

Supporting Information

Enantioselective synthesis of enecaline-derived potent antimalarial agents

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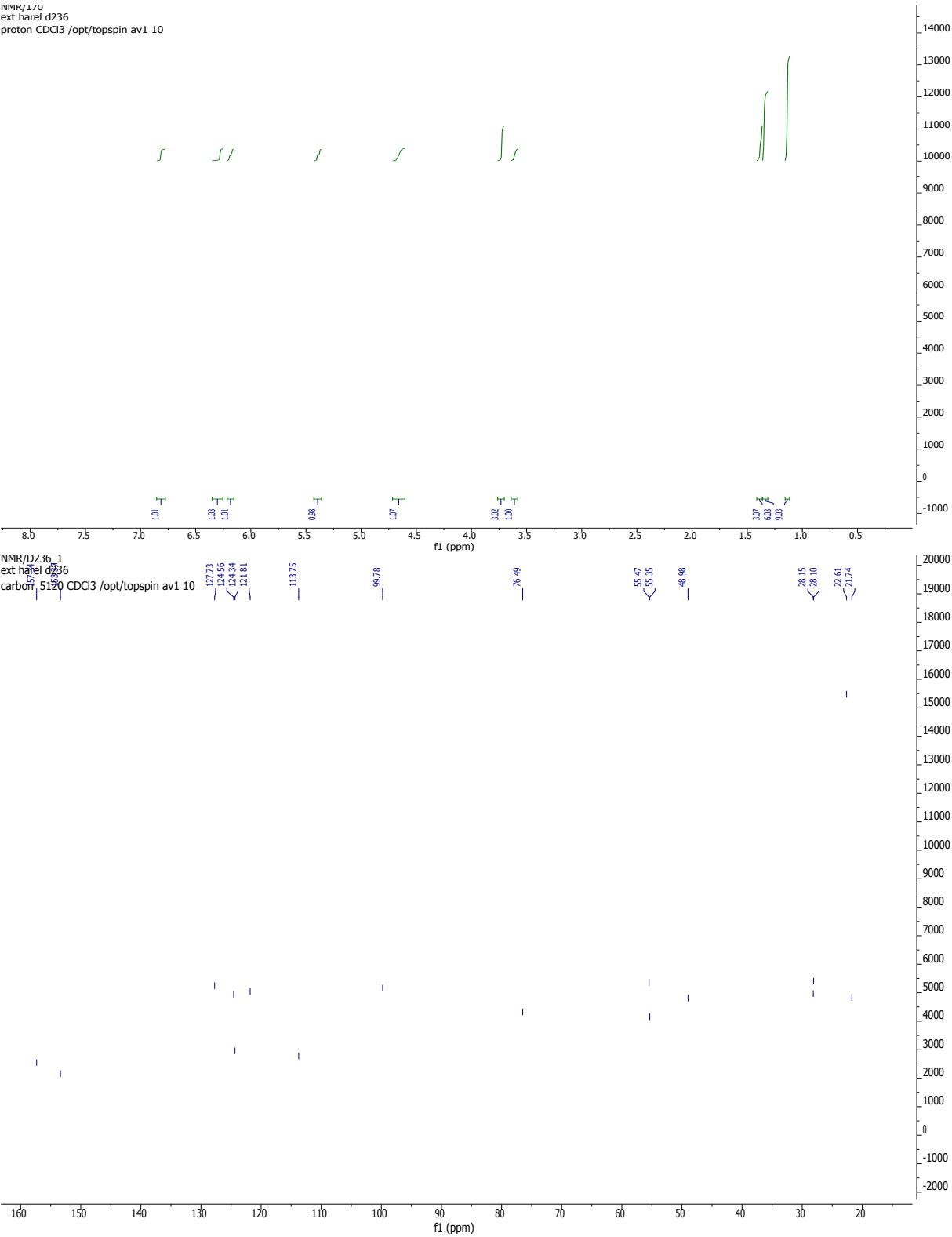
^{b)} Swiss Tropical and Public Health Institute (Swiss TPH), Socinstraße 57, CH-4002 Basel, Switzerland

^{c)} Institut für Pharmazeutische Biologie und Phytochemie der Westfälischen Wilhelms-Universität Münster, Corrensstraße 48, D-48149 Münster, Germany

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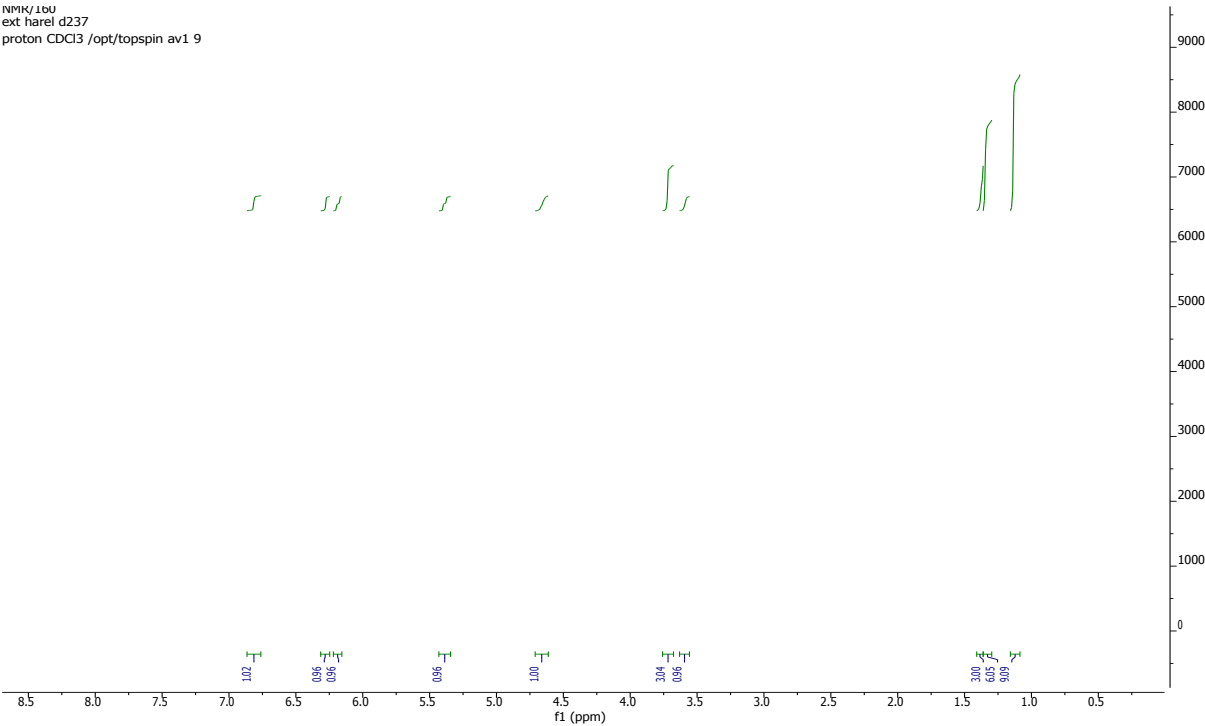
¹H and ¹³C NMR spectra of all new compounds

(*S*)-N-[(*R*)-1-(7-Methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethyl]-2-methylpropane-2-sulfinamide ((*S,R*)-8)

