

Electronic Supporting Information

Impact of Substituent Position on the DSSC Performances of New 1,1'-bis(diphenylphosphino)ferrocene appended Nickel(II) methoxy cyanodithiolates

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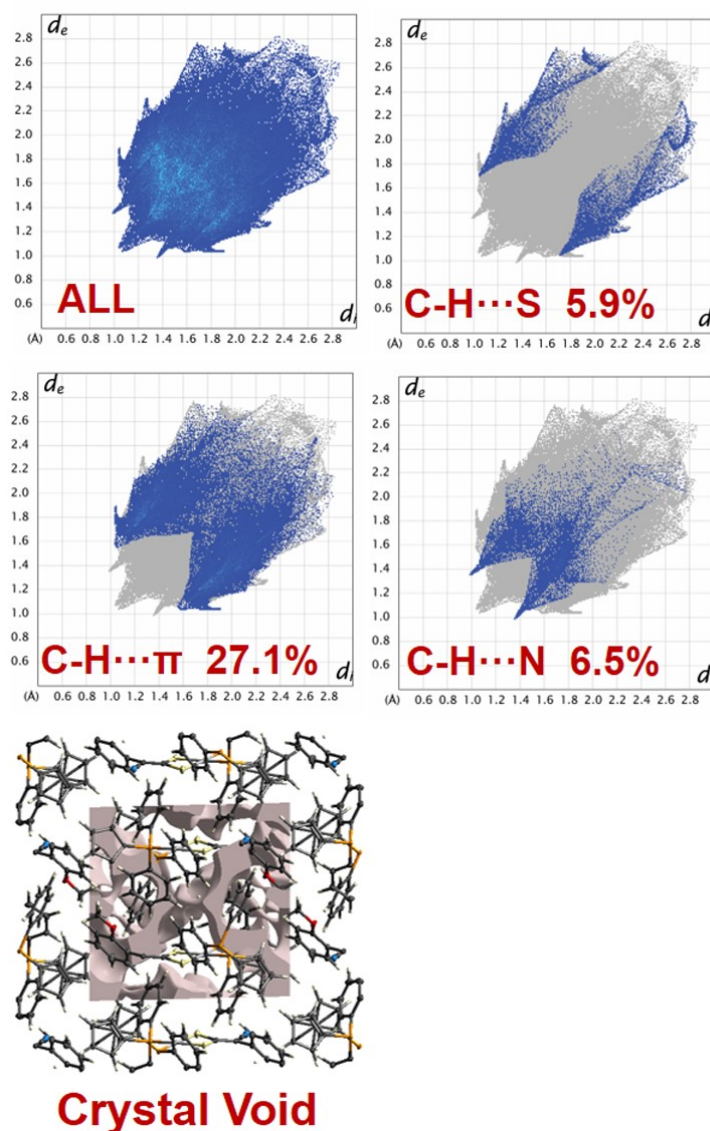
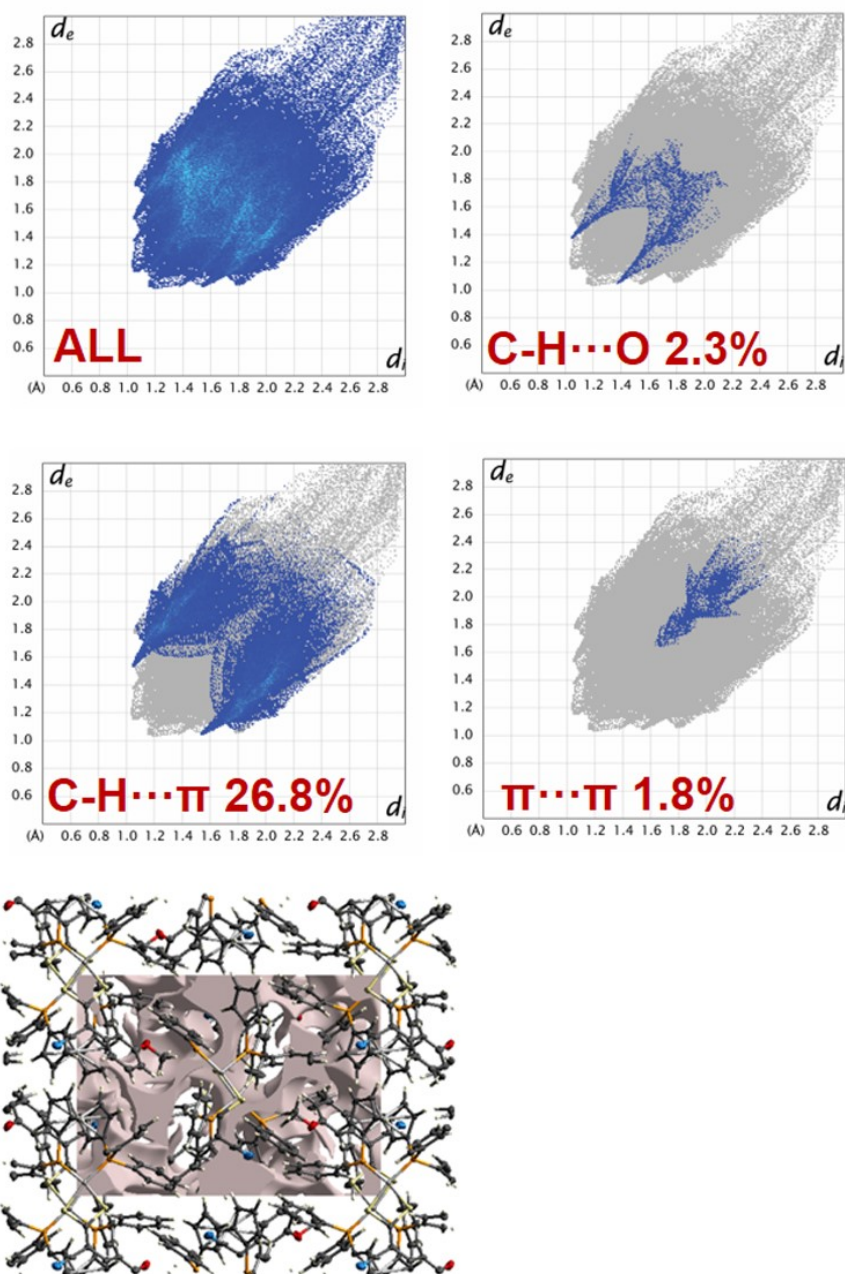
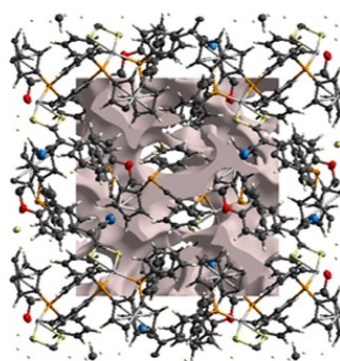
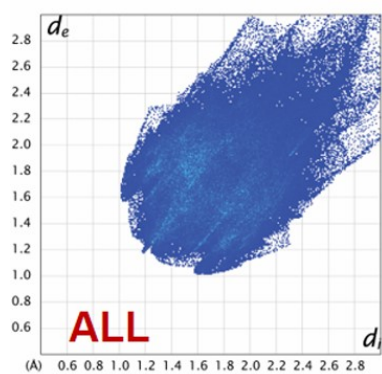


Fig. S1 Fingerprint plots for *o*-NiL.



Crystal Void

Fig. S2 Fingerprint plots for *m*-NiL.



Crystal Void

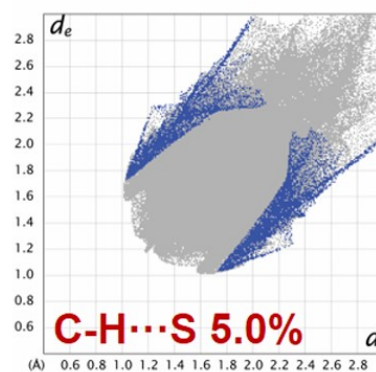
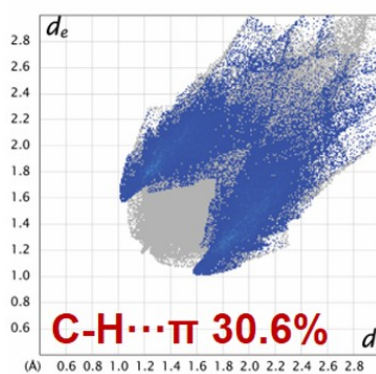


Fig. S3 Fingerprint plots for *p*-NiL.

