Supporting Information for "NDI and DAN DNA: Nucleic Acid Directed Assembly of NDI and DAN"

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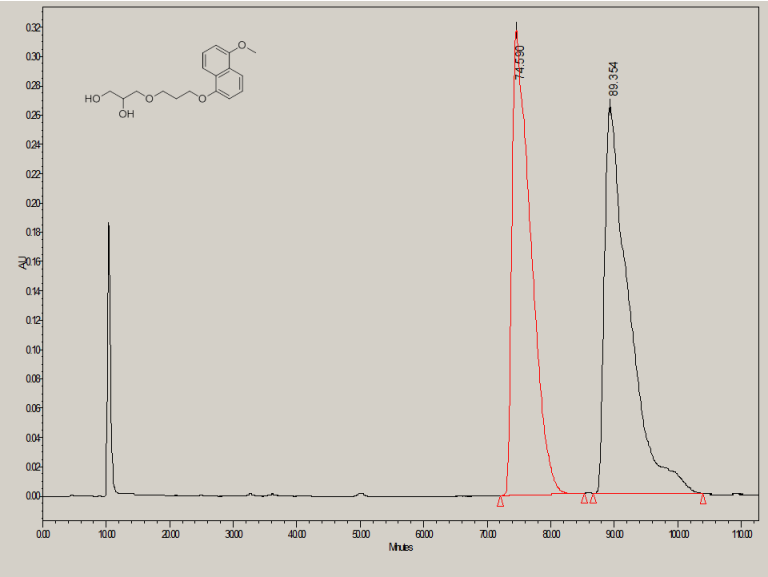
CONTENTS

General Procedures and Reagents

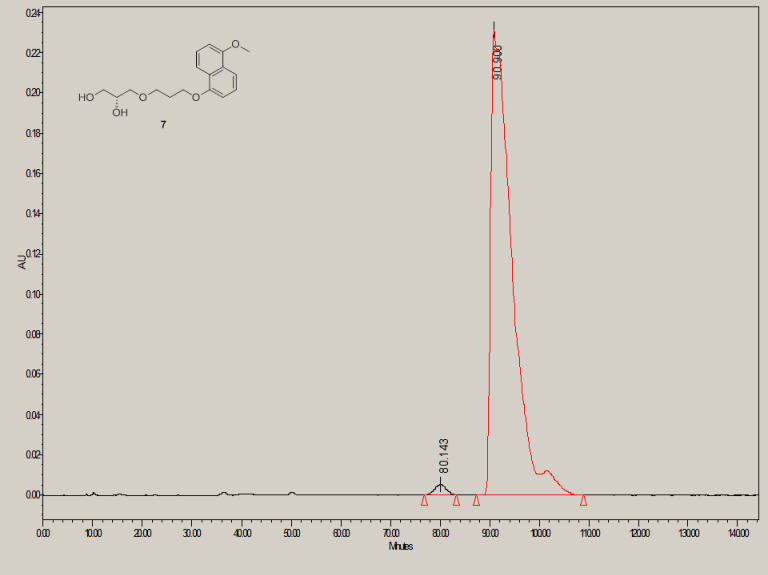
High-resolution mass spectra were analyzed by Q-TOF. Reactions were performed under an atmosphere of argon unless otherwise specified. All microwave reactions were conducted in a C.E.M. MARS microwave reactor at a power of 300W in an open vessel or C.E.M. Explorer 48 microwave reactor in a sealed vessel at a power of 300W.

Figure S1. [a] Chiral HPLC Chromatograms of 7 and 10.

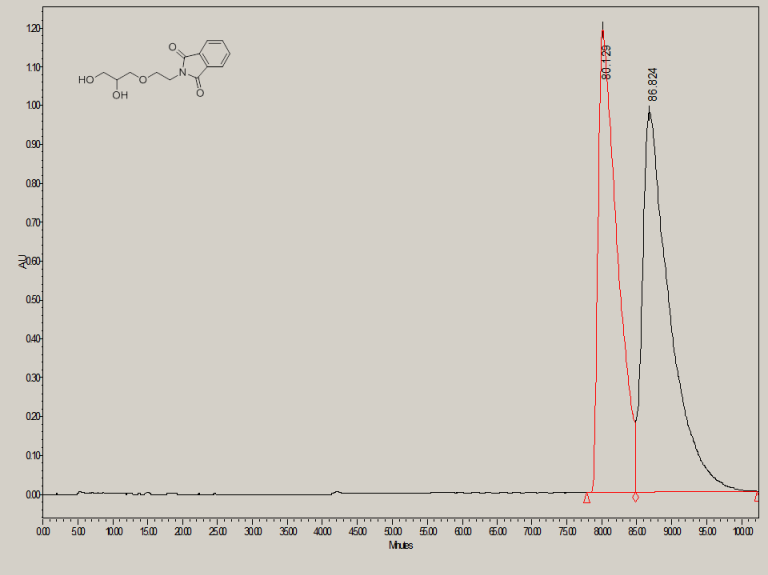


Racemic Sample

	Retention Time	Area	% Area	Height
1	80.129	226355648	45.90	1189756
2	86.824	266826823	54.10	976579

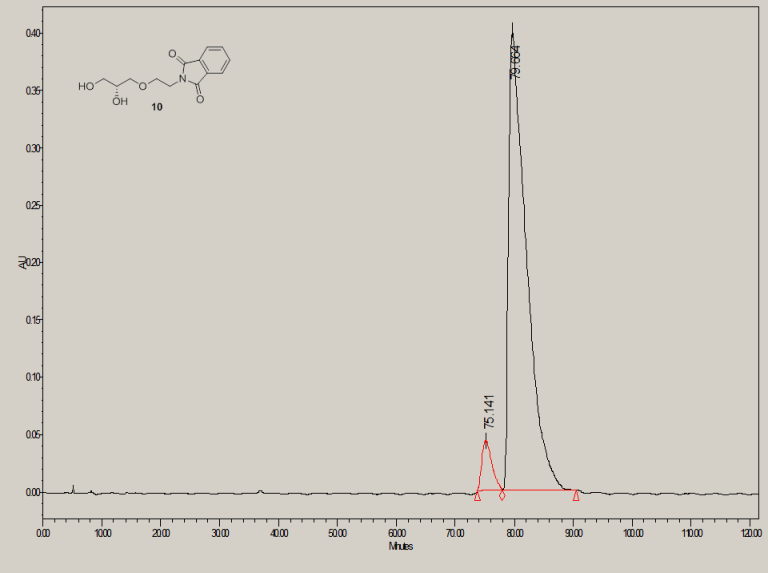


	Retention Time	Area	% Area	Height
1	75.141	5187344	5.82	43704
2	79.664	83915537	94.18	401161



Racemic Sample

	Retention Time	Area	% Area	Height
1	74.590	65668561	48.10	316870
2	89.354	70865309	51.90	263866



	Retention Time	Area	% Area	Height
1	80.143	824716	1.19	5290
2	90.900	68763657	98.81	231161

[a] Enantiomeric excess was determined by HPLC on a Chiralcel ODH column (0.46 cm I.D. x 25 cmL); eluent, hexane:*i*-PrOH, 95:5 v/v; flow rate, 1.0 mL/min; UV at 254 nm; room temperature.

