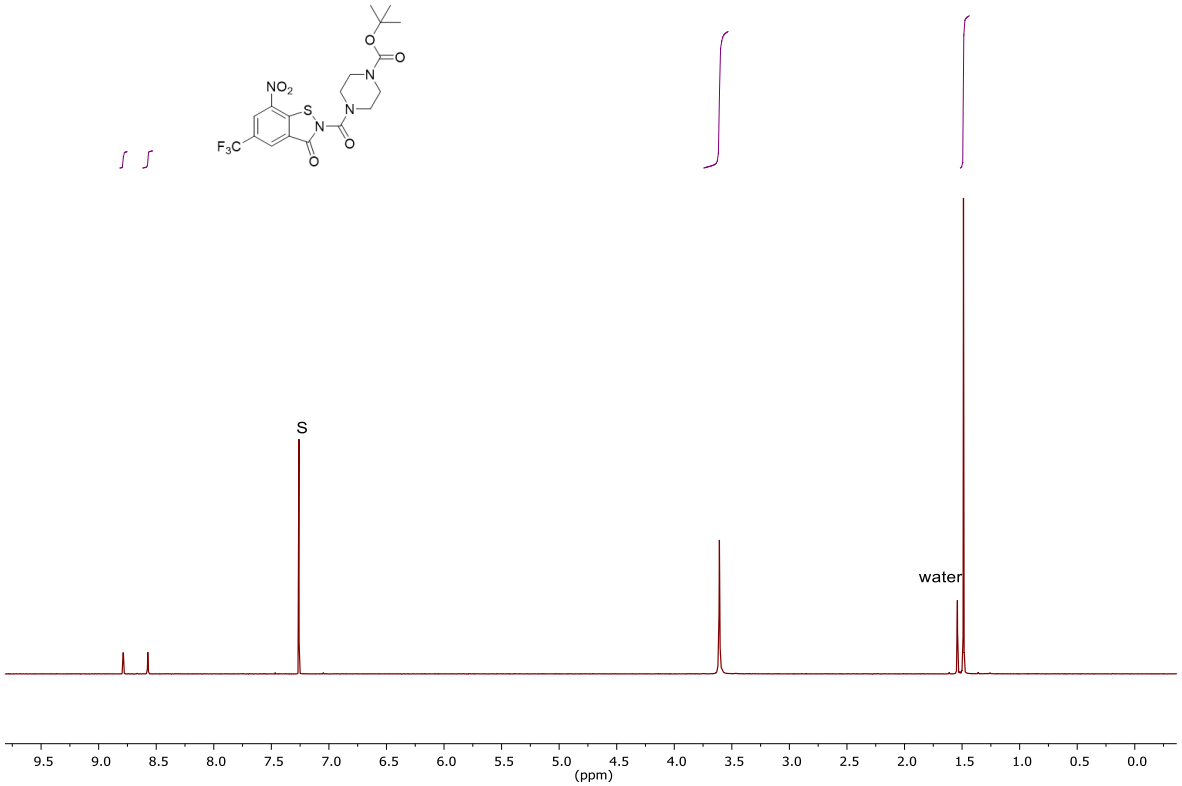


Figure S1 ^{1}H NMR spectrum of 2-(4-Boc-piperazine-1-carbonyl)-7-nitro-5-(trifluoromethyl)-benzo[*d*]isothiazol-3(2*H*)-one in chloroform-*d*. S denotes the residual solvent signal.

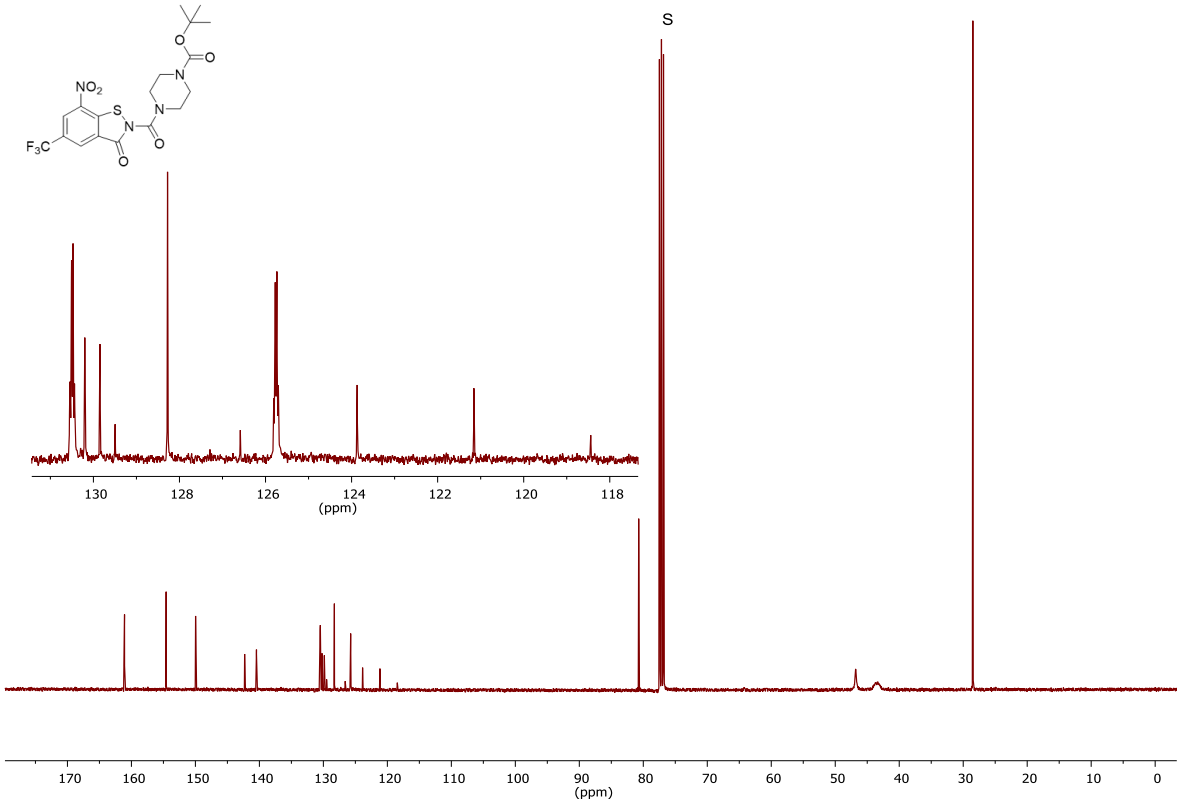


Figure S2 ^{13}C NMR spectrum of 2-(4-Boc-piperazine-1-carbonyl)-7-nitro-5-(trifluoromethyl)-benzo[*d*]isothiazol-3(2*H*)-one in chloroform-*d*. S denotes the residual solvent signal.