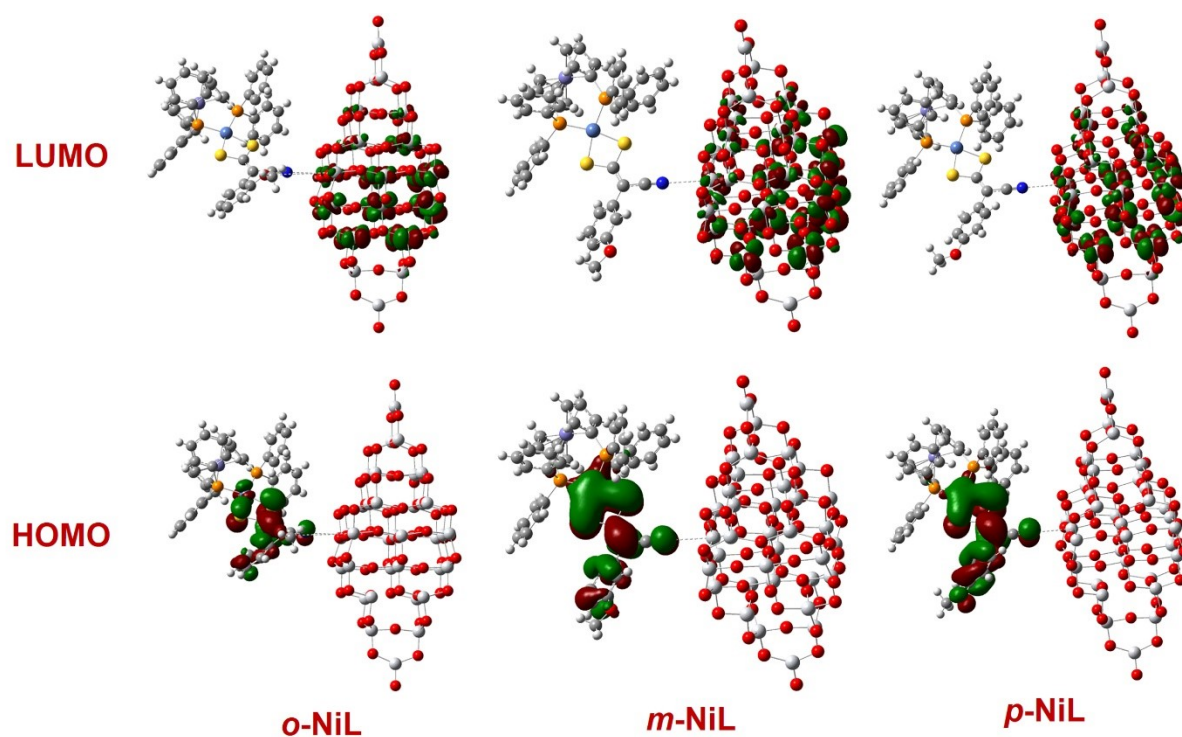


Fig. S4 HOMO-LUMO plots for *o*-NiL@TiO₂, *m*-NiL@TiO₂ and *p*-NiL@TiO₂.

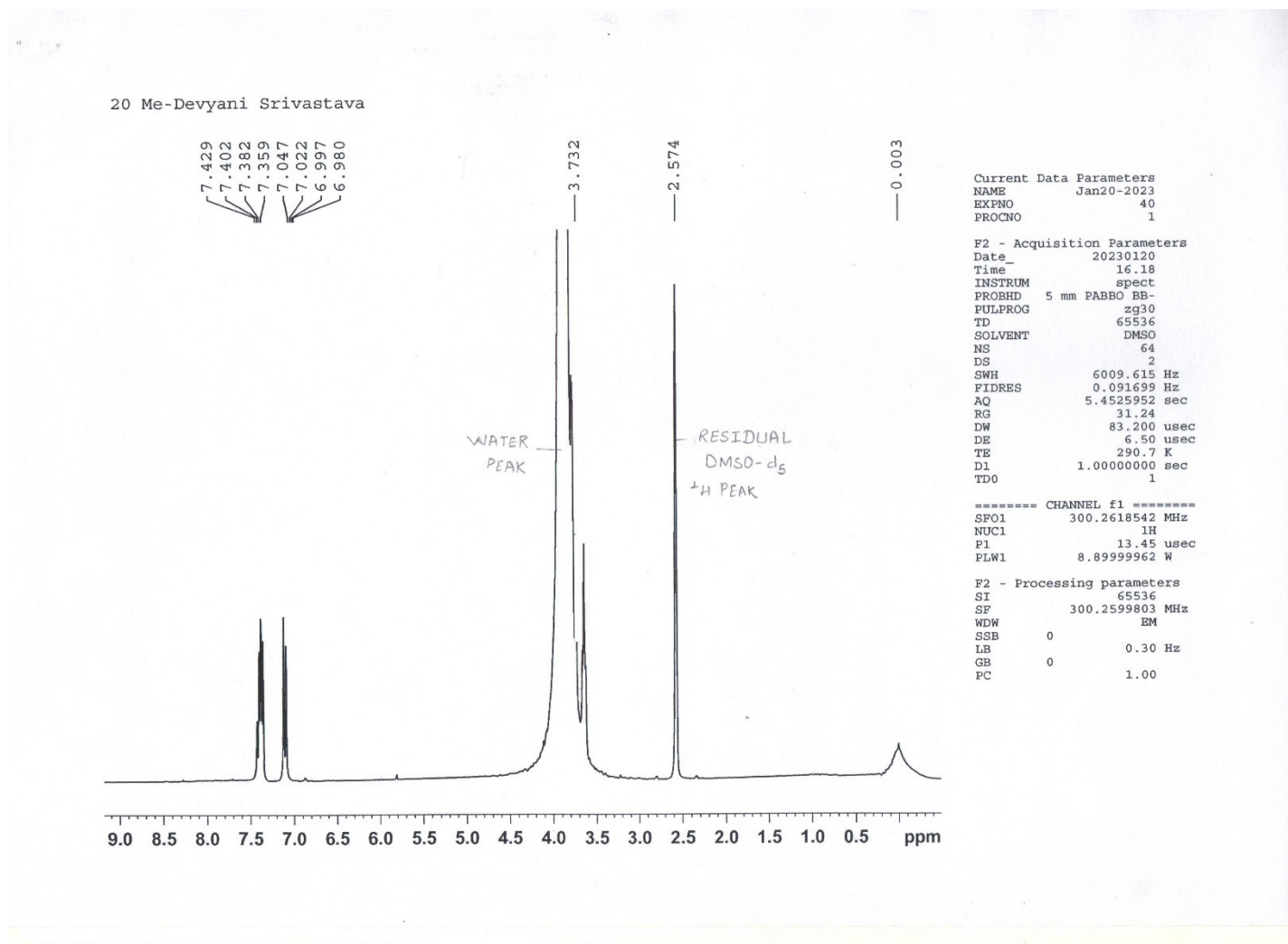


Fig. S5 1H NMR spectrum of *o*-L.

