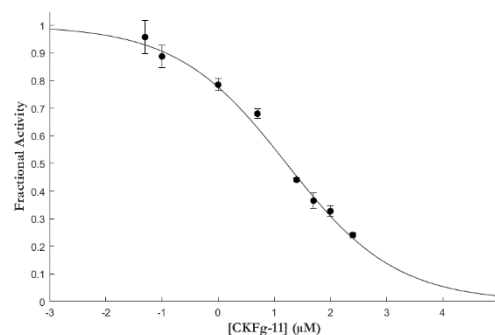
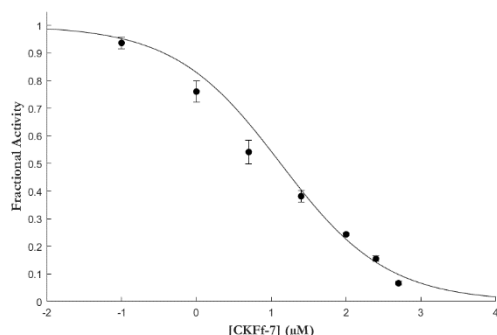
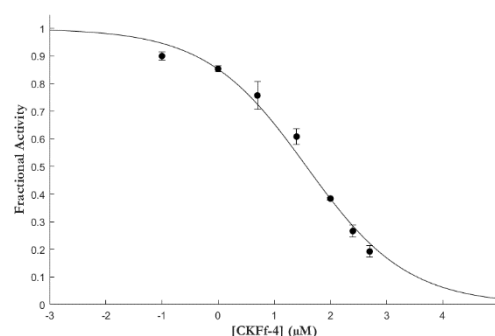
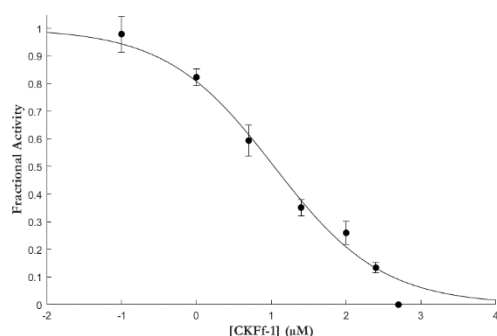
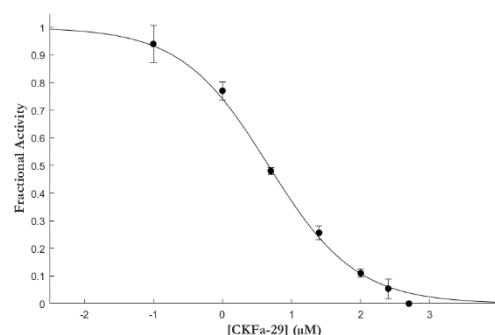
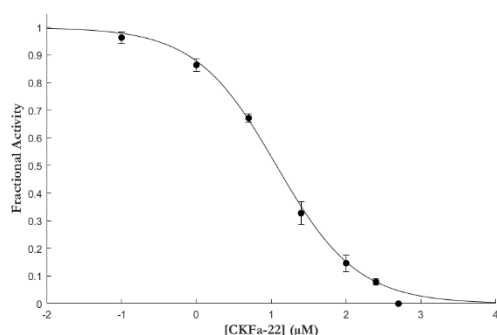


Supplementary Materials: New Compounds with Bioisosteric Replacement of Classic Choline Kinase Inhibitors Show Potent Antiplasmodial Activity

Francisco José Aguilar-Troyano, Archimede Torretta, Gianluca Rubbini, Alberto Fasiolo, Pilar María Luque-Navarro, María Paz Carrasco-Jimenez, Guiomar Pérez-Moreno, Cristina Bosch-Navarrete, Dolores González-Pacanowska, Emilio Parisini and Luisa Carlota Lopez-Cara



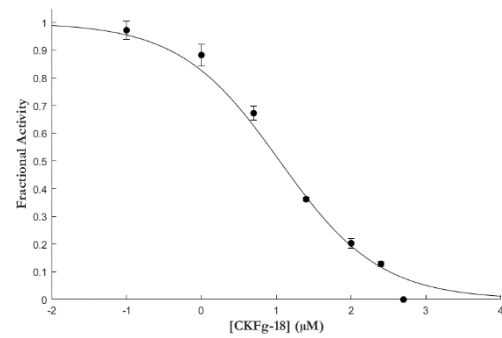
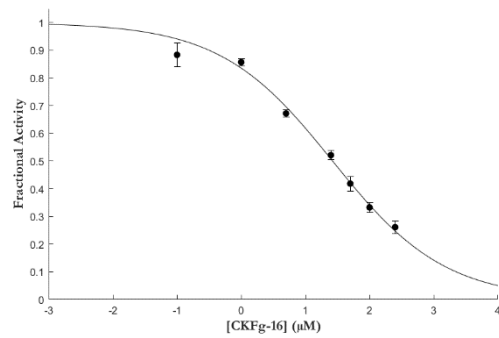
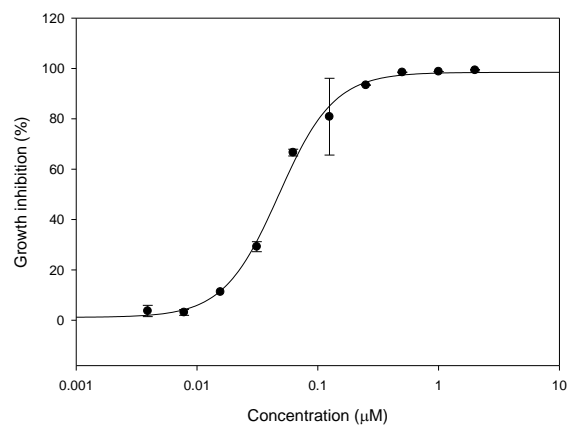
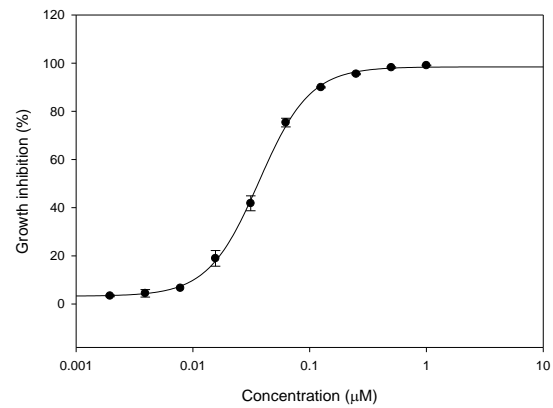


Figure S1. IC₅₀ Curves Inhibition of *Pf*CK.

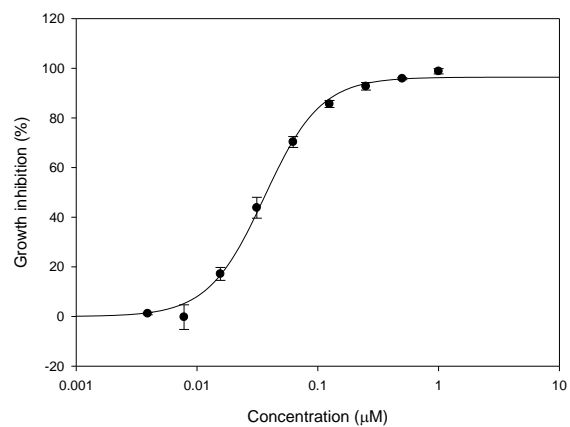
CKF-aM2



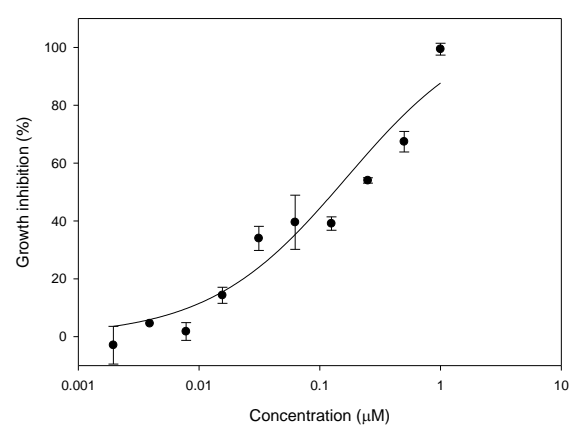
CKF-aM1



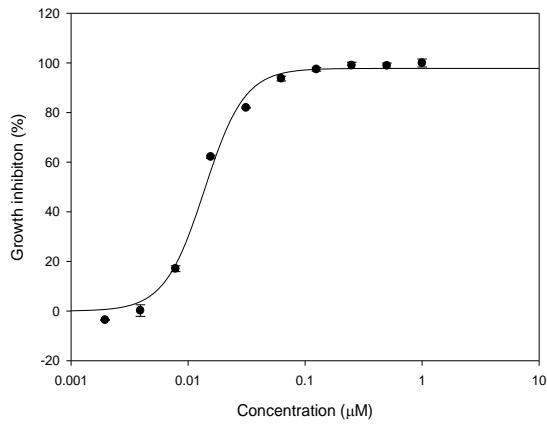
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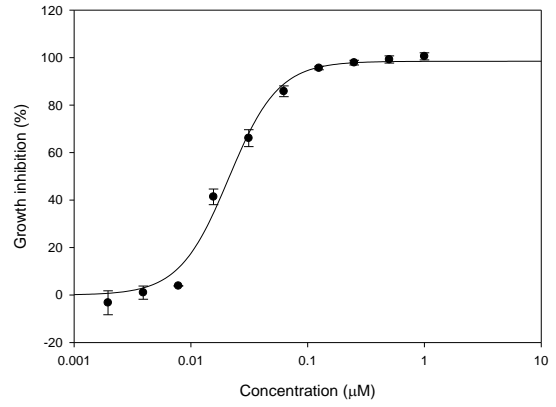
CKFg-9



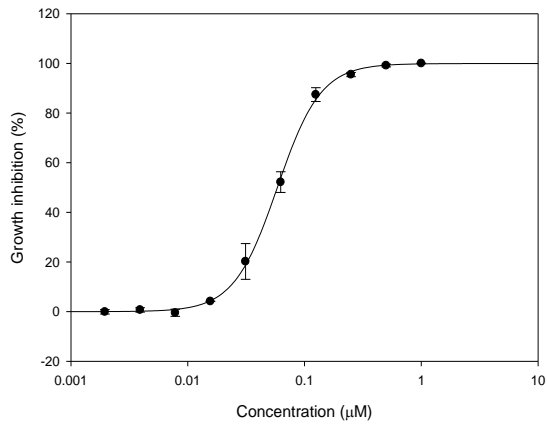
CKFa-21



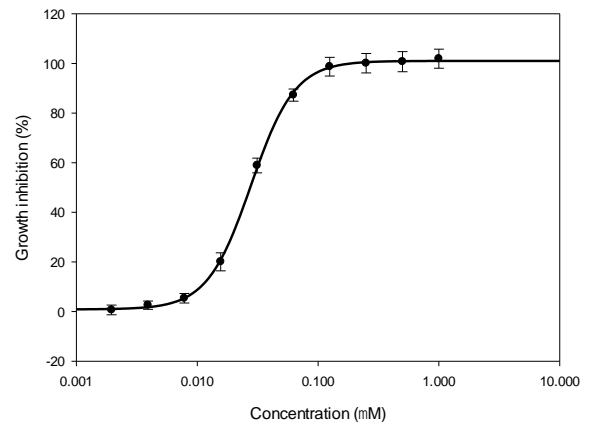
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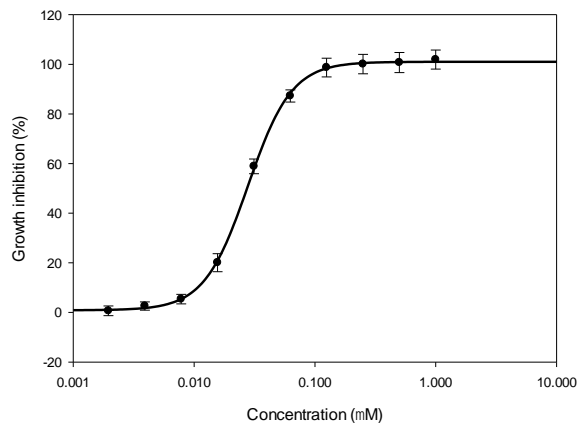
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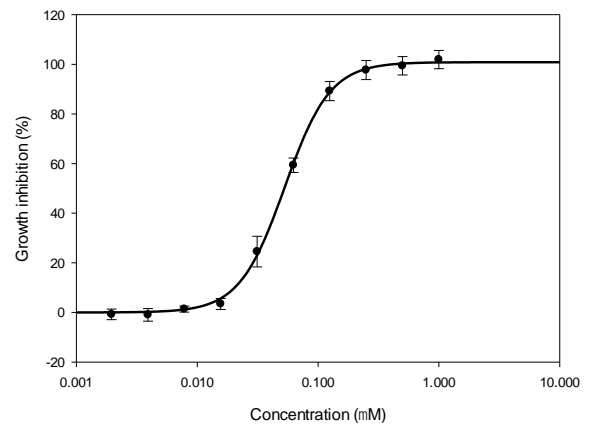
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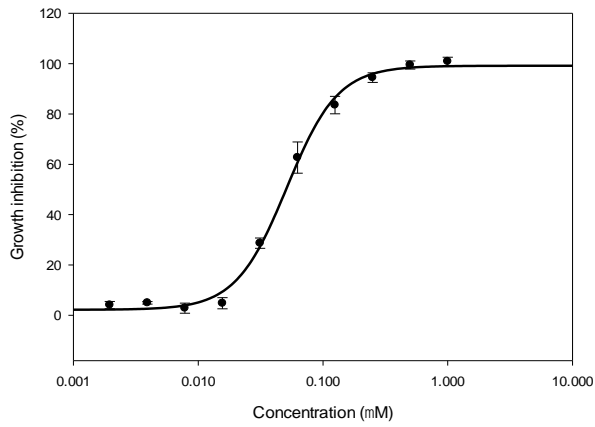
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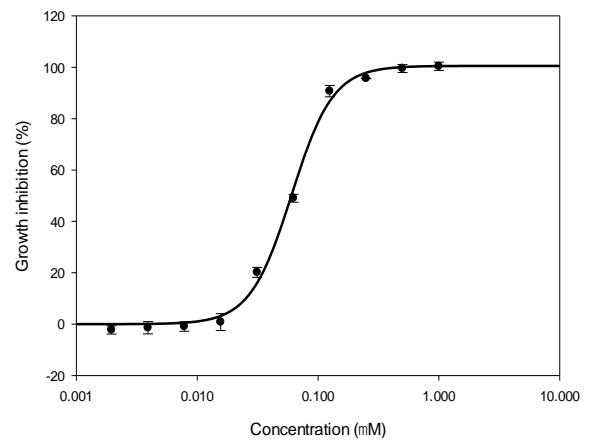
CKF-g10



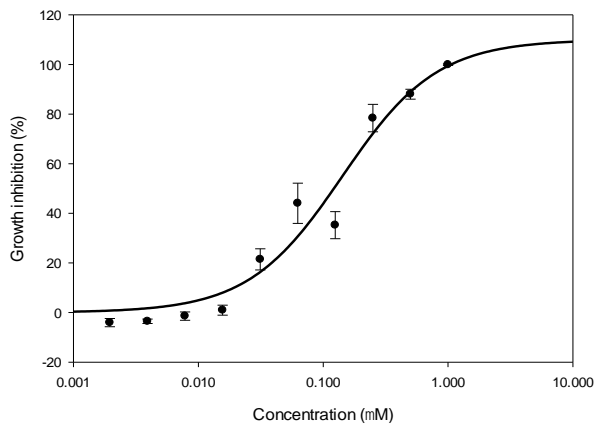
CKF-a22



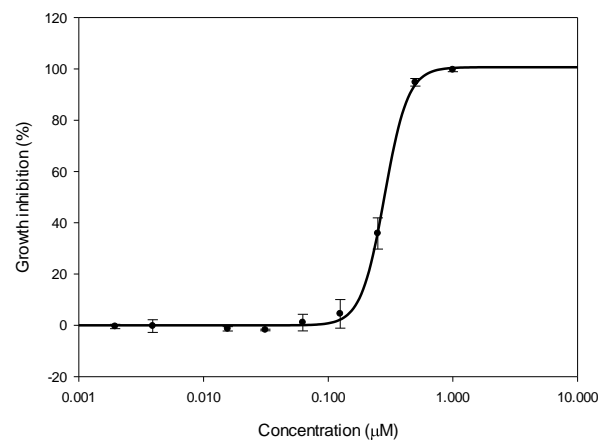
14CKF-g18



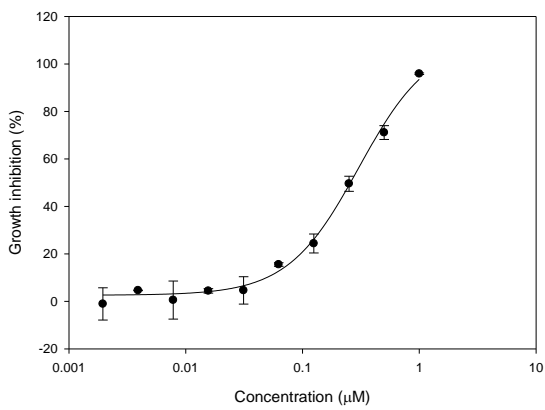
CKFp-1



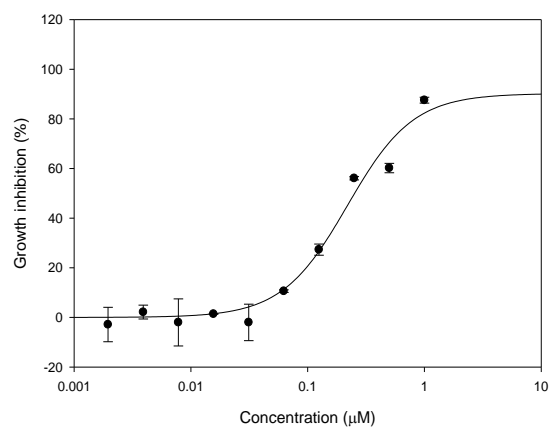
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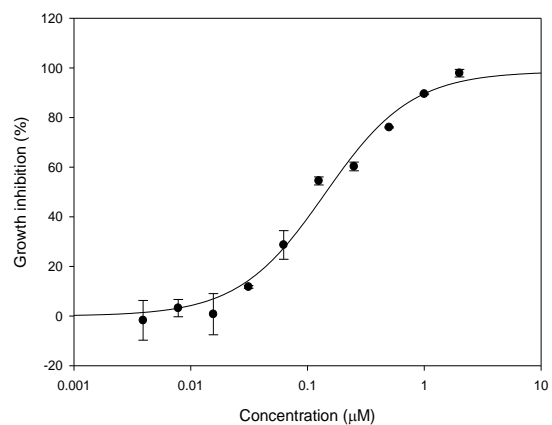
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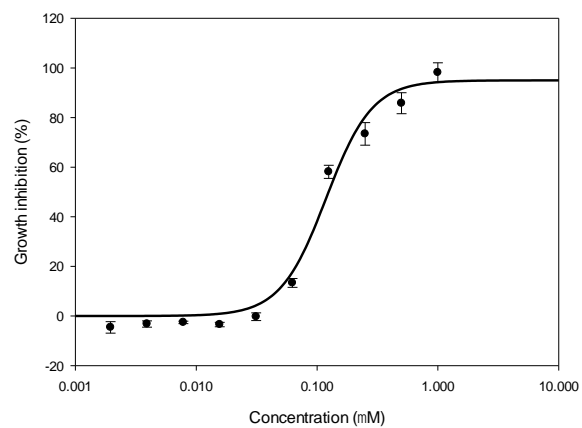
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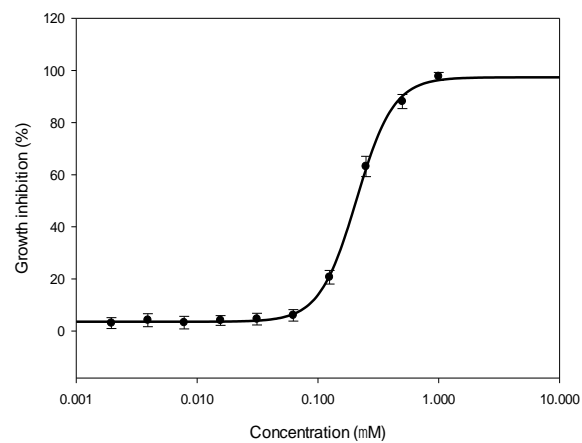
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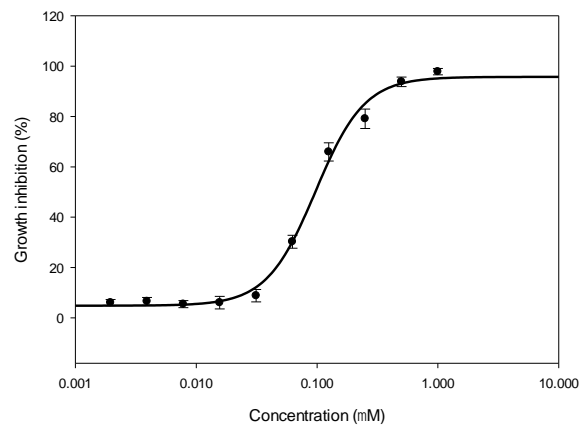
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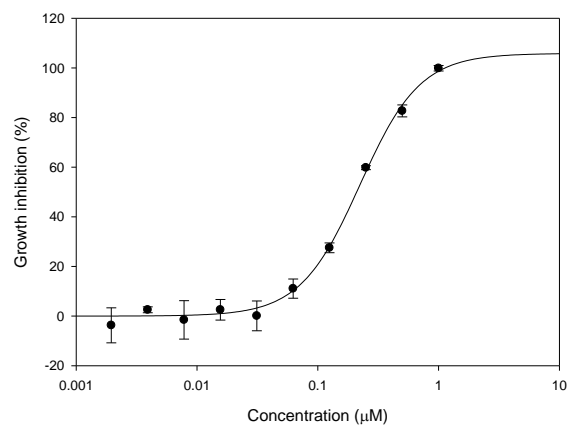
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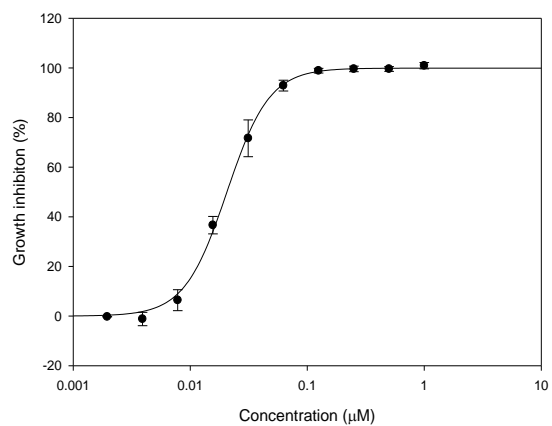
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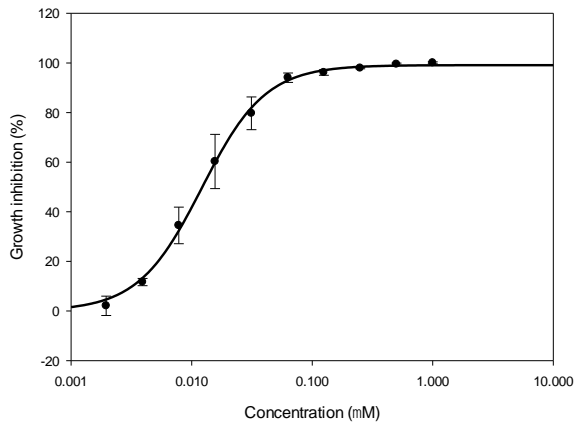
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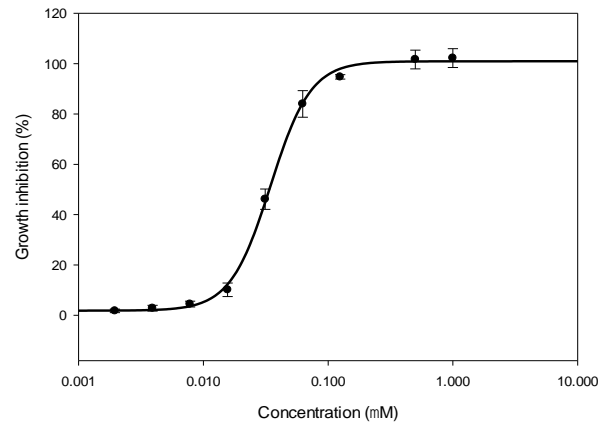
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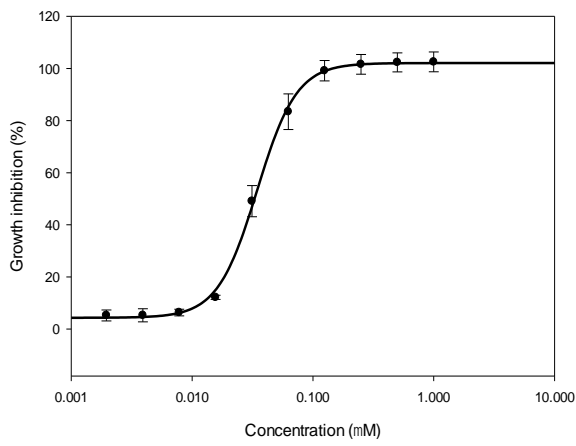
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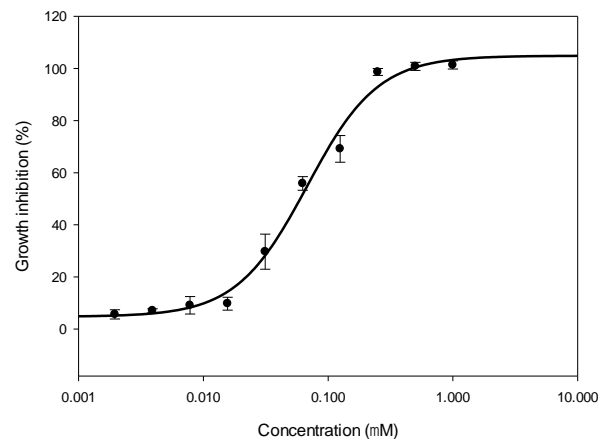
CKF-a25



