

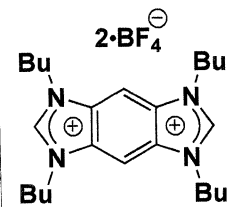
Modular Fluorescent Benzobis(imidazolium) Salts: Syntheses, Photophysical Analyses, and Applications

Andrew J. Boydston, Peter D. Vu[†], Olga L. Dykhno[†], Vicki Chang[†], Alvin R. Wyatt, II[†], Adam S. Stockett, Eric T. Ritschdorff, Jason B. Shear, and Christopher W. Bielawski*

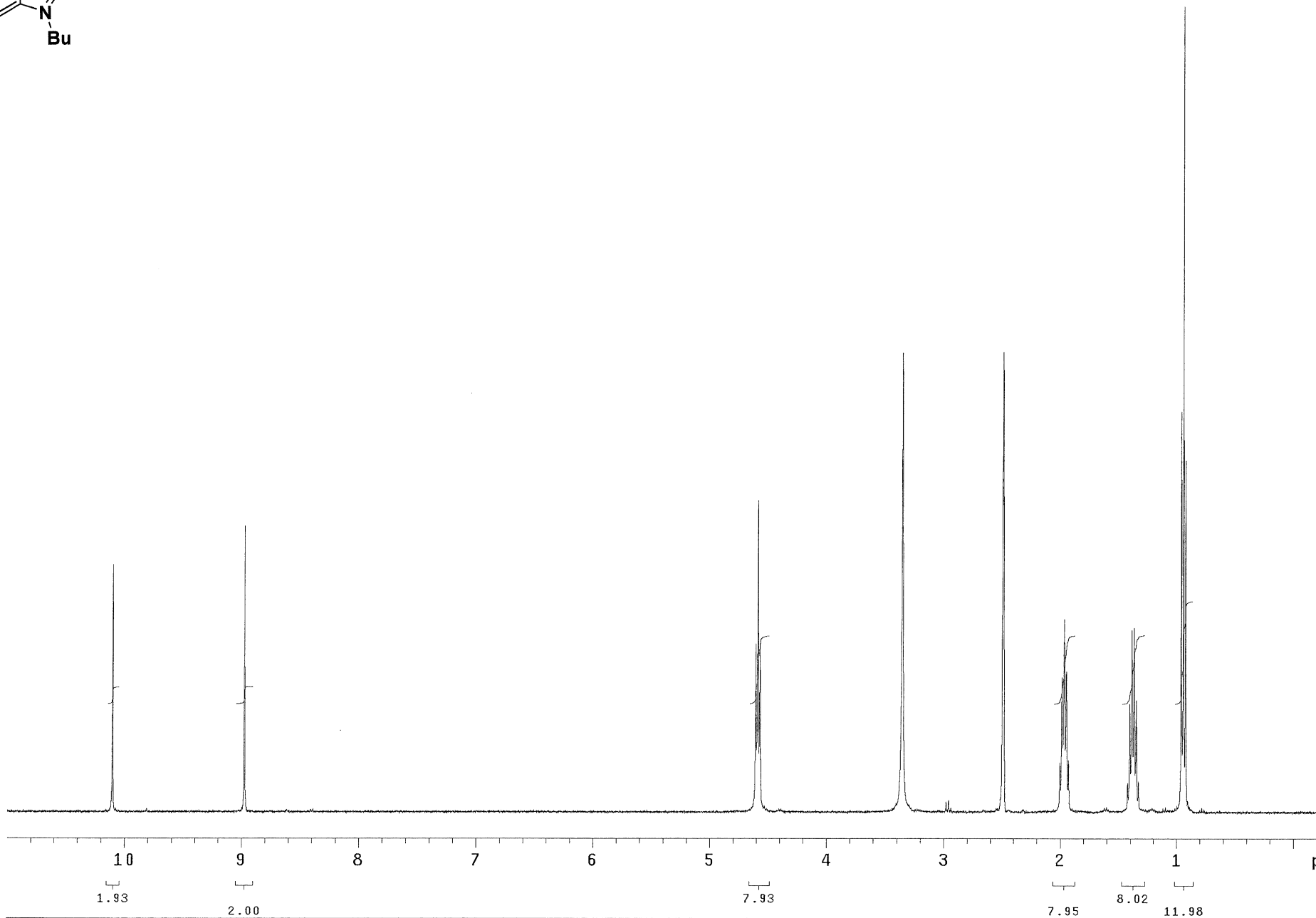
Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712
bielawski@cm.utexas.edu

SUPPORTING INFORMATION

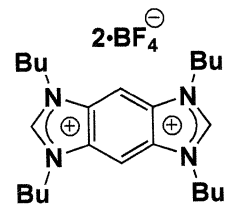
Reference 24a: Xin, Z.; Serby, M. D.; Zhao, H.; Kosogof, C.; Szczaepankiewicz, B. G.; Liu, M.; BoLiu; Hutchins, C. W.; Sarris, K. A.; Hoff, E. D.; Falls, H. D.; Lin, C. W.; Ogiela, C. A.; Collins, C. A.; Brune, M. E.; Bush, E. N.; Droz, B. A.; Fey, T. A.; Knourek-Segel, V. E.; Shapiro, R.; Jaconsen, P. B.; Beno, D. W. A.; Turner, T. M.; Sham, H. L.; Liu, G. *J. Med. Chem.* **2006**, *49*, 4459.



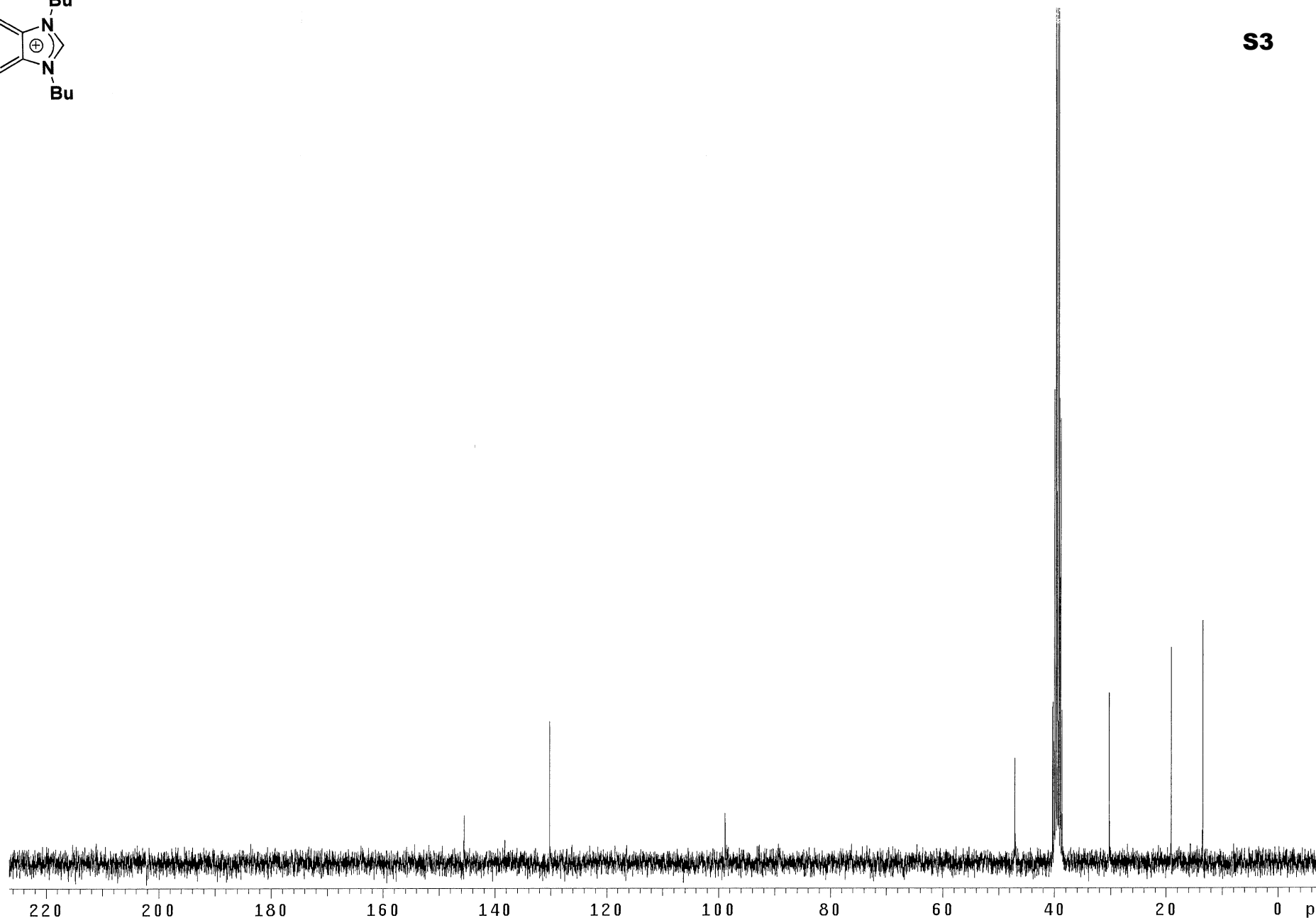
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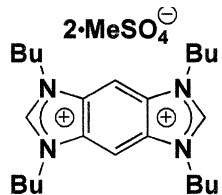
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 2 repetitions	OBSERVE H1, 400.2688767	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			B5AB229 Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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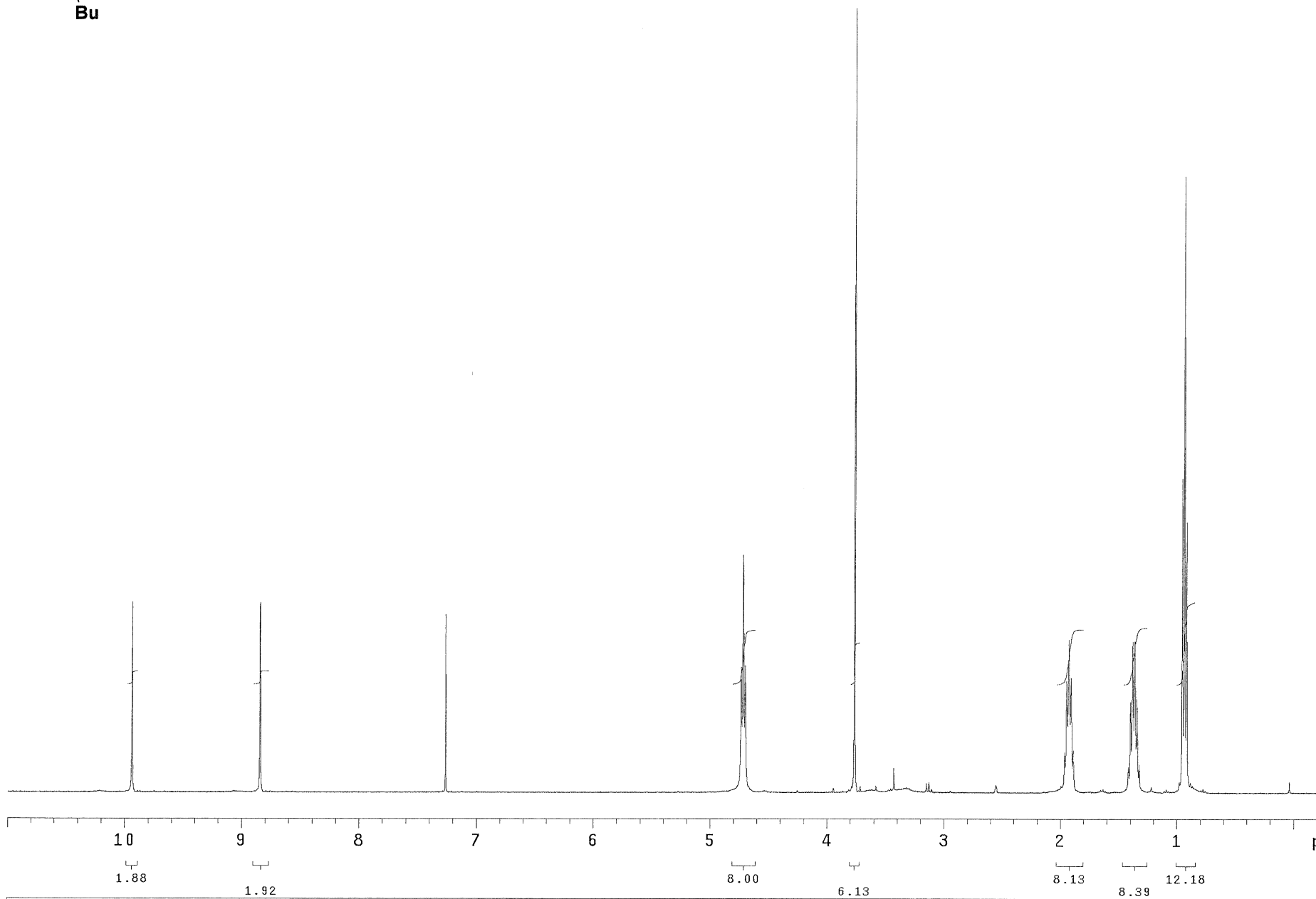
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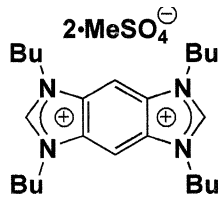
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 213 repetitions	OBSERVE C13, 75.4704115 DECOUPLE H1, 300.1423516 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 13 minutes	B5AB229-13C Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature UNITYplus-300 "nmr2"
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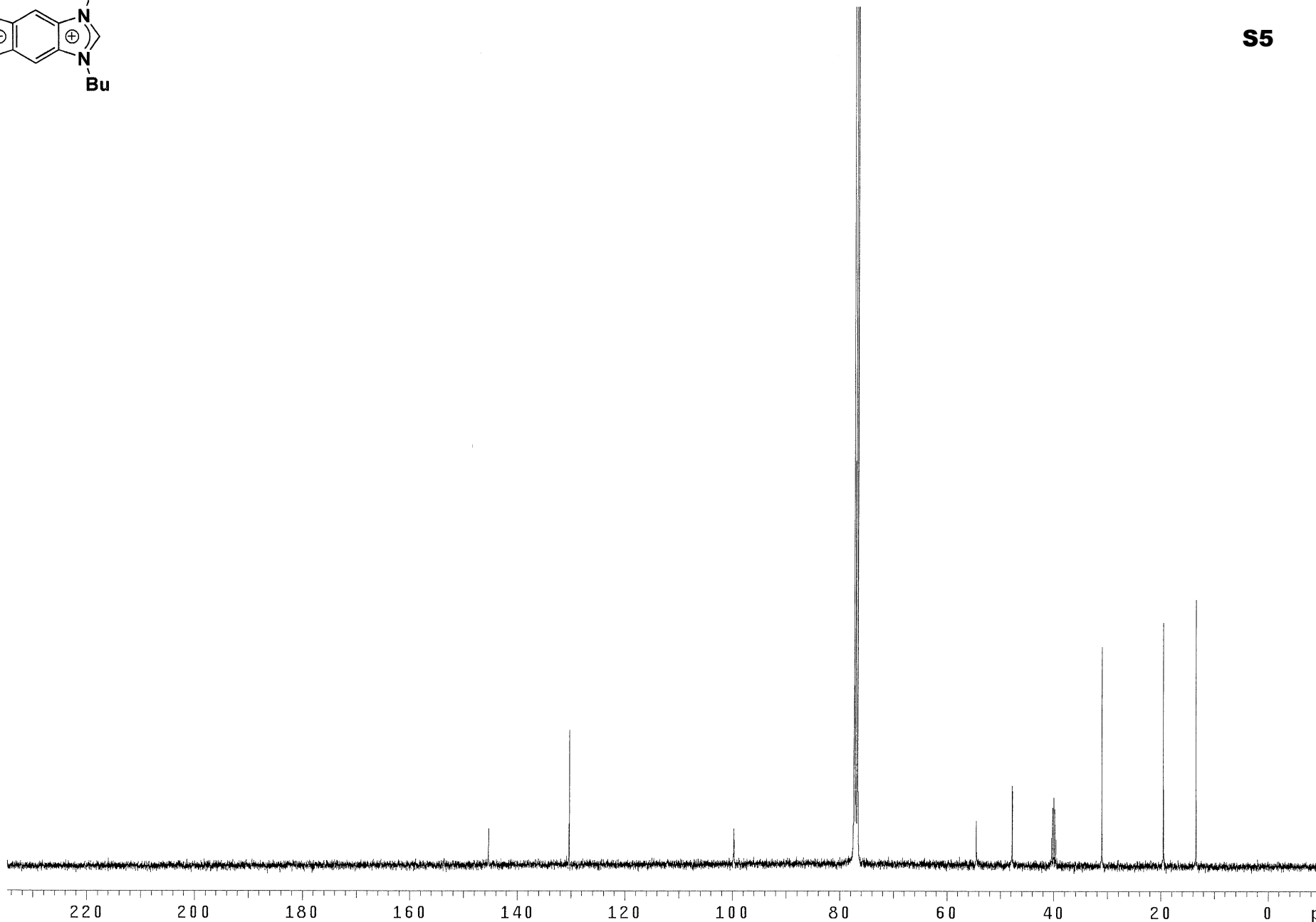
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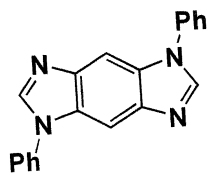
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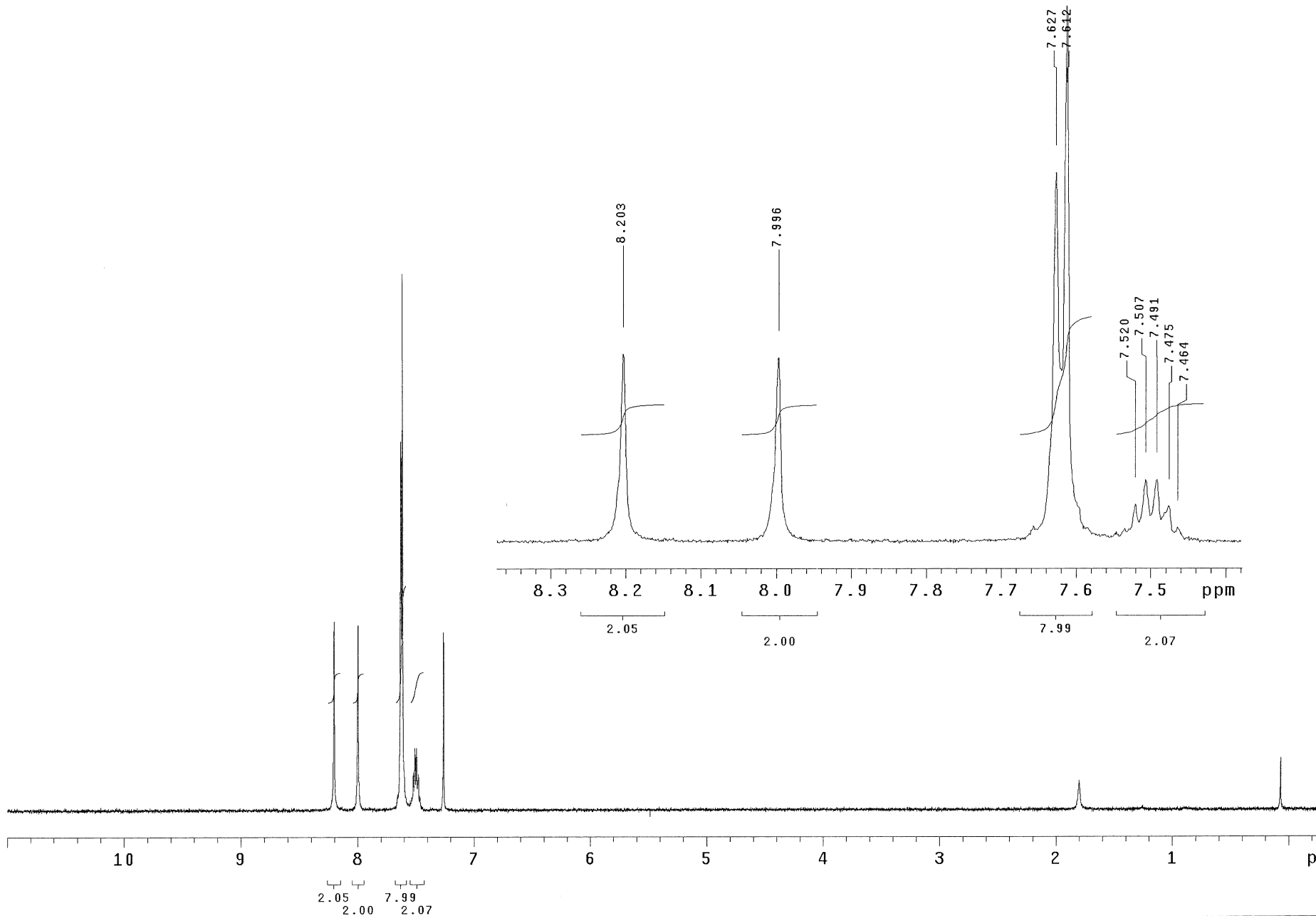
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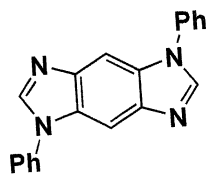
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 10000 repetitions	OBSERVE C13, 100.6472184 DECOUPLE H1, 400.2689955 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 9.1 hours	B6AB283+DMSO-13C Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"
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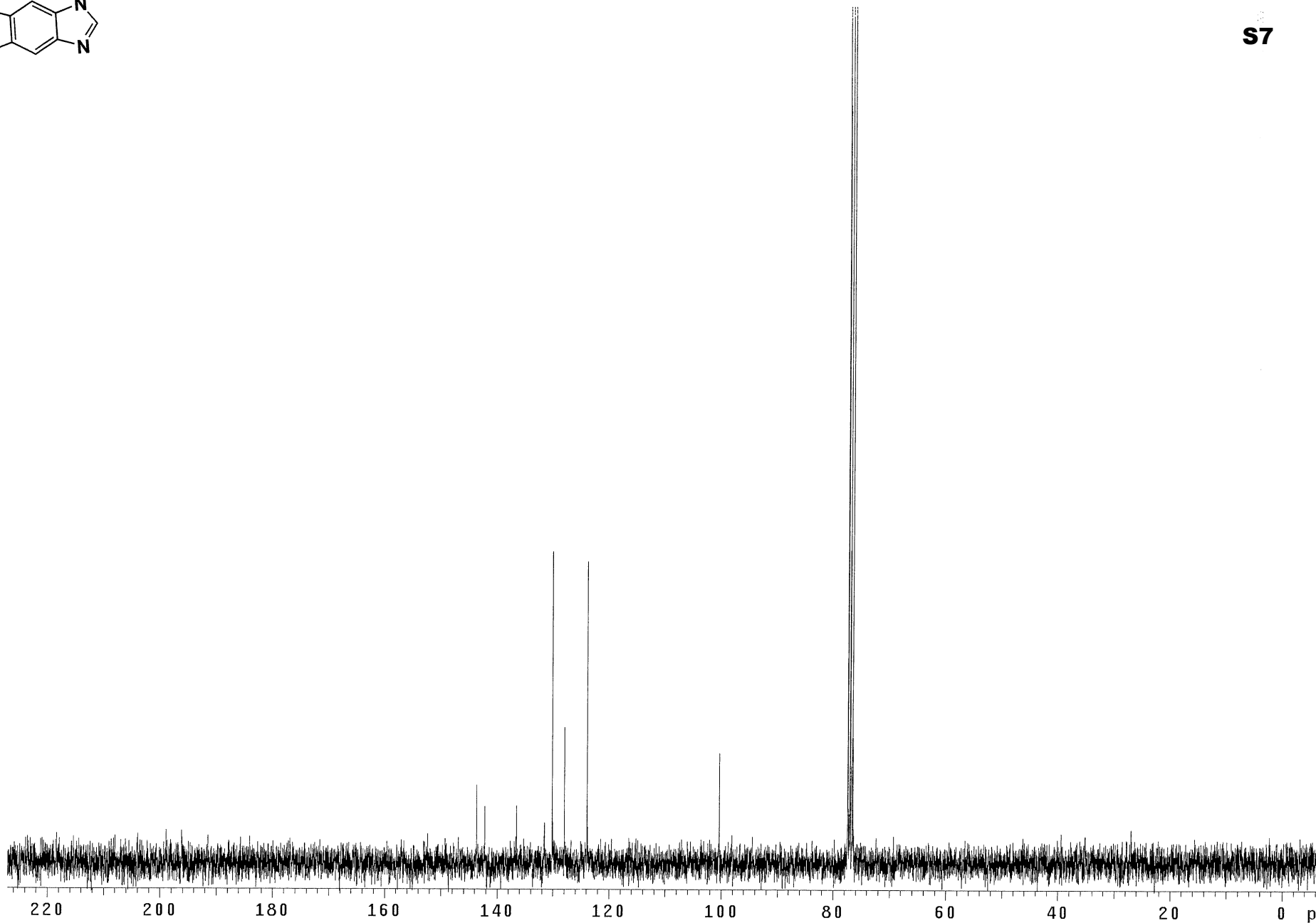
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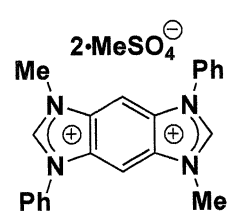
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 15 repetitions	OBSERVE H1, 300.1390321	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute	1PV116 Pulse Sequence: s2pu1 Solvent: CDCl ₃ Ambient temperature UNITYplus-300 "nmr2"
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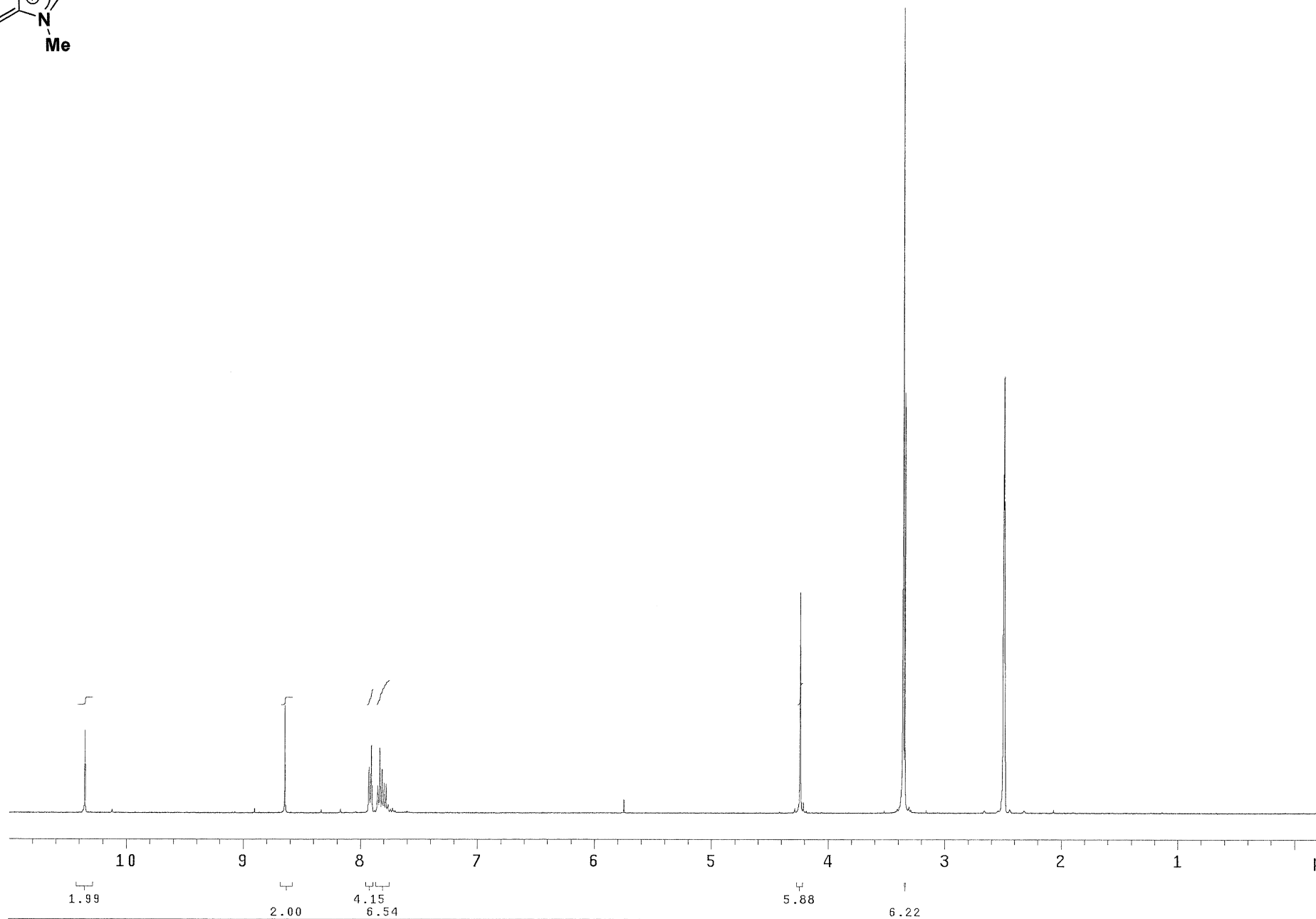
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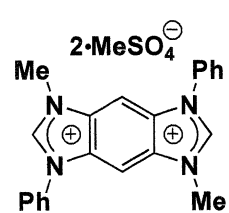
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 200 repetitions	OBSERVE C13, 75.4700205 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 18 minutes	1PV116-13C <hr/> Pulse Sequence: s2pul Solvent: CDCl3 Ambient temperature UNITYplus-300 "nmr2"	
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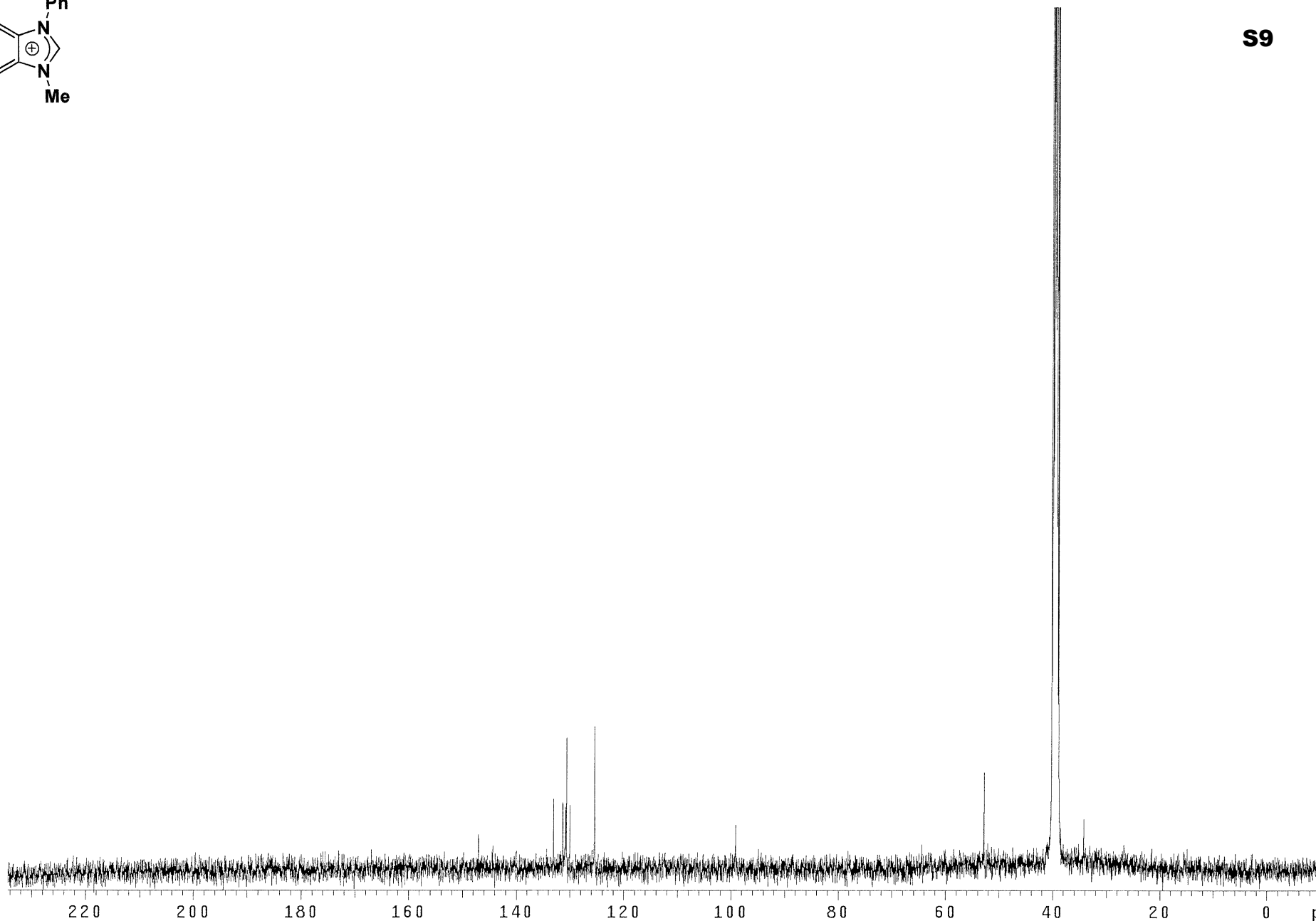
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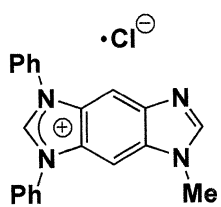
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 20 repetitions	OBSERVE H1, 400.2688771	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minutes	B6AB-CC-MS Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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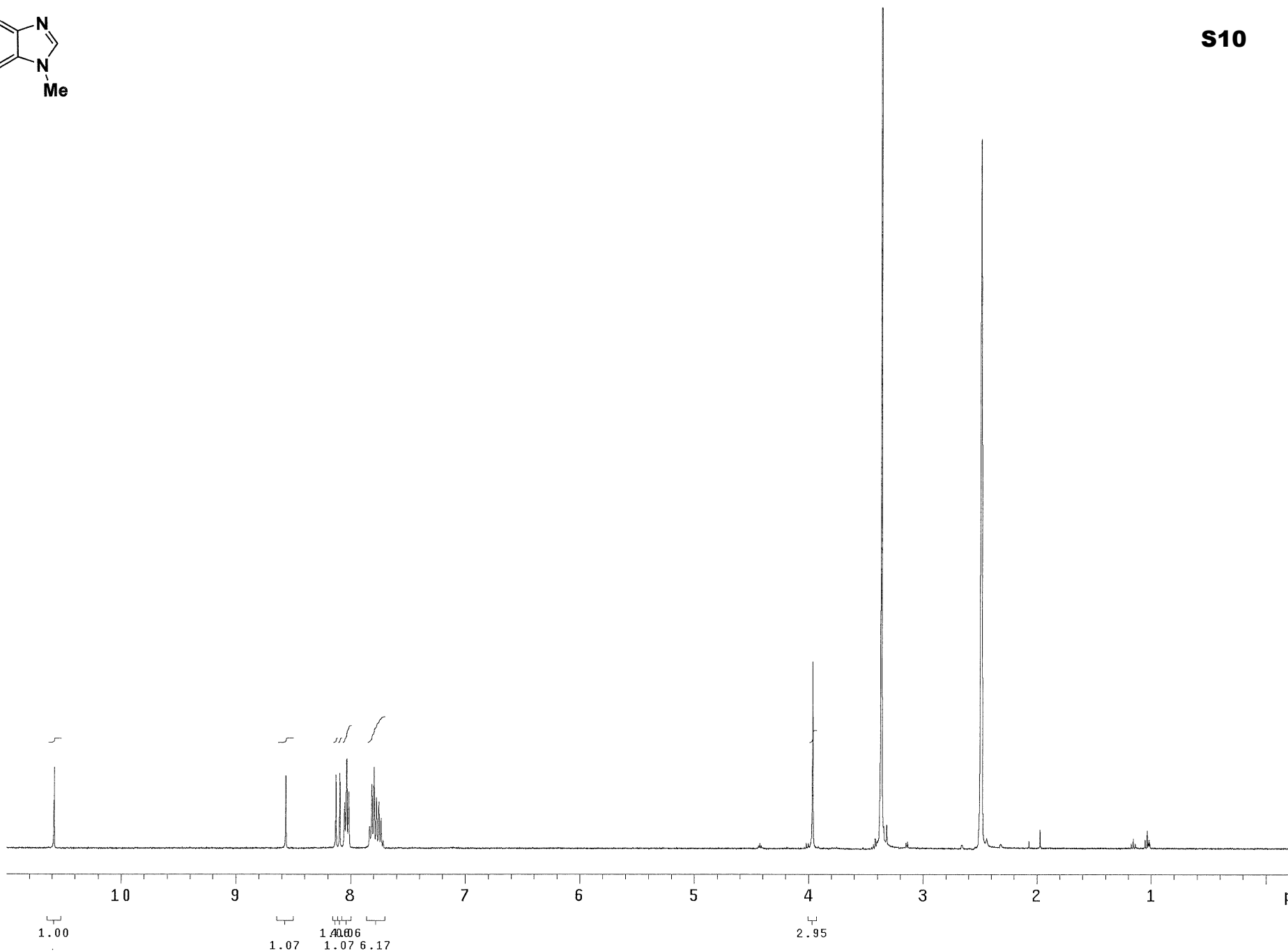
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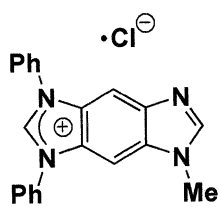
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 3515 repetitions	OBSERVE C13, 100.6477349 DECOUPLE H1, 400.2708968 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.0 Hz FT size 65536 Total time 3.2 hours		B6AB-CC-MS-13C Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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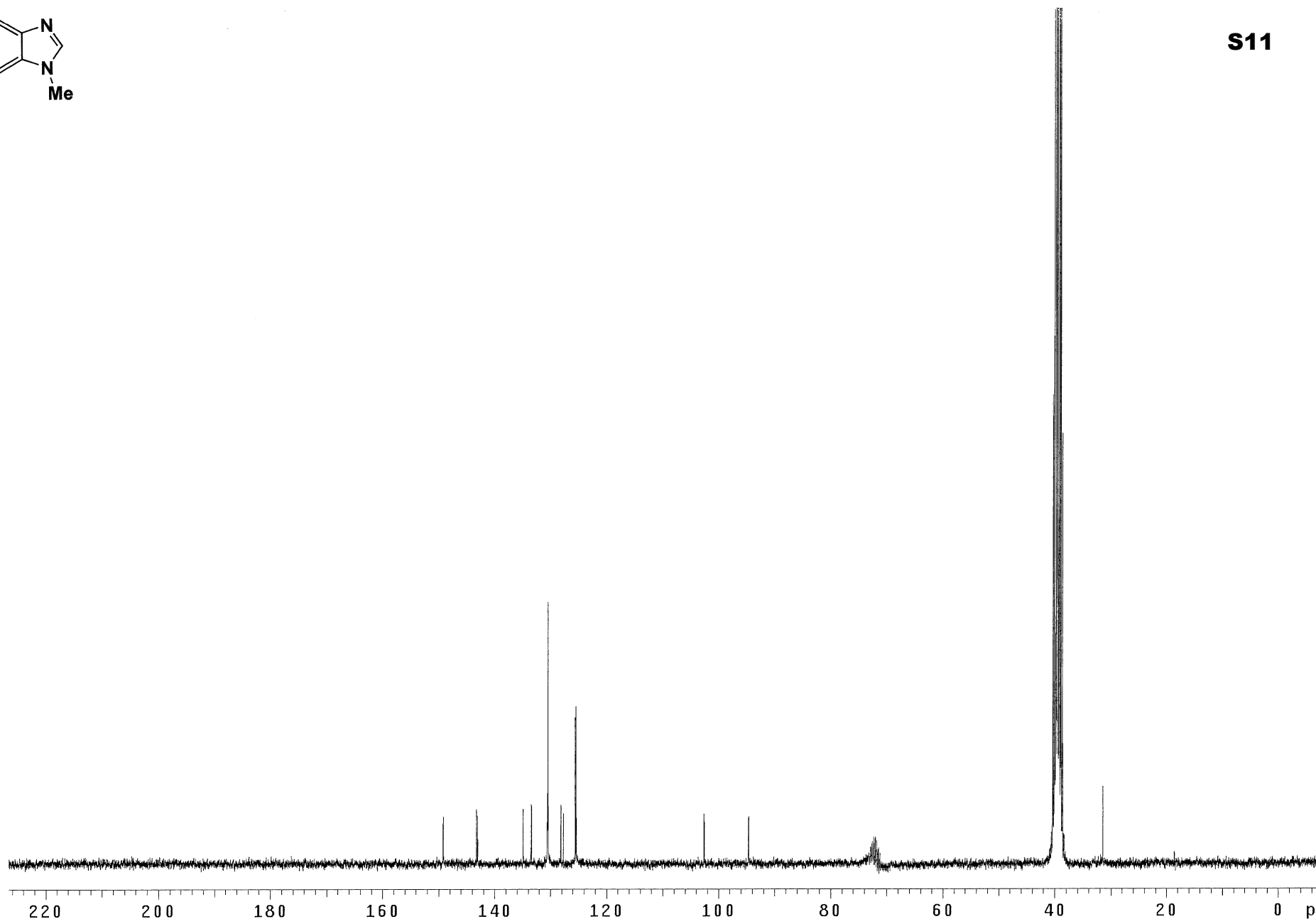
S10