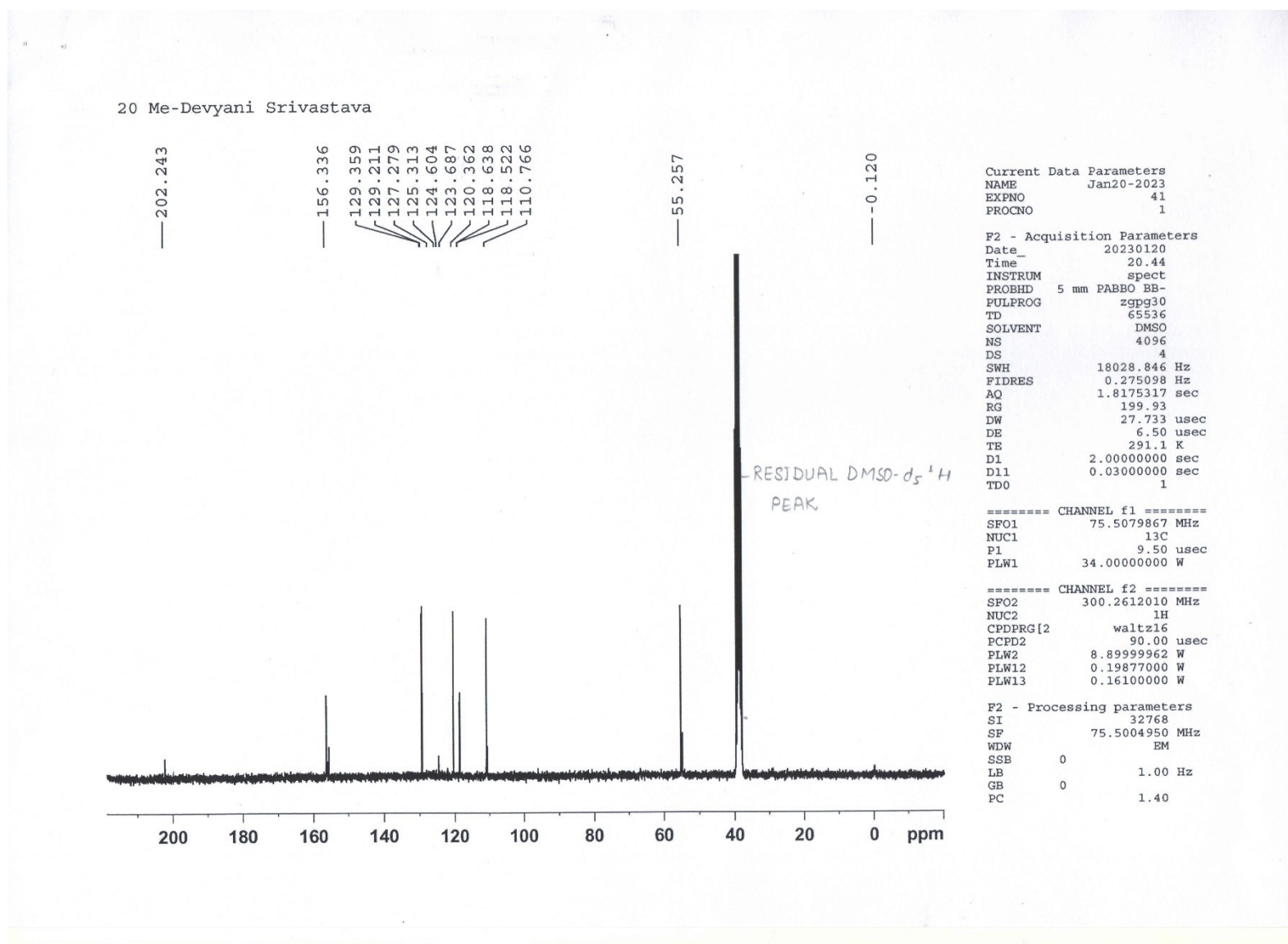


Fig. S6 ^{13}C NMR spectrum of *o*-L.

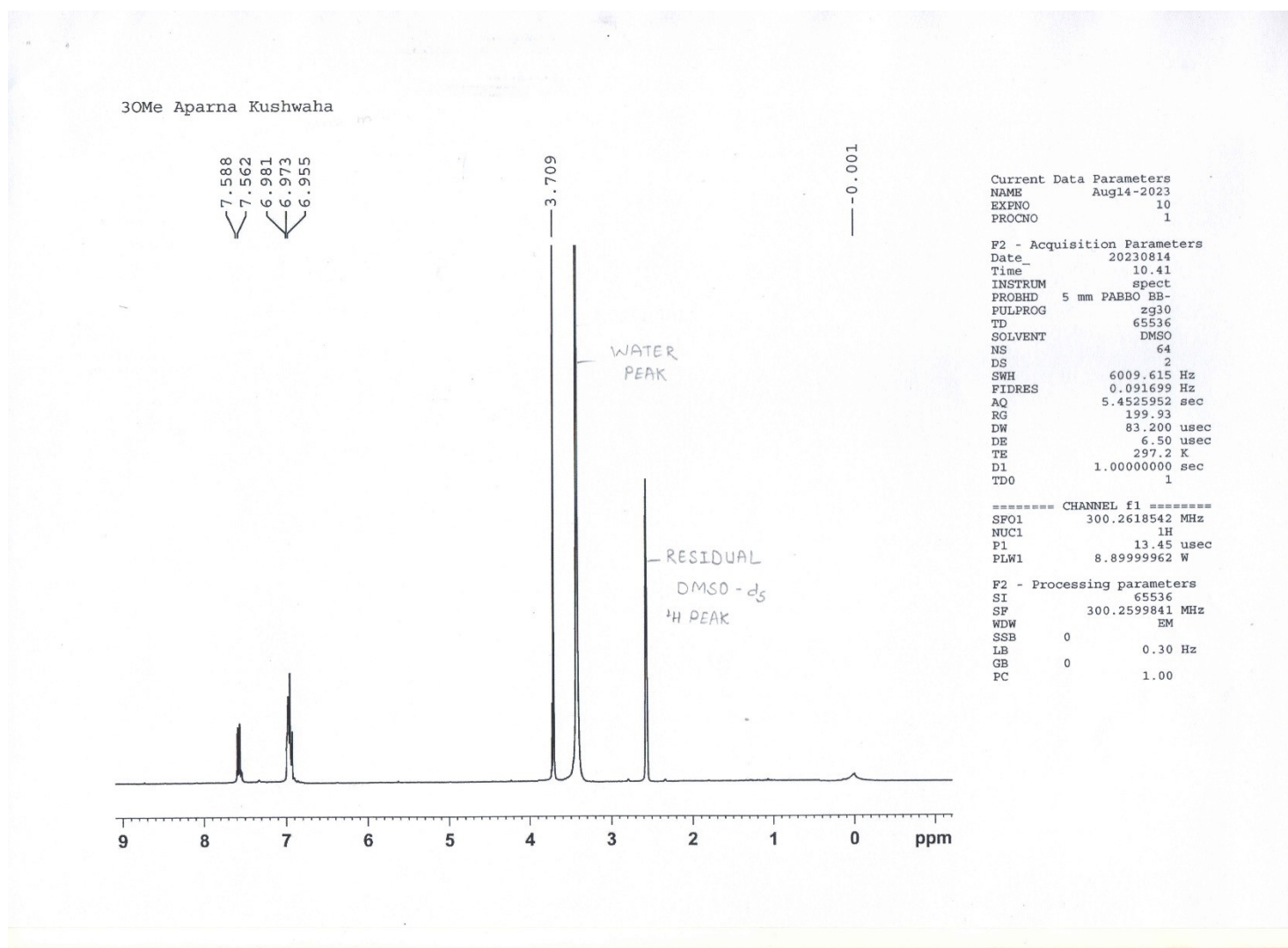


Fig. S7 ^1H NMR spectrum of *m*-L.