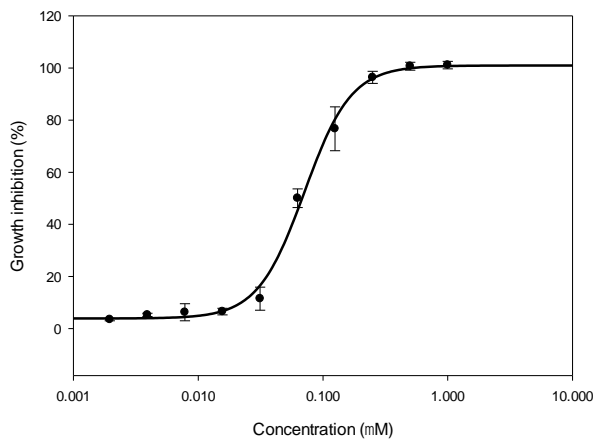
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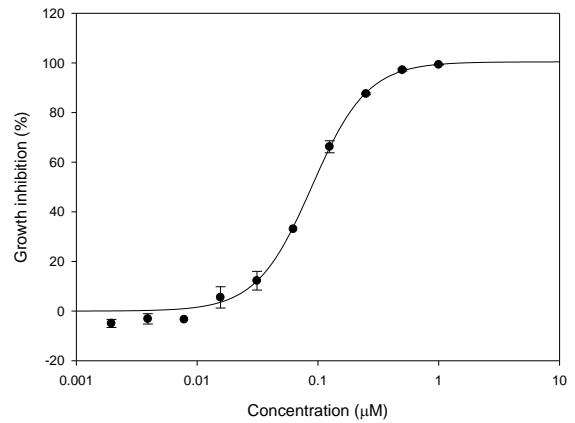
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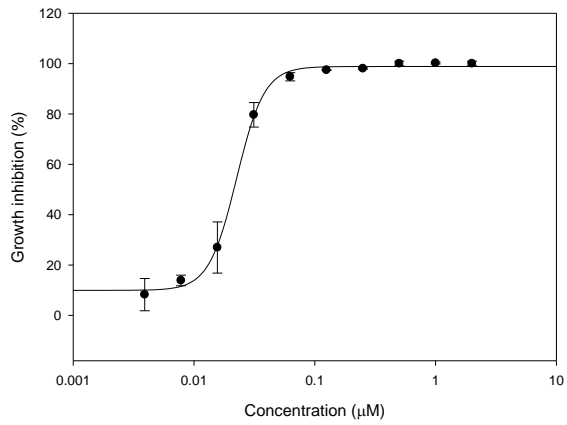
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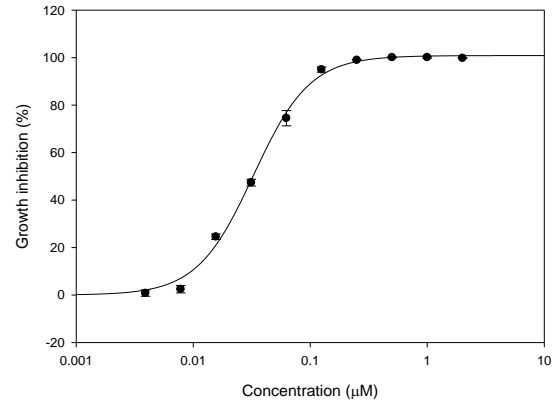
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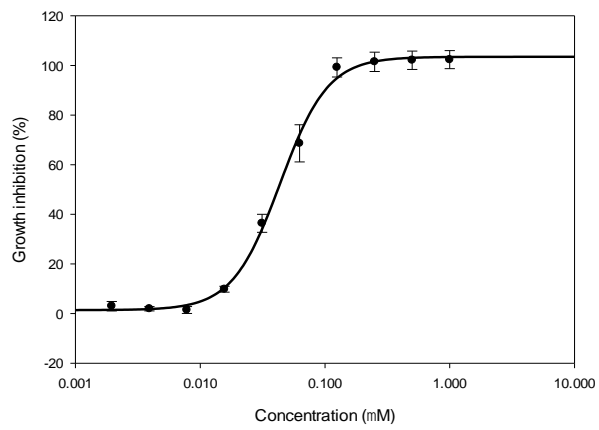
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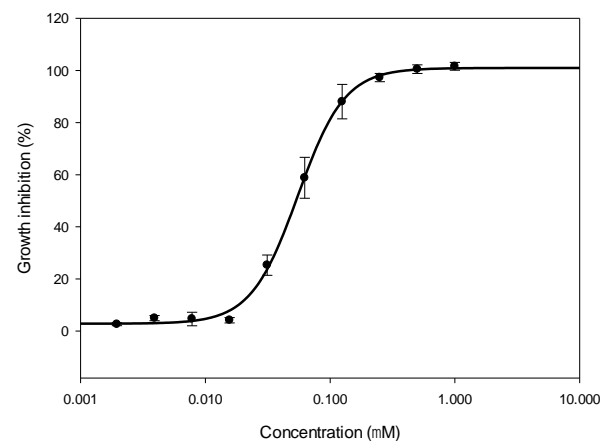
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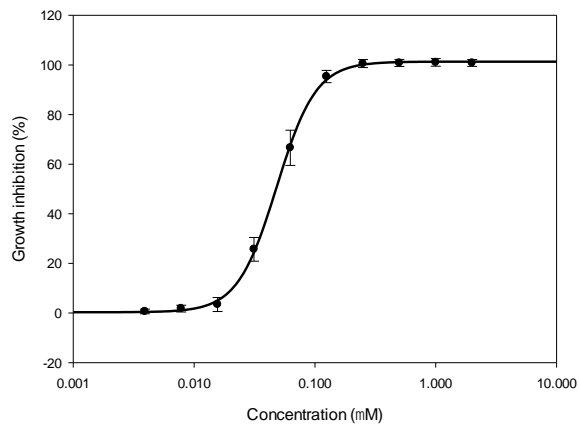
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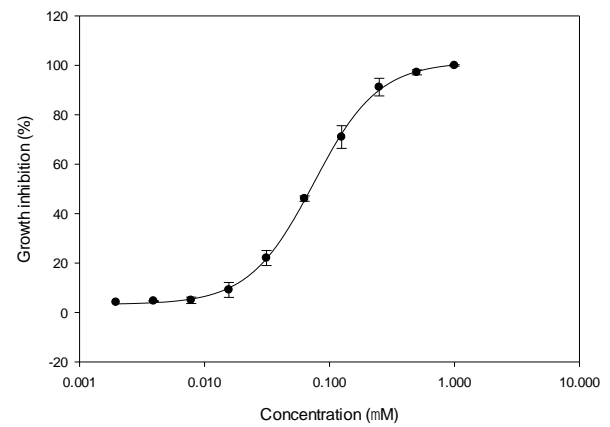
CKFa-29



CKFf-35



CKFf-2



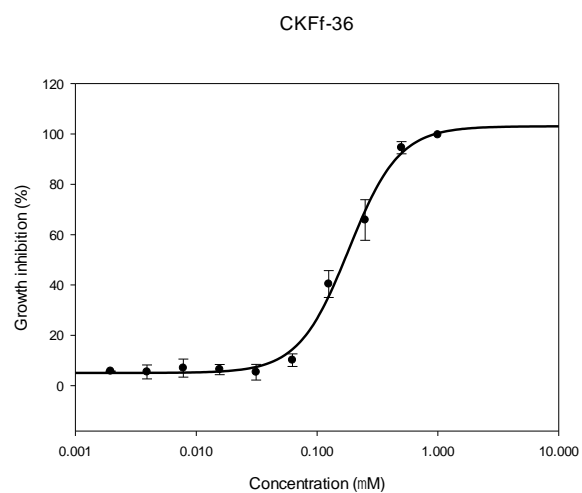
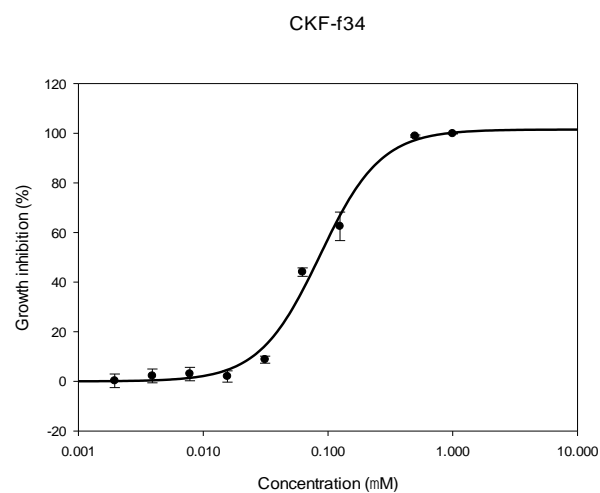
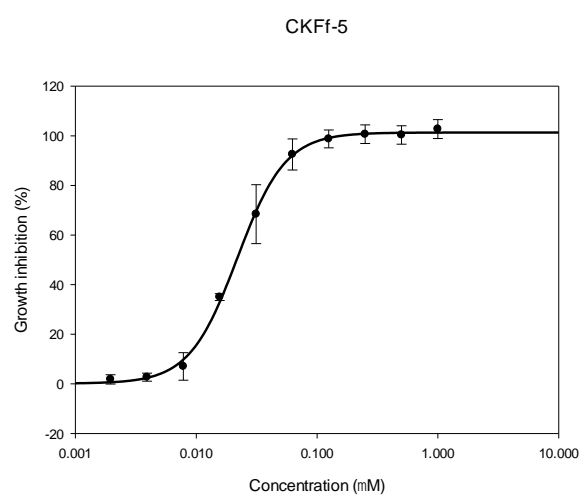
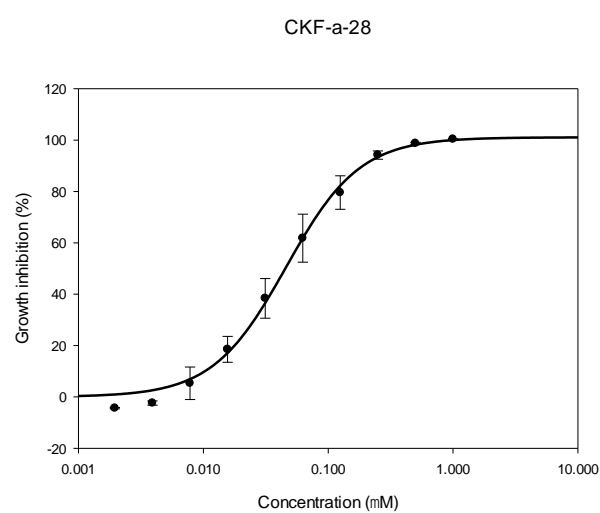
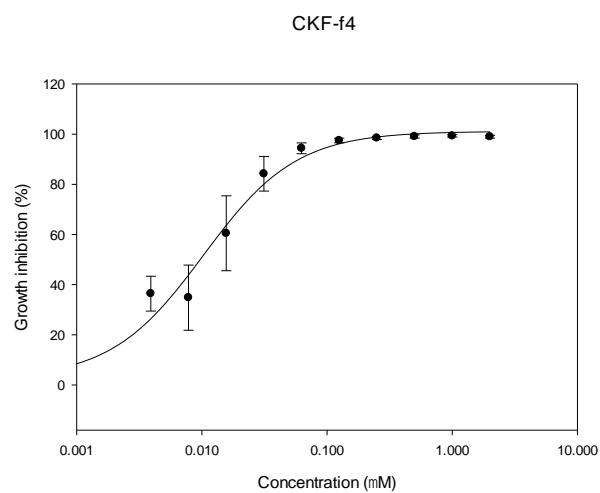
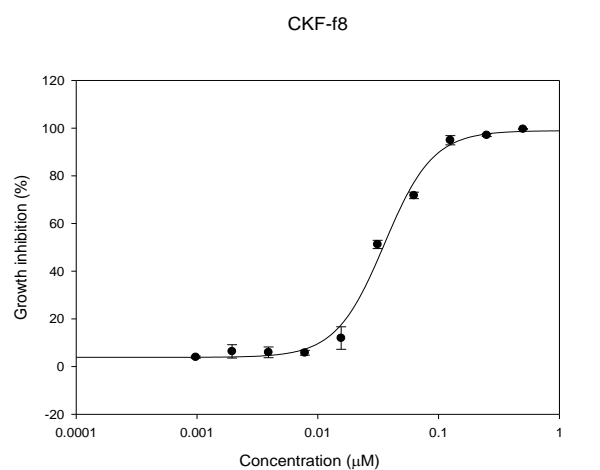
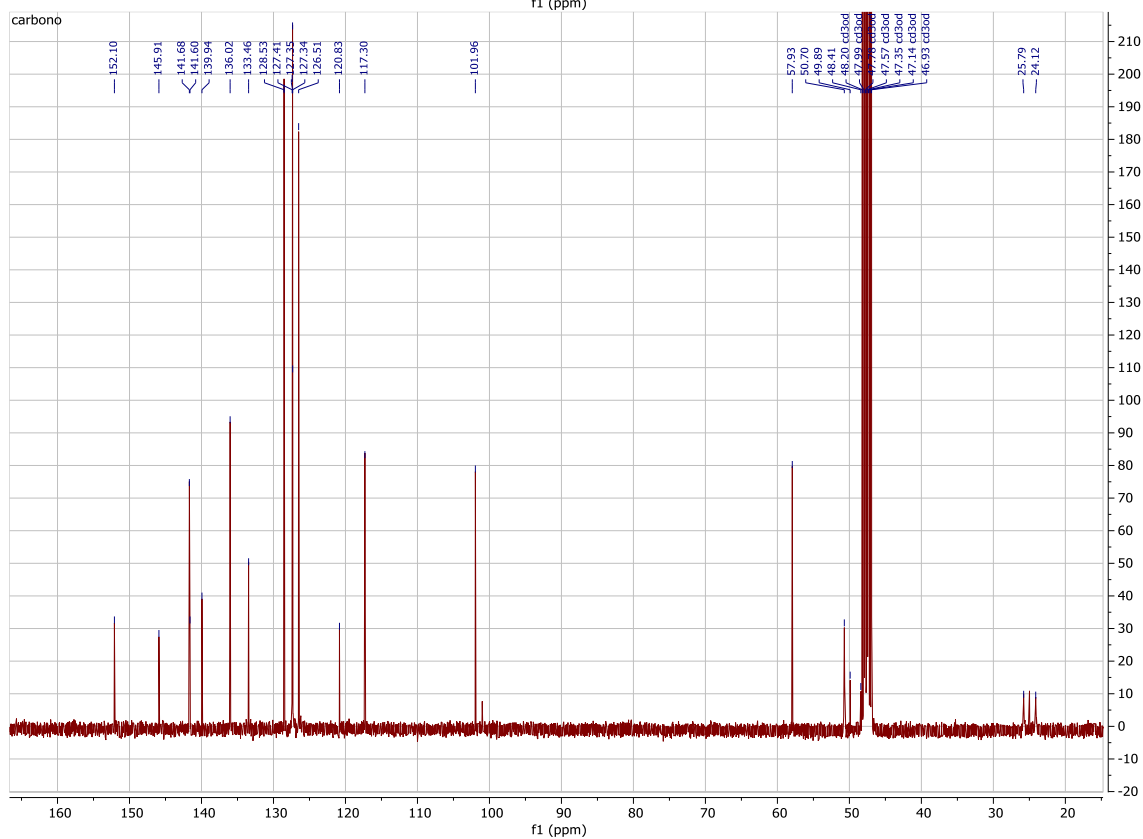
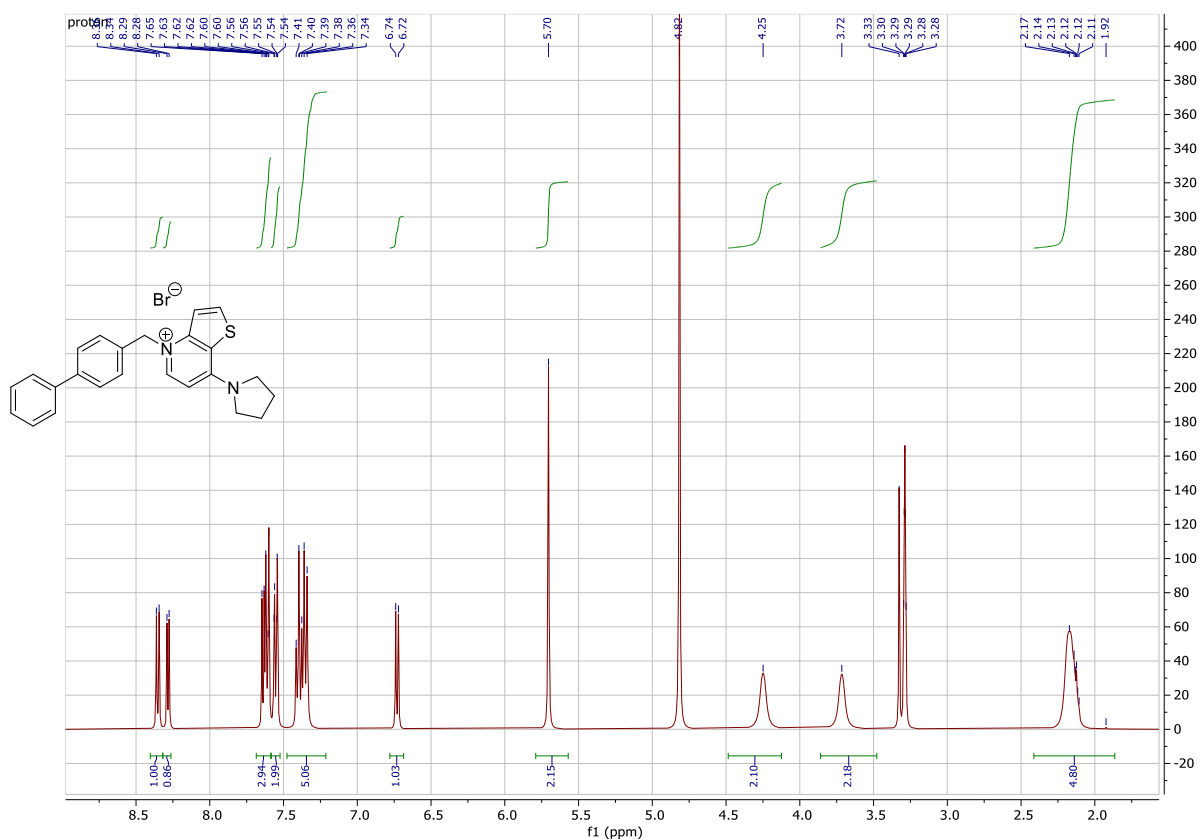
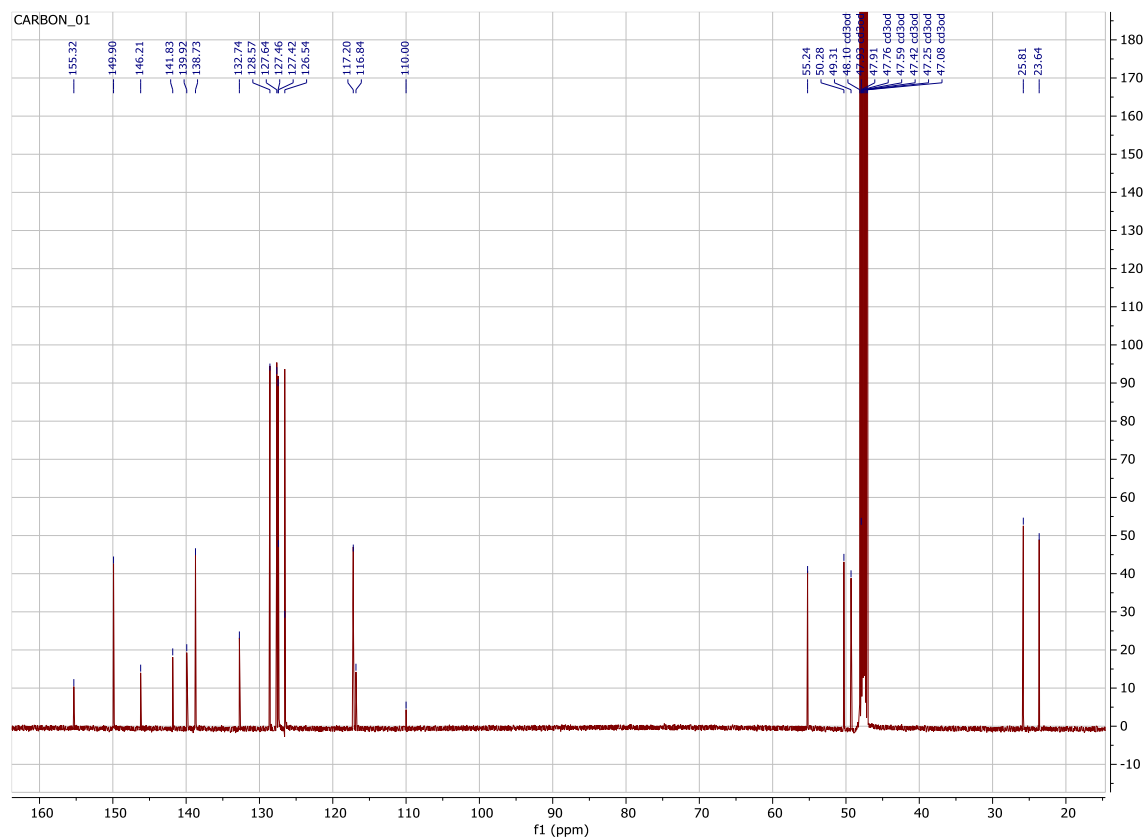
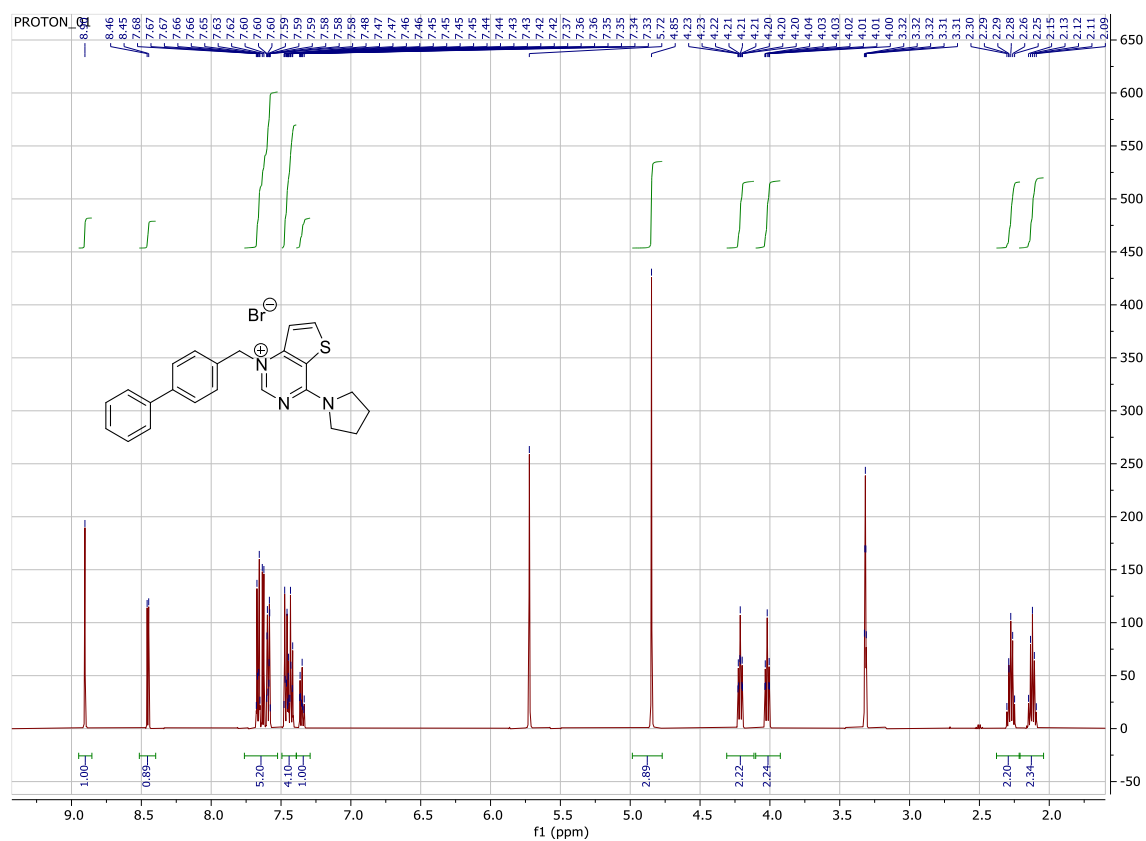


Figure S2. IC₅₀ Curves.

