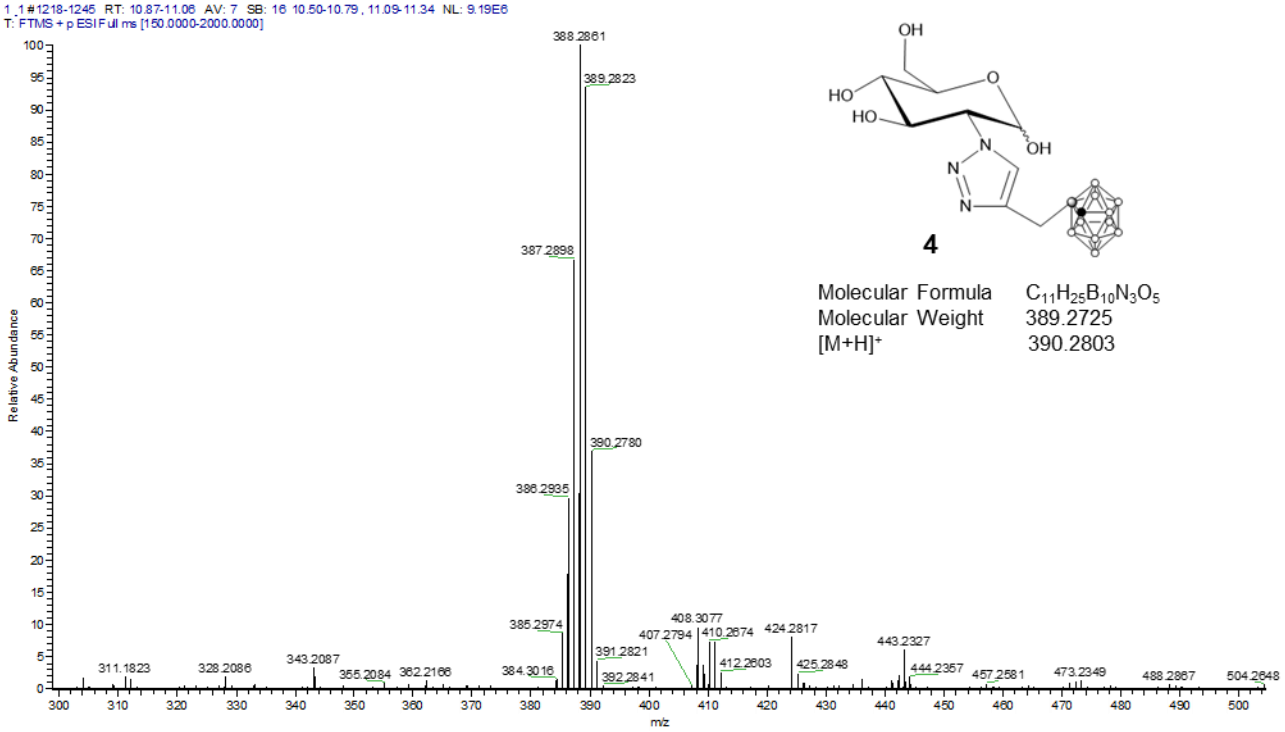
Supporting Information

A Novel *Closo*-*Ortho*-Carborane-Based Glucosamine Derivative as a Promising Agent for Boron Neutron Capture Therapy

