

Pyrrolo[3,2-*e*][1,4]diazepin-2-one Supported Synthesis

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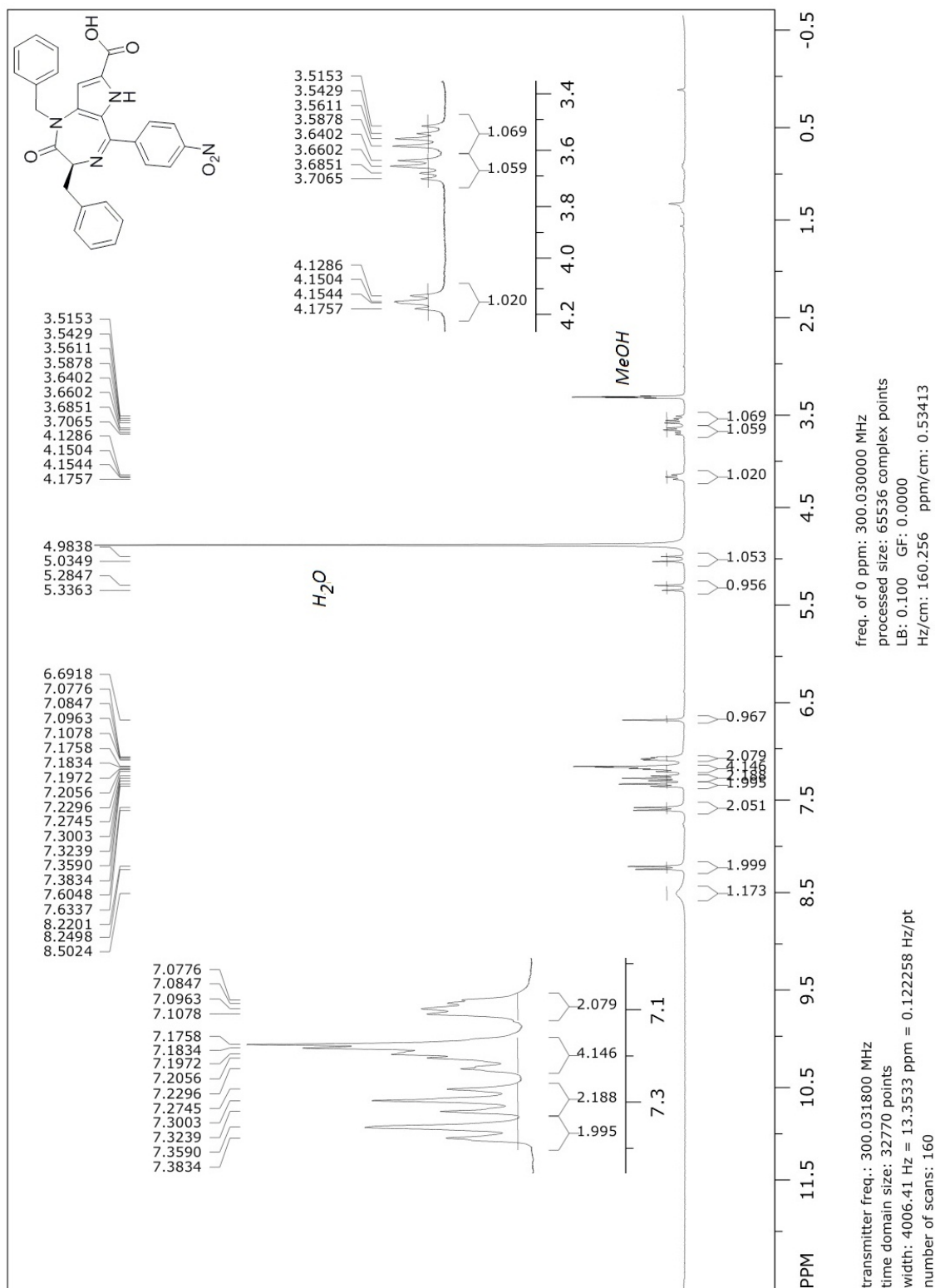
¹H NMR and ¹³C NMR spectra were recorded on 300, 400 and 500 MHz spectrometers with chemical shift values in ppm relative to residual chloroform (δ_{H} 7.26 & δ_{C} 77.2), acetone (δ_{H} 2.05 & δ_{C} 29.84), or DMSO (δ_{H} 2.50 & δ_{C} 39.52) as standards. Coupling constant *J* values are given in Hz, with splitting described as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet).

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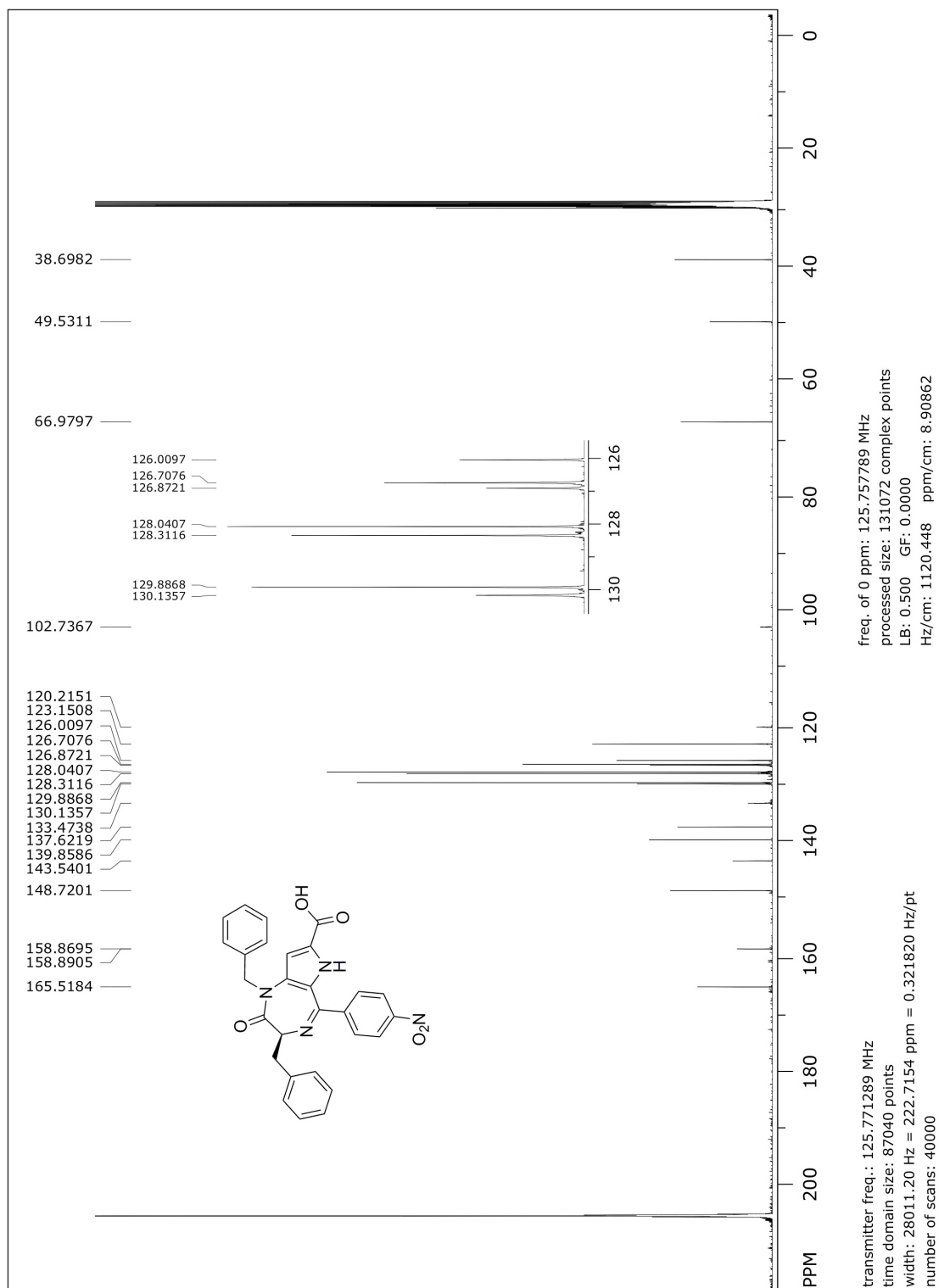
RMN ¹ H (300 MHz, CD ₃ OD): (<i>S</i>)-1,3-Dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2- <i>e</i>][1,4]diazepine-7-carboxylic acid 46.....	3
RMN ¹³ C [125 MHz, (CD ₃) ₂ CO]: (<i>S</i>)-1,3-Dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2- <i>e</i>][1,4]diazepine-7-carboxylic acid 46.....	4

