

Synthesis, Characterization, and Anticancer Activity of New N,N'-Diarylthiourea Derivative against Breast Cancer Cells

Mohamed A. El-Atawy ^{1,2}, Mai S. Alsubaie ¹, Mohammed L. Alazmi ¹, Ezzat A. Hamed ^{1,*},
Demiana H. Hanna ^{3,*}, Hoda A. Ahmed ³ and Alaa Z. Omar ¹

¹ Chemistry Department, Faculty of Science, Alexandria University, P.O. Box 426 Ibrahemia, Alexandria 21321, Egypt; mohamed.elatawi@alexu.edu.eg (M.A.E.-A.); maisaudalsubaie@gmail.com (M.S.A.); mohammadalazmmi@gmail.com (M.L.A.); alazaki@alexu.edu.eg (A.Z.O.)

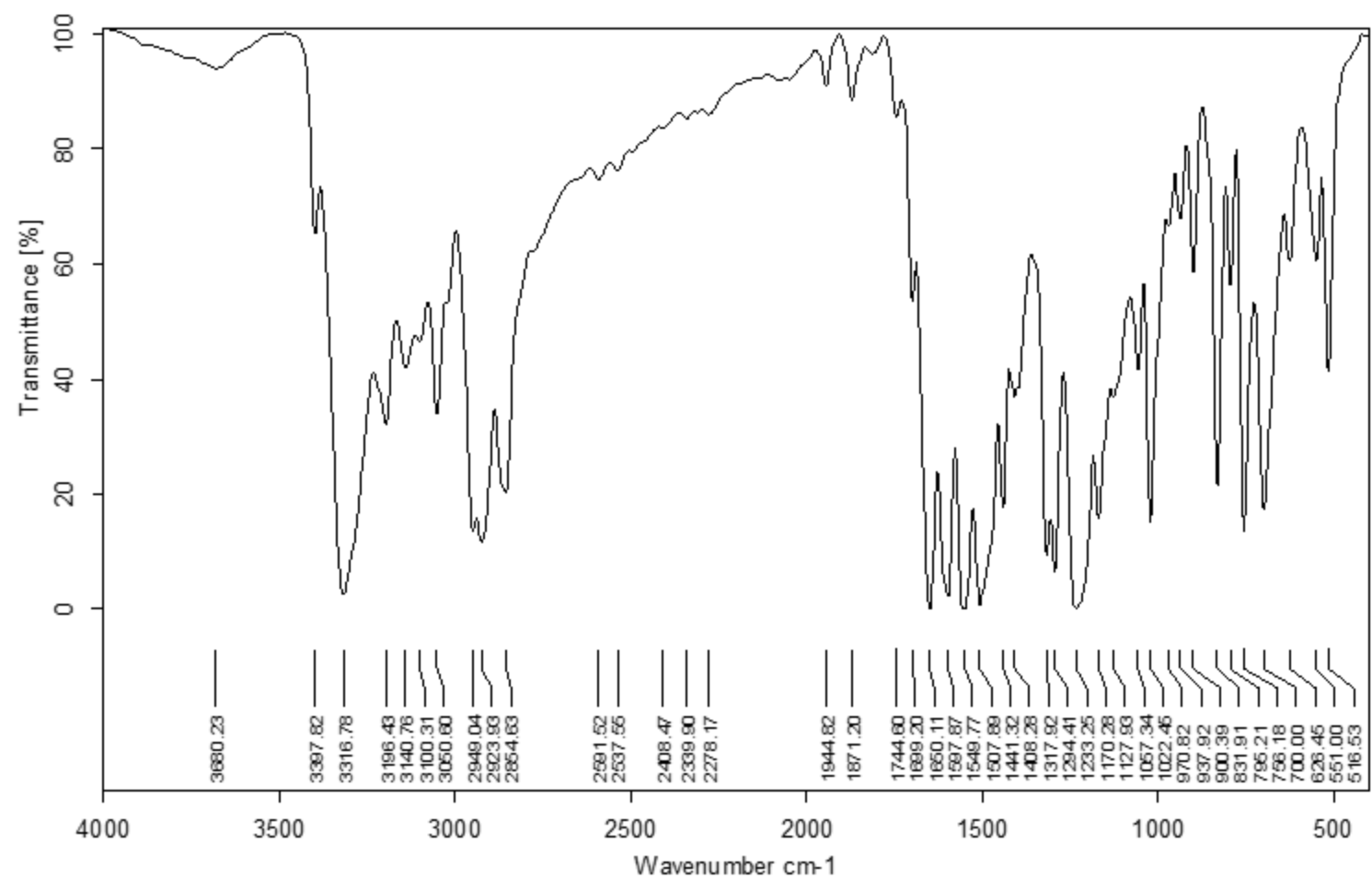
² Chemistry Department, Faculty of Science, Taibah University, Yanbu 46423, Saudi Arabia

³ Department of Chemistry, Faculty of Science, Cairo University, Giza 12613, Egypt; ahoda@sci.cu.edu.eg

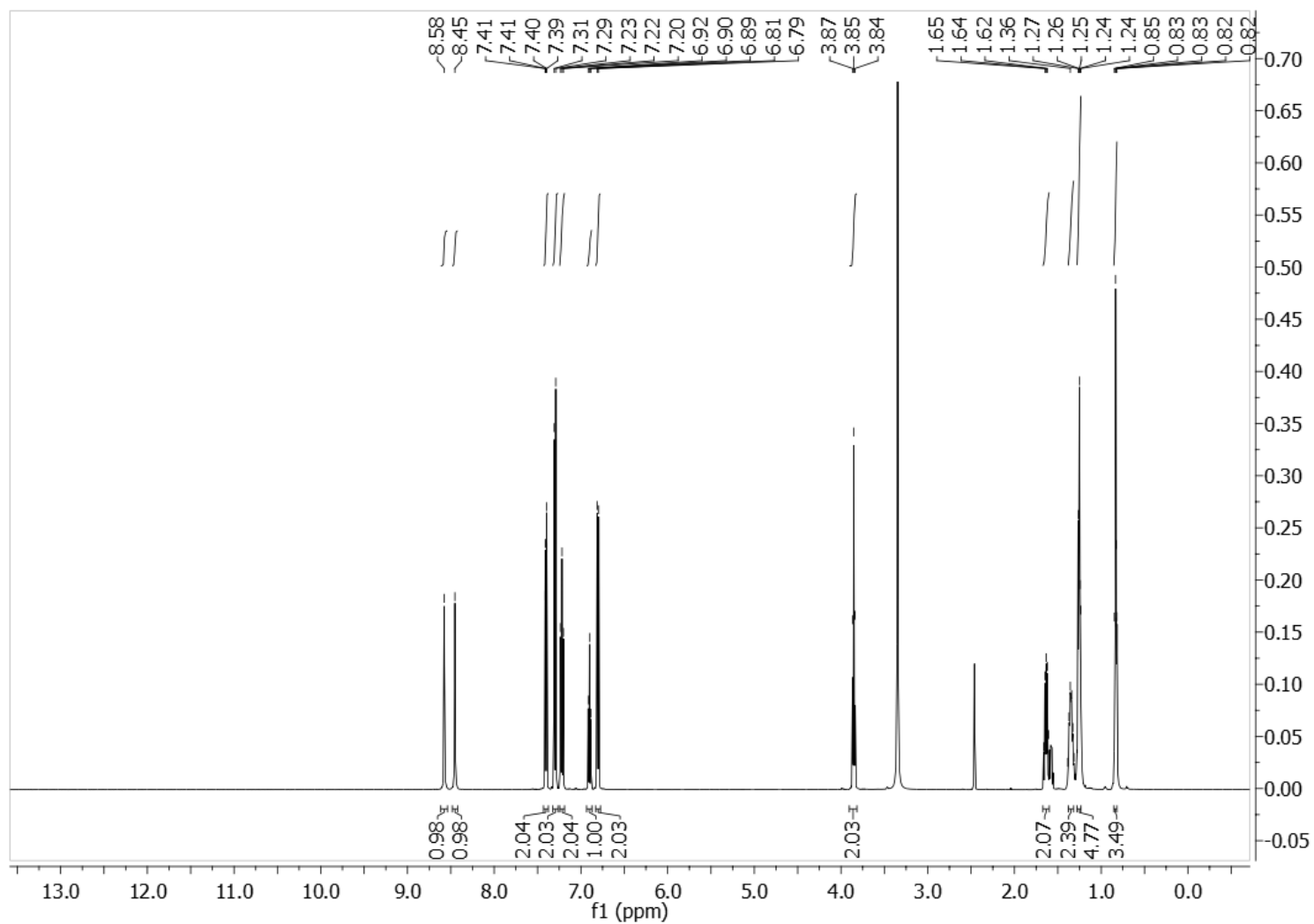
* Correspondence: ezzat.awad@alexu.edu.eg (E.A.H.); dhelmy@sci.cu.edu.eg (D.H.H.)

Table S1: Effect of the tested compounds (1- 6) on MCF-7 cell viability through the different doses (50 to 1000 μ M) for 24 h incubation.

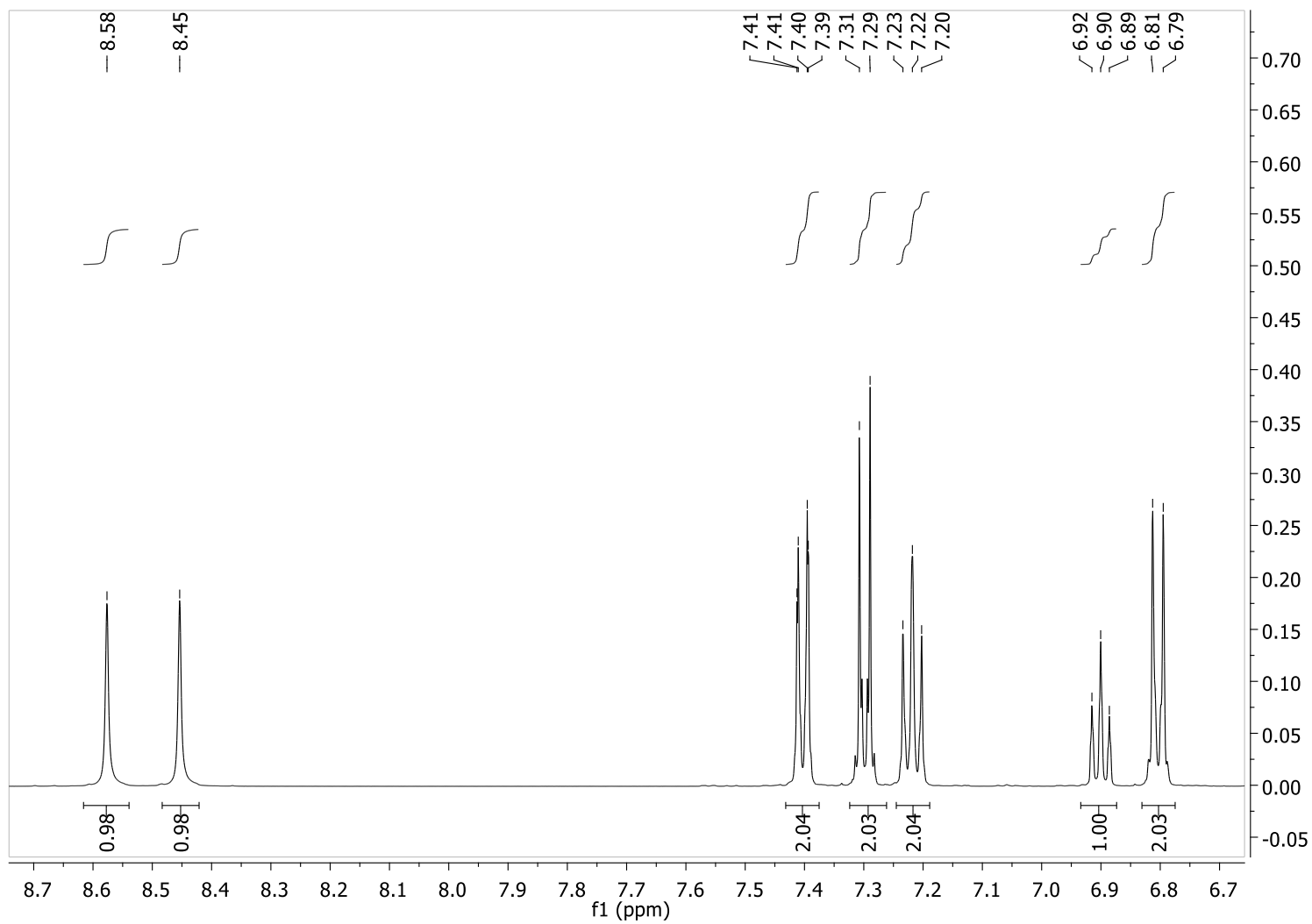
Dose (μM)	Cell Viability %					
	Compound 1	Compound 2	Compound 3	Compound 4	Compound 5	Compound 6
1000	36.41 \pm 1.34	23.32 \pm 2.33	20.93 \pm 2.75	7.28 \pm 2.56	17.98 \pm 1.45	36.73 \pm 1.66
600	57.24 \pm 2.44	38.27 \pm 1.97	56.73 \pm 2.55	18.31 \pm 1.92	45.37 \pm 2.74	46.91 \pm 2.34
300	67.17 \pm 1.13	49.86 \pm 1.77	64.92 \pm 1.66	21.21 \pm 1.66	61.98 \pm 1.84	79.23 \pm 2.64
150	80.62 \pm 2.76	72.24 \pm 2.13	80.68 \pm 2.44	48.14 \pm 1.15	79.45 \pm 1.92	84.11 \pm 1.83
100	87.32 \pm 1.34	88.57 \pm 2.22	93.59 \pm 1.82	90.23 \pm 2.78	96.45 \pm 2.33	91.71 \pm 2.47
50	98.58 \pm 2.21	98.76 \pm 2.26	97.28 \pm 2.45	99.95 \pm 2.24	98.64 \pm 2.53	96.44 \pm 2.63



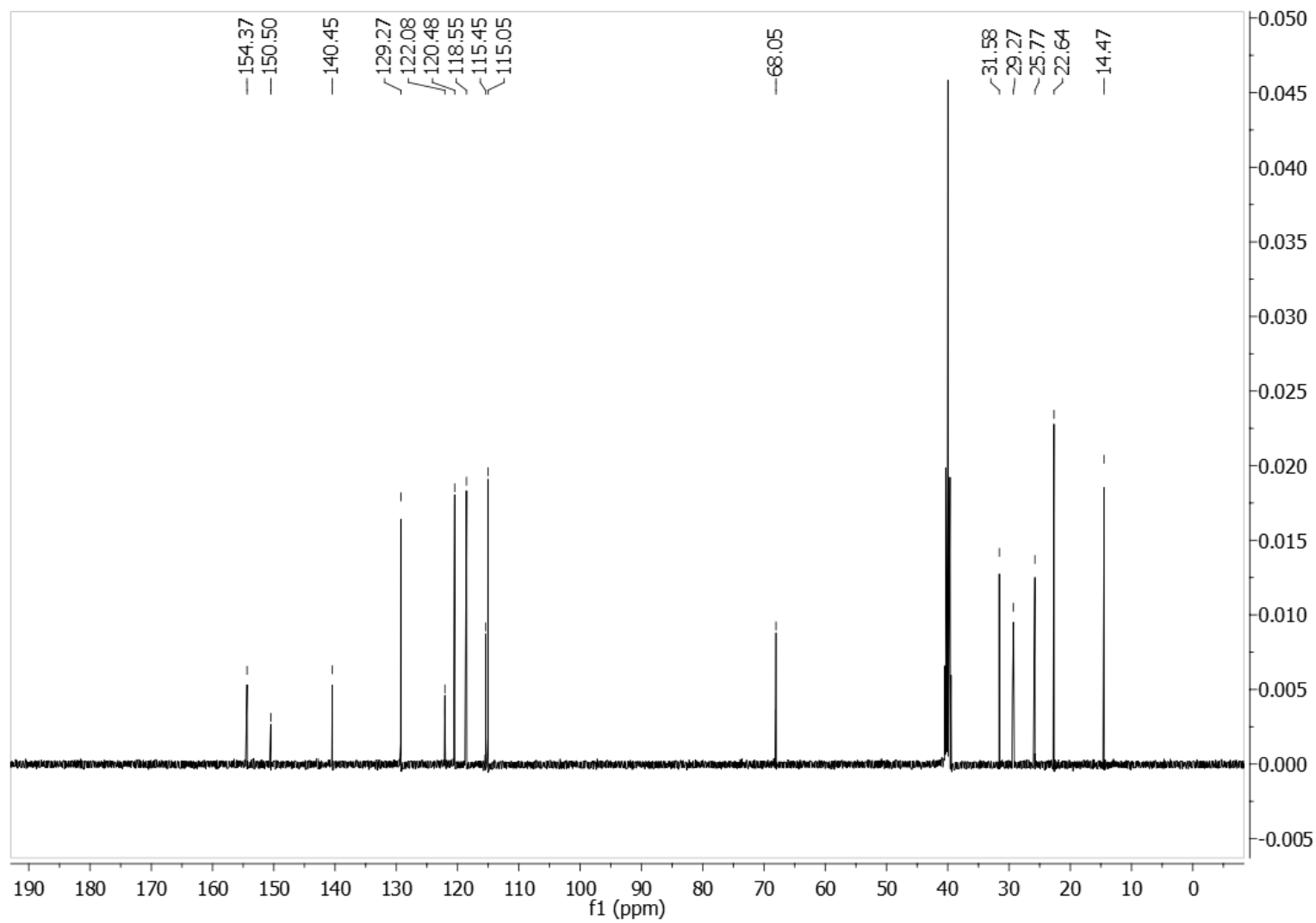
IR (KBr) spectrum of 1-(4-(hexyloxy)phenyl)-3-phenylurea **1**



