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Synthesis, characterization, and DFT studies of *N*-(3,5-*bis*(trifluoromethyl)benzyl)stearamide

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SUPPORTING INFORMATION

Content

1. Copy of the MS spectrum for compound 3

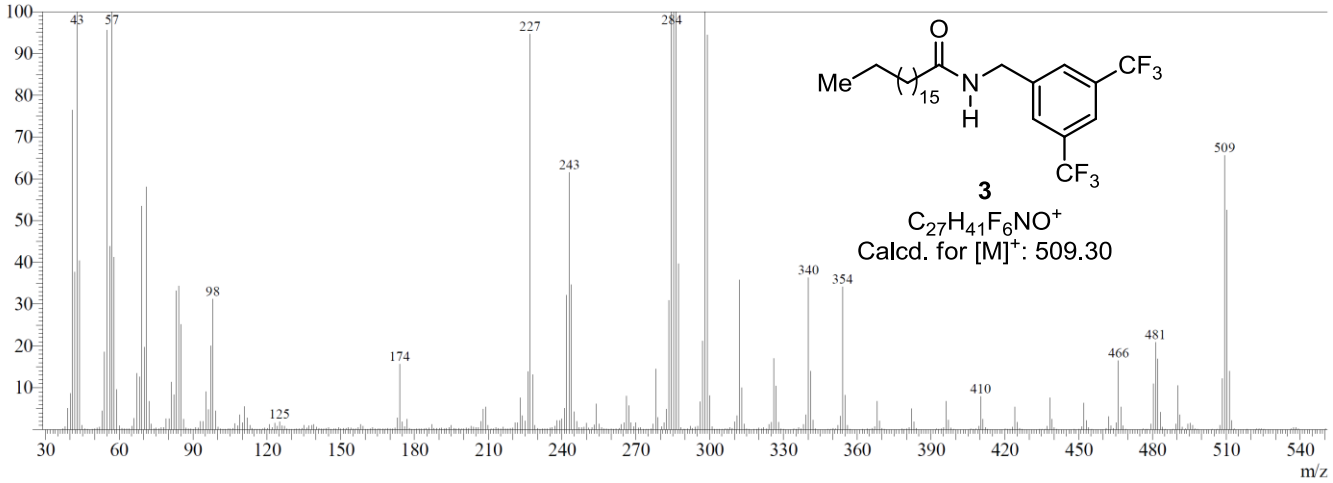

Figure S1. MS spectrum of the compound **3**.

