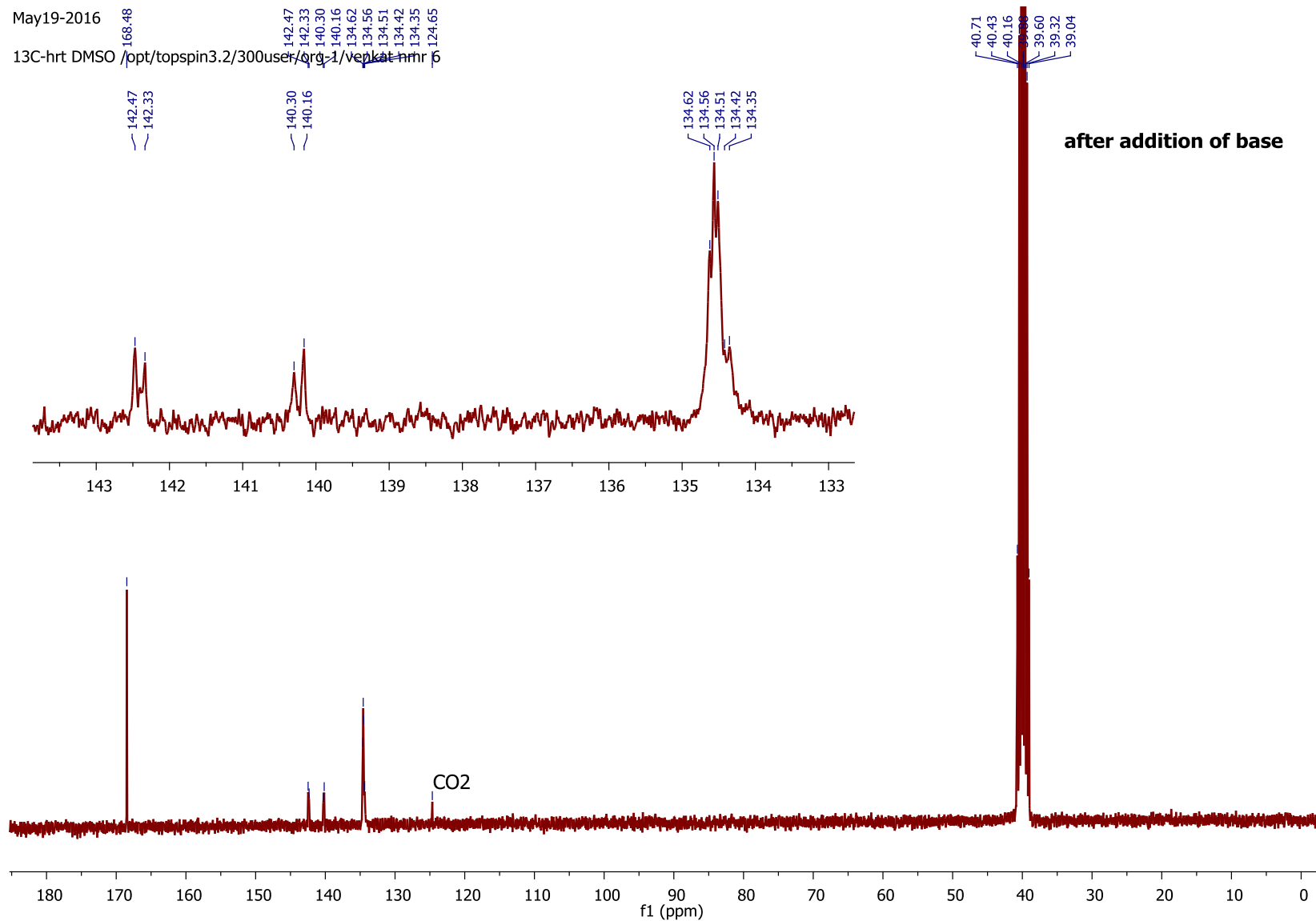
May19-2016

31P-DMSO DMSO /opt/topspin3.2/300user/org-1/venkat nmr 6

10.00  
9.88  
9.81  
9.74  
9.61



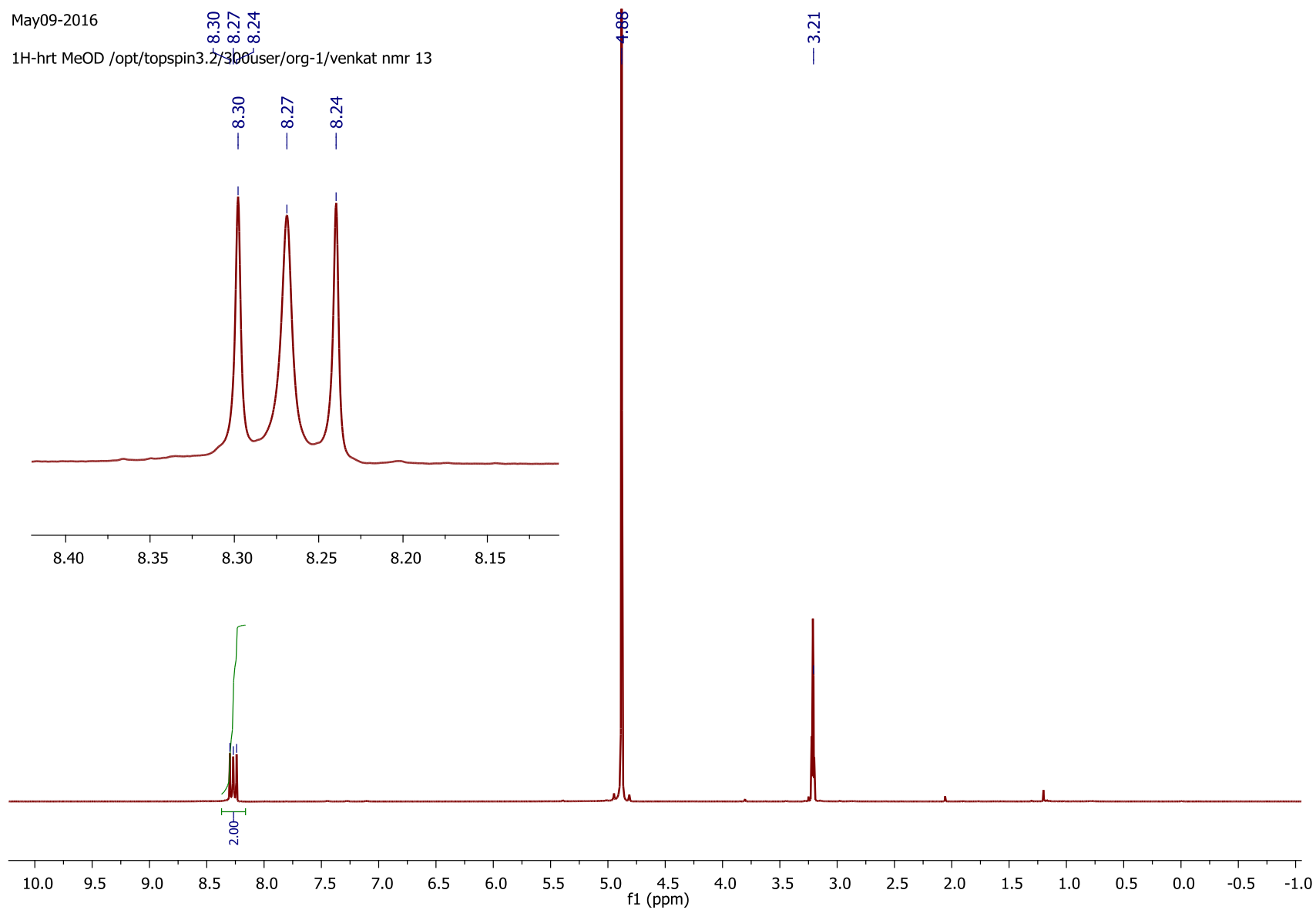
**Figure S5** -  $^{31}\text{P}$  NMR (121.49 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) upon the addition of  $\text{K}_2\text{CO}_3$  in  $\text{DMSO-}d_6$ .



