Electronic Supplementary Material (ESI) for Dalton Transactions.

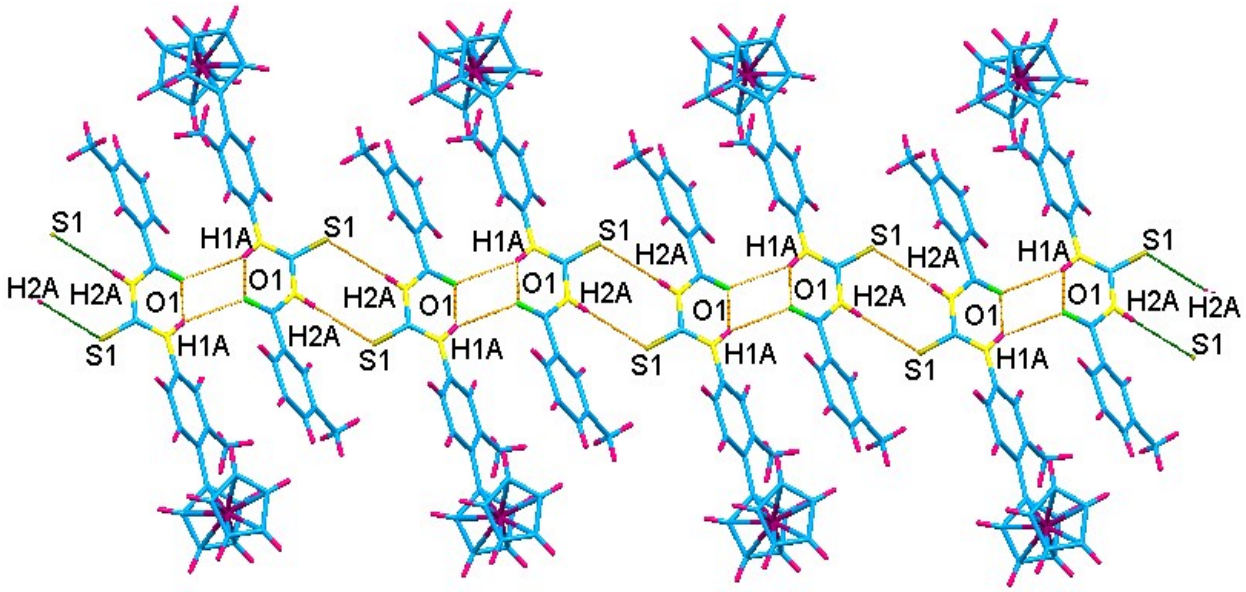


Figure S1. Secondary non-covalent interactions in **A8** leading to supramolecular structure.

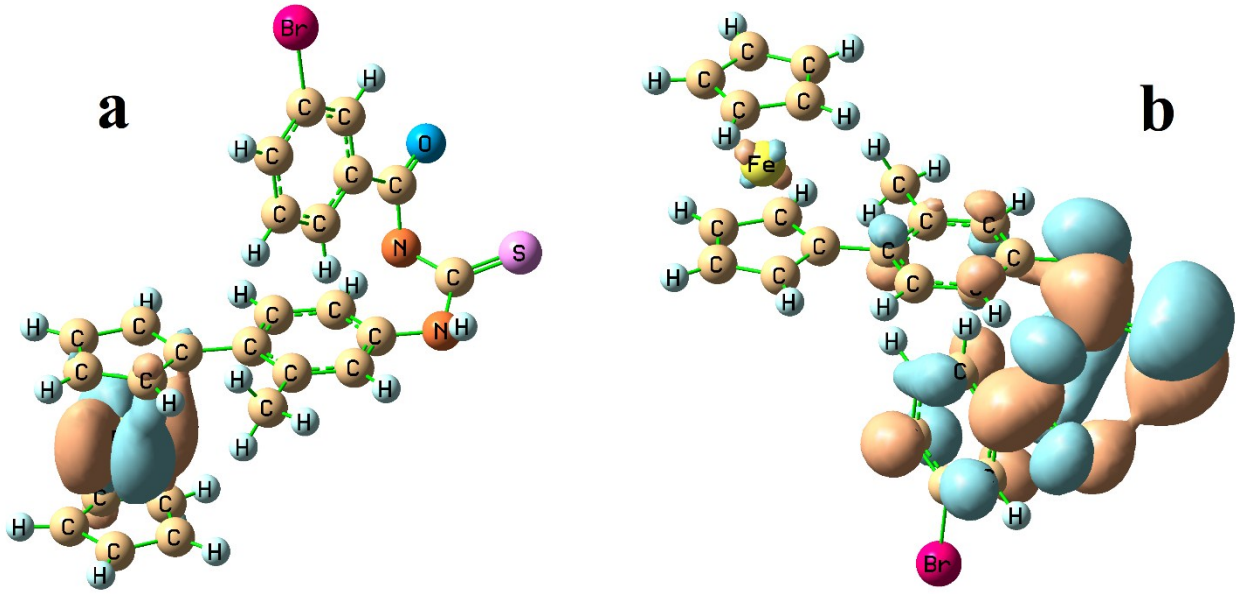


Figure S2. (a) Representative graphical demonstration of HOMO of **A5**. (b) Representative graphical demonstration of LUMO orbitals of **A5**.

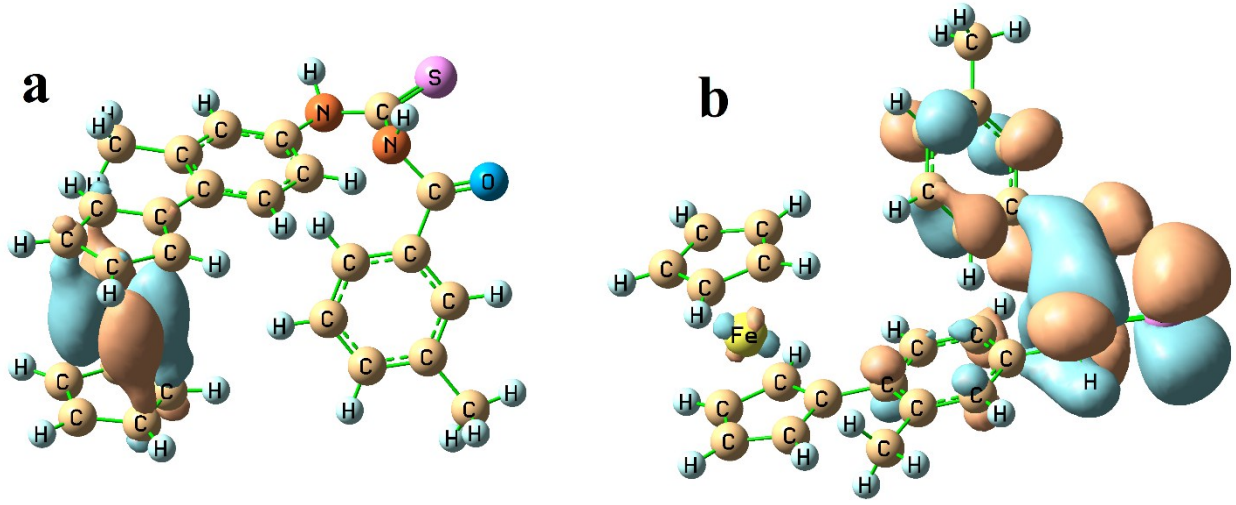


Figure S3. (a) Representative graphical demonstration of HOMO of **A8**. (b) Representative graphical demonstration of LUMO orbitals of **A8**.

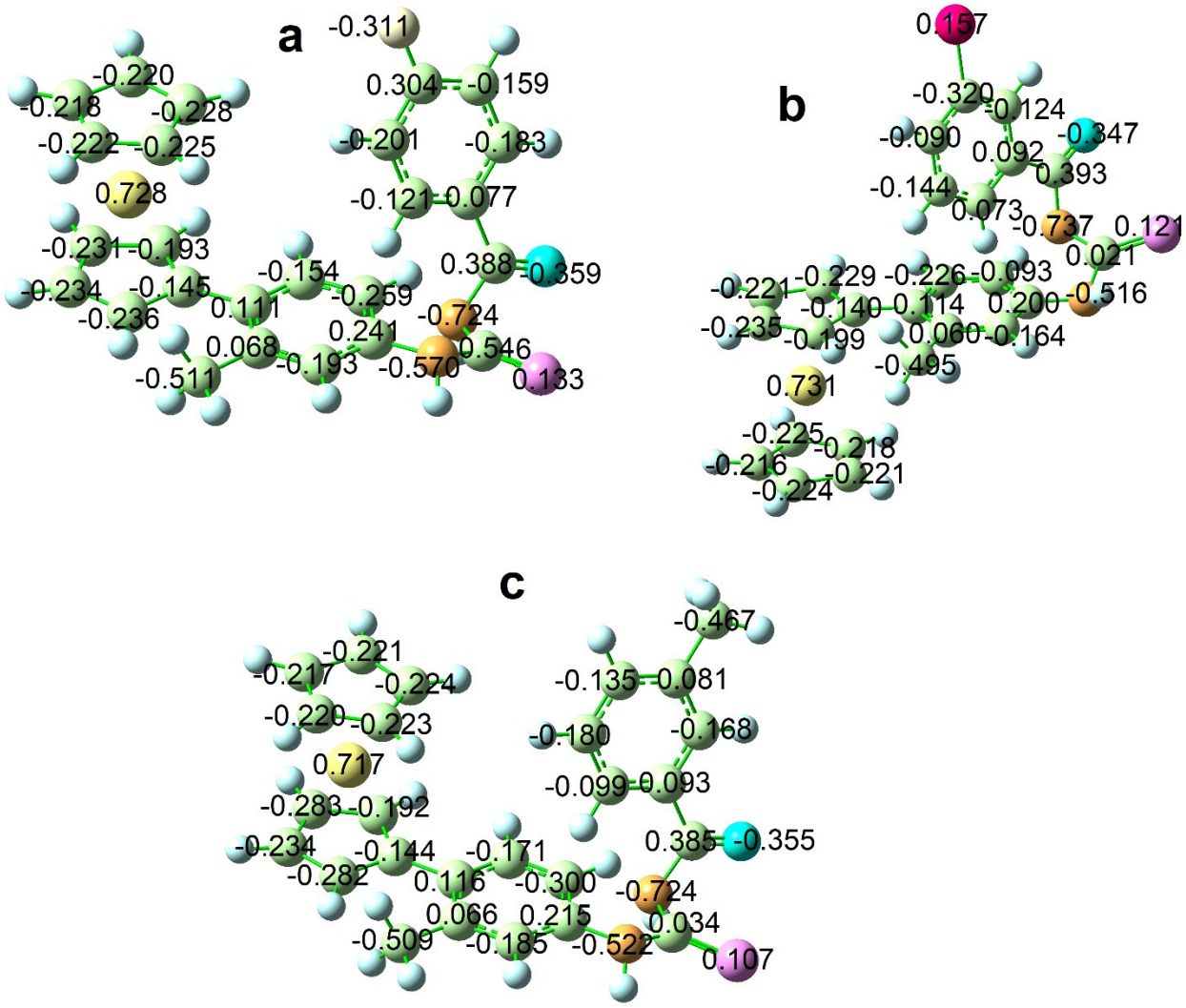


Figure S4. Graphical representation of charge distribution on the molecular structures (a) **A3**, (b) **A5**, and (c) **A8**.

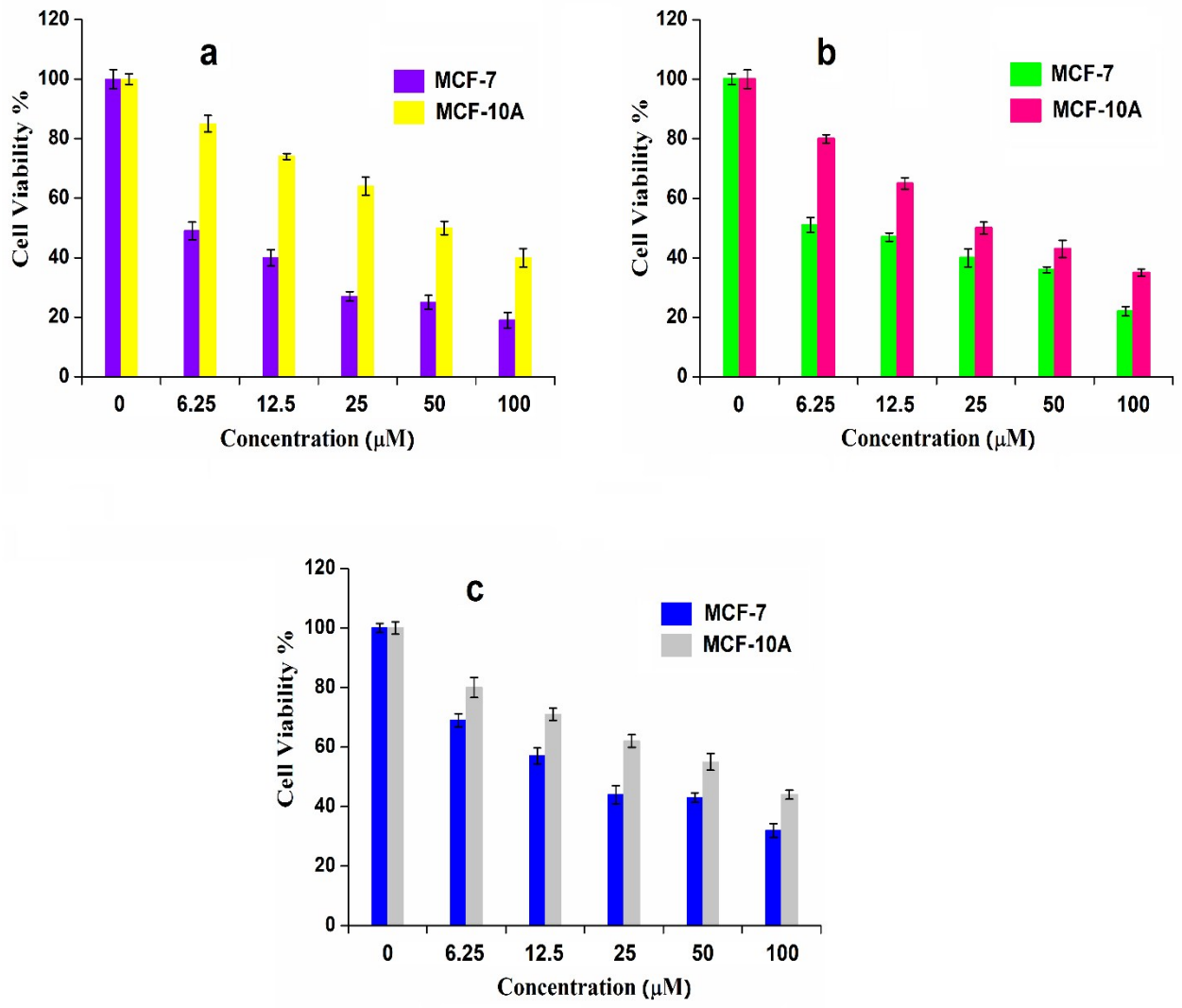


Figure S5. Cell viability (%) of cancerous and non-cancerous cells at various concentrations of (a) **A3**, (b) **A5**, and (c) **A8**, after 72 h of incubation.