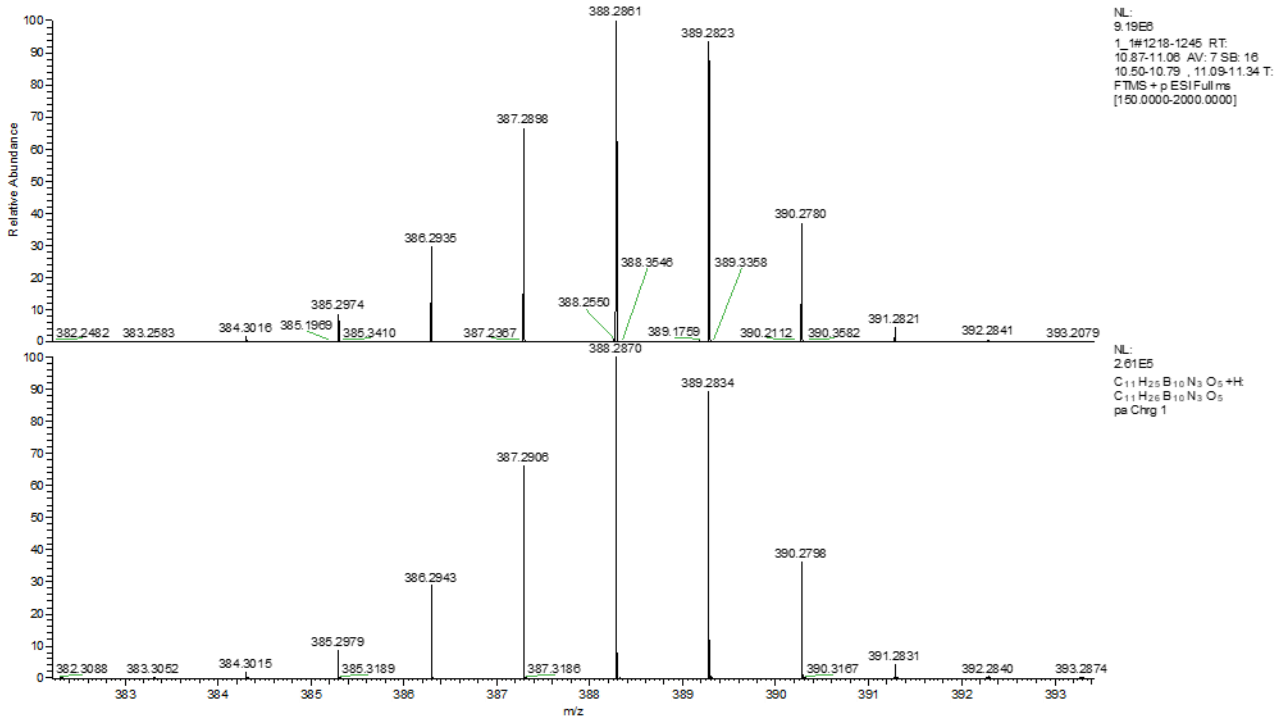
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a)


1_1#1218-1245 RT: 10.87-11.06 AV: 7 SB: 16 10.50-10.79 , 11.09-11.34 NL: 9.19E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]
Relative Abundance
m/z
388.2861
389.2823
387.2898
390.2780
386.2935
385.2974
408.3077
407.2794
410.2674
424.2817
443.2327
391.2821
412.2603
425.2848
444.2357
311.1823
328.2086
343.2087
355.2084
362.2166
384.3016
392.2841
457.2581
473.2349
488.2867
504.2648
OH
HO
HO
O
OH
N
N
N
4
Molecular Formula C11H25B10N3O5
Molecular Weight 389.2725
[M+H]+ 390.2803

b)


Relative Abundance
m/z
NL:
9.19E6
1_1#1218-1245 RT:
10.87-11.06 AV: 7 SB: 16
10.50-10.79 , 11.09-11.34 T:
FTMS + p ESI Full ms
[150.0000-2000.0000]
388.2861
389.2823
387.2898
390.2780
386.2935
388.3546
389.3358
385.2974
388.2550
382.2482
383.2583
384.3016
385.1969
385.3410
387.2367
389.1759
390.2112
390.3582
391.2821
392.2841
393.2079
NL:
2.61E5
C11H25B10N3O5+H
C11H26B10N3O5
pa Chrg 1
388.2870
389.2834
387.2906
390.2798
386.2943
385.2979
382.3088
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384.3015
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390.3167
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392.2840
393.2874

c)

