Supporting Information

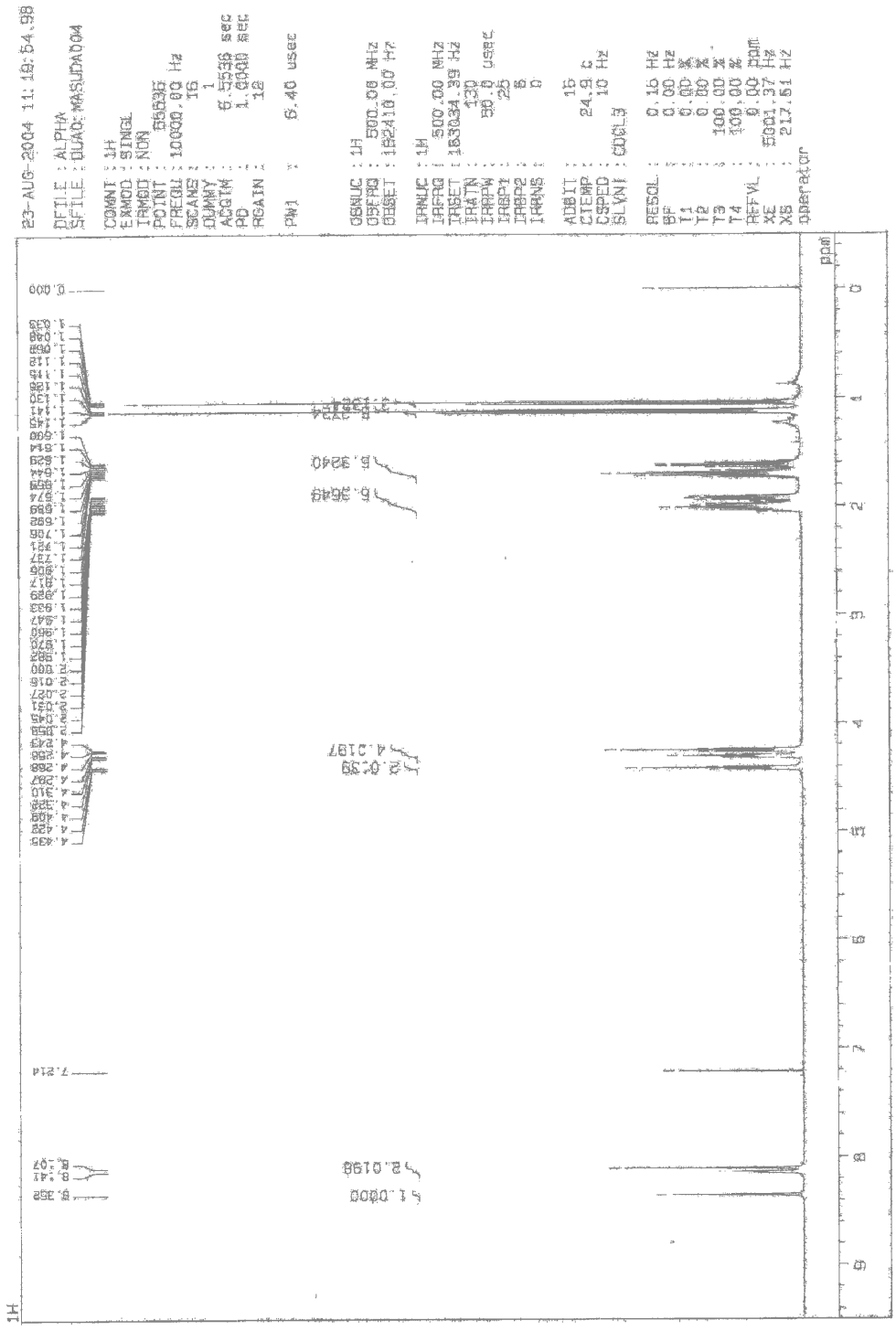
Computational details

The GAUSSIAN03 program[1] was used to perform DFT calculations. First the geometry was optimized within the B3LYP/3-21G level, and single point (or time-dependent) calculations were performed using the B3LYP with 6-31G(d) basis set. TAC-C_{60} and the constituting components, i.e. 1,2-C_{60} and TAC, were constrained to have the C_{2v} symmetry.