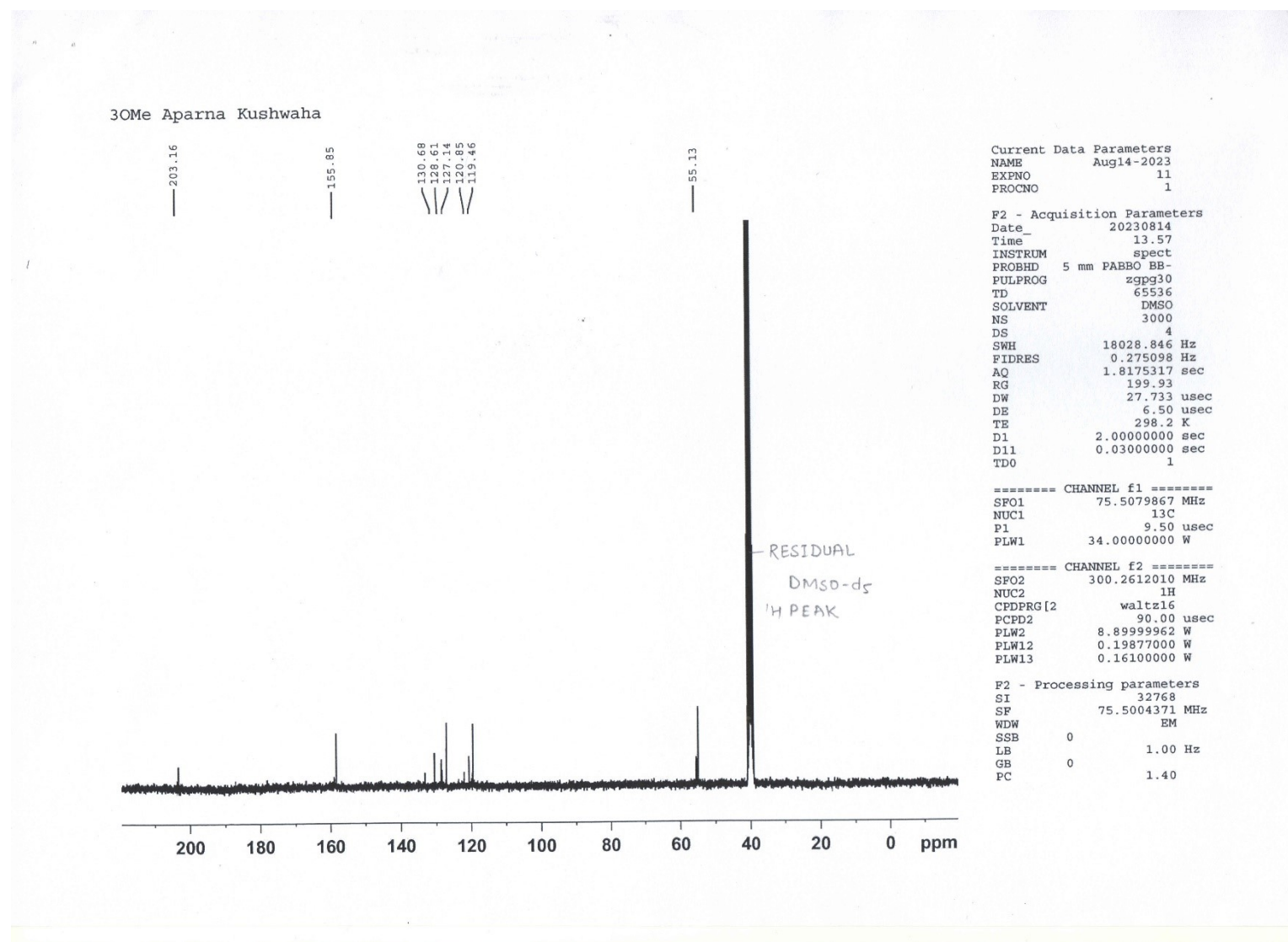


Fig. S8 ^{13}C NMR spectrum of *m*-L.

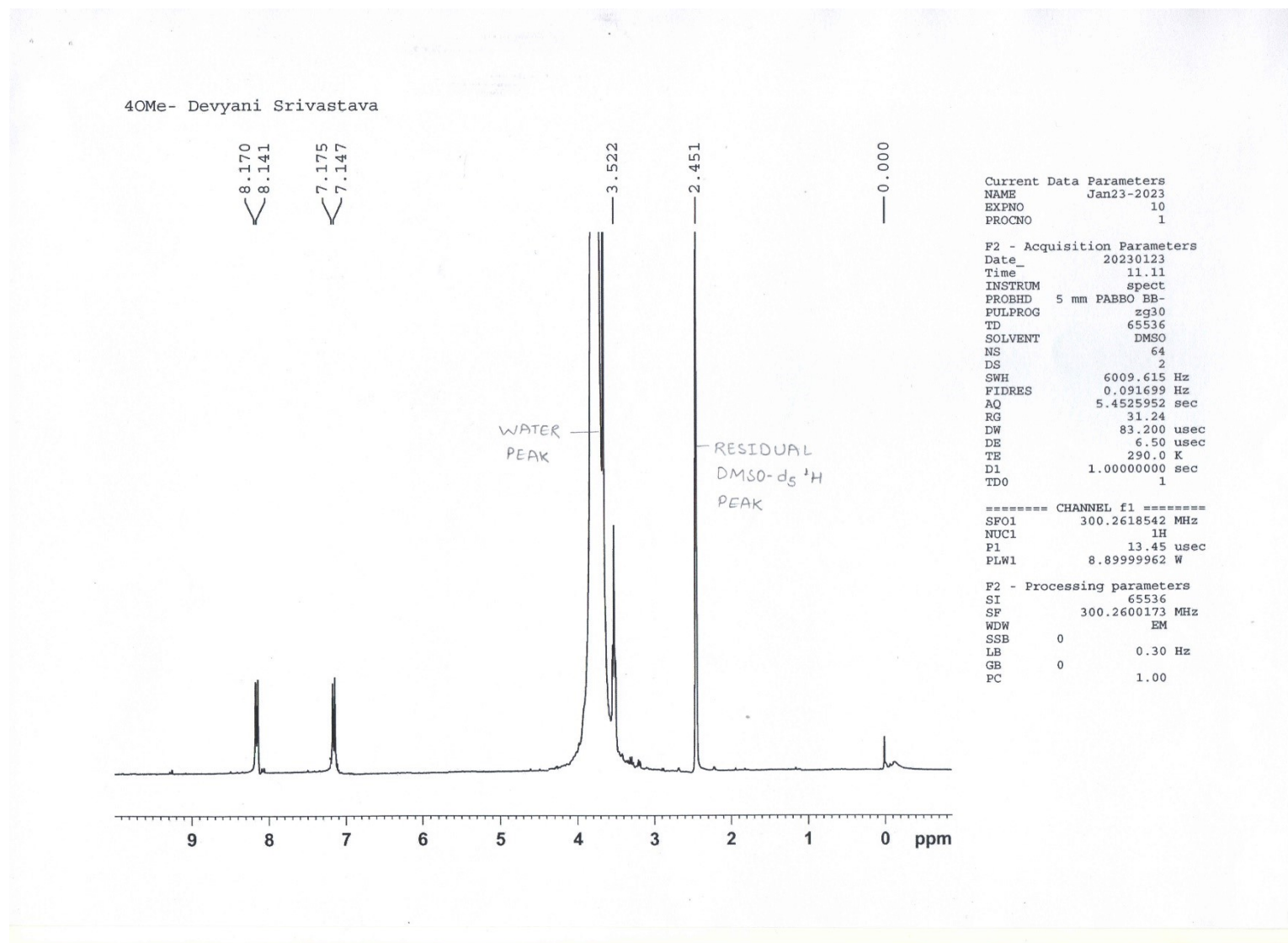


Fig. S9 ¹H NMR spectrum of *p*-L.

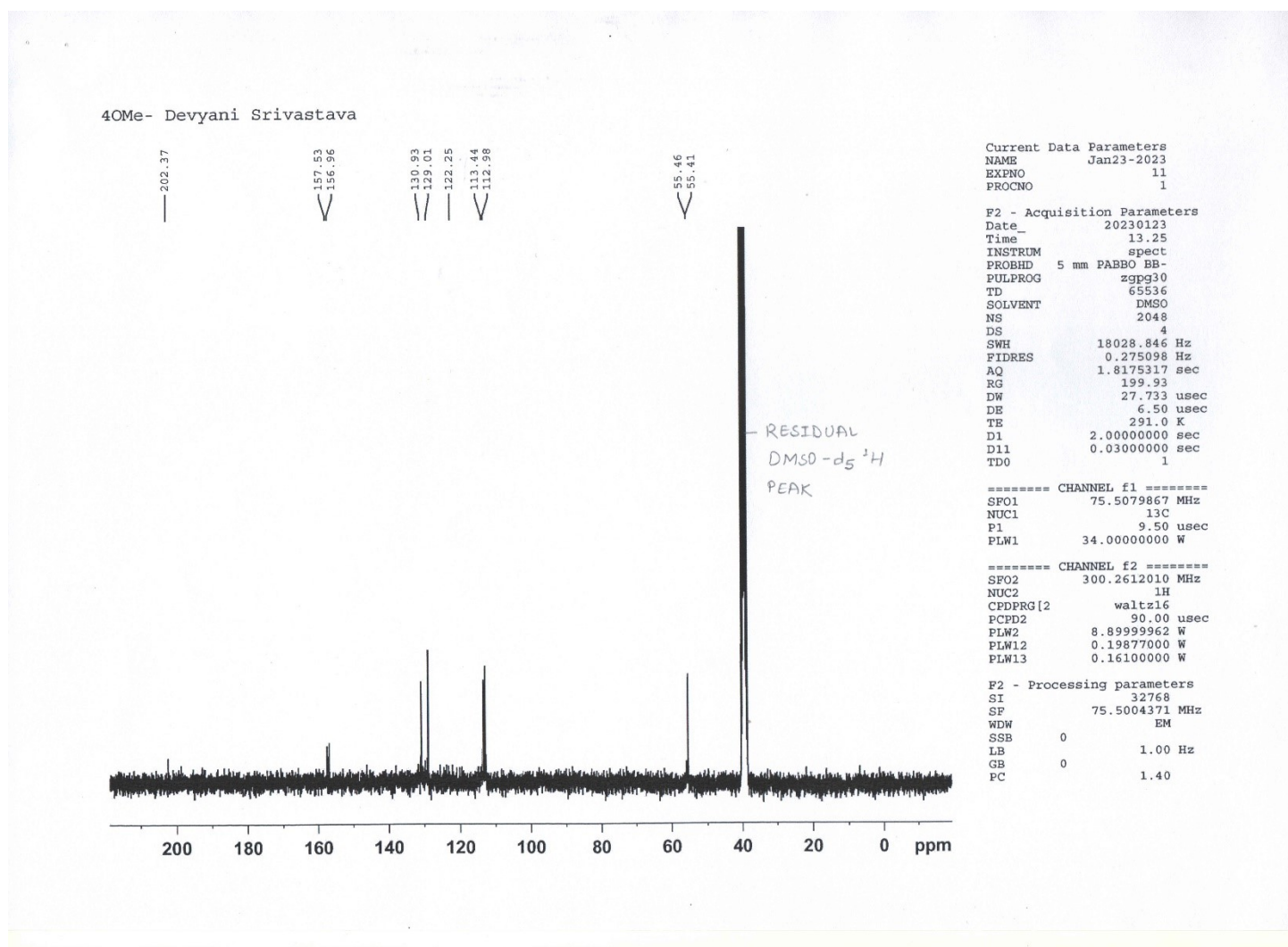


Fig. S10 ^{13}C NMR spectrum of *p*-L.