2. Copy of the IR spectrum for compound 3

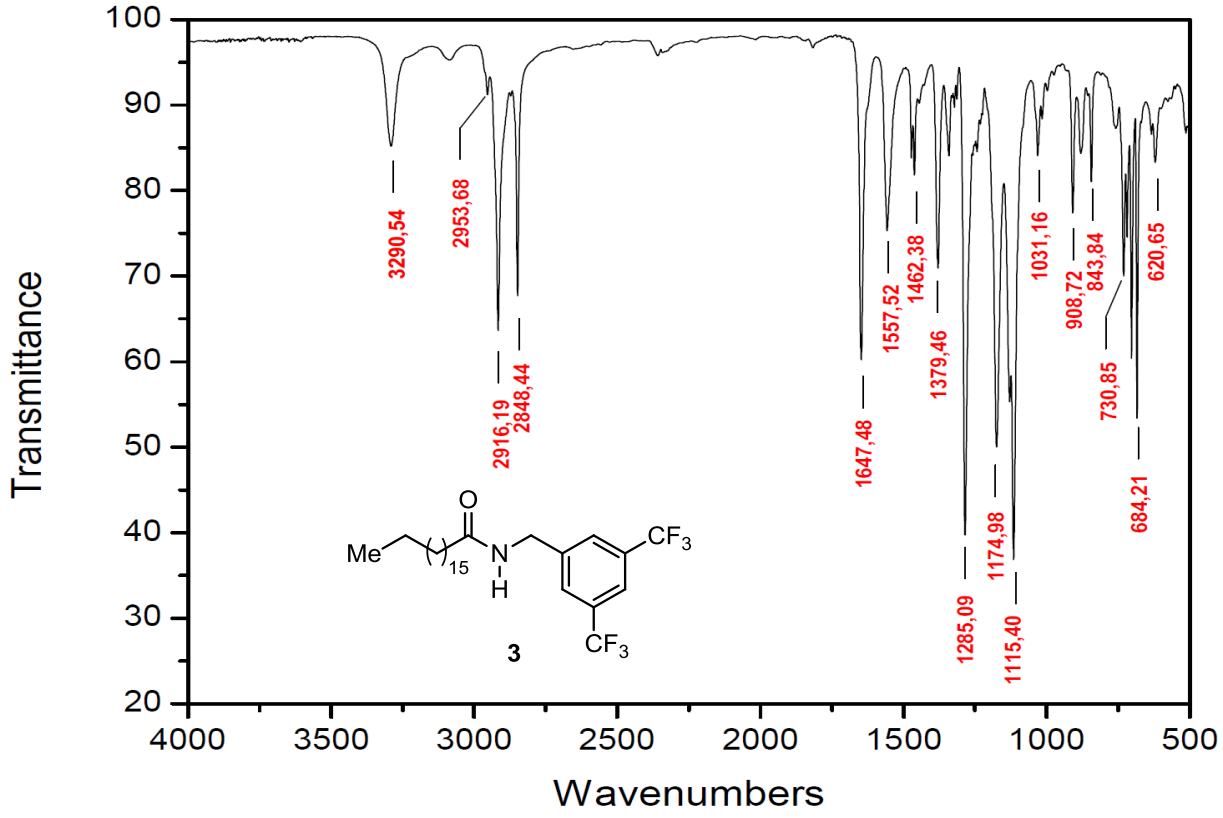

Figure S2. IR spectrum of the compound **3**.

3. Copy of the ^{1}H-NMR spectrum for compound 3

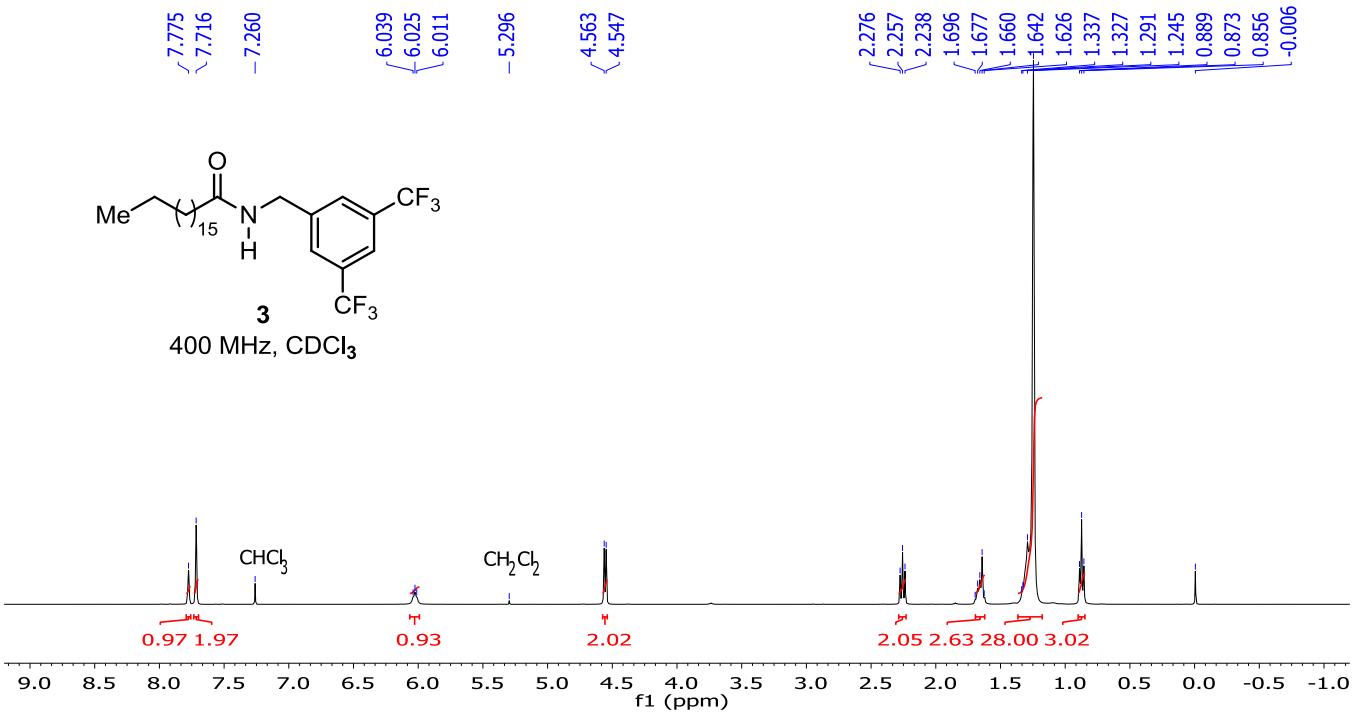

Figure S3. ^{1}H-NMR spectrum of the compound **3**.