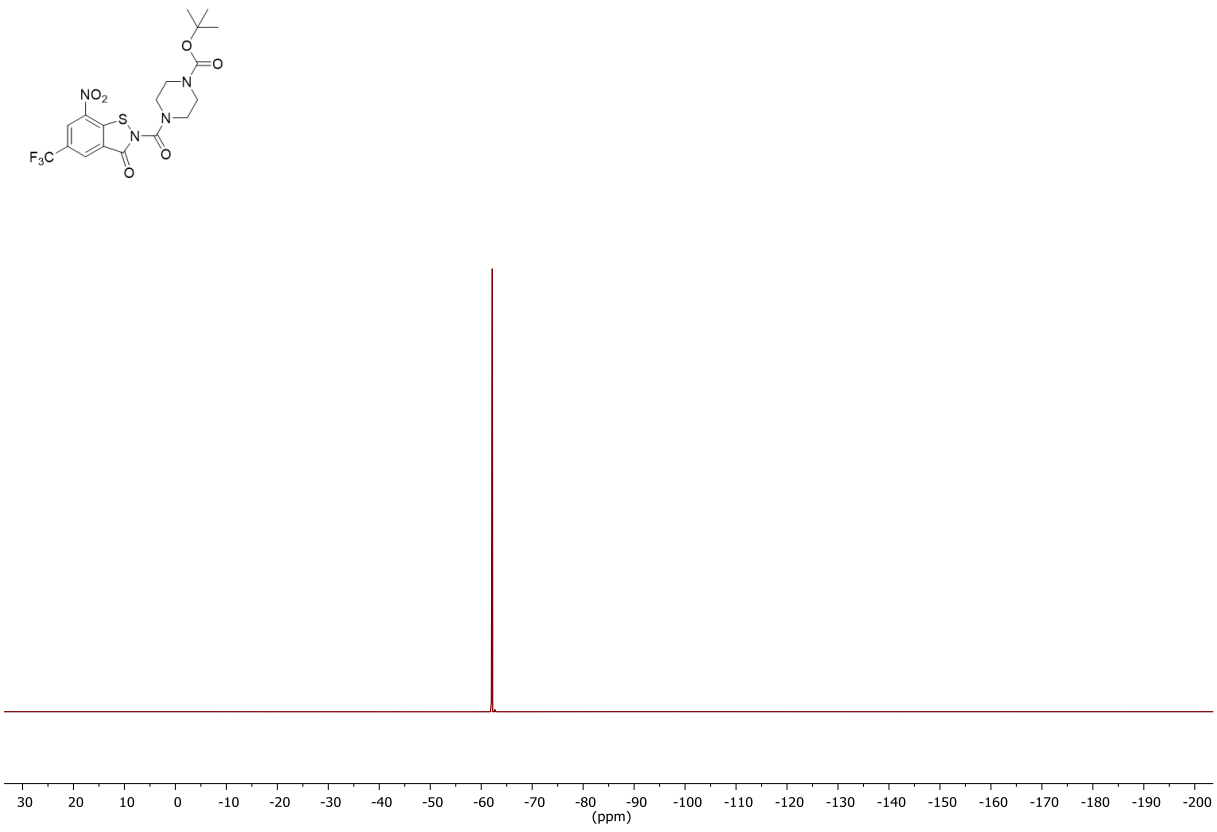


Figure S3 ^{19}F NMR spectrum of 2-(4-Boc-piperazine-1-carbonyl)-7-nitro-5-(trifluoromethyl)-benzo[*d*]isothiazol-3(2*H*)-one in chloroform-*d*.

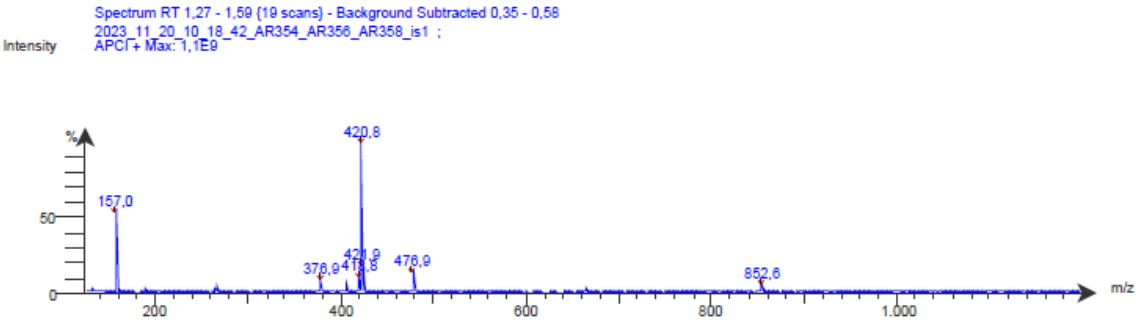


Figure S4 APCI$^+$ mass spectrum of 2-(4-Boc-piperazine-1-carbonyl)-7-nitro-5-(trifluoro-methyl)benzo[*d*]isothiazol-3(2*H*)-one.