Fa-M2



Fa-M1



FMa-3

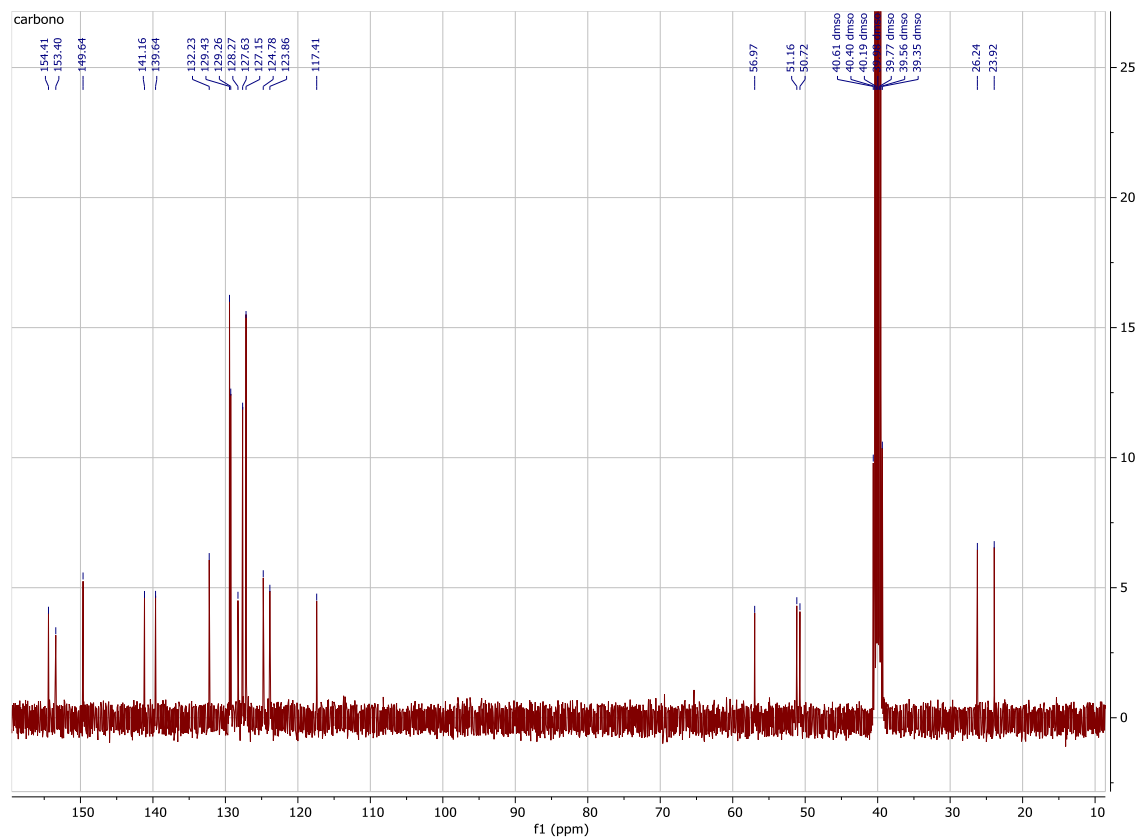
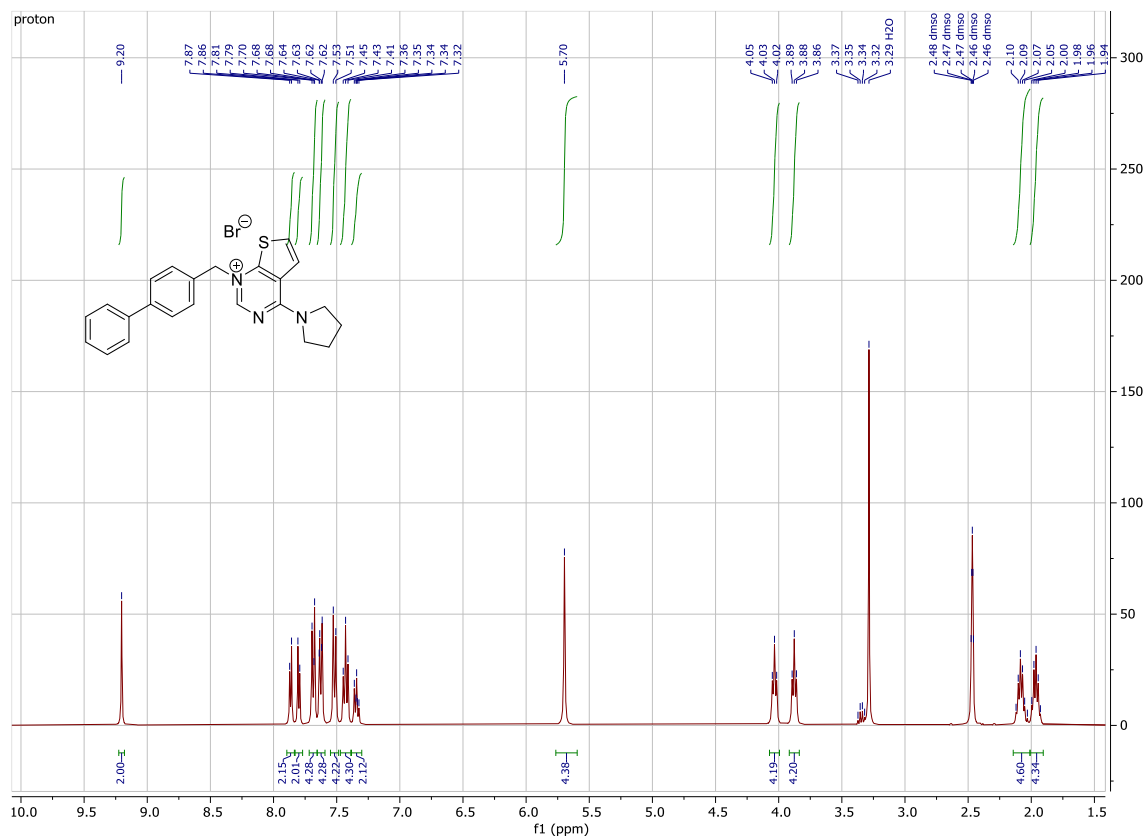
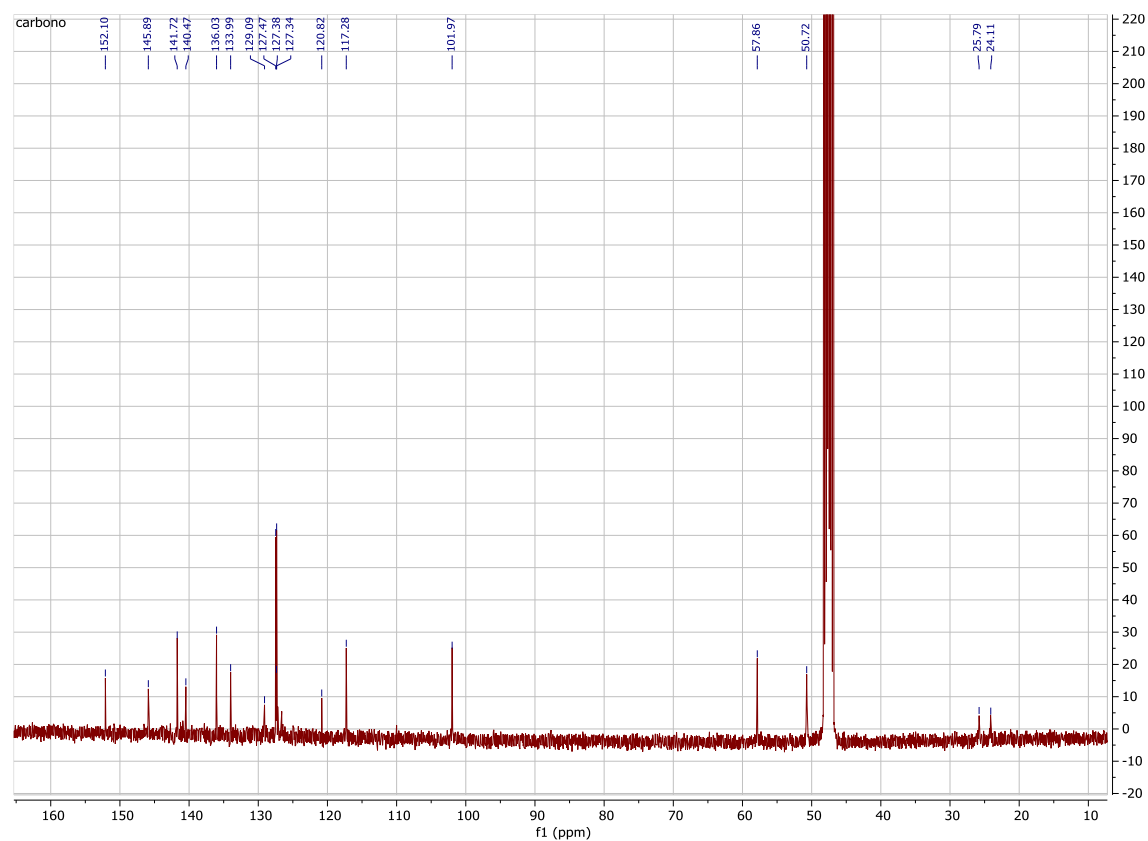
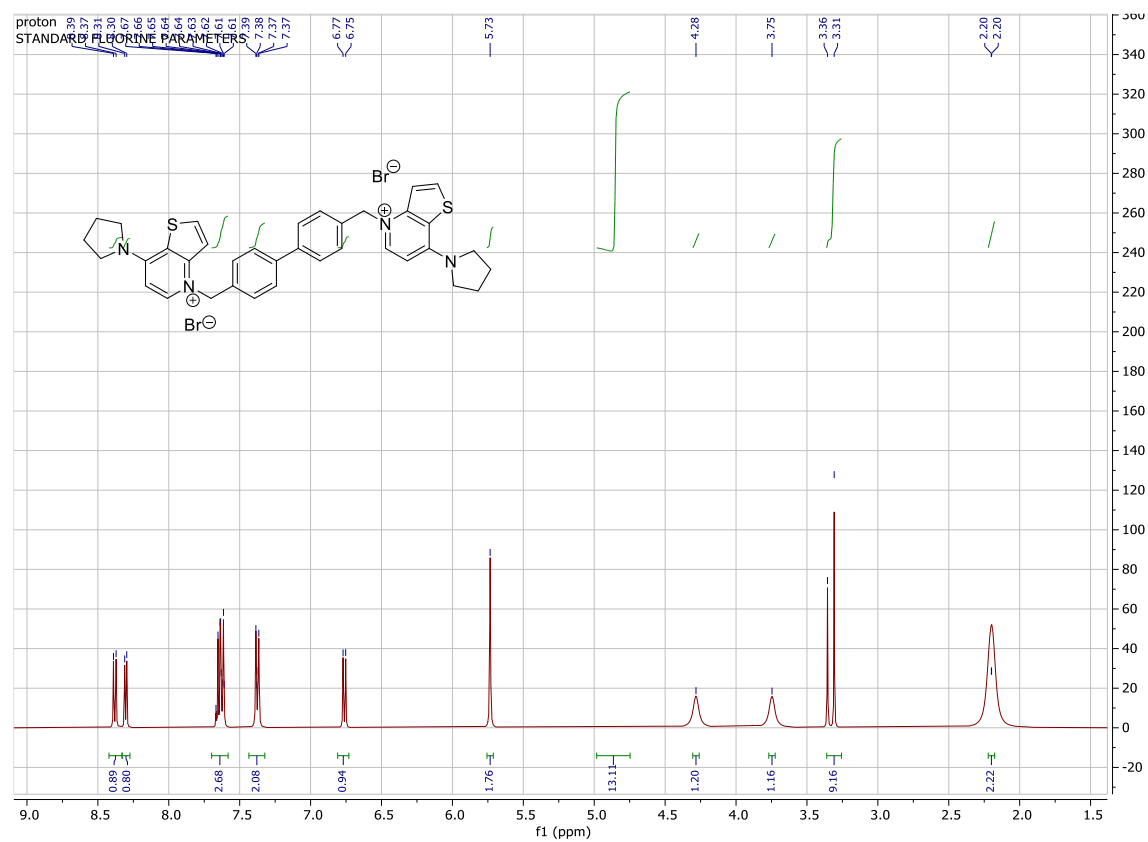
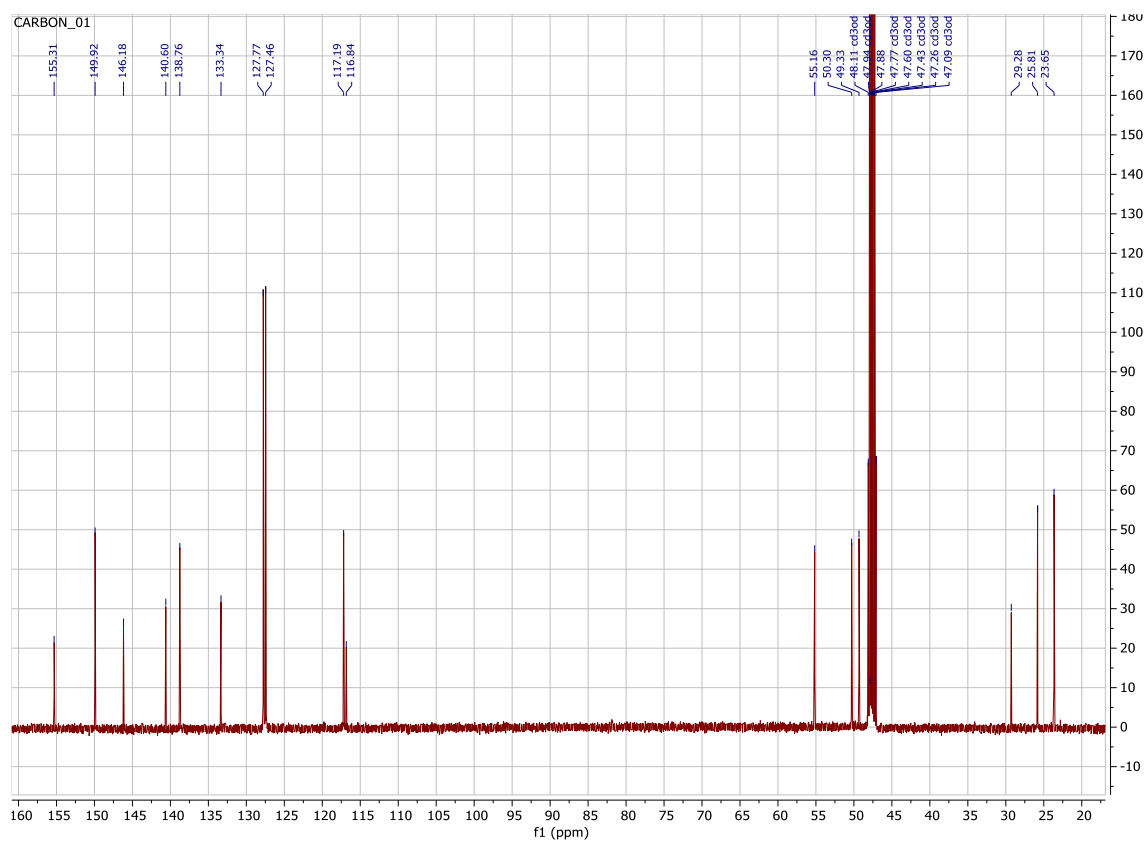
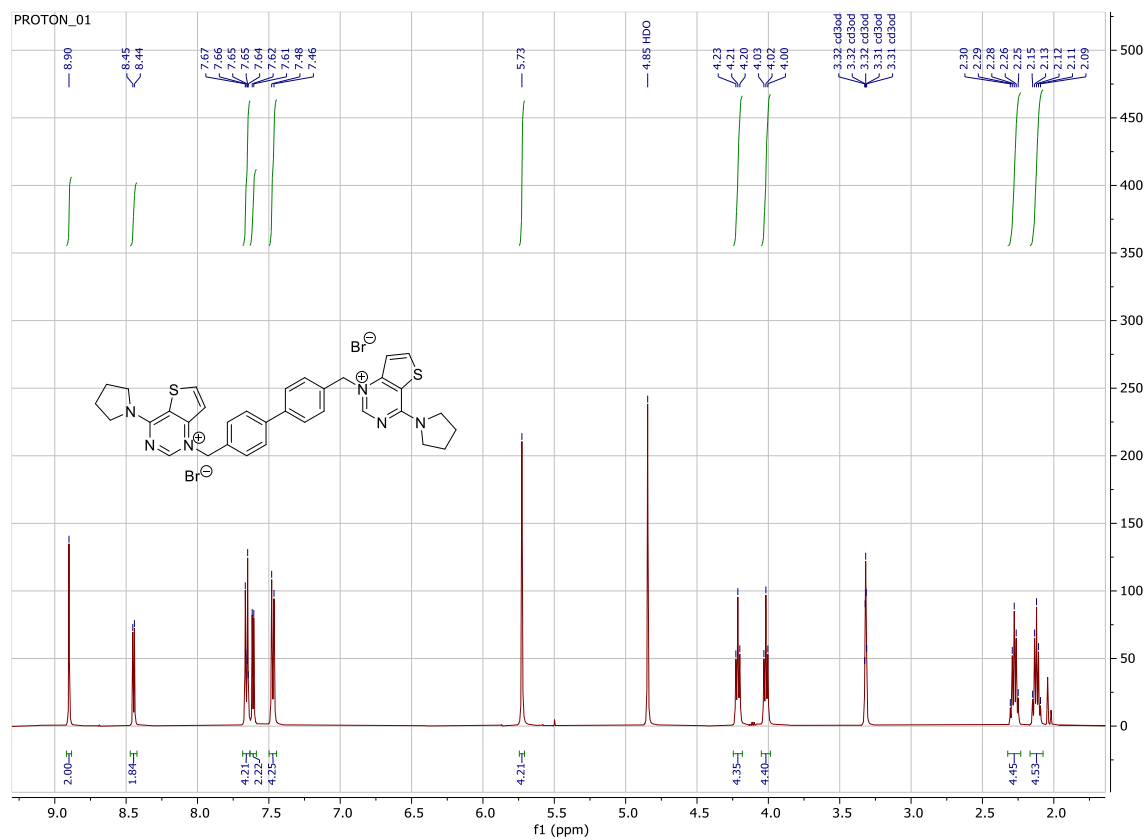


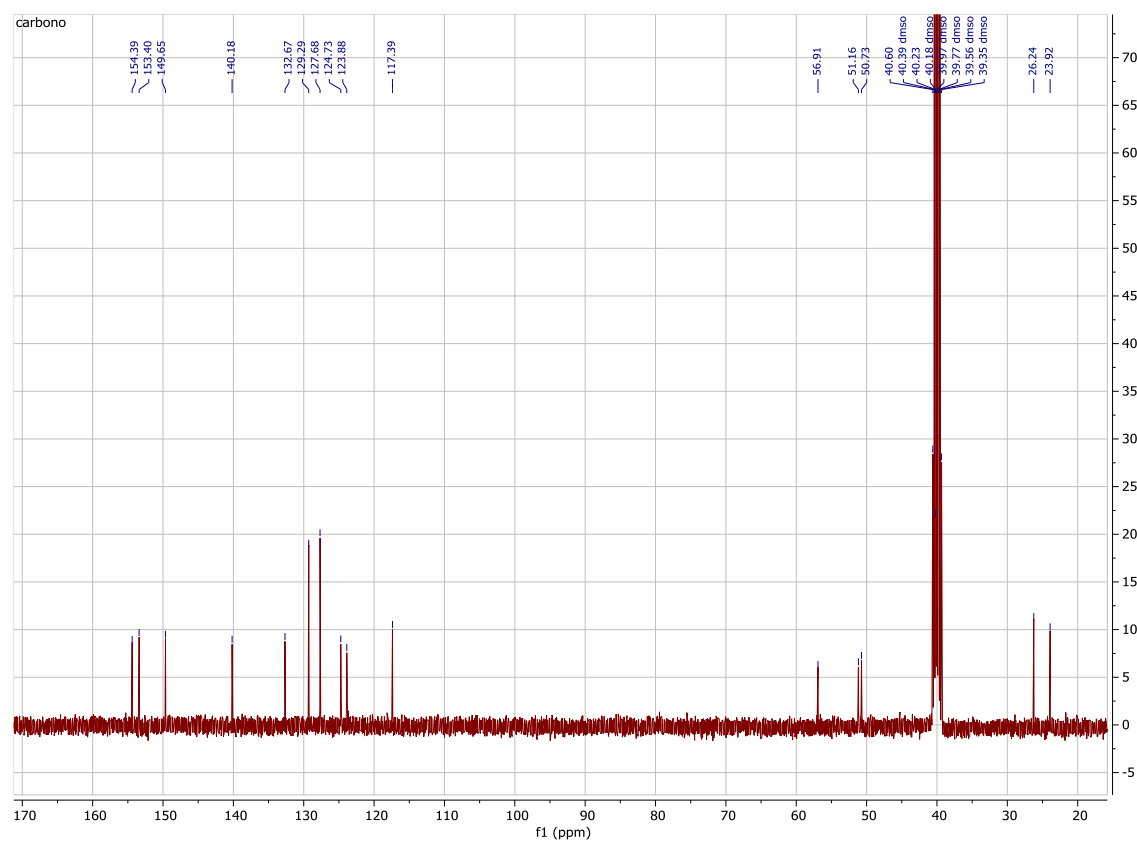
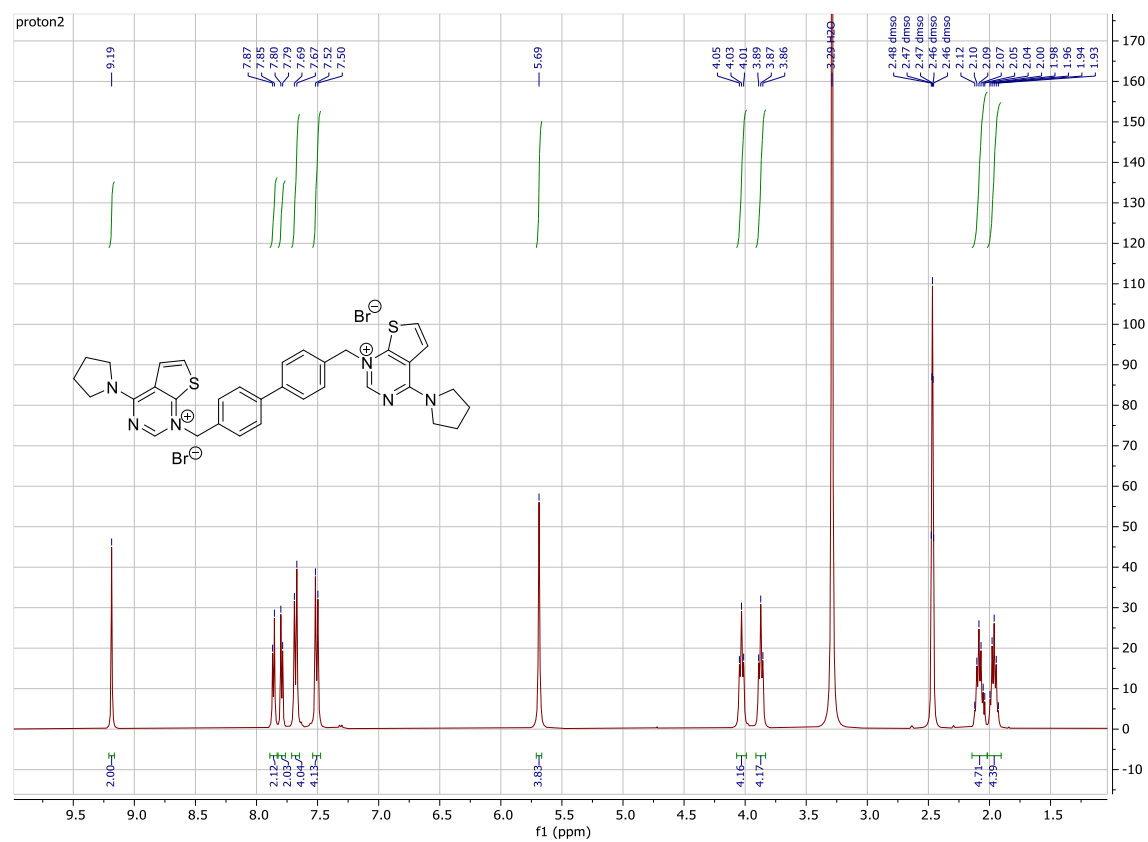
Fig-9