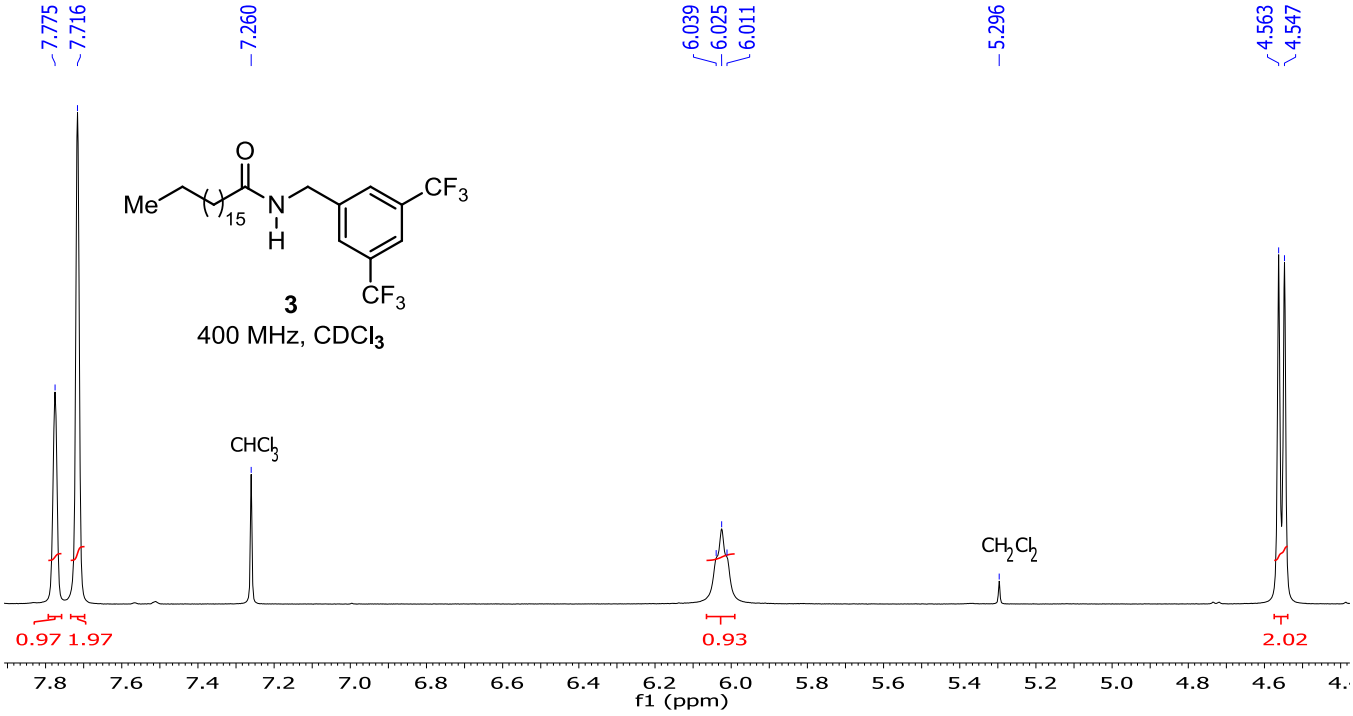

Figure S4. Expansion ^{1}H-NMR spectrum of the compound **3**.

