Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information for DOI: 10.1039/b811086g

Development of a method for the parallel synthesis and purification of *N*-substituted pantothenamides, known inhibitors of Coenzyme A biosynthesis and utilization

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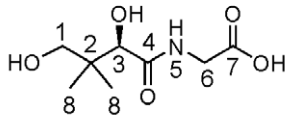
Synthetic preparation of pantothenic acid thioesters

The thiopantothenate precursors were prepared synthetically according to a method modified from Yamada *et al.*[1]

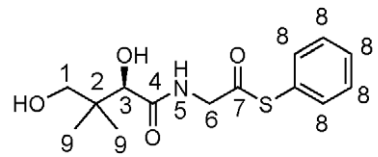
***S*-Phenyl thio-α-pantothenate (*1a*)**

α-Pantothenic acid



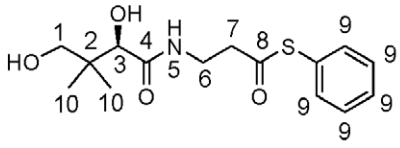
L-glycine (2.20 g; 29.3 mmol) was dissolved in 29.3 ml 1M NaOH, and the solution was lyophilized. Pantolactone (4.20 g; 32.2 mmol) was added to the resulting salt and the mixture was heated under nitrogen for 17 hours at 130°C. The resulting orange, sticky oil was dissolved in water and loaded onto a column of Amberlite IR-120 (H^+-form) ion exchange resin. The free acid of α-pantothenic acid was eluted with deionized water. Unreacted pantolactone present in the eluate was removed by extraction with dichloromethane (5×100 ml). The aqueous layer was lyophilized to give the pure acid as a yellow sticky solid (5.61 g; 93%). δ_H (300 MHz; D_2O; 25°C) δ 0.79 (3H, s, -CH_3[8]), 0.82 (3H, s, -CH_3[8]), 3.28 (1H, d, *J* 11.1, -CH-[1]), 3.39 (1H, d, *J* 11.1, -CH-[1]), 3.75 (1H, d, *J* 17.6, -CH-[6]), 3.83 (1H, d, *J* 17.6, -CH-[6]) and 3.91 (1H, s, -CH-[3]); *m/z* (ESI–MS) $[M–H]^-$ 204 (Calculated $[C_8H_{14}NO_5]^-$ = 204.09).

S-Phenyl thio-α-pantothenate ***1a***



The α-pantothenic acid prepared above (27.4 mmol) was dissolved in 24 ml DMF followed by the addition of diphenylphosphoryl azide (9.70 ml; 54.7 mmol) and thiophenol (3.37 ml; 32.8 mmol). After cooling to 0°C, triethylamine (7.63 ml; 54.7 mmol) was added and the solution was stirred for 10 minutes at 0°C followed by stirring for 3 hours at room temperature. Ethyl acetate (250 ml) was added and the solution was washed with 1M HCl (2×50 ml), 1M $NaHCO_3$ (2×50 ml) and saturated NaCl (1×50 ml). The solution was dried over Na_2SO_4 and the solvent was removed *in vacuo*. The residue was purified by flash chromatography (silica gel; ethyl acetate/hexane 2:1 to 4:1) to give *S*-phenyl thio-α-pantothenate **1a** as a orange oil (2.06 g; 25%). δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s, -CH_3[9]), 1.05 (3H, s, -CH_3[9]), 3.51 (2H, d, *J* 11.2, -CH_2-[1]), 3.57 (2H, d, *J* 11.2, -CH_2-[1]), 4.11 (1H, s, -CH-[3]), 4.28 (1H, dd, *J* 17.9, 6.1, -CH-[6]), 4.36 (1H, dd, *J* 17.9, 6.1, -CH-[6]), 7.42 (5H, s, arom.[8]) and 7.43 (1H, br s, -NH-[5]); δ_C (75MHz; $CDCl_3$; 25°C): δ 20.5, 21.5, 39.4, 48.5, 71.3, 77.6, 129.4, 129.8, 134.7, 173.6 and 195.3; *m/z* (ESI–MS) $[M+H]^+$ 298 (Calculated $[C_{14}H_{20}NO_4S]^+$ = 298.11).

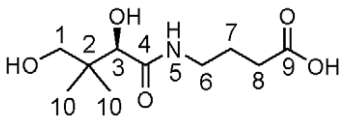
***S*-Phenyl thiopantothenate (*1b*)**



Sodium pantothenate (1.00 g; 4.15 mmol) was exchanged to the free acid by dissolving the salt in water and passing the solution through a column of Amberlite IR-120 (H^+-form) ion exchange resin. The free acid of pantothenic acid was eluted with deionized water, followed by lyophilization of the collected column eluate. The resulting syrup was dissolved in 5 ml DMF and diphenylphosphoryl azide (1.47 ml; 8.30 mmol) and thiophenol (0.513 ml; 5.00 mmol) were added. After cooling to 0°C triethylamine (1.15 ml; 8.25 mmol) was added. The solution was stirred for 10 minutes at 0°C and then at room temperature for 3 hours. Ethyl acetate (50 ml) was added and the solution was sequentially washed with 1M HCl (2×10 ml), 1M $NaHCO_3$ (2×10 ml) and saturated NaCl (1×10 ml). The solution was dried over Na_2SO_4 and the solvent was removed *in vacuo*. The residue was purified by flash chromatography (silica gel; ethyl acetate/hexane 2:1 to 4:1) to give *S*-phenyl thiopantothenate **1b** as a yellow oil (0.550 g; 42%). δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s, -CH_3[10]), 1.02 (3H, s, -CH_3[10]), 2.91–2.95 (2H, m, -CH_2-[7]), 3.47 (1H, d, *J* 11.2, -CH-[1]), 3.52 (1H, d, *J* 11.2, -CH-[1]), 3.56–3.69 (2H, m, -CH_2-[6]), 4.01 (1H, s, -CH-[3]), 7.10 (1H, br s, -NH-[5]) and 7.38–7.44 (5H, m, arom.[9]); δ_C (100 MHz; $CDCl_3$; 25°C): δ 20.3, 21.2, 34.9, 39.2, 42.8, 71.2, 77.5, 127.0, 129.3, 129.7, 134.4, 173.2 and 196.9; *m/z* (ESI–MS) $[M+H]^+$ 312 (Calculated $[C_{15}H_{22}NO_4S]^+$ = 312.13).

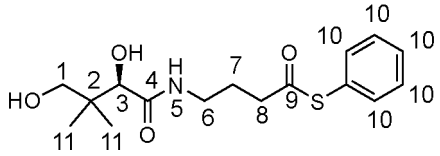
_S_-Phenyl thiohomopantothenate (*1c*)

Homopantothenic acid



4-Amino butyric acid (0.500 g; 4.80 mmol) was dissolved in 4.80 ml 1M NaOH, followed by lyophilization of the solution. Pantolactone (0.500 g; 3.84 mmol) was added to the resulting white salt and the mixture was heated under nitrogen for 17 hours at 130°C. The resulting colourless sticky oil was dissolved in water and loaded onto a column of Amberlite IR-120 (H^+-form) ion exchange resin. The free acid of homopantothenic acid was eluted with deionized water. Unreacted pantolactone present in the eluate was removed by extraction with dichloromethane (3×20 ml). The aqueous layer was lyophilized to give the pure acid as a colourless sticky solid (0.877 g; 99%). δ_H (400 MHz; D_2O; 25°C) δ 0.76 (3H, s, -CH_3[10]), 0.79 (3H, s, -CH_3[10]), 1.66 (2H, tt, *J* 7.4, 6.9, -CH_2-[7]), 2.19 (2H, t, *J* 7.4, -CH_2-[8]), 3.29 (2H, t, *J* 6.9, -CH_2-[6]), 3.25 (1H, d, *J* 11.3, -CH-[1]), 3.37 (1H, d, *J* 11.3 -CH-[1]) and 3.84 (1H, s, -CH-[3]); *m/z* (ESI–MS) $[M–H]^-$ 232 (Calculated $[C_{10}H_{18}NO_5]^-$ = 232.12).

*S-Phenyl thiohomopantothenate **1c***

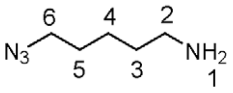


The homopantothenic acid prepared above was dissolved in 3.8 ml DMF followed by the addition of diethyl cyanophosphonate (1.14 ml; 7.60 mmol) and thiophenol (0.493 ml; 4.80 mmol). After cooling to 0°C, triethylamine (1.06 ml; 7.60 mmol) was added and the solution was stirred for 10 minutes at 0°C followed by stirring for 3 hours at room temperature. Ethyl acetate (50 ml) was added and the solution was washed with 5% citric acid (3×10 ml), 1M $NaHCO_3$ (3×10 ml) and saturated NaCl (2×10 ml). The solution was dried over Na_2SO_4 and the solvent was removed *in vacuo*. The residue was purified by flash chromatography (silica gel; ethyl acetate/hexane 2:1 to 4:1) to give *S*-phenyl thiohomopantothenate **1c** as a orange oil (0.761 g; 61%). δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, s, -CH_3[11]), 1.00 (3H, s, -CH_3[11]), 1.93 (2H, q, *J* 7.0, -CH_2-[7]), 2.71 (2H, t, *J* 7.1, -CH_2-[8]), 3.29–3.42 (2H, m, -CH_2-[6]), 3.47 (1H, d, *J* 11.4 -CH-[1]), 3.51 (1H, d, *J* 11.4 -CH-[1]), 4.01 (1H, s, -CH-[3]), 6.90 (1H, br s, -NH-[5]) and 7.40 (5H, s, arom.[10]); δ_C (75 MHz; $CDCl_3$; 25°C): δ 20.2, 21.3, 25.3, 38.1, 39.3, 40.8, 71.3, 77.6, 129.2, 129.5, 134.4, 173.4 and 197.3; *m/z* (ESI–MS) $[M+H]^+$ 326 (Calculated $[C_{16}H_{24}NO_4S]^+$ = 326.14).

Synthetic preparation of 5-azidopentan-1-amine

5-Azidopentan-1-amine was prepared by modification of the method of Lee *et al.*[2]

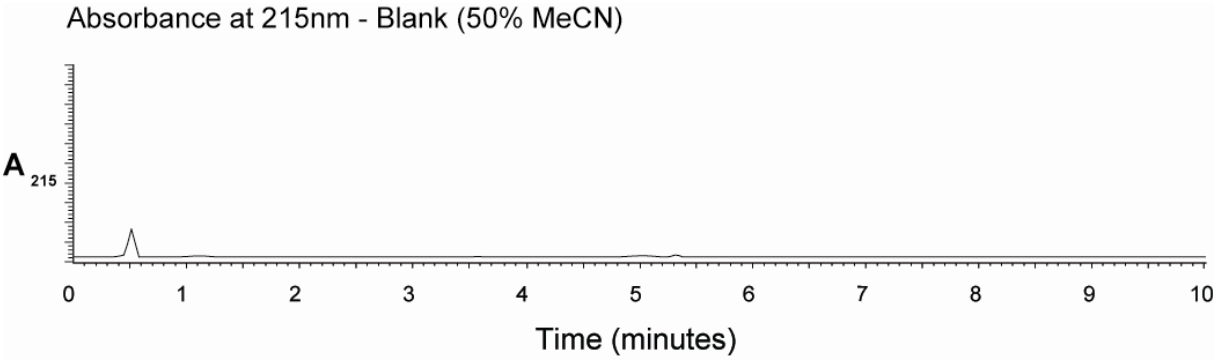
*5-Azidopentan-1-amine **28m***



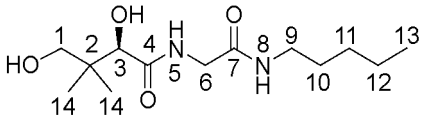
1,5-Dibromopentane (2.30 g; 10.0 mmol) was dissolved in DMF (50 ml) and sodium azide (2.60 g; 40.0 mmol) was carefully added while the solution was heated. The reaction was subsequently stirred for 20 hours at 80 °C. A mixture of ether (50 ml) and water (50 ml) was added to the reaction and mixture was left to separate. The organic phase was removed and 1,5-diazidopentane was extracted from the aqueous phase with ether (2×25 ml). The combined organic phases were washed thoroughly with water (5×12 ml) and dried over $MgSO_4$. After filtration the organic phase was reduced to ~7 ml by evaporation. Ethyl acetate (7 ml) was added to the resulting 1,5-diazidopentane/ether mixture, followed by addition of a 5% HCl solution (10 ml). The reaction was cooled to 0°C, and triphenylphosphine (2.56 g; 9.75 mmol) was added slowly over 2 hours. The reaction was allowed to warm to room tempeature and subsequently stirred for a further 18 hours. The organic layer was removed and the aqueous phase was washed with dichloromethane (2×10 ml). The pH of the aqueous phase was adjusted to pH 12 by addition of NaOH, and the product was extracted with dichloromethane (4×25 ml). Evaporation of the solvent gave 5-azidopentan-1-amine **28m** (470 mg; 37%). δ_H (300 MHz; $CDCl_3$; 25°C) δ 1.35–1.51 (4H, m, -CH_2-[4+5]), 1.60 (2H, tt, *J* 6.8, 7.1, -CH_2-[3]), 1.64 (2H, s, -NH_2[1]), 2.69 (2H, t, *J* 7.1, -CH_2-[6]) and 3.26 (2H, t, *J* 6.8, -CH_2-[2]); δ_C (75 MHz; $CDCl_3$; 25°C): δ 24.0, 28.7, 33.1, 41.9 and 51.4; *m/z* (EI–MS) $[M+H]^+$ 129 (Calculated $[C_5H_{13}N_4]^+$ = 129.11).

Characterization of N-substituted pantothenamides 4 and 45

Pantothenamides **4a-c** and **45a-c** were thoroughly characterized by ^{1}H NMR, ^{13}C NMR, and by LC-MS analysis, the latter giving single peaks with the reported retention times. The small peak visible at 0.6 minutes in all the LC-MS chromatograms is also present in the chromatogram for a blank injection of the solvent used to prepare the samples for LC-MS analysis, as shown below. All other pantothenamides were characterized by ^{1}H NMR.

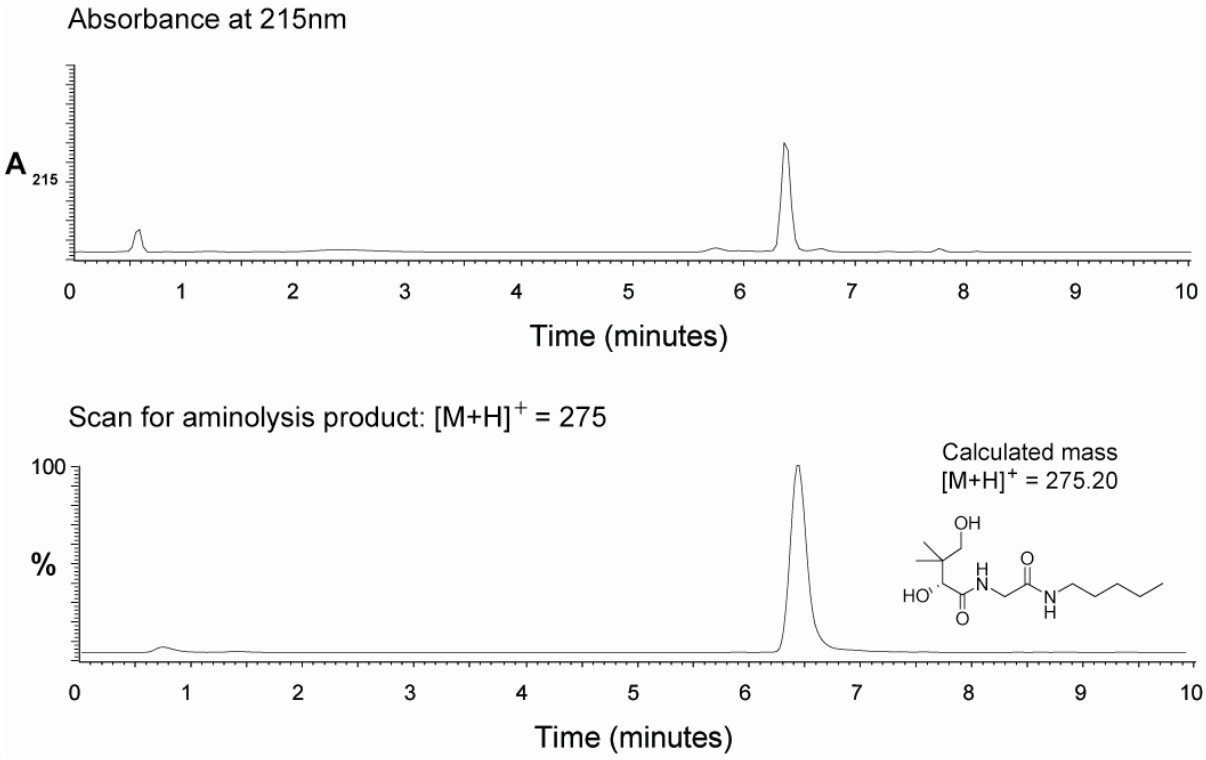


N-Pentyl α-pantothenamide (*4a*)

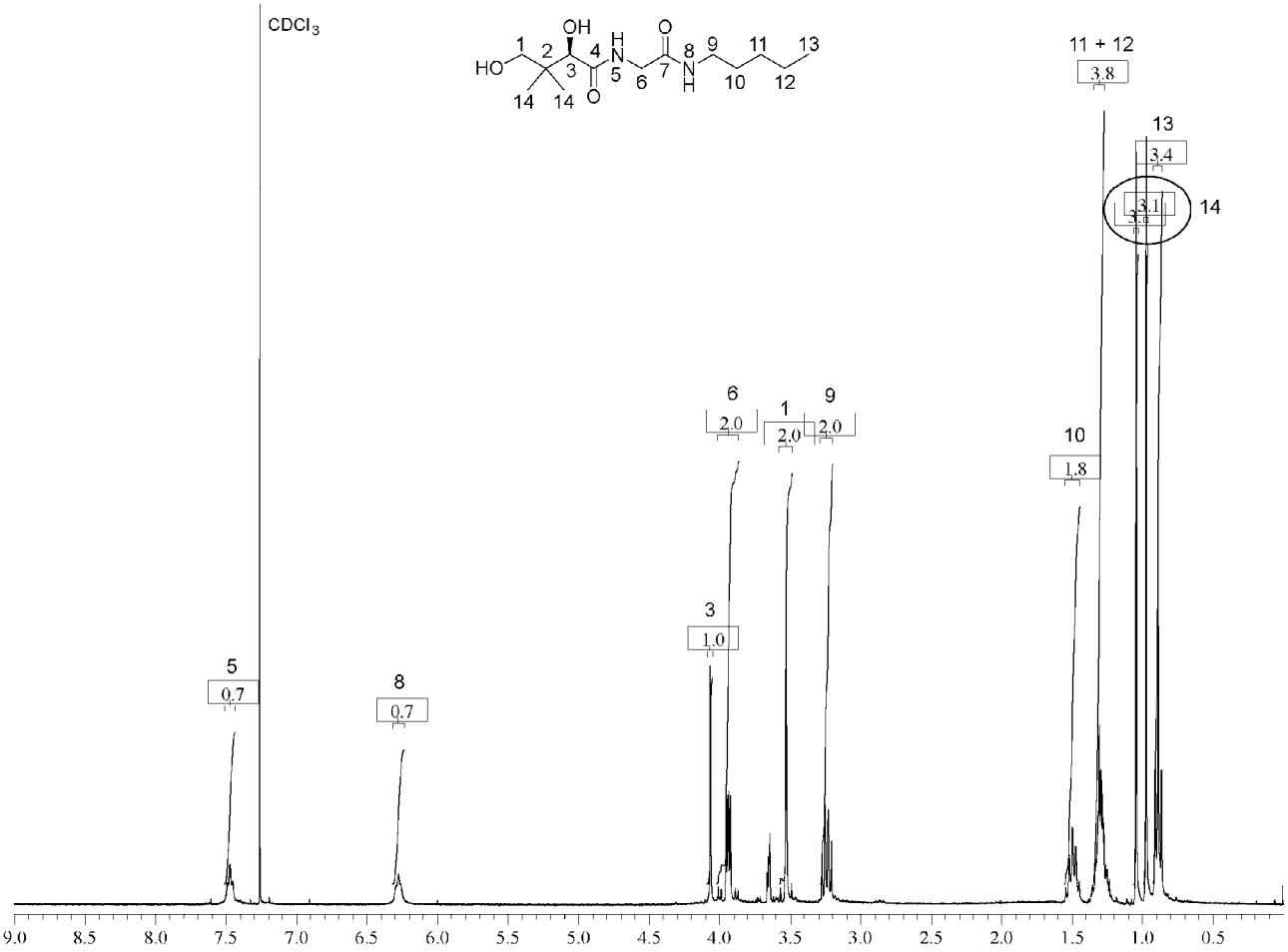


δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, t, *J* 6.9, -CH_3[13]), 0.97 (3H, s, -CH_3[14]), 1.05 (3H, s, -CH_3[14]), 1.23–1.35 (4H, m, -CH_2-[11+12]), 1.45–1.54 (2H, m, -CH_2-[10]), 3.23 (1H, t, *J* 7.0 -CH-[9]), 3.25 (1H, t, *J* 6.6 -CH-[9]), 3.52 (2H, s, -CH_2-[1]), 3.90 (1H, dd, *J* 16.3, 5.9 -CH-[6]), 3.97 (1H, d, *J* 16.3, 5.9 -CH-[6]), 4.06 (1H, s, -CH-[3]), 6.27 (1H, br s, -NH-[8]) and 7.47 (1H, br s, -NH-[5]); δ_C (100 MHz; $CDCl_3$; 25°C) δ 13.9, 21.0, 21.1, 22.3, 29.0, 29.0, 39.4, 39.7, 42.7, 70.4, 91.6, 169.2 and 174.5; *m/z* (ESI–MS) $[M+H]^+$ 275 (Calculated $[C_{13}H_{27}N_2O_4]^+$ = 275.20); LC retention time 6.40 min.