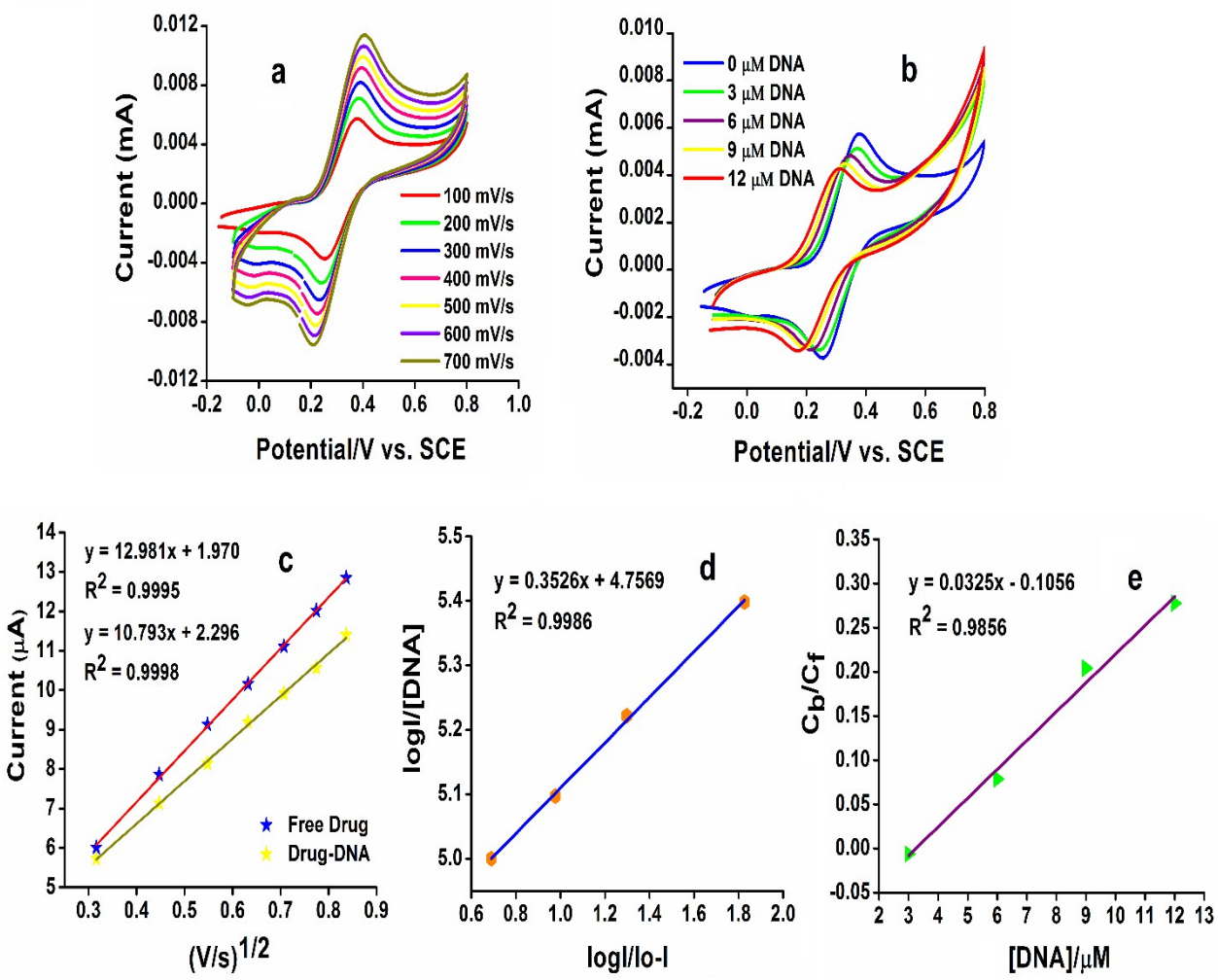


Figure S6. (a) Representative plots of Current *vs*. Potential/V (SCE) at different scan rates for **A8**. (b) Cyclic voltammogram of 1 mM **A8** with 1 mL of 0.5 M TBAP as supporting electrolyte in the absence and presence of 3-12 μM DNA showing a decrease in I from I_o and a concentration dependent -ve shift in potential showing electrostatic interactions. (c) Representative plot of current *vs*. $(V/s)^{1/2}$, for the determination of diffusion coefficient of free **A8** and **A8**-3 μM DNA. (d) Representative plot of log (I/I_o-I) *vs*. log (1/[DNA] for determination of binding constant of **A8**. (e) Plot of C_b/C_f *vs*. [DNA]/μM for determination of binding site size of 3-12 μM DNA concentrations **A8**.

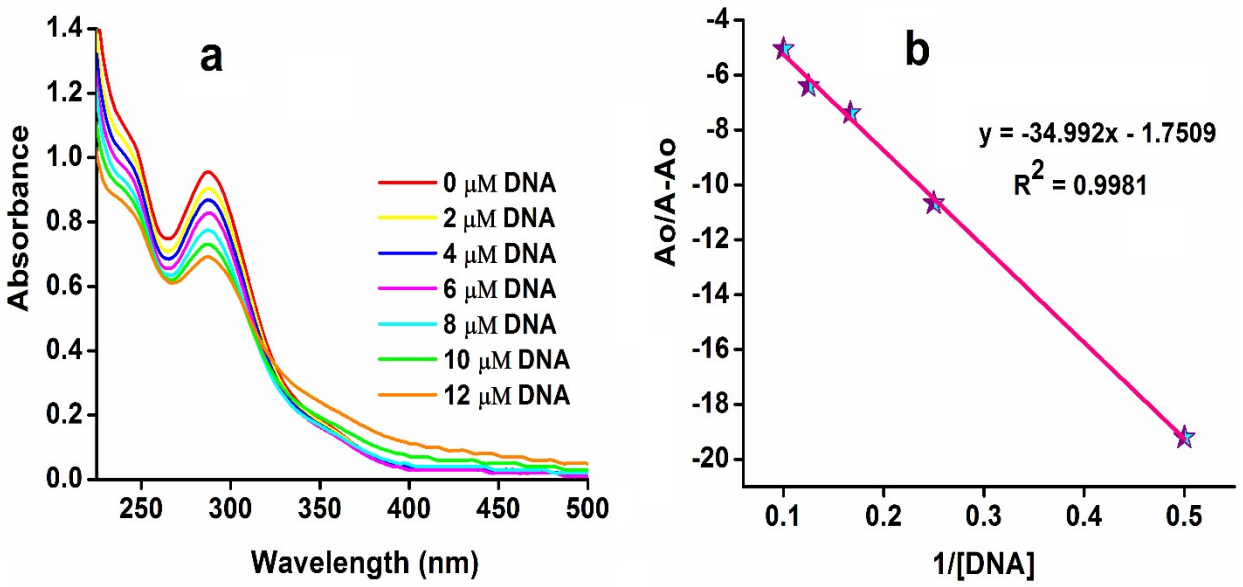


Figure S7. (a) Representative plots of absorbance *vs*. wavelength of 25 μM **A8** in ethanol with increasing concentration of DNA (2-12 μM). (b) Plot of $A_o/A\text{-}A_o$ *vs*. 1/[DNA] for determination of DNA binding constant of **A8**.

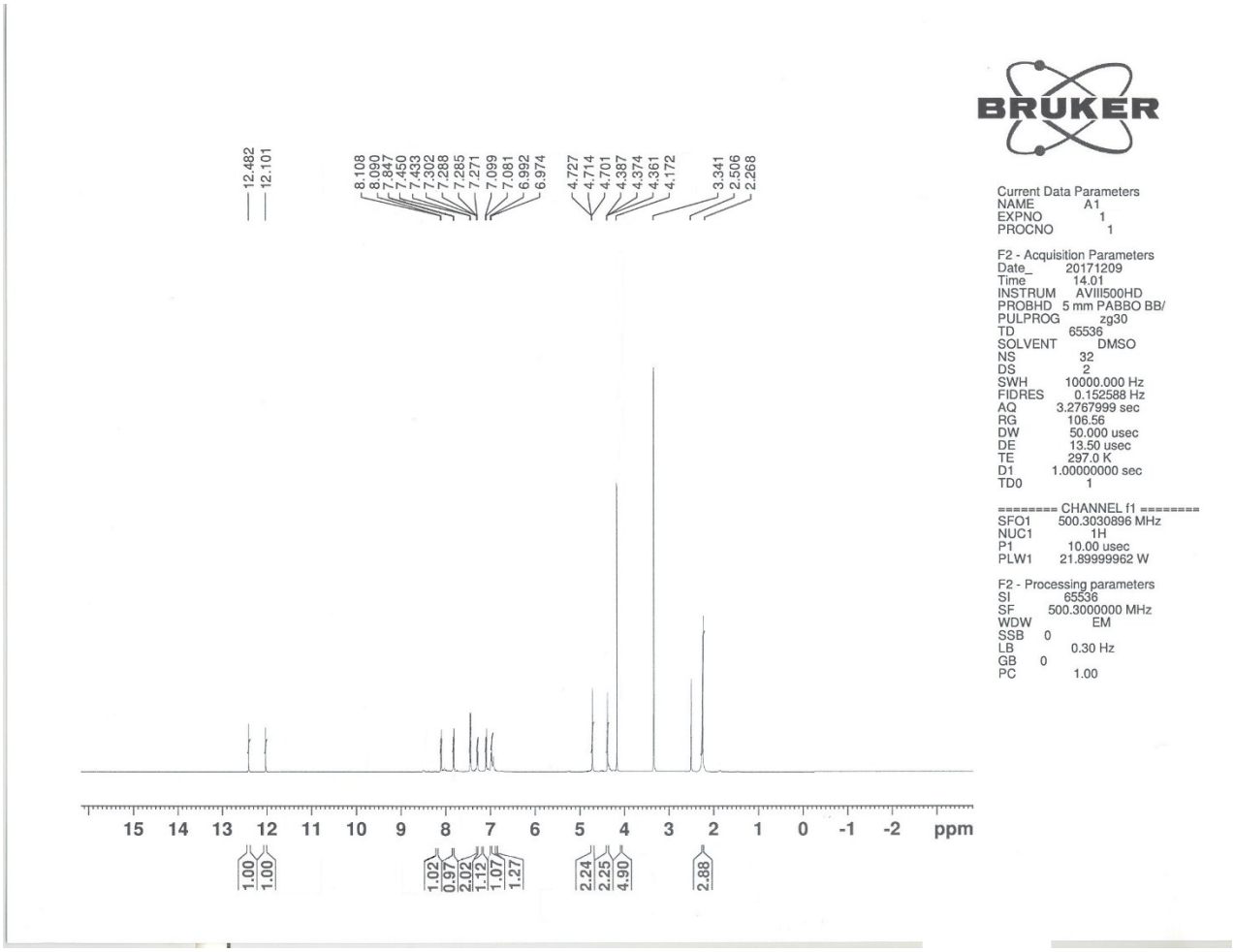
Table S1. Selected bond lengths [Å] and angles [°] for **A8**.

Bond Lengths (Å)	
C(1)-C(2)	1.408(3)
C(6)-C(7)	1.415(3)
Fe(1)-C(5)	2.042(2)
Fe(1)-C(10)	2.056(17)
C(10)-C(11)	1.479(2)
C(11)-C(12)	1.392(2)
C(11)-C(16)	1.399(2)
N(1)-C(14)	1.423(2)
N(1)-C(18)	1.324(2)
S(1)-C(18)	1.659(18)
N(2)-C(18)	1.392(2)
N(2)-C(19)	1.377(2)
O(1)-C(19)	1.217(2)
C(19)-C(20)	1.486(2)
C(22)-C(26)	1.502(3)
Bond Angles (°)	
C(1)-C(2)-Fe(1)	40.47(9)
C(6)-C(7)-Fe(1)	40.82(8)
C(9)-C(10)-C(11)	127.6(17)
C(10)-C(11)-C(12)	119.8(15)
C(11)-C(16)-C(17)	123.2(15)
C(15)-C(16)-C(17)	118.2(15)
N(1)-C(14)-C(15)	116.6(15)
C(14)-N(1)-C(18)	127.9(15)
N(1)-C(18)-S(1)	126.4(13)
N(2)-C(18)-S(1)	118.2(12)
N(1)-C(18)-N(2)	115.4(15)
C(18)-N(2)-C(19)	128.2(14)
N(2)-C(19)-O(1)	122.7(16)
N(2)-C(19)-C(20)	115.9(15)
C(19)-C(20)-C(25)	117.1((16)
C(21)-C(22)-C(26)	120.9(19)

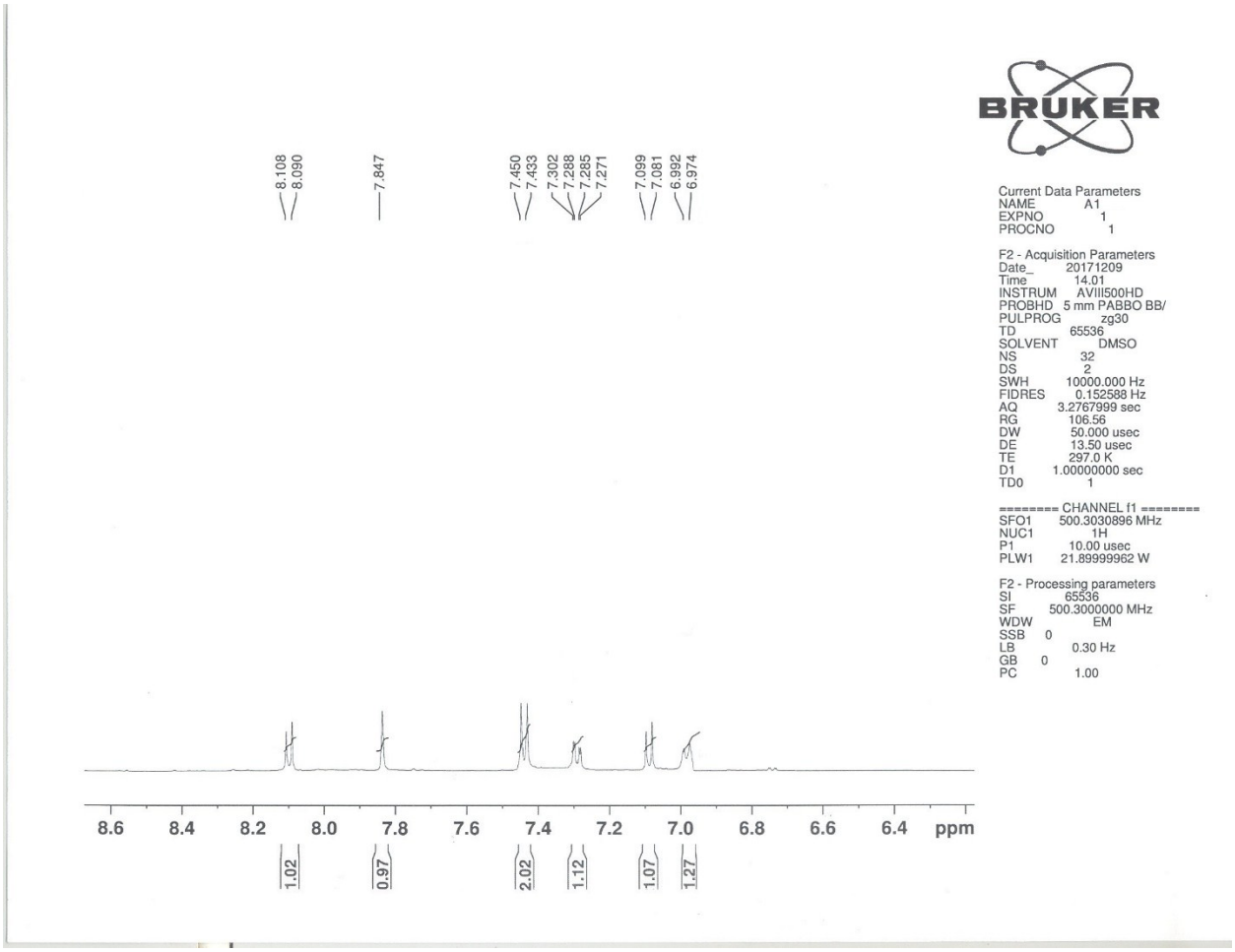
Table S2. The intramolecular and intermolecular hydrogen bond interactions in **A8**.