4. Copies of $^{13}C\{^1H\}$-NMR and DEPT-135 spectra for compound 3

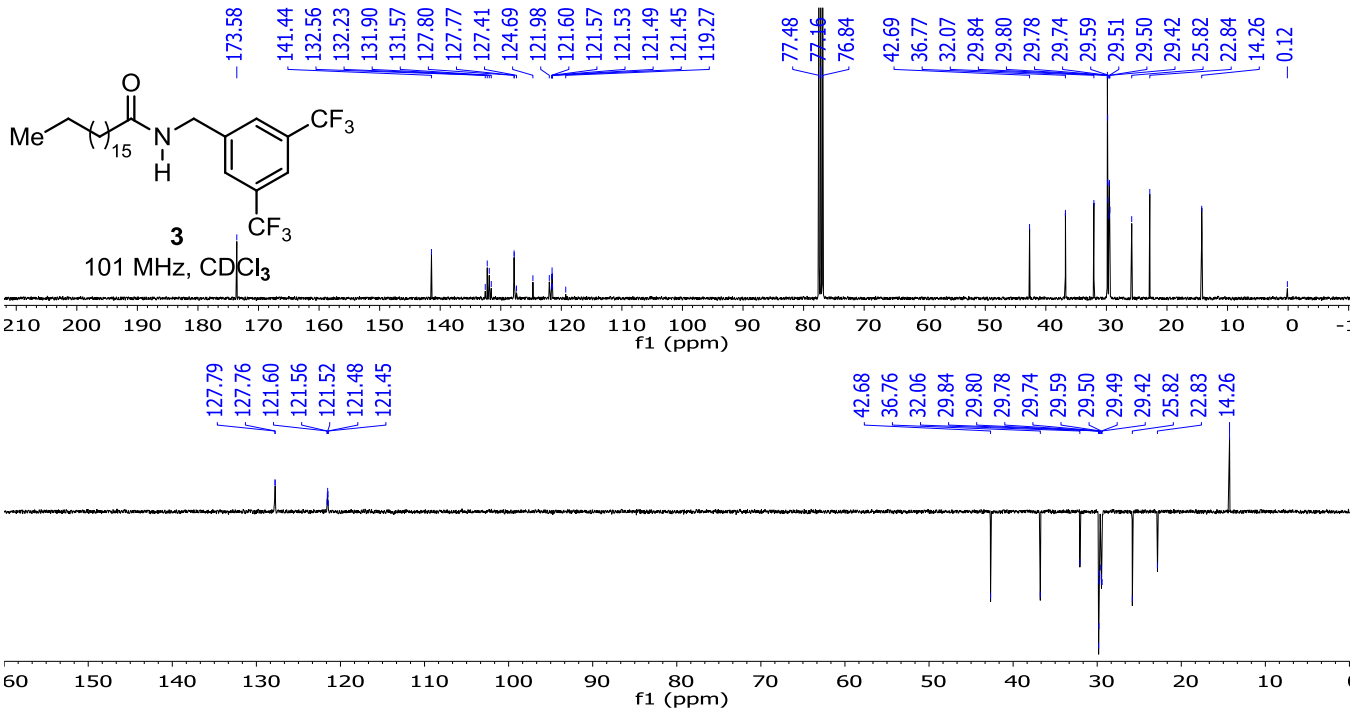

Figure S5. $^{13}C\{^1H\}$-NMR and DEPT-135 spectra of the compound **3**.

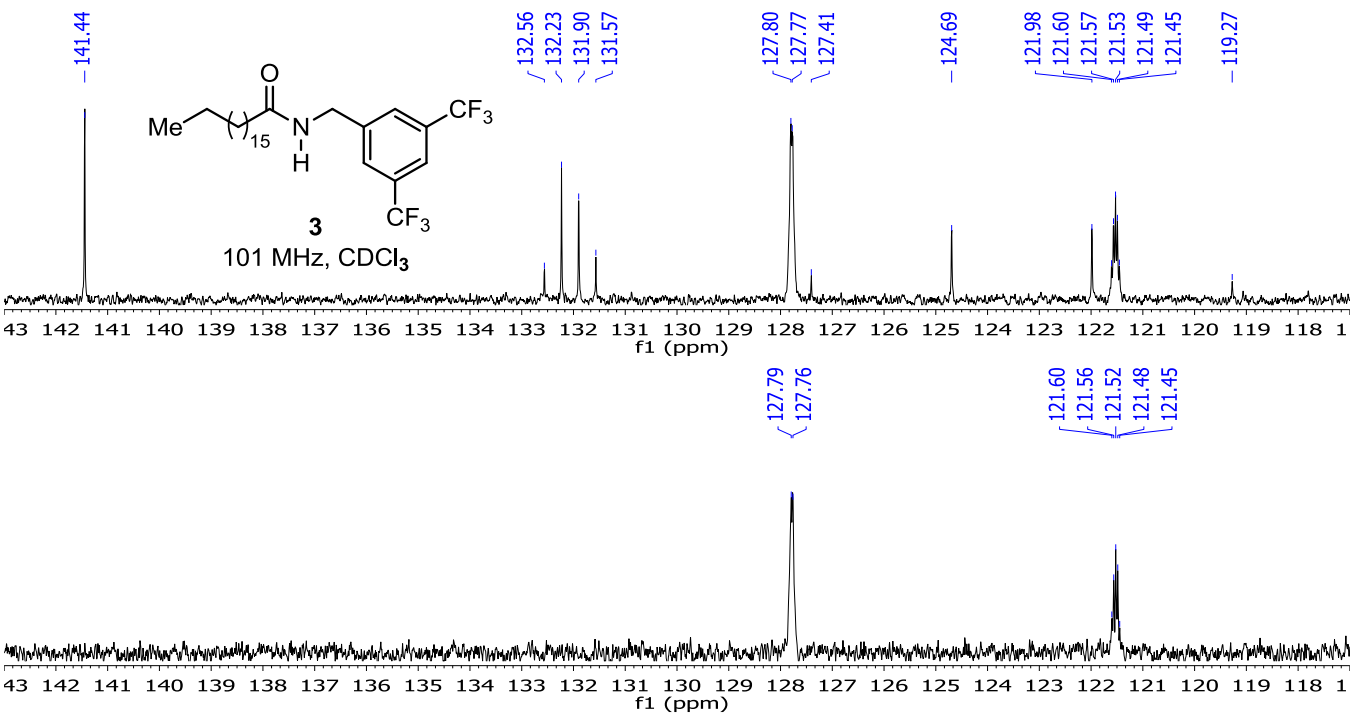

Figure S6. Expansion $^{13}C\{^1H\}$-NMR and DEPT-135 spectra of the compound **3**.