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 18 repetitions	OBSERVE H1, 400.2688771	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			B6AB269-Rx1 Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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S11



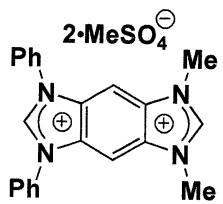
PULSE SEQUENCE
 Relax. delay 2.000 sec
 Pulse 36.0 degrees
 Acq. time 1.777 sec
 Width 18009.9 Hz
 11652 repetitions

OBSERVE C13, 75.4704115
 DECOUPLE H1, 300.1423516
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 Single precision data

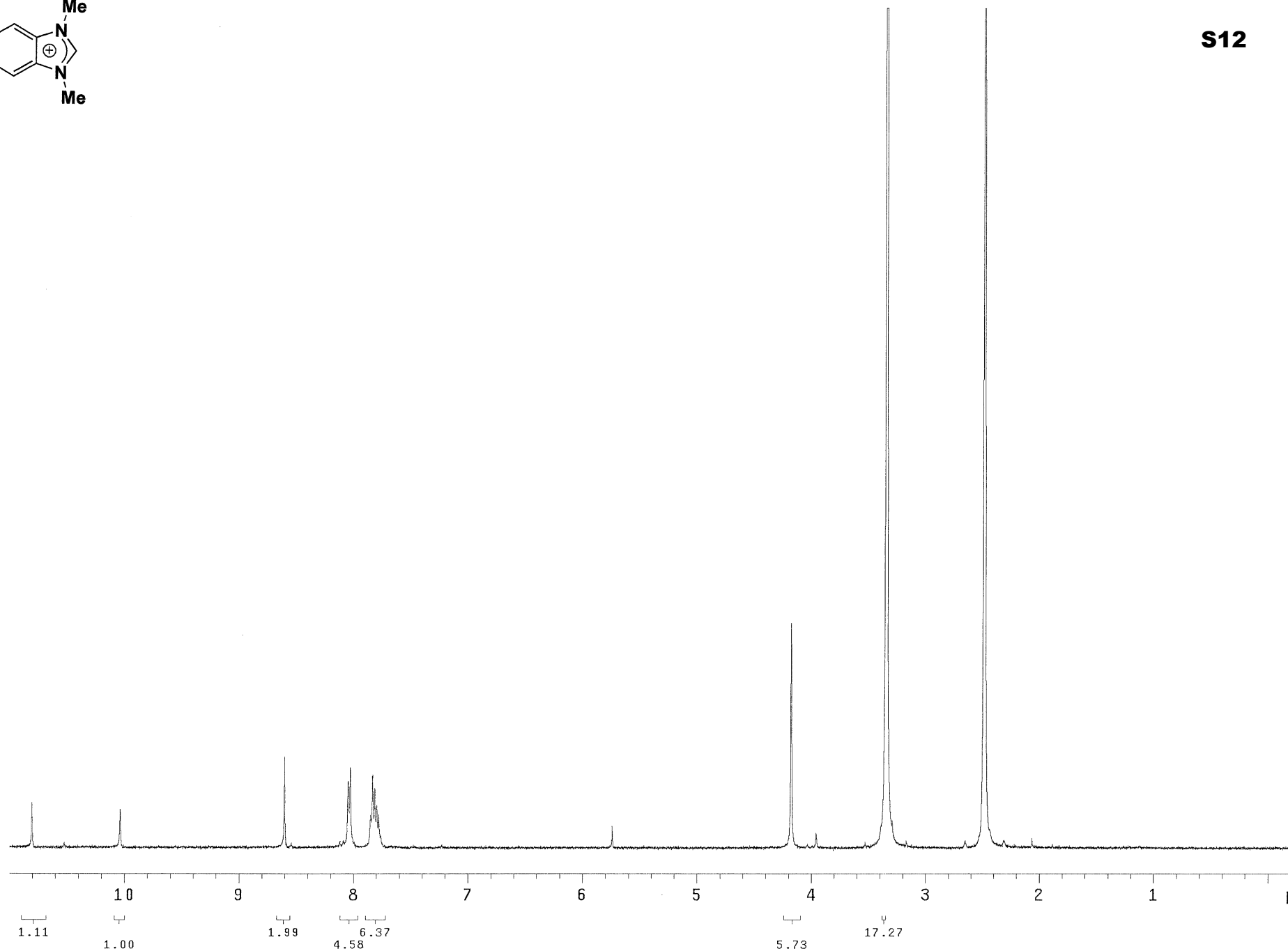
DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 12.2 hours

B6AB269-13C

Pulse Sequence: s2pu1
 Solvent: DMSO
 Ambient temperature
 UNITYplus-300 "nmr2"



S12



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
34 repetitions

OBSERVE H1, 400.2688797

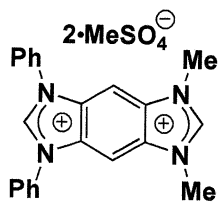
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 2 minutes

B6AB300-2

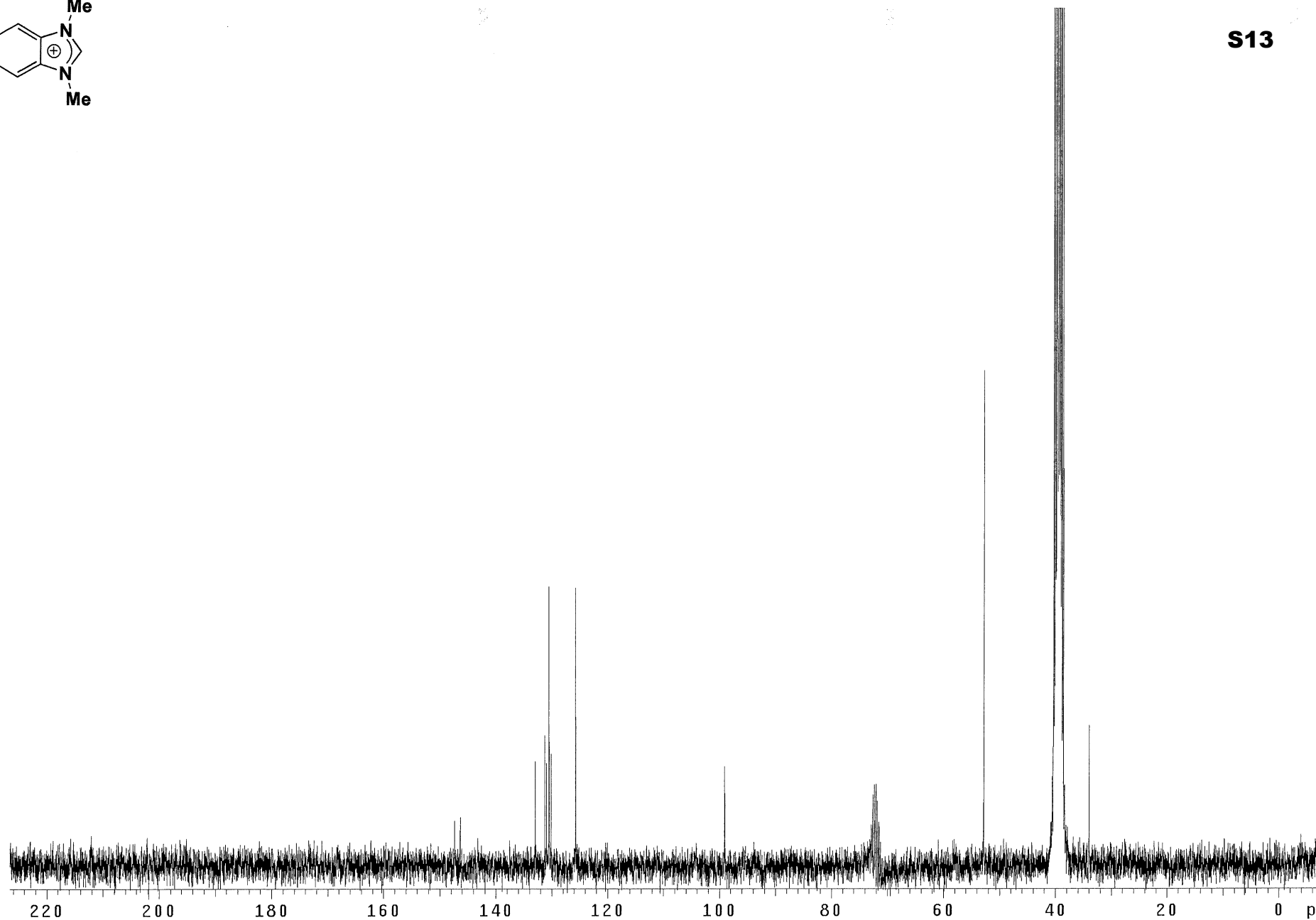
Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature
Mercury-400 "nmr6"



S13



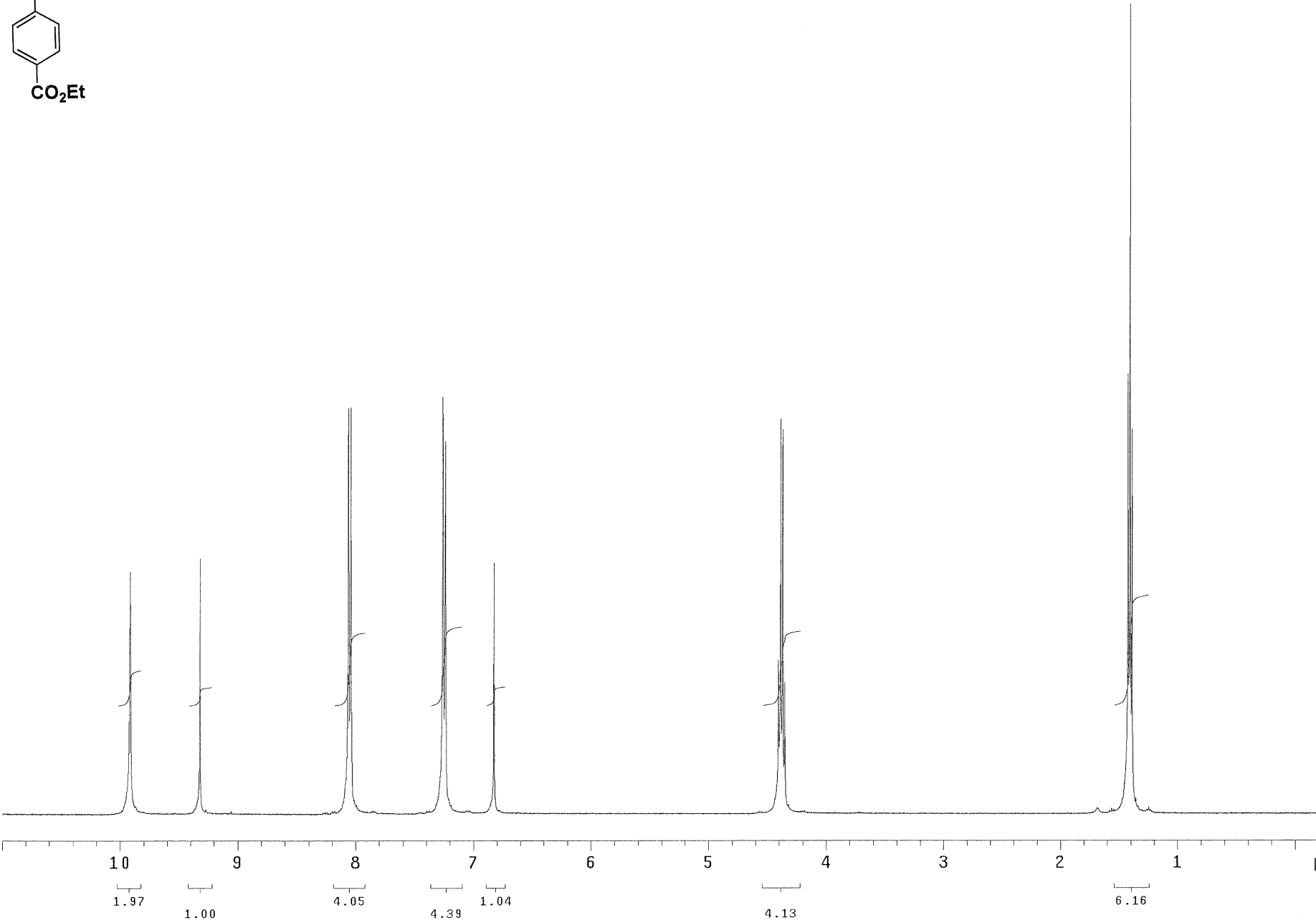
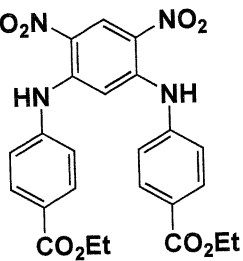
PULSE SEQUENCE
 Relax. delay 2.000 sec
 Pulse 36.0 degrees
 Acq. time 1.777 sec
 Width 18009.9 Hz
 9759 repetitions

OBSERVE C13, 75.4704115
 DECOUPLE H1, 300.1423516
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 Single precision data

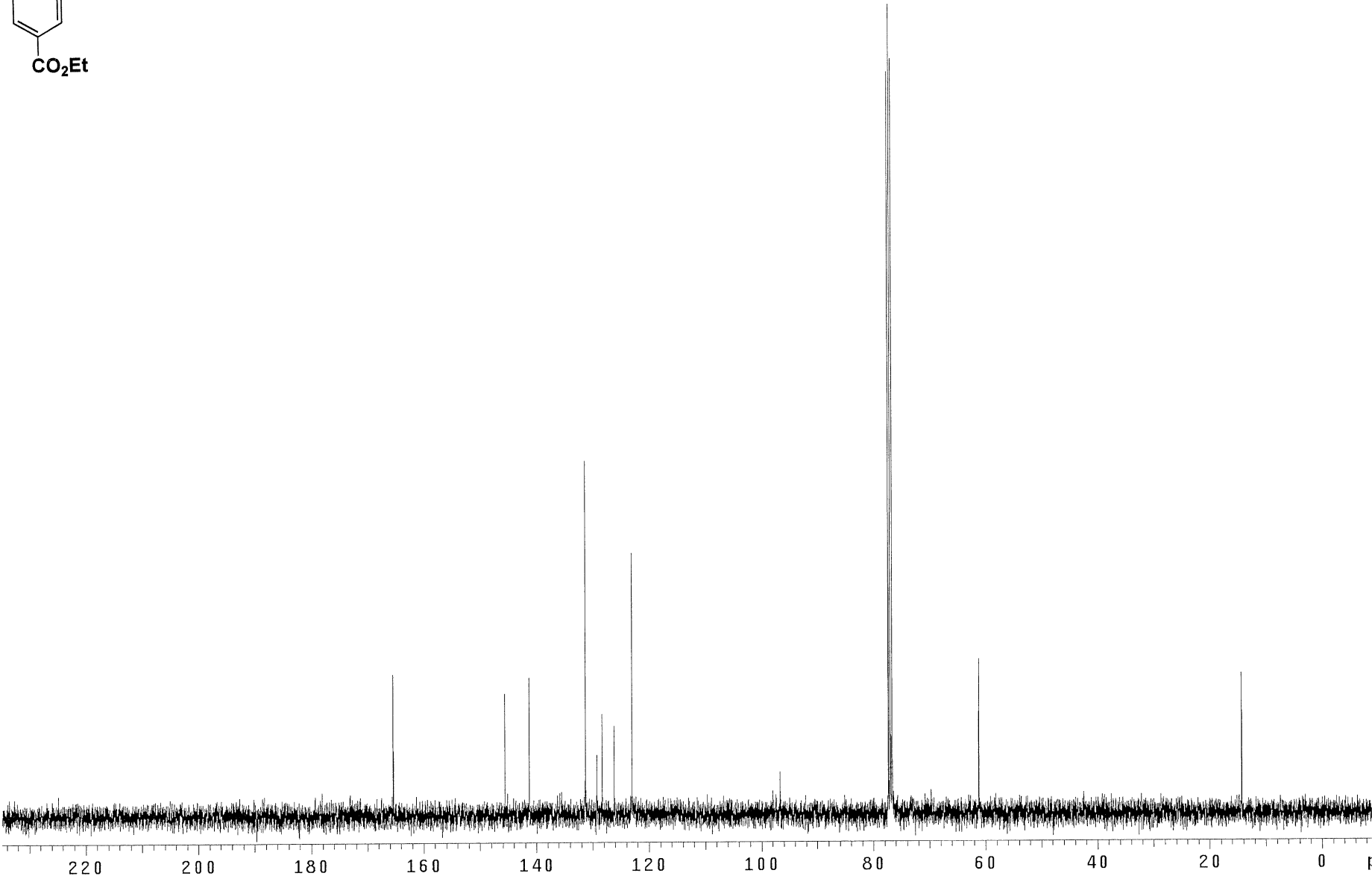
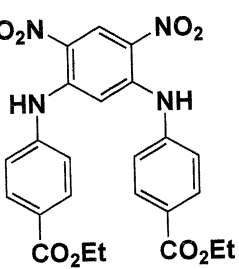
DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 10.2 hours

B6AB300-MS-13C
 Pulse Sequence: s2pu1
 Solvent: DMSO
 Ambient temperature
 UNITYplus-300 "nmr2"

S14

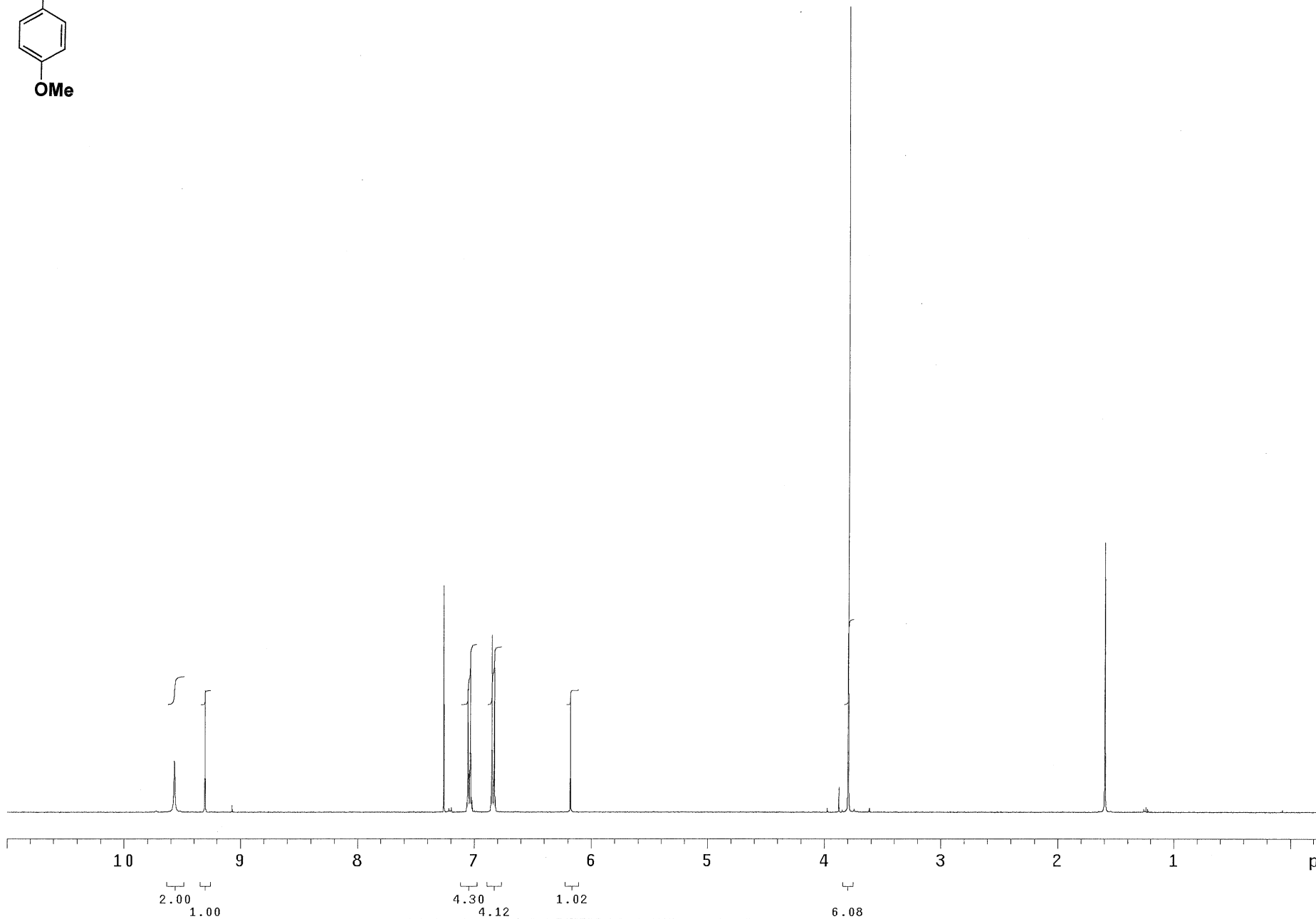
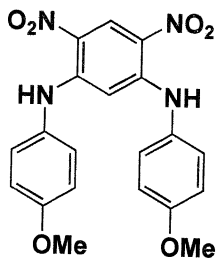


PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 12 repetitions	OBSERVE	H1, 400.2669755	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			B6AB220-Rx1
						Pulse Sequence: s2pu1
						Solvent: CDCl3
						Ambient temperature Mercury-400 "nmr5"



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 91 repetitions	OBSERVE C13, 100.6472161 DECOUPLE H1, 400.2689955 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 5 minutes			B6AB220-13C
					Pulse Sequence: s2pul
					Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"

S16



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
12 repetitions

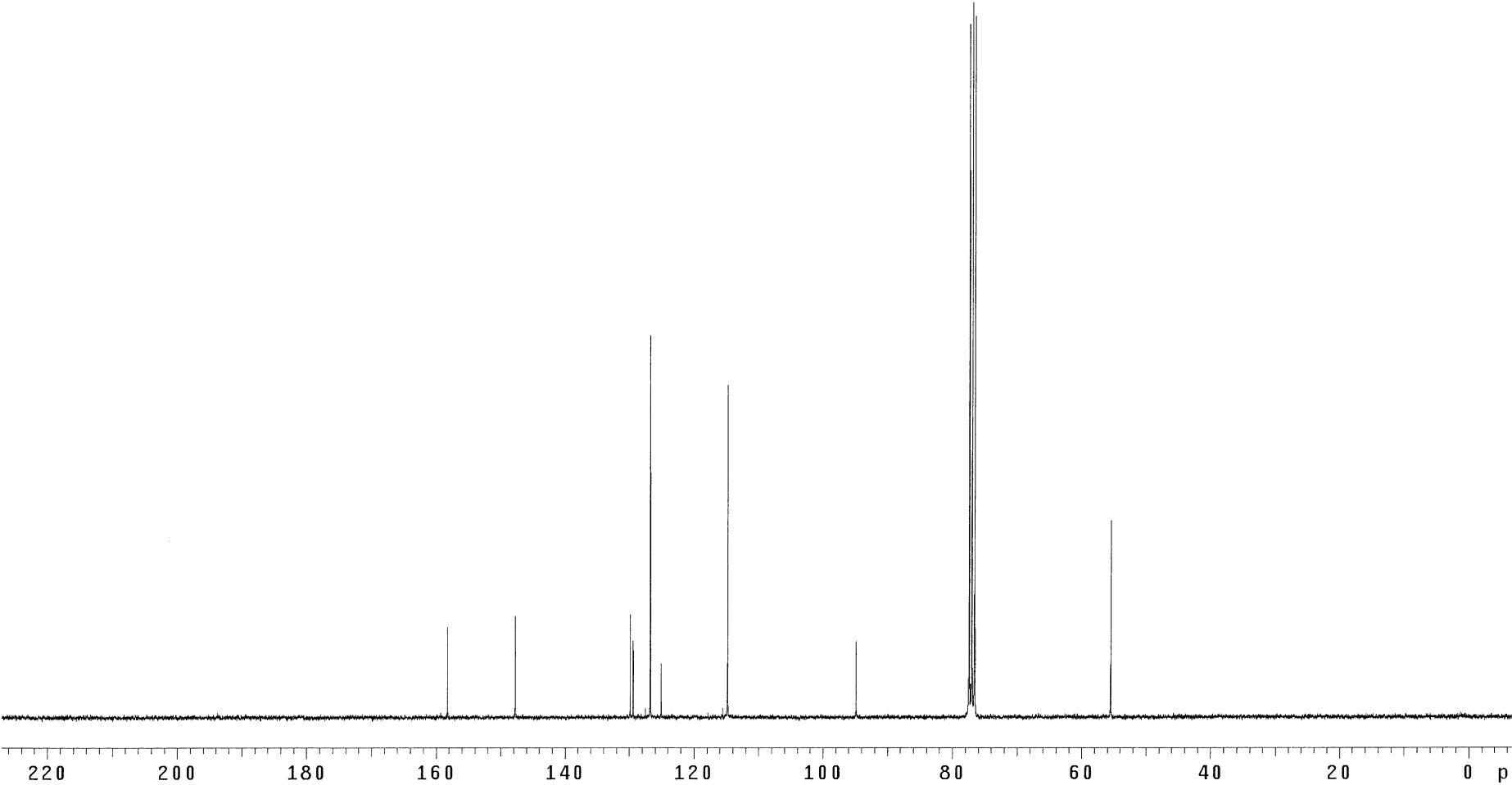
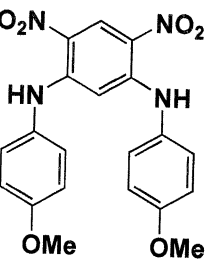
OBSERVE H1, 400.2669783

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute

ASS1-189

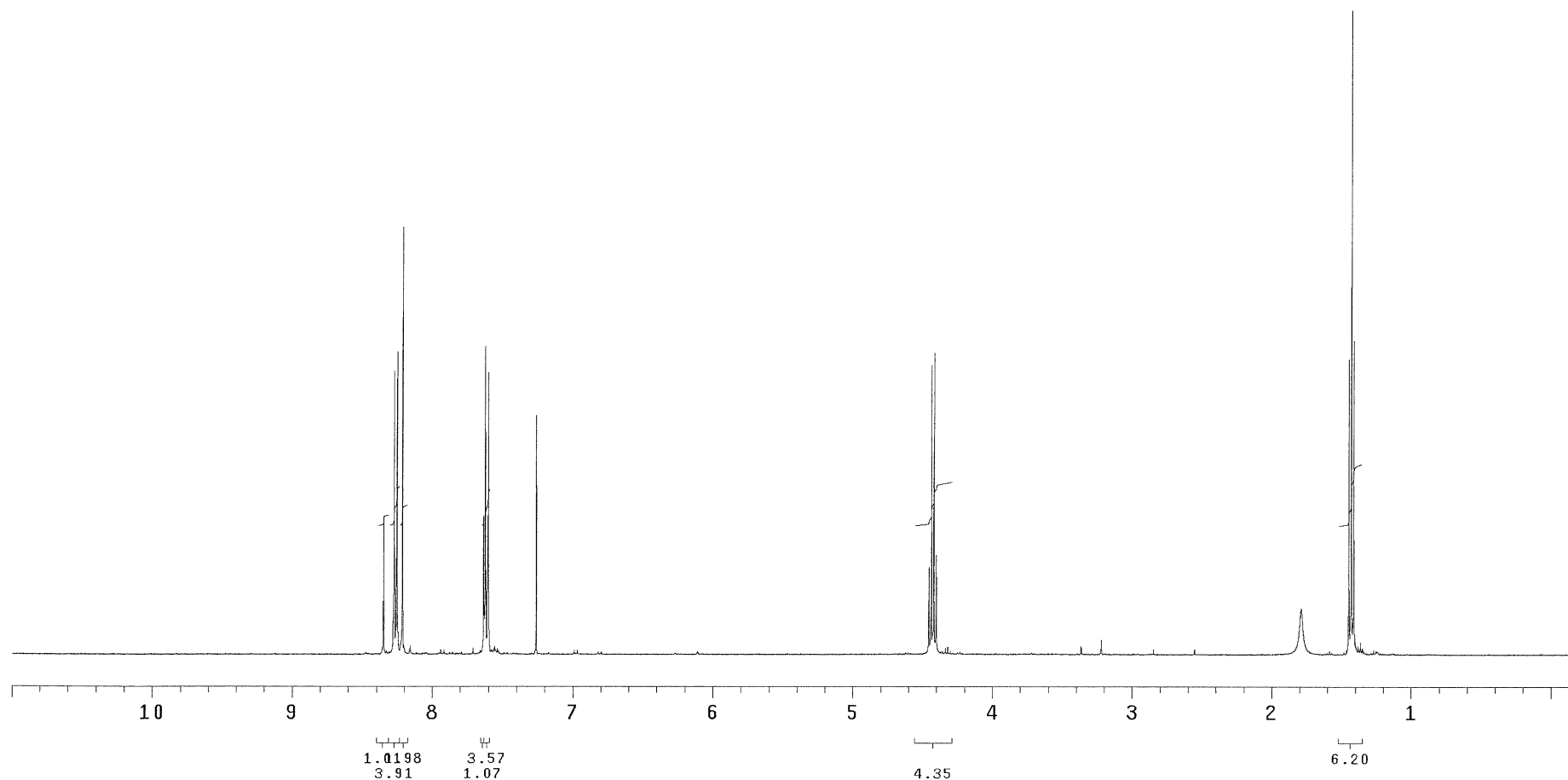
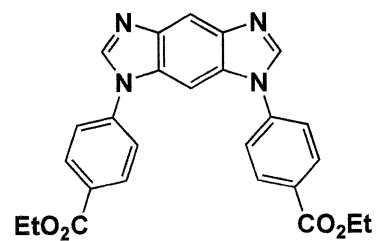
Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
Mercury-400 "nmr6"



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 11998 repetitions	OBSERVE C13, 75.4700205 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 12.6 hours			ASS189-13C Pulse Sequence: s2pu1 Solvent: CDC13 Ambient temperature UNITYplus-300 "nmr2"
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S18



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
13 repetitions

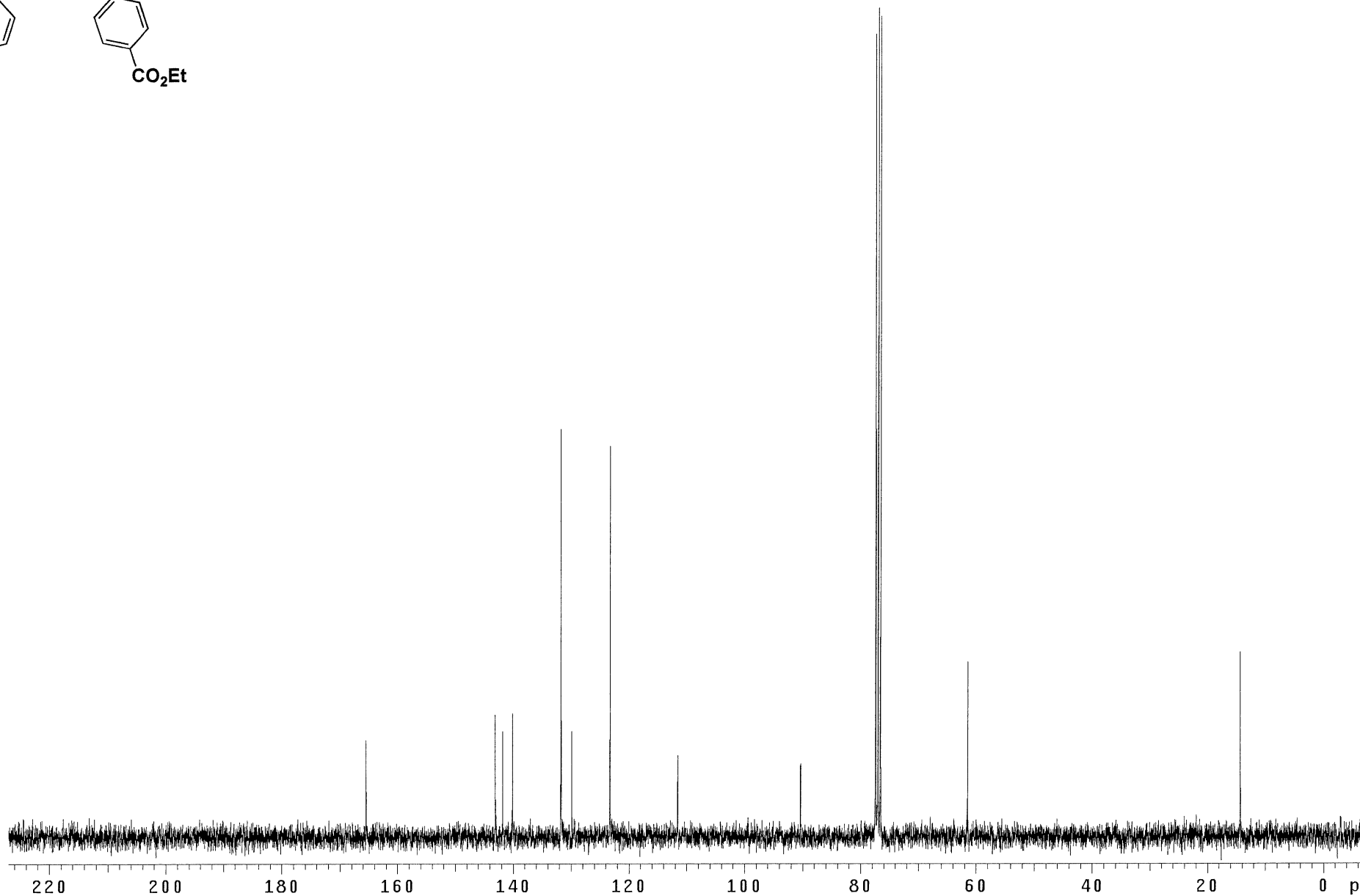
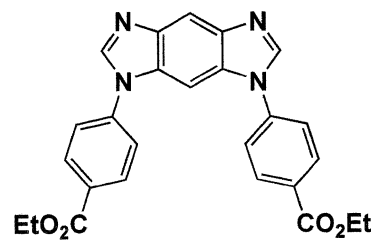
OBSERVE H1, 400.2669779

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute

B6AB227

Pulse Sequence: s2pul
Solvent: CDCl₃
Ambient temperature
Mercury-400 "nmr6"

S19



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
464 repetitions

OBSERVE C13, 75.4700211
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 29 minutes

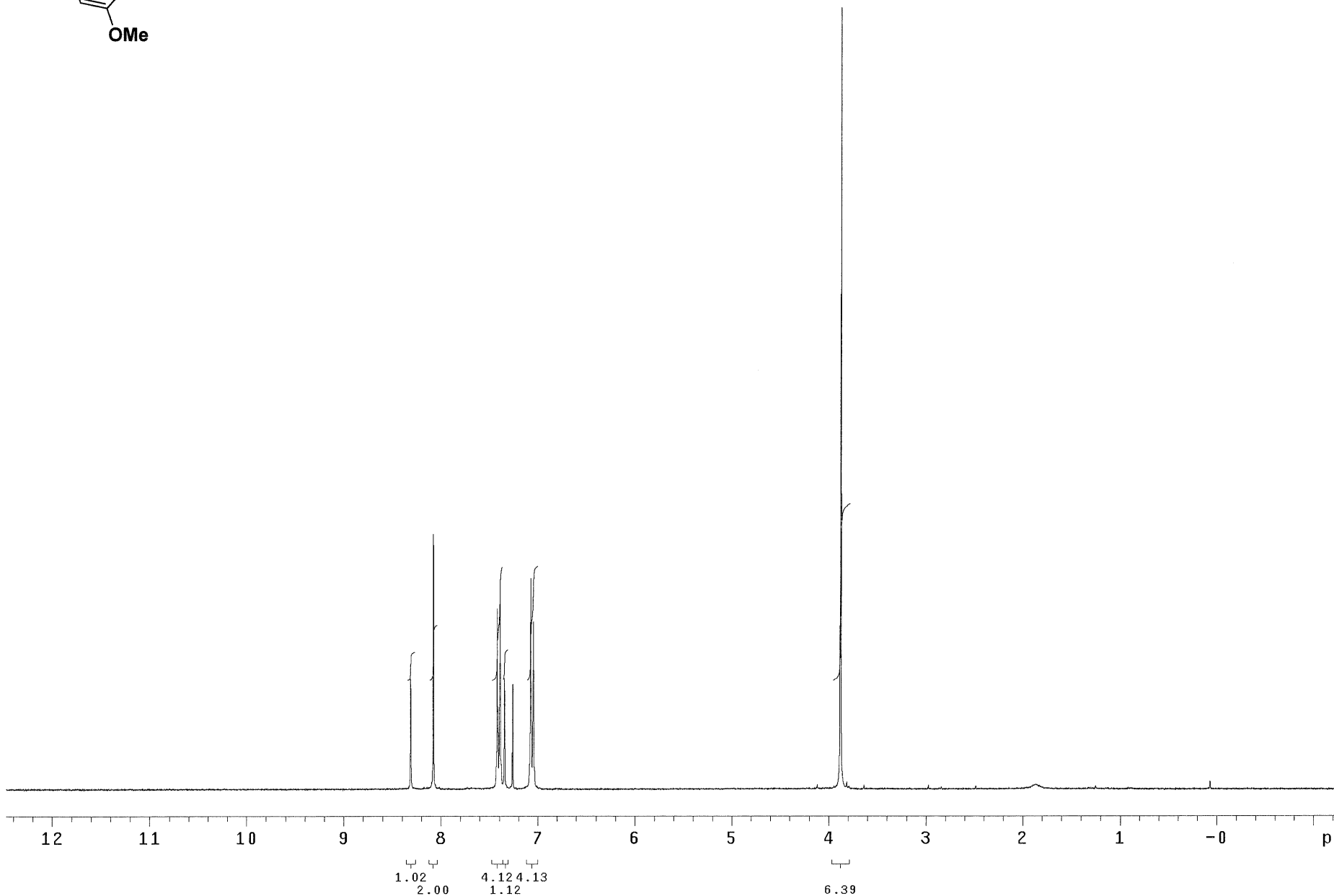
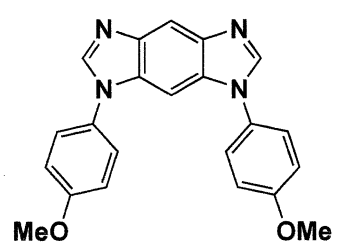
B6AB227-13C