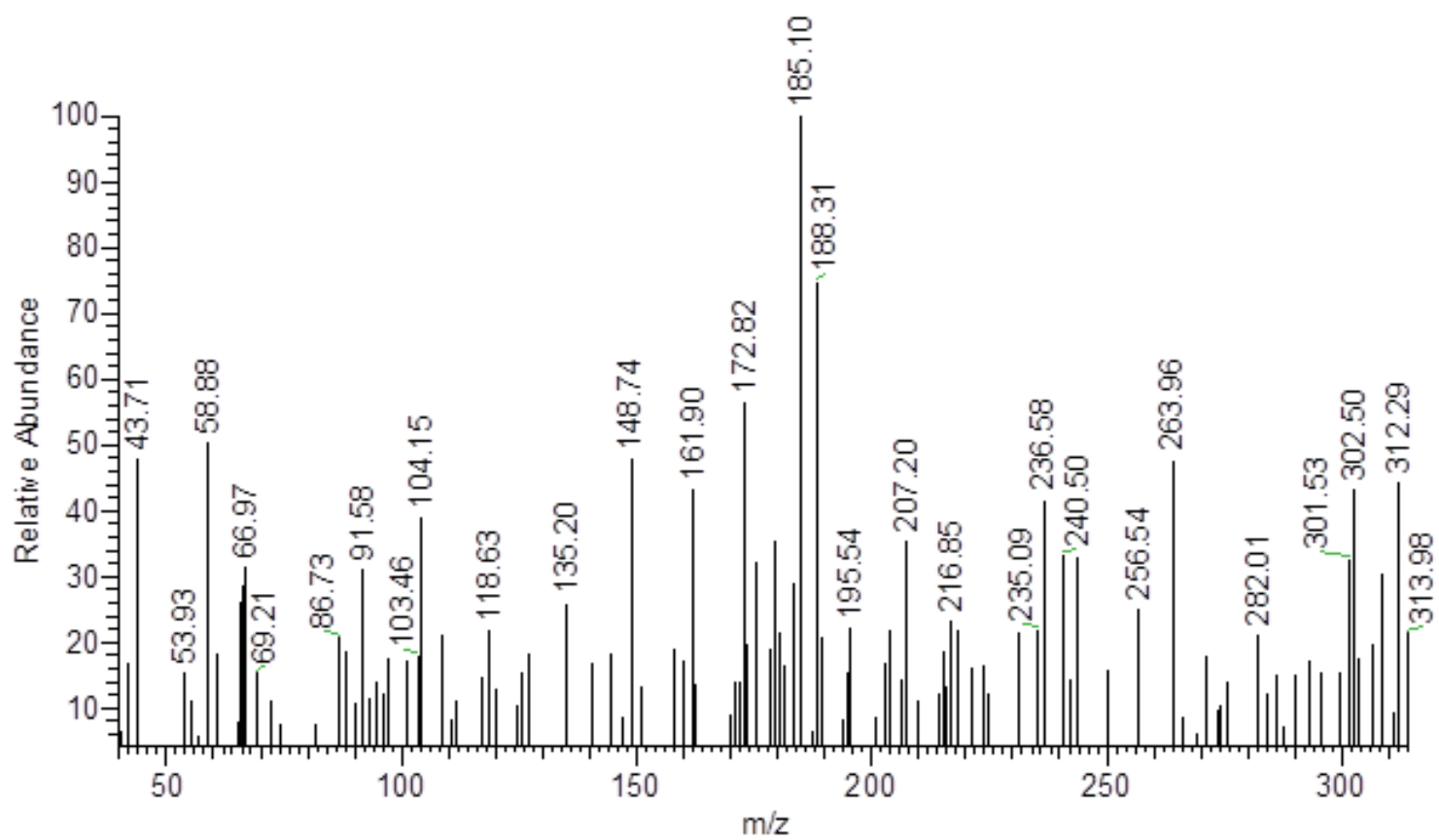
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-(hexyloxy)phenyl)-3-phenylurea **1**



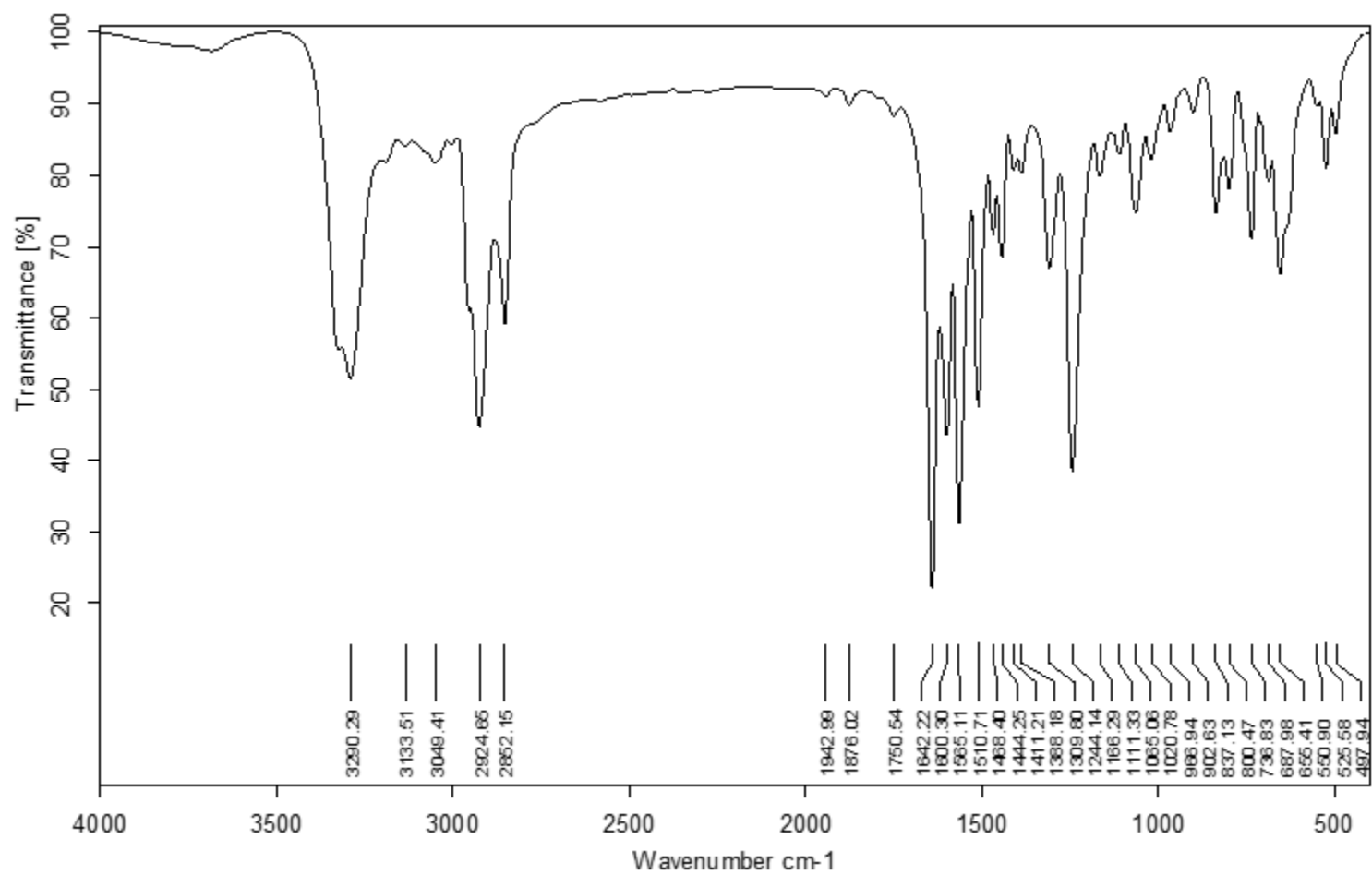
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-(hexyloxy)phenyl)-3-phenylurea **1**



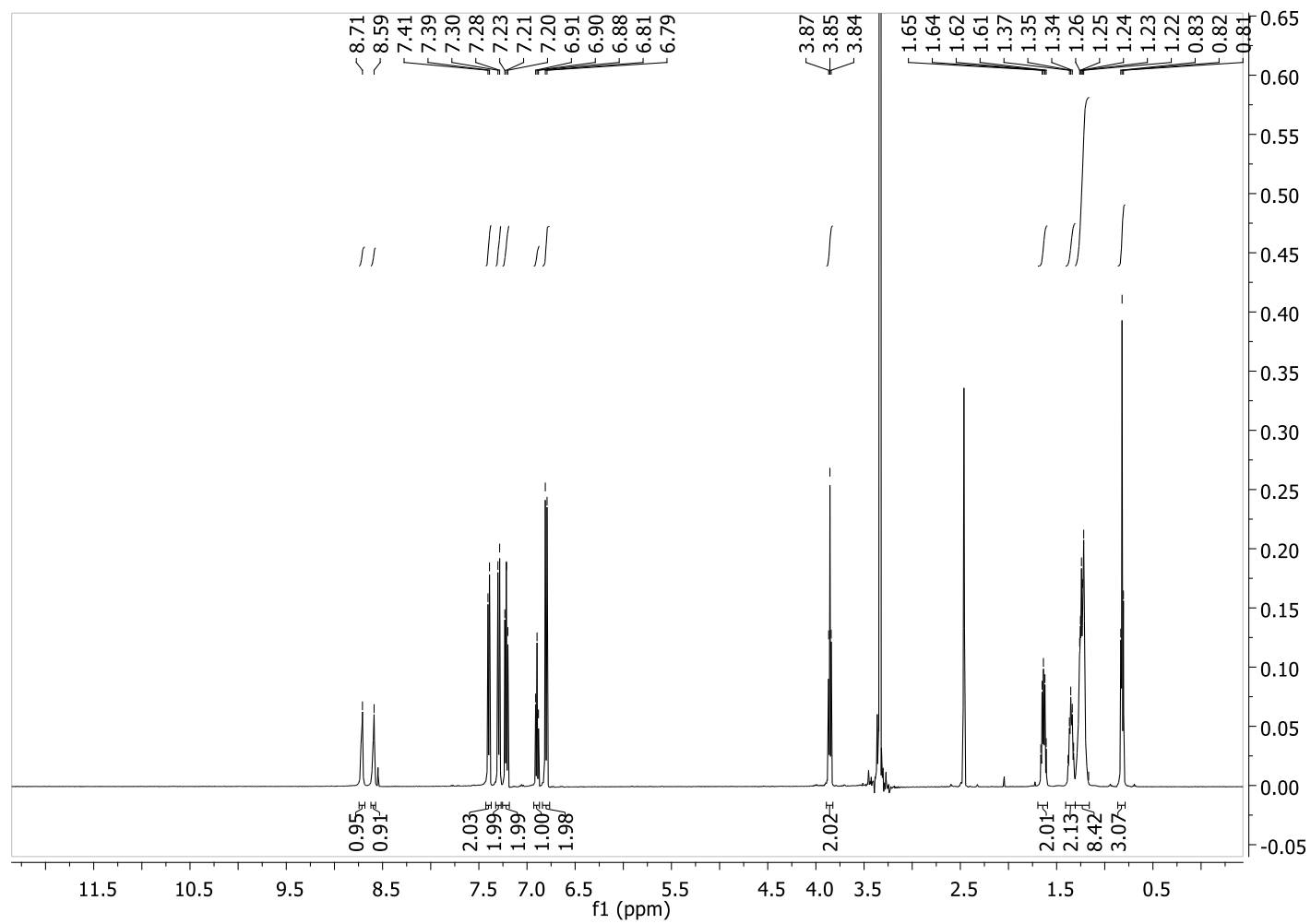
¹³C NMR (DMSO-*d*₆) of 1-(4-(hexyloxy)phenyl)-3-phenylurea **1**



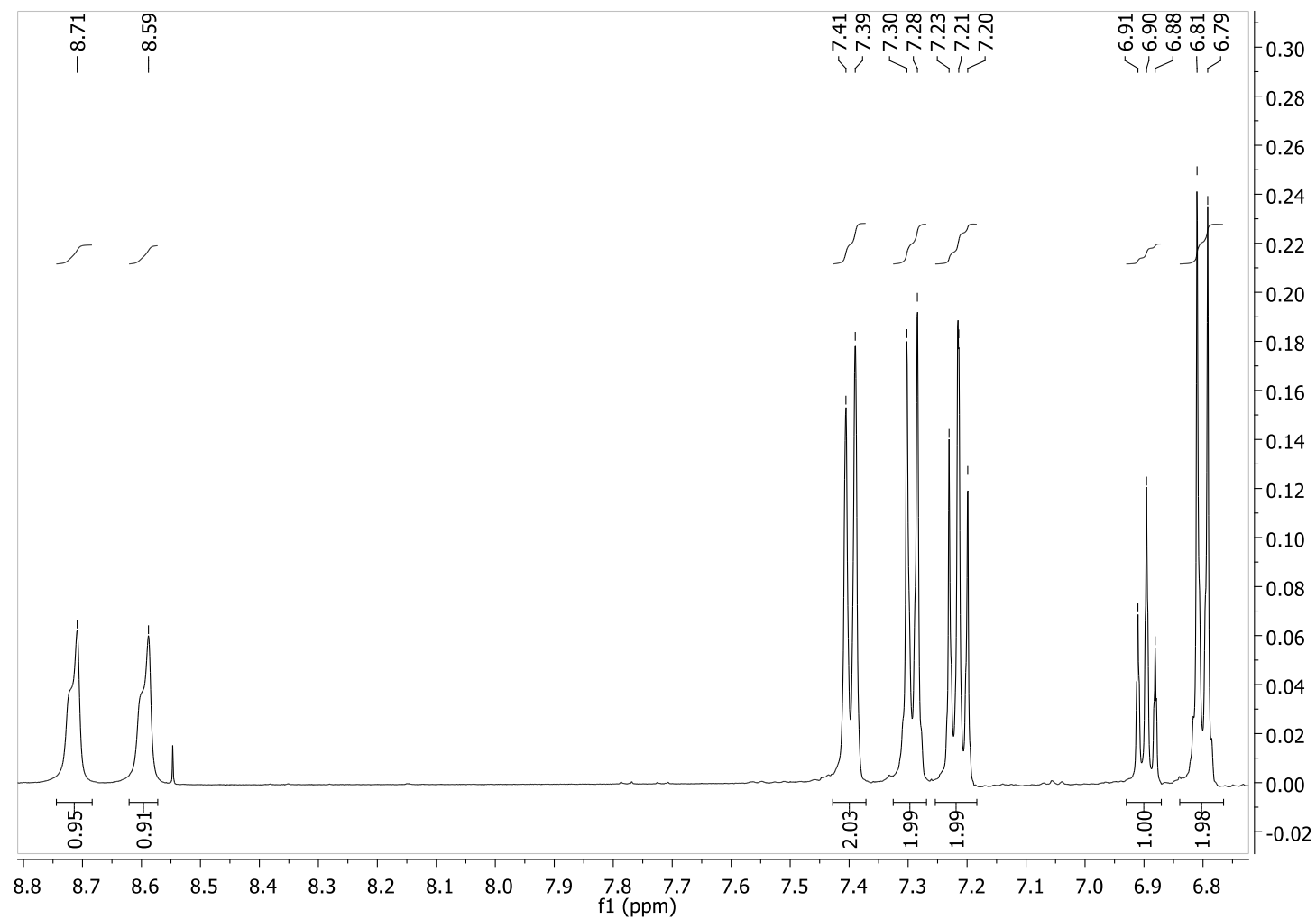
Mass spectrum of 1-(4-(hexyloxy)phenyl)-3-phenylurea **1**



