

Supporting Information

(R)-8-methylsulfinyloctyl isothiocyanate from *Nasturtium officinale* inhibits LPS-induced immunoinflammatory response in mouse peritoneal macrophages: chemical synthesis and molecular signaling pathways involved

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¹H-NMR, ¹³C-NMR of selected compounds

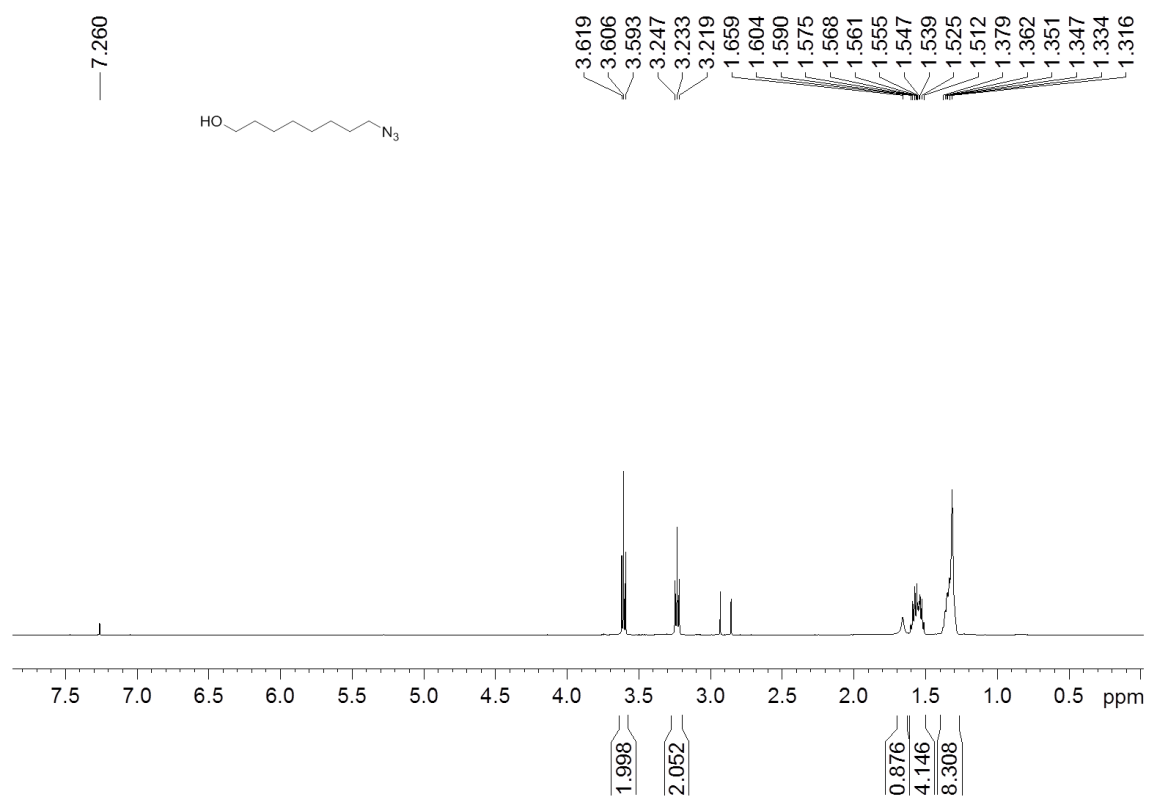


Figure S1. ¹H-NMR (500 MHz, CDCl₃) of 8-Azidoctan-1-ol (**2**)

