

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

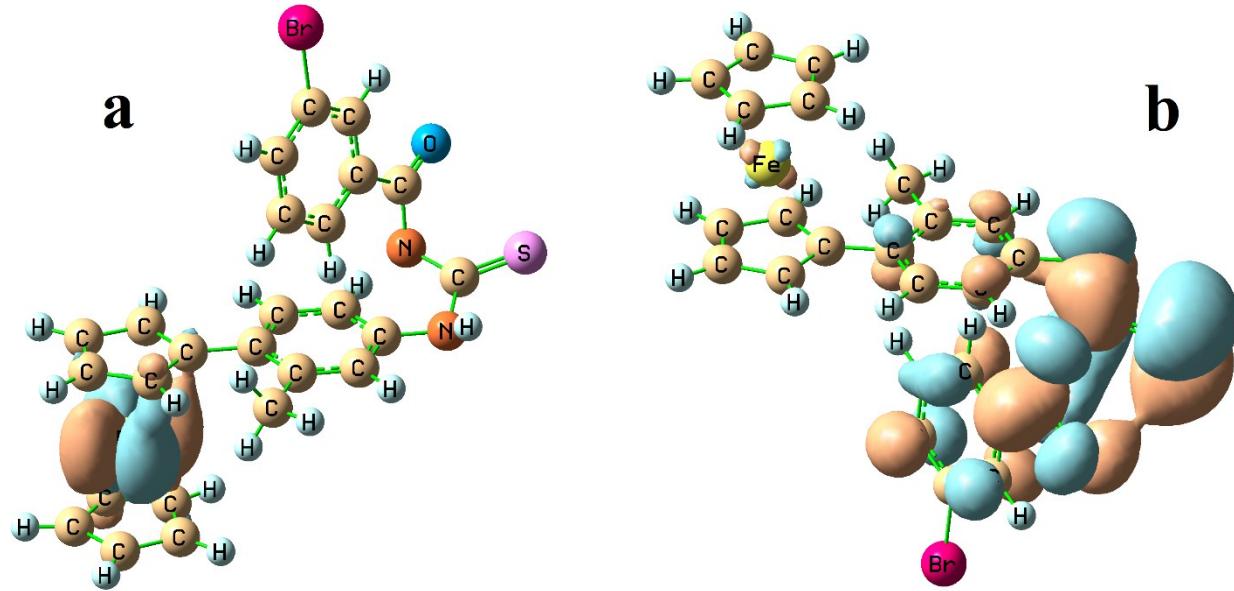


Figure S2. (a) Representative graphical demonstration of HOMO of **A5**. (b) Representative graphical demonstration of LUMO orbitals of **A5**.

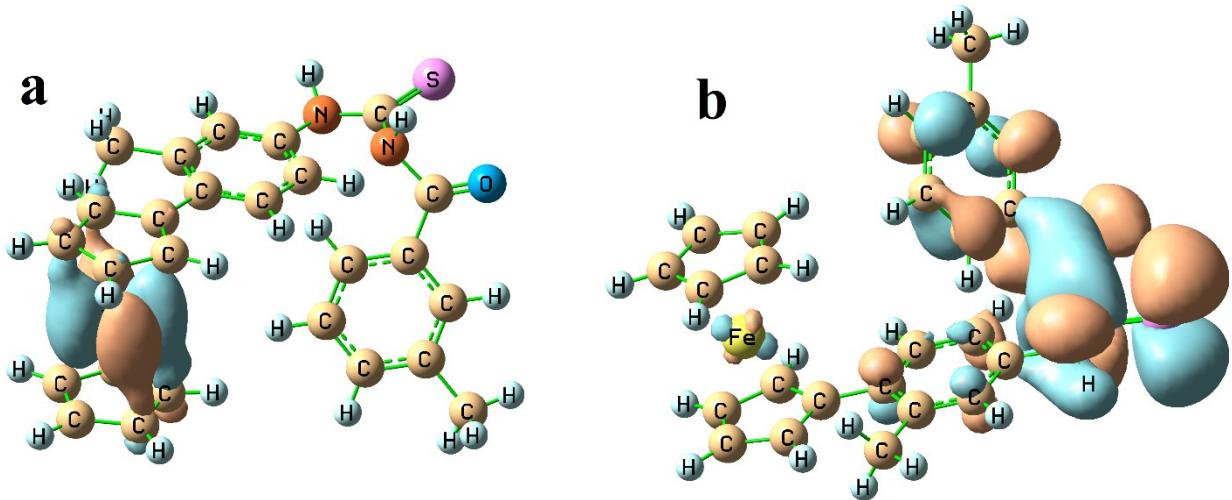


Figure S3. (a) Representative graphical demonstration of HOMO of **A8**. (b) Representative graphical demonstration of LUMO orbitals of **A8**.

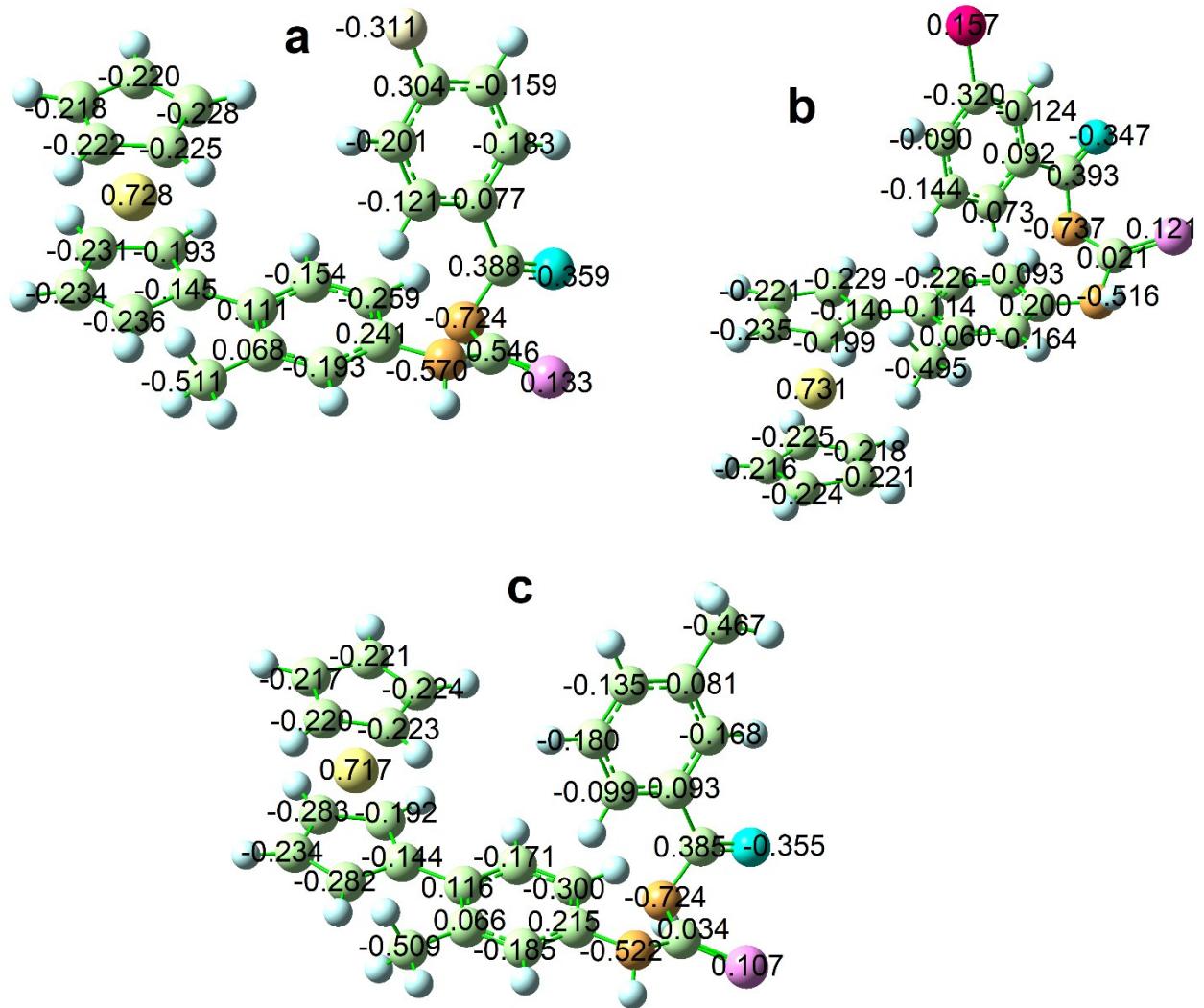


Figure S4. Graphical representation of charge distribution on the molecular structures (a) A3, (b) A5, and (c) A8.

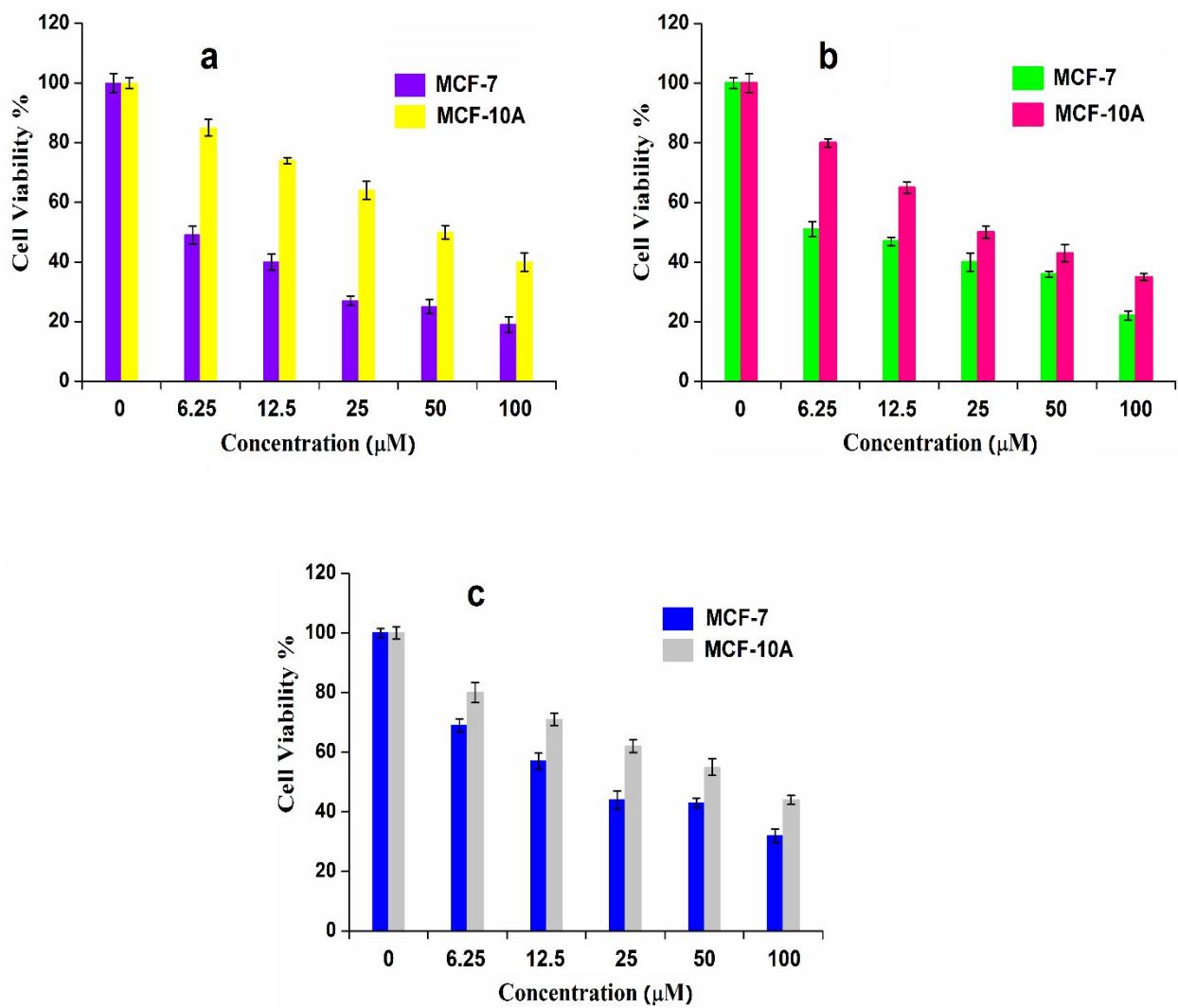


Figure S5. Cell viability (%) of cancerous and non-cancerous cells at various concentrations of (a) A3, (b) A5, and (c) A8, after 72 h of incubation.

