

Electronic Supplementary Information

Synthesis and properties of ionic liquids based on mecoprop

Juliusz Pernak,^{a*} Adrian Luboiński^b, Agnieszka Łacka^c, Tadeusz Praczyk^b

^aDepartment of Chemical Technology, Poznan University of Technology, Poznan 60-965, Poland

^bInstitute of Plant Protection, National Research Institute, Poznan 60-318, Poland

^cDepartment of Mathematical and Statistical Methods, Poznan University of Life Sciences, Poznan 60-637, Poland

* Corresponding author at: E-mail: juliusz.pernak@put.poznan.pl

1-Ethyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**1**) 98% yield. ¹H NMR (300 MHz, CDCl₃) δ [ppm] = 1.20 (t, *J* = 7.1 Hz, 3H); 1.57 (m, 3H); 1.62 (m, 2H); 1.71 (m, 4H); 2.22 (s, 3H); 2.96 (s, 3H); 3.31 (m, 4H); 3.40 (m, 2H); 4.48 (m, 1H); 6.78 (d, *J* = 8.5 Hz, 1H); 6.95 (m, 1H); 7.04 (d, *J* = 2.1 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ [ppm] = 155.7; 129.6; 128.5; 125.7; 123.7; 113.2; 75.6; 59.9; 57.9; 46.9; 20.5; 19.7; 19.1; 16.1; 7.2. Elemental analysis calcd for C₁₈H₂₈ClNO₃ (M_{mol} = 341.9 g mol⁻¹) (%): C = 63.24; H = 8.26; N = 4.10; found: C = 63.01; H = 8.43; N = 4.27.

1-Methyl-1-propylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**2**) 96% yield. ¹H NMR (300 MHz, CDCl₃) δ [ppm] = 0.92 (t, *J* = 7.2 Hz, 3H); 1.55 (m, 5H); 1.61 (m, 2H); 1.67 (m, 4H); 2.21 (s, 3H); 2.93 (s, 3H); 3.17 (m, 4H); 3.26 (m, 2H); 4.47 (m, 1H); 6.76 (d, *J* = 7.6 Hz, 1H); 6.96 (d, *J* = 6.4 Hz, 1H); 7.03 (d, *J* = 2.2 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ [ppm] = 155.6; 129.6; 128.5; 125.8; 123.8; 113.2; 75.3; 63.8; 60.4; 47.9; 20.5; 19.7; 19.1; 16.1; 14.9; 10.5. Elemental analysis calcd for C₁₉H₃₀ClNO₃ (M_{mol} = 355.9 g mol⁻¹) (%): C = 64.12; H = 8.50; N = 3.94; found: C = 63.85; H = 8.17; N = 4.23.

1-Butyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**3**) 94% yield. ¹H NMR (300 MHz, CDCl₃) δ [ppm] = 0.90 (t, *J* = 7.0 Hz, 3H); 1.30 (m, 2H); 1.57 (m, 4H); 1.62 (m, 3H); 1.67 (m, 4H); 2.20 (s, 3H); 3.09 (s, 3H); 3.38 (m, 4H); 3.49 (m, 2H); 4.47 (m, 1H); 6.77 (d, *J*

= 7.2 Hz, 1H); 6.96 (d, J = 6.2 Hz, 1H); 7.03 (d, J = 2.1 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 155.7; 129.6; 128.2; 125.7; 123.7; 113.2; 62.2; 60.3; 47.9; 31.4; 29.0; 28.8; 22.3; 19.8; 14.2; 13.8. Elemental analysis calcd for $\text{C}_{20}\text{H}_{32}\text{ClNO}_3$ (M_{mol} = 369.2 g mol $^{-1}$) (%): C = 64.94; H = 8.72; N = 3.79; found: C = 65.18; H = 8.55; N = 3.98.

1-Methyl-1-pentylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**4**) 97% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.91 (t, J = 7.1 Hz, 3H); 1.33 (m, 4H); 1.56 (m, 4H); 1.63 (m, 3H); 1.74 (m, 4H); 2.22 (s, 3H); 3.09 (s, 3H); 3.38 (m, 4H); 3.48 (m, 2H); 4.46 (m, 1H); 6.79 (d, J = 8.5 Hz, 1H); 6.94 (dd, J = 2.4; 8.5 Hz, 1H); 7.03 (d, J = 2.5 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 176.1; 155.6; 129.5; 128.3; 125.6; 123.6; 113.2; 75.7; 62.4; 60.3; 47.7; 28.0; 21.9; 21.2; 20.4; 19.8; 19.1; 16.1; 14.9; 13.5. Elemental analysis calcd for $\text{C}_{21}\text{H}_{34}\text{ClNO}_3$ (M_{mol} = 383.9 g mol $^{-1}$) (%): C = 65.69; H = 8.93; N = 3.65; found: C = 65.92; H = 8.61; N = 3.85.

1-Hexyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**5**) 95% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.89 (t, J = 6.6 Hz, 3H); 1.30 (m, 6H); 1.58 (m, 4H); 1.63 (m, 3H); 1.74 (m, 4H); 2.23 (s, 3H); 3.06 (s, 3H); 3.34 (m, 4H); 3.43 (m, 2H); 4.47 (m, 1H); 6.79 (d, J = 8.6 Hz, 1H); 6.94 (dd, J = 2.4; 8.4 Hz, 1H); 7.03 (d, J = 2.63 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 176.2; 155.7; 129.6; 128.4; 125.6; 123.6; 113.5; 75.6; 62.5; 60.4; 47.9; 31.0; 25.7; 22.1; 21.6; 20.4; 19.8; 19.1; 16.1; 13.6. Elemental analysis calcd for $\text{C}_{22}\text{H}_{36}\text{ClNO}_3$ (M_{mol} = 397.9 g mol $^{-1}$) (%): C = 66.39; H = 9.12; N = 3.52; found: C = 66.22; H = 8.87; N = 3.76.

1-Heptyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**6**) 94% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.89 (t, J = 6.9 Hz, 3H); 1.30 (m, 8H); 1.57 (m, 4H); 1.63 (m, 3H); 1.74 (m, 4H); 2.22 (s, 3H); 3.06 (s, 3H); 3.36 (m, 4H); 3.43 (m, 2H); 4.47 (m, 1H); 6.76 (d, J = 8.6 Hz, 1H); 6.94 (dd, J = 2.2; 8.6 Hz, 1H); 7.04 (d, J = 2.0 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 155.5; 129.5; 128.3; 125.6; 123.6; 113.0; 75.5; 62.4; 60.3; 47.7; 31.2; 28.5; 25.9; 22.1; 21.5; 20.3; 19.7; 19.0; 16.1; 13.7. Elemental analysis calcd for $\text{C}_{23}\text{H}_{38}\text{ClNO}_3$ (M_{mol} = 412.0 g mol $^{-1}$) (%): C = 67.05; H = 9.30; N = 3.40; found: C = 67.35; H = 9.52; N = 3.59.

1-Methyl-1-octylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**7**) 96% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.89 (t, J = 6.9 Hz, 3H); 1.30 (m, 10H); 1.57 (m, 4H); 1.63 (m, 3H); 1.74 (m, 4H); 2.22 (s, 3H); 3.05 (s, 3H); 3.36 (m, 4H); 3.43 (m, 2H); 4.47 (m, 1H); 6.76 (d, J = 8.6 Hz, 1H); 6.94 (dd, J = 2.3; 8.5 Hz, 1H); 7.04 (d, J = 2.0 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 176.0; 155.6; 129.5; 128.3; 125.6;

123.5; 113.1; 75.5; 62.2; 60.2; 47.7; 31.3; 28.8; 28.7; 26.0; 22.2; 21.5; 20.3; 19.7; 19.0; 16.1; 13.7. Elemental analysis calcd for $C_{24}H_{40}ClNO_3$ ($M_{mol} = 426.0 \text{ g mol}^{-1}$) (%): C = 67.66; H = 9.46; N = 3.29; found: C = 67.91; H = 9.17; N = 3.42.

1-Methyl-1-nonylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**8**) 92% yield. 1H NMR (300 MHz, $CDCl_3$) δ [ppm] = 0.88 (t, $J = 6.7$ Hz, 3H); 1.26 (m, 12H); 1.56 (m, 4H); 1.63 (m, 3H); 1.76 (m, 4H); 2.23 (s, 3H); 3.08 (s, 3H); 3.36 (m, 4H); 3.46 (m, 2H); 4.50 (m, 1H); 6.79 (d, $J = 8.7$ Hz, 1H); 6.94 (dd, $J = 2.4$; 8.6 Hz, 1H); 7.04 (d, $J = 1.95$ Hz, 1H) ^{13}C NMR (75 MHz, $CDCl_3$) δ [ppm] = 176.2; 155.7; 129.6; 128.5; 125.7; 123.7; 113.2; 75.7; 62.3; 60.4; 48.0; 31.5; 29.1; 29.0; 28.9; 26.2; 22.4; 21.7; 20.5; 19.9; 19.2; 16.2; 13.9. Elemental analysis calcd for $C_{25}H_{42}ClNO_3$ ($M_{mol} = 440.0 \text{ g mol}^{-1}$) (%): C = 68.23; H = 9.62; N = 3.18; found: C = 67.93; H = 9.38; N = 3.40.

1-Decyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**9**) 98% yield. 1H NMR (300 MHz, $CDCl_3$) δ [ppm] = 0.88 (t, $J = 6.7$ Hz, 3H); 1.26 (m, 14H); 1.57 (m, 4H); 1.64 (m, 3H); 1.76 (m, 4H); 2.22 (s, 3H); 3.07 (s, 3H); 3.36 (m, 4H); 3.44 (m, 2H); 4.47 (m, 1H); 6.79 (d, $J = 8.4$ Hz, 1H); 6.95 (d, $J = 6.1$ Hz, 1H); 7.03 (d, $J = 2.47$ Hz, 1H) ^{13}C NMR (75 MHz, $CDCl_3$) δ [ppm] = 176.1; 155.7; 129.6; 128.4; 125.7; 123.7; 113.2; 75.6; 62.4; 60.4; 47.9; 31.5; 29.1; 29.1; 29.0; 28.9; 26.1; 22.3; 21.6; 20.4; 19.8; 19.1; 16.1; 13.8. Elemental analysis calcd for $C_{26}H_{44}ClNO_3$ ($M_{mol} = 454.0 \text{ g mol}^{-1}$) (%): C = 68.77; H = 9.77; N = 3.08; found: C = 68.44; H = 9.61; N = 3.33.

1-Methyl-1-undecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**10**) 95% yield. 1H NMR (300 MHz, $CDCl_3$) δ [ppm] = 0.88 (t, $J = 6.8$ Hz, 3H); 1.26 (m, 16H); 1.56 (m, 4H); 1.65 (m, 3H); 1.74 (m, 4H); 2.23 (s, 3H); 3.08 (s, 3H); 3.36 (m, 4H); 3.45 (m, 2H); 4.50 (m, 1H); 6.79 (d, $J = 8.6$ Hz, 1H); 6.94 (dd, $J = 2.5$; 8.6 Hz, 1H); 7.03 (d, $J = 3.3$ Hz, 1H) ^{13}C NMR (75 MHz, $CDCl_3$) δ [ppm] = 176.0; 155.6; 129.5; 128.4; 125.6; 123.6; 113.1; 75.5; 62.3; 60.3; 47.8; 31.5; 29.2; 29.1; 29.0; 28.9; 26.0; 22.3; 21.6; 20.4; 19.7; 19.0; 16.1; 13.8. Elemental analysis calcd for $C_{27}H_{46}ClNO_3$ ($M_{mol} = 468.1 \text{ g mol}^{-1}$) (%): C = 69.28; H = 9.90; N = 2.99; found: C = 69.56; H = 10.21; N = 3.12.

1-Dodecyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**11**) 99% yield. 1H NMR (300 MHz, $CDCl_3$) δ [ppm] = 0.88 (t, $J = 6.8$ Hz, 3H); 1.26 (m, 18H); 1.56 (m, 4H); 1.63 (m, 3H); 1.76 (m, 4H); 2.22 (s, 3H); 3.07 (s, 3H); 3.30 (m, 4H); 3.45 (m, 2H); 4.46 (m, 1H); 6.76 (d, $J = 8.6$ Hz, 1H); 6.95 (dd, $J = 2.6$; 8.6 Hz, 1H); 7.03 (d, $J = 2.6$ Hz, 1H) ^{13}C NMR (75 MHz, $CDCl_3$) δ [ppm] = 176.4; 155.7; 129.6; 128.5; 125.8; 123.7; 113.2; 75.8; 62.2; 60.4; 48.1; 31.7; 29.4; 29.3; 29.2; 29.1; 29.0; 26.2; 22.5; 21.7; 20.5; 19.8. 19.2; 16.2; 13.9. Elemental analysis calcd for $C_{28}H_{48}ClNO_3$ ($M_{mol} = 482.1 \text{ g mol}^{-1}$) (%): C = 69.75; H = 10.03; N = 2.91; found: C = 69.48; H = 9.88; N = 3.17.

1-Methyl-1-tetradecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**12**) 93% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.88 (t, J = 6.8 Hz, 3H); 1.26 (m, 22H); 1.56 (m, 4H); 1.67 (m, 3H); 1.75 (m, 4H); 2.23 (s, 3H); 3.08 (s, 3H); 3.36 (m, 4H); 3.47 (m, 2H); 4.48 (m, 1H); 6.79 (d, J = 8.7 Hz, 1H); 6.94 (dd, J = 2.4; 8.5 Hz, 1H); 7.04 (d, J = 2.6 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 176.1; 155.7; 129.6; 128.4; 123.6; 113.1; 75.5; 62.3; 60.3; 47.9; 31.6; 29.4; 29.3; 29.2; 29.1; 29.0; 28.9; 26.1; 22.4; 21.6; 20.4; 19.8; 19.1; 16.1; 13.9 Elemental analysis calcd for $\text{C}_{30}\text{H}_{52}\text{ClNO}_3$ (M_{mol} = 510.1 g mol $^{-1}$) (%): C = 70.62; H = 10.27; N = 2.75; found: C = 70.45; H = 10.49; N = 2.90.

1-Hexadecyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**13**) 92% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.88 (t, J = 6.6 Hz, 3H); 1.26 (m, 24H); 1.58 (m, 4H); 1.64 (m, 3H); 1.75 (m, 4H); 2.23 (s, 3H); 3.09 (s, 3H); 3.33 (m, 4H); 3.46 (m, 2H); 4.51 (m, 1H); 6.79 (d, J = 8.6 Hz, 1H); 6.95 (dd, J = 2.5; 8.6 Hz, 1H); 7.03 (d, J = 2.6 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 176.2; 155.8; 129.7; 128.6; 125.8; 123.8; 113.2; 75.6; 62.3; 60.4; 48.1; 31.7; 29.5; 29.4; 29.3; 29.2; 29.1; 29.0; 26.3; 22.5; 21.7; 20.5; 19.9; 19.2; 16.2; 13.9 Elemental analysis calcd for $\text{C}_{32}\text{H}_{56}\text{ClNO}_3$ (M_{mol} = 538.2 g mol $^{-1}$) (%): C = 71.41; H = 10.49; N = 2.60; found: C = 71.71; H = 10.11; N = 2.82.

1-Methyl-1-octadecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**14**) 94% yield. ^1H NMR (300 MHz, CDCl_3) δ [ppm] = 0.88 (t, J = 6.7 Hz, 3H); 1.26 (m, 28H); 1.58 (m, 4H); 1.64 (m, 3H); 1.73 (m, 4H); 2.22 (s, 3H); 3.09 (s, 3H); 3.37 (m, 4H); 3.49 (m, 2H); 4.46 (m, 1H); 6.80 (d, J = 8.6 Hz, 1H); 6.94 (dd, J = 2.4; 8.6 Hz, 1H); 7.03 (d, J = 2.0 Hz, 1H) ^{13}C NMR (75 MHz, CDCl_3) δ [ppm] = 176.0; 155.7; 129.5; 128.4; 125.7; 123.6; 113.2; 75.7; 62.2; 60.2; 47.8; 31.6; 29.3; 29.2; 29.1; 29.0; 28.9; 26.1; 22.4; 21.6; 20.4; 19.8; 19.1; 16.1; 13.8; Elemental analysis calcd for $\text{C}_{34}\text{H}_{60}\text{ClNO}_3$ (M_{mol} = 566.3 g mol $^{-1}$) (%): C = 72.11; H = 10.68; N = 2.47; found: C = 72.39; H = 10.95; N = 2.62.

Greenhouse experiments

Due to the fact that commercial preparations comprising MCPP-P were not available on the market, the herbicidal effects were compared with a commercial herbicide: MCPA in the form of sodium and potassium salts (Chwastox Extra 300 SL). The samples were dissolved in water in an amount, which equalled 400 g of active substance per 1 ha. The test plants included common lambsquarters (*Chenopodium album* L.), cornflower (*Centaurea cyanus* L.) and white mustard (*Sinapis alba* L.). The seeds were planted to pots (volume of 0.82 L) filled with a slightly acidic (pH 5.2 – 6.3) substrate for growing plants. After growing of leaves the plants were thinned to 5 per pot. After reaching the BBCH 14/16 stage, the plants were treated with a spray, which included the studied compounds. A cabin sprayer equipped with a Tee Jet XR 110/02 VP spraying nozzle

was used. The sprayer was placed 50 cm from the plant tops and moved at a constant velocity of 3.36 km/h. The liquid pressure in the sprayer was at 0.15 MPA, the working solution was applied at 200 L per 1 ha. After treatment the plants in the pots were placed in the greenhouse. The greenhouse tests were carried out under the following conditions: temperature – 20°C ($\pm 2^\circ\text{C}$), humidity – 60%, photoperiod day/night – 16/8 hours. The efficacy of the studied compounds was evaluated visually 1 week, 2 weeks and 3 after treatment (WAT) in comparison to control (plants not treated with herbicides). The results of the evaluation were expressed in a percentage scale, where 100% refers to total destruction of weeds, whereas 0% refers to a lack of effect of the tested compounds. All tests were conducted using 4 repetitions.