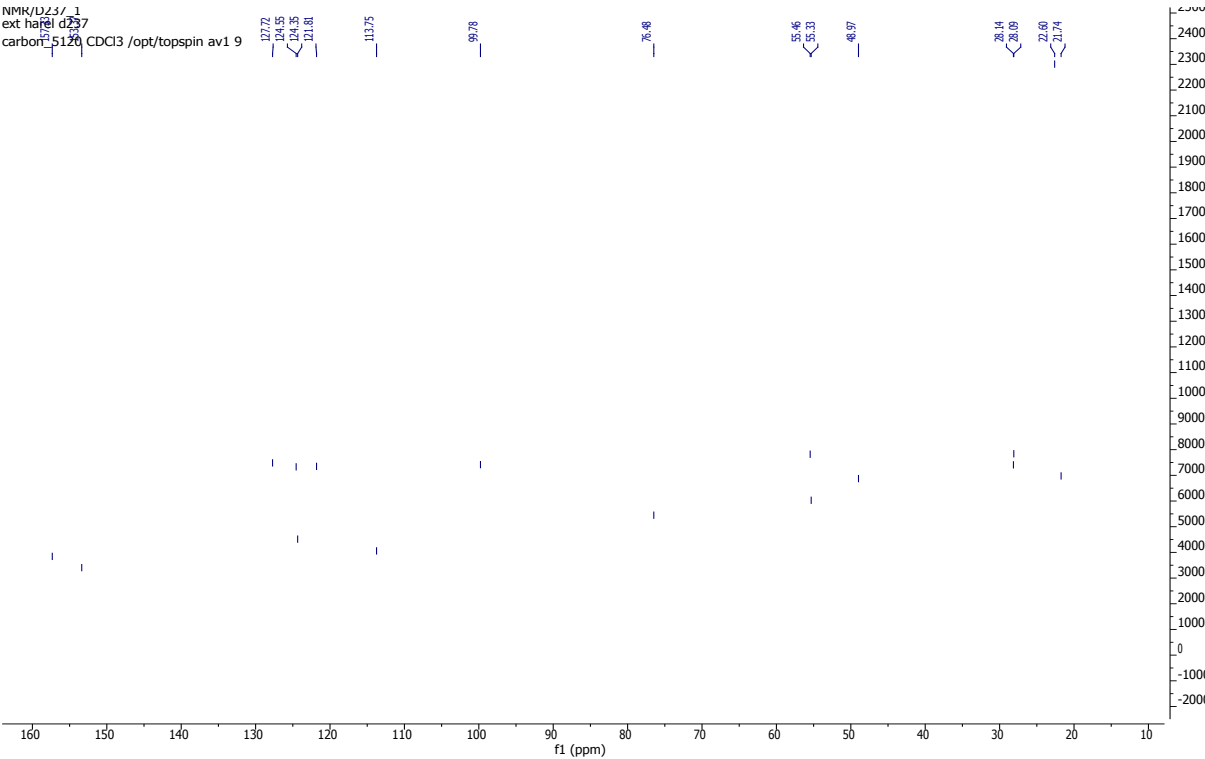


(R)-N-[(S)-1-(7-Methoxy-2,2-dimethyl-2H-chromen-6-yl)ethyl]-2-methylpropane-2-sulfonamide (R,S)-8