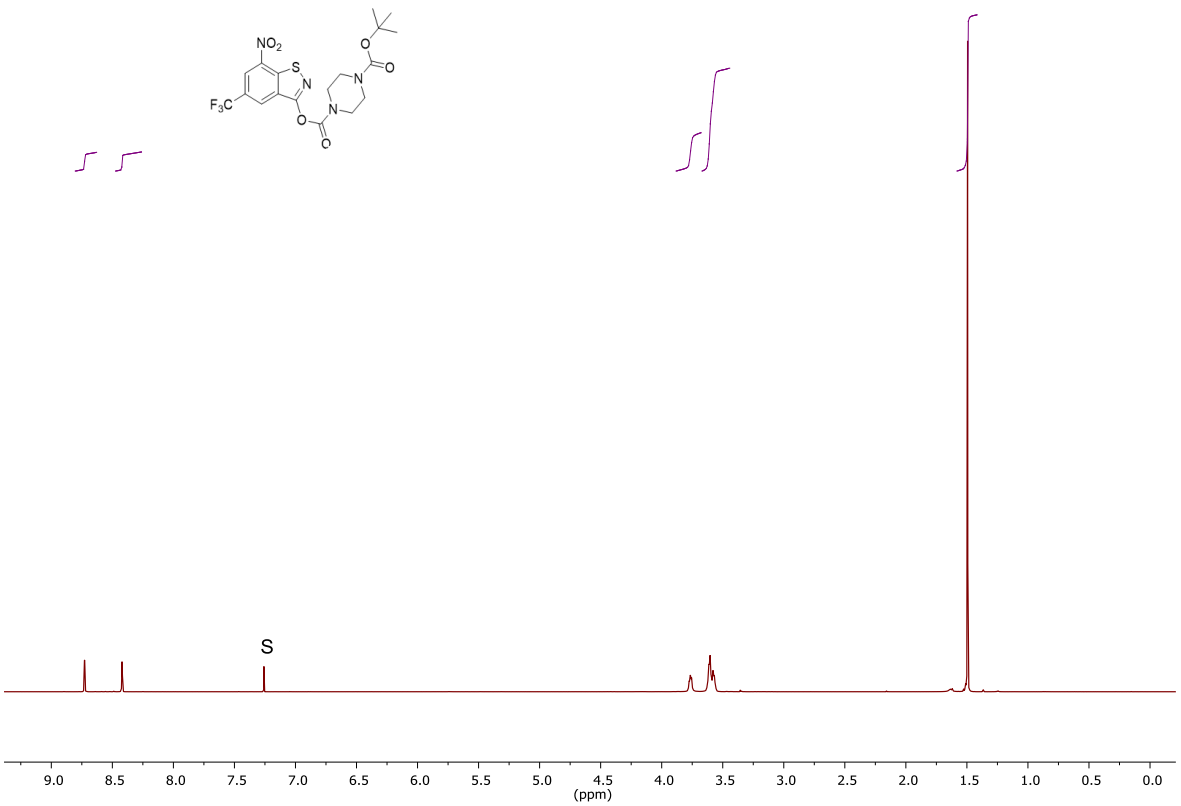


Figure S5 ^{1}H NMR spectrum of 7-nitro-5-(trifluoromethyl)benzo[*d*]isothiazol-3-yl 4-Boc-piperazine-1-carboxylate in chloroform-*d*. S denotes the residual solvent signal.

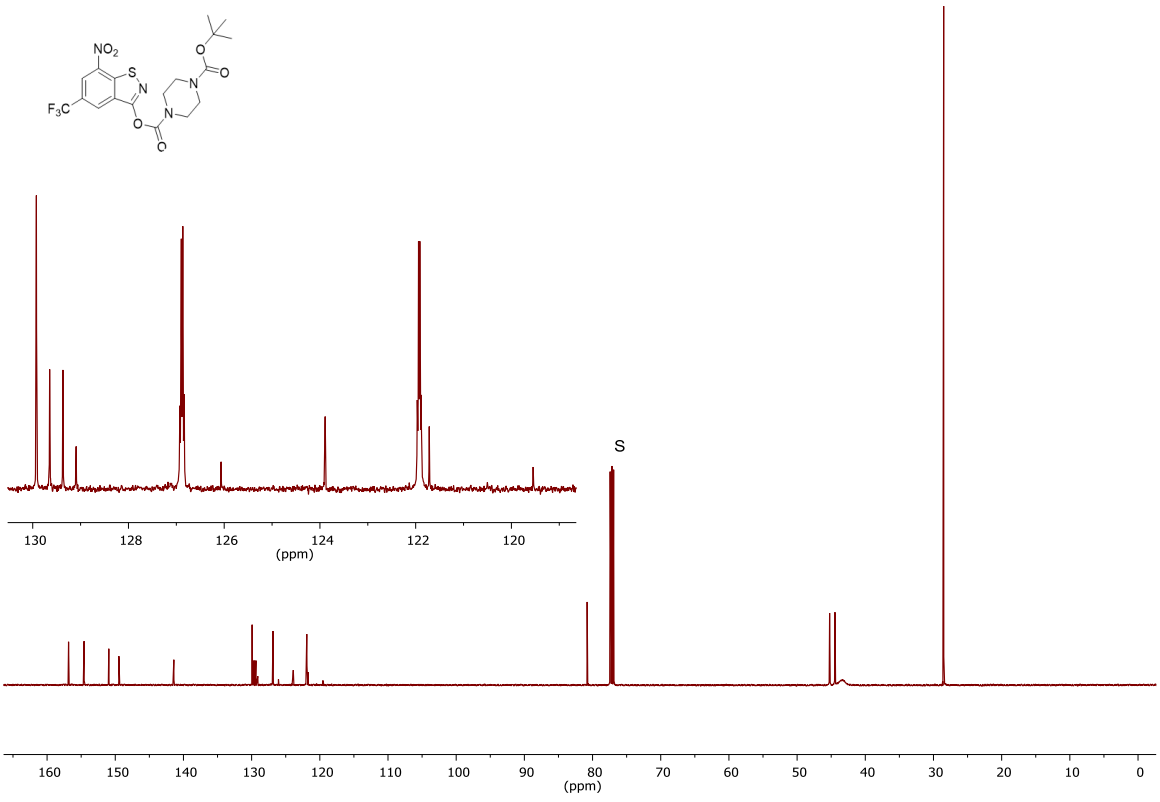


Figure S6 ^{13}C NMR spectrum of 7-nitro-5-(trifluoromethyl)benzo[*d*]isothiazol-3-yl 4-Boc-piperazine-1-carboxylate in chloroform-*d*. S denotes the residual solvent signal.