Acquisition Time (sec)	4.9999	Comment	AB 27	Date	Apr 16 2015	Date Stamp	Apr 16 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB27-H1.fid\AB27-H1.fid\fid			Frequency (MHz)	300.07	Nucleus	¹ H
Number of Transients	64	Original Points Count	16458	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Receiver Gain	6.00	Spectrum Type	STANDARD
Temperature (degree C)	AMBIENT TEMPERATURE			Spectrum Offset (Hz)	1505.5831	Sweep Width (Hz)	3291.64

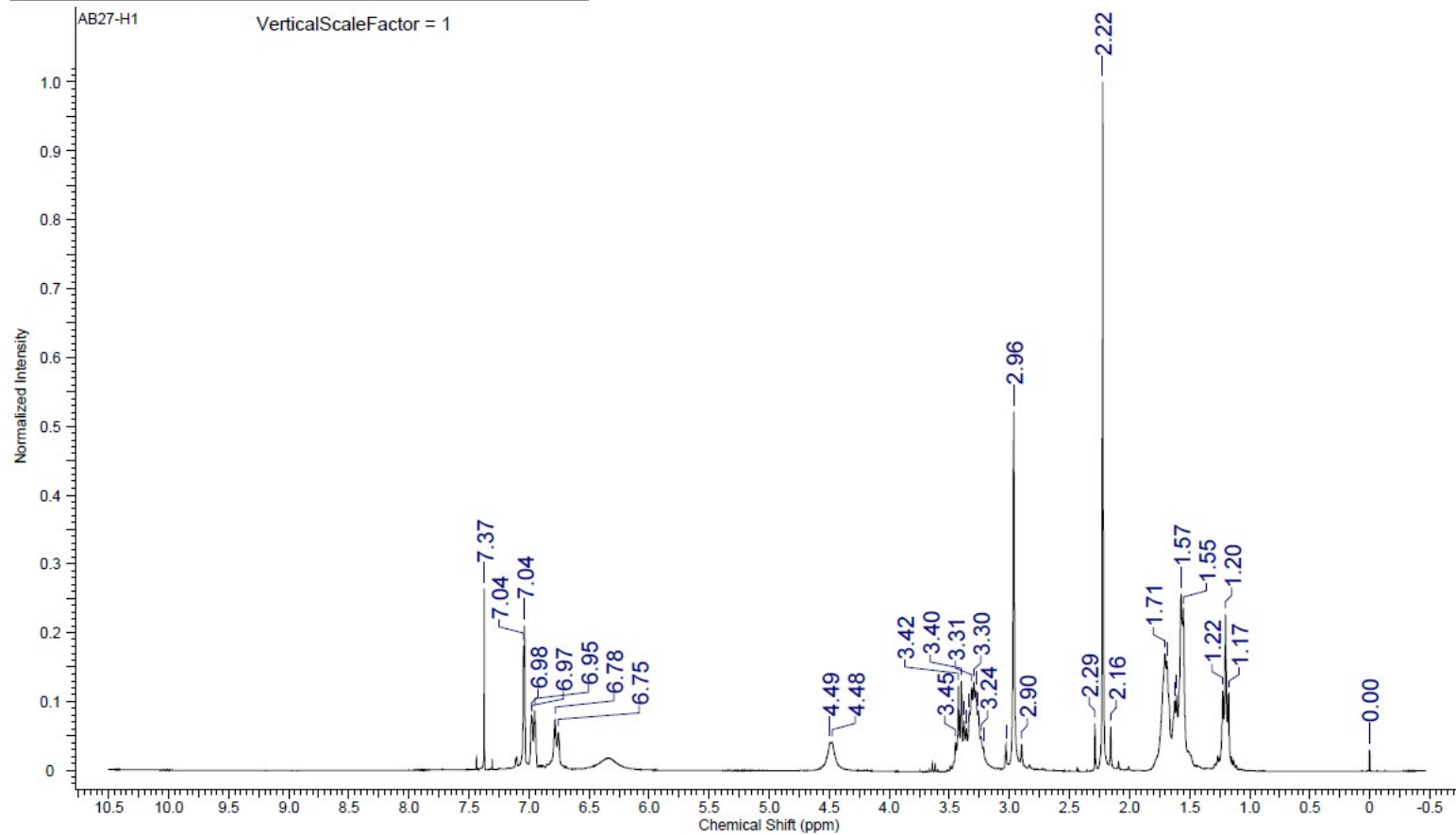


Figure S1. ¹H NMR spectrum of 1-ethyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**1**)

Acquisition Time (sec)	0.6400	Comment	AB 27	Date	Apr 16 2015	Date Stamp	Apr 16 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB27-C13.fid\AB27-C13.fid\fid				Frequency (MHz)	75.46	
Nucleus	¹³ C	Number of Transients	1628	Original Points Count	12191	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	34.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7947.3286	Spectrum Type	STANDARD	Sweep Width (Hz)	19047.62	Temperature (degree C) AMBIENT TEMPERATURE	

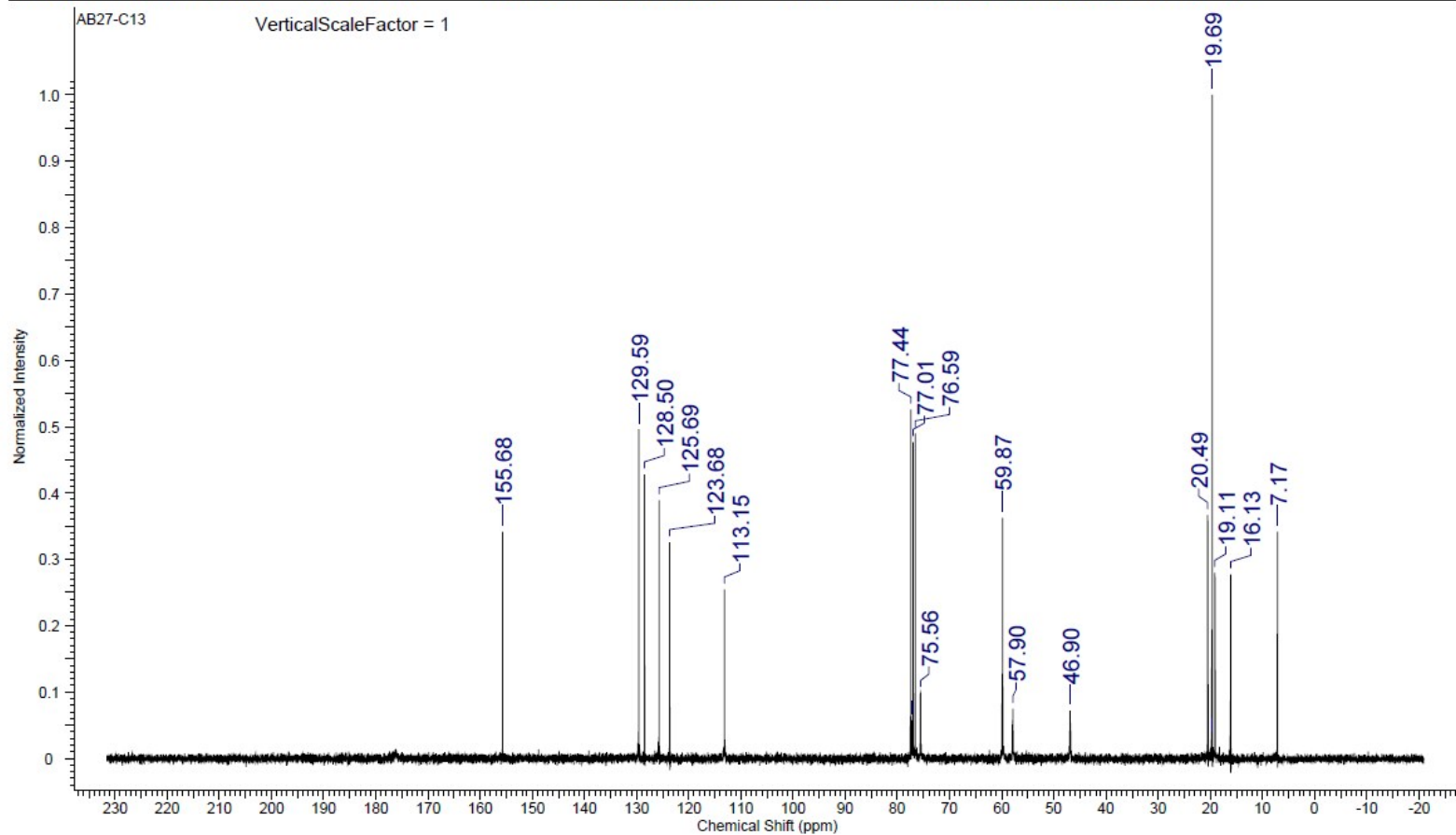


Figure S2. ¹³C NMR spectrum of 1-ethyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**1**)

Acquisition Time (sec)	4.5002	Comment	AB-28	Date	Apr 23 2015	Date Stamp	Apr 23 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-28.fid\AB-28.fid\fid					Frequency (MHz)	402.64	Nucleus	1H
Number of Transients	64	Original Points Count	20090	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	24.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	1978.6017	Spectrum Type	STANDARD	Sweep Width (Hz)	4464.29
Temperature (degree C)	AMBIENT TEMPERATURE								

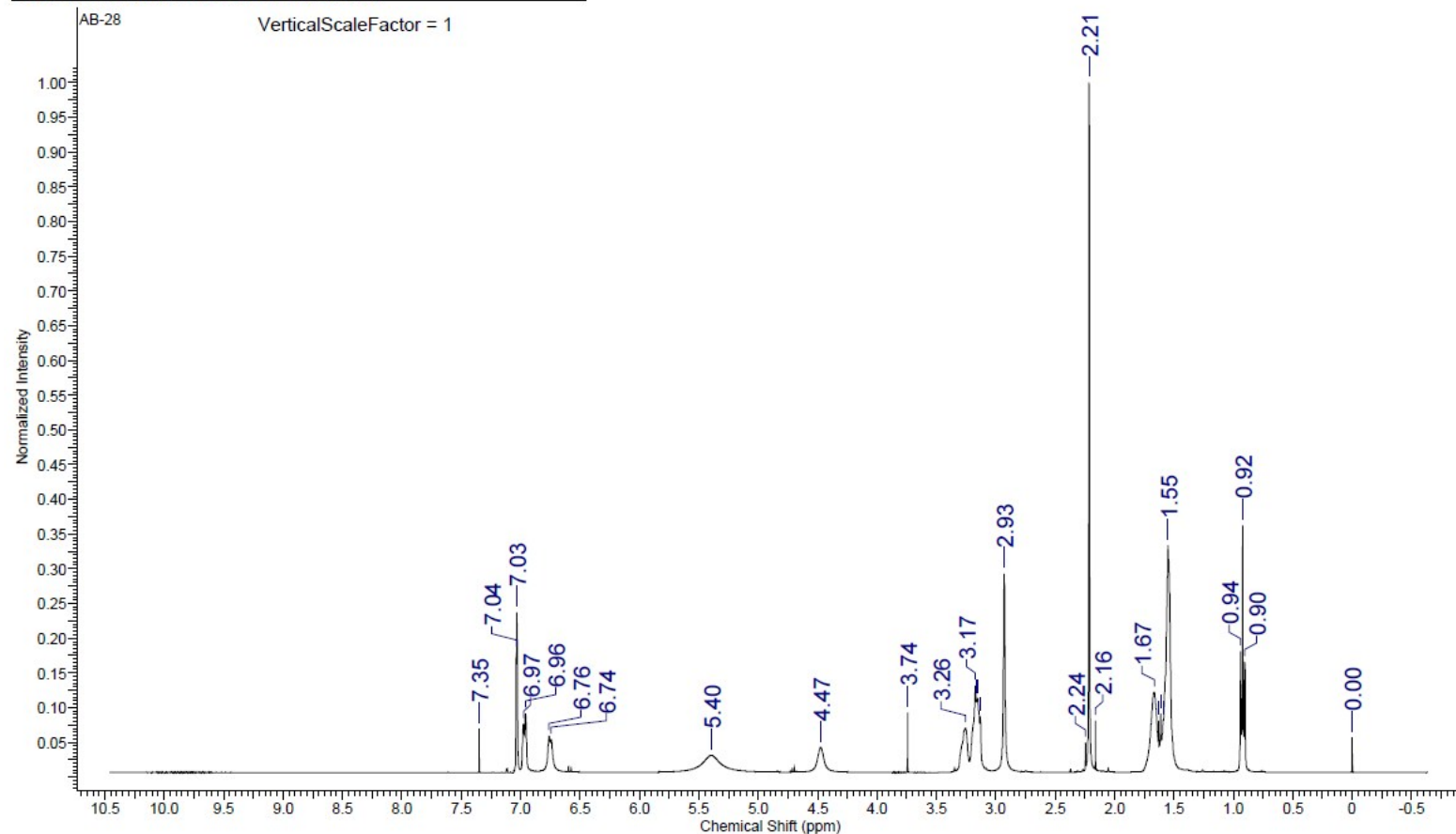


Figure S3. ^1H NMR spectrum of 1-methyl-1-propylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**2**)

Acquisition Time (sec)	1.3010	Comment	AB-28	Date	Apr 23 2015	Date Stamp	Apr 23 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-28-C13.fid\AB-28-C13.fid\fid					Frequency (MHz)	101.25
Nucleus	¹³ C	Number of Transients	1436	Original Points Count	28039	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9601.1943	Spectrum Type	STANDARD	Sweep Width (Hz)	21551.72	Temperature (degree C)	AMBIENT TEMPERATURE

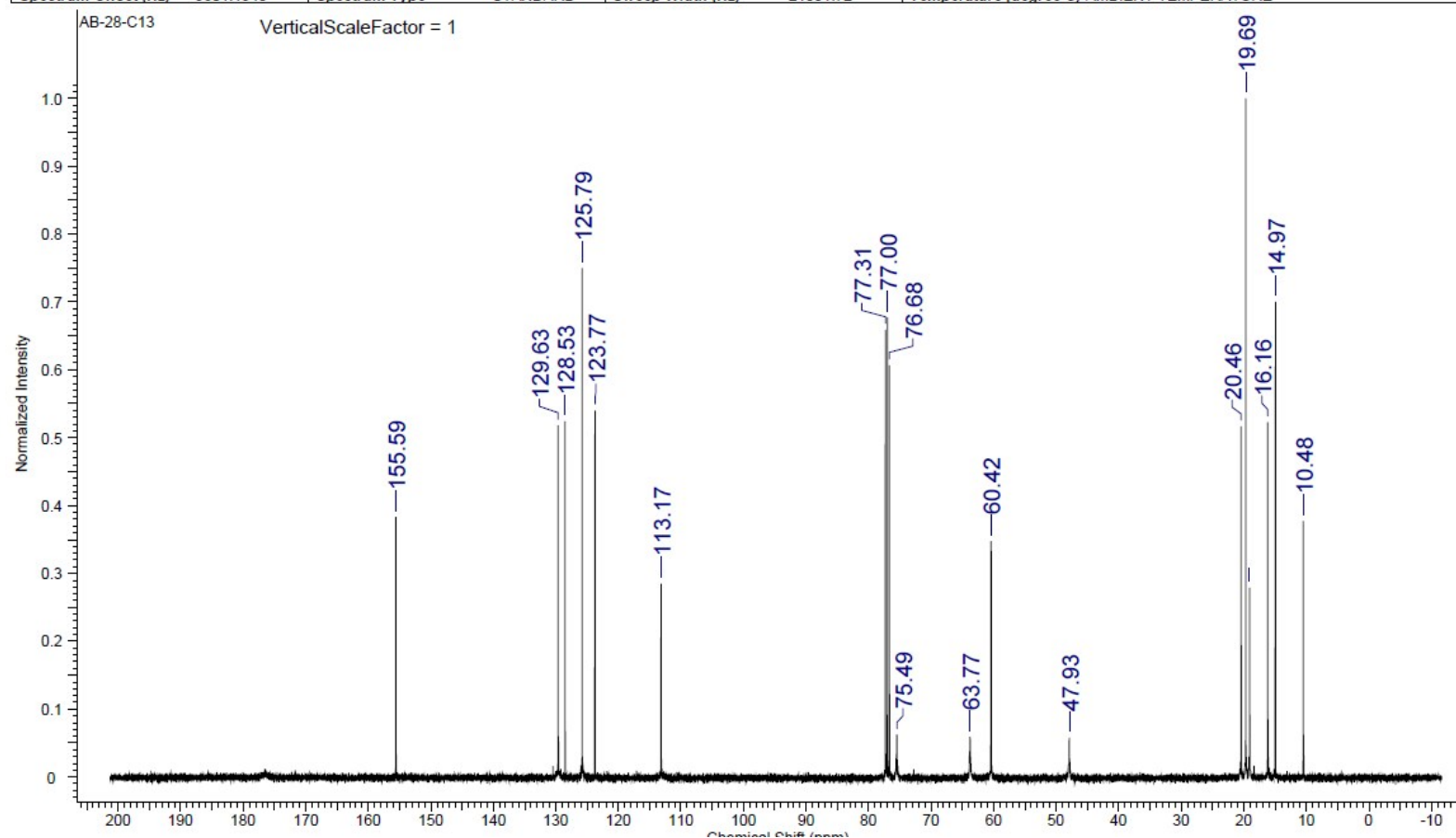


Figure S4. ¹³C NMR spectrum of 1-methyl-1-propylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**2**)