**Figure S6** -  $^{13}\text{C}$  NMR (75.47 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) upon the addition of  $\text{K}_2\text{CO}_3$  in  $\text{DMSO-}d_6$ .

May09-2016

1H-hrt MeOD /opt/topspin3.2/300user/org-1/venkat nmr 13



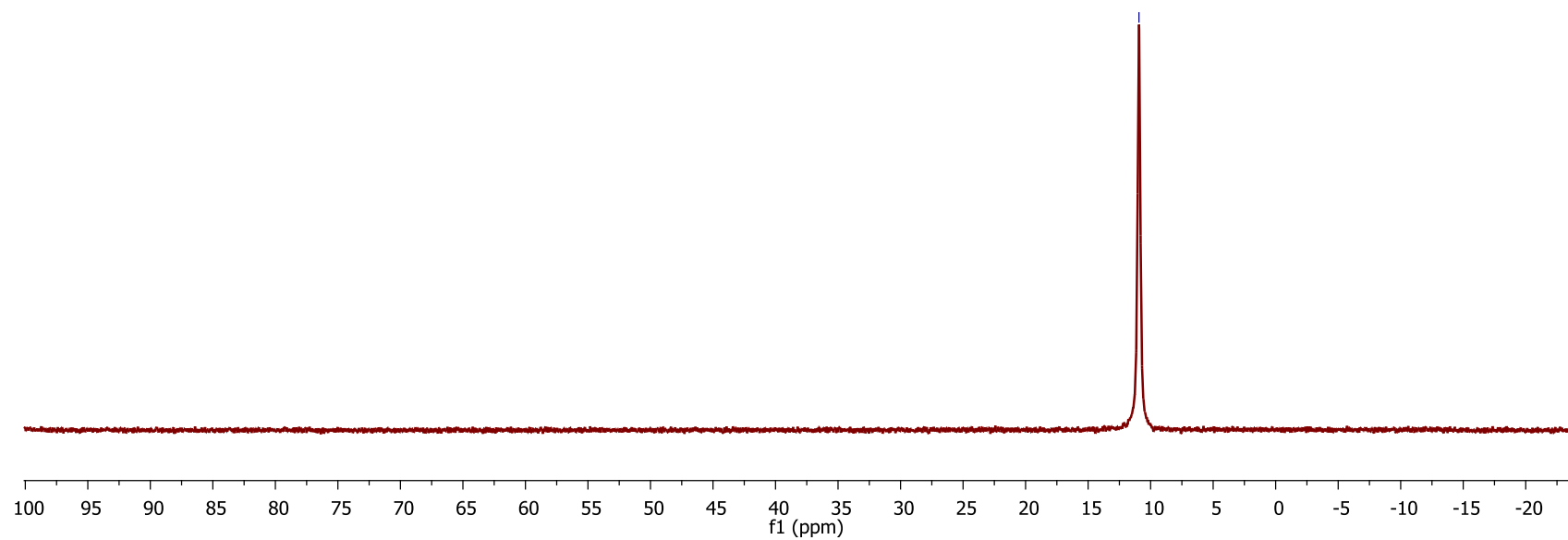
**Figure S7** - <sup>1</sup>H NMR (300.13 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) in methanol-*d*<sub>4</sub>.