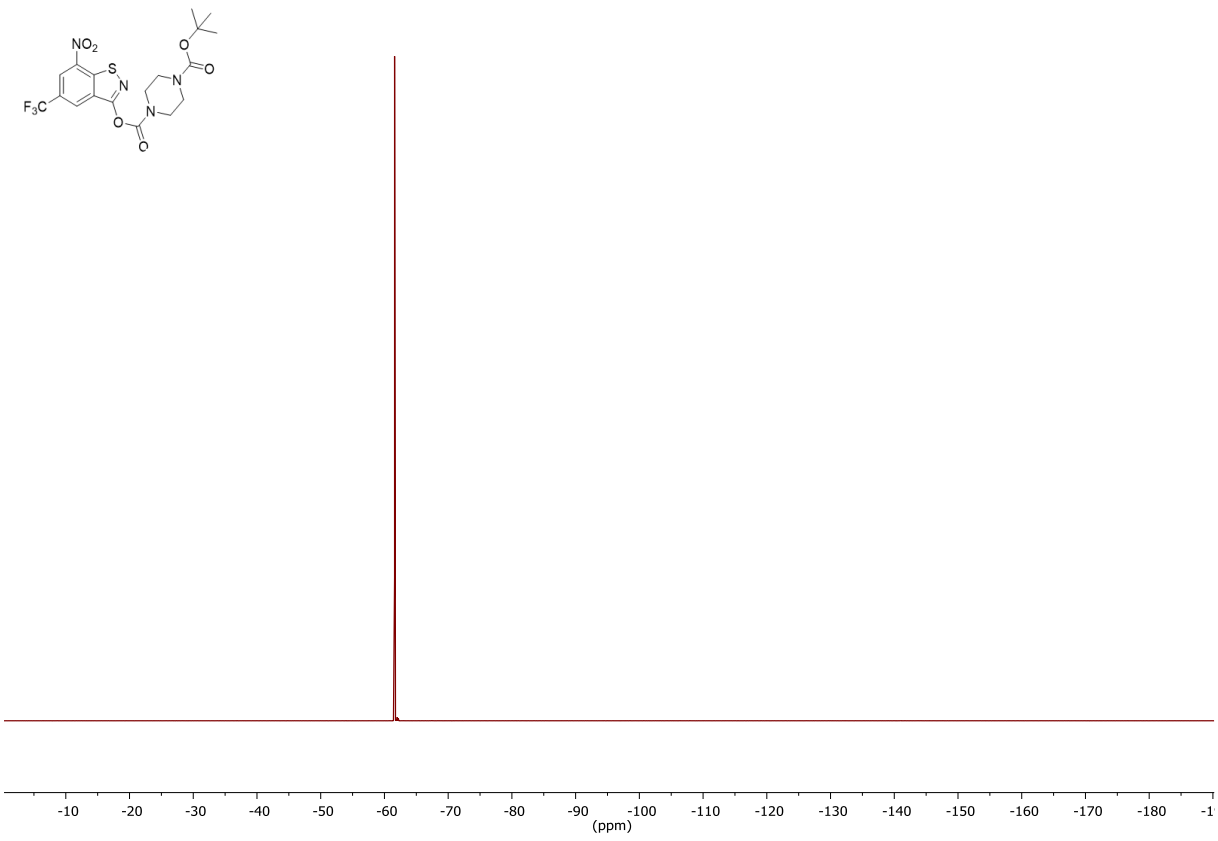


Figure S7 ^{19}F NMR spectrum of 7-nitro-5-(trifluoromethyl)benzo[*d*]isothiazol-3-yl 4-Boc-piperazine-1-carboxylate in chloroform-*d*.

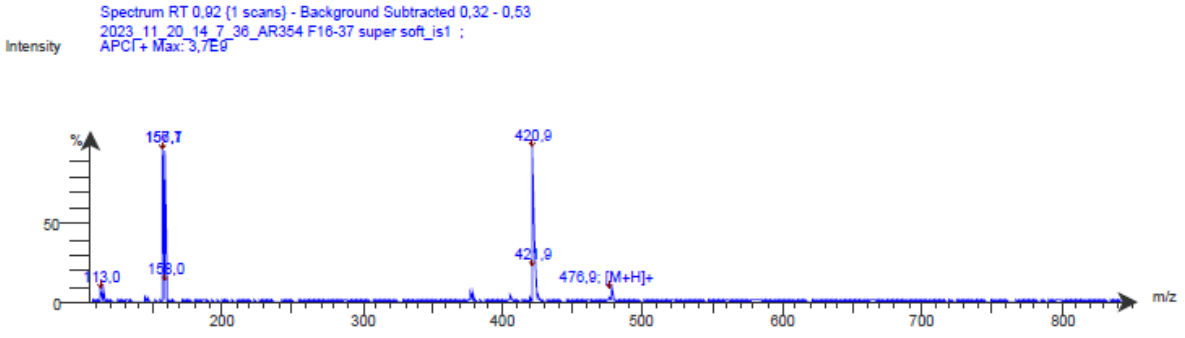


Figure S8 APCI$^+$ mass spectrum of 7-nitro-5-(trifluoromethyl)benzo[*d*]isothiazol-3-yl 4-Boc-piperazine-1-carboxylate.