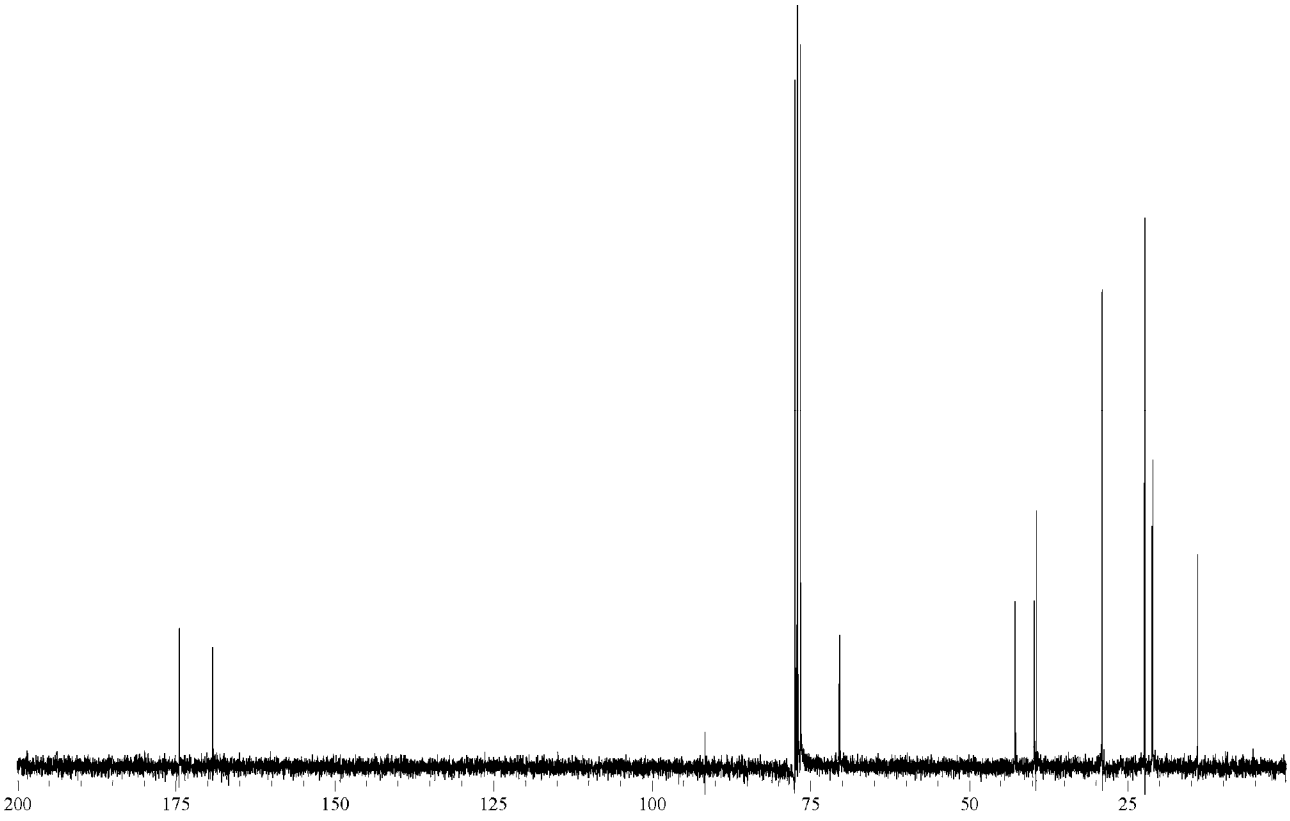
LC-MS analysis:



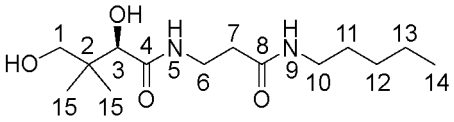
^{1}H NMR (300 MHz):



^{13}C NMR (100 MHz):

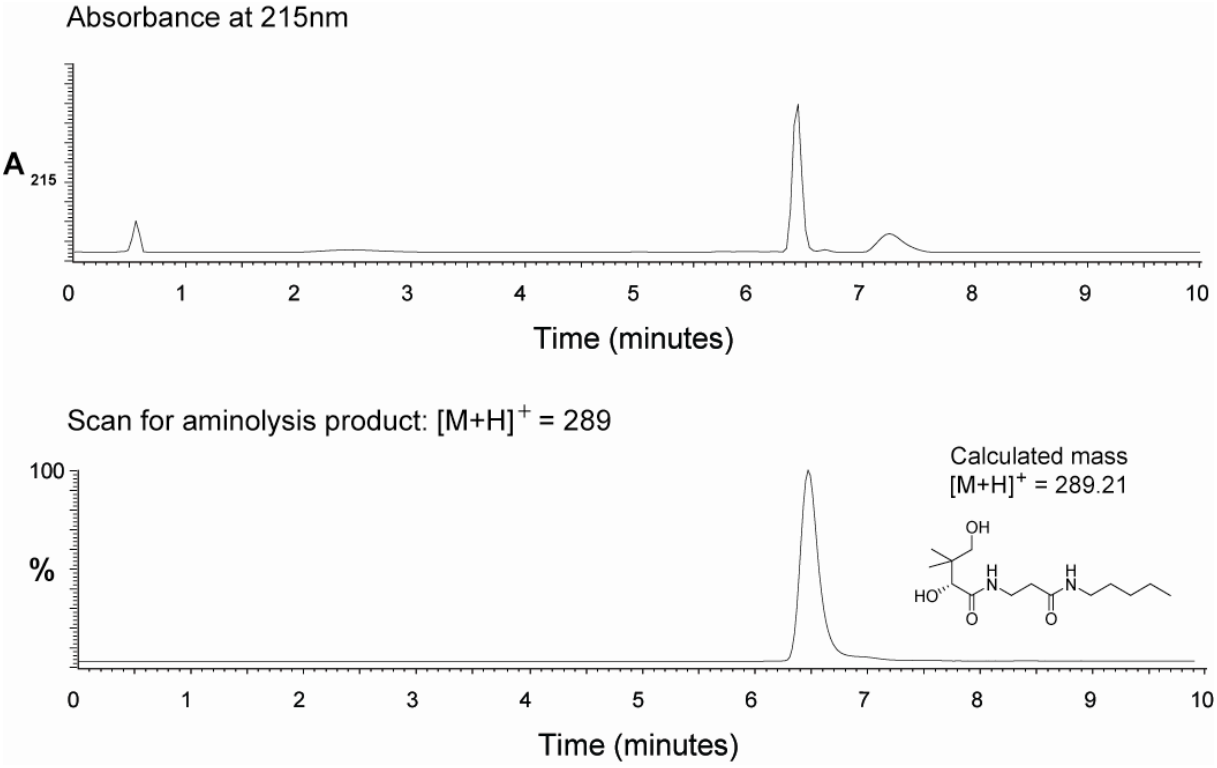


_N_-Pentyl pantothenamide (*4b*)

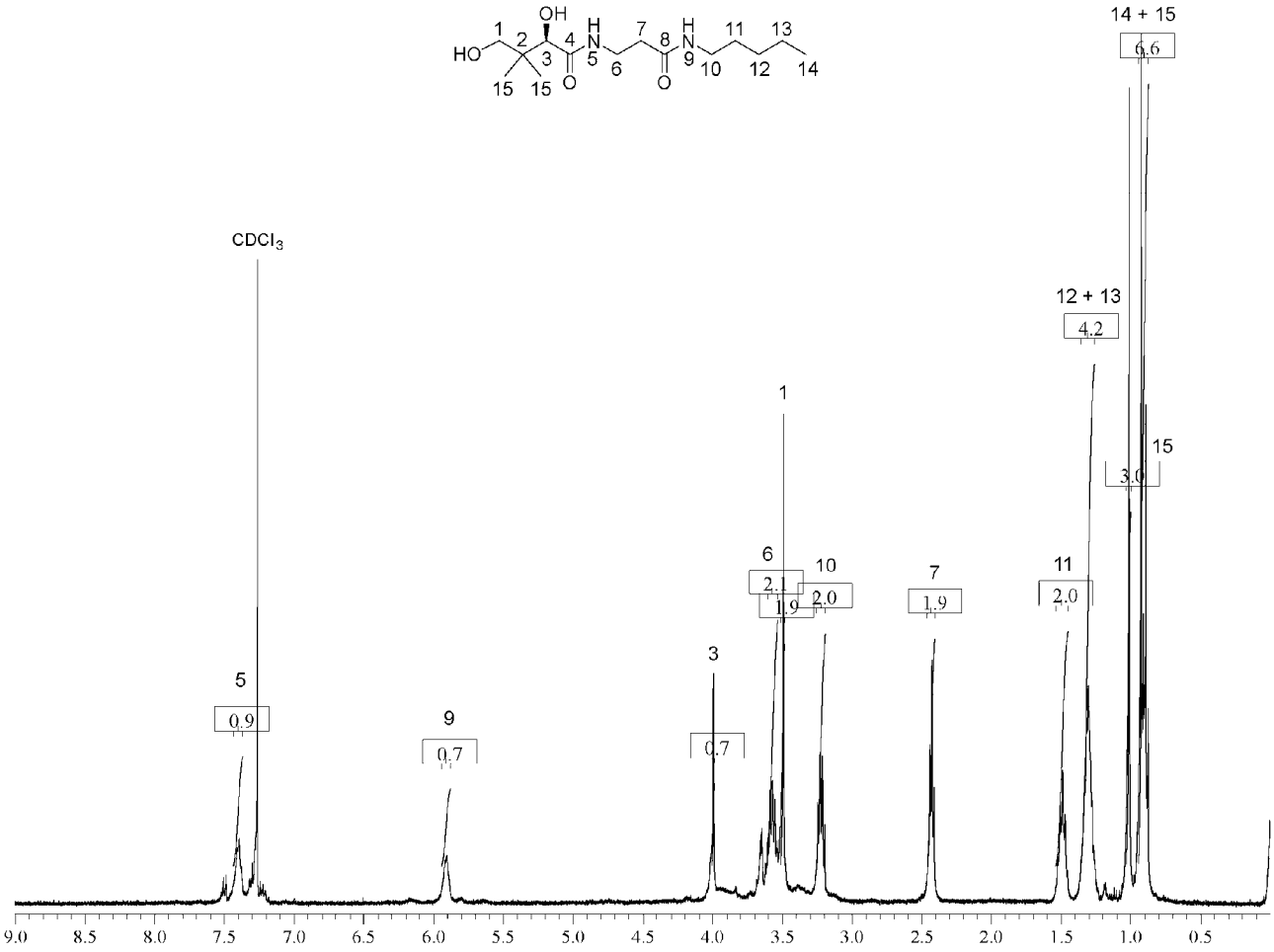


δH (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, t, *J* 7.1, -CH_3[14]), 0.92 (3H, s, -CH_3[15]), 1.01 (3H, s, -CH_3[15]), 1.27–1.34 (4H, m, -CH_2-[12+13]), 1.46–1.52 (2H, m, -CH_2-[11]), 2.43 (2H, t, *J* 6.1, -CH_2-[7]), 3.21 (1H, t, *J* 7.3, -CH-[10]), 3.23 (1H, t, *J* 7.1, -CH-[10]), 3.49 (2H, s, -CH_2-[1]), 3.53–3.60 (2H, m, -CH_2-[6]), 3.99 (1H, s, -CH-[3]), 5.92 (1H, br s, -NH-[9]) and 7.40 (1H, br s, -NH-[5]); δC (100 MHz; $CDCl_3$; 25°C) δ 13.9, 20.5, 21.2, 22.3, 29.0, 29.1, 35.3, 35.8, 39.2, 39.6, 70.7, 77.2, 171.4 and 173.9; m/z (ESI–MS) $[M+H]^+$ 289 (Calculated $[C_{14}H_{29}N_2O_4]^+$ = 289.21); LC retention time 6.48 min.

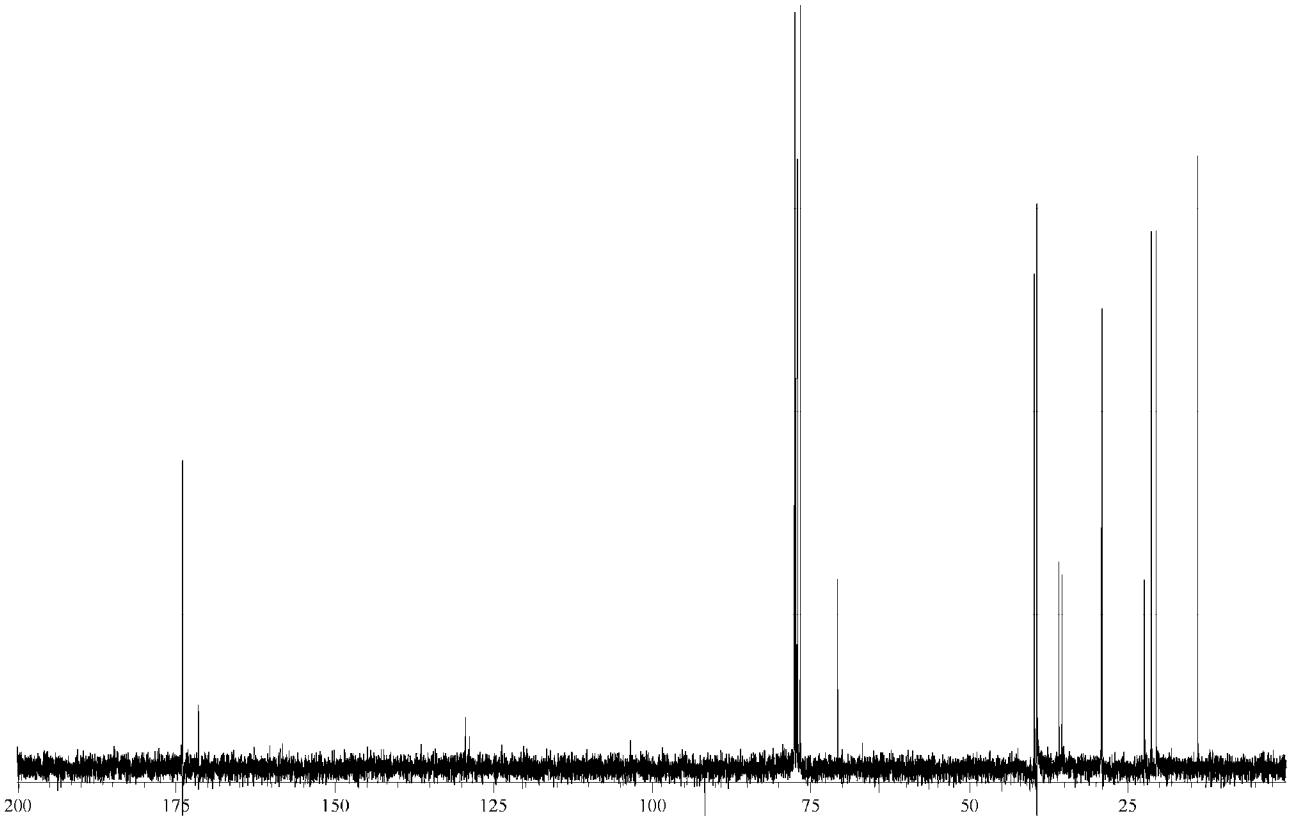
LC-MS analysis:



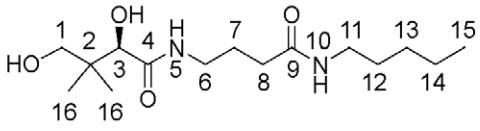
^{1}H NMR (400 MHz):



^{13}C NMR (100 MHz):