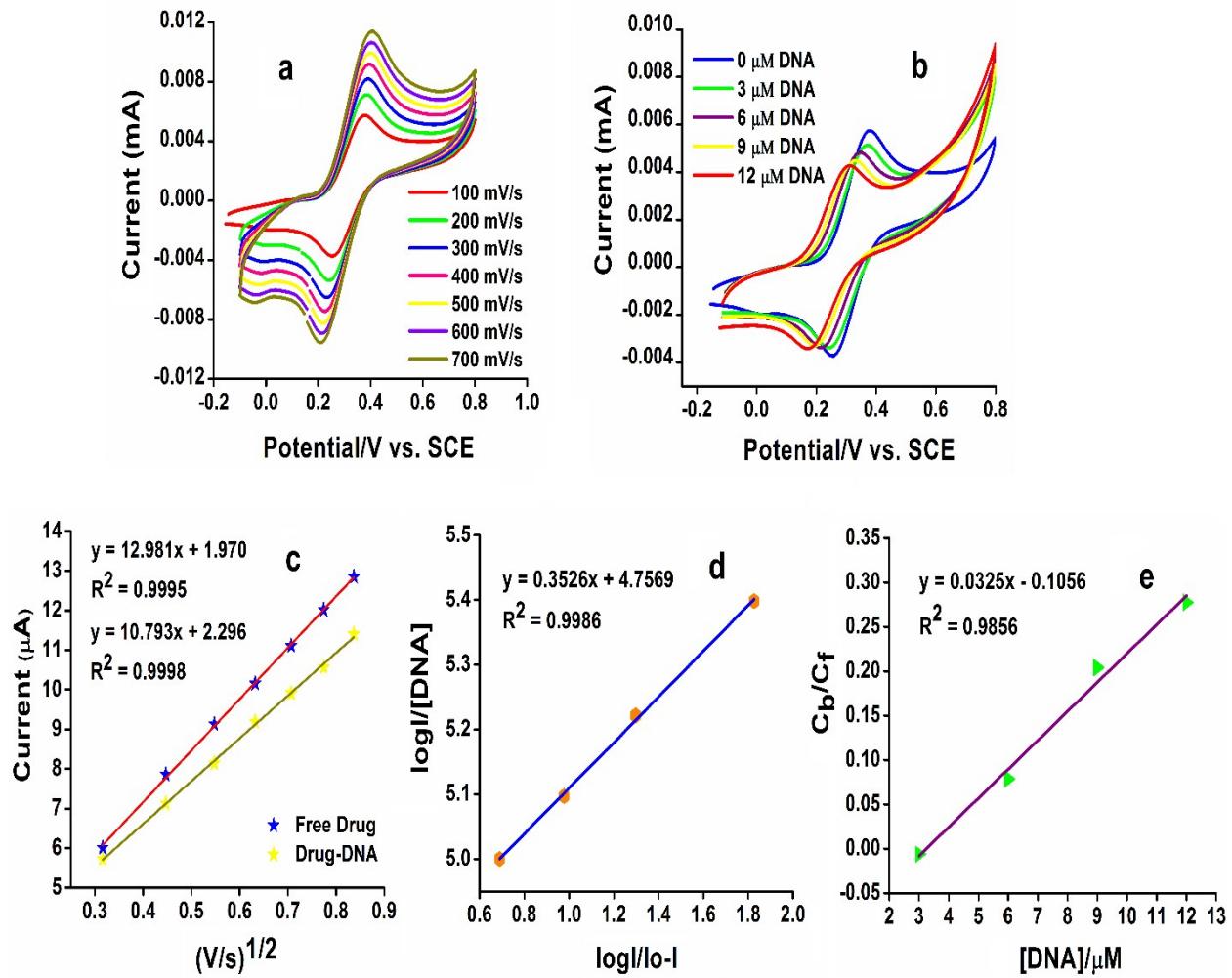


Figure S6. (a) Representative plots of Current vs. Potential/V (SCE) at different scan rates for **A8**. (b) Cyclic voltammogram of 1 mM **A8** with 1 mL of 0.5 M TBAP as supporting electrolyte in the absence and presence of 3-12 μM DNA showing a decrease in I from I_0 and a concentration dependent -ve shift in potential showing electrostatic interactions. (c) Representative plot of current vs. $(\text{V}/\text{s})^{1/2}$, for the determination of diffusion coefficient of free **A8** and **A8**-3 μM DNA. (d) Representative plot of $\log(I/I_0 - I)$ vs. $\log(1/\text{[DNA]})$ 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**.

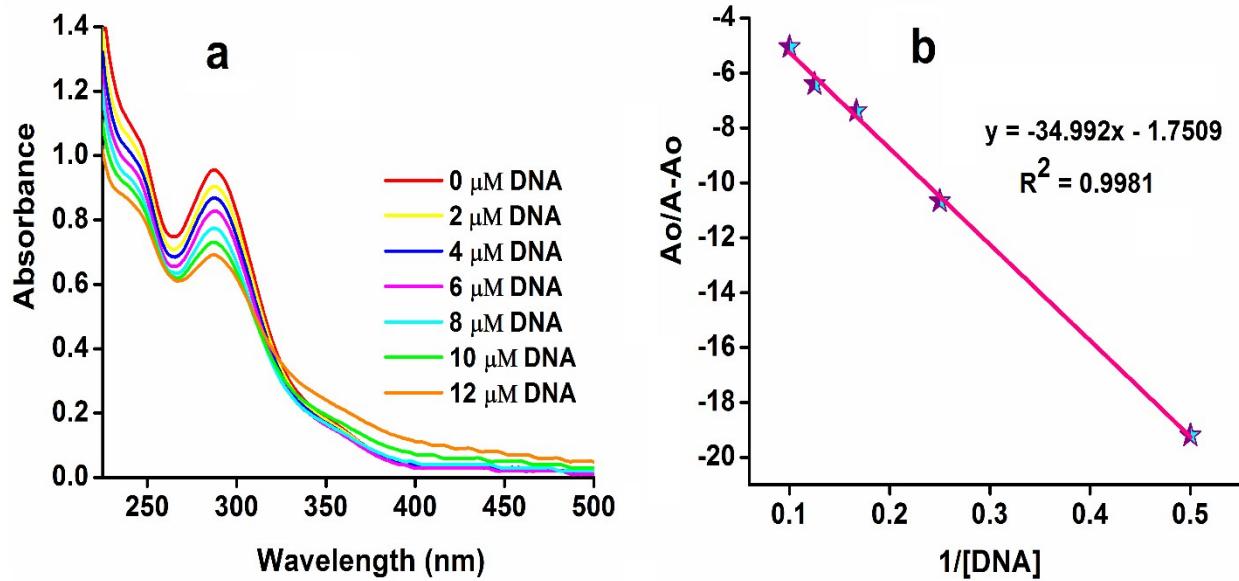


Figure S7. (a) Representative plots of absorbance *vs.* wavelength of 25 μM **A8** in ethanol with increasing concentration of DNA (2-12 μM). (b) Plot of $A_o/A - A_o$ *vs.* $1/[\text{DNA}]$ for determination of DNA binding constant of **A8**.

Table S1. Selected bond lengths [\AA] and angles [$^\circ$] for **A8**.

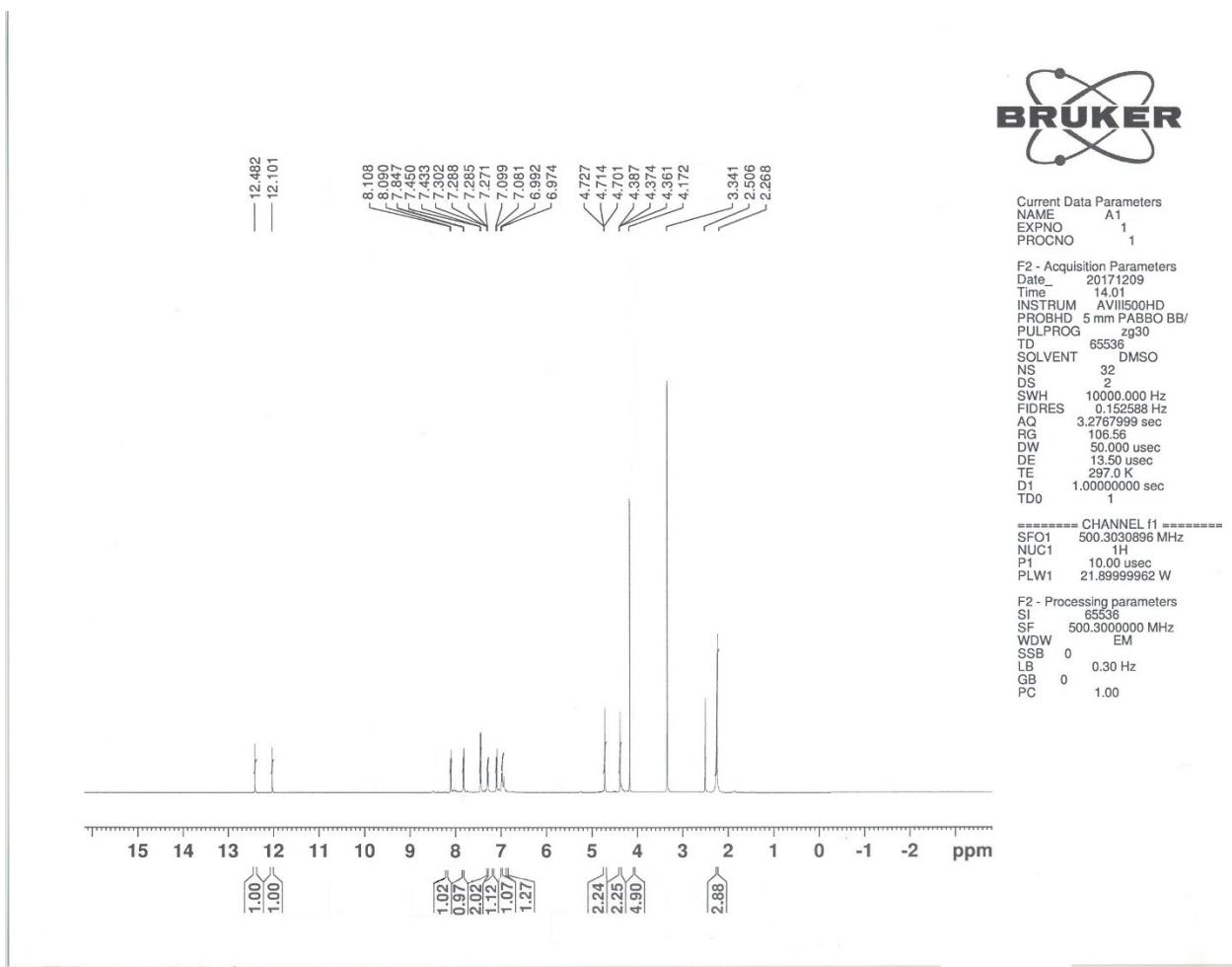
Bond Lengths (\AA)	
C(1)-C(2)	1.408(3)
C(6)-C(7)	1.415(3)
Fe(1)-C(5)	2.042(2)
Fe(1)-C(10)	2.056(17)
C(10)-C(11)	1.479(2)
C(11)-C(12)	1.392(2)
C(11)-C(16)	1.399(2)
N(1)-C(14)	1.423(2)
N(1)-C(18)	1.324(2)
S(1)-C(18)	1.659(18)
N(2)-C(18)	1.392(2)
N(2)-C(19)	1.377(2)
O(1)-C(19)	1.217(2)
C(19)-C(20)	1.486(2)
C(22)-C(26)	1.502(3)

Bond Angles ($^\circ$)	
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)

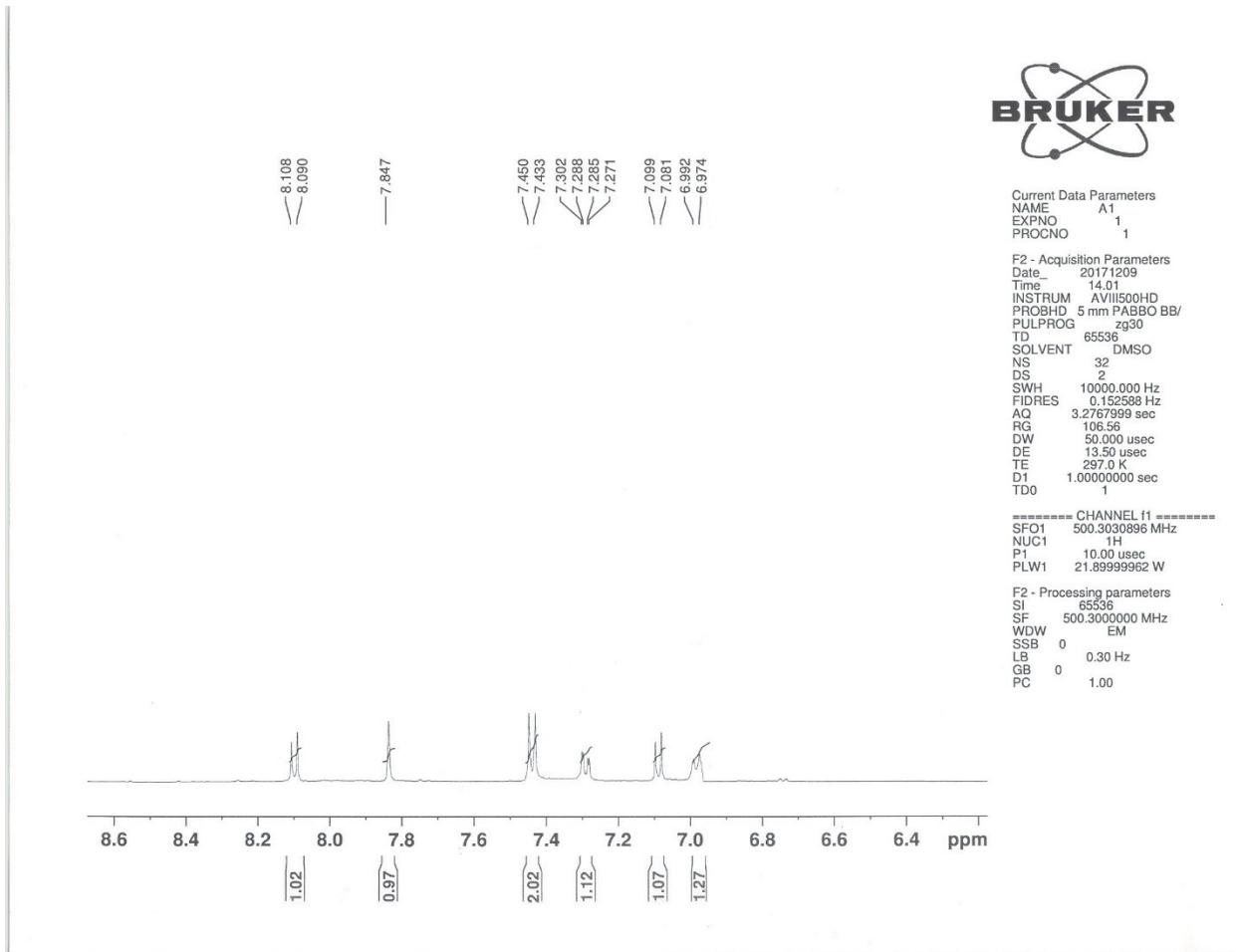
Table S2. The intramolecular and intermolecular hydrogen bond interactions in **A8**.