Figure S2. ^{1}H NMR ($CDCl_3$) of **1**

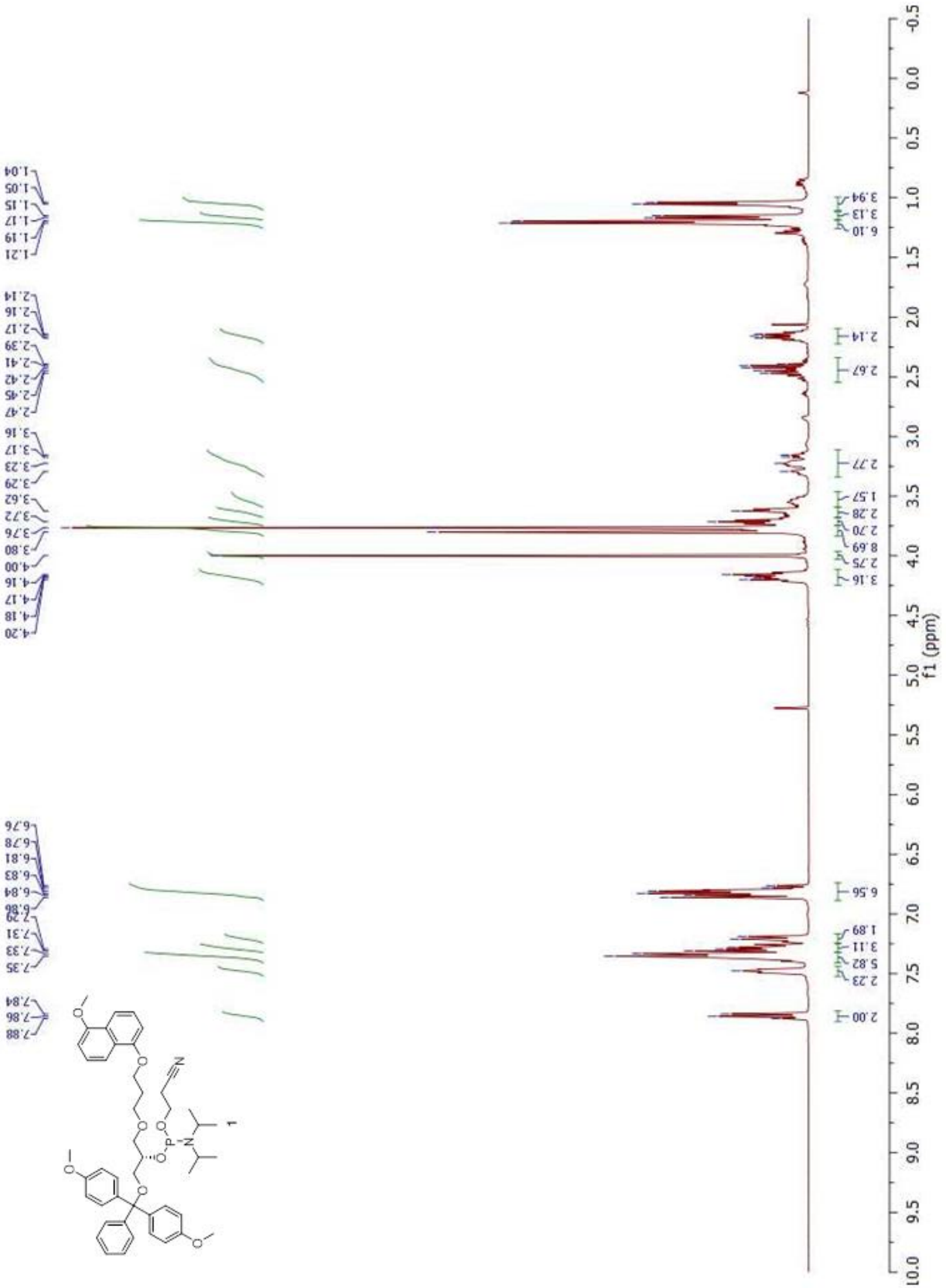


Figure S3. ^{1}H NMR ($CDCl_3$) of **2**

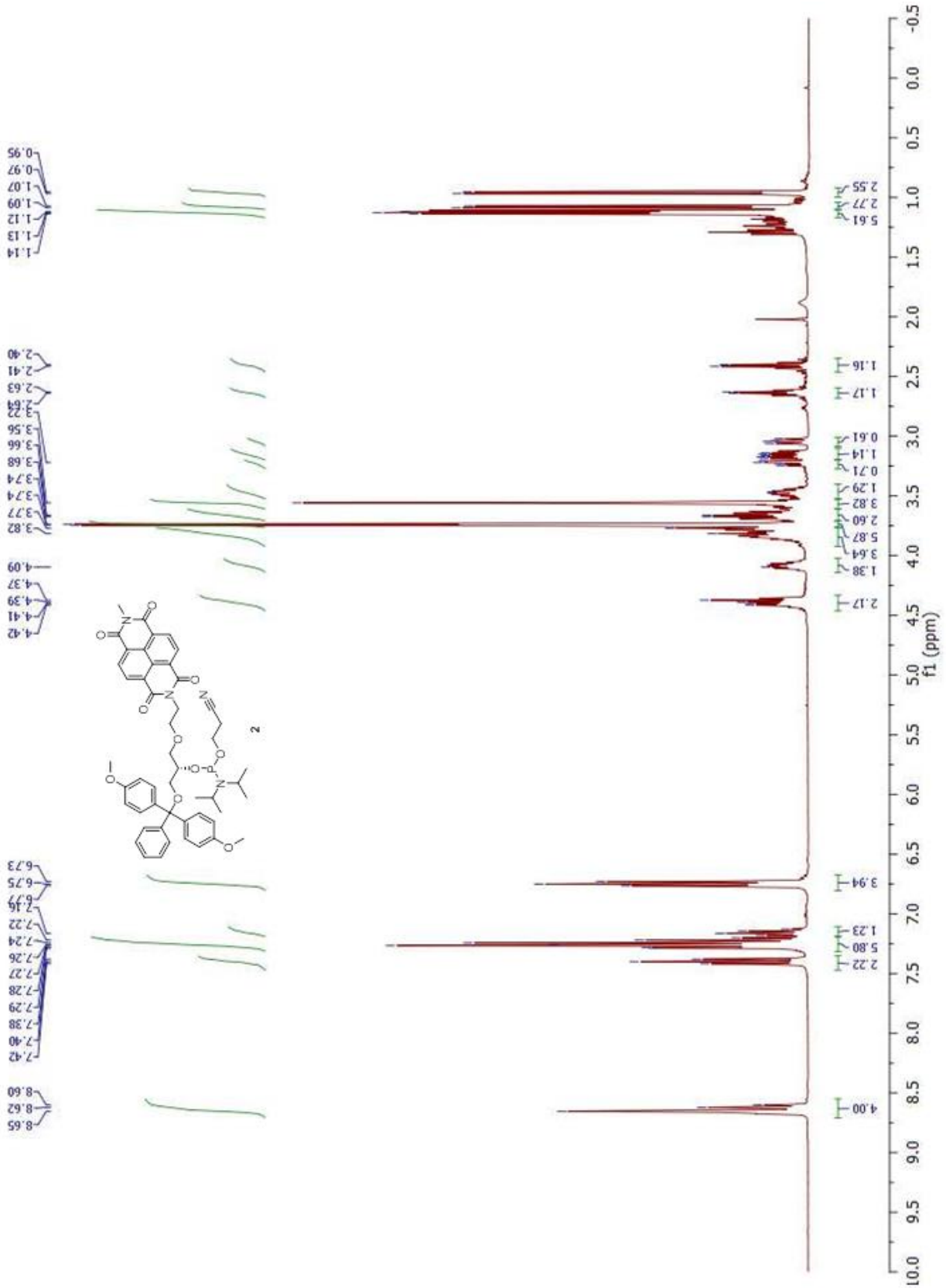


Figure S4. ^{1}H NMR ($CDCl_3$) of **3**

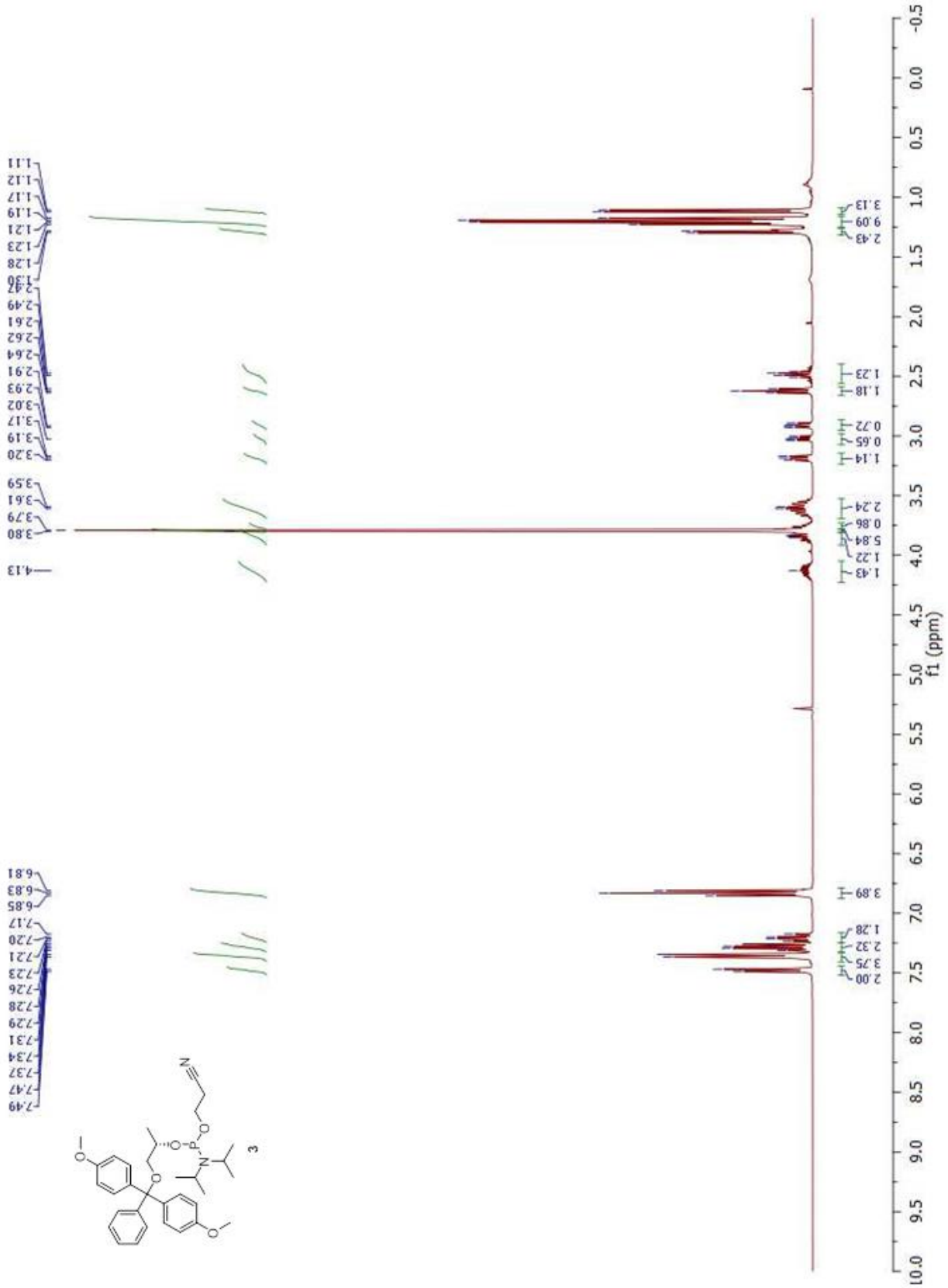


Figure S5. ^{1}H NMR ($CDCl_3$) of **5**

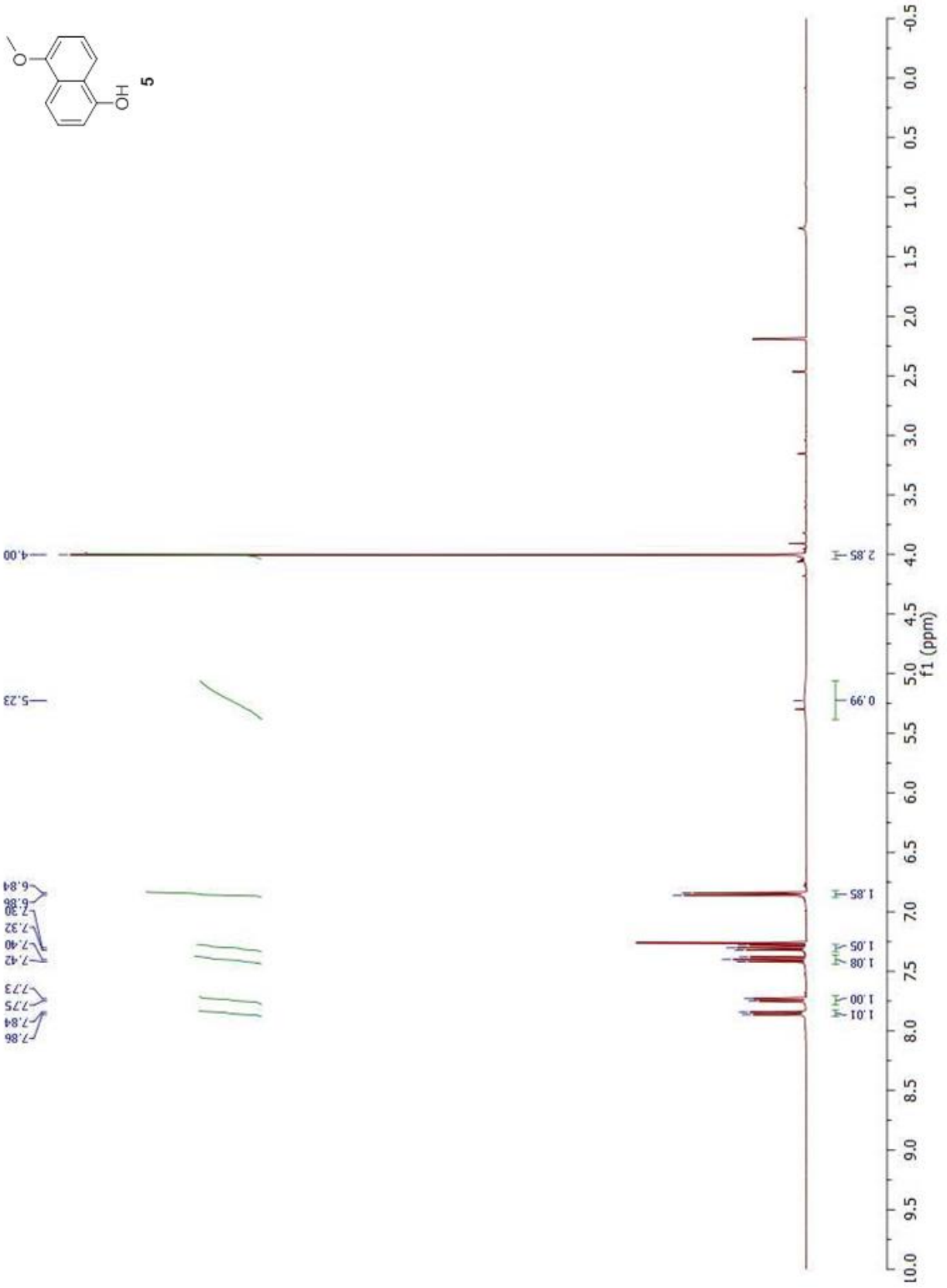


Figure S6. ^{1}H NMR ($CDCl_3$) of **6**

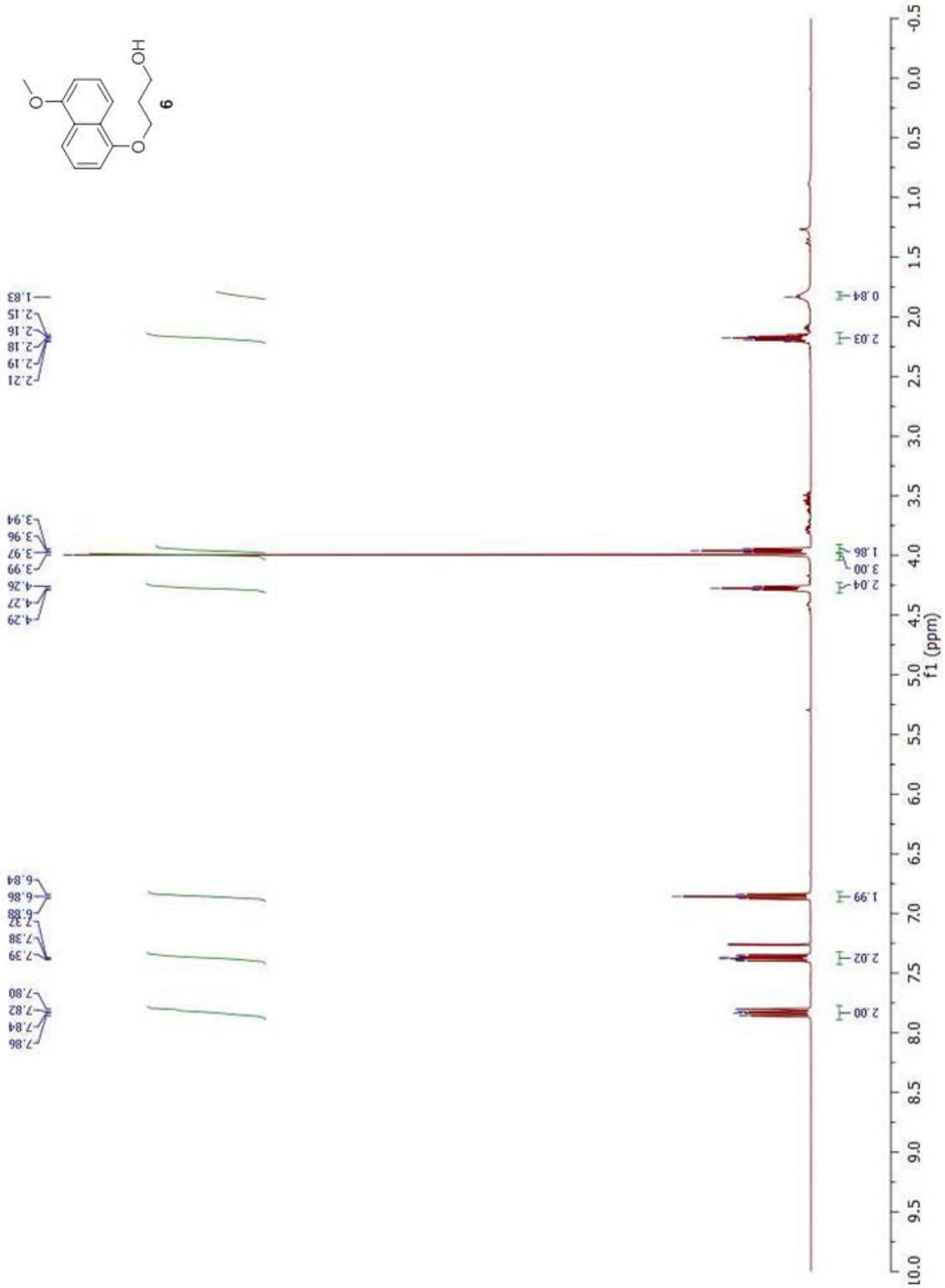


Figure S7. ^{1}H NMR ($CDCl_3$) of **7**

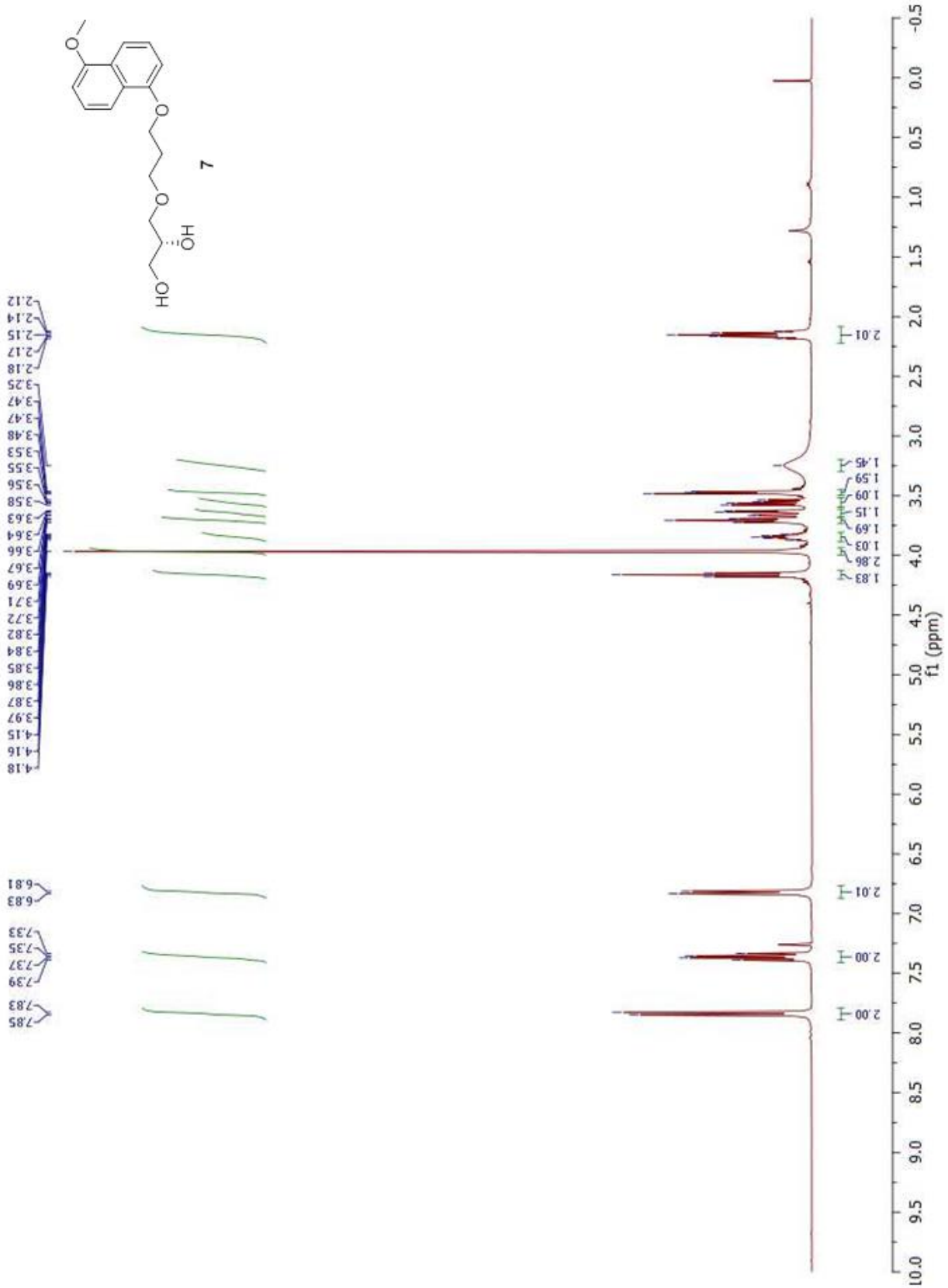


Figure S8. ^{1}H NMR ($CDCl_3$) of **8**

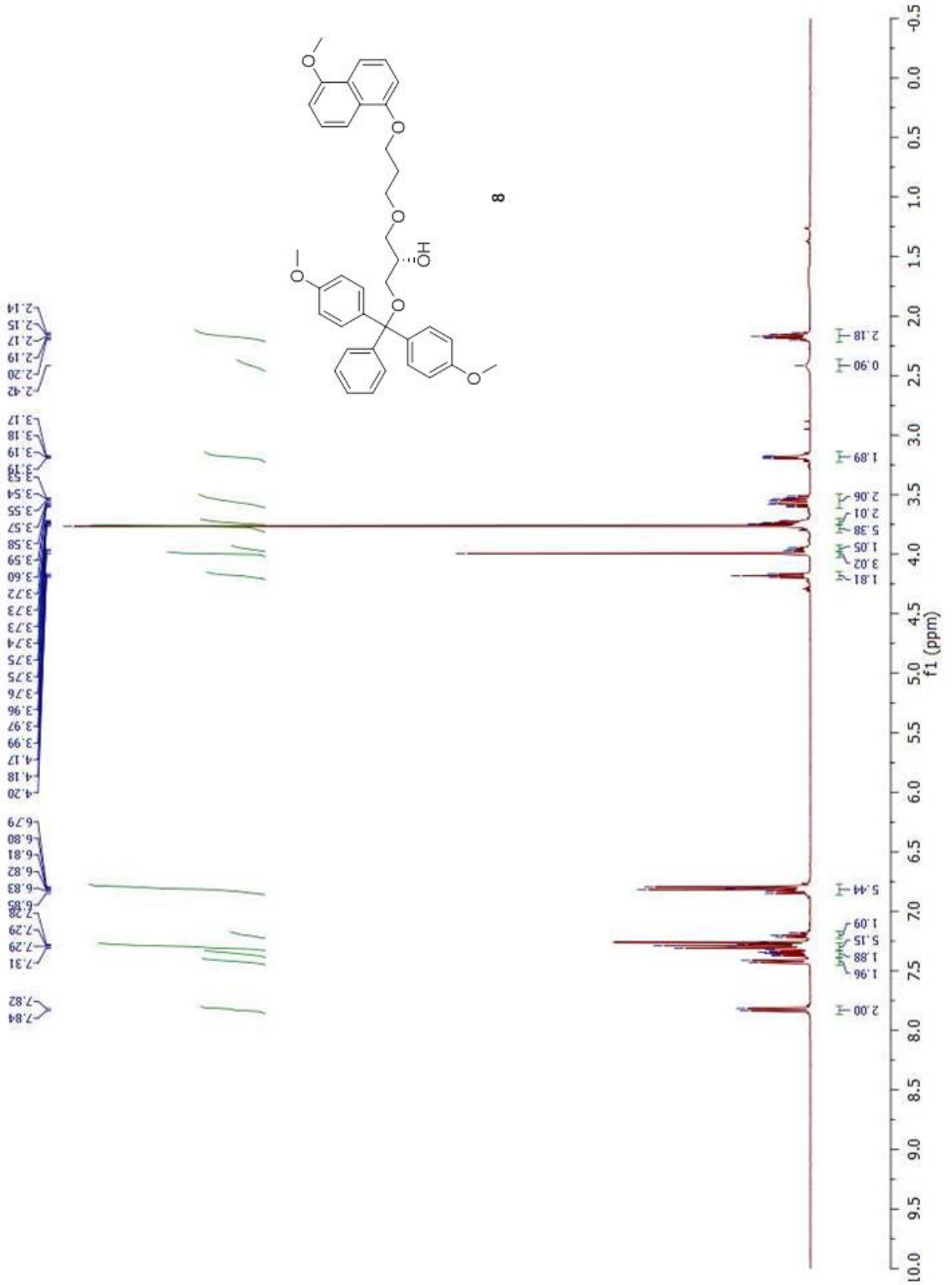


Figure S9. ^{1}H NMR ($CDCl_3$) of **10**