5. Copies of 2D NMR spectra for compound 3

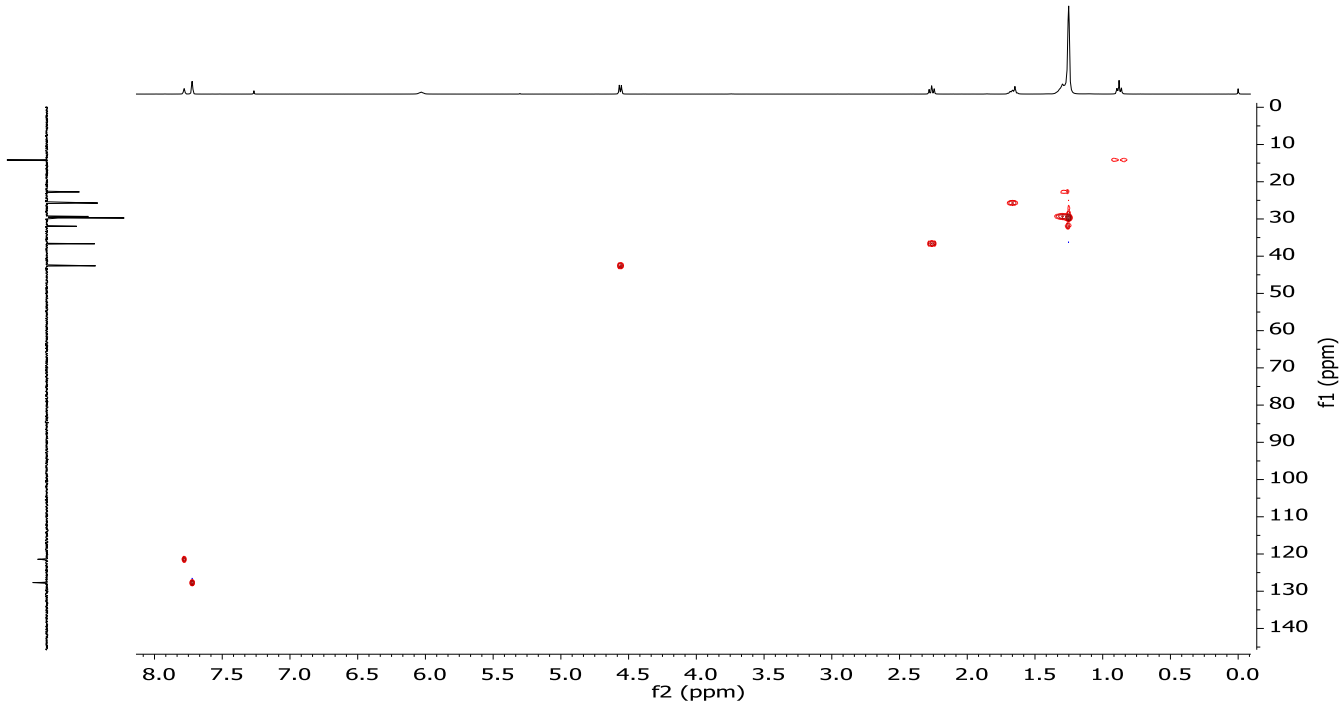

Figure S7. HSQC 2D C–H correlation spectrum of the compound **3**.