H-Bonding	D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
Intramolecular	N1	H1A	O1	0.86	1.98	2.646(2)	133.6
Intermolecular	N1	H1A	O1	0.86	2.54	3.254(2)	141.4
Intermolecular	N2	H2A	S1	0.86	2.90	3.759(15)	175.5

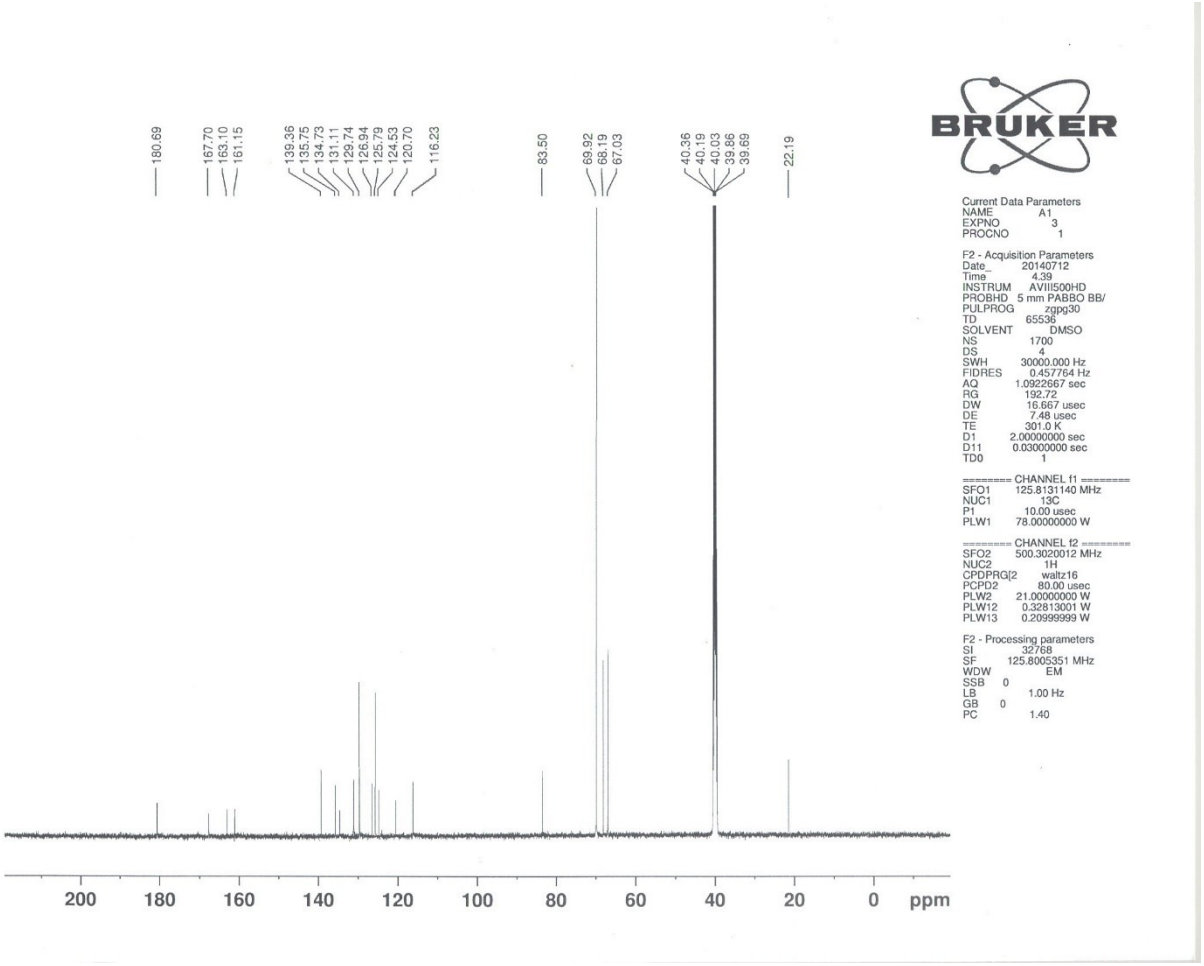
^{1}H-NMR Spectrum of A1



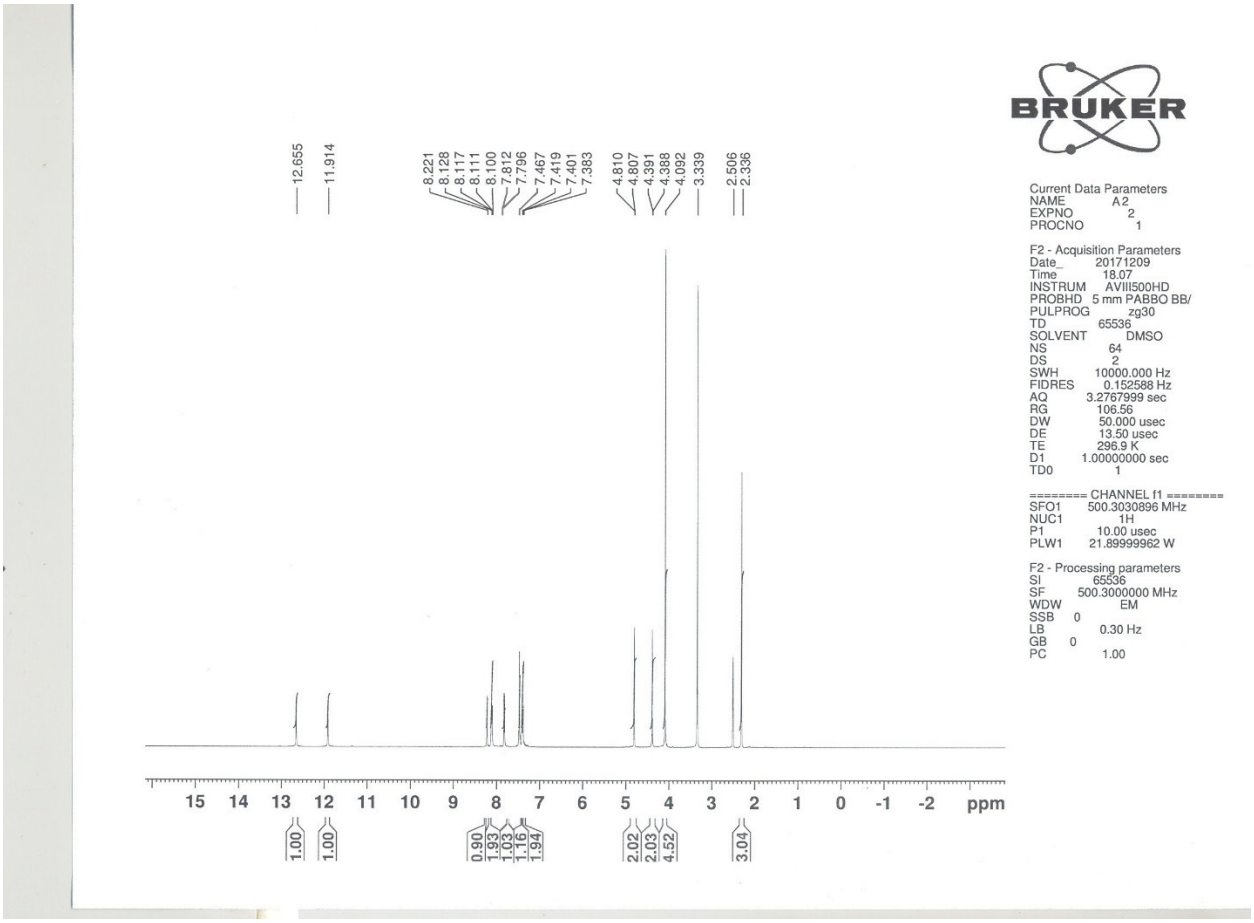
^{1}H-NMR Spectrum of A1



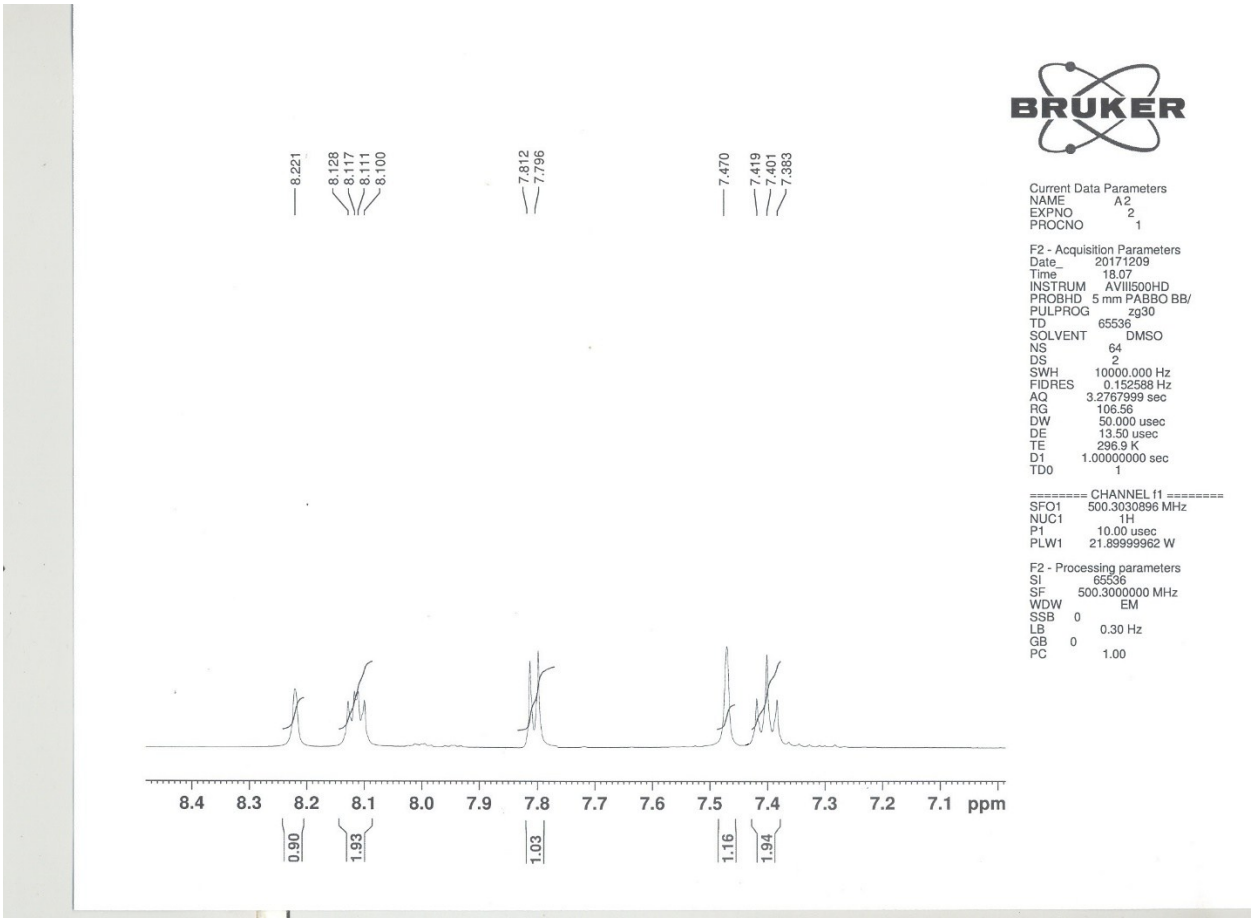