Acquisition Time (sec)	5.0001	Comment	AB 29	Date	Jan 30 2015	Date Stamp	Jan 30 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-29.fid\AB-29.fid					Frequency (MHz)	402.64	Nucleus	1H
Number of Transients	40	Original Points Count	29905	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	24.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2698.3052	Spectrum Type	STANDARD	Sweep Width (Hz)	5980.86
Temperature (degree C)	AMBIENT TEMPERATURE								

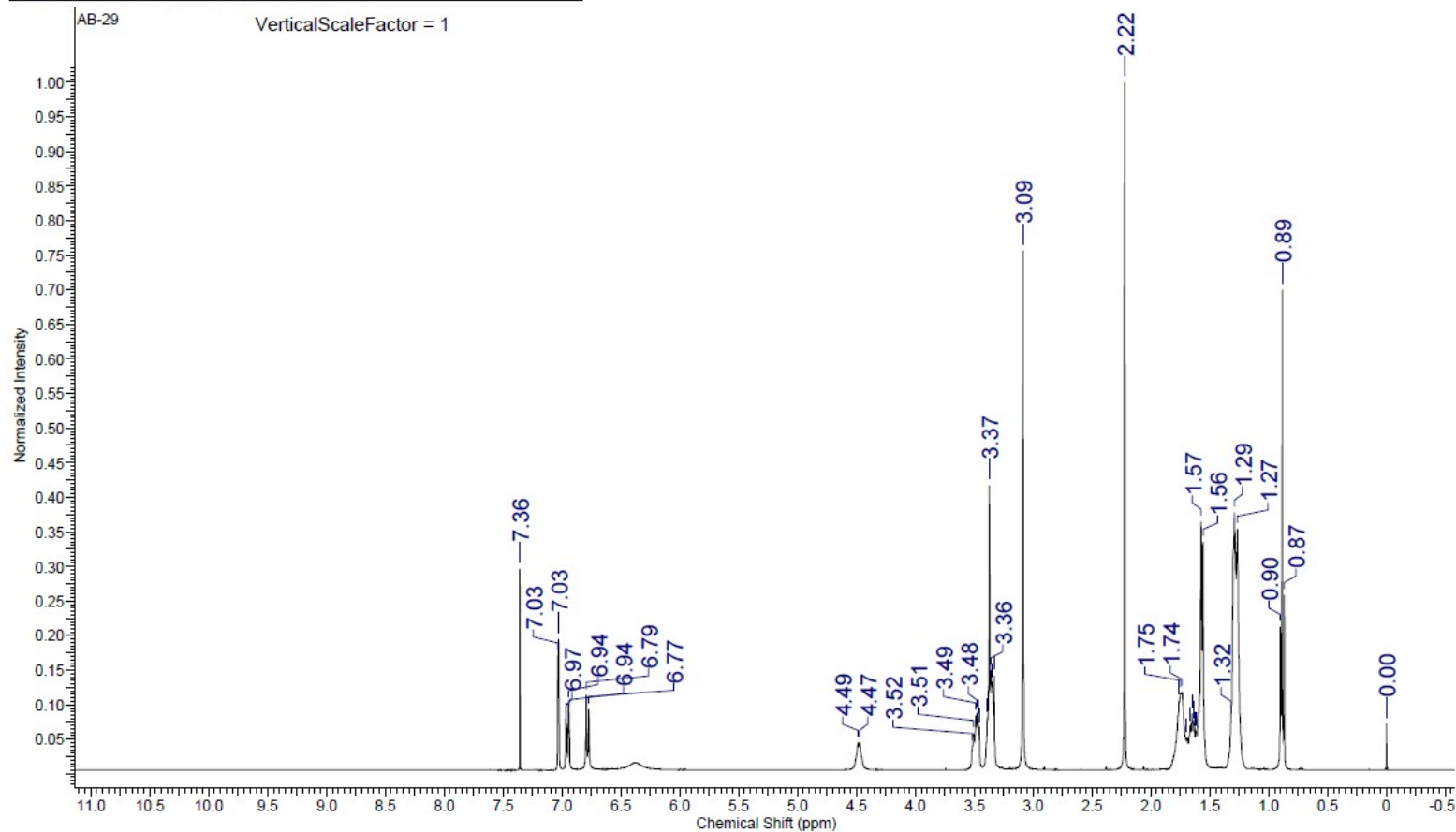


Figure S5. ¹H NMR spectrum of 1-butyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**3**)

Acquisition Time (sec)	1.3010	Comment	AB 29	Date	Jan 30 2015	Date Stamp	Jan 30 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-29-c13.fid\AB-29-c13.fid\fid				Frequency (MHz)	101.25	
Nucleus	¹³ C	Number of Transients	808	Original Points Count	28039	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9601.8525	Spectrum Type	STANDARD	Sweep Width (Hz)	21551.72	Temperature (degree C) AMBIENT TEMPERATURE	

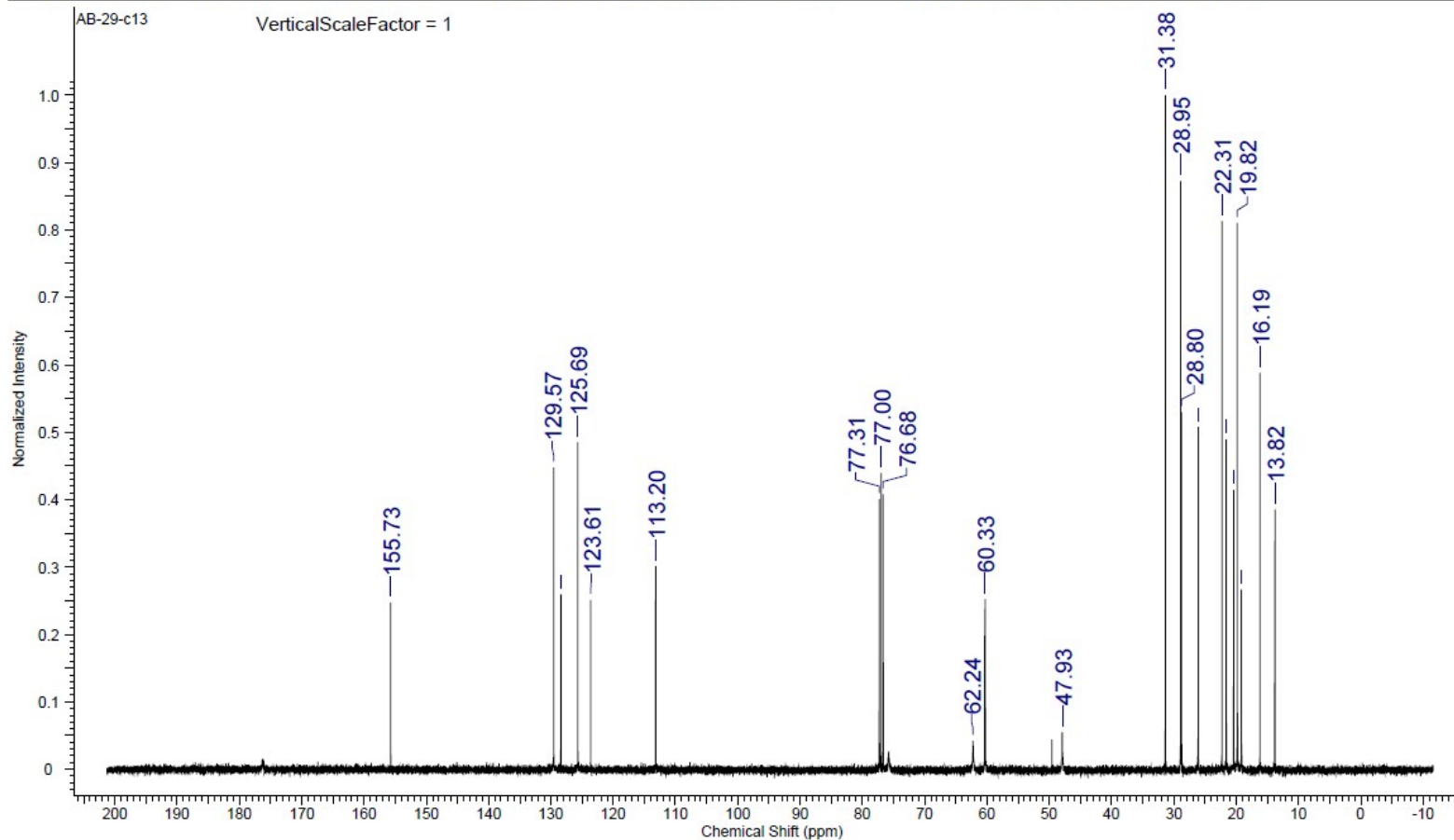


Figure S6. ¹³C NMR spectrum of 1-butyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**3**)

Acquisition Time (sec)	5.0001	Comment	AB-30	Date	Jan 30 2015	Date Stamp	Jan 30 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-30.fid\AB-30.fid.fid					Frequency (MHz)	402.64	Nucleus	1H
Number of Transients	44	Original Points Count	29905	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	20.00
Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2716.4661	Spectrum Type	STANDARD	Sweep Width (Hz)	5980.86	
Temperature (degree C)	AMBIENT TEMPERATURE								

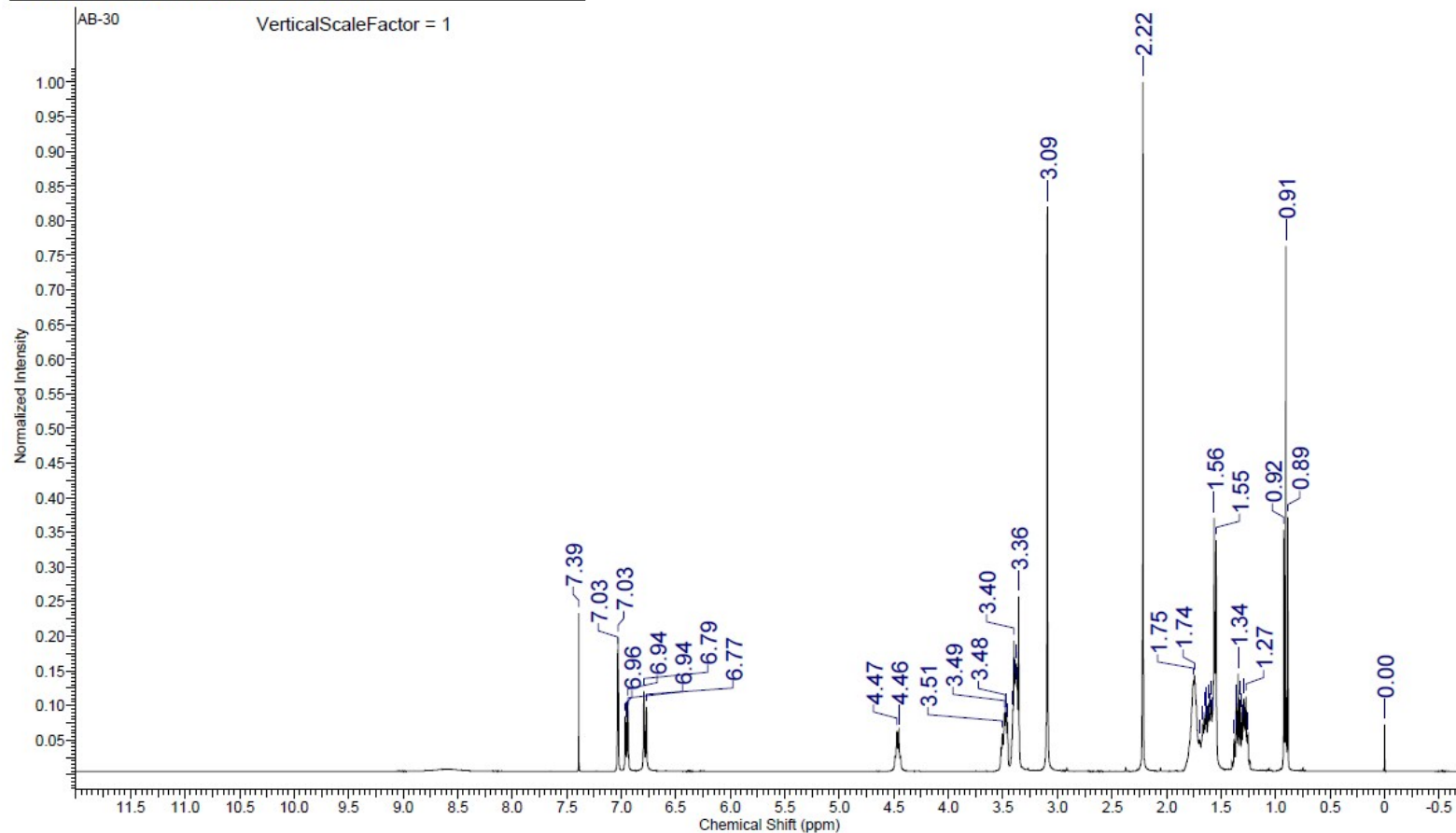


Figure S7. ^1H NMR spectrum of 1-methyl-1-pentylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**4**)

Acquisition Time (sec)	1.3010	Comment	AB-30	Date	Jan 30 2015	Date Stamp	Jan 30 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-30-c13.fid\AB-30-c13.fid\fid				Frequency (MHz)	101.25	
Nucleus	¹³ C	Number of Transients	420	Original Points Count	30684	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10608.9492	Spectrum Type	STANDARD	Sweep Width (Hz)	23584.91	Temperature (degree C) AMBIENT TEMPERATURE	

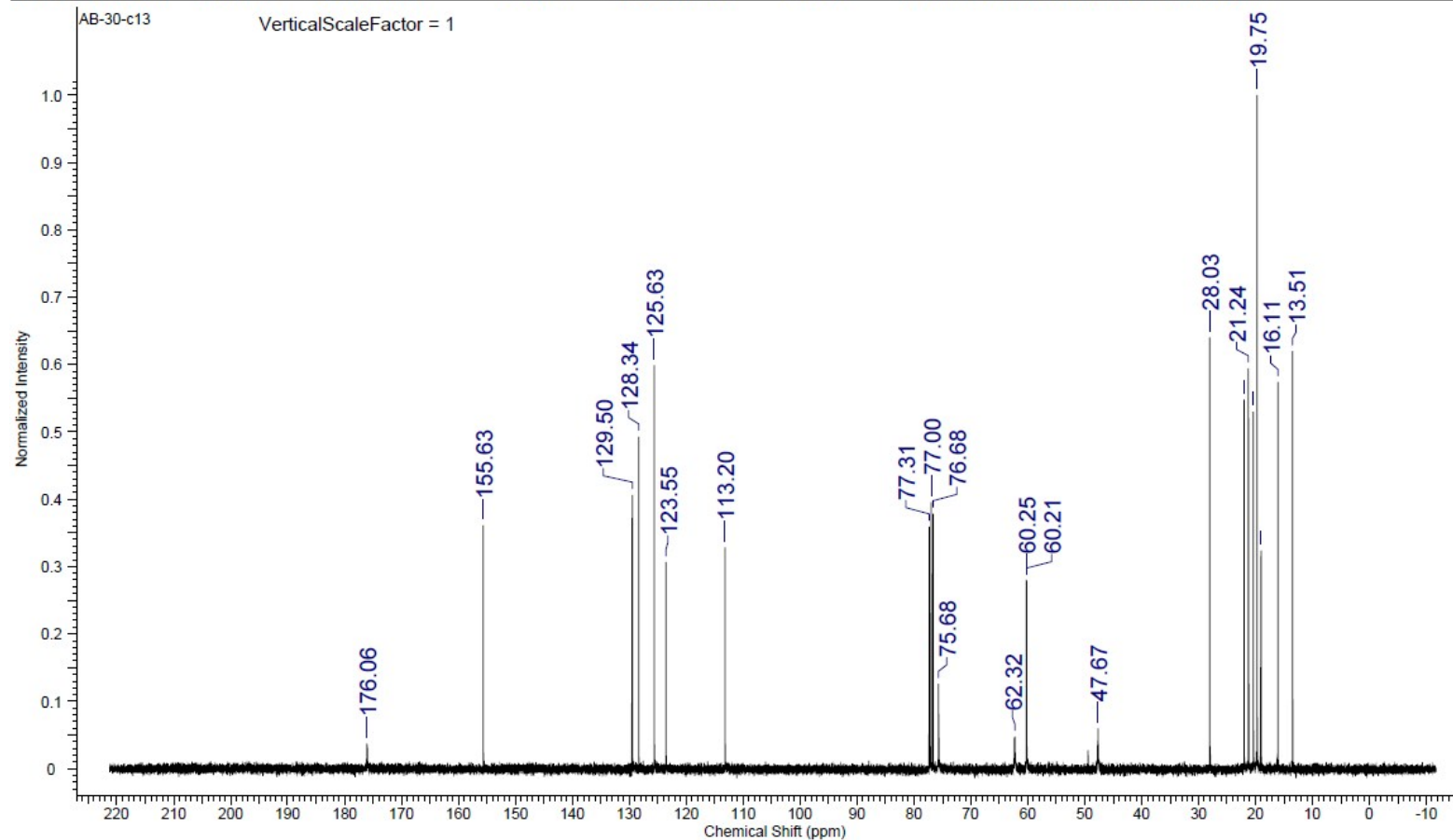


Figure S8. ¹³C NMR spectrum of 1-methyl-1-pentylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**4**)