Fa-21



Fg-14



Fa-24

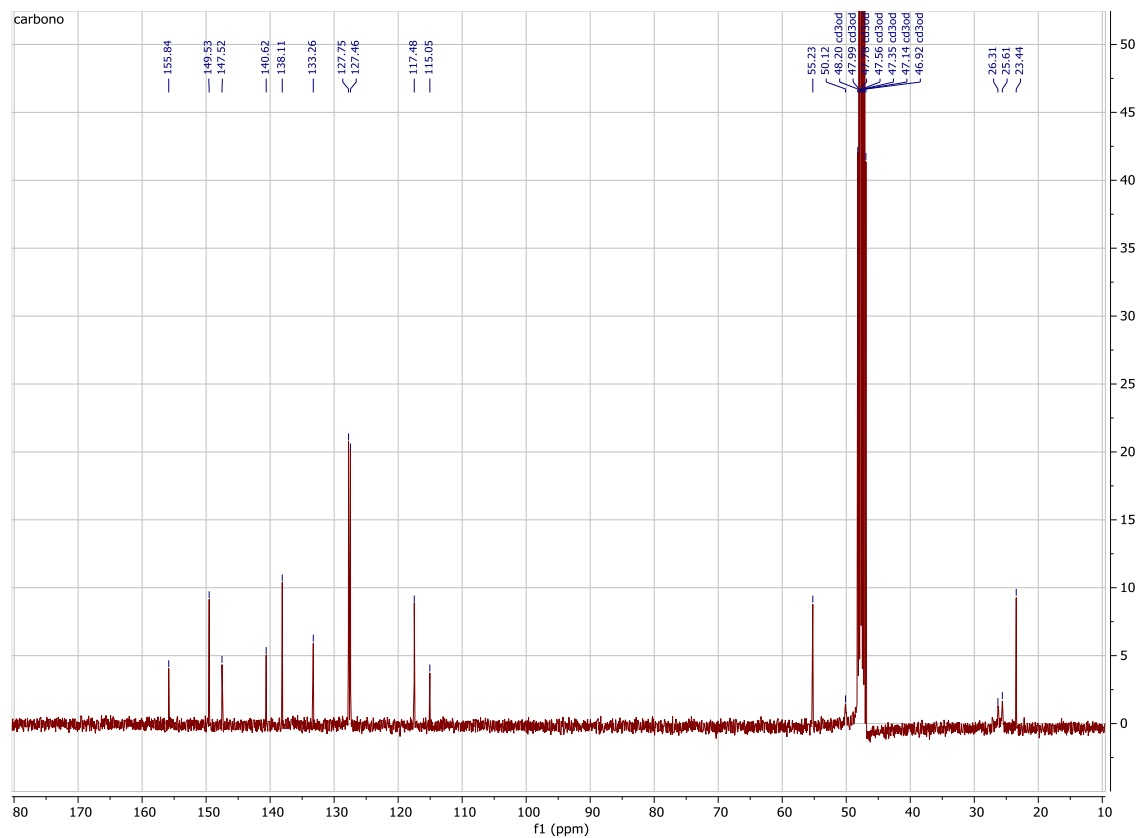
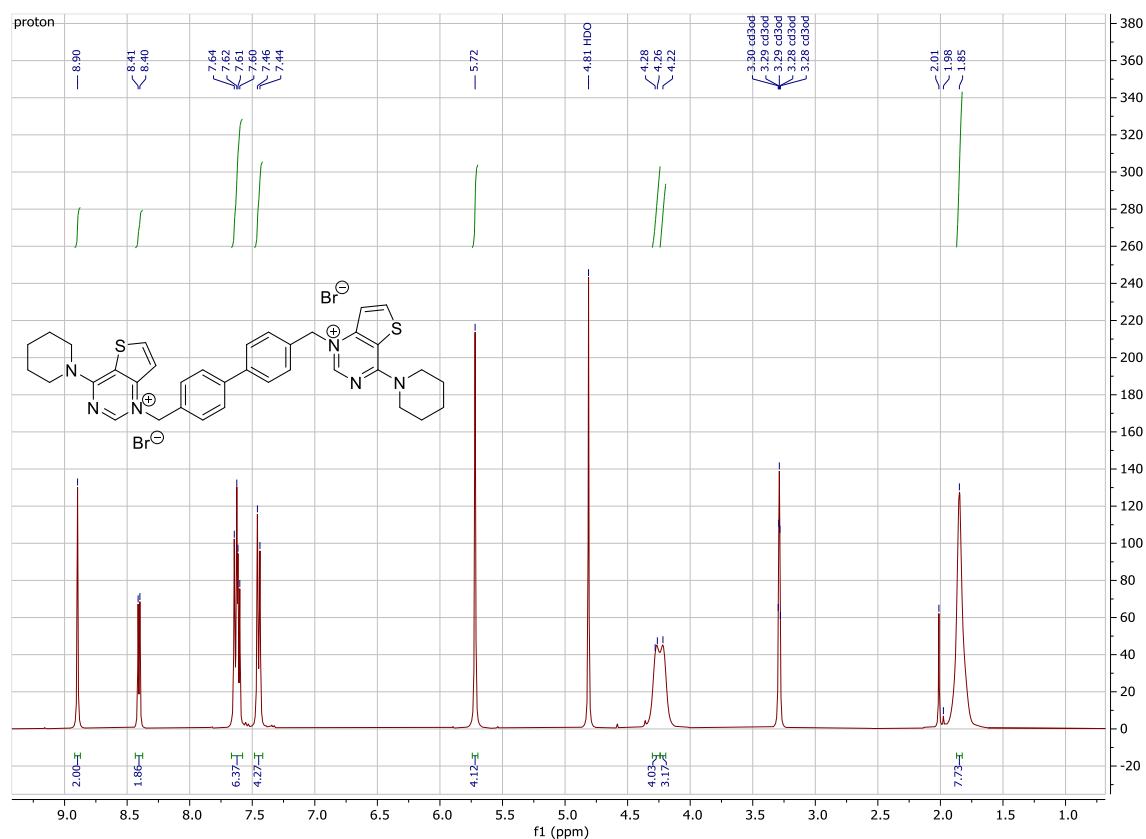
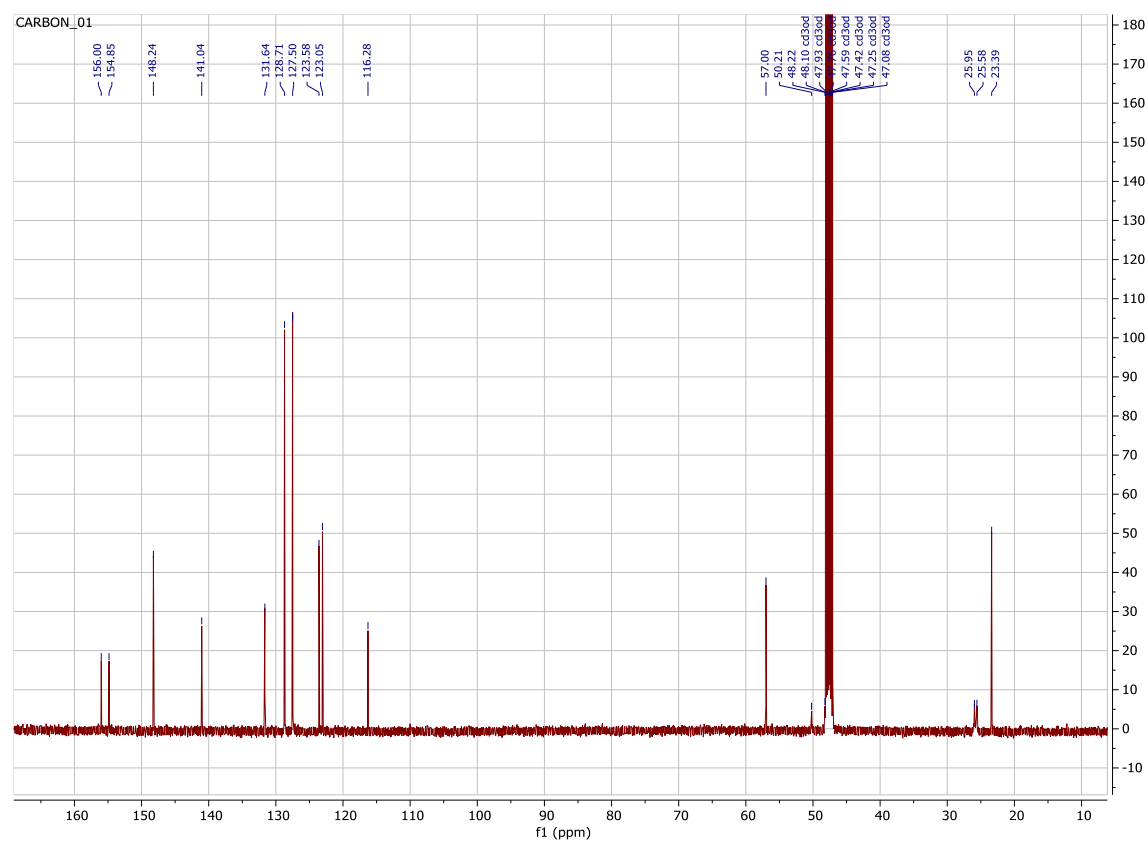
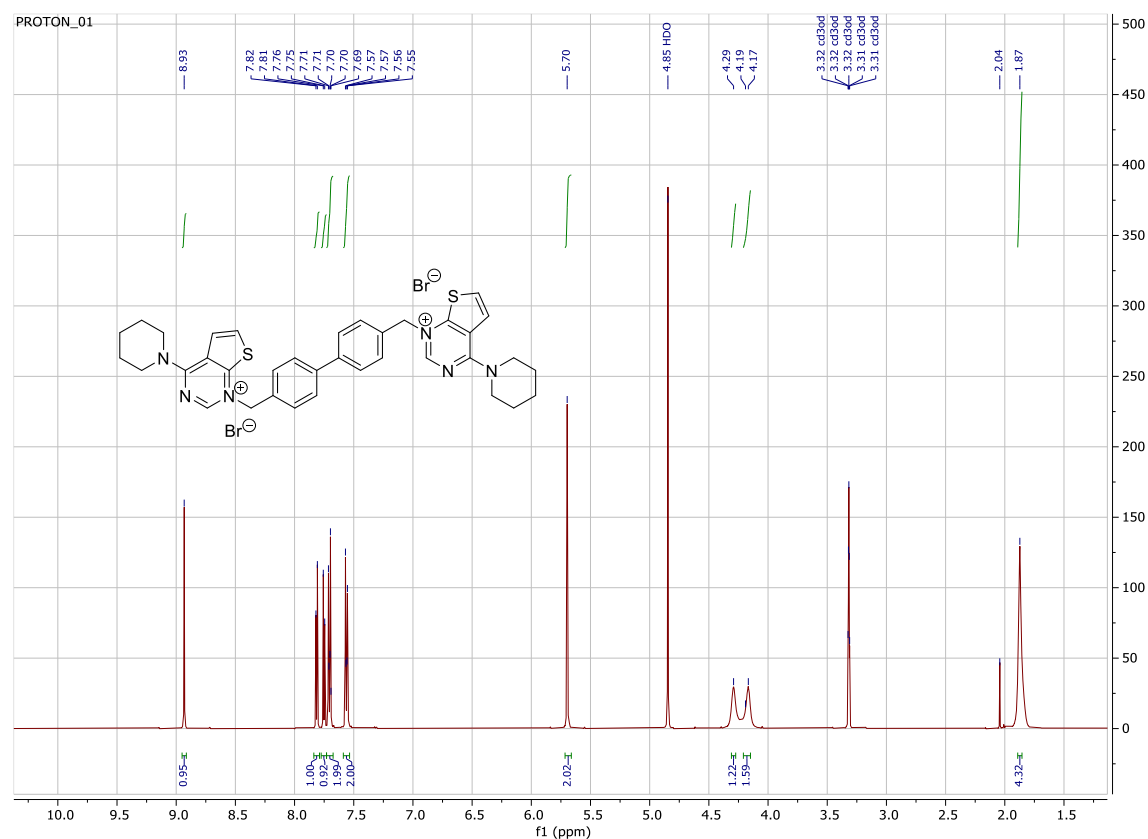
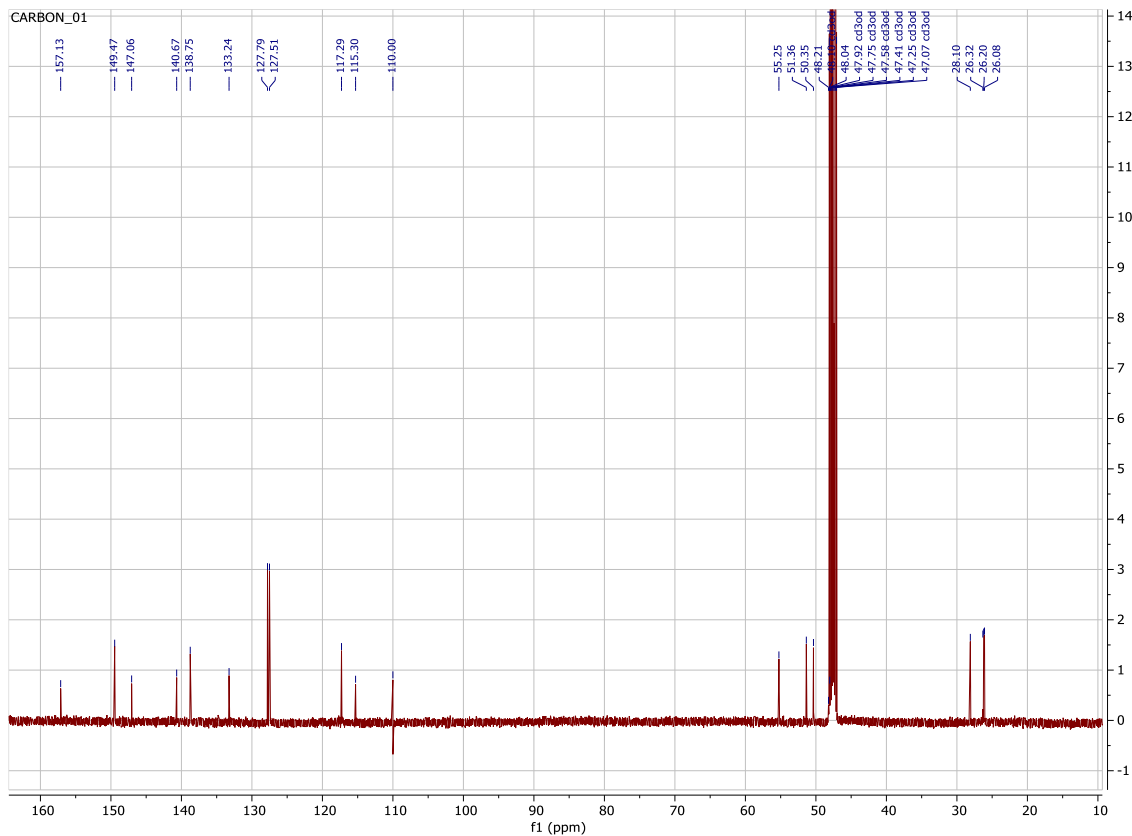
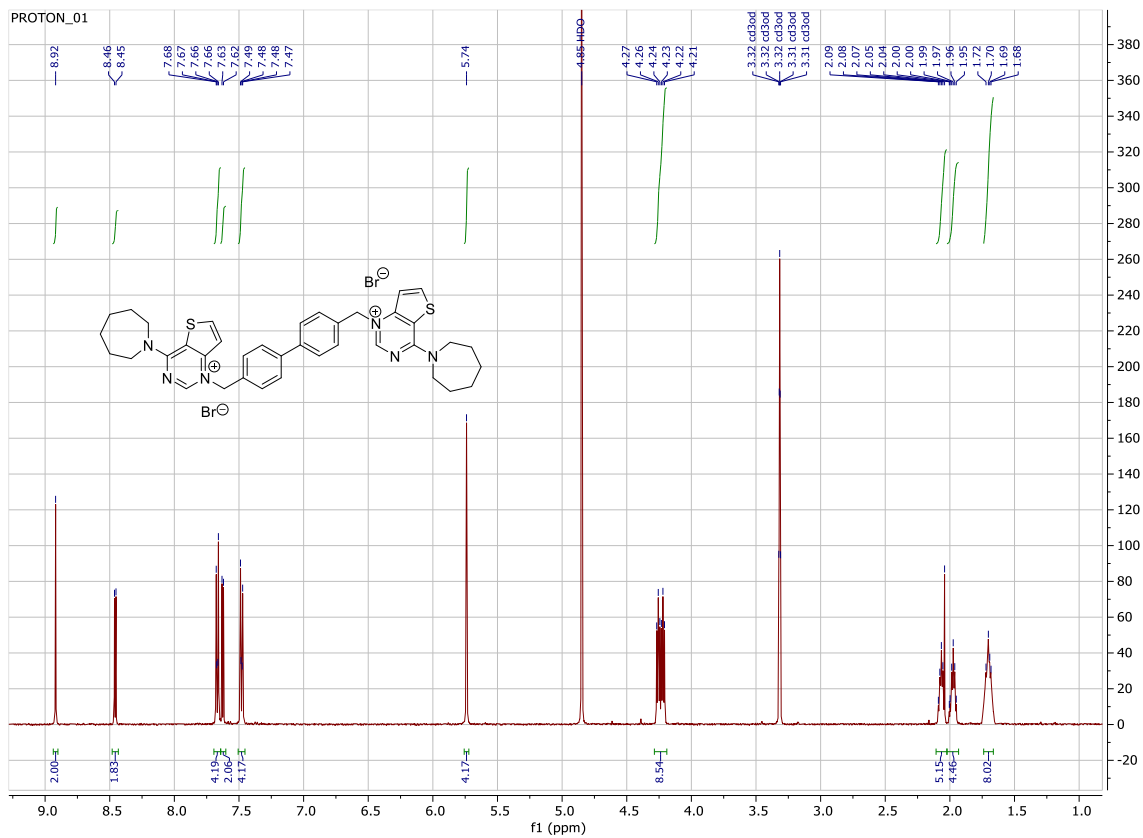
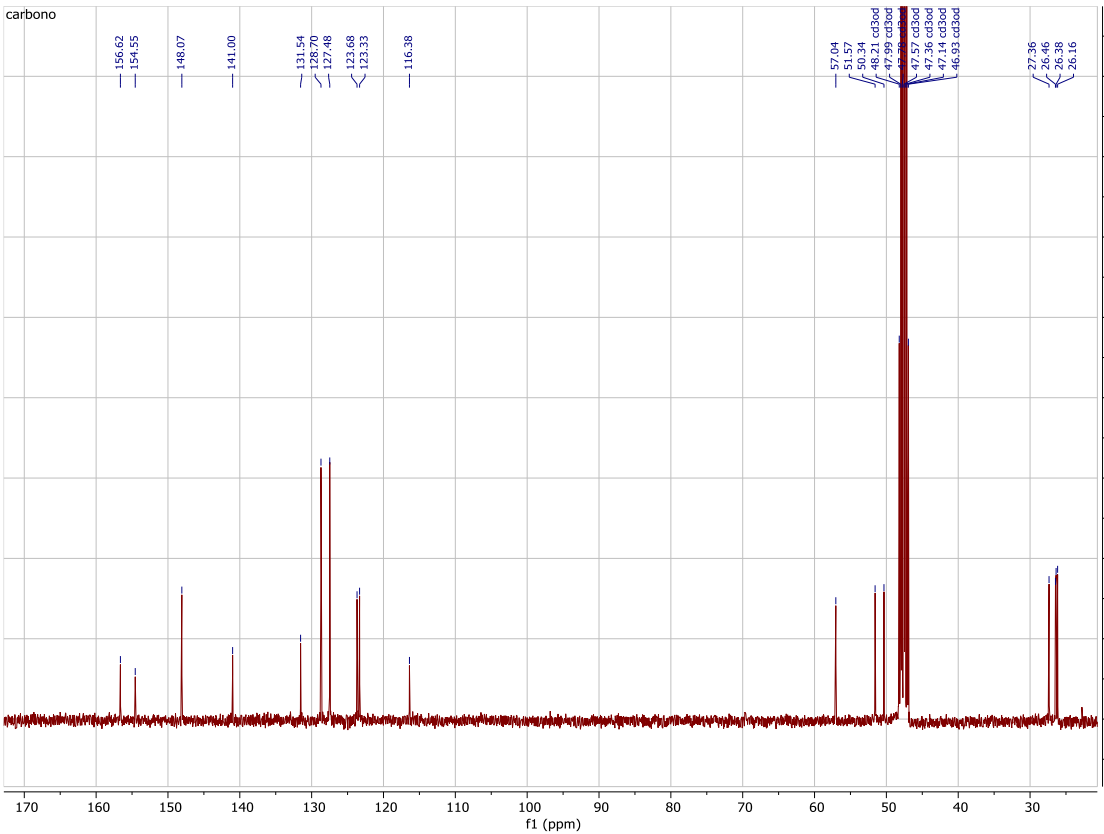
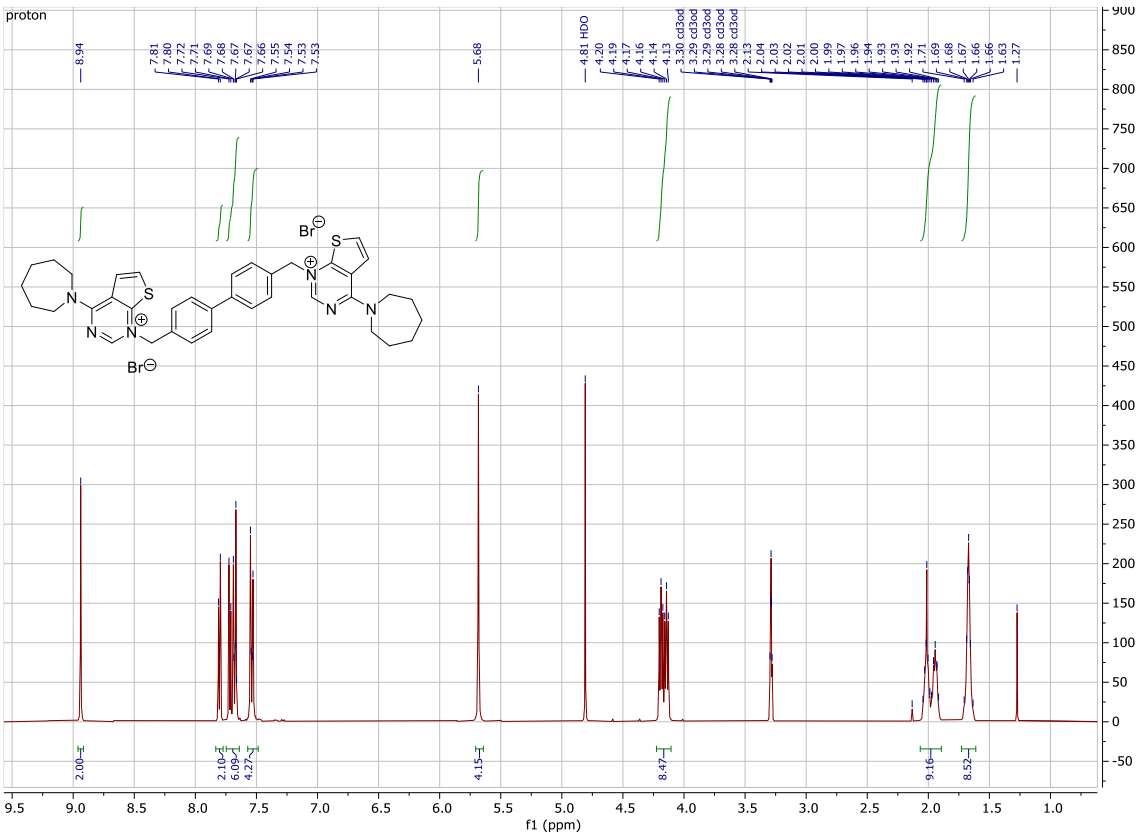