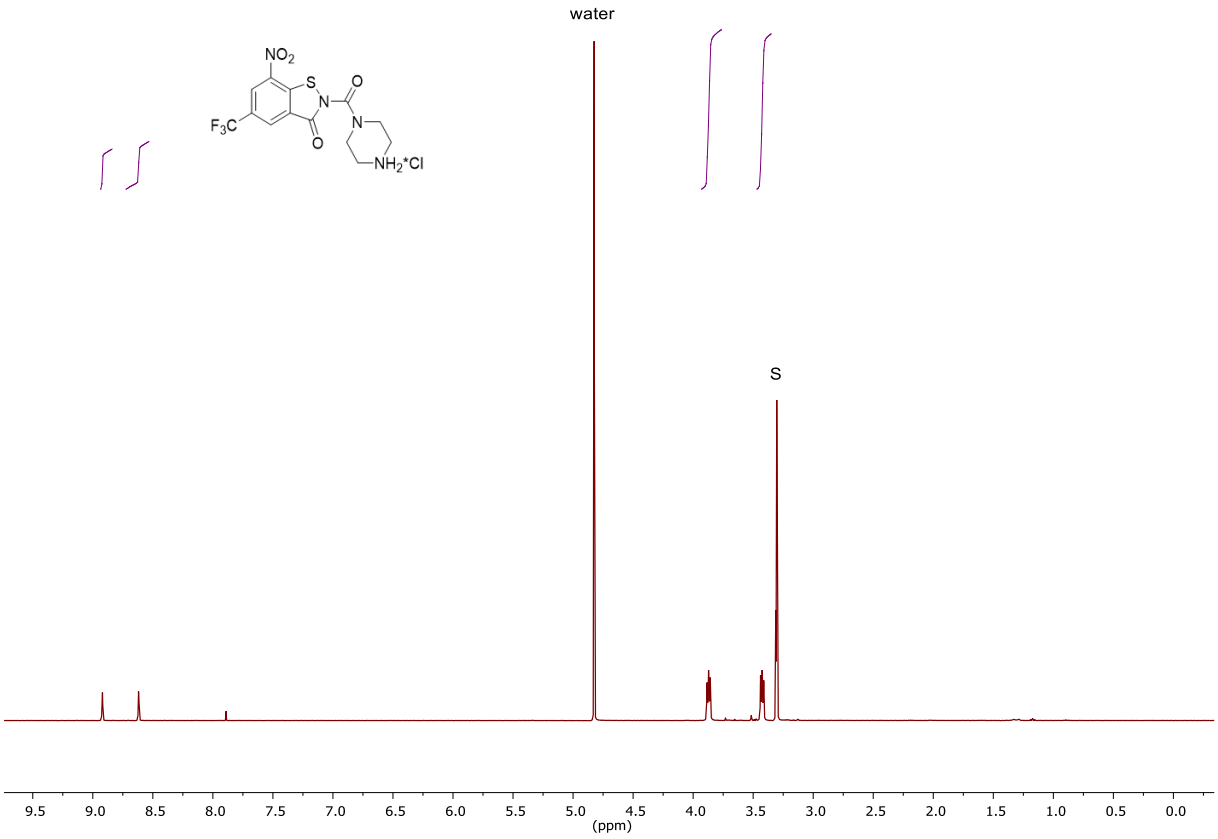


Figure S9 ^{1}H NMR spectrum of 4-(7-nitro-3-oxo-5-(trifluoromethyl)-2,3-dihydrobenzo[*d*]-isothiazole-2-carbonyl)piperazin-1-ium chloride (**2**) in methanol-d_4. S denotes the residual solvent signal.

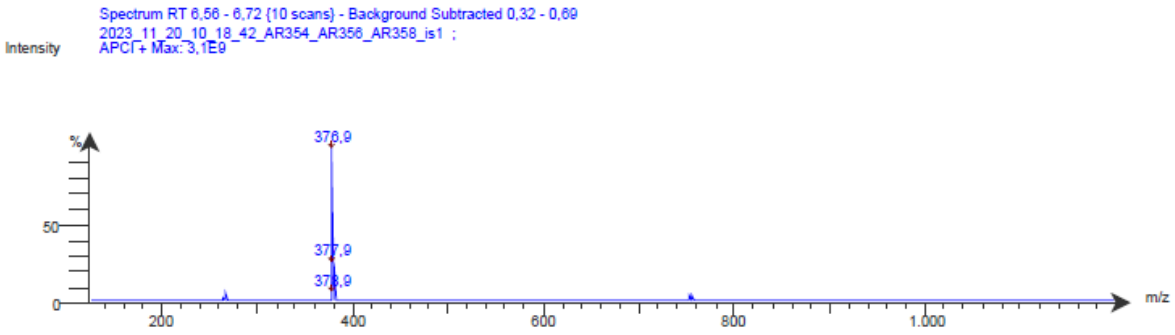


Figure S10 APCI^{+} mass spectrum of 4-(7-nitro-3-oxo-5-(trifluoromethyl)-2,3-dihydro-benzo[*d*]-isothiazole-2-carbonyl)piperazin-1-ium chloride (**2**).