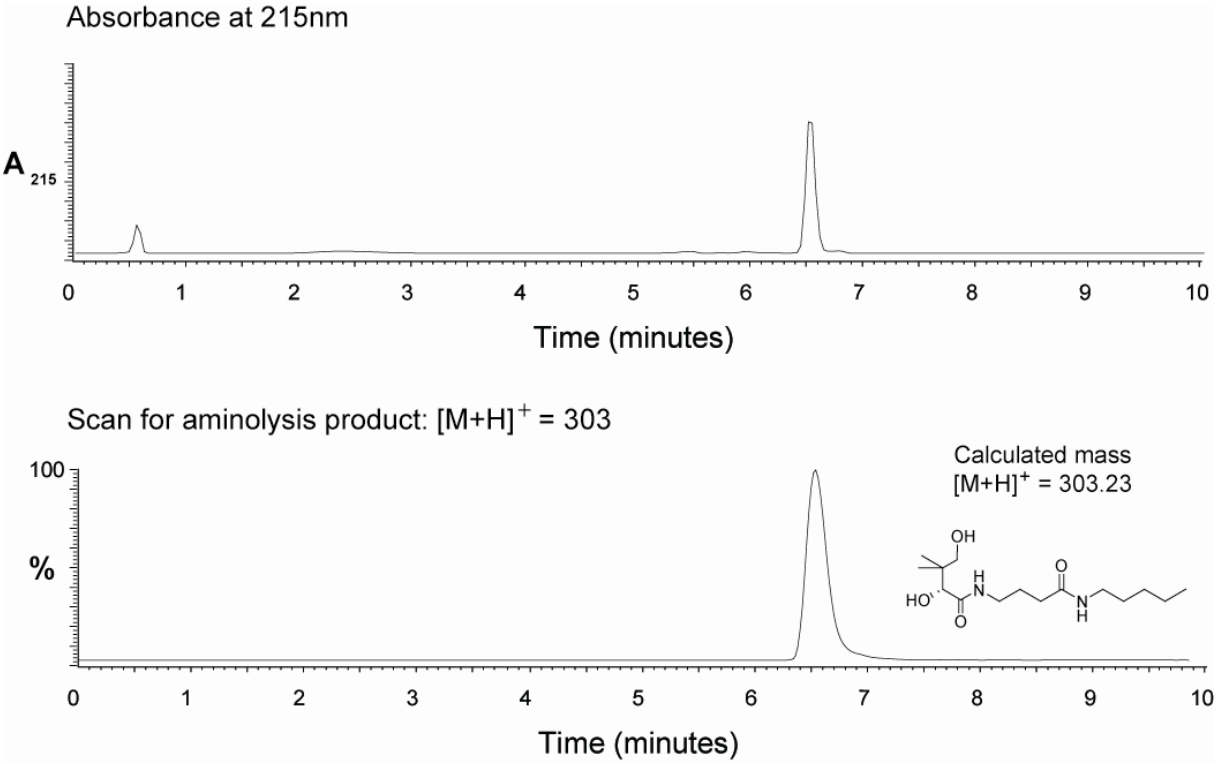


***N*-Pentyl homopantothenamide (*4*c)**

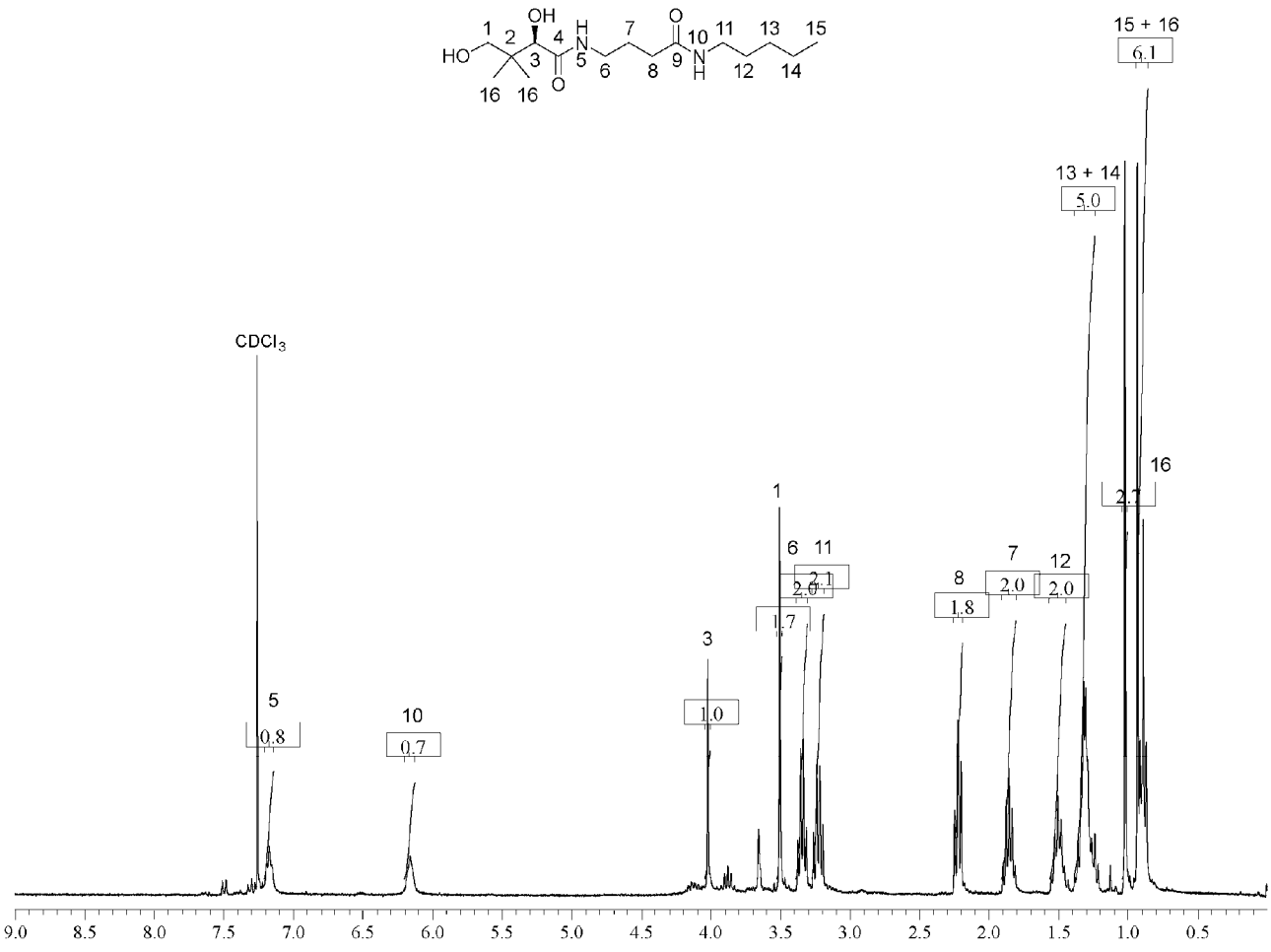


δH (300 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, t, *J* 6.7, -CH_3[15]), 0.93 (3H, s, -CH_3[16]), 1.02 (3H, s, -CH_3[16]), 1.22–1.38 (4H, m, -CH_2-[13+14]), 1.46–1.55 (2H, m, -CH_2-[12]), 1.81–1.90 (2H, m, -CH_2-[7]), 2.22 (2H, t, *J* 6.7, -CH_2-[8]), 3.22 (1H, t, *J* 6.5 -CH-[11]), 3.24 (1H, t, *J* 7.0 -CH-[11]), 3.33 (1H, t, *J* 6.4, -CH-[6]), 3.36 (1H, t, *J* 6.5, -CH-[6]), 3.51 (2H, s, -CH_2-[1]), 4.02 (1H, s, -CH-[3]), 6.20 (1H, br s, -NH-[10]) and 7.20 (1H, br s, -NH-[5]); δC (100 MHz; $CDCl_3$; 25°C) δ 14.0, 20.5, 21.3, 22.3, 25.8, 29.1, 29.1, 33.8, 38.4, 39.3, 39.7, 71.0, 77.3, 172.8 and 174.0; m/z (ESI–MS) $[M+H]^+$ 303 (Calculated $[C_{15}H_{31}N_2O_4]^+$ = 303.23); LC retention time 6.55 min.

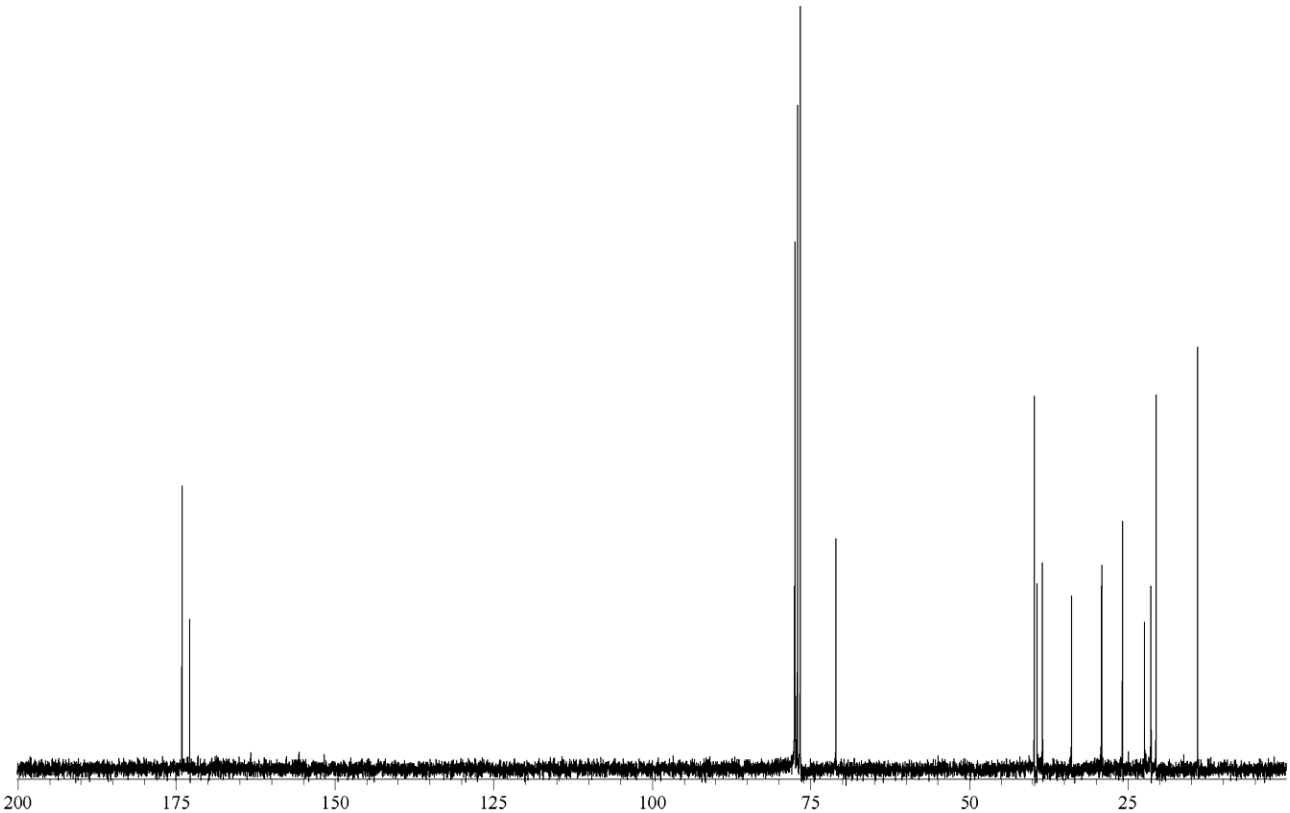
LC-MS analysis:



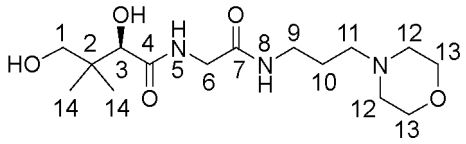
^{1}H NMR (300 MHz):



^{13}C NMR (100 MHz):

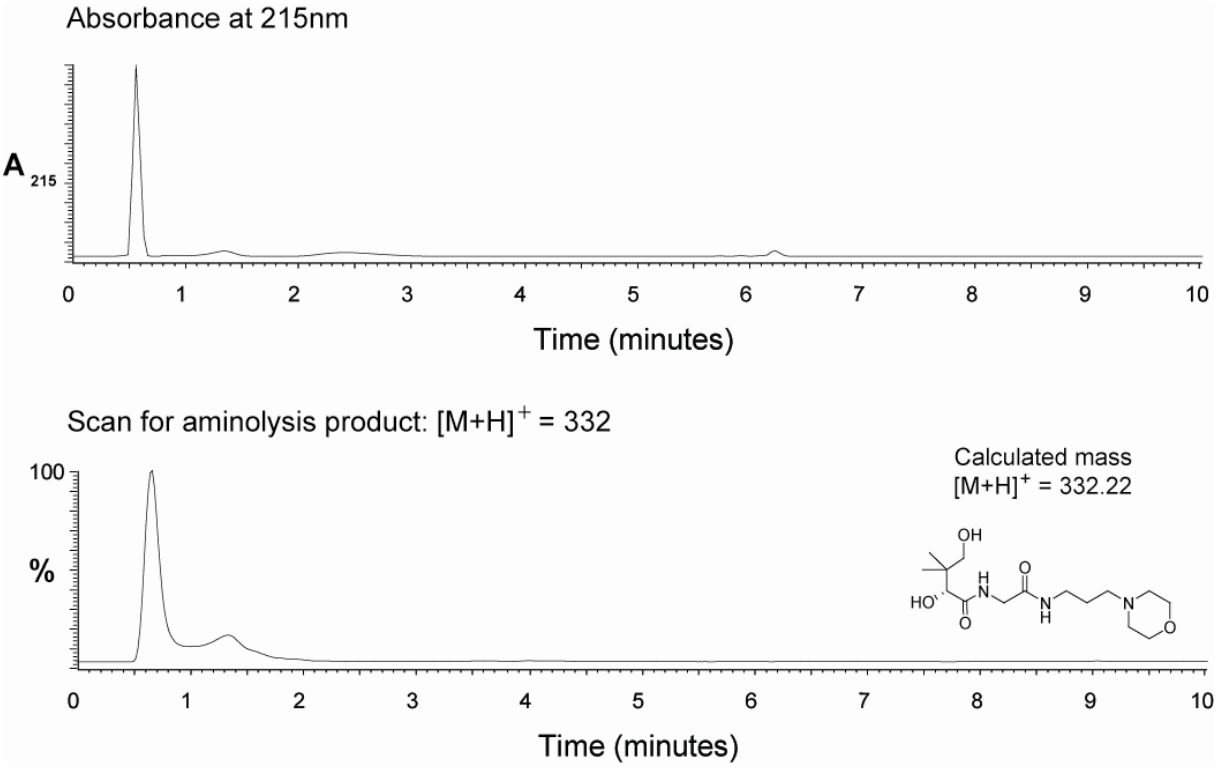


_N_-(3-Morpholin-4-yl-propyl) α-pantothenamide (45a)

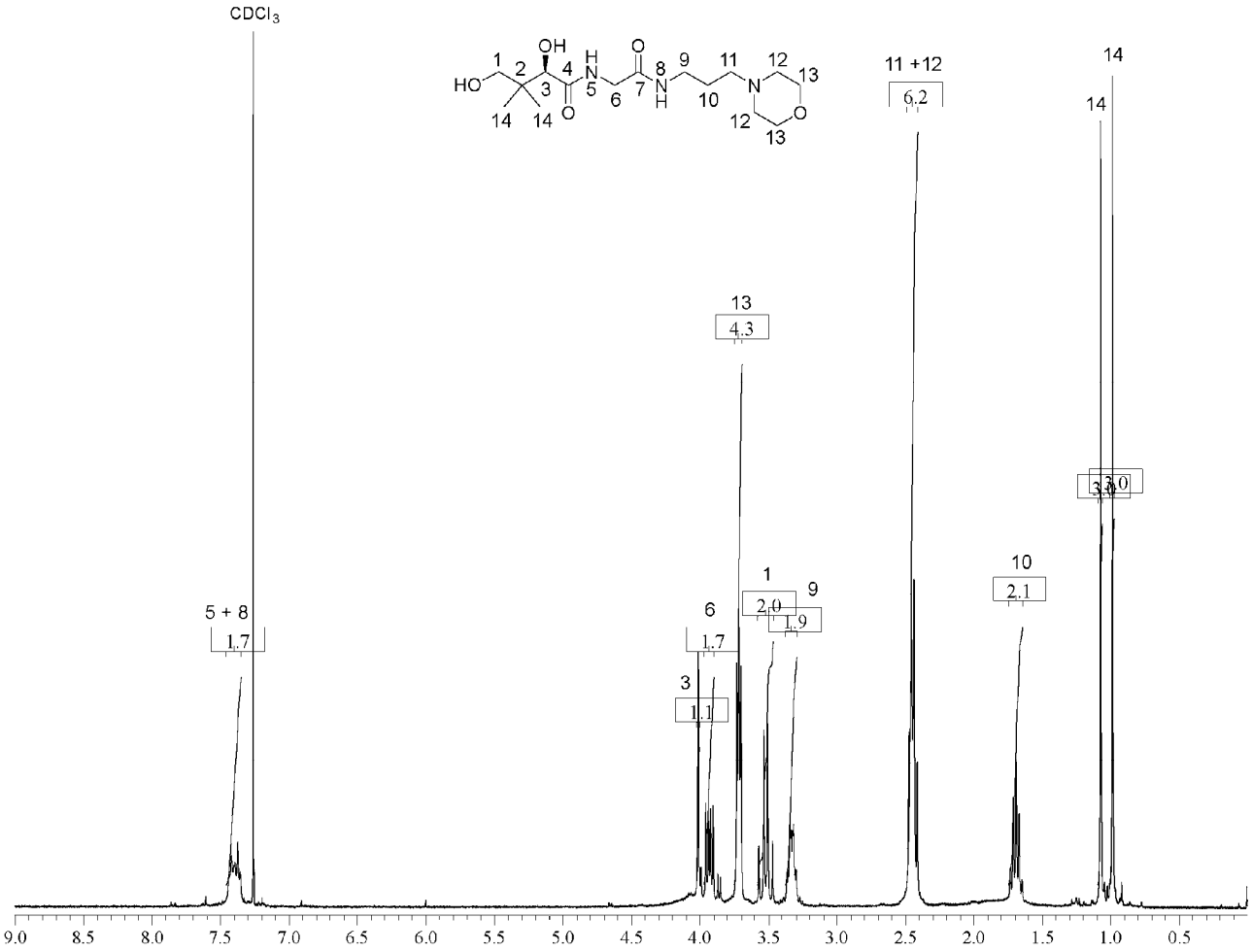


δ_H (300MHz; $CDCl_3$; 25°C) δ 0.99 (3H, s, -CH_3[14]), 1.07 (3H, s, -CH_3[14]), 1.65–1.73 (2H, m, -CH_2-[10]), 2.39–2.51 (6H, m, -CH_2-[11+12]), 3.29–3.36 (2H, m, -CH_2-[9]), 3.48 (1H, d, *J* 11.0, -CH-[1]), 3.53 (1H, d, *J* 11.0, -CH-[1]), 3.71 (4H, t, *J* 4.7, -CH_2-[13]), 3.89 (1H, dd, *J* 16.3, 5.9 -CH-[6]), 3.98 (1H, dd, *J* 16.3, 5.9 -CH-[6]), 4.01 (1H, s, -CH-[3]) and 7.35–7.43 (2H, m, -NH-[5+8]); δ_C (100MHz; $CDCl_3$; 25°C): δ 21.3, 21.6, 25.0, 38.7, 39.5, 42.6, 53.5, 56.8, 66.9, 70.0, 77.3, 169.1 and 174.2; *m/z* (ESI–MS) $[M+H]^+$ 332 (Calculated $[C_{15}H_{30}N_3O_5]^+$ = 332.22); LC retention time 0.67 min.

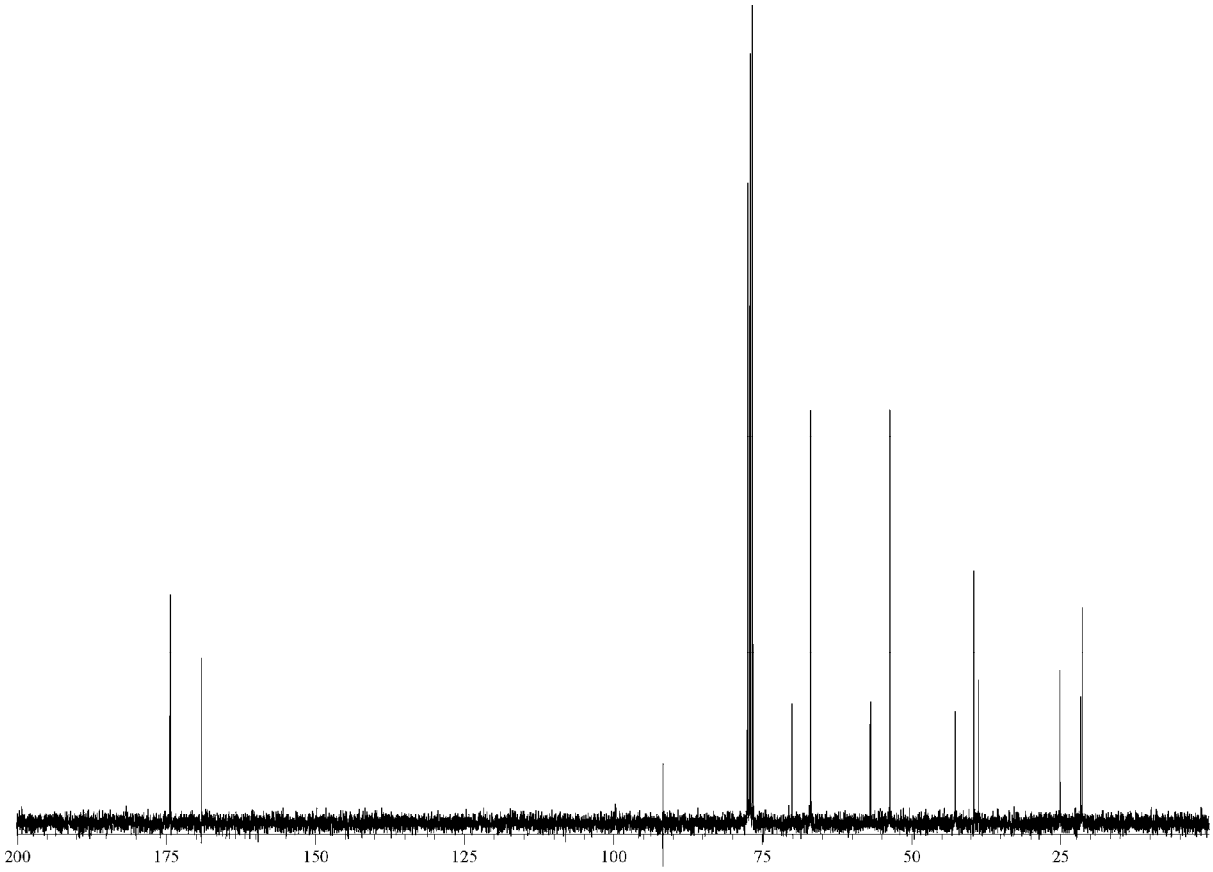
LC-MS analysis:



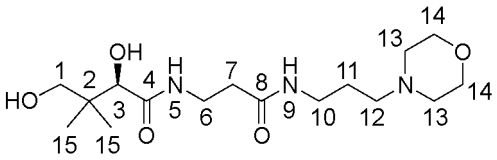
^{1}H NMR (300 MHz):



^{13}C NMR (100 MHz):

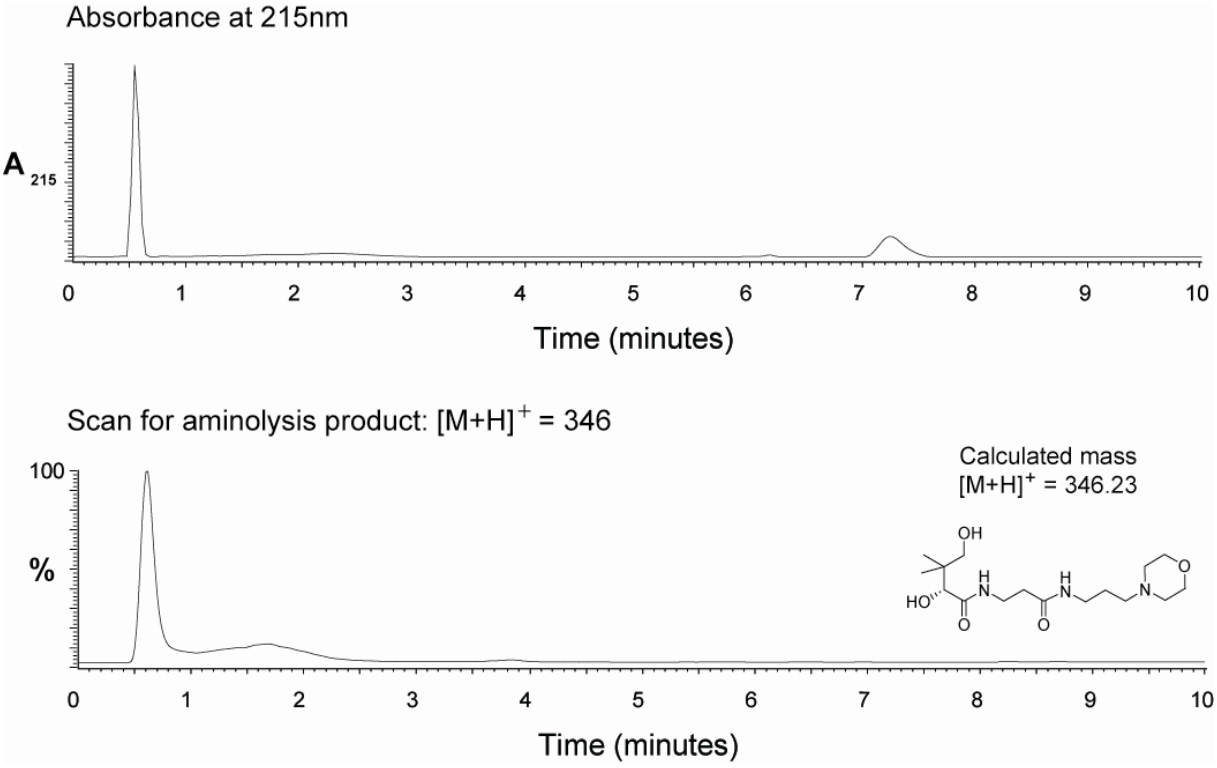


***N*-(3-Morpholin-4-yl-propyl) pantothenamide (45b)**

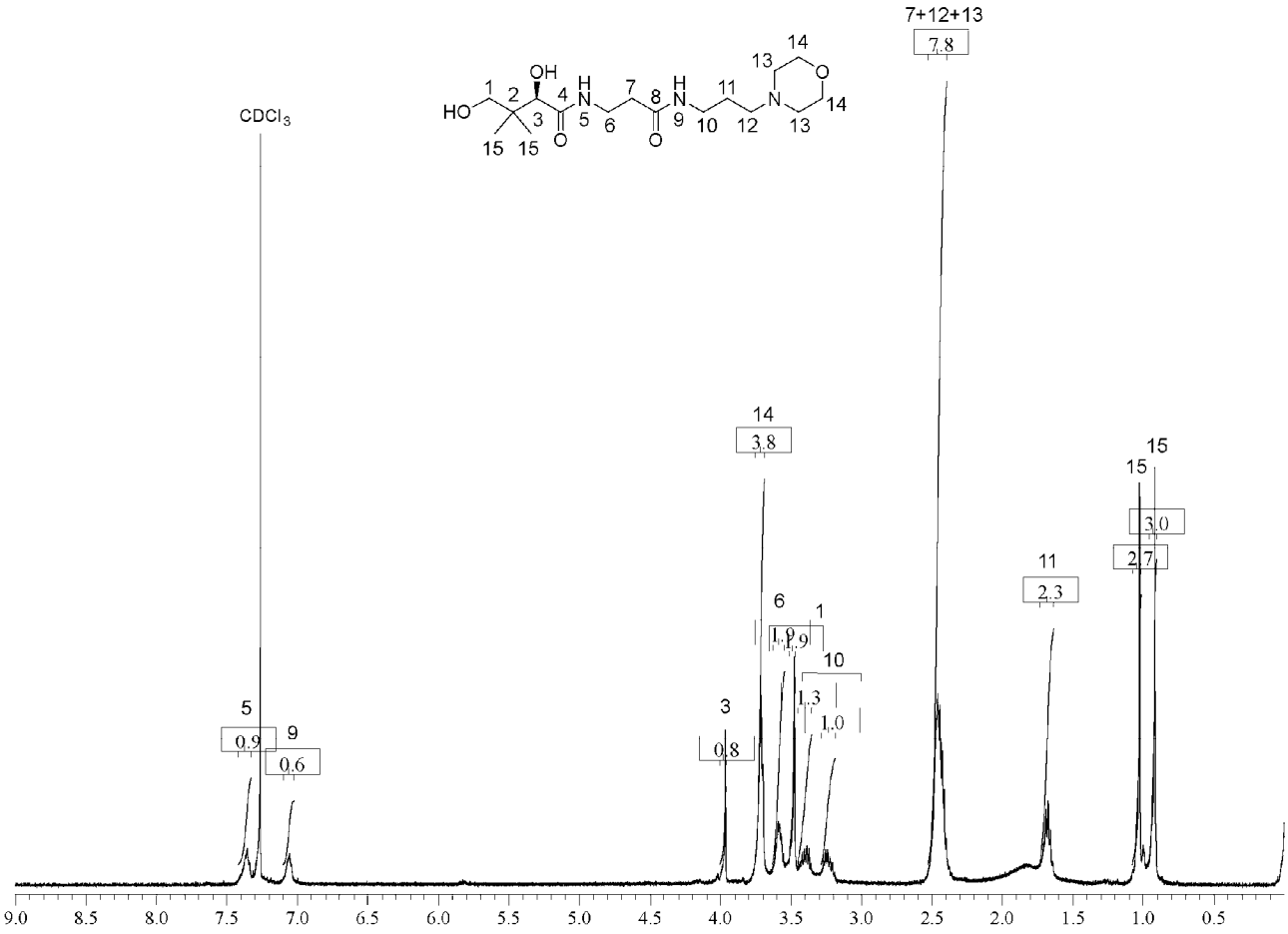


δH (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s, -CH_3[15]), 1.02 (3H, s, -CH_3[15]), 1.65–1.73 (2H, m, -CH_2[11]), 2.40–2.52 (8H, m, -CH_2-[7+12+13]), 3.19–3.27 (1H, m, -CH-[10]), 3.35–3.45 (1H, m, -CH-[10]), 3.47 (2H, s, -CH_2-[1]), 3.55–3.62 (2H, m, -CH_2-[6]), 3.67–3.78 (4H, m, -CH_2-[14]), 3.96 (2H, s, -CH-[3]), 7.05 (1H, br s, -NH-[9]) and 7.35 (1H, br s, -NH-[5]); δC (100 MHz; $CDCl_3$; 25°C) δ 20.4, 21.5, 25.2, 35.4, 35.8, 38.8, 39.3, 53.5, 57.2, 66.8, 70.5, 77.1, 171.3 and 174.0; m/z (ESI–MS) $[M+H]^+$ 346 (Calculated $[C_{16}H_{32}N_3O_5]^+$ = 346.23); LC retention time 0.67 min.

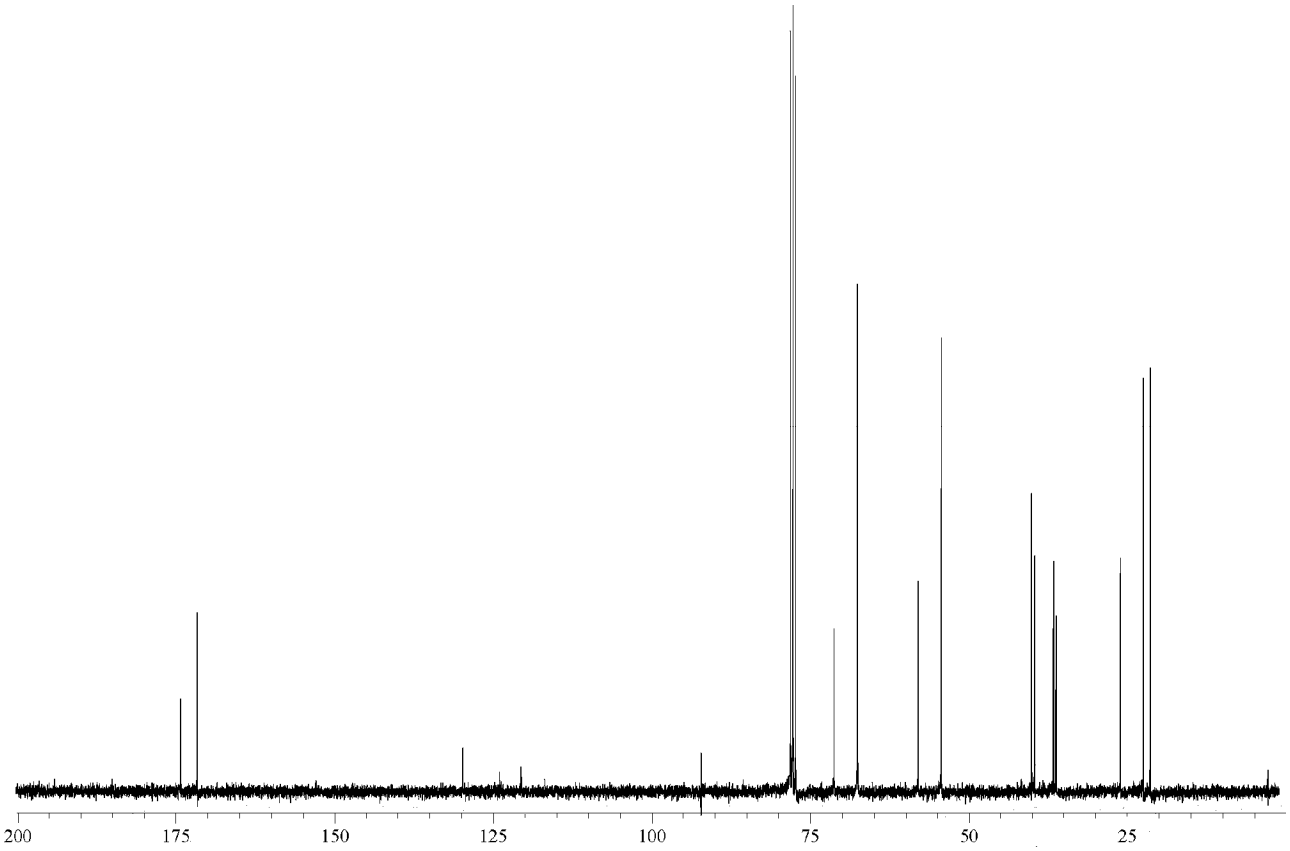
LC-MS analysis:



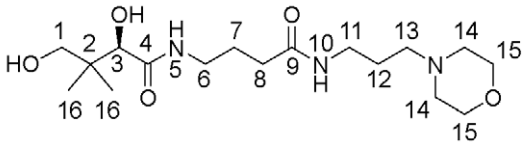
^{1}H NMR (400 MHz):



^{13}C NMR (100 MHz):

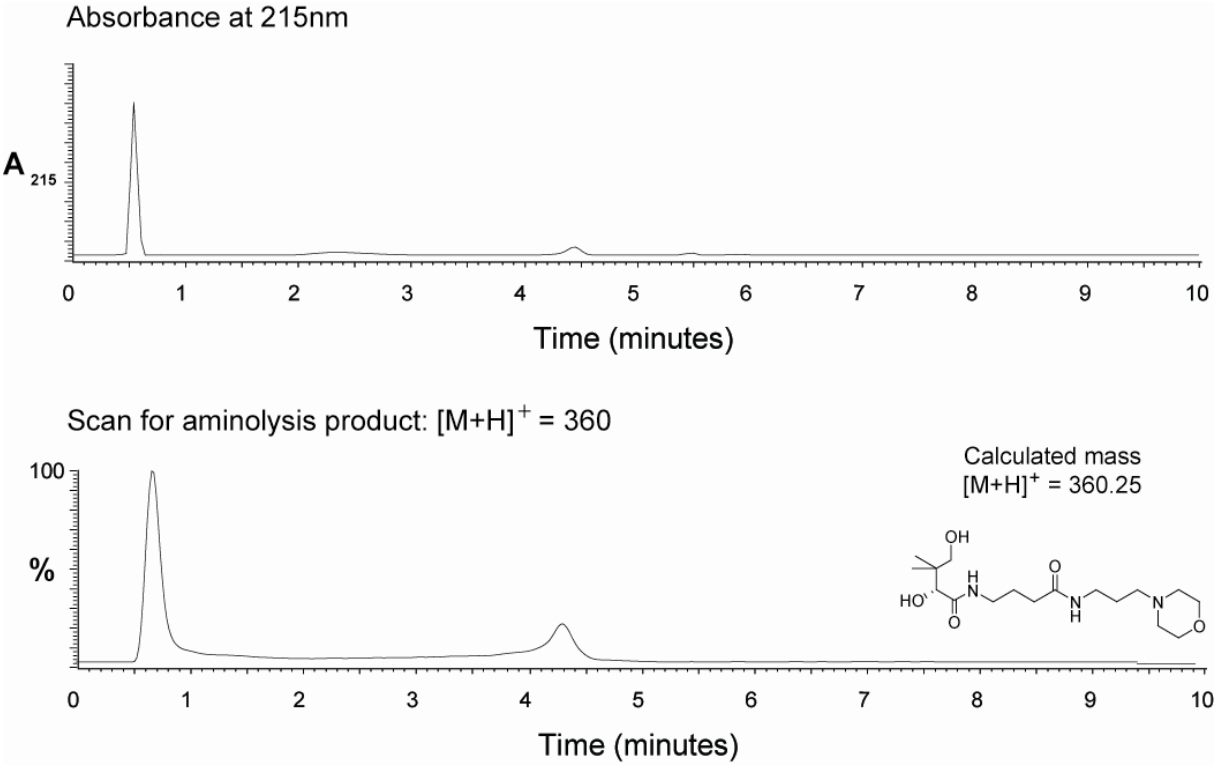


***N*-(3-Morpholin-4-yl-propyl) homopantothenamide (45c)**

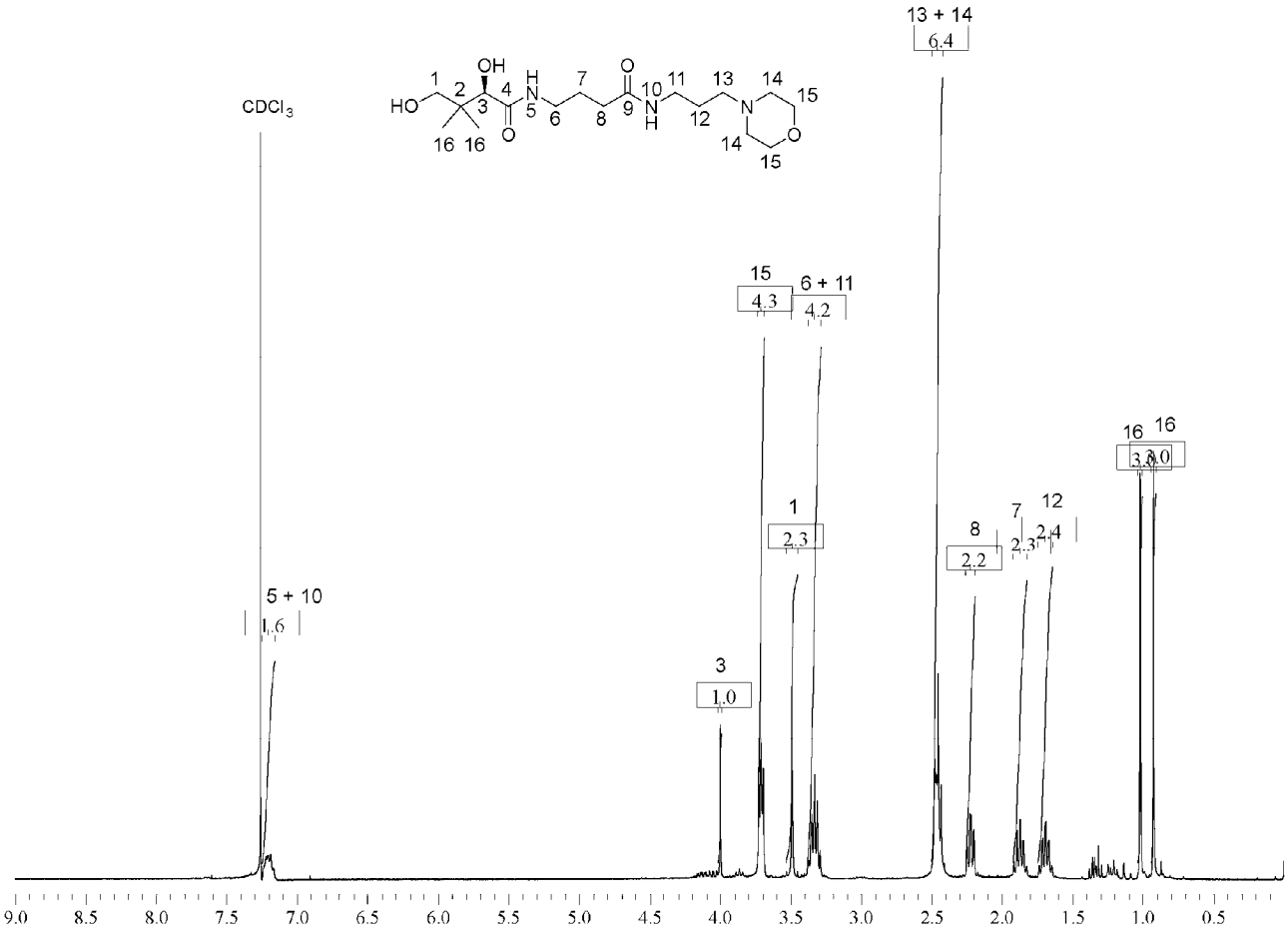


δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s, -CH_3[16]), 1.02 (3H, s, -CH_3[16]), 1.65–1.73 (2H, m, -CH_2-[12]), 1.82–1.91 (2H, m, -CH_2-[7]), 2.23 (2H, t, *J* 7.0, -CH_2-[8]), 2.41–2.48 (6H, m, -CH_2-[13+14]), 3.29–3.39 (4H, m, -CH_2-[6+11]), 3.49 (2H, s, -CH_2-[1]), 3.71 (4H, t, *J* 9.1, -CH_2-[15]), 4.00 (1H, s, -CH-[3]), 7.19 (1H, br s, -NH-[10]) and 7.22 (1H, br s, -NH-[5]); δ_C (100 MHz; $CDCl_3$; 25°C) δ 20.5, 21.4, 25.0, 25.5, 34.0, 38.6, 39.0, 39.3, 53.6, 57.3, 66.9, 70.6, 77.4, 172.7 and 173.9; *m/z* (ESI–MS) $[M+H]^+$ 360 (Calculated $[C_{17}H_{34}N_3O_5]^+$ = 360.25); LC retention time 0.68 min.