RMN ^1H (400 MHz, CDCl_3): (<i>S</i>)-Methyl 1,3-dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2- <i>e</i>][1,4]diazepine-7-carboxylate 53.....	5
RMN ^{13}C (125 MHz, CDCl_3): (<i>S</i>)-Methyl 1,3-dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2- <i>e</i>][1,4]diazepine-7-carboxylate 53.....	6
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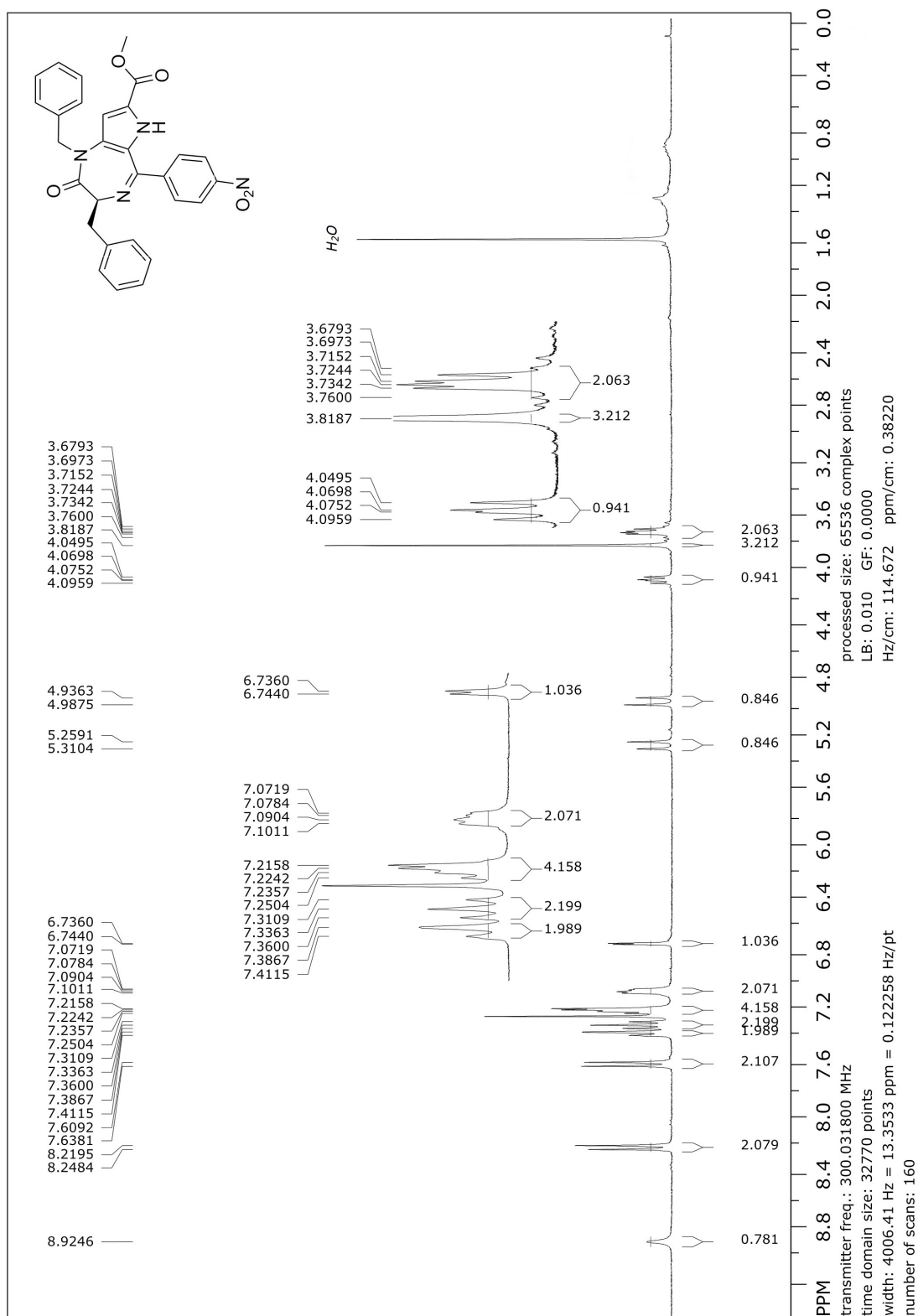
RMN ^1H (300 MHz, CD_3OD): (S)-1,3-Dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2-e][1,4]diazepine-7-carboxylic acid 46.