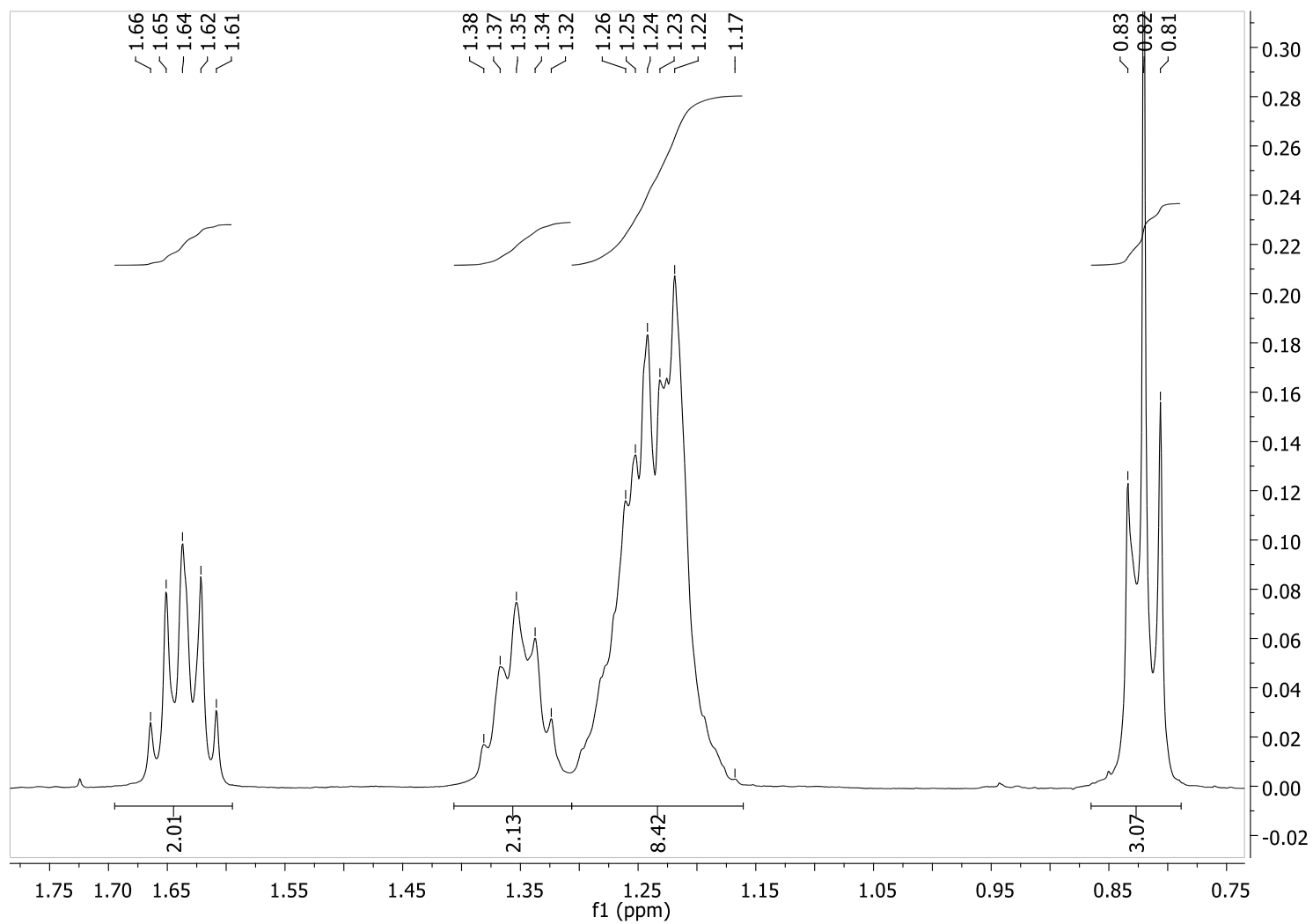
IR (KBr) spectrum of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



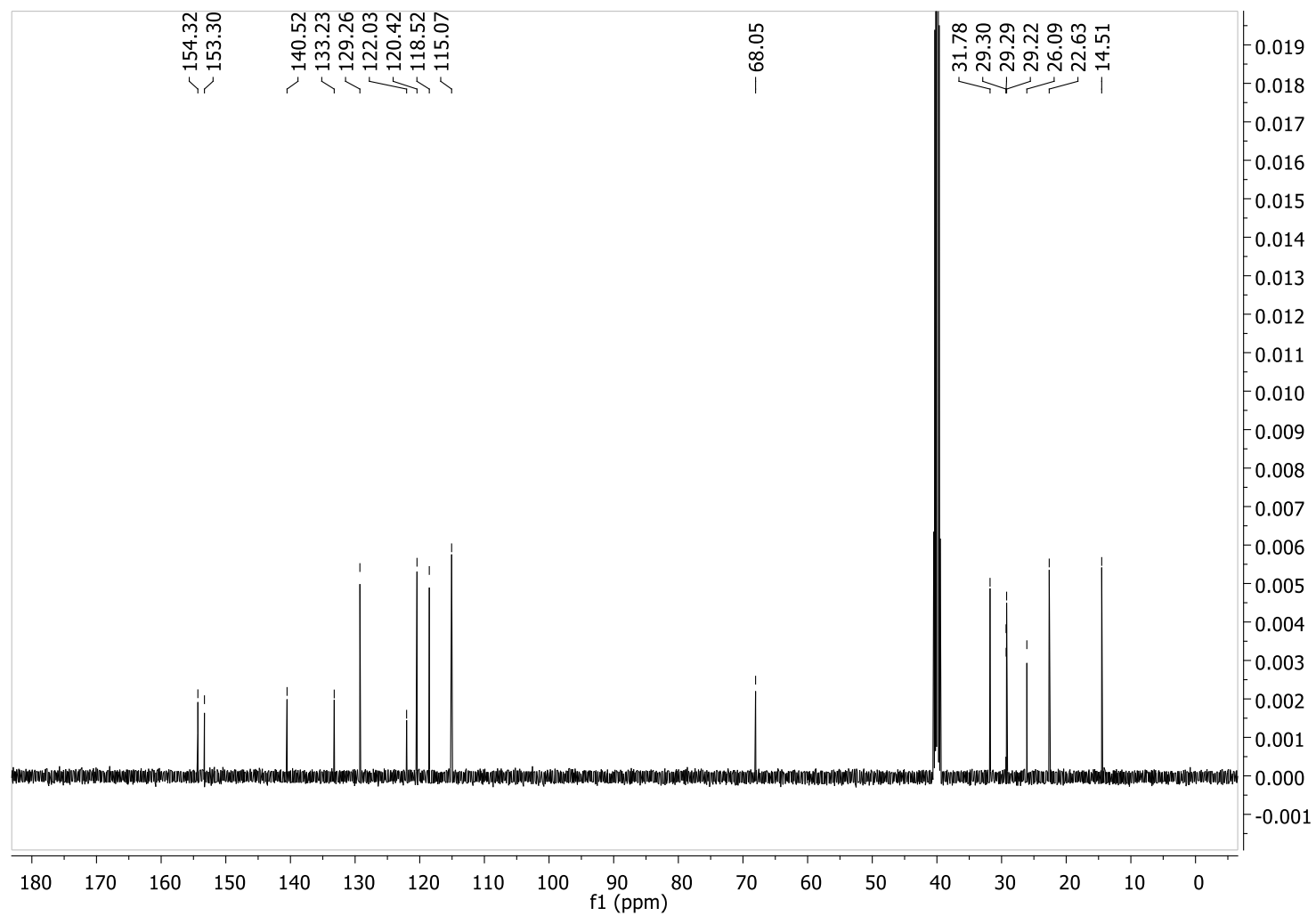
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



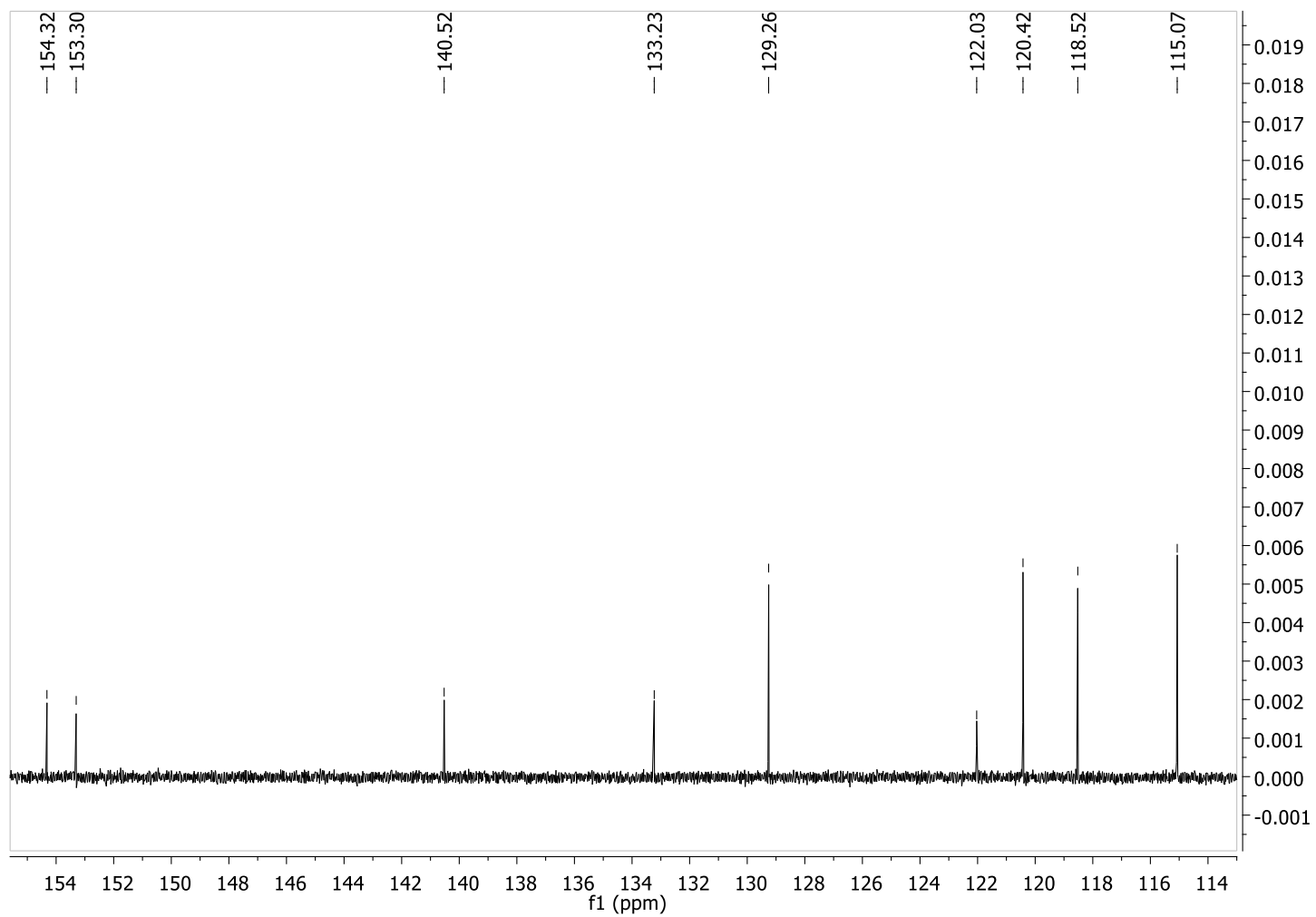
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



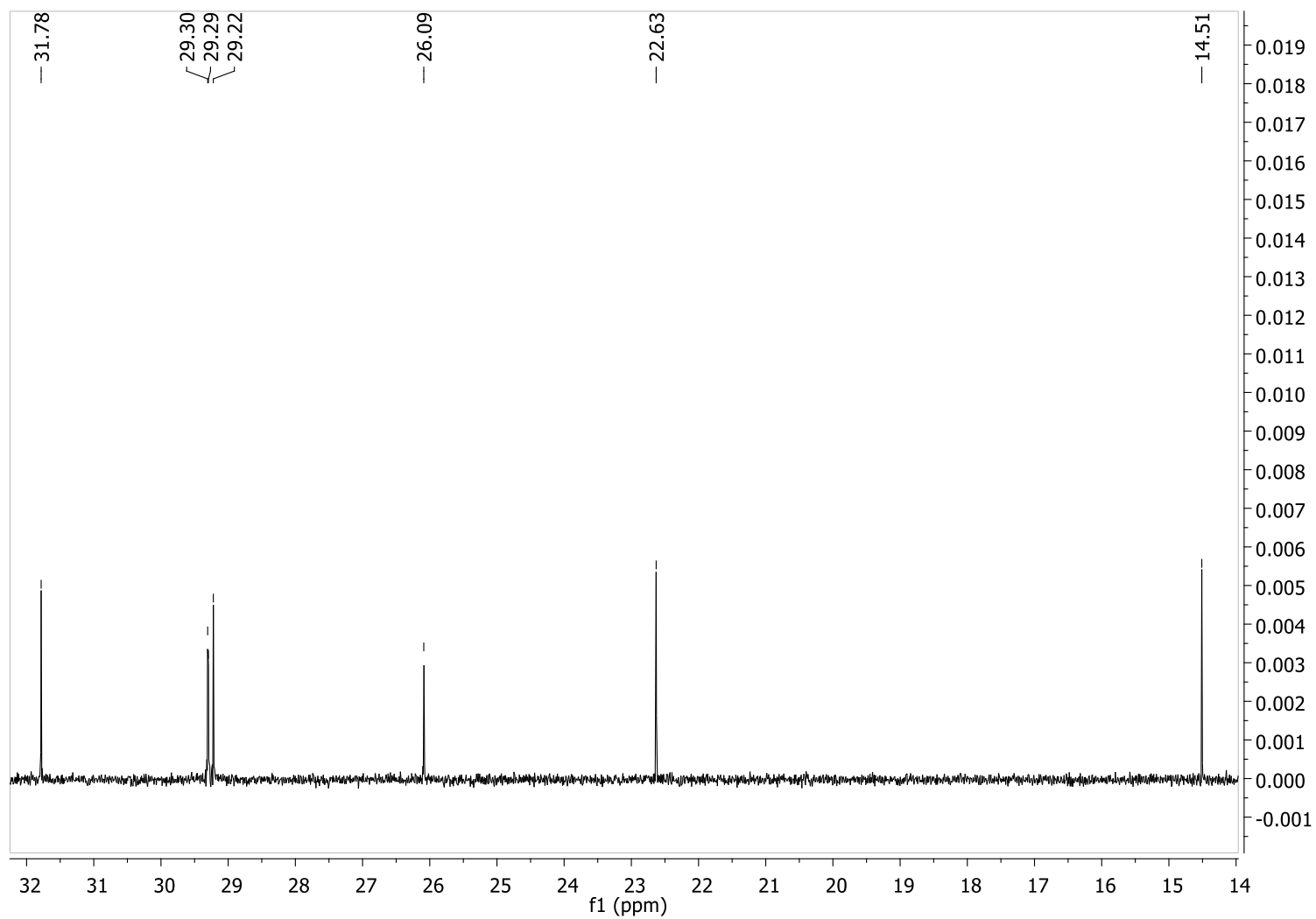
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