NMR/100
ext harel d237
proton CDCl3 /opt/topspin av1 9

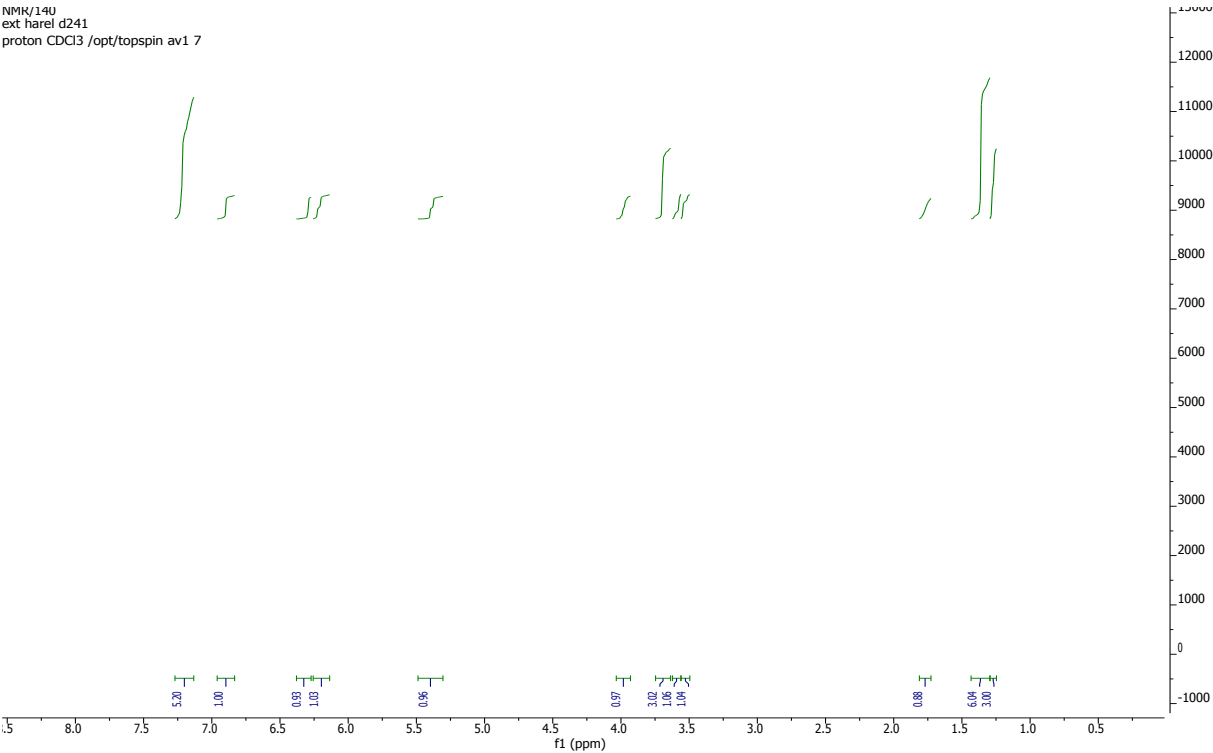


NMR/100
ext harel d237
carbon 125
CDCl3 /opt/topspin av1 9

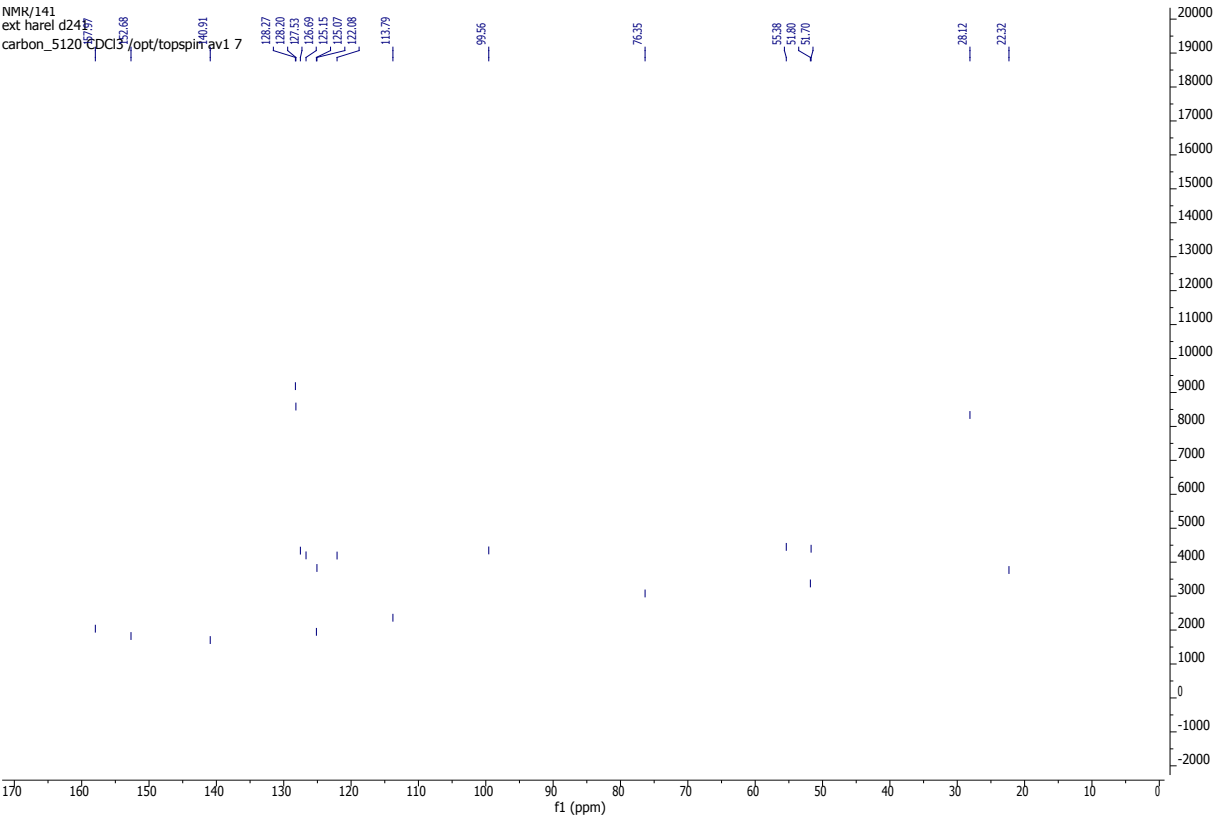


(*R*)-N-Benzyl-1-(7-methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethanamine ((*R*)-1)

NMR/140
ext harel d241
proton CDCl3 /opt/topspin av1 7

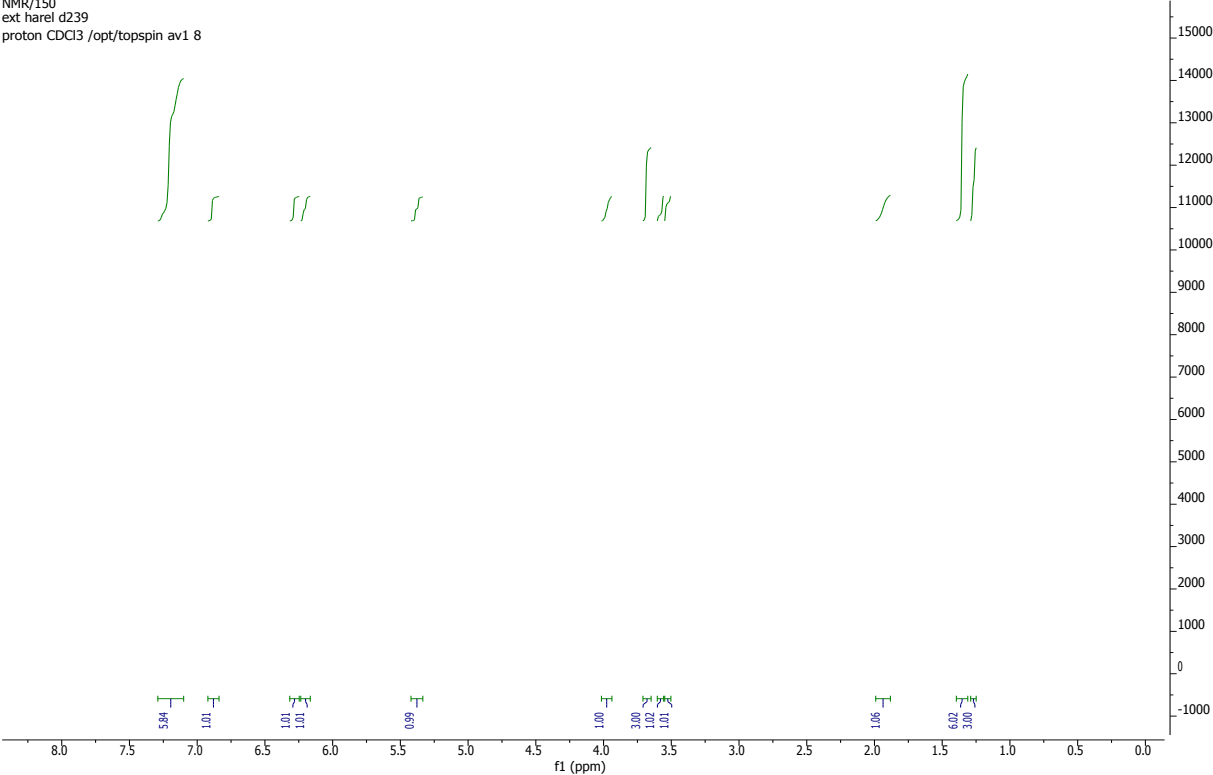


NMR/141
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carbon_5120 CDCl3 /opt/topspin av1 7

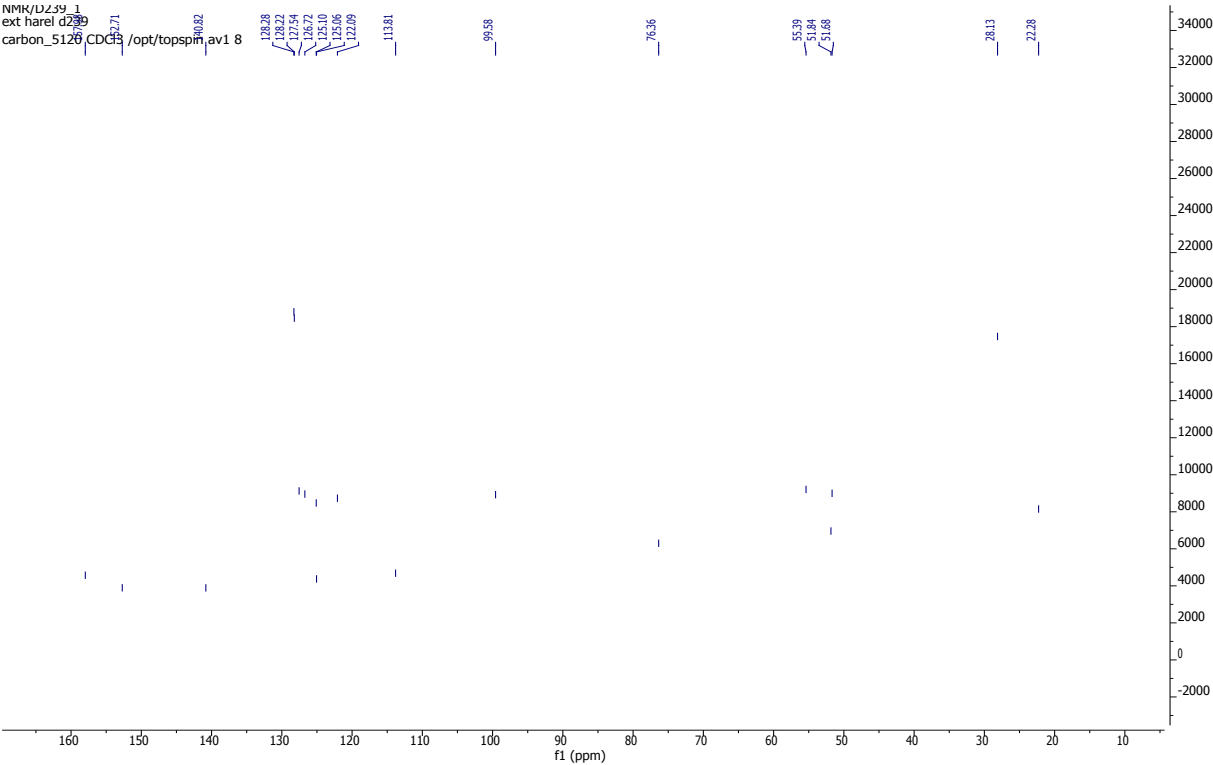


(S)-N-Benzyl-1-(7-methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethanamine ((S)-1)