Pulse Sequence: s2pu1

Solvent: CDCl3

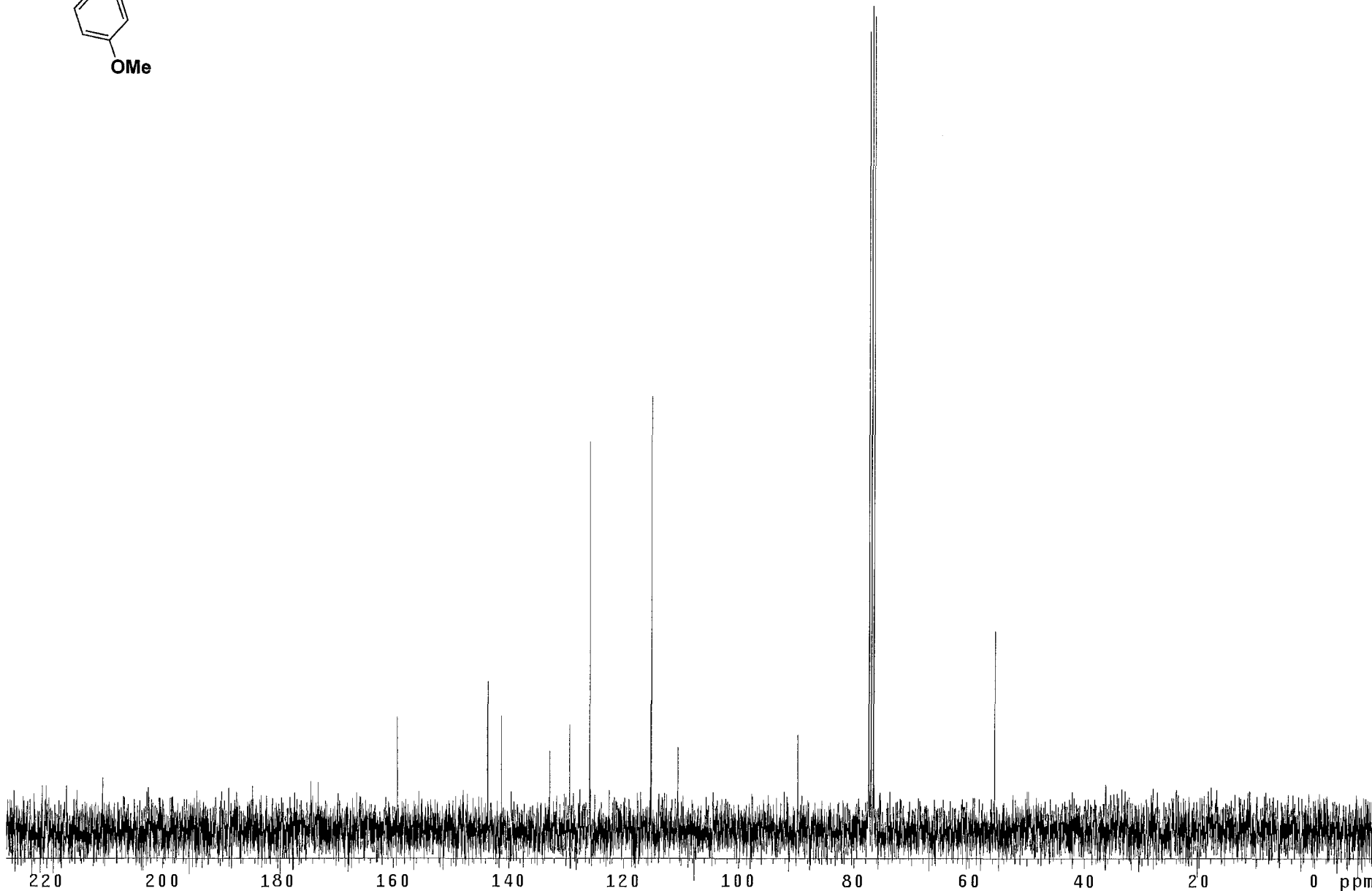
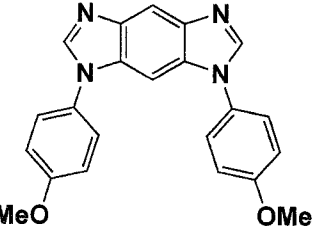
Ambient temperature
UNITYplus-300 "nmr2"

S20

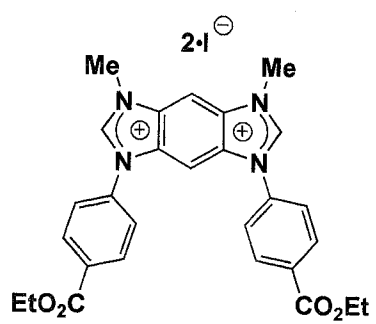


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 19 repetitions	OBSERVE H1, 300.1390318	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minutes			1PV161 Pulse Sequence: s2pu1 Solvent: CDC13 Ambient temperature UNITYplus-300 "nmr2"
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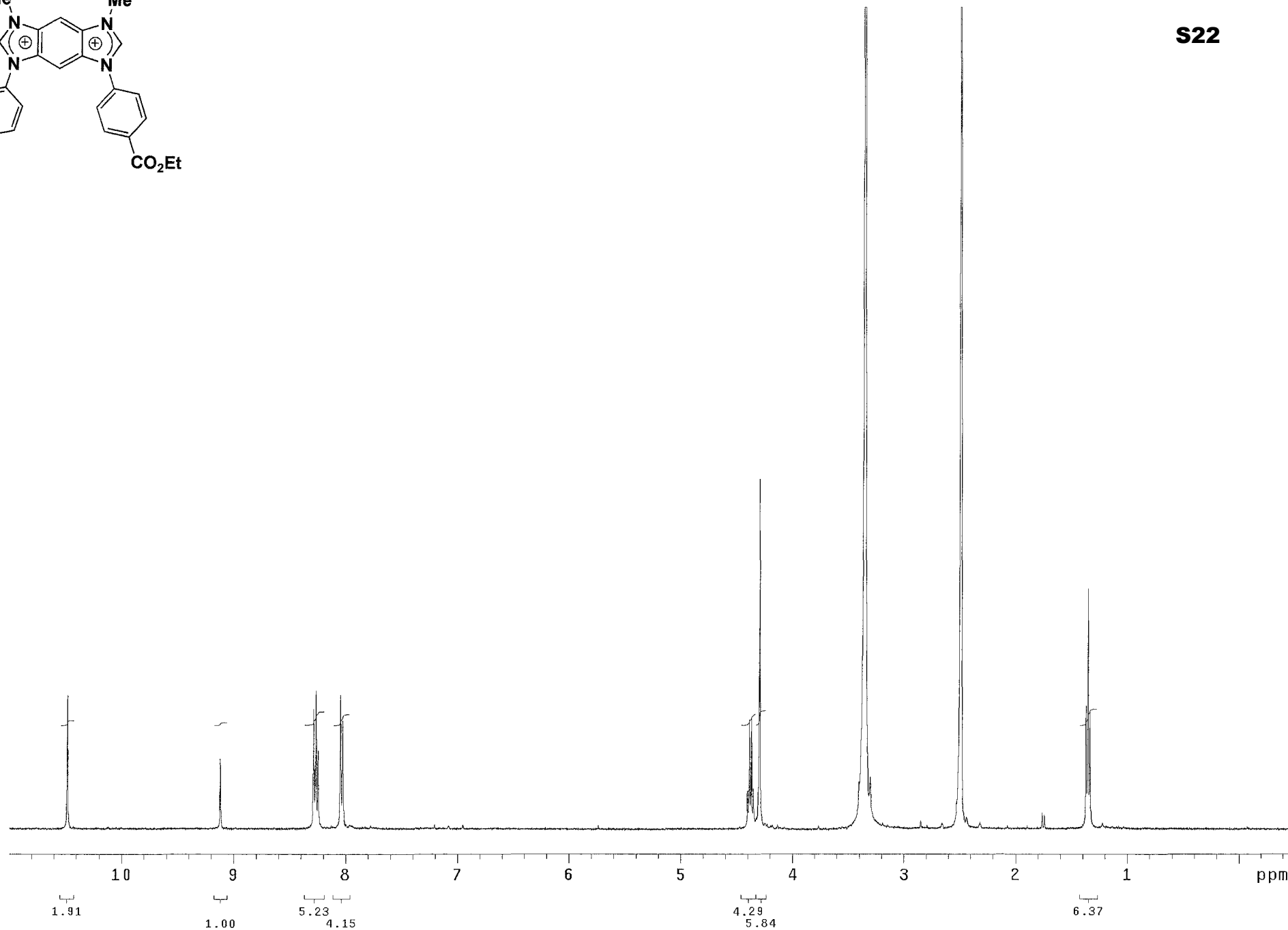
S21



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 53 repetitions	OBSERVE C13, 75.4700216 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 3 minutes			1PV161-13C Pulse Sequence: s2pu1 Solvent: CDC13 Ambient temperature UNITYplus-300 "nmr2"
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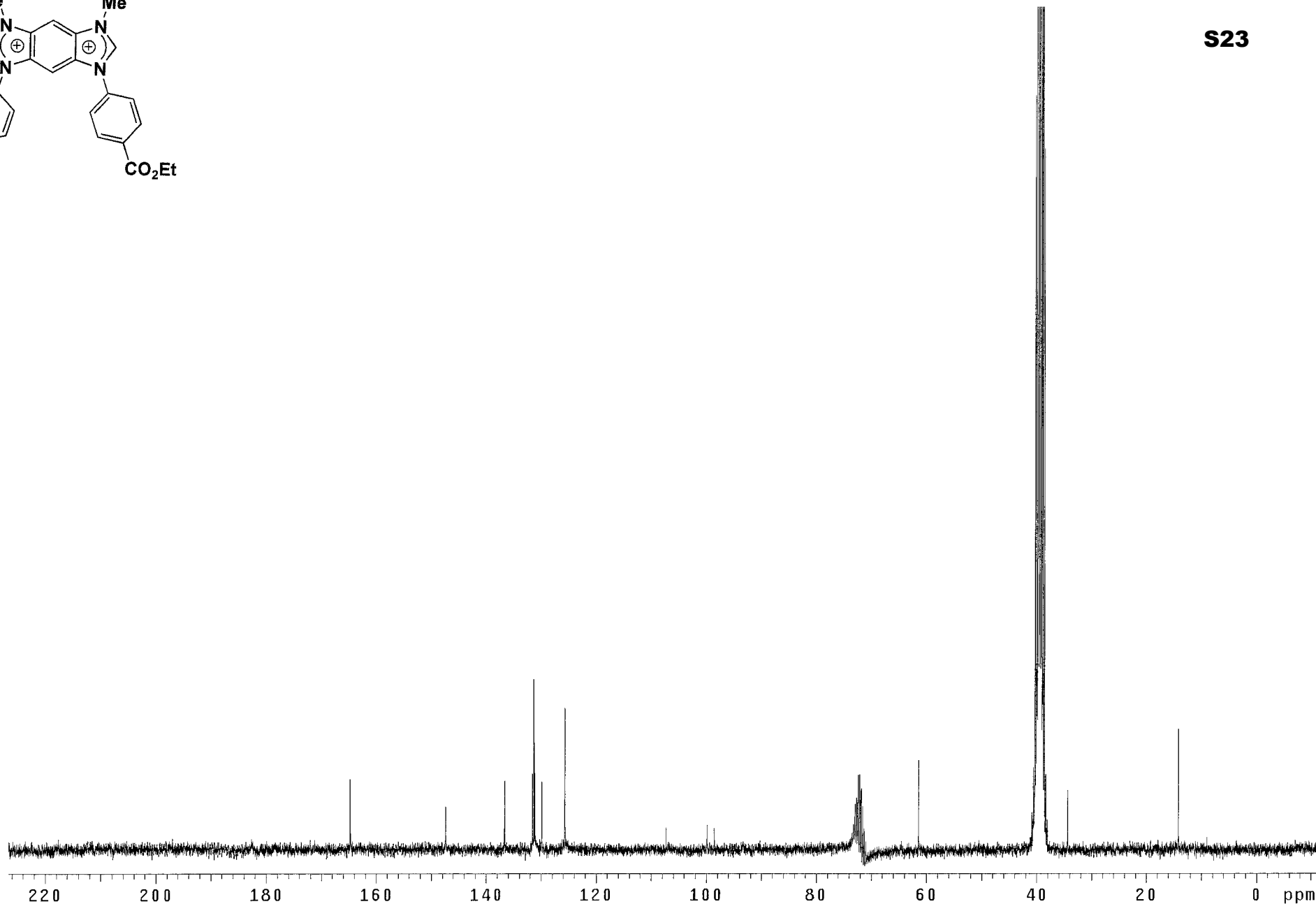
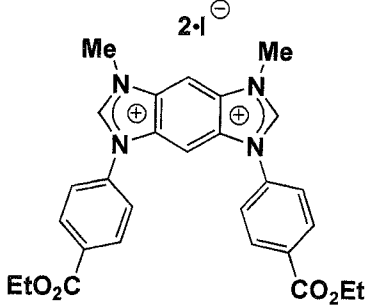


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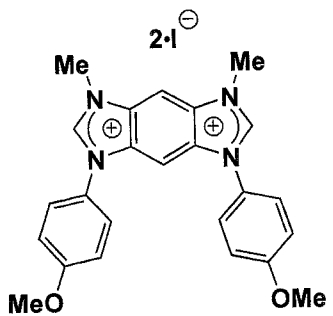


<p>PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 17 repetitions</p>	<p>OBSERVE H1, 400.2688760</p>	<p>DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute</p>			<p>B6AB238 Pulse Sequence: s2pul Solvent: DMSO Ambient temperature File: B6AB238 Mercury-400 "nmr6"</p>
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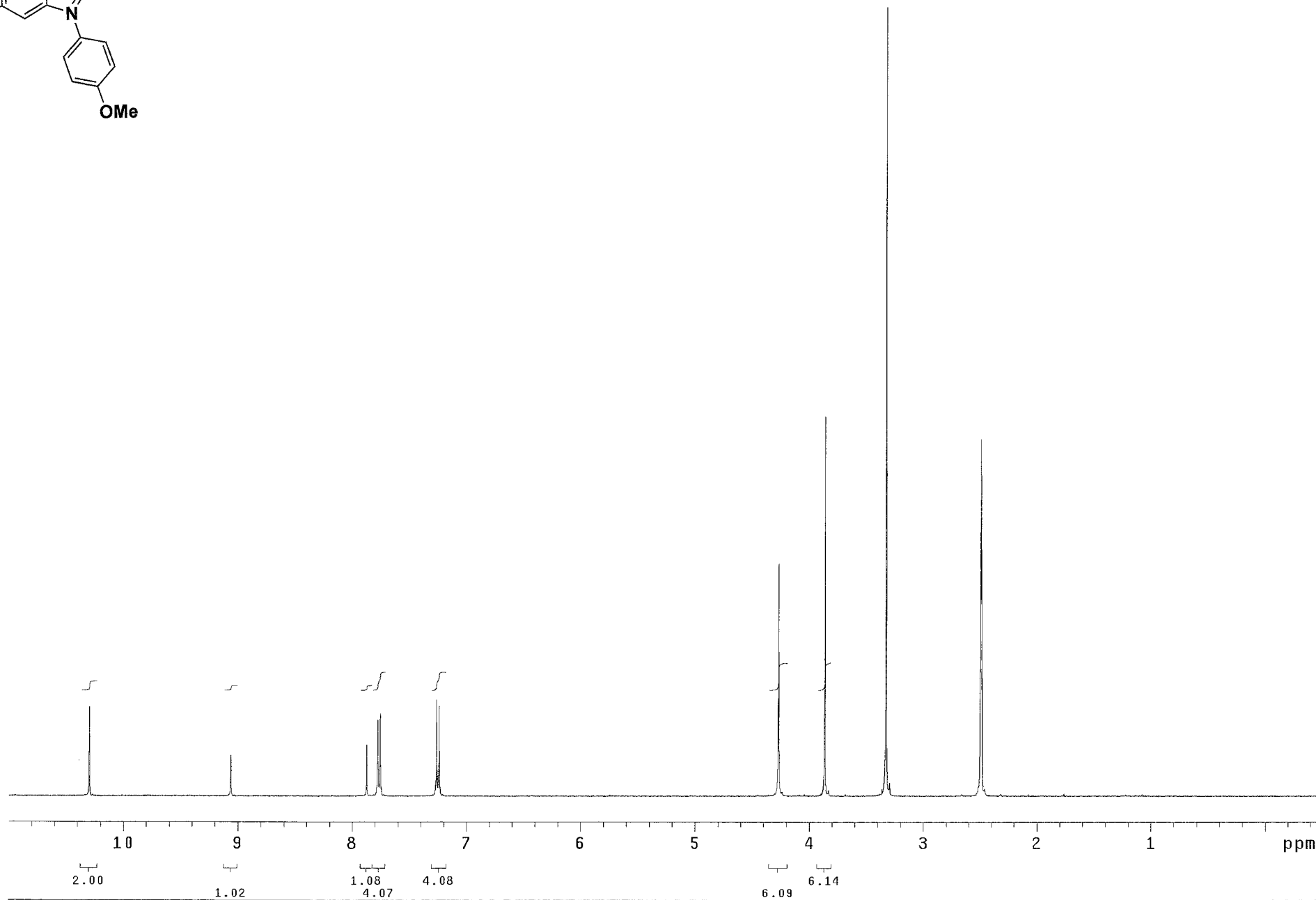
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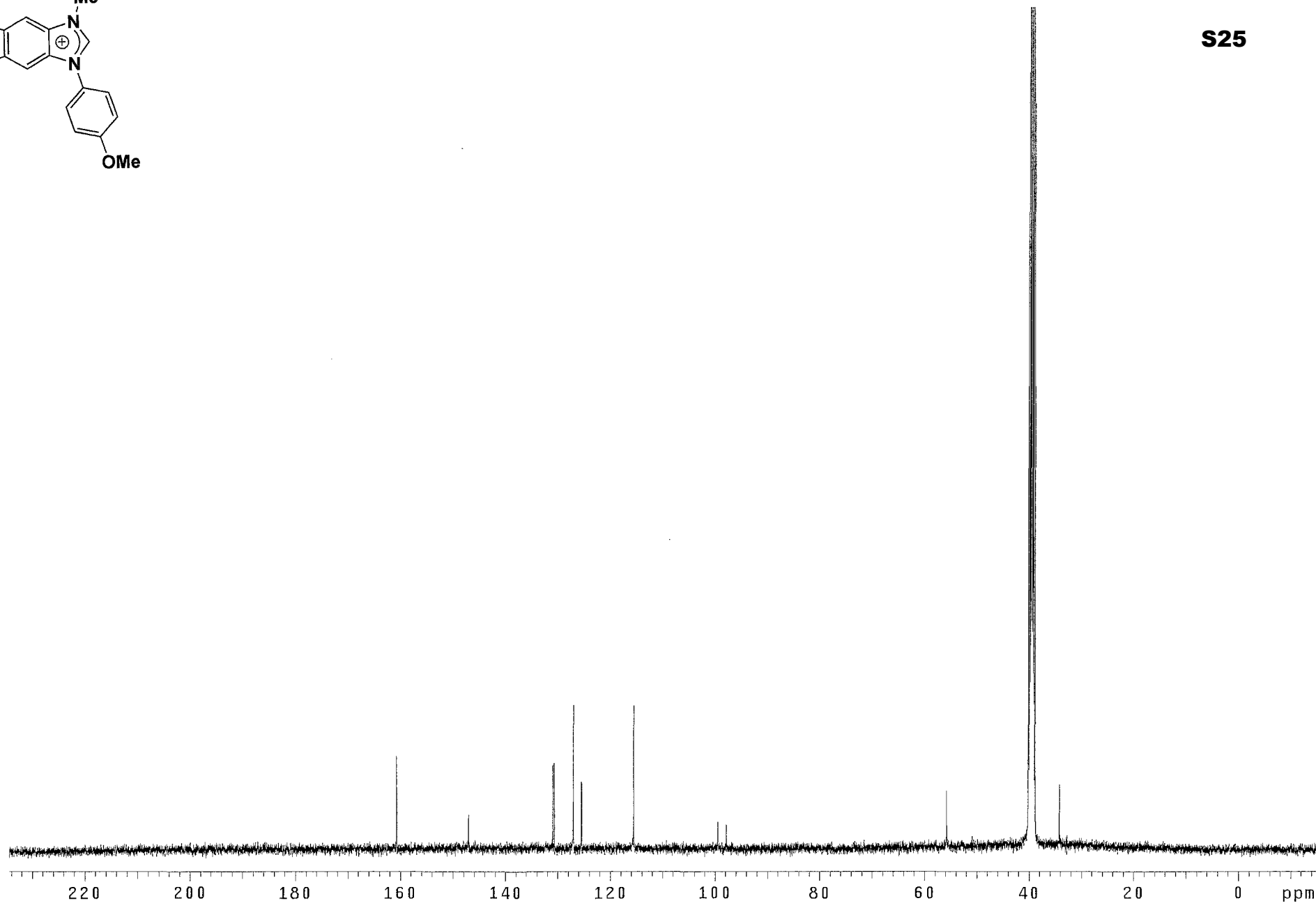
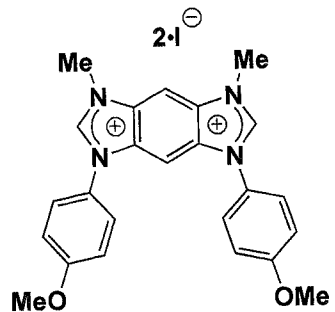
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 12219 repetitions	OBSERVE C13, 75.4704109 DECOUPLE H1, 300.1423516 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 12.8 hours	B6AB238-13C Pulse Sequence: s2pul Solvent: DMSO Ambient temperature UNITYplus-300 "nmr2"
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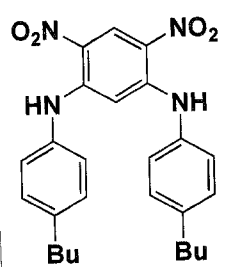
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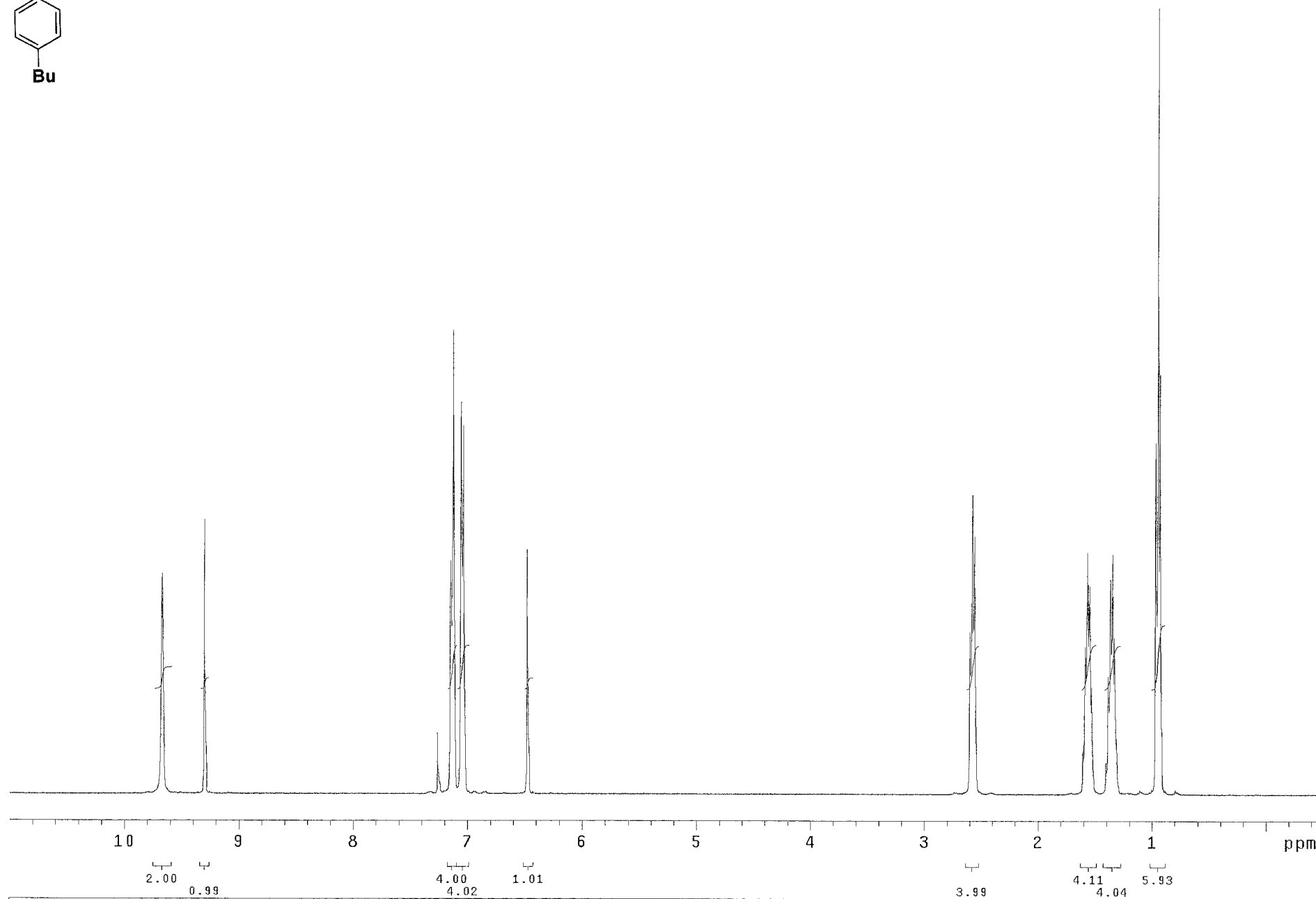
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 9 repetitions	OBSERVE H1, 400.2688764	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			ASS-201 Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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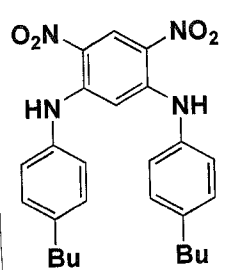
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 13925 repetitions	OBSERVE C13, 100.6477364 DECOUPLE H1, 400.2708968 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 12.7 hours			ASS201-13C Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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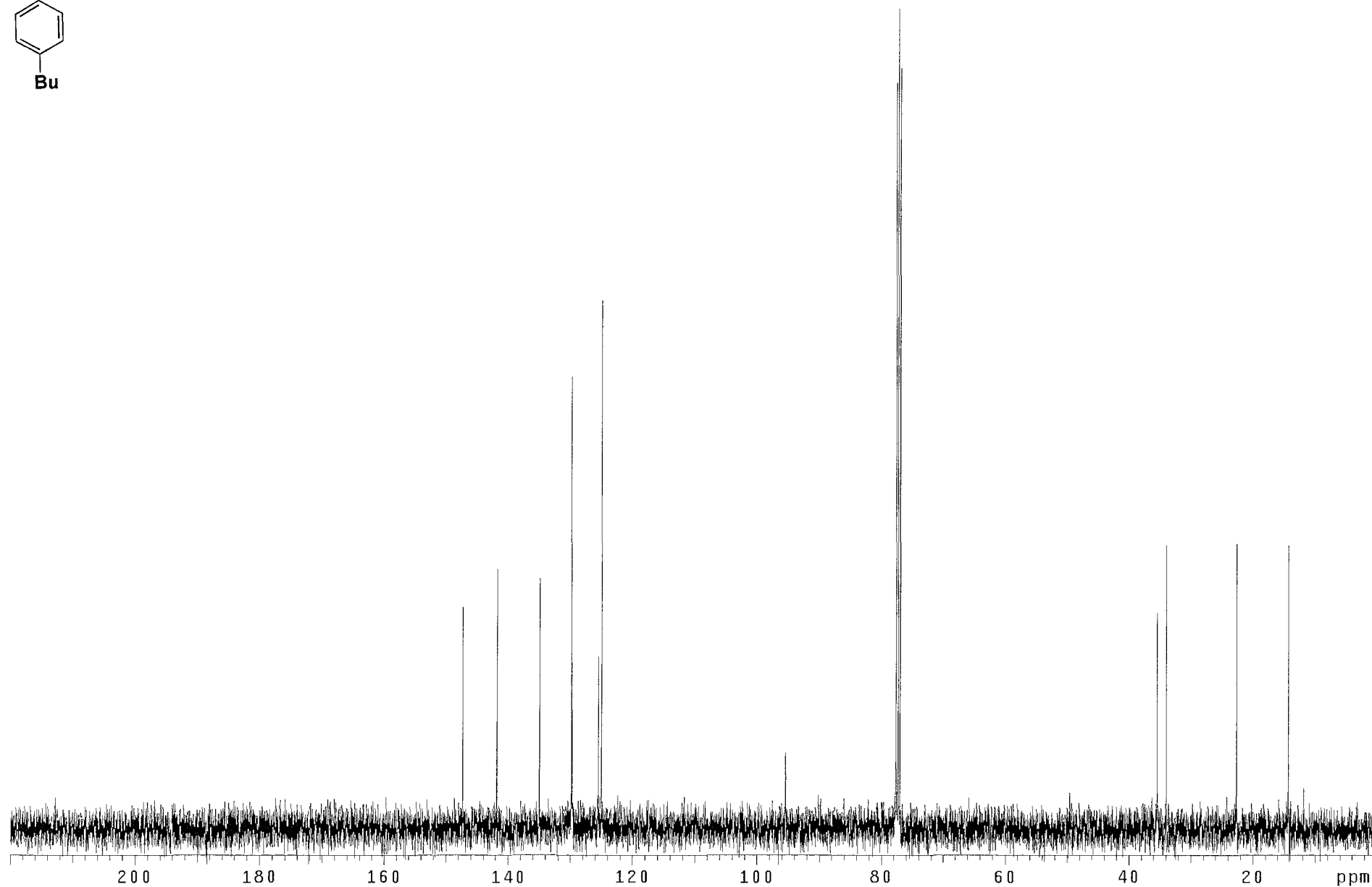
S26



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 7 repetitions	OBSERVE H1, 400.2669784	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute		1PV166 Pulse Sequence: s2pul Solvent: CDCl ₃ Ambient temperature Mercury-400 "nmr6"
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S27

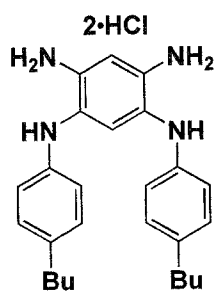


PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 22.5 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
53 repetitions

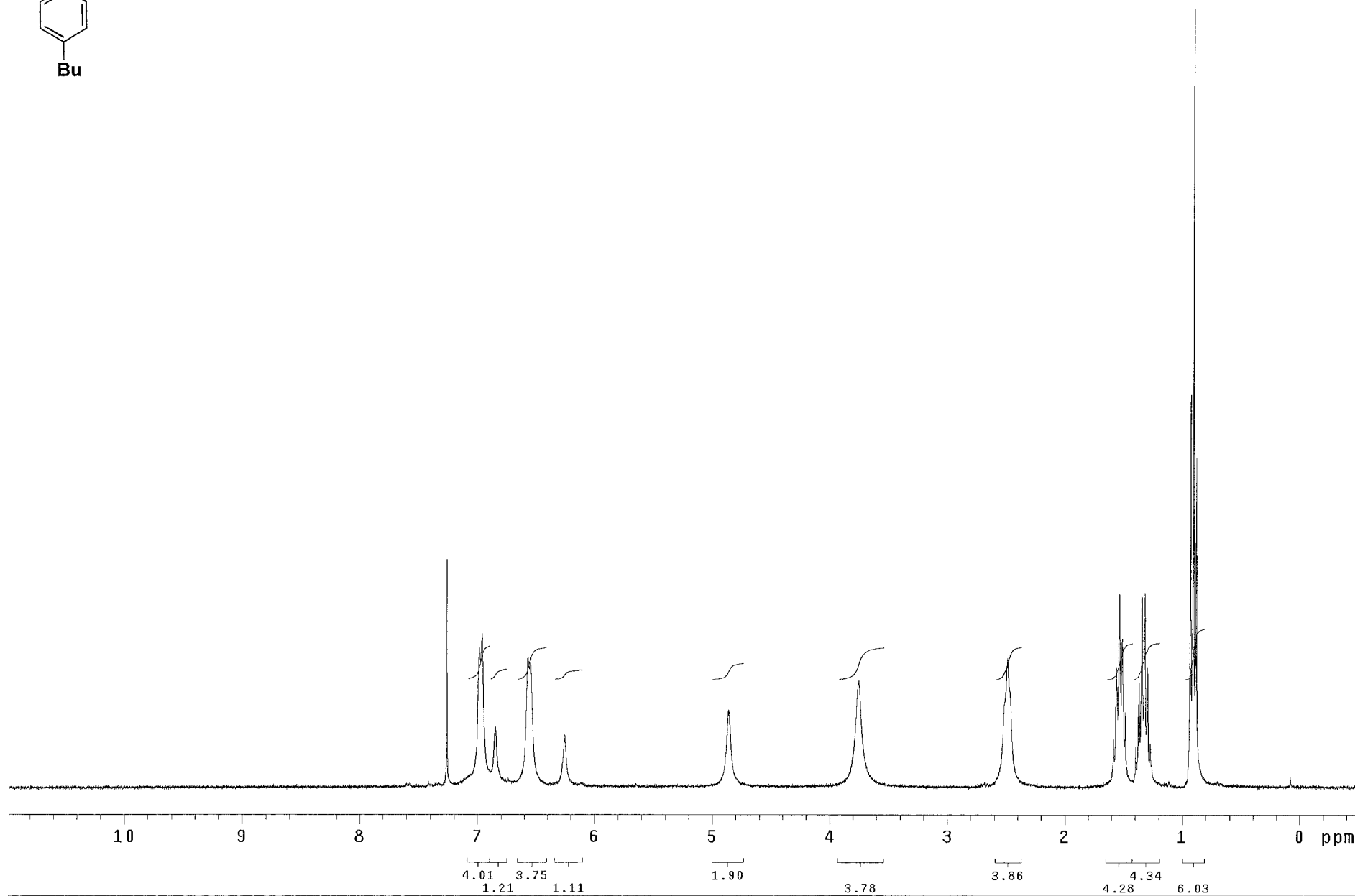
OBSERVE C13, 100.6471877
DECOUPLE H1, 400.2689955
Power 38 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 minutes

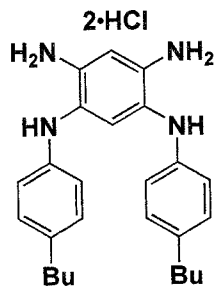
1PV166
Pulse Sequence: s2pul
Solvent: CDCl₃
Ambient temperature
Mercury-400 "nmr6"



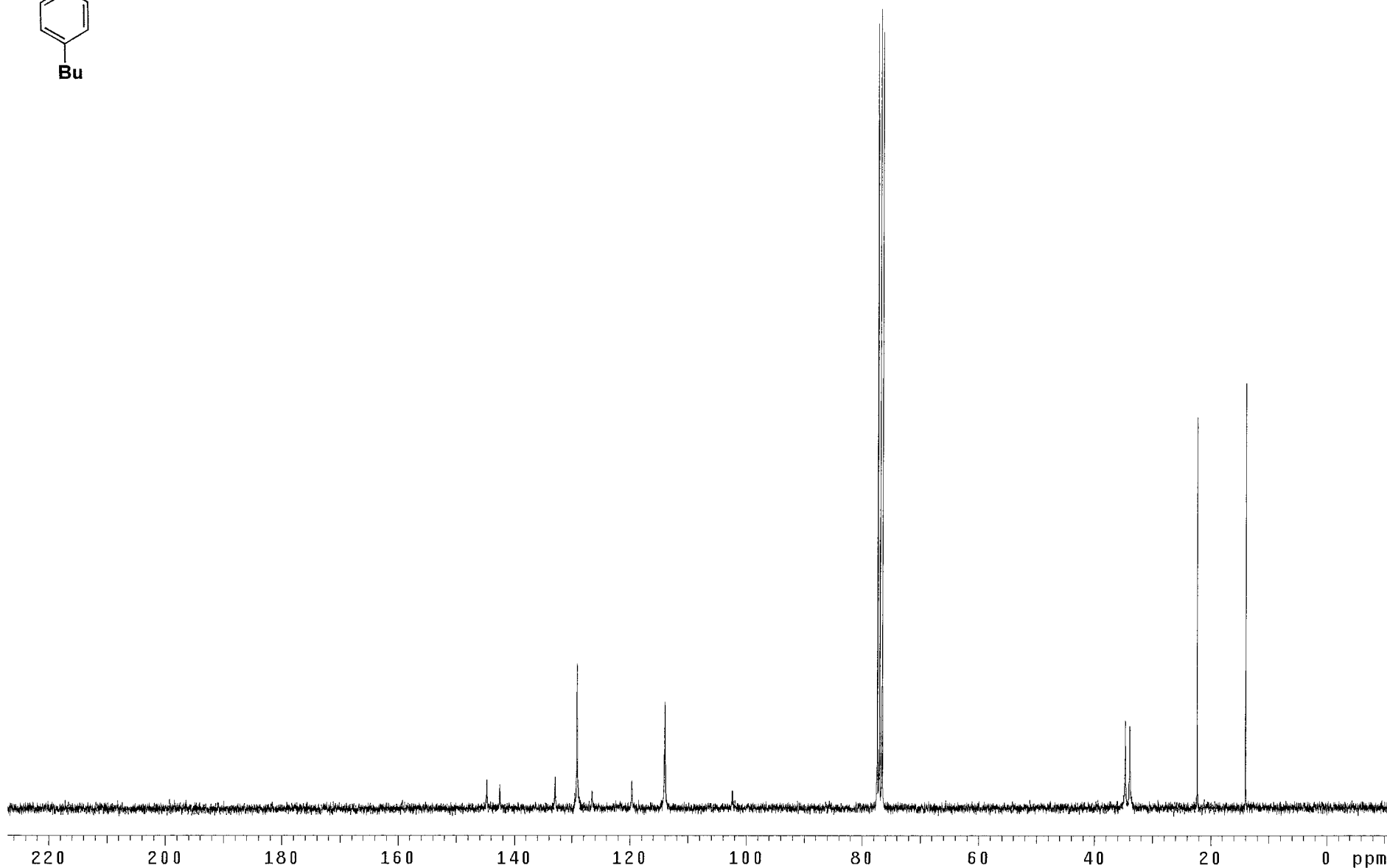
S28



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 27 repetitions	OBSERVE H1, 300.1390321	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 2 minutes			1PV150 Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature UNITYplus-300 "nmr2"
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S29



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
9175 repetitions

OBSERVE C13, 75.4700205
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9.6 hours

1PV50-13C

Pulse Sequence: s2pu1

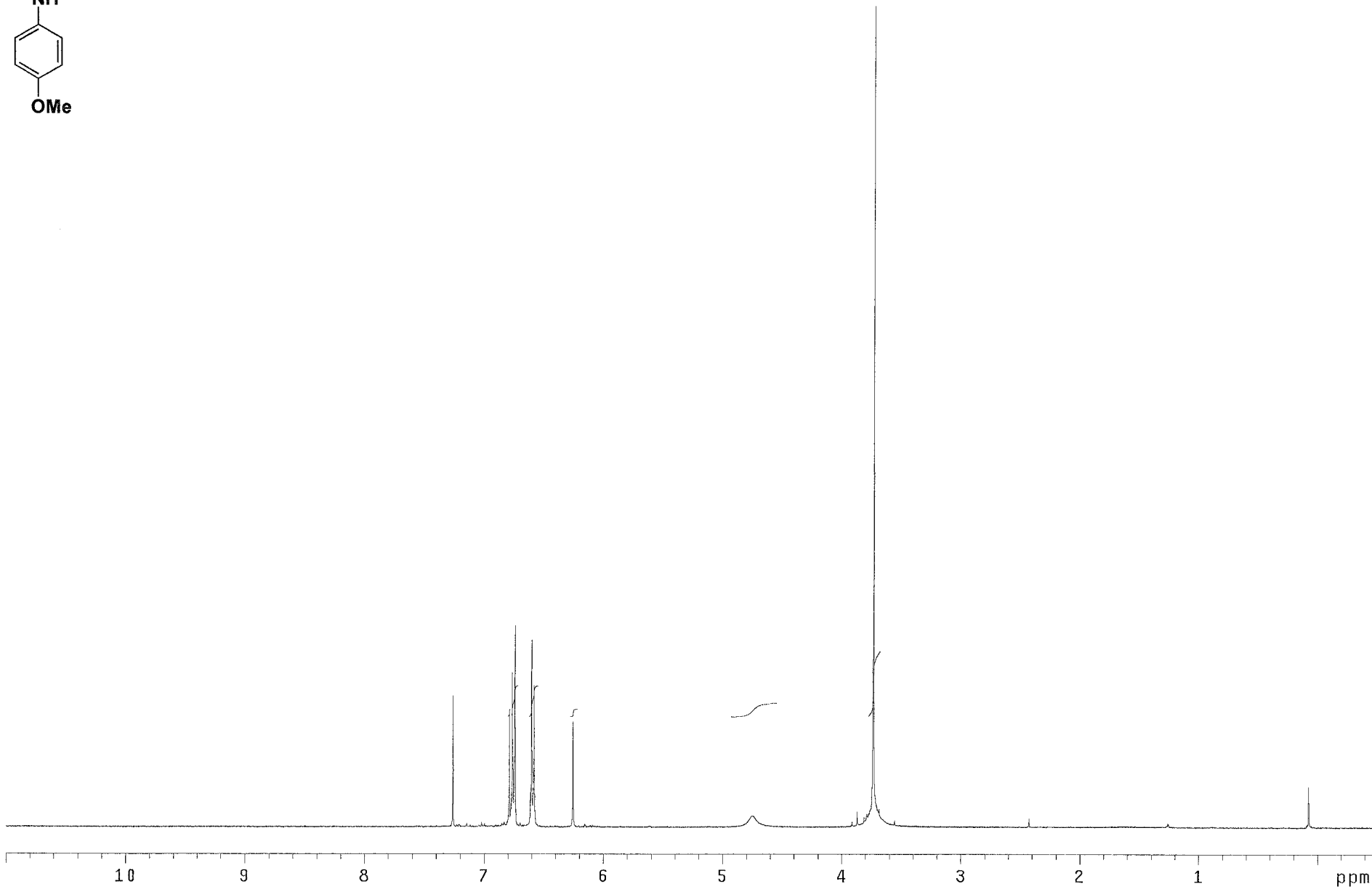
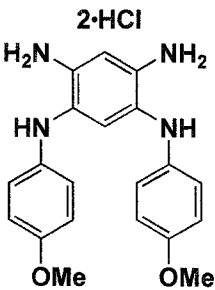
Solvent: CDCl₃