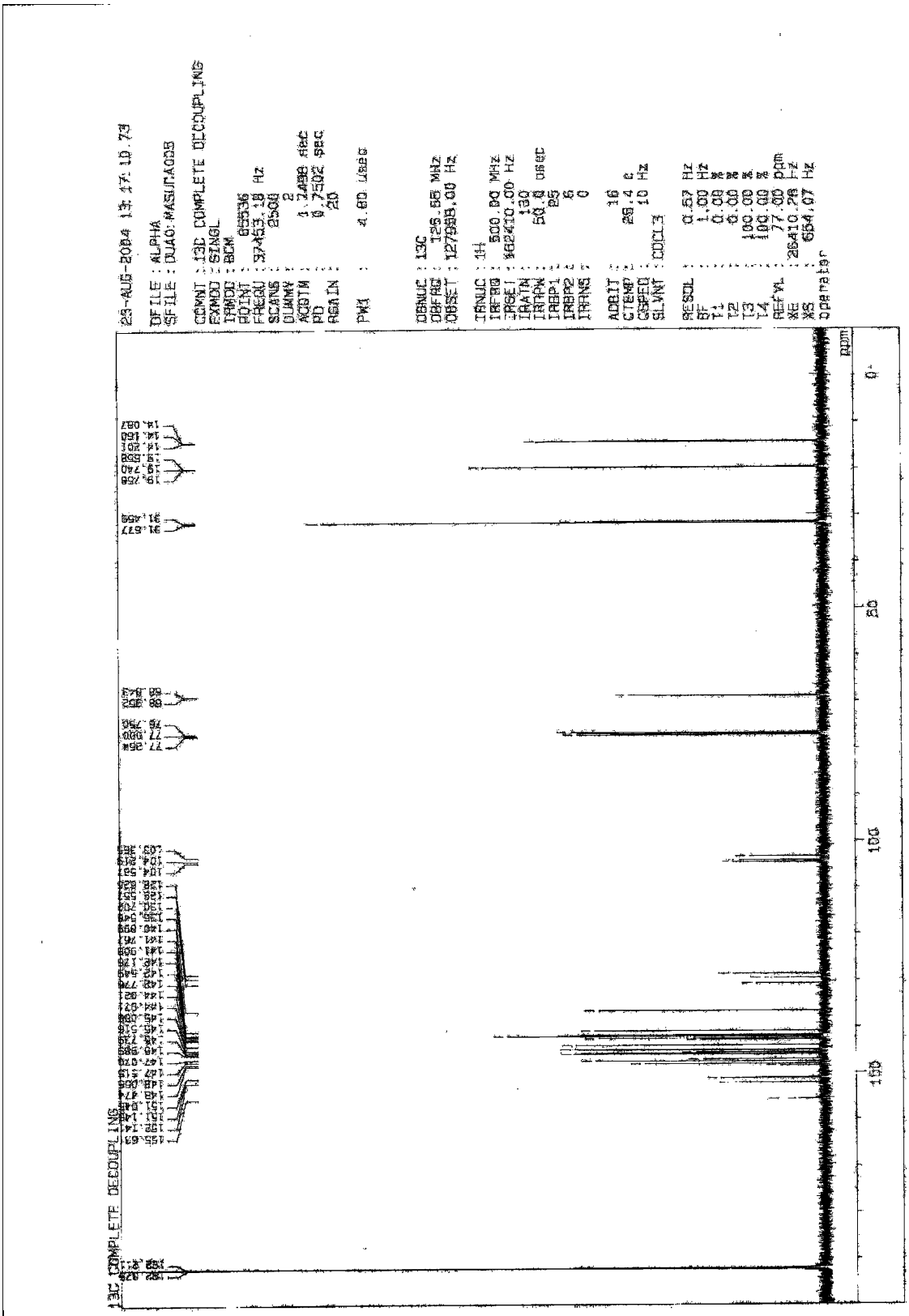
Reference

1 Frisch M. J.; Trucks G. W.; Schlegel H. B.; Scuseria G. E.; Robb M. A.; Cheeseman J. R.; Montgomery J. A.; Vreven Jr., T.; Kudin K. N.; Burant J. C.; Millam J. M.; Iyengar S. S.; Tomasi J.; Barone V.; Mennucci B.; Cossi M.; Scalmani G.; Rega N.; Petersson G. A.; Nakatsuji