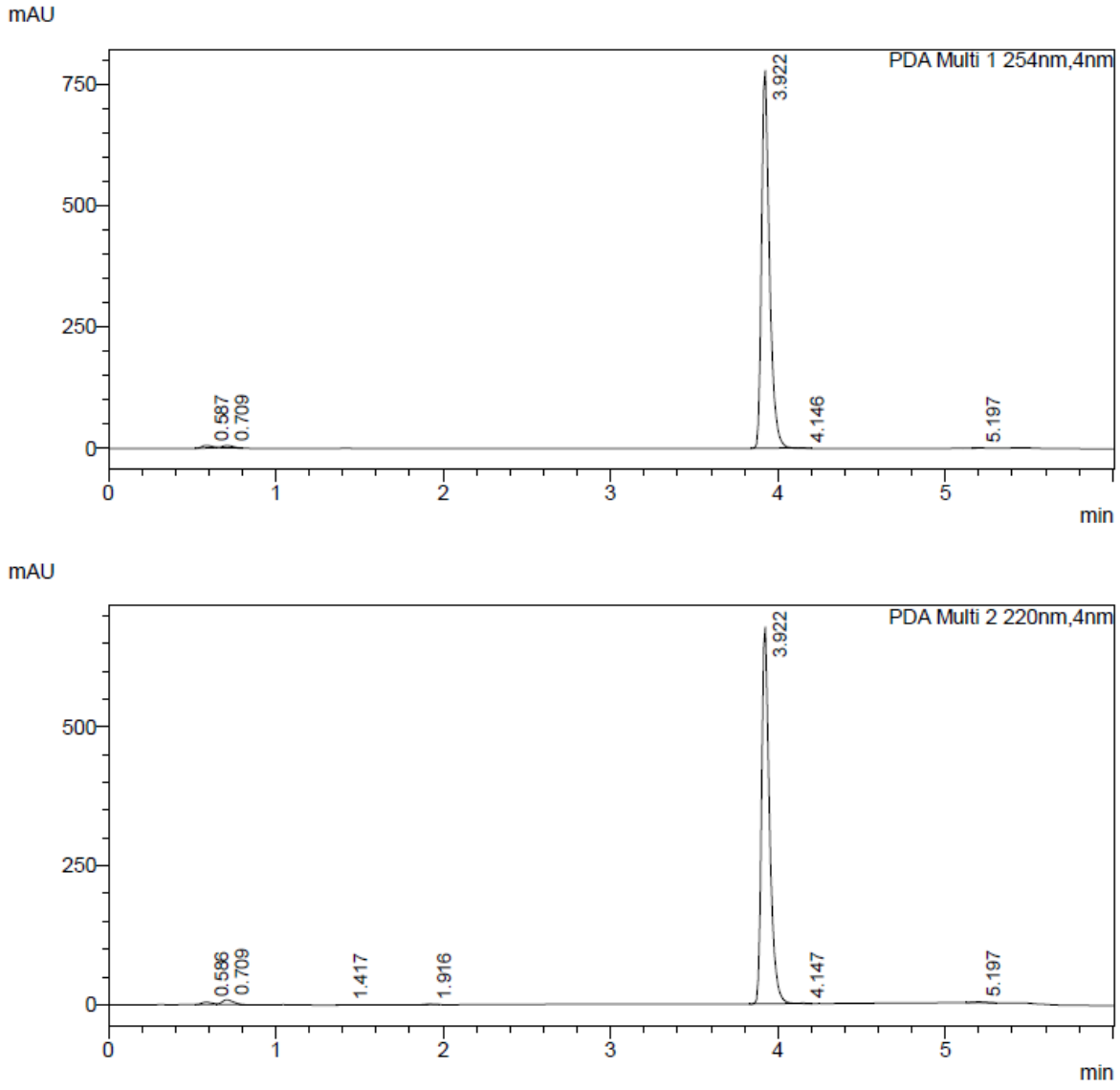


Figure S11 HPLC traces of 2-(cyclohexylmethyl)-7-nitro-5-(trifluoromethyl)benzo[*d*]-isothiazol-3(2*H*)-one (**4**) at 254 nm (top) and 220 nm (bottom).