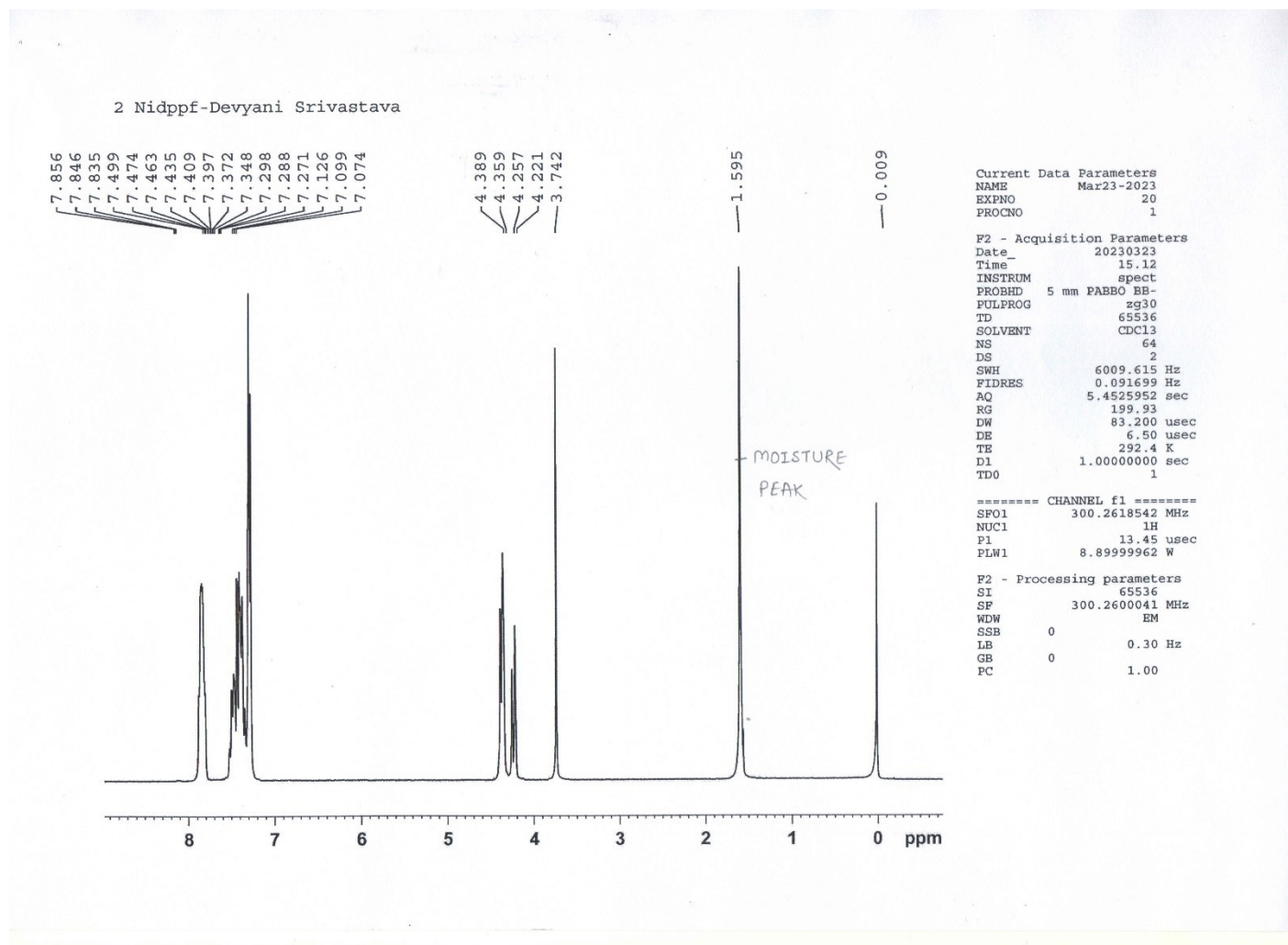
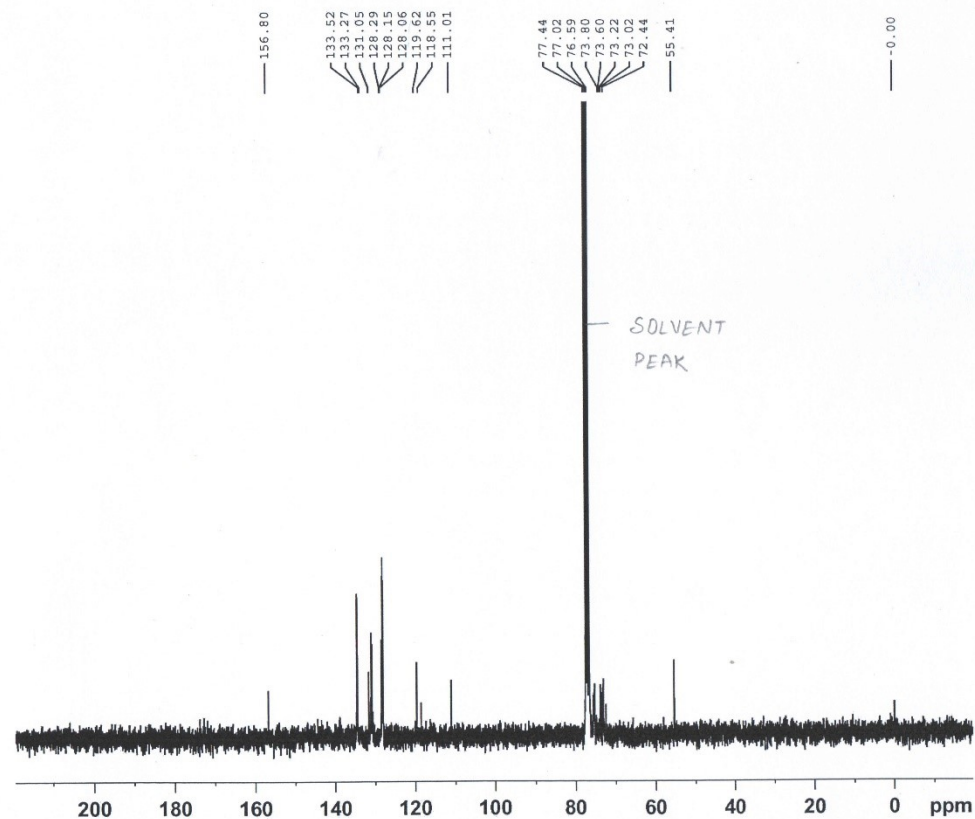


Fig. S11 ^1H NMR spectrum of *o*-NiL.