^{13}C-NMR Spectrum of A1



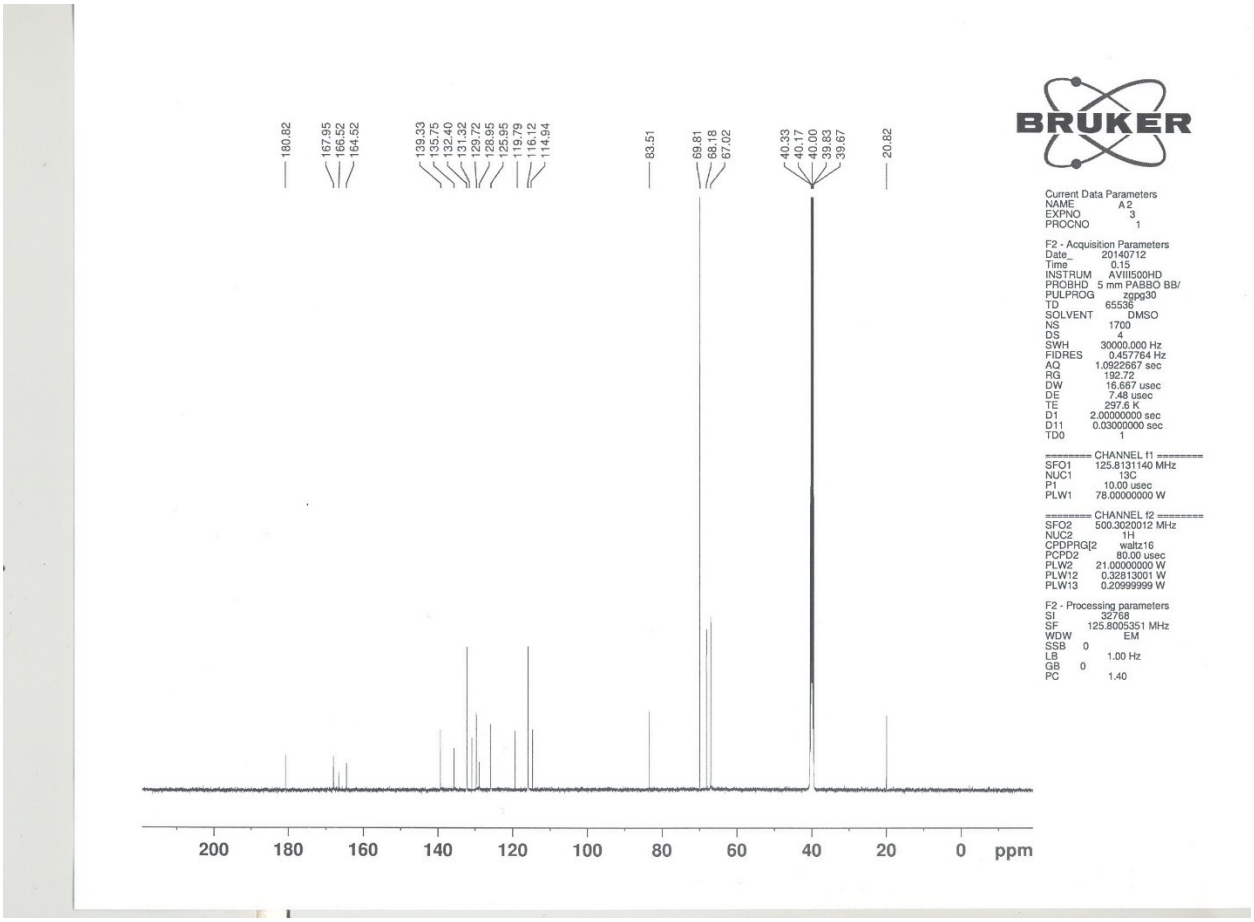
^{1}H-NMR Spectrum of A2



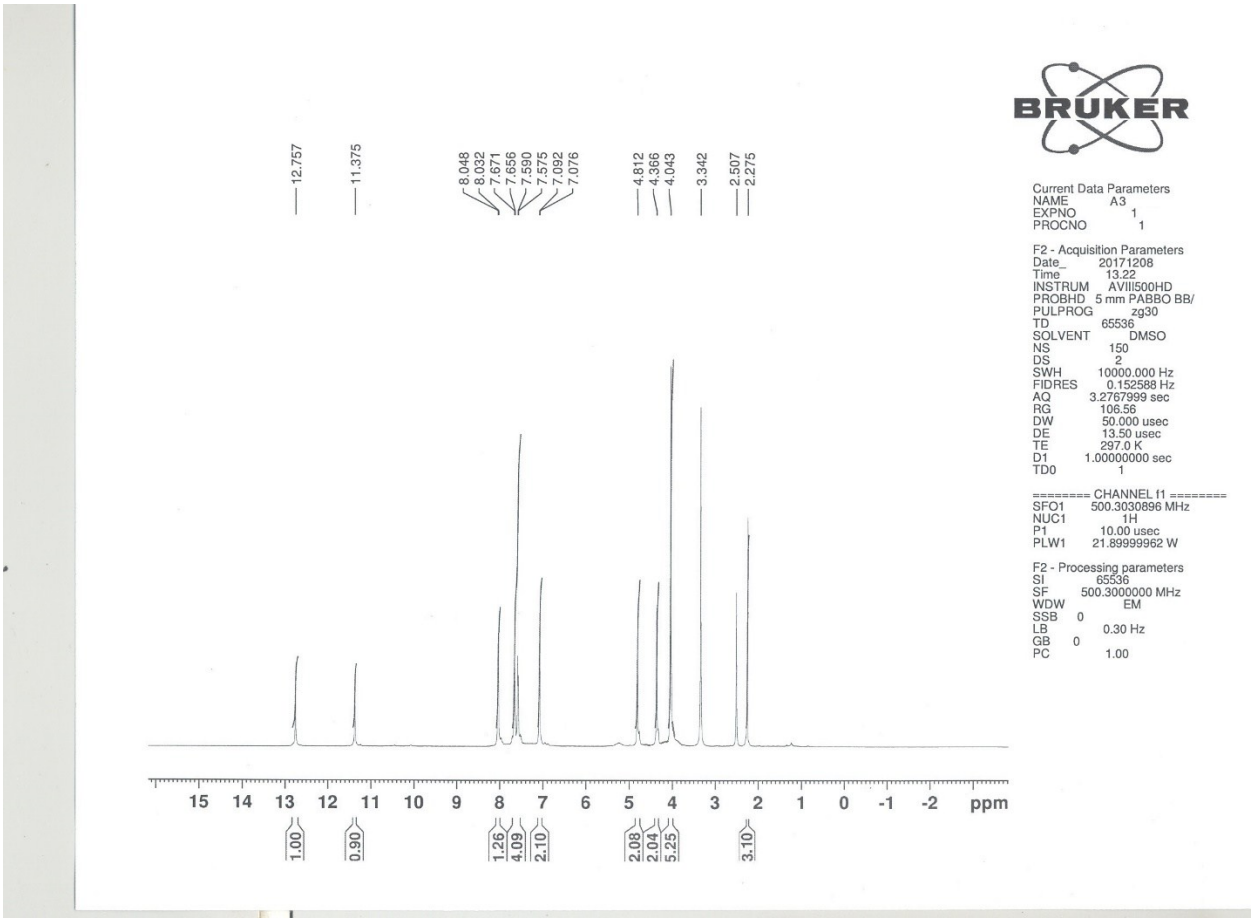
^{1}H-NMR Spectrum of A2



^{13}C-NMR Spectrum of A2



^{1}H-NMR Spectrum of A3



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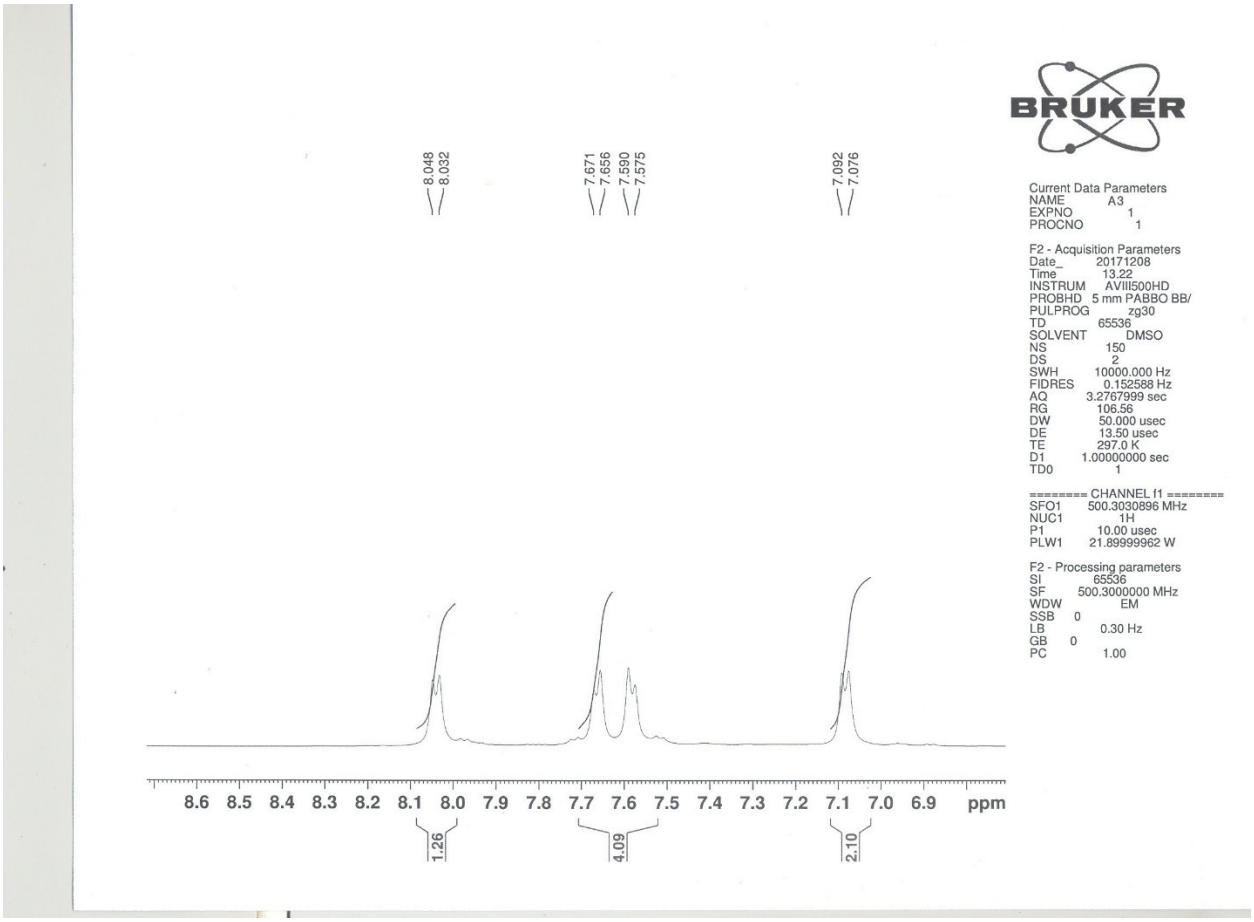
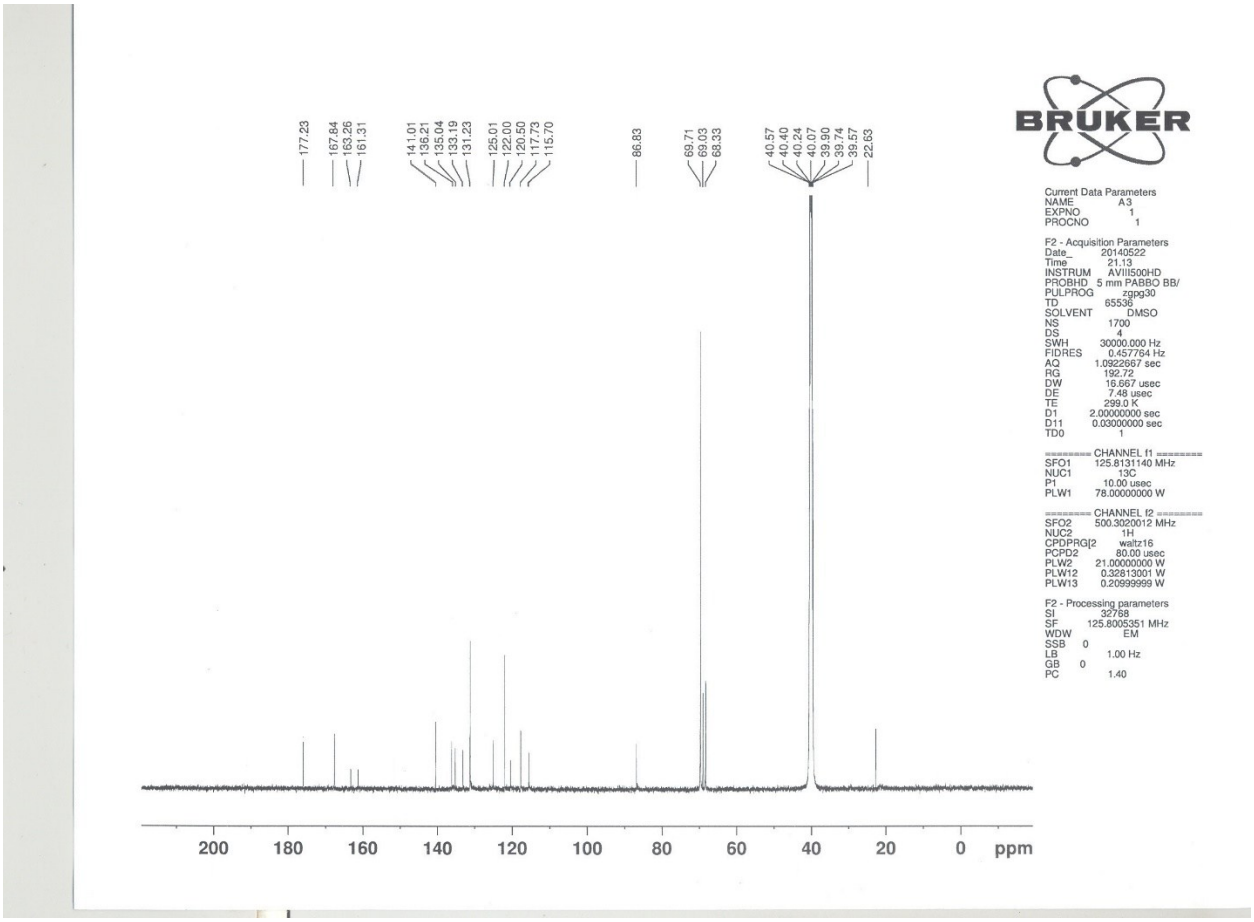