Fig-30

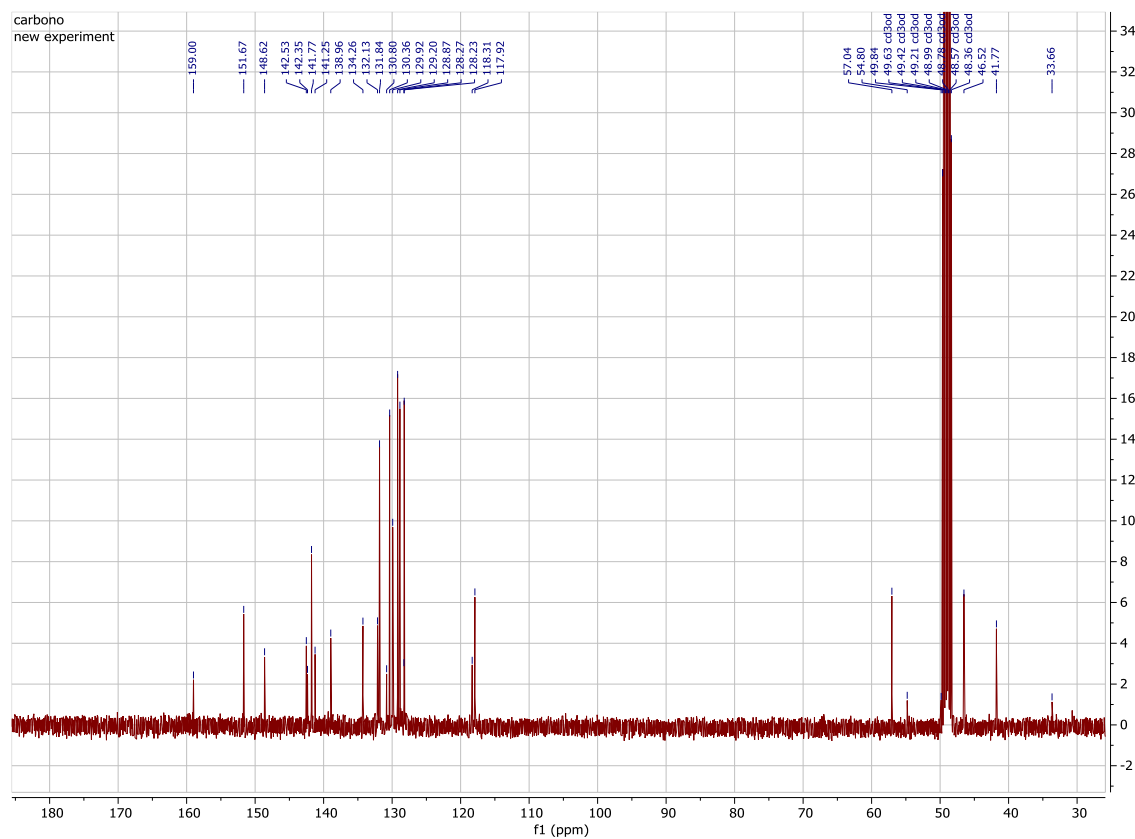
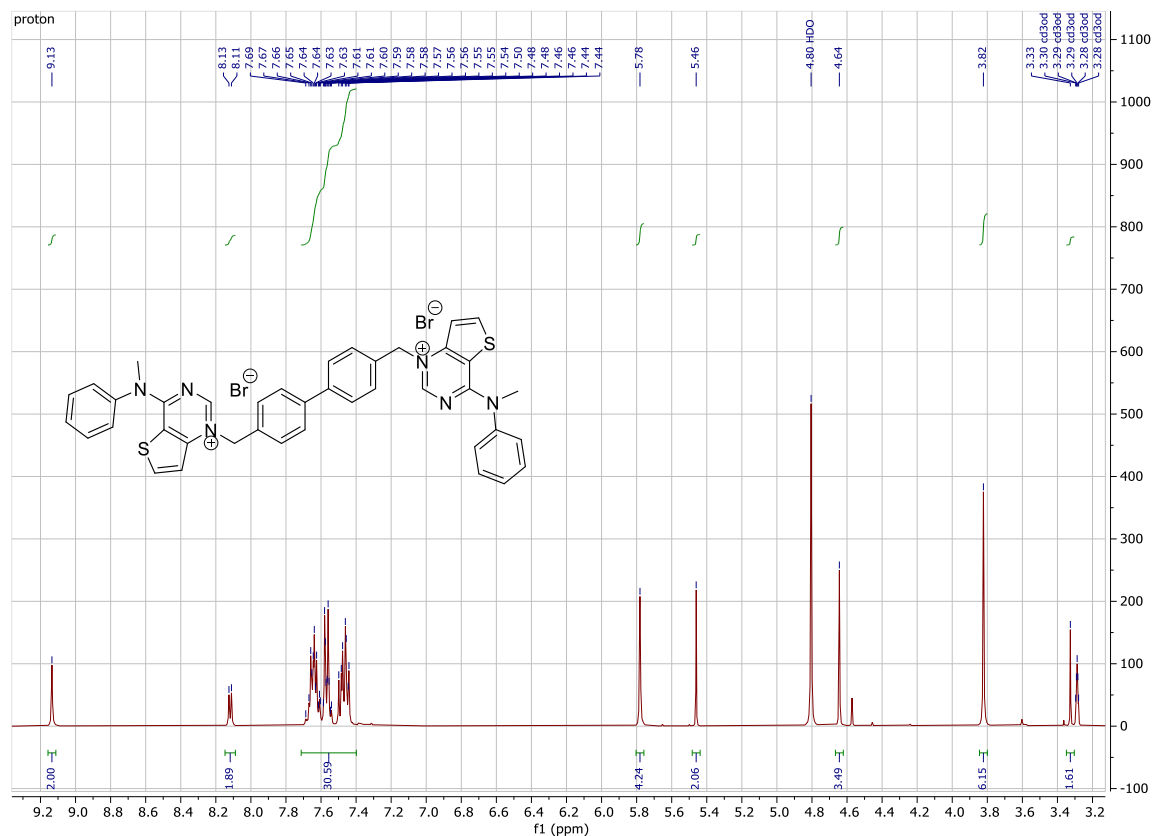




Fg-18



Fp-1



Fp-8

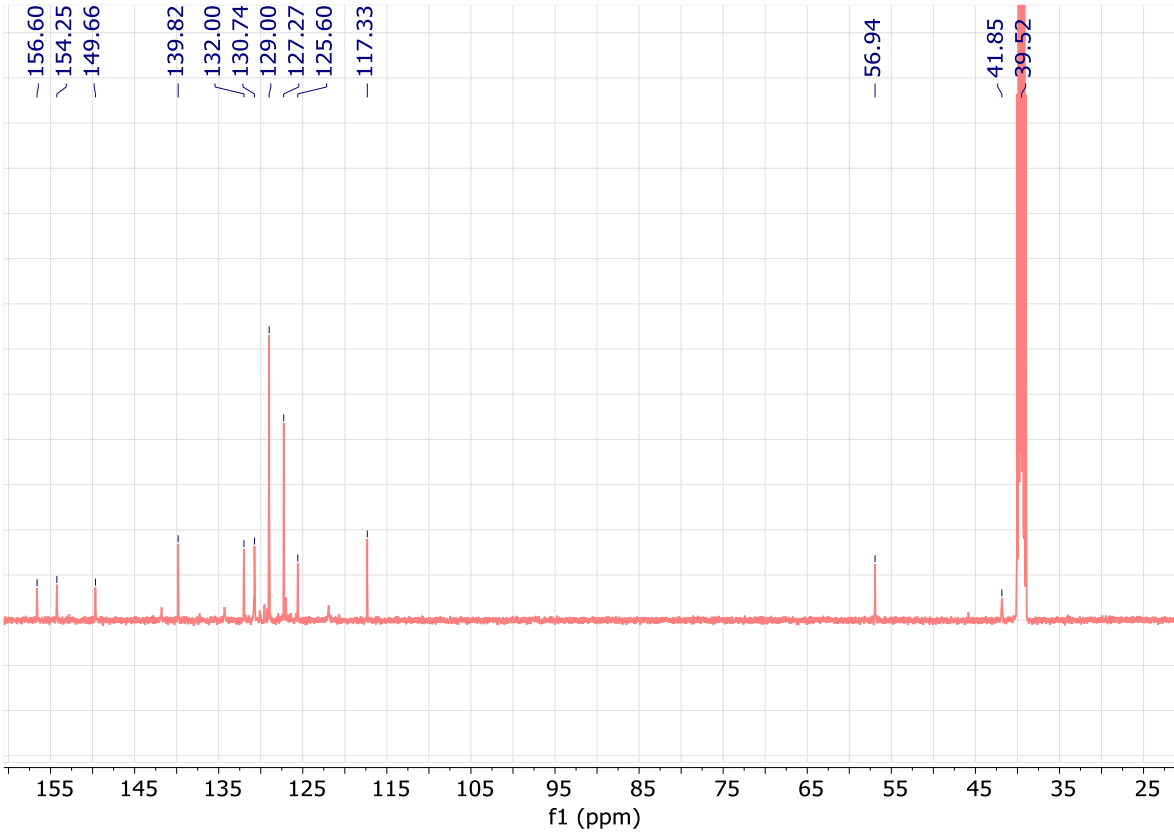
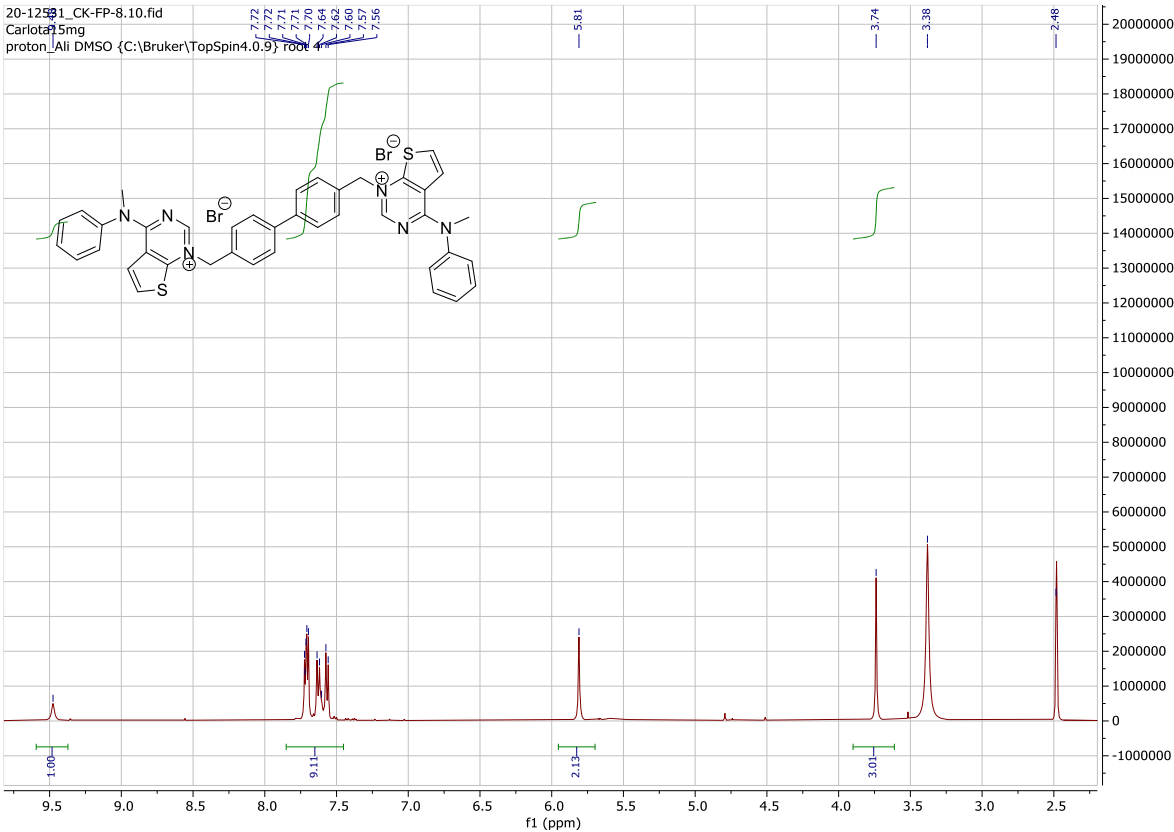


Fig-12

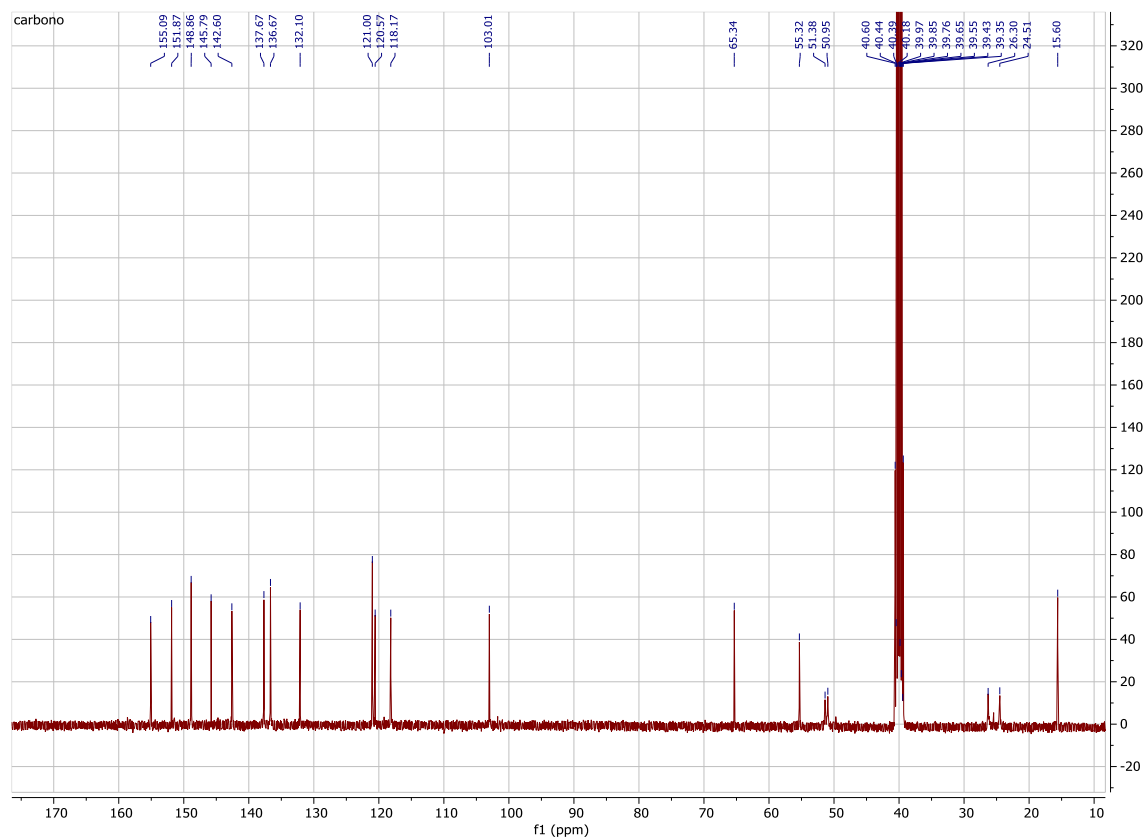
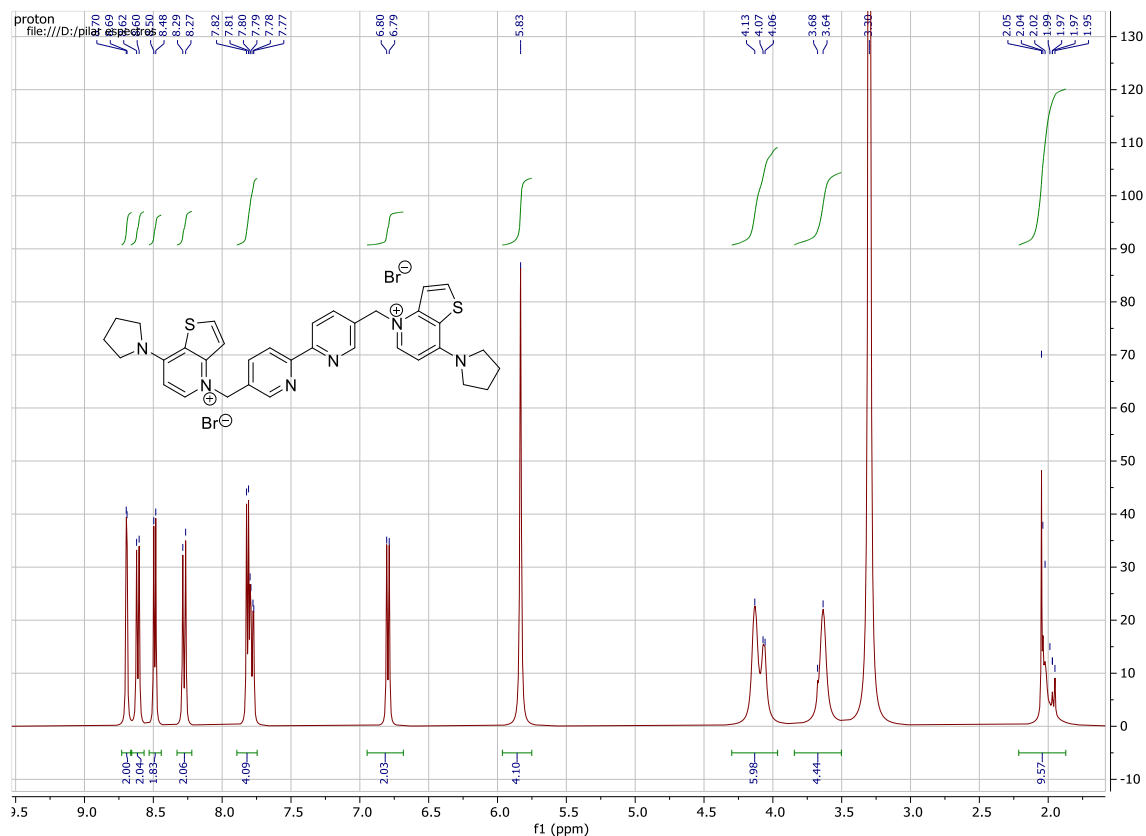
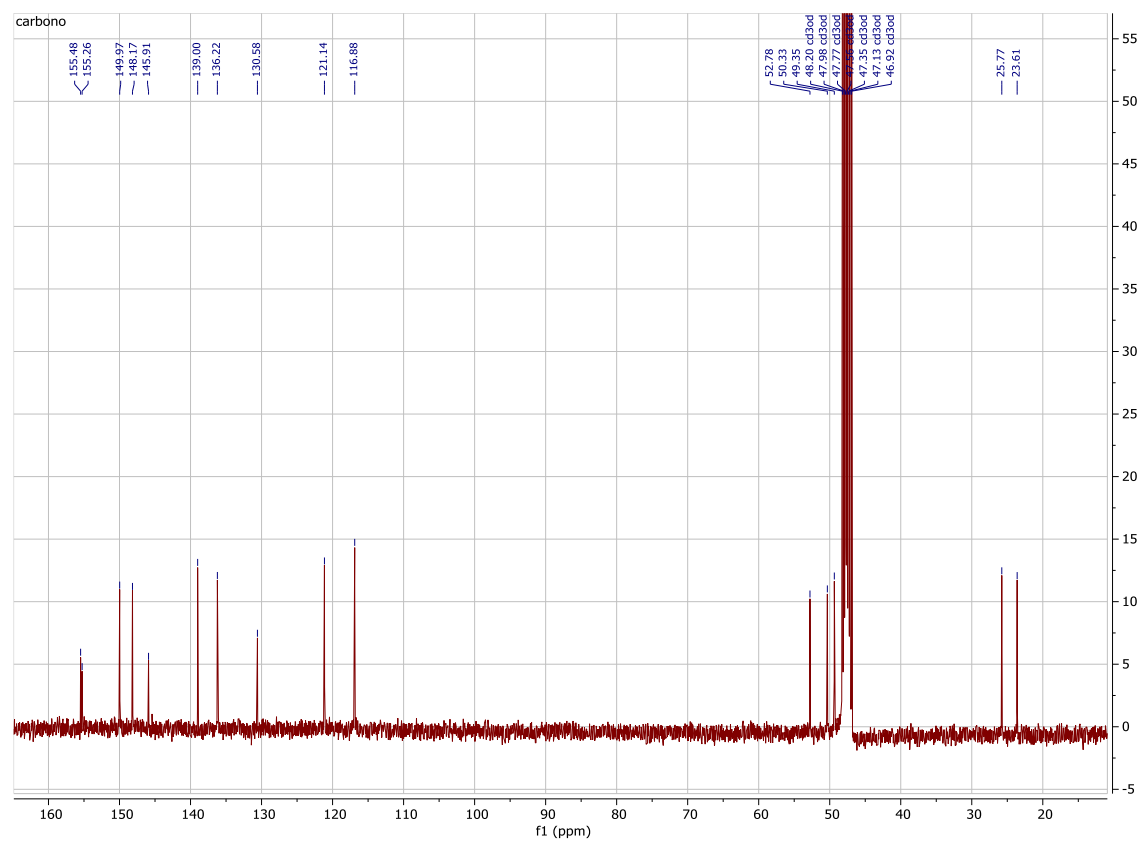
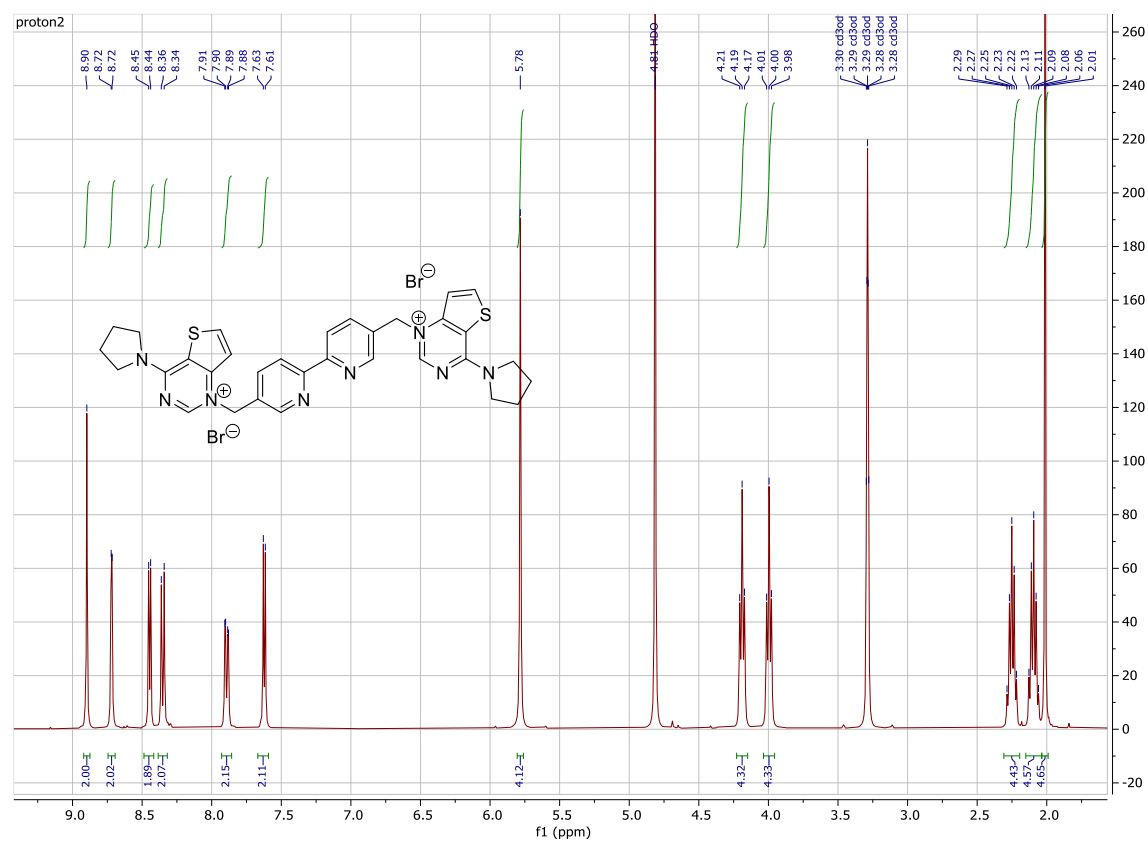
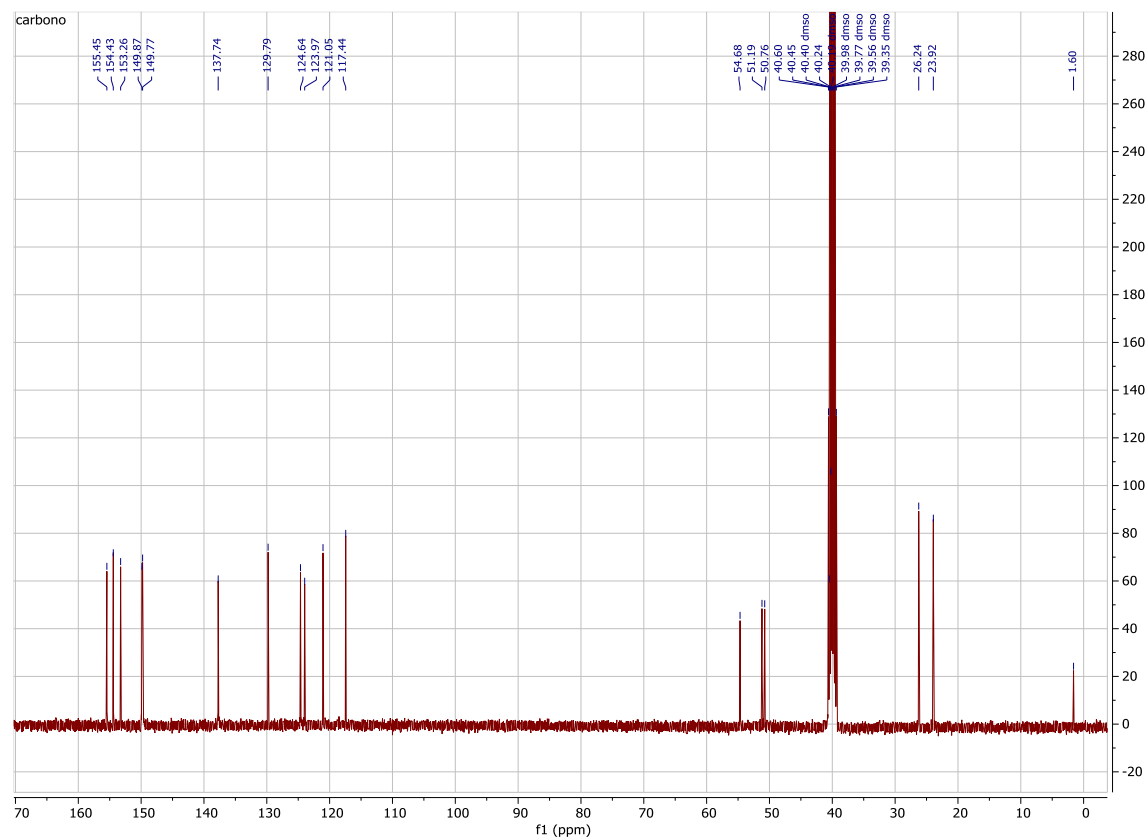
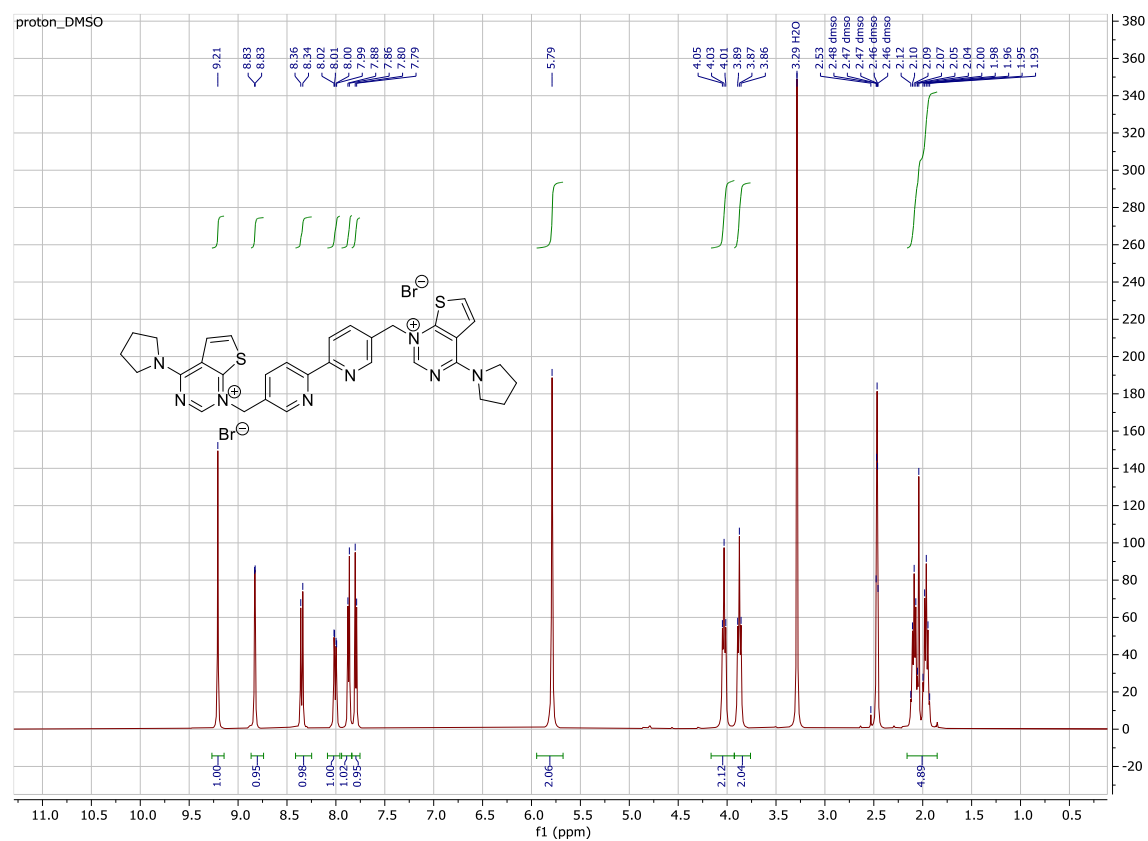