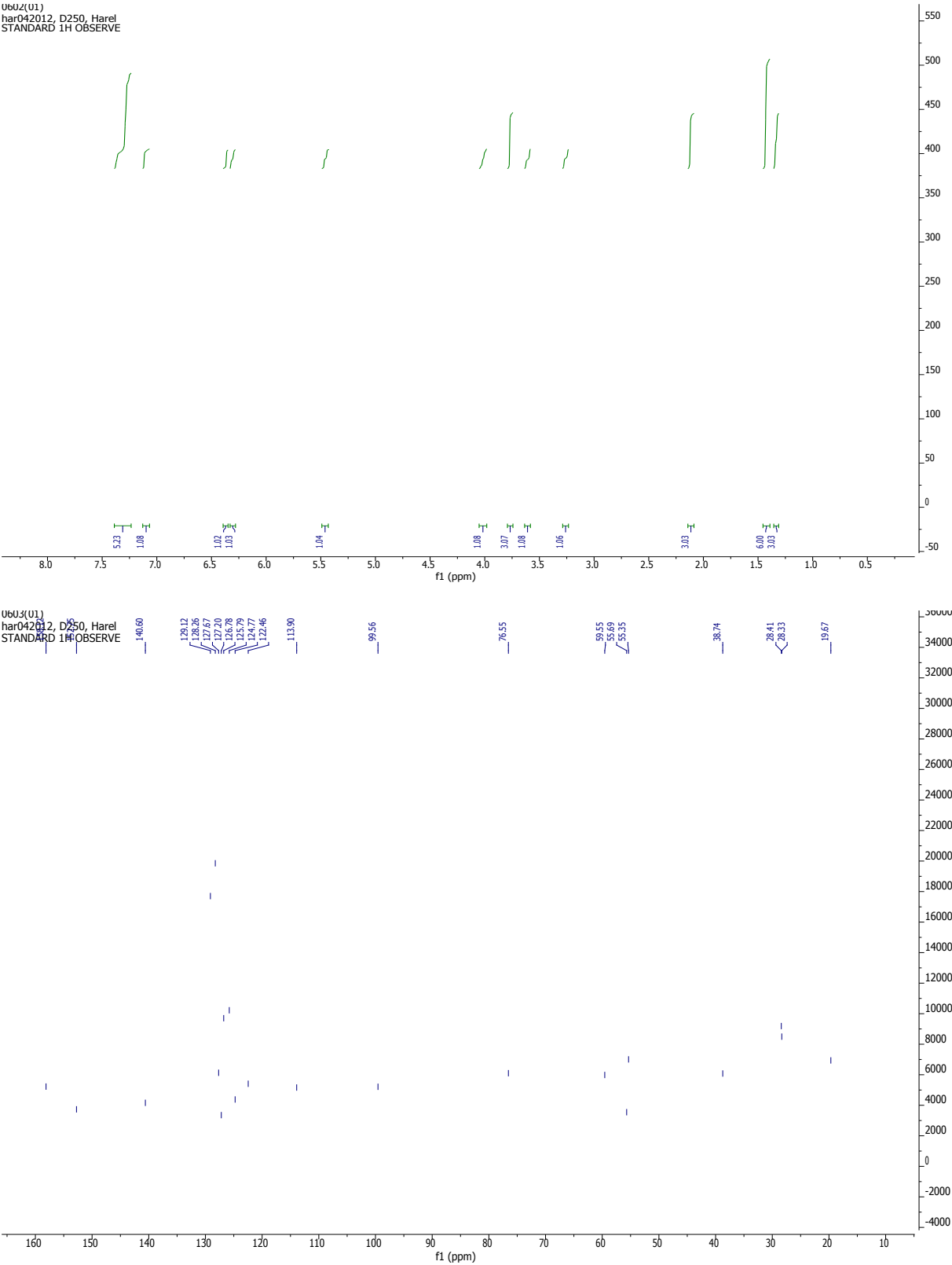
NMR/150
ext harel d239
proton CDCl3 /opt/topspin av1 8



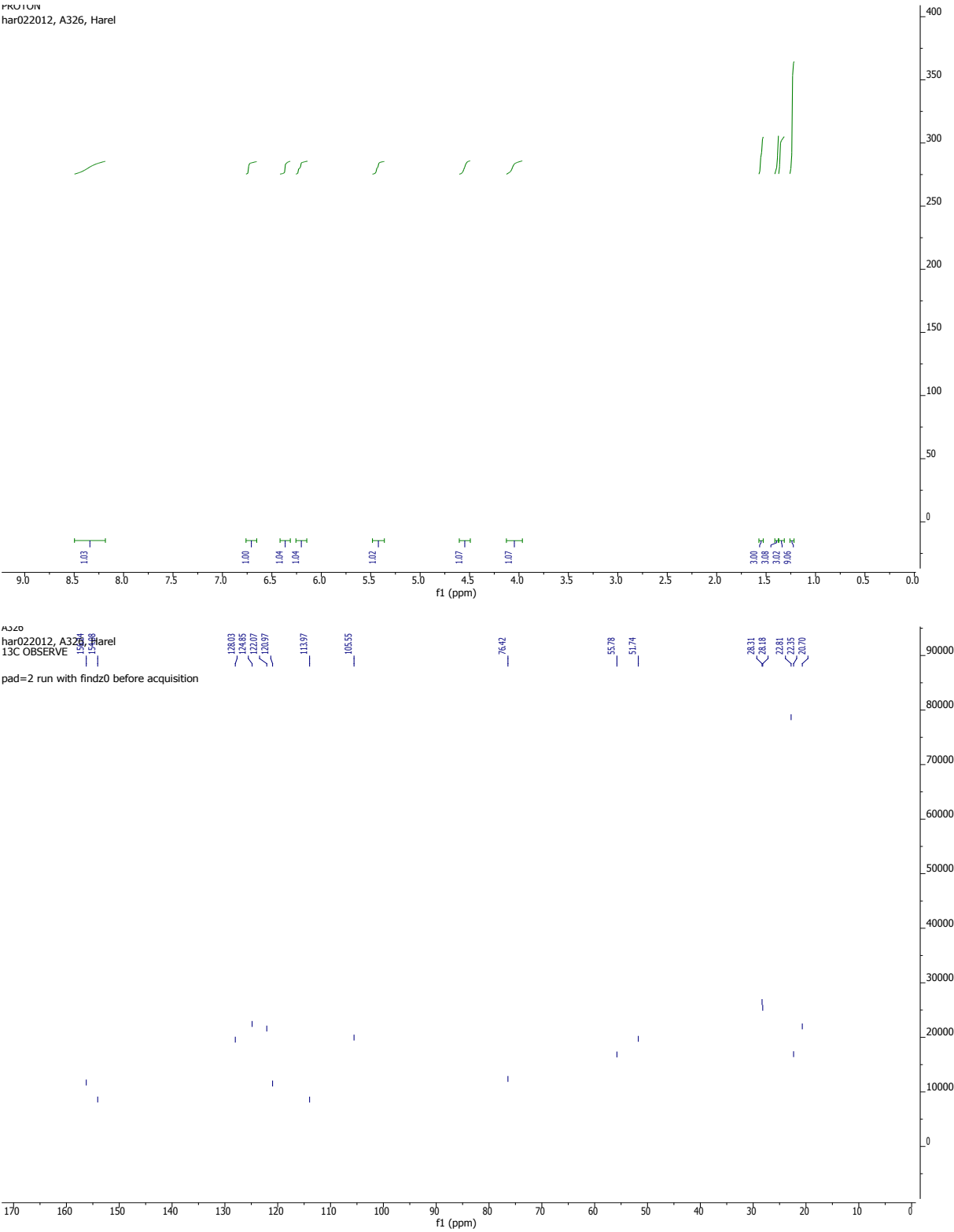
NMR/150
ext harel d239
carbon_5126 CDCl3 /opt/topspin av1 8