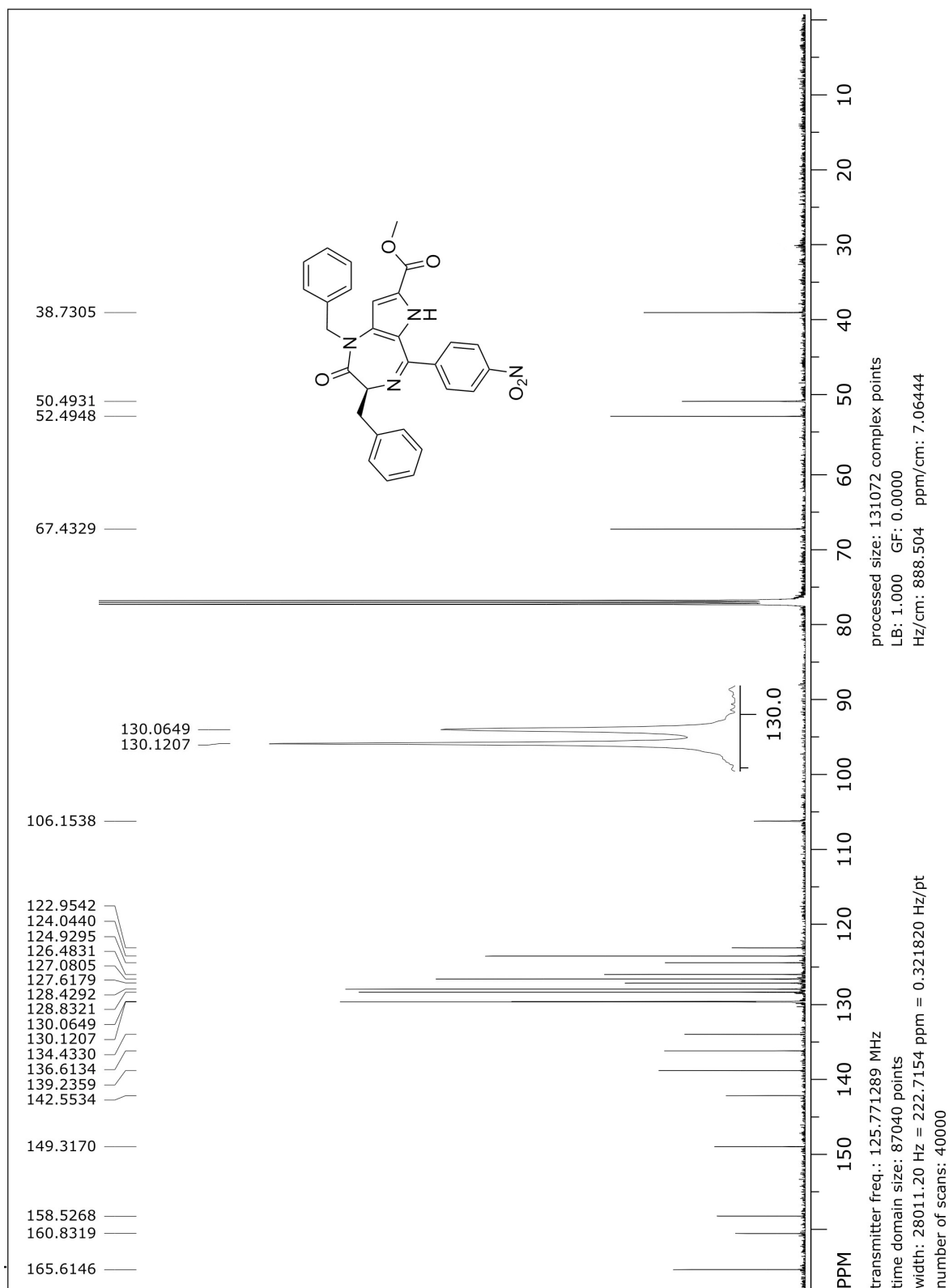
RMN ^{13}C [125 MHz, $(\text{CD}_3)_2\text{CO}$]: (S)-1,3-Dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2-e][1,4]diazepine-7-carboxylic acid 46.



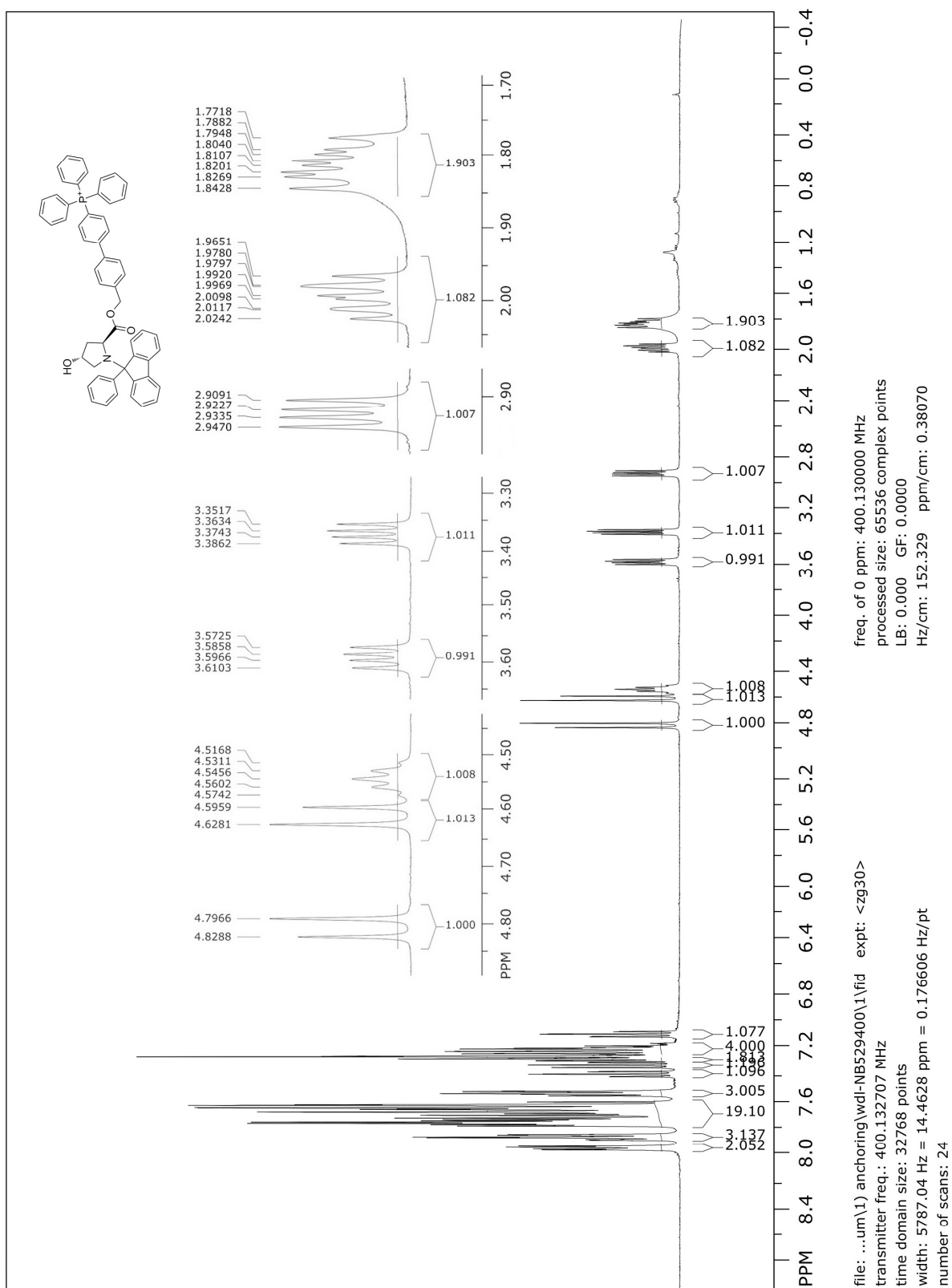
RMN ^1H (400 MHz, CDCl_3): (S)-Methyl 1,3-dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2-e][1,4]diazepine-7-carboxylate 53.