H.; Hada M.; Ehara M.; Toyota K.; Fukuda R.; Hasegawa J.; Ishida M.; Nakajima T.; Honda Y.; Kitao O.; Nakai H.; Klene M.; Li X.; Knox J. E.; Hratchian H. P.; Cross J. B.; Adamo C.; Jaramillo J.; Gomperts R.; Stratmann R. E.; Yazyev O.; Austin A. J.; Cammi R.; Pomelli C.; Ochterski J. W.; Ayala P. Y.; Morokuma K.; Voth G. A.; Salvador P.; Dannenberg J. J.; Zakrzewski V. G.; Dapprich S.; Daniels A. D.; Strain M. C.; Farkas O.; Malick D. K.; Rabuck A. D.; Raghavachari K.; Foresman J. B.; Ortiz J. V.; Cui Q.; Baboul A. G.; Clifford S.; Cioslowski J.; Stefanov B. B.; Liu G.; Liashenko A.; Piskorz P.; Komaromi I.; Martin R. L.; Martin D. J.; Fox D. J.; Keith T.; Al-Laham M. A.; Peng C. Y.; Nanayakkara A.; Challacombe M.; Gill P. M. W.; Johnson B.; Chen W.; Wong M. W.; Gonzalez C.; Pople J. A. *Gaussian 03, Revision B.05*, Gaussian, Inc., Pittsburgh, PA, **2003**.

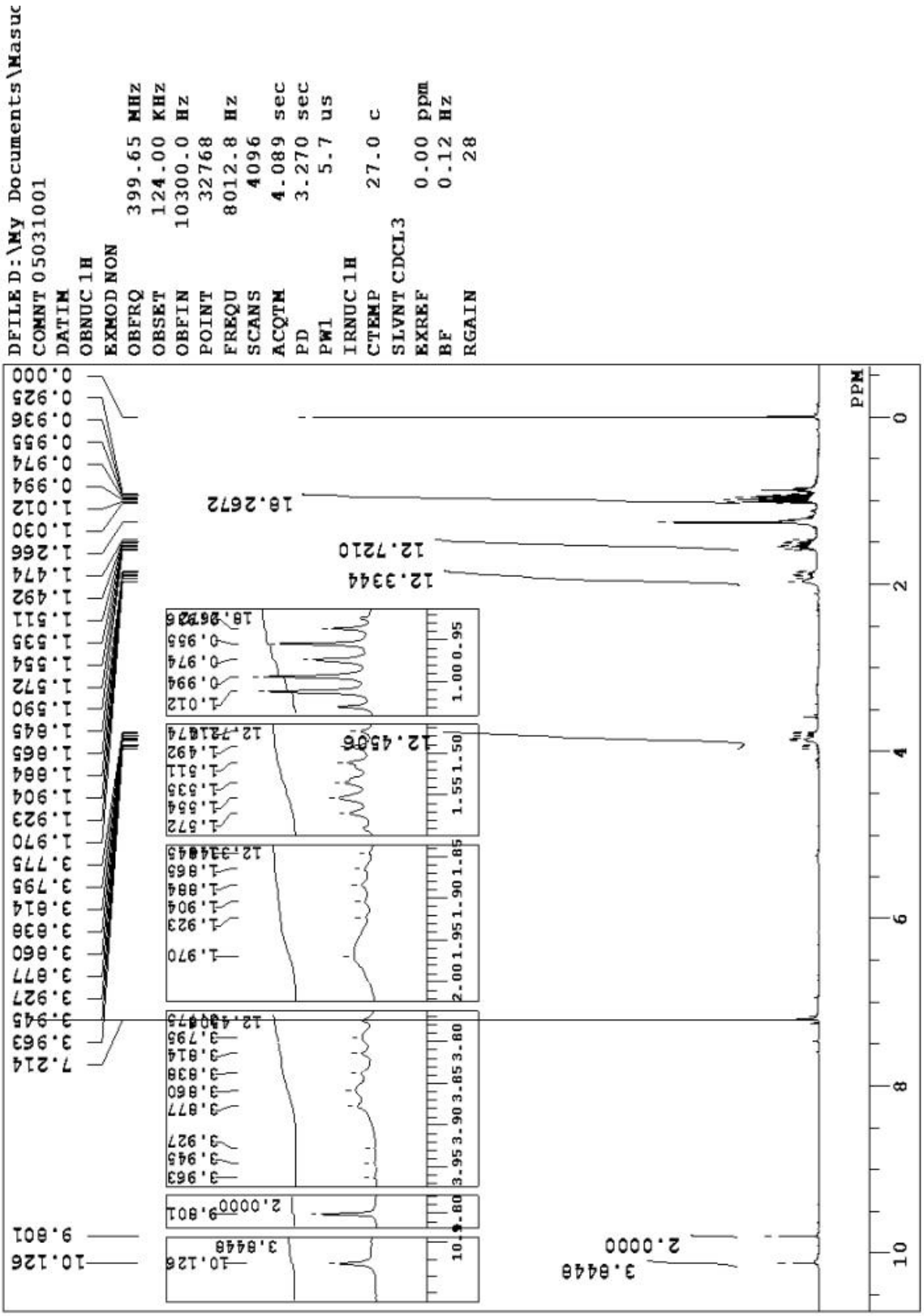
500 MHz ^{1}H NMR of 3a in CS_2:$CDCl_3$ = 4:1