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31P-DMSO MeOD /opt/topspin3.2/300user/org-1/venkat nmr 13

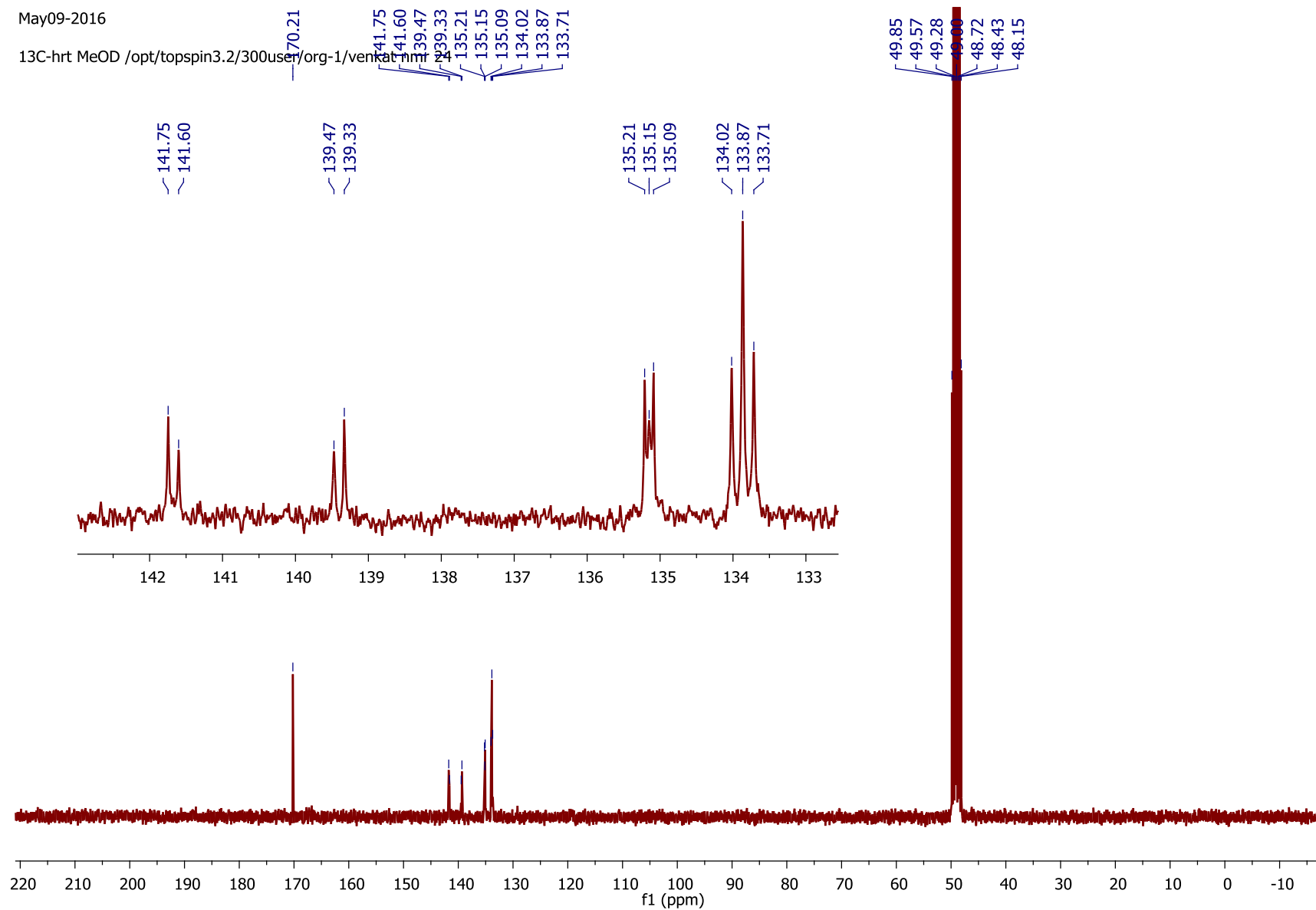
— 10.93