^{13}C-NMR Spectrum of A3



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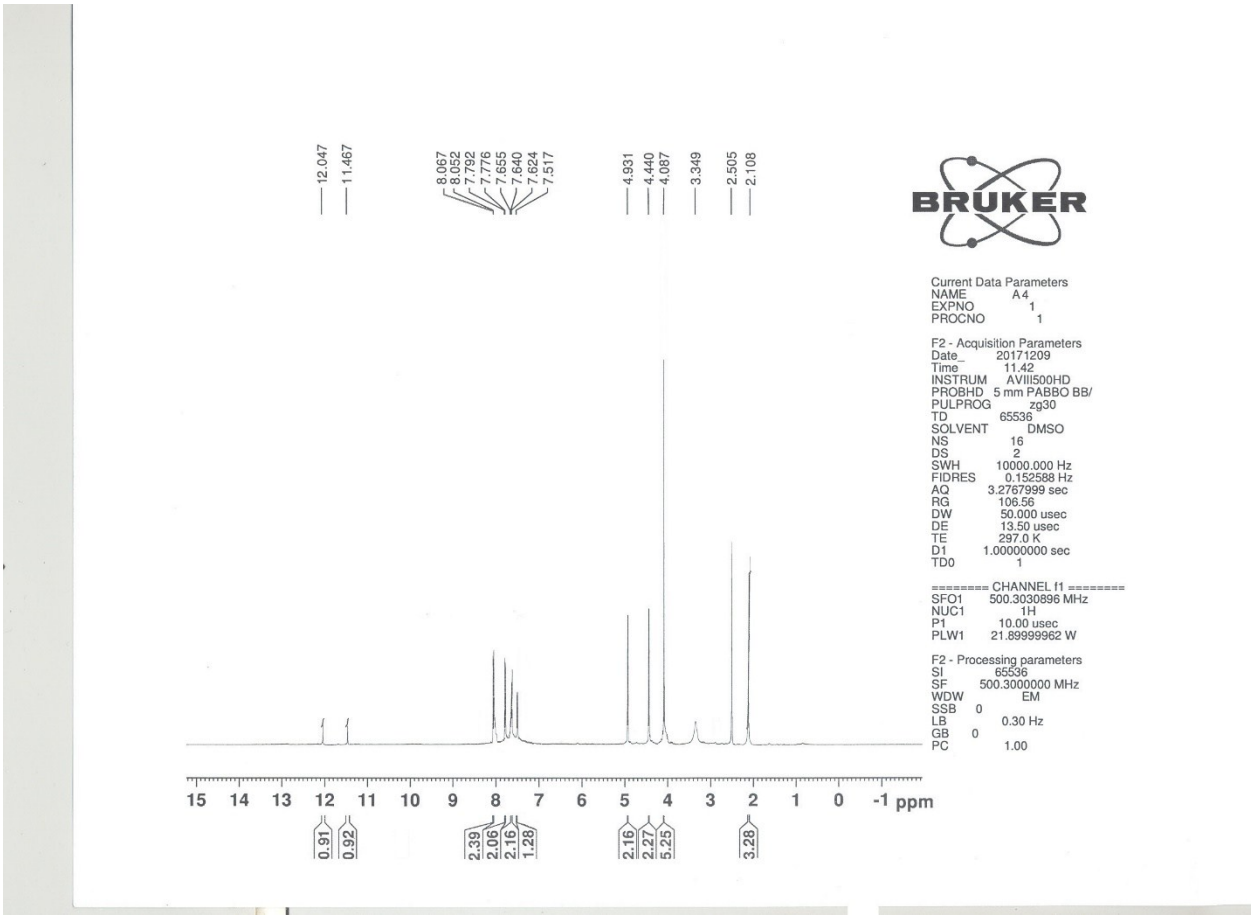
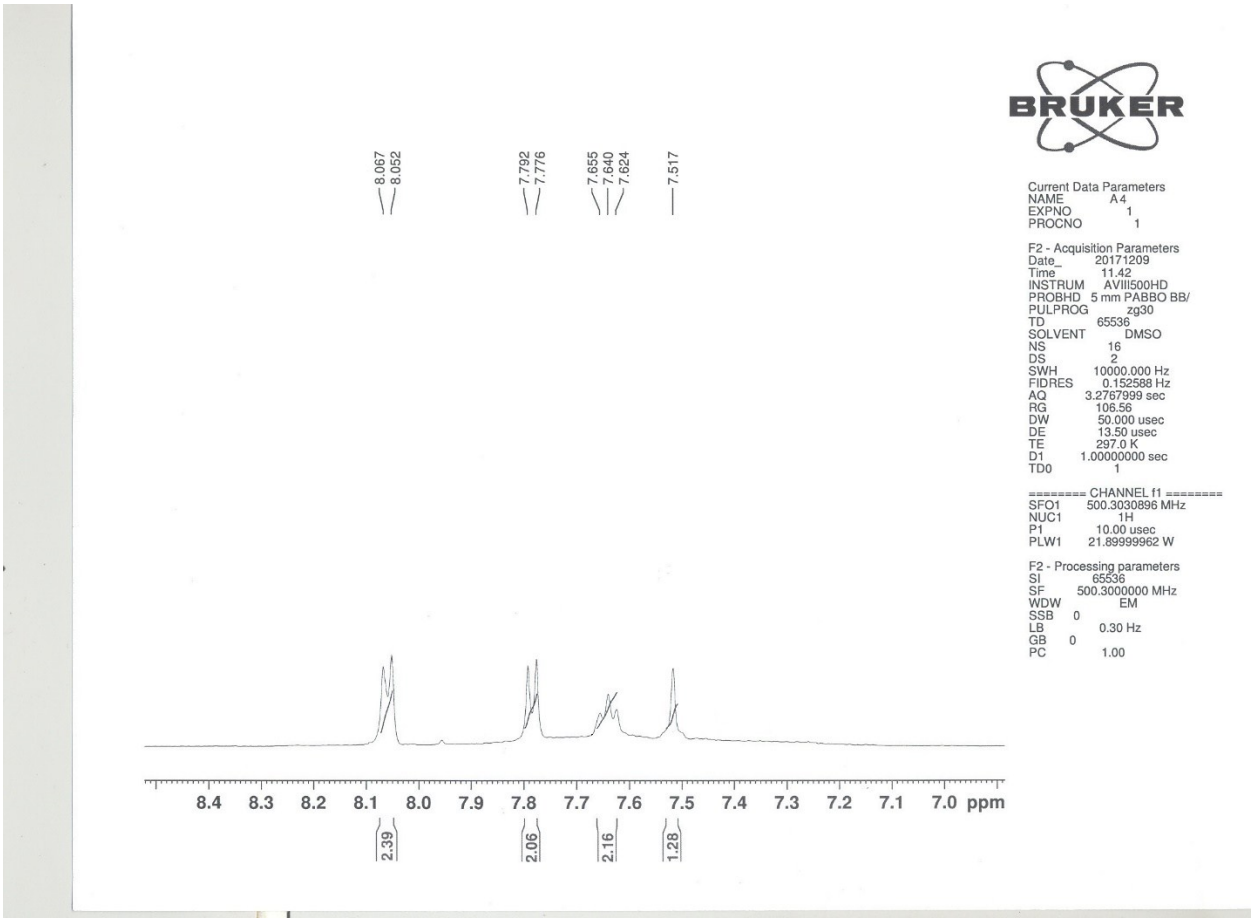


^{1}H-NMR Spectrum of A4



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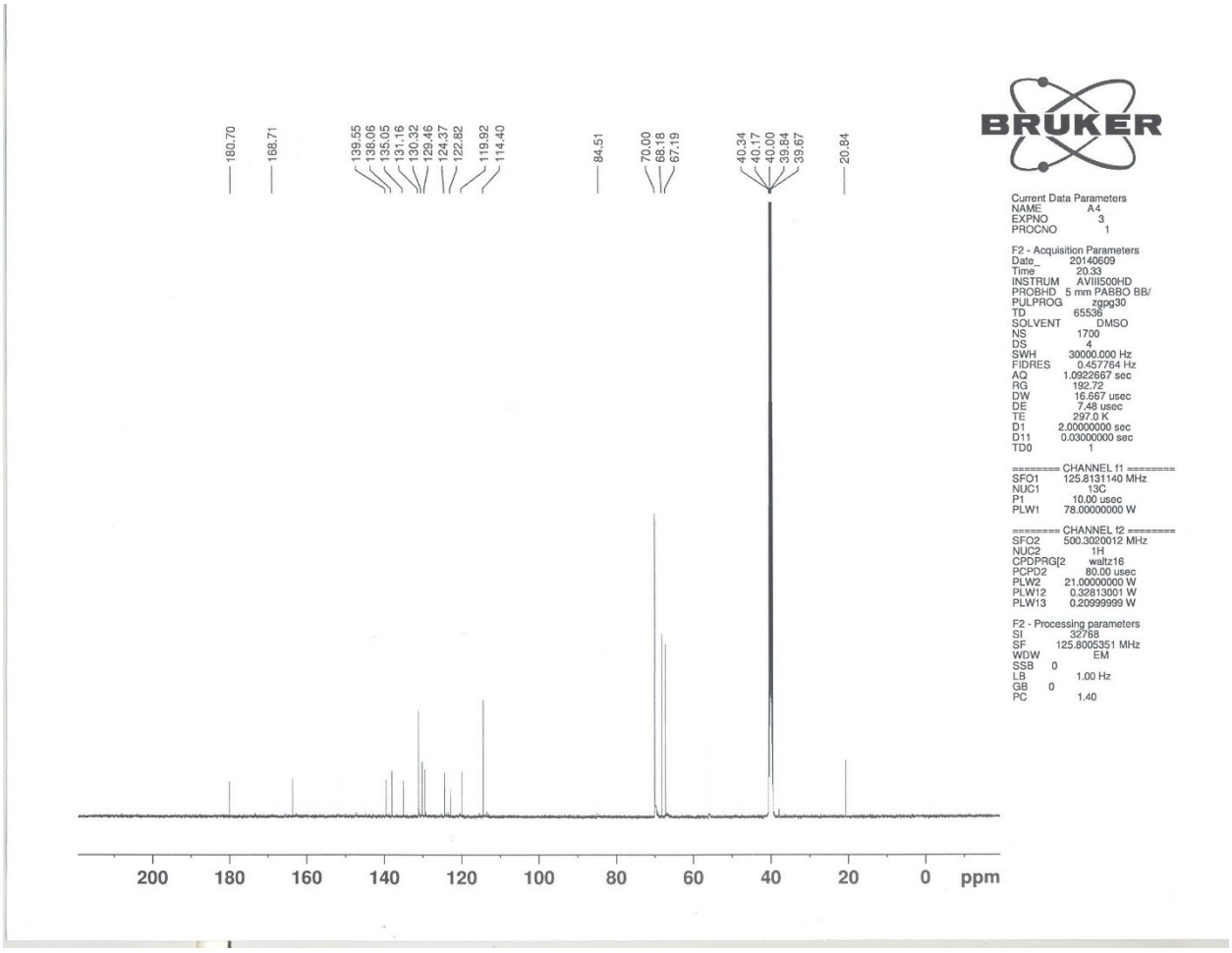

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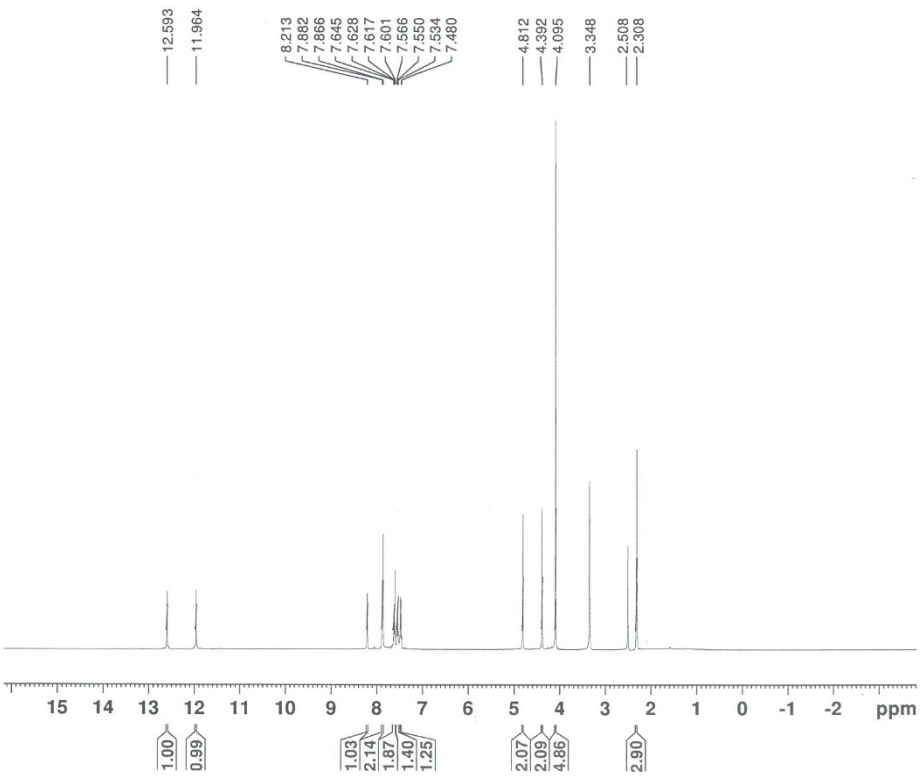

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DE 13.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

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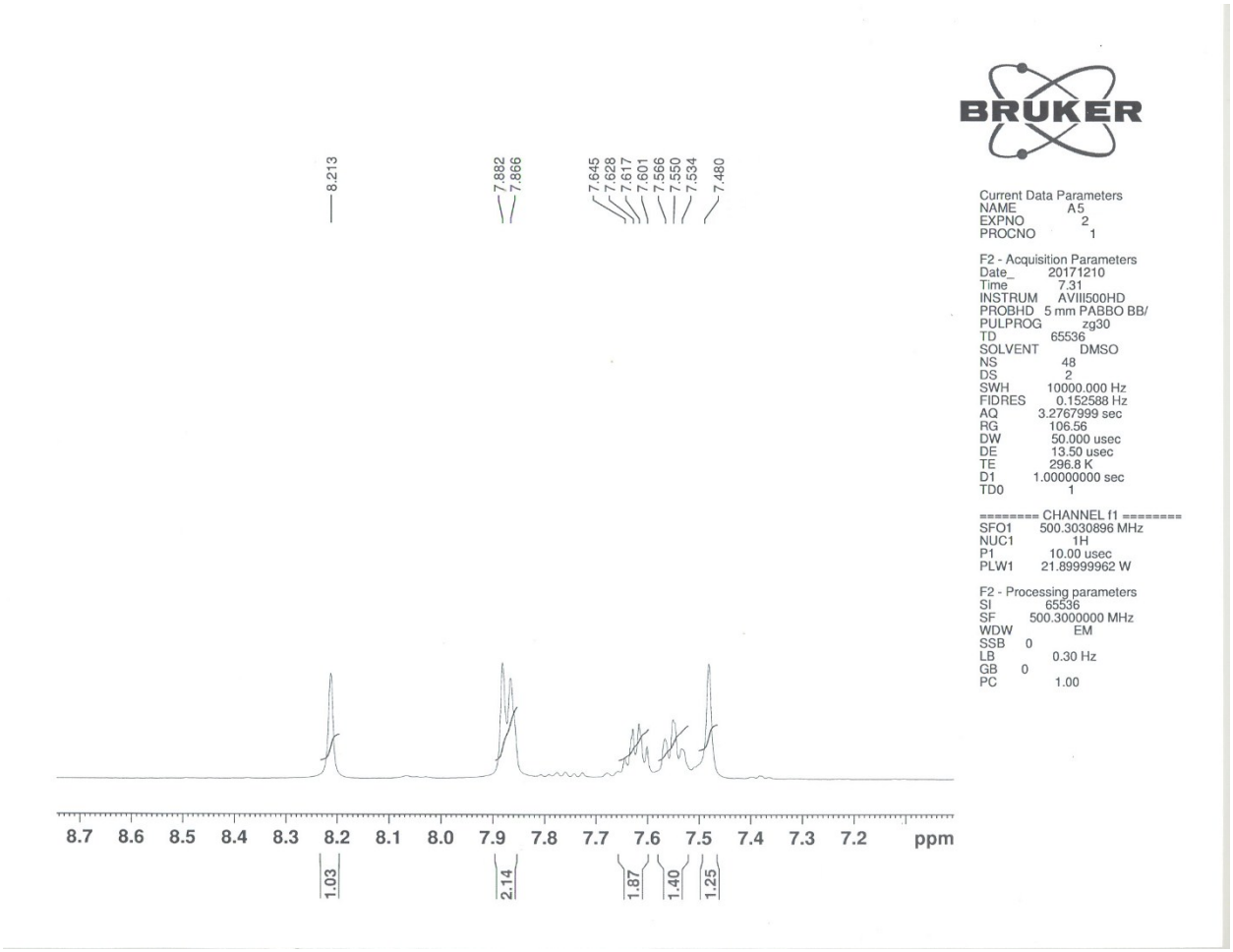