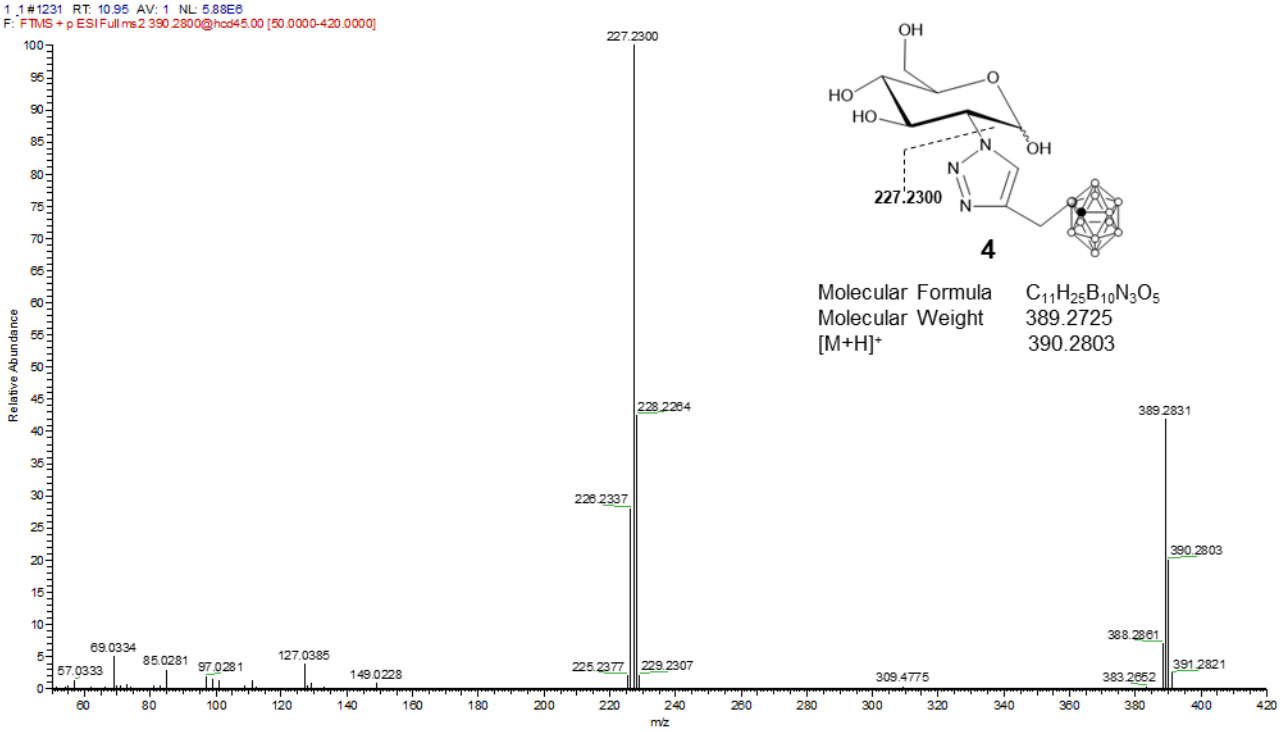


Figure S1. **a)** Full-MS(+), **b)**MS^2 Spectra of **4** and **c)** comparison with calculated mass distribution of the isotopic cluster. To capture the complete isotopic pattern, an isolation window of ±4 m/z was applied, centring on the precursor ion at *m/z* 390.2803. This setting accounts for the natural isotopic distribution of carbon and boron in compound **4**. The base peak observed is the product ion at *m/z* 227.2300, which arises from cleavage of

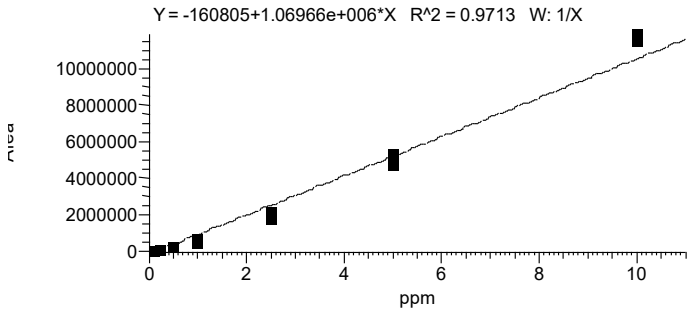


Figure S2. Compound **4** calibration curve in neat H_2O:ACN (7:3, v/v) solvent, ranging from 0.250 to 10 ppm. The LLOD was 0.100 ppm, with no detection at lower concentrations. The coefficient of determination (R^2) was 0.9713.