(R)-N-Benzyl-1-(7-methoxy-2,2-dimethyl-2*H*-chromen-6-yl)-N-methylethanamine ((R)-10)

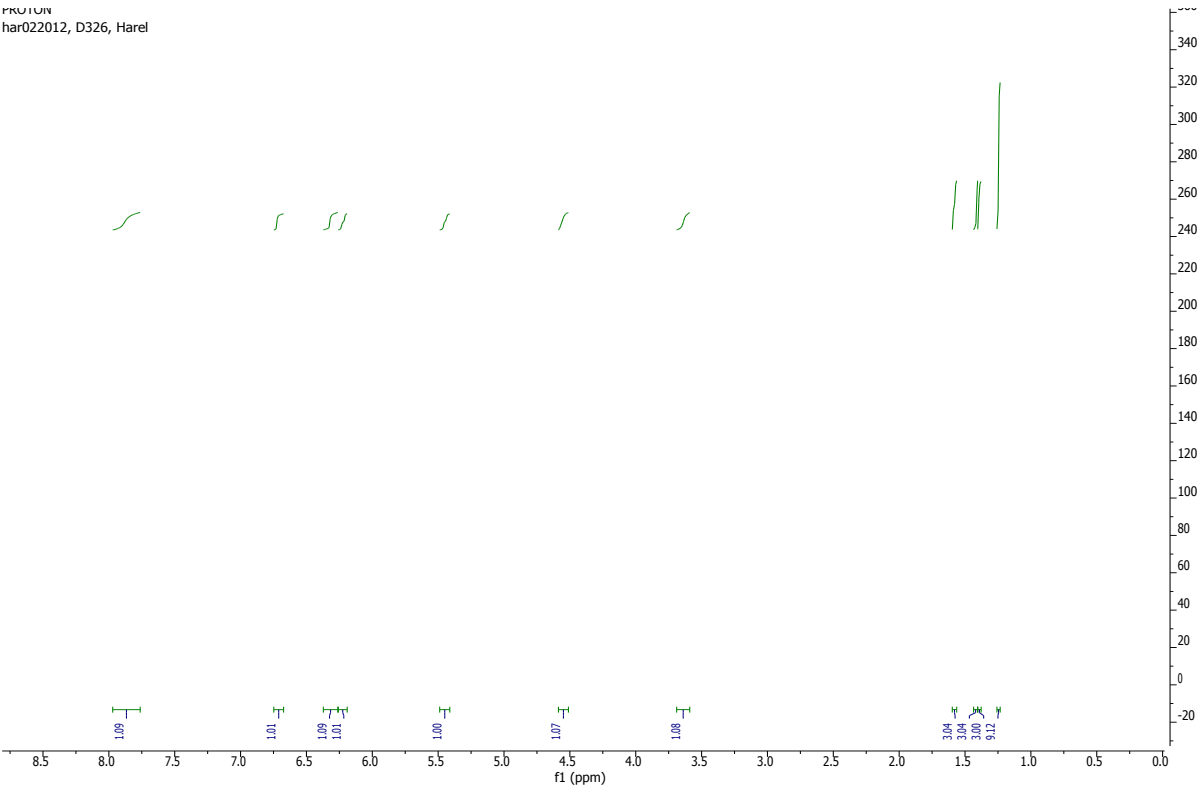


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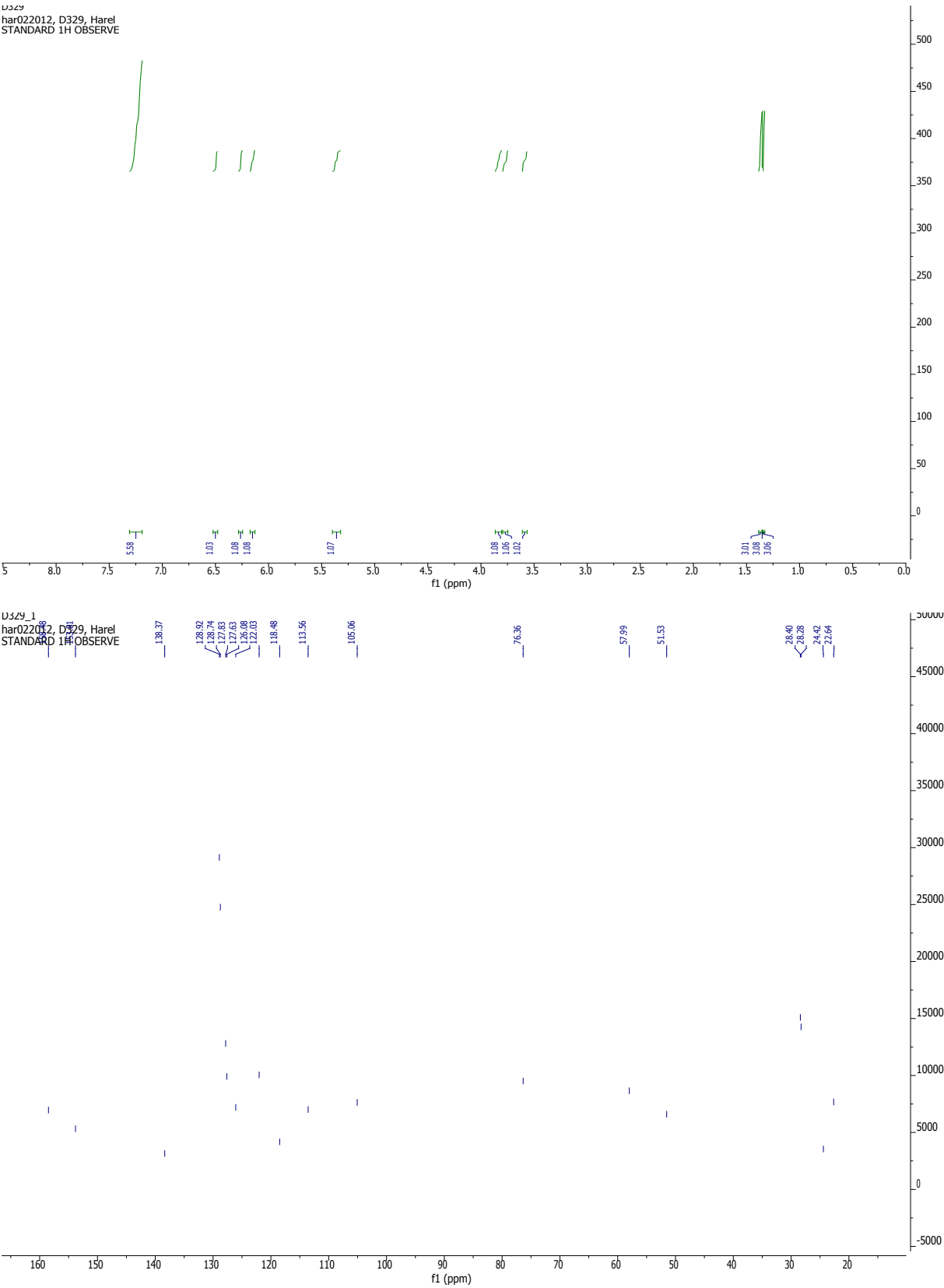