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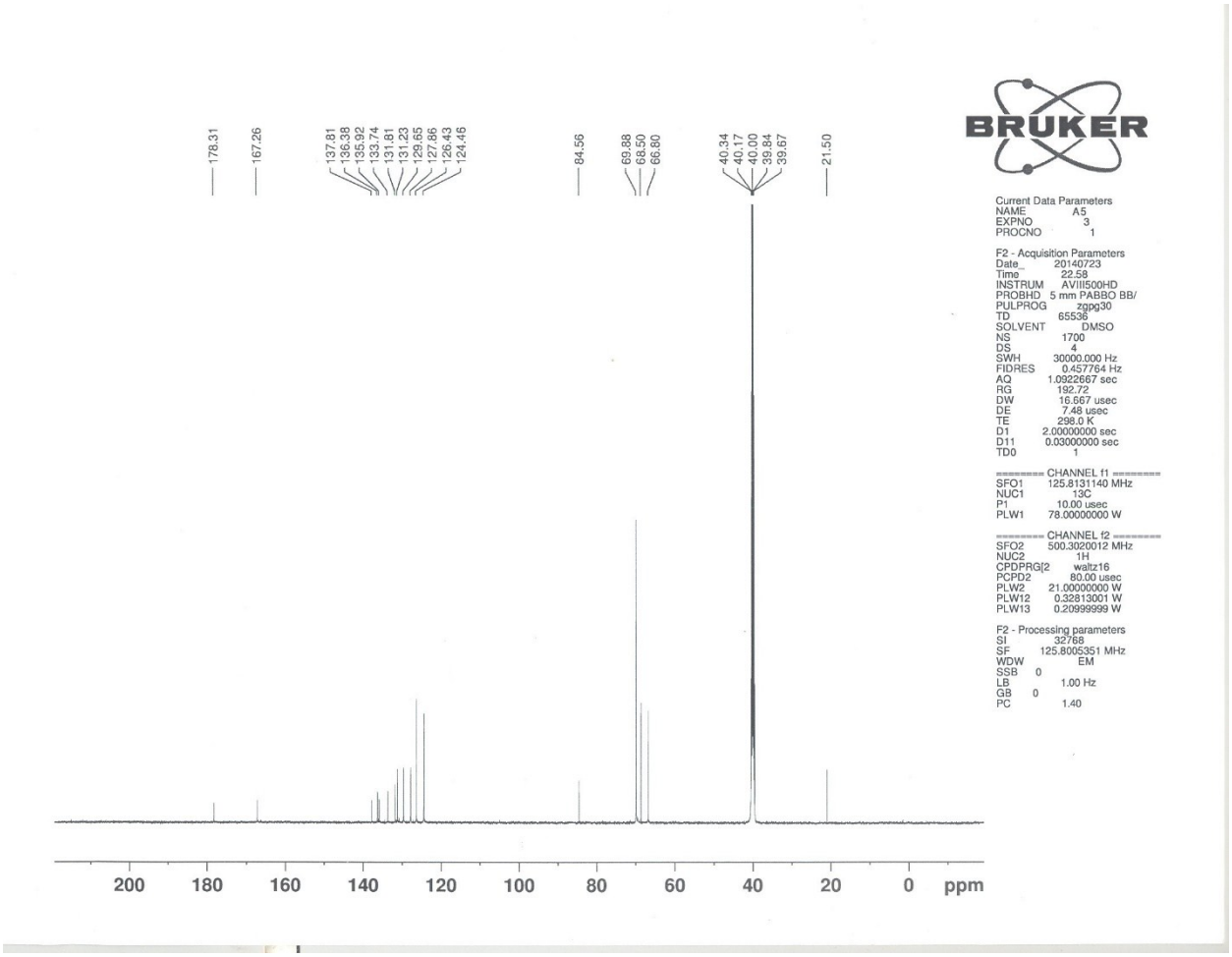

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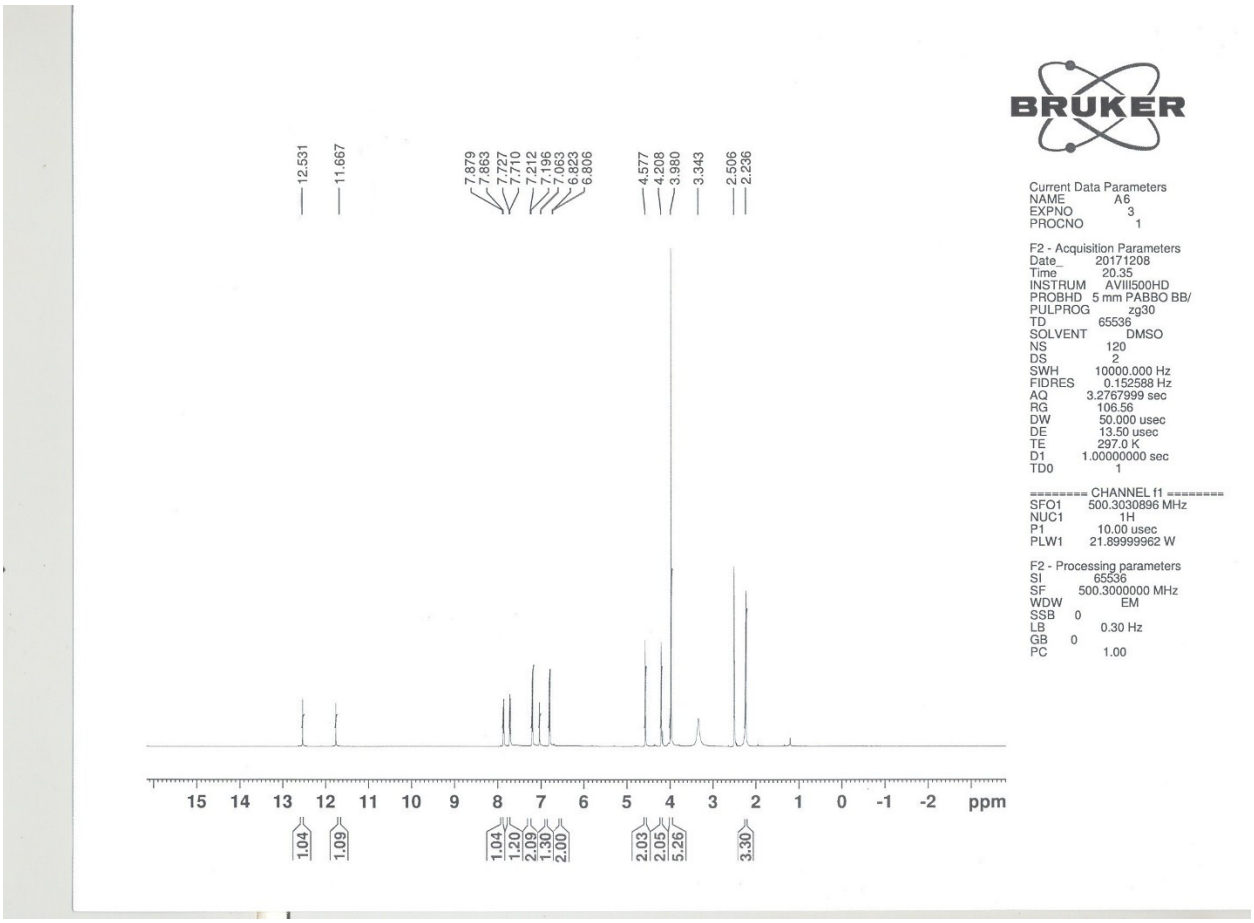
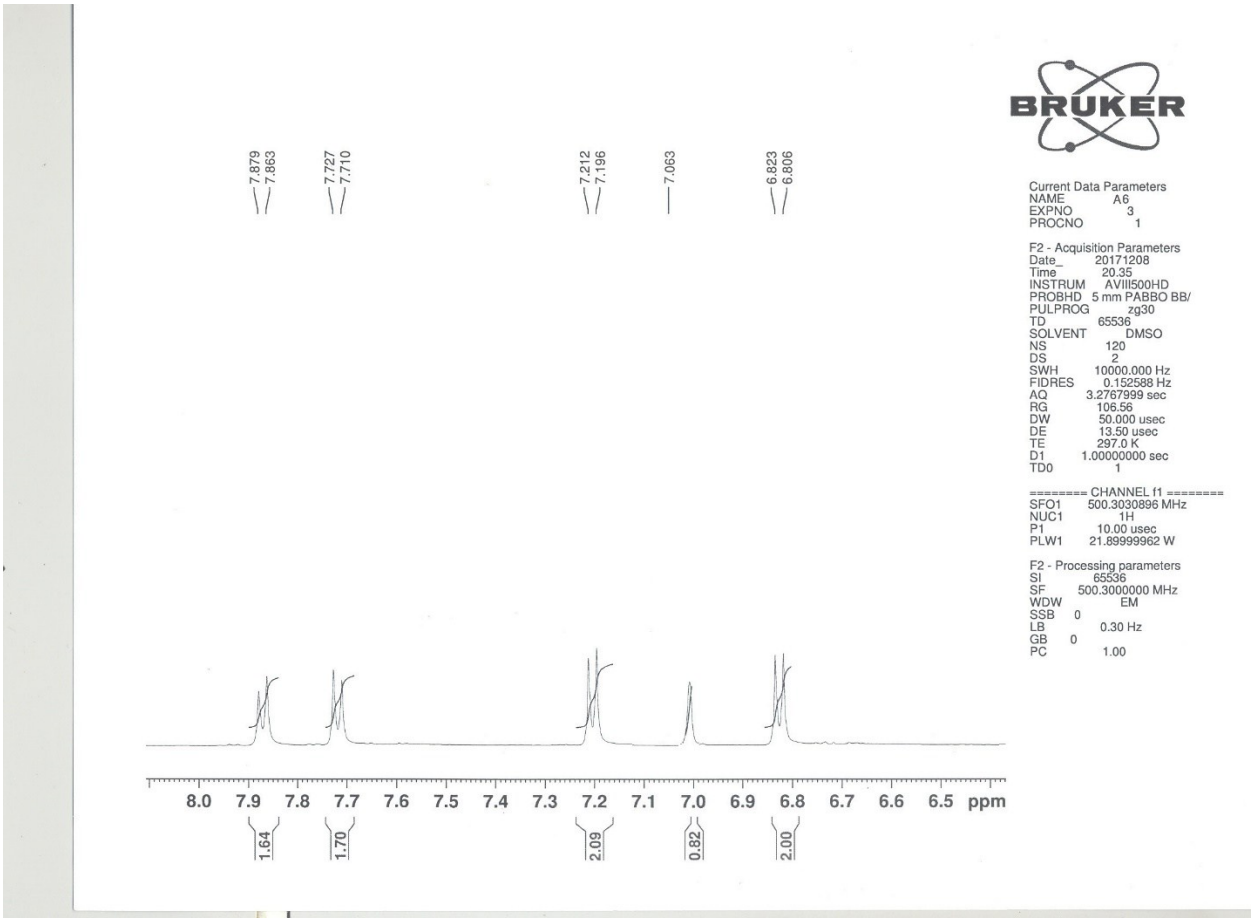


^{1}H-NMR Spectrum of A6



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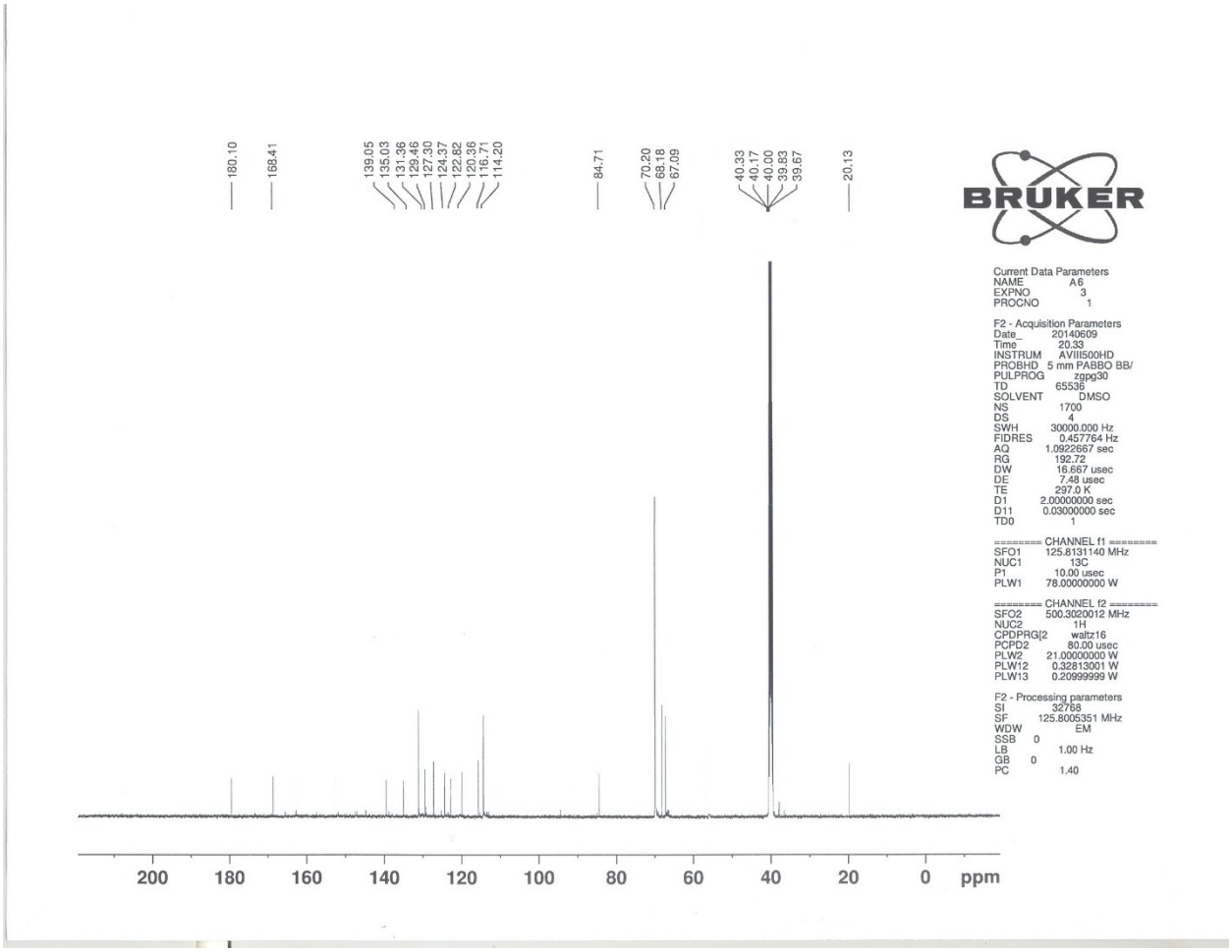