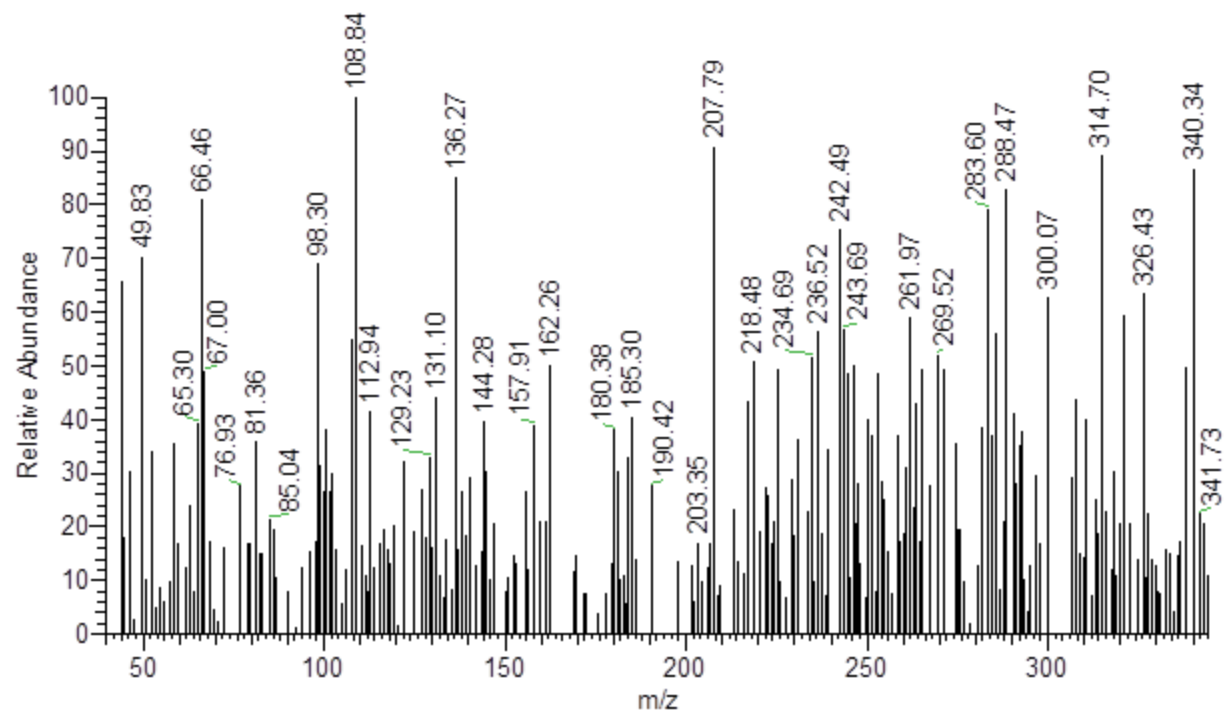
^{13}C NMR (DMSO- d_6) of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



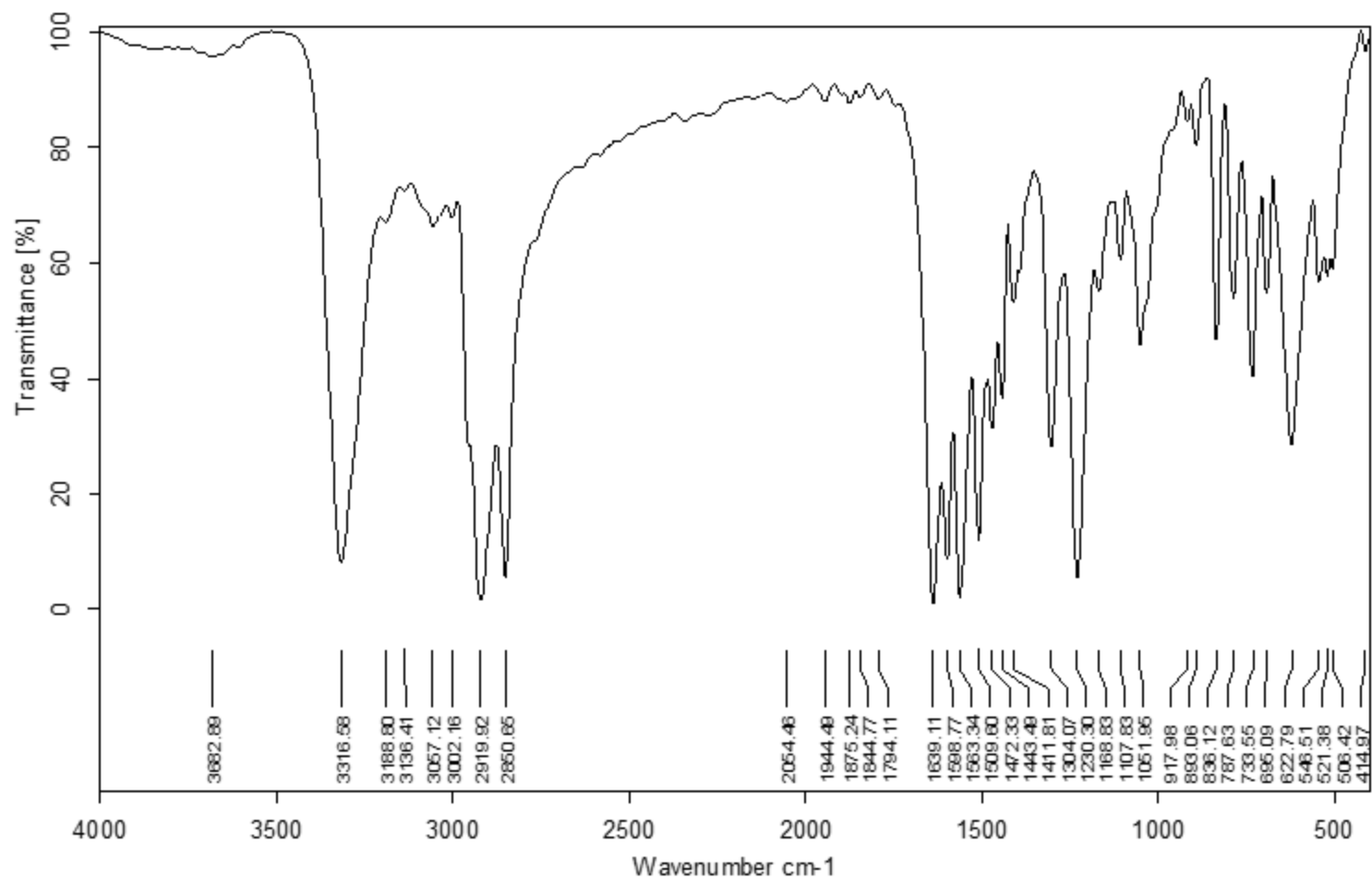
¹³C NMR (DMSO-*d*₆) of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



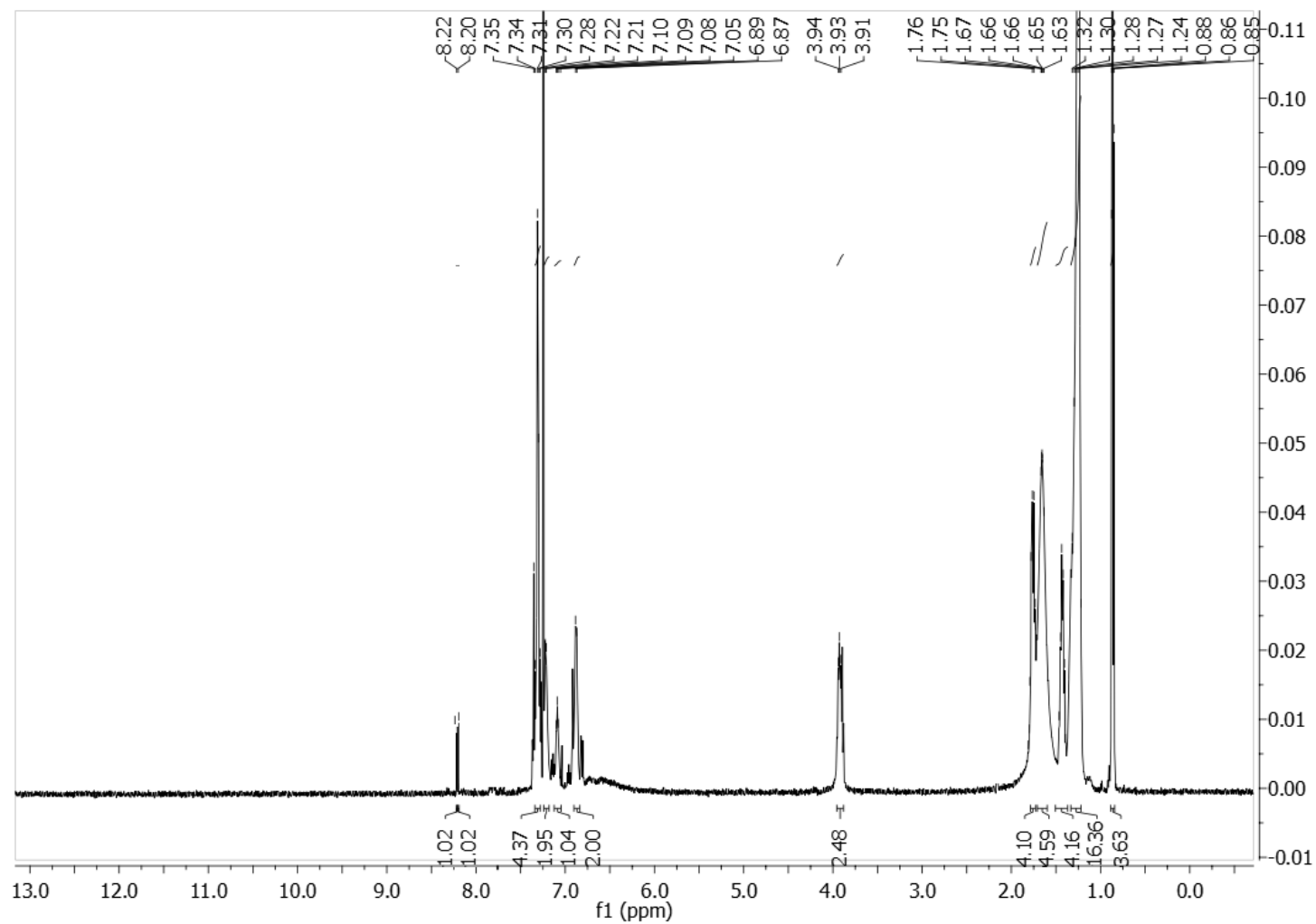
¹³C NMR (DMSO-*d*₆) of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



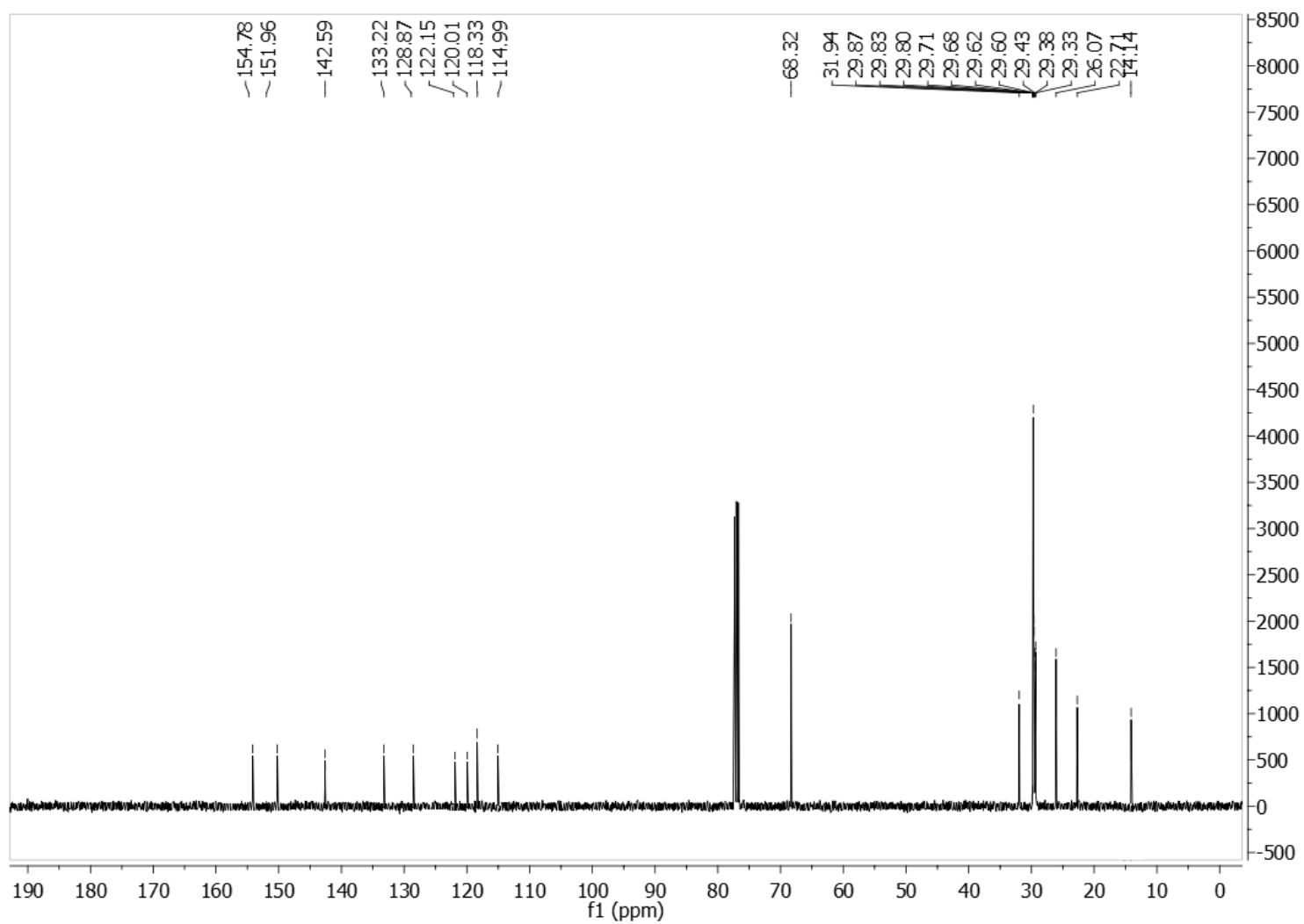
Mass spectrum of 1-(4-(octyloxy)phenyl)-3-phenylurea **2**



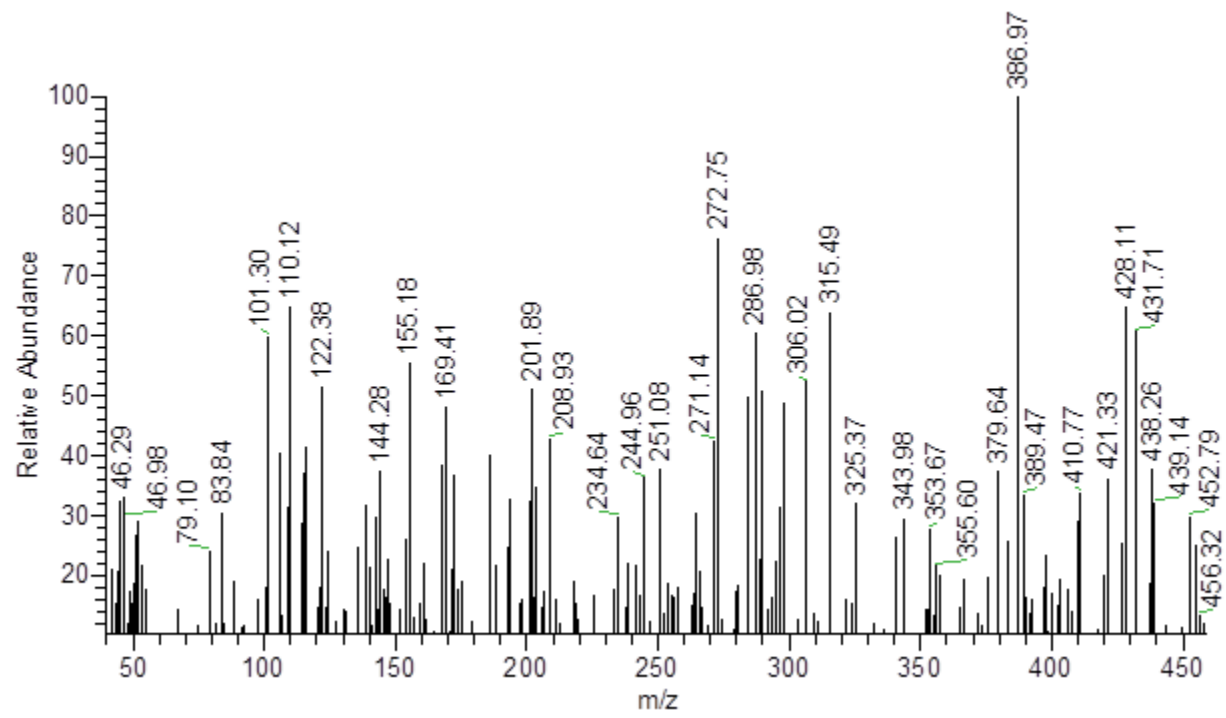
IR (KBr) spectrum of 1-(4-(hexadecyloxy)phenyl)-3-phenylurea **3**