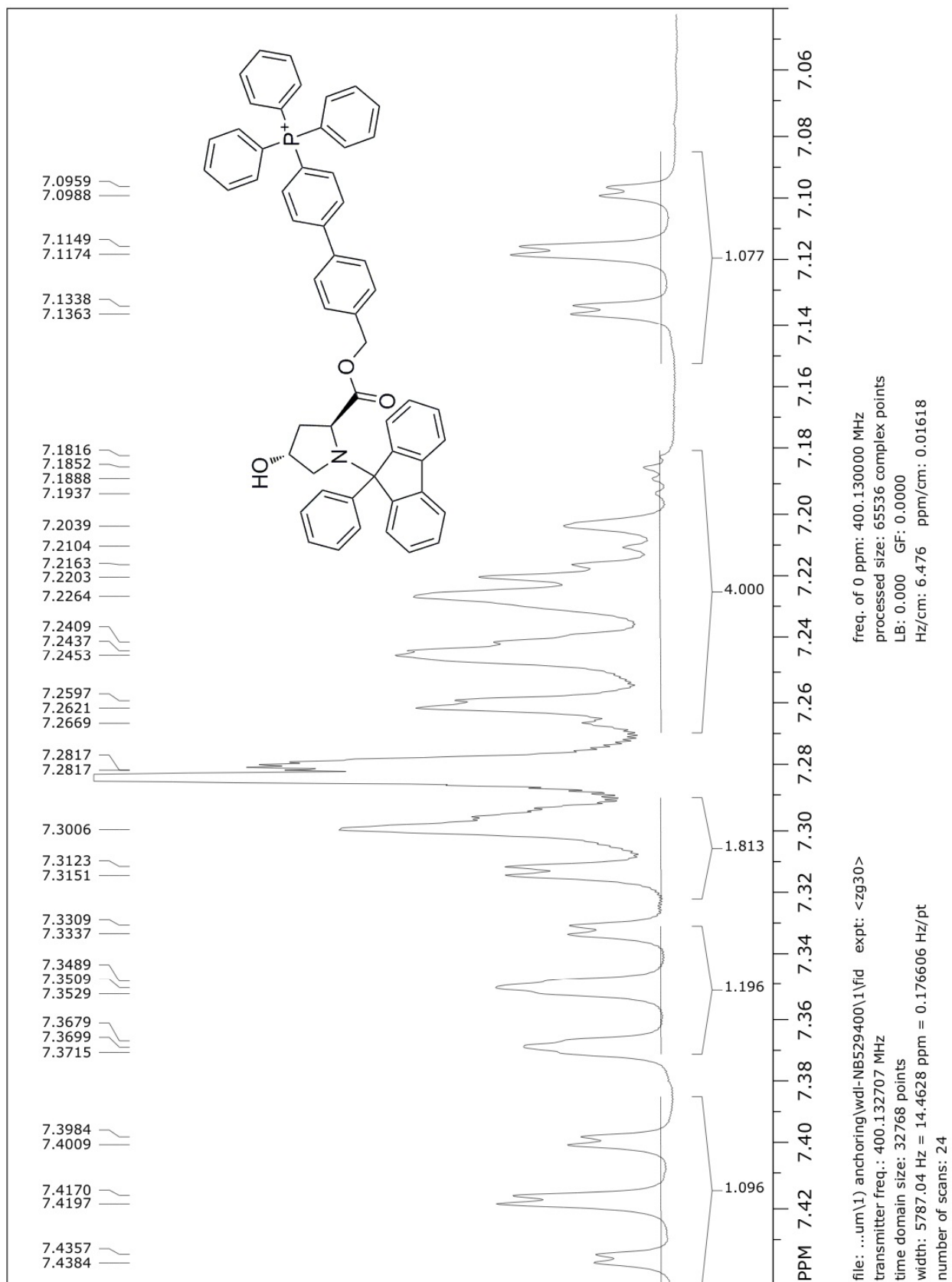


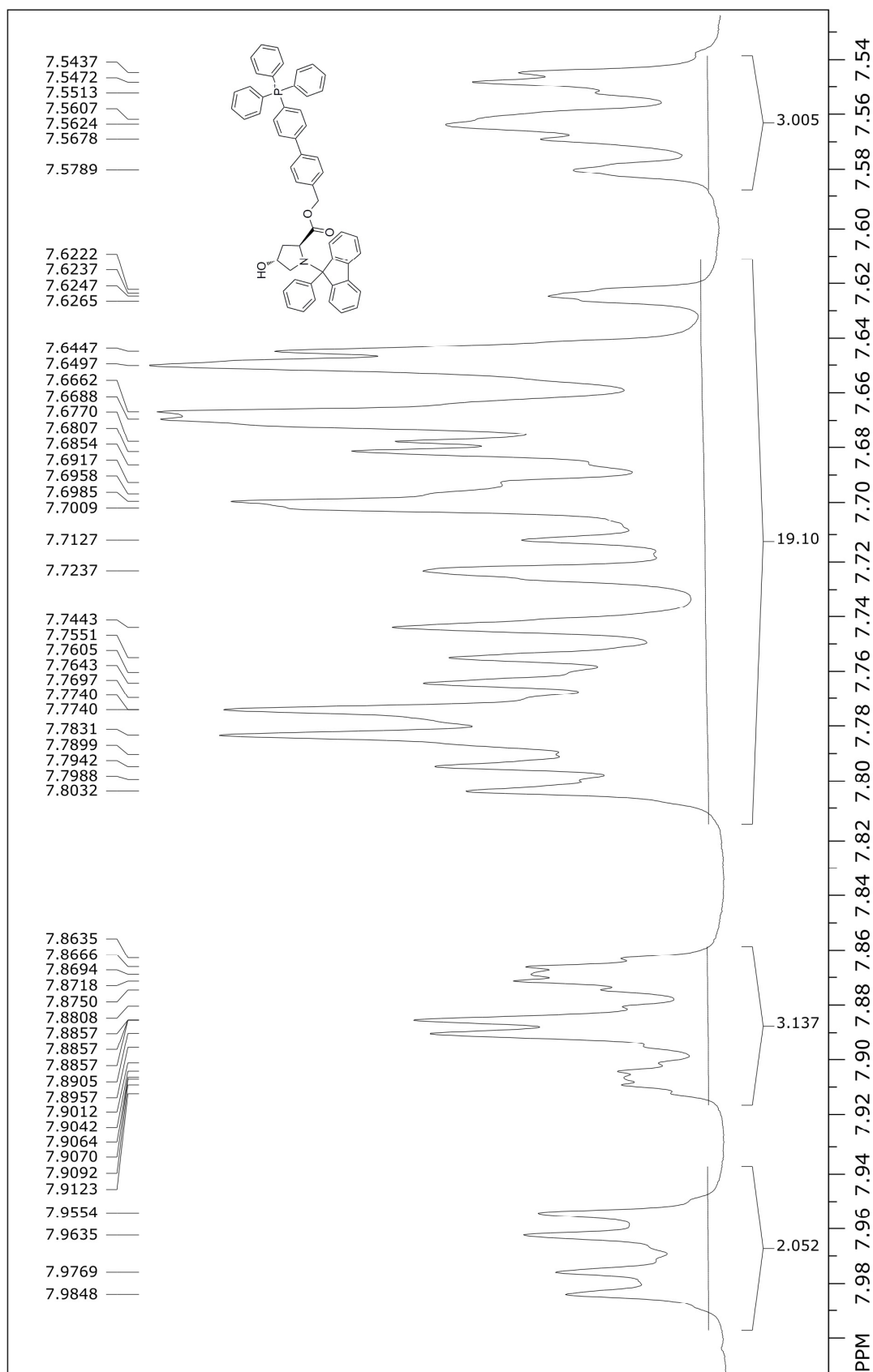
RMN ^{13}C (125 MHz, CDCl_3): (S)-Methyl 1,3-dibenzyl-5-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrrolo[3,2-e][1,4]diazepine-7-carboxylate **53.**