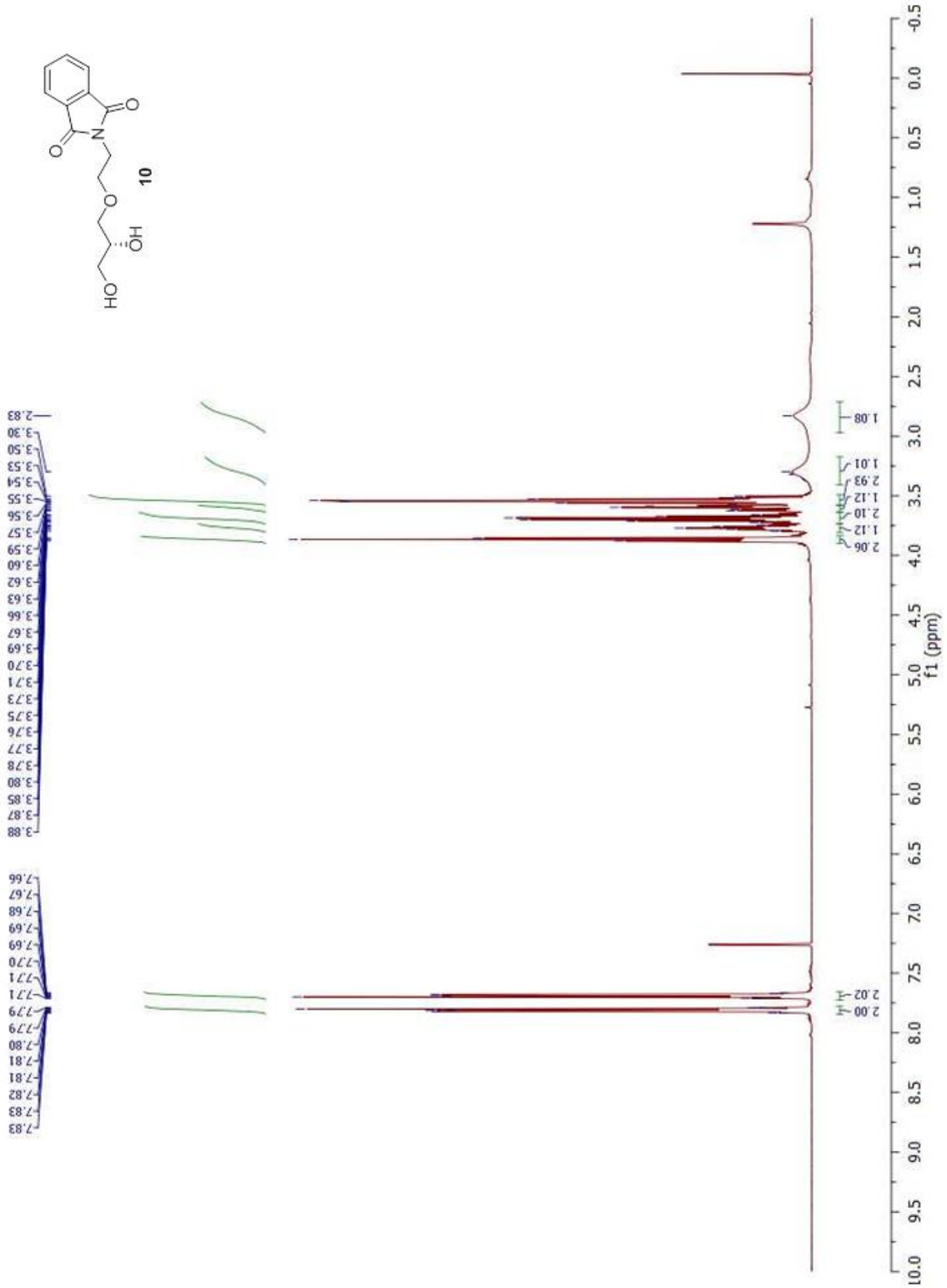


Figure S10. ^{1}H NMR ($CDCl_3$) of **11**

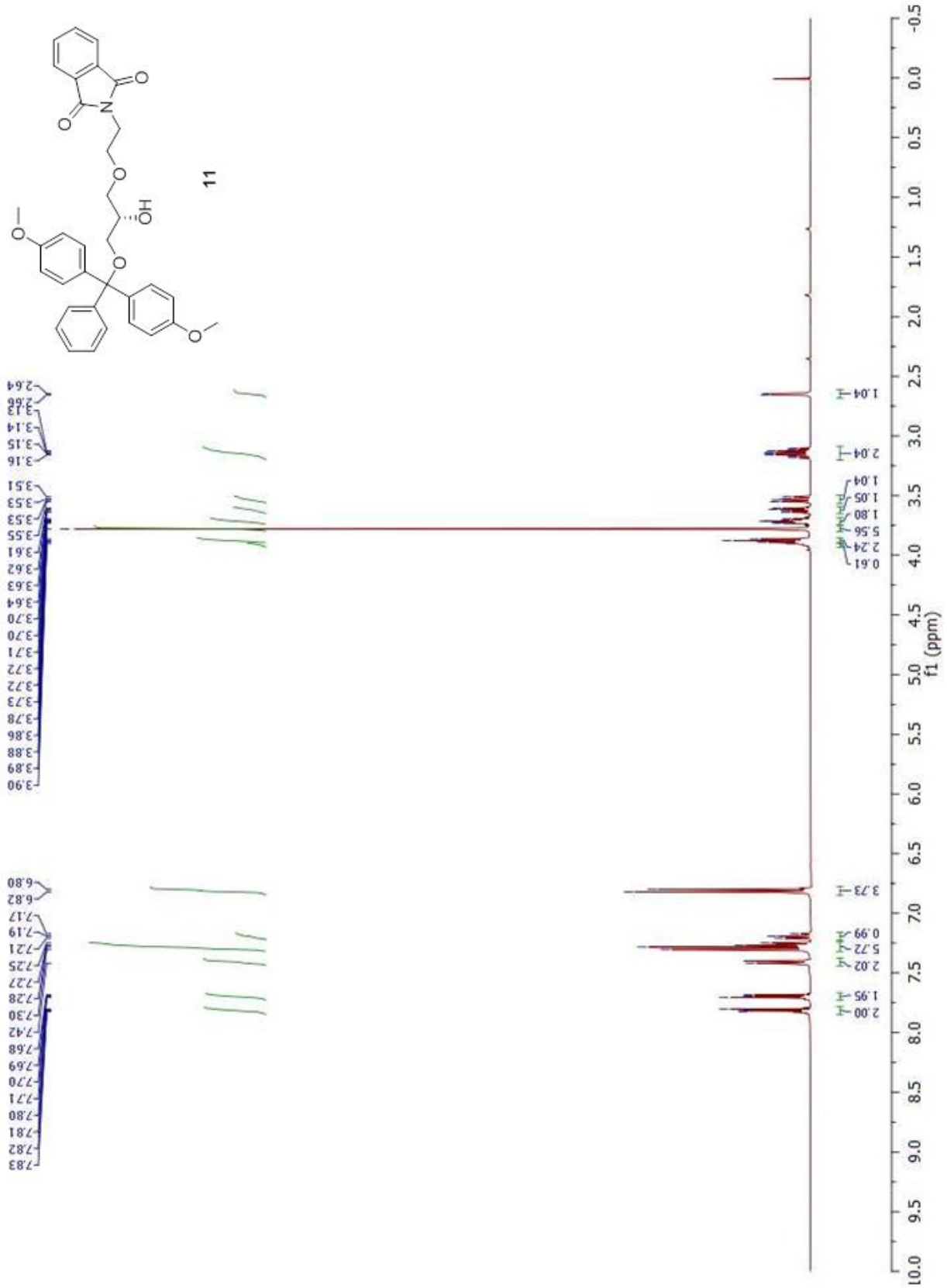


Figure S11. ^{1}H NMR ($CDCl_3$) of **12**

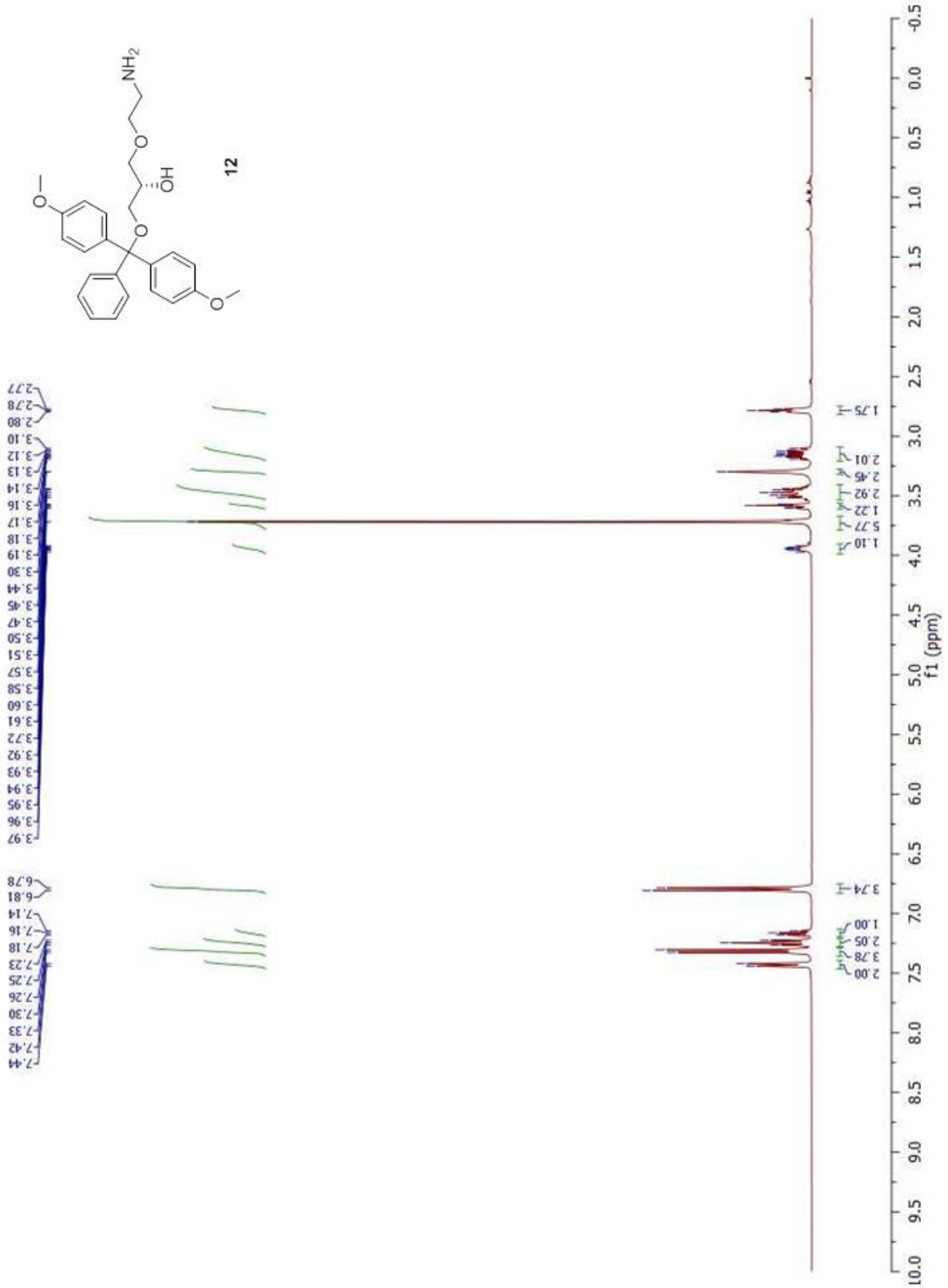


Figure S12. ^{1}H NMR ($CDCl_3$) of **14**

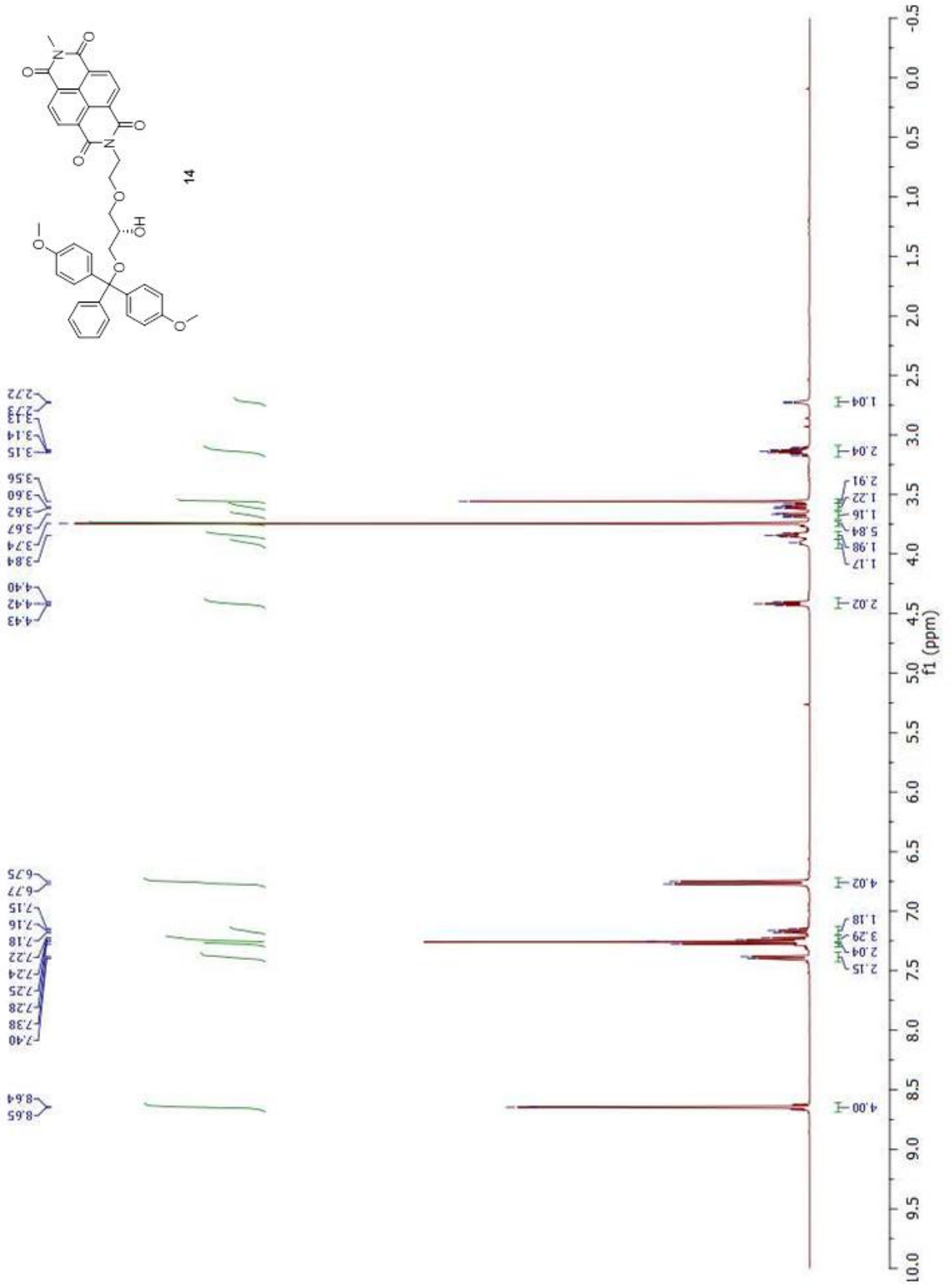


Figure S13. ^{13}C NMR ($CDCl_3$) of **1**

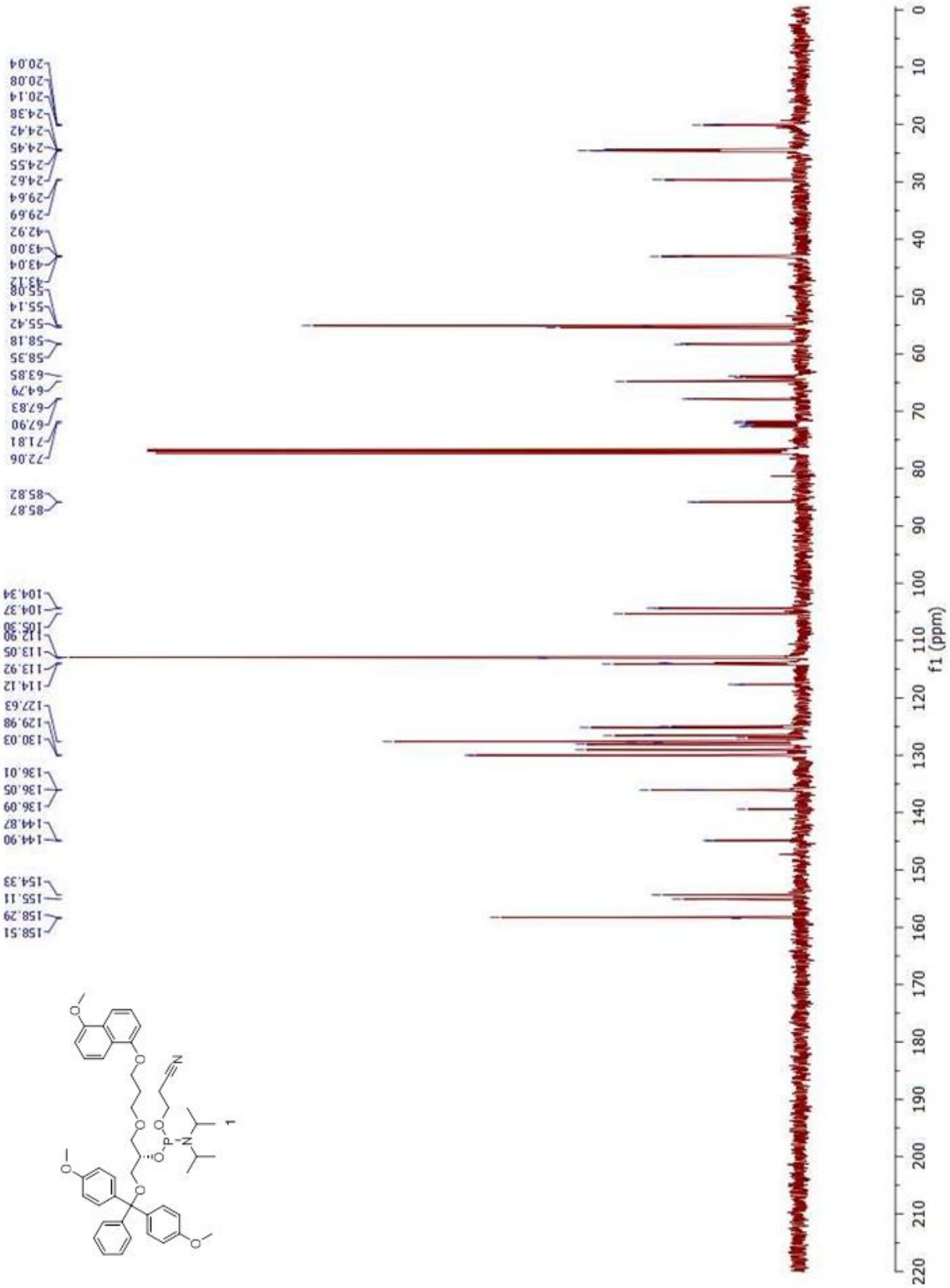


Figure S14. ^{13}C NMR ($CDCl_3$) of **2**

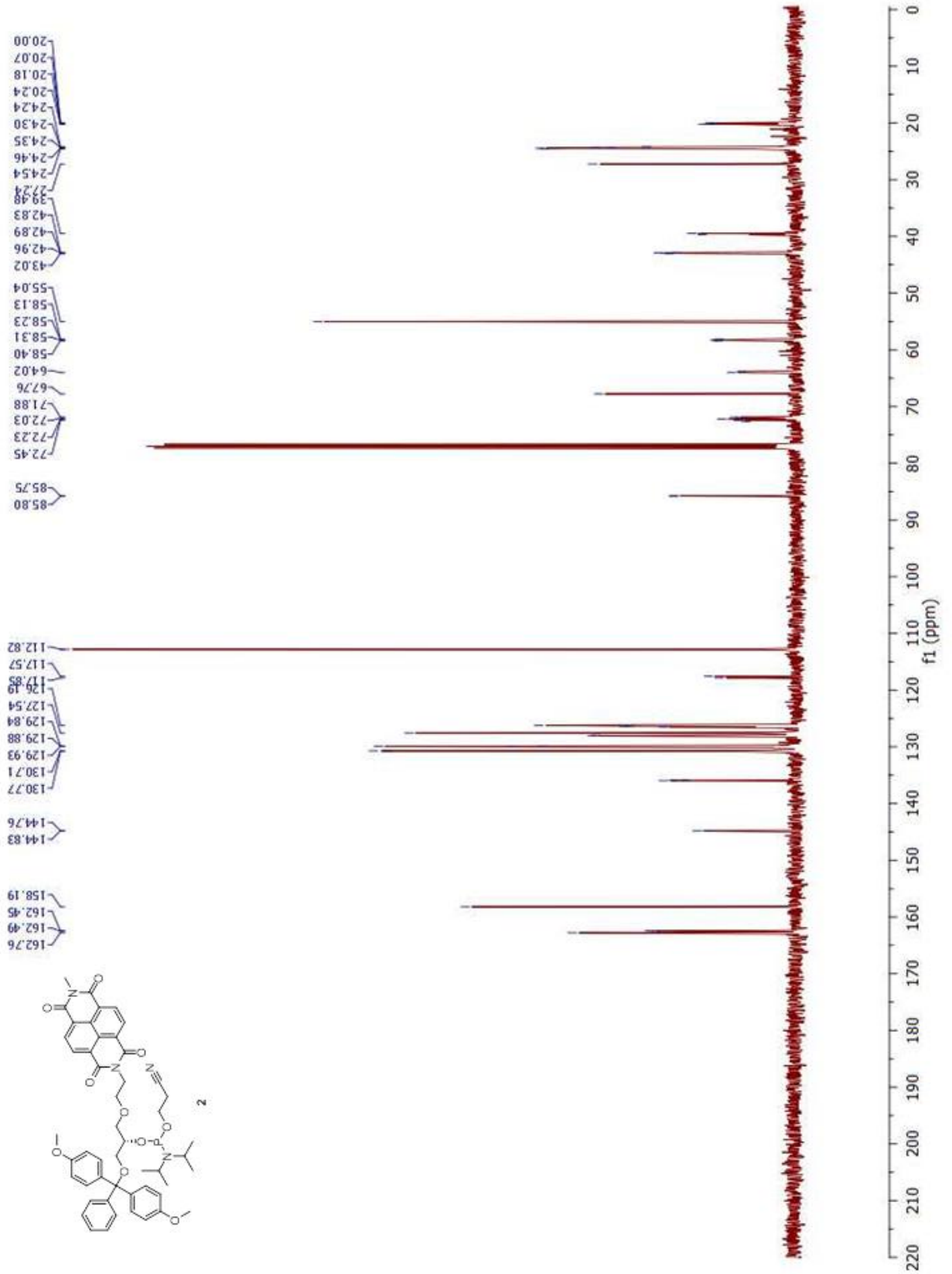


Figure S15. ^{13}C NMR ($CDCl_3$) of **3**

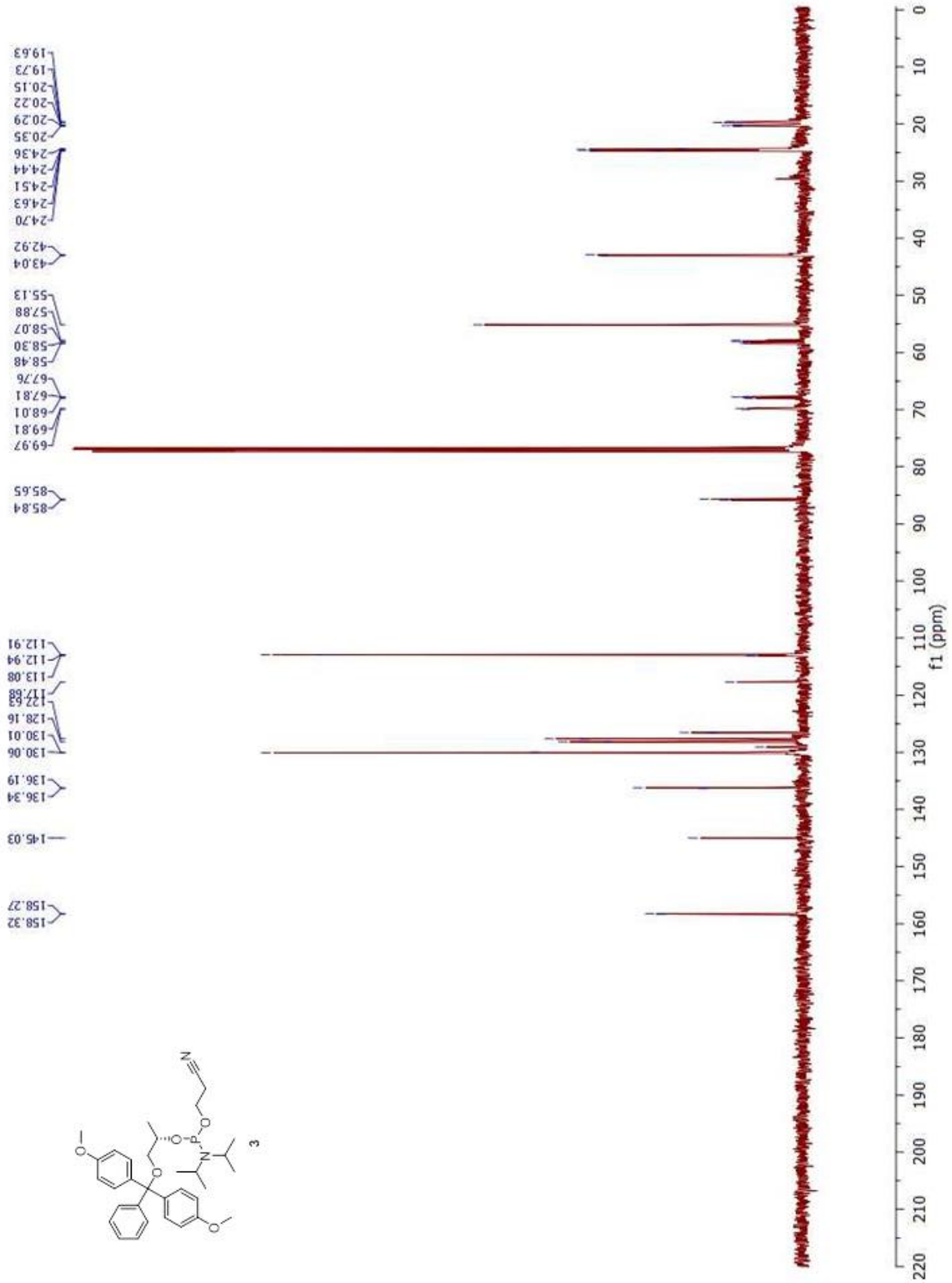


Figure S16. ^{13}C NMR ($CDCl_3$) of **5**

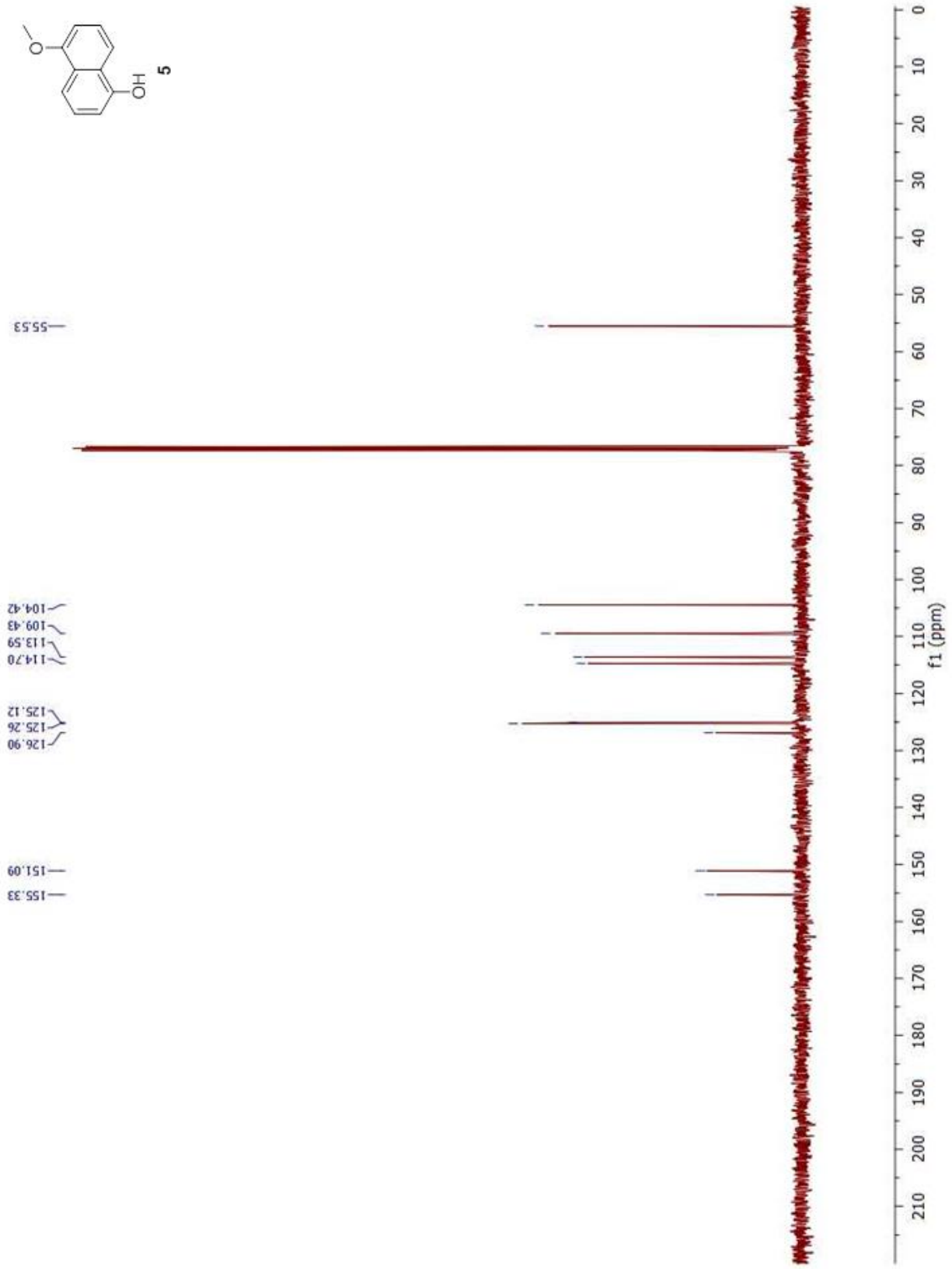