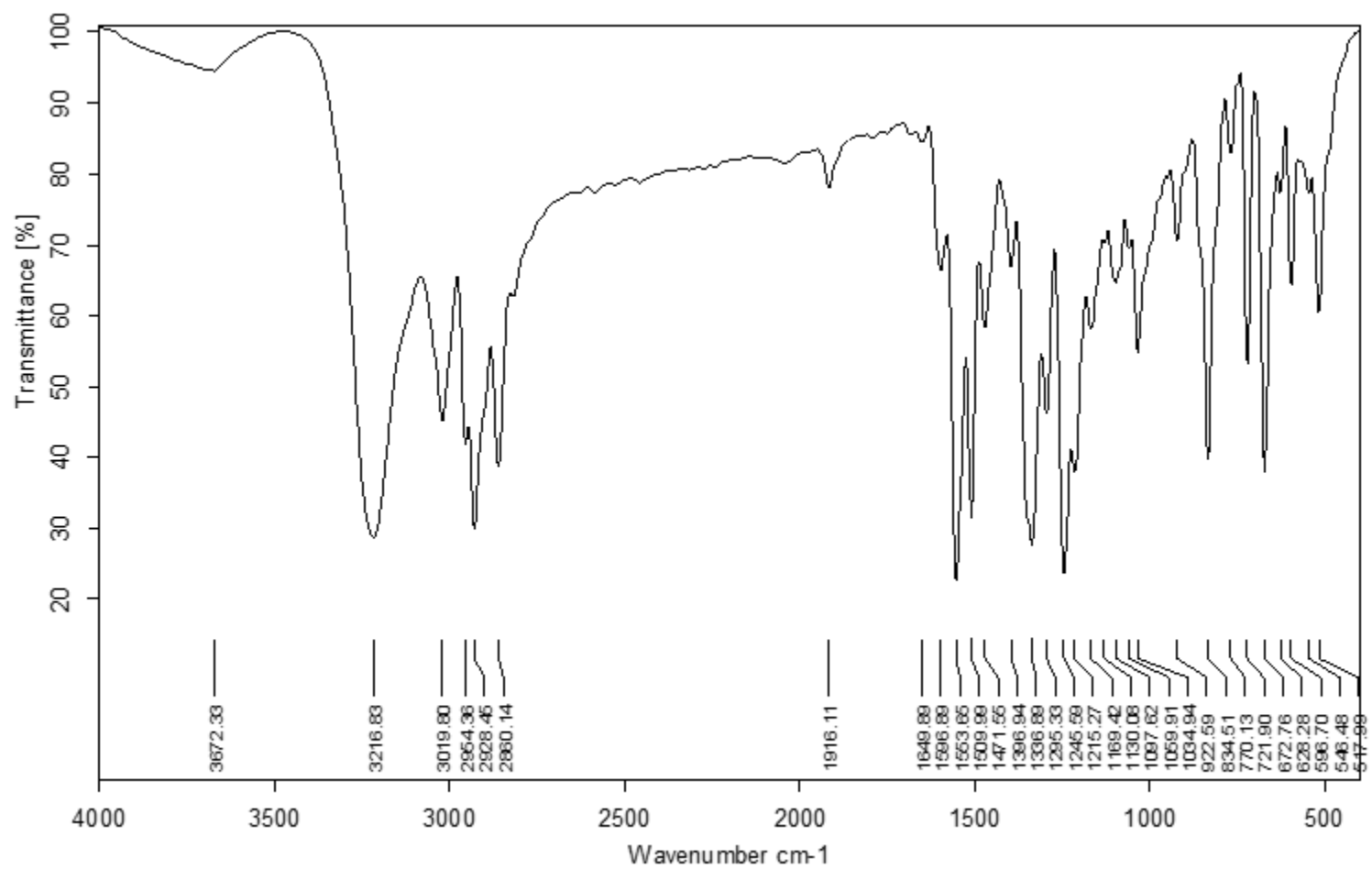
^1H NMR (CDCl_3) spectrum of 1-(4-(hexadecyloxy)phenyl)-3-phenylurea **3**



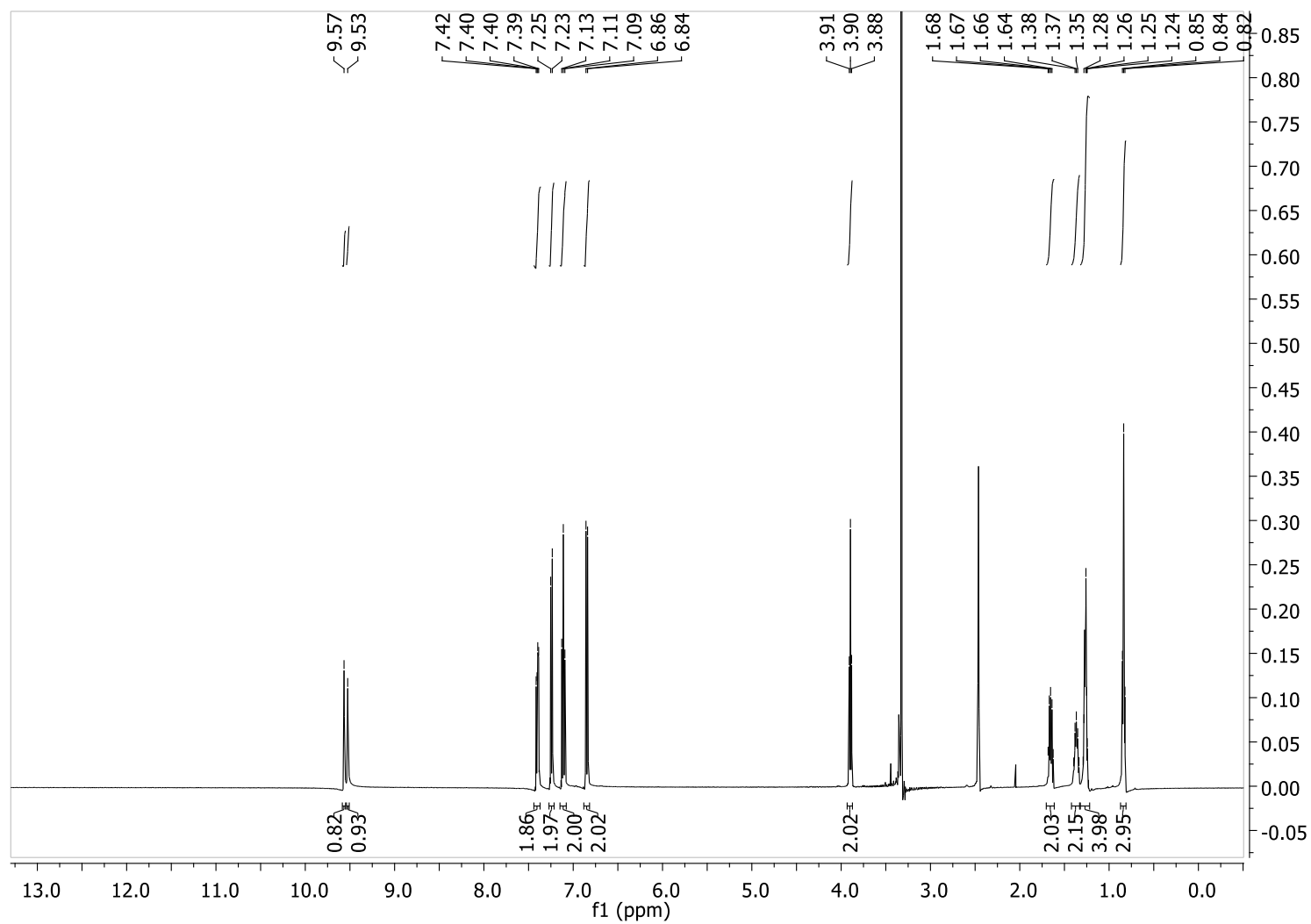
¹³C NMR (CDCl₃) of 1-(4-(hexadecyloxy)phenyl)-3-phenylurea **3**



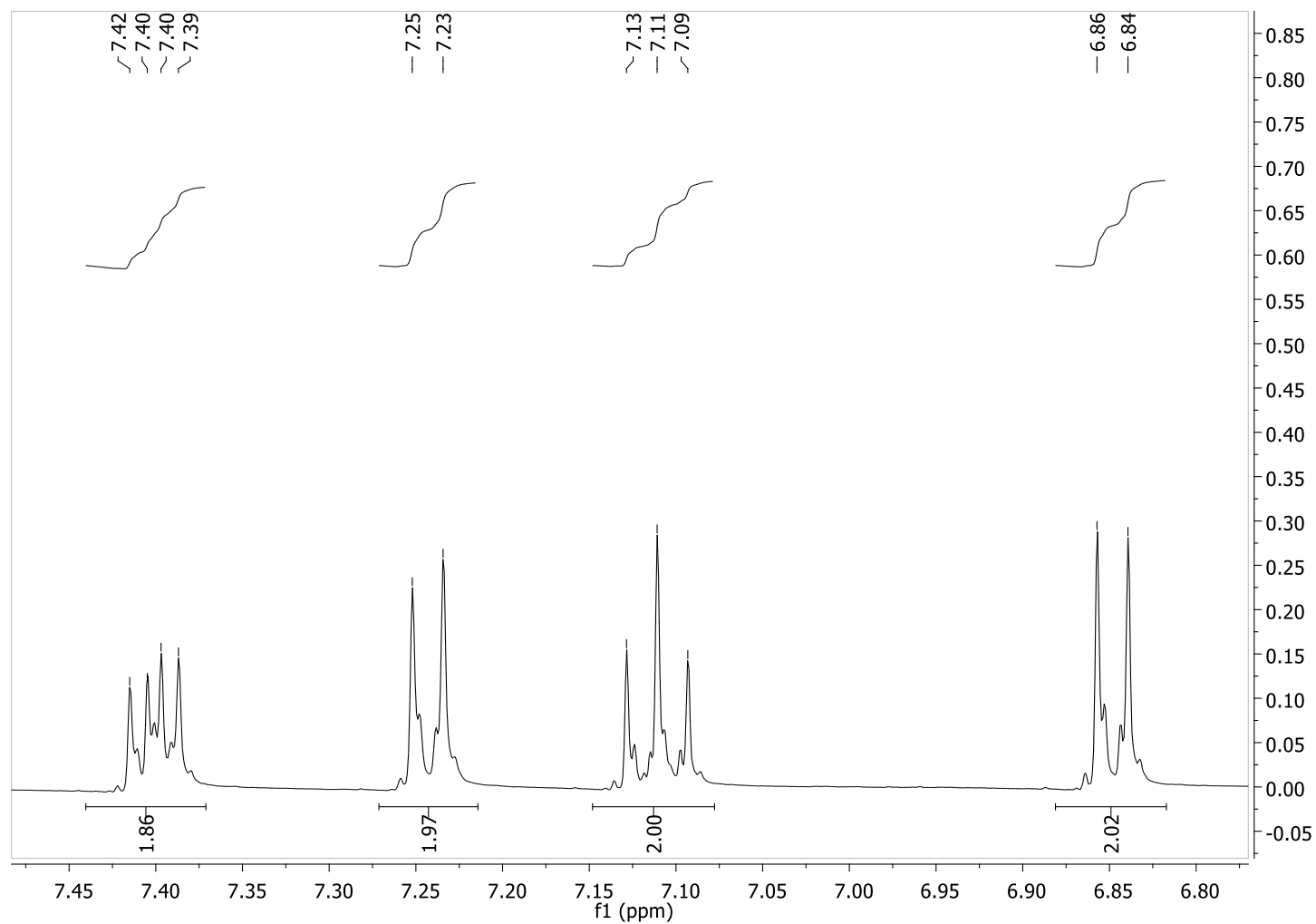
Mass spectrum of 1-(4-(hexadecyloxy)phenyl)-3-phenylurea **3**



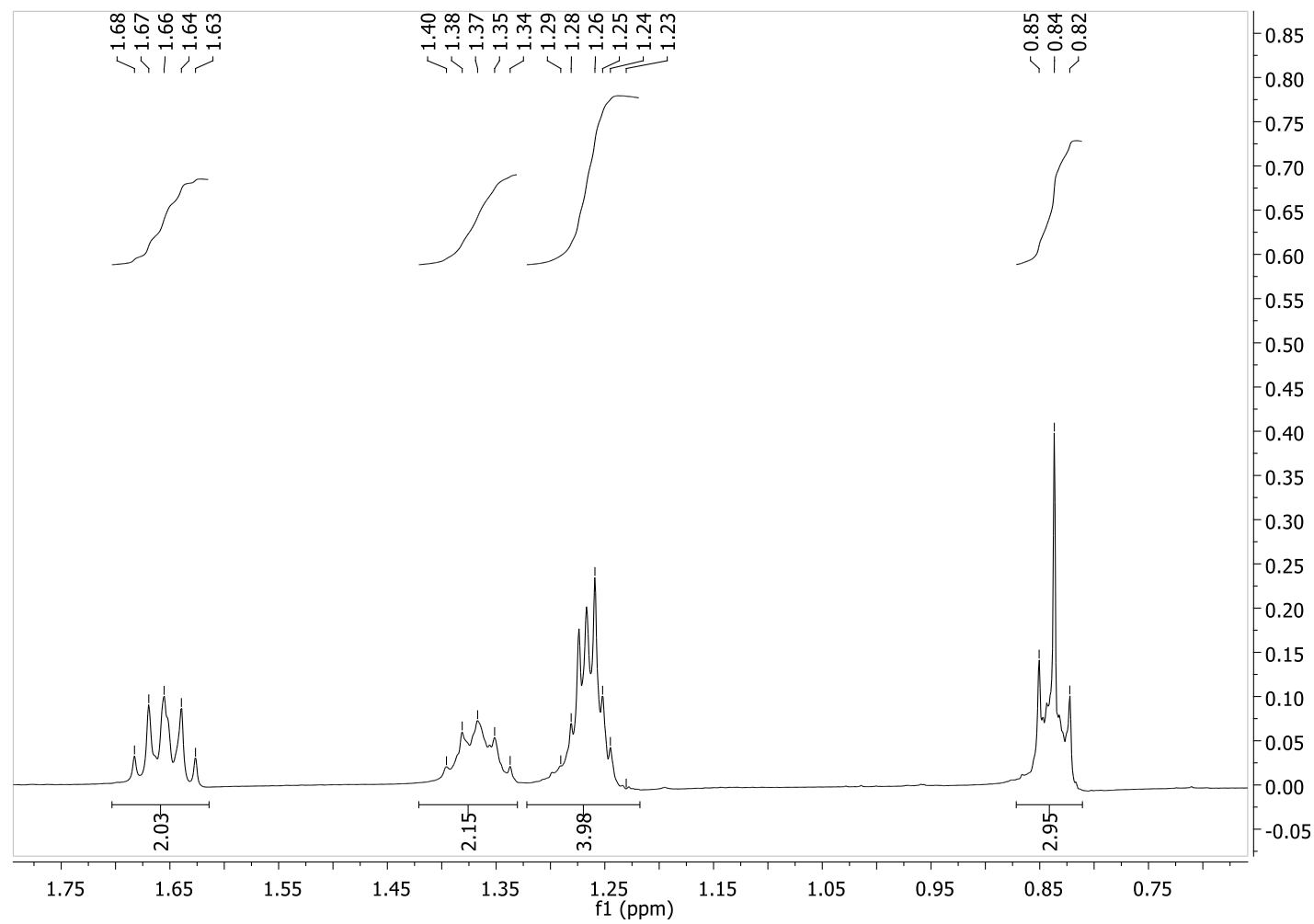
IR (KBr) spectrum of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