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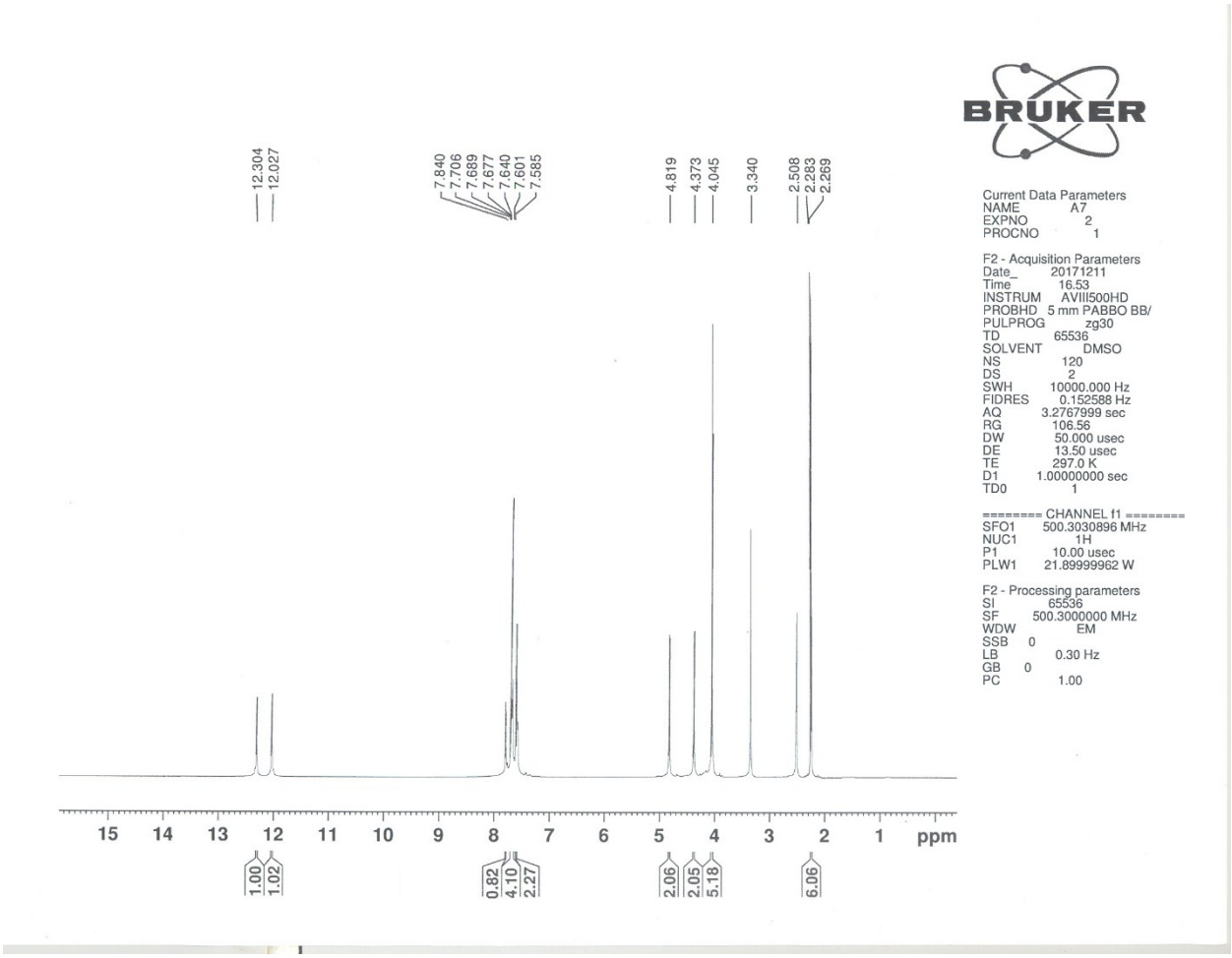

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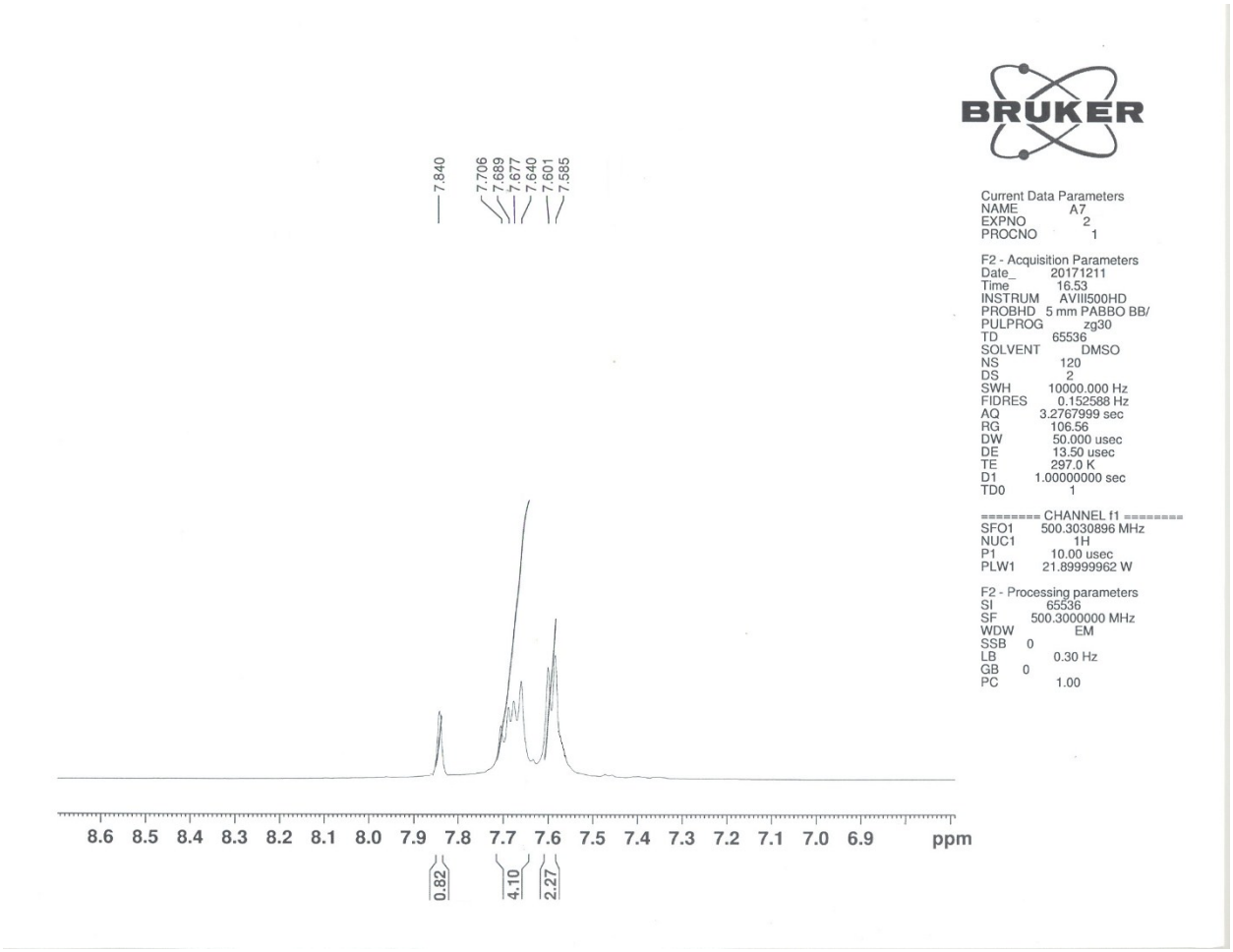

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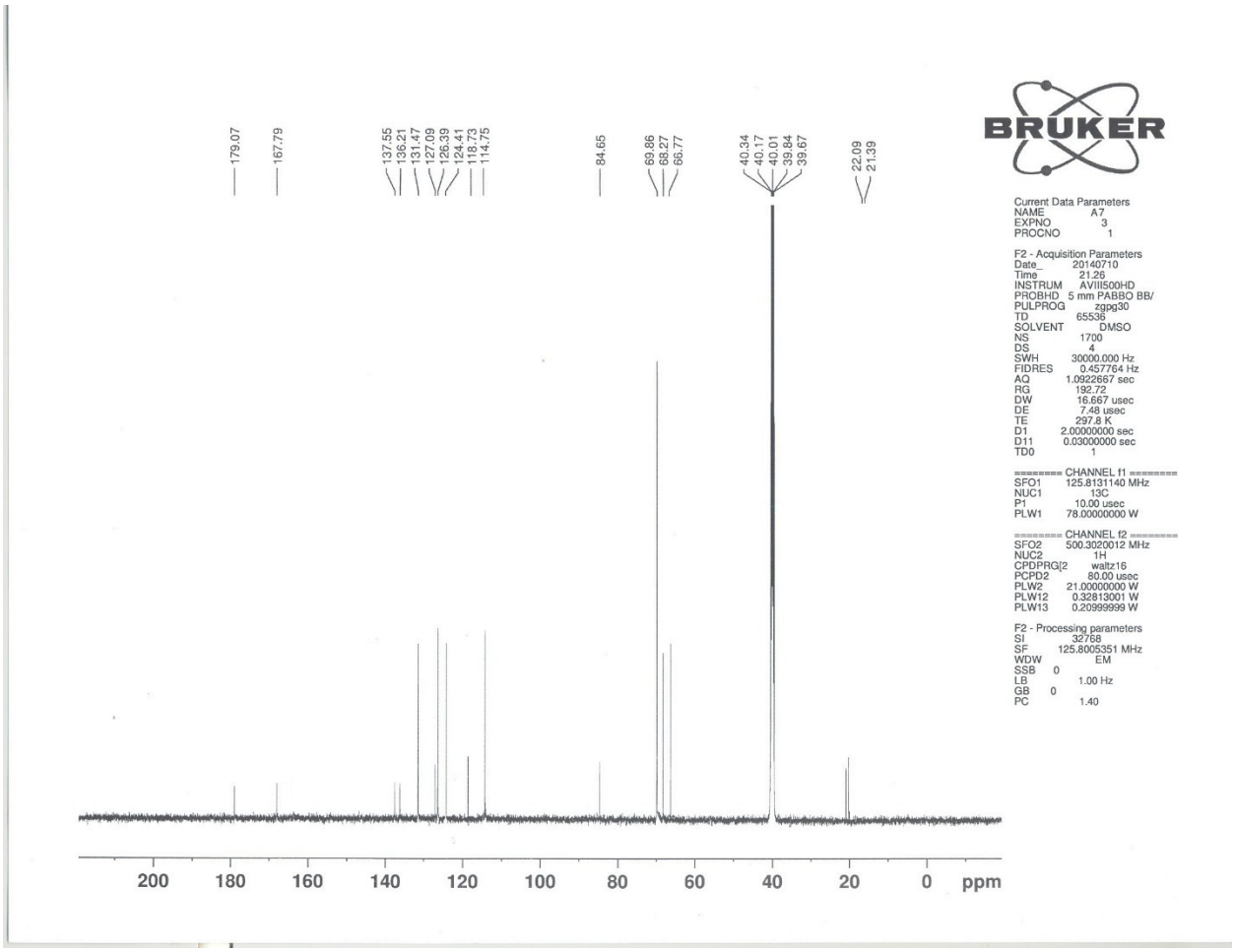

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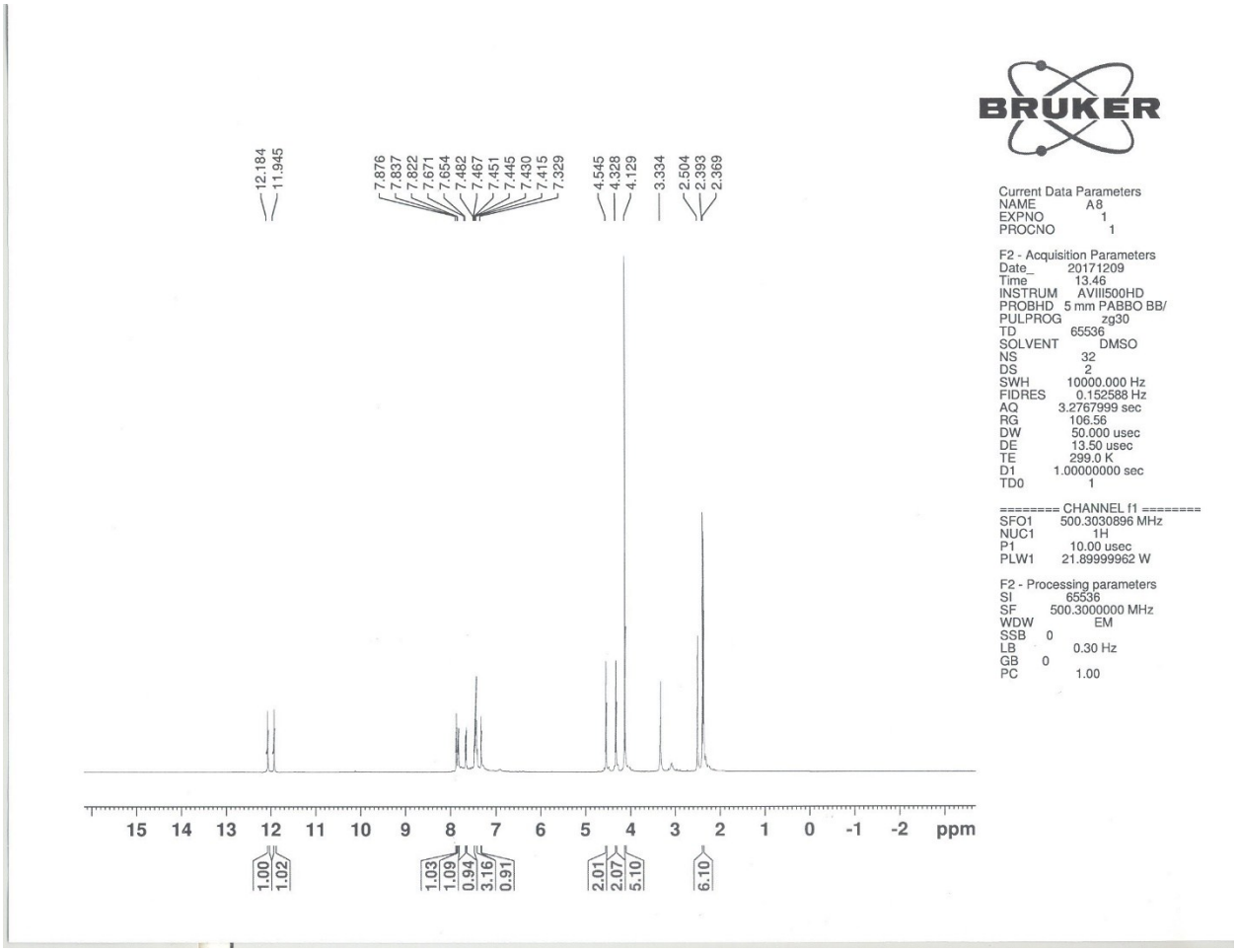