Acquisition Time (sec)	5.0001	Comment	AB 31	Date	Apr 17 2015	Date Stamp	Apr 17 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB31-H1.fid\AB31-H1.fid\fid					Frequency (MHz)	300.07	Nucleus	1H
Number of Transients	64	Original Points Count	25304	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	6.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2298.1584	Spectrum Type	STANDARD	Sweep Width (Hz)	5060.73
Temperature (degree C)	AMBIENT TEMPERATURE								

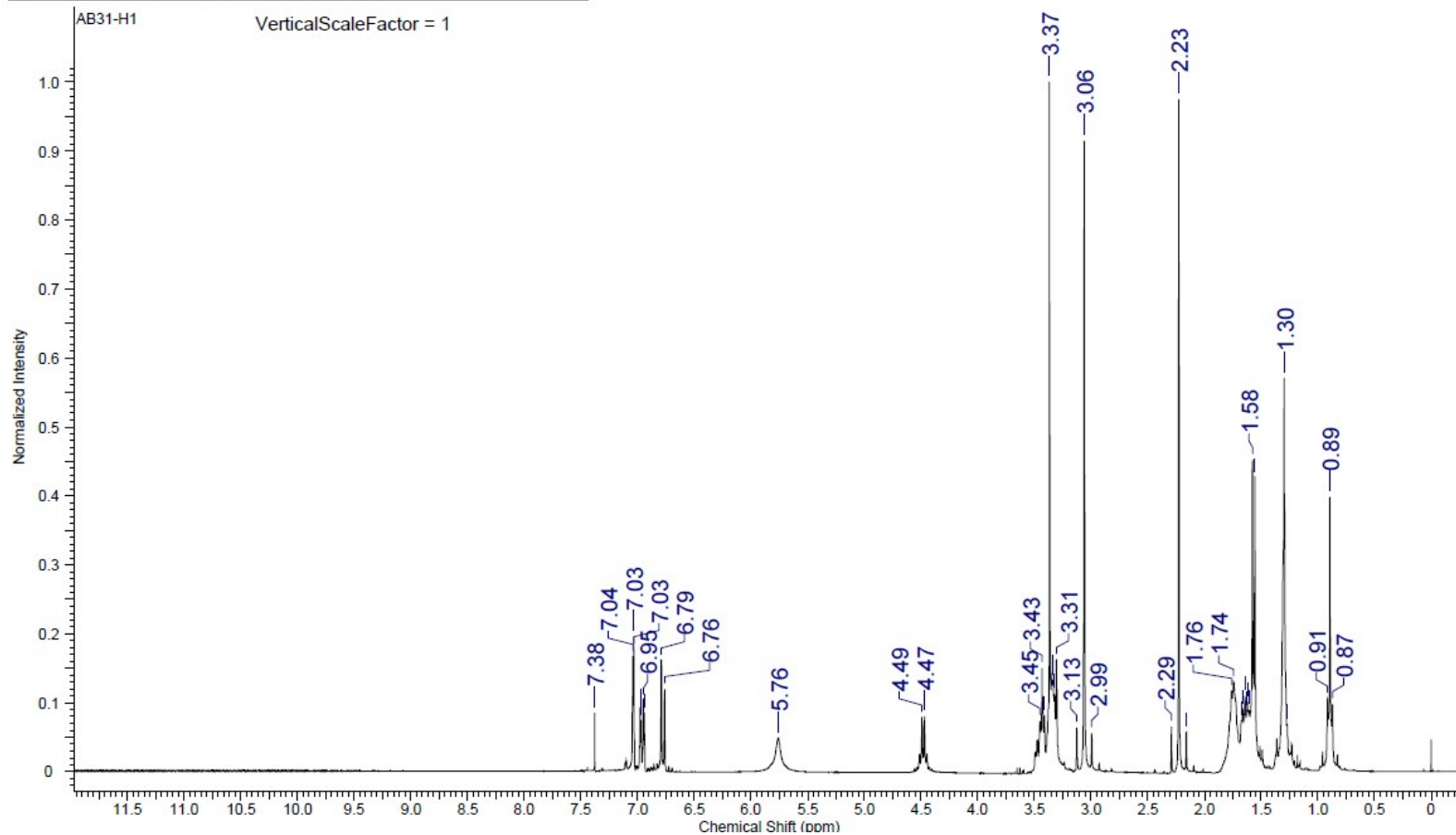


Figure S9. ^1H NMR spectrum of 1-hexyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**5**)

Acquisition Time (sec)	0.6400	Comment	AB 31	Date	Apr 17 2015	Date Stamp	Apr 17 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB31-C13.fid\AB31-C13.fid\fid				Frequency (MHz)	75.46	
Nucleus	¹³ C	Number of Transients	2148	Original Points Count	12191	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7946.1660	Spectrum Type	STANDARD	Sweep Width (Hz)	19047.62	Temperature (degree C) AMBIENT TEMPERATURE	

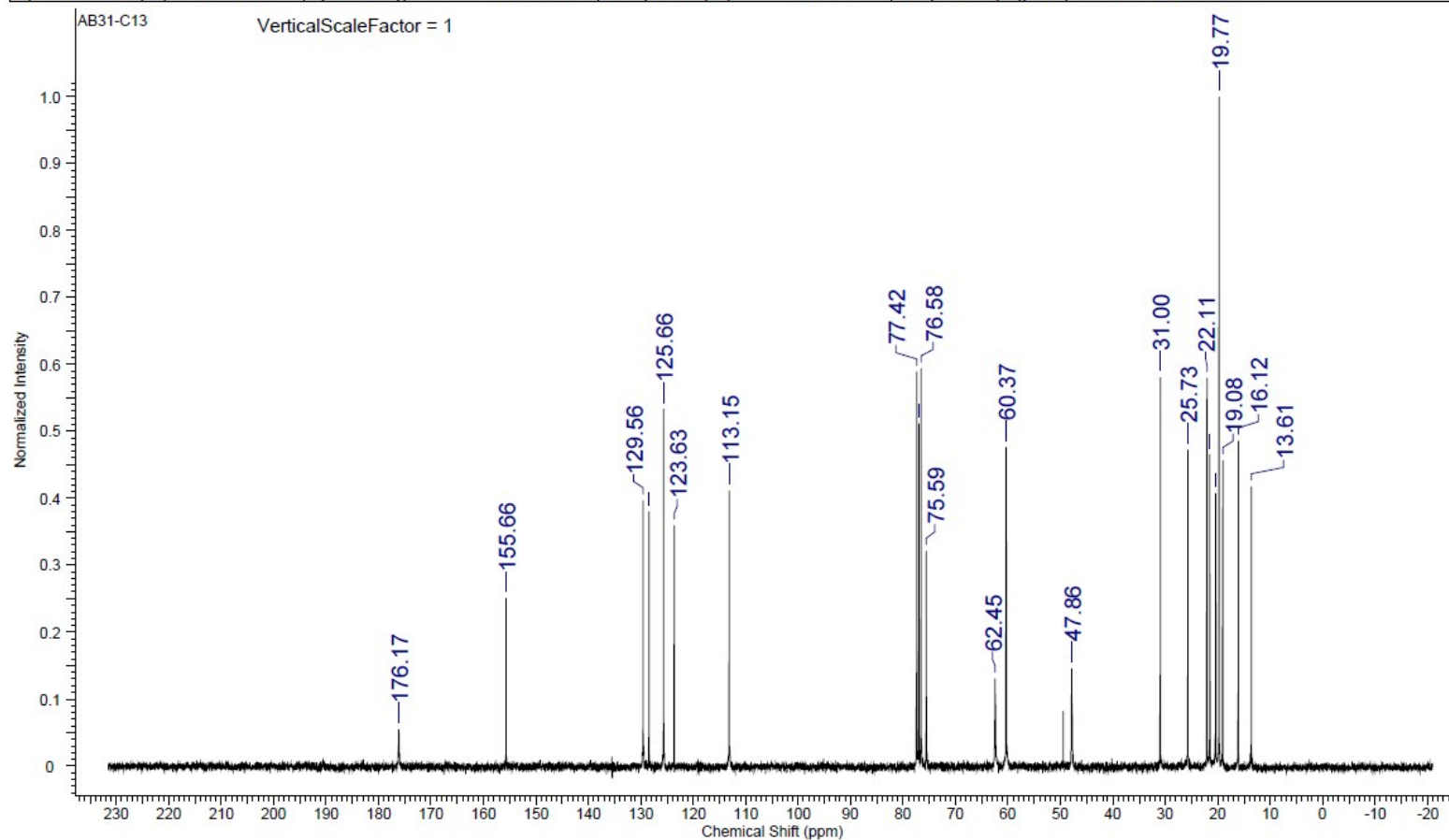


Figure S10. ¹³C NMR spectrum 1-hexyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**5**)

Acquisition Time (sec)	4.5003	Comment	AB-32	Date	Apr 24 2015	Date Stamp	Apr 24 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-32.fid\AB-32.fid\fid			Frequency (MHz)	402.64	Nucleus	¹ H
Number of Transients	64	Original Points Count	21148	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2117.4438	Spectrum Type	STANDARD
Temperature (degree C)	AMBIENT TEMPERATURE					Receiver Gain	18.00
						Sweep Width (Hz)	4699.25

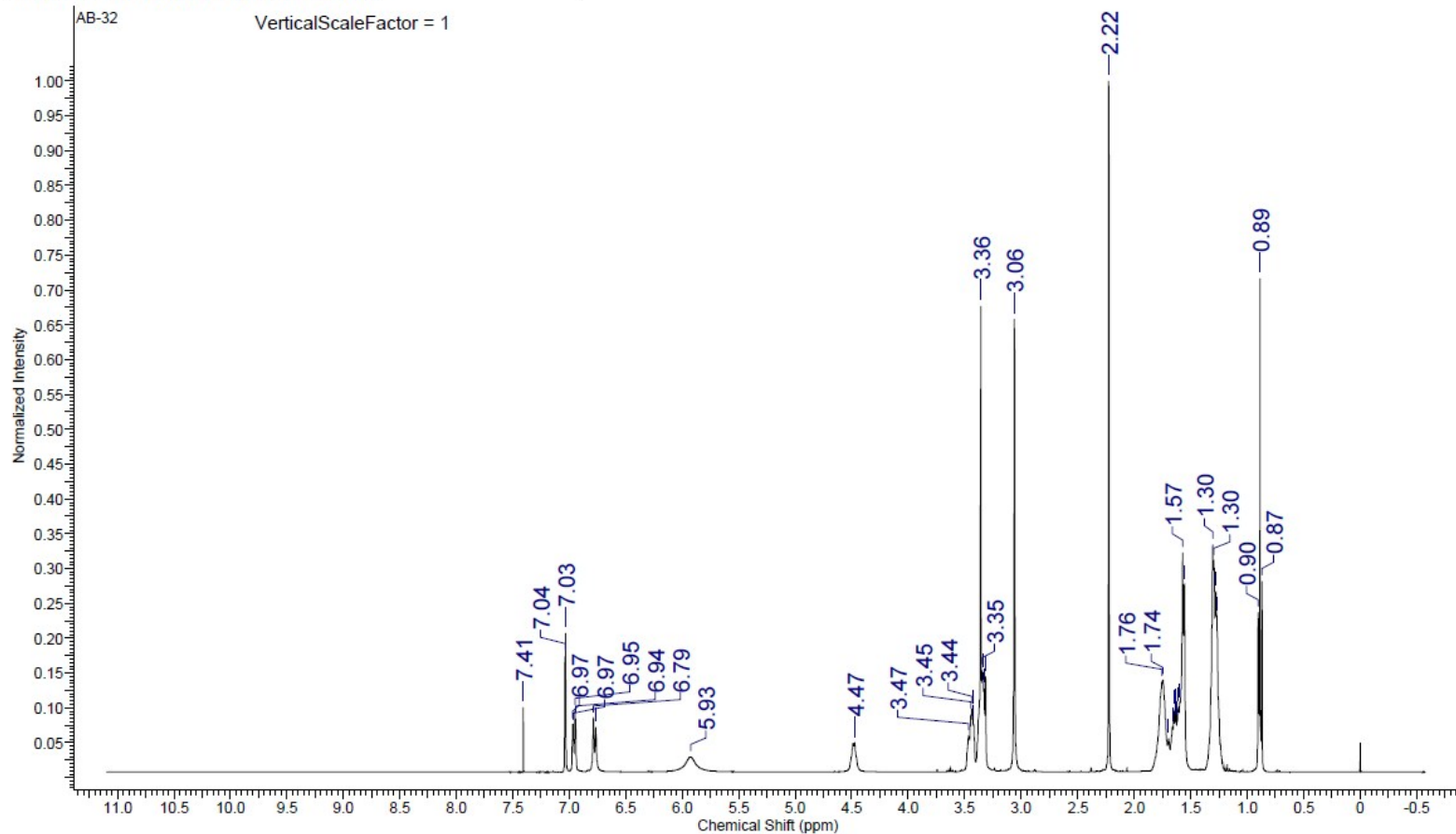


Figure S11. ¹H NMR spectrum of heptyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**6**)

Acquisition Time (sec)	1.3010	Comment	AB-32	Date	Apr 24 2015	Date Stamp	Apr 24 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-32-c13.fid\AB-32-c13.fid\fid				Frequency (MHz)	101.25	
Nucleus	¹³ C	Number of Transients	1228	Original Points Count	28039	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9590.6719	Spectrum Type	STANDARD	Sweep Width (Hz)	21551.72	Temperature (degree C) AMBIENT TEMPERATURE	

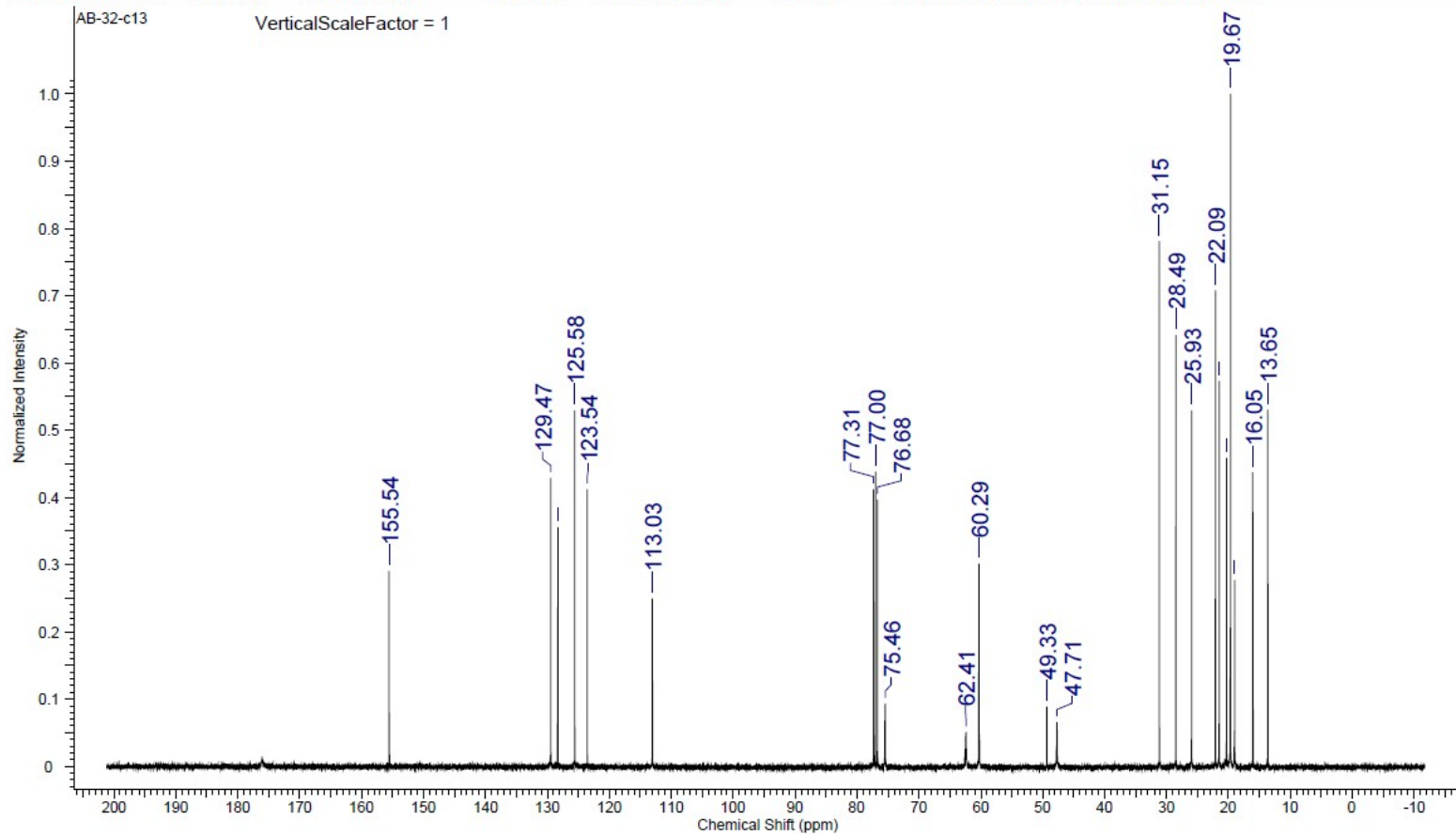


Figure S12. ¹³C NMR spectrum of heptyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**6**)