RMN ^1H (400 MHz, CDCl_3): (2S,4R)-4-Hydroxy-N-(PhF)proline TAP 19.



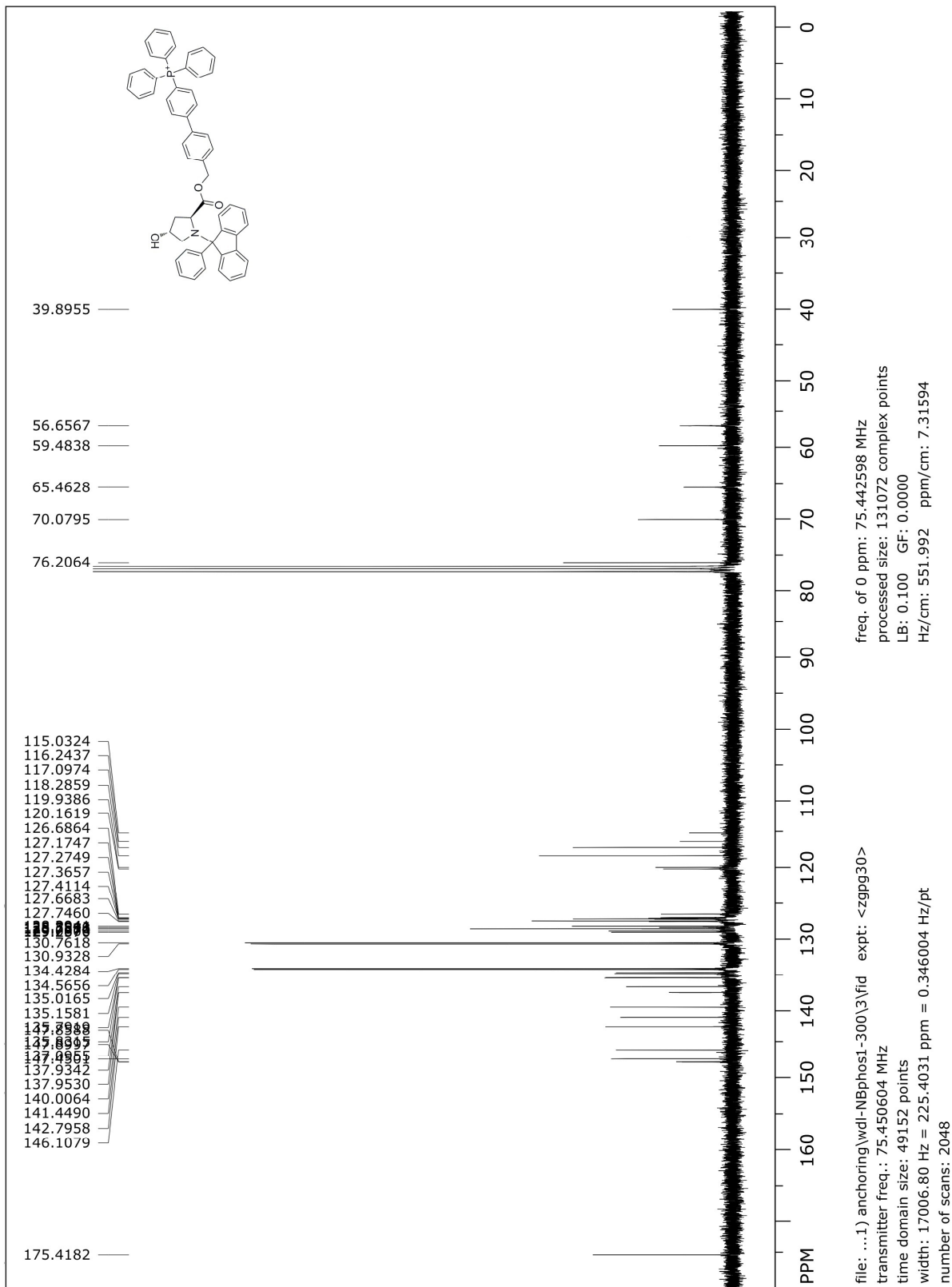


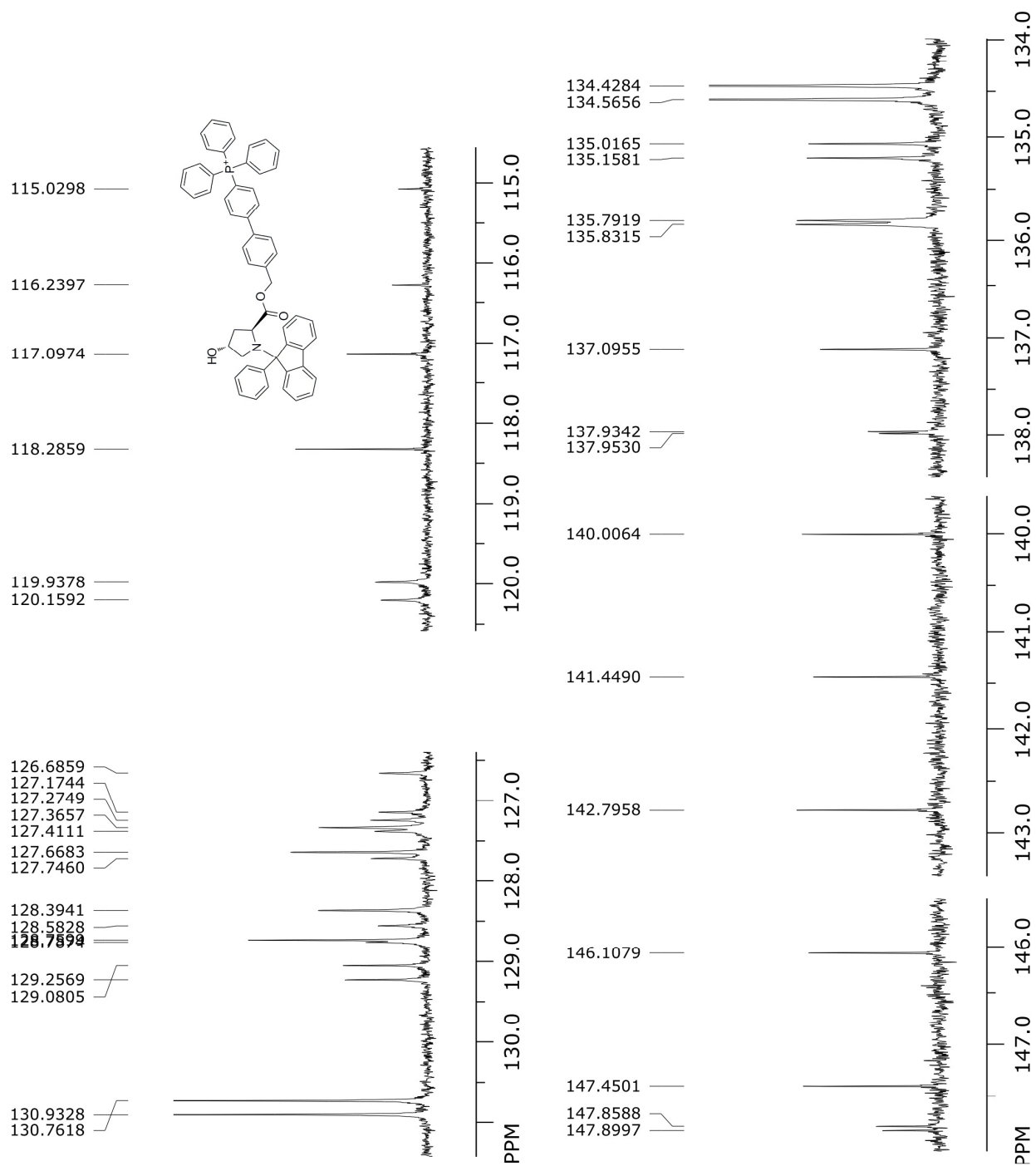


freq. of 0 ppm: 400.130000 MHz
 processed size: 65536 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 7.859 ppm/cm: 0.01964