Ambient temperature

File: BOYDA

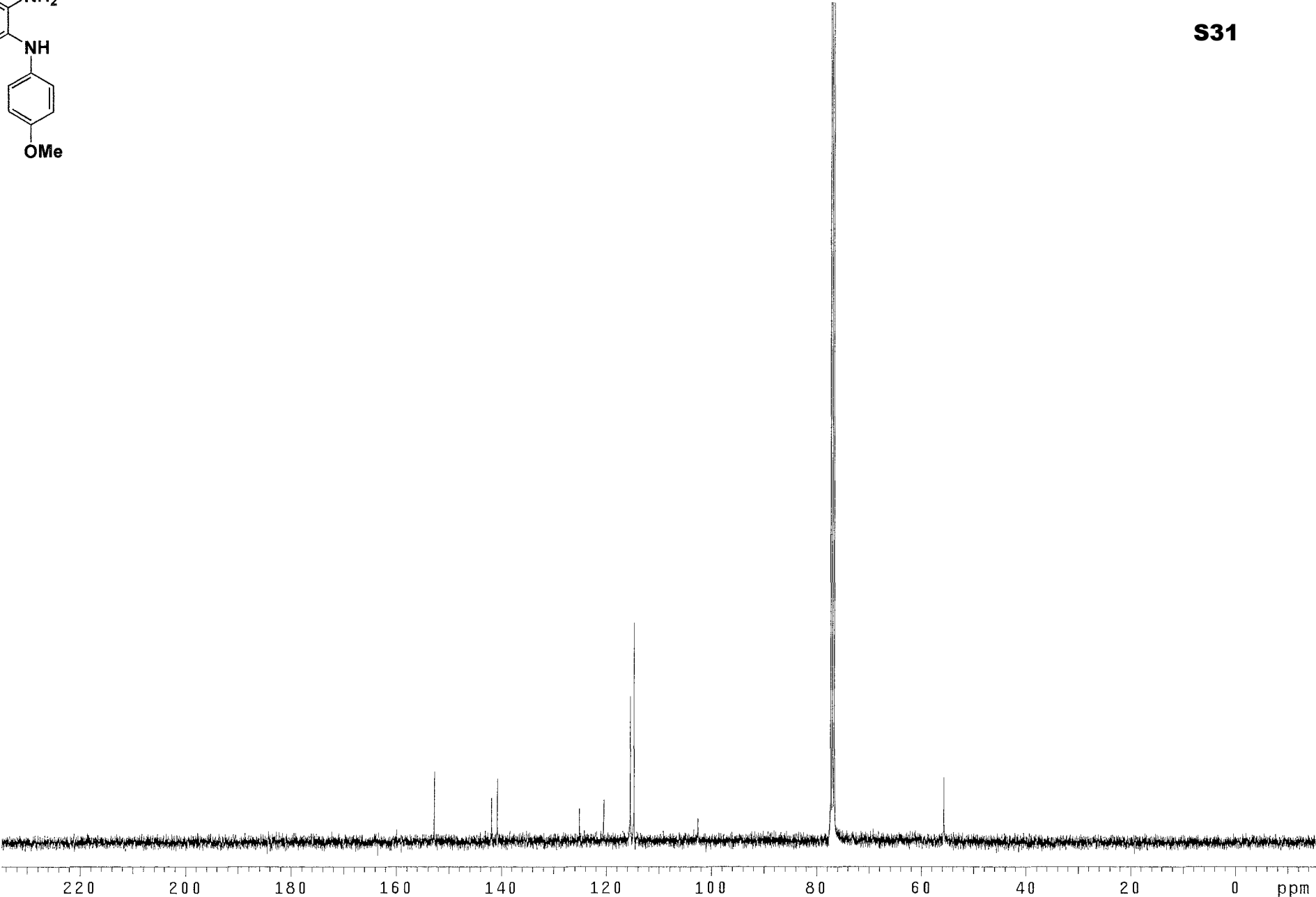
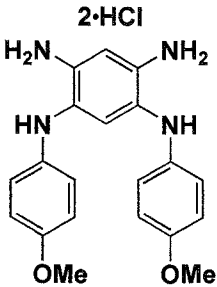
UNITYplus-300 "nmr2"

S30

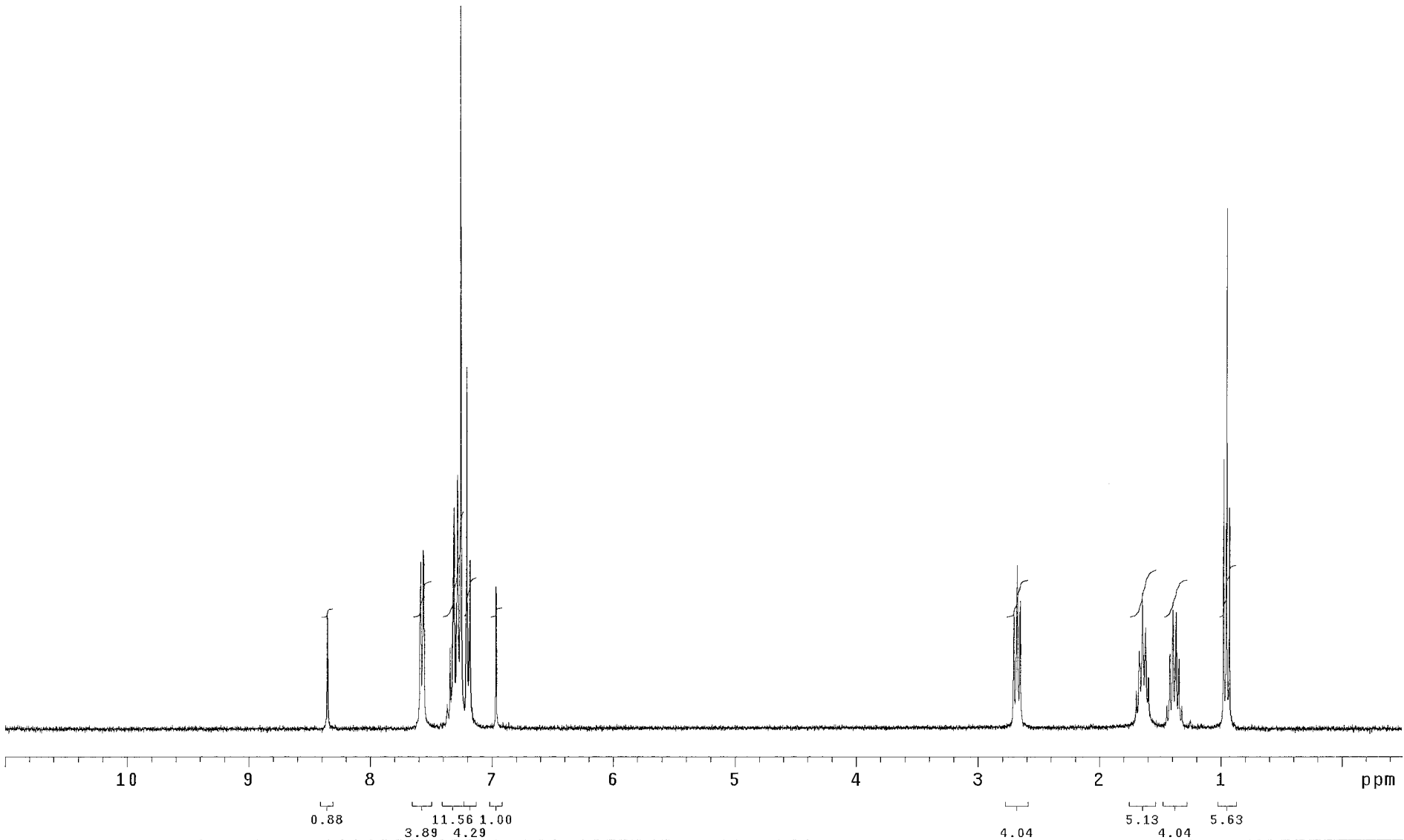
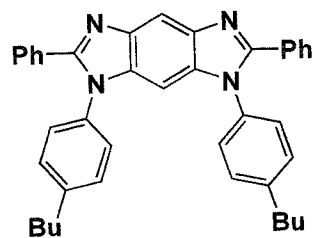


PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 8 repetitions	OBSERVE H1, 400.2669779	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			1PV171 Pulse Sequence: s2pul Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"
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S31

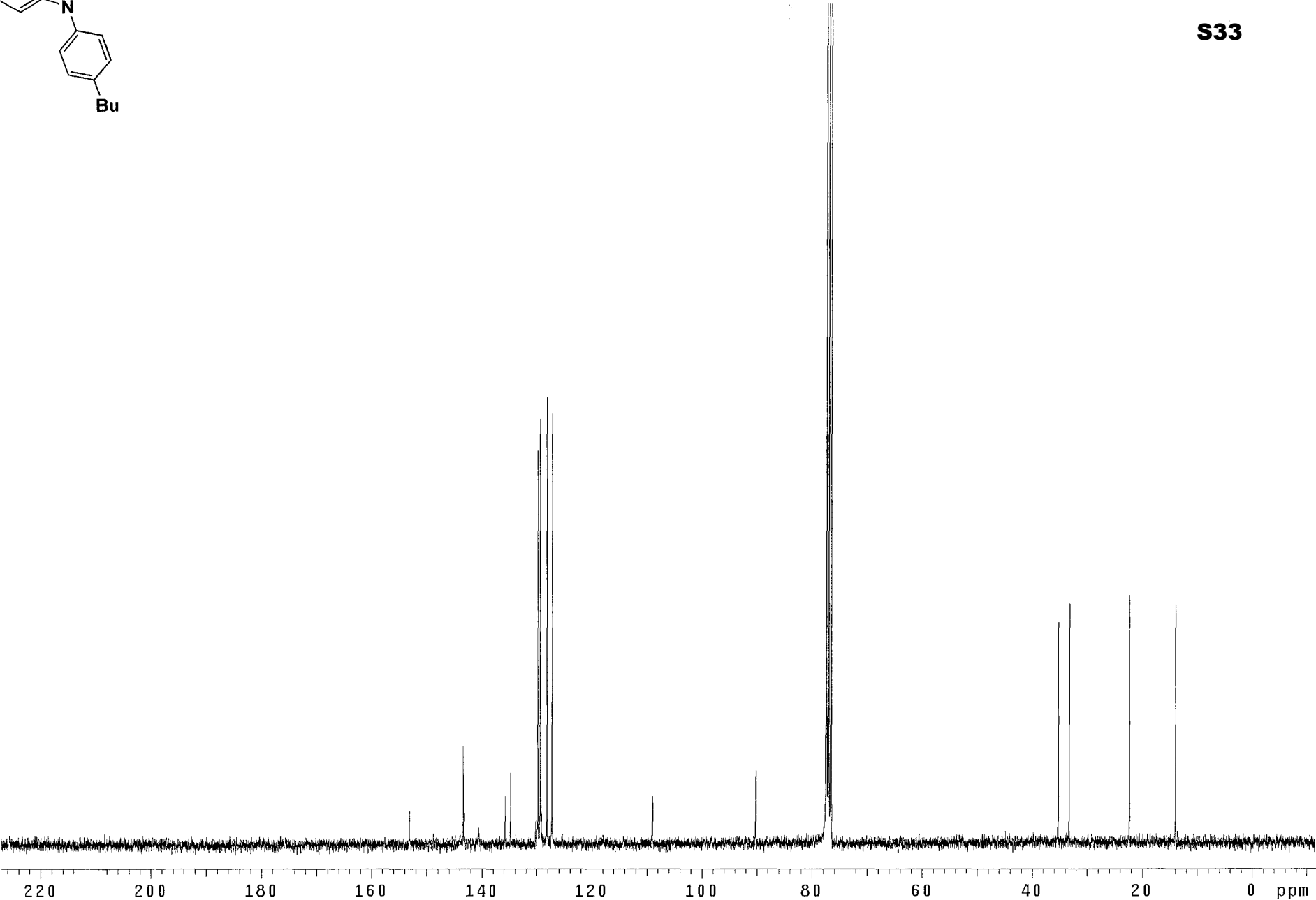
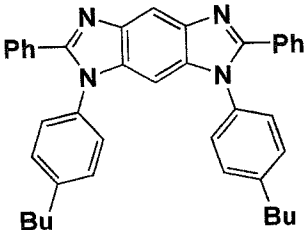


PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 4035 repetitions	OBSERVE C13, 100.6472130 DECOUPLE H1, 400.2689955 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 3.7 hours			1PV171-13C Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"
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<p>PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 37 repetitions</p>	<p>OBSERVE H1, 300.1390321</p>	<p>DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 2 minutes</p>			<p>1PV155-Rx1 Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature UNITYplus-300 "nmr2"</p>
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S33

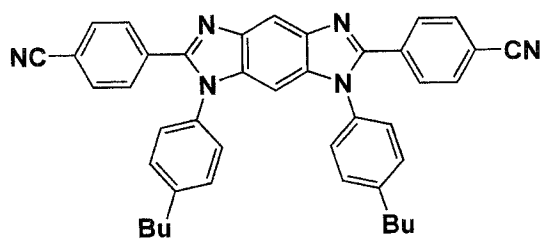


PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
20962 repetitions

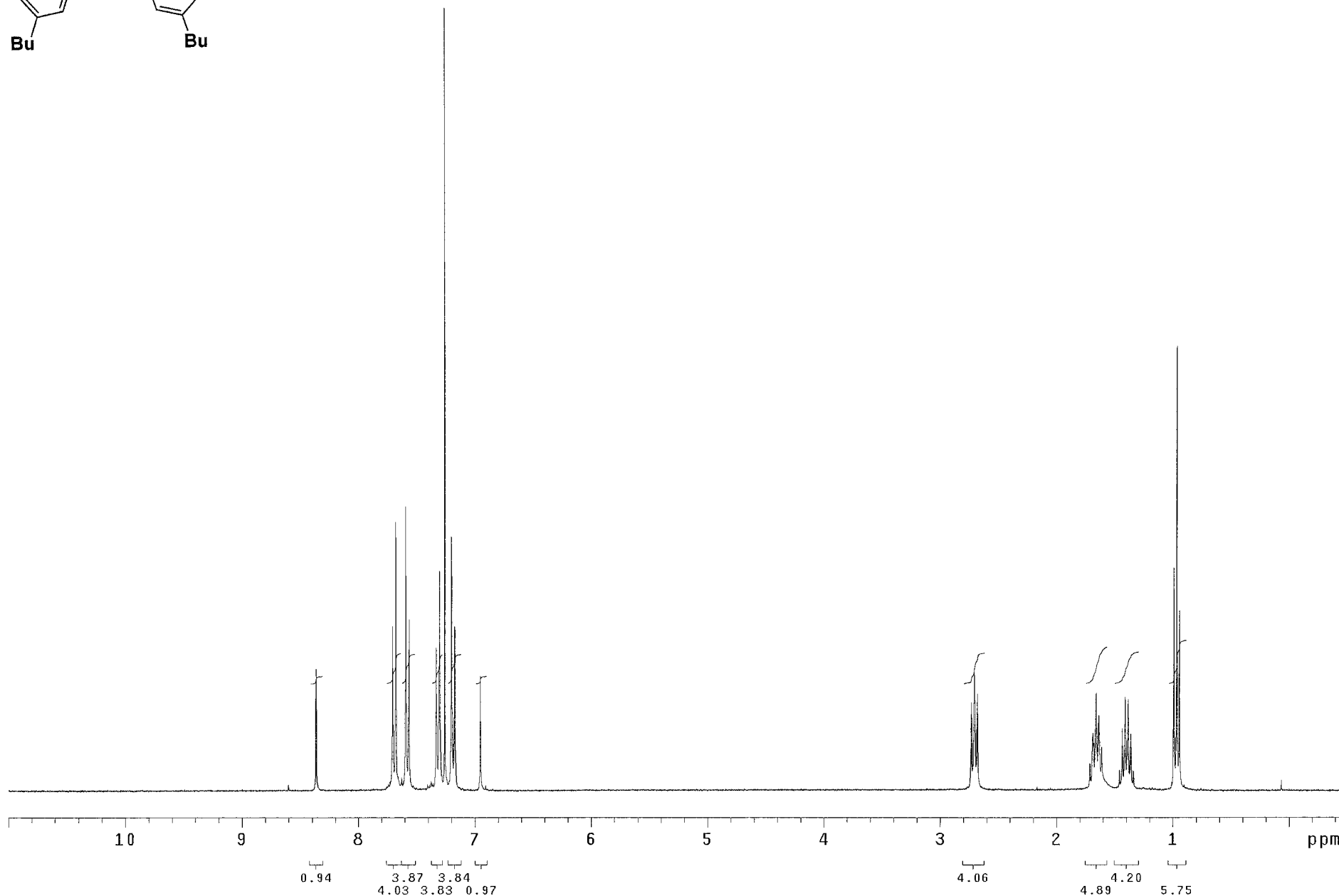
OBSERVE C13, 75.4700200
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 22.0 hours

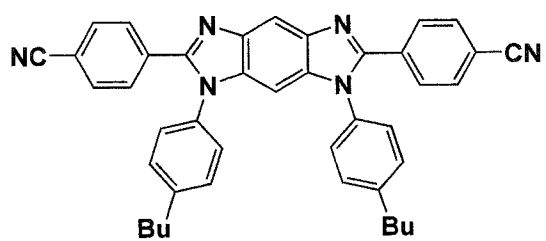
1PV155-13C
Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
UNITYplus-300 "nmr2"



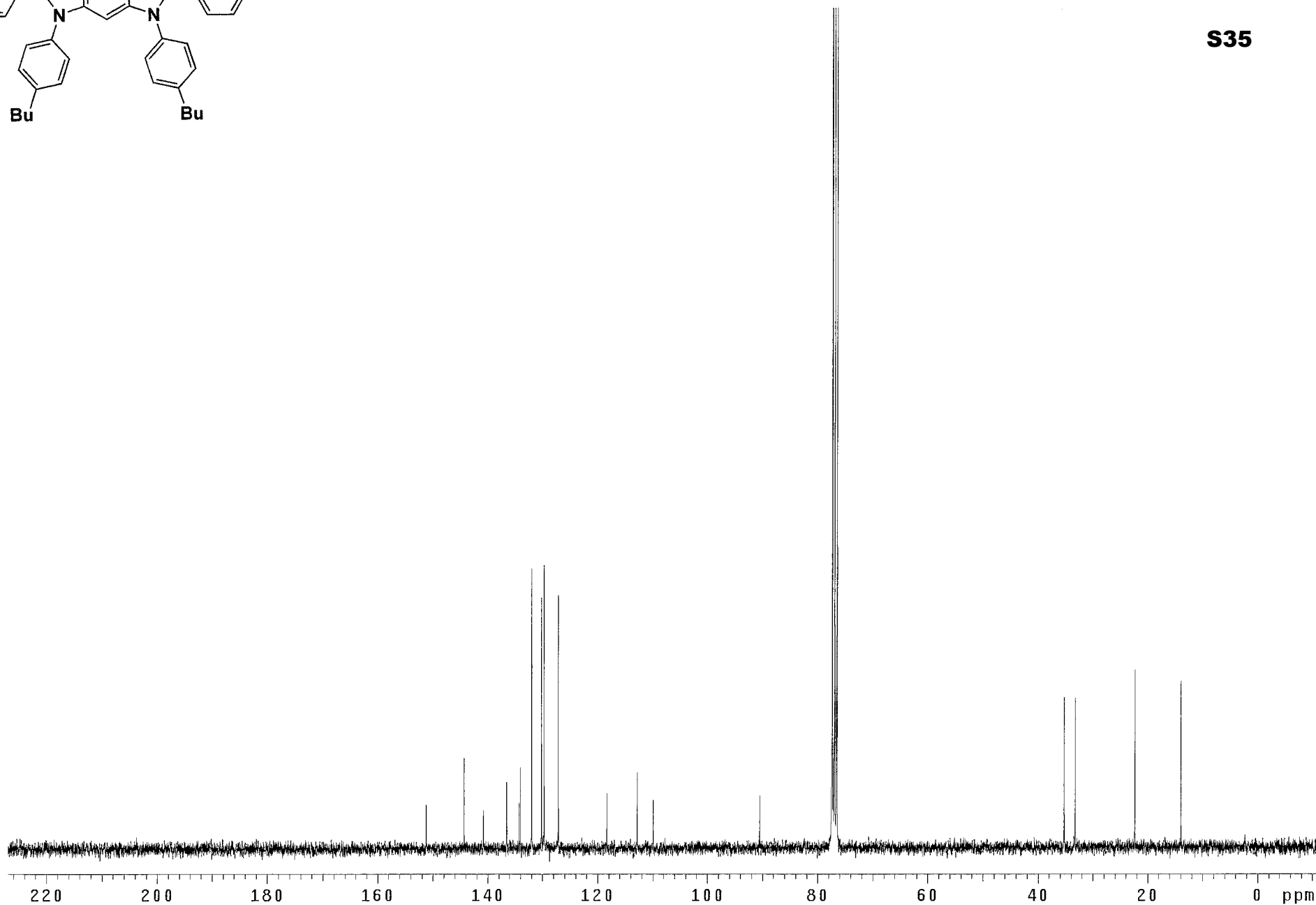
S34



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 276 repetitions	OBSERVE H1, 300.1390321	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 22 minutes			B6AB287-Rx1 Pulse Sequence: s2pu1 Solvent: CDC13 Ambient temperature UNITYplus-300 "nmr2"
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S35



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
9232 repetitions

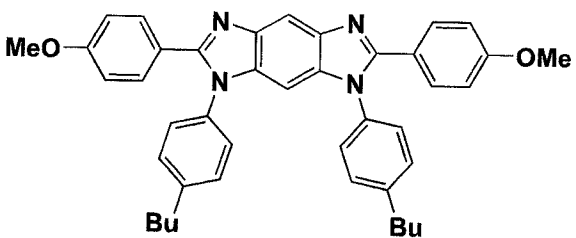
OBSERVE C13, 75.4700200
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9.7 hours

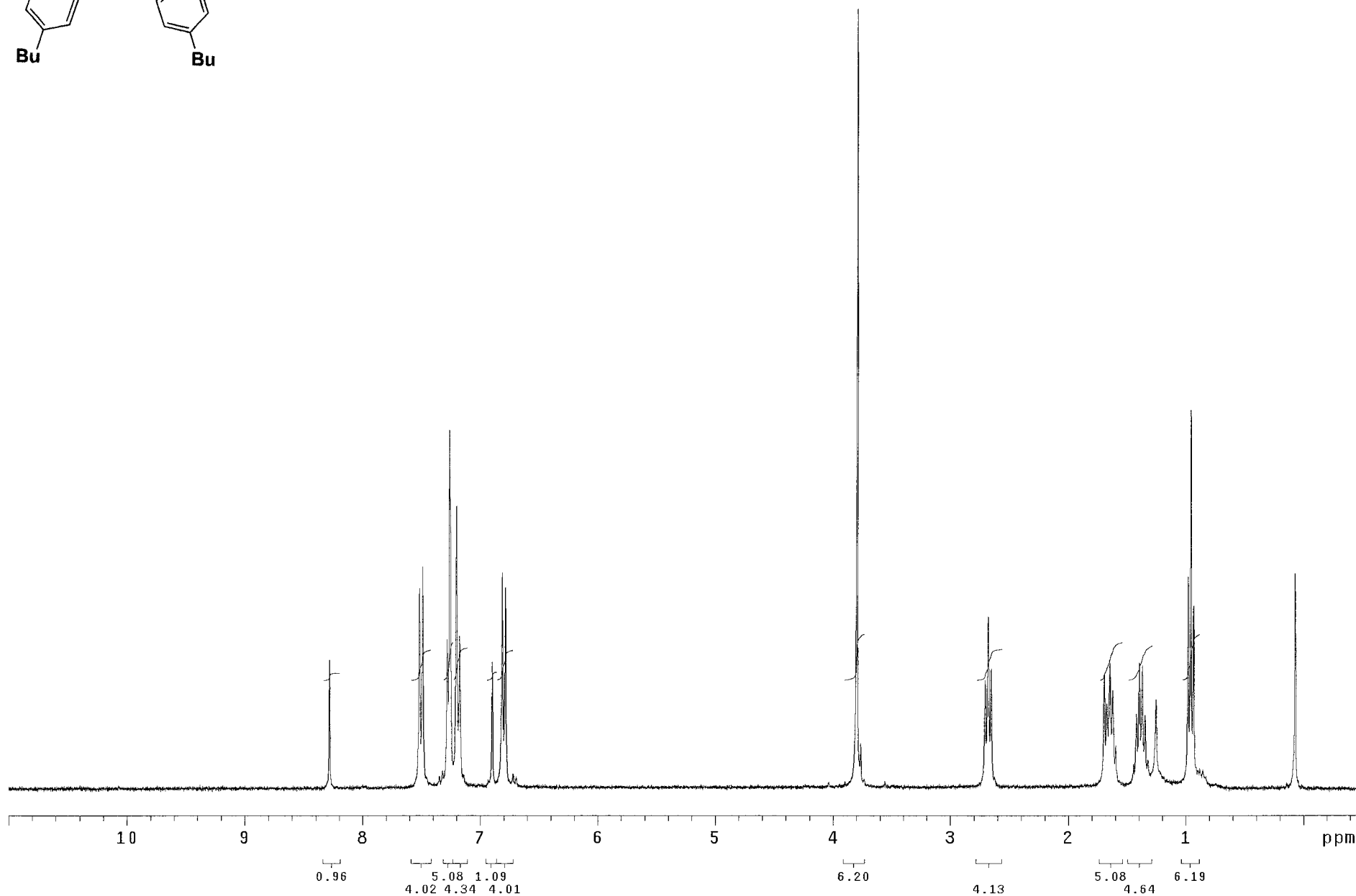
B6AB287-13C

Pulse Sequence: s2pu1

Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"



S36



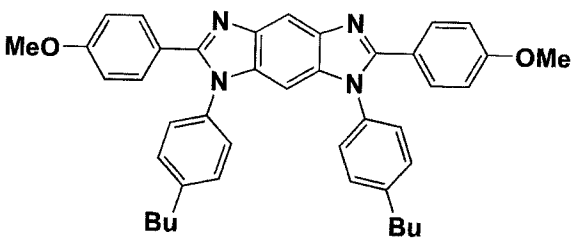
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
36 repetitions

OBSERVE H1, 300.1390316

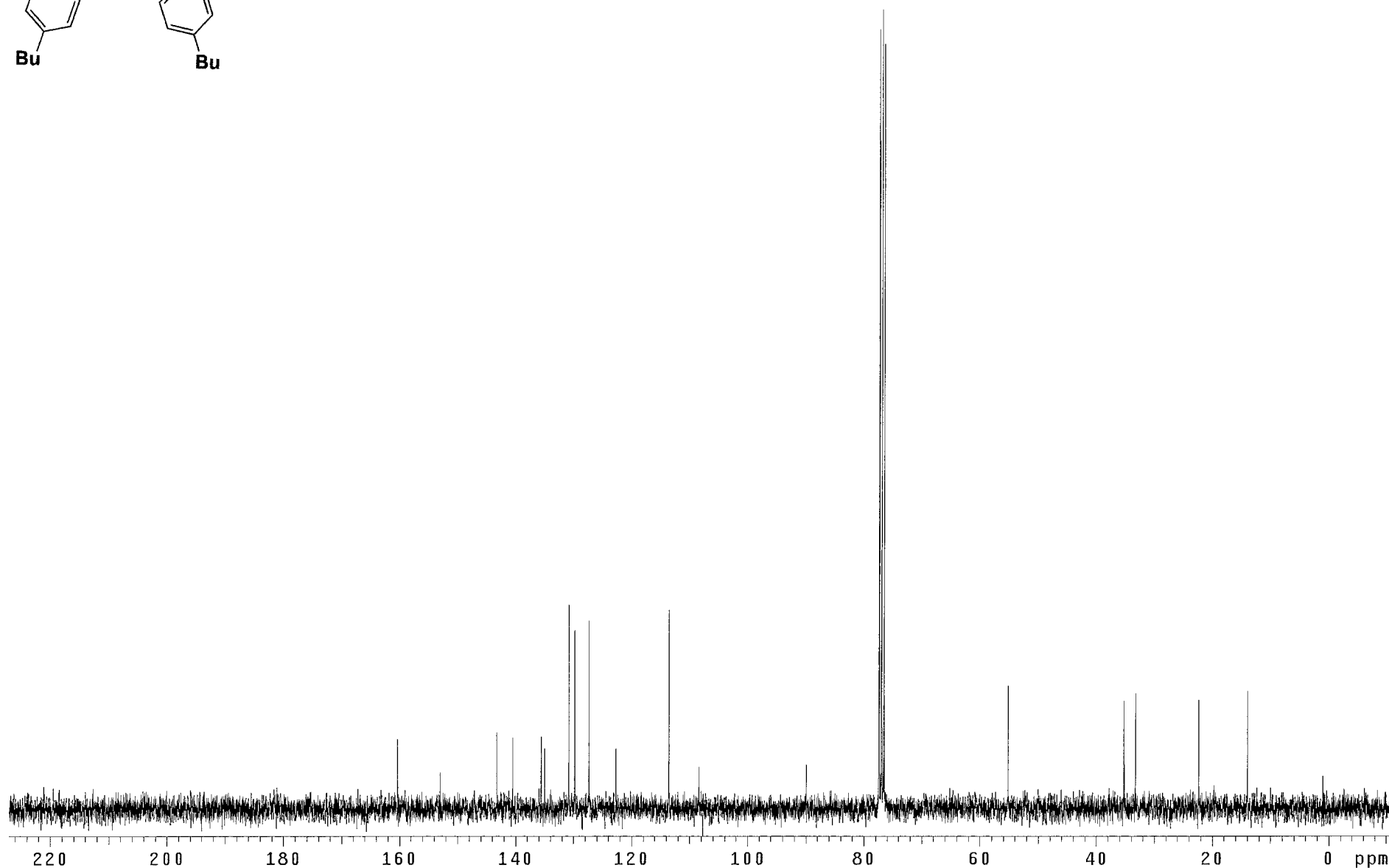
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 2 minutes

1PV157-Rx1

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"



S37



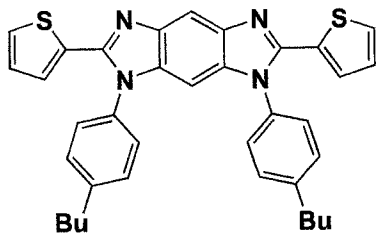
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
393 repetitions

OBSERVE C13, 75.4700205
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

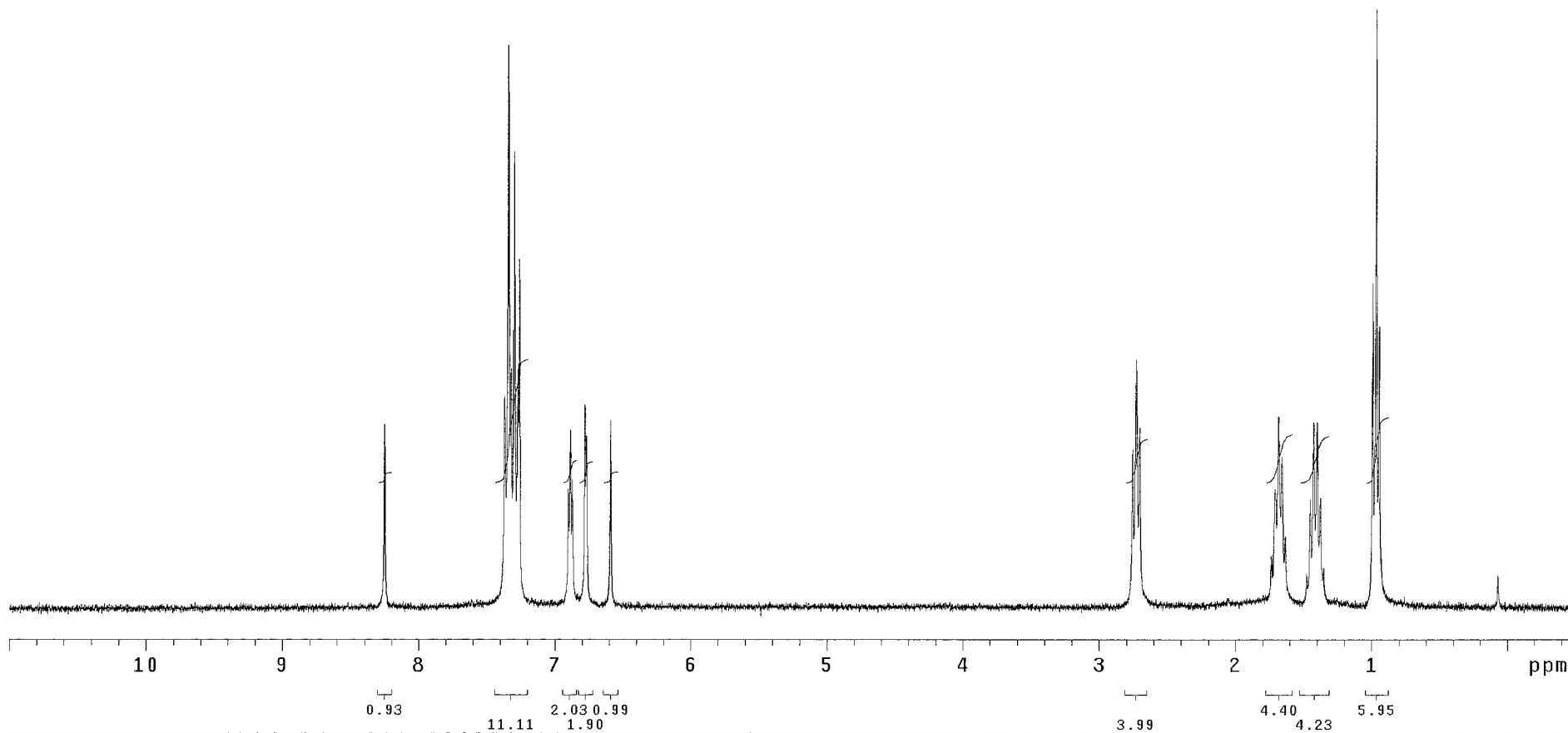
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 minutes

1PV157-13C

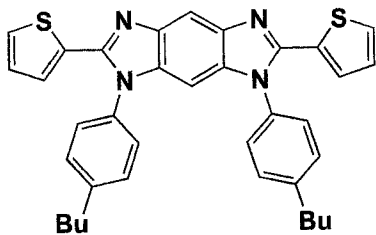
Pulse Sequence: s2pu1
Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"



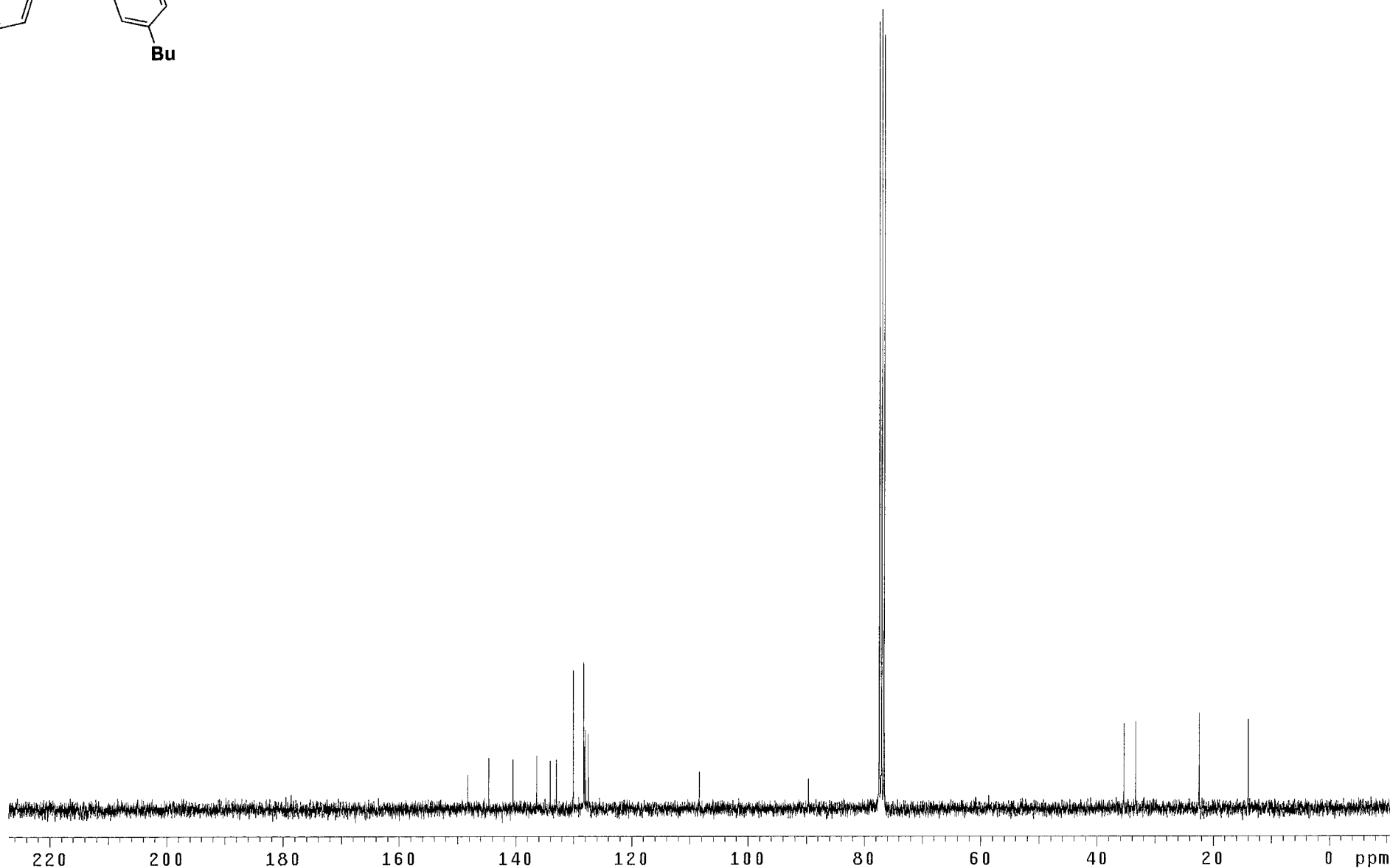
S38



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 18 repetitions	OBSERVE H1, 300.1390324	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			1PV158 Pulse Sequence: s2pu1 Solvent: CDCl ₃ Ambient temperature UNITYplus-300 "nmr2"
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S39