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

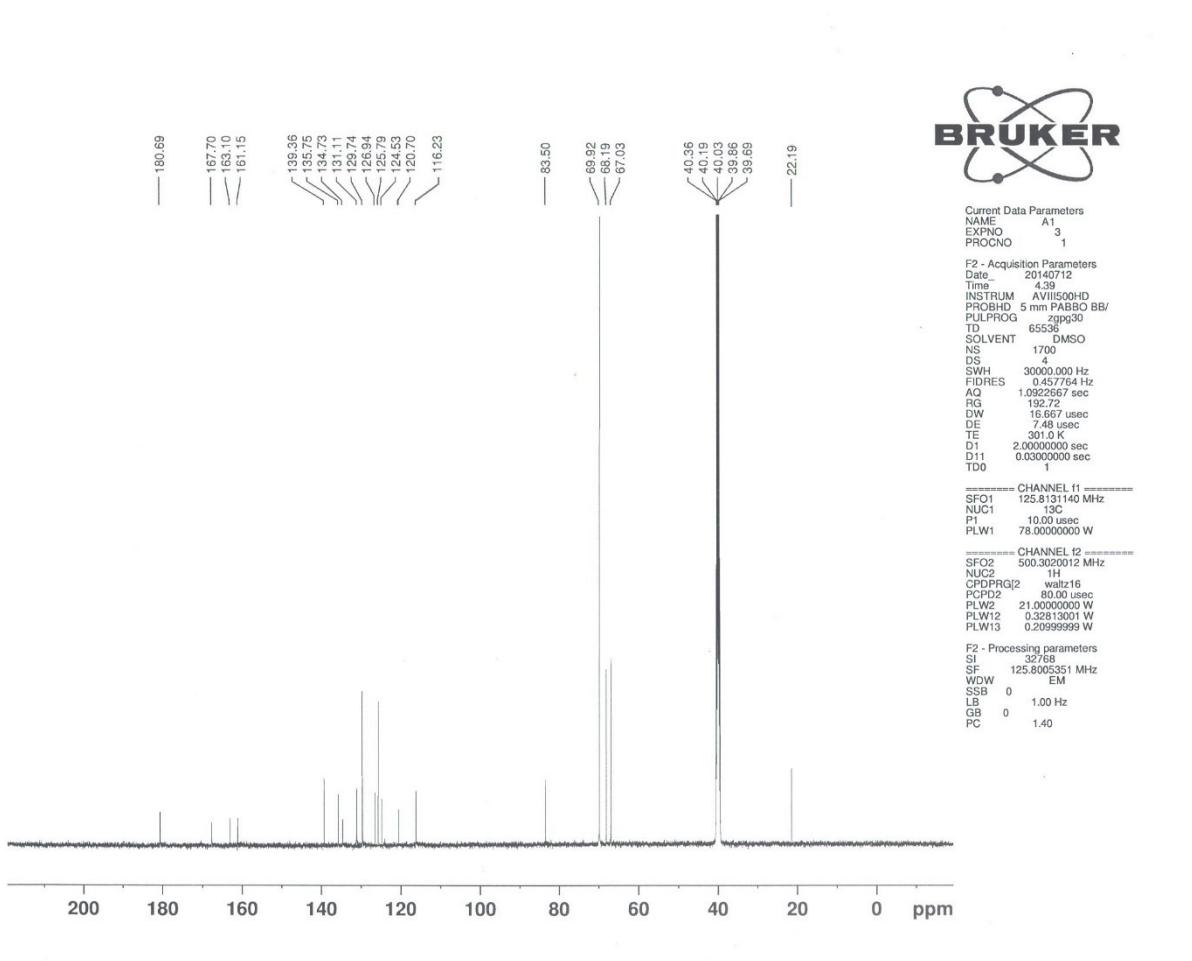
¹H-NMR Spectrum of A1



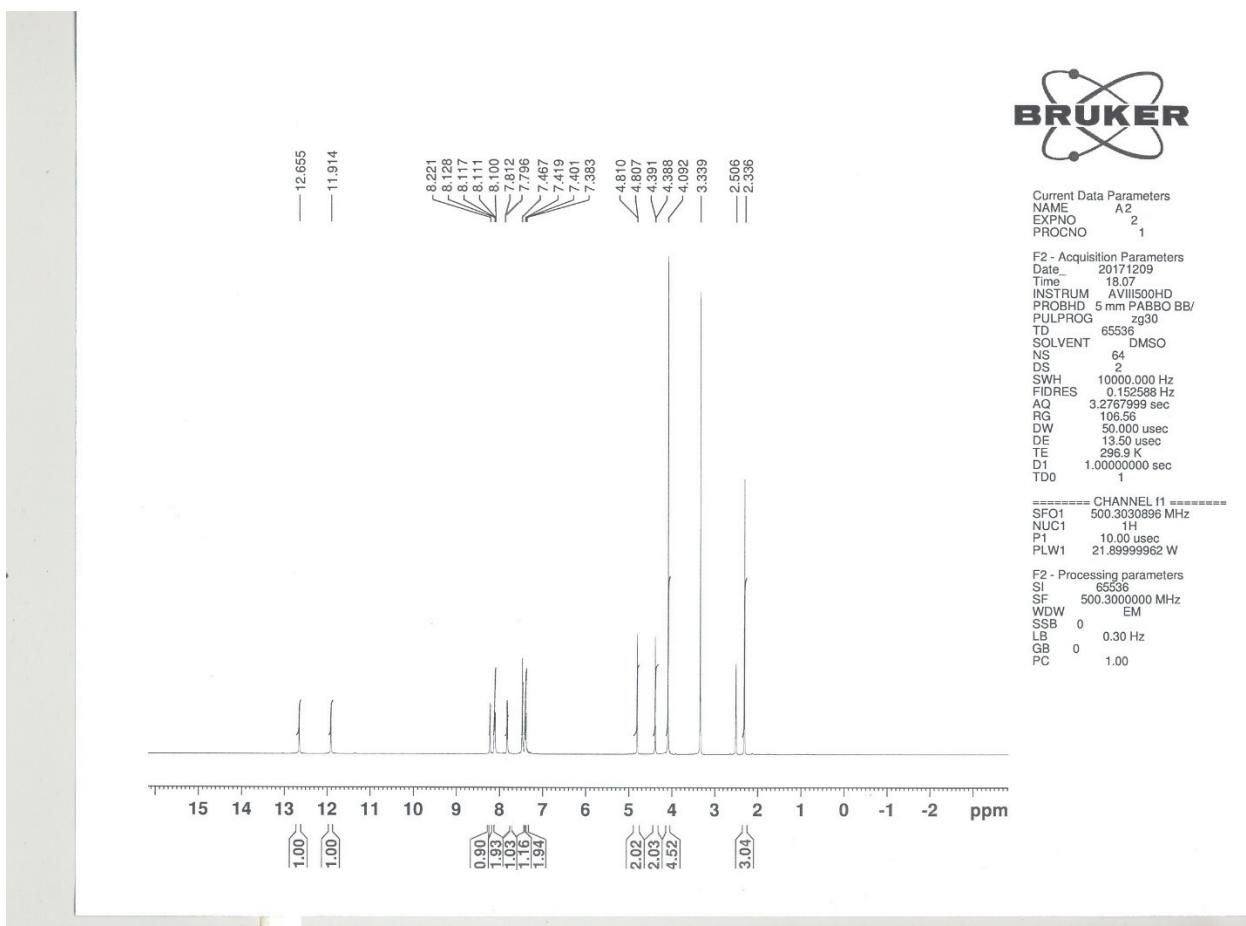
¹H-NMR Spectrum of A1



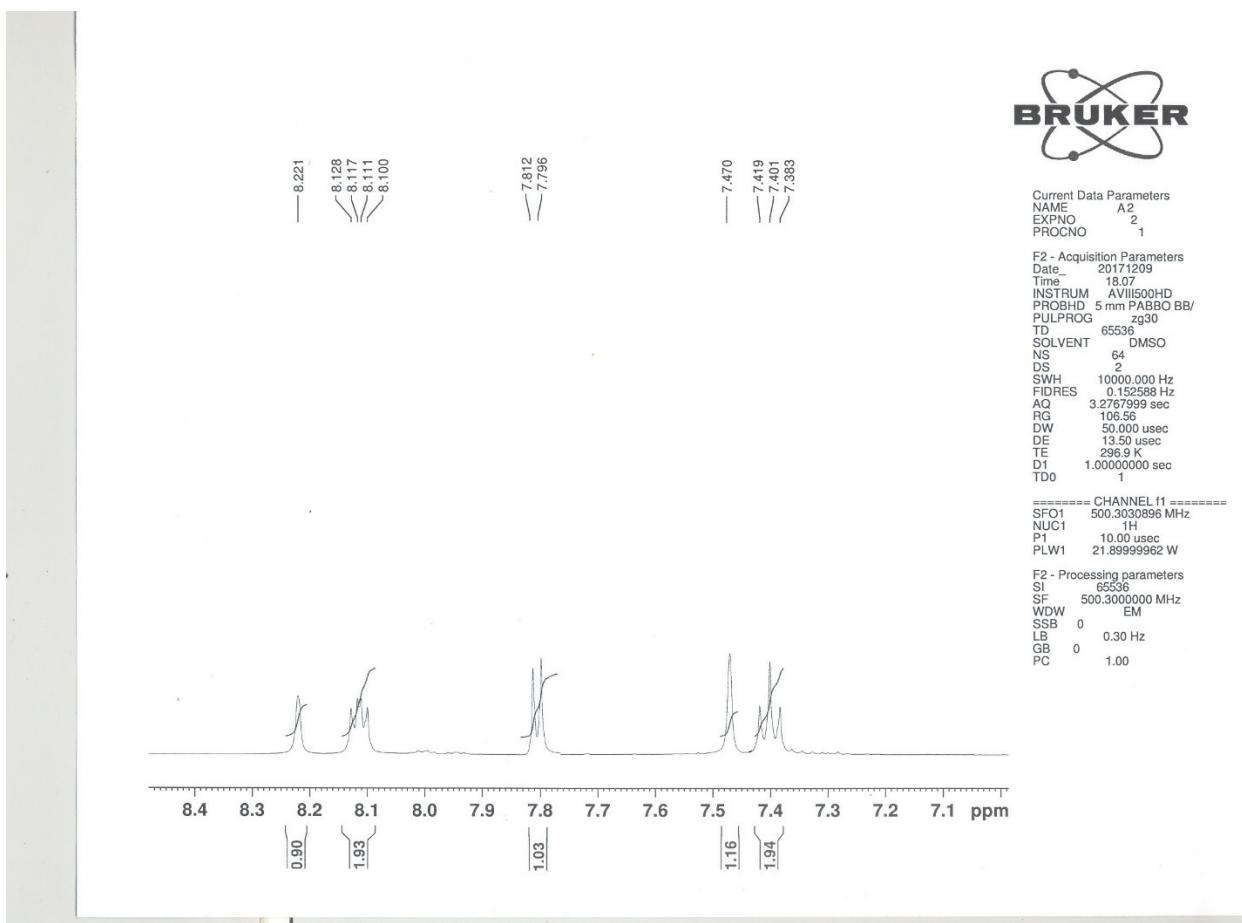
¹³C-NMR Spectrum of A1



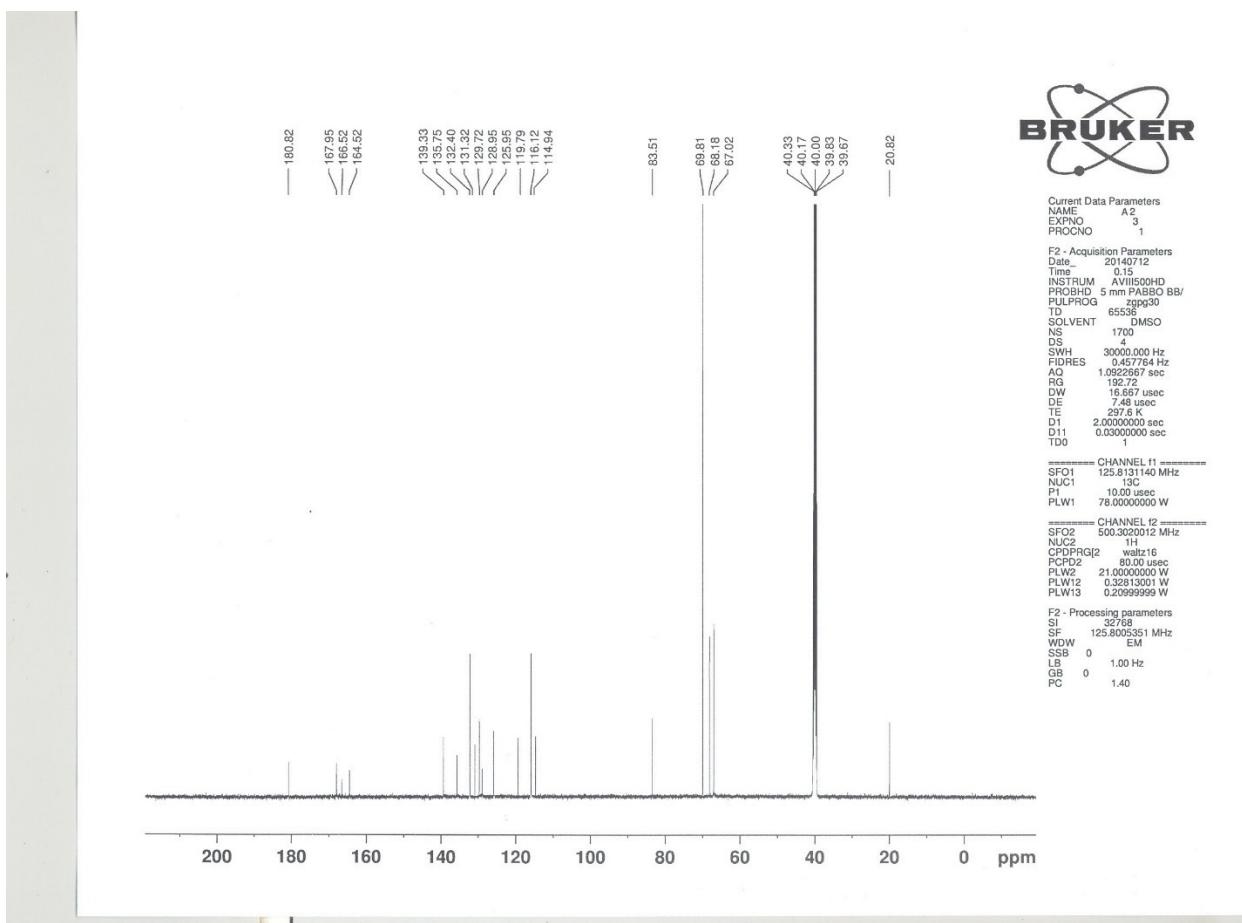
¹H-NMR Spectrum of A2



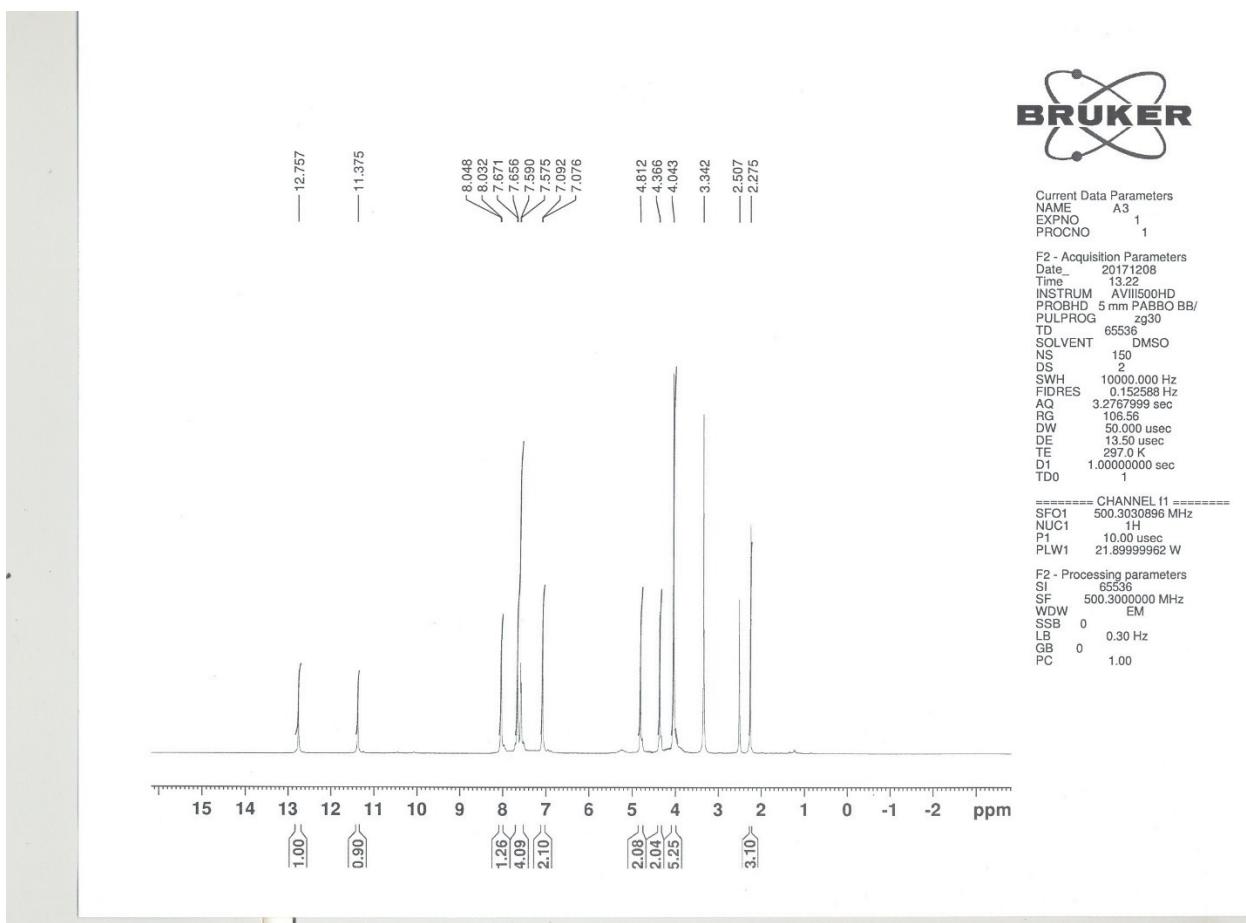
¹H-NMR Spectrum of A2



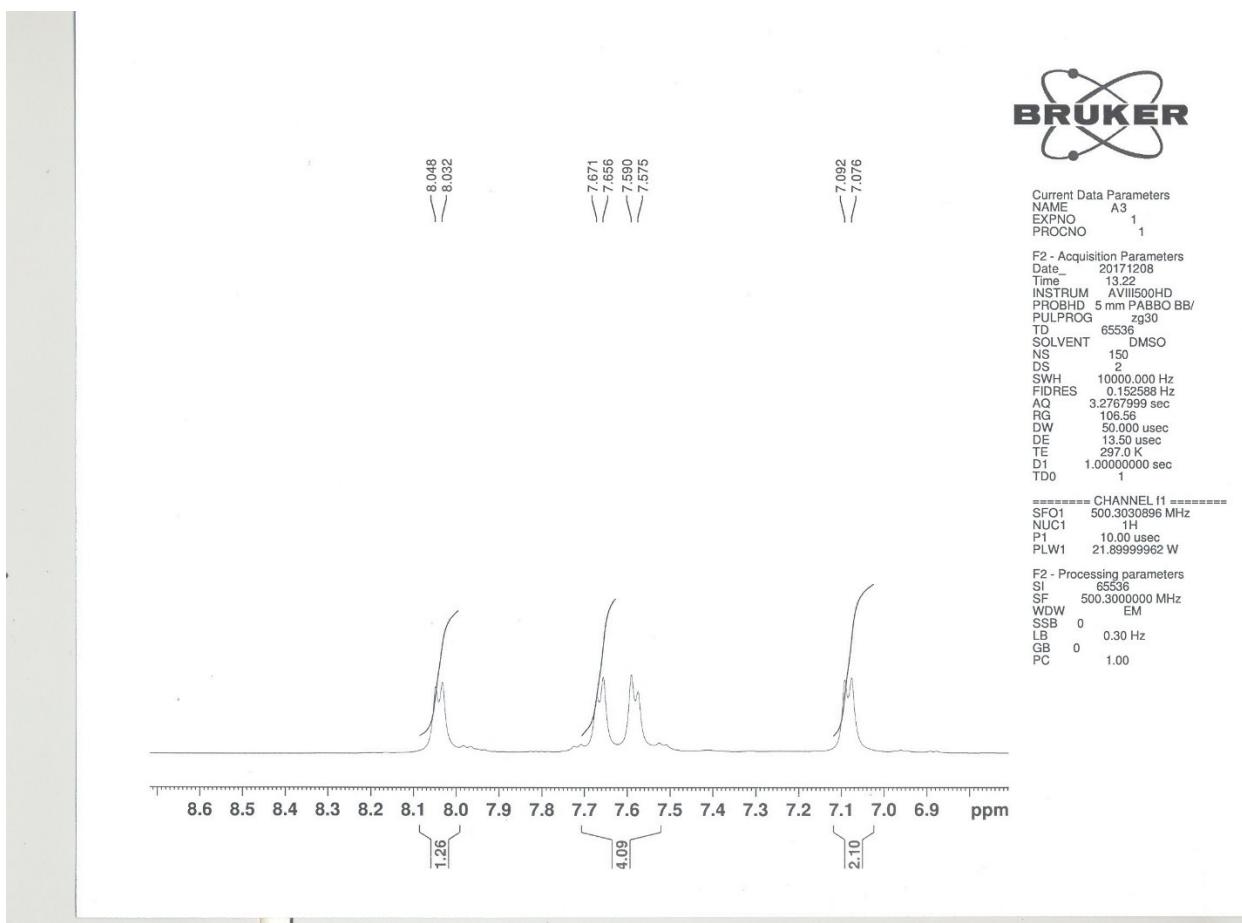
¹³C-NMR Spectrum of A2



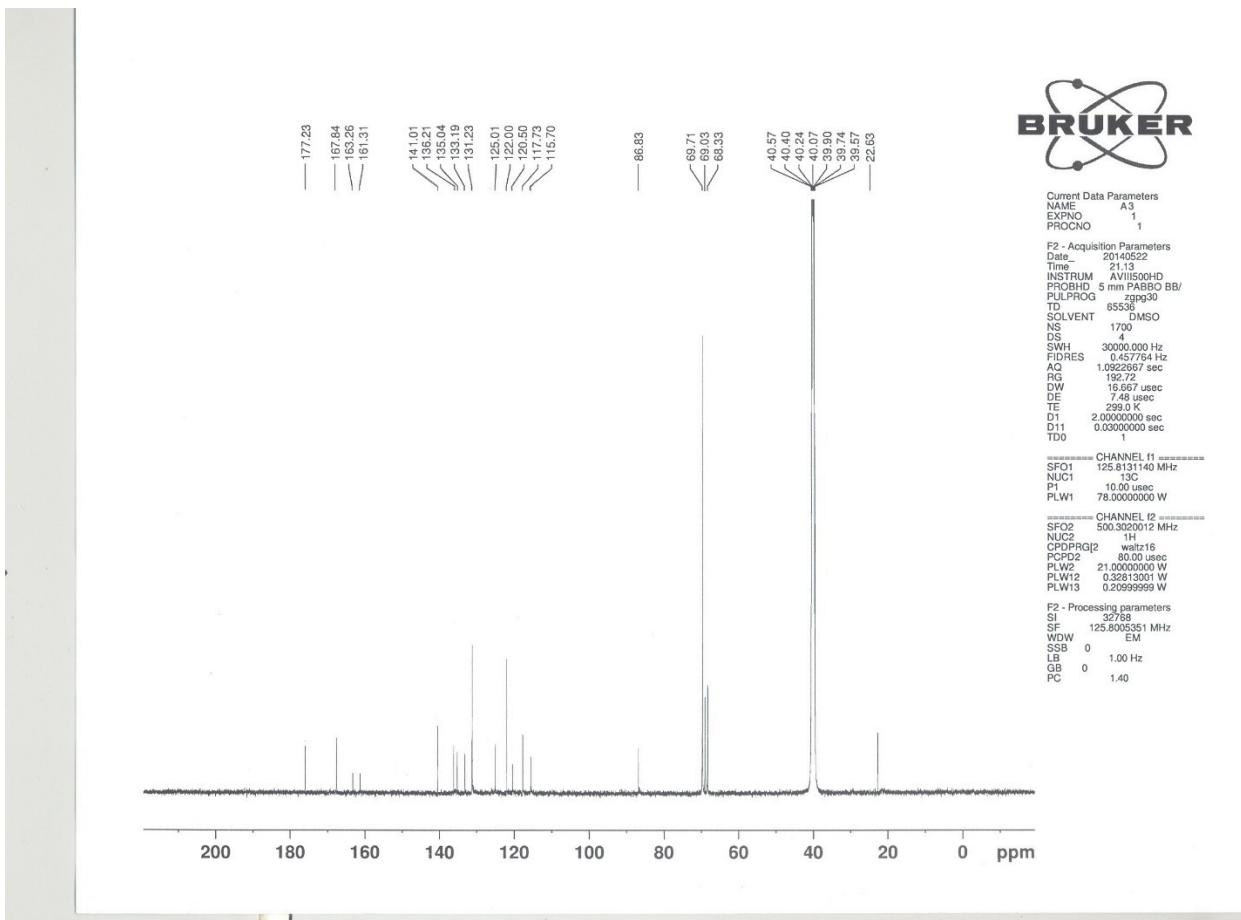