Fig-17



Fg-13



Fa-27

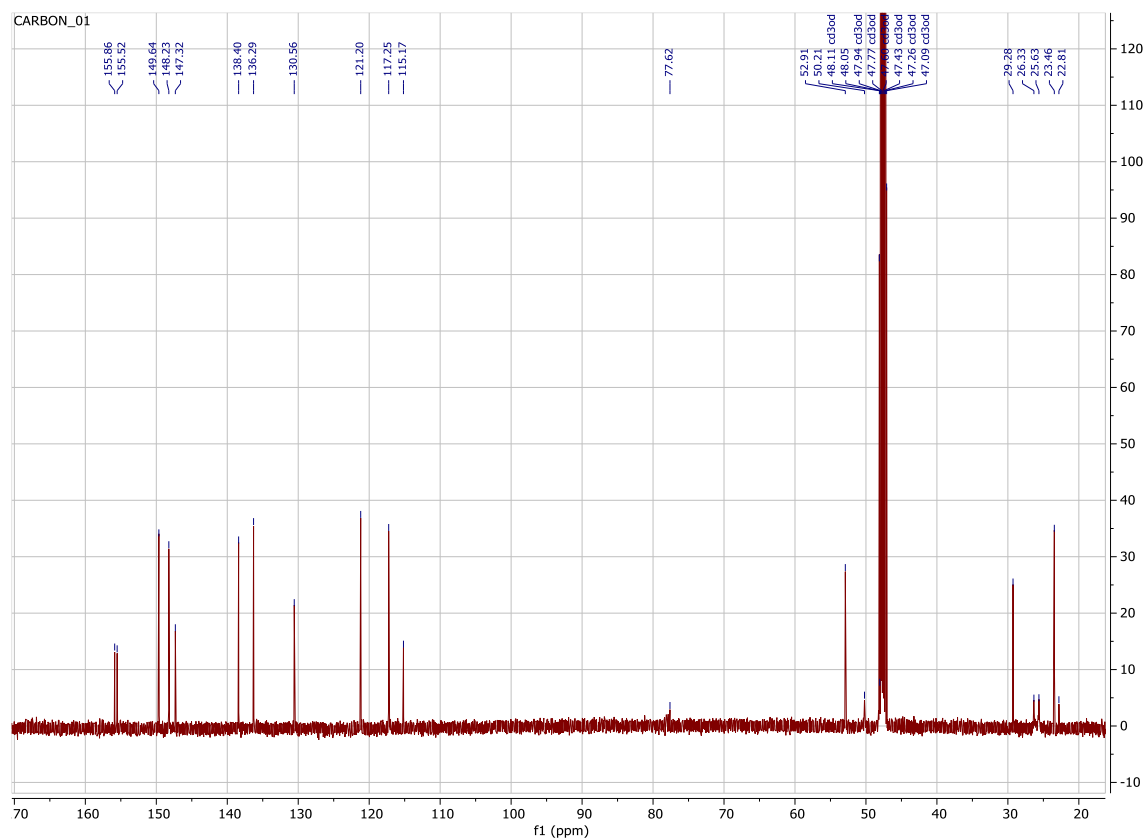
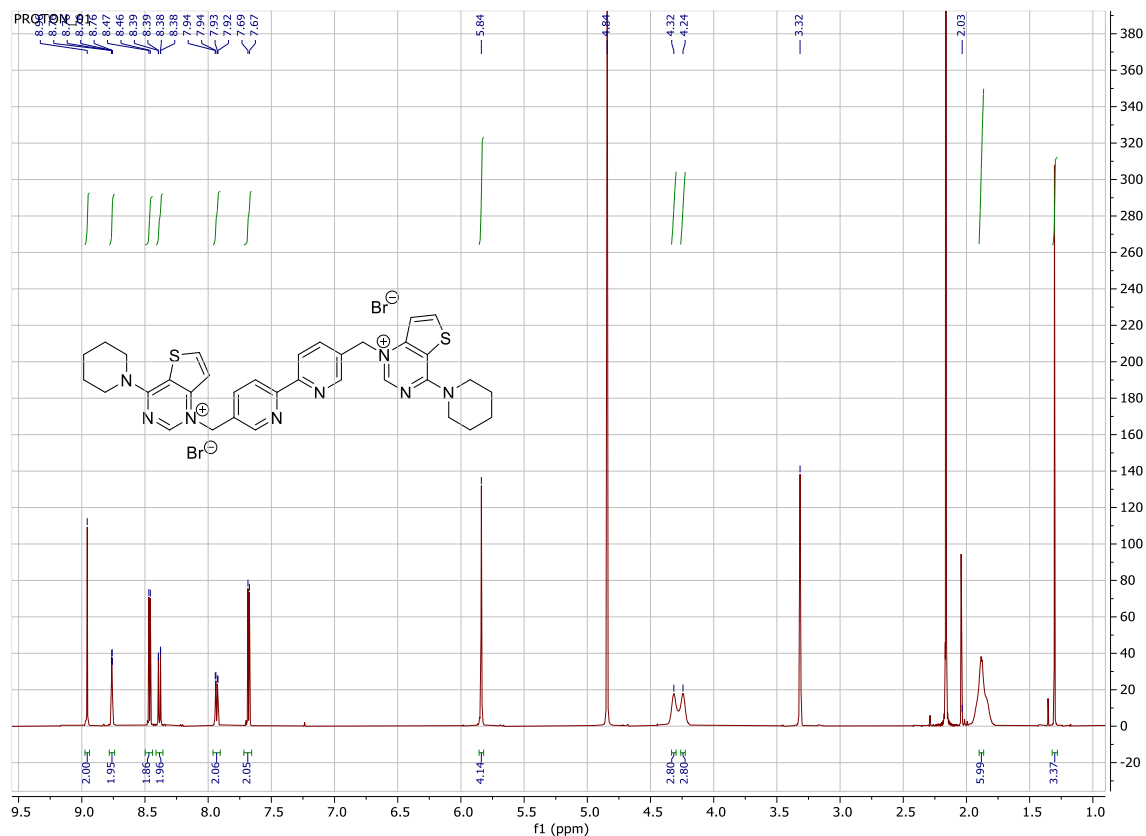
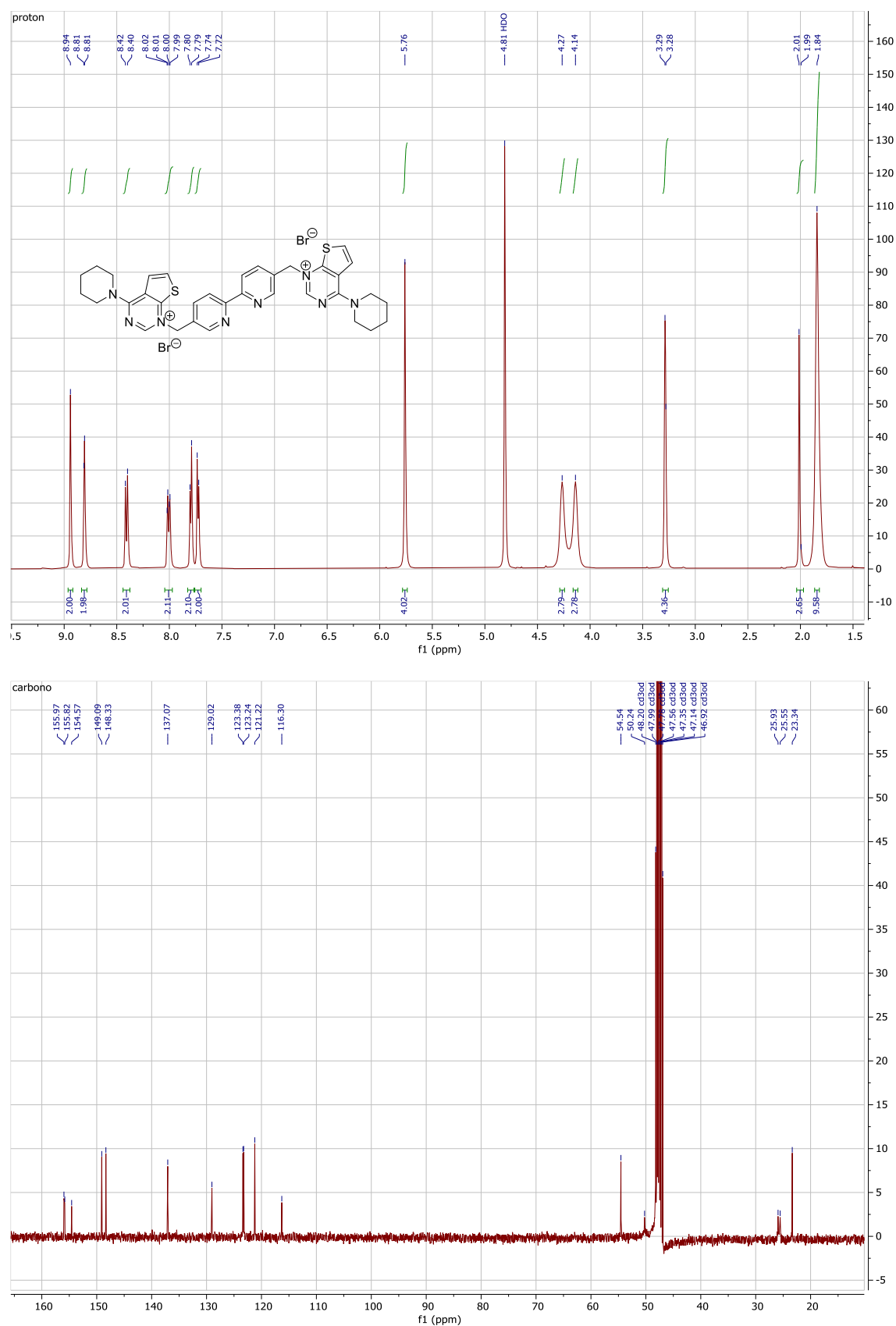


Fig-32



Fa-26

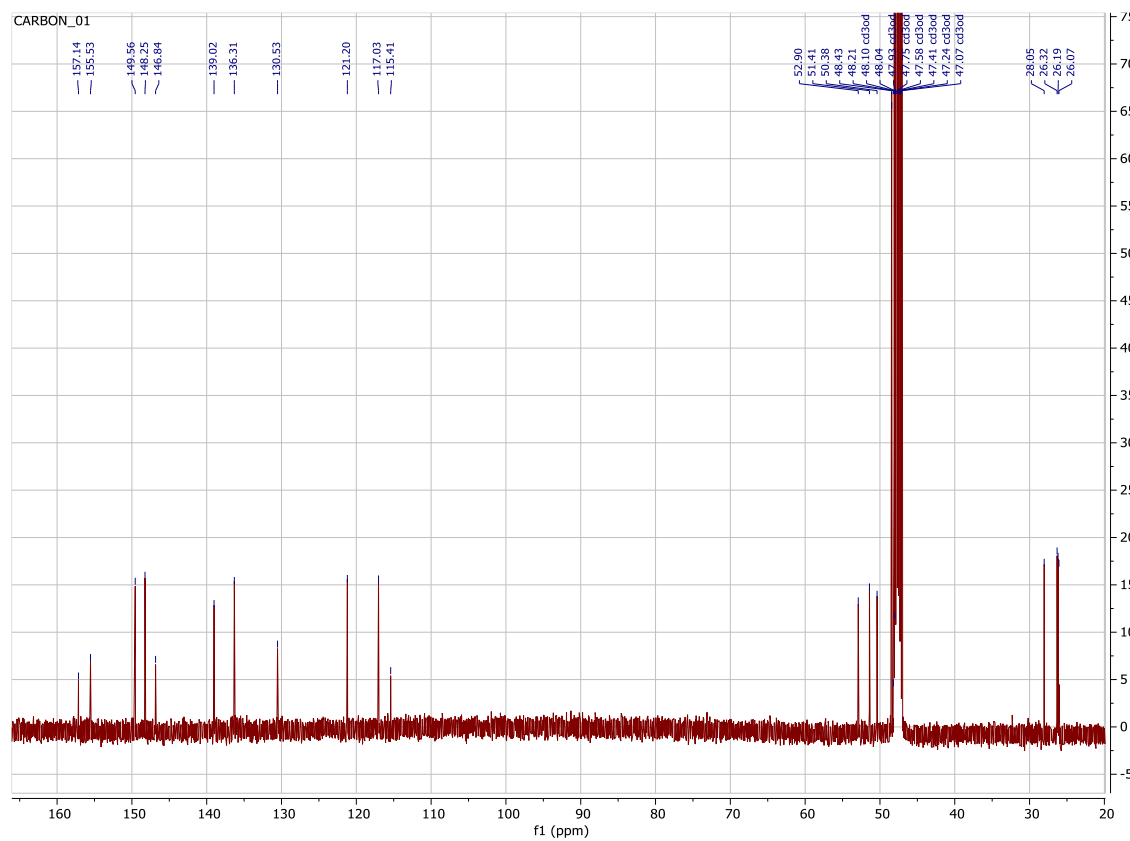
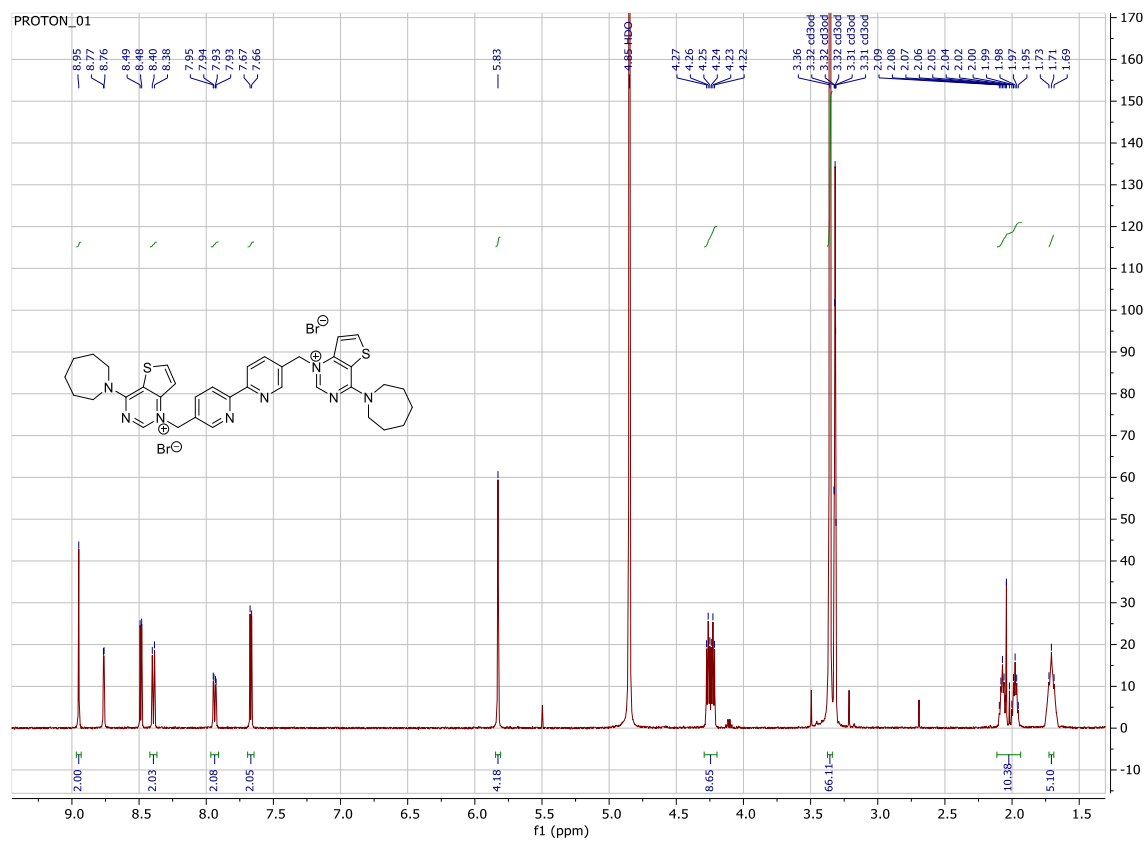