(S)-N-[(S)-1-(7-hydroxy-2,2-dimethyl-2*H*-chromen-6-yl)ethyl]-2-methylpropane-2-sulfinamide ((S,S)-12)

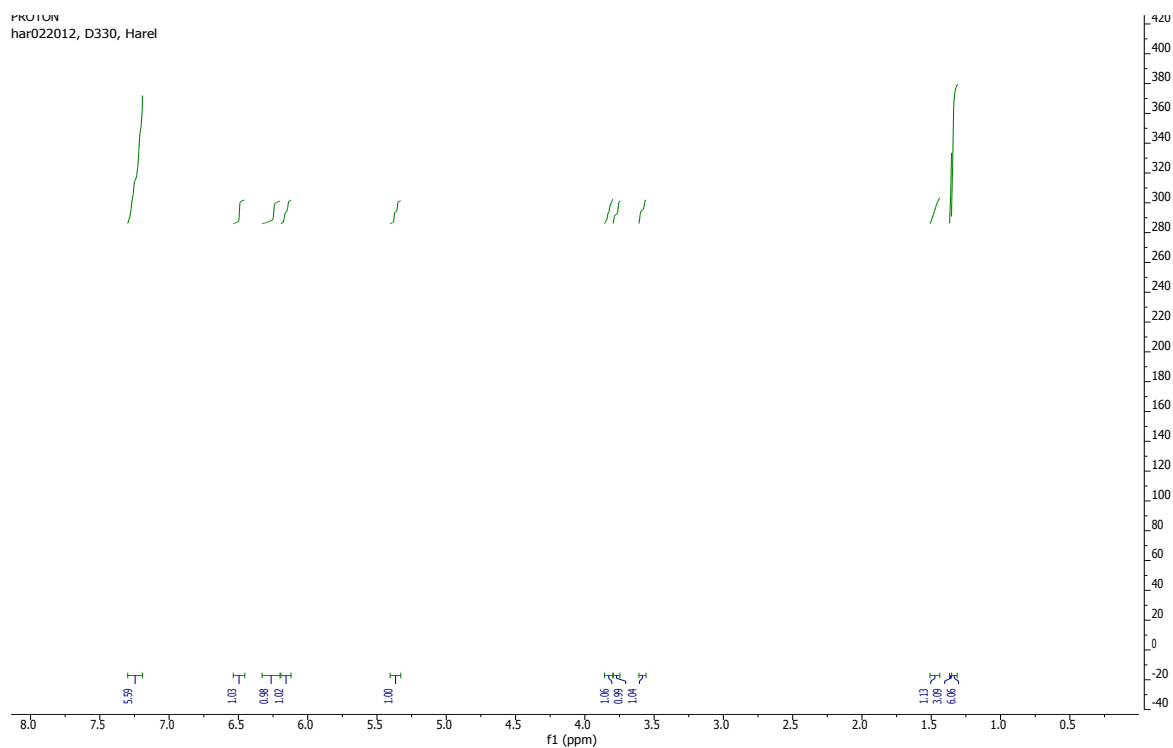
PR001010
har022012, D326, Harel



(R)-6-[1-(Benzylamino)ethyl]-2,2-dimethyl-2H-chromen-7-ol ((R)-2)

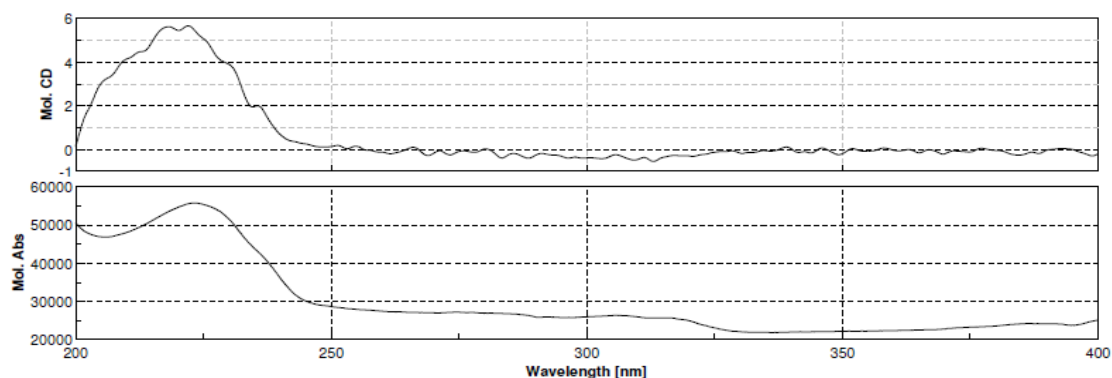


PROTON
har022012, D330, Harel



CD and UV-spectra of enantiomerically pure compounds

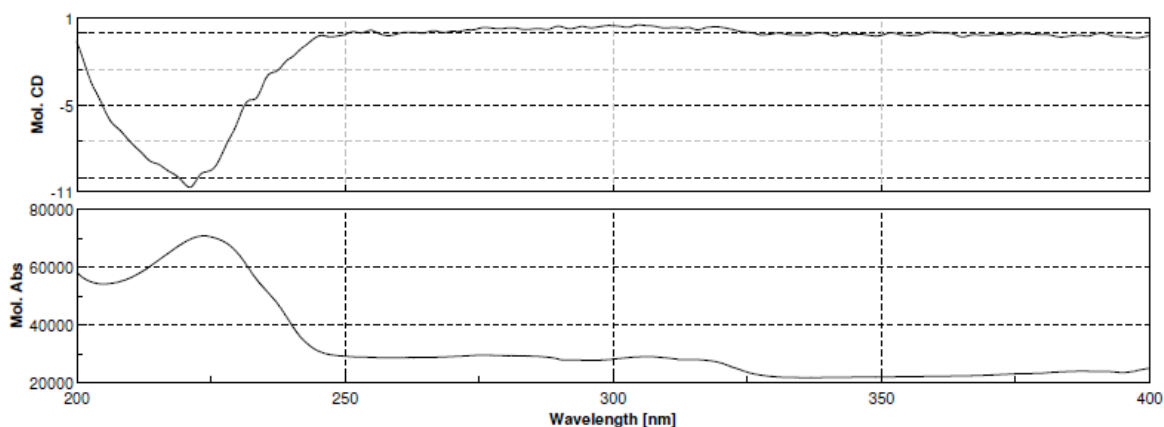
(S)-N-[(*R*)-1-(7-Methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethyl]-2-methylpropane-2-sulfinamide (*(S,R)*-8)



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Sensitivity Standard
Measurement range 450 - 190 nm
Data pitch 0.1 nm
Scanning speed 100 nm/min
Accumulation 5
Cell Length 0.1 cm
Concentration 0.0003 mol/L
Solvent H₂O
Temperature Room Temperature
Sample name D236 1zu10 MeoH 18.8.2011 490-190nm