¹H-NMR Spectrum of A3



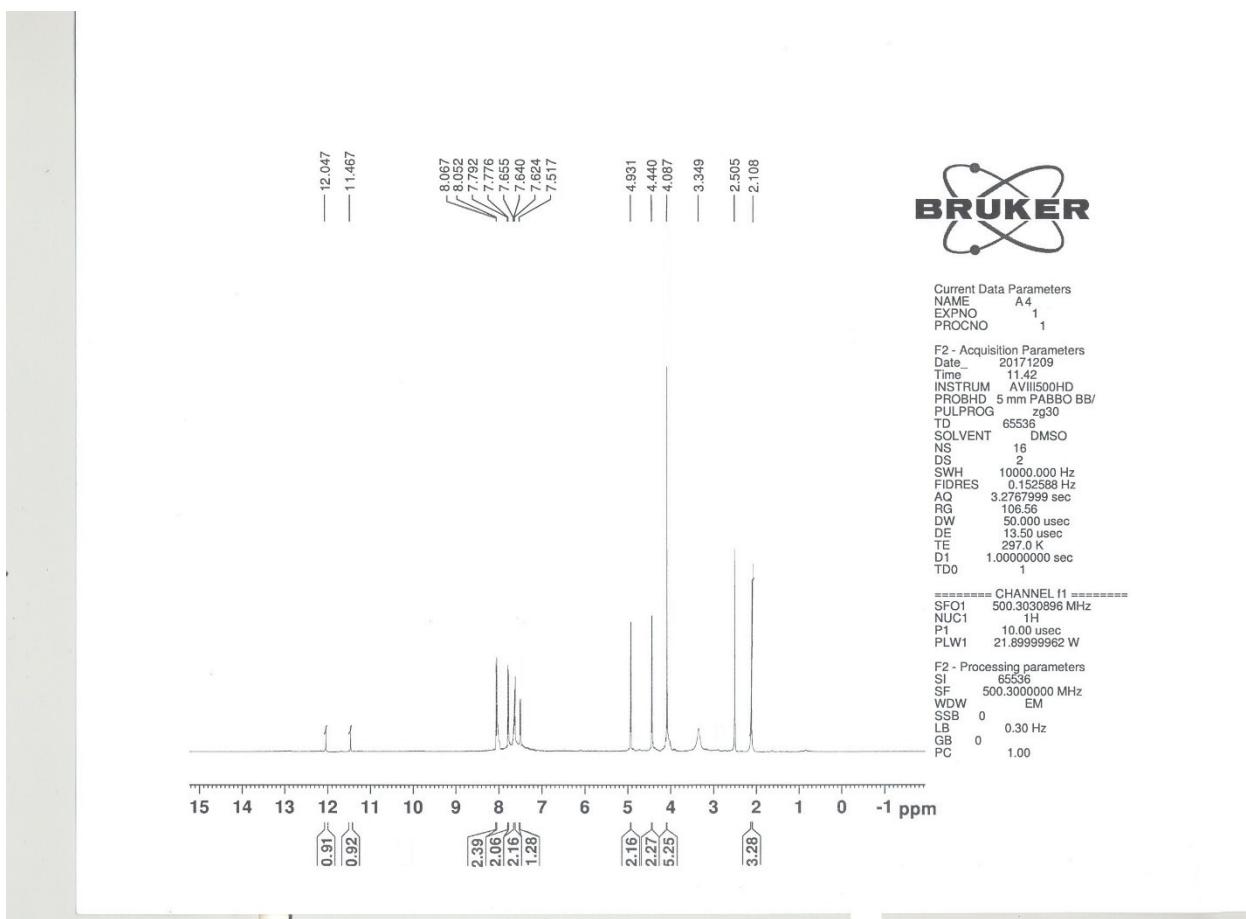
¹H-NMR Spectrum of A3



¹³C-NMR Spectrum of A3



¹H-NMR Spectrum of A4



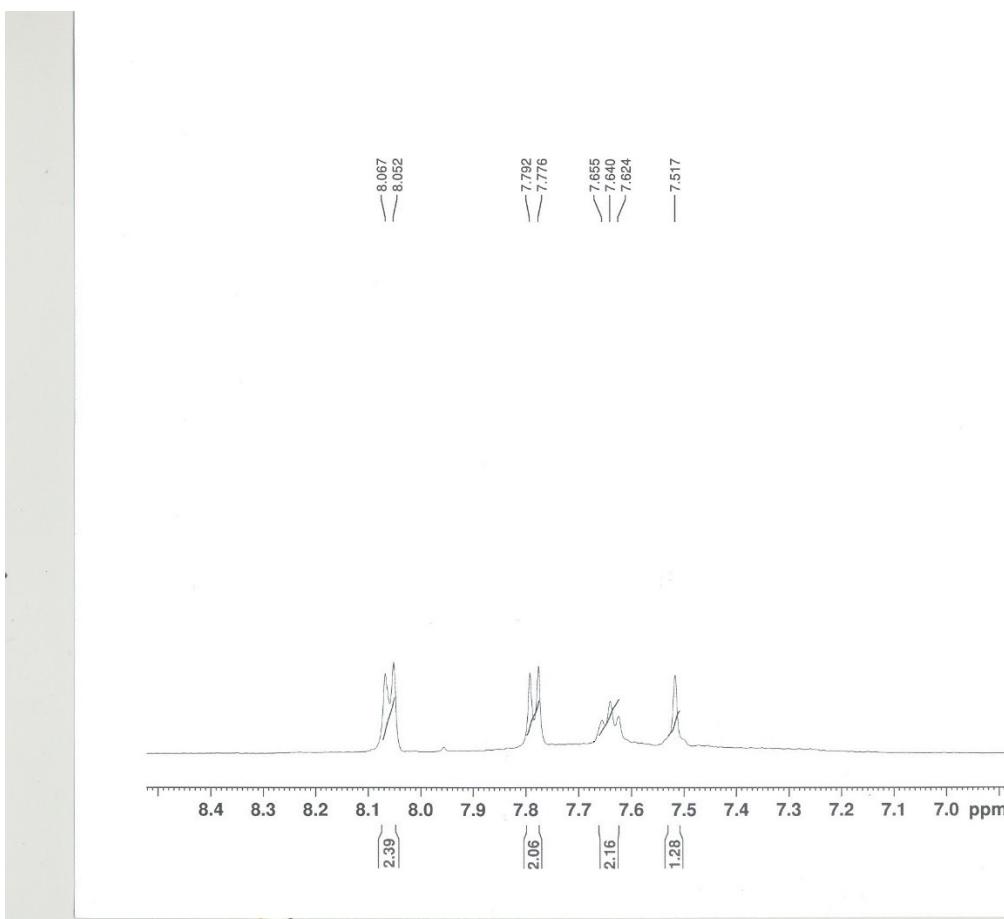
¹H-NMR Spectrum of A4



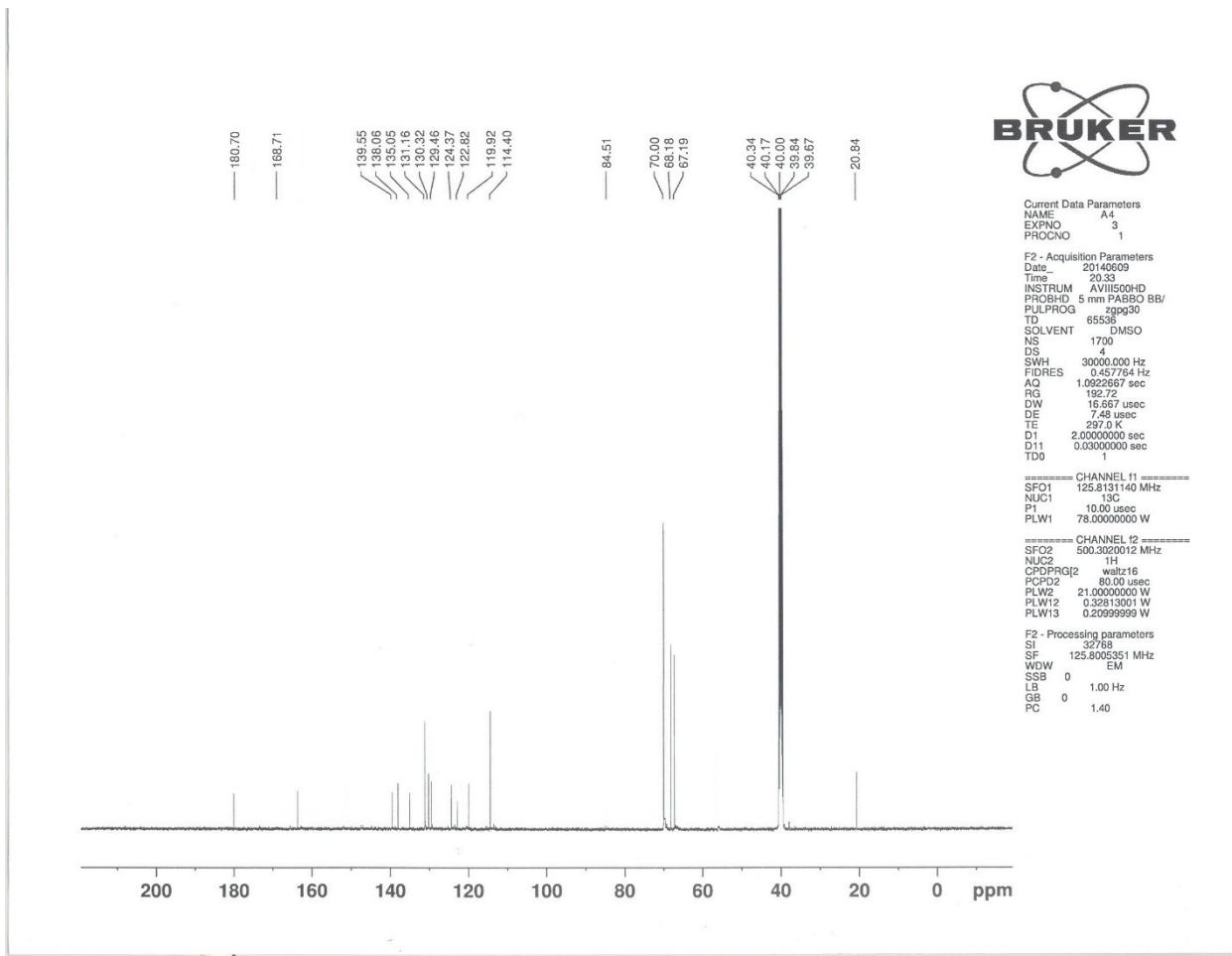
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PROCNO 1

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PULPROG zg30
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SOLVENT DMSO