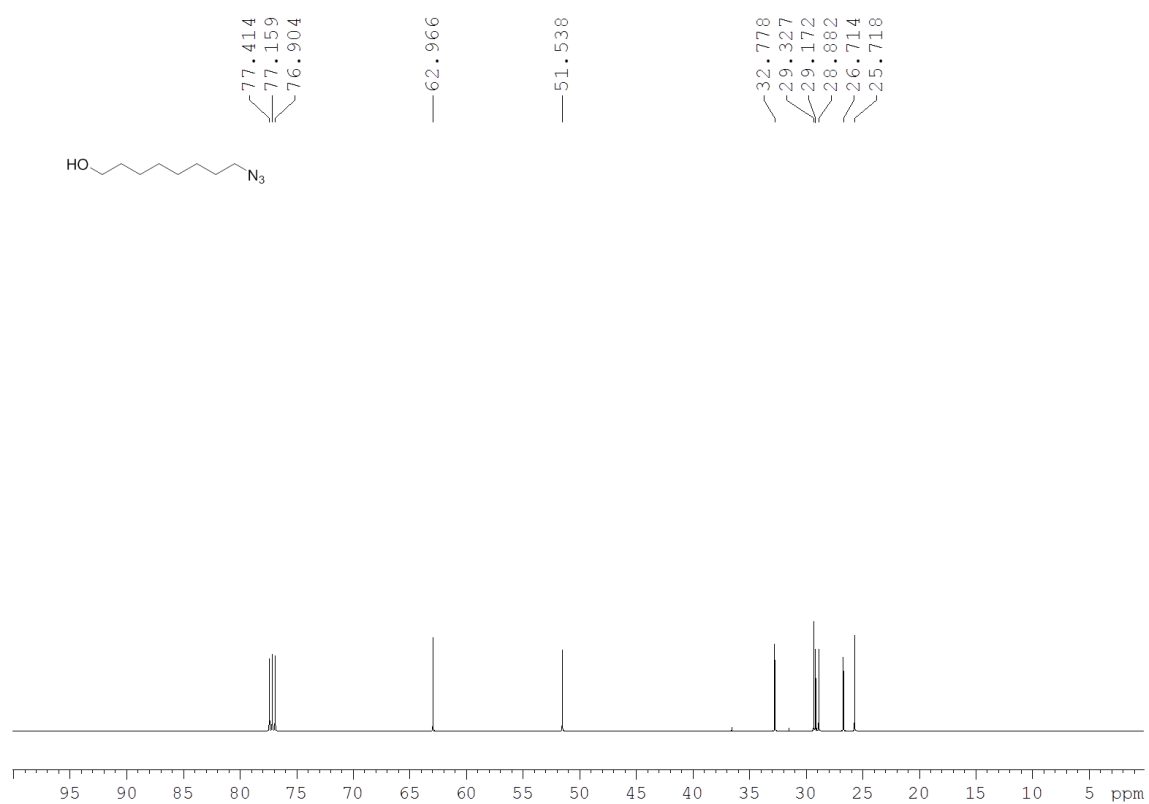


Figure S2. ¹³C-NMR (500 MHz, CDCl₃) of 8-Azidoctan-1-ol (**2**)

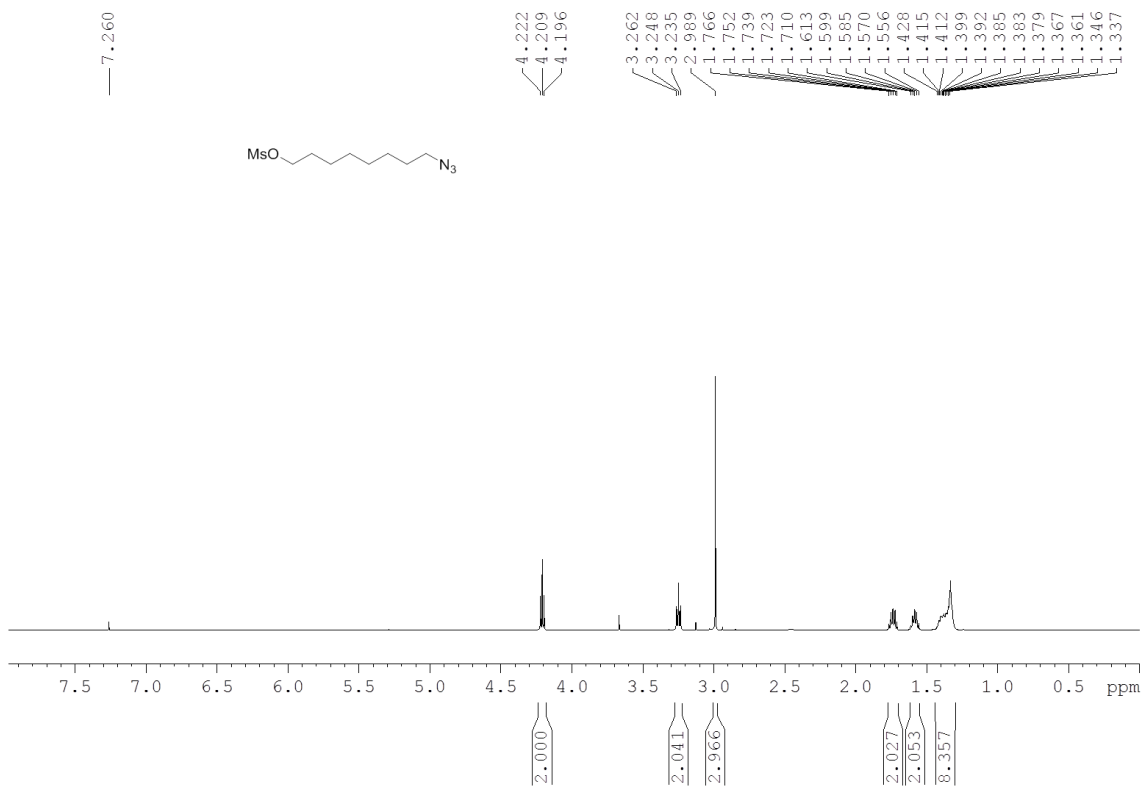


Figure S3. $^1\text{H-NMR}$ (500 MHz, CDCl_3) of 8-Azidoctyl methanesulfonate (**3**)