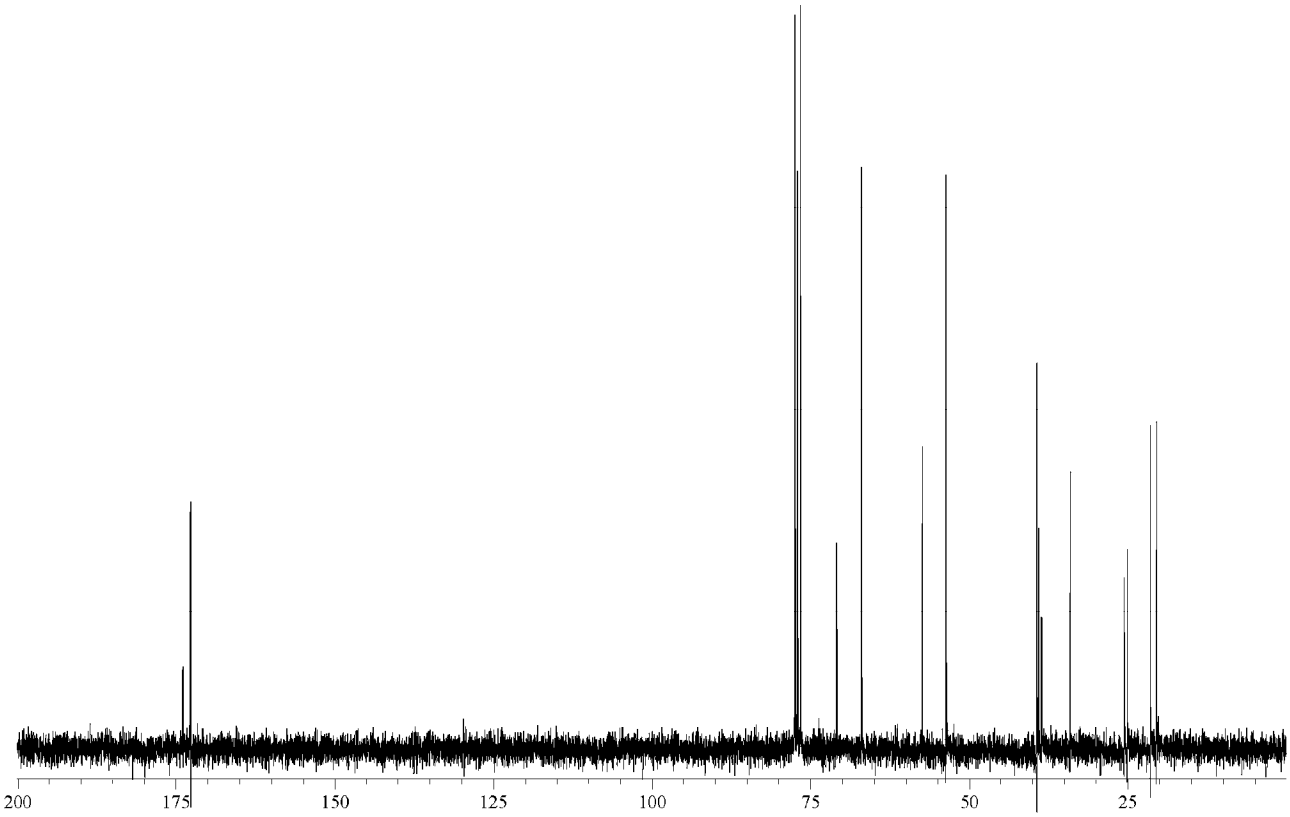
LC-MS analysis:



^{1}H NMR (300 MHz):



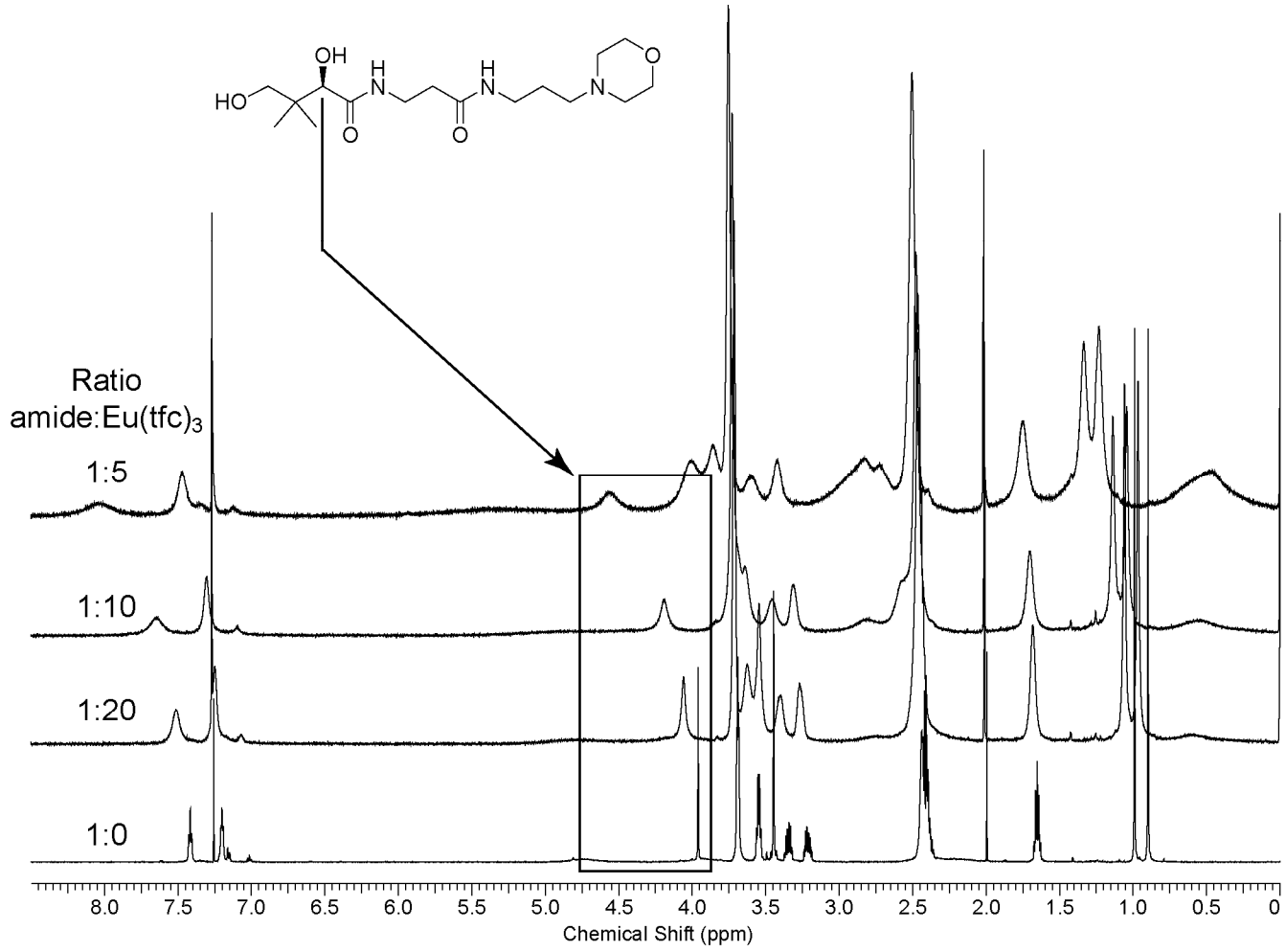
^{13}C NMR (100 MHz):



Optical purity of pantothenamides 4b and 45b

To confirm that the pantothenamides prepared and purified by the two described methods do not racemize during the workup and purification procedures, pantothenamides **4b** and **45b** – each representing one of the two purification methods – were analyzed by ^{1}H NMR in the presence of increasing amounts of the chiral shift reagent tris-[3-(trifluoromethylhydroxymethylene)-(+)-camphorato]europium ($Eu(tfc)_3$). The spectra resulting from the experiment with the amide **45b** are shown below. While the singlet peak at 3.96 ppm representing the proton on the chiral carbon atom (boxed signal below) shifts significantly downfield as the amount of $Eu(tfc)_3$ is increased, no separate peak can be observed, confirming the optical purity of the pantothenamide product.

A similar experiment with the amide **4b** gave identical results.



Characterization of all other N-substituted pantothenamides

All other pantothenamides were characterized by ^{1}H NMR; the corresponding data are reported below.

***N*-Propyl α-pantothenamide (*2a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, t, *J* 7.5), 0.97 (3H, s), 1.05 (3H, s), 1.47–1.58 (2H, m), 3.20 (1H, t, *J* 6.3), 3.22 (1H, t, *J* 6.8), 3.50 (1H, d, *J* 11.4), 3.55 (1H, d, *J* 11.4), 3.91 (1H, dd, *J* 5.9, 16.1), 3.98 (1H, dd, *J* 5.9, 16.1), 4.06 (1H, s), 6.31 (1H, br s) and 7.47 (1H, br s).

***N*-Propyl pantothenamide (*2b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, t, *J* 7.6), 0.92 (3H, s), 1.01 (3H, s), 1.47–1.58 (2H, m), 2.43 (2H, t, *J* 5.9), 3.19 (1H, t, *J* 7.2), 3.20 (1H, t, *J* 6.0), 3.49 (2H, s), 3.53–3.61 (2H, m), 3.99 (1H, s), 5.93 (1H, br s) and 7.39 (1H, br s).

***N*-Propyl homopantothenamide (*2c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, t, *J* 7.5), 0.93 (3H, s), 1.02 (3H, s), 1.47–1.58 (2H, m), 1.81–1.90 (2H, m), 2.23 (2H, t, *J* 6.8), 3.19 (1H, t, *J* 5.8), 3.22 (1H, t, *J* 7.0), 3.33 (1H, t, *J* 6.0), 3.36 (1H, t, *J* 6.2), 3.51 (2H, s), 4.02 (1H, s), 6.19 (1H, br s) and 7.17 (1H, br s).

***N*-Butyl α-pantothenamide (*3a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, t, *J* 7.3), 0.97 (3H, s), 1.04 (3H, s), 1.29–1.39 (2H, m), 1.43–1.53 (2H, m), 3.24 (1H, t, *J* 7.1), 3.26 (1H, t, *J* 7.0), 3.50 (1H, d, *J* 11.2), 3.54 (1H, d, *J* 11.2), 3.91 (1H, dd, *J* 5.9, 16.1), 3.98 (1H, dd, *J* 5.9, 16.1), 4.06 (1H, s), 6.29 (1H, br s) and 7.48 (1H, br s).

***N*-Butyl pantothenamide (*3b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, t, *J* 7.3), 0.92 (3H, s), 1.01 (3H, s), 1.30–1.36 (2H, m), 1.47 (2H, dt, *J* 6.8, 7.3), 2.43 (2H, t, *J* 6.1), 3.22 (1H, t, *J* 7.3), 3.24 (1H, t, *J* 6.0), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.99 (1H, s), 5.93 (1H, br s) and 7.40 (1H, br s).

***N*-Butyl homopantothenamide (*3c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, t, *J* 7.2), 0.93 (3H, s), 1.03 (3H, s), 1.31–1.41 (2H, m), 1.44–1.54 (2H, m), 1.81–1.90 (2H, m), 2.23 (2H, t, *J* 6.9), 3.23 (1H, t, *J* 6.0), 3.25 (1H, t, *J* 7.1), 3.33 (1H, t, *J* 6.1), 3.36 (1H, t, *J* 6.5), 4.02 (1H, s), 6.14 (1H, br s) and 7.16 (1H, br s).

***N*-Hexyl α-pantothenamide (*5a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 6.7), 0.98 (3H, s), 1.05 (3H, s), 1.24–1.35 (6H, m), 1.44–1.54 (2H, m), 3.23 (1H, t, *J* 7.1), 3.25 (1H, t, *J* 6.7), 3.51 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.91 (1H, dd, *J* 5.9, 16.1), 3.98 (1H, dd, *J* 5.9, 16.1), 4.07 (1H, s), 6.23 (1H, br s) and 7.45 (1H, br s).

***N*-Hexyl pantothenamide (*5b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 6.8), 0.92 (3H, s), 1.01 (3H, s), 1.26–1.32 (6H, m), 1.45–1.50 (2H, m), 2.42 (2H, t, *J* 6.1), 3.21 (1H, t, *J* 7.2), 3.23 (1H, t, *J* 5.9), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.99 (1H, s), 5.90 (1H, br s) and 7.39 (1H, br s).

***N*-Hexyl homopantothenamide (*5c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 6.6), 0.93 (3H, s), 1.02 (3H, s), 1.22–1.38 (6H, m), 1.43–1.54 (2H, m), 1.81–1.90 (2H, m), 2.22 (2H, t, *J* 6.9), 3.23 (1H, t, *J* 7.1), 3.25 (1H, t, *J* 6.6), 3.33 (1H, t, *J* 6.5), 3.36 (1H, t, *J* 6.2), 3.51 (2H, s), 4.02 (1H, s), 6.12 (1H, br s) and 7.17 (1H, br s).

***N*-Heptyl α-pantothenamide (*6a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 6.9), 0.98 (3H, s), 1.05 (3H, s), 1.24–1.28 (8H, m), 1.44–1.54 (2H, m), 3.23 (1H, t, *J* 6.7), 3.25 (1H, t, *J* 6.2), 3.51 (1H, d, *J* 11.4), 3.54 (1H, d, *J* 11.4), 3.91 (1H, dd, *J* 5.9, 16.4), 3.97 (1H, dd, *J* 5.9, 16.4), 4.07 (1H, s), 6.22 (1H, br s) and 7.44 (1H, br s).

***N*-Heptyl pantothenamide (*6b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 7.1), 0.92 (3H, s), 1.01 (3H, s), 1.23–1.30 (8H, m), 1.46–1.50 (2H, m), 2.42 (2H, t, *J* 6.1), 3.23 (1H, t, *J* 7.0), 3.25 (2H, t, *J* 6.7), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.99 (2H,

s), 5.91 (1H, br s) and 7.40 (1H, br s).

***N*-Heptyl homopantothenamide (*6c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 6.6), 0.93 (3H, s), 1.03 (3H, s), 1.22–1.36 (8H, m), 1.43–1.54 (2H, m), 1.81–1.90 (2H, m), 2.22 (2H, t, *J* 6.8), 3.23 (1H, t, *J* 6.4), 3.25 (1H, t, *J* 7.2), 3.33 (1H, t, *J* 6.2), 3.36 (1H, t, *J* 6.2), 3.59 (2H, dd, *J* 11.4, 12.9), 4.02 (1H, s), 6.12 (1H, br s) and 7.15 (1H, br s).

***N*-Octyl α-pantothenamide (*7a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 6.7), 0.98 (3H, s), 1.05 (3H, s), 1.19–1.31 (10H, m), 1.44–1.53 (2H, m), 3.23 (1H, t, *J* 5.9), 3.25 (1H, t, *J* 6.9), 3.51 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.91 (1H, dd, *J* 5.9, 16.4), 3.98 (1H, dd, *J* 5.9, 16.4) and 4.07 (1H, s).

***N*-Octyl pantothenamide (*7b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, t, *J* 7.1), 0.92 (3H, s), 1.01 (3H, s), 1.23–1.30 (10H, m), 1.45–1.50 (2H, m), 2.42 (2H, t, *J* 6.1), 3.21 (1H, t, *J* 6.0), 3.22 (1H, t, *J* 7.1), 3.49 (2H, s), 3.53–3.61 (2H, m), 3.99 (1H, s), 5.87 (1H, br s) and 7.38 (1H, br s).

***N*-Octyl homopantothenamide (*7c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.87 (3H, t, *J* 6.7), 0.93 (3H, s), 1.03 (3H, s), 1.22–1.33 (10H, m), 1.43–1.55 (2H, m), 1.81–1.90 (2H, m), 2.22 (2H, t, *J* 6.7), 3.23 (1H, t, *J* 7.1), 3.25 (1H, t, *J* 6.7), 3.33 (1H, t, *J* 6.3), 3.36 (1H, t, *J* 6.2), 3.51 (2H, s), 4.02 (1H, s), 6.14 (1H, br s) and 7.16 (1H, br s).

***N-tert*-Butyl α-pantothenamide (*8a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.05 (3H, s), 1.35 (9H, s), 3.53 (2H, s), 3.81 (1H, dd, *J* 5.9, 16.1), 3.92 (1H, dd, *J* 5.9, 16.1), 4.07 (1H, s), 5.82 (1H, br s) and 7.40 (1H, br s).

***N-tert*-Butyl pantothenamide (*8b*)**
No product formed

***N-tert*-Butyl homopantothenamide (*8c*)**
No product formed

***N*-Isopropyl α-pantothenamide (*9a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.06 (3H, s), 1.15 (6H, d, *J* 6.5), 3.51 (1H, d, *J* 11.2), 3.56 (1H, d, *J* 11.2), 3.87 (1H, dd, *J* 5.9, 16.4), 3.97 (1H, dd, *J* 5.9, 16.4), 3.98–4.11 (1H, m), 4.08 (1H, s), 5.93 (1H, br s) and 7.39 (1H, br s).

***N*-Isopropyl pantothenamide (*9b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.01 (3H, s), 1.14 (6H, d, *J* 6.3), 2.40 (2H, t, *J* 6.1), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.99 (1H, s), 3.98–4.08 (1H, m), 5.71 (1H, br s) and 7.38 (1H, br s).

***N*-Isopropyl homopantothenamide (*9c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.94 (3H, s), 1.03 (3H, s), 1.16 (6H, d, *J* 6.7), 1.81–1.90 (2H, m), 2.20 (2H, t, *J* 6.9), 3.32 (1H, t, *J* 5.1), 3.37 (1H, t, *J* 6.5), 3.49 (1H, d, *J* 11.1), 3.53 (1H, d, *J* 11.1), 4.02 (1H, s), 4.02–4.09 (1H, m), 5.88 (1H, br s) and 7.16 (1H, br s).

***N-sec*-Butyl α-pantothenamide (*10a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, t, *J* 7.4), 0.97 (3H, s), 1.04 (3H, s), 1.12 (3H, d, *J* 6.7), 1.46 (2H, q, *J* 7.4), 3.52 (2H, s), 3.83–4.00 (3H, m), 4.07 (1H, s), 6.04 (1H, br s) and 7.48 (1H, br s).

***N-sec*-Butyl pantothenamide (*10b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, t, *J* 7.3), 0.92 (3H, s), 1.01 (3H, s), 1.11 (3H, d, *J* 6.3), 1.45 (2H, q, *J* 7.3), 2.42 (2H, t, *J* 5.9), 3.49 (2H, s), 3.53–3.61 (2H, m), 3.86–3.90 (1H, m), 3.99 (1H, s), 5.64 (1H, br s) and 7.40 (1H, br s).

***N-sec*-Butyl homopantothenamide (*10c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, t, *J* 7.5), 0.94 (3H, s), 1.03 (3H, s), 1.13 (3H, d, *J* 6.5), 1.42–1.52

(2H, m), 1.82–1.91 (2H, m), 2.22 (2H, t, *J* 6.9), 3.33 (1H, t, *J* 6.1), 3.37 (1H, t, *J* 6.4), 3.49 (1H, d, *J* 11.3), 3.53 (1H, d, *J* 11.3), 3.86–3.94 (1H, m), 4.03 (1H, s), 5.84 (1H, br s) and 7.16 (1H, br s).

_N_-Isobutyl α-pantothenamide (*11a*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.90 (6H, d, *J* 6.7), 0.97 (3H, s), 1.04 (3H, s), 1.70–1.83 (1H, m), 3.07 (1H, d, *J* 6.1), 3.09 (1H, d, *J* 6.8), 3.53 (2H, s), 3.93 (1H, dd, *J* 5.9, 16.4), 3.99 (1H, dd, *J* 5.9, 16.4), 4.07 (1H, s), 6.35 (1H, br s) and 7.49 (1H, br s).