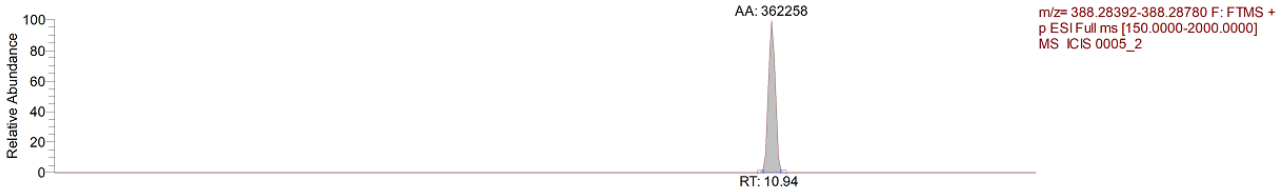


Figure S3. Extracted ion chromatogram (EIC) of compound 4 at 5 ppm, obtained from Full-MS(+) acquisition. The EIC was generated by extracting the base peak at m/z 388.2862 within a 5 ppm mass tolerance.

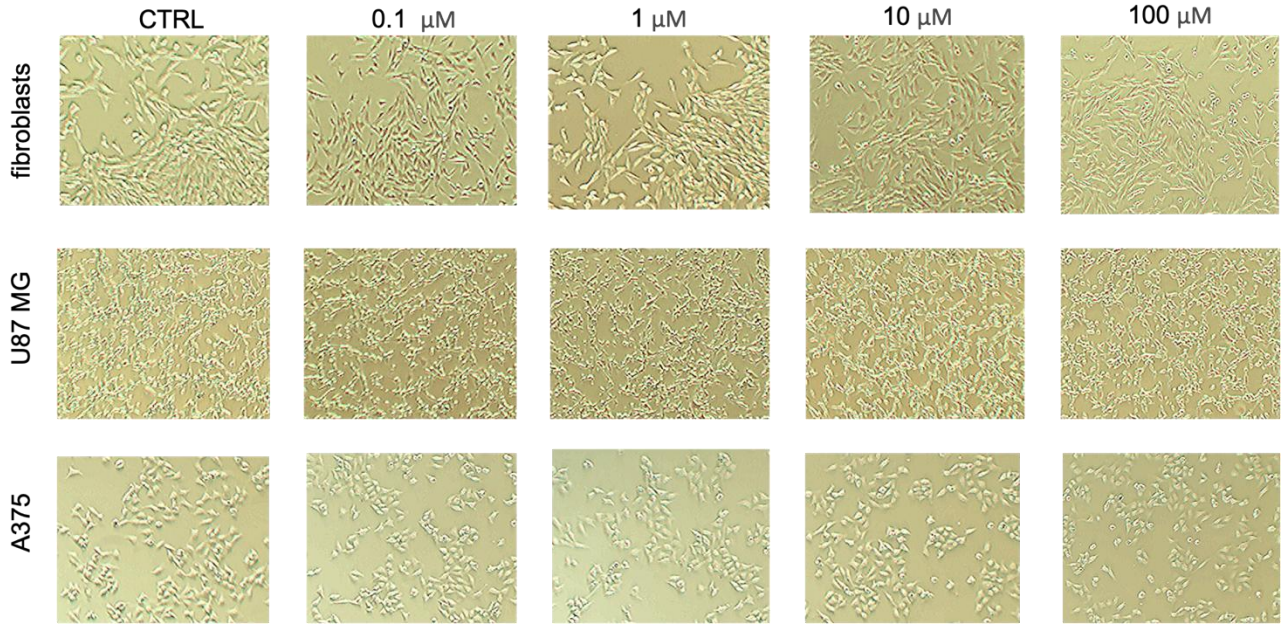


Figure S4. Cell morphology of human fibroblasts, U87 MG glioblastoma, and A375 melanoma cell lines after compound **4** treatment. Bright field Images were taken after 72h of treatment with increasing concentrations of compound **4** with an inverted microscope using a 4X objective. Only images of non-toxic concentration are taken to observe the cell morphology of cell treated/untreated with compound **4**.