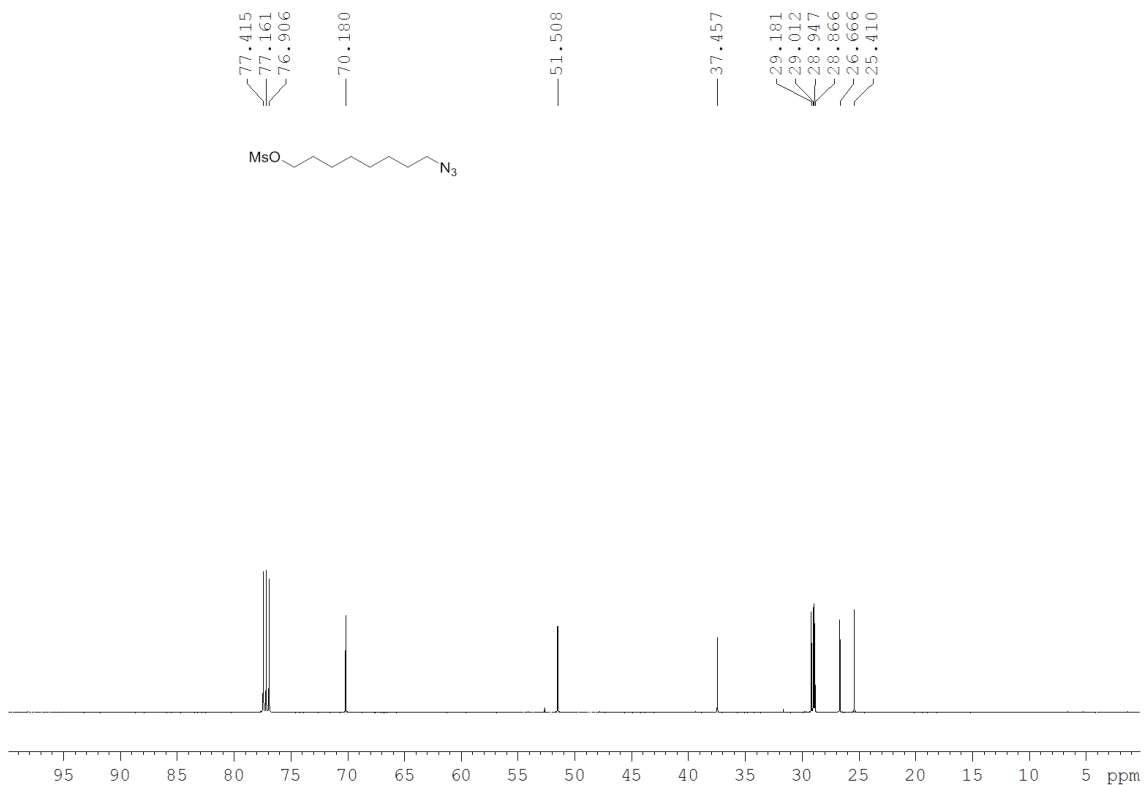


Figure S4. $^{13}\text{C-NMR}$ (500 MHz, CDCl_3) of 8-Azidoctyl methanesulfonate (**3**)