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DS 2
SWH 10000.000 Hz
FIDRES 0.152581 Hz
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RG 108.56
DW 50.000 usec
DE 13.50 usec
TE 297.0 K
D1 1.0000000 sec
TD0 1

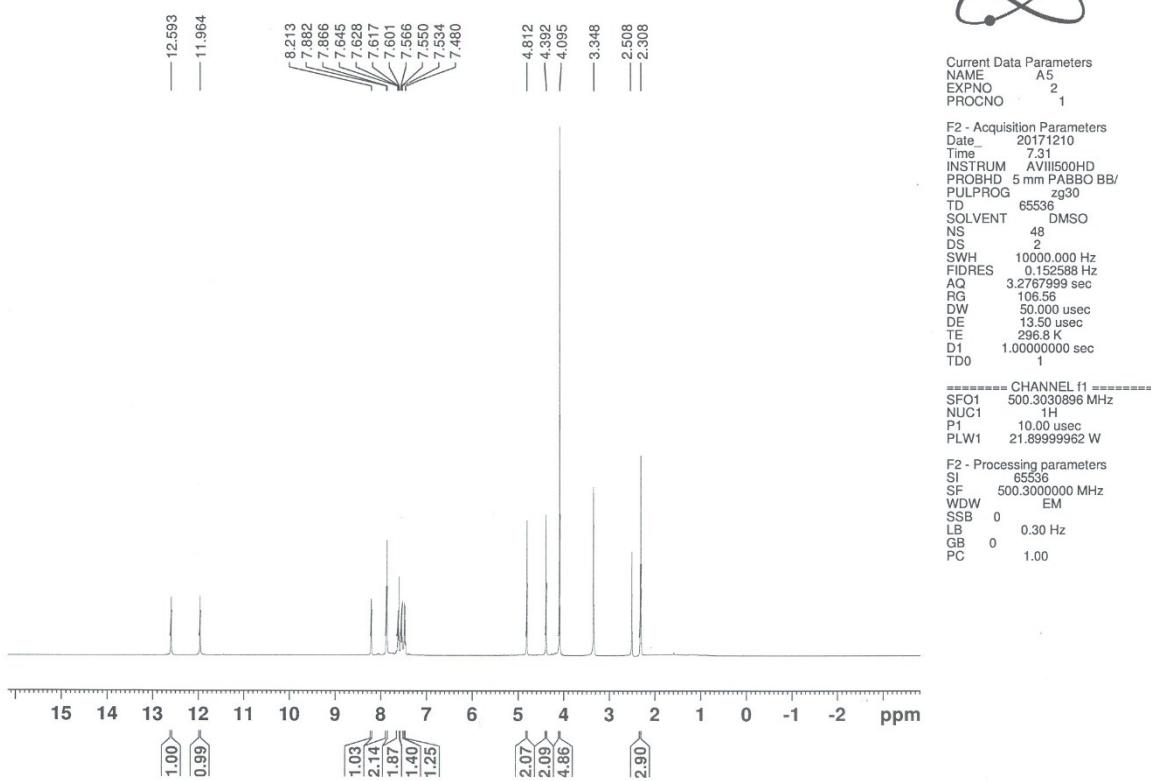
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NUC1 1H
P1 10.00 usec
PLW1 21.89999962 W
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SF 500.3000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C-NMR Spectrum of A4