Acquisition Time (sec)	5.5000	Comment	AB-33	Date	Apr 24 2015	Date Stamp	Apr 24 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-33.fid\AB-33.fid\fid					Frequency (MHz)	402.64	Nucleus	1H
Number of Transients	40	Original Points Count	27067	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	18.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2138.4082	Spectrum Type	STANDARD	Sweep Width (Hz)	4921.26
Temperature (degree C)	AMBIENT TEMPERATURE								

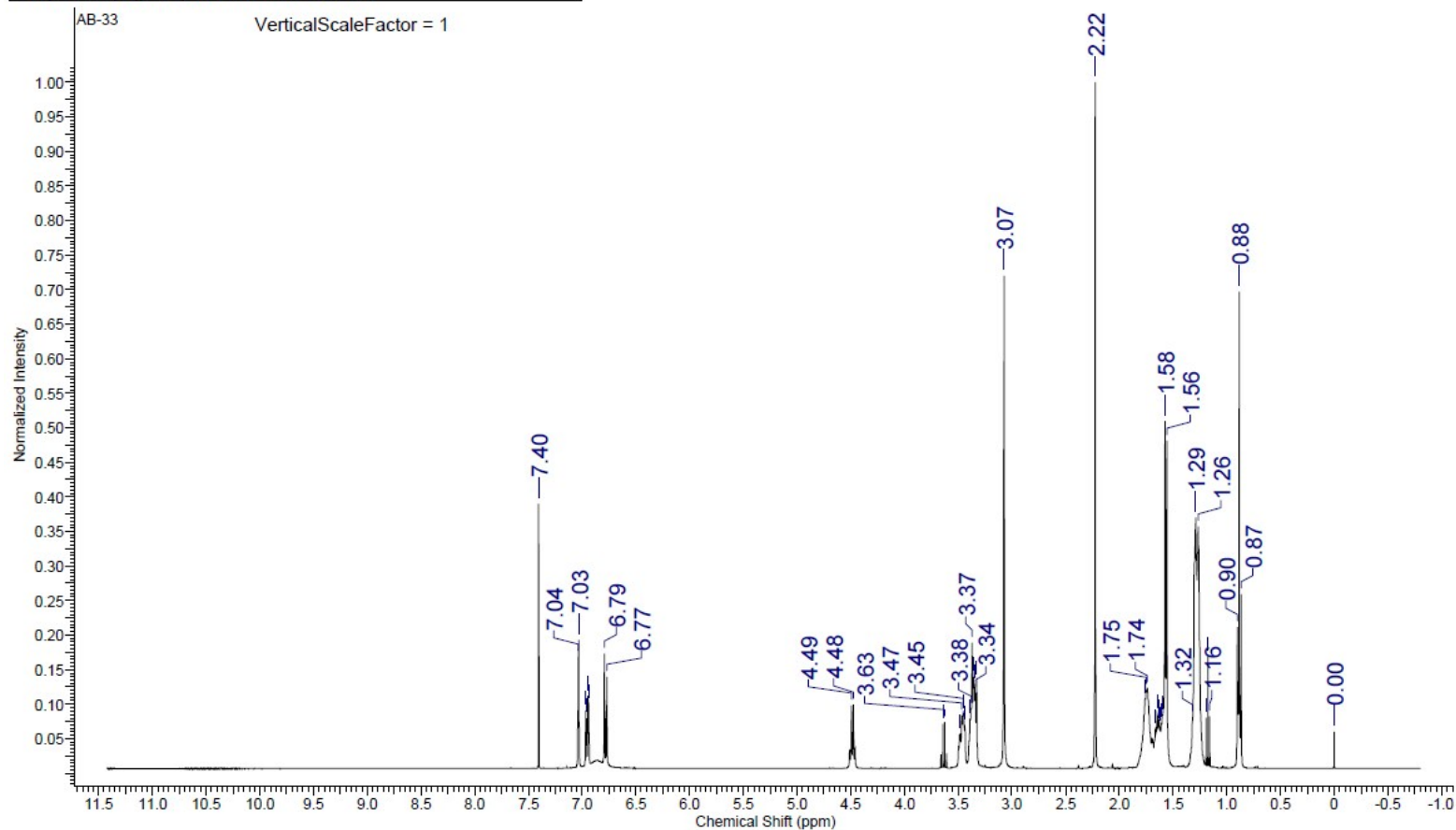


Figure S13. ¹H NMR spectrum of 1-methyl-1-octylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (7)

Acquisition Time (sec)	1.5010	Comment	AB-33	Date	Apr 24 2015	Date Stamp	Apr 24 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-33-C13.fid\AB-33-C13.fid\fid				Frequency (MHz)	101.25	
Nucleus	13C	Number of Transients	688	Original Points Count	32349	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	44.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9591.3301	Spectrum Type	STANDARD	Sweep Width (Hz)	21551.72	Temperature (degree C) AMBIENT TEMPERATURE	

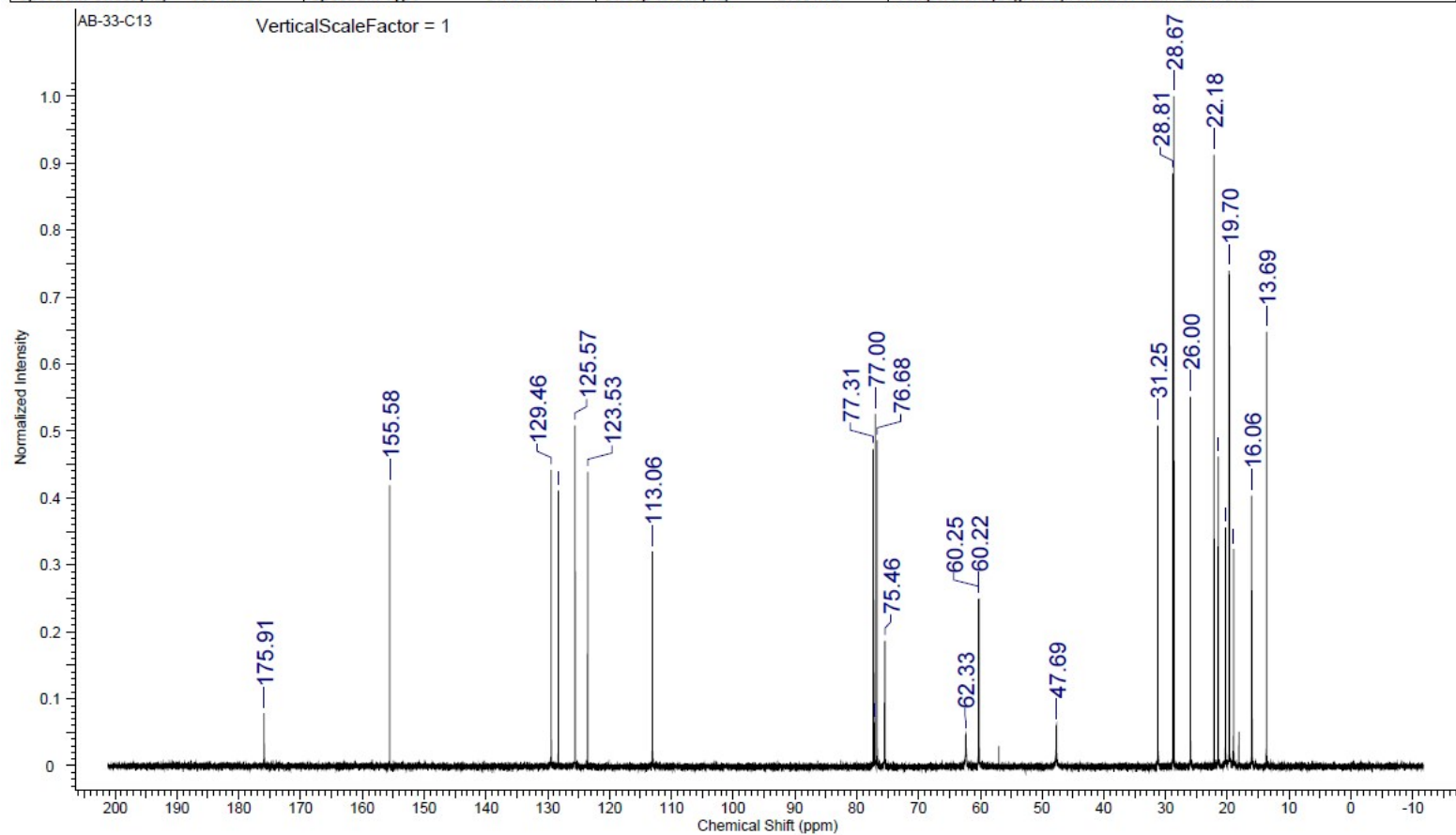


Figure S14. ^{13}C NMR spectrum of 1-methyl-1-octylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (7)

Acquisition Time (sec)	6.0000	Comment	AB 34	Date	Apr 27 2015	Date Stamp	Apr 27 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-34-H1.fid\AB-34-H1.fid\fid			Frequency (MHz)			402.64
Nucleus	¹ H	Number of Transients	64	Original Points Count	31915	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	22.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2254.4048	Spectrum Type	STANDARD	Sweep Width (Hz)	5319.15	Temperature (degree C) AMBIENT TEMPERATURE	

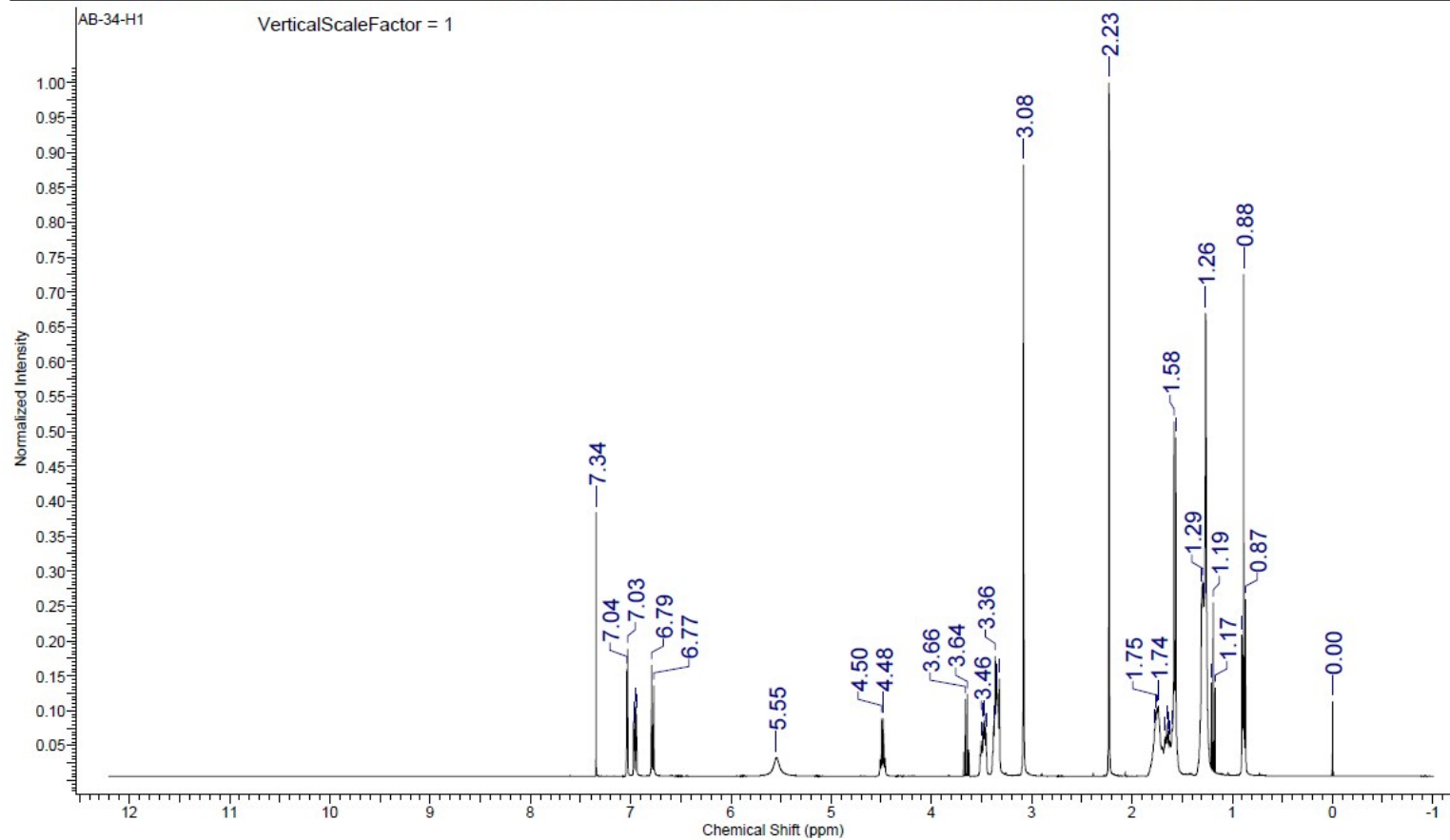


Figure S15. ¹H NMR spectrum of 1-methyl-1-nonylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**8**)

Acquisition Time (sec)	1.3010	Comment	AB 34	Date	Apr 27 2015	Date Stamp	Apr 27 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-34-C13.fid\AB-34-C13.fid.fid					Frequency (MHz)	101.25
Nucleus	¹³ C	Number of Transients	1004	Original Points Count	31274	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10869.5557	Spectrum Type	STANDARD	Sweep Width (Hz)	24038.46	Temperature (degree C)	AMBIENT TEMPERATURE

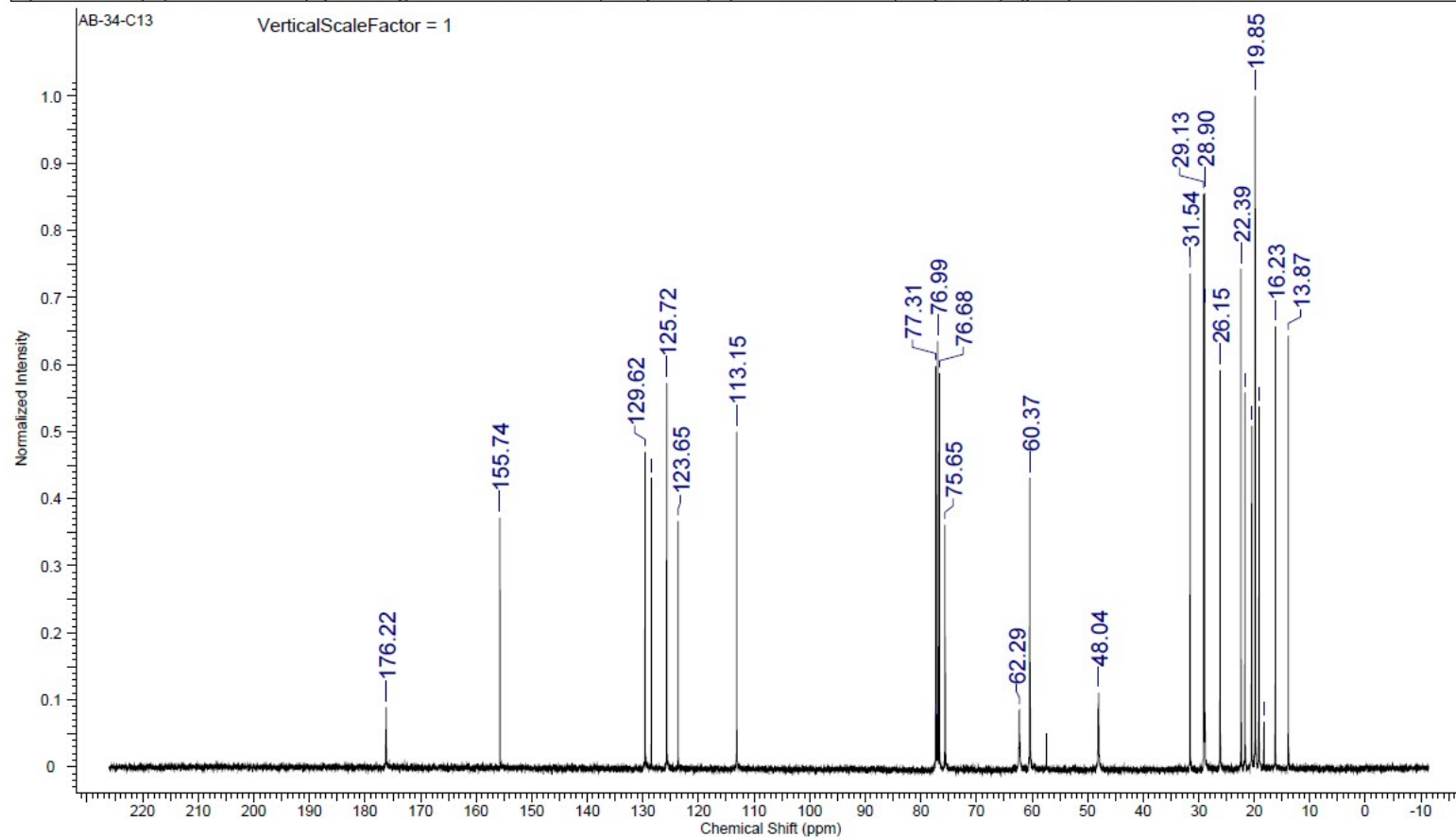


Figure S16. ¹³C NMR spectrum of 1-methyl-1-nonylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**8**)