Fig-20

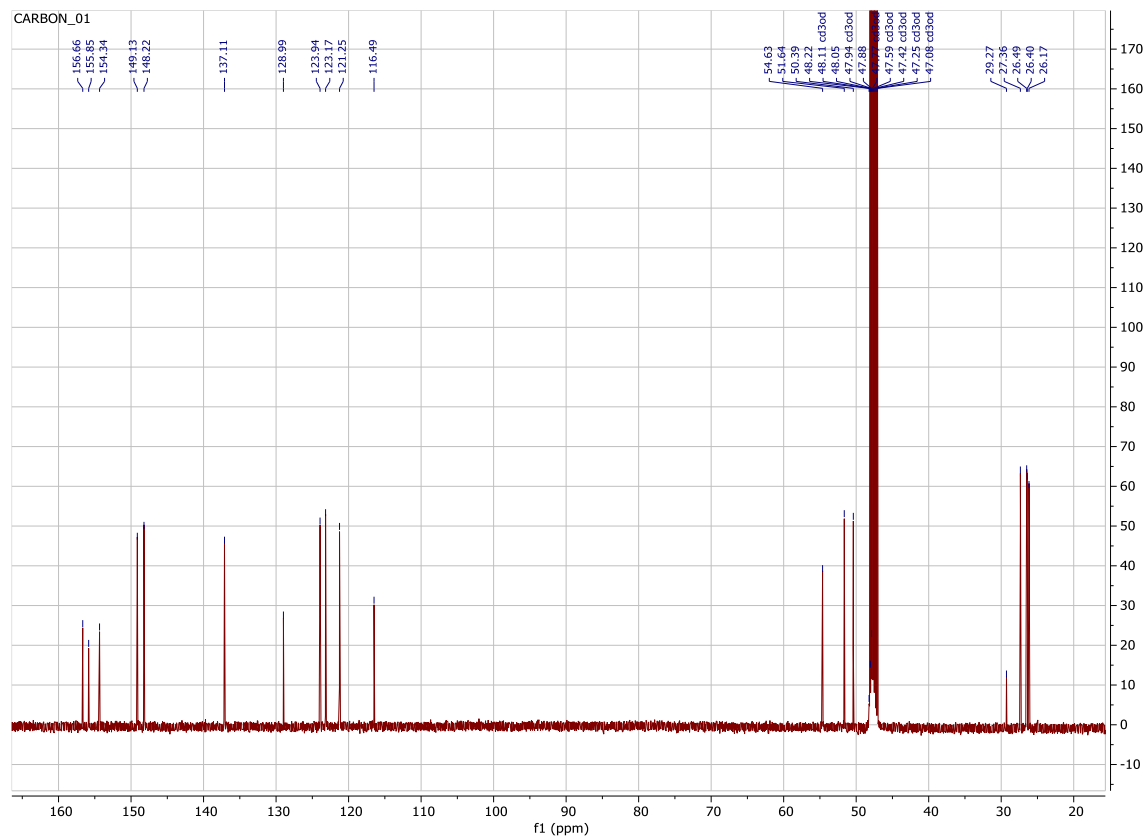
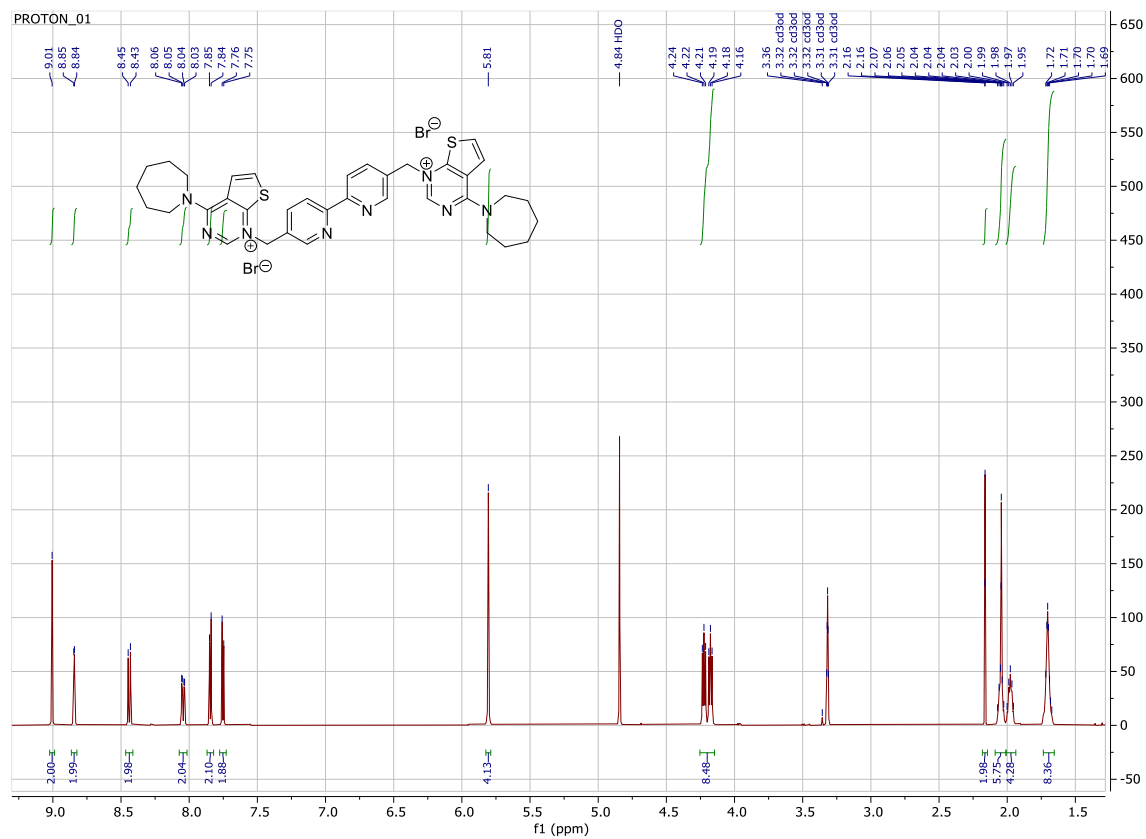
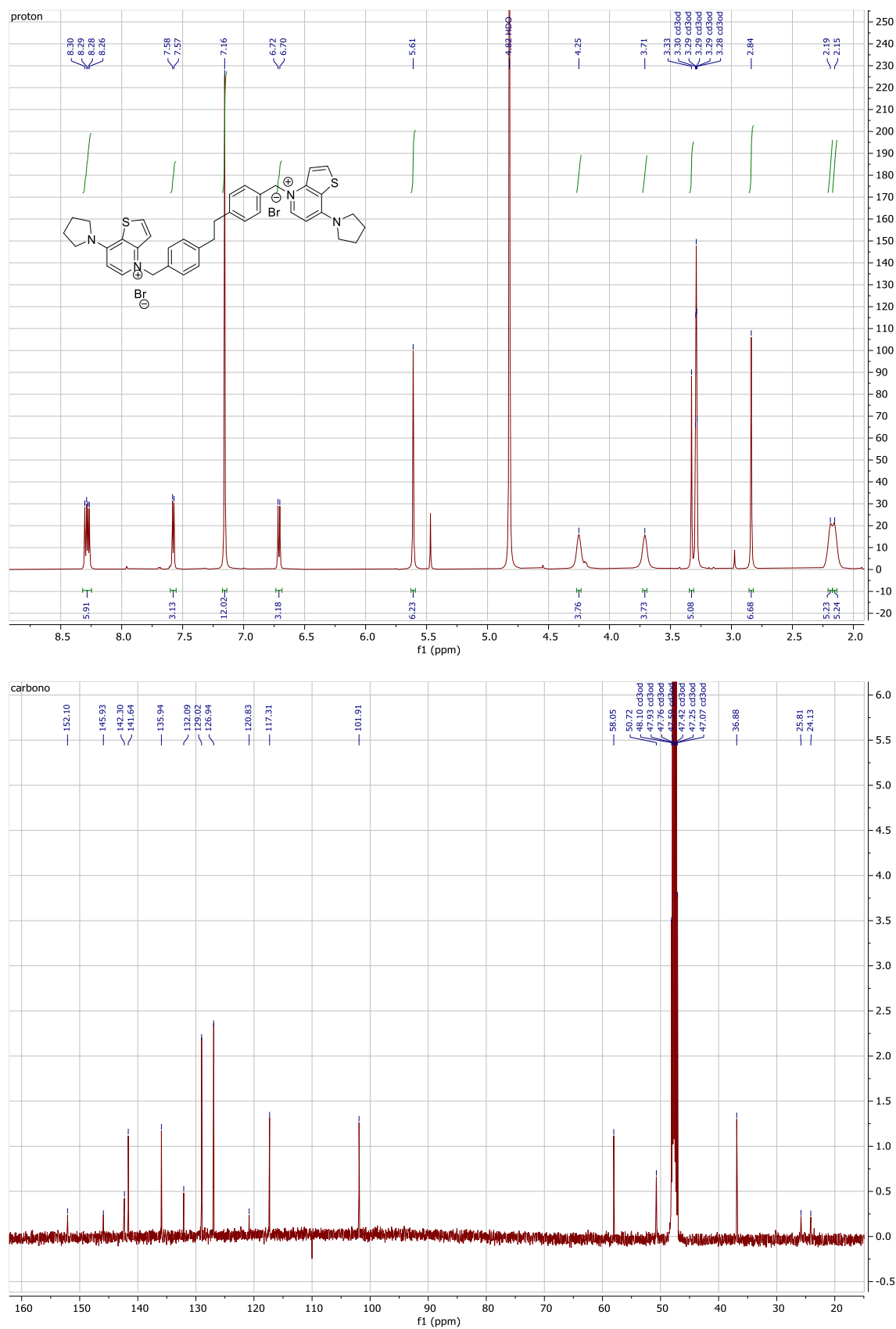


Fig-11



Chemical structure of compound 10:

C1CCN1c2nc3cc(Cc4ccc(Cc5ccc(cc5)C6=NC7C(=N6)N(CCN7)S8C=CC=C8)cc4)cc3s2.[Br-]

¹H NMR (400 MHz, CDCl₃) data:

Chemical Shift (ppm)	Integration
8.81	2.00
8.43, 8.41	2.01
7.55, 7.53, 7.25, 7.24, 7.23, 7.19, 7.17, 7.16	2.03, 4.10, 4.08
5.60	4.02
4.81 (H ₂ O)	
4.20, 4.18, 4.16, 3.99, 3.98, 3.96	4.20, 4.23
3.30, 3.29, 3.28, 3.28, 3.28, 3.28 (CDCl ₃)	
2.85	4.07
2.28, 2.24, 2.24, 2.23, 2.21, 2.12, 2.10, 2.07, 2.05, 2.01, 2.01	4.27, 8.17

¹³C NMR (100 MHz, CDCl₃) data:

Chemical Shift (ppm)
155.27
149.77, 146.17, 142.44, 138.64
131.33, 129.11, 127.17
117.18, 116.78
55.31, 50.24, 49.28, 48.94, 48.64, 47.78, 47.57, 47.36, 47.14, 46.93, 46.82
25.78, 23.62

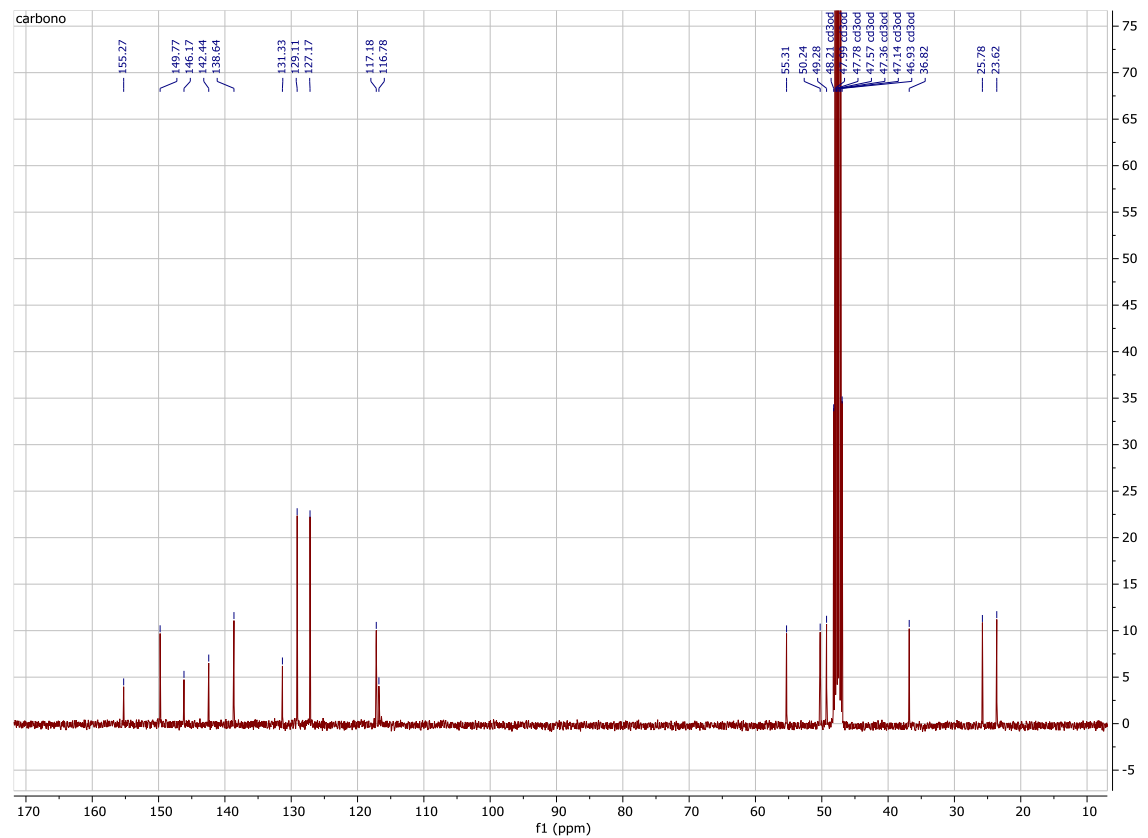
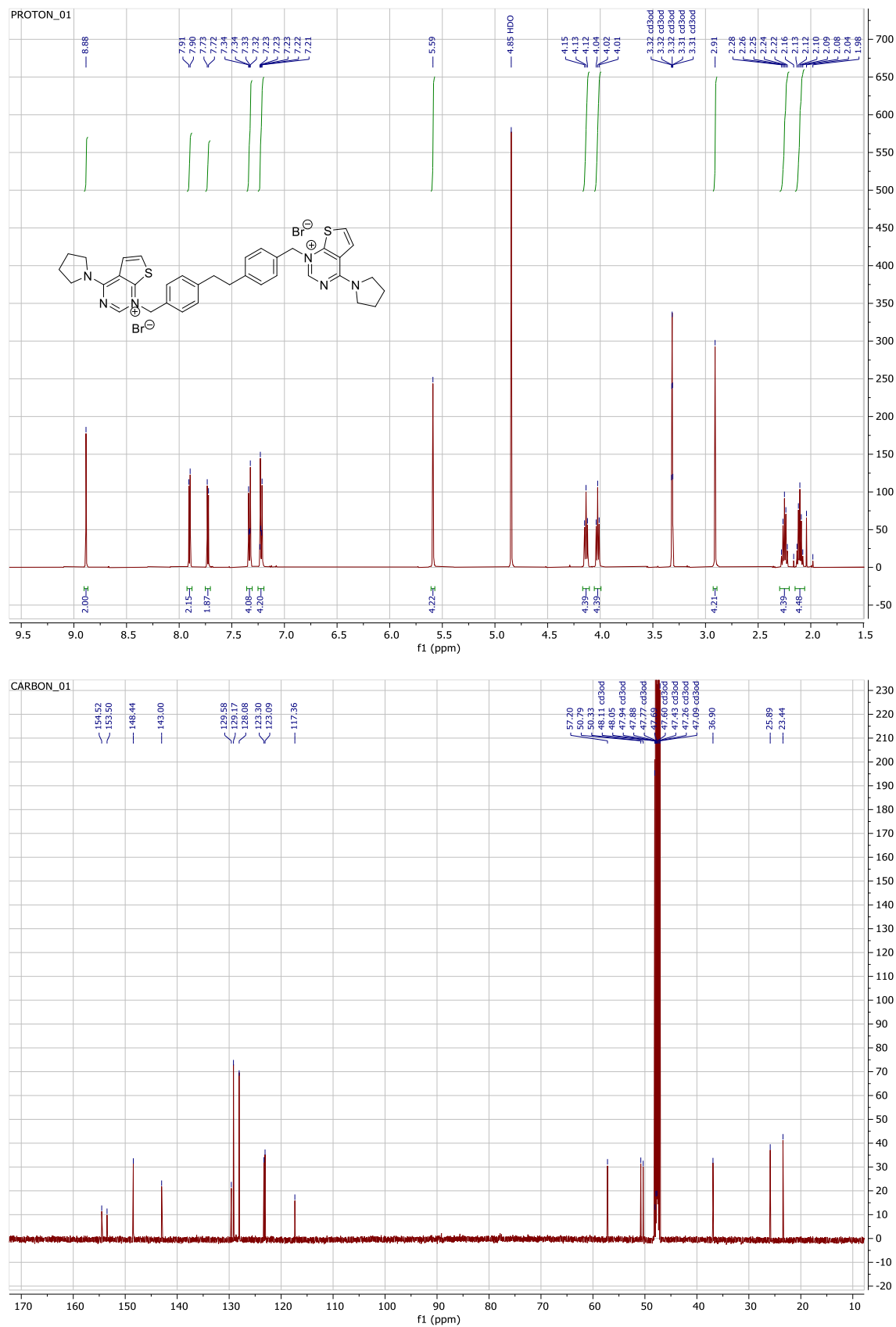