— DHarel_D236_proc01.jws

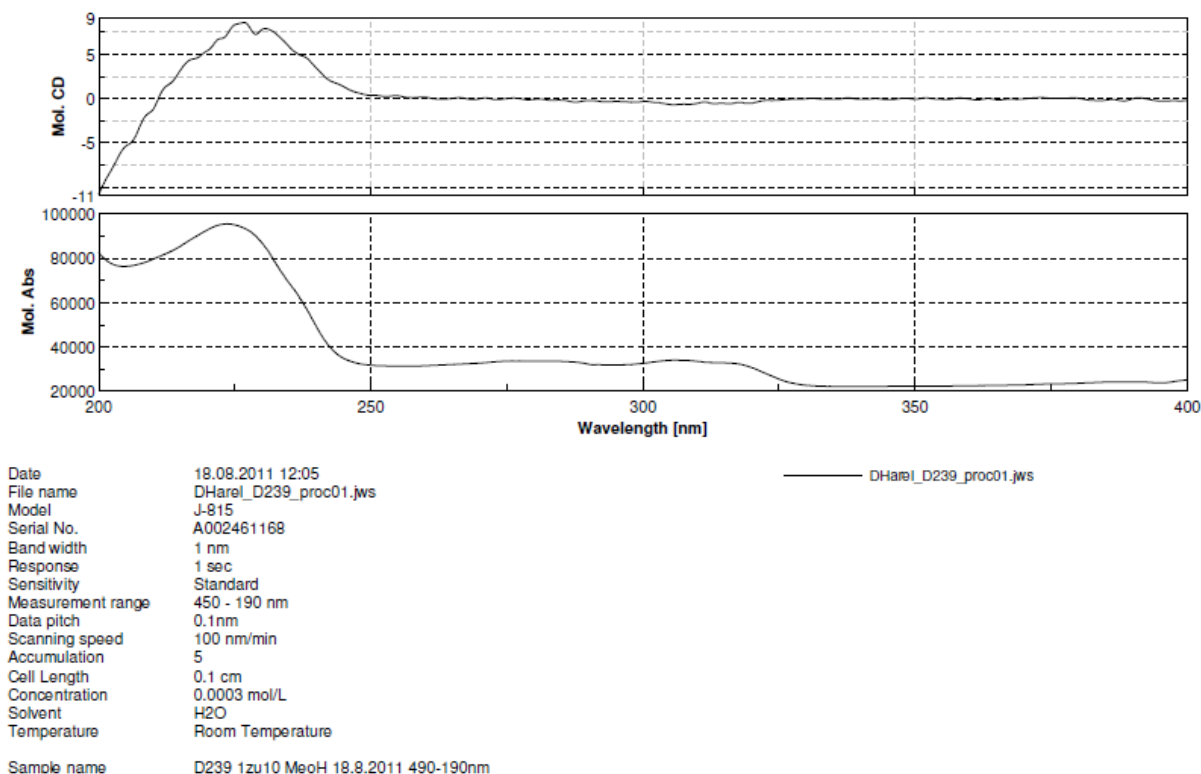
(R)-N-[(*S*)-1-(7-Methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethyl]-2-methylpropane-2-sulfinamide (*(R,S)*-8)



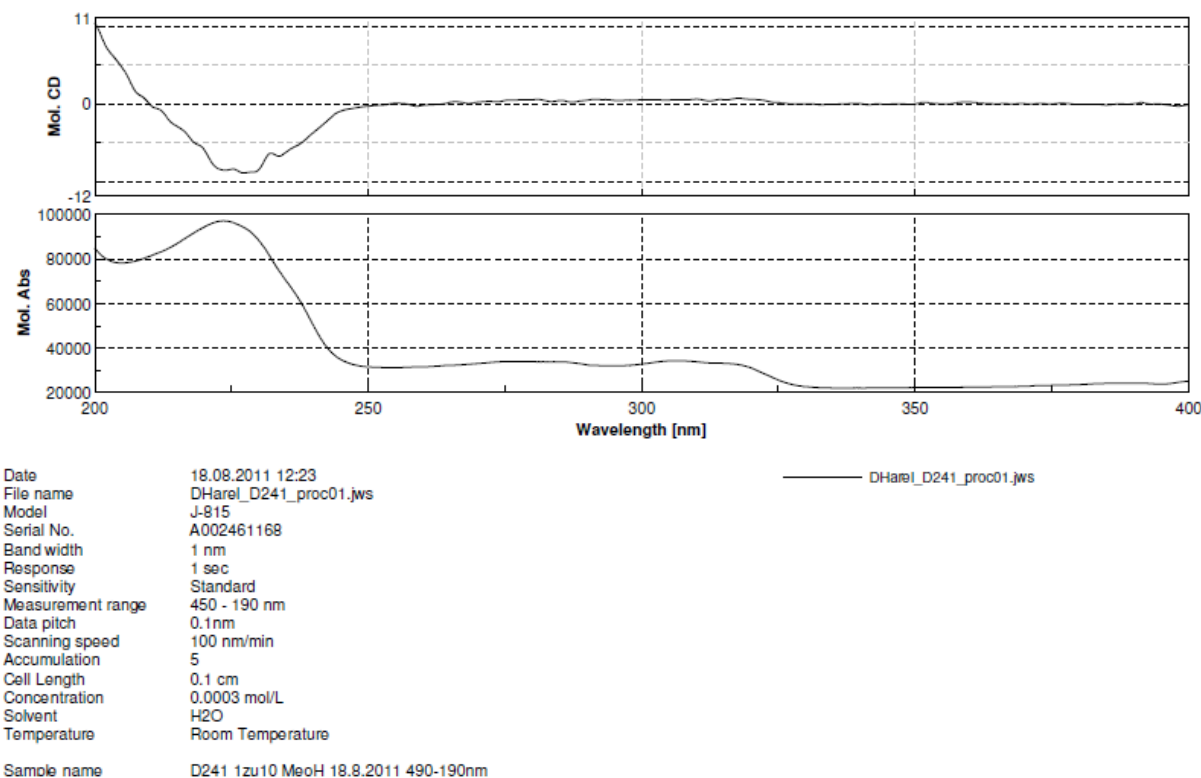
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Sensitivity Standard
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Scanning speed 100 nm/min
Accumulation 5
Cell Length 0.1 cm
Concentration 0.0003 mol/L
Solvent H₂O
Temperature Room Temperature
Sample name D237 1zu10 MeoH 18.8.2011 490-190nm

— DHarel_D237_proc01.jws

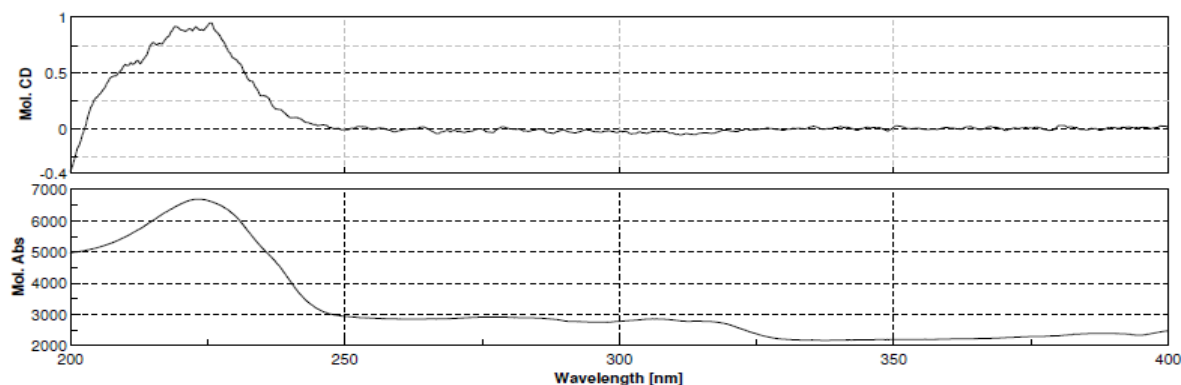
(*R*)-N-Benzyl-1-(7-methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethanamine ((*R*)-1)