Acquisition Time (sec)	5.0001	Comment	AB 35	Date	Apr 17 2015	Date Stamp	Apr 17 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB35-H1.fid\AB35-H1.fid\fid					Frequency (MHz)	300.07	Nucleus	1H
Number of Transients	64	Original Points Count	25304	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	6.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2298.9307	Spectrum Type	STANDARD	Sweep Width (Hz)	5060.73
Temperature (degree C)	AMBIENT TEMPERATURE								

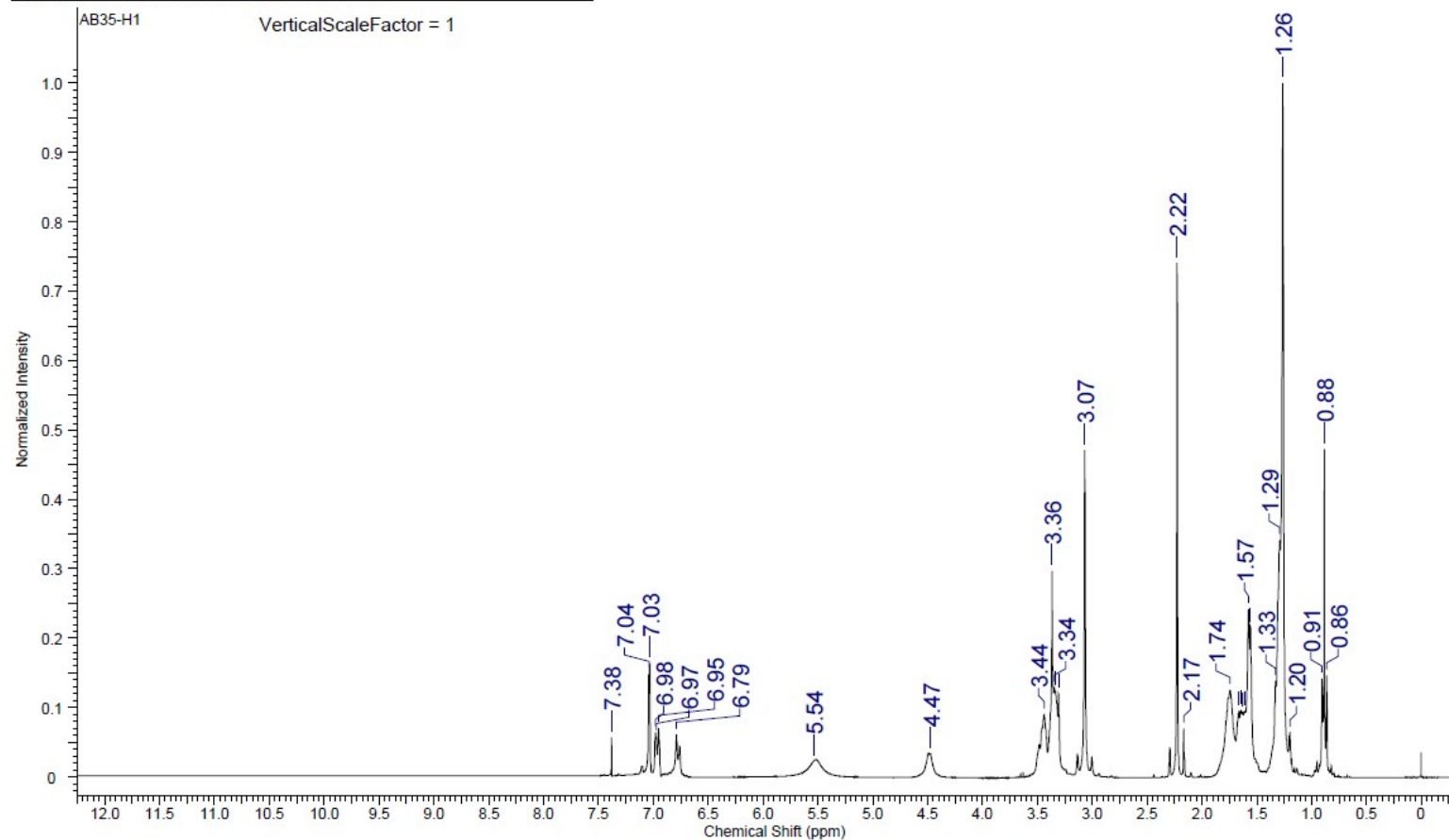


Figure S17. ^1H NMR spectrum of 1-decyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**9**)

Acquisition Time (sec)	0.6400	Comment	AB 35	Date	Apr 17 2015	Date Stamp	Apr 17 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB35-C13.fid\AB35-C13.fid\fid				Frequency (MHz)	75.46	
Nucleus	¹³ C	Number of Transients	1988	Original Points Count	12191	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7946.1660	Spectrum Type	STANDARD	Sweep Width (Hz)	19047.62	Temperature (degree C)	AMBIENT TEMPERATURE

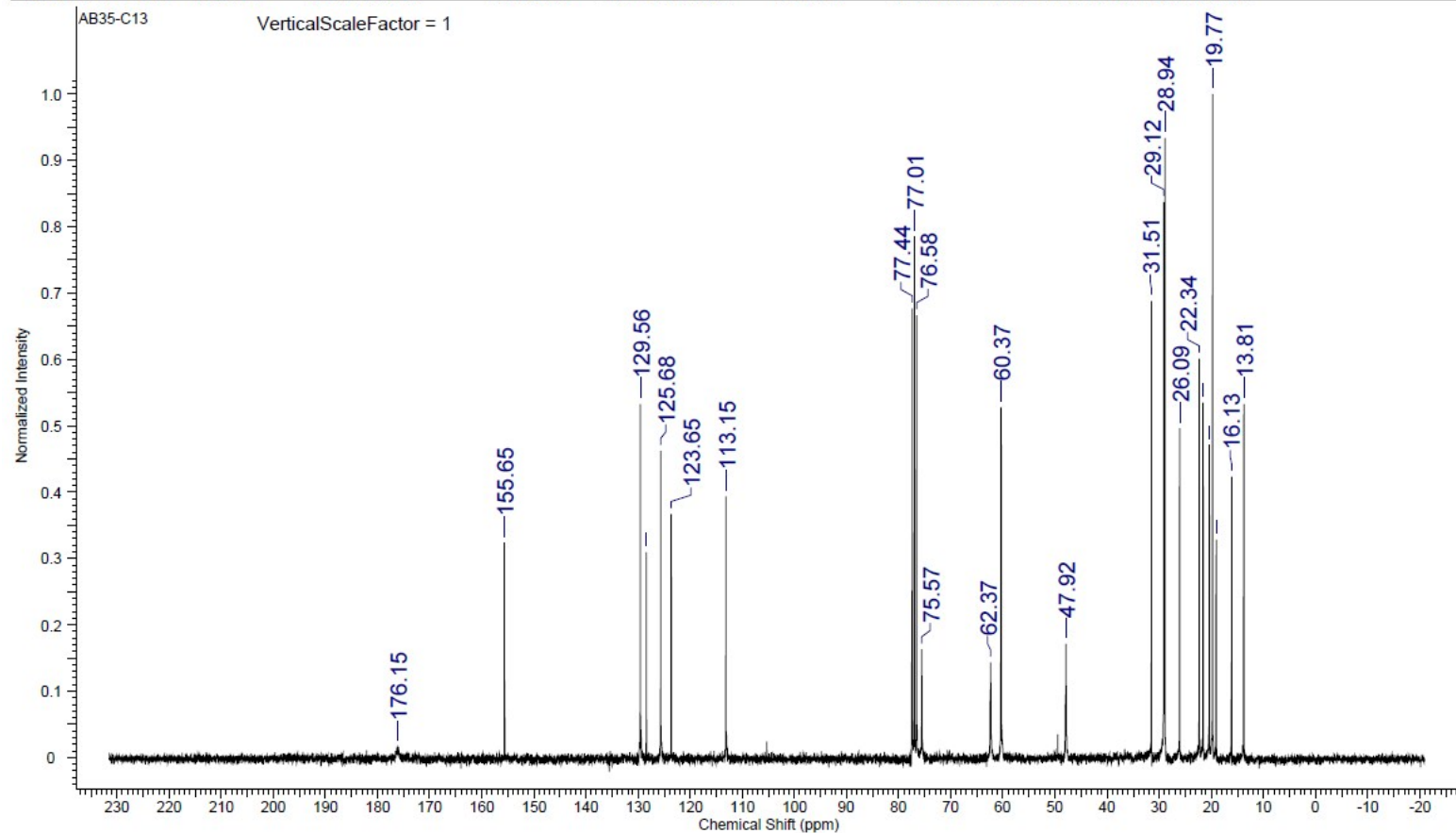


Figure S18. ¹³C NMR spectrum of 1-decyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**9**)

Acquisition Time (sec)	6.4999	Comment	AB 36	Date	Apr 27 2015	Date Stamp	Apr 27 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-36-H1.fid\AB-36-H1.fid\fid				Frequency (MHz)	402.64	
Nucleus	¹ H	Number of Transients	64	Original Points Count	34574	Points Count	65536
Pulse Sequence	s2pul	Receiver Gain	22.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2270.6377	Spectrum Type	STANDARD	Sweep Width (Hz)	5319.15	Temperature (degree C) AMBIENT TEMPERATURE	

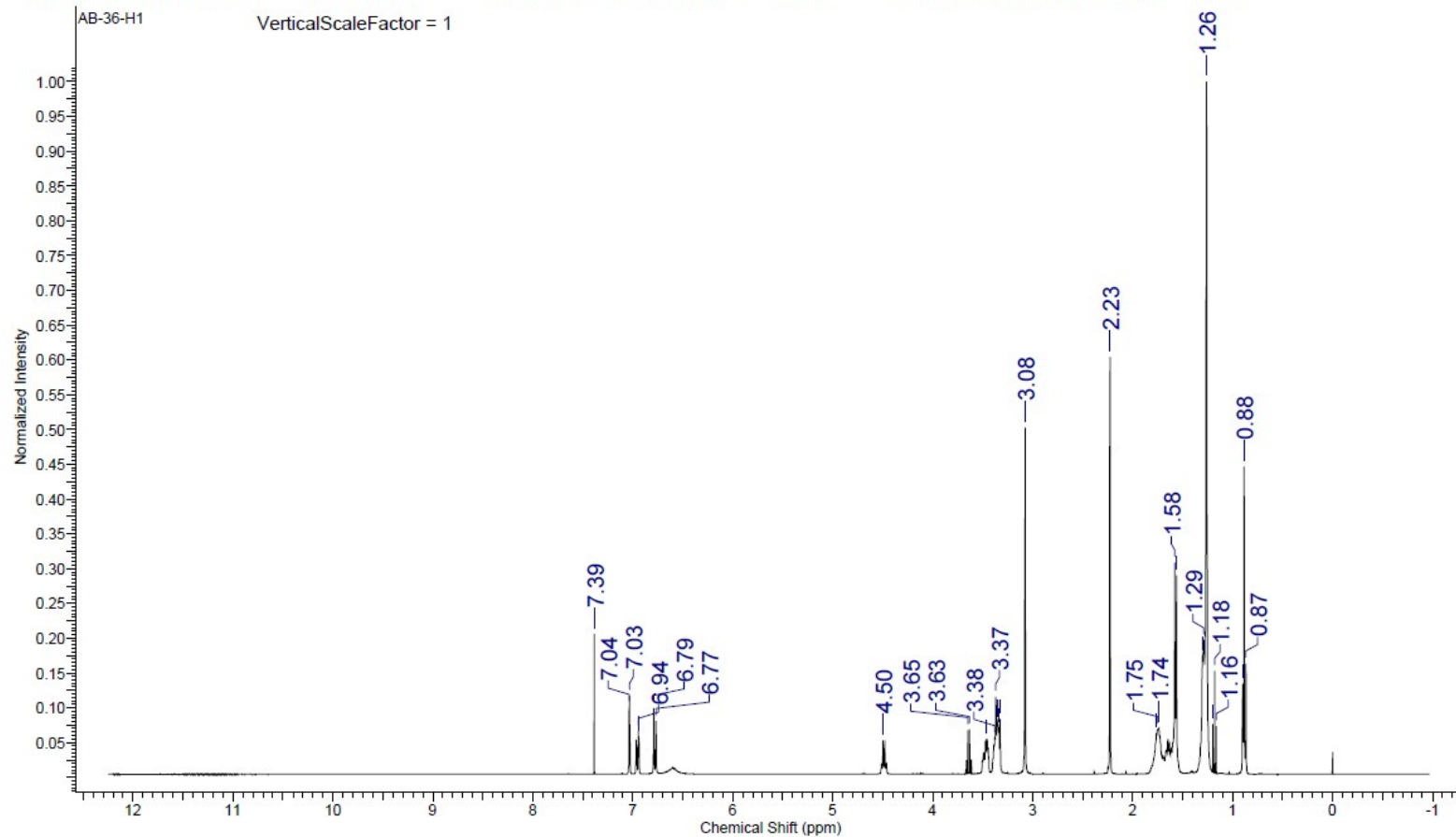


Figure S19. ¹H NMR spectrum of 1-methyl-1-undecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**10**)

Acquisition Time (sec)	1.3010	Comment	AB 36	Date	Apr 27 2015	Date Stamp	Apr 27 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-36-C13.fid\AB-36-C13.fid\fid				Frequency (MHz)	101.25	
Nucleus	¹³ C	Number of Transients	1212	Original Points Count	31274	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10862.2207	Spectrum Type	STANDARD	Sweep Width (Hz)	24038.46	Temperature (degree C) AMBIENT TEMPERATURE	

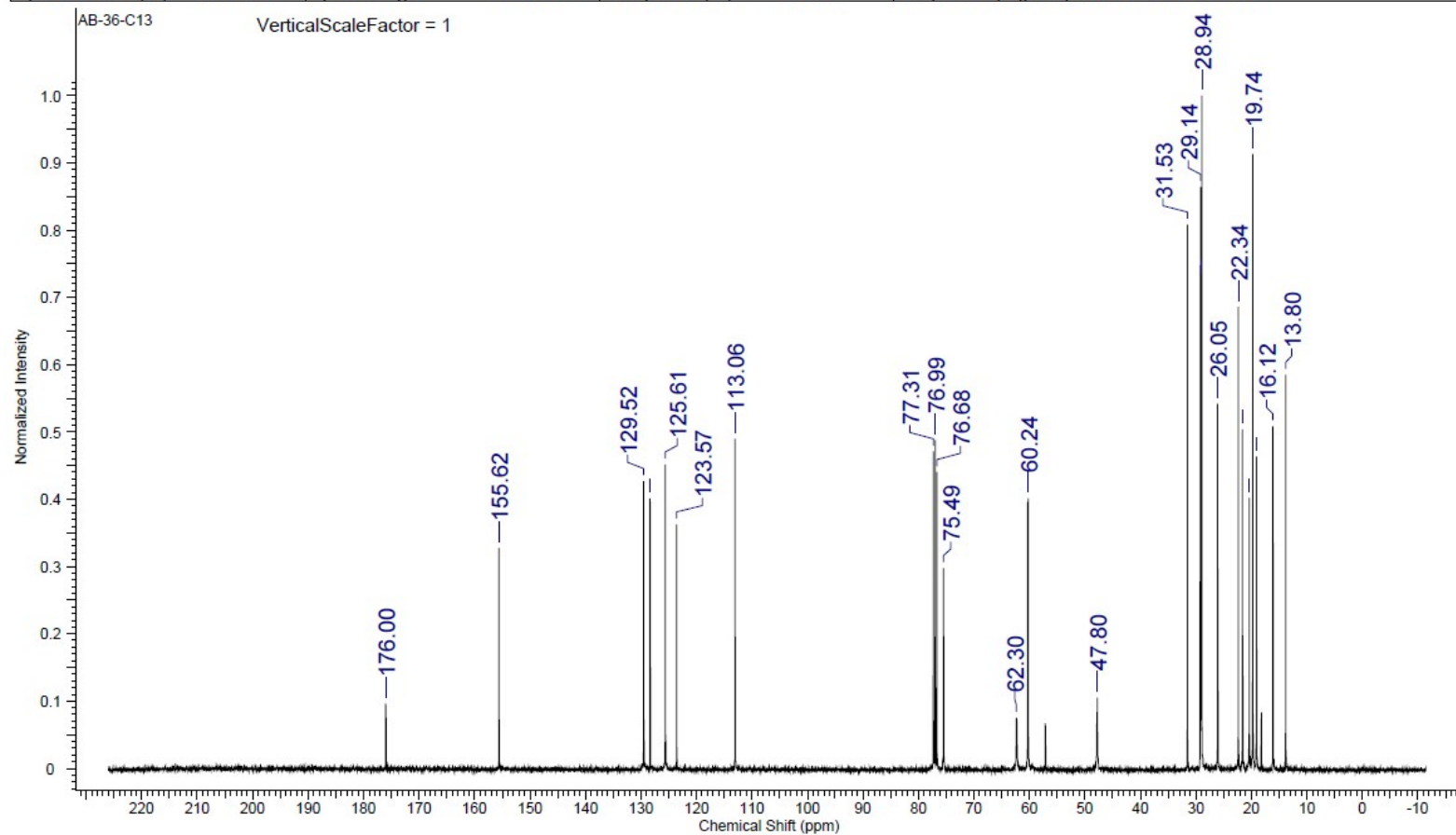


Figure S20. ¹³C NMR spectrum of 1-methyl-1-undecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**10**)