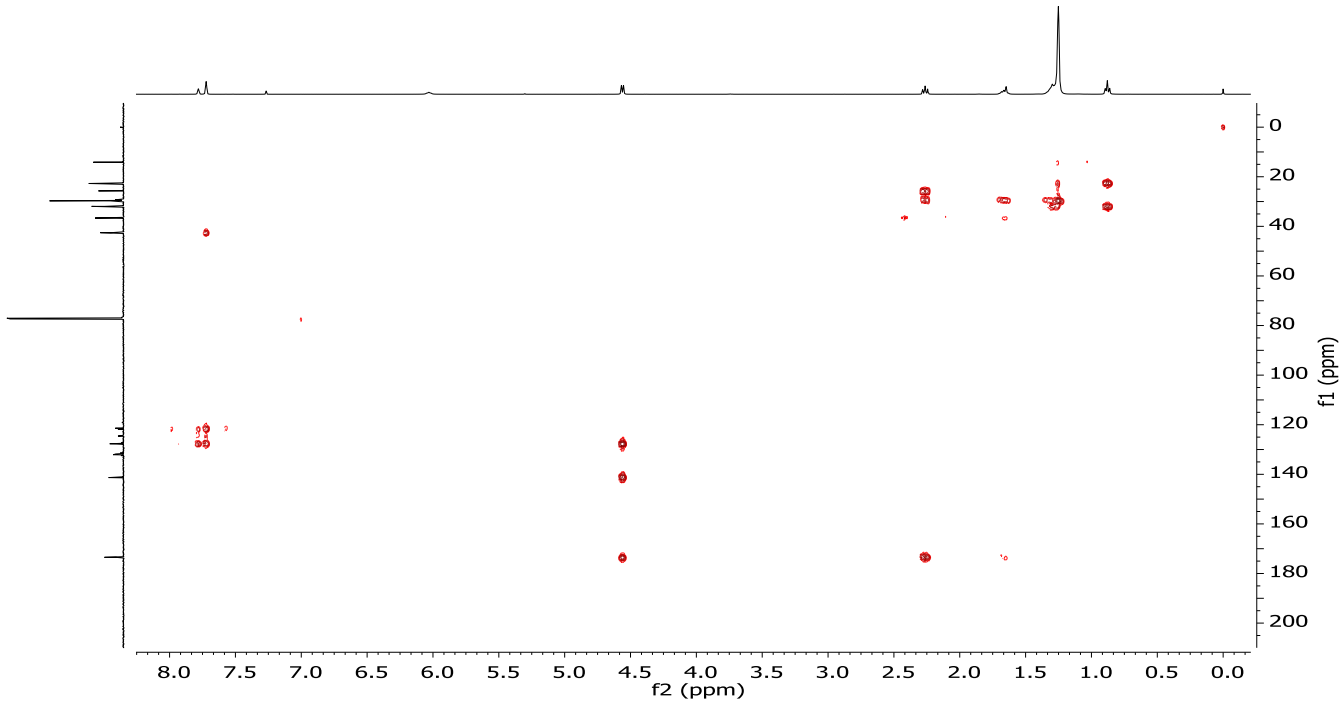

Figure S8. HMBC 2D C–H correlation spectrum of the compound **3**.

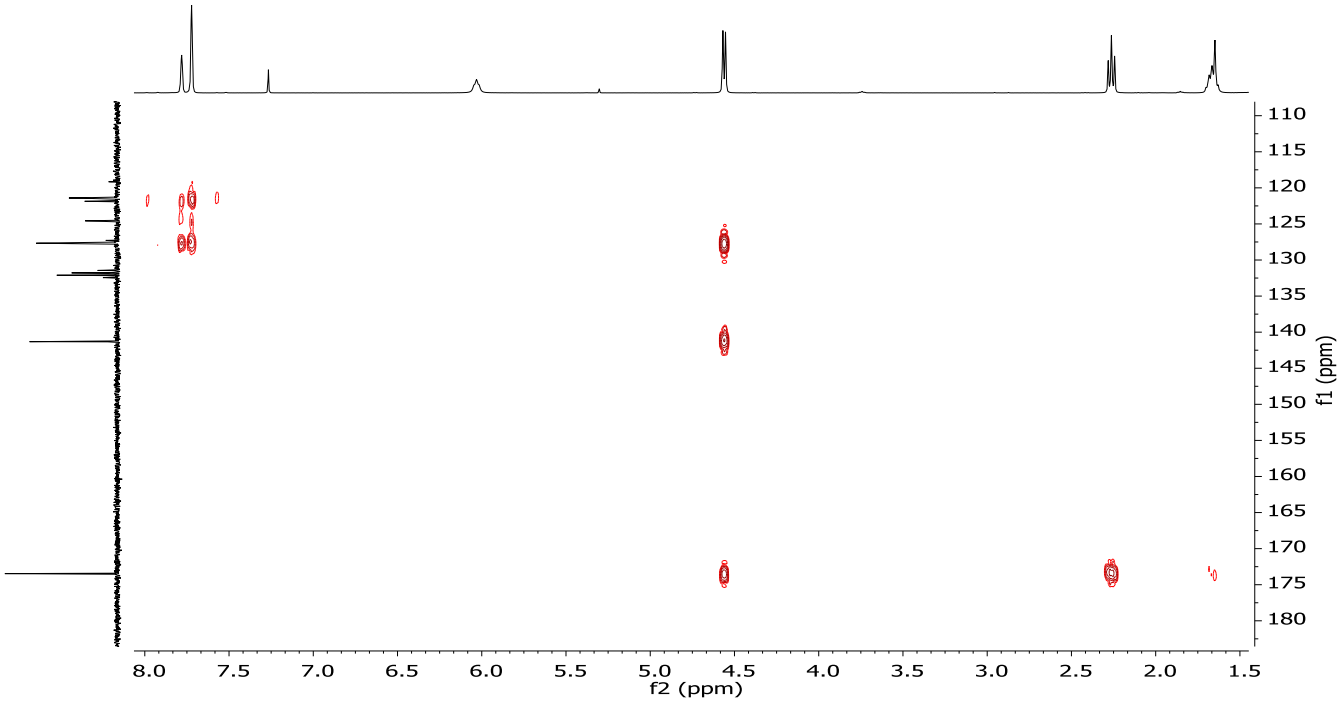

Figure S9. Expansion HMBC 2D C–H correlation spectrum of the compound **3**.