Figure S17. ^{13}C NMR ($CDCl_3$) of **6**

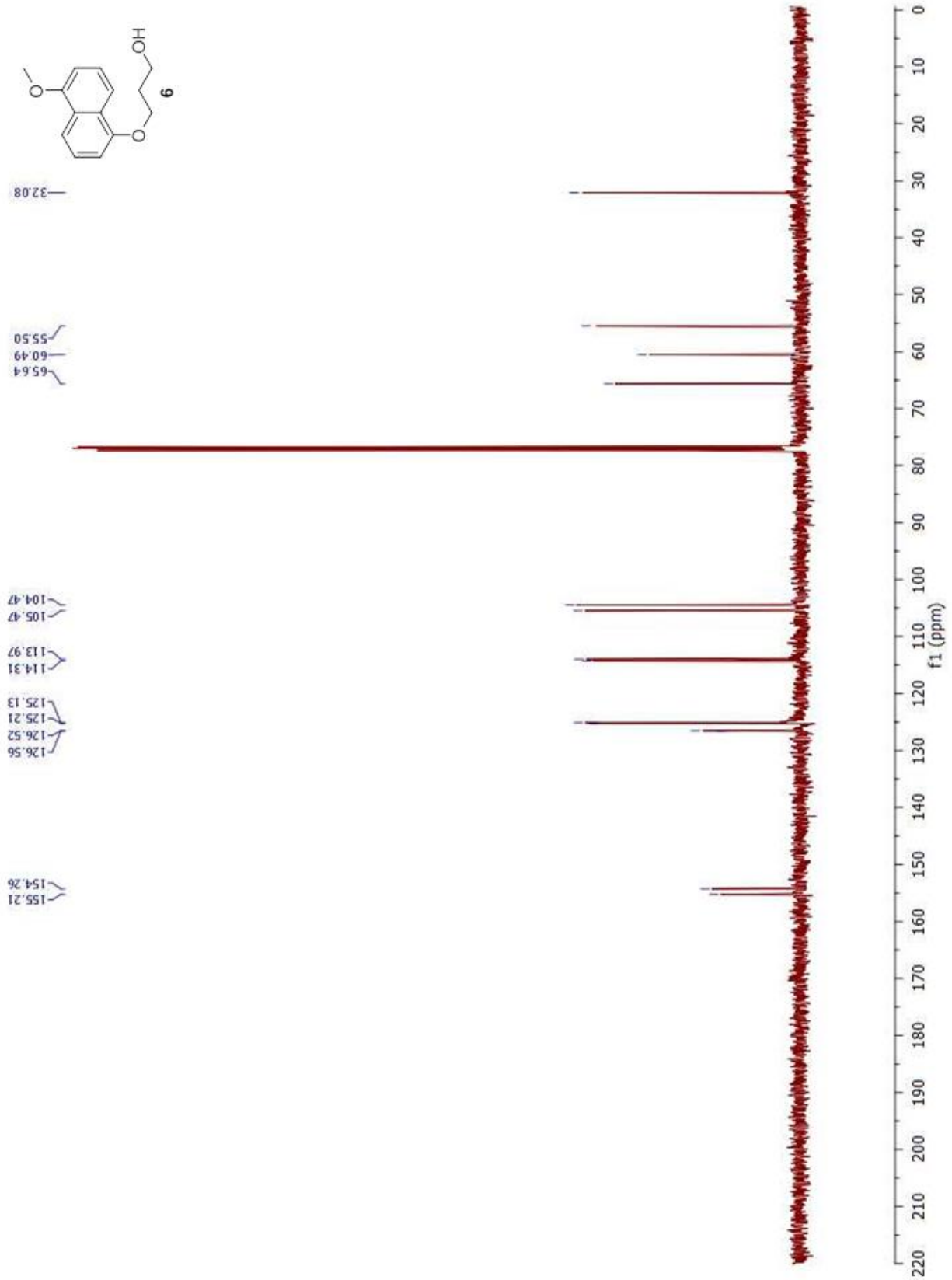


Figure S18. ^{13}C NMR ($CDCl_3$) of **7**

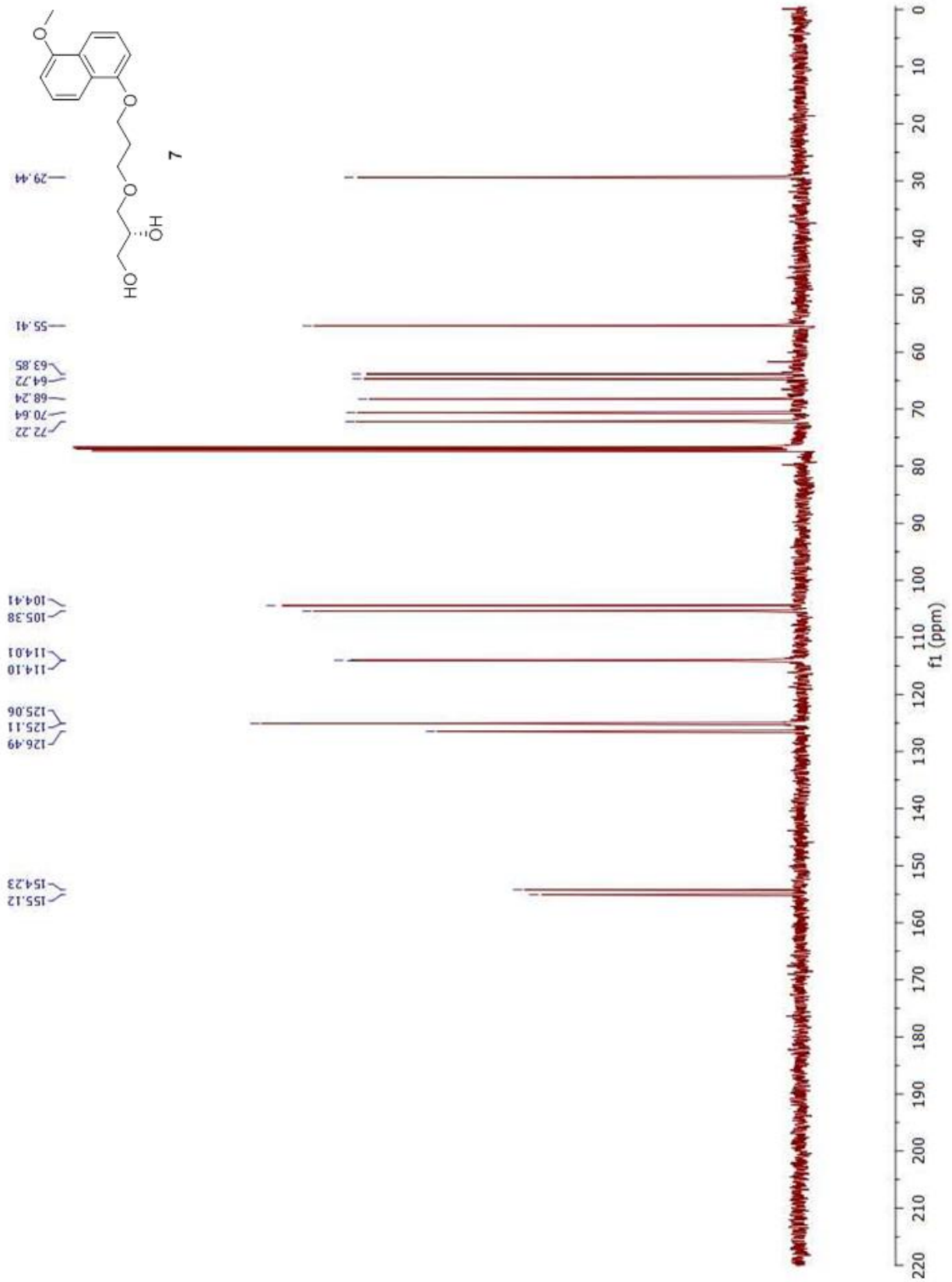


Figure S19. ^{13}C NMR ($CDCl_3$) of **8**

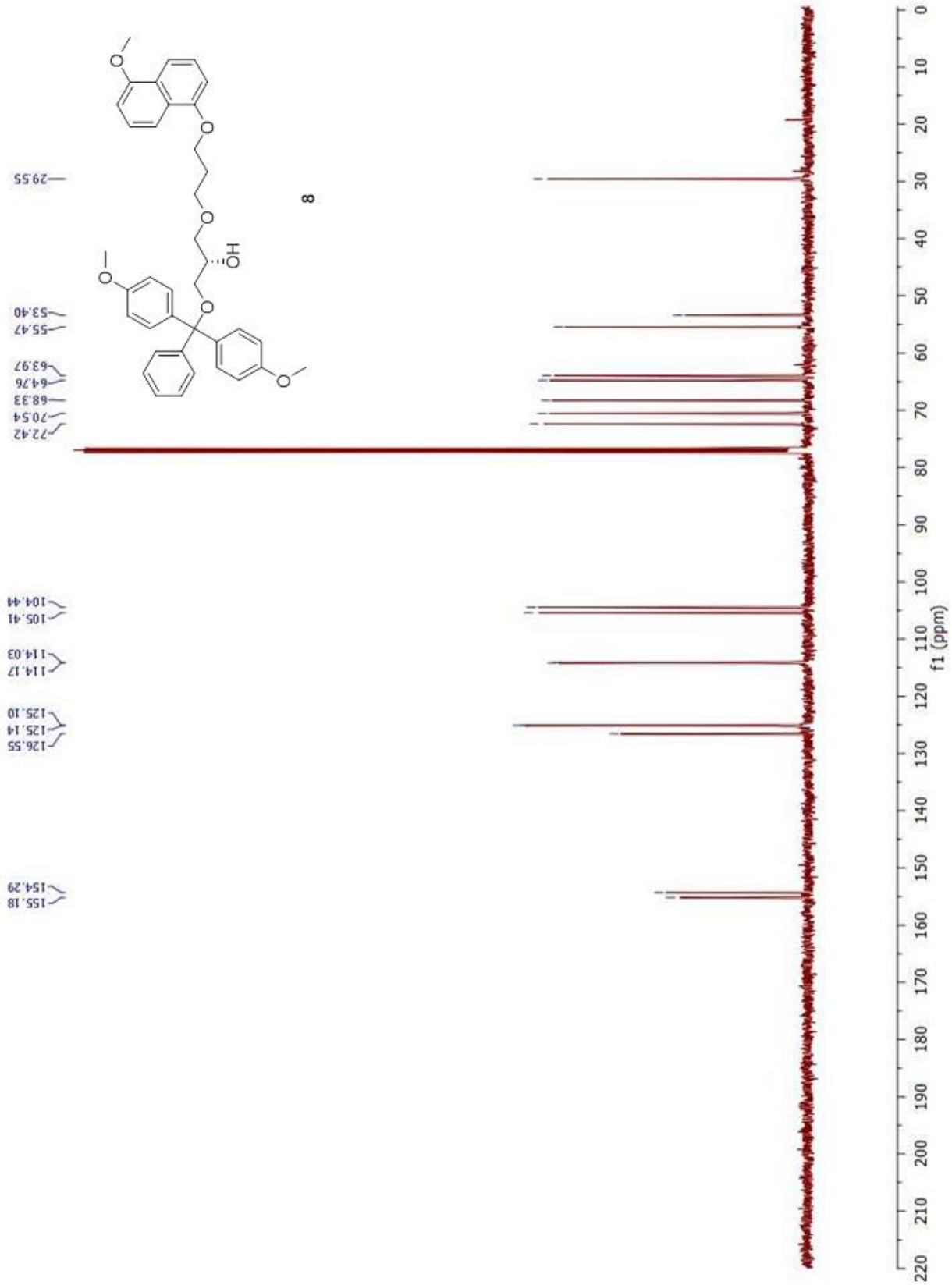


Figure S20. ^{13}C NMR ($CDCl_3$) of **10**

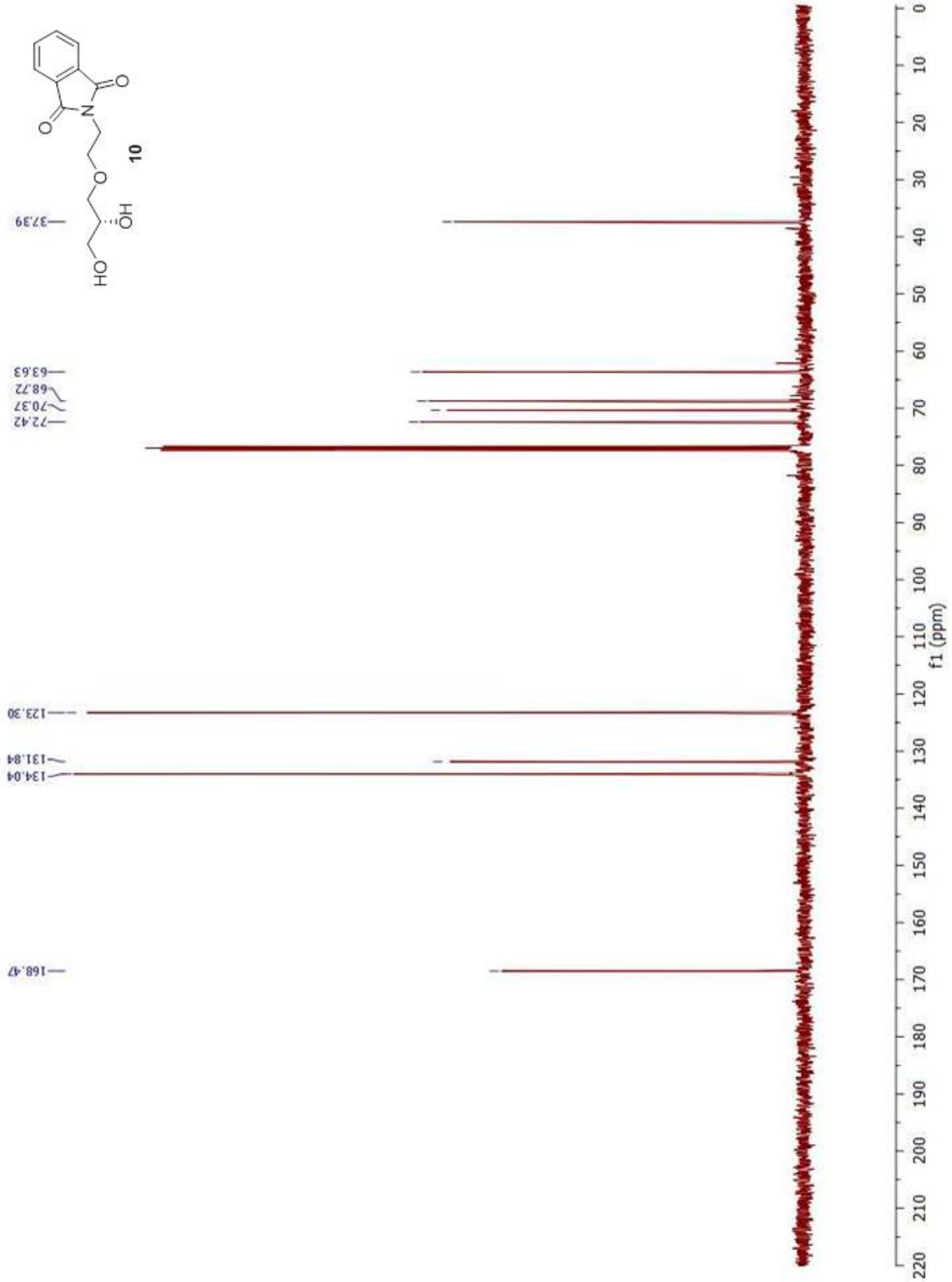


Figure S21. ^{13}C NMR ($CDCl_3$) of **11**

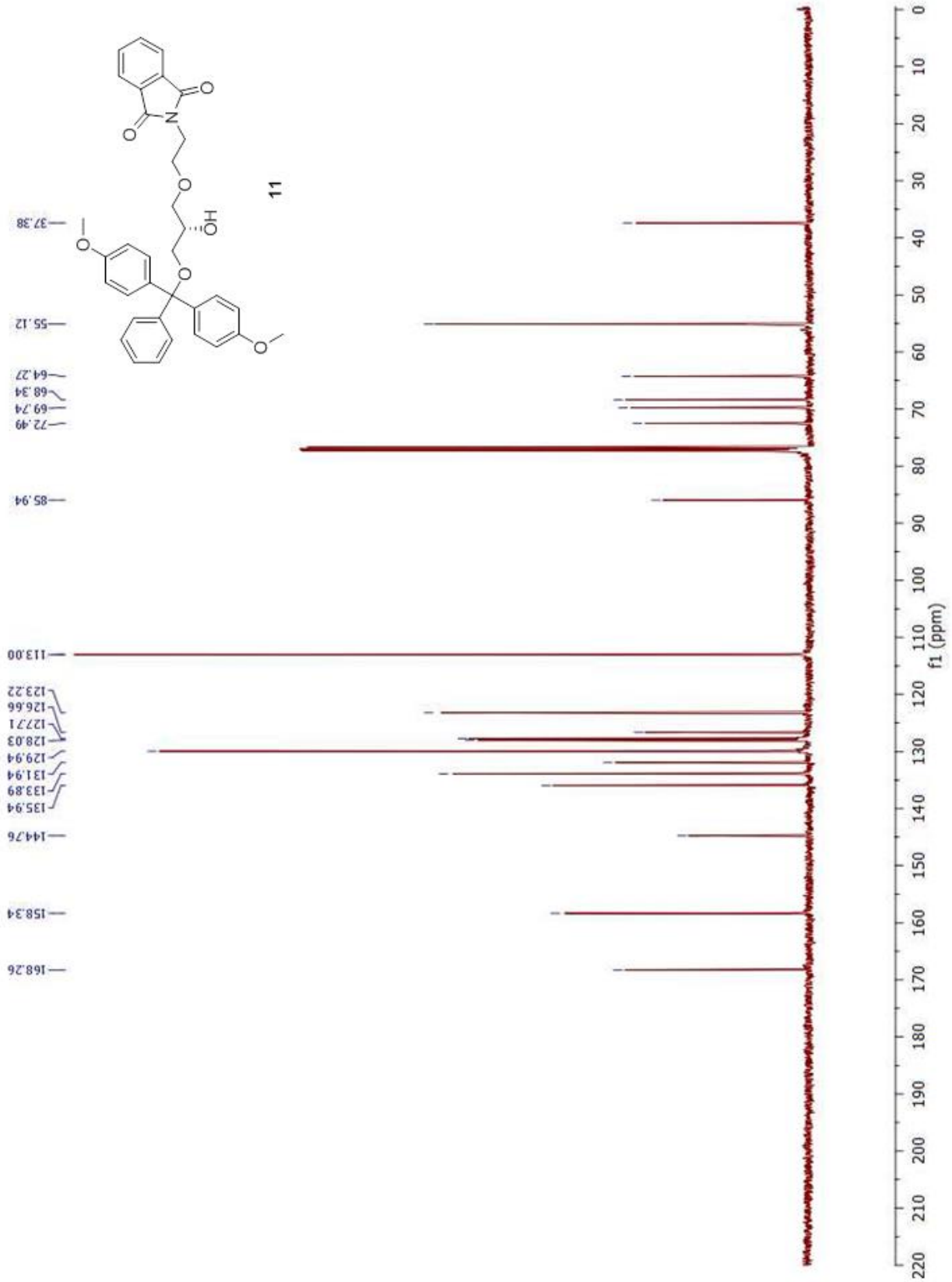


Figure S22. ^{13}C NMR ($CDCl_3$) of **12**

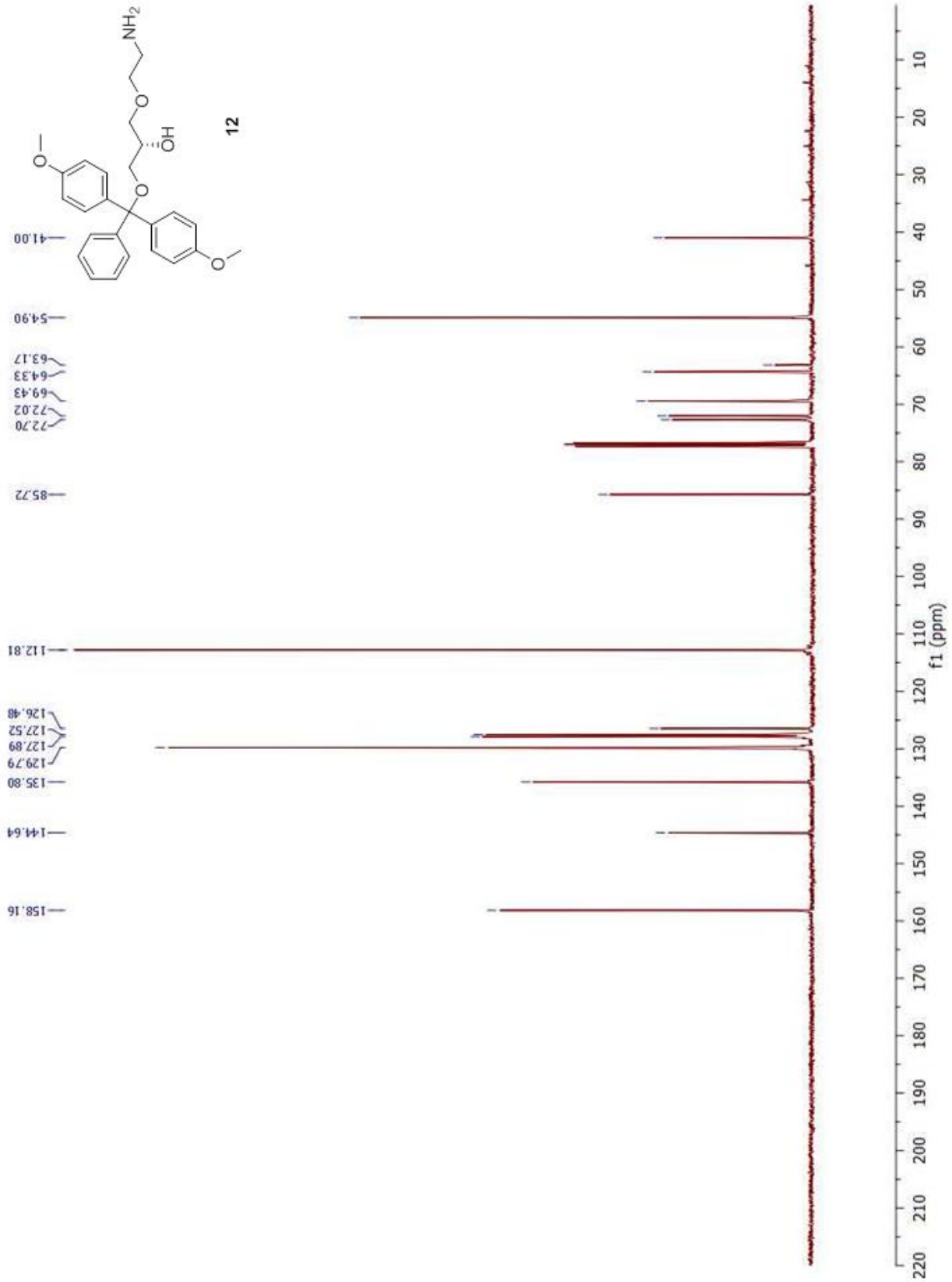


Figure S23. ^{13}C NMR ($CDCl_3$) of **14**

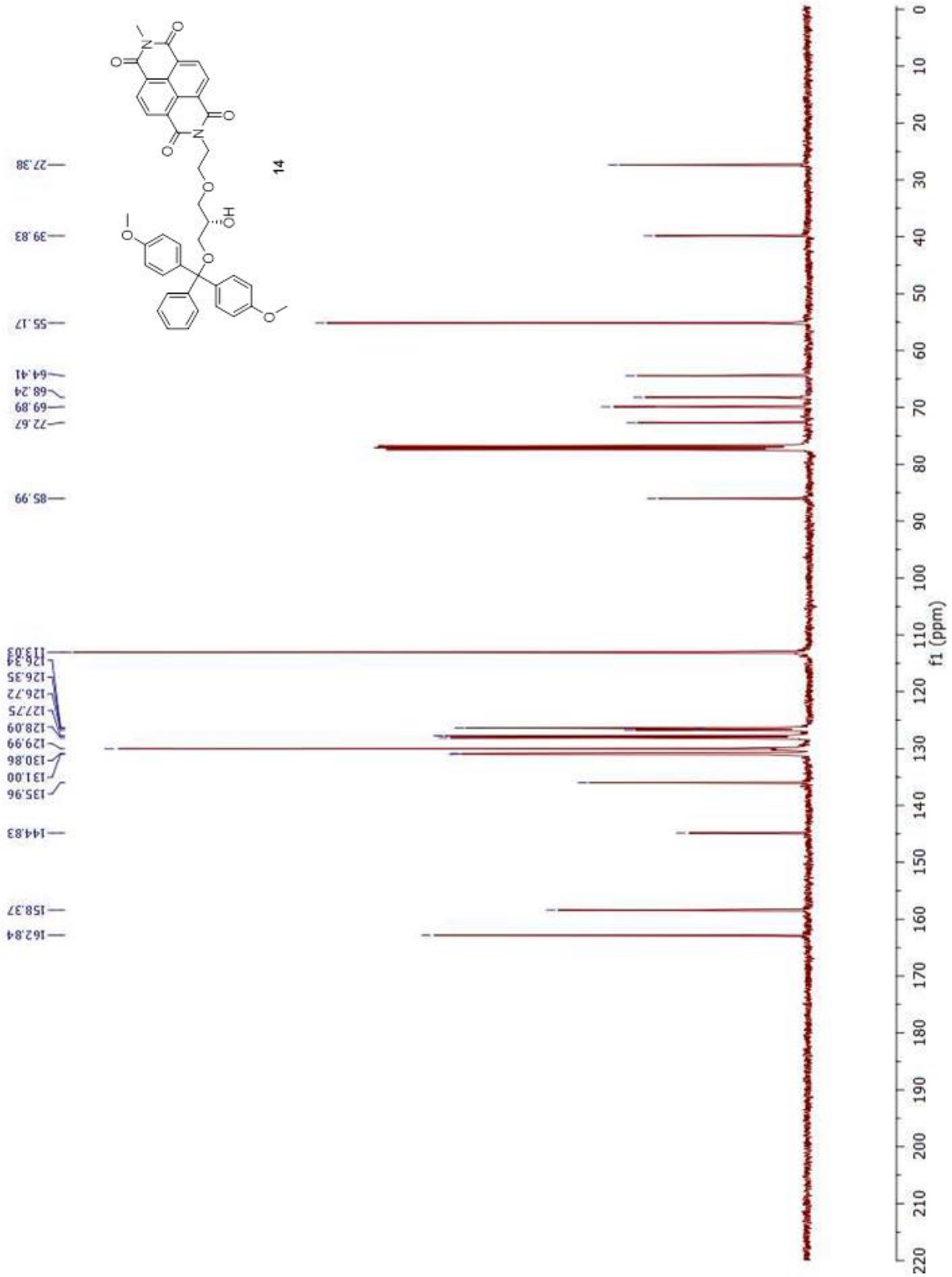


Figure S24. ^{31}P NMR ($CDCl_3$) of **1**