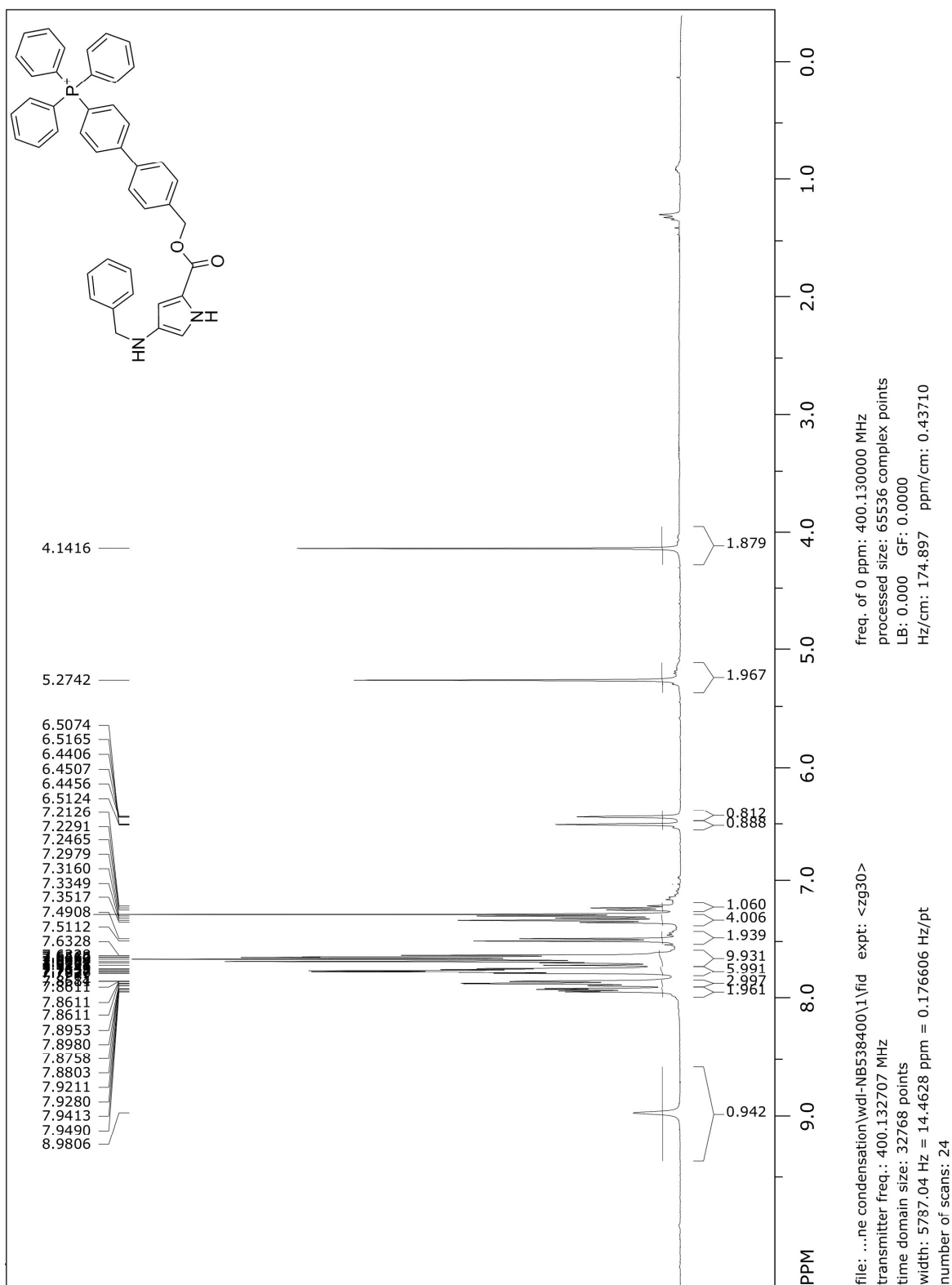
file: ...um\1) anchoring wdl-NB529400\1\fid expt: <zg30>
 transmitter freq.: 400.132707 MHz
 time domain size: 32768 points
 width: 5787.04 Hz = 14.4628 ppm = 0.176606 Hz/pt
 number of scans: 24