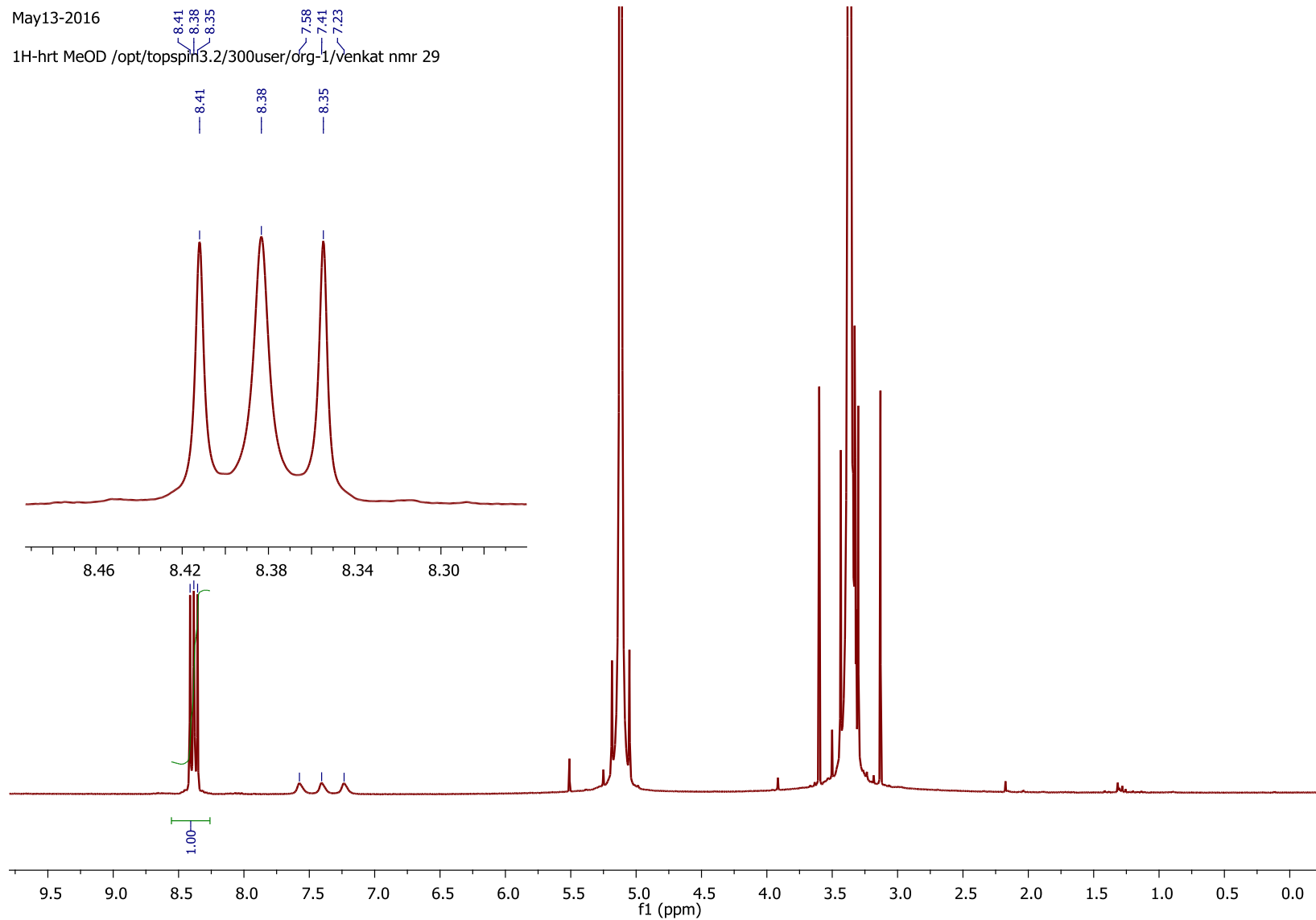
**Figure S8** -  $^{31}\text{P}$  NMR (121.49 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) in methanol- $d_4$ .