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
550 repetitions

OBSERVE C13, 75.4700211
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

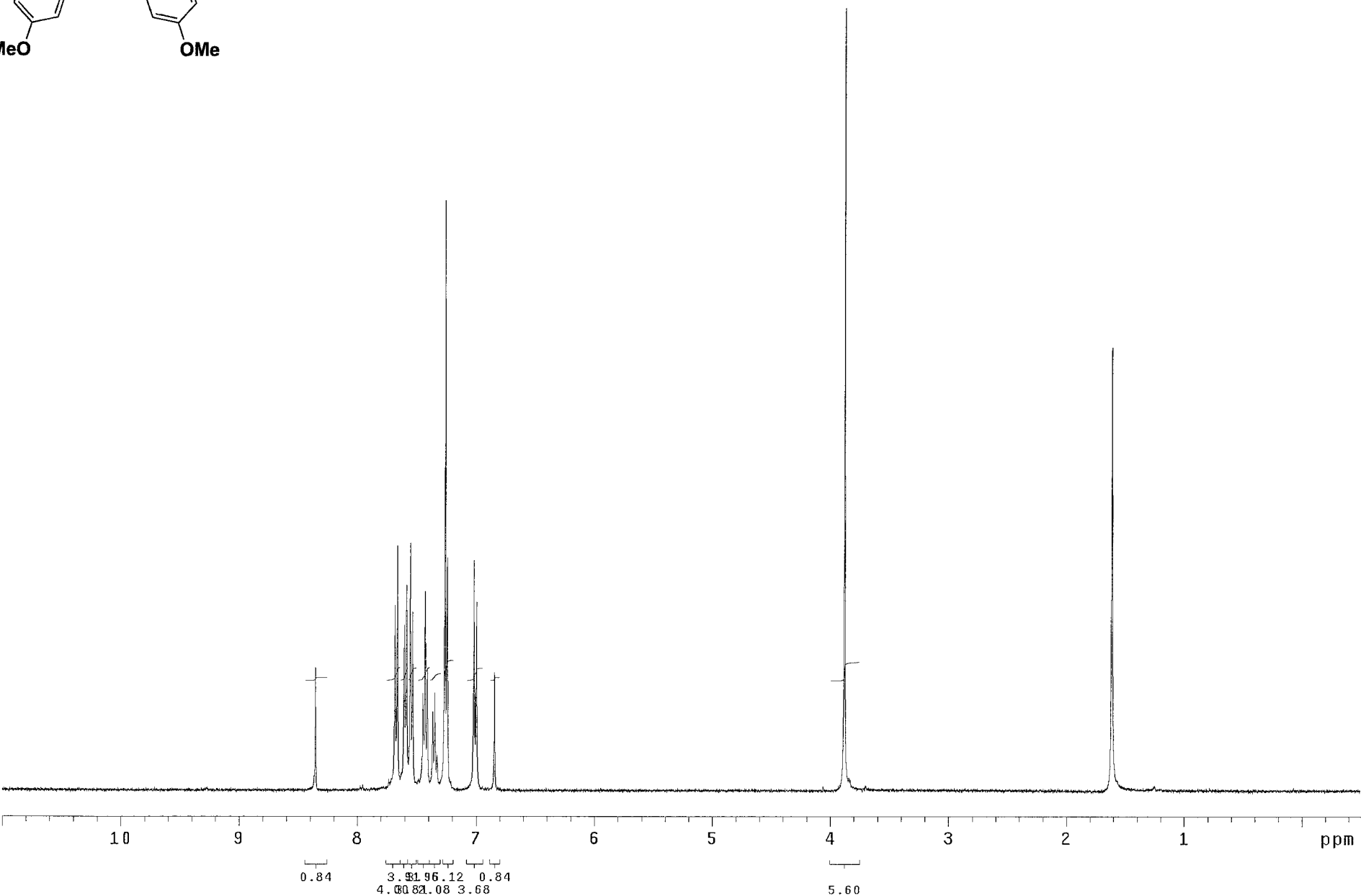
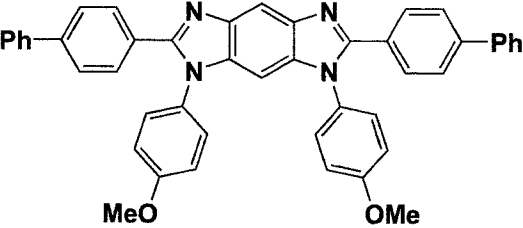
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 34 minutes

1PV158-13C

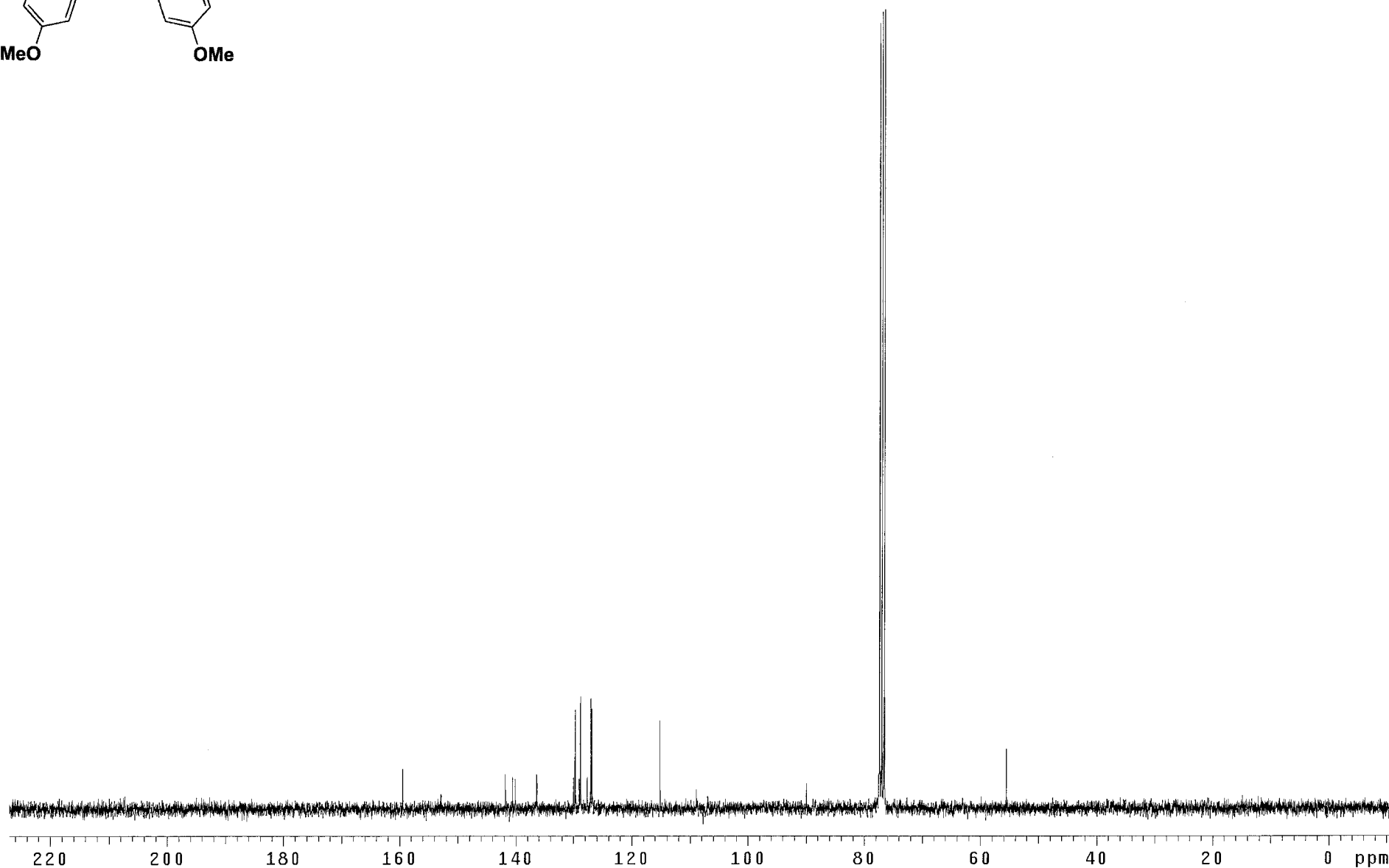
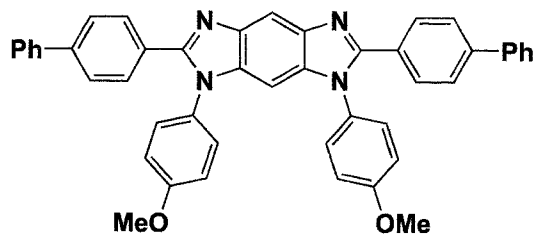
Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"

S40



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 26 repetitions	OBSERVE H1, 400.2669776	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 2 minutes			B6AB180
					Pulse Sequence: s2pul
					Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"

S41

PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
1353 repetitions

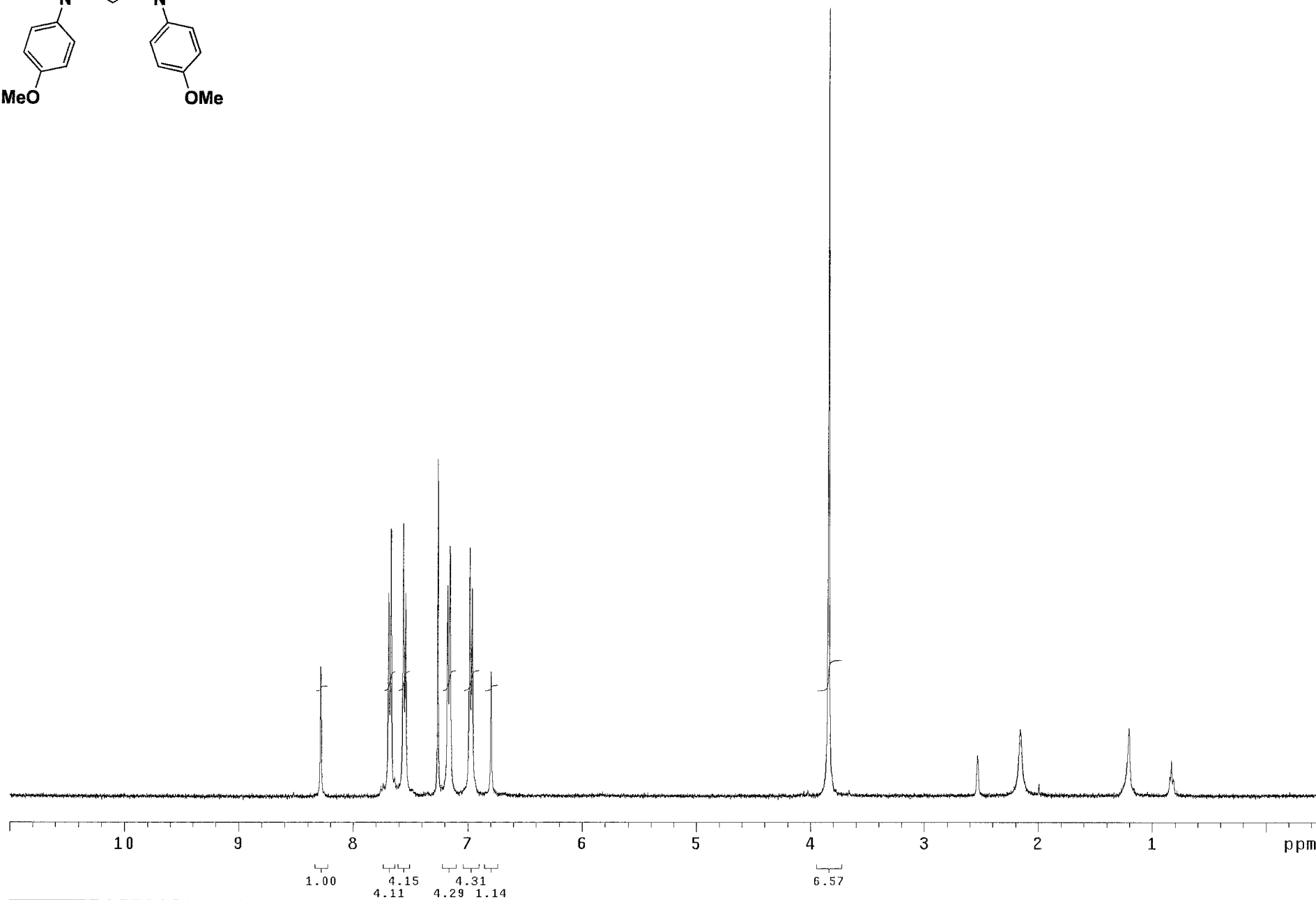
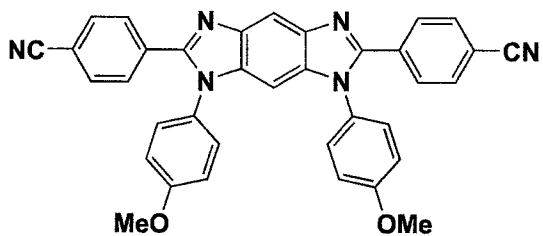
OBSERVE C13, 75.4700200
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 85 minutes

B6AB180-13C

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"

S42



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
13 repetitions

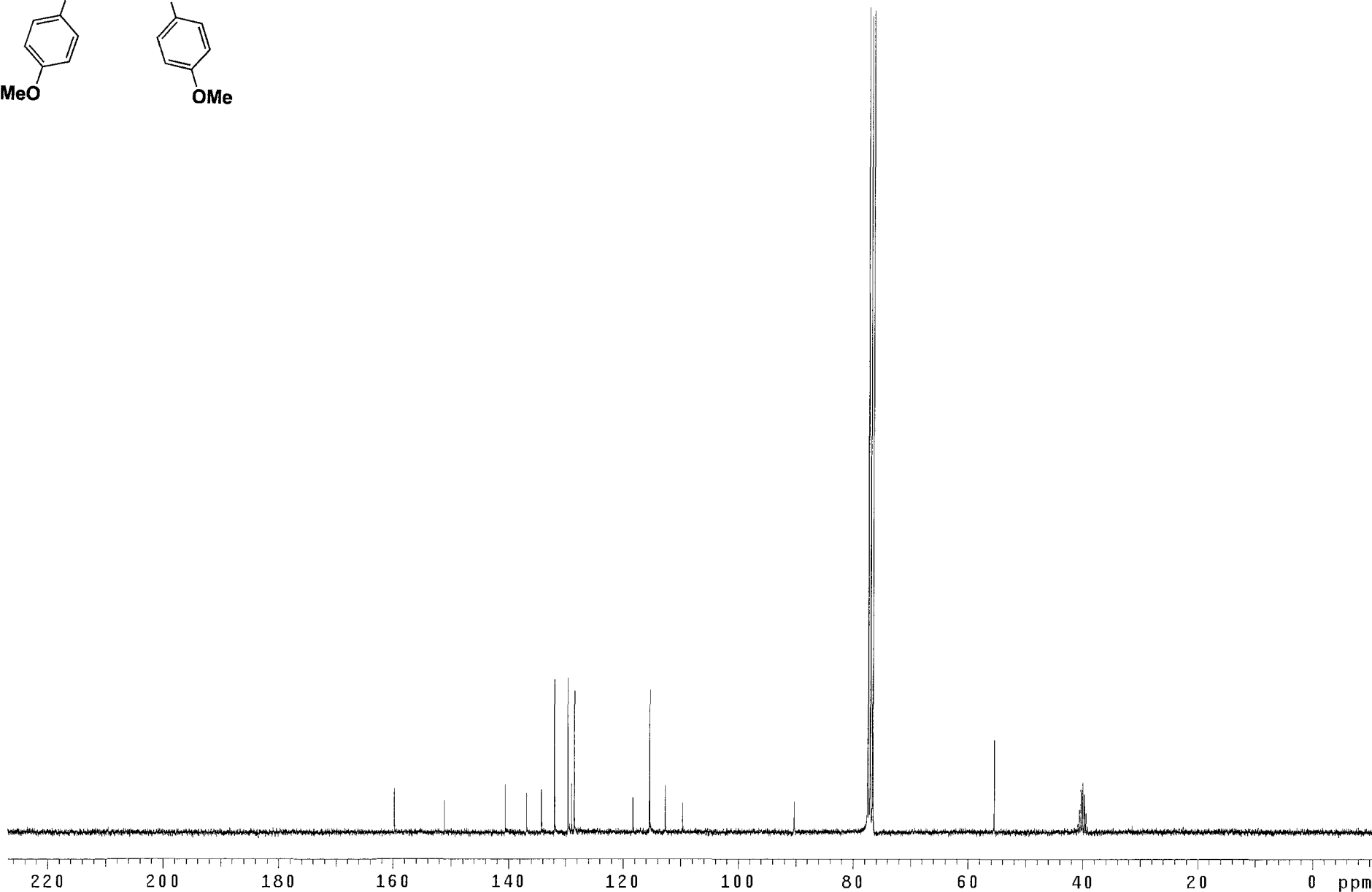
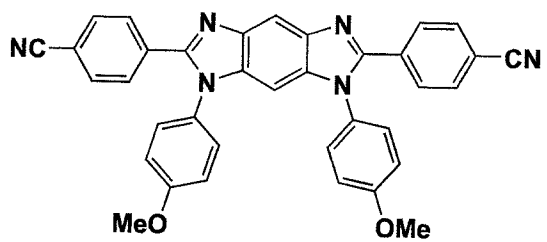
OBSERVE H1, 400.2669776

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute

B6AB181

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
Mercury-400 "nmr6"

S43



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
8599 repetitions

OBSERVE C13, 75.4700271
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

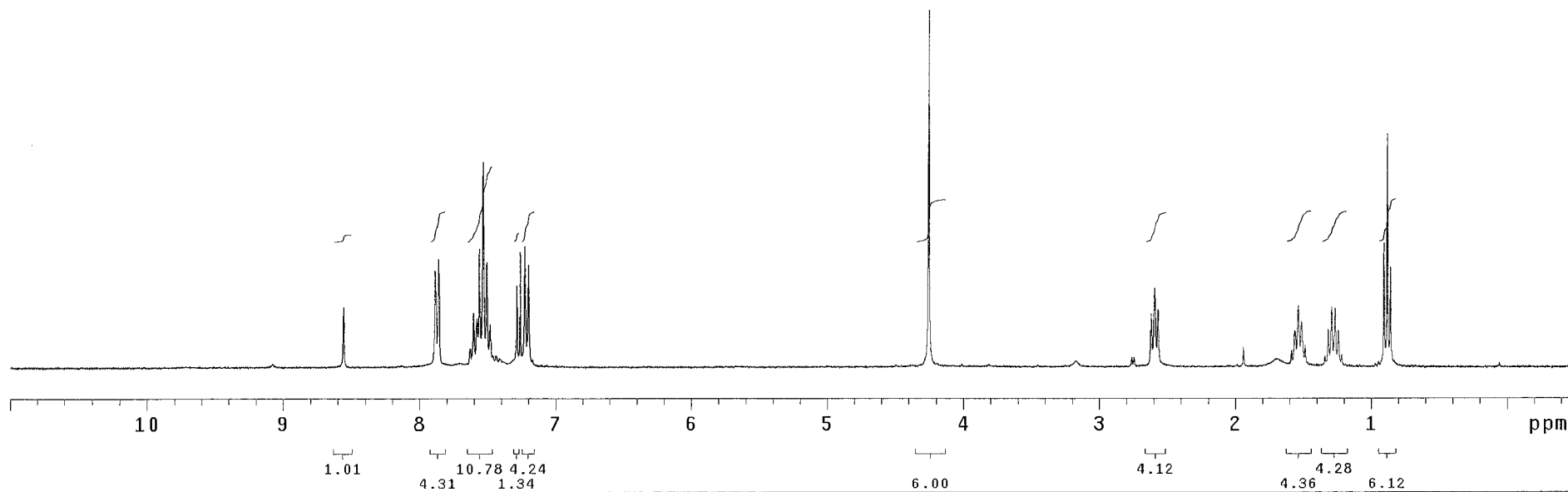
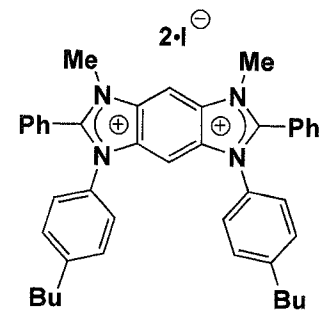
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9.0 hours

B6AB181-13C

Pulse Sequence: s2pul

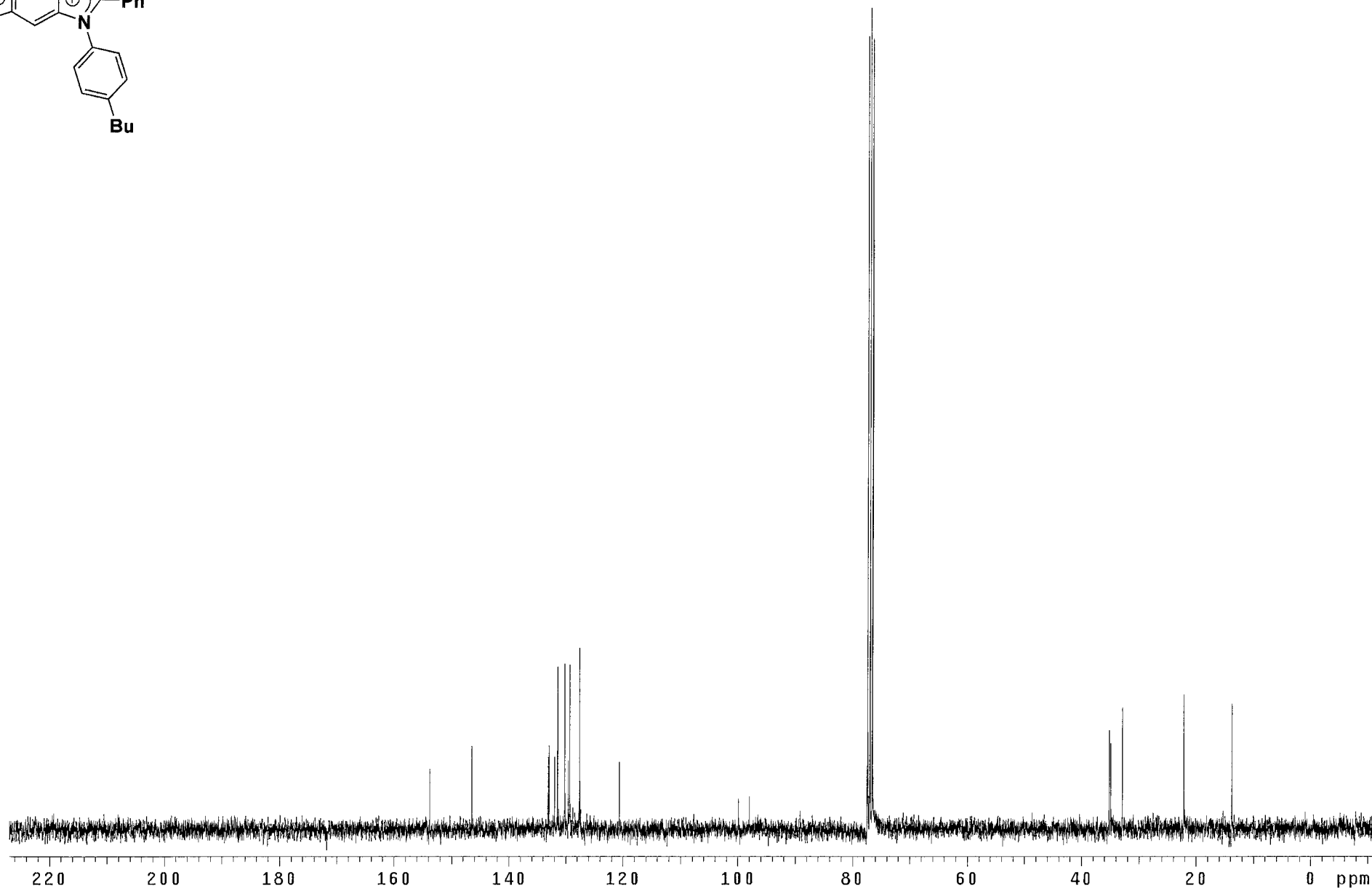
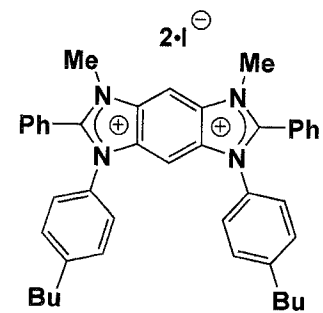
Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"

S44

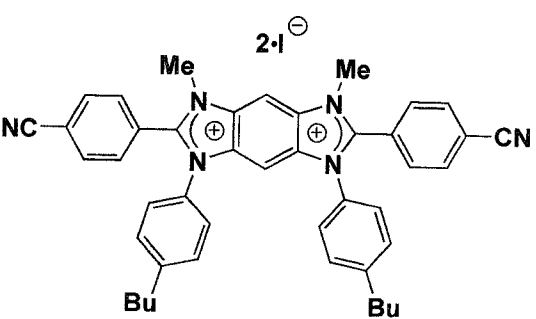


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 15.0 degrees Acq. time 3.813 sec Width 4196.4 Hz 20 repetitions	OBSERVE H1, 300.1390321	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minutes			STANDARD 1H OBSERVE Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature UNITYplus-300 "nmr2"
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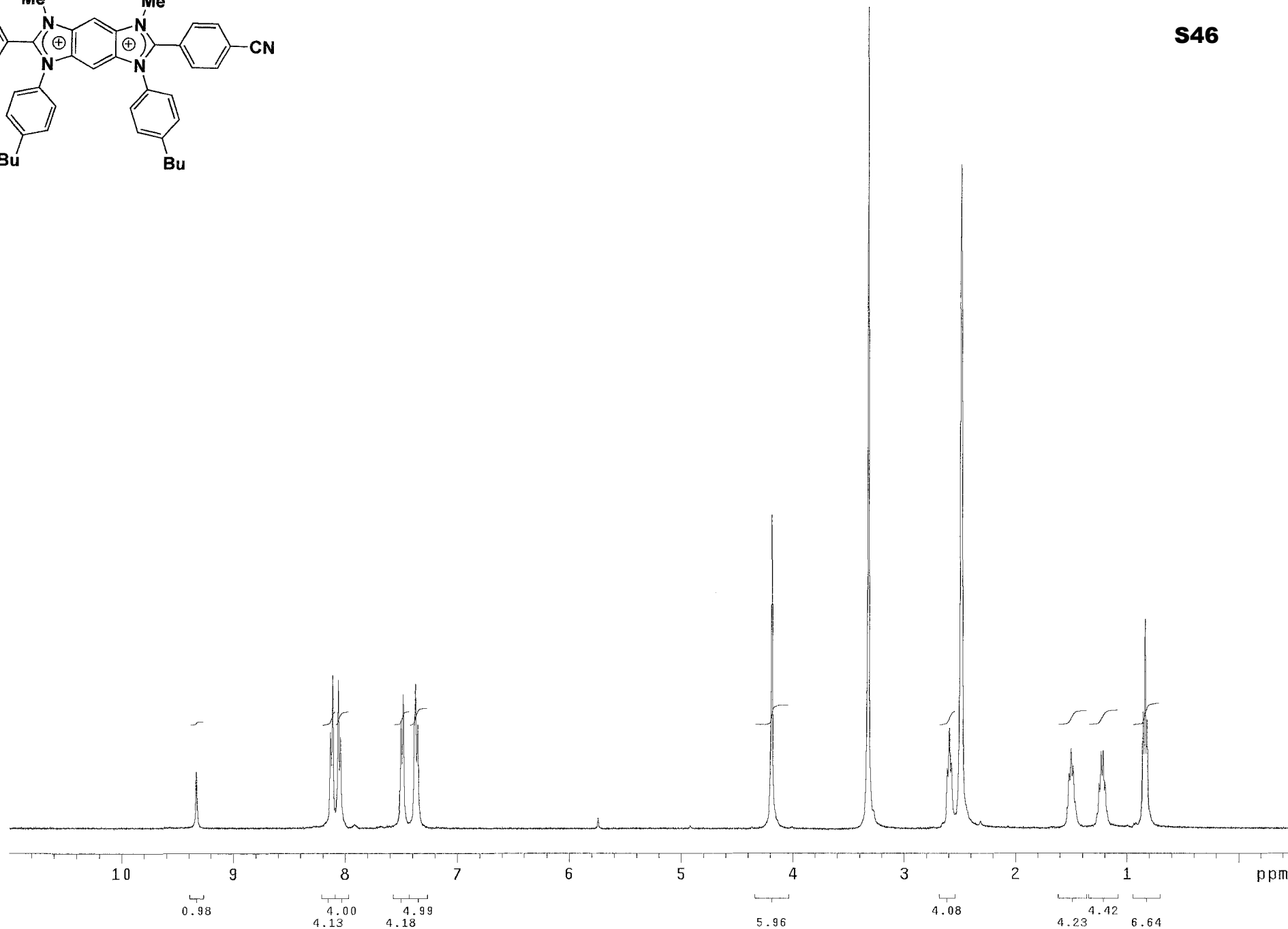
S45



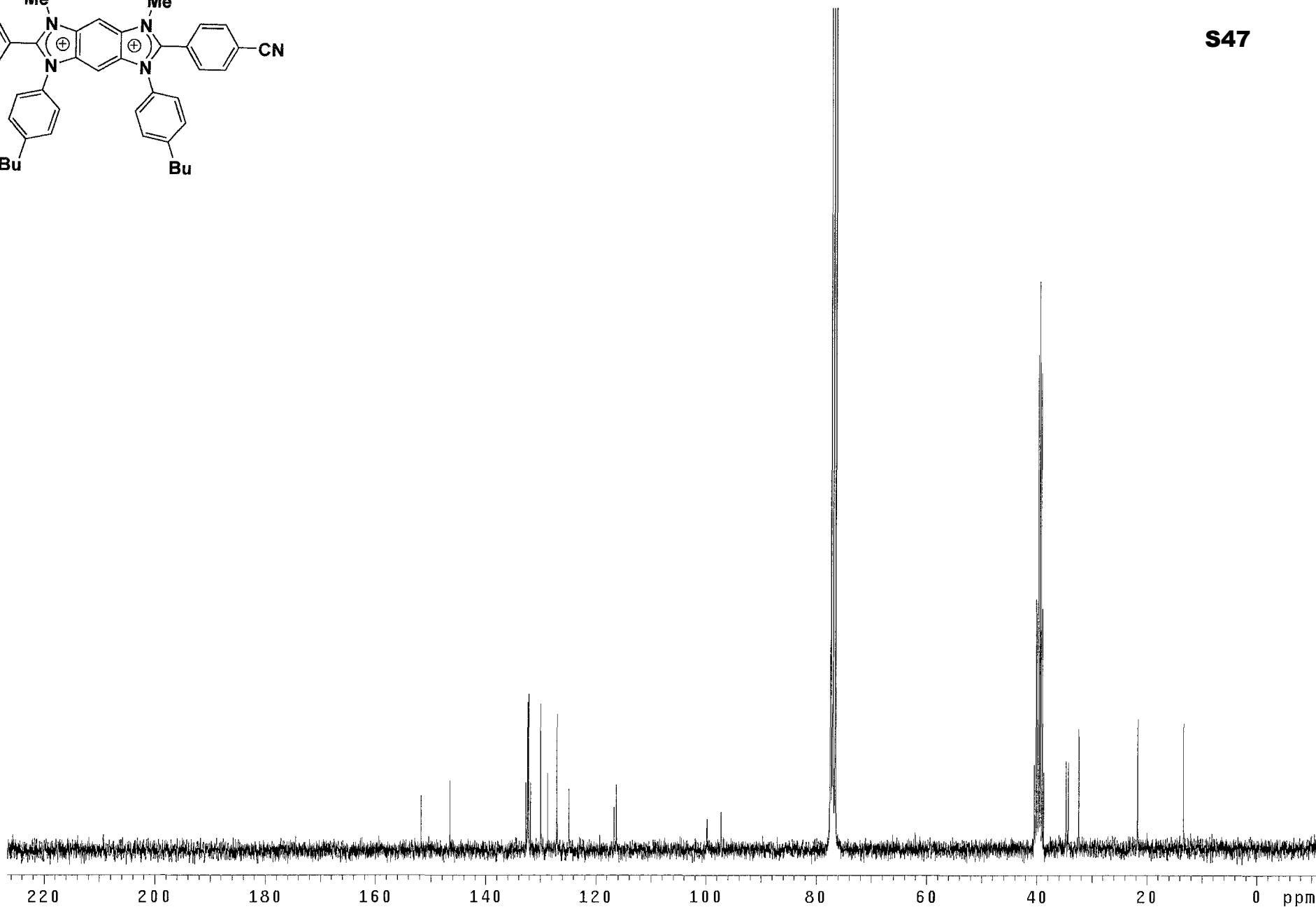
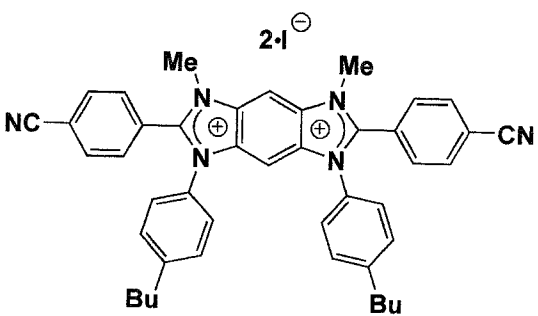
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 544 repetitions	OBSERVE C13, 75.4700238 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 34 minutes	B6AB264-13C Pulse Sequence: s2pu1 Solvent: CDC13 Ambient temperature UNITYplus-300 "nmr2"	
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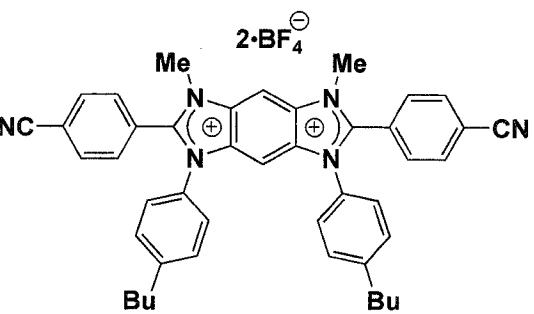
S46



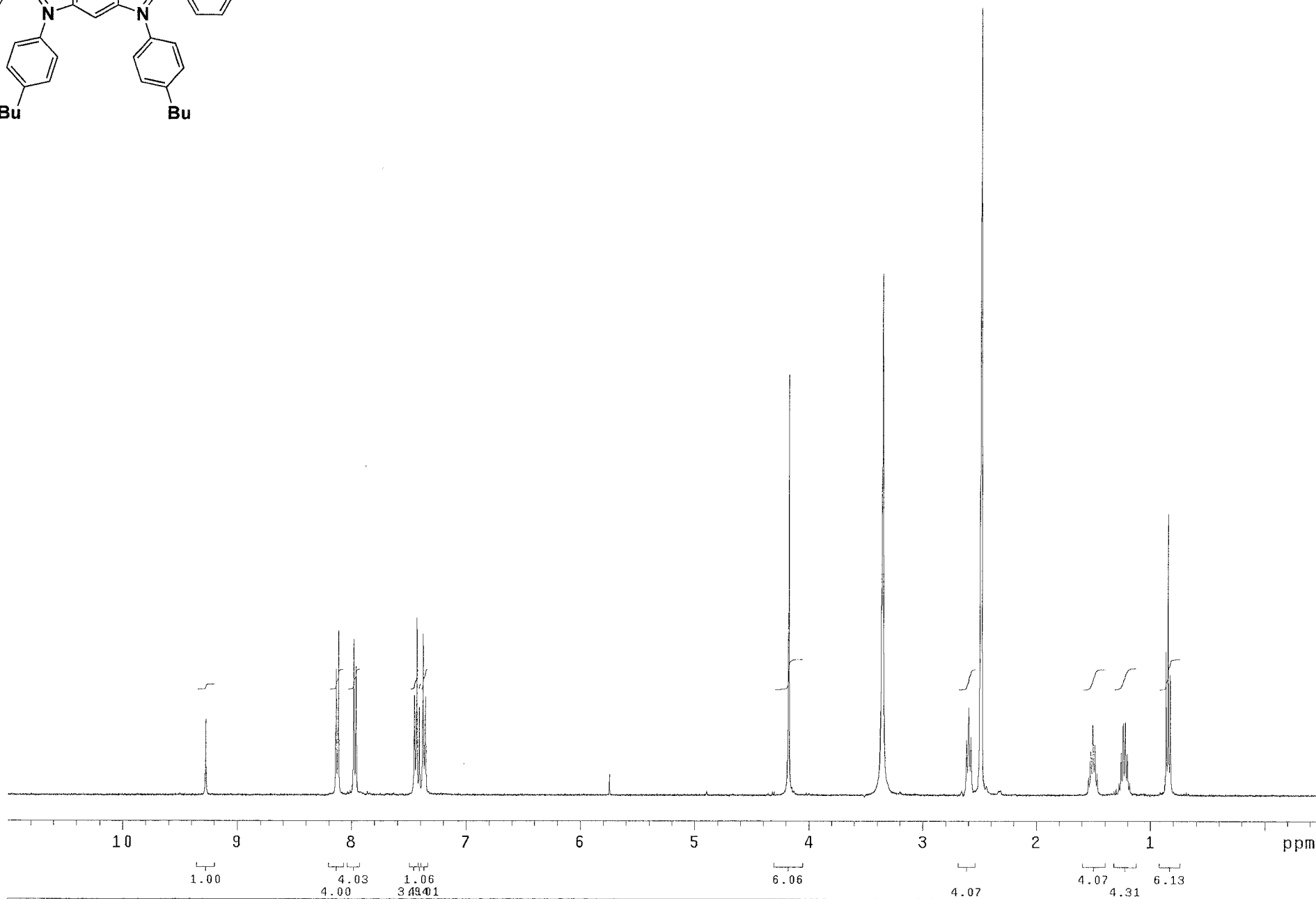
<p>PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 21 repetitions</p>	<p>OBSERVE H1, 400.2688767</p>	<p>DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minutes</p>			<p>B6AB290-2nd Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature Mercury-400 "nmr6"</p>
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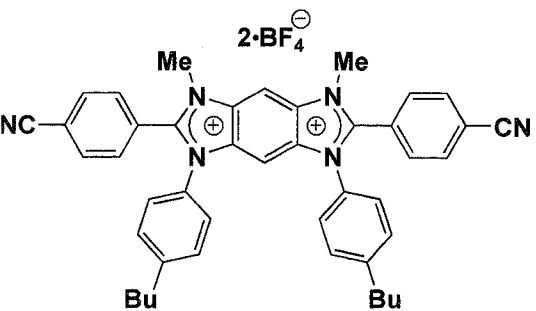
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 10946 repetitions	OBSERVE C13, 75.4700469 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 11.5 hours	B6AB290+DMSO-13C Pulse Sequence: s2pul Solvent: CDC13 Ambient temperature UNITYplus-300 "nmr2"
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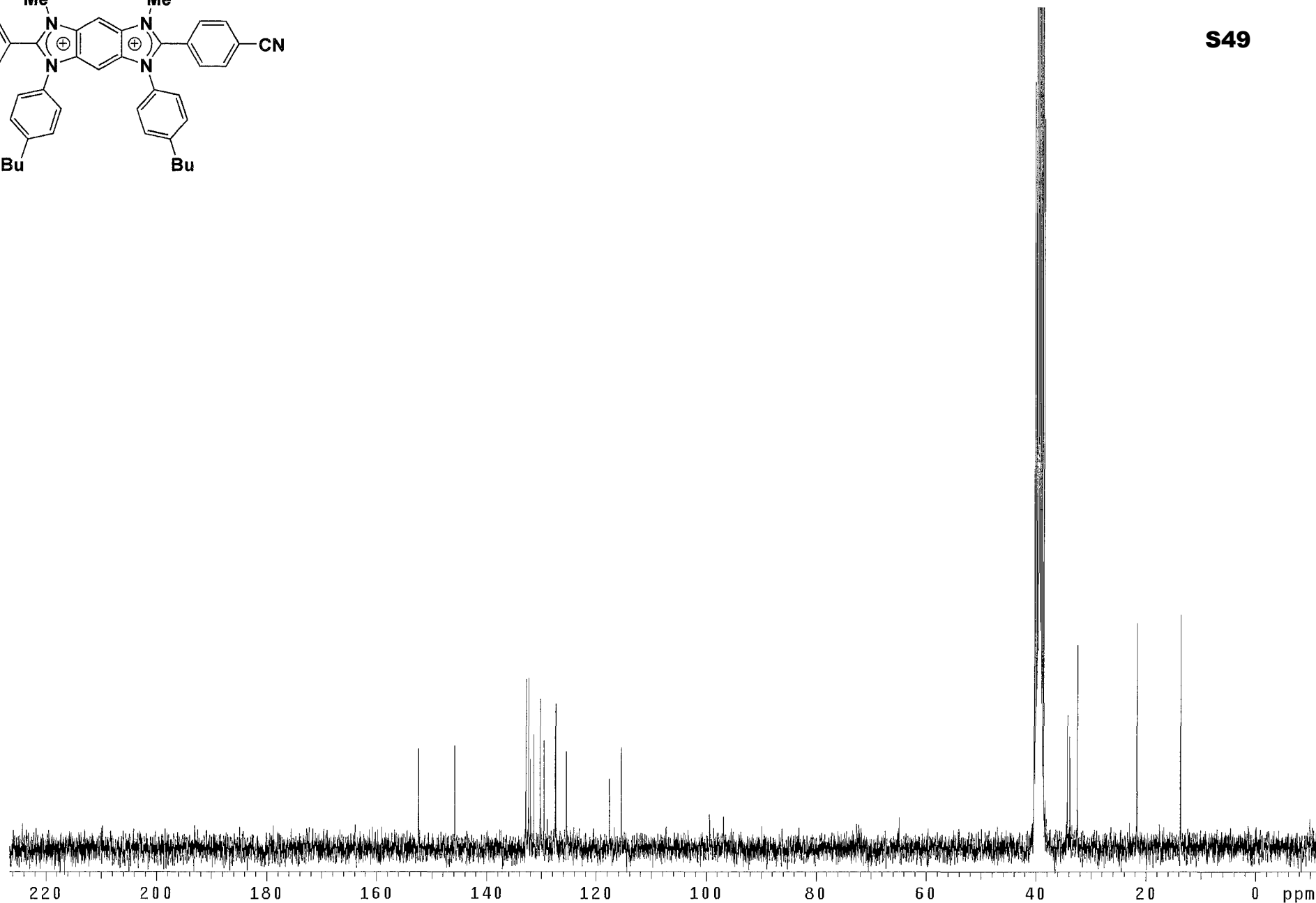
S48