2 Nidppf-Devyani Srivastava



Current Data Parameters
 NAME Mar23-2023
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230323
 Time 18.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3072
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 199.93
 DW 27.733 usec
 DE 6.50 usec
 TE 293.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

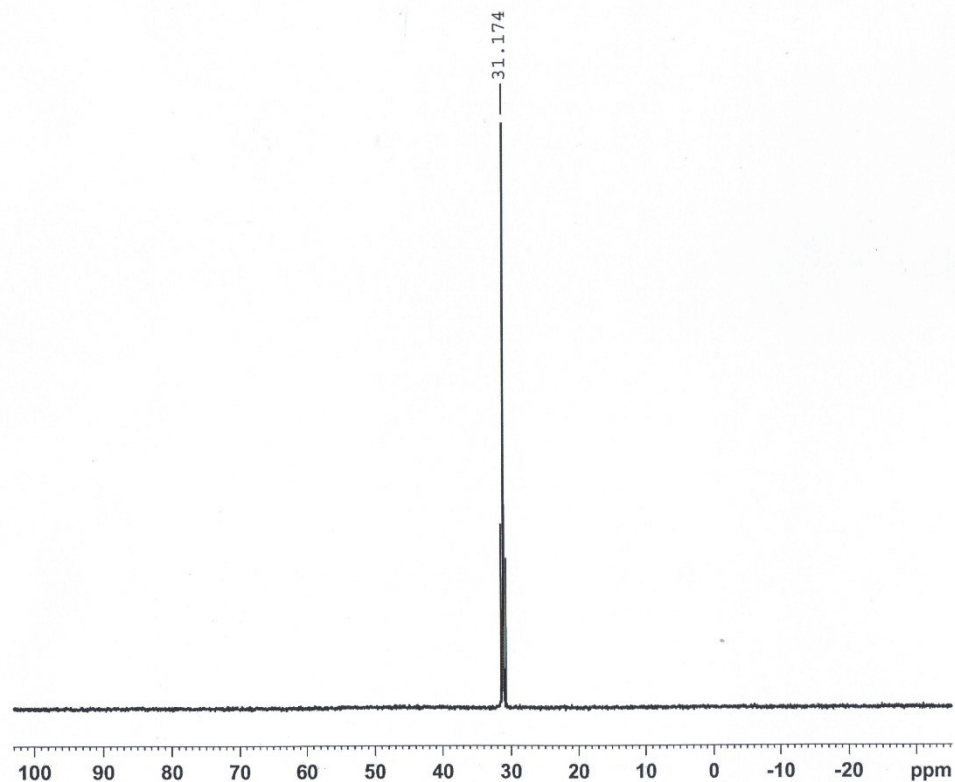
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 P1 9.50 usec
 PLW1 34.00000000 W

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 8.89999962 W
 PLW12 0.19877000 W
 PLW13 0.16100000 W

F2 - Processing parameters
 SI 32768
 SF 75.5004389 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Fig. S12 ^{13}C NMR spectrum of *o*-NiL.

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Current Data Parameters
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EXPNO     22
PROCNO    1

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PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        3000
DS        4
SWH       49019.609 Hz
FIDRES    0.747980 Hz
AQ        0.6684672 sec
RG        199.93
DW        10.200 usec
DE        6.50 usec
TE        293.9 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1      121.5413986 MHz
NUC1      31P
P1        12.00 usec
PLW1      12.00000000 W

===== CHANNEL f2 =====
SFO2      300.2612010 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      8.89999962 W
PLW12     0.19877000 W
PLW13     0.16100000 W

F2 - Processing parameters
SI        32768
SF        121.5474759 MHz
WDW       EM
SSB       0
LB        1.00 Hz
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PC        1.40
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Fig S13 ^{31}P NMR spectrum of *o*-NiL.

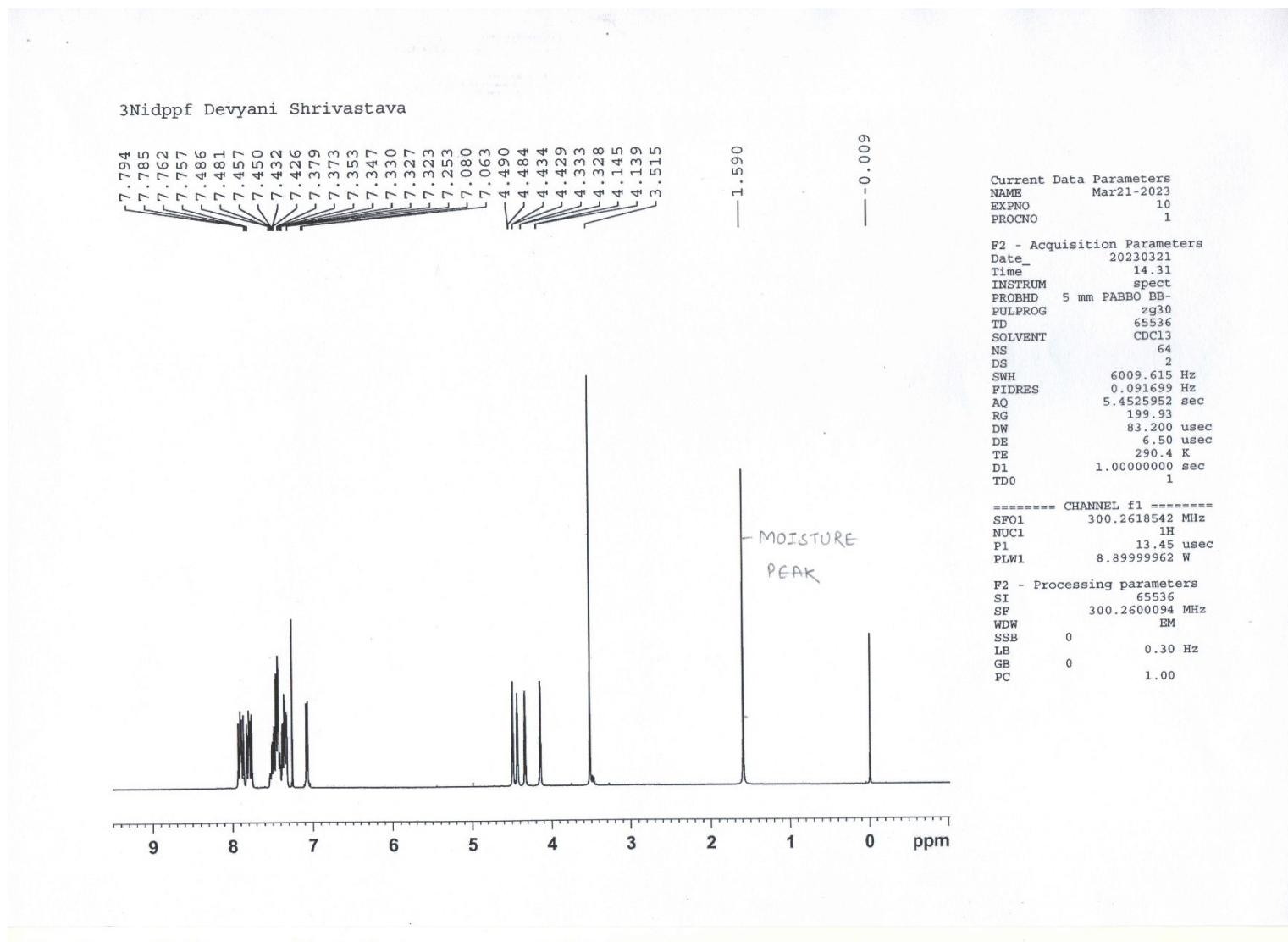


Fig. S14 ^1H NMR spectrum of *m*-NiL.