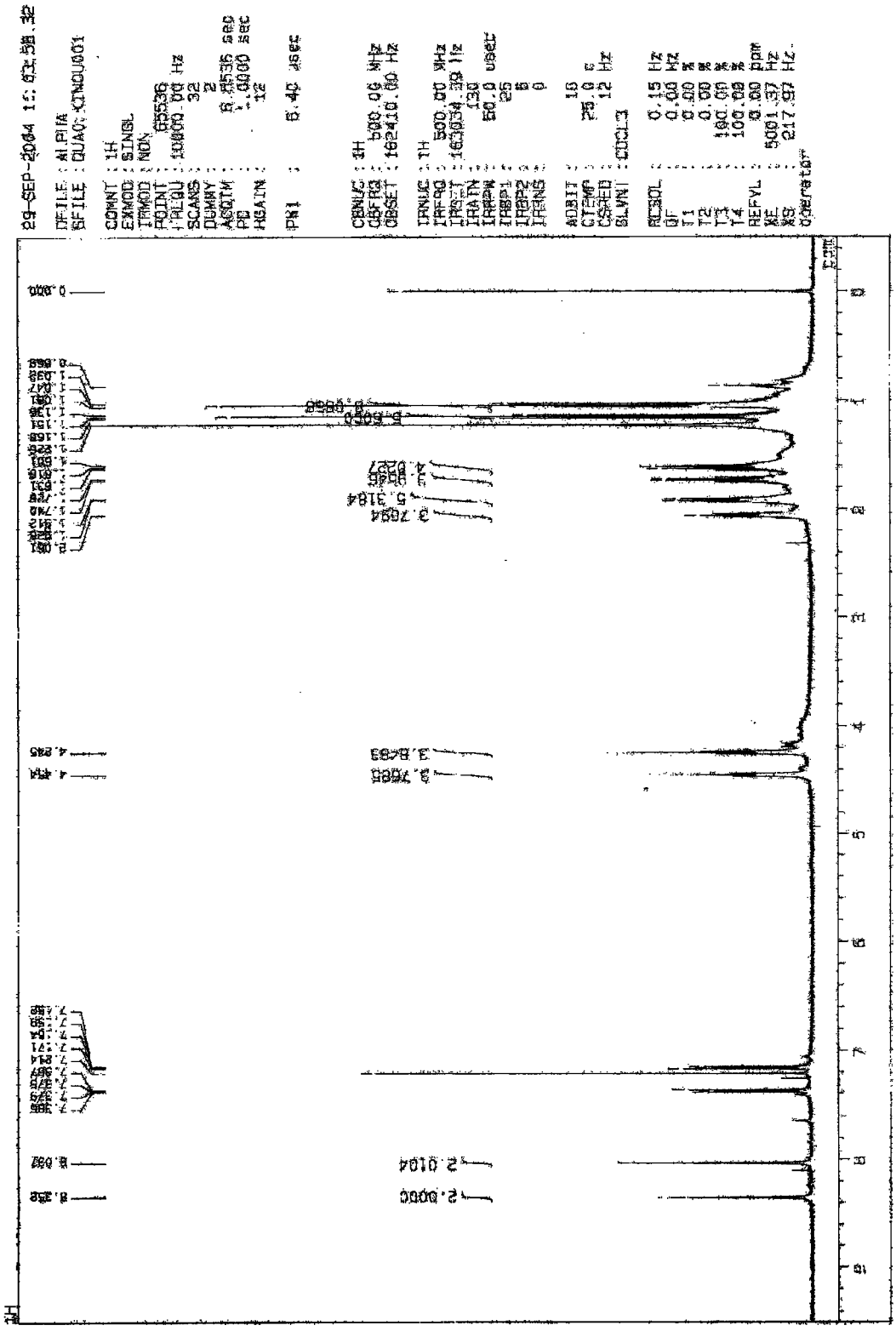
125 MHz ^{13}C NMR of 3a in CS_2:$CDCl_3$ = 4:1



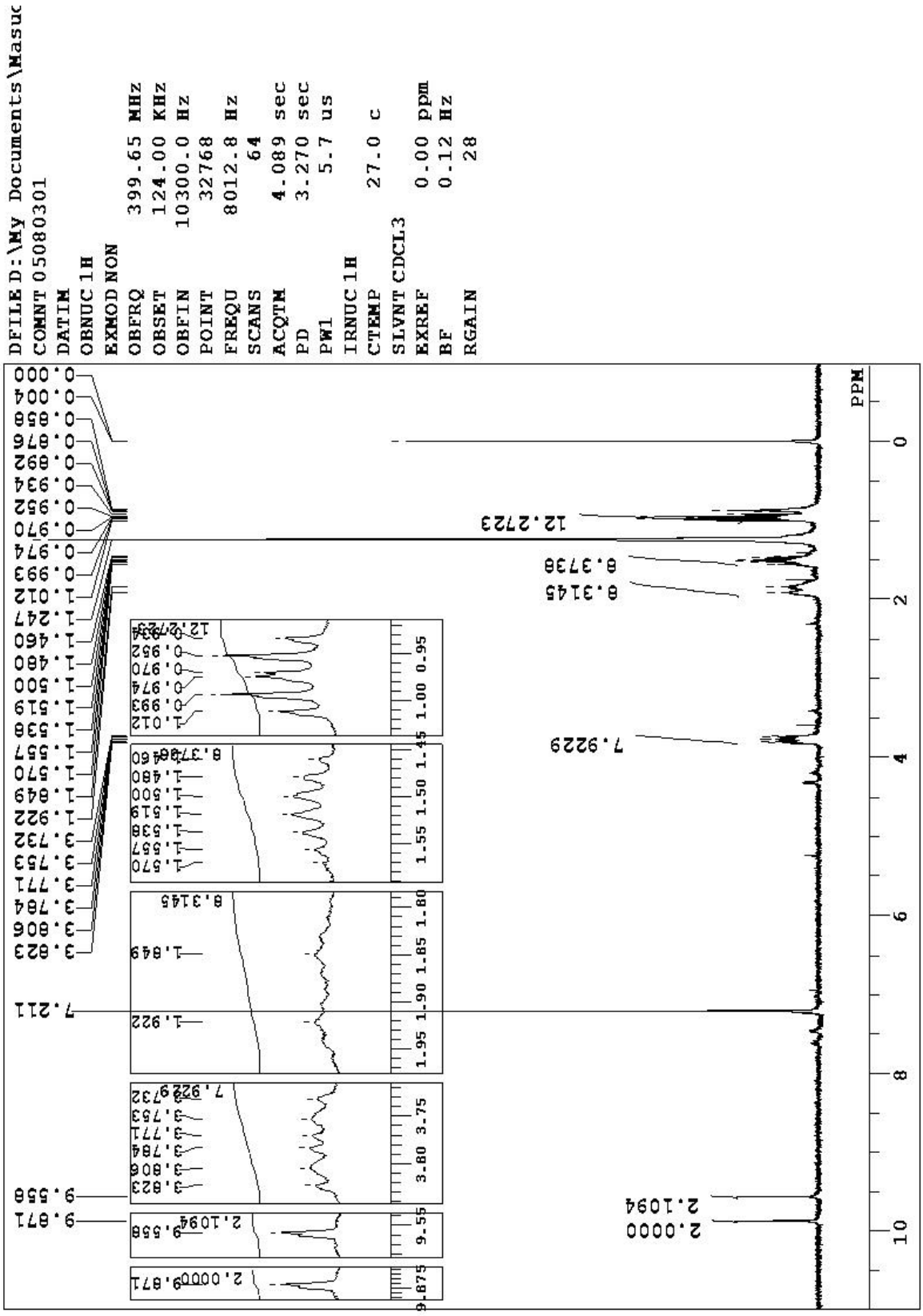
400 MHz ^{1}H NMR of 3b in CS_2:$CDCl_3$ = 4:1



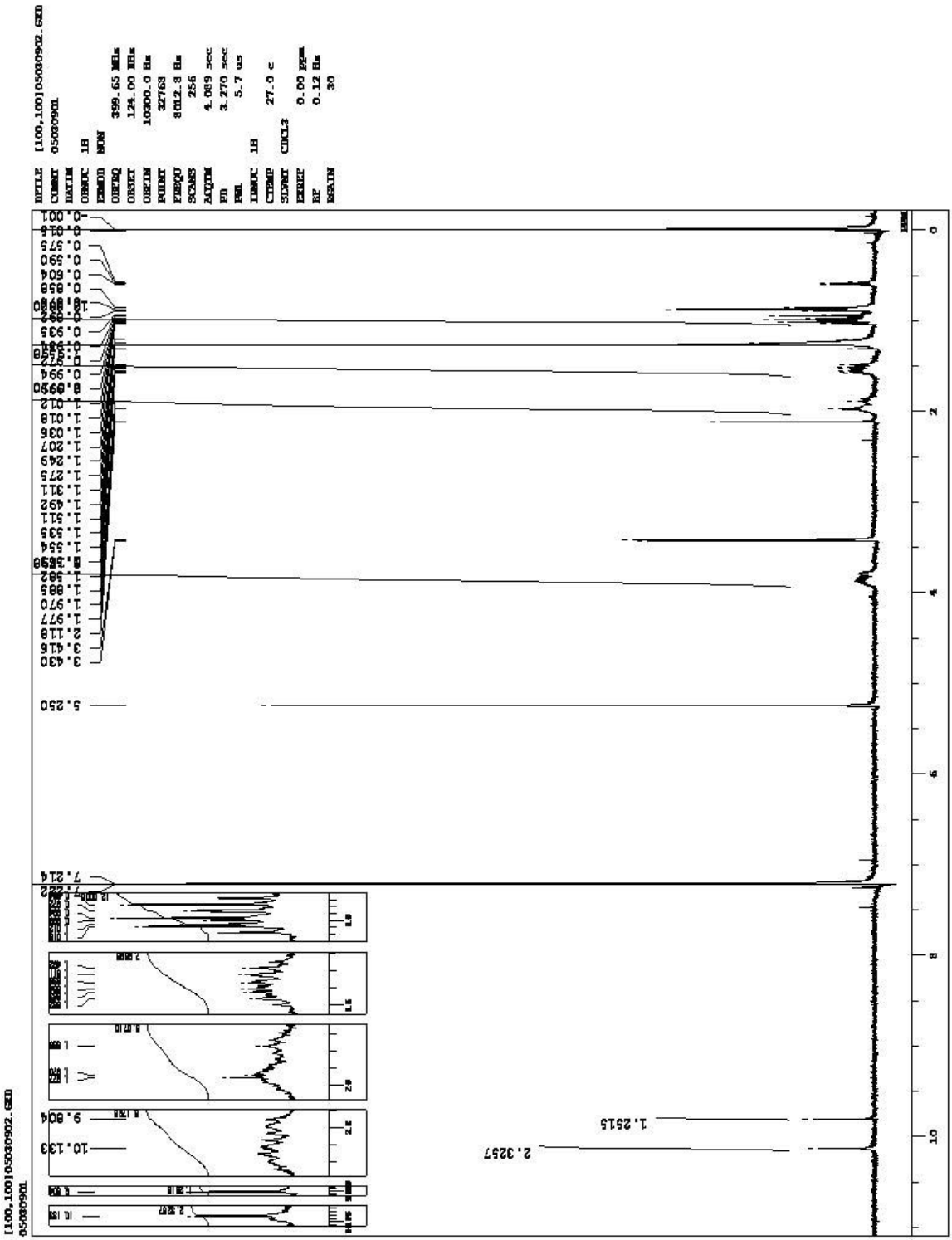
400 MHz ^{1}H NMR of 4a in CS_2:$CDCl_3$ = 4:1



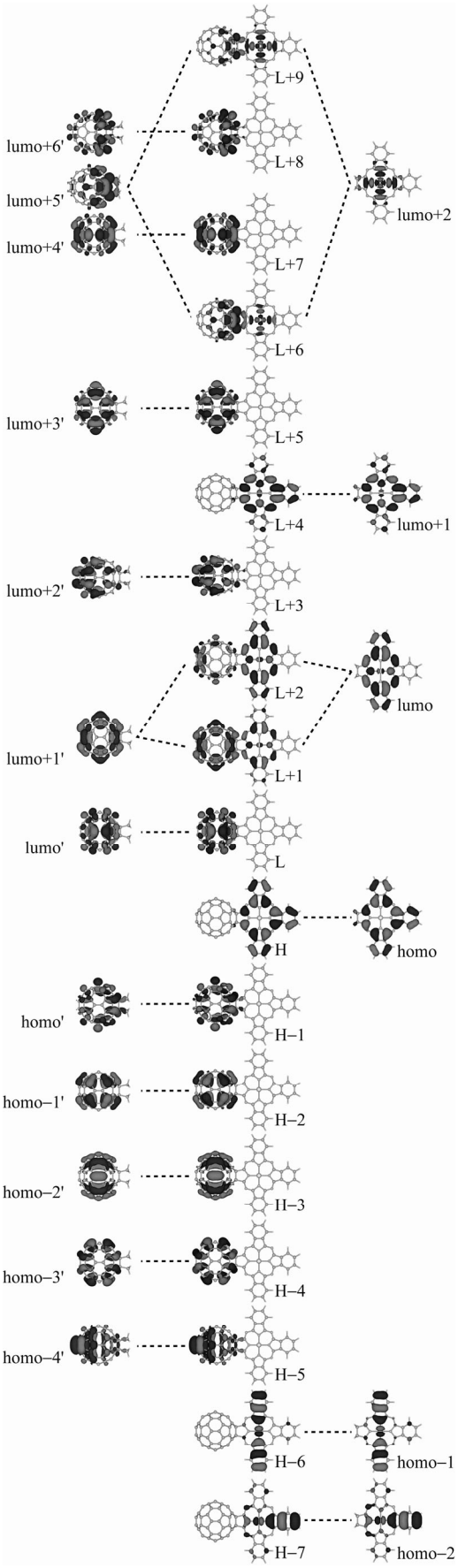
400 MHz ^{1}H NMR of 4b in CS_2:$CDCl_3$ = 4:1



400 MHz ^{1}H NMR of 5b in CS_2:$CDCl_3$ = 3:2



M O s


L+9
lumo+6'
L+8
lumo+5'
lumo+2
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L+7
L+6
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L+5
L+4
lumo+1
lumo+2'
L+3
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