Fig-15



Fa-25

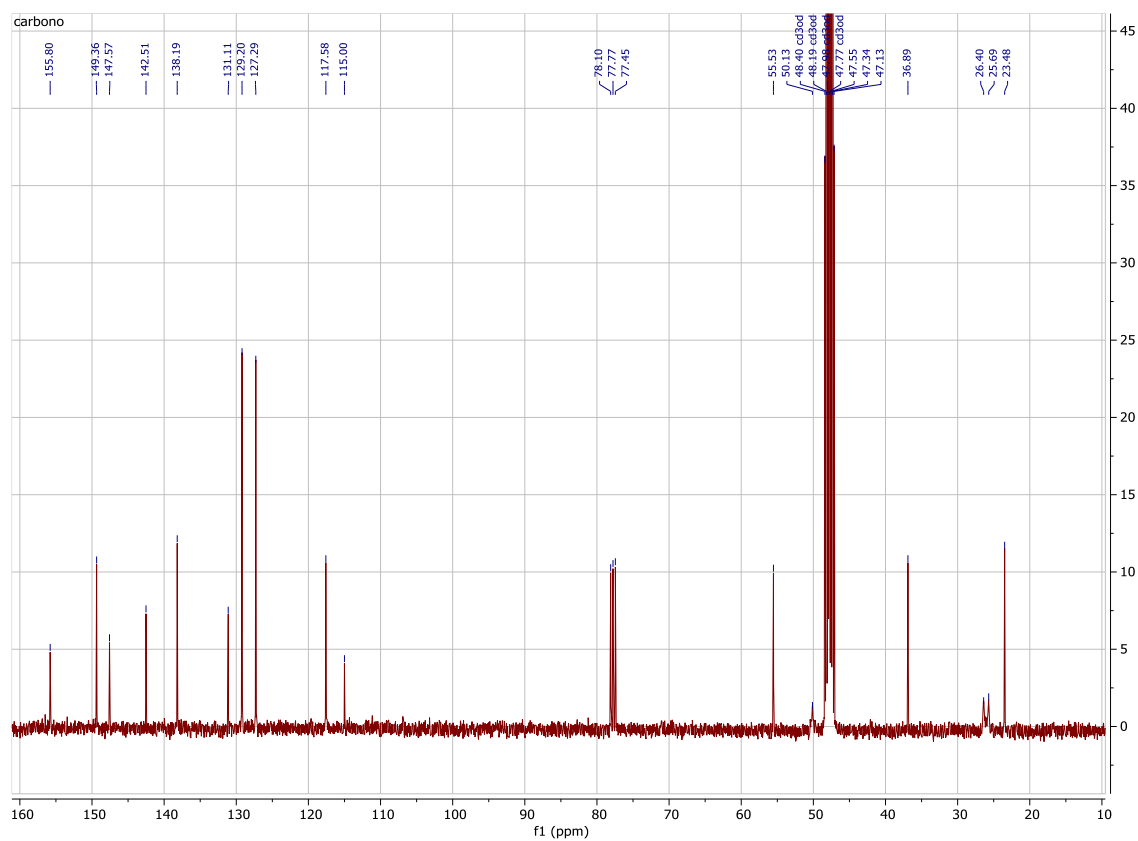
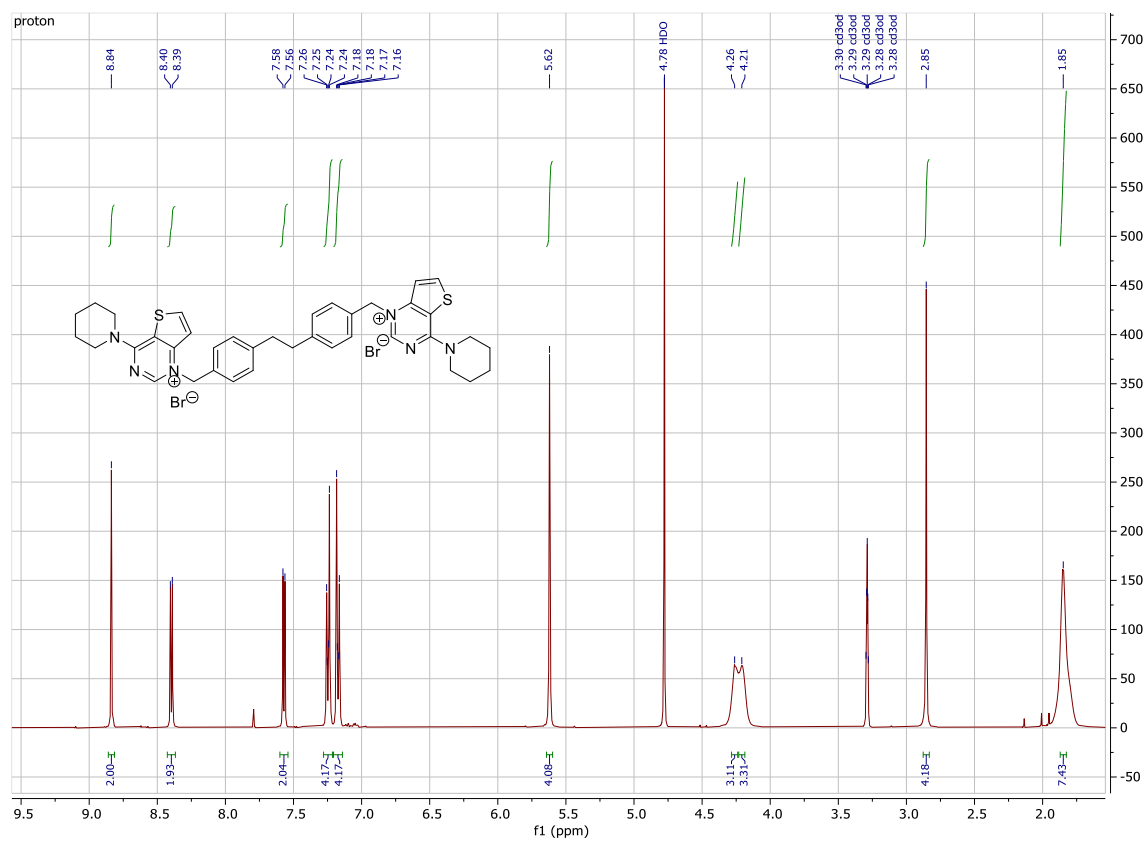
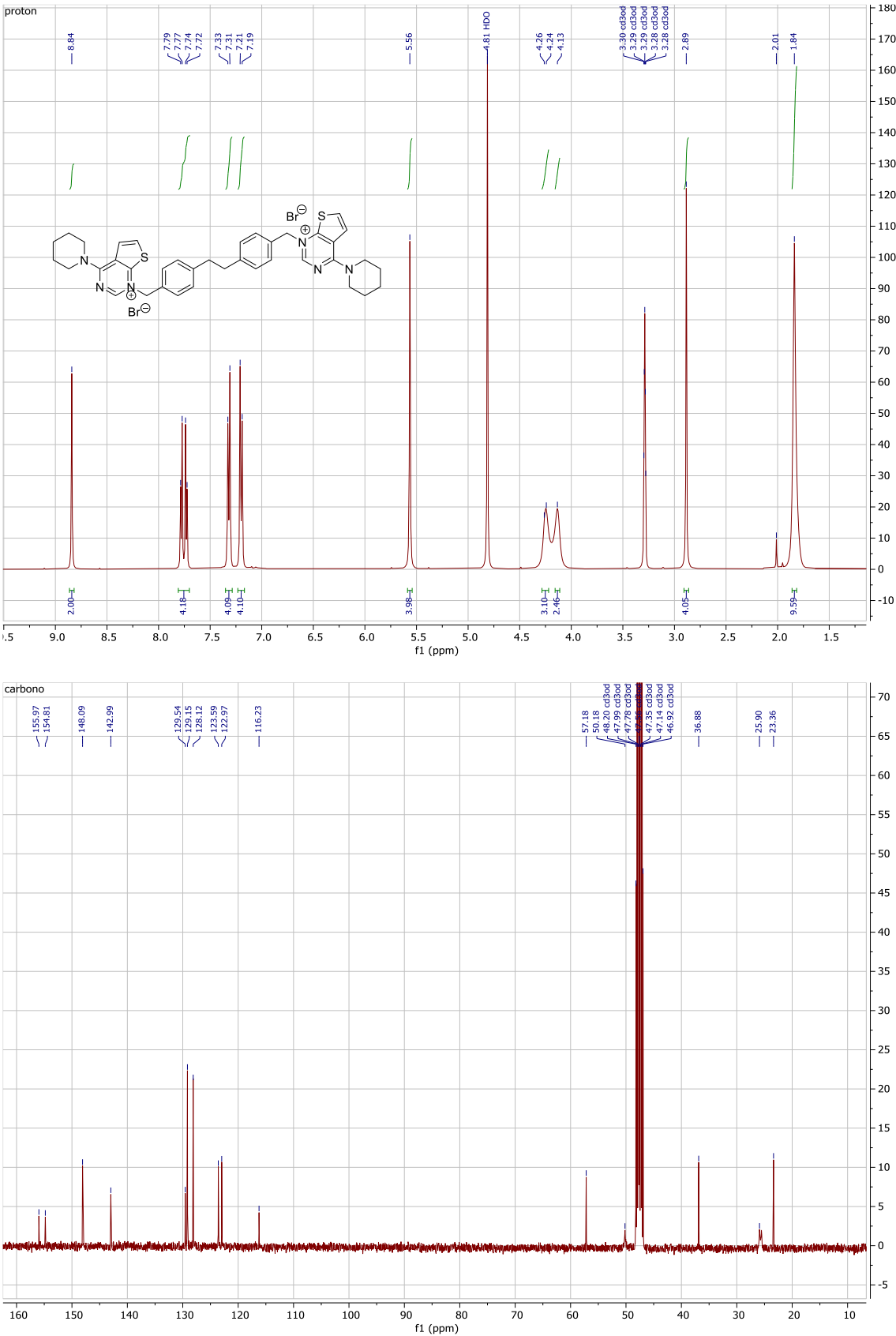
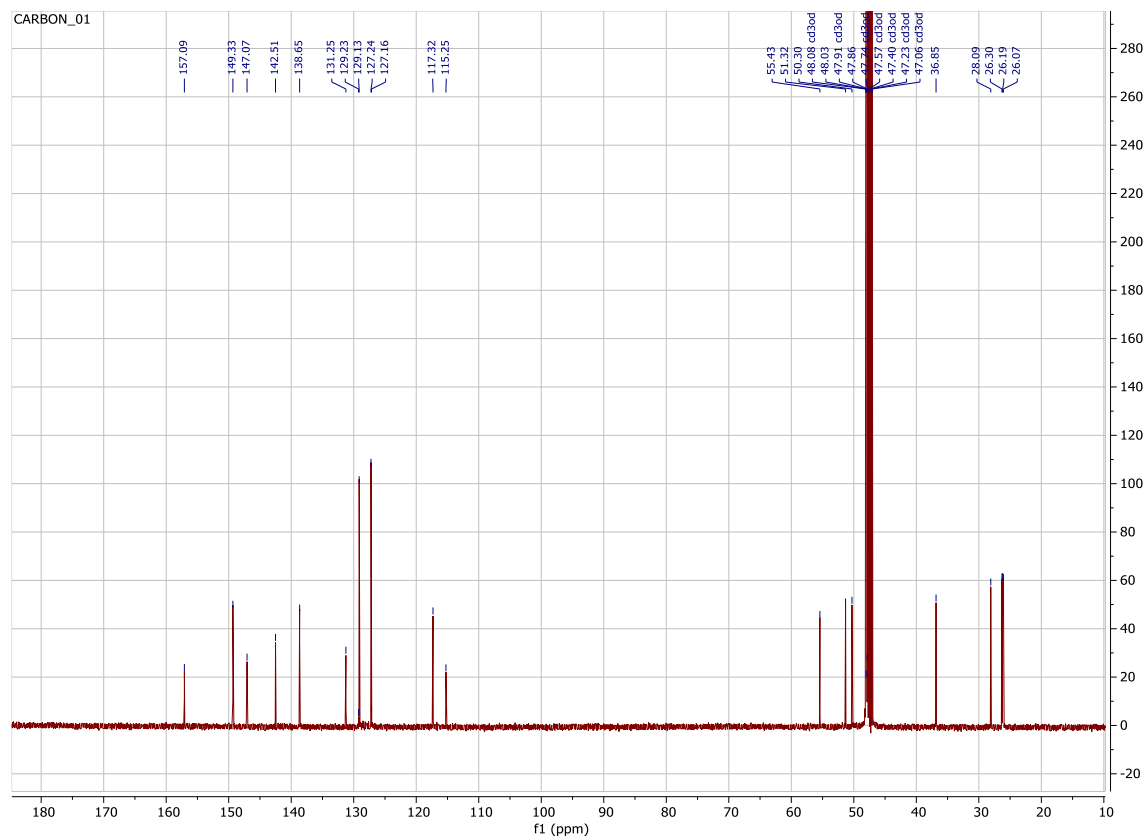
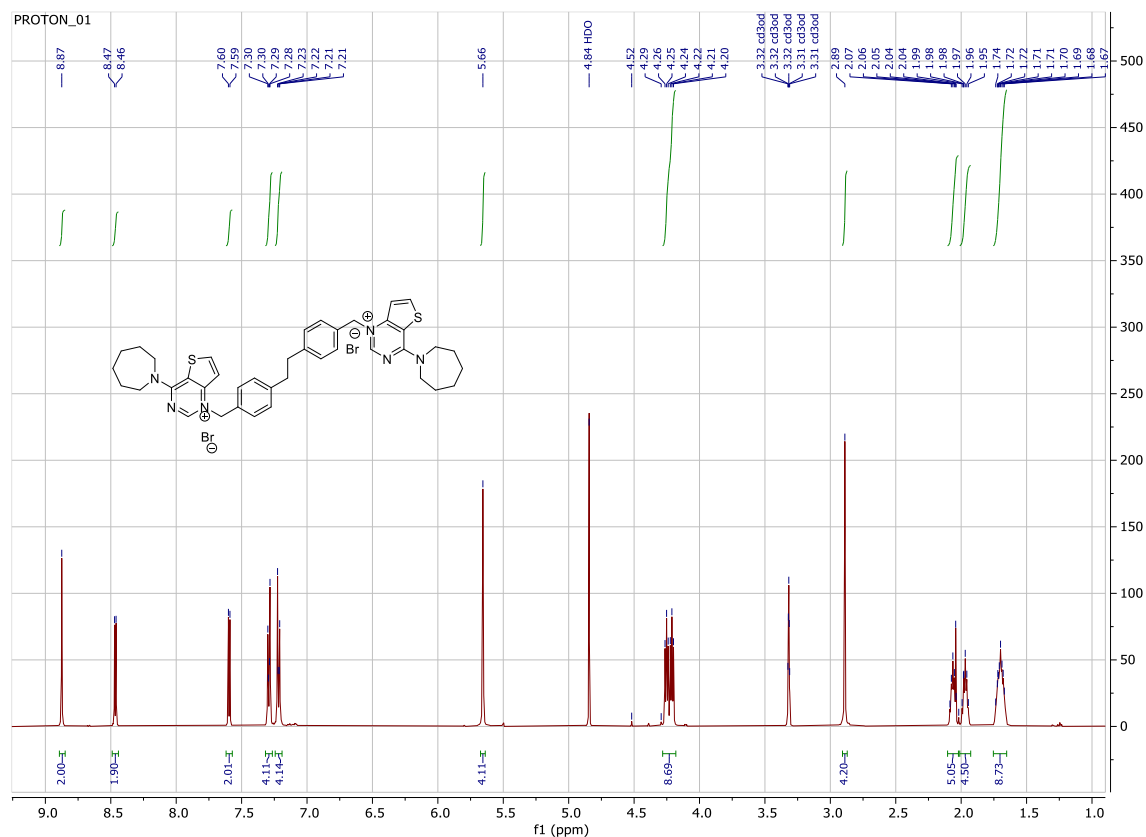


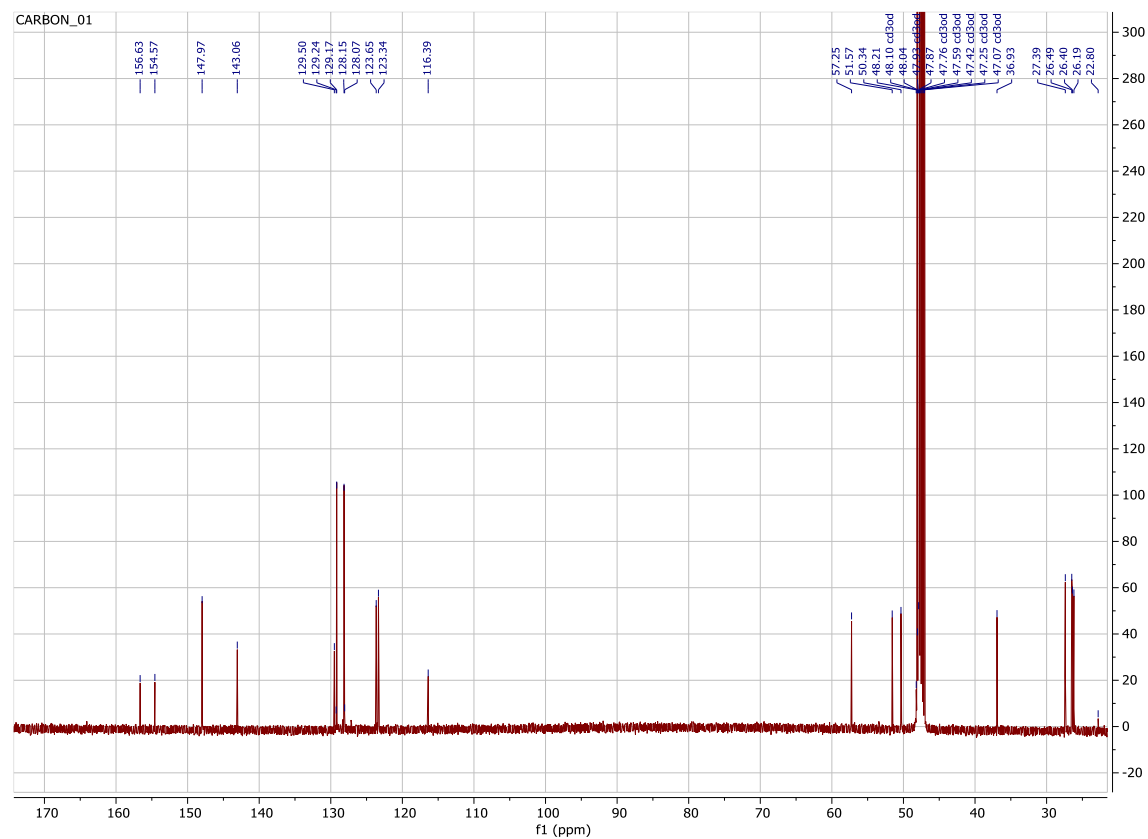
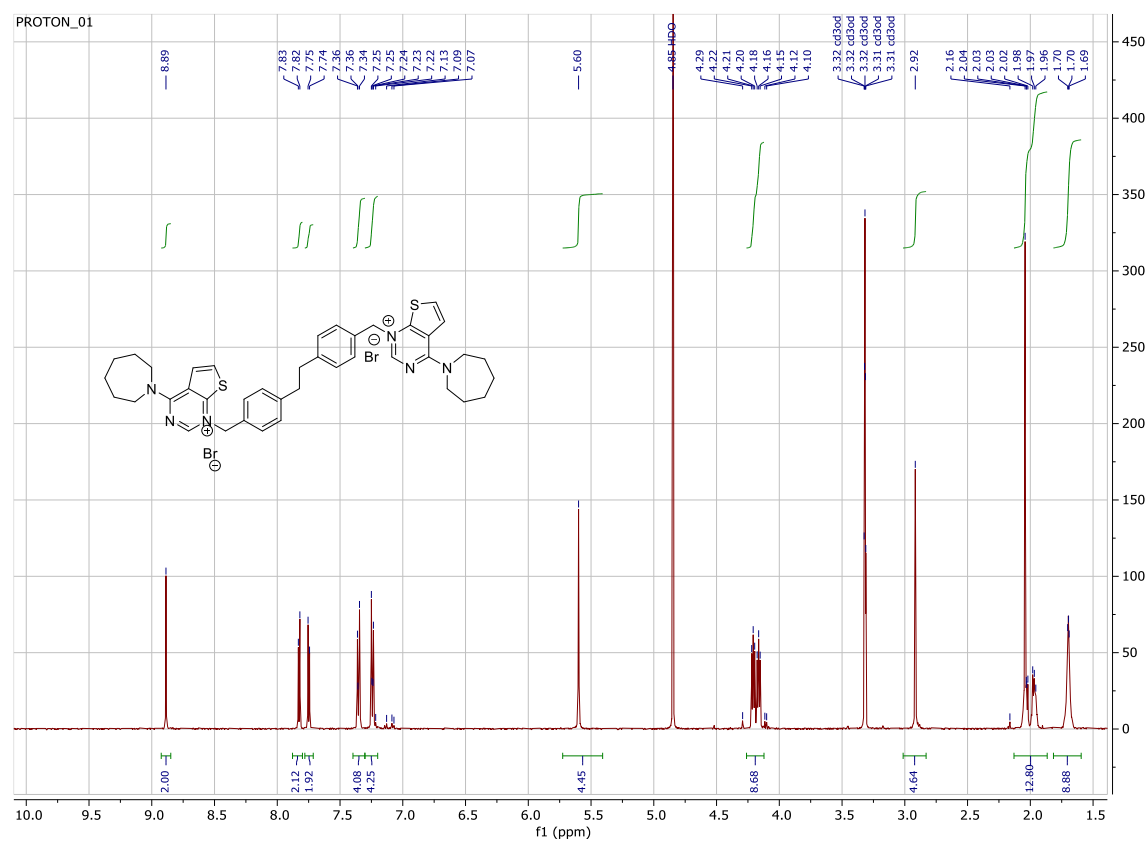
Fig-31



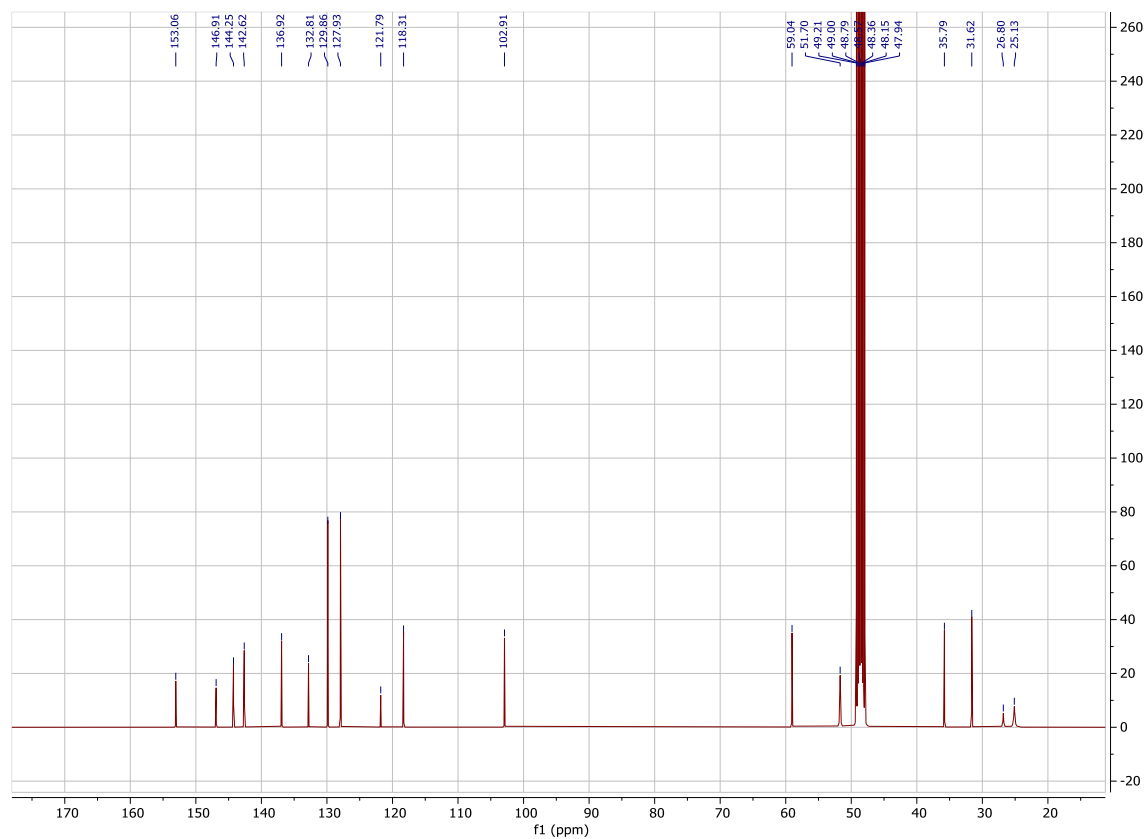
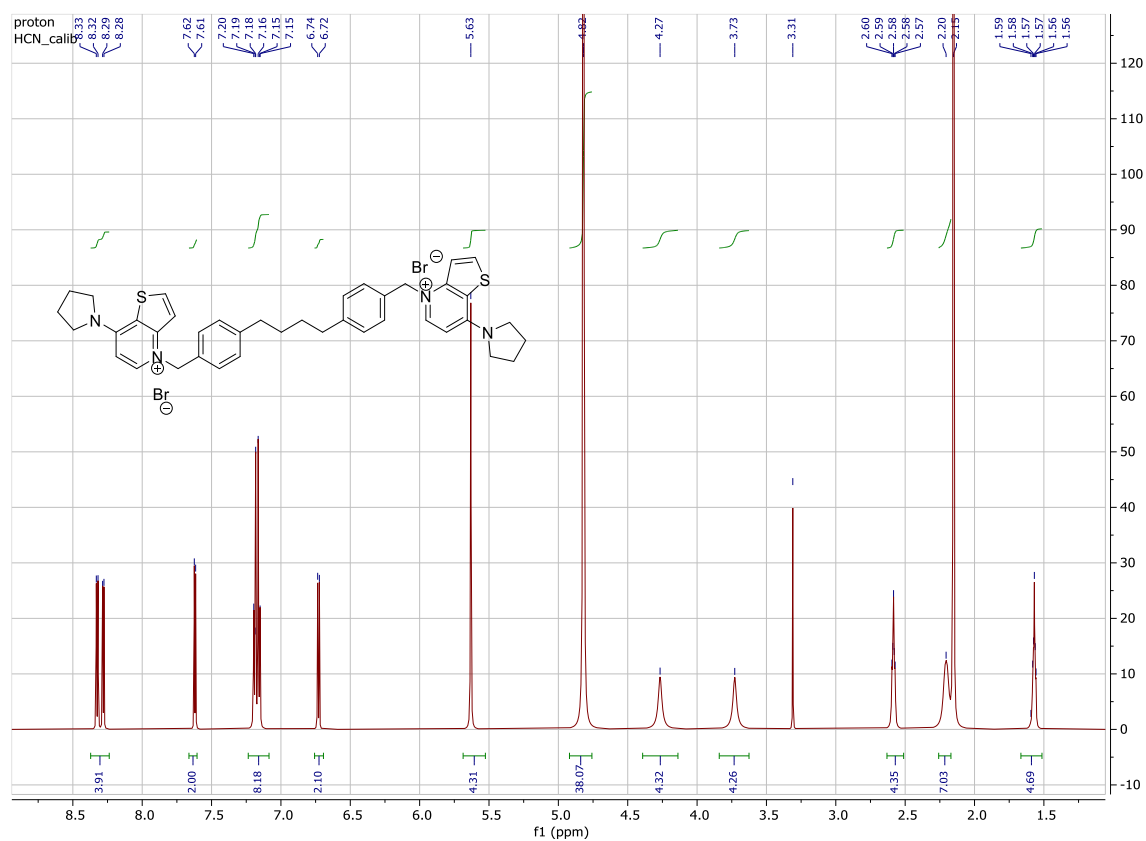
Fa-23



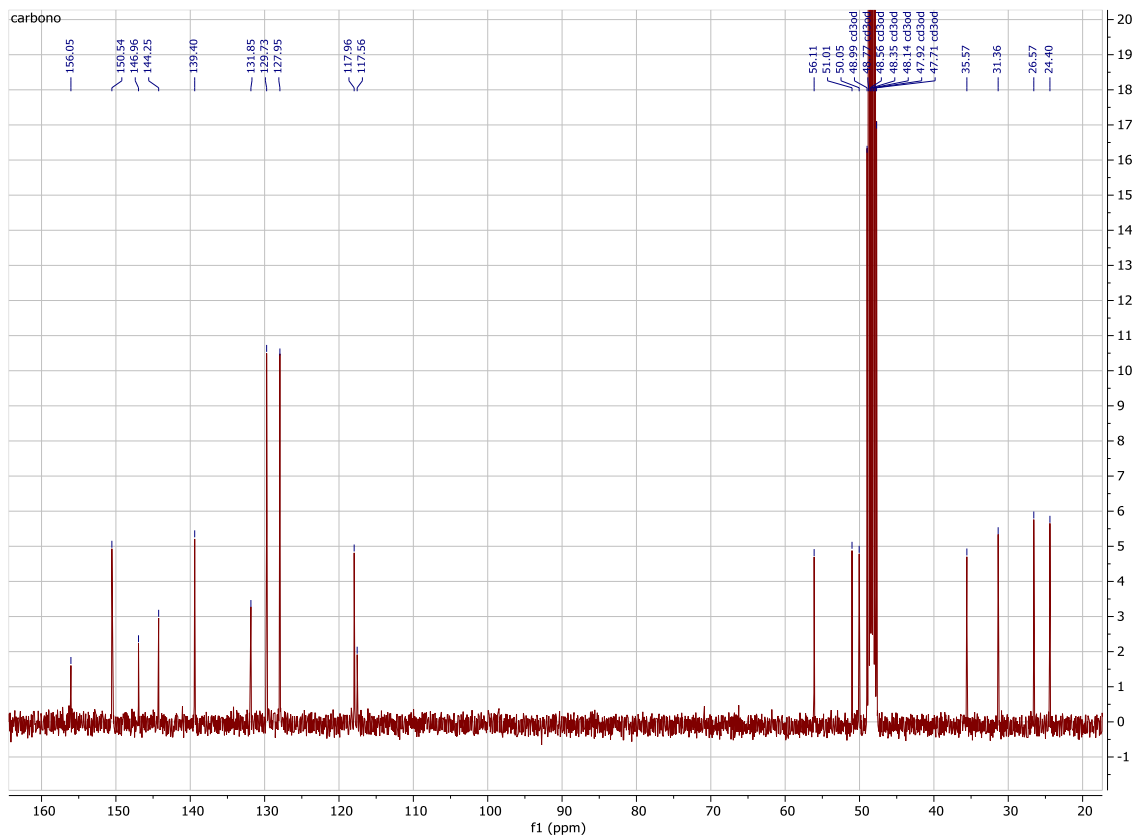