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 12 repetitions	OBSERVE H1, 400.2688771	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute	B6AB299-pump Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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S49



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
2327 repetitions

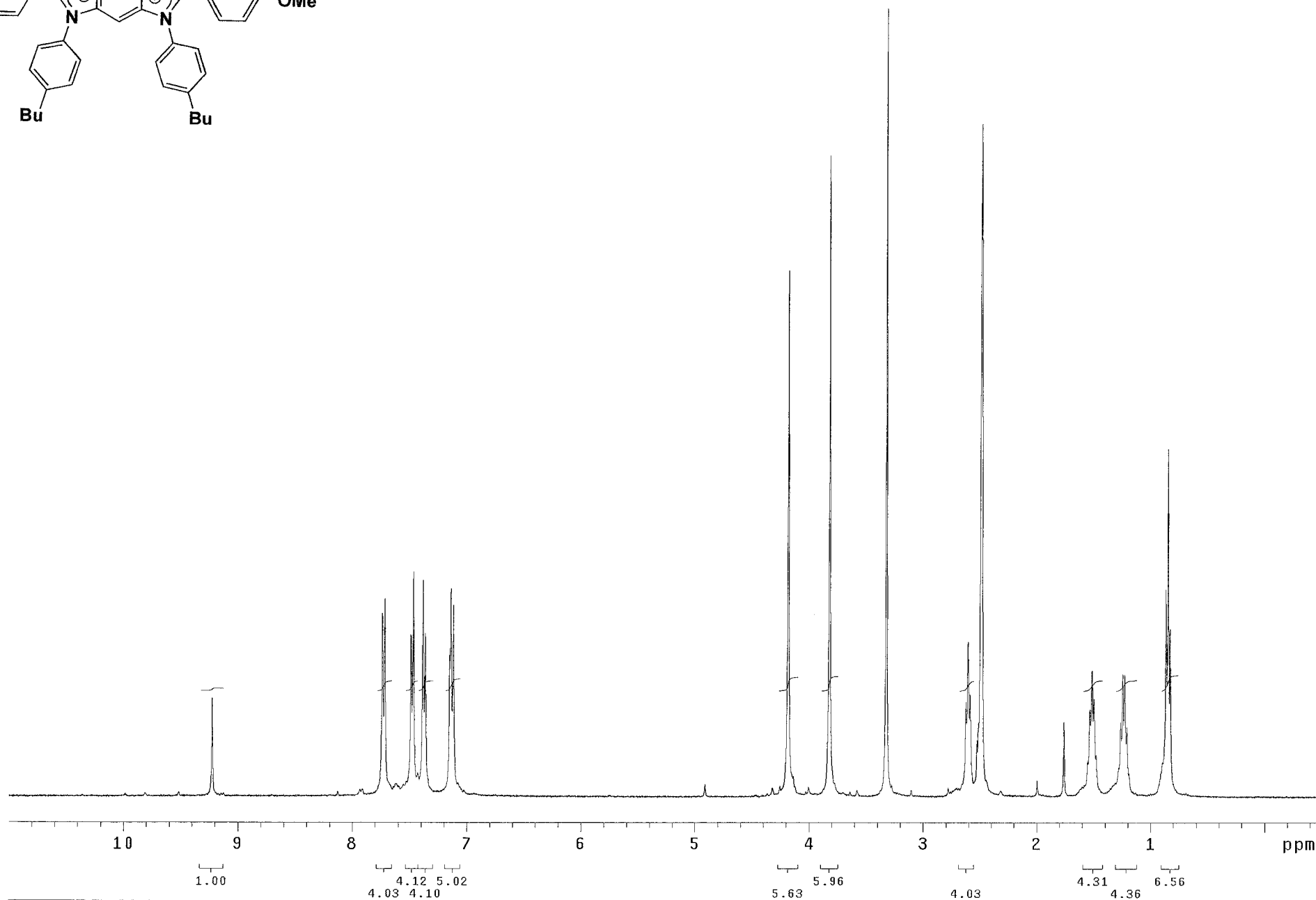
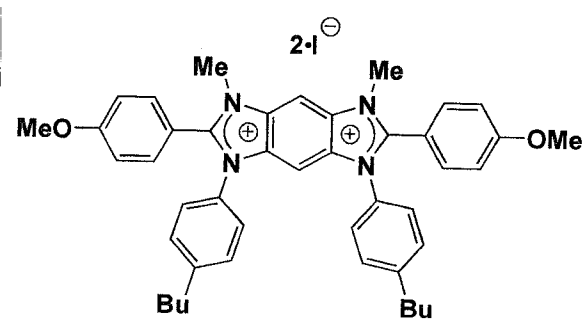
OBSERVE C13, 75.4704126
DECOUPLE H1, 300.1423516
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2.4 hours

B6AB299-13C

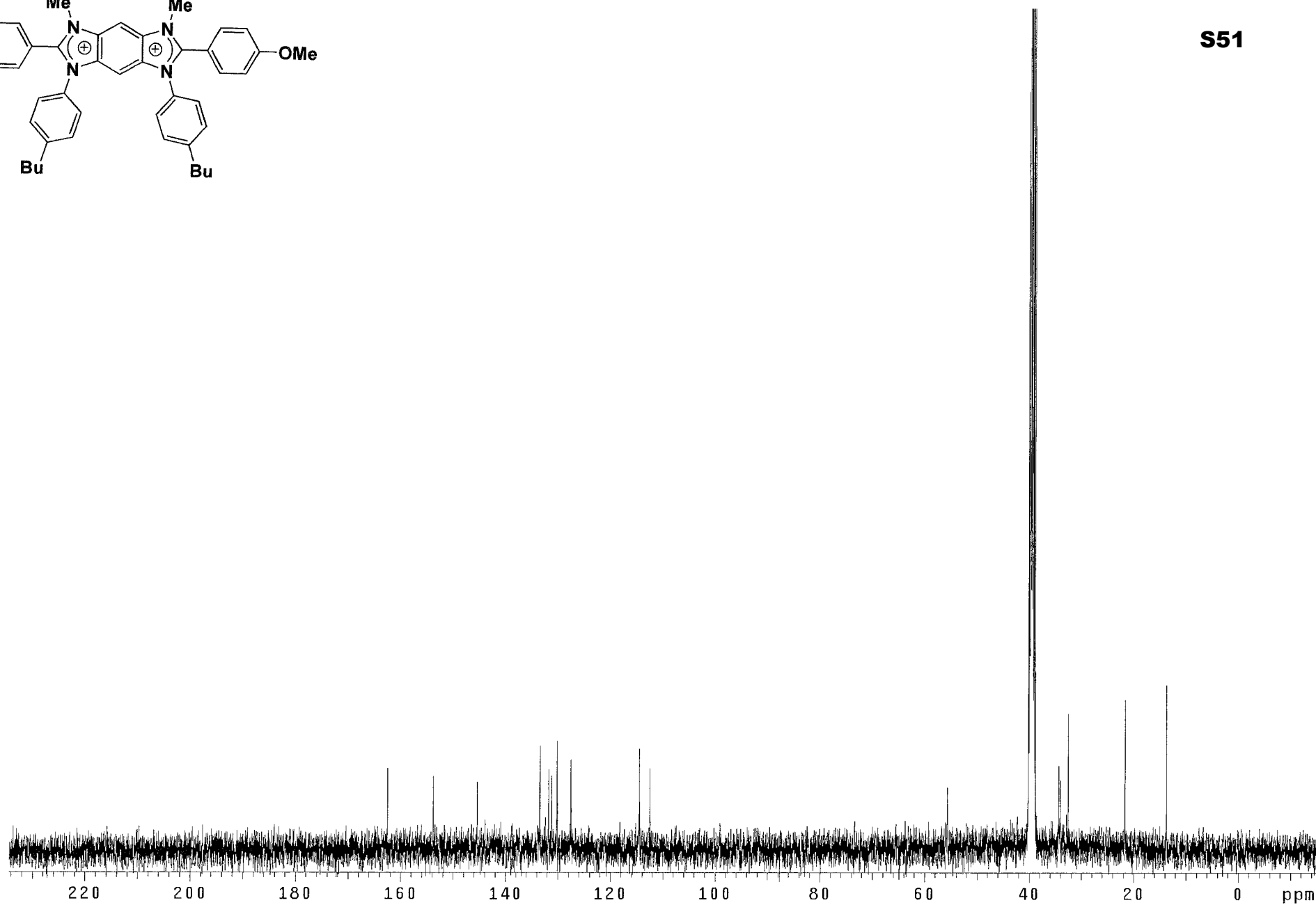
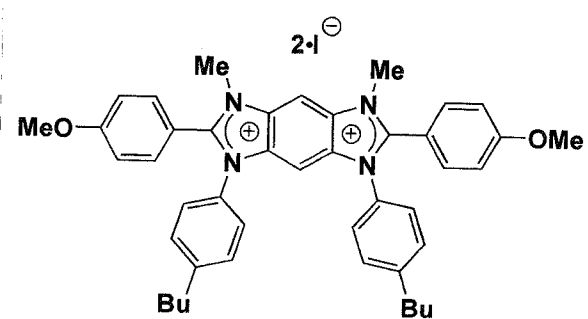
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
UNITYplus-300 "nmr2"

S50



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 18 repetitions	OBSERVE H1, 400.2688764	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute	10D176 Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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S51



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 22.5 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
1138 repetitions

OBSERVE C13, 100.6477380
DECOUPLE H1, 400.2708968
Power 38 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 62 minutes

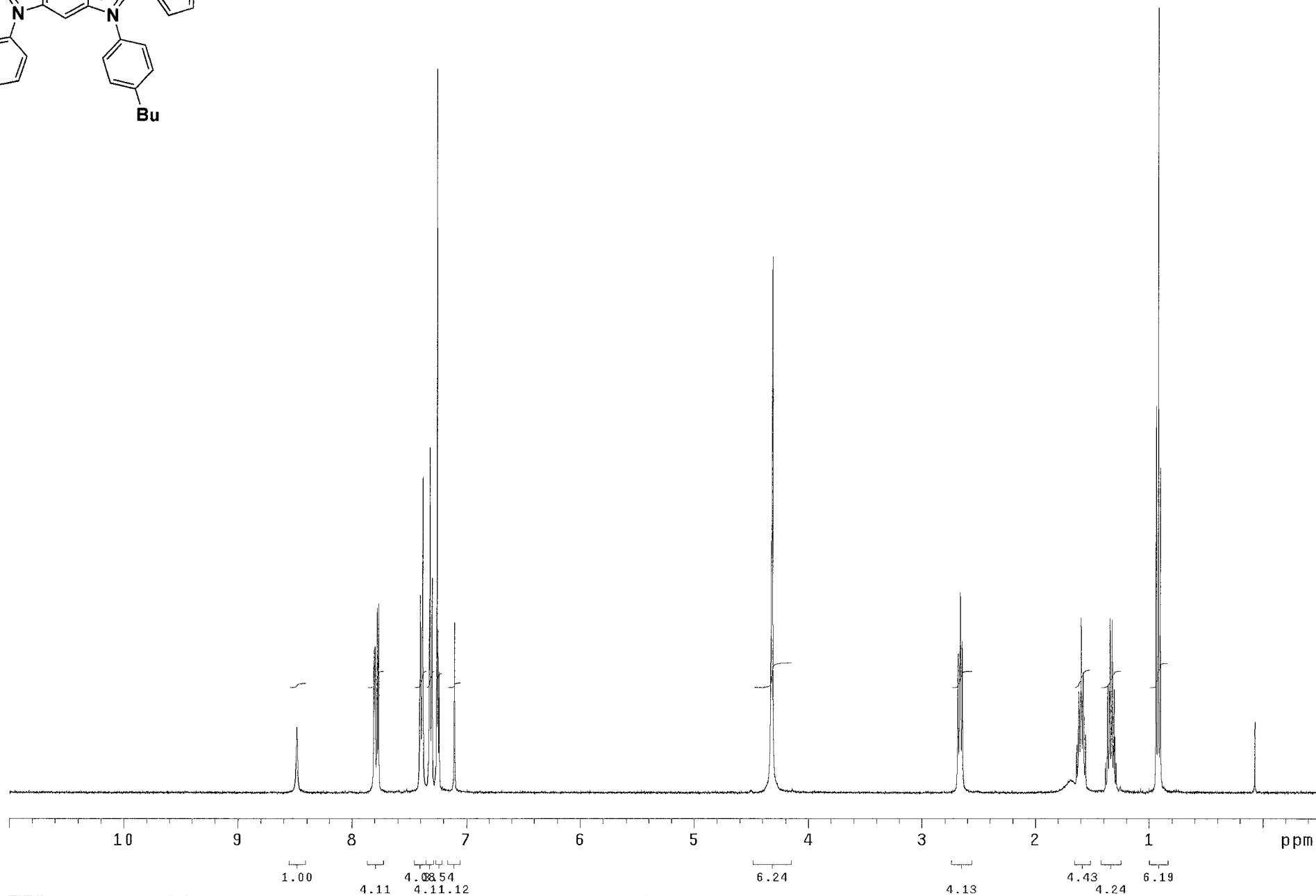
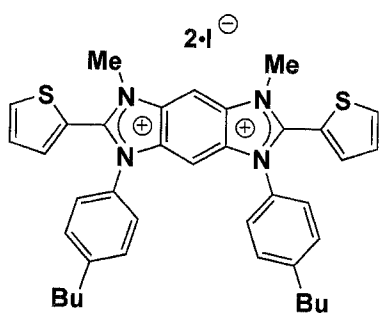
10D176-13C

Pulse Sequence: s2pu1

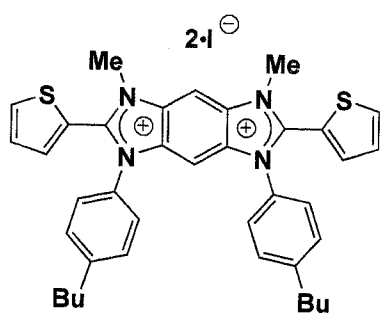
Solvent: DMSO

Ambient temperature

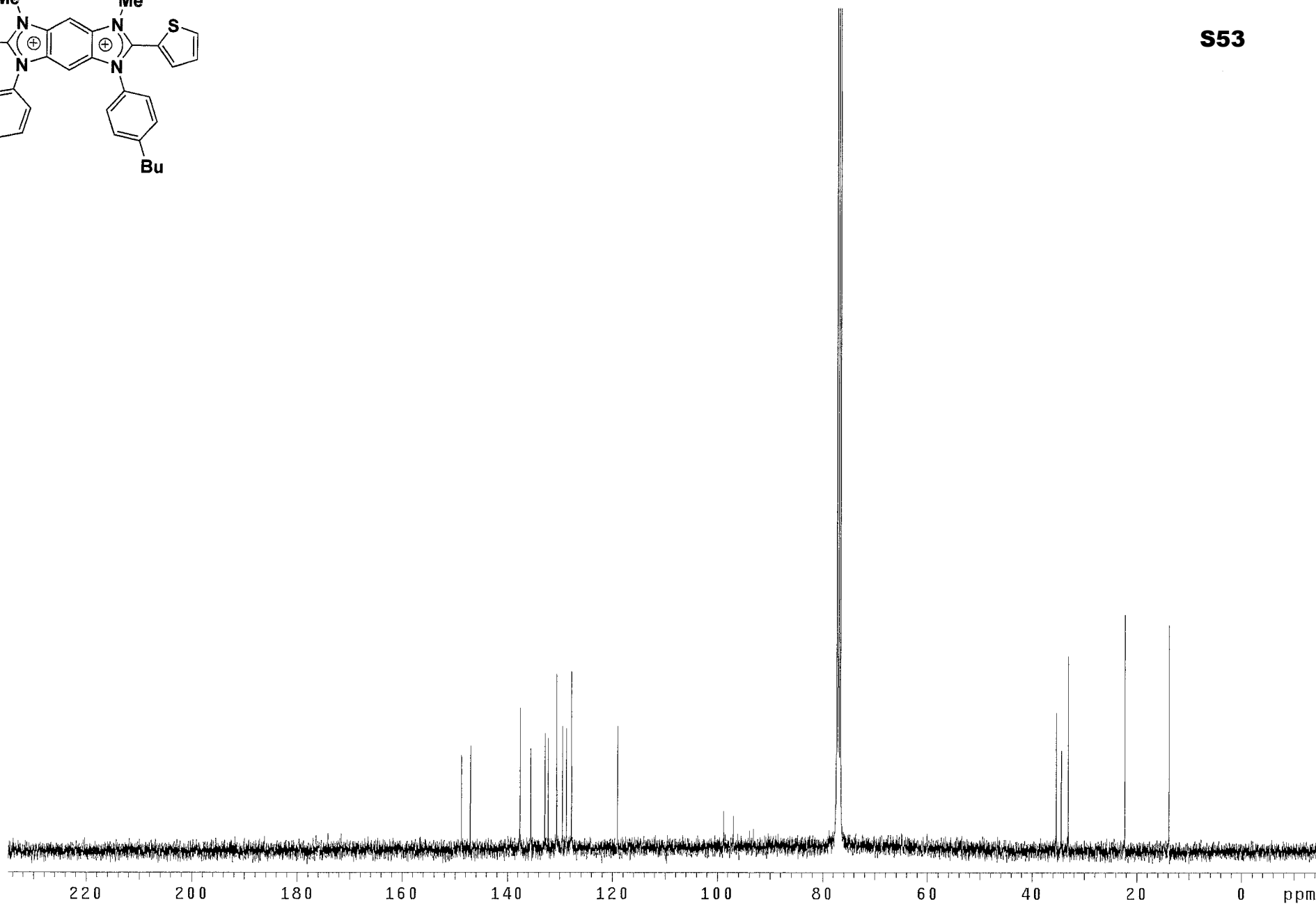
Mercury-400 "nmr6"



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 16 repetitions	OBSERVE H1, 400.2669779	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute	B6AB173-Rx3 Pulse Sequence: s2pul Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"

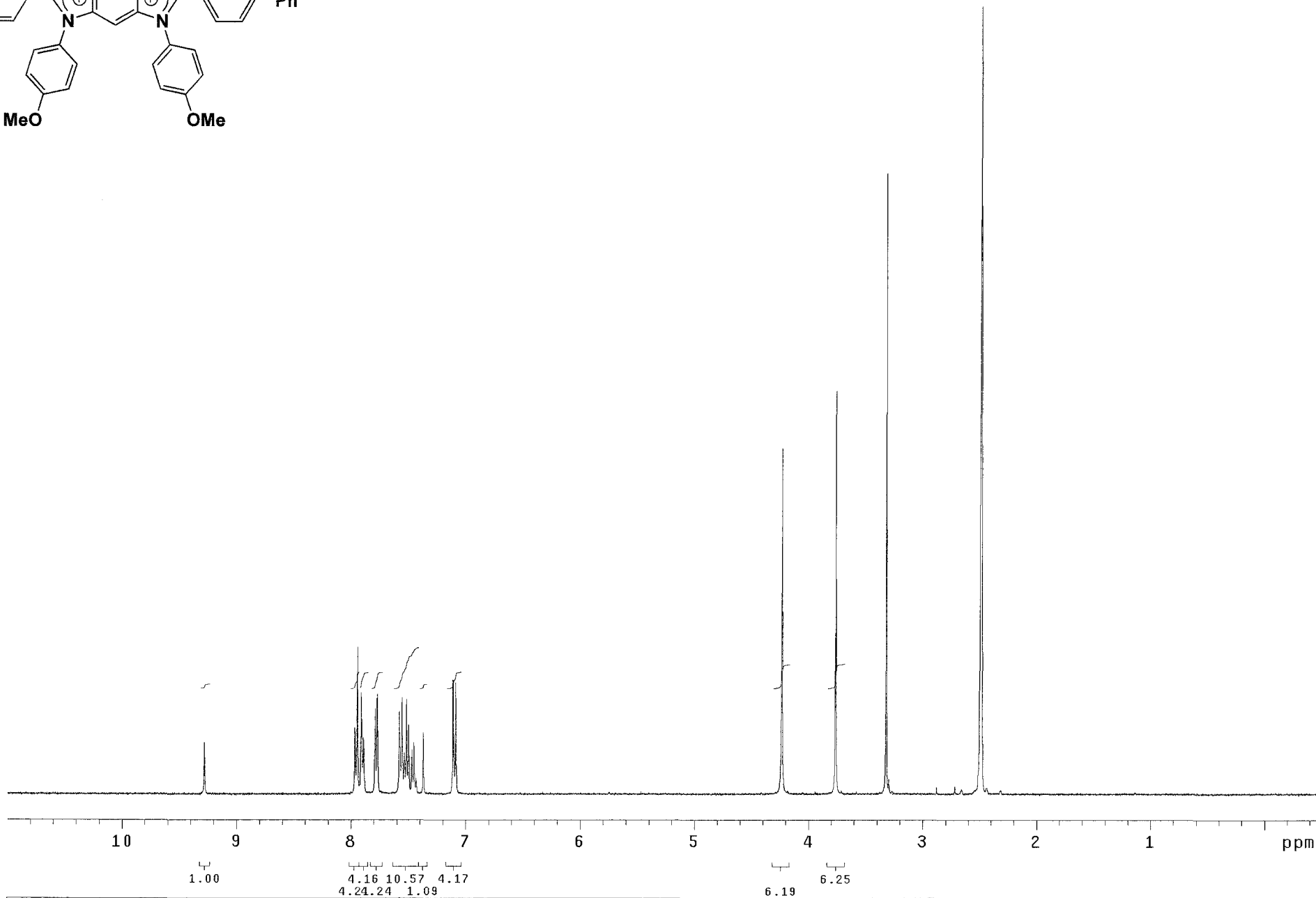
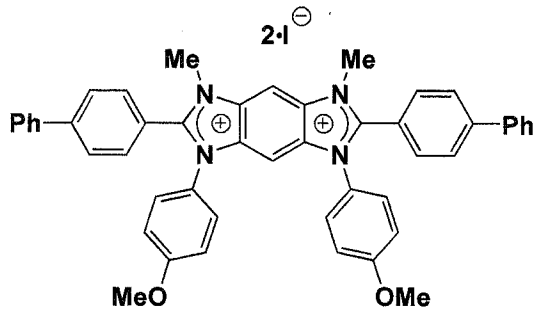


S53

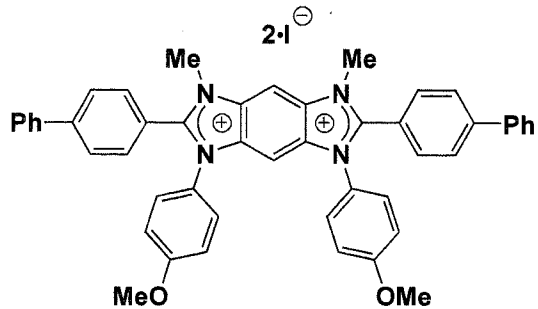


PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 12328 repetitions	OBSERVE C13, 100.6472138 DECOUPLE H1, 400.2689955 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 11.2 hours	B6AB173-13C Pulse Sequence: s2pu1 Solvent: CDC13 Ambient temperature Mercury-400 "nmr6"	
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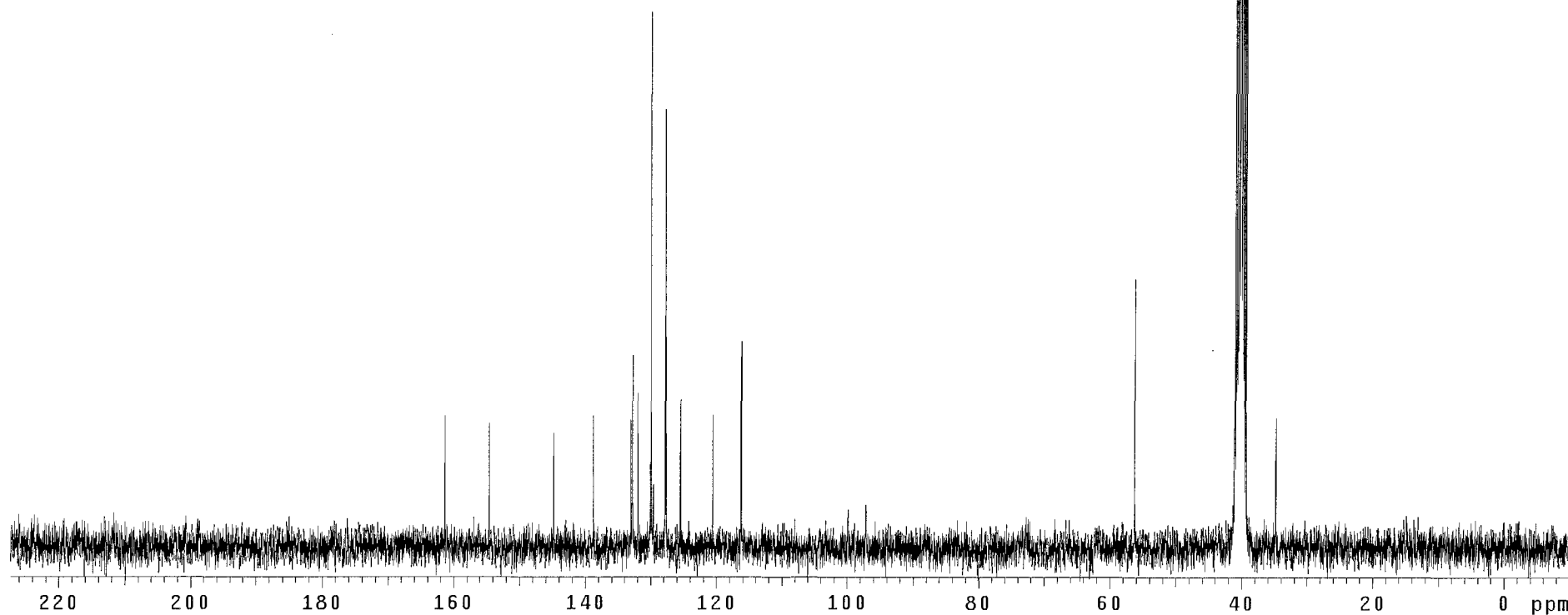
S54



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 12 repetitions	OBSERVE H1, 400.2688767	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute	B6AB190 Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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S55



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
4696 repetitions

OBSERVE C13, 75.4703584
DECOUPLE H1, 300.1423516
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 4.9 hours

B6AB190-13C

Pulse Sequence: s2pu1

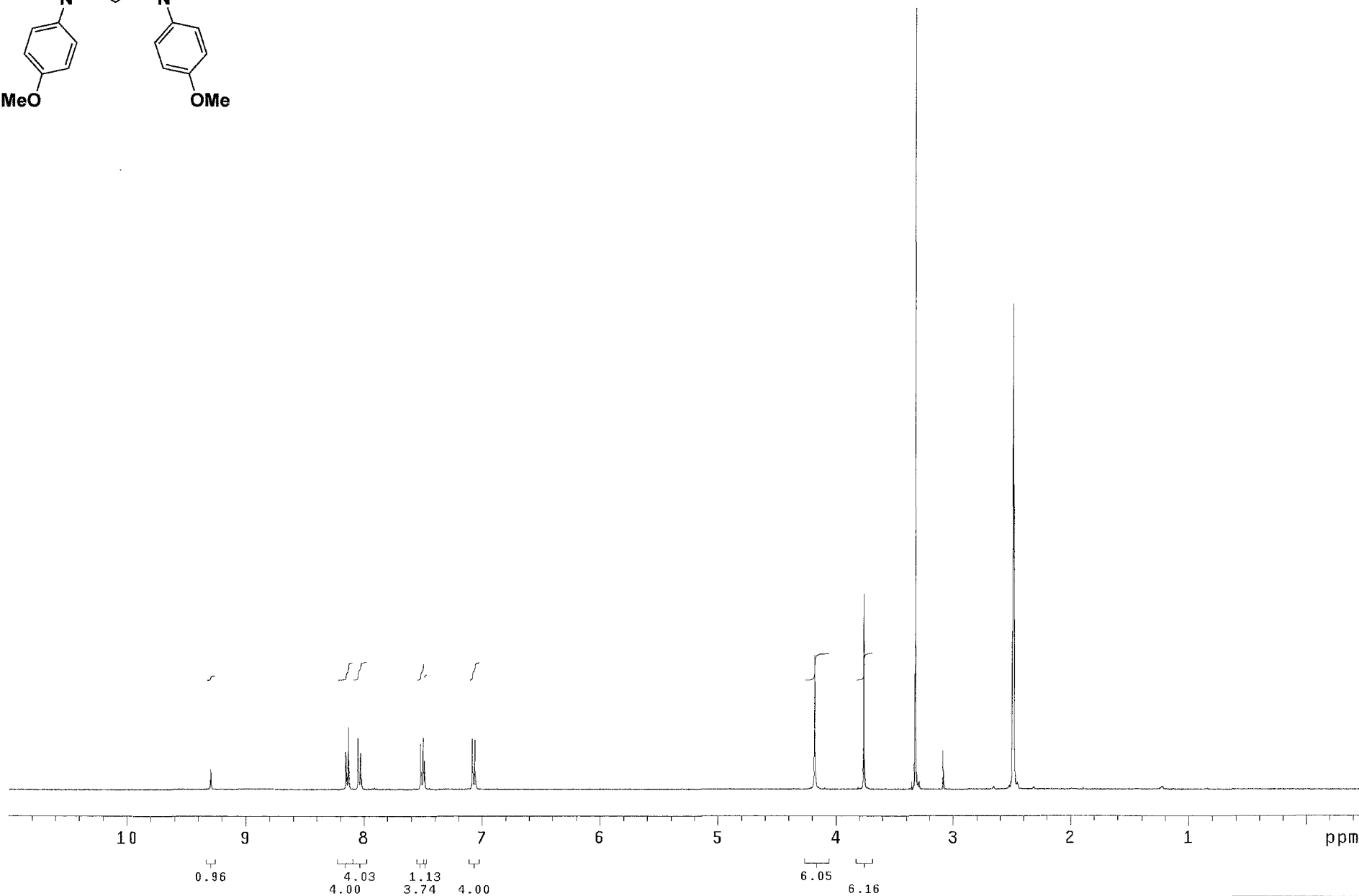
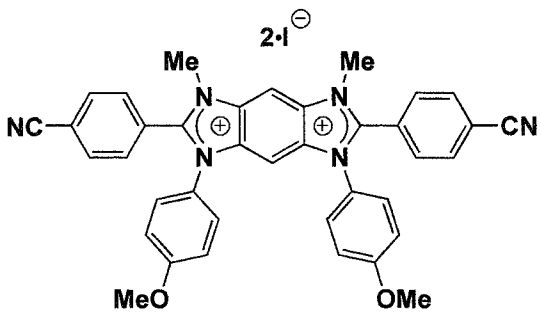
Solvent: DMSO

Ambient temperature

File: B6AB190-13C

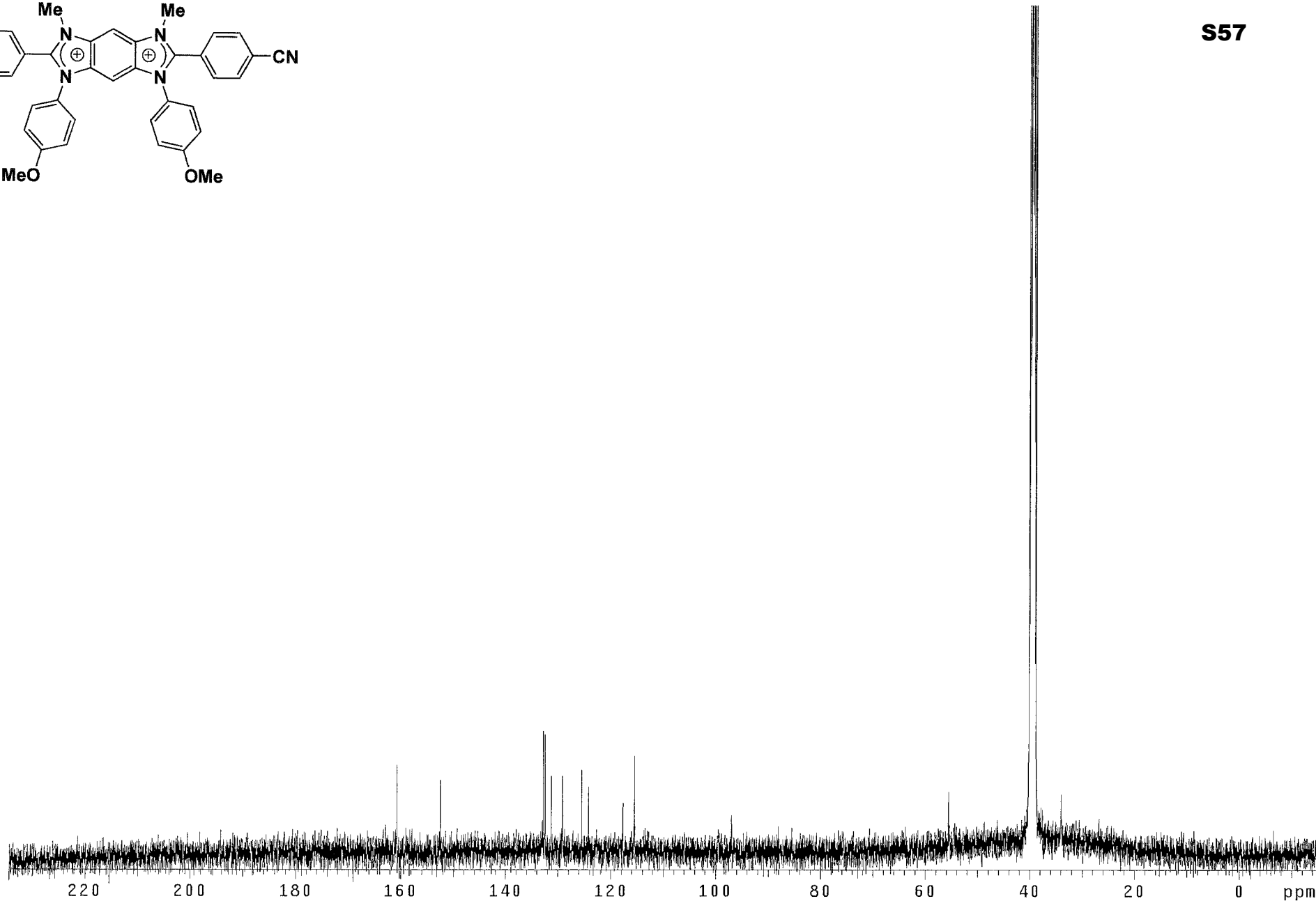
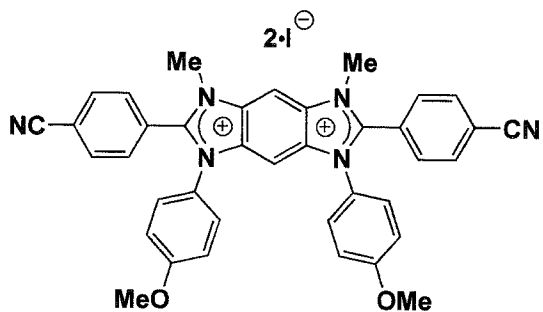
UNITYplus-300 "nmr2"

S56

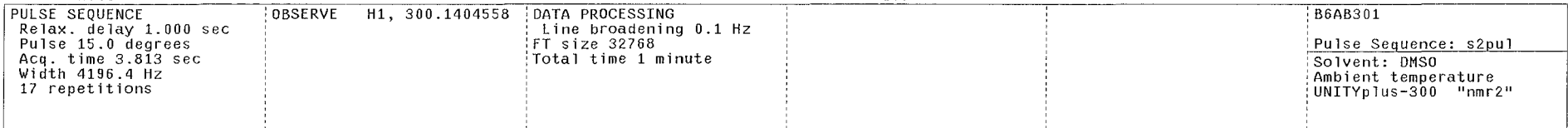


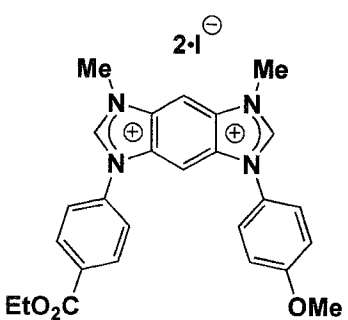
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 18 repetitions	OBSERVE H1, 400.2688764	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			B6AB191 Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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S57

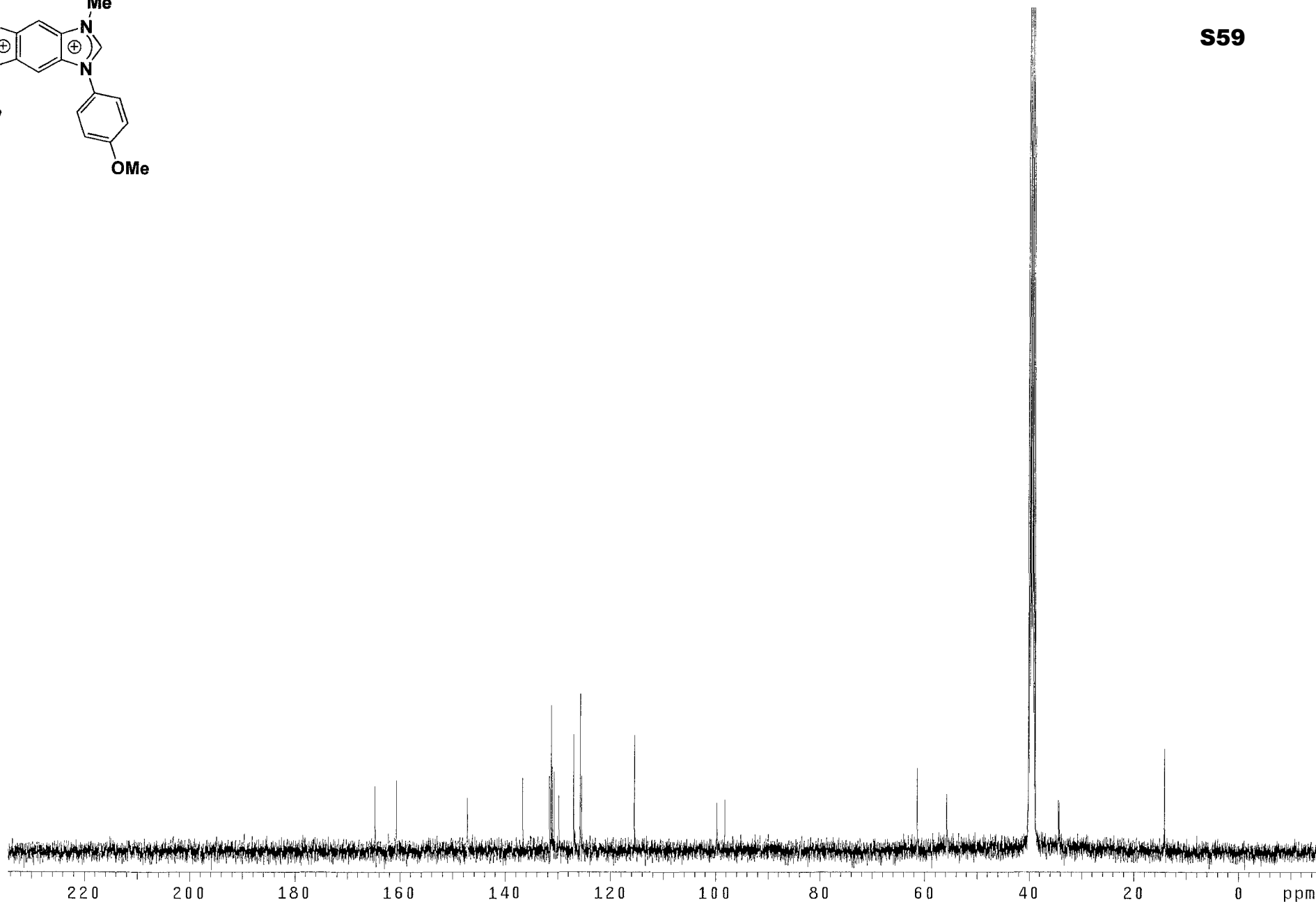


PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 11398 repetitions	OBSERVE C13, 100.6477357 DECOUPLE H1, 400.2708968 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 10.4 hours			B6AB191-13C Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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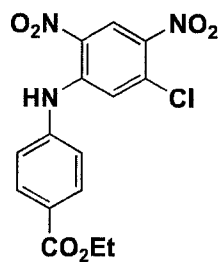