Figure S5: NMR ^{1}H spectrum of compound **4** (400 MHz, CD_3OD anomeric α,β mixture)

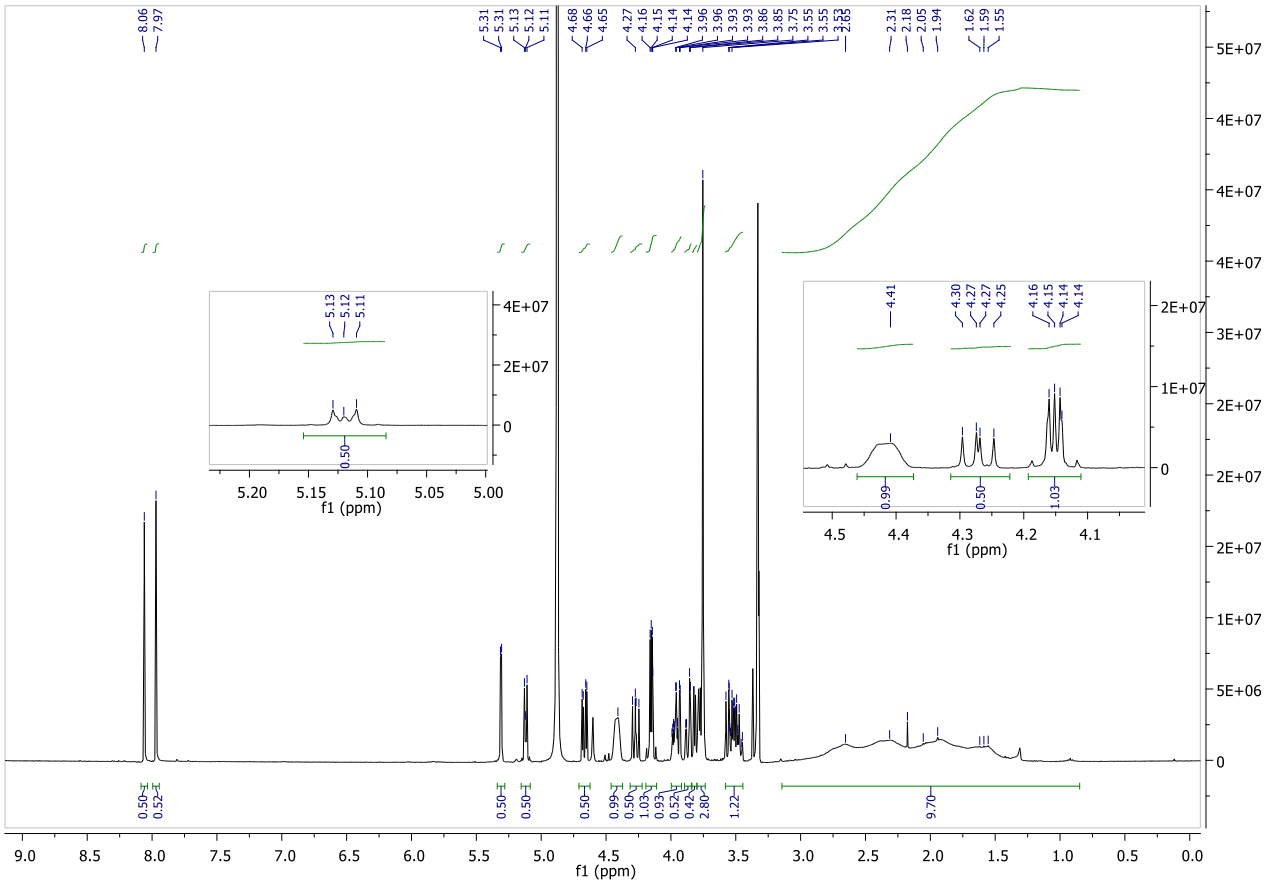


Figure S6: NMR ^{13}C spectrum of compound **4** (101 MHz, CD_3OD)