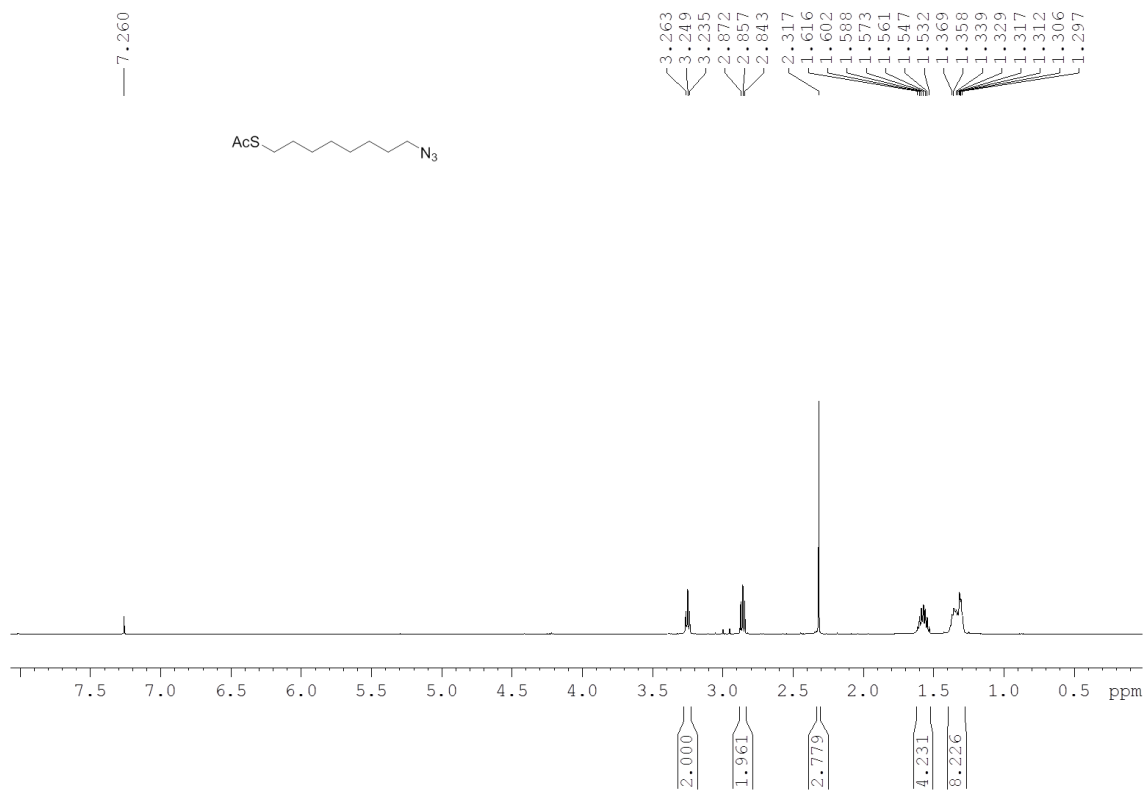


Figure S5. $^1\text{H-NMR}$ (500 MHz, CDCl_3) of 8-Azido-octyl-1-thioacetate (**4**)

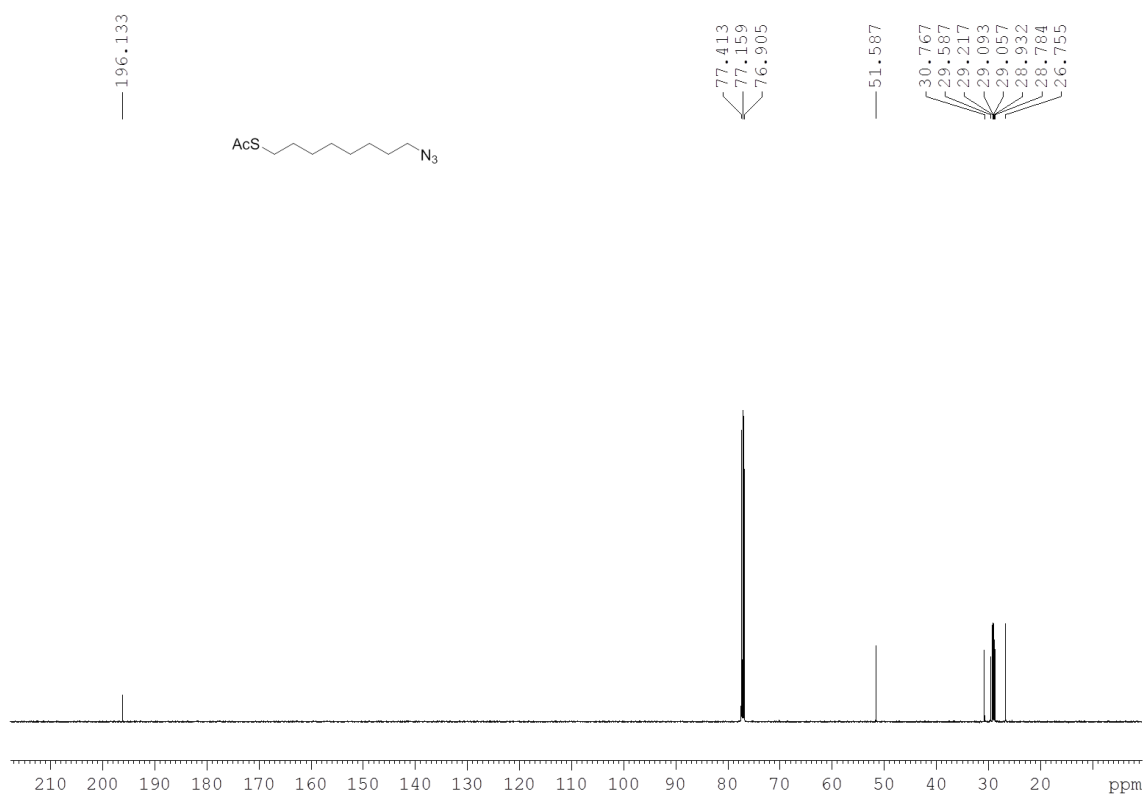


Figure S6. $^{13}\text{C-NMR}$ (500 MHz, CDCl_3) of 8-Azido-octyl-1-thioacetate (**4**)