¹H-NMR Spectrum of A5



¹H-NMR Spectrum of A5

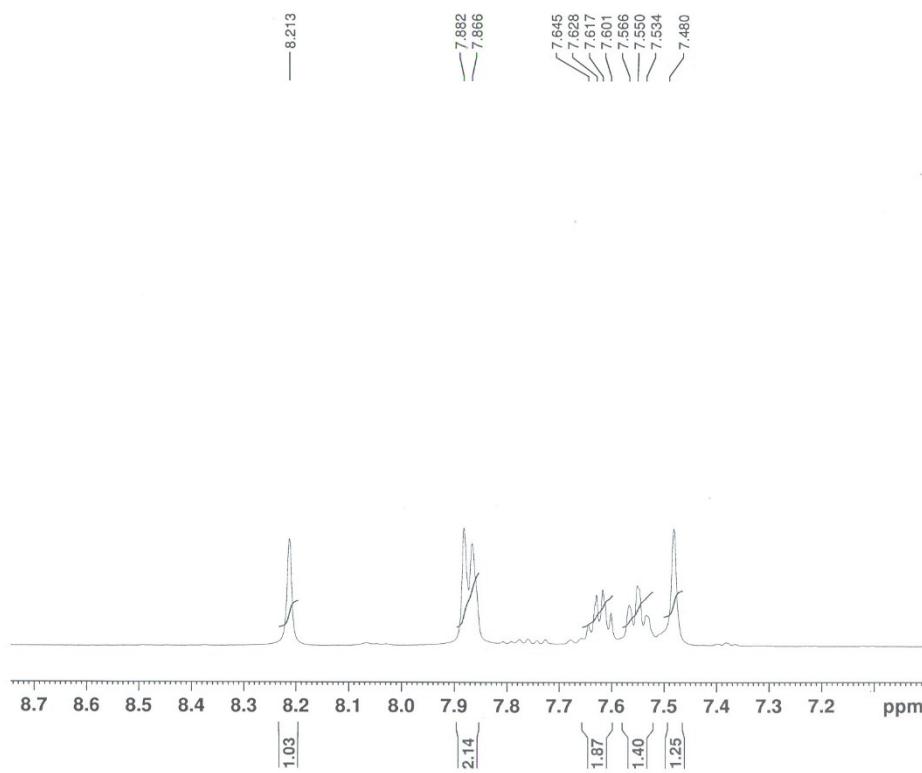


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PROCNO 1

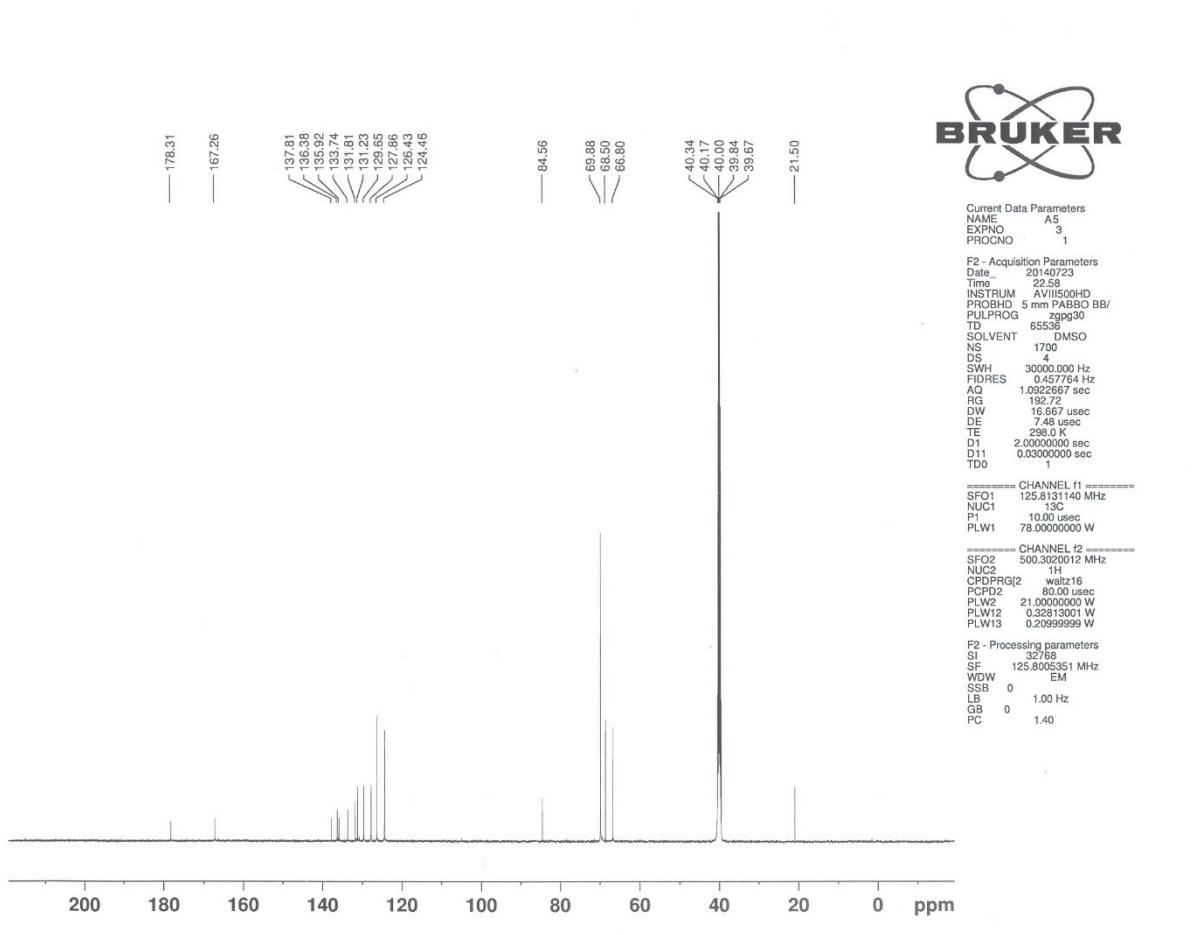
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SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 106.56
DW 50.000 usec
DE 13.50 usec
TE 296.8 K
D1 1.0000000 sec
TD0 1

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P1 10.00 usec
PLW1 21.89999962 W

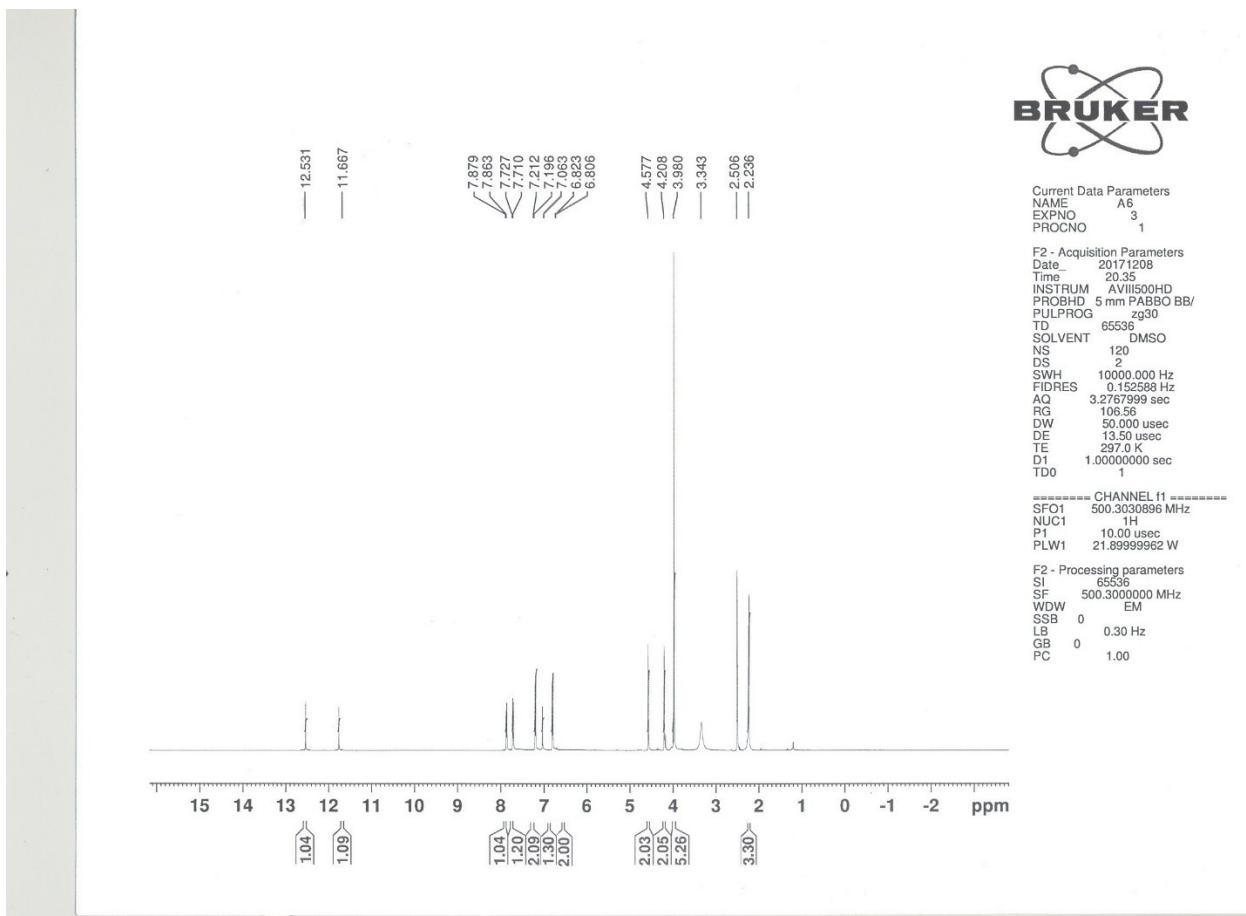
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LB 0.30 Hz
GB 0
PC 1.00