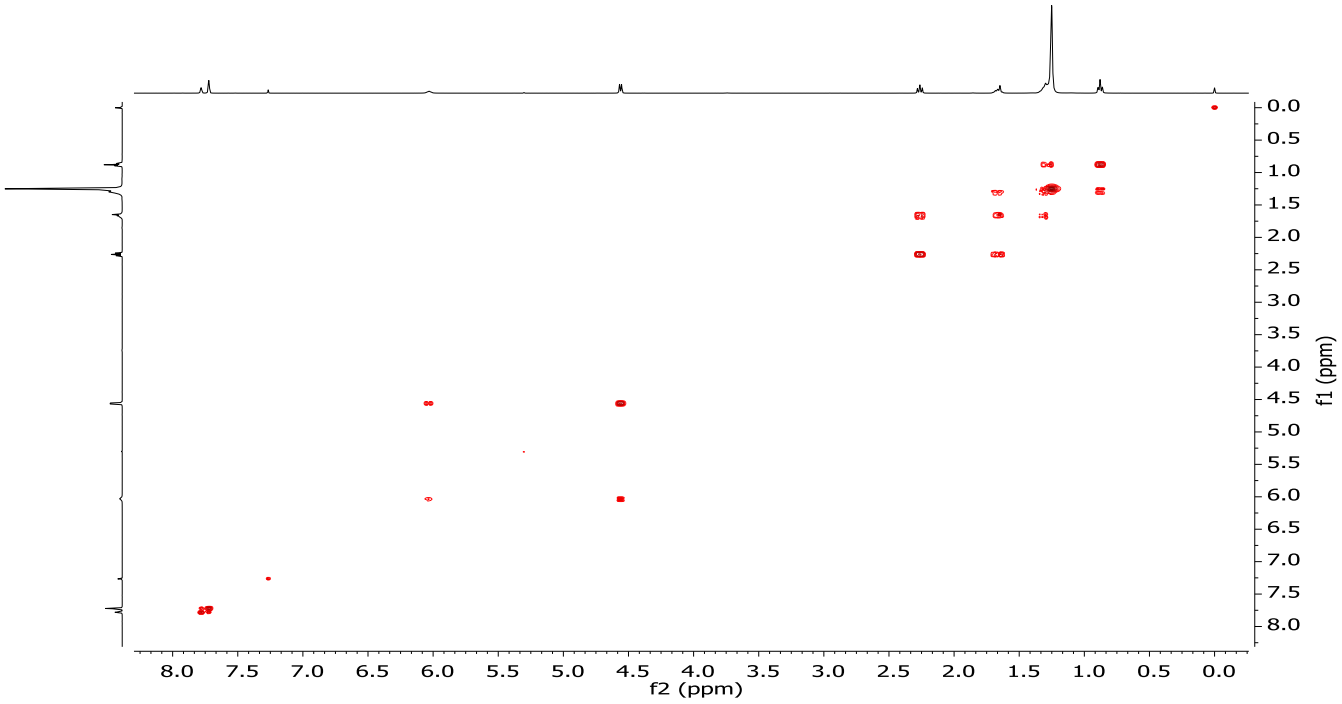

Figure S10. COSY 2D H–H correlation spectrum of the compound **3**.

6. Copy of the UV-Vis spectrum for compound 3

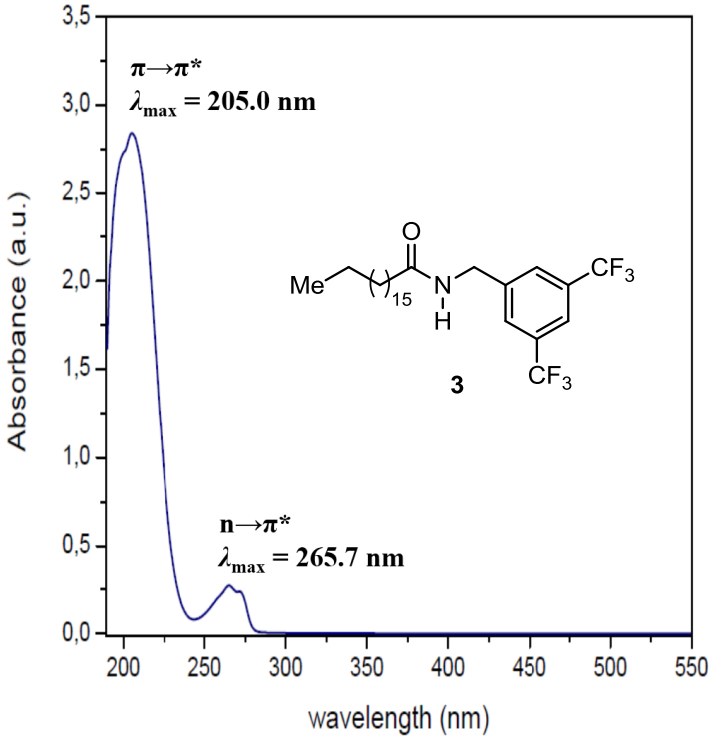

Figure S11. UV–Vis spectrum of the compound **3**.