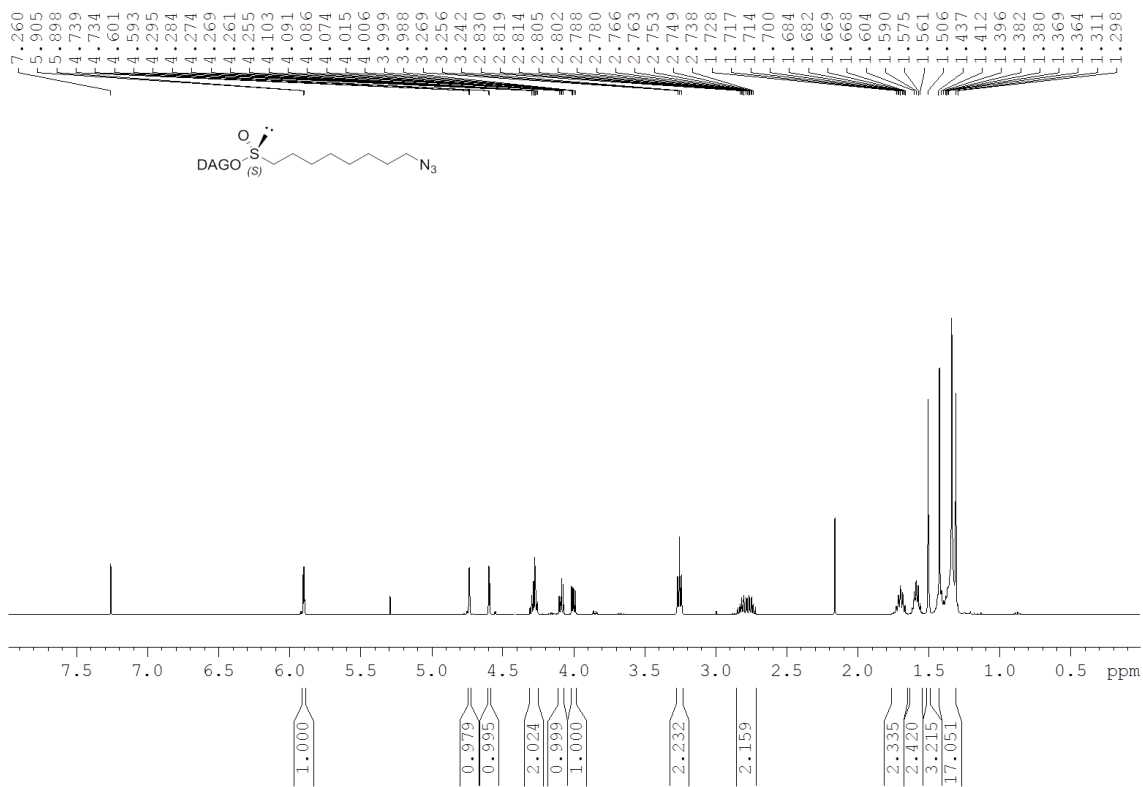


Figure S7. ¹H-NMR (500 MHz, CDCl₃) of (*S*)-(1,2:5,6-Di-*O*-isopropylidene- α -d-glucofuranosyl) 8-azido-octanesulfinate (**6-(S₅)**)

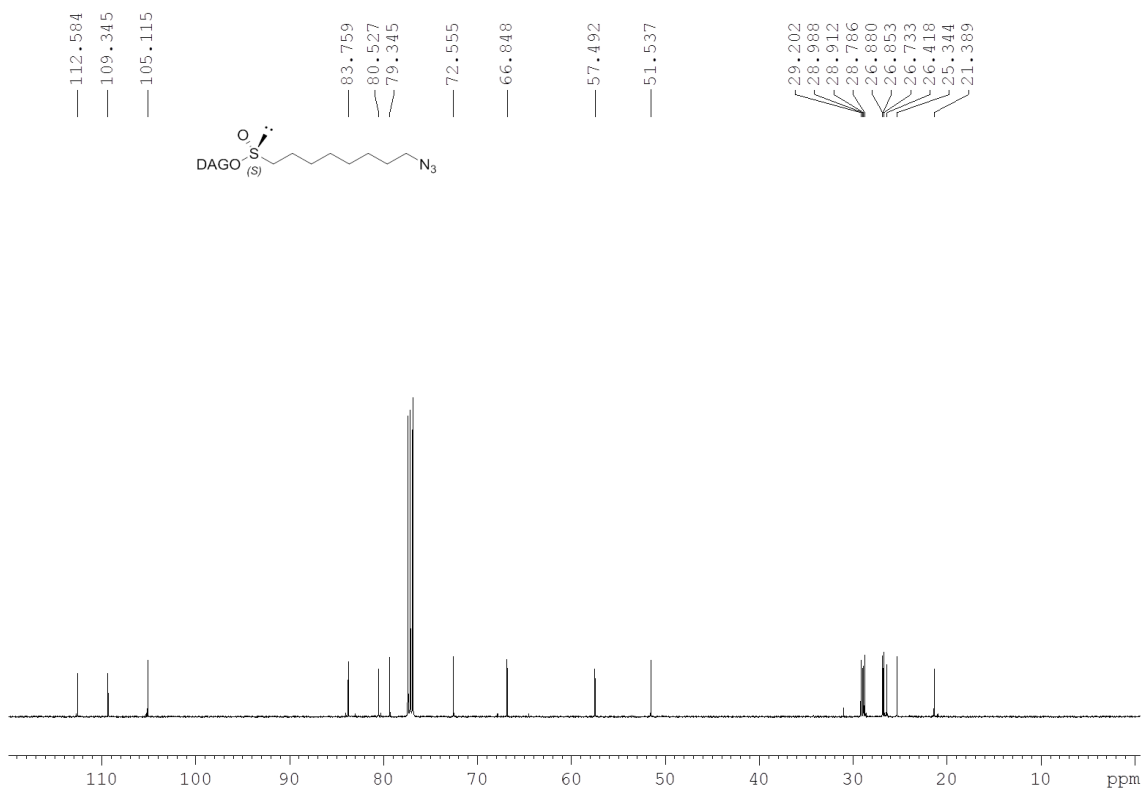


Figure S8. ¹³C-NMR (500 MHz, CDCl₃) of (*S*)-(1,2:5,6-Di-*O*-isopropylidene- α -d-glucofuranosyl) 8-azido-octanesulfinate (**6-(S₅)**)