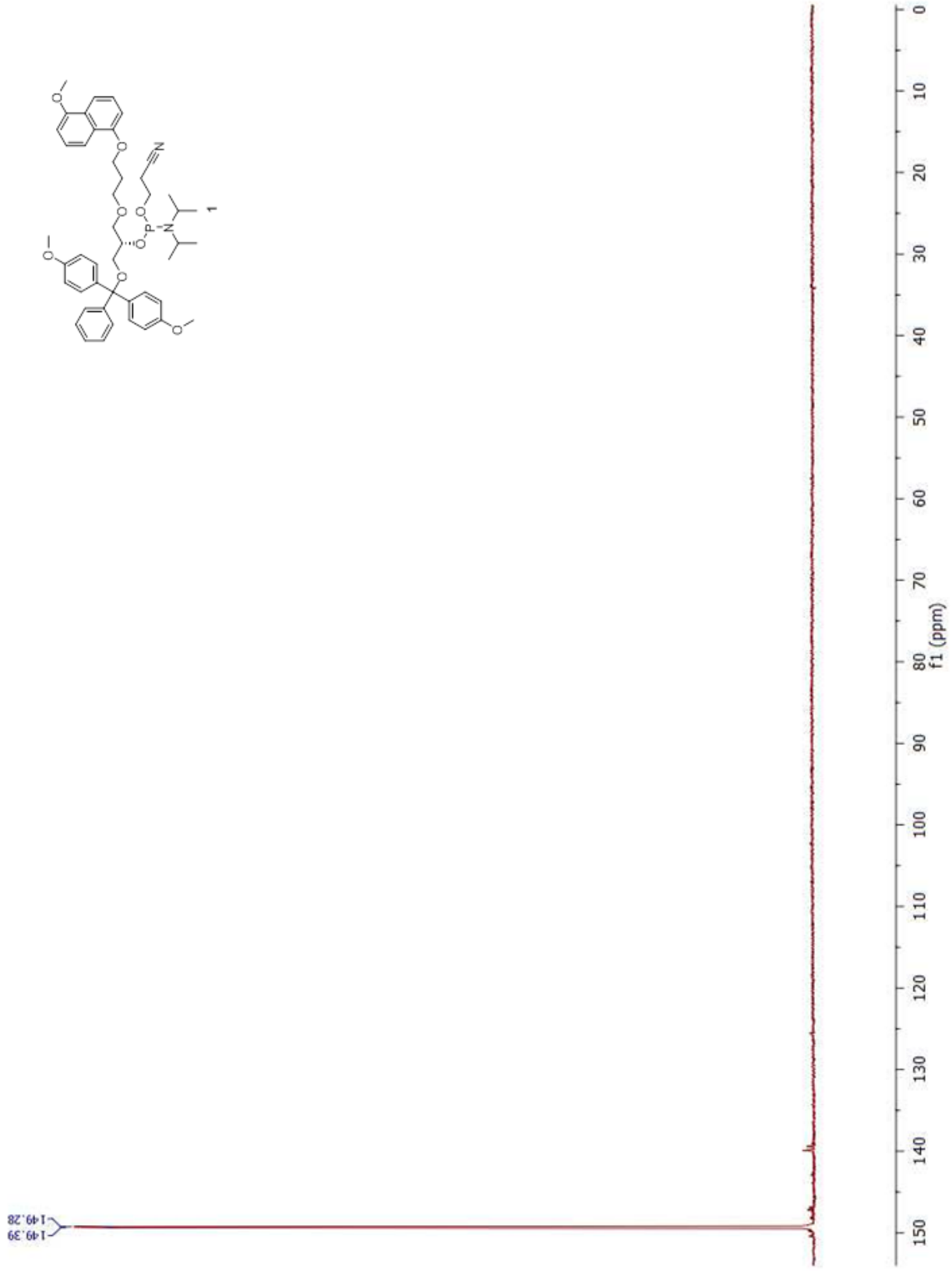


Figure S25. ^{31}P NMR ($CDCl_3$) of **2**

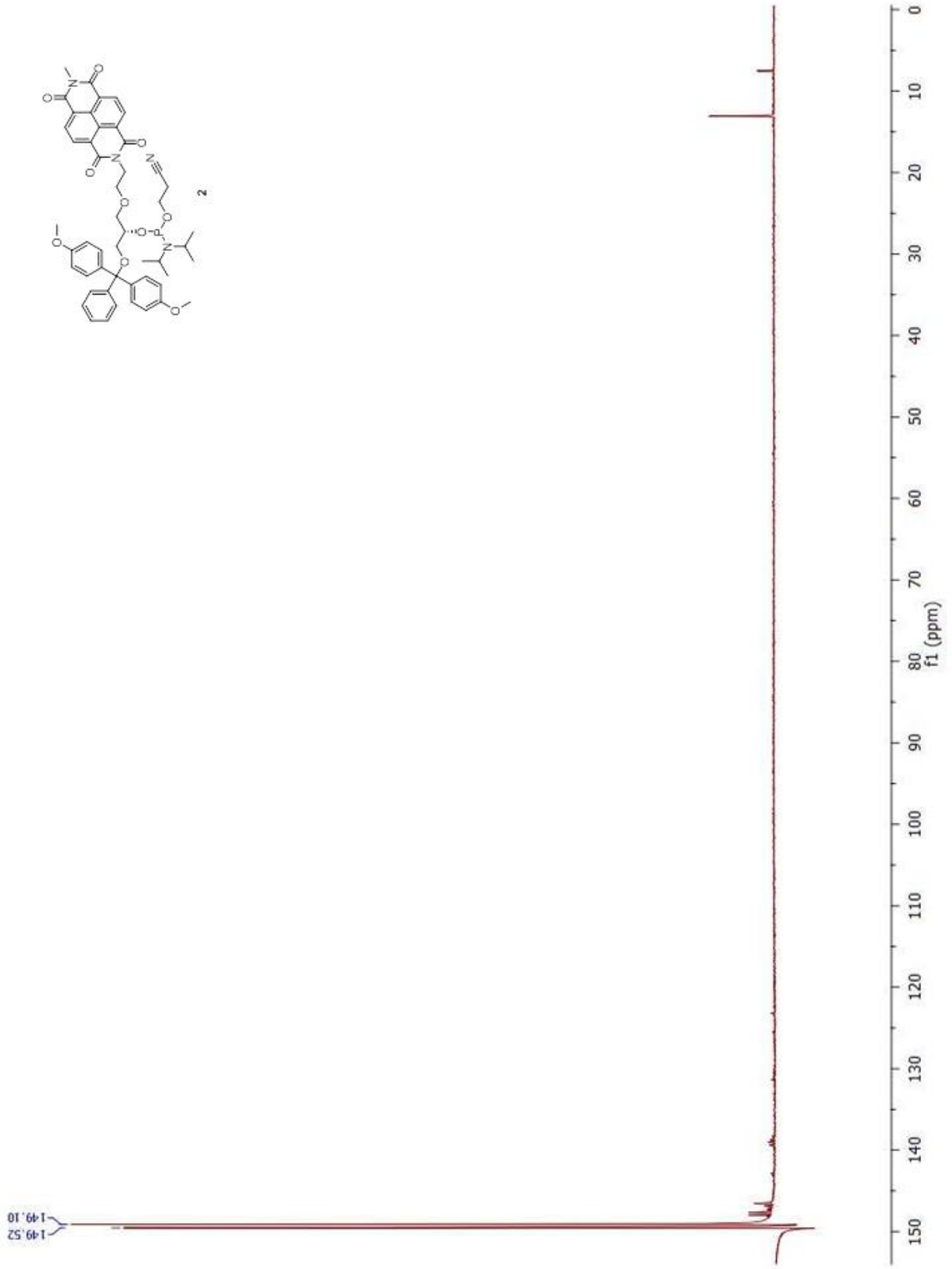


Figure S26. ^{31}P NMR ($CDCl_3$) of **3**

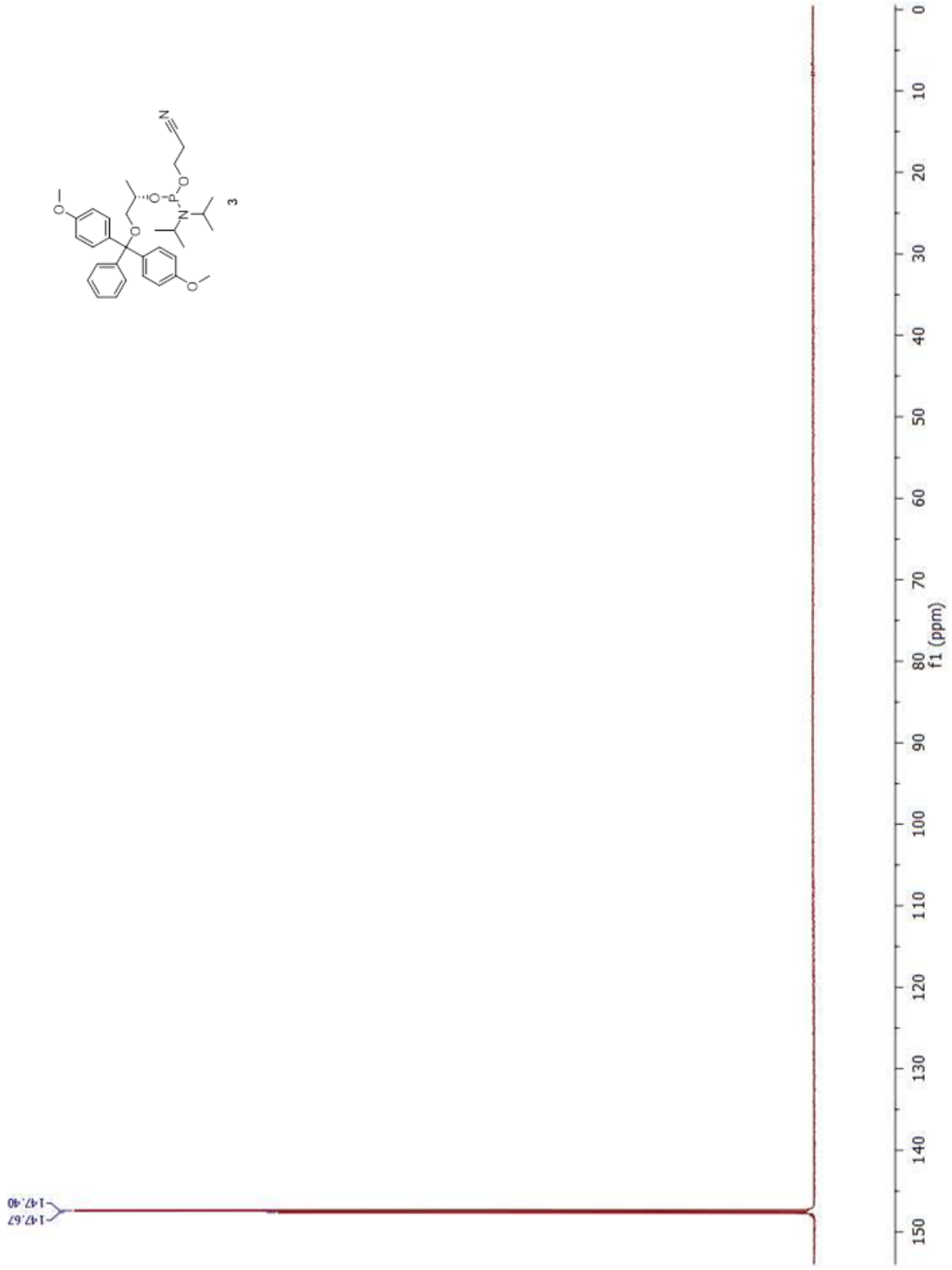
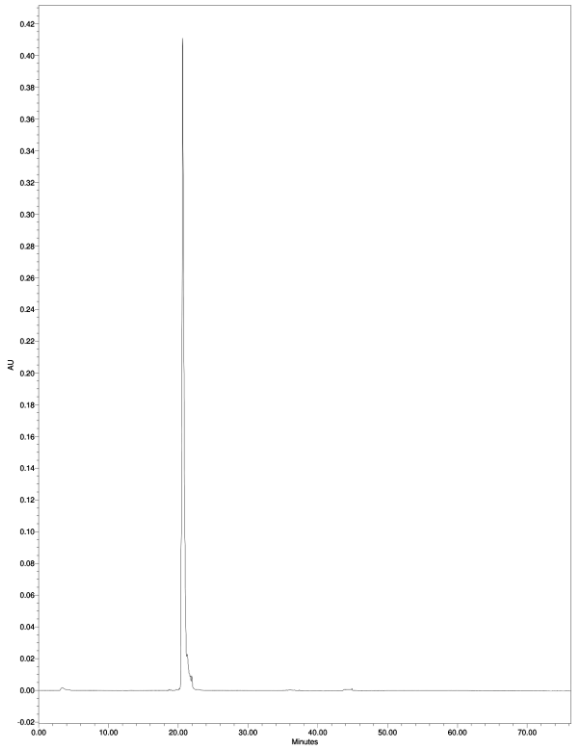


Table S1. HRMS-ESI of individual oligonucleotides.

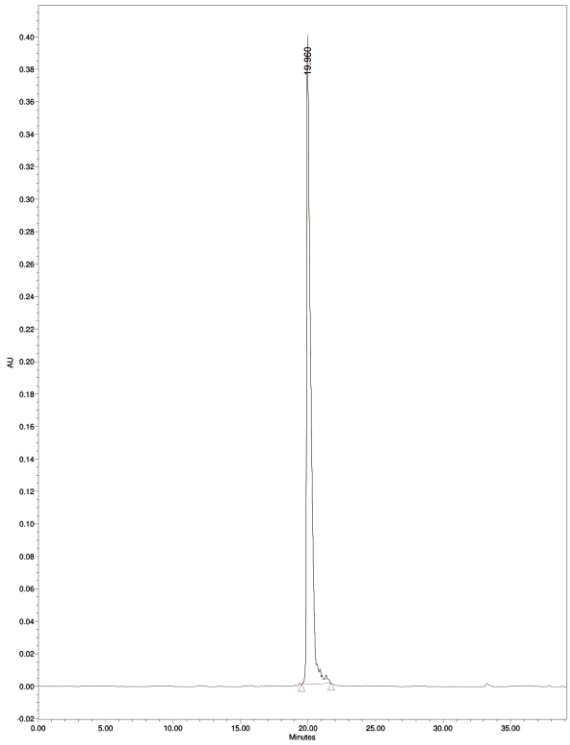
Sequence	Ion	Mass (calcd)	Mass (found)
5′-GACTGACCTGCG-3′	$[M-4H]^{-4}$	910.1545	910.1540
5′-CGCAGGTCAGTC-3′	$[M-4H]^{-4}$	910.1545	910.1537
5′-GACTGAAAACCTGCG-3′	$[M-5H]^{-5}$	915.7567	915.7570
5′-CGCAGGTTTTCAGTC-3′	$[M-3H]^{-3}$	1517.9211	1517.9144
5′-GACTGAGCGCCTGCG-3′	$[M-5H]^{-5}$	917.3524	917.3528