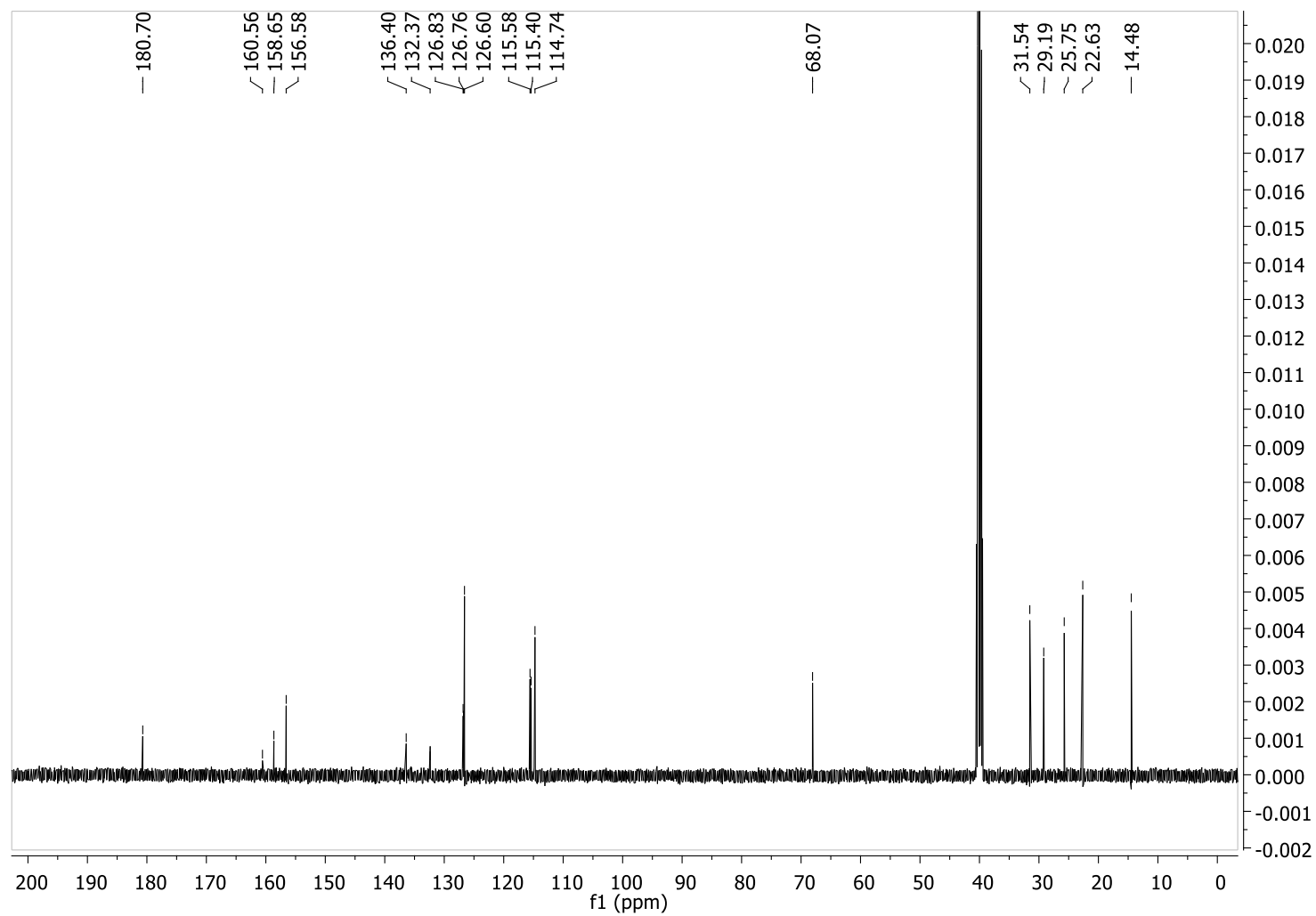
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



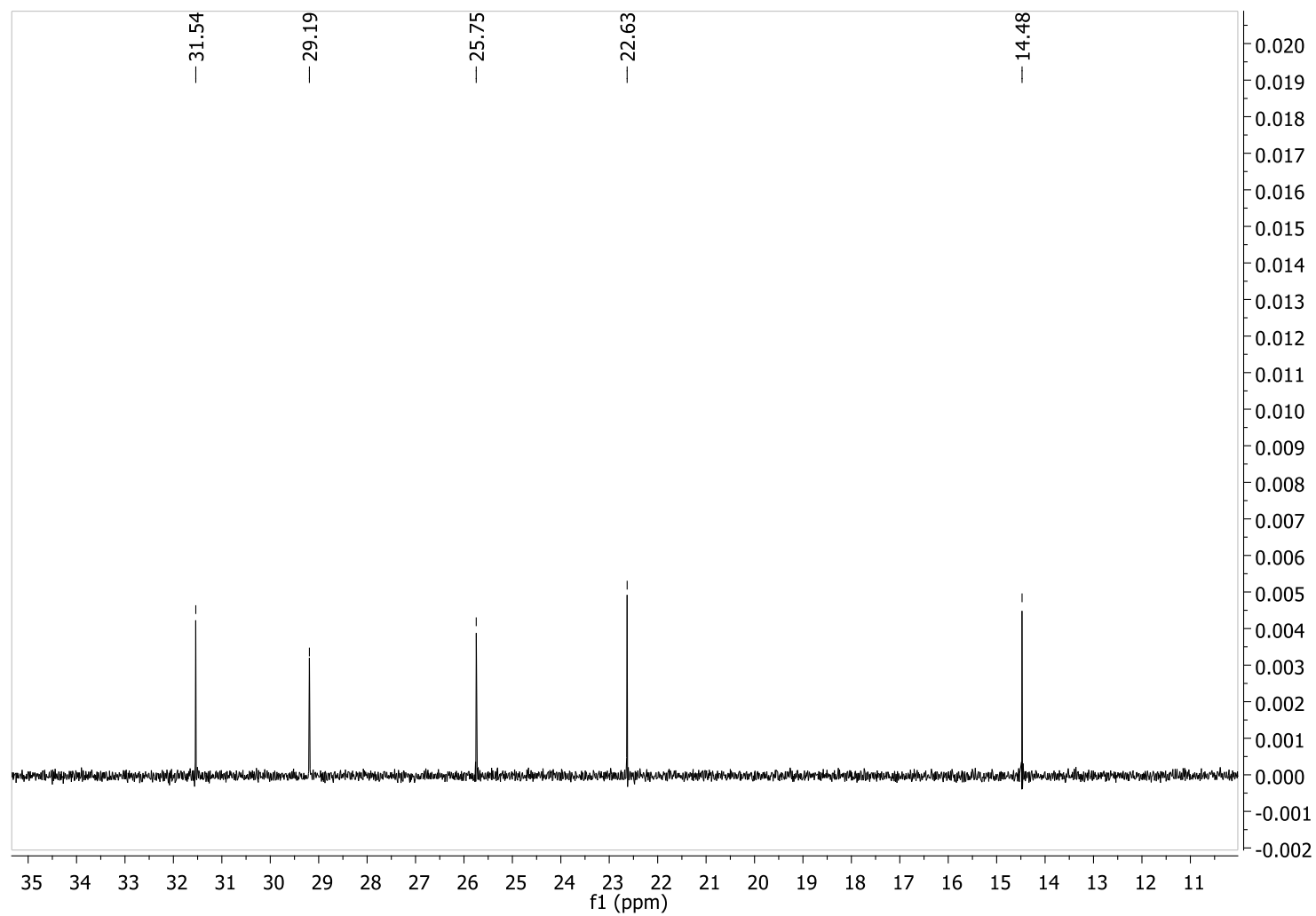
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



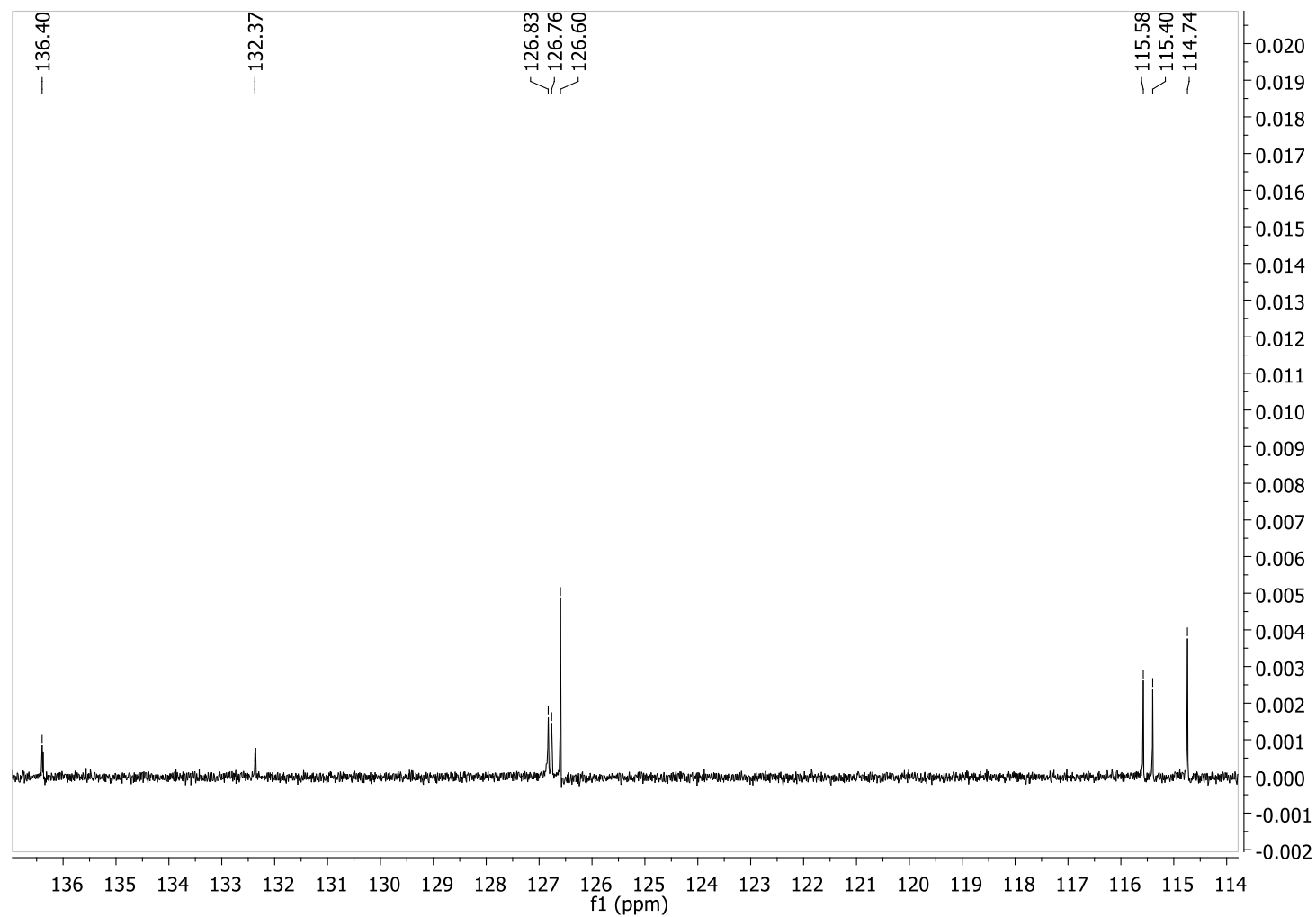
^1H NMR ($\text{DMSO-}d_6$) spectrum of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



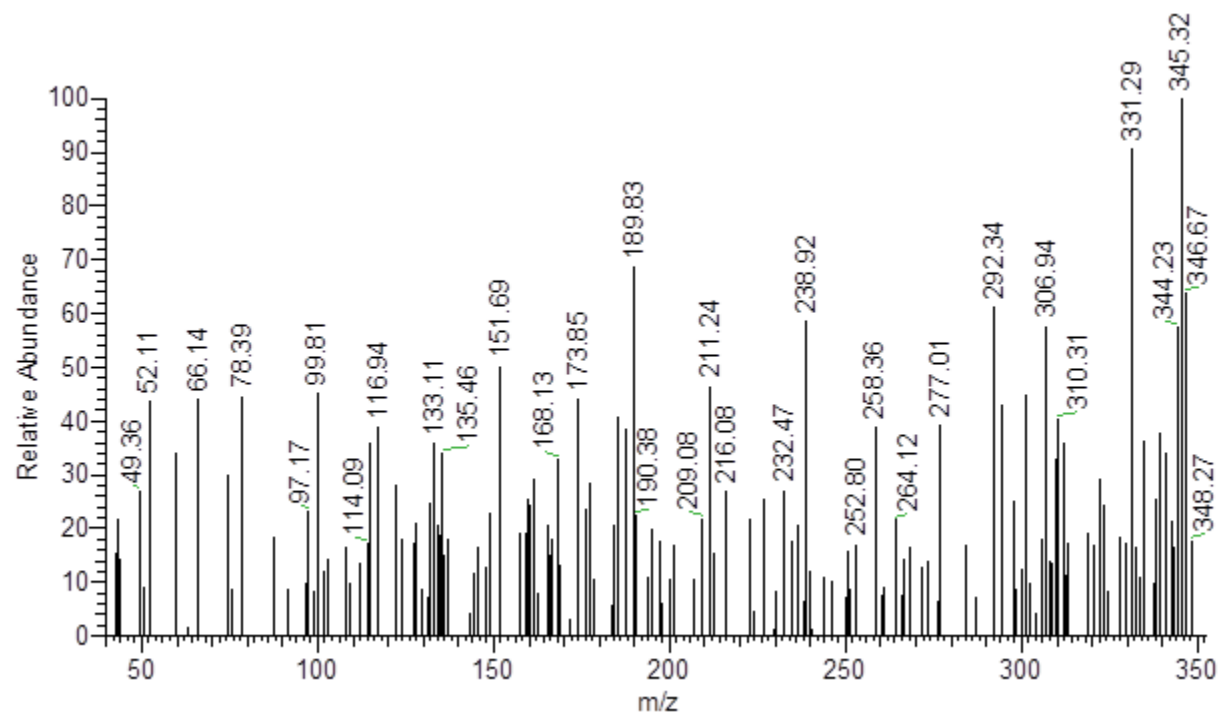
¹³C NMR (DMSO-*d*₆) of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



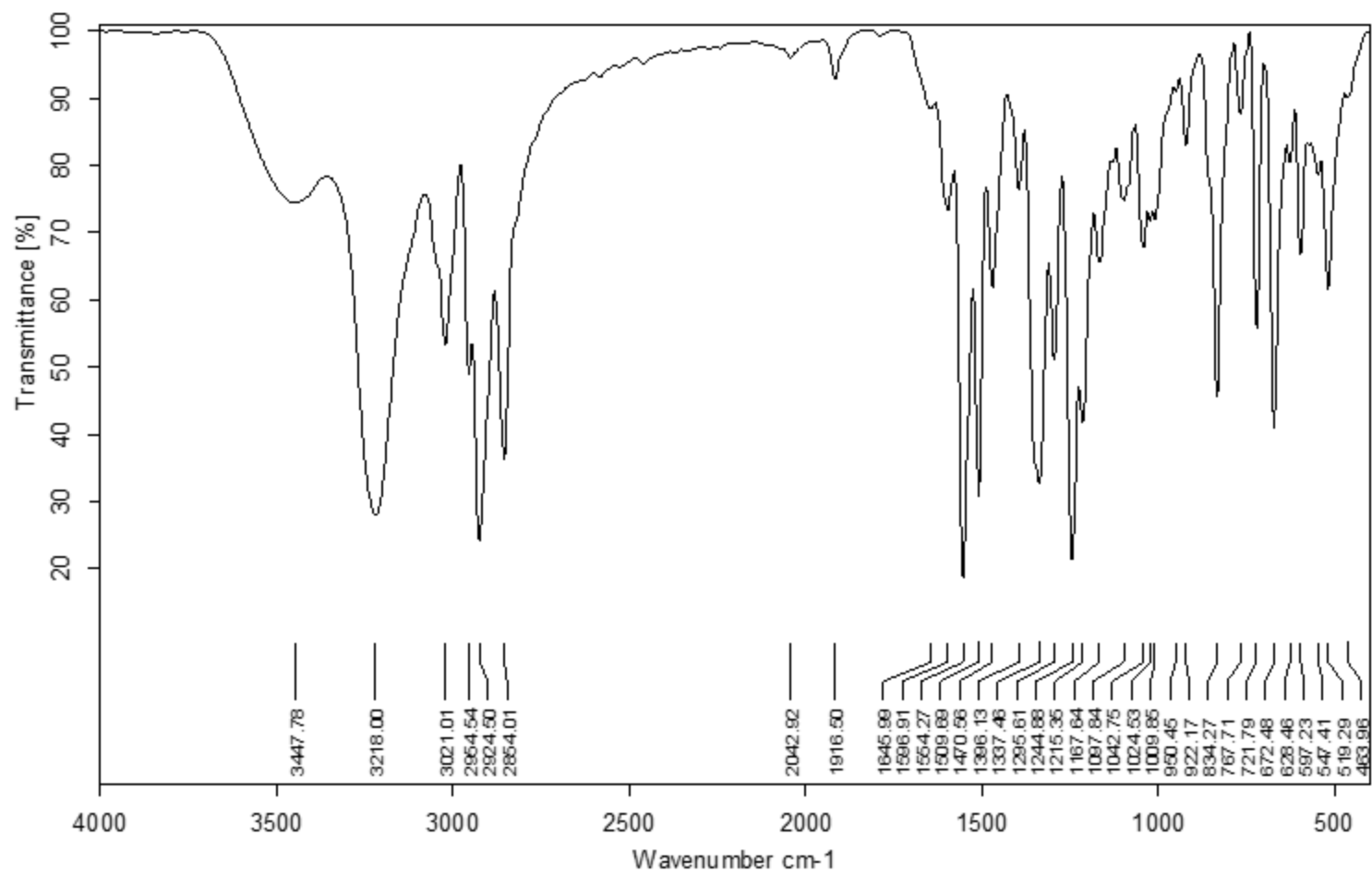
¹³C NMR (DMSO-*d*₆) of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