Acquisition Time (sec)	6.4999	Comment	AB 37	Date	Apr 27 2015	Date Stamp	Apr 27 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-37-H1.fid\AB-37-H1.fid\fid				Frequency (MHz)	402.64	
Nucleus	¹ H	Number of Transients	64	Original Points Count	34574	Points Count	65536
Pulse Sequence	s2pul	Receiver Gain	22.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2253.2686	Spectrum Type	STANDARD	Sweep Width (Hz)	5319.15	Temperature (degree C) AMBIENT TEMPERATURE	

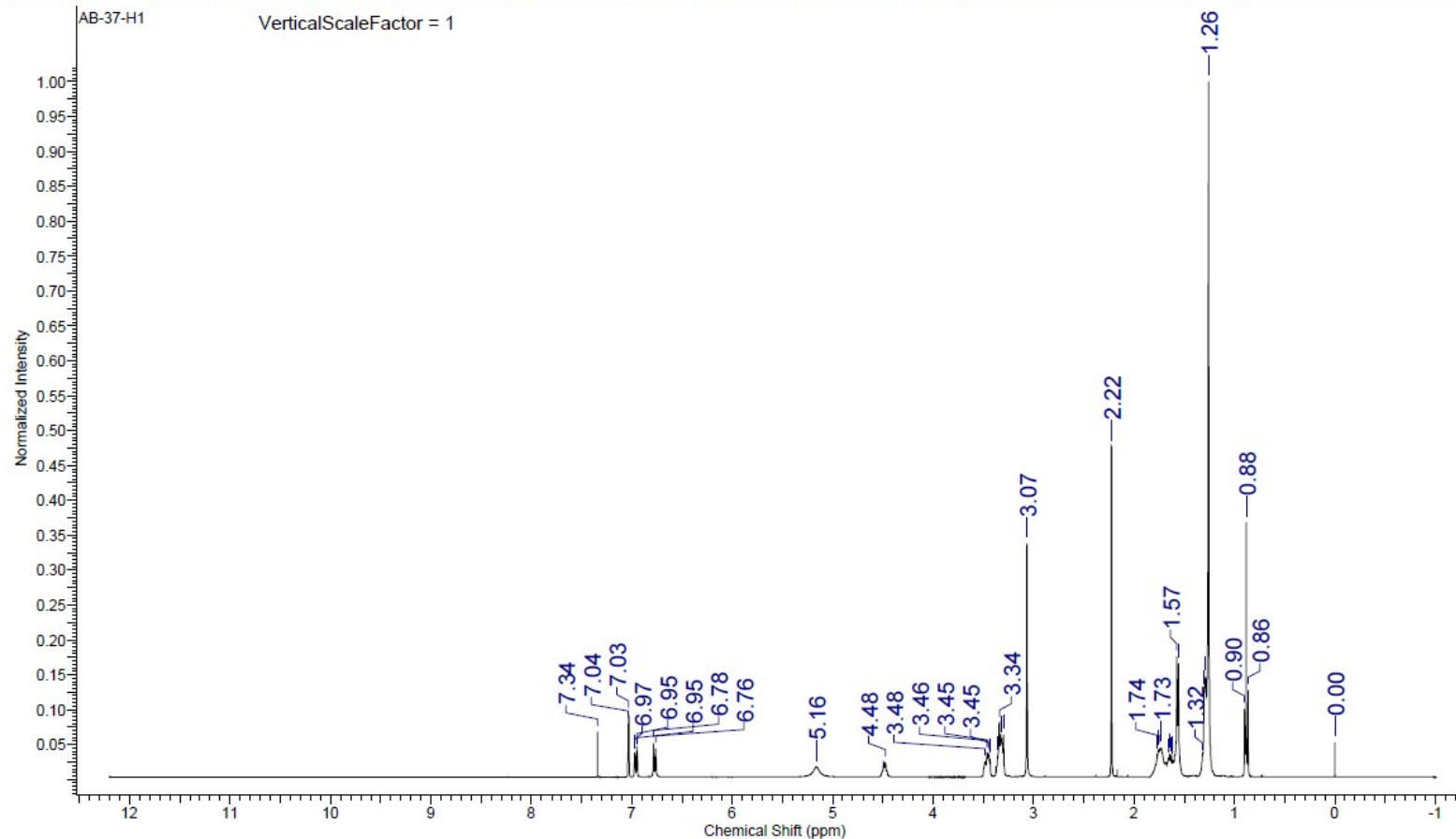


Figure S21. ¹H NMR spectrum of 1-dodecyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**11**)

Acquisition Time (sec)	1.3010	Comment	AB 37	Date	Apr 27 2015	Date Stamp	Apr 27 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-37-C13.fid\AB-37-C13.fid\fid				Frequency (MHz)	101.25	
Nucleus	¹³ C	Number of Transients	1864	Original Points Count	31274	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10869.5557	Spectrum Type	STANDARD	Sweep Width (Hz)	24038.46	Temperature (degree C)	AMBIENT TEMPERATURE

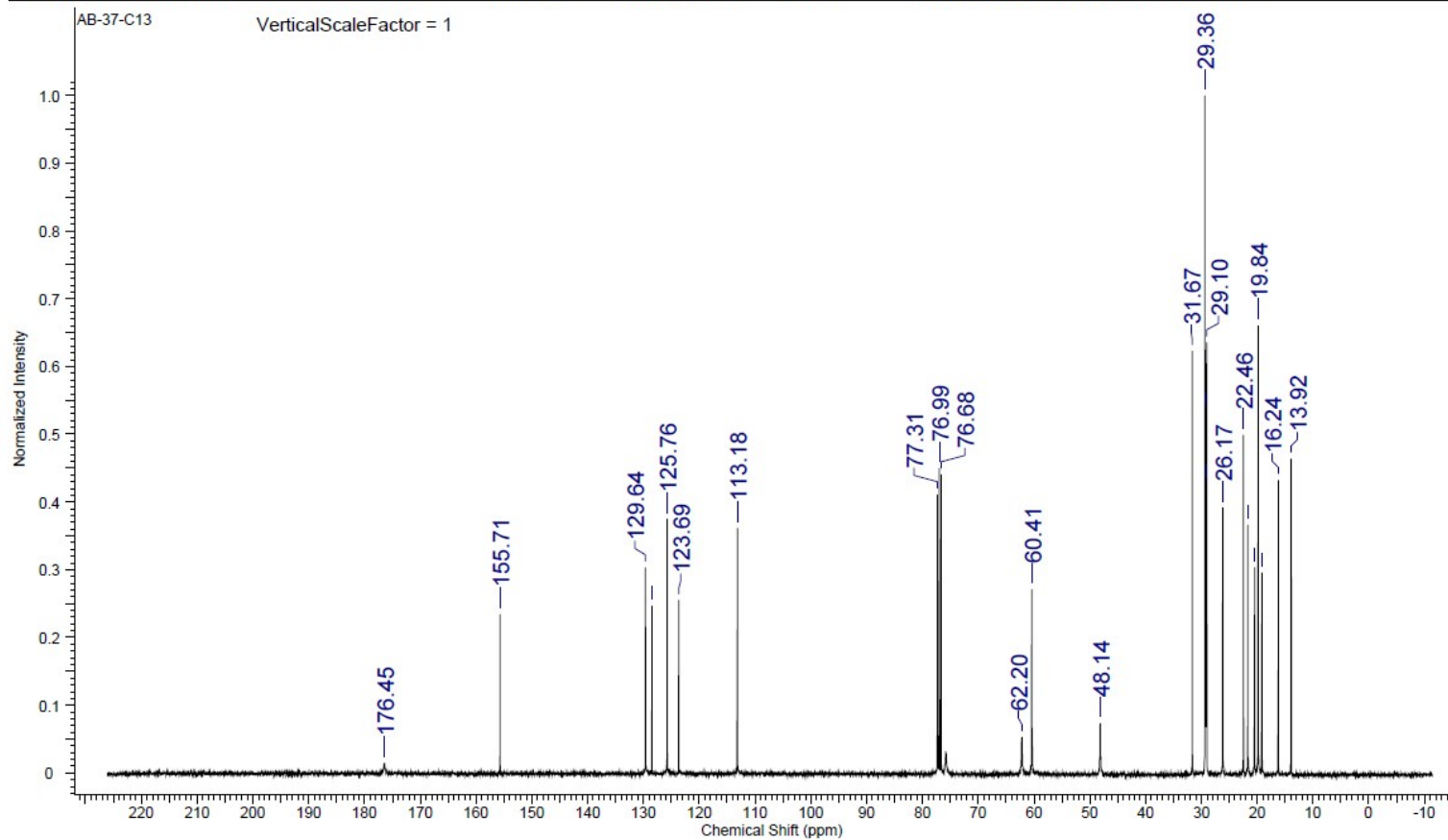


Figure S22. ¹³C NMR spectrum of 1-dodecyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**11**)

Acquisition Time (sec)	4.4999	Comment	AB-38	Date	Apr 28 2015	Date Stamp	Apr 28 2015		
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-38.fid\AB-38.fid					Frequency (MHz)	402.64	Nucleus	1H
Number of Transients	64	Original Points Count	21469	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	18.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2095.8267	Spectrum Type	STANDARD	Sweep Width (Hz)	4770.99
Temperature (degree C)	AMBIENT TEMPERATURE								

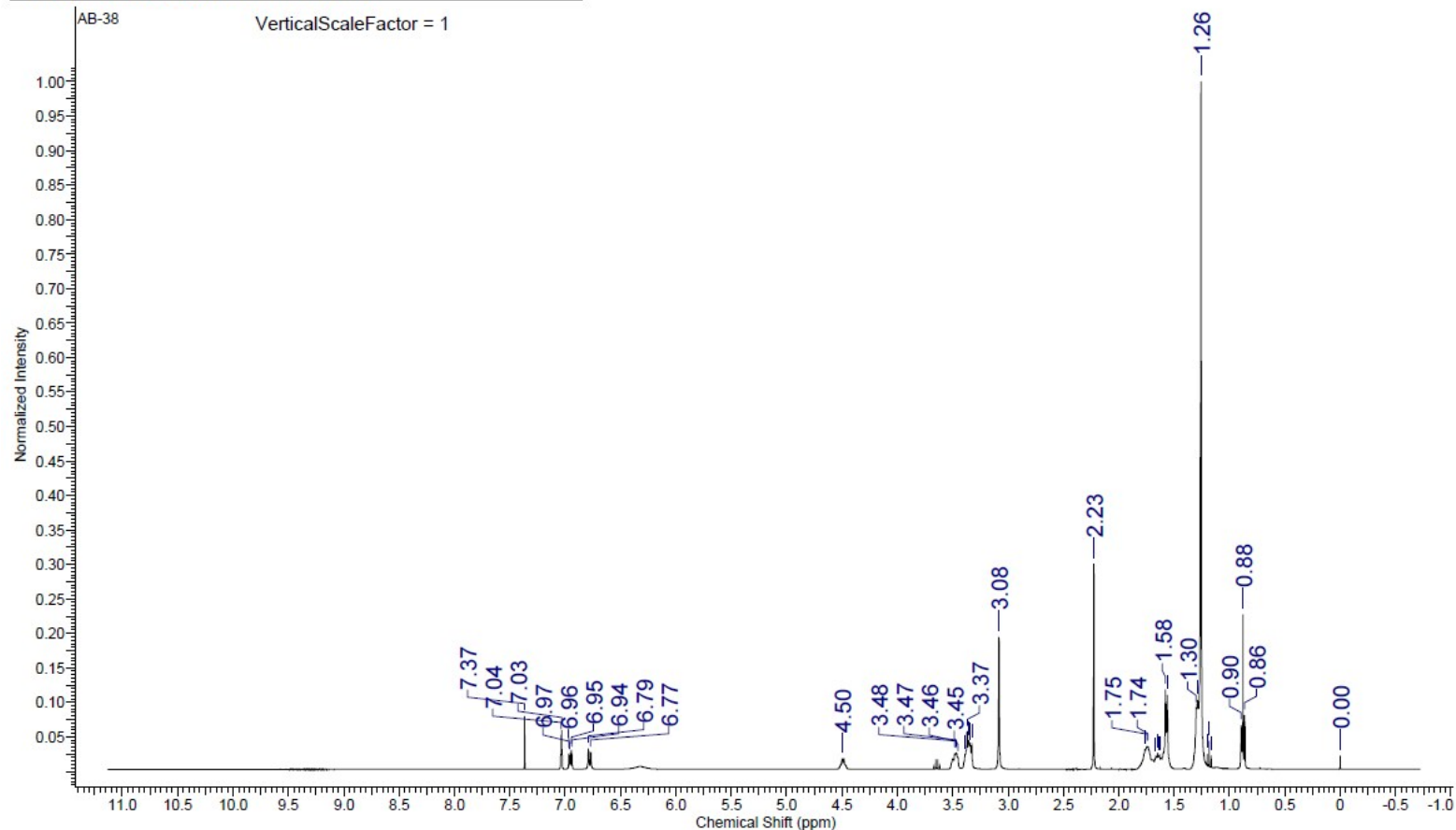


Figure S23. ¹H NMR spectrum of 1-methyl-1-tetradecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**12**)

Acquisition Time (sec)	1.3010	Comment	AB-38	Date	Apr 28 2015	Date Stamp	Apr 28 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-38-c13.fid\AB-38-c13.fid				Frequency (MHz)	101.25	
Nucleus	¹³ C	Number of Transients	608	Original Points Count	28039	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9600.2080	Spectrum Type	STANDARD	Sweep Width (Hz)	21551.72	Temperature (degree C)	AMBIENT TEMPERATURE

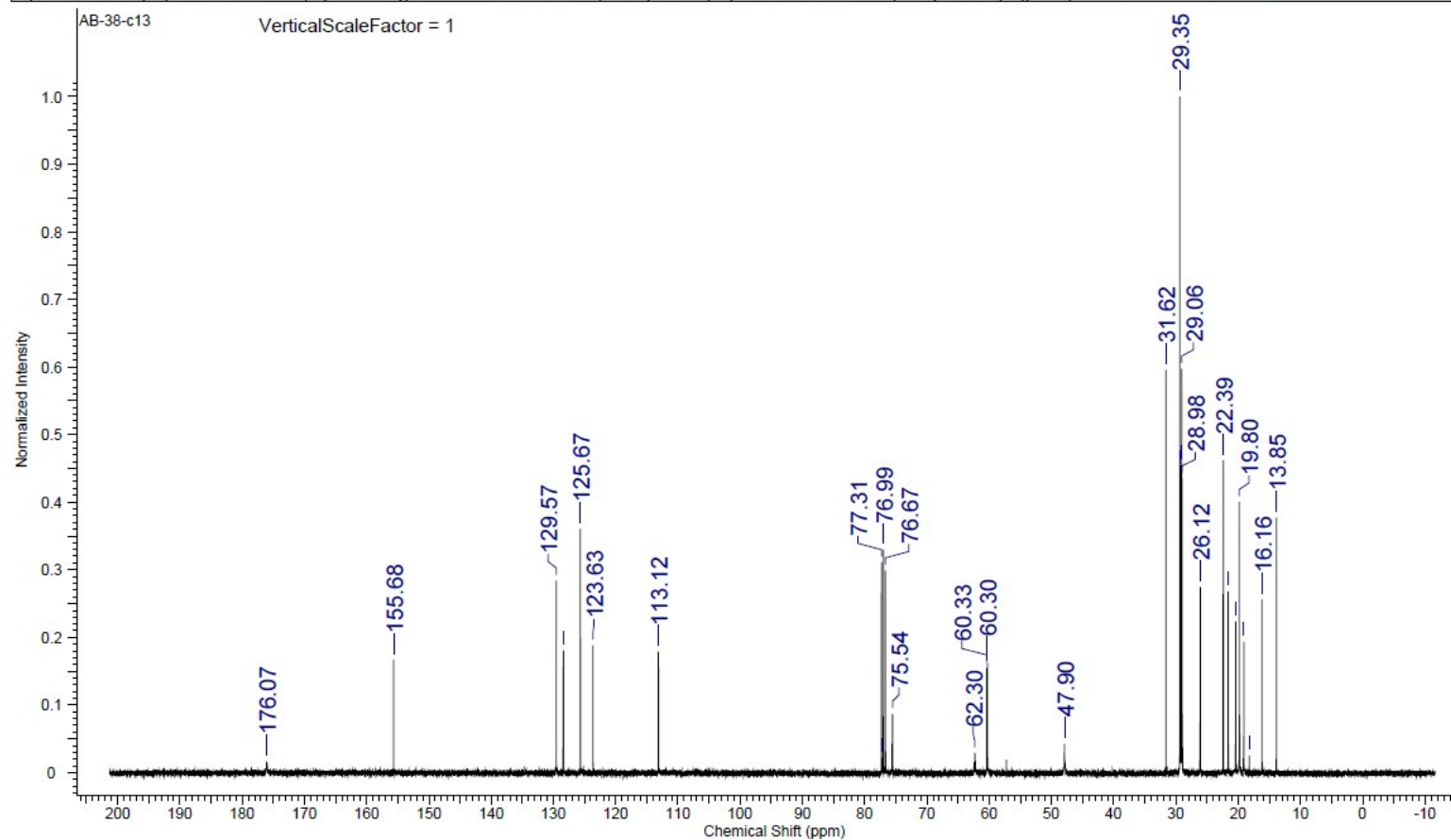


Figure S24. ¹³C NMR spectrum of 1-methyl-1-tetradecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**12**)

Acquisition Time (sec)	4.5000	Comment	AB 39	Date	Apr 26 2015	Date Stamp	Apr 26 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB39-H1.fid\AB39-H1.fid\fid				Frequency (MHz)	300.07	
Nucleus	¹ H	Number of Transients	64	Original Points Count	18711	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-d	Spectrum Offset (Hz) 1658.7224			
Spectrum Type	STANDARD	Sweep Width (Hz)	4158.00	Temperature (degree C) AMBIENT TEMPERATURE			