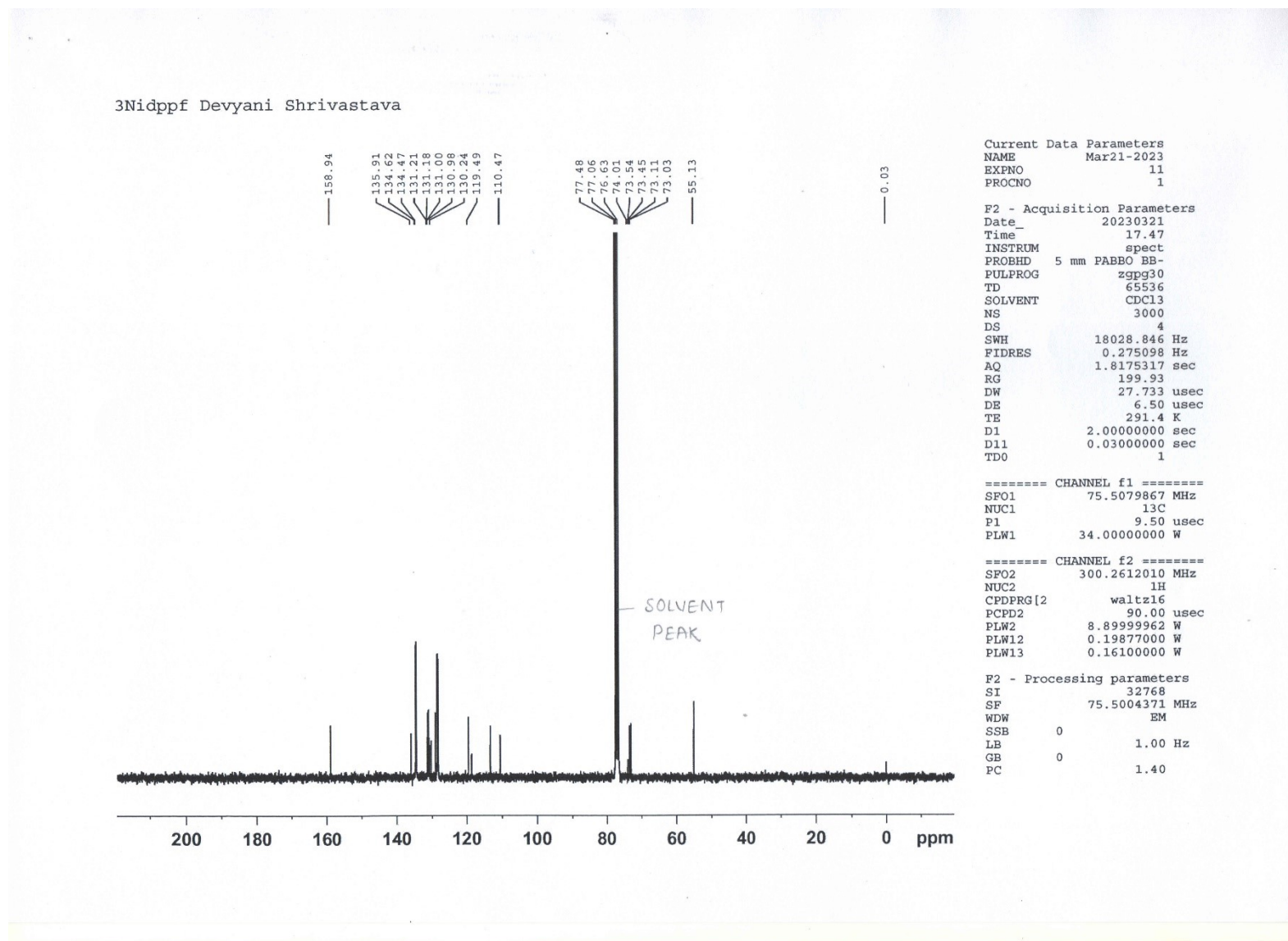
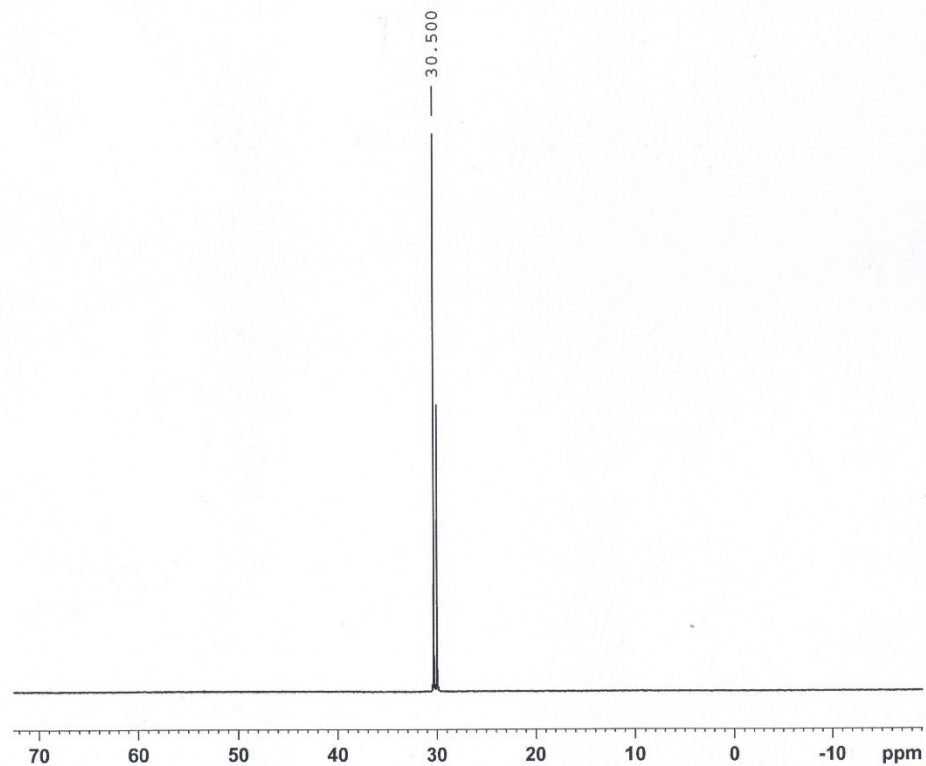


Fig. S15 ^{13}C NMR spectrum of *m*-NiL.

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Current Data Parameters
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PROCNO    1

F2 - Acquisition Parameters
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TD        65536
SOLVENT   CDCl3
NS        1024
DS         4
SWH       49019.609 Hz
FIDRES    0.747980 Hz
AQ        0.6684672 sec
RG        199.93
DW        10.200 usec
DE        6.50 usec
TE        291.3 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
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NUC1      31P
P1        12.00 usec
PLW1     12.00000000 W

===== CHANNEL f2 =====
SFO2     300.2612010 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2     8.89999962 W
PLW12    0.19877000 W
PLW13    0.16100000 W

F2 - Processing parameters
SI        32768
SF        121.5474759 MHz
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SSB       0
LB        1.00 Hz
GB        0
PC        1.40
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Fig. S16 ^{31}P NMR spectrum of *m*-NiL.

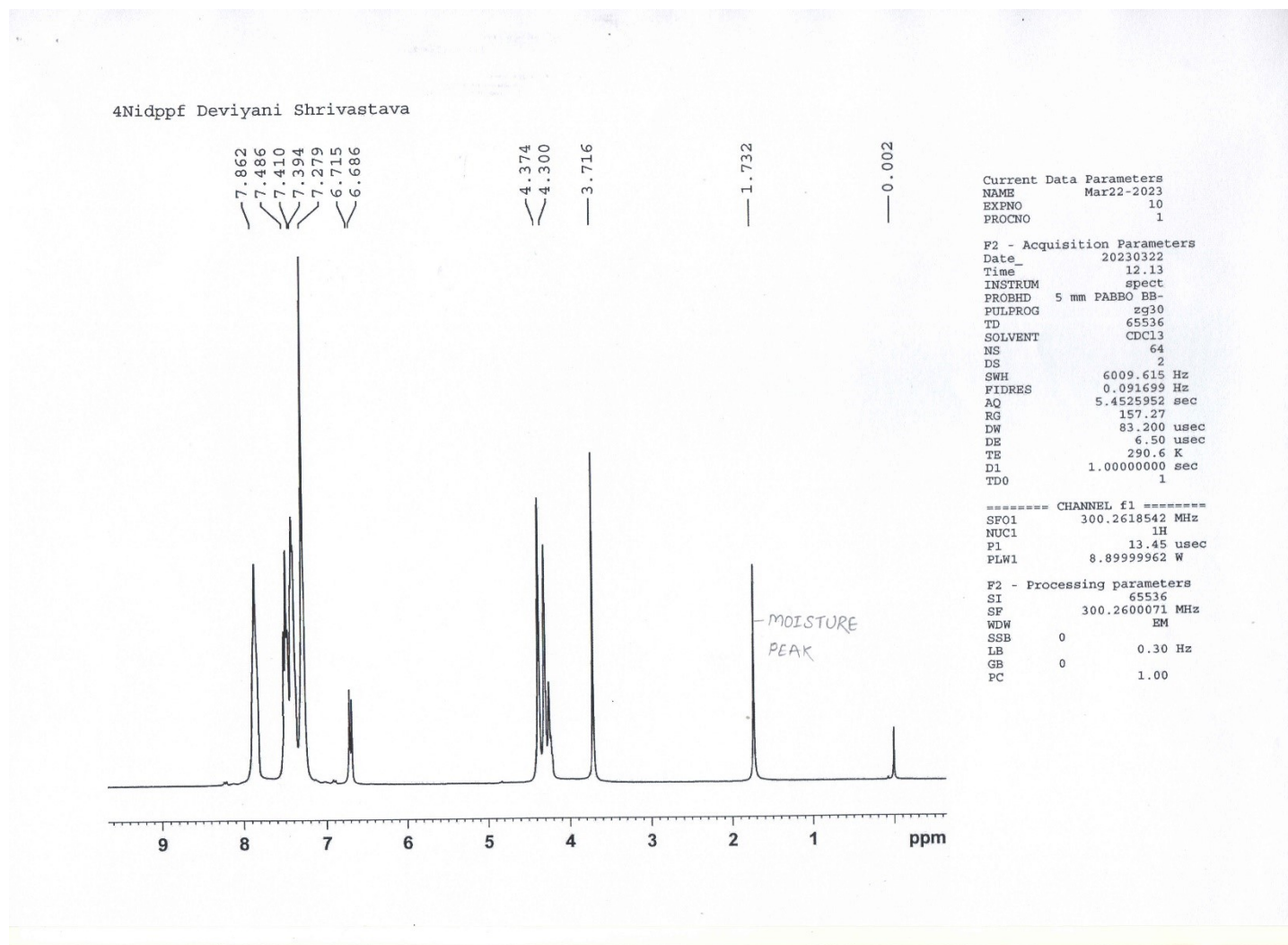


Fig. S17 ^1H NMR spectrum of *p*-NiL.