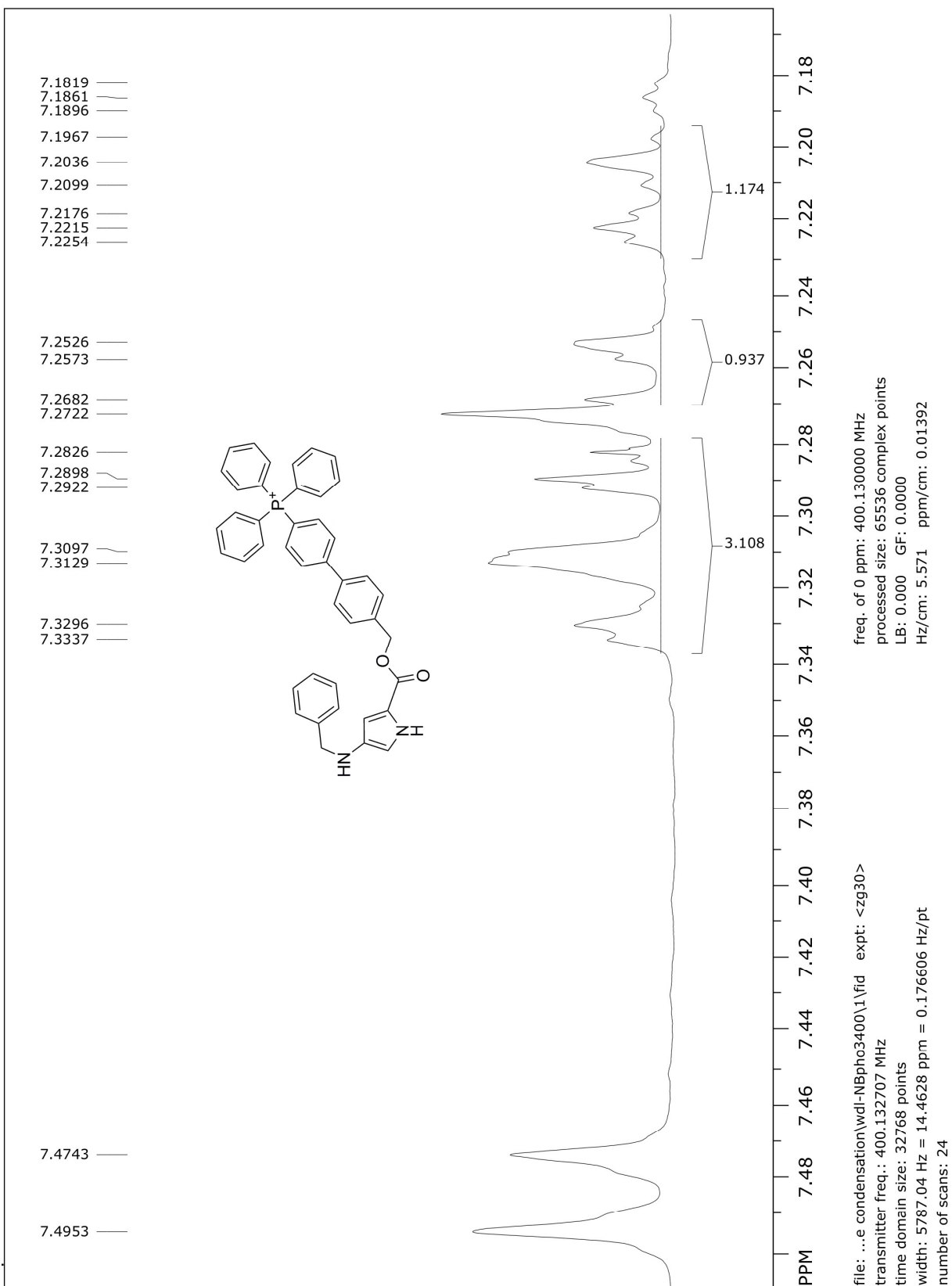
RMN ¹³C (75 MHz, CDCl₃): (2*S*,4*R*)-4-Hydroxy-*N*-(PhF)proline TAP 19.