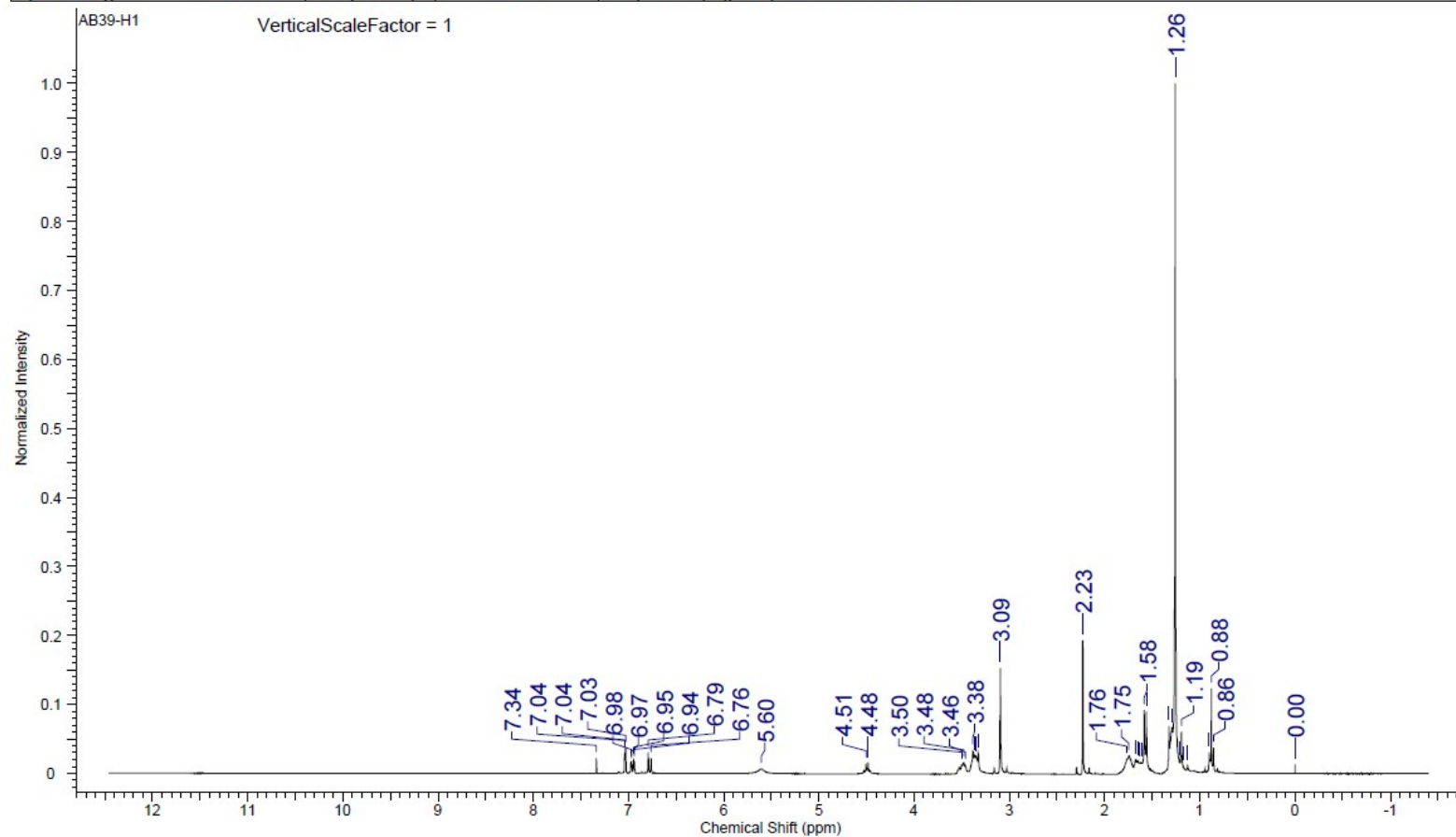


Figure S25. ¹H NMR spectrum of 1-hexadecyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**13**)

Acquisition Time (sec)	0.6400	Comment	AB 39	Date	Apr 26 2015	Date Stamp	Apr 26 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB39-C13.fid\AB39-C13.fid\fid					Frequency (MHz)	75.46
Nucleus	¹³ C	Number of Transients	3088	Original Points Count	10257	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	34.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7202.2539	Spectrum Type	STANDARD	Sweep Width (Hz)	16025.64	Temperature (degree C) AMBIENT TEMPERATURE	

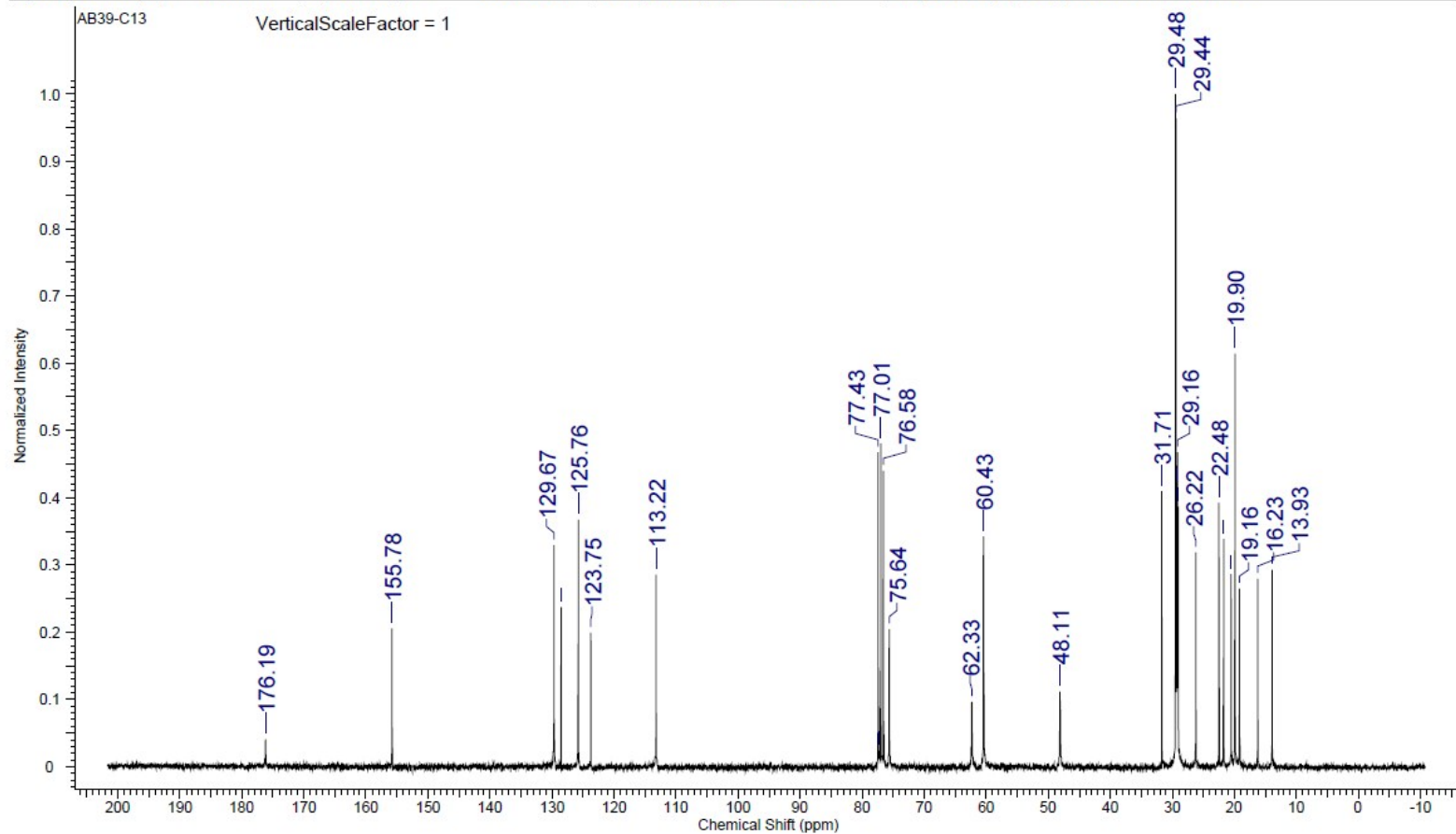


Figure S26. ¹³C NMR spectrum of 1-hexadecyl-1-methylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**13**)

Acquisition Time (sec)	5.0001	Comment	AB 40	Date	Apr 17 2015	Date Stamp	Apr 17 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB40-H1.fid\AB40-H1.fid\fid				Frequency (MHz)	300.07	
Nucleus	¹ H	Number of Transients	64	Original Points Count	25304	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-d	Spectrum Offset (Hz) 2298.5405			
Spectrum Type	STANDARD	Sweep Width (Hz)	5060.73	Temperature (degree C) AMBIENT TEMPERATURE			

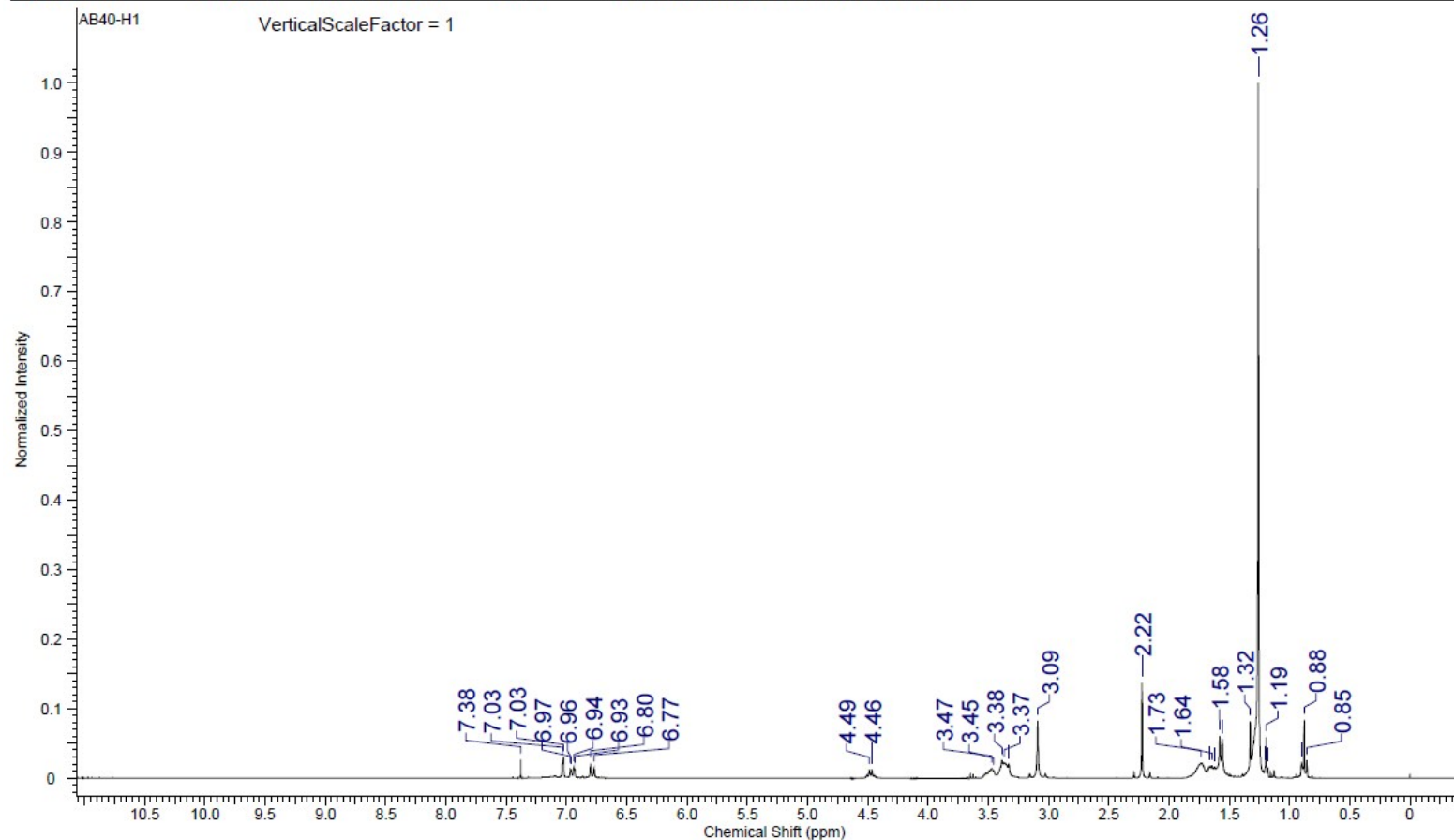


Figure S27. ¹H NMR spectrum of 1-methyl-1-octadecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**14**)

Acquisition Time (sec)	0.6400	Comment	AB 40	Date	Apr 17 2015	Date Stamp	Apr 17 2015
File Name	C:\Users\Niemcz\Desktop\Nowy folder\AB-40-C13.fid\AB-40-C13.fid\fid					Frequency (MHz)	75.46
Nucleus	¹³ C	Number of Transients	1964	Original Points Count	12191	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	34.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7946.1660	Spectrum Type	STANDARD	Sweep Width (Hz)	19047.62	Temperature (degree C)	AMBIENT TEMPERATURE

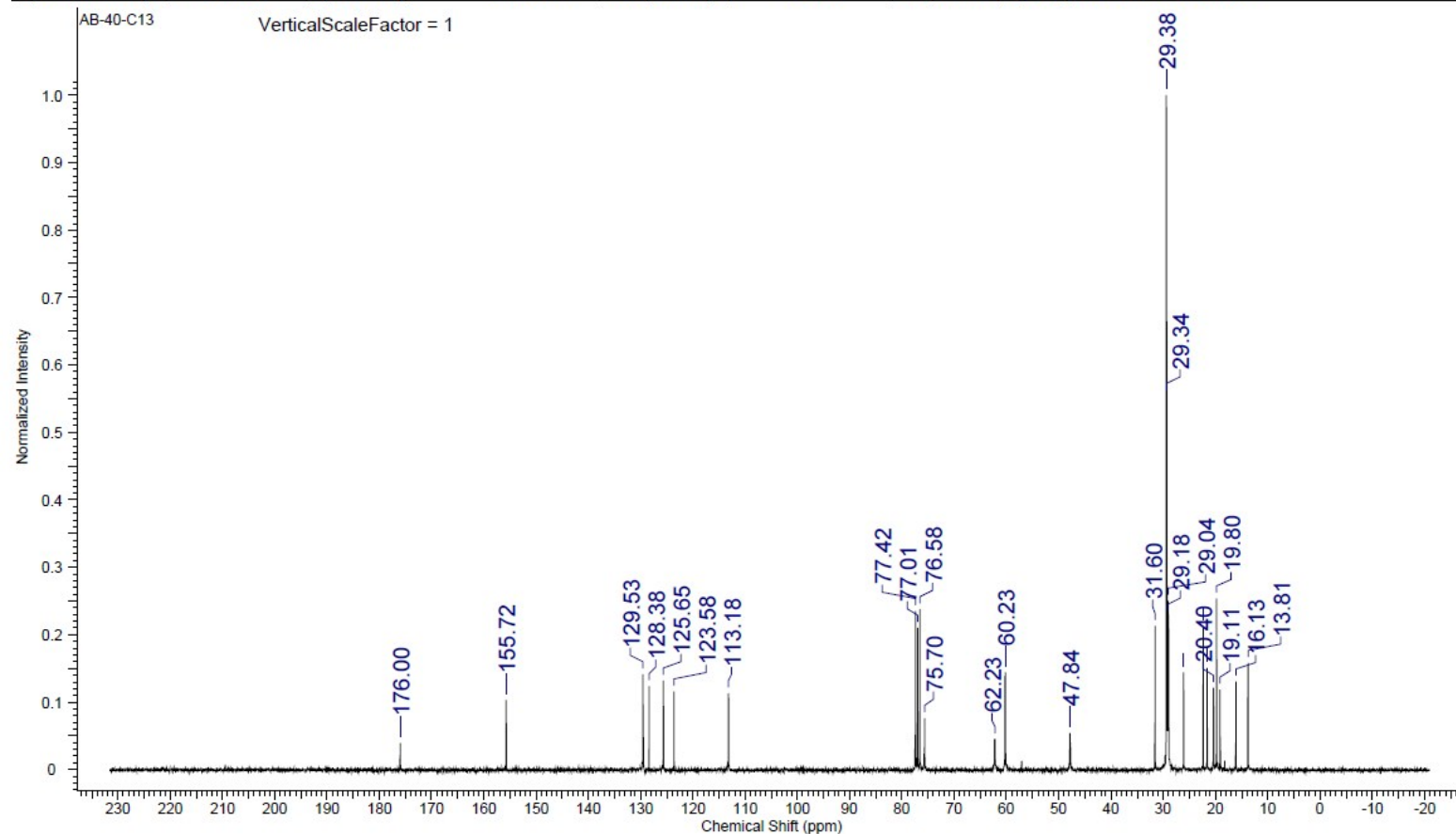


Figure S28. ¹³C NMR spectrum of 1-methyl-1-octadecylpiperidinium 2-(4-chloro-2-methylphenoxy)propionate (**14**)

The following abbreviations were used to explain the multiplicities:

s = singlet, d = doublet, dd = doublet of doublets, t = triplet, m = multiplet.