_N_-Isobutyl pantothenamide (*11b*)
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.91 (6H, d, *J* 6.3), 0.92 (3H, s), 1.01 (3H, s), 1.72–1.79 (1H, m), 2.45 (2H, t, *J* 5.9), 3.06 (1H, d, *J* 6.2), 3.07 (1H, d, *J* 6.6), 3.49 (2H, s), 3.54–3.61 (2H, m), 3.99 (1H, s), 5.95 (1H, br s) and 7.40 (1H, br s).

_N_-Isobutyl homopantothenamide (*11c*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, s), 0.93 (3H, s), 0.94 (3H, s), 1.02 (3H, s), 1.70–1.84 (1H, m), 1.82–1.91 (2H, m), 2.24 (2H, t, *J* 6.9), 3.07 (1H, t, *J* 6.1), 3.08 (1H, t, *J* 5.8), 3.34 (1H, t, *J* 6.4), 3.36 (1H, t, *J* 6.4), 3.51 (2H, s), 4.02 (1H, s), 6.23 (1H, br s) and 7.18 (1H, br s).

_N_-(1-Methyl-butyl) α-pantothenamide (*12a*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, t, *J* 7.0), 0.98 (3H, s), 1.05 (3H, s), 1.12 (3H, d, *J* 6.7), 1.23–1.45 (4H, m), 3.53 (2H, s), 3.84–4.01 (3H, m), 4.07 (1H, s), 6.00 (1H, br s) and 7.46 (1H, br s).

_N_-(1-Methyl-butyl) pantothenamide (*12b*)
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, t, *J* 7.1), 0.92 (3H, s), 1.01 (3H, s), 1.10 (3H, d, *J* 6.8), 1.29–1.35 (2H, m), 1.37–1.42 (2H, m), 2.41 (2H, t, *J* 5.9), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.94–3.98 (1H, m), 3.99 (1H, s), 5.63 (1H, br s) and 7.40 (1H, br s).

_N_-(1-Methyl-butyl) homopantothenamide (*12c*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, t, *J* 7.6), 0.93 (3H, s), 1.03 (3H, s), 1.13 (3H, d, *J* 6.5), 1.29–1.46 (4H, m), 1.82–1.91 (2H, m), 2.12 (2H, t, *J* 6.7), 3.33 (1H, t, *J* 6.3), 3.36 (1H, t, *J* 6.2), 3.49 (1H, d, *J* 11.4), 3.52 (1H, d, *J* 11.4), 3.92–3.99 (1H, m), 5.84 (1H, br s) and 7.17 (1H, br s).

_N_-Isopentyl α-pantothenamide (*13a*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.90 (6H, d, *J* 6.5), 0.97 (3H, s), 1.04 (3H, s), 1.38 (2H, dt, *J* 7.0, 7.7), 1.54–1.67 (1H, m), 3.25 (1H, t, *J* 5.8), 3.28 (1H, t, *J* 5.8), 3.52 (2H, s), 3.90 (1H, dd, *J* 5.9, 16.1), 3.97 (1H, dd, *J* 5.9, 16.1), 4.06 (1H, s), 6.24 (1H, br s) and 7.47 (1H, br s).

_N_-Isopentyl pantothenamide (*13b*)
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.91 (6H, d, *J* 6.3), 0.92 (3H, s), 1.01 (3H, s), 1.38 (2H, dt, *J* 7.1, 7.6), 1.56–1.63 (1H, m), 2.42 (2H, t, *J* 5.9), 3.24 (1H, t, *J* 5.8), 3.26 (1H, t, *J* 5.8), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.99 (1H, s), 5.88 (1H, br s) and 7.40 (1H, br s).

_N_-Isopentyl homopantothenamide (*13c*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, s), 0.92 (3H, s), 0.93 (3H, s), 1.02 (3H, s), 1.34–1.43 (2H, m), 1.55–1.68 (1H, m), 1.81–1.90 (2H, m), 2.22 (2H, t, *J* 6.9), 3.24 (1H, t, *J* 5.9), 3.27 (1H, t, *J* 6.1), 3.33 (1H, t, *J* 6.1), 3.35 (1H, t, *J* 6.1), 3.50 (2H, s), 4.02 (1H, s), 6.12 (1H, br s) and 7.17 (1H, br s).

_N_-Cyclopentyl α-pantothenamide (*14a*)
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s), 1.04 (3H, s), 1.33–1.44 (2H, m), 1.54–1.71 (4H, m), 1.91–2.02 (2H, m), 3.53 (2H, s), 3.87 (1H, dd, *J* 5.9, 16.1), 3.96 (1H, dd, *J* 5.9, 16.1), 4.06 (1H, s), 4.11–4.23 (1H, m), 6.25 (1H, br s) and 7.48 (1H, br s).

_N_-Cyclopentyl pantothenamide (*14b*)
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.33–1.39 (2H, m), 1.57–1.62 (2H, m), 1.64–1.68 (2H, m), 1.94–1.99 (2H, m), 2.40 (2H, t, *J* 6.1), 3.49 (2H, s), 3.52–3.59 (2H, m), 3.99 (1H, s), 4.13–4.19 (1H, m), 5.89 (1H, br s) and 7.40 (1H, br s).

***N*-Cyclopentyl homopantothenamide (*14c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.94 (3H, s), 1.03 (3H, s), 1.34–1.45 (2H, m), 1.55–1.71 (4H, m), 1.80–1.89 (2H, m), 1.92–2.03 (2H, m), 2.20 (2H, t, *J* 6.9), 3.24 (1H, t, *J* 6.2), 3.33 (1H, t, *J* 6.2), 3.35 (2H, s), 4.03 (1H, s), 4.12–4.23 (1H, m), 6.15 (1H, br s) and 7.18 (1H, br s).

***N*-Cyclohexyl α-pantothenamide (*15a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.05 (3H, s), 1.11–1.42 (5H, m), 1.58–1.74 (3H, m), 1.87–1.92 (2H, m), 3.53 (2H, s), 3.69–3.79 (1H, m), 3.87 (1H, dd, *J* 5.9, 16.1), 3.98 (1H, dd, *J* 5.9, 16.1), 4.07 (1H, s), 6.05 (1H, br s) and 7.43 (1H, br s).

***N*-Cyclohexyl pantothenamide (*15b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.10–1.18 (3H, m), 1.31–1.38 (2H, m), 1.60–1.63 (1H, m), 1.69–1.72 (2H, m), 1.87–1.89 (2H, m), 2.40 (2H, t, *J* 6.1), 3.49 (2H, s), 3.53–3.60 (2H, m), 3.70–3.80 (1H, m), 3.99 (1H, s), 5.72 (1H, br s) and 7.4 (1H, br s).

***N*-Cyclohexyl homopantothenamide (*15c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.03 (3H, s), 1.13–1.39 (7H, m), 1.56–1.64 (1H, m), 1.66–1.76 (2H, m), 1.80–1.92 (4H, m), 2.20 (2H, t, *J* 6.7), 3.33 (1H, t, *J* 6.4), 3.35 (1H, t, *J* 6.1), 3.48 (1H, d, *J* 11.9), 3.53 (1H, d, *J* 11.9), 3.70–3.80 (1H, m), 4.02 (1H, s), 5.99 (1H, br s) and 7.17 (1H, br s).

***N*-Cyclopropylmethyl α-pantothenamide (*16a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.16–0.28 (2H, m), 0.48–0.57 (2H, m), 0.87–0.98 (1H, m), 0.98 (3H, s), 1.05 (3H, s), 3.10 (1H, d, *J* 6.7), 3.12 (1H, d, *J* 5.9), 3.53 (2H, s), 3.92 (1H, dd, *J* 5.9, 16.1), 4.01 (1H, dd, *J* 5.9, 16.1), 4.07 (1H, s), 6.35 (1H, br s) and 7.47 (1H, br s).

***N*-Cyclopropylmethyl pantothenamide (*16b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ0.17–0.22 (2H, m), 0.48–0.54 (2H, m), 0.90–0.95 (1H, m), 0.93 (3H, s), 1.01 (3H, s), 2.45 (2H, t, *J* 6.1), 3.09 (1H, d, *J* 5.4), 3.10 (1H, d, *J* 5.6), 3.49 (2H, s), 3.54–3.62 (2H, m), 3.99 (1H, s), 5.97 (1H, br s) and 7.38 (1H, br s).

***N*-Cyclopropylmethyl homopantothenamide (*16c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.17–0.23 (2H, m), 0.47–0.54 (2H, m), 0.93 (3H, s), 0.90–0.95 (1H, m), 1.02 (3H, s), 1.82–1.91 (2H, m), 2.25 (2H, t, *J* 6.9), 3.09 (1H, d, *J* 7.0), 3.11 (1H, d, *J* 7.0), 3.34 (1H, t, *J* 6.1), 3.36 (1H, t, *J* 6.1), 3.50 (2H, s), 4.02 (1H, s), 6.22 (1H, br s) and 7.18 (1H, br s).

***N*-Cyclohexylmethyl α-pantothenamide (*17a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.83–0.97 (2H, m), 0.97 (3H, s), 1.05 (3H, s), 1.11–1.28 (3H, m), 1.38–1.50 (1H, m), 1.63–1.76 (5H, m), 3.08 (1H, d, *J* 6.5), 3.10 (1H, d, *J* 6.4), 3.53 (2H, s), 3.92 (1H, dd, *J* 5.9, 16.1), 3.98 (1H, dd, *J* 5.9, 16.1), 4.07 (1H, s), 6.29 (1H, br s) and 7.46 (1H, br s).

***N*-Cyclohexylmethyl pantothenamide (*17b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.11–1.25 (4H, m), 1.40–1.47 (1H, m), 1.65–1.73 (6H, m), 2.44 (2H, t, *J* 5.9), 3.07 (1H, d, *J* 6.4), 3.09 (1H, d, *J* 6.1), 3.49 (2H, s), 3.53–3.61 (2H, m), 3.99 (1H, s), 5.90 (1H, br s) and 7.40 (1H, br s).

***N*-Cyclohexylmethyl homopantothenamide (*17c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.02 (3H, s), 1.12–1.27 (4H, m), 1.41–1.52 (1H, m), 1.62–1.73 (6H, m), 1.81–1.90 (2H, m), 2.23 (2H, t, *J* 6.7), 3.07 (1H, d, *J* 6.4), 3.09 (1H, d, *J* 6.5), 3.33 (1H, t, *J* 6.2), 3.36 (1H, t, *J* 6.2), 3.50 (2H, s), 4.02 (1H, s), 6.18 (1H, br s) and 7.17 (1H, br s).

***N*-Tetrahydrofurfuryl α-pantothenamide (*18a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 1.03 (3H, s), 1.10 (3H, s), 1.47–1.59 (1H, m), 1.85–2.05 (3H, m), 3.02–3.13 (1H, m), 3.54 (2H, s), 3.58–3.99 (5H, m), 4.00 (1H, s), 4.07–4.17 (1H, m), 6.77 (1H, br s) and 7.41 (1H, br s).

***N*-Tetrahydrofurfuryl pantothenamide (*18b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, d, *J* 13.7), 1.03 (3H, s), 1.48–1.57 (3H, m), 1.87–1.96 (2H, m), 1.96–

2.04 (1H, m), 2.37–2.52 (2H, m), 2.94–3.16 (2H, m), 3.48 (1H, s), 3.57–3.64 (4H, m), 3.73–3.79 (1H, m), 3.80–3.88 (1H, m), 3.97 (1H, s), 3.98–4.06 (1H, m), 6.15 (1H, br s) and 7.34 (1H, br s).

***N*-Tetrahydrofurfuryl homopantothenamide (*18c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.03 (3H, s), 1.47–1.58 (1H, m), 1.83–1.94 (4H, m), 1.93–2.04 (1H, m), 2.26 (2H, t, *J* 7.2), 3.05–3.20 (1H, m), 3.28–3.42 (2H, m), 3.47 (1H, d, *J* 12.4), 3.51 (1H, d, *J* 12.4), 3.52–3.60 (1H, m), 3.72–3.79 (1H, m), 3.82–3.92 (2H, m), 4.00 (1H, s), 6.25 (1H, br s) and 7.16 (1H, br s).

***N*-(2-Methoxy-ethyl) α-pantothenamide (*19a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 1.00 (3H, s), 1.07 (3H, s), 3.35 (3H, s), 3.44–3.49 (4H, m), 3.53 (2H, s), 3.90 (1H, dd, *J* 5.9, 16.4), 4.05 (1H, dd, *J* 5.9, 16.4), 4.03 (1H, s), 6.74 (1H, br s) and 7.45 (1H, br s).

***N*-(2-Methoxy-ethyl) pantothenamide (*19b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 2.45 (2H, t, *J* 6.3), 3.36 (3H, s), 3.39–3.47 (6H, m), 3.48 (2H, s), 3.56–3.60 (2H, m), 3.98 (1H, s), 6.13 (1H, br s) and 7.34 (1H, br s).

***N*-(2-Methoxy-ethyl) homopantothenamide (*19c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.03 (3H, s), 1.83–1.92 (2H, m), 2.26 (2H, t, *J* 6.6), 3.29–3.40 (2H, m), 3.36 (3H, s), 3.42–3.48 (4H, m), 3.48 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 4.01 (1H, s), 6.27 (1H, br s) and 7.15 (1H, br s).

***N*-(2-(Ethylthio)-ethyl) α-pantothenamide (*20a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.05 (3H, s), 1.26 (3H, t, *J* 7.3), 2.55 (2H, q, *J* 7.3), 2.67 (2H, t, *J* 6.5), 3.44 (1H, t, *J* 6.2), 3.46 (1H, t, *J* 6.5), 3.53 (2H, s), 3.94 (1H, dd, *J* 5.9, 16.4), 4.01 (1H, dd, *J* 5.9, 16.4), 4.06 (1H, s), 6.73 (1H, br s) and 7.47 (1H, br s).

***N*-(2-(Ethylthio)-ethyl) pantothenamide (*20b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 1.26 (3H, t, *J* 7.5), 2.45 (2H, t, *J* 6.3), 2.55 (2H, q, *J* 7.5), 2.67 (2H, t, *J* 6.5), 3.41–3.49 (2H, m), 3.49 (2H, s), 3.55–3.60 (2H, m), 4.00 (1H, s), 6.23 (1H, br s) and 7.35 (1H, br s).

***N*-(2-(Ethylthio)-ethyl) homopantothenamide (*20c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.02 (3H, s), 1.26 (3H, t, *J* 7.3), 1.82–1.91 (2H, m), 2.25 (2H, t, *J* 6.9), 2.56 (2H, q, *J* 7.3), 2.68 (2H, t, *J* 6.5), 3.34 (1H, t, *J* 6.2), 3.37 (1H, t, *J* 6.4), 3.43 (1H, t, *J* 6.4), 3.45 (1H, t, *J* 6.5), 3.49 (1H, d, *J* 11.6), 3.52 (1H, d, *J* 11.6), 4.02 (1H, s), 6.47 (1H, br s) and 7.14 (1H, br s).

***N*-(3-Methoxy-propyl) α-pantothenamide (*21a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.05 (3H, s), 1.77 (2H, q, *J* 5.9), 3.34 (3H, s), 3.35 (2H, t, *J* 6.2), 3.37 (2H, t, *J* 6.2), 3.47 (2H, t, *J* 5.9), 3.49 (1H, d, *J* 11.2), 3.55 (1H, d, *J* 11.2), 3.91 (1H, dd, *J* 5.9, 16.3), 3.97 (1H, dd, *J* 5.9, 16.3), 4.04 (1H, s), 6.72 (1H, br s) and 7.42 (1H, br s).

***N*-(3-Methoxy-propyl) pantothenamide (*21b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 1.76 (2H, q, *J* 6.0), 2.41 (2H, t, *J* 6.1), 3.29–3.39 (2H, m), 3.34 (3H, s), 3.47 (2H, t, *J* 6.0), 3.48 (2H, s), 3.57 (2H, q, *J* 6.6), 3.98 (1H, s), 6.35 (1H, br s) and 7.39 (1H, br s).

***N*-(3-Methoxy-propyl) homopantothenamide (*21c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.02 (3H, s), 1.73–1.81 (2H, m), 1.81–1.90 (2H, m), 2.22 (2H, t, *J* 6.9), 3.31–3.38 (4H, m), 3.34 (3H, s), 3.47 (2H, t, *J* 5.9), 3.50 (2H, s), 4.01 (1H, s), 6.49 (1H, br s) and 7.20 (1H, br s).

***N*-(3-(Methylthio)-propyl) α-pantothenamide (*22a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.06 (3H, s), 1.82 (2H, q, *J* 7.0), 2.10 (3H, s), 2.53 (2H, t, *J* 7.0), 3.36 (1H, t, *J* 6.8), 3.38 (1H, t, *J* 6.5), 3.51 (1H, d, *J* 11.2), 3.57 (1H, d, *J* 11.2), 3.93 (1H, dd, *J* 5.9, 16.3), 3.98 (1H, dd, *J* 5.9, 16.3), 4.06 (1H, s), 6.62 (1H, br s) and 7.50 (1H, br s).

***N*-(3-(Methylthio)-propyl) pantothenamide (*22b*)**

δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.80 (2H, q, *J* 7.0), 2.10 (3H, s), 2.44 (2H, t, *J* 6.0), 2.52 (2H, t, *J* 7.0), 3.31–3.38 (2H, m), 3.49 (2H, s), 3.54–3.60 (2H, m), 3.99 (1H, s), 6.19 (1H, br s) and 7.38 (1H, br s).

***N*-(3-(Methylthio)-propyl) homopantothenamide (*22c*)**

δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.02 (3H, s), 1.77–1.90 (4H, m), 2.10 (3H, s), 2.23 (2H, t, *J* 6.9), 2.54 (2H, t, *J* 7.0), 3.31–3.39 (4H, m), 3.51 (2H, s), 4.02 (1H, s), 6.47 (1H, br s) and 7.16 (1H, br s).

***N*-(3-Isopropoxypropyl) α-pantothenamide (*23a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.06 (3H, s), 1.15 (3H, s), 1.17 (3H, s), 1.75 (2H, q, *J* 6.0), 3.36 (1H, t, *J* 5.9), 3.38 (1H, t, *J* 5.8), 3.48–3.56 (2H, m), 3.51 (2H, s), 3.57 (1H, t, *J* 6.0), 3.90 (1H, dd, *J* 5.9, 16.4), 3.96 (1H, dd, *J* 5.9, 16.4), 4.04 (1H, s), 6.80 (1H, br s) and 7.41 (1H, br s).

***N*-(3-Isopropoxypropyl) pantothenamide (*23b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 1.15 (3H, s), 1.17 (3H, s), 1.75 (2H, q, *J* 5.7), 2.39 (2H, t, *J* 5.9), 3.30–3.40 (2H, m), 3.48 (2H, s), 3.52 (2H, t, *J* 5.9), 3.54–3.58 (3H, m), 3.99 (1H, s), 6.52 (1H, br s) and 7.40 (1H, br s).

***N*-(3-Isopropoxypropyl) homopantothenamide (*23c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.02 (3H, s), 1.15 (3H, s), 1.17 (3H, s), 1.75 (2H, q, *J* 6.0), 1.82–1.91 (2H, m), 2.22 (2H, t, *J* 6.7), 3.31–3.38 (4H, m), 3.50 (2H, s), 3.50–3.60 (3H, m), 4.00 (1H, s), 6.63 (1H, br s) and 7.20 (1H, br s).

***N*-(2-Hydroxy-ethyl) α-pantothenamide (*24a*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.97 (6H, s), 3.37 (2H, t, *J* 5.6), 3.48 (1H, d, *J* 11.4), 3.52 (1H, d, *J* 11.4), 3.60 (2H, t, *J* 5.6), 3.97 (2H, s) and 4.06 (1H, s).

***N*-(2-Hydroxy-ethyl) pantothenamide (*24b*) (also known as Oxypantetheine)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, s), 0.93 (3H, s), 2.53 (2H, t, *J* 6.3), 3.33 (2H, t, *J* 5.5), 3.40 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 10.3), 3.49–3.57 (2H, m), 3.66 (2H, t, *J* 5.5) and 3.99 (1H, s).