(*S*)-N-Benzyl-1-(7-methoxy-2,2-dimethyl-2*H*-chromen-6-yl)ethanamine ((*S*)-1)



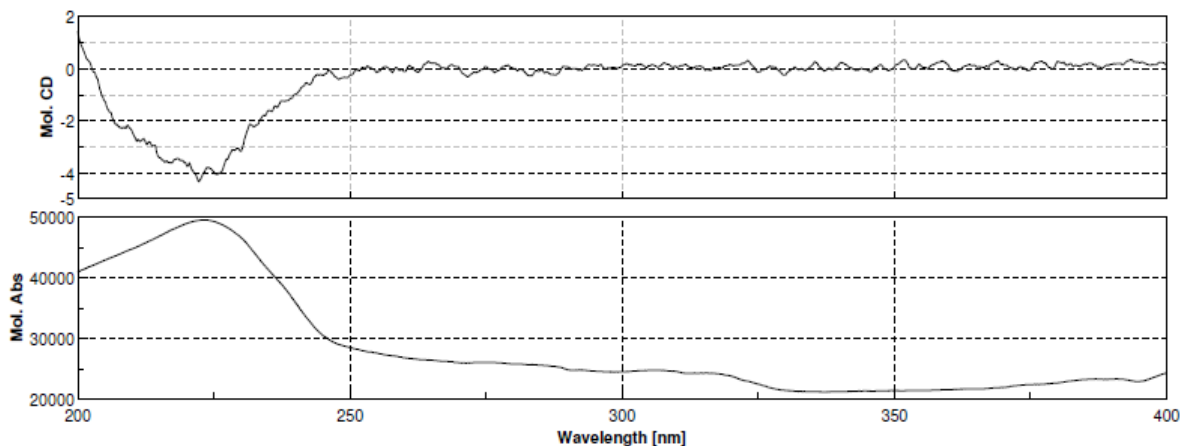
(*S*)-*N*-[(*R*)-1-(7-Hydroxy-2,2-dimethyl-2*H*-chromen-6-yl)ethyl]-2-methylpropane-2-sulfonamide ((*S,R*)-12)



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Sensitivity Standard
Measurement range 400 - 200 nm
Data pitch 0.1nm
Scanning speed 100 nm/min
Accumulation 5
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Concentration 0.0031 mol/L
Solvent Acetonitril
Temperature Room Temperature
Sample name A326 0 1mg ml 26042012

— A326_0_1mg_mL_processed.jws

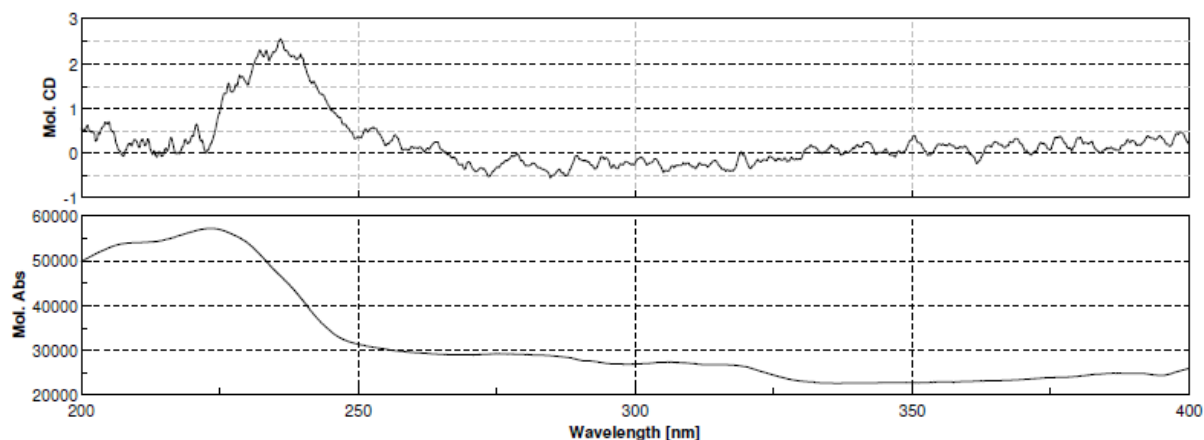
(*S*)-*N*-[(*S*)-1-(7-hydroxy-2,2-dimethyl-2*H*-chromen-6-yl)ethyl]-2-methylpropane-2-sulfonamide ((*S,S*)-12)



Date 26.04.2012 12:35
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Model J-815
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Band width 1 nm
Response 1 sec
Sensitivity Standard
Measurement range 400 - 200 nm
Data pitch 0.1nm
Scanning speed 100 nm/min
Accumulation 5
Cell Length 0.1 cm
Concentration 0.00031 mol/L
Solvent Acetonitril
Temperature Room Temperature
Sample name D326 0 1mg ml 26042012

— D326_0_1mg_mL_processed.jws

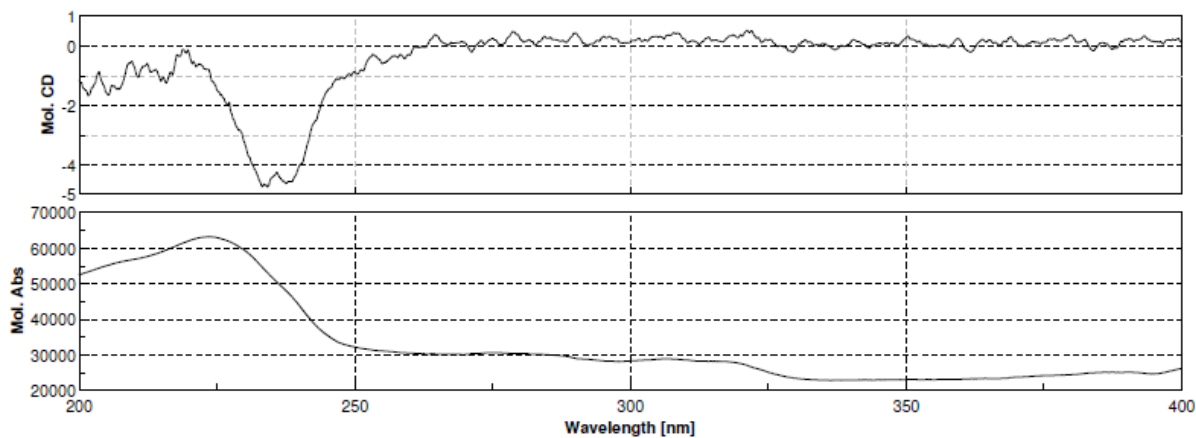
(R)-6-[1-(Benzylamino)ethyl]-2,2-dimethyl-2H-chromen-7-ol ((R)-2)



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Sensitivity Standard
Measurement range 400 - 200 nm
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Scanning speed 100 nm/min
Accumulation 5
Cell Length 0.1 cm
Concentration 0.00029 mol/L
Solvent Acetonitril
Temperature Room Temperature
Sample name D329 0 1mg mL 26042012

— D329_0_1mg_mL_processed.jws

(S)-6-[1-(Benzylamino)ethyl]-2,2-dimethyl-2H-chromen-7-ol ((S)-2)



Date 26.04.2012 12:48
File name D330_0_1mg_mL_processed.jws
Model J-815
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Band width 1 nm
Response 1 sec
Sensitivity Standard
Measurement range 400 - 200 nm
Data pitch 0.1nm
Scanning speed 100 nm/min
Accumulation 5
Cell Length 0.1 cm
Concentration 0.00029 mol/L
Solvent Acetonitril
Temperature Room Temperature
Sample name D330 0 1mg mL 26042012

— D330_0_1mg_mL_processed.jws