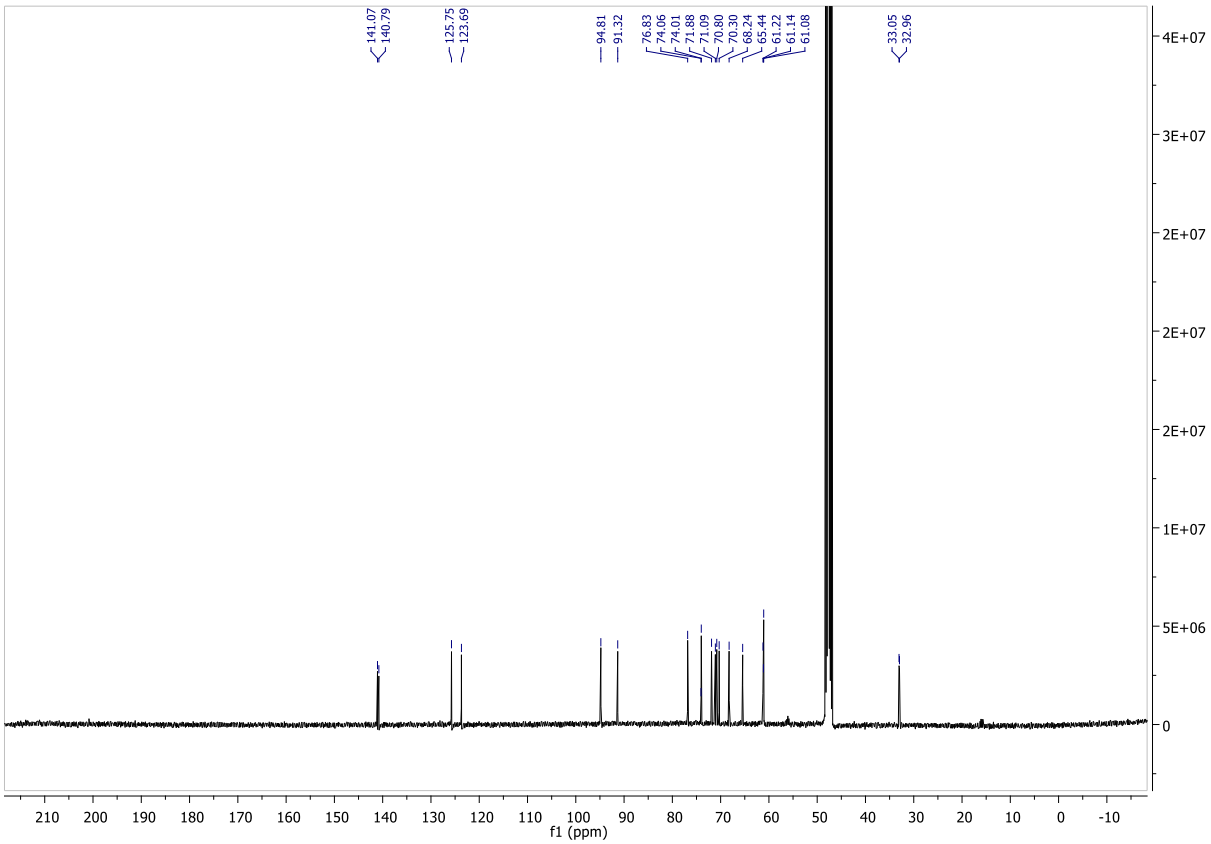


Figure S7: NMR ^{11}B spectrum of compound **4** (128 MHz, CD_3OD)