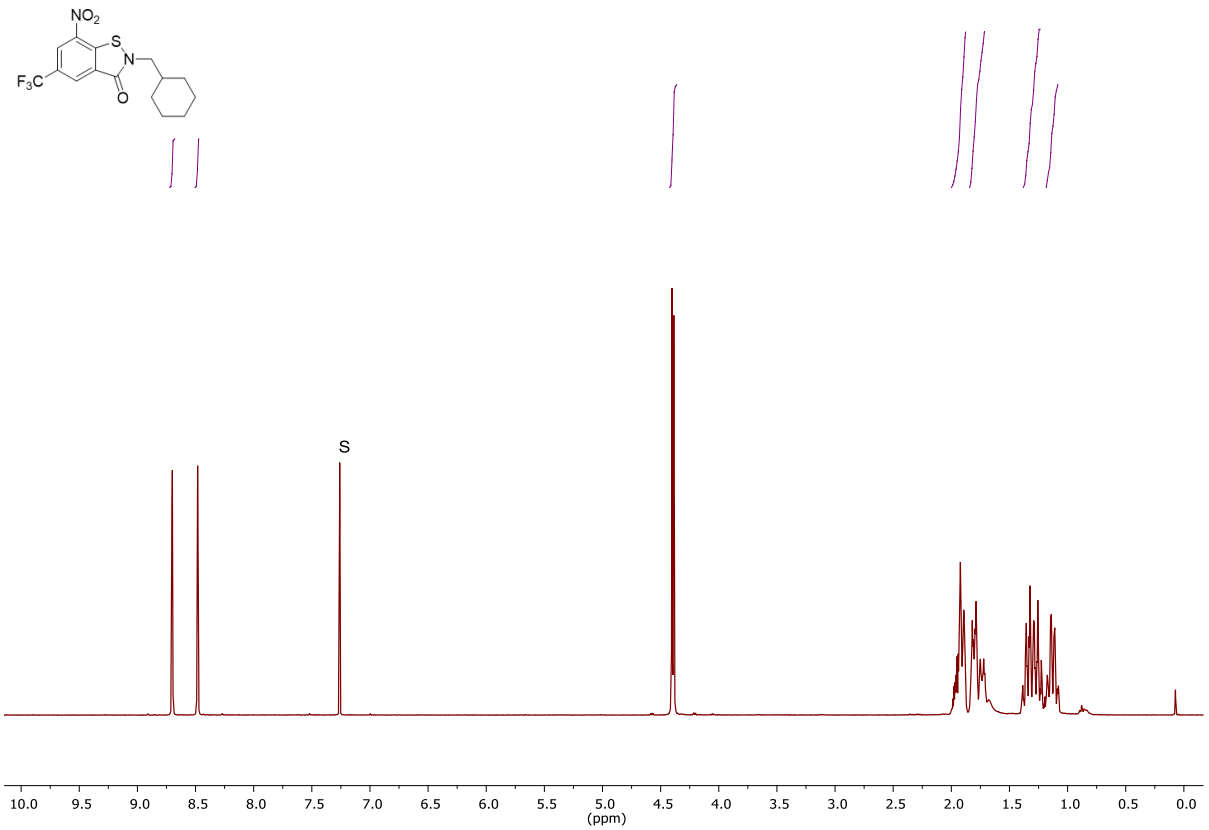


Figure S12 ^{1}H NMR spectrum of 2-(cyclohexylmethyl)-7-nitro-5-(trifluoromethyl)benzo[*d*]-isothiazol-3(2*H*)-one (**4**) in chloroform-*d*. S denotes the residual solvent signal.

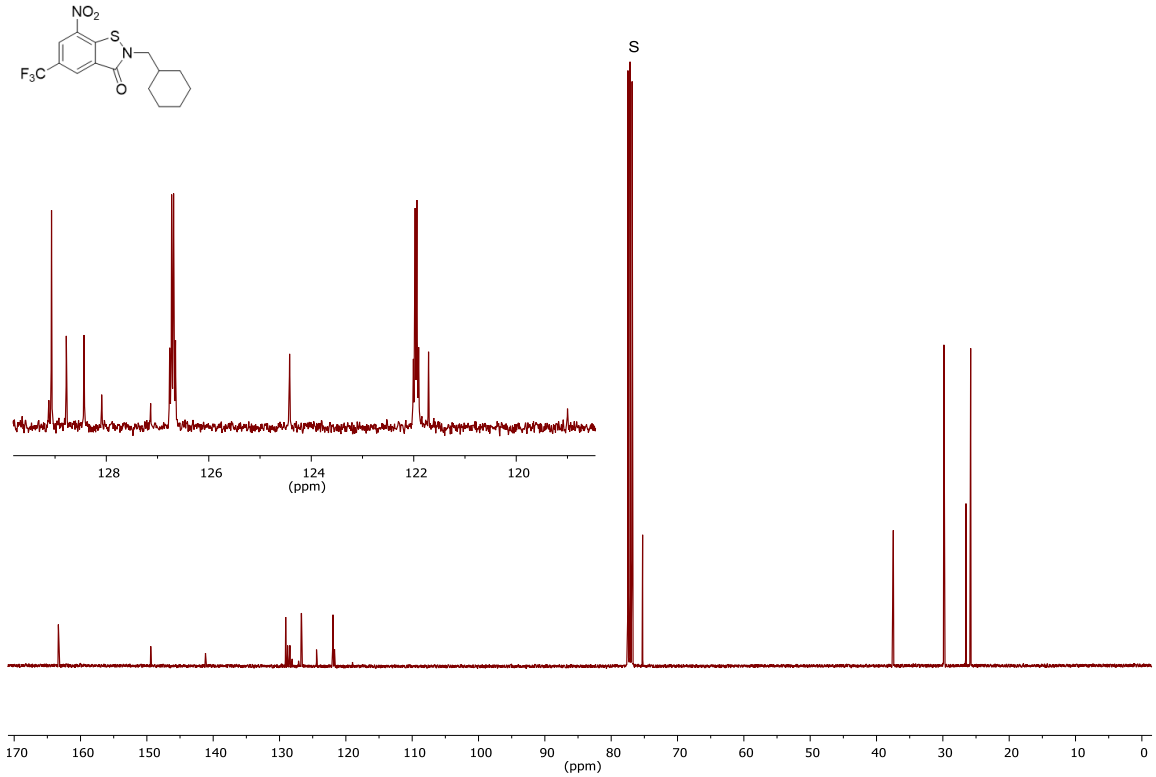
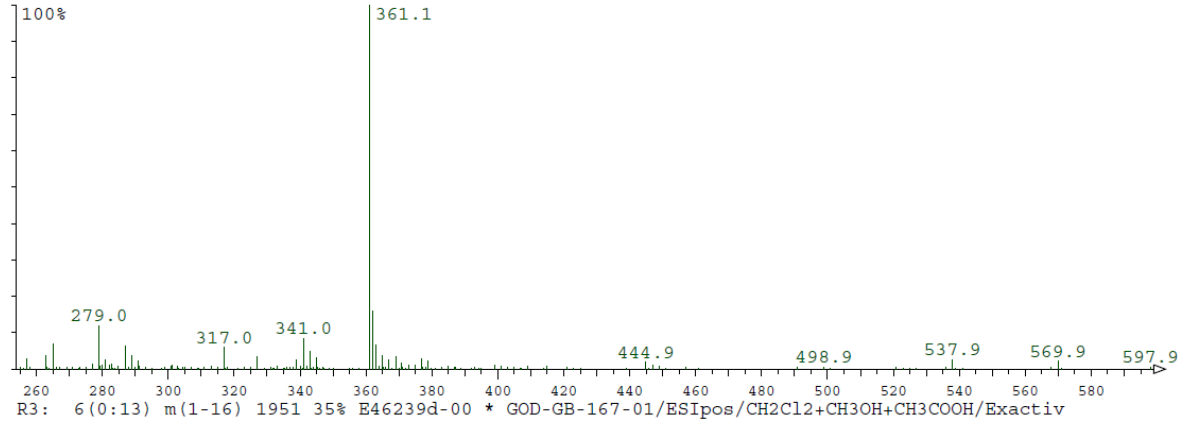


Figure S13 ^{13}C NMR spectrum of 2-(cyclohexylmethyl)-7-nitro-5-(trifluoromethyl)benzo[*d*]-isothiazol-3(2*H*)-one (**4**) in chloroform-*d*. S denotes the residual solvent signal.