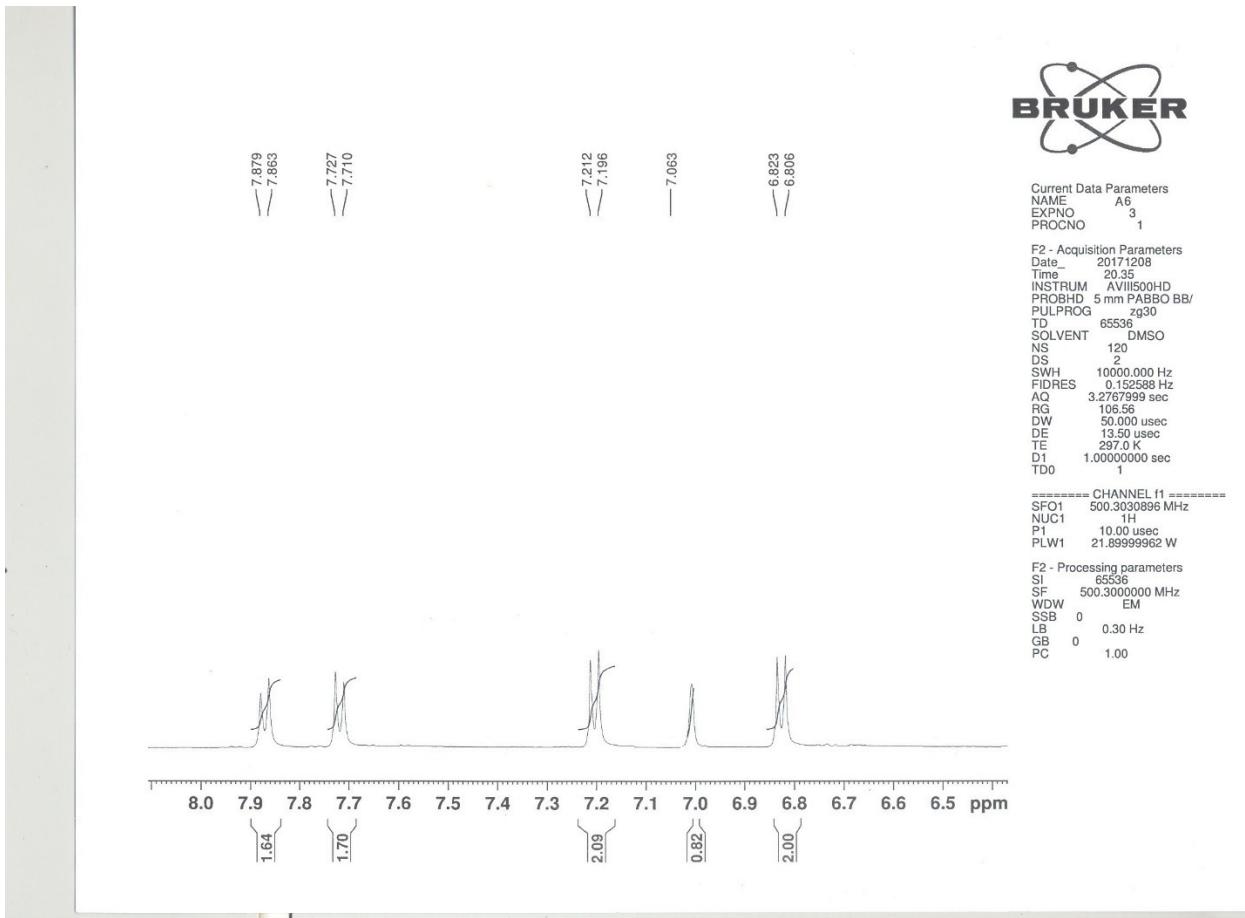
¹³C-NMR Spectrum of A5



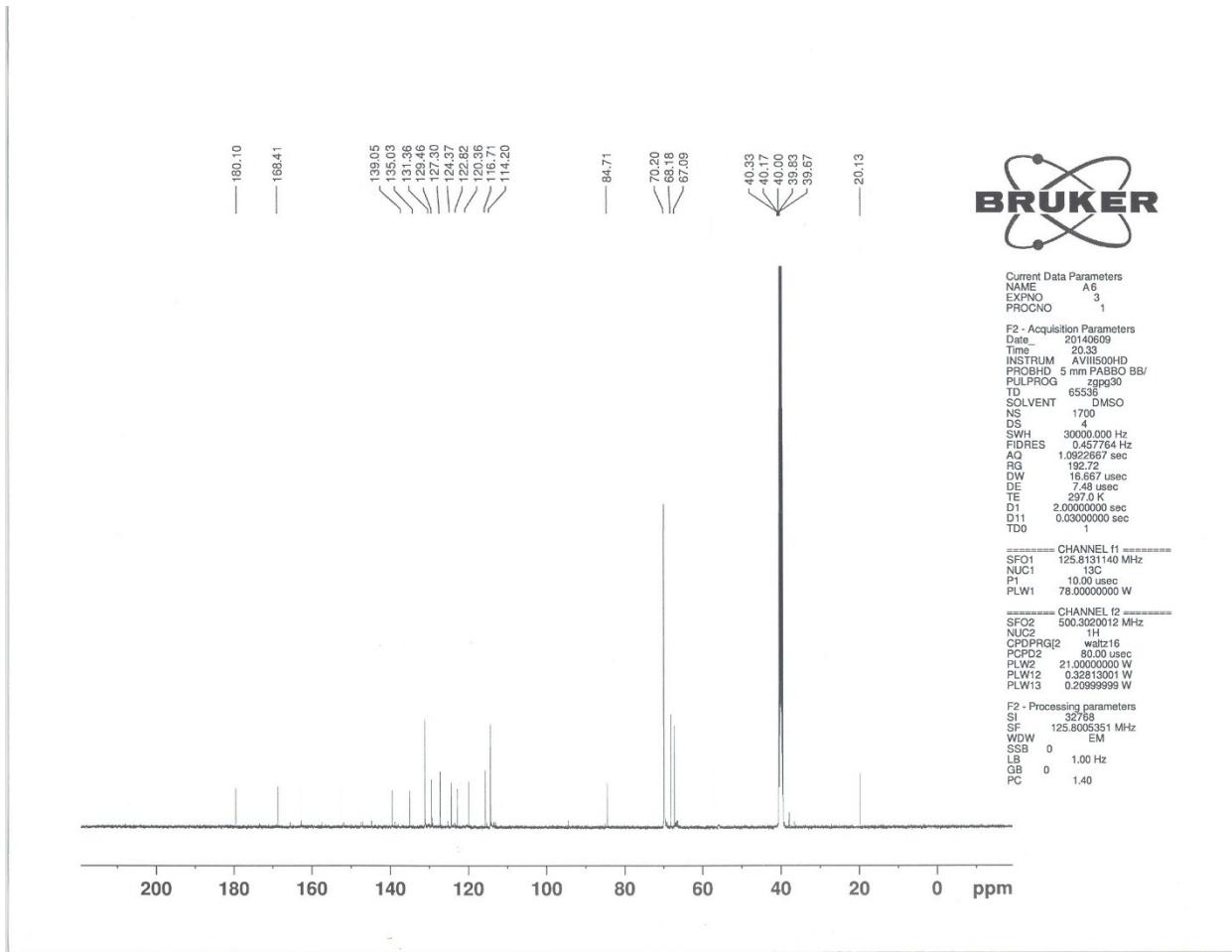
¹H-NMR Spectrum of A6



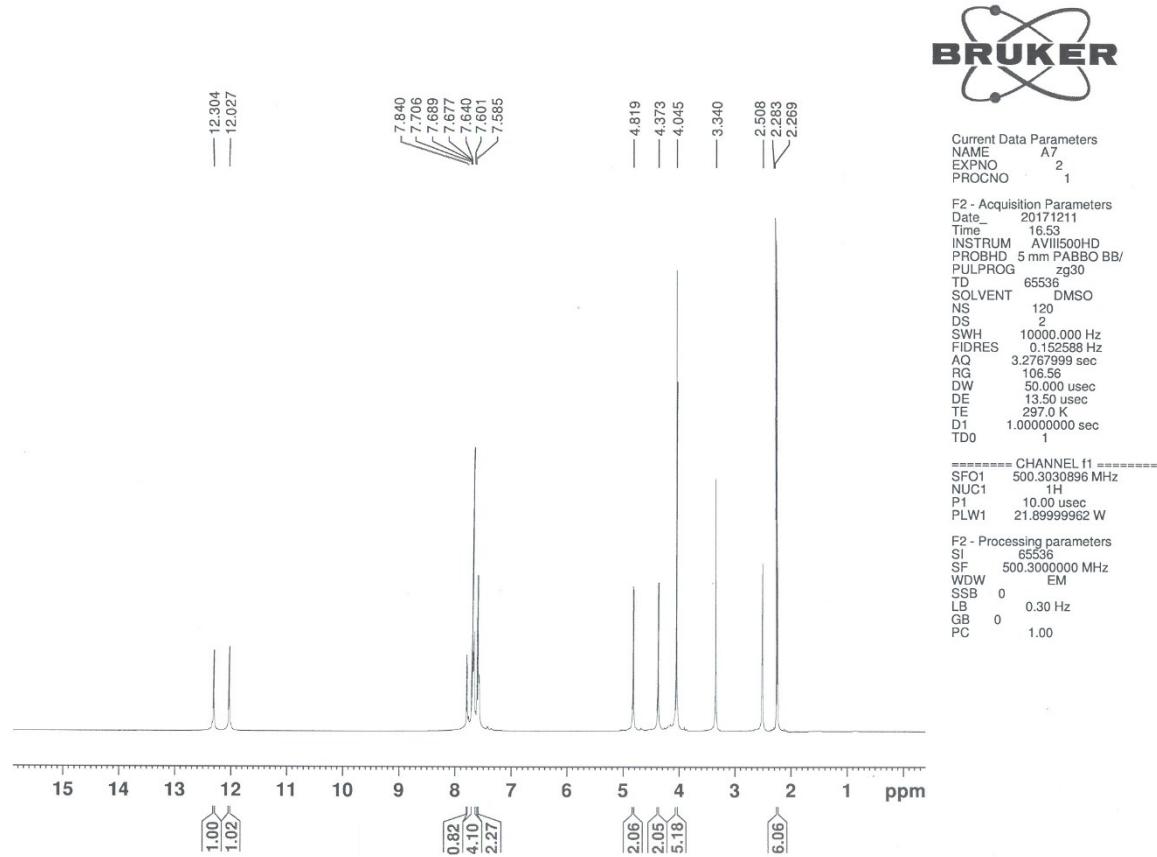
¹H-NMR Spectrum of A6



¹³C-NMR Spectrum of A6



¹H-NMR Spectrum of A7



¹H-NMR Spectrum of A7

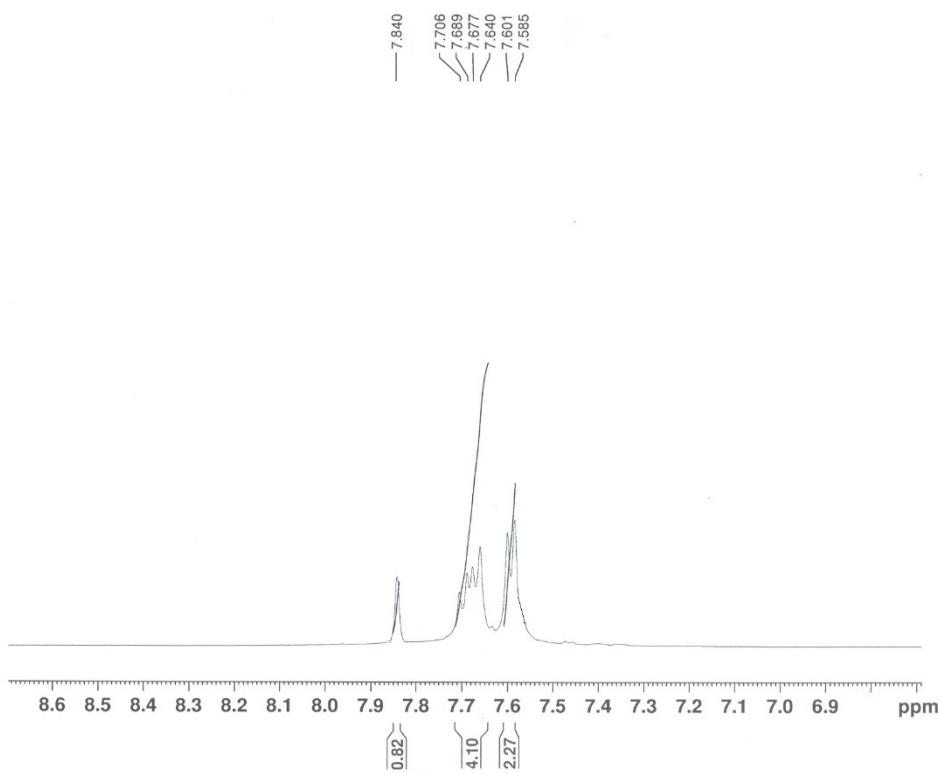


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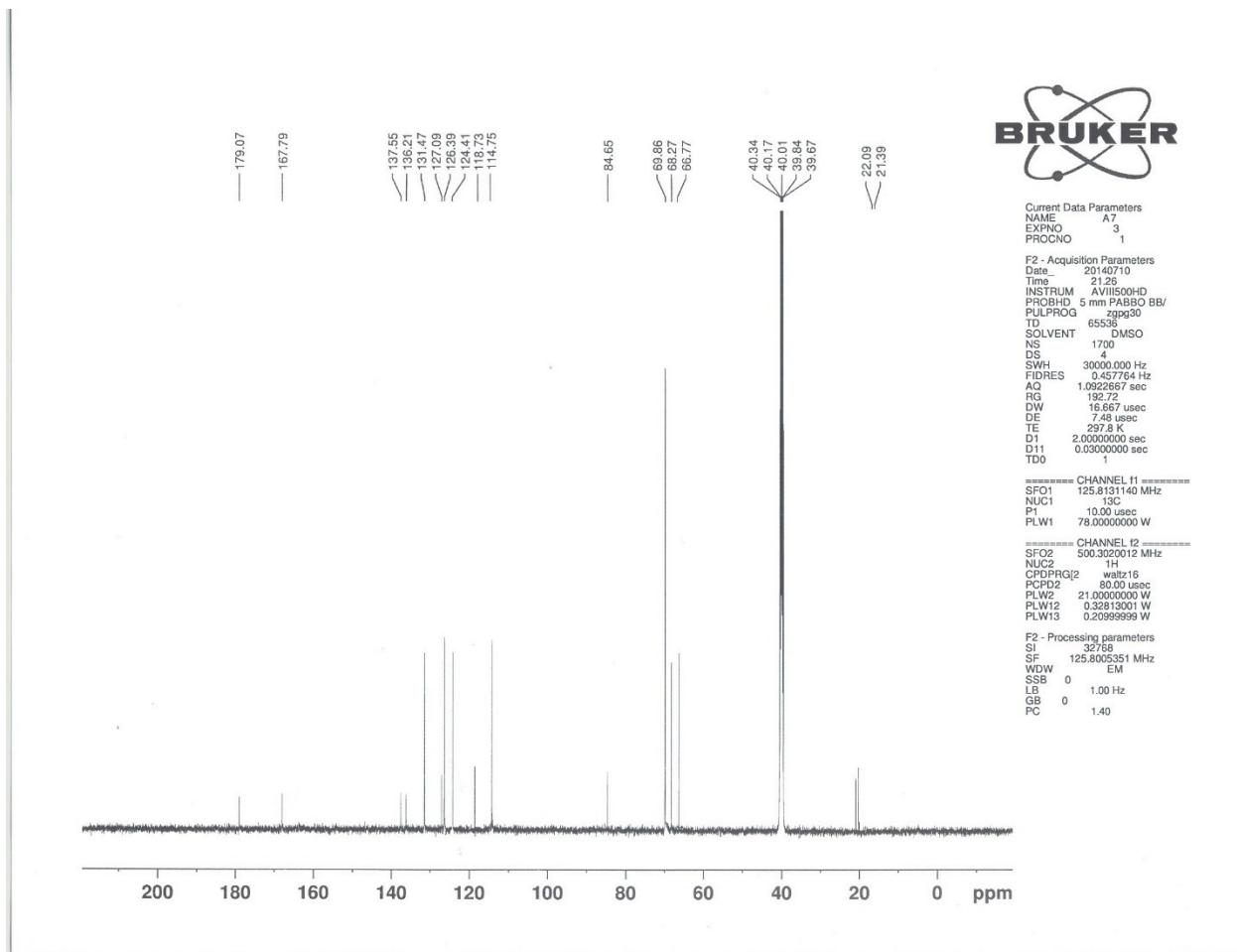
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TD 65536
SOLVENT DMSO
NS 120
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 106.56
DW 50.000 usec
DE 13.50 usec
TE 297.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 ¹H
P1 10.00 usec
PLW1 21.89999962 W

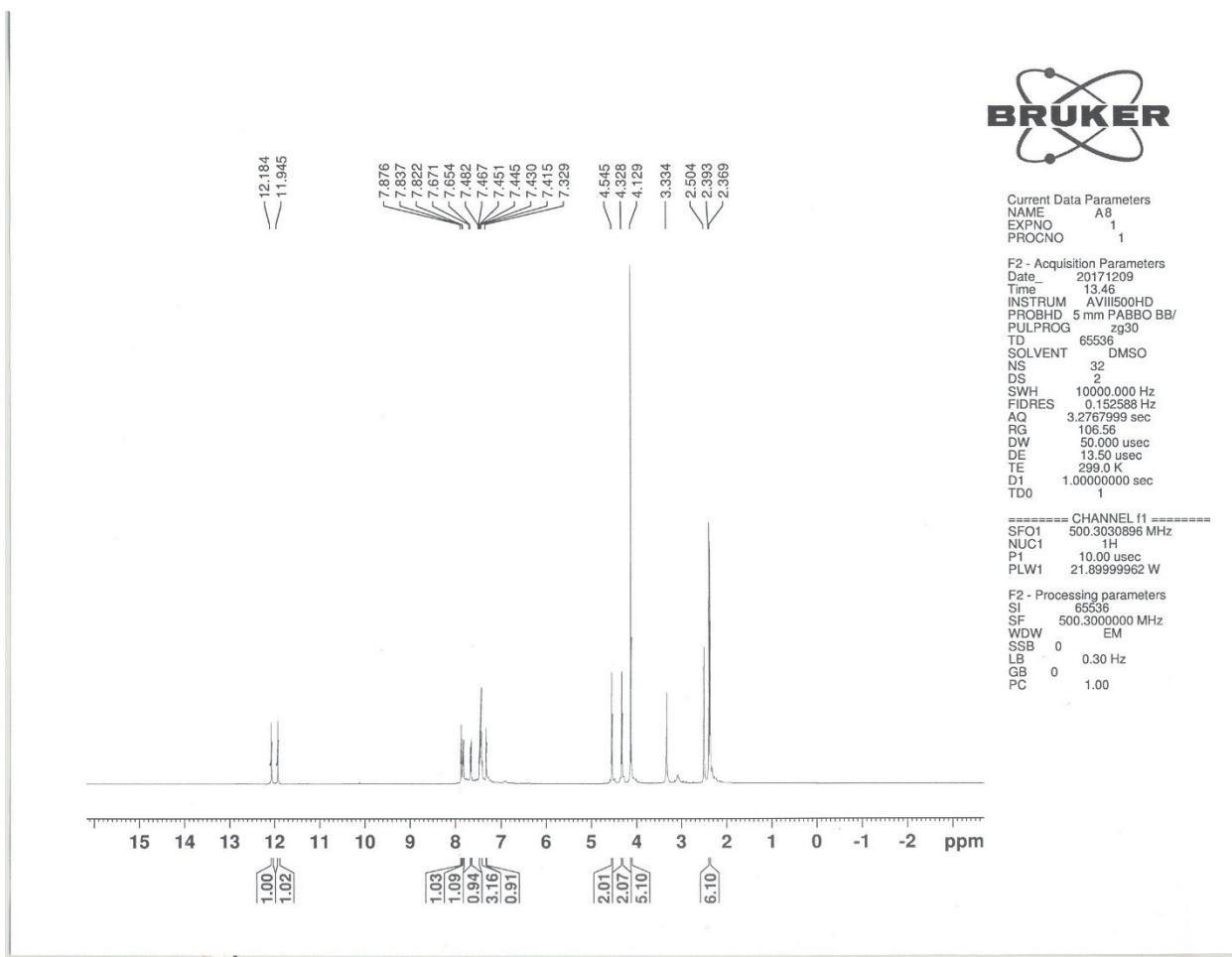
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LB 0 0.30 Hz
GB 0 1.00
PC 1.00