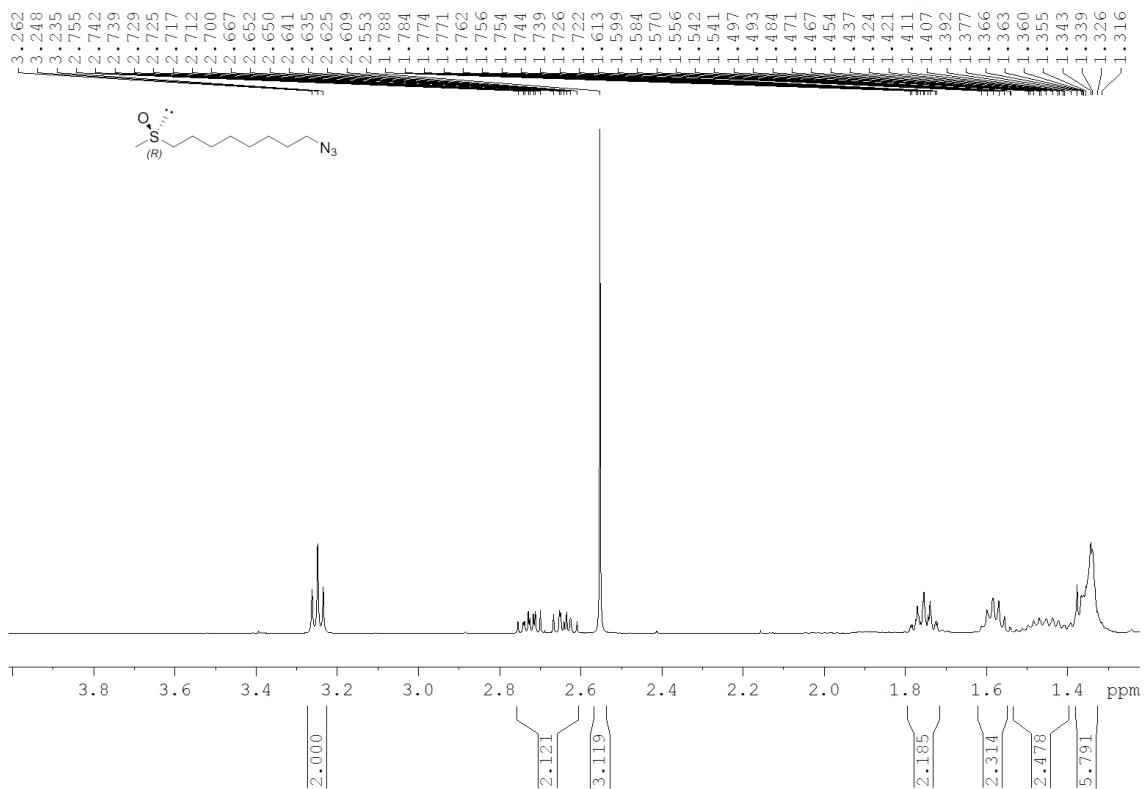


Figure S9. $^1\text{H-NMR}$ (500 MHz, CDCl_3) of (R)-(-)-1-Azido-8-(methylsulfinyl)octane (6-R)