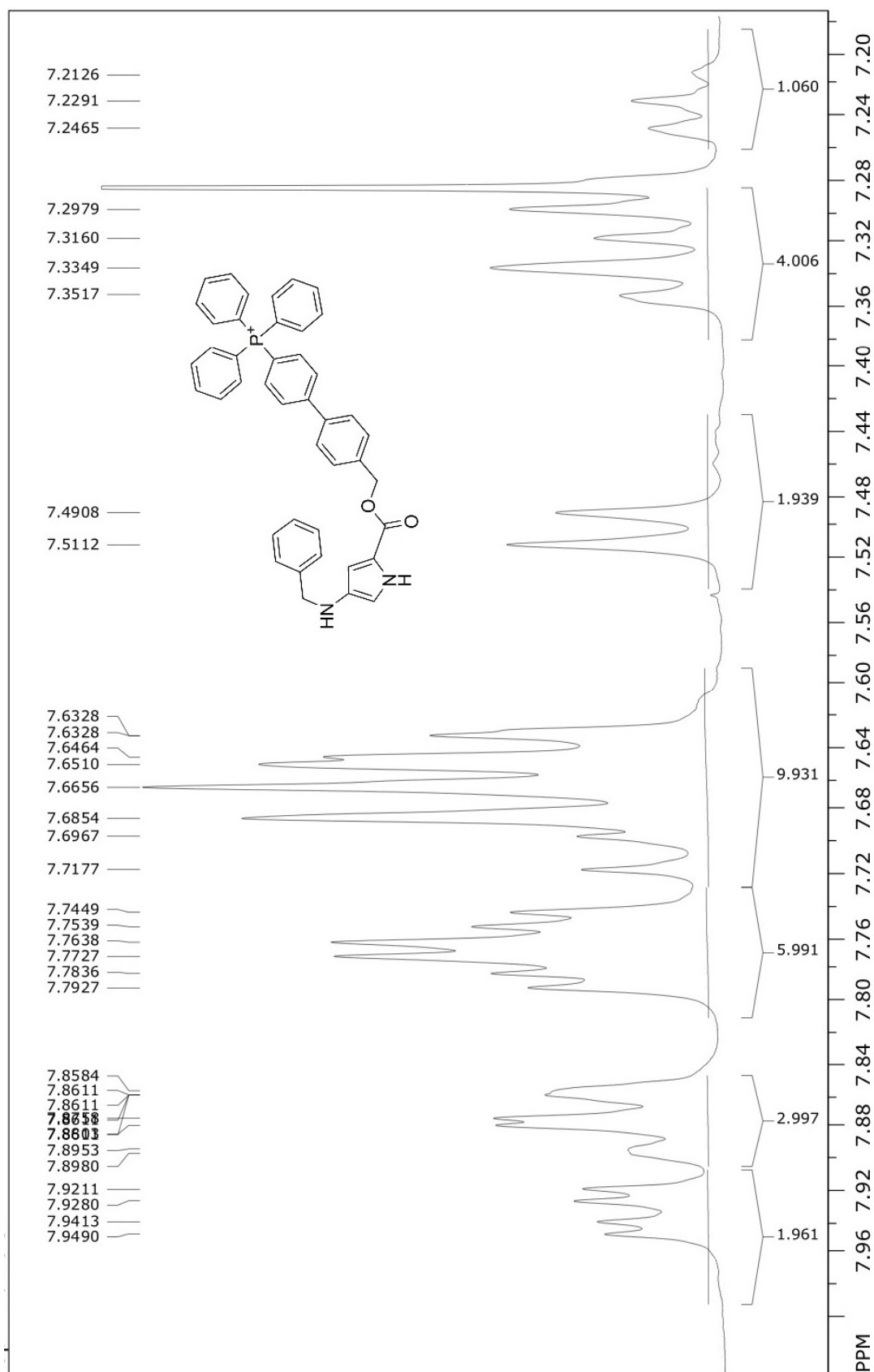




RMN ^1H (400 MHz, CDCl_3): 4-Benzylamino-1H-pyrrole-2-carboxylate
TAP 25.



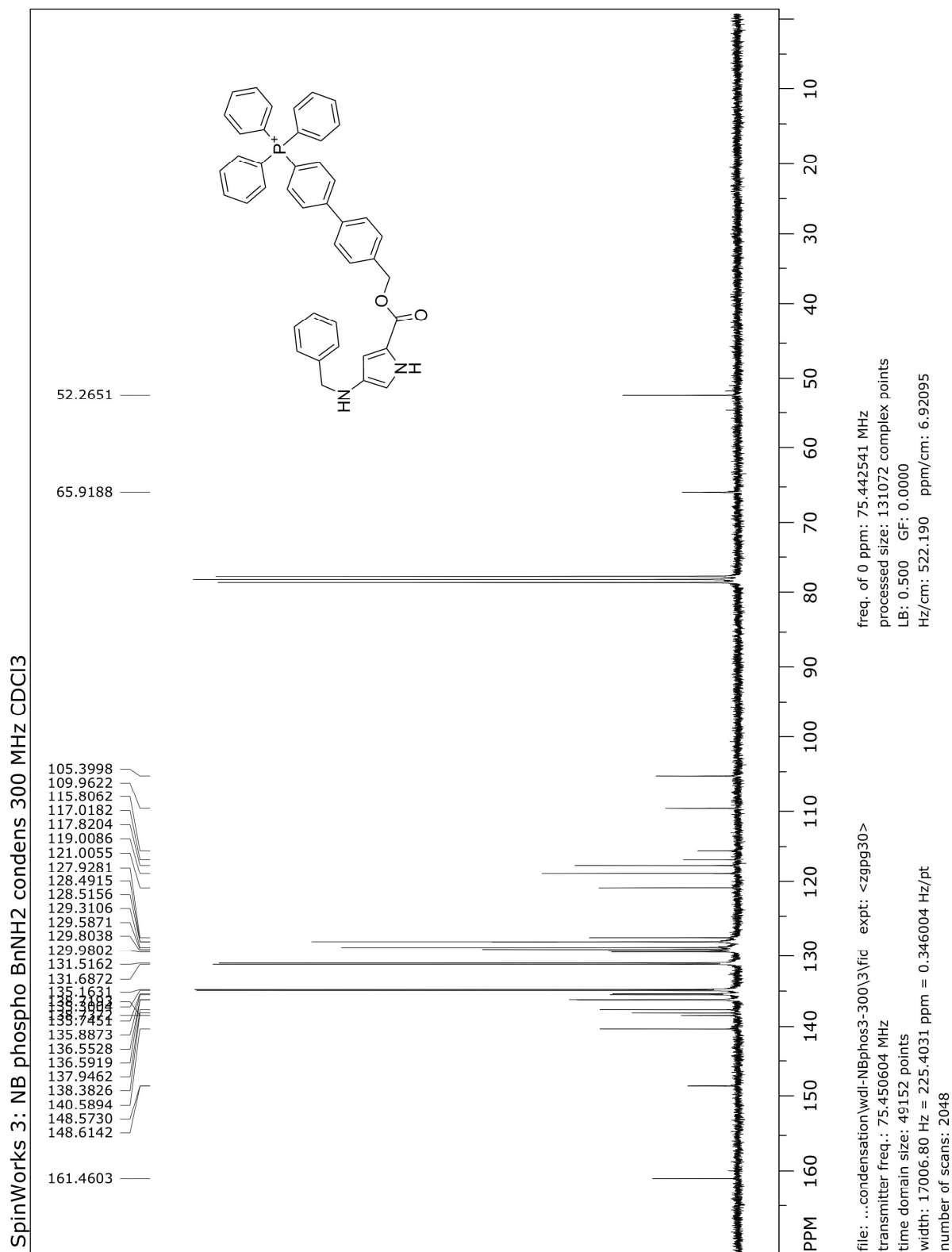




file: ...ne condensation\wdl-NB538400\1\fid expt: <zg30>
 transmitter freq.: 400.132707 MHz
 time domain size: 32768 points
 width: 5787.04 Hz = 14.4628 ppm = 0.176606 Hz/pt
 number of scans: 24

freq. of 0 ppm: 400.130000 MHz
 processed size: 65536 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 13.832 ppm/cm: 0.03457

**RMN ^{13}C (75 MHz, CDCl_3): 4-Benzylamino-1H-pyrrole-2-carboxylate
TAP 25.**



Chemical structure of compound 10: c1ccc(cc1)CNC2=CC=C(C(=O)OCC3=CC=CC=C3C4=CC=CC=C4C5(C(=C(C=C5)C6=CC=CC=C6)C7(C(=C(C=C7)C8=CC=CC=C8)C9(C(=C(C=C9)C10=CC=CC=C10)C11(C(=C(C=C11)C12=CC=CC=C12)C13=CC=CC=C13)C14=CC=CC=C14)C15=CC=CC=C15)C16=CC=CC=C16)C17=CC=CC=C17)C18=CC=CC=C18)C19=CC=CC=C19)C20=CC=CC=C20

¹³C NMR spectrum (CDCl₃):

Chemical Shift (ppm)
127.9281
128.4915
128.5156
129.3106
129.5871
129.8038
129.9802
131.5162
131.6872
135.1631
135.3004
135.7451
135.8873
136.5528
136.5919
137.9462
138.3826
138.7193
138.7372

S16