May09-2016

13C-hrt MeOD /opt/topspin3.2/300user/org-1/venkat.nmr



**Figure S9** -  $^{13}\text{C}$  NMR (75.47 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) in methanol- $d_4$ .

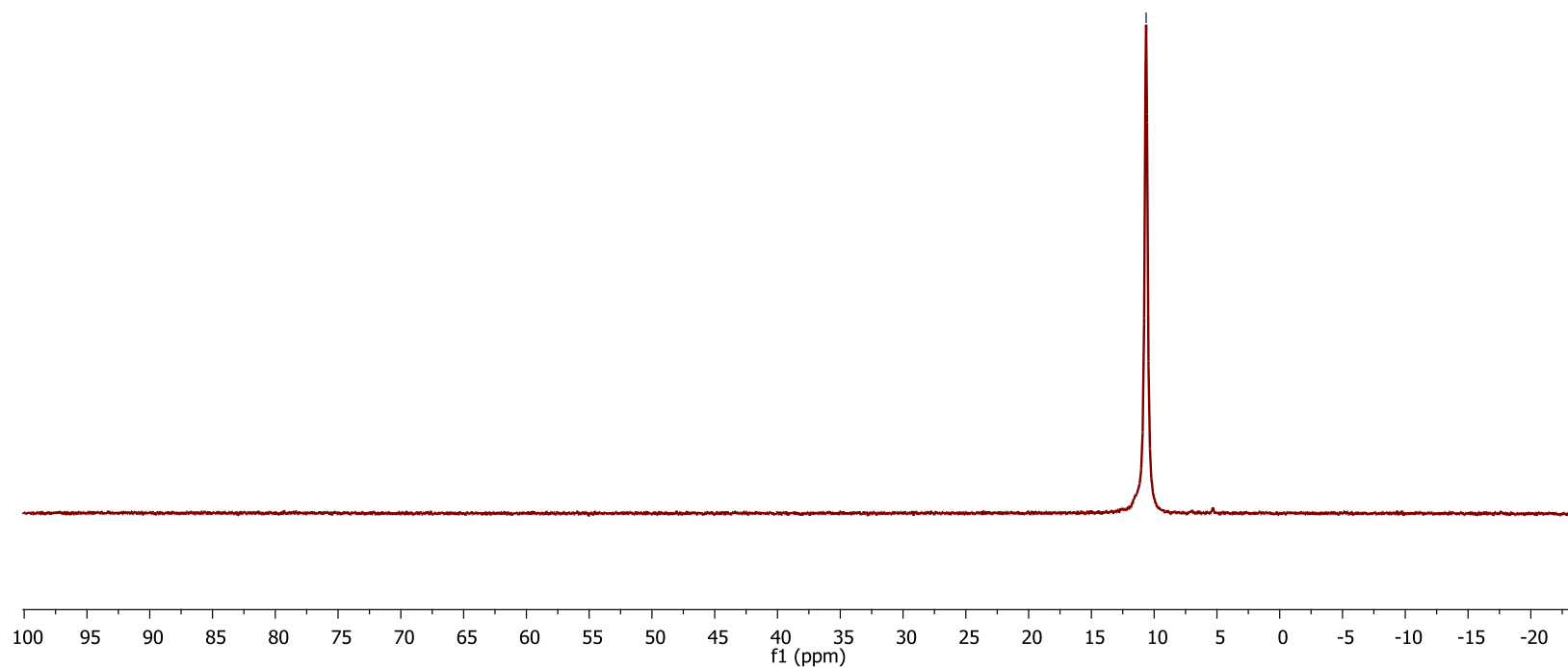


**Figure S10** -  $^1\text{H}$  NMR (300.13 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) upon the addition of few drops of methanolic ammonia (7M) in methanol- $d_4$ .