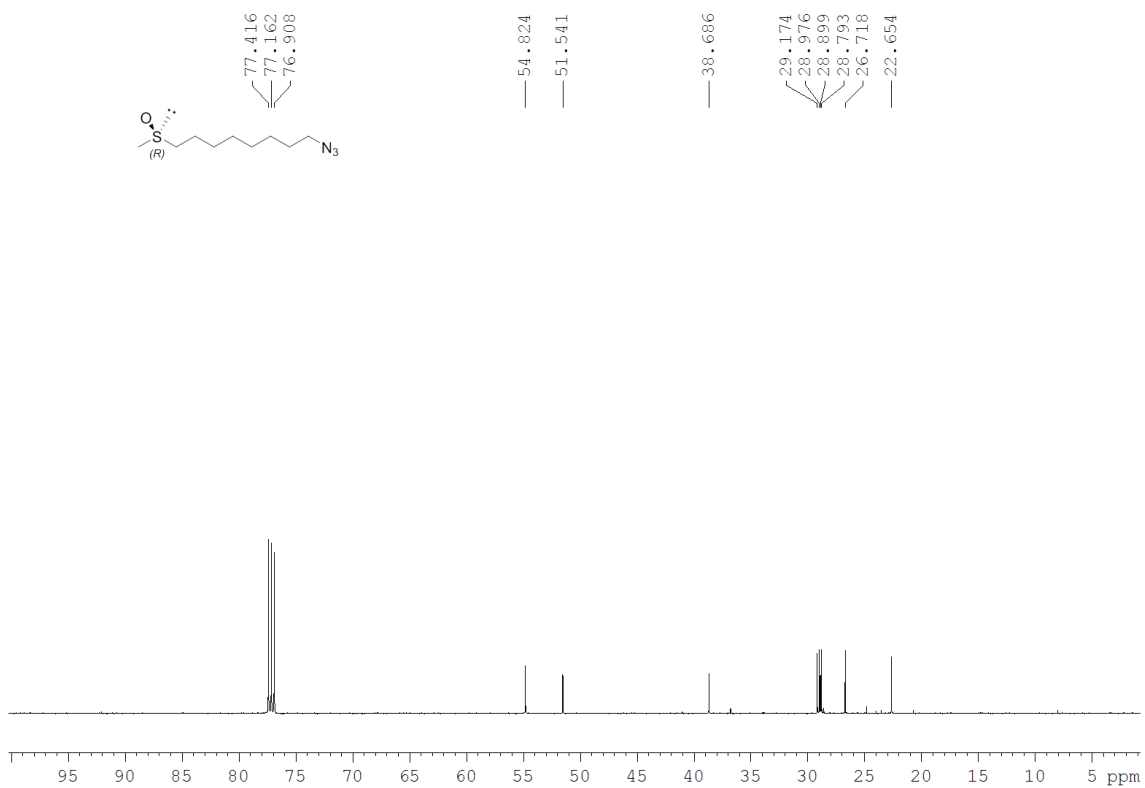


Figure S10. $^{13}\text{C-NMR}$ (500 MHz, CDCl_3) of (R)-(-)-1-Azido-8-(methylsulfinyl)octane (6-R)

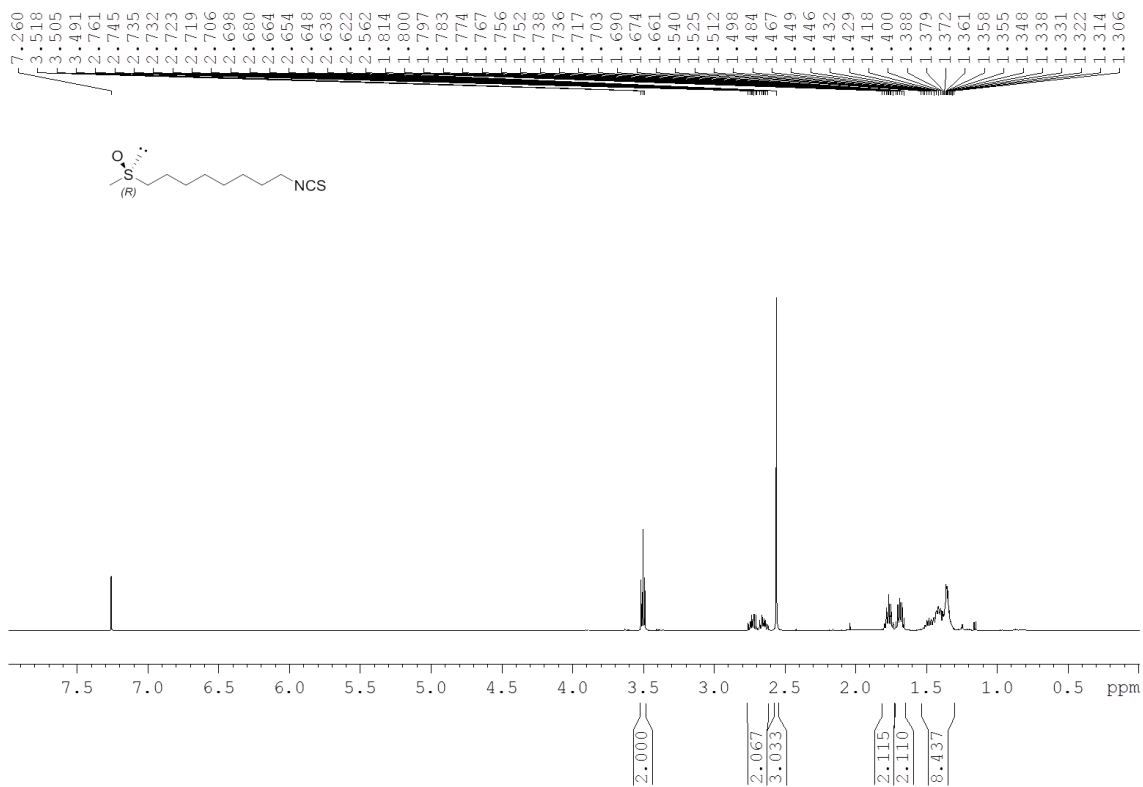


Figure S11. ¹H-NMR (500 MHz, CDCl₃) of *(R)*-(-)-1-Isothiocyanato-8-(methylsulfinyl)octane (*(R)*-8-OITC)