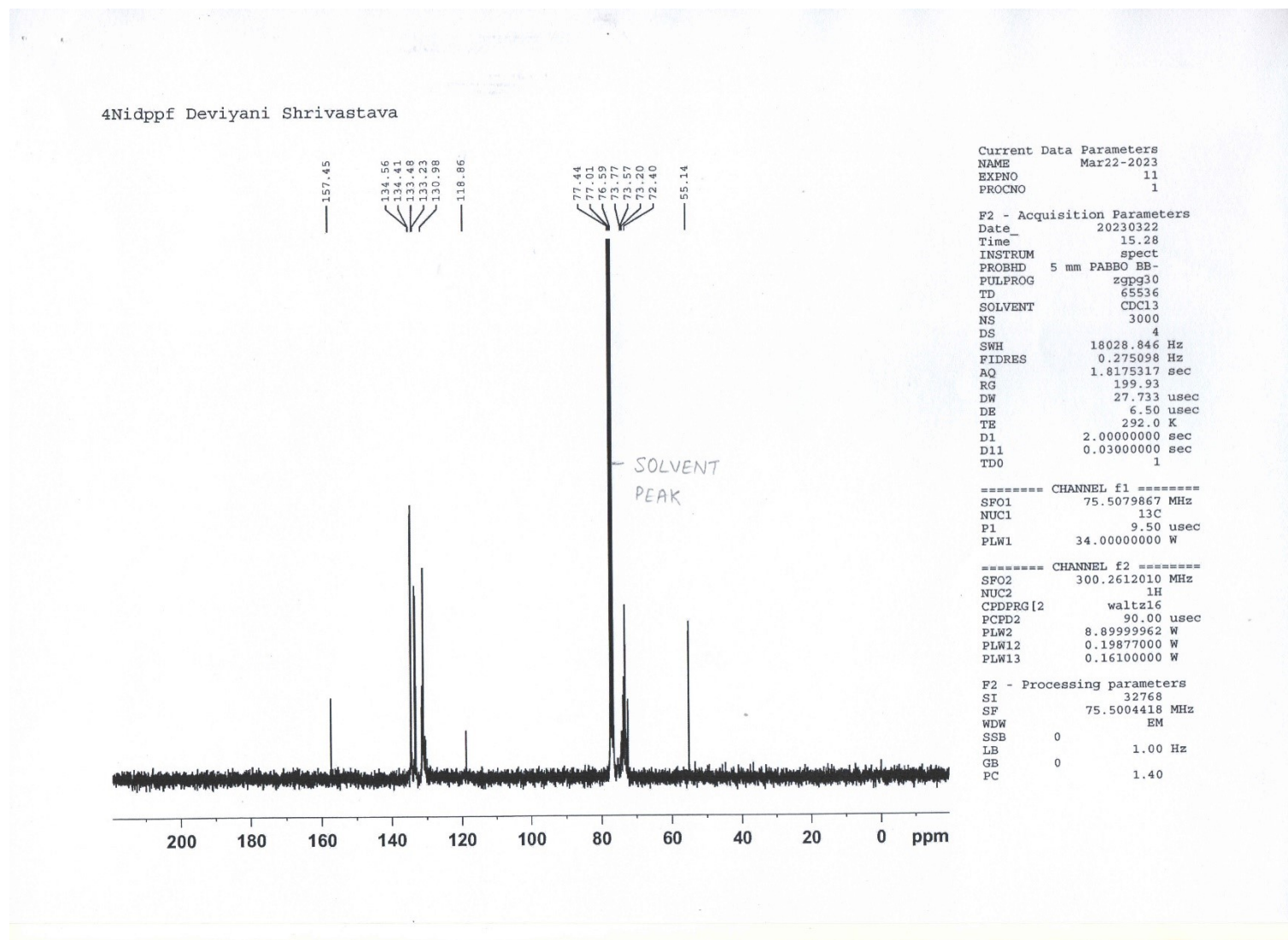


Fig. S18 ^{13}C NMR spectrum of *p*-NiL.

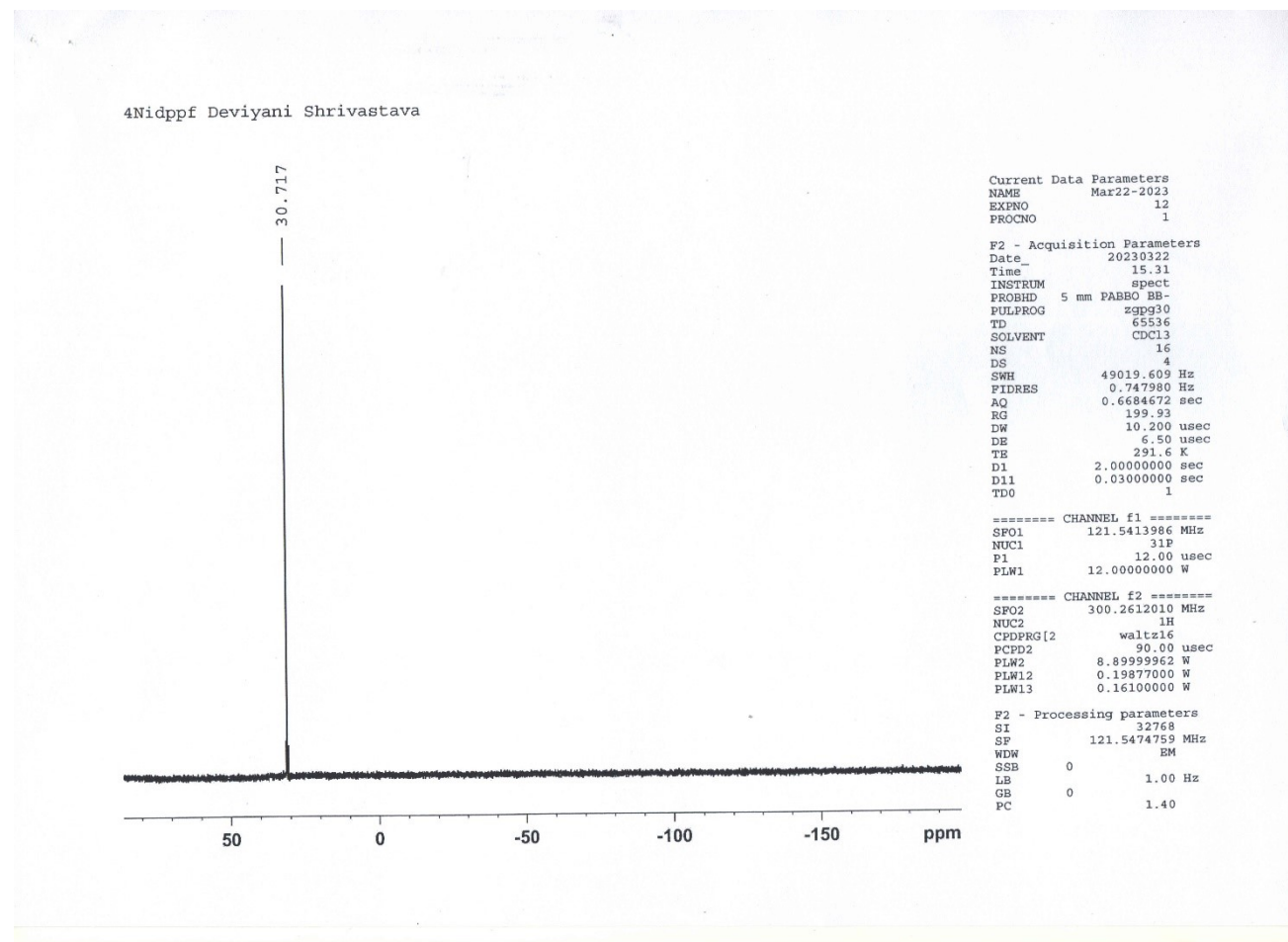


Fig. S19 ^{31}P NMR spectrum of *p*-NiL.