7. TLC analysis for compound 3

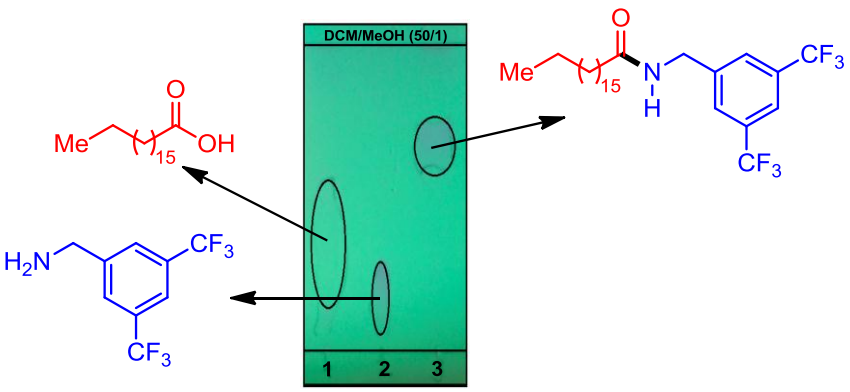

Figure S12. TLC analysis of amide **3** compared to stearic acid **1** and 3,5-*bis*(trifluoromethyl)benzylamine **2** using DCM/MeOH (50/1) as mobile phase under UV lamp, 254 nm.

8. Computational calculations

Table S1. Atomic coordinates of the optimized structure of **3** calculated at the B3LYP/6-311+G(d,p) level theory in gas phase.

C	8.40756000	0.82276400	-0.91880000

C	8.06685400	-0.53061600	-0.79461800
C	7.11127500	-0.93933200	0.13621500
C	6.50001300	0.02613300	0.95260200
C	6.84367700	1.37121100	0.82370600
C	7.79881900	1.78161600	-0.11388000
H	8.55592300	-1.26581400	-1.42777300
H	5.76420800	-0.28726400	1.68670600
H	8.06567100	2.82717100	-0.20632000
C	4.31033100	-2.74077100	0.69793800
C	2.96287900	-3.09848400	0.08629100
C	1.85561000	-2.11526900	0.49887800
H	2.71135900	-4.10412000	0.44842100
H	3.03152100	-3.16231300	-1.00714500
C	0.46984300	-2.53292500	-0.00824600
H	1.85078300	-2.03969700	1.59171300
H	2.09982800	-1.11407600	0.11803800
H	0.49040300	-2.62626600	-1.10415000
H	0.22977900	-3.53382300	0.37919100
C	-0.64181300	-1.55447200	0.39387400
C	-2.03353900	-1.97126400	-0.09995900
H	-0.40280100	-0.55458800	0.00374900
H	-0.65881100	-1.45797800	1.48882100
C	-3.14561400	-0.99282500	0.30073300
H	-2.01535000	-2.06991600	-1.19528600
H	-2.27230300	-2.97080900	0.29178000
H	-3.16179700	-0.89235100	1.39570000
H	-2.90788700	0.00625100	-0.09269300
C	-4.53849700	-1.41074200	-0.18898100
C	-5.65050700	-0.43185600	0.21083400
H	-4.77627600	-2.40947200	0.20553900
H	-4.52212100	-1.51238500	-1.28403200
C	-7.04399400	-0.85075600	-0.27635300
H	-5.66563000	-0.32894300	1.30568500
H	-5.41348200	0.56651500	-0.18494900
H	-7.02883500	-0.95447900	-1.37121400
H	-7.28115600	-1.84883200	0.12021700
C	-8.15586200	0.12855500	0.12282600
C	-9.54974700	-0.29137200	-0.36233400
H	-7.91943700	1.12633100	-0.27487000
H	-8.17003900	0.23335600	1.21754500
C	-10.66159500	0.68811400	0.03648300
H	-9.53562300	-0.39666500	-1.45705200
H	-9.78624300	-1.28896400	0.03585400
H	-10.67510800	0.79419200	1.13110200

H	-10.42574100	1.68550600	-0.36254100
C	-12.05565100	0.26719700	-0.44732600
C	-13.16775000	1.24662500	-0.04898200
H	-12.29154600	-0.73005000	-0.04794200
H	-12.04214300	0.16072000	-1.54192500
C	-14.56185000	0.82506700	-0.53179900
H	-13.18090600	1.35363700	1.04557600
H	-12.93237300	2.24375800	-0.44899700
H	-14.54975200	0.71789700	-1.62649500
H	-14.79828000	-0.17194800	-0.13173500
O	4.44795000	-2.51781700	1.89974000
C	-15.67475400	1.80388700	-0.13410900
H	-15.43957400	2.79989400	-0.53454200
H	-15.68737600	1.91105400	0.95952700
C	6.14578600	2.40857800	1.66835700
C	9.45080200	1.21430500	-1.93347000