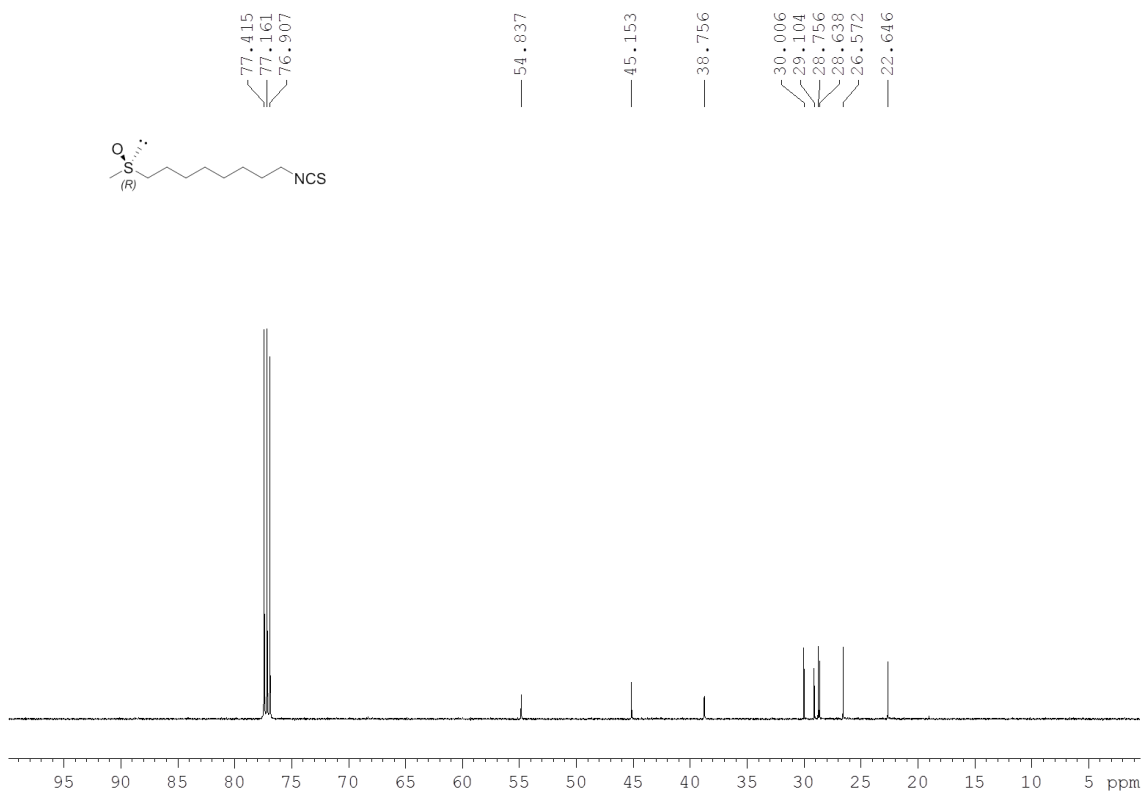
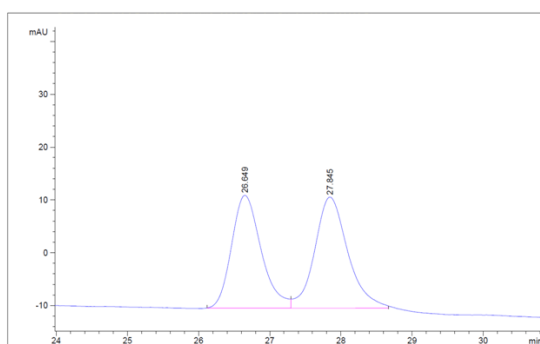


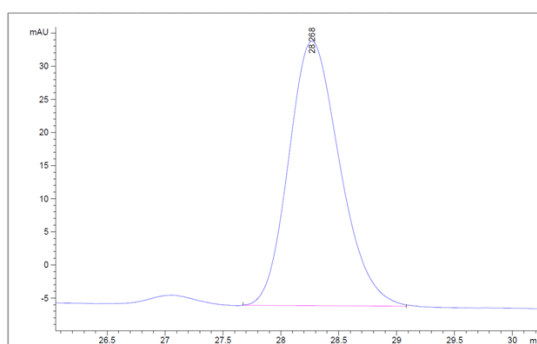
Figure S12. ¹³C-NMR (500 MHz, CDCl₃) of *(R)*-(-)-1-Isothiocyanato-8-(methylsulfinyl)octane (*(R)*-8-OITC)

(rac)-8-OITC



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.649	BV	0.4415	618.08533	21.36637	47.6274
2	27.845	VB	0.4830	679.66620	21.03182	52.3726

(R)-8-OITC



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.269	BB	0.4699	588.19452	19.27943	100.0000

Figure S13. HPLC chromatogram of the racemic form of 8-OITC and its enantiopure form **(R)-8-OITC**