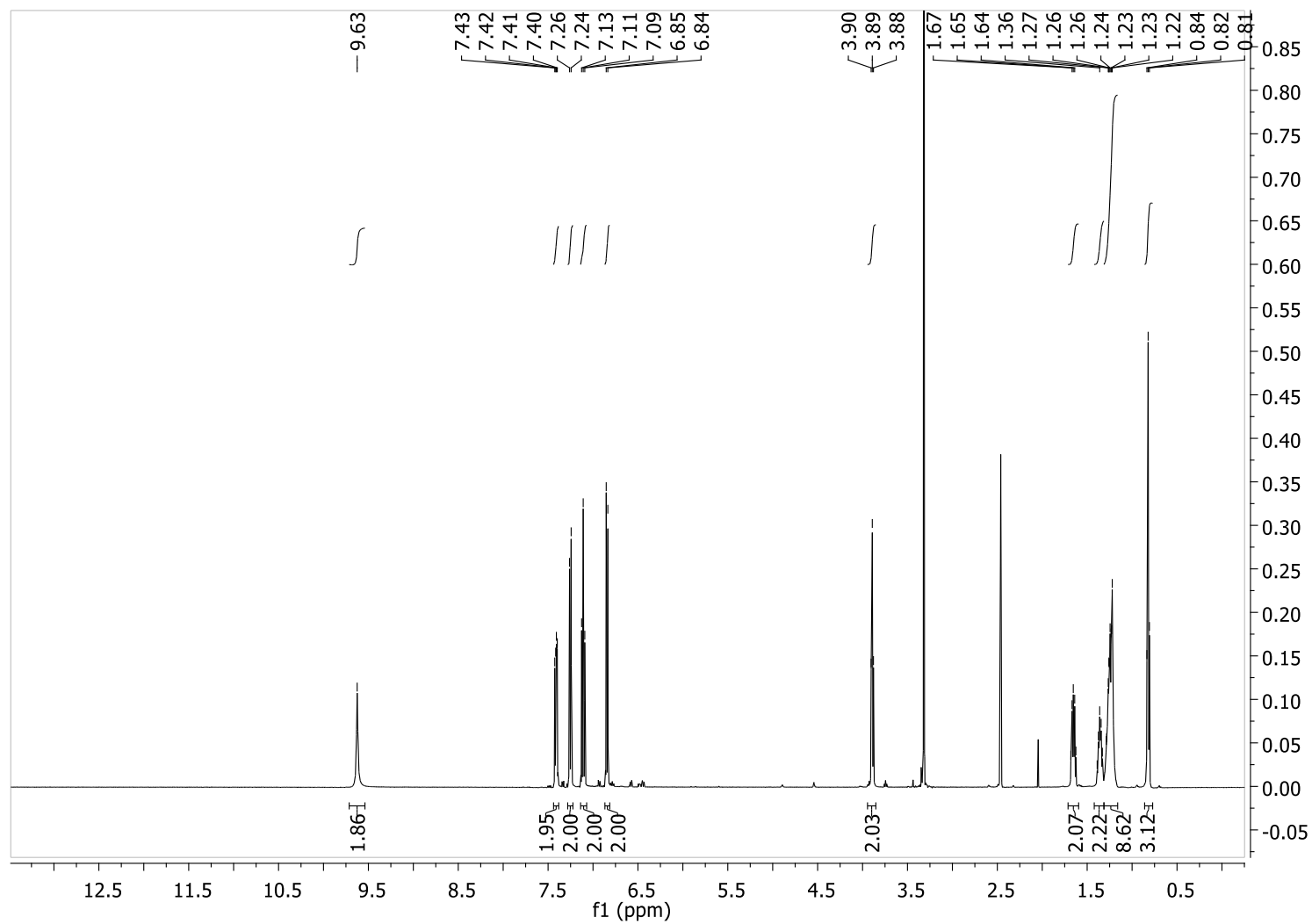
¹³C NMR (DMSO-*d*₆) of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



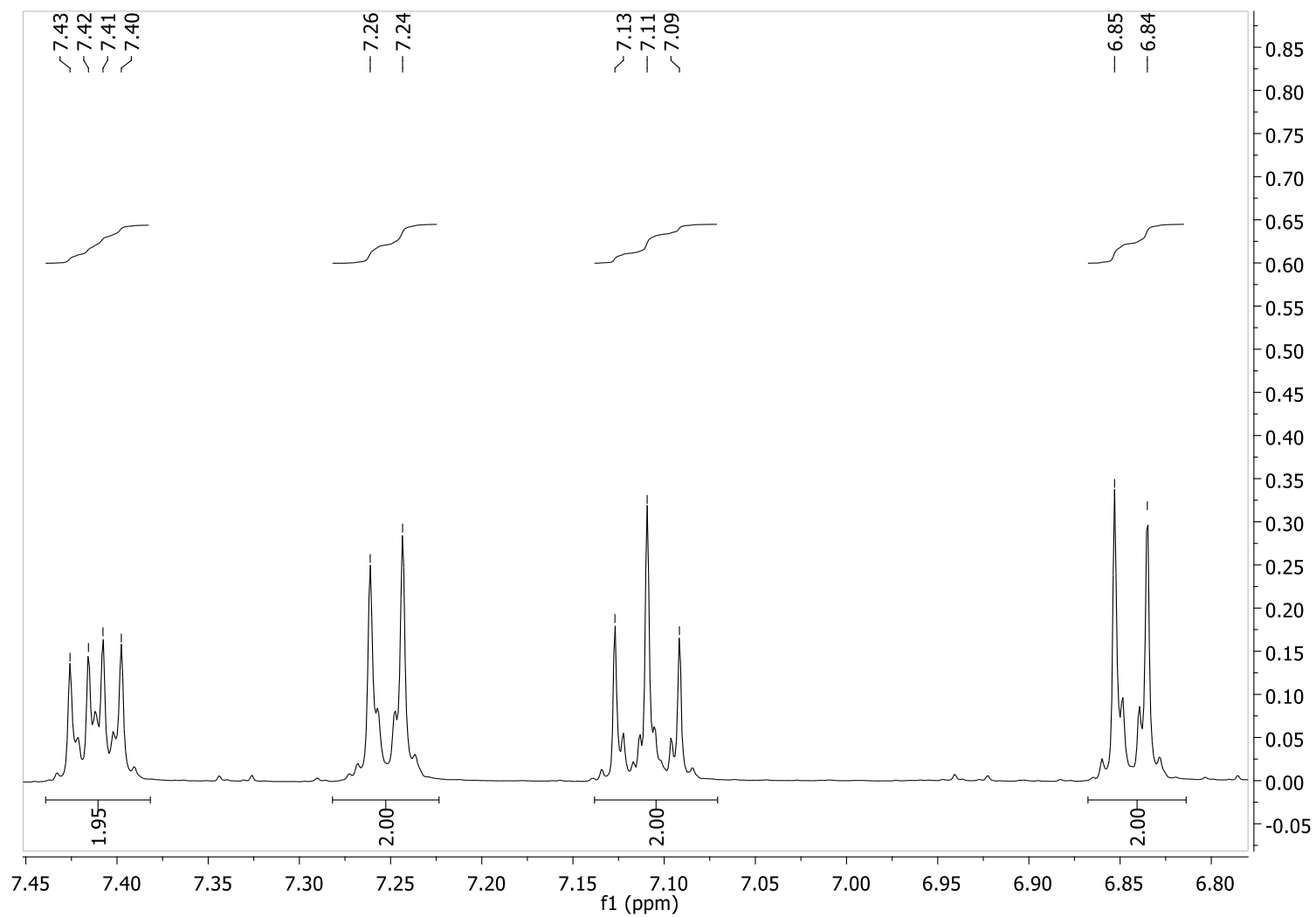
Mass spectrum of 1-(4-fluorophenyl)-3-(4-(hexyloxy)phenyl)thiourea **4**



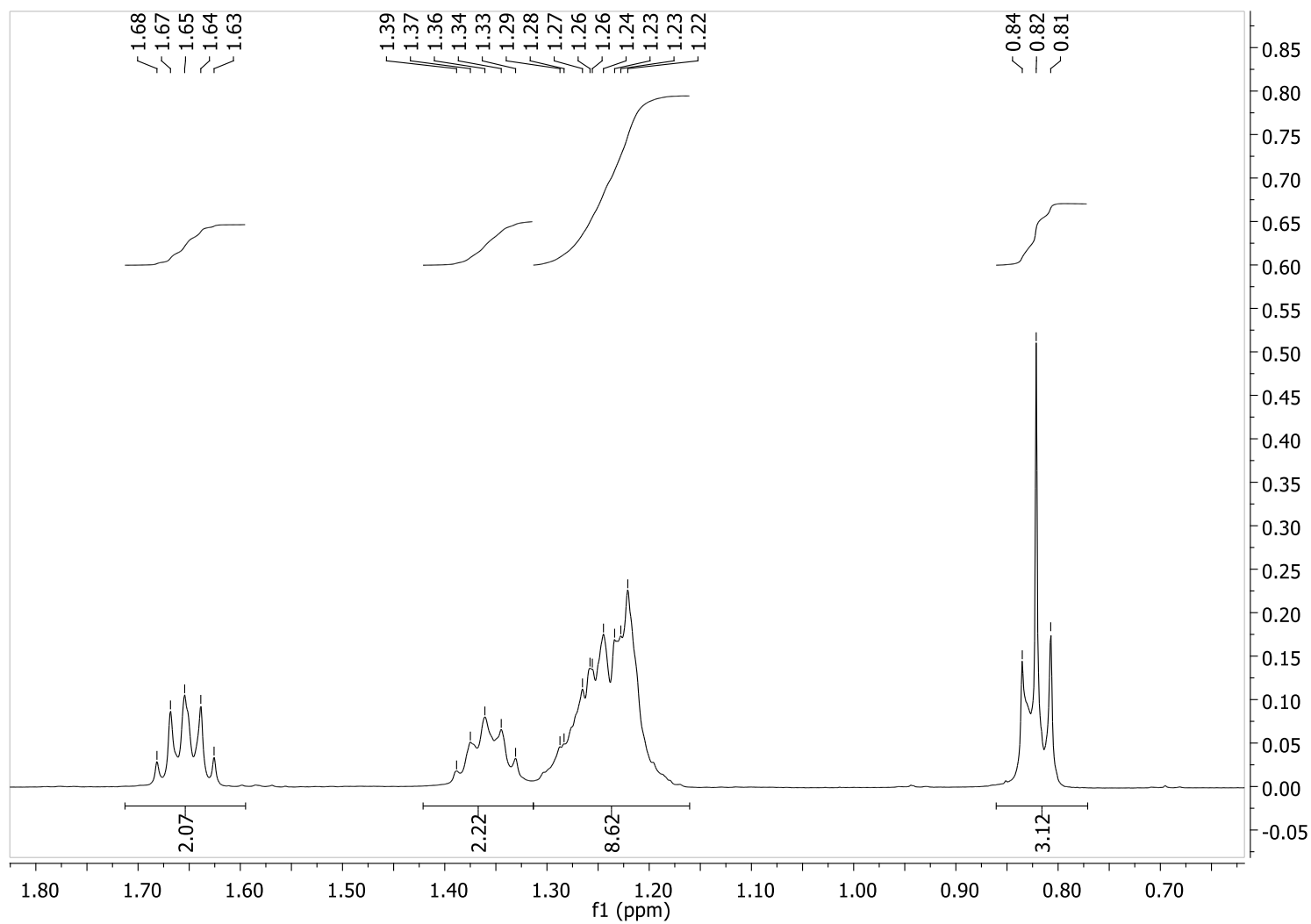
IR (KBr) spectrum of 1-(4-fluorophenyl)-3-(4-(octyloxy)phenyl)thiourea **5**



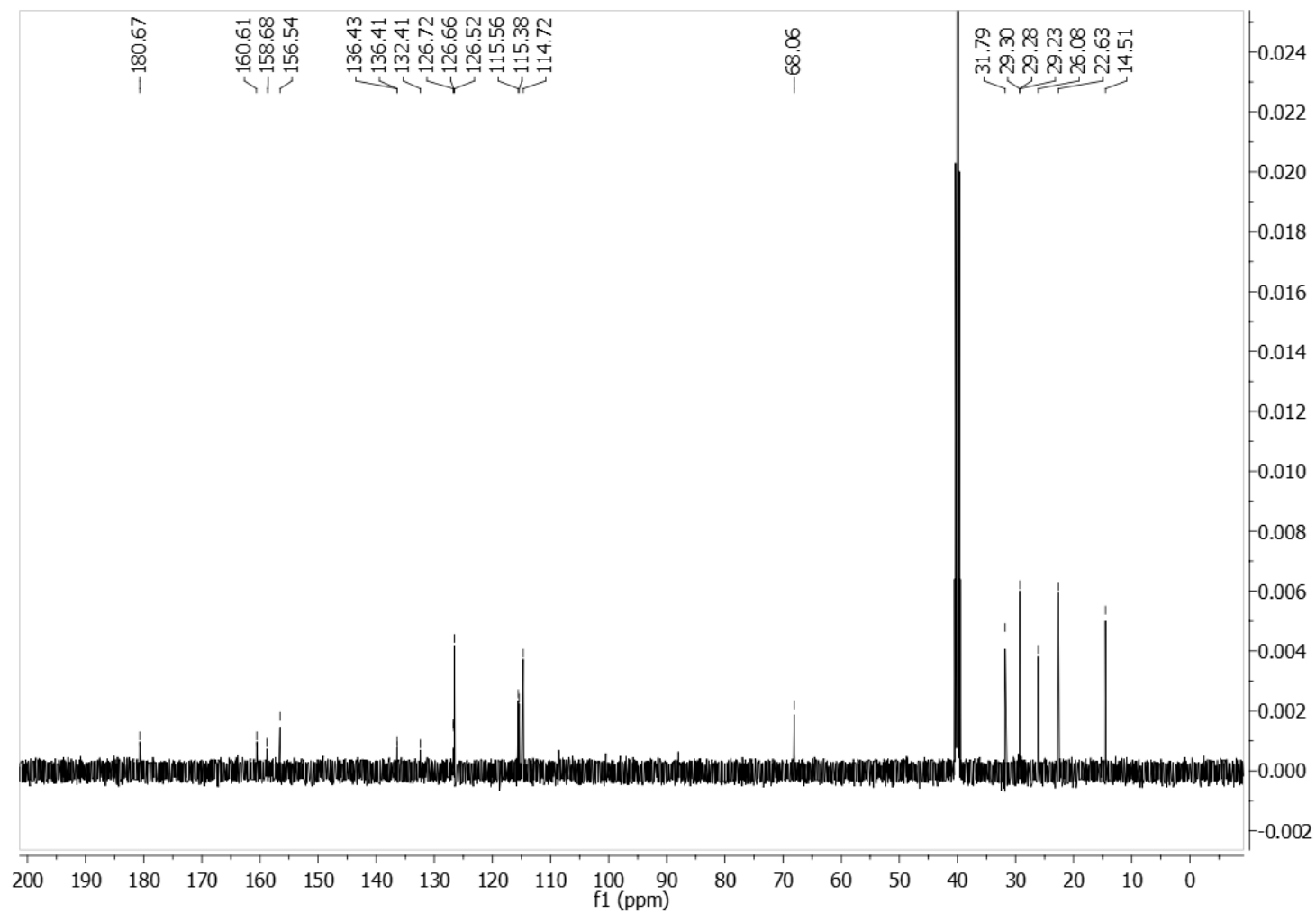
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-fluorophenyl)-3-(4-(octyloxy)phenyl)thiourea **5**