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Mass tolerance: ±0.002
restriction of atom numbers:
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   1-100   1-100     0-2    0-10     0-3     1-1
Number of calculated formulas: 4
Formula             Diff. (ppm)  theor. m/z
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C15 H16 F3 N2 O3 S1        0.50   361.08282  <-
C18 H15 F2 N2 O2 S1       -2.66   361.08168
C11 H20 F1 N1 O9 S1        3.02   361.08373
```

Figure S14 High resolution ESI$^+$ mass spectrum of 2-(cyclohexylmethyl)-7-nitro-5-(trifluoromethyl)benzo[*d*]-isothiazol-3(2*H*)-one (**4**) in dichloromethane/methanol/acetic acid.

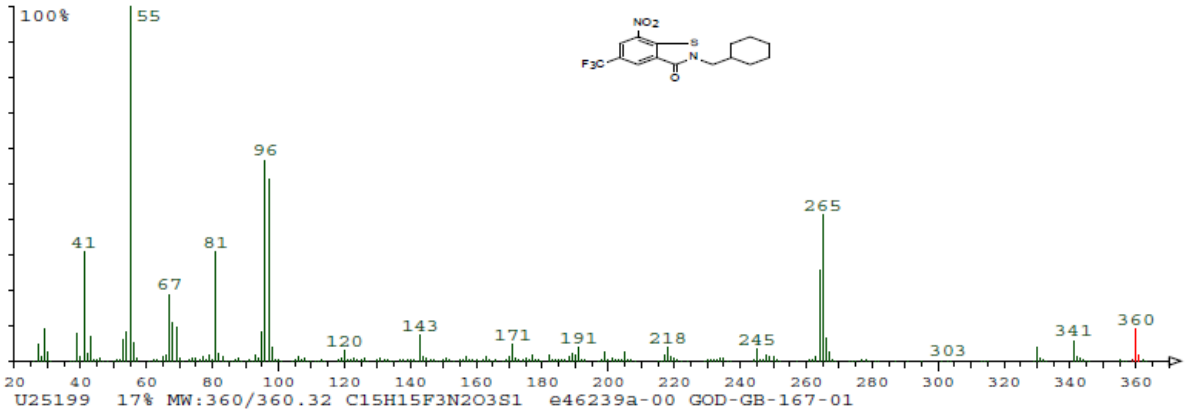

Figure S15 EI mass spectrum of 2-(cyclohexylmethyl)-7-nitro-5-(trifluoromethyl)benzo[*d*]-isothiazol-3(2*H*)-one (**4**).

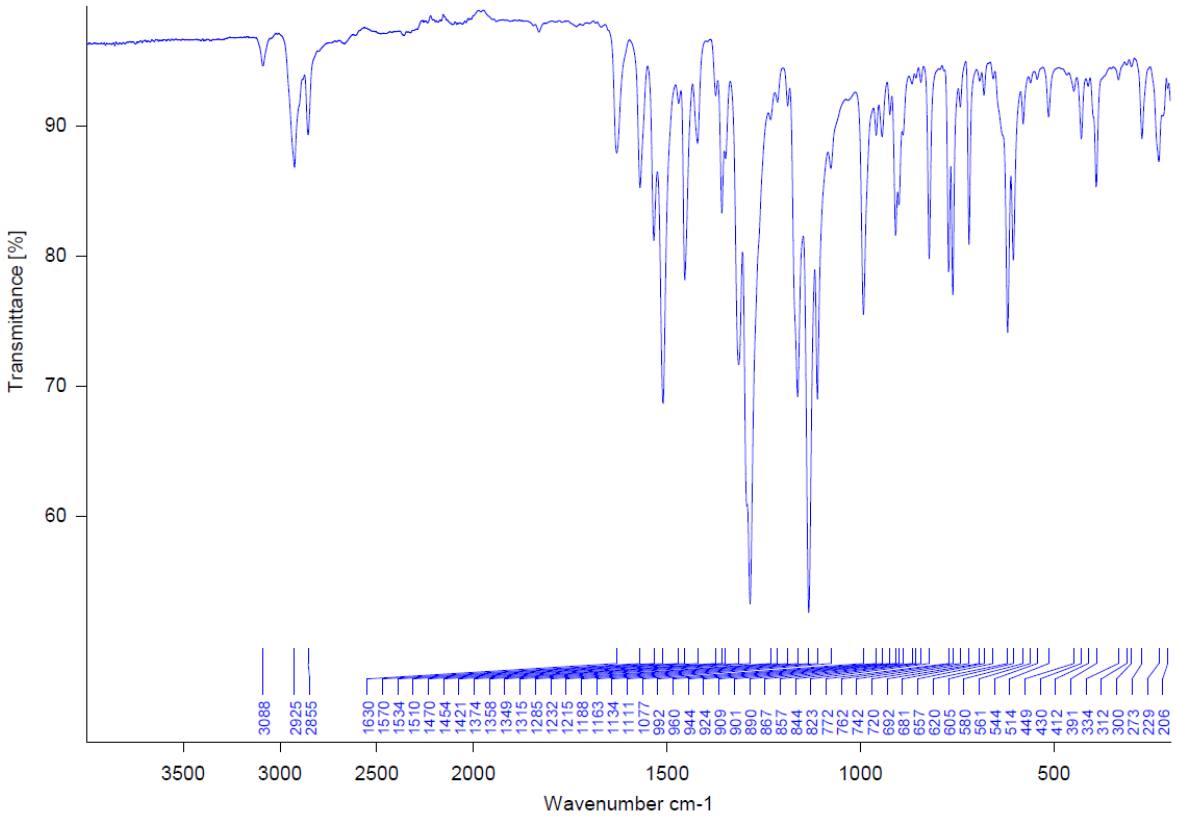

Figure S16 ATR-FT-IR spectrum of 2-(cyclohexylmethyl)-7-nitro-5-(trifluoromethyl)-benzo[*d*]-isothiazol-3(2*H*)-one (**4**).