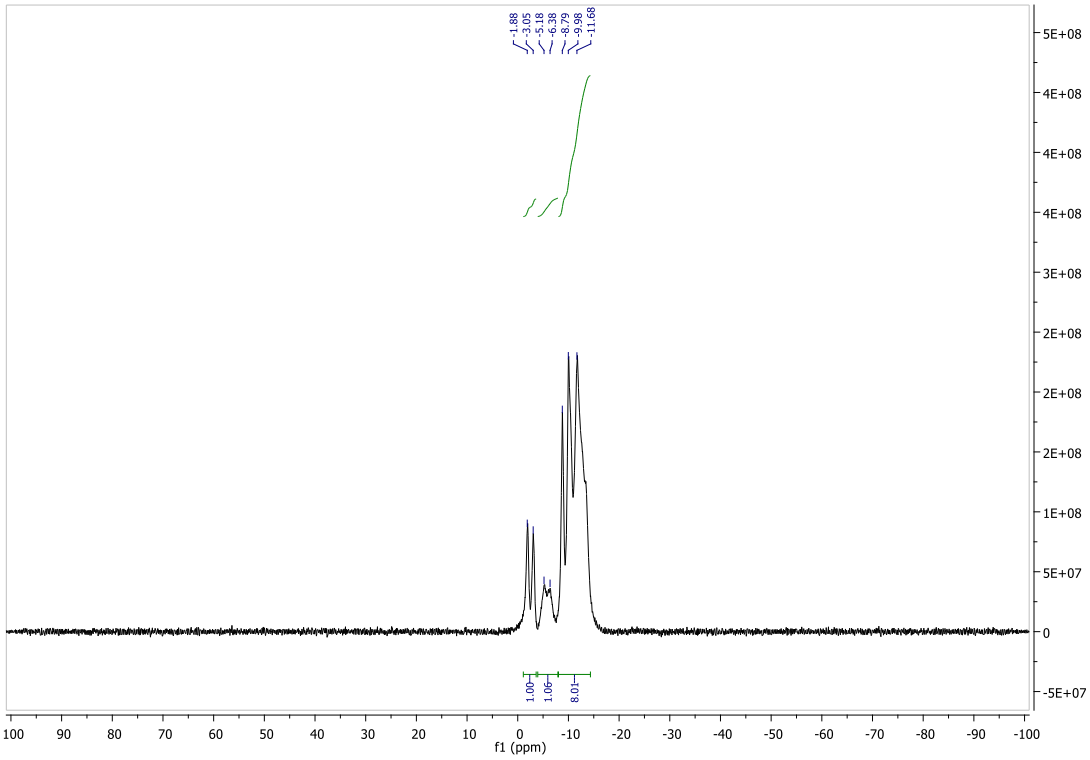


Figure S8: NMR ^{11}B decoupling spectrum of compound **4** (128 MHz, CD_3OD)