***N*-(2-Hydroxy-ethyl) homopantothenamide (*24c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.91 (3H, s), 0.95 (3H, s), 1.78–1.88 (2H, m), 2.32 (2H, t, *J* 7.5), 3.27 (2H, t, *J* 6.9), 3.34 (2H, t, *J* 5.6), 3.41 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.67 (2H, t, *J* 5.6) and 4.00 (1H, s).

***N*-(1-Hydroxymethyl-propyl) α-pantothenamide (*25a*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.89 (3H, t, *J* 7.5), 0.96 (3H, s), 0.97 (3H, s), 1.33–1.48 (1H, m), 1.54–1.69 (1H, m), 3.43–3.55 (2H, m), 3.51–3.66 (2H, m), 3.79–3.87 (1H, m), 3.97 (2H, s) and 4.06 (1H, s).

***N*-(1-Hydroxymethyl-propyl) pantothenamide (*25b*)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, t, *J* 7.5), 0.90 (3H, s), 0.93 (3H, s), 1.36–1.44 (1H, m), 1.55–1.63 (1H, m), 2.54 (2H, t, *J* 6.3), 3.40 (1H, d, *J* 11.1), 3.52 (1H, d, *J* 11.1), 3.52–3.55 (4H, m), 3.61 (1H, dd, *J* 4.7, 10.1), 3.77–3.82 (1H, m) and 3.99 (1H, s).

***N*-(1-Hydroxymethyl-propyl) homopantothenamide (*25c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.90 (3H, t, *J* 7.6), 0.92 (3H, s), 0.95 (3H, s), 1.54–1.73 (2H, m), 1.66–1.75 (2H, m), 2.33 (2H, t, *J* 7.5), 3.13 (2H, t, *J* 6.9), 3.27 (1H, d, *J* 11.2), 3.38 (1H, d, *J* 11.2), 3.35–3.52 (5H, m), 3.75–3.82 (1H, m) and 4.00 (1H, s).

***N*-(3-Hydroxy-propyl) α-pantothenamide (*26a*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.95 (6H, s), 1.76 (2H, q, *J* 6.7), 3.30 (2H, t, *J* 6.7), 3.46 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 3.63 (2H, t, *J* 6.7), 3.93 (2H, s) and 4.05 (1H, s).

***N*-(3-Hydroxy-propyl) pantothenamide (*26b*)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, s), 0.93 (3H, s), 1.75 (2H, q, *J* 6.6), 2.50 (2H, t, *J* 6.3), 3.25 (2H, t, *J* 7.1), 3.40 (2H, d, *J* 11.2), 3.52 (2H, d, *J* 11.7), 3.47–3.56 (2H, m), 3.63 (2H, t, *J* 6.6) and 3.99 (1H, s).

***N*-(3-Hydroxy-propyl) homopantothenamide (*26c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.91 (3H, s), 0.95 (3H, s), 1.71–1.80 (2H, m), 1.78–1.87 (2H, m), 2.29 (2H, t, *J* 7.5), 3.26 (2H, t, *J* 7.0), 3.41 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.64 (2H, t, *J* 6.5) and 4.00 (1H, s).

***N*-(2,3-Dihydroxy-propyl) α-pantothenamide (*27a*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.96 (6H, s), 3.26 (1H, dd, *J* 7.0, 13.8), 3.38 (1H, dd, *J* 7.0, 13.8), 3.45 (1H, d, *J* 11.3), 3.52 (1H, d, *J* 11.3), 3.54 (1H, dd, *J* 4.1, 11.7), 3.62 (1H, dd, *J* 4.1, 11.7), 3.78–3.87 (1H, m), 3.97 (2H, s) and 4.06 (1H, s).

***N*-(2,3-Dihydroxy-propyl) pantothenamide (*27b*)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, s), 0.93 (3H, s), 2.53 (2H, t, *J* 6.6), 3.22 (1H, dd, *J* 7.2, 14.1), 3.35 (1H, dd, *J* 7.2, 14.1), 3.41 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 3.49–3.66 (3H, m), 3.61 (1H, dd, *J* 3.9, 11.7), 3.78–3.83 (1H, m) and 3.99 (1H, s).

***N*-(2,3-Dihydroxy-propyl) homopantothenamide (*27c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.91 (3H, s), 0.95 (3H, s), 1.79–1.88 (2H, m), 2.33 (2H, t, *J* 7.6), 3.17–3.35 (4H, m), 3.42 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.49–3.66 (2H, m), 3.78–3.86 (1H, m) and 4.00 (1H, s).

***N*-(5-Azido-pentyl) α-pantothenamide (*28a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s), 1.03 (3H, s), 1.36–1.55 (4H, m), 1.53–1.65 (2H, m), 3.20–3.34 (4H, m), 3.52 (2H, s), 3.94 (2H, d, *J* 5.9), 4.06 (1H, s), 6.55 (1H, br s) and 7.53 (1H, br s).

***N*-(5-Azido-pentyl) pantothenamide (*28b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 1.37–1.44 (2H, m), 1.49–1.57 (2H, m), 1.58–1.65 (2H, m), 2.44 (2H, t, *J* 6.0), 3.21–3.30 (4H, m), 3.49 (2H, s), 3.54–3.59 (2H, m), 4.00 (1H, s), 6.07 (1H, br s) and 7.39 (1H, br s).

***N*-(5-Azido-pentyl) homopantothenamide (*28c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.94 (3H, s), 1.01 (3H, s), 1.38–1.46 (2H, m), 1.50–1.67 (4H, m), 1.81–1.90 (2H, m), 2.23 (2H, t, *J* 6.7), 3.22–3.30 (4H, m), 3.33 (1H, t, *J* 5.9), 3.35 (1H, t, *J* 6.5), 3.50 (2H, s), 4.03 (1H, s), 6.39 (1H, br s) and 7.18 (1H, br s).

***N*-(2-Acetylamino-ethyl) α-pantothenamide (*29a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.96 (6H, s), 1.99 (3H, s), 3.28–3.37 (4H, m), 3.46 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 3.93 (2H, s) and 4.06 (1H, s).

***N*-(2-Acetylamino-ethyl) pantothenamide (*29b*)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, s), 0.93 (3H, s), 1.99 (3H, s), 2.49 (2H, t, *J* 6.6), 3.30 (4H, s), 3.40 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.46–3.55 (2H, m) and 3.99 (1H, s).

***N*-(2-Acetylamino-ethyl) homopantothenamide (*29c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.91 (3H, s), 0.95 (3H, s), 1.76–1.86 (2H, m), 1.98 (3H, s), 2.82 (2H, t, *J* 7.5), 3.26 (2H, t, *J* 6.9), 3.32 (4H, s), 3.41 (1H, d, *J* 11.4), 3.52 (1H, d, *J* 11.2) and 3.72 (1H, s).

***N*-(6-*Boc*-amino-hexyl) α-pantothenamide (*30a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.98 (3H, s), 1.05 (3H, s), 1.29–1.34 (4H, m), 1.43 (9H, s), 1.43–1.52 (4H, m), 3.07 (1H, t, *J* 6.4), 3.10 (1H, t, *J* 6.8), 3.18–3.35 (2H, m), 3.52 (2H, s), 3.91 (1H, dd, *J* 5.9, 16.4), 4.00 (1H, dd, *J* 5.9, 16.4), 4.06 (1H, s), 4.63 (1H, br s), 6.55 (1H, br s) and 7.48 (1H, br s).

***N*-(6-*Boc*-amino-hexyl) pantothenamide (*30b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.01 (3H, s), 1.32–1.33 (4H, m), 1.43 (9H, s), 1.46–1.50 (4H, m), 2.43 (2H, td, *J* 6.0, 2.4), 3.07–3.10 (2H, m), 3.17–3.23 (1H, m), 3.24–3.30 (1H, m), 3.49 (2H, s), 3.57 (2H, q, *J* 6.0), 4.00 (1H, s), 4.63 (1H, br s), 6.13 (1H, br s) and 7.40 (1H, br s).

***N*-(6-*Boc*-amino-hexyl) homopantothenamide (*30c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.03 (3H, s), 1.30–1.36 (4H, m), 1.43 (9H, s), 1.46–1.53 (4H, m), 1.82–1.91 (2H, m), 2.24 (2H, t, *J* 6.7), 3.06–3.12 (2H, m), 3.22 (1H, t, *J* 6.5), 3.24 (1H, t, *J* 5.9), 3.36 (1H, t, *J* 6.2), 3.37 (1H, t, *J* 6.2), 3.50 (2H, s), 4.02 (1H, s), 4.61 (1H, br s), 6.35 (1H, br s) and 7.18 (1H, br s).

***N*-Phenethyl α-pantothenamide (*31a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.94 (3H, s), 1.02 (3H, s), 2.81 (2H, t, *J* 6.9), 3.44 (1H, d, *J* 11.2), 3.49 (1H, d, *J* 11.2), 3.51 (1H, t, *J* 4.5), 3.53 (1H, t, *J* 6.5), 3.87 (1H, dd, *J* 5.9, 16.4), 3.94 (1H, dd, *J* 5.9, 16.4), 4.01 (1H, s), 6.28 (1H, br s), 7.17–7.34 (5H, m) and 7.37 (1H, br s).

***N*-Phenethyl pantothenamide (*31b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 2.38 (2H, t, *J* 6.1), 2.81 (2H, t, *J* 6.8), 3.48 (2H, s), 3.46–3.58 (4H, m), 3.97 (1H, s), 5.86 (1H, br s), 7.18 (2H, d, *J* 6.8), 7.23 (1H, t, *J* 7.6), 7.31 (2H, t, *J* 7.3) and 7.34 (1H, br s).

***N*-Phenethyl homopantothenamide (*31c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (s, 3H), 1.03 (s, 3H), 1.78–1.87 (2H, m), 2.19 (2H, t, *J* 6.7), 2.83 (2H, t, *J* 7.0), 3.22 (1H, t, *J* 6.5), 3.28 (1H, t, *J* 6.5), 3.46–3.54 (4H, m), 4.01 (1H, s), 6.06 (1H, br s), 7.09 (1H, br s), 7.18–7.34 (5H, m).

***N*-Benzyl α-pantothenamide (*32a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 3.44 (1H, d, *J* 11.2), 3.49 (1H, d, *J* 11.2), 3.93 (1H, dd, *J* 5.9, 16.4), 4.00 (1H, dd, *J* 5.9, 16.4), 4.03 (1H, s), 4.41 (2H, d, *J* 5.9), 6.69 (1H, br s), 7.23–7.35 (5H, m) and 7.45 (1H, br s).

***N*-Benzyl pantothenamide (*32b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, s), 0.99 (3H, s), 2.47 (2H, t, *J* 6.1), 3.45 (2H, s), 3.54–3.61 (2H, m), 3.96 (1H, s), 4.40 (2H, d, *J* 5.7), 6.28 (1H, br s), 7.25 (2H, d, *J* 7.3), 7.27 (1H, t, *J* 7.3), 7.33 (2H, t, *J* 7.3) and 7.37 (1H, br s).

***N*-Benzyl homopantothenamide (*32c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.84–1.93 (2H, m), 2.28 (2H, t, *J* 6.9), 3.33 (1H, td, *J* 6.2, 1.8), 3.35 (1H, td, *J* 6.2, 1.8), 3.49 (2H, s), 3.99 (1H, s), 4.43 (2H, d, *J* 5.6), 6.52 (1H, br s), 7.16 (1H, br s) and 7.28–7.37 (5H, m).

***N*-(4-Methoxy-benzyl) α-pantothenamide (*33a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.01 (3H, s), 3.44 (1H, d, *J* 11.2), 3.50 (1H, d, *J* 11.2), 3.78 (3H, s), 3.94 (2H, t, *J* 5.5), 3.95 (2H, t, *J* 4.9), 4.02 (1H, s), 4.33 (2H, d, *J* 5.9), 6.59 (1H, br s), 6.83 (2H, d, *J* 8.8), 7.17 (2H, d, *J* 8.8) and 7.44 (1H, br s).

***N*-(4-Methoxy-benzyl) pantothenamide (*33b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, s), 0.99 (3H, s), 2.44 (2H, t, *J* 5.9), 3.46 (2H, s), 3.53–3.60 (2H, m), 3.79 (3H, s), 3.96 (1H, s), 4.34 (2H, d, *J* 5.6), 6.19 (1H, br s), 6.85 (2H, d, *J* 8.8), 7.18 (2H, d, *J* 8.8) and 7.37 (1H, br s).

***N*-(4-Methoxy-benzyl) homopantothenamide (*33c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, s), 1.04 (3H, s), 1.82–1.92 (2H, m), 2.25 (2H, t, *J* 6.9), 3.33 (1H, td, *J* 6.4, 2.9), 3.35 (1H, td, *J* 6.4, 2.9), 3.48 (2H, s), 3.79 (3H, s), 3.98 (1H, s), 4.34 (2H, d, *J* 5.6), 6.36 (1H, br s), 6.85 (2H, d, *J* 8.5), 7.13 (1H, br s) and 7.20 (2H, d, *J* 8.8).

***N*-(3-Methoxy-benzyl) α-pantothenamide (*34a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 3.45 (1H, d, *J* 11.2), 3.48 (1H, d, *J* 11.2), 3.78 (3H, s), 3.95 (1H, d, *J* 5.9), 3.97 (1H, d, *J* 5.9), 4.02 (1H, s), 4.37 (2H, d, *J* 5.9), 6.74 (1H, br s), 6.79–6.84 (3H, m), 7.20–7.25 (1H, m) and 7.47 (1H, br s).

***N*-(3-Methoxy-benzyl) pantothenamide (*34b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, s), 1.00 (3H, s), 2.43–2.53 (2H, m), 3.44 (1H, d, *J* 11.5), 3.48 (1H, d, *J* 11.5), 3.59 (2H, q, *J* 5.5), 3.80 (3H, s), 3.96 (1H, s), 4.32 (1H, dd, *J* 5.6, 14.6), 4.46 (1H, dd, *J* 5.8, 14.9), 6.27 (1H, br s), 6.79 (1H, s), 6.80 (1H, d, *J* 7.8), 6.84 (1H, d, *J* 7.8), 7.24 (1H, t, *J* 7.8) and 7.39 (1H, br s).

***N*-(3-Methoxy-benzyl) homopantothenamide (*34c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, s), 1.00 (3H, s), 1.83–1.93 (2H, m), 2.28 (2H, t, *J* 6.9), 3.30–3.38 (2H, m), 3.48 (2H, s), 3.79 (3H, s), 3.98 (1H, s), 4.39 (2H, d, *J* 5.9), 6.48 (1H, br s), 6.79–6.87 (3H, m), 7.14 (1H, br s) and 7.23 (1H, dd, *J* 7.6, 1.2).

***N*-(3,4,5,-Trimethoxy-benzyl) α-pantothenamide (*35a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 3.45 (1H, d, *J* 11.2), 3.50 (1H, d, *J* 11.2), 3.81 (3H, s), 3.84 (6H, s), 3.91–3.97 (2H, m), 4.02 (1H, s), 4.34 (2H, d, *J* 5.6), 6.48 (2H, s), 6.73 (1H, br s) and 7.43

(1H, br s).

***N*-(3,4,5,-Trimethoxy-benzyl) pantothenamide (*35b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, s), 0.98 (3H, s), 2.47 (2H, t, *J* 5.4), 3.46 (2H, s), 3.55–3.62 (2H, m), 3.81 (3H, s), 3.84 (6H, s), 3.95 (1H, s), 4.30–4.36 (2H, m), 6.32 (1H, br s), 6.49 (2H, s) and 7.36 (1H, br s).

***N*-(3,4,5,-Trimethoxy-benzyl) homopantothenamide (*35c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, s), 1.00 (3H, s), 1.83–1.93 (2H, m), 2.27 (2H, t, *J* 6.9), 3.33 (1H, td, *J* 6.2, 1.2), 3.35 (1H, td, *J* 6.2, 1.2), 3.49 (2H, s), 3.82 (3H, s), 3.84 (3H, s), 3.99 (1H, s), 4.35 (2H, d, *J* 5.9), 6.52 (2H, s), 6.60 (1H, br s) and 7.12 (1H, br s).

***N*-Piperonyl α-pantothenamide (*36a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.01 (3H, s), 3.46 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.93 (1H, d, *J* 5.9, 16.3), 3.99 (1H, d, *J* 5.9, 16.3), 4.03 (1H, s), 4.28 (1H, dd, *J* 5.8, 14.7), 4.32 (1H, dd, *J* 5.8, 14.7), 5.93 (2H, s), 6.68 (1H, br s), 6.69–6.75 (3H, m) and 7.47 (1H, br s).

***N*-Piperonyl pantothenamide (*36b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.90 (3H, s), 0.99 (3H, s), 2.46 (2H, t, *J* 5.4), 3.47 (2H, s), 3.66–3.61 (2H, m), 3.97 (1H, s), 4.28 (1H, dd, *J* 5.6, 14.2), 4.33 (1H, dd, *J* 5.6, 14.2), 5.94 (2H, s), 6.24 (1H, br s), 6.70–6.75 (3H, m) and 7.37 (1H, br s).

***N*-Piperonyl homopantothenamide (*36c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.83–1.92 (2H, m), 2.26 (2H, t, *J* 6.9), 3.33 (1H, td, *J* 6.2, 2.3), 3.35 (1H, td, *J* 6.2, 2.3), 3.49 (2H, s), 3.99 (1H, s), 4.32 (2H, d, *J* 5.6), 5.94 (2H, s), 6.44 (1H, br s), 6.74 (2H, s), 6.78 (1H, s) and 7.12 (1H, br s).

***N*-(4-Trifluoromethoxy-benzyl) α-pantothenamide (*37a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 3.46 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.94 (1H, dd, *J* 5.9, 16.4), 4.03 (1H, dd, *J* 5.9, 16.4), 4.04 (1H, s), 4.39 (1H, dd, *J* 5.8, 14.8), 4.44 (1H, dd, *J* 5.8, 14.8), 6.83 (1H, br s), 7.15–7.40 (4H, m) and 7.46 (1H, br s).

***N*-(4-Trifluoromethoxy-benzyl) pantothenamide (*37b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, s), 0.98 (3H, s), 2.49 (2H, t, *J* 5.9), 3.46 (1H, d, *J* 11.2), 3.49 (1H, d, *J* 11.2), 3.55–3.67 (2H, m), 3.97 (1H, s), 4.41 (2H, d, *J* 6.3), 3.82 (1H, br s), 7.17 (2H, d, *J* 8.7), 7.29 (2H, d, *J* 8.7) and 7.33 (1H, br s).

***N*-(4-Trifluoromethoxy-benzyl) homopantothenamide (*37c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.03 (3H, s), 1.83–1.93 (2H, m), 2.29 (2H, t, *J* 6.7), 3.34 (1H, t, *J* 6.1), 3.37 (1H, t, *J* 6.1), 3.49 (H, d, *J* 11.2), 3.53 (H, d, *J* 11.2), 4.02 (1H, s), 4.44 (2H, dd, *J* 5.9), 6.62 (1H, br s), 7.07 (1H, br s) and 7.19–7.31 (4H, m).

***N*-(4-Trifluoromethyl-benzyl) α-pantothenamide (*38a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 3.46 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.96 (2H, dd, *J* 5.4, 16.4), 4.02 (2H, dd, *J* 5.4, 16.4), 4.04 (1H, s), 4.43 (1H, dd, *J* 5.9, 16.0), 4.48 (1H, dd, *J* 5.9, 16.0), 6.95 (1H, br s), 7.36 (2H, d, *J* 7.9), 7.47 (1H, br s) and 7.56 (2H, d, *J* 8.2).

***N*-(4-Trifluoromethyl-benzyl) pantothenamide (*38b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.89 (3H, s), 0.98 (3H, s), 2.50 (2H, t, *J* 5.6), 3.46 (2H, s), 3.55–3.63 (2H, m), 3.96 (1H, s), 4.47 (2H, d, *J* 5.8), 6.54 (1H, br s), 7.35 (1H, br s), 7.38 (2H, d, *J* 8.3) and 7.58 (2H, d, *J* 8.3).

***N*-(4-Trifluoromethyl-benzyl) homopantothenamide (*38c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.84–1.93 (2H, m), 2.30 (2H, t, *J* 6.7), 3.34 (1H, t, *J* 6.5), 3.36 (1H, t, *J* 6.3), 3.48 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 4.02 (1H, s), 4.49 (2H, d, *J* 5.9), 6.88 (1H, br s), 7.10 (1H, br s) and 7.41–7.55 (4H, m).