5′-CGCAGGCGCTCAGTC-3′	$[M-3H]^{-3}$	1516.2568	1516.2541
5′-GACTGASSSCCTGCG-3′	$[M-4H]^{-4}$	1013.6607	1013.6586
5′-CGCAGGSSSTCAGTC-3′	$[M-5H]^{-5}$	810.7271	810.7270
5′-GACTGADSDCCTGCG-3′	$[M-3H]^{-3}$	1505.2795	1505.2785
5′-CGCAGGSNSTCAGTC-3′	$[M-5H]^{-5}$	875.1389	875.1373
5′-GACTGANSNCCTGCG-3′	$[M-5H]^{-5}$	939.5506	939.5497
5′-CGCAGGSDSTCAGTC-3′	$[M-4H]^{-4}$	1071.1842	1071.1818

Figure S27. HPLC Chromatograms of oligonucleotides made with 1, 2, and/or 3.

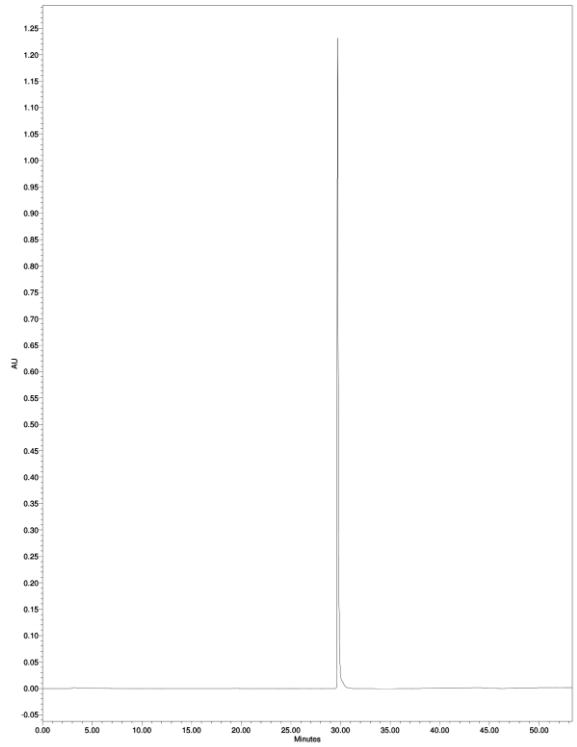
5′-GACTGA**SSS**CCTGCG-3′



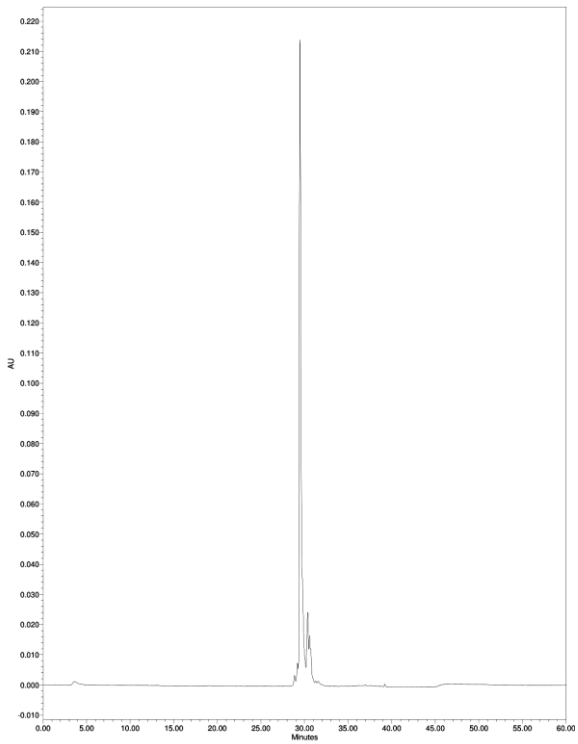
5′-CGCAGG**SSS**TCAGTC-3′



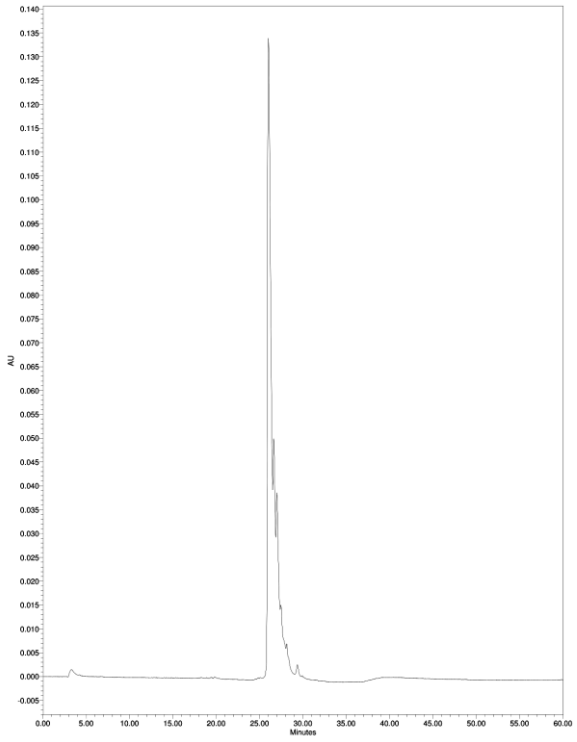
5′-GACTGA**DSD**CCTGCG-3′