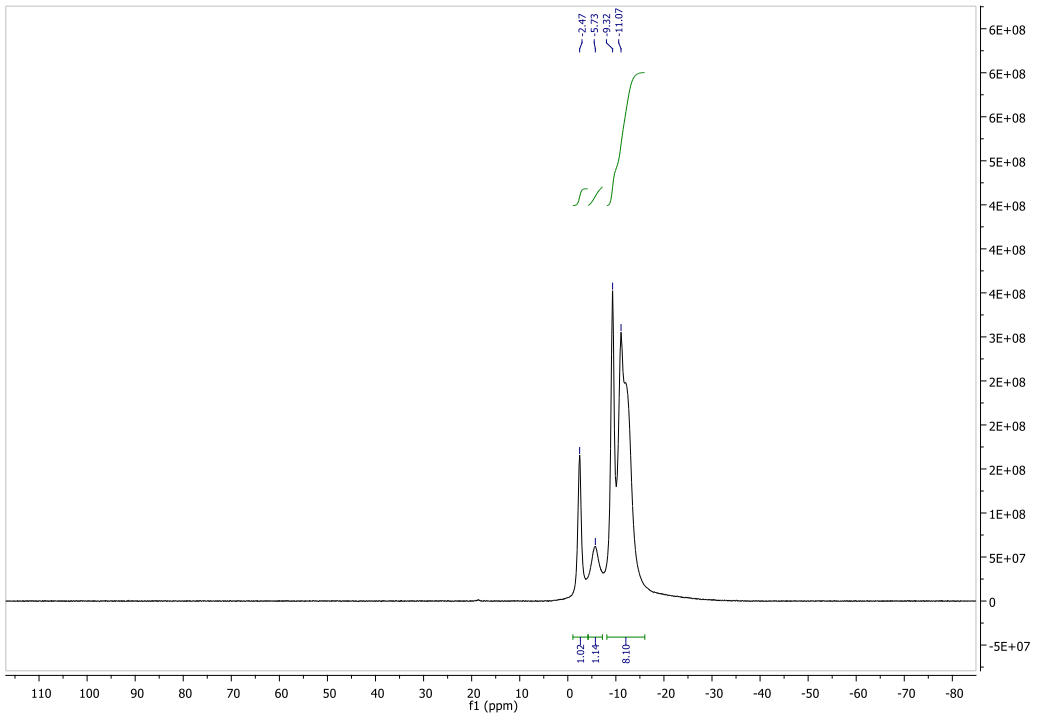


Figure S9: NMR COSY spectrum of compound **4**

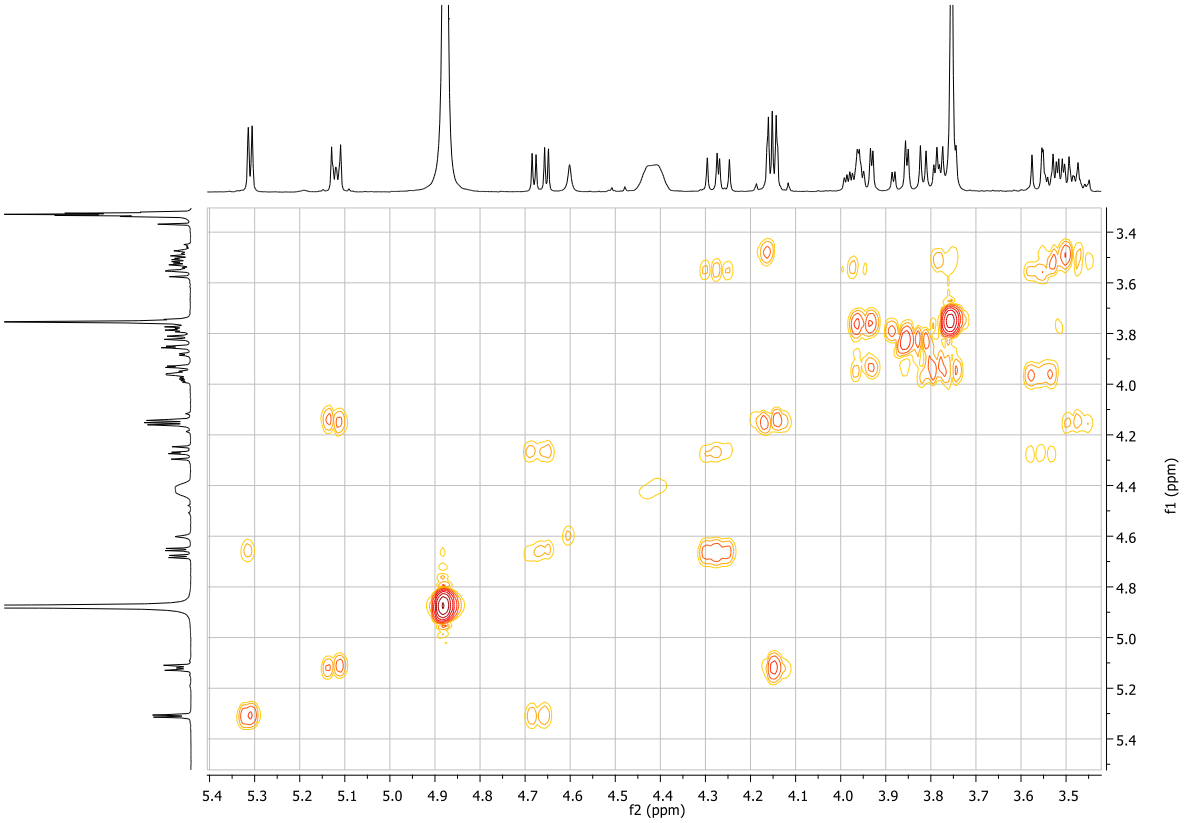


Figure S10: NMR HSQC spectrum of compound **4**