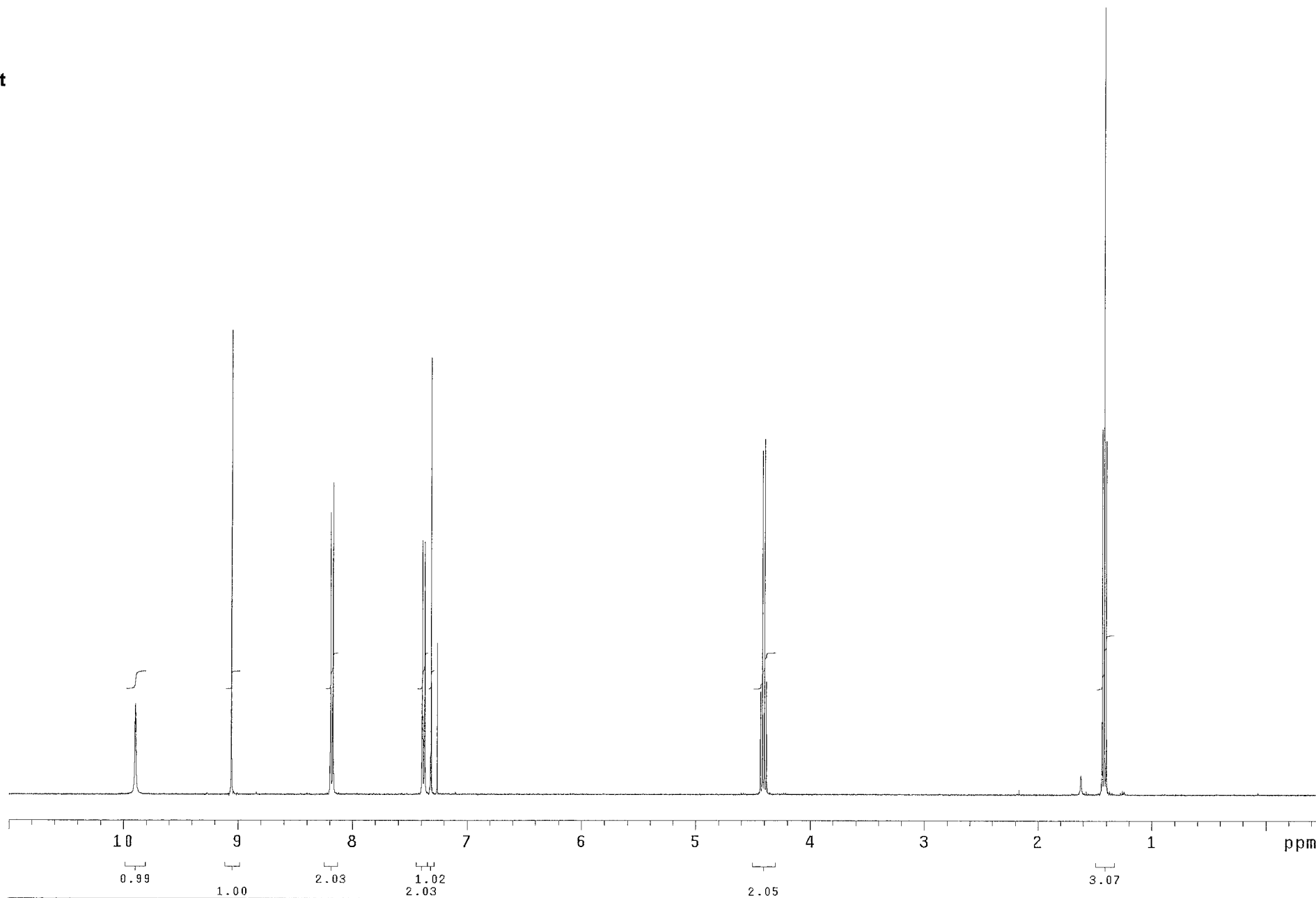
S59



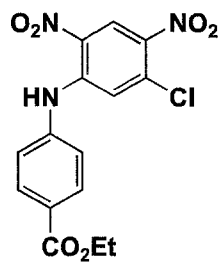
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 3408 repetitions	OBSERVE C13, 100.6477364 DECOUPLE H1, 400.2708968 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 3.1 hours	B6AB301-13C Pulse Sequence: s2pu1 Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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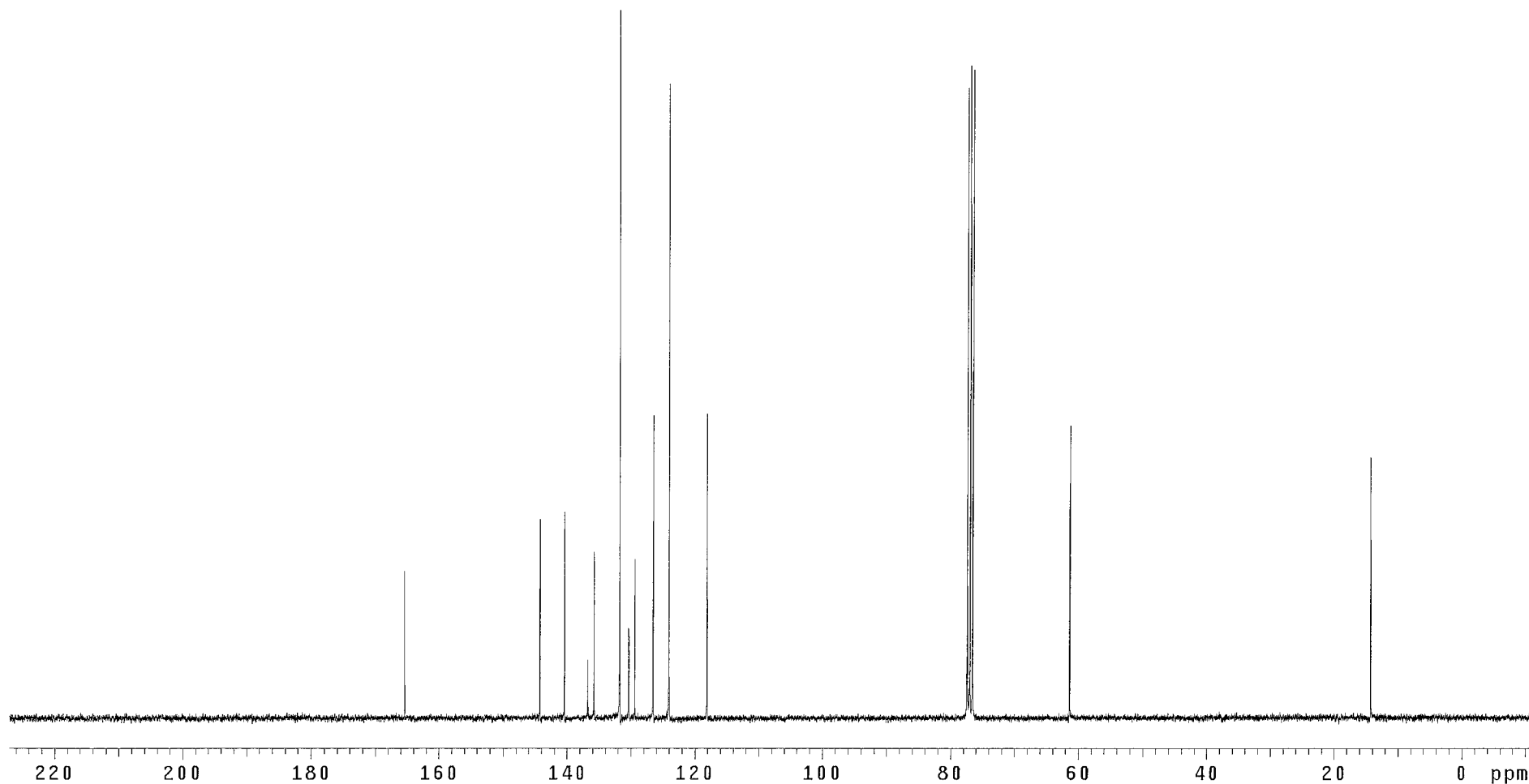
S60



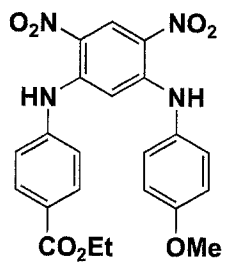
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 4 repetitions	OBSERVE H1, 400.2669779	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minute			B6AB284 Pulse Sequence: s2pul Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"
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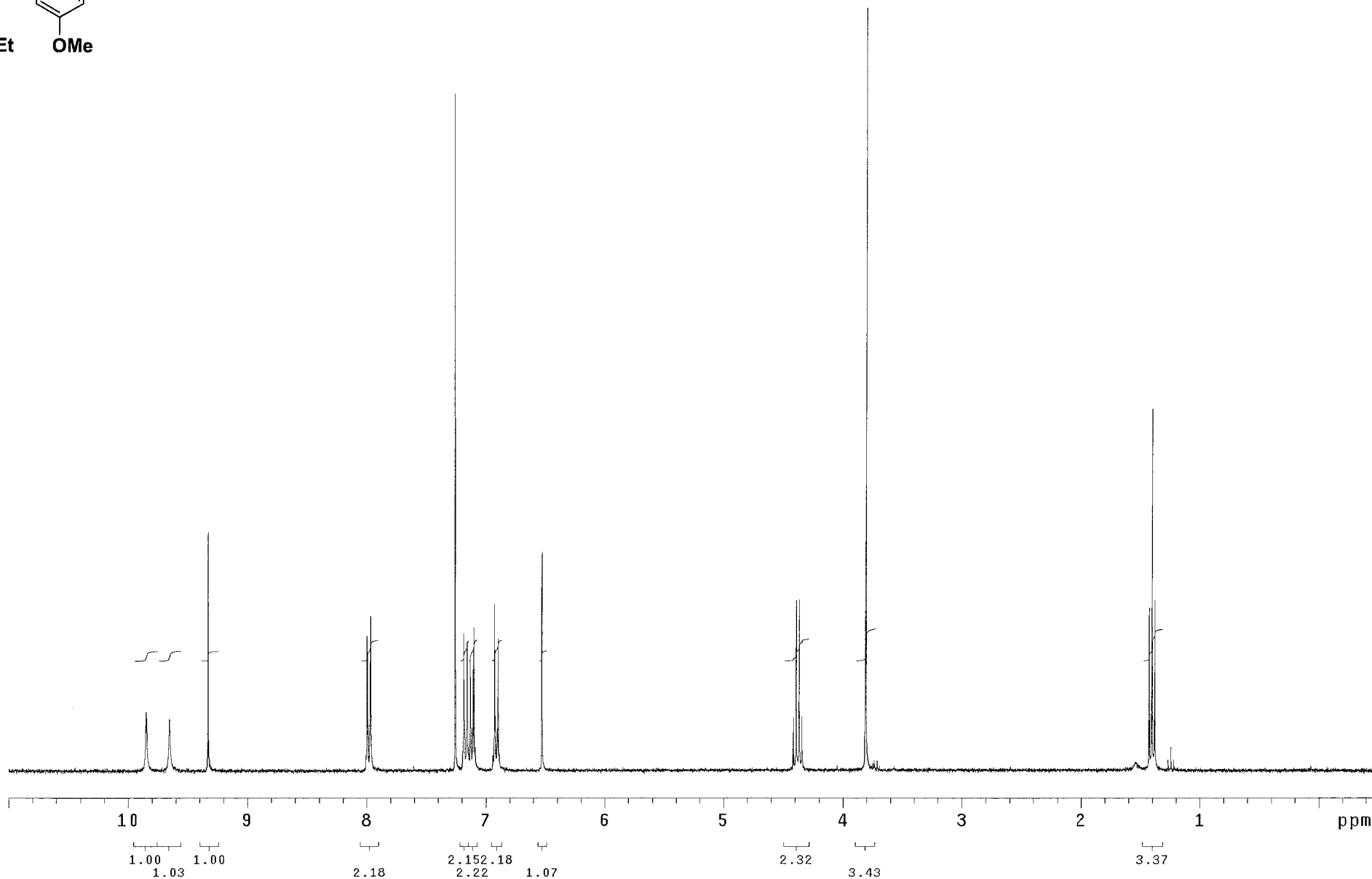
S61



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 10000 repetitions	OBSERVE C13, 75.4700222 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 10.5 hours			13C OBSERVE Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature UNITYplus-300 "nmr2"
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S62



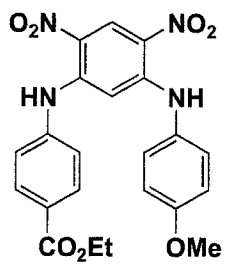
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
31 repetitions

OBSERVE H1, 300.1390321

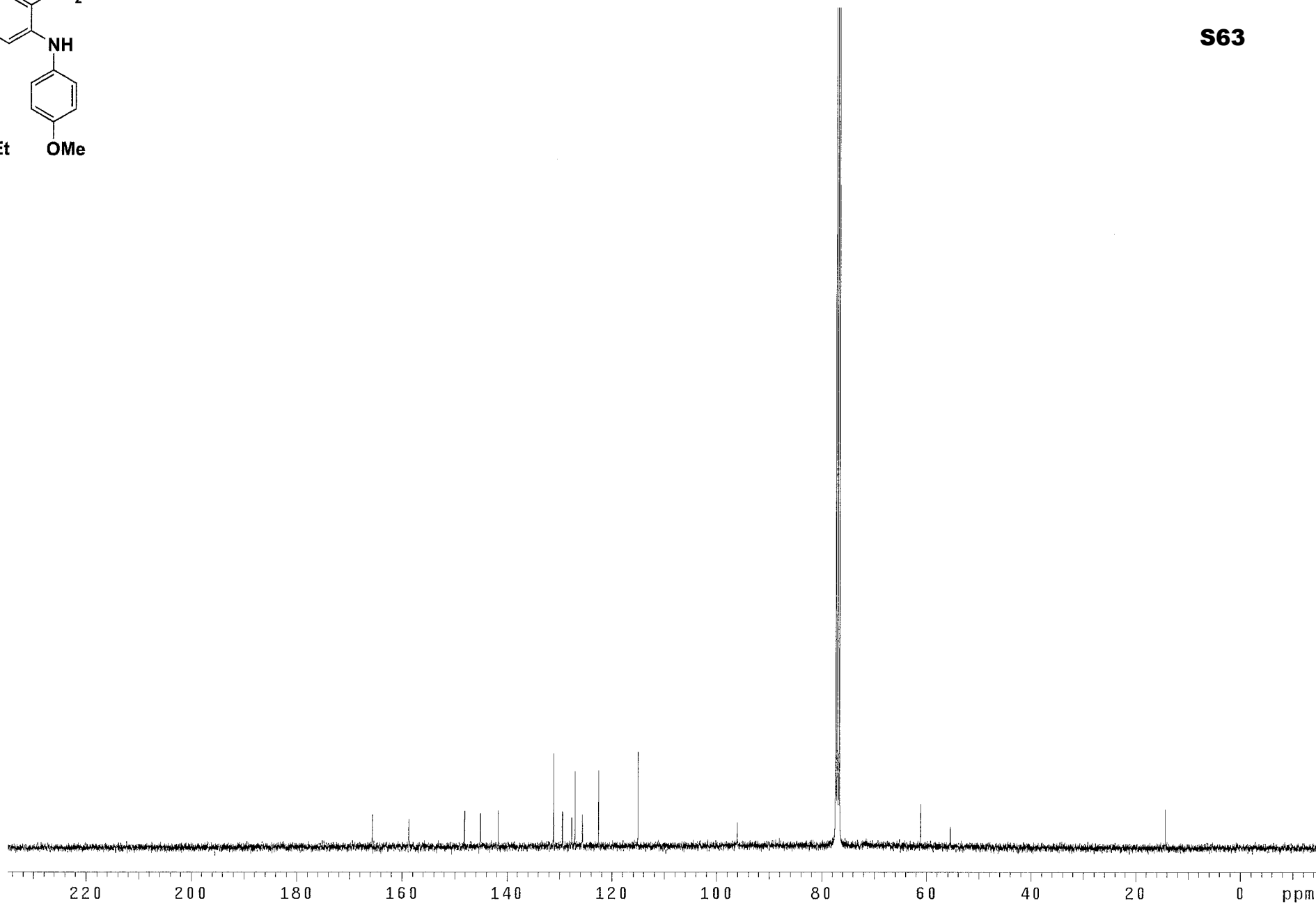
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 2 minutes

B6AB288

Pulse Sequence: s2pu1
Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"

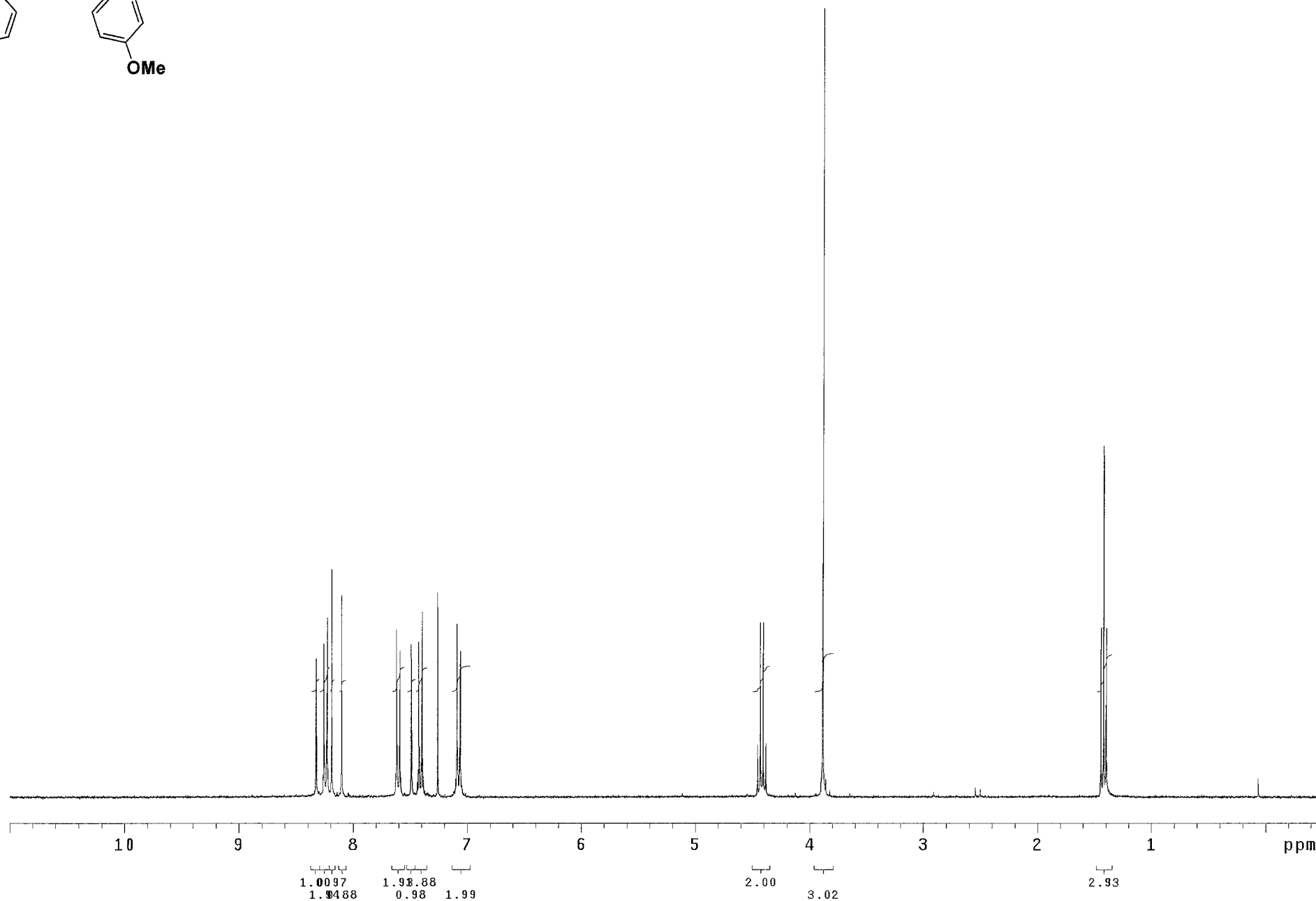
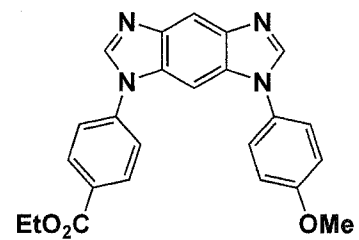


S63



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 22.5 degrees Acq. time 1.280 sec Width 25188.9 Hz 10919 repetitions	OBSERVE C13, 100.6472123 DECOUPLE H1, 400.2689955 Power 38 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 9.9 hours	B6AB288-13C Pulse Sequence: s2pu1 Solvent: CDCl3 Ambient temperature Mercury-400 "nmr6"
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S64



PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
11 repetitions

OBSERVE H1, 300.1390321

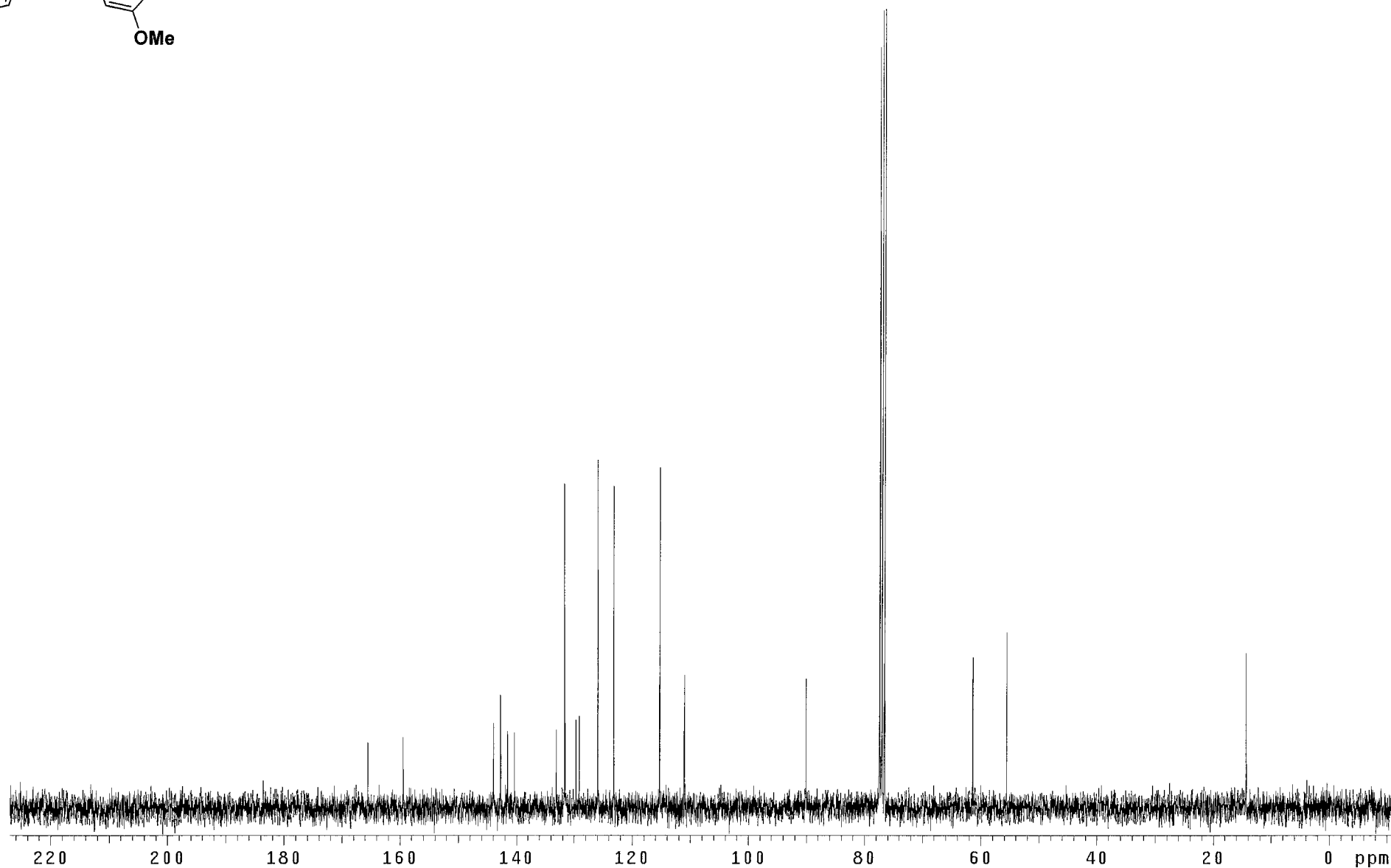
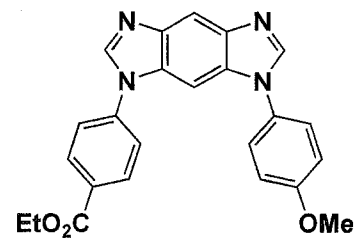
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute

B6AB289-pump

Pulse Sequence: s2pu1

Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"

S65



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
504 repetitions

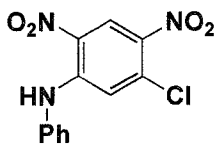
OBSERVE C13, 75.4700205
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 minutes

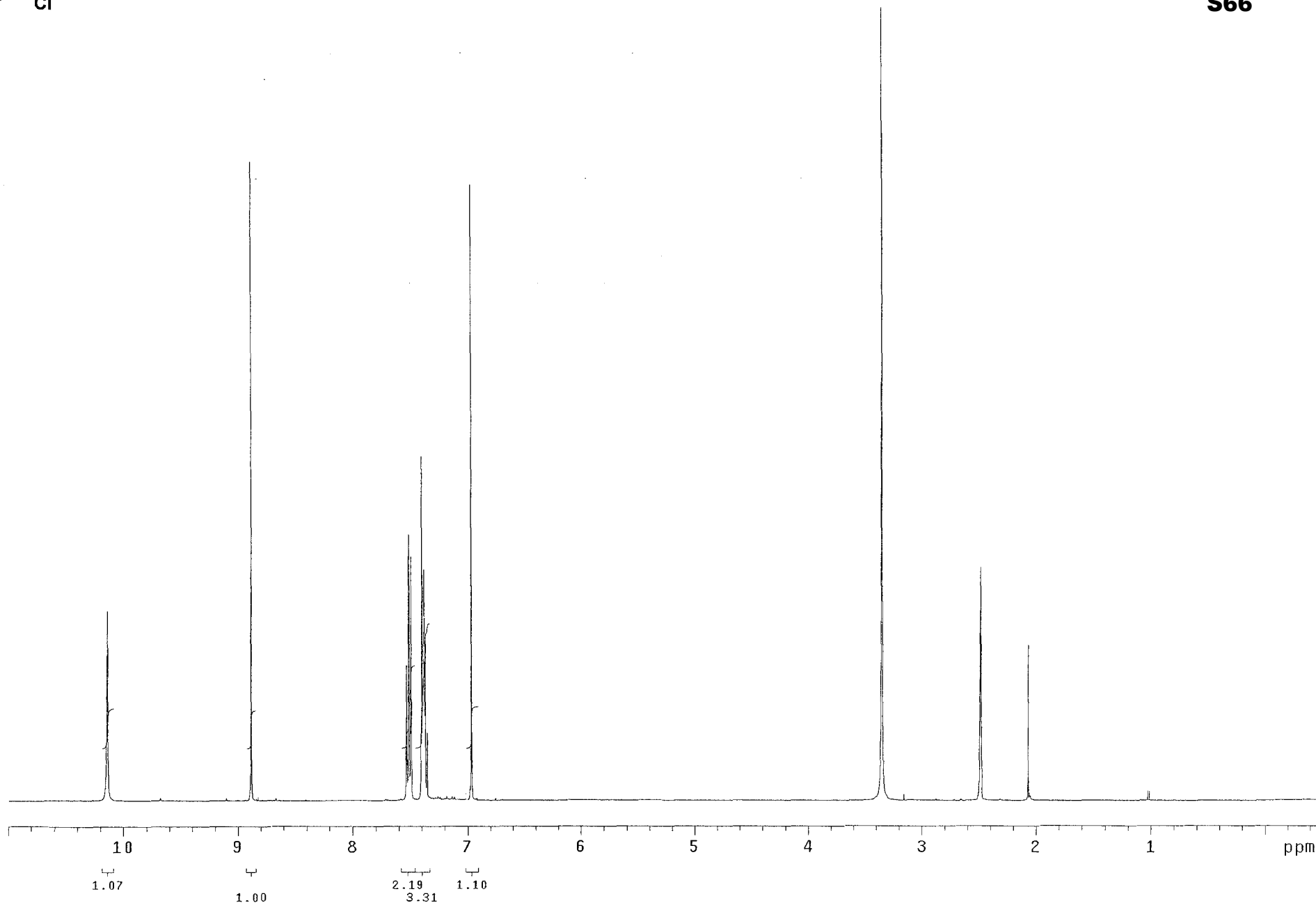
B6AB289-13C

Pulse Sequence: s2pu1

Solvent: CDCl₃
Ambient temperature
UNITYplus-300 "nmr2"



S66



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 4.049 sec
Width 4807.7 Hz
8 repetitions

OBSERVE H1, 399.8065869

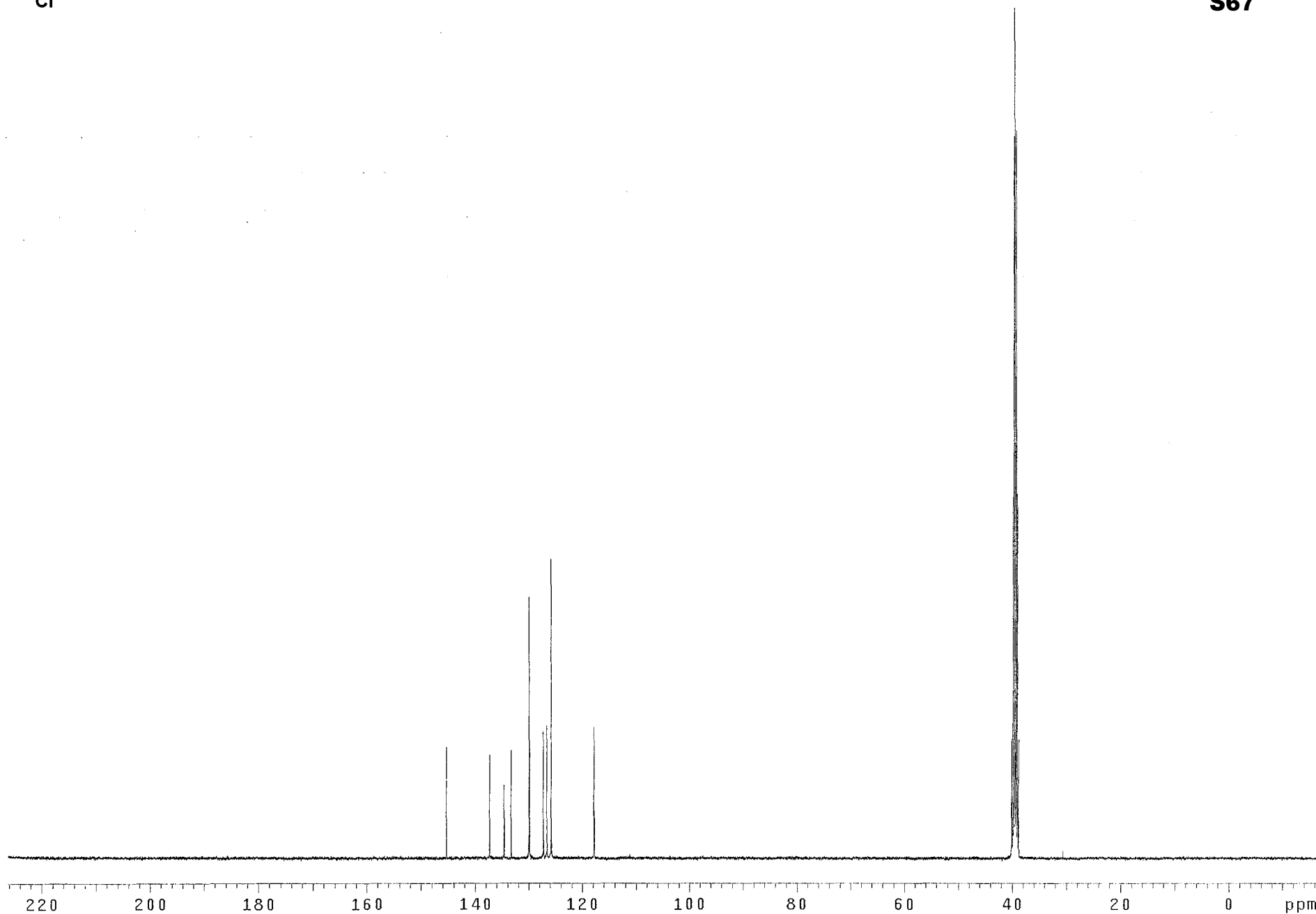
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 1 minute

Archive directory:
Sample directory:

Pulse Sequence: s2pul
Solvent: dmsd
Temp. 27.0 C / 300.1 K



S67



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
5000 repetitions

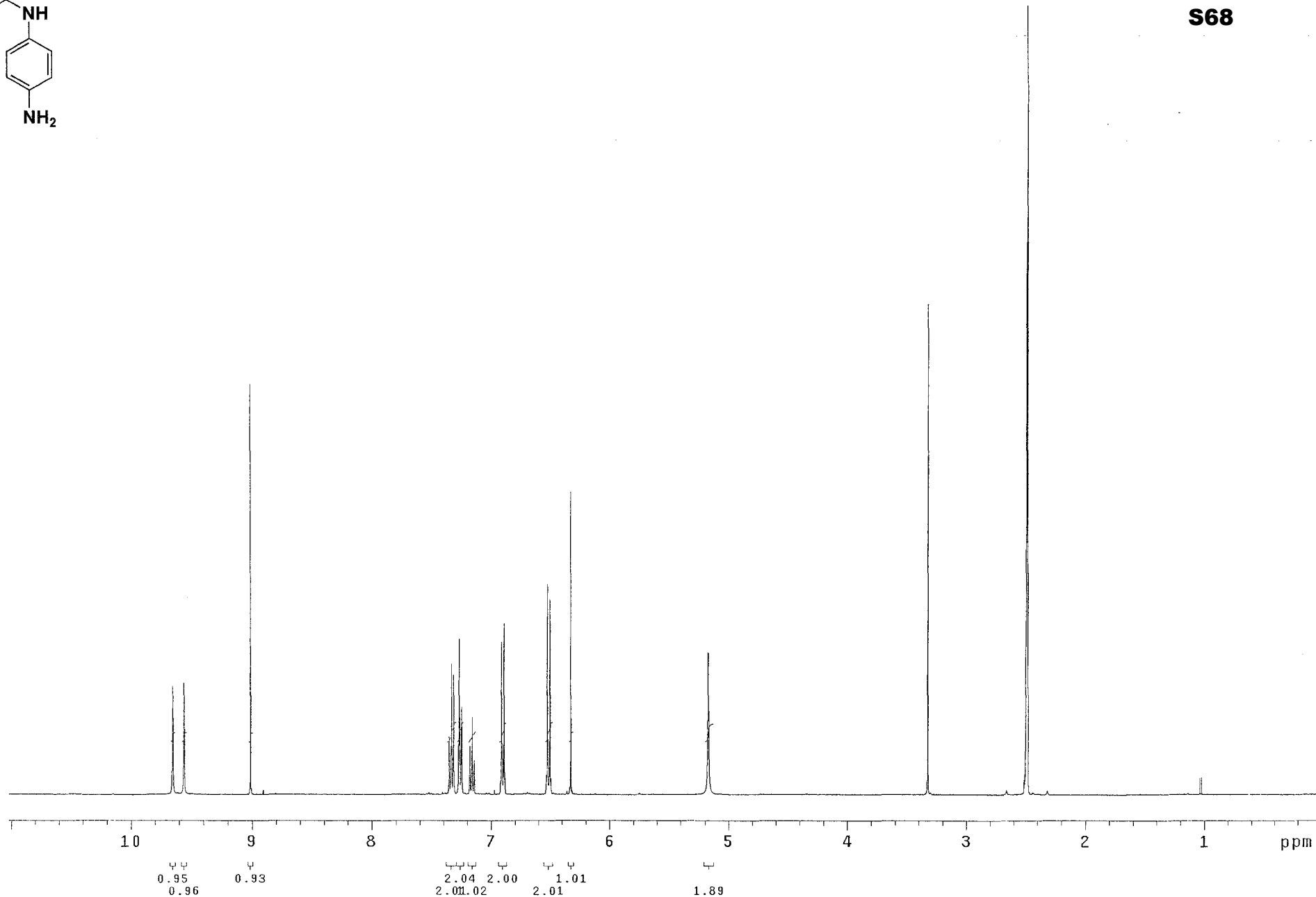
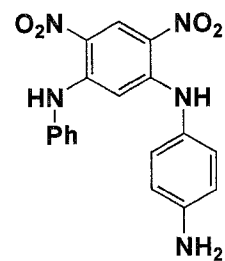
OBSERVE C13, 100.5314915
DECOUPLE H1, 399.8085923
Power 44 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 4.6 hours

Archive directory:
Sample directory:

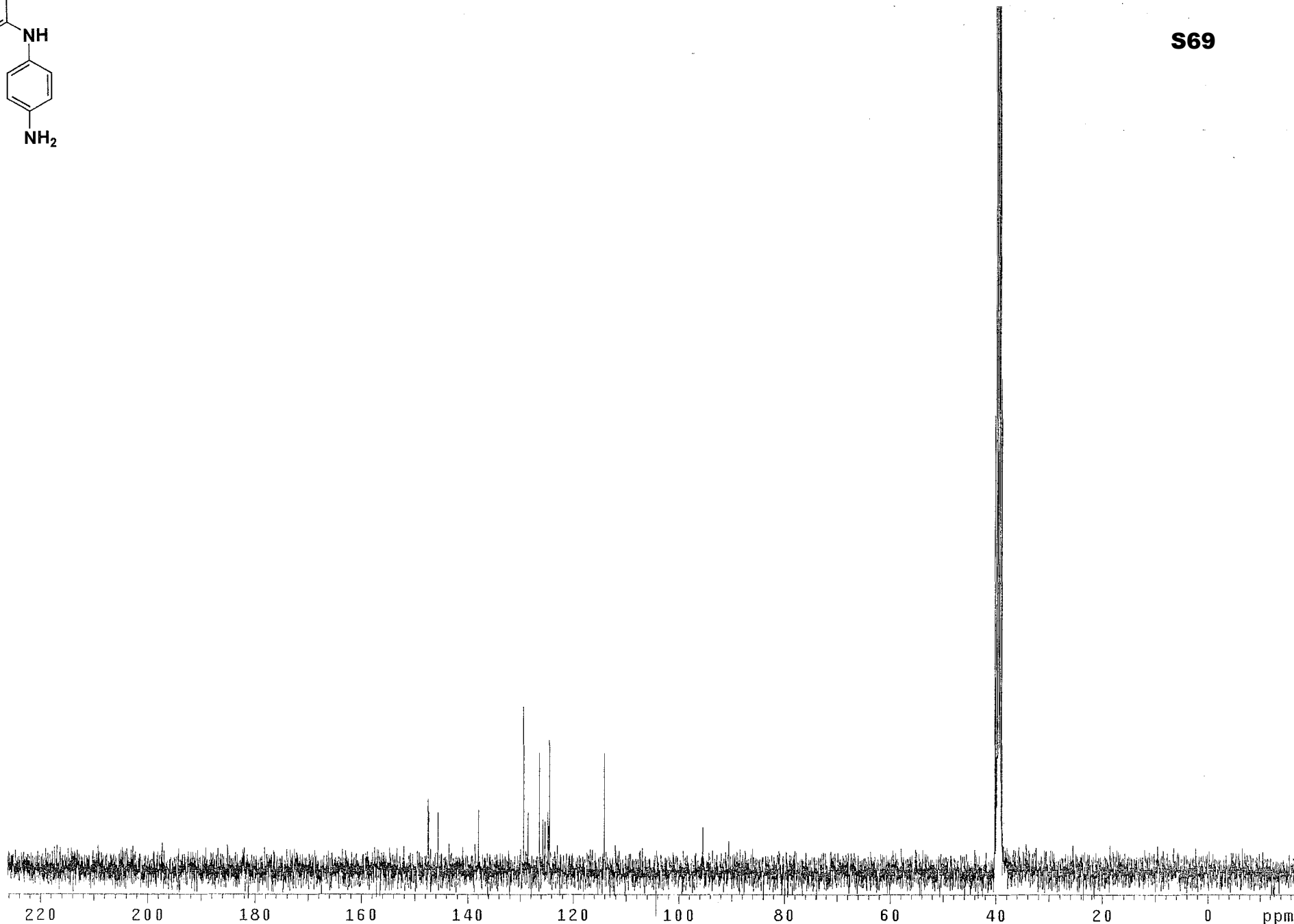
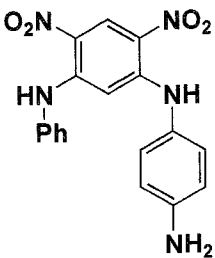
Pulse Sequence: s2pul
Solvent: dmsd
Temp. 27.0 C / 300.1 K