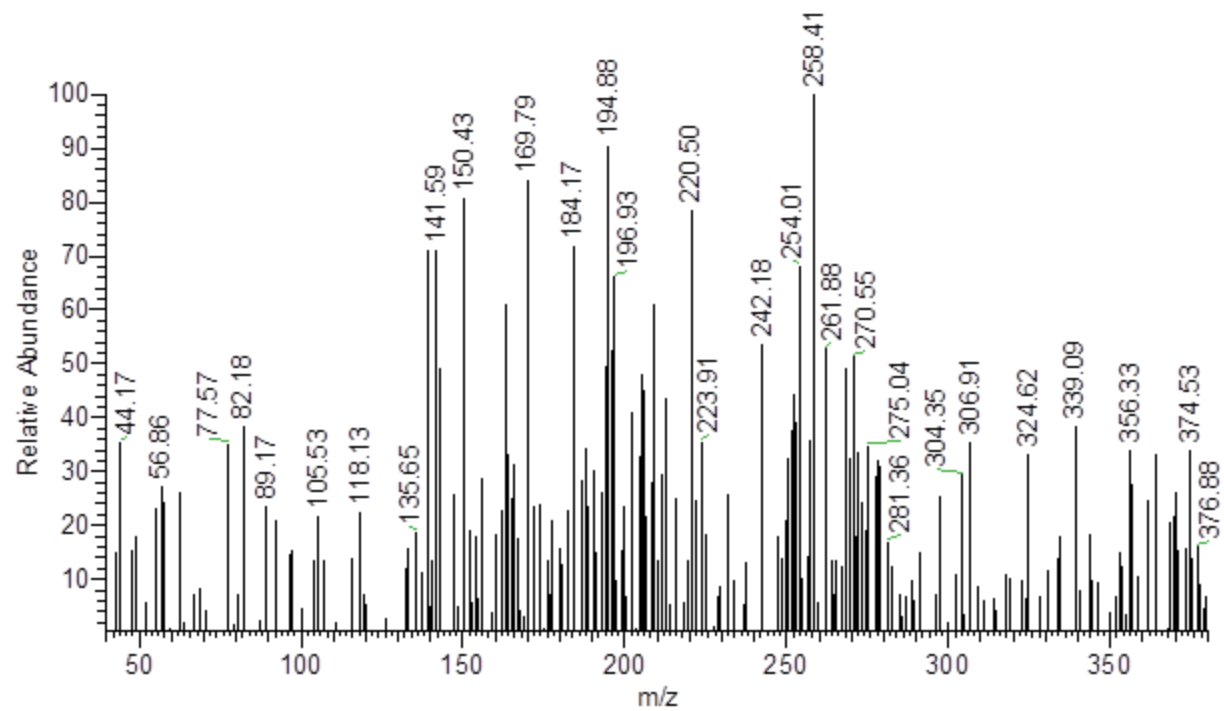
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-fluorophenyl)-3-(4-(octyloxy)phenyl)thiourea **5**



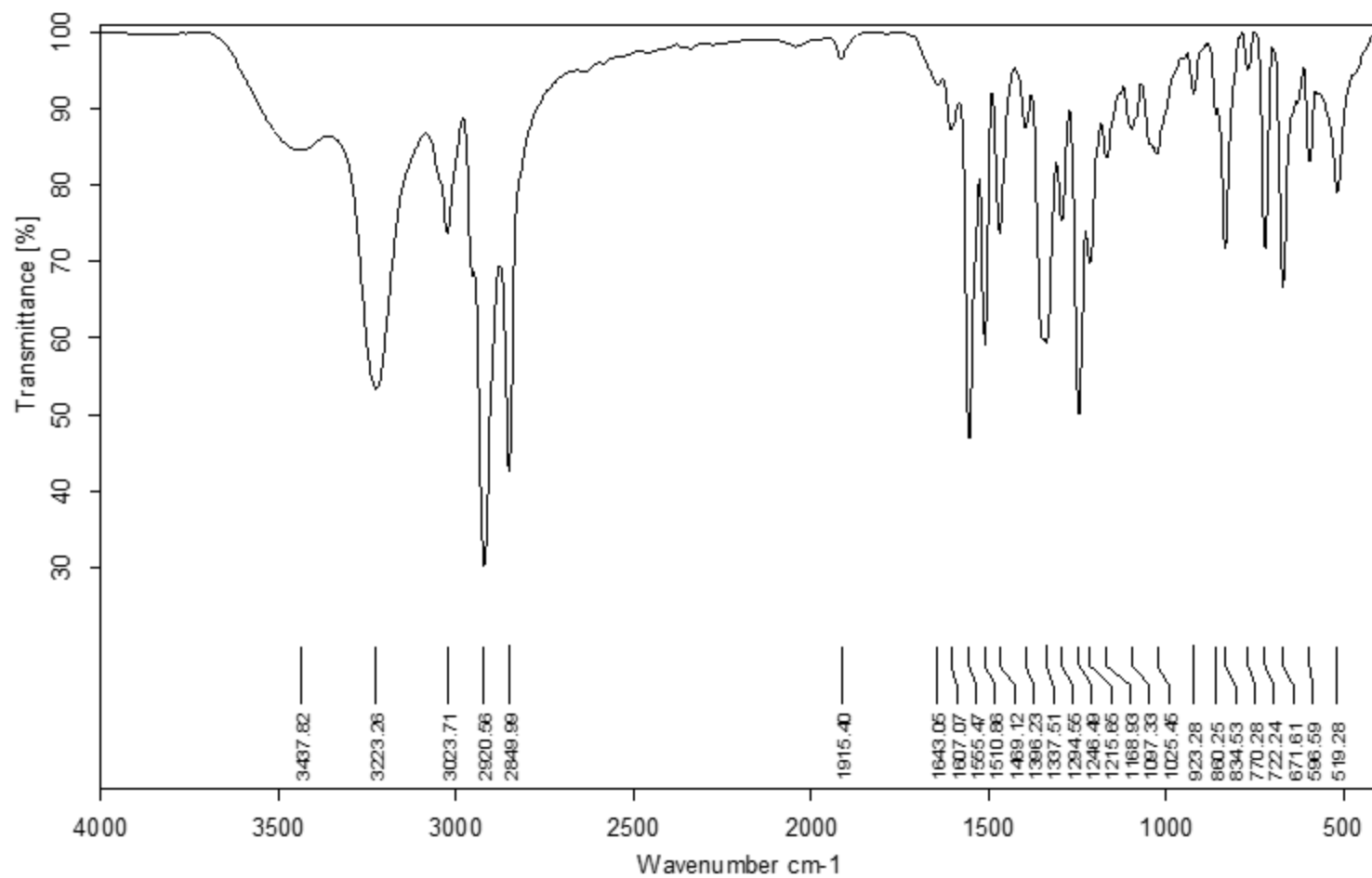
¹H NMR (DMSO-*d*₆) spectrum of 1-(4-fluorophenyl)-3-(4-(octyloxy)phenyl)thiourea **5**



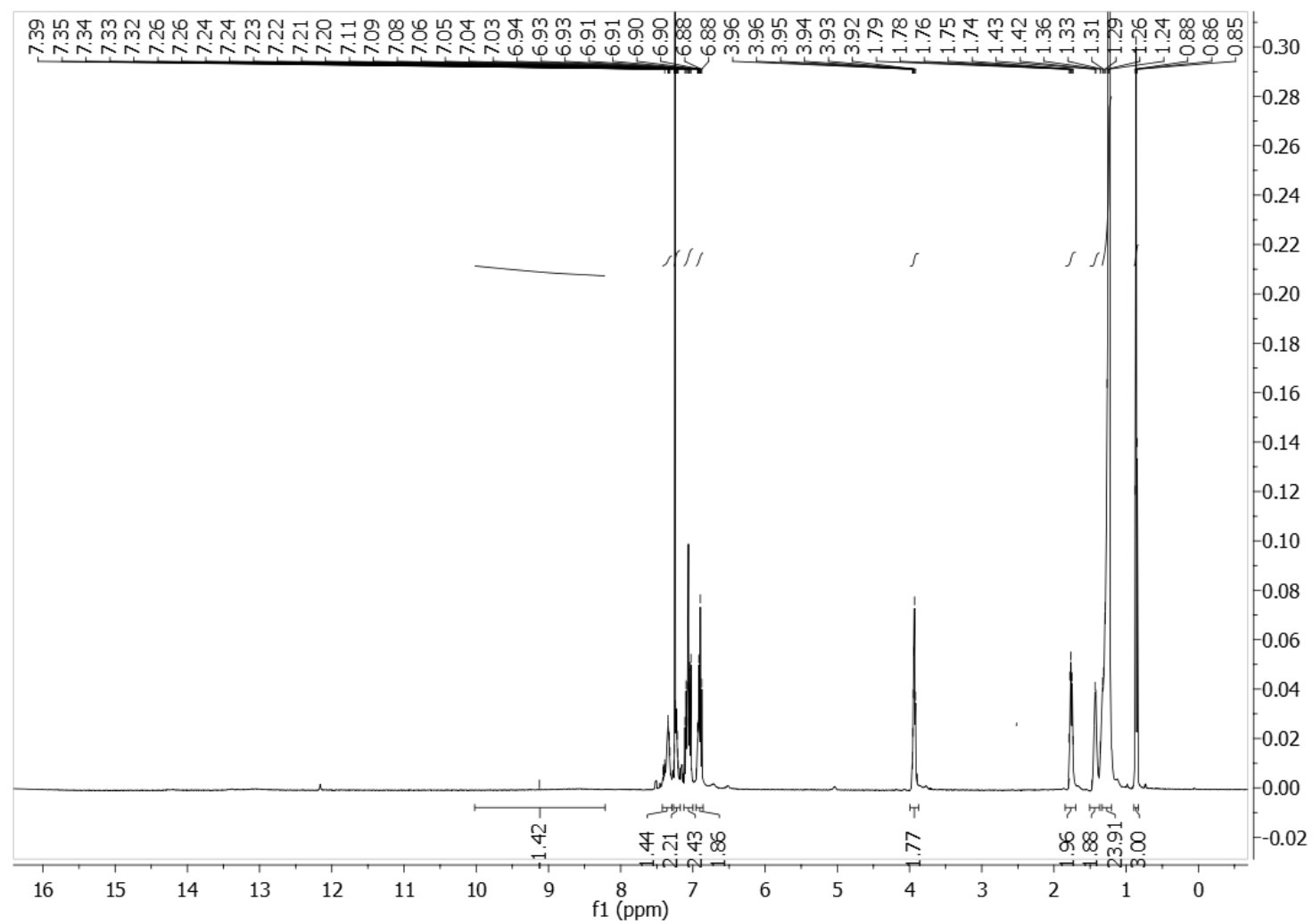
¹³C NMR (DMSO-*d*₆) of 1-(4-fluorophenyl)-3-(4-(octyloxy)phenyl)thiourea **5**



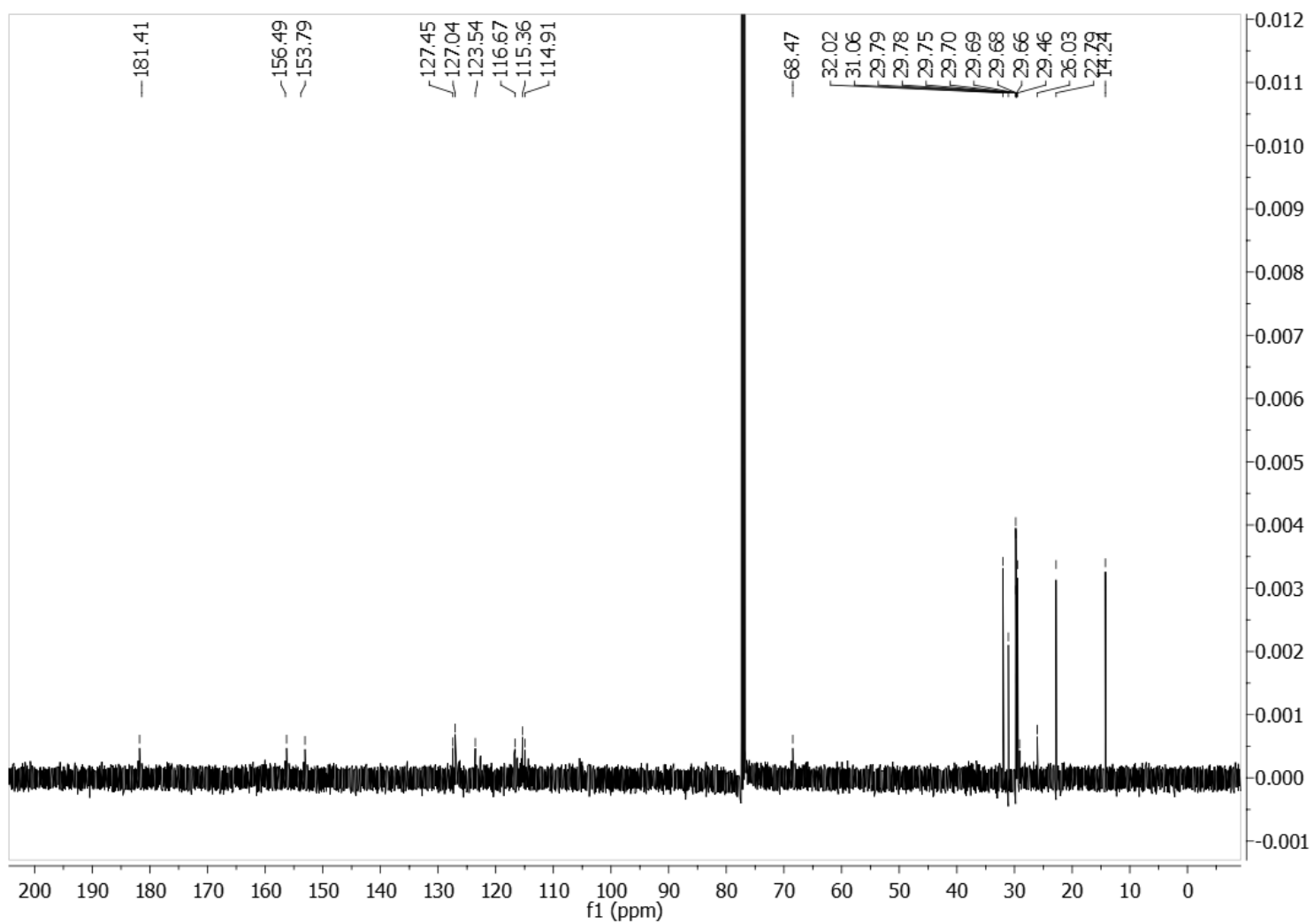
Mass spectrum of 1-(4-fluorophenyl)-3-(4-(octyloxy)phenyl)thiourea **5**



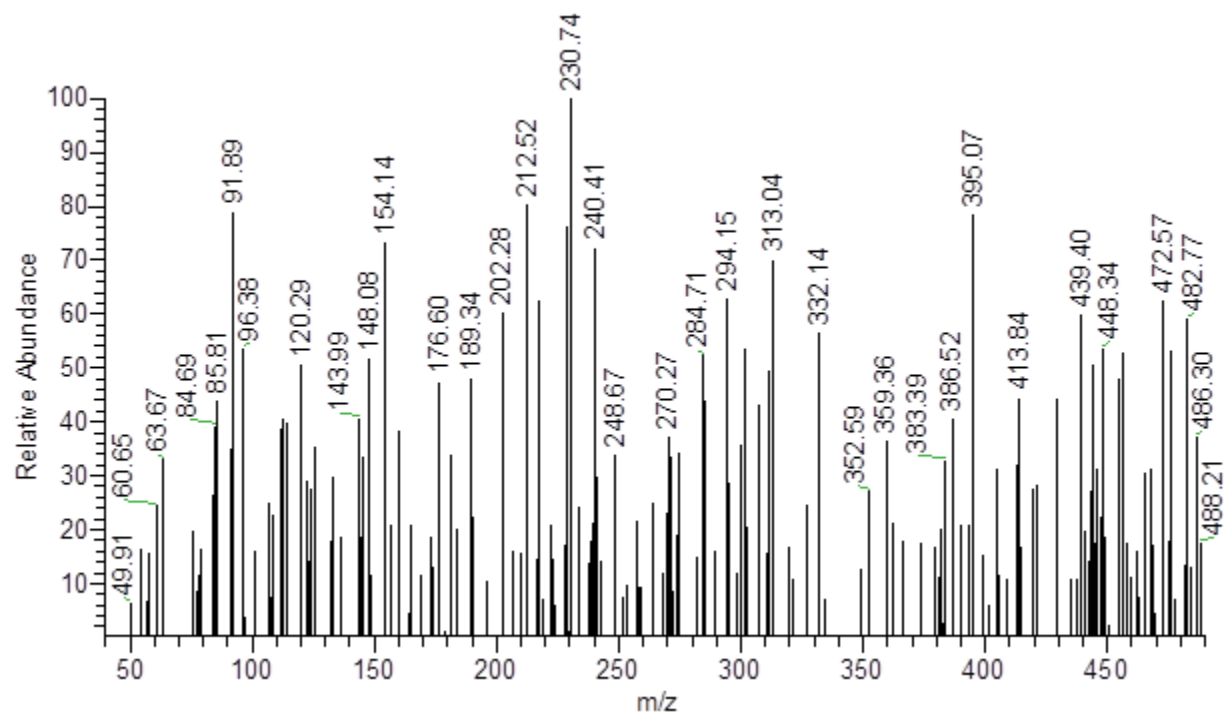
IR (KBr) spectrum of 1-(4-fluorophenyl)-3-(4-(hexadecyloxy)phenyl)thiourea **6**



¹H NMR (CDCl₃) spectrum of 1-(4-fluorophenyl)-3-(4-(hexadecyloxy)phenyl)thiourea **6**



¹³C NMR (CDCl₃) of 1-(4-fluorophenyl)-3-(4-(hexadecyloxy)phenyl)thiourea **6**



Mass spectrum of 1-(4-fluorophenyl)-3-(4-(hexadecyloxy)phenyl)thiourea **6**