***N*-(3-Trifluoromethyl-benzyl) α-pantothenamide (*39a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.00 (3H, s), 3.46 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.96 (2H,

dd, *J* 5.4, 16.4), 4.02 (2H, dd, *J* 5.4, 16.4), 4.04 (1H, s), 4.46 (2H, d, *J* 5.8), 6.94 (1H, br s) and 7.43–7.54 (5H, m).

***N*-(3-Trifluoromethyl-benzyl) pantothenamide (*39b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.88 (3H, s), 0.98 (3H, s), 2.50 (2H, t, *J* 5.9), 3.46 (2H, s), 3.54–3.63 (2H, m), 3.97 (1H, s), 4.47 (2H, d, *J* 5.9), 6.54 (1H, br s), 7.35 (1H, br s), 7.44–7.47 (2H, m), 7.51 (1H, s) and 7.53 (1H, d, *J* 6.8).

***N*-(3-Trifluoromethyl-benzyl) homopantothenamide (*39c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 1.84–1.93 (2H, m), 2.30 (2H, t, *J* 6.7), 3.34 (1H, t, *J* 6.2), 3.36 (1H, t, *J* 6.2), 3.47 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 4.02 (1H, s), 4.49 (2H, d, *J* 5.9), 6.88 (1H, br s), 7.10 (1H, br s) and 7.41–7.54 (4H, m).

***N*-Dansylcadaverinyl α-pantothenamide (*40a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s), 1.03 (3H, s), 1.23–1.44 (6H, m), 2.82–2.88 (2H, m), 2.88 (6H, s), 3.10–3.24 (2H, m), 3.52 (2H, s), 3.94 (1H, dd, *J* 5.9, 16.4), 4.03 (1H, dd, *J* 5.9, 16.4), 4.09 (1H, s), 5.59 (1H, br s), 6.63 (1H, br s), 7.17 (1H, dd, *J* 7.6), 7.48–7.57 (2H, m), 7.62 (1H, br s), 8.20 (1H, d, *J* 7.3), 8.30 (1H, d, *J* 8.5) and 8.53 (1H, d, *J* 8.5).

***N*-Dansylcadaverinyl pantothenamide (*40b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 1.25–1.46 (6H, m), 2.46 (2H, t, *J* 6.1), 2.87 (2H, m), 2.88 (6H, s), 3.01–3.21 (2H, m), 3.49 (2H, s), 3.56–3.62 (2H, m), 4.02 (1H, s), 5.57 (1H, br s), 6.26 (1H, br s), 7.18 (1H, d, *J* 7.7), 7.47 (1H, br s), 7.49–7.57 (2H, m), 8.21 (1H, d, *J* 7.3), 8.31 (1H, d, *J* 8.5) and 8.53 (1H, d, *J* 8.5).

***N*-Dansylcadaverinyl homopantothenamide (*40c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.00 (3H, s), 1.30–1.43 (6H, m), 1.83–1.92 (2H, m), 2.24 (2H, t, *J* 6.6), 2.68 (2H, t, *J* 6.6), 2.88 (6H, s), 3.10–3.19 (2H, m), 3.35 (1H, t, *J* 6.4), 3.37 (1H, t, *J* 6.4), 3.50 (2H, s), 4.06 (1H, s), 5.58 (1H, br s), 6.46 (1H, br s), 7.17 (1H, m), 7.24 (1H, br s), 7.48–7.56 (2H, m), 8.20 (1H, d, *J* 7.3), 8.30 (1H, d, *J* 8.5) and 8.52 (1H, d, *J* 8.5).

***N*-(1-Morpholin-4-yl) α-pantothenamide (*41a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s), 1.06 (3H, s), 3.44 (2H, t, *J* 4.8), 3.53 (2H, s), 3.61–3.68 (2H, m), 3.68–3.74 (4H, m), 4.08 (1H, s), 4.12 (2H, d, *J* 5.0) and 7.54 (1H, br s).

***N*-(1-Morpholin-4-yl) pantothenamide (*41b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.01 (3H, s), 2.55 (2H, t, *J* 5.8), 3.52–3.42 (4H, m), 3.58–3.68 (8H, m), 3.98 (1H, s) and 7.35 (1H, br s).

***N*-(1-Morpholin-4-yl) homopantothenamide (*41c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 1.85–1.94 (2H, m), 2.39 (2H, t, *J* 6.9), 3.34 (1H, t, *J* 6.0), 3.36 (1H, t, *J* 6.4), 3.45 (2H, t, *J* 4.8), 3.49 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.57–3.62 (2H, m), 3.62–3.69 (4H, m), 4.00 (1H, s) and 7.14 (1H, br s).

***N*-(1-Thiomorpholin-4-yl) α-pantothenamide (*42a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s), 1.06 (3H, s), 2.61–2.68 (4H, m), 3.53 (2H, s), 3.68–3.73 (2H, m), 3.88–3.98 (2H, m), 4.08 (1H, s), 4.11 (2H, d, *J* 4.7) and 7.55 (1H, br s).

***N*-(1-Thiomorpholin-4-yl) pantothenamide (*42b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 2.55 (2H, t, *J* 5.7), 2.59–2.63 (4H, m), 3.49 (1H, d, *J* 11.2), 3.50 (1H, d, *J* 11.2), 3.58–3.63 (2H, m), 3.71–3.75 (2H, m), 3.85–3.93 (2H, m), 3.98 (1H, s) and 7.32 (1H, br s).

***N*-(1-Thiomorpholin-4-yl) homopantothenamide (*42c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.03 (3H, s), 1.85–1.94 (2H, m), 2.39 (2H, t, *J* 6.9), 2.59–2.63 (4H, m), 3.34 (1H, td, *J* 6.7, 1.8), 3.36 (1H, td, *J* 6.4, 1.8), 3.48 (1H, d, *J* 11.4), 3.51 (1H, d, *J* 11.4), 3.71–3.75 (2H, m), 3.85–3.93 (2H, m), 4.00 (1H, s) and 7.11 (1H, br s).

***N*-(1-Pyrrolidin-1-yl-ethyl) α-pantothenamide (*43a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 1.11 (3H, s), 1.16 (3H, s), 1.80–1.86 (4H, m), 2.53–2.61 (4H, m), 2.65 (2H, t, *J* 7.3), 3.46 (1H, d, *J* 9.9), 3.52 (1H, d, *J* 9.9), 3.82–3.91 (5H, m), 7.33 (1H, br s) and 7.43 (1H, br s).

***N*-(1-Pyrrolidin-1-yl-ethyl) pantothenamide (*43b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.04 (3H, s), 1.82–1.84 (4H, m), 2.40–2.49 (2H, m), 2.56–2.71 (6H, m), 3.27–3.35 (2H, m), 3.42–3.57 (4H, m), 3.60–3.68 (2H, m), 3.93 (1H, s), 6.39 (1H, br s) and 7.39 (1H, br s).

***N*-(1-Pyrrolidin-1-yl-ethyl) homopantothenamide (*43c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.03 (3H, s), 1.77–1.85 (4H, m), 1.83–1.93 (2H, m), 2.26 (2H, td, *J* 6.6, 2.6), 2.56–2.66 (6H, m), 3.26–3.45 (4H, m), 3.49 (1H, d, *J* 11.2), 3.50 (1H, d, *J* 11.2), 3.97 (1H, s), 6.62 (1H, br s) and 7.18 (1H, br s).

***N*-(2-Morpholin-4-yl-ethyl) α-pantothenamide (*44a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 1.06 (3H, s), 1.14 (3H, s), 2.43–2.49 (4H, m), 2.51 (2H, t, *J* 5.9), 3.33–3.45 (2H, m), 3.52 (1H, d, *J* 10.6), 3.58 (1H, d, *J* 10.6), 3.72 (4H, t, *J* 4.7), 3.80 (1H, dd, *J* 5.3, 16.8), 3.95 (1H, s), 4.20 (1H, dd, *J* 7.0, 16.8), 7.09 (1H, br s) and 7.29 (1H, br s).

***N*-(2-Morpholin-4-yl-ethyl) pantothenamide (*44b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 2.43–2.49 (8H, m), 3.28–3.43 (2H, m), 3.48 (2H, s), 3.57 (1H, t, *J* 6.3), 3.59 (1H, t, *J* 6.0), 3.71 (4H, t, *J* 4.6), 3.98 (1H, s), 6.24 (1H, br s) and 7.38 (1H, br s).

***N*-(2-Morpholin-4-yl-ethyl) homopantothenamide (*44c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.93 (3H, s), 1.02 (3H, s), 1.83–1.92 (2H, m), 2.26 (2H, t, *J* 6.9), 2.45–2.51 (6H, m), 3.34 (1H, t, *J* 5.0), 3.37 (1H, t, *J* 6.0), 3.48 (1H, d, *J* 11.2), 3.51 (1H, d, *J* 11.2), 3.71 (4H, t, *J* 4.7), 4.00 (1H, s), 6.46 (1H, br s) and 7.14 (1H, br s).

***N*-(2-Dimethylamino-ethyl) α-pantothenamide (*46a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 1.13 (3H, s), 1.16 (3H, s), 2.25 (6H, s), 2.47 (2H, t, *J* 5.6), 3.31–3.45 (2H, m), 3.48 (1H, d, *J* 10.0), 3.58 (1H, d, *J* 10.0), 3.69 (1H, dd, *J* 5.0, 17.1), 3.88 (1H, s), 4.34 (1H, dd, *J* 7.9, 17.1), 7.17 (1H, br s) and 7.40 (1H, br s).

***N*-(2-Dimethylamino-ethyl) pantothenamide (*46b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.04 (3H, s), 2.25 (6H, br s), 2.38–2.51 (4H, m), 3.24–3.31 (1H, m), 3.42–3.50 (3H, m), 3.51–3.65 (2H, m), 3.94 (1H, s), 6.26 (1H, br s) and 7.39 (1H, br s).

***N*-(2-Dimethylamino-ethyl) homopantothenamide (*46c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.03 (3H, s), 1.83–1.92 (2H, m), 2.21–2.28 (2H, m), 2.26 (6H, s), 2.45 (2H, t, *J* 5.7), 3.23–3.45 (4H, m), 3.46 (1H, d, *J* 11.4), 3.49 (1H, d, *J* 11.4), 3.97 (1H, s), 6.45 (1H, br s) and 7.19 (1H, br s).

***N*-(2-Diethylamino-ethyl) α-pantothenamide (*47a*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.95 (3H, s), 0.96 (3H, s), 1.05 (6H, t, *J* 7.2), 2.62 (4H, q, *J* 7.2), 2.67 (2H, t, *J* 6.9), 3.37 (2H, t, *J* 7.0), 3.46 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 3.93 (2H, s) and 4.05 (1H, s).

***N*-(2-Diethylamino-ethyl) pantothenamide (*47b*)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, s), 0.93 (3H, s), 1.05 (6H, t, *J* 7.3), 2.50 (2H, t, *J* 6.4), 2.62 (4H, q, *J* 7.3), 2.66 (2H, t, *J* 7.3), 3.33 (1H, t, *J* 6.6), 3.33 (1H, t, *J* 6.3), 3.40 (1H, d, *J* 11.2), 3.52 (1H, d, *J* 11.2), 3.45–3.58 (2H, m) and 3.99 (1H, s).

***N*-(2-Diethylamino-ethyl) homopantothenamide (*47c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.91 (3H, s), 0.95 (3H, s), 1.05 (6H, t, *J* 7.2), 1.77–1.87 (2H, m), 2.29 (2H, t, *J* 7.6), 2.62 (4H, q, *J* 7.3), 2.65 (2H, t, *J* 7.0), 3.26 (2H, t, *J* 6.9), 3.34 (2H, t, *J* 7.0), 3.40 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.4) and 4.00 (1H, s).

***N*-(2-(4-Ethyl-piperazin-1-yl)-ethyl) α-pantothenamide (*48a*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.97 (3H, s), 1.06 (3H, s), 1.10 (3H, t, *J* 7.2), 2.41–2.49 (6H, m), 3.45 (2H, dd, *J* 5.1, 5.3), 3.50 (1H, d, *J* 11.9), 3.54 (1H, d, *J* 11.9), 3.66 (2H, dd, *J* 5.1, 5.3), 4.07 (1H, s), 4.12 (2H, d, *J* 4.7) and 7.53 (1H, br s).

***N*-(2-(4-Ethyl-piperazin-1-yl)-ethyl) pantothenamide (*48b*)**
δ_H (400 MHz; $CDCl_3$; 25°C) δ 0.91 (3H, s), 1.01 (3H, s), 1.09 (3H, t, *J* 7.3), 2.38–2.45 (6H, m), 2.55 (2H, t, *J* 5.7), 3.44–3.68 (4H, m), 3.56–3.68 (4H, m), 3.98 (1H, s) and 7.37 (1H, br).

***N*-(2-(4-Ethyl-piperazin-1-yl)-ethyl) homopantothenamide (*48c*)**
δ_H (300 MHz; $CDCl_3$; 25°C) δ 0.92 (3H, s), 1.02 (3H, s), 1.09 (3H, t, *J* 7.2), 1.84–1.93 (2H, m), 2.38–2.46 (8H, m), 3.33 (1H, t, *J* 6.6), 3.36 (1H, t, *J* 6.5), 3.44–3.50 (4H, m), 3.62 (1H, d, *J* 5.1), 3.63 (1H, d, *J* 5.1) and 3.99 (1H, s).

***N*-(2-(4-Hydroxymethyl-piperazin-1-yl)-ethyl) α-pantothenamide (*49a*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.95 (3H, s), 0.96 (3H, s), 2.58–2.67 (6H, m), 3.44 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.57–3.62 (4H, m), 3.76 (2H, t, *J* 6.2), 4.08 (1H, s) and 4.19 (2H, s).

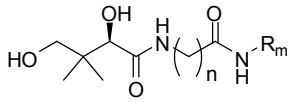
***N*-(2-(4-Hydroxymethyl-piperazin-1-yl)-ethyl) pantothenamide (*49b*)**
δ_H (400 MHz; D_2O; 25°C) δ 0.89 (3H, s), 0.93 (3H, s), 2.52–2.64 (6H, m), 2.71 (2H, t, *J* 6.6), 2.90 (2H, t, *J* 4.9), 3.40 (1H, d, *J* 11.0), 3.51–3.53 (3H, m), 3.60 (2H, m), 3.74 (1H, t, *J* 5.9), 3.75 (1H, t, *J* 6.2) and 3.99 (1H, s).

***N*-(2-(4-Hydroxymethyl-piperazin-1-yl)-ethyl) homopantothenamide (*49c*)**
δ_H (300 MHz; D_2O; 25°C) δ 0.92 (3H, s), 0.95 (3H, s), 1.77–1.87 (2H, m), 2.49 (2H, t, *J* 7.6), 2.55–2.63 (6H, m), 3.26–3.33 (2H, m), 3.41 (1H, d, *J* 11.2), 3.53 (1H, d, *J* 11.2), 3.60 (4H, t, *J* 4.5), 3.76 (2H, t, *J* 6.2) and 4.00 (1H, s).

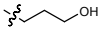
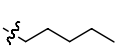
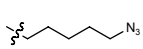
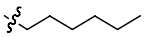
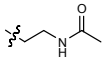
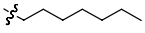
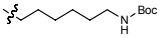
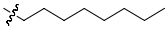
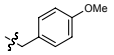
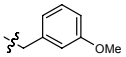
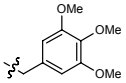
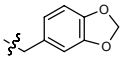
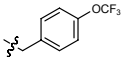
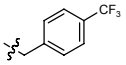
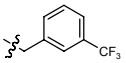
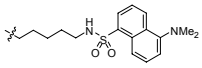
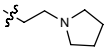
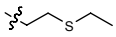
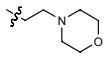
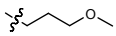
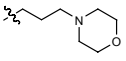
Inhibitory effects of N-substituted pantothenamides

Inhibition assays were performed by preparing a starter culture of *Escherichia coli* K12 in 1% tryptone containing four separate colonies grown on LB agar plates. The starter culture was grown to mid-log phase and then diluted 30 000-fold in the same medium. A 10 µl aliquot of the diluted cell suspension was used to inoculate each well of a 96-well flat-bottomed plate containing 100 µl of 1% tryptone broth supplemented with a specific *N*-substituted pantothenamide (final concentration 50 µM). The plates were incubated at 37ºC for 20 hours before the cell densities were measured by reading the absorbance in each well at 600 nm. The extent of growth in each well was determined by normalizing the OD_{600} values relative to those of the negative control (containing 3% acetonitrile instead of pantothenamide), which were taken as 100% growth. Each compound was tested in quadruplicate and the average % growth and standard deviations were determined from these experiments. The results are reported in Table 1.

Table 1 Average % growth of *N*-substituted pantothenamides at 50µM final concentration.



2a-49a (n=1)
2b-49b (n=2)
2c-49c (n=3)

Entry	R-group	Average growth (%) a (n=1)	b (n=2)	c (n=3)	Entry	R-group	Average growth (%) a (n=1)	b (n=2)	c (n=3)
2		134 ± 16	94 ± 8	157 ± 22	**26**		107 ± 23	96 ± 18	106 ± 5
3		134 ± 20	56 ± 11	135 ± 25	**27**		118 ± 26	62 ± 18	105 ± 5
4		104 ± 11	**-2 ± 2**	129 ± 23	**28**		114 ± 18	71 ± 29	110 ± 7
5		114 ± 8	75 ±14	183 ± 10	**29**		85 ± 15	72 ± 18	96 ± 4
6		76 ± 13	122 ± 45	151 ± 27	**30**		101 ± 9	87 ± 28	92 ± 9
7		112 ± 27	125 ± 16	143 ± 2	**31**		97 ± 14	75 ± 23	101 ± 17
-	No inhibitor/Control	100 ± 11	100 ± 9	100 ± 8	**32**		153 ± 49	62 ± 17	106 ± 15
9		112 ± 31	110 ± 6	176 ± 15	**33**		123 ± 15	115 ± 23	104 ± 14
10		94 ± 15	107 ± 21	115 ± 18	**34**		85 ± 4	108 ± 28	139 ± 18
11		57 ± 13	94 ± 15	152 ± 27	**35**		83 ± 4	99 ± 16	96 ± 25
12		75 ± 11	94 ± 27	125 ± 17	**36**		68 ± 12	116 ± 25	94 ± 10
13		76 ± 4	79 ± 14	136 ± 26	**37**		66 ± 18	83 ± 25	85 ± 22
14		**-2 ± 5**	40 ± 8	130 ± 29	**38**		73 ± 16	85 ± 4	110 ± 10
15		89 ± 10	83 ± 11	126 ± 21	**39**		90 ± 10	92 ± 30	88 ± 8
16		**-3 ± 1**	69 ± 13	126 ± 29	**40**		86 ± 24	75 ± 25	107 ± 31
17		112 ± 41	155 ± 19	158 ± 19	**41**		99 ± 13	98 ± 25	109 ± 29
18		124 ± 14	101 ± 11	150 ± 27	**42**		60 ± 8	98 ± 18	100 ± 15
19		106 ± 30	84 ± 32	129 ± 18	**43**		66 ± 4	100 ± 14	82 ± 8
20		87 ± 12	60 ± 28	120 ± 22	**44**		77 ± 17	95 ± 14	66 ± 9
21		82 ± 31	95 ± 17	103 ± 26	**45**		71 ± 4	110 ± 16	84 ± 7
22		90 ± 25	118 ± 41	83 ± 23	**46**		82 ± 19	91 ± 14	75 ± 7
23		121 ± 26	88 ± 32	94 ± 20	**47**		84 ± 6	105 ± 10	77 ± 18
24		108 ± 8	70 ± 16	97 ± 21	**48**		81 ± 25	95 ± 15	86 ± 8
25		149 ± 43	131 ± 17	114 ± 12	**49**		110 ± 19	109 ± 22	119 ± 9

References:

1. S. Yamada, Y. Yokoyama and T. Shioiri, *J. Org. Chem.*, 1974, **39**, 3302.
2. J. W. Lee, S. I. Jun and K. Kim, *Tetrahedron Lett.*, 2001, **42**, 2709.