S68

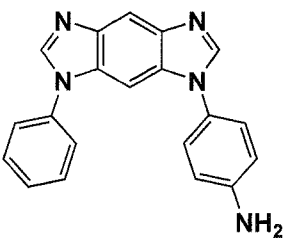


PULSE SEQUENCE Relax. delay 2.000 sec Pulse 30.0 degrees Acq. time 4.049 sec Width 4807.7 Hz 8 repetitions	OBSERVE H1, 399.8065879	DATA PROCESSING Line broadening 0.1 Hz FT size 65536 Total time 1 minute	Archive directory: Sample directory: Pulse Sequence: s2pul Solvent: dms Temp. 27.0 C / 300.1 K
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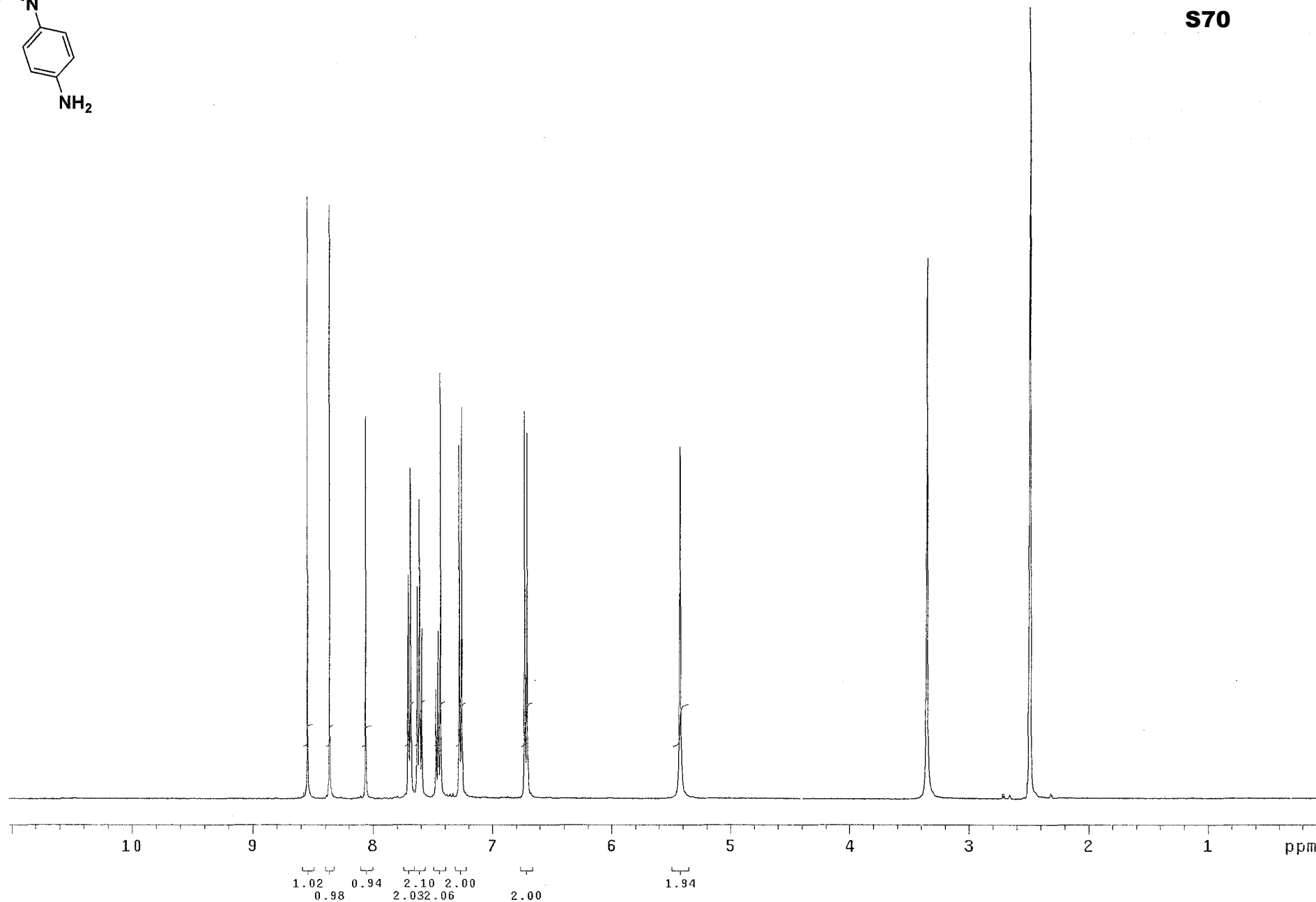
S69



<p>PULSE SEQUENCE Relax. delay 2.000 sec Pulse 30.0 degrees Acq. time 1.300 sec Width 24509.8 Hz 1000 repetitions</p>	<p>OBSERVE C13, 100.5314930 DECOUPLE H1, 399.8085923 Power 44 dB continuously on WALTZ-16 modulated</p>	<p>DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 55 minutes</p>			<p>Archive directory: Sample directory: Pulse Sequence: s2pul Solvent: dmsO Temp. 27.0 C / 300.1 K</p>
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S70



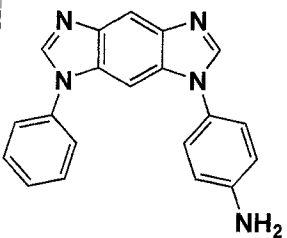
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 4.049 sec
Width 4807.7 Hz
8 repetitions

OBSERVE H1, 399.8065879

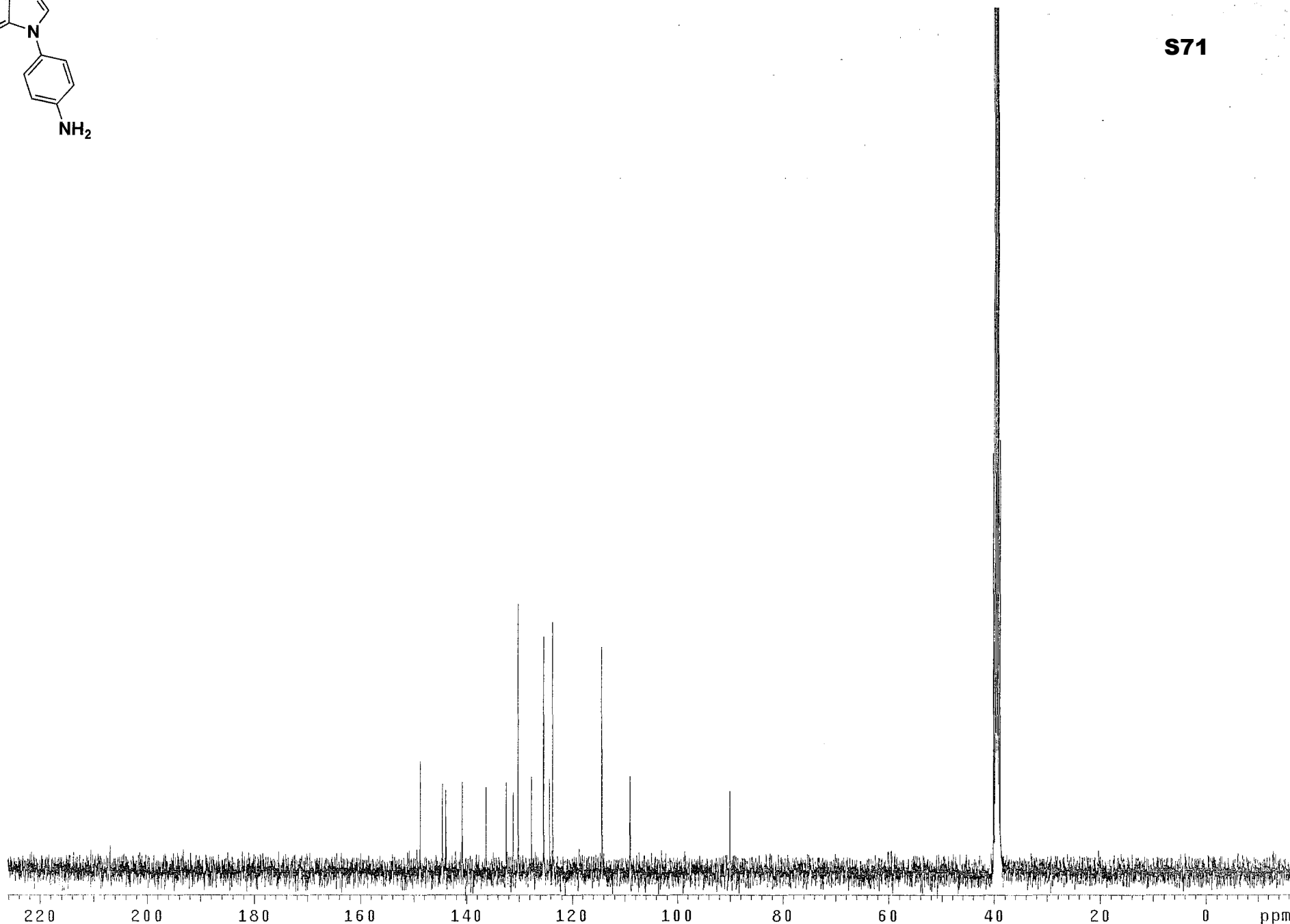
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 1 minute

Archive directory:
Sample directory:

Pulse Sequence: s2pu1
Solvent: dms0
Temp. 27.0 C / 300.1 K



S71



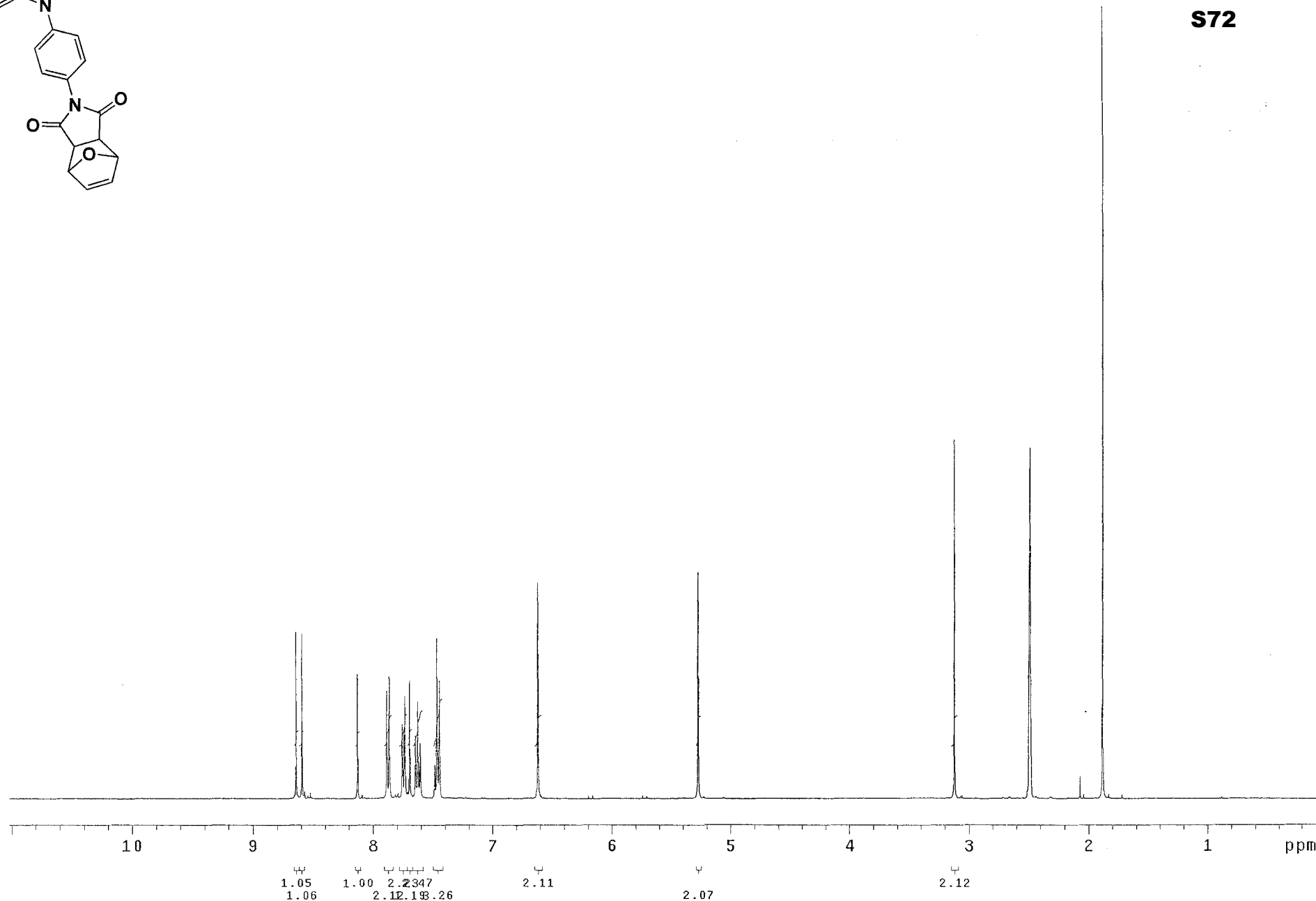
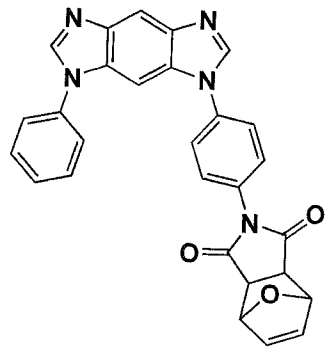
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
1000 repetitions

OBSERVE C13, 100.5314930
DECOUPLE H1, 399.8085923
Power 44 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 55 minutes

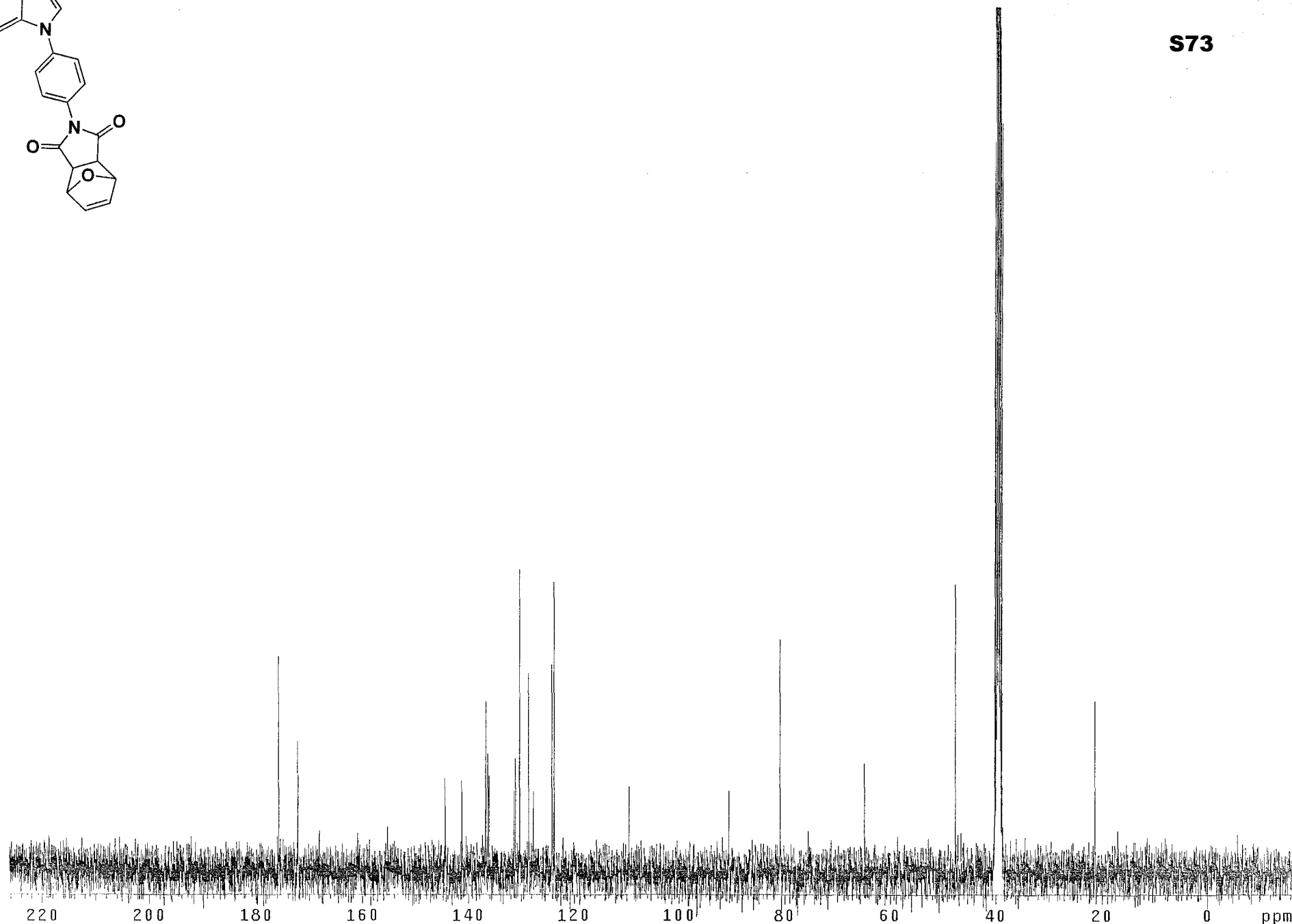
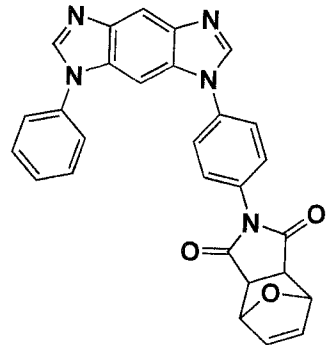
Archive directory:
Sample directory:
Pulse Sequence: s2pul
Solvent: dmsd
Temp. 27.0 C / 300.1 K

S72



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 30.0 degrees Acq. time 4.049 sec Width 4807.7 Hz 8 repetitions	OBSERVE H1, 399.8065878	DATA PROCESSING Line broadening 0.1 Hz FT size 65536 Total time 1 minute			Archive directory: Sample directory: Pulse Sequence: s2pul Solvent: dmsd Temp. 27.0 C / 300.1 K
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S73



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
1000 repetitions

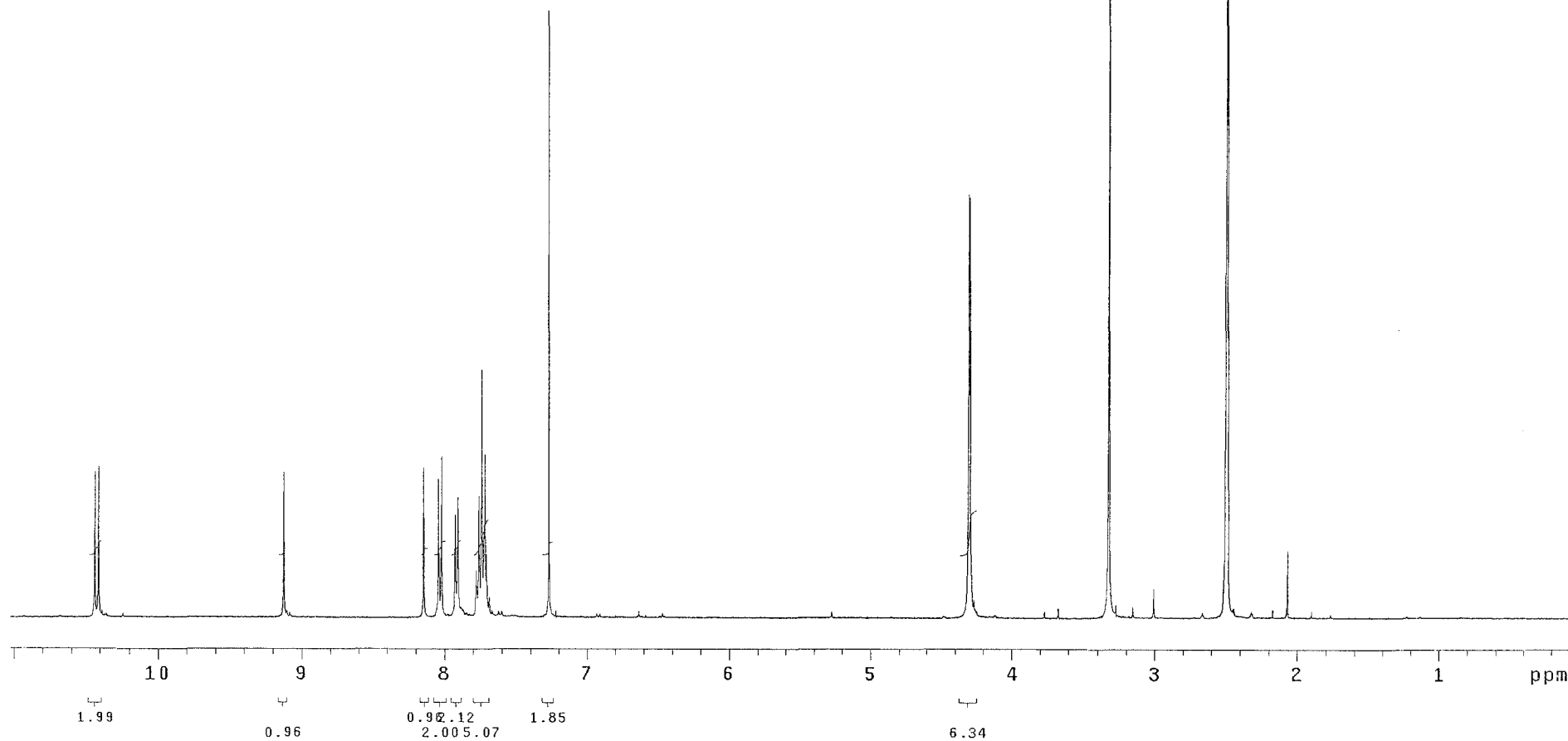
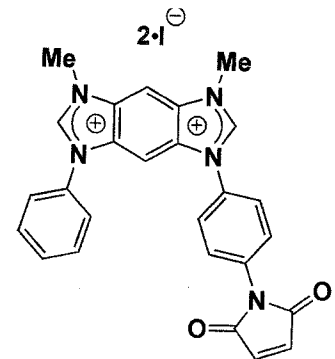
OBSERVE C13, 100.5314922
DECOUPLE H1, 399.8085923
Power 44 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 55 minutes

Archive directory:
Sample directory:

Pulse Sequence: s2pul
Solvent: dmsd
Temp. 27.0 C / 300.1 K

S74



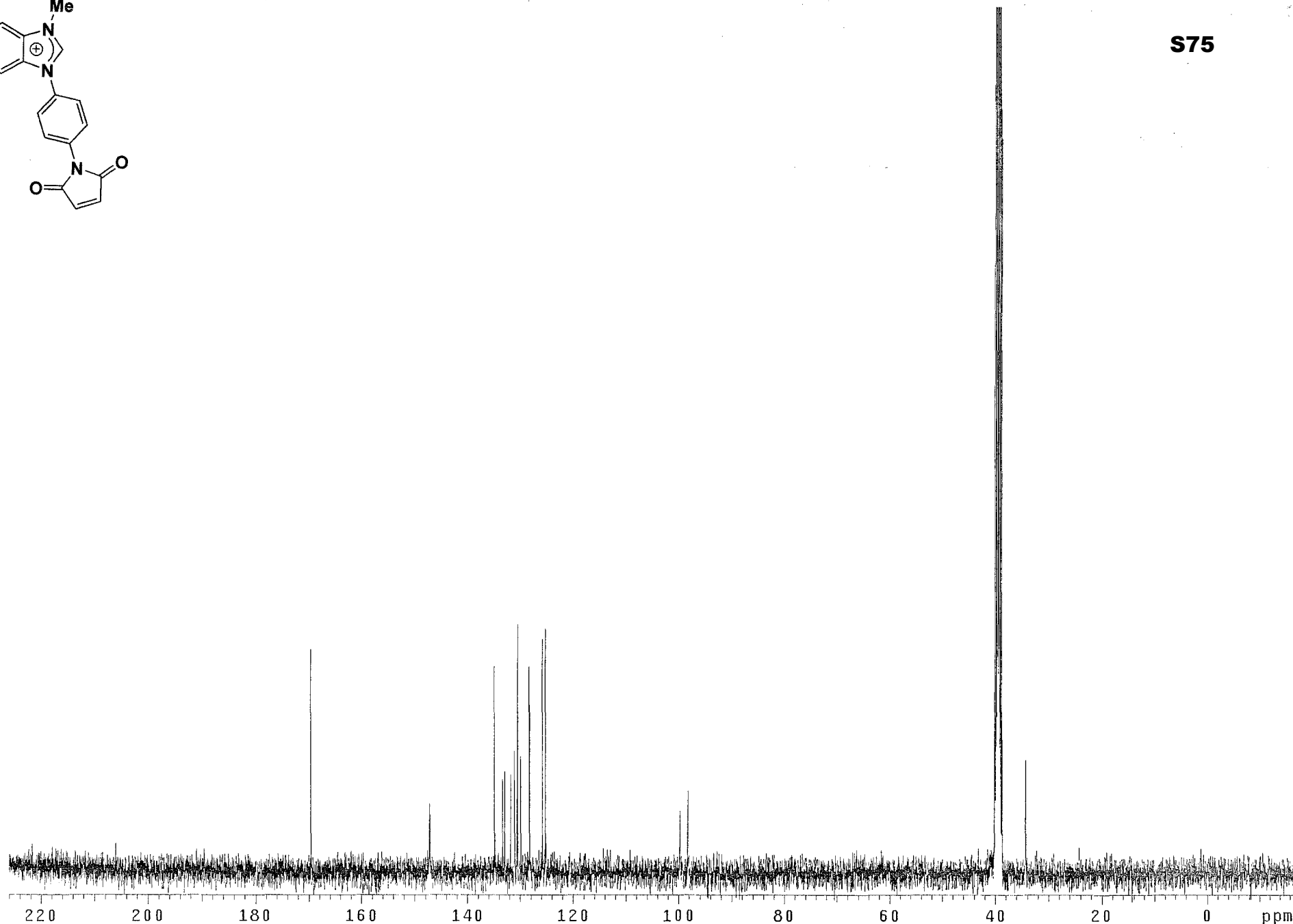
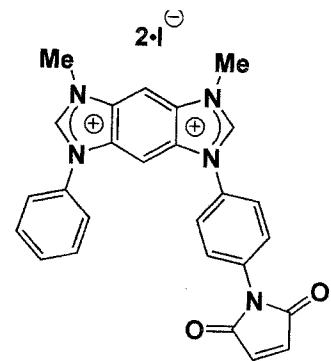
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 4.049 sec
Width 4807.7 Hz
8 repetitions

OBSERVE H1, 399.8065868

DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 1 minute

Archive directory:
Sample directory:
Pulse Sequence: s2pul
Solvent: dmsd
Temp. 27.0 C / 300.1 K

S75



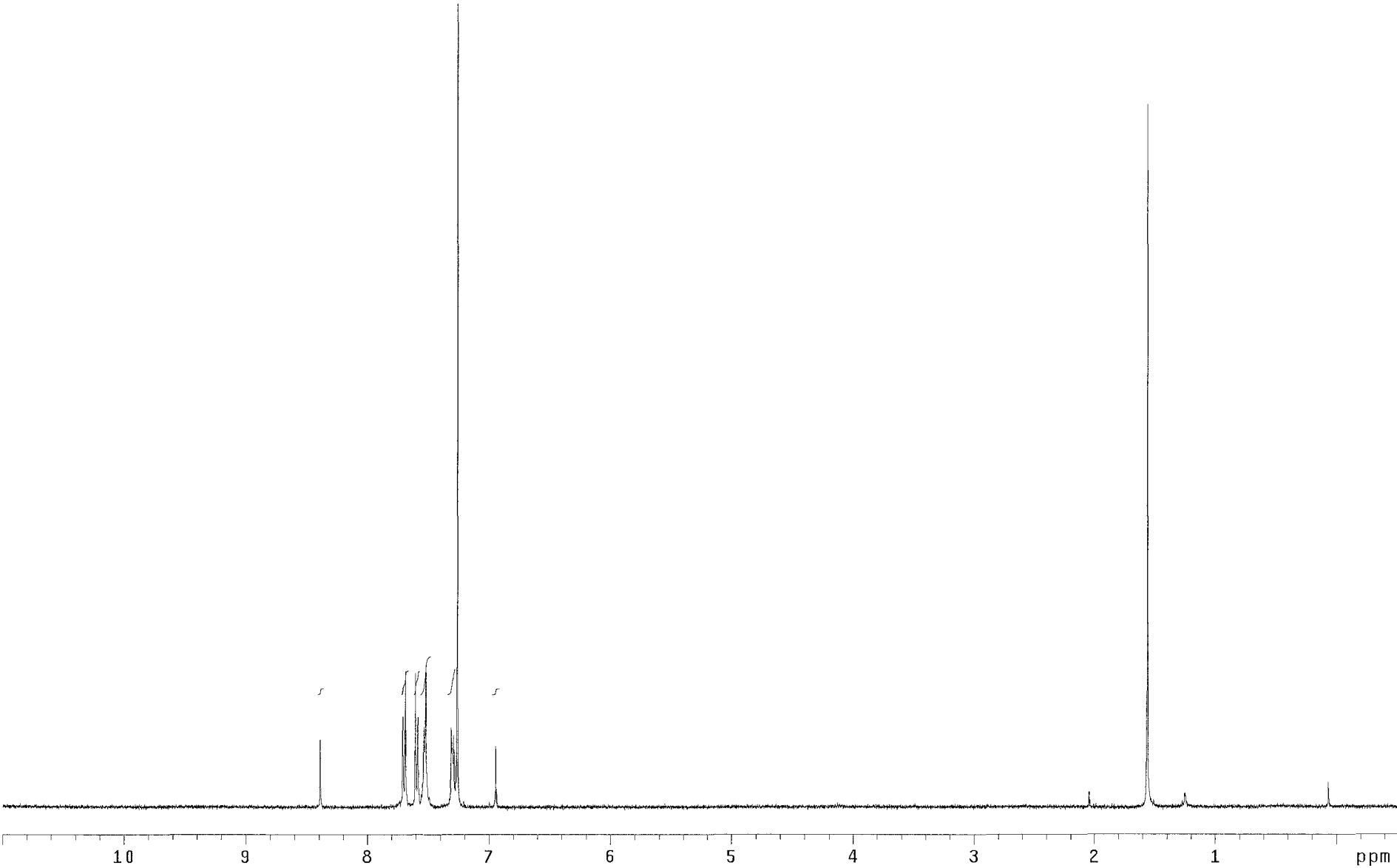
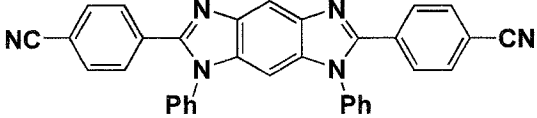
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
5000 repetitions

OBSERVE C13, 100.5314967
DECOUPLE H1, 399.8085923
Power 44 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 4.6 hours

Archive directory:
Sample directory:
Pulse Sequence: s2pul
Solvent: dmsd
Temp. 27.0 C / 300.1 K

S78

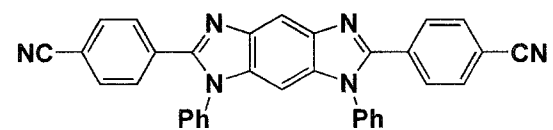


PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
29 repetitions

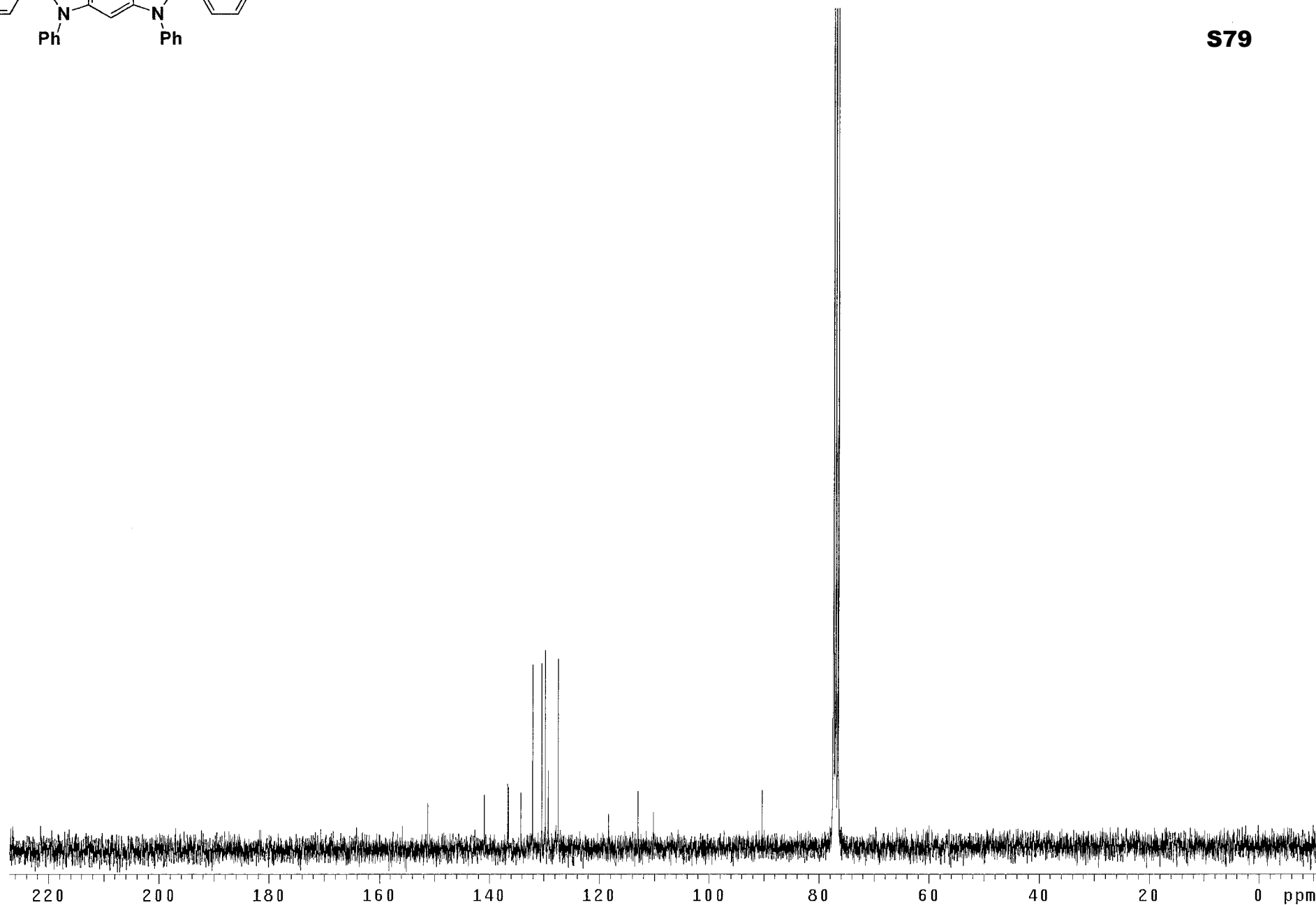
OBSERVE H1, 400.2669779

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 2 minutes

B6AB196-Rx3
Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
Mercury-400 "nmr6"



S79



PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
10329 repetitions

OBSERVE C13, 75.4700200
DECOUPLE H1, 300.1409259
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data

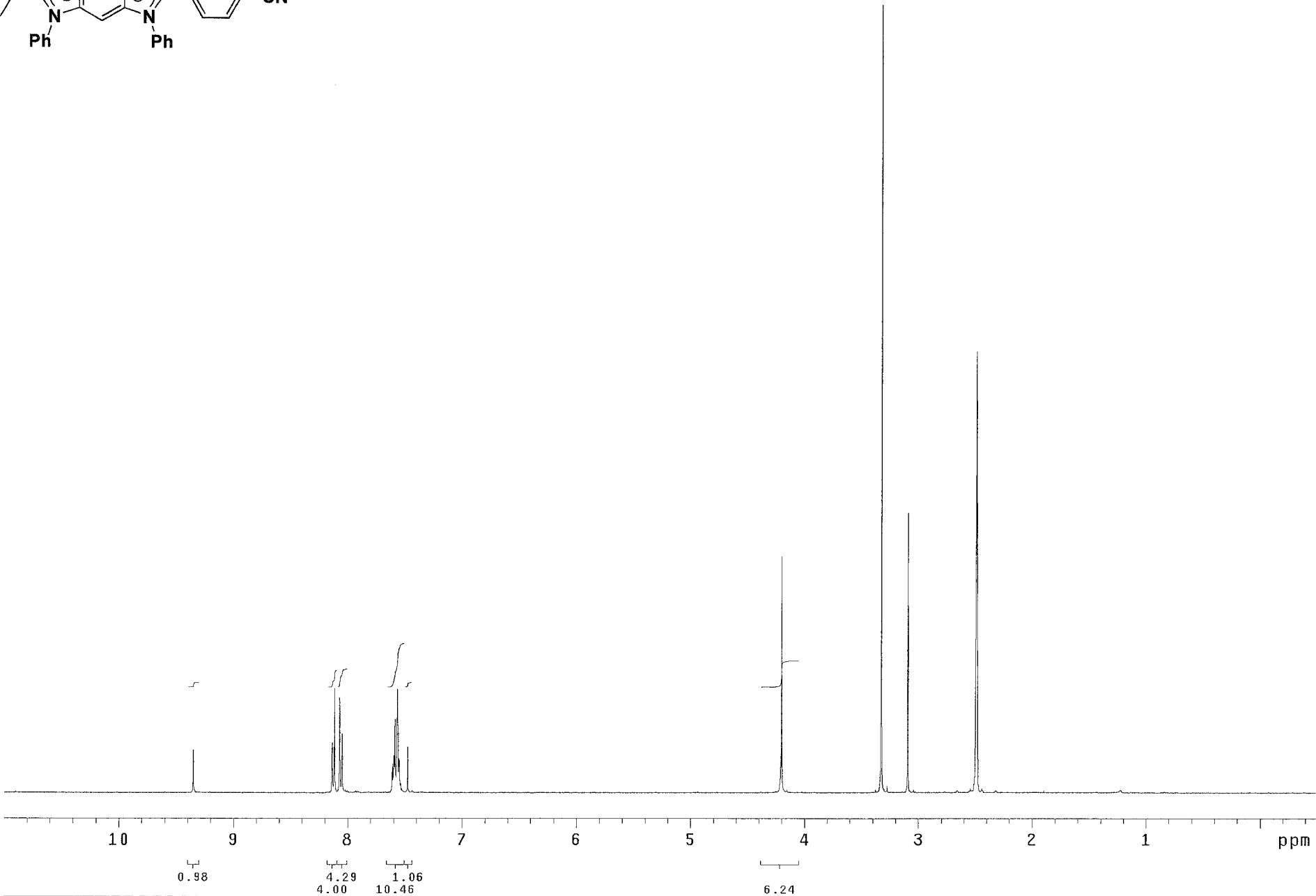
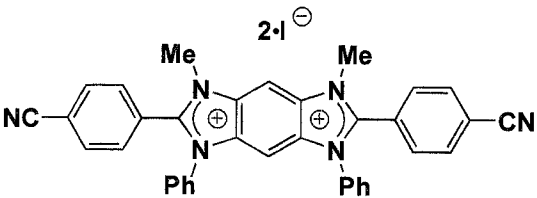
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 10.8 hours

B6AB196-13C

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"

S80



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 16.4 degrees Acq. time 2.856 sec Width 5602.2 Hz 24 repetitions	OBSERVE H1, 400.2688764	DATA PROCESSING Line broadening 0.1 Hz FT size 32768 Total time 1 minutes	B6AB201 Pulse Sequence: s2pul Solvent: DMSO Ambient temperature Mercury-400 "nmr6"
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