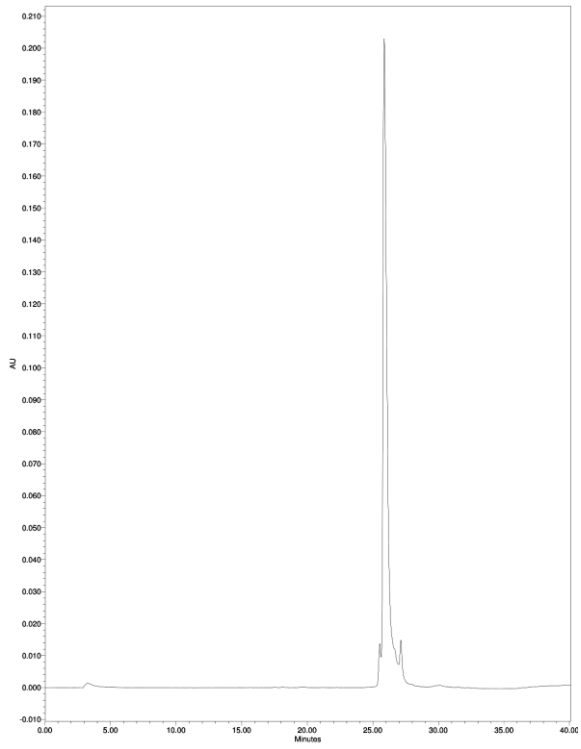
5′-CGCAGG**SNS**TCAGTC-3′



5′-GACTGA**NSN**CCTGCG-3′

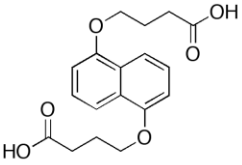


5′-CGCAGG**SDS**TCAGTC-3′

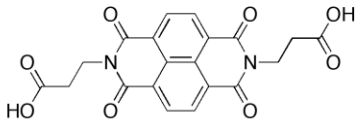


Method for Determining Extinction Coefficient of 1 and 2

The extinction coefficient of **1** and **2** were determined based on dilutions and UV measurements of water-soluble DAN and NDI analogues (**Figure S28**). The DAN and NDI analogues were diluted with a phosphate buffer (pH 7, 100 mM NaCl, 10 mM NaH_2PO_4, 0.1 mM EDTA) and UV absorbance measurements were taken at 260 nm. The resulting extinction coefficients (2504 and 1955 $M^{-1} \bullet cm^{-1}$) were used as an estimate for the corresponding phosphoramidites **1** and **2**, respectively. Because the content of the non-natural DNA base analogues is small compared to the amount of naturally occurring DNA bases, this approximation is unlikely to cause any major discrepancies in DNA concentration.



4,4'-(naphthalene-1,5-diylbis(oxy))dibutanoic acid



3,3'-(1,3,6,8-tetraoxobenzo[*lmn*][3,8]phenanthroline-2,7(1*H*,3*H*,6*H*,8*H*)-diyl)dipropanoic acid

Figure S28. Structures of DAN and NDI analogues used to determine extinction coefficients for **1** and **2**.

Figure S29. UV melting curves of DNA duplexes.