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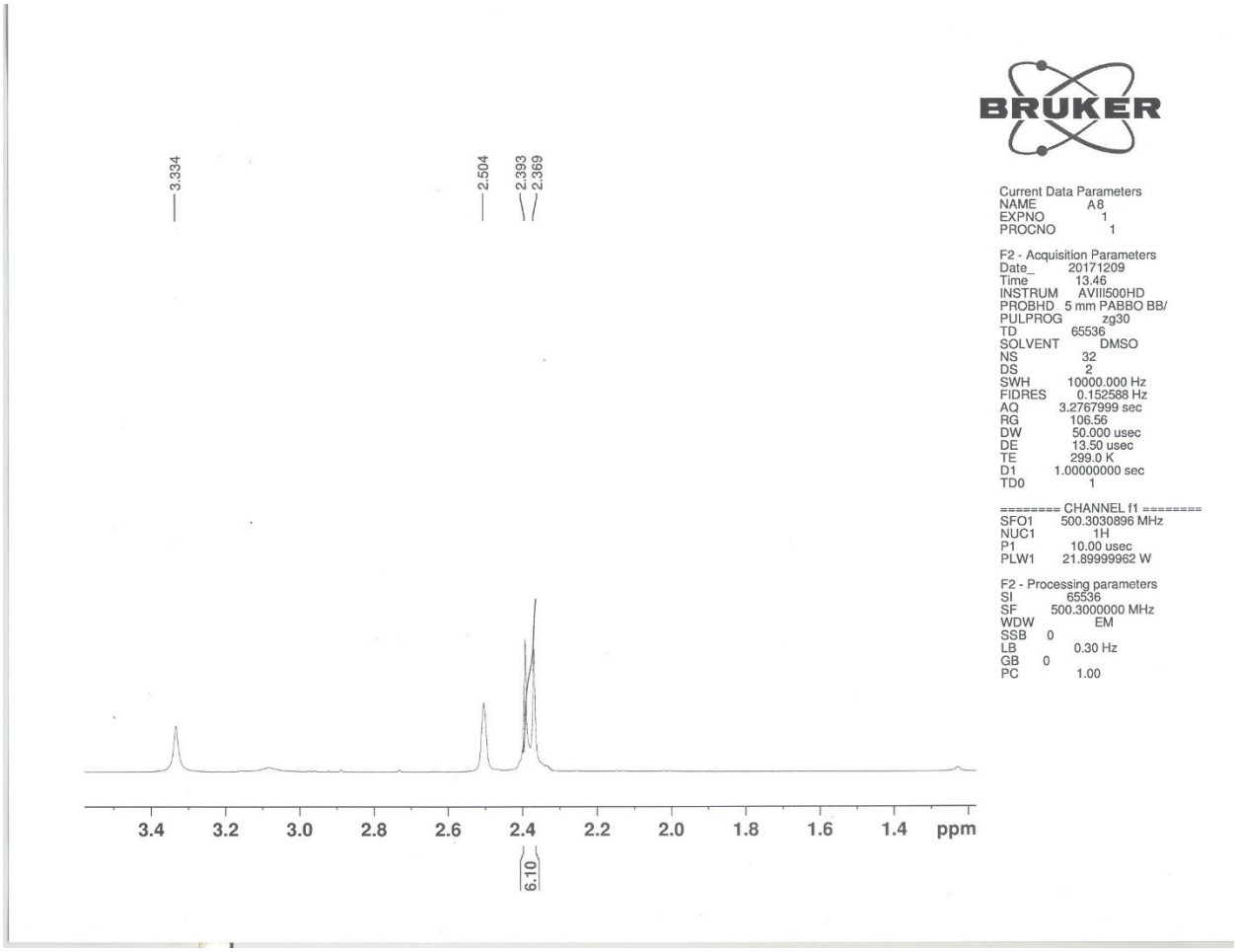
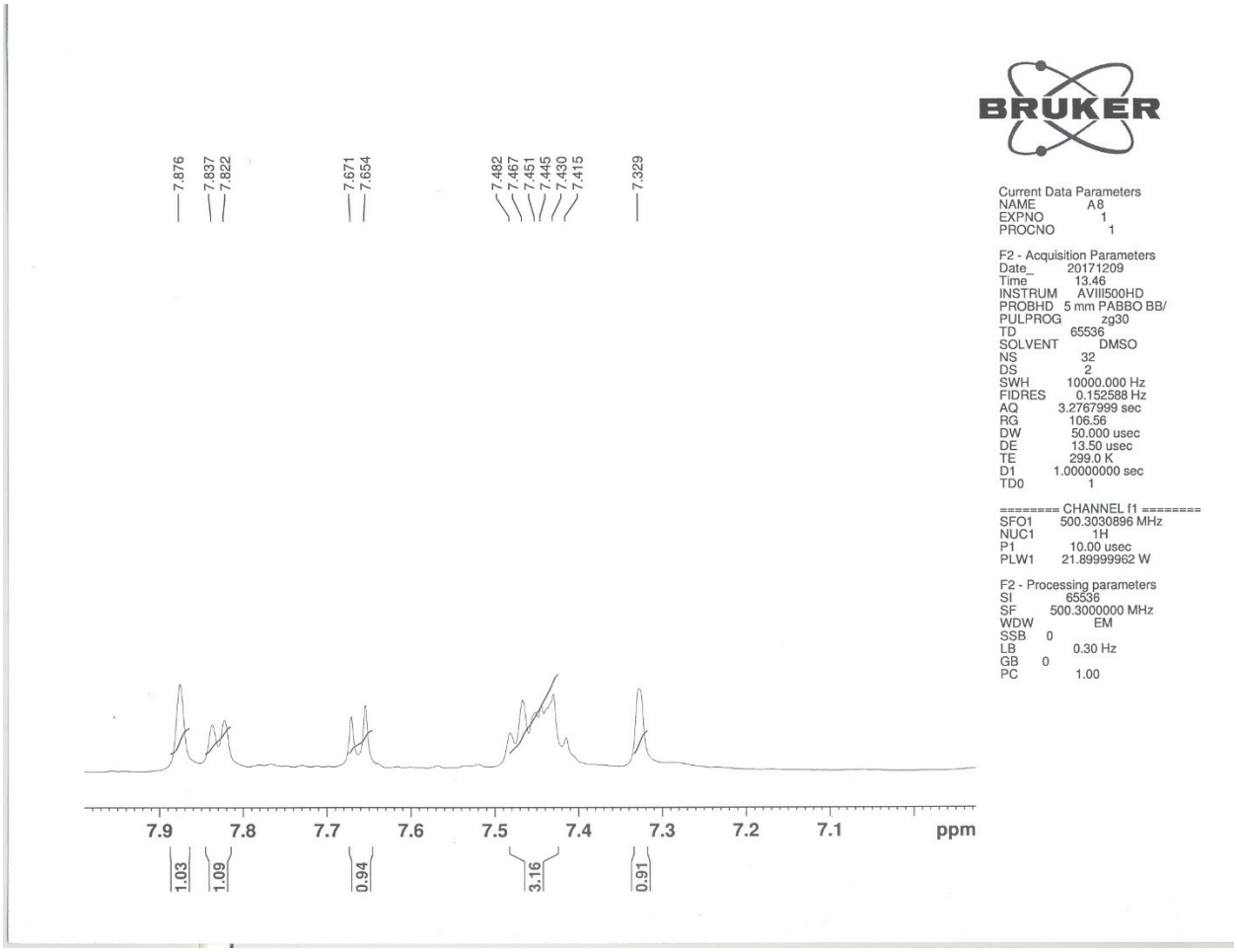


^{1}H-NMR Spectrum of A8



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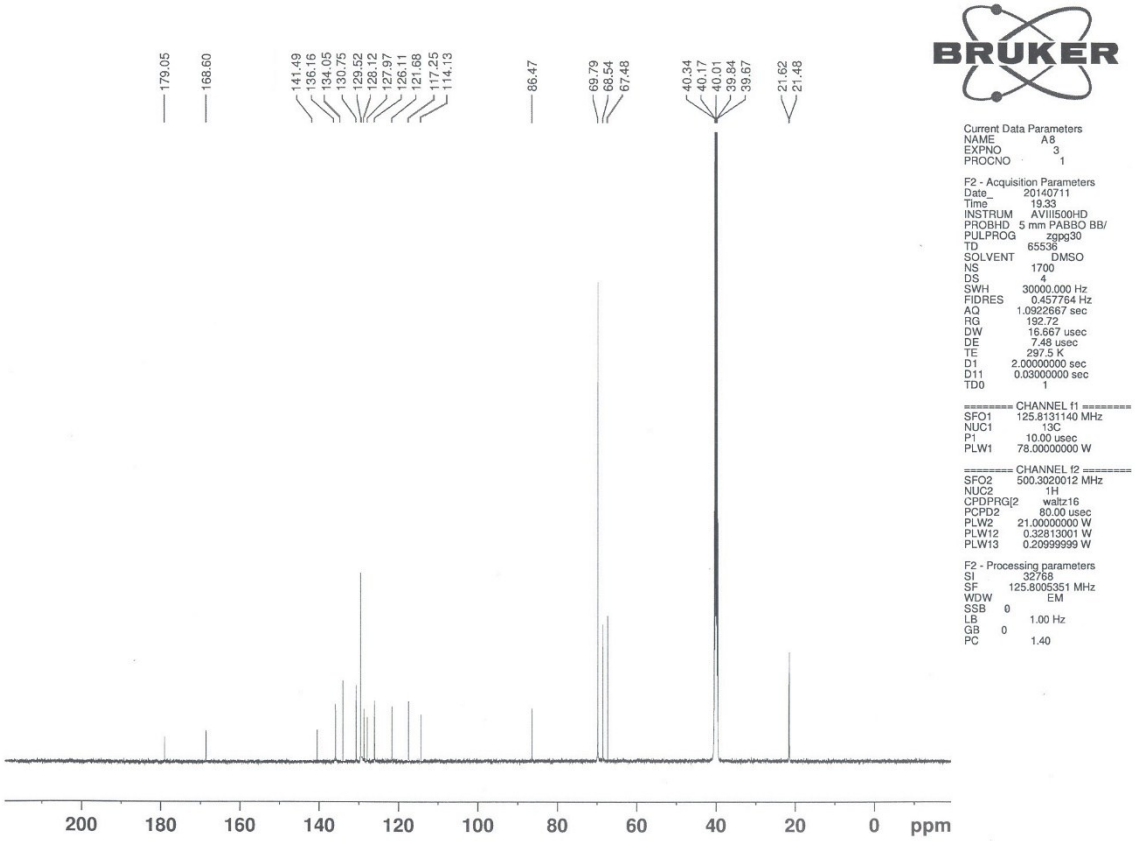
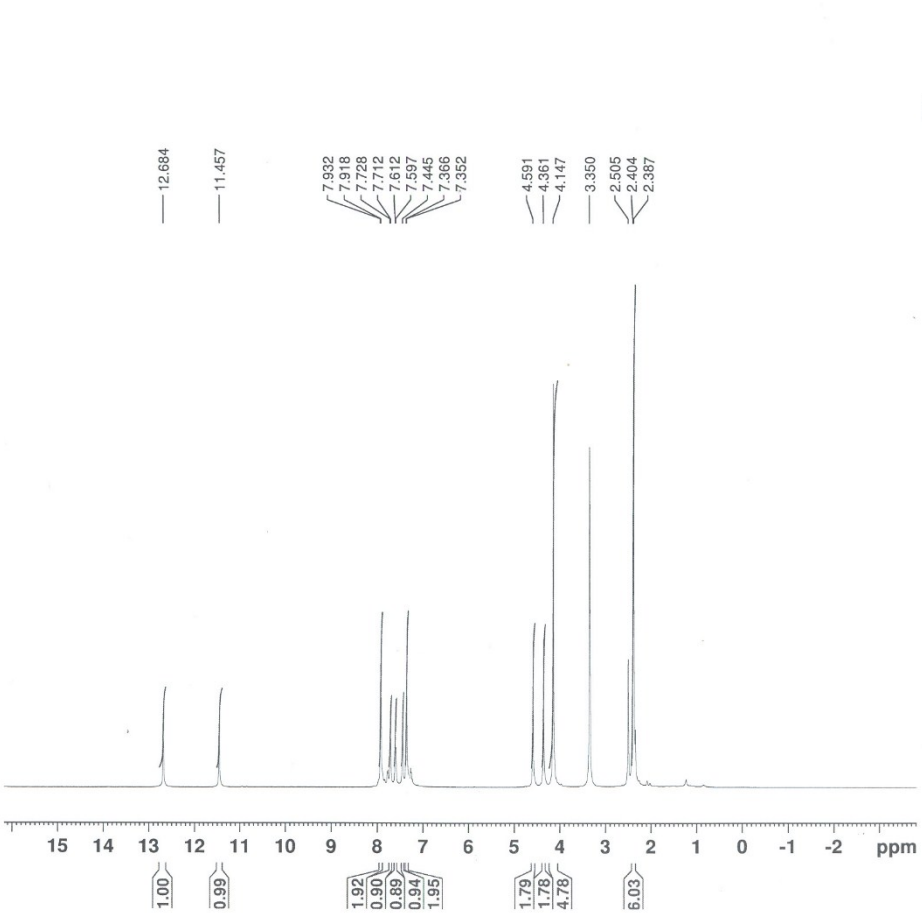


^{1}H-NMR Spectrum of A9



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DE 13.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

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P1 10.00 usec
PLW1 21.89999962 W

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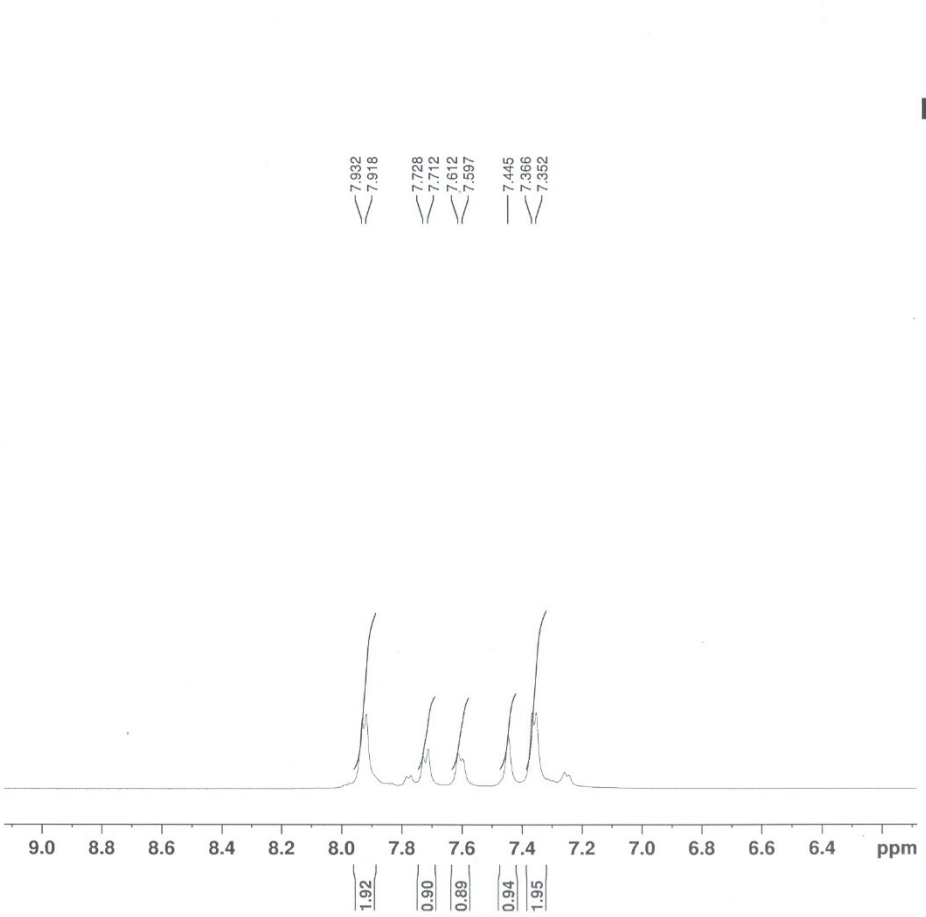
^{1}H-NMR Spectrum of A9



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FIDRES 0.152588 Hz
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RG 106.56
DW 50.000 usec
DE 13.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 10.00 usec
PLW1 21.89999962 W

F2 - Processing parameters
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^{13}C-NMR Spectrum of A9