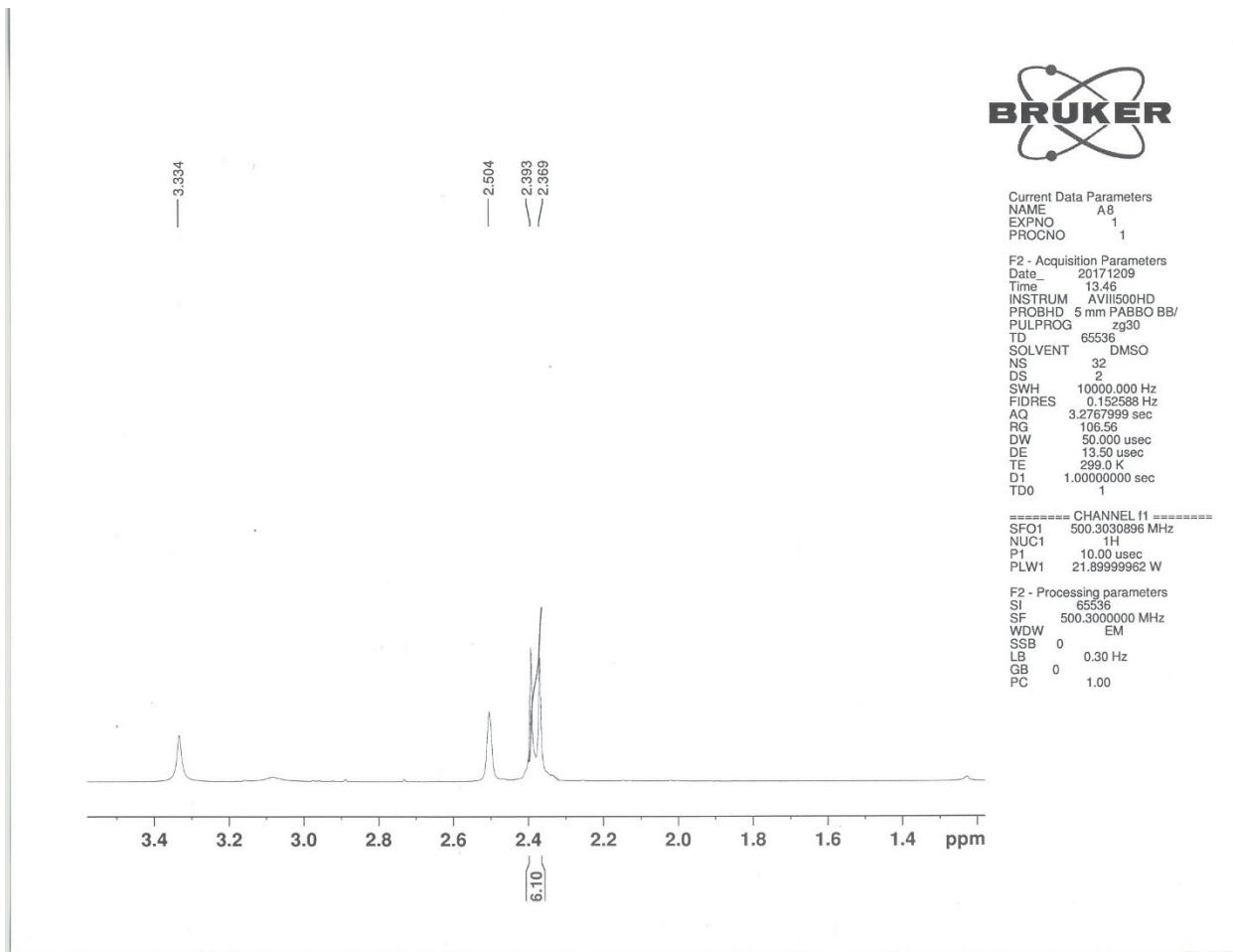
¹³C-NMR Spectrum of A7



¹H-NMR Spectrum of A8



¹H-NMR Spectrum of A8



¹H-NMR Spectrum of A8

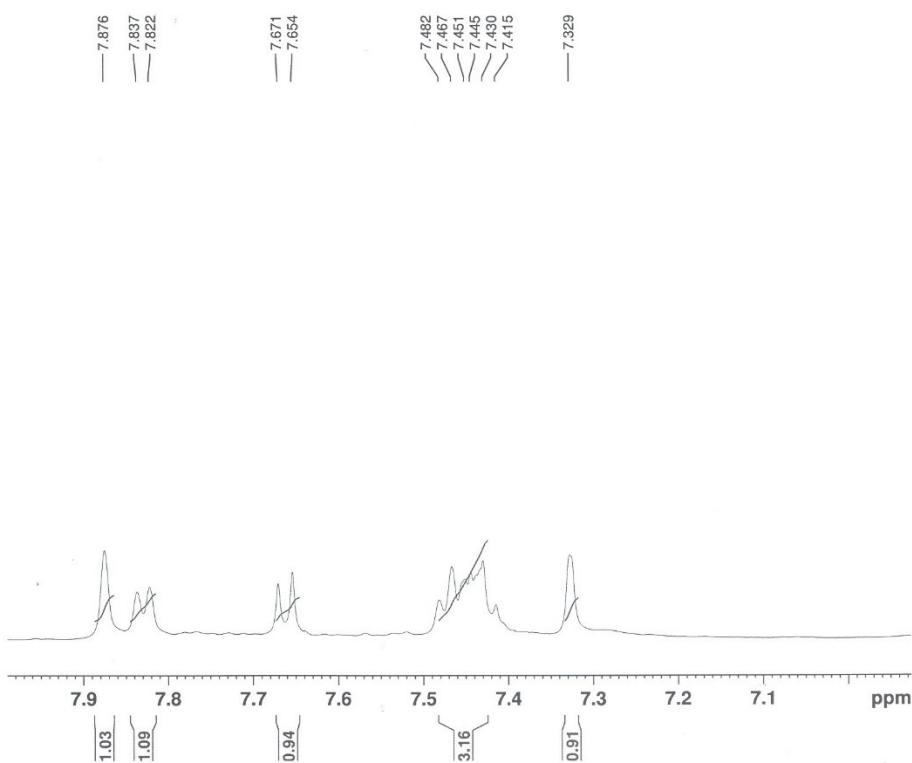


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PROCNO 1

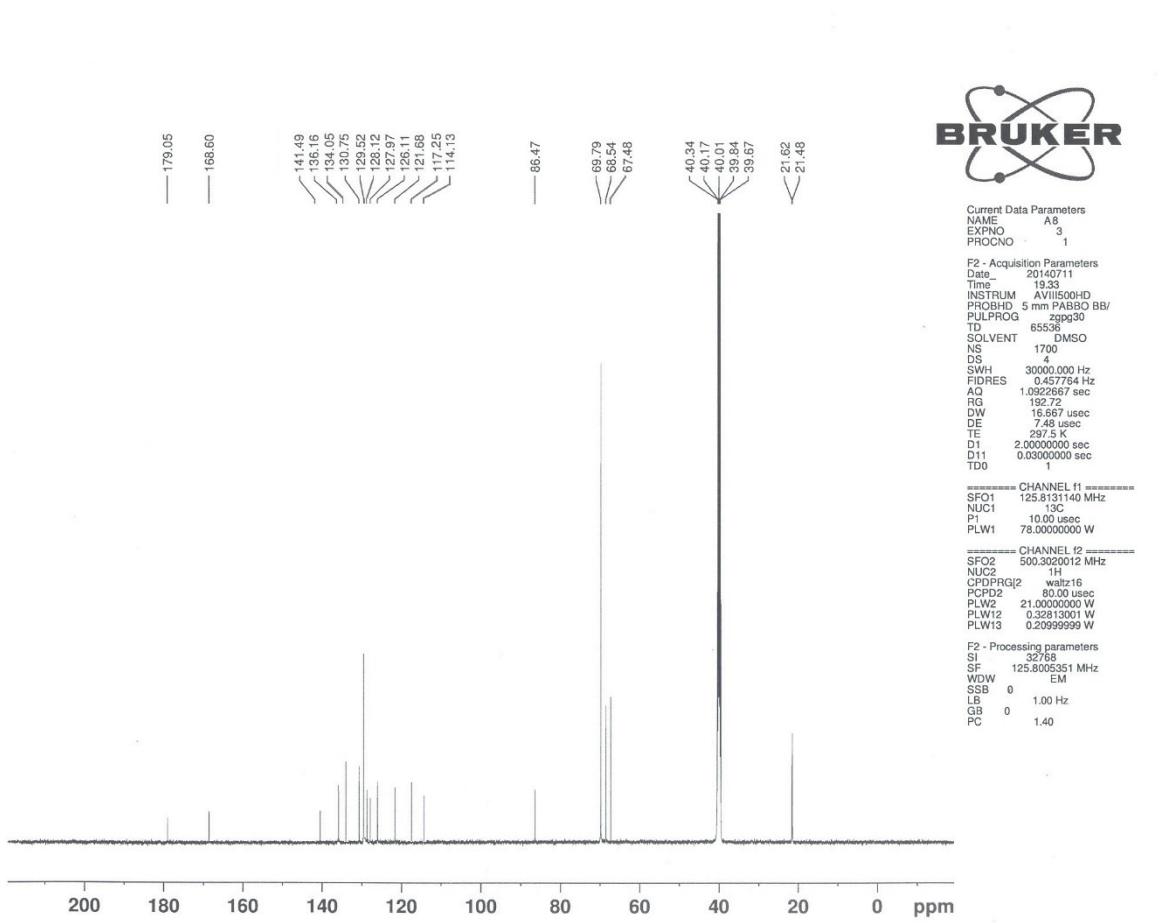
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AO 3.2767999 sec
RG 100
DW 50.000 usec
DE 13.50 usec
TE 299.0 usec
D1 1.0000000 sec
TD0 1

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NUC1 ¹H
P1 10.00 usec
PLW1 21.89999952 W

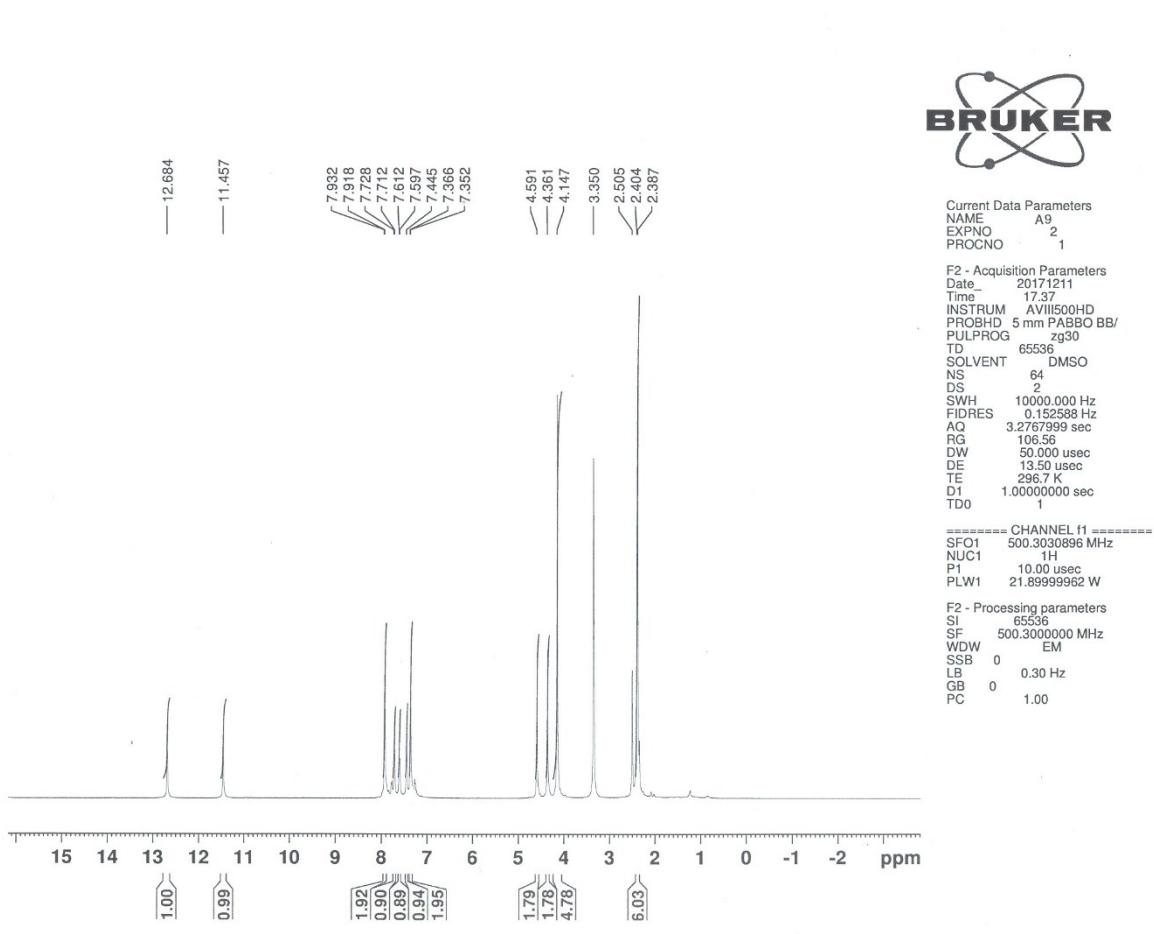
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SF 500.3000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C-NMR Spectrum of A8



¹H-NMR Spectrum of A9



¹H-NMR Spectrum of A9

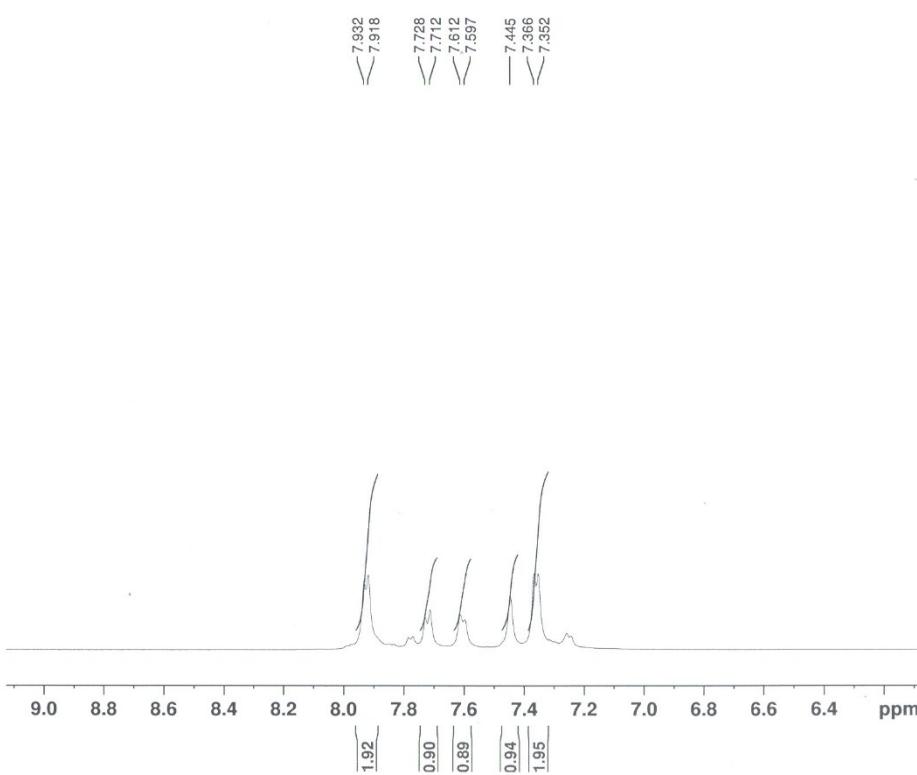


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EXPNO 2
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 106.56
DW 50.000 usec
DE 13.50 usec
TE 298.7 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 ¹H
P1 10.00 usec
PLW1 21.89999962 W

F2 - Processing parameters
SI 65536
SF 500.3000000 MHz
WDW EM
SSB 0 0.30 Hz
LB 0.30 Hz
GB 0 1.00
PC 1.00



¹³C-NMR Spectrum of A9