May19-2016

31P-DMSO MeOD /opt/topspin3.2/300user/org-1/venkat nmr 4

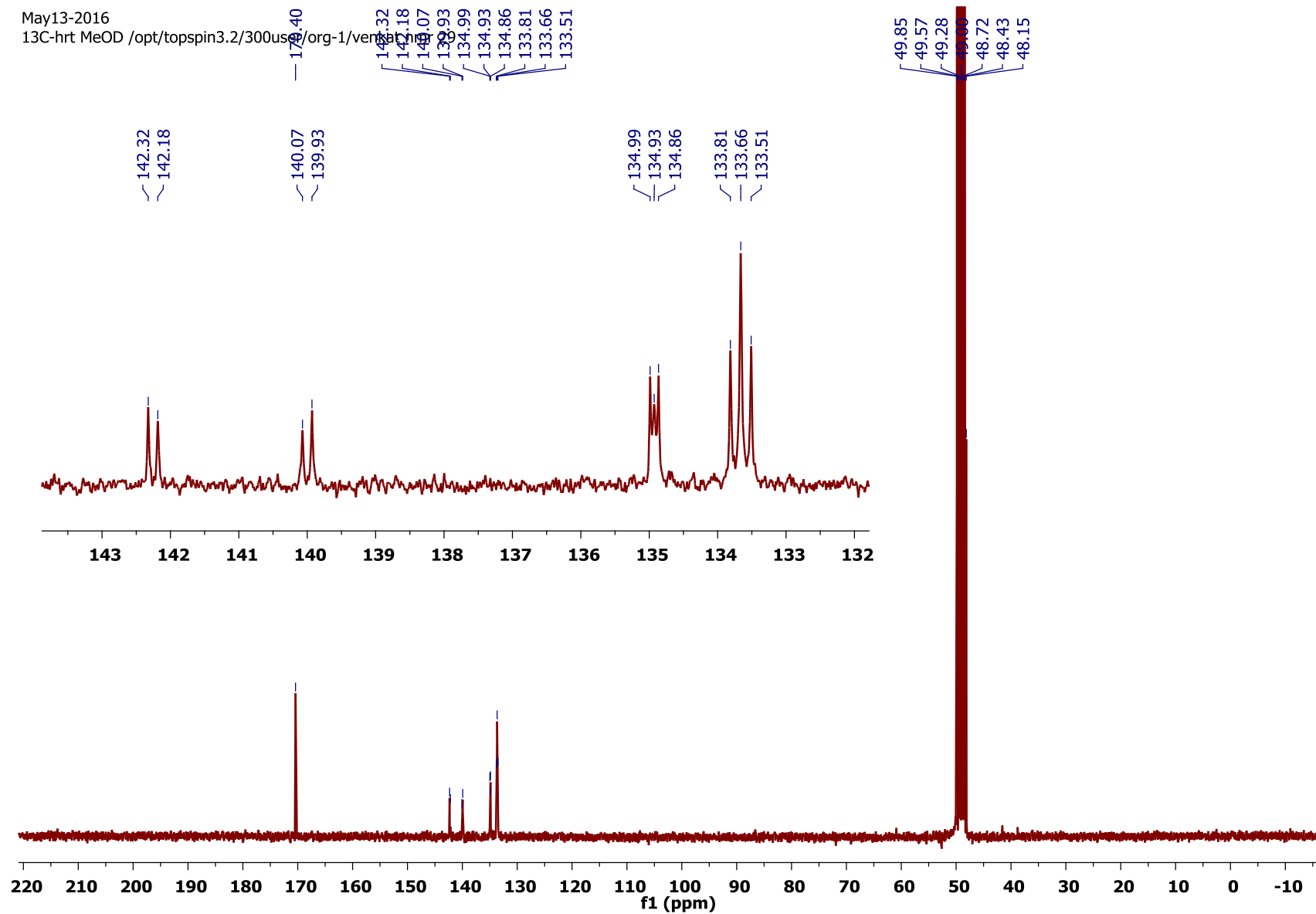
— 10.64



**Figure S11** -  $^{31}\text{P}$  NMR (121.49 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) spectrum of  $\text{H}_4\text{CPP}$  upon the addition of few drops of methanolic ammonia (7M) in methanol- $d_4$ .

May13-2016

13C-hrt MeOD /opt/topspin3.2/300use/org-1/ventat/



**Figure S12** -  $^{13}\text{C}$  NMR (75.47 MHz) spectrum of (4,5-dicyano-1,2-phenylene)bis(phosphonic acid) upon the addition of few drops of methanolic ammonia (7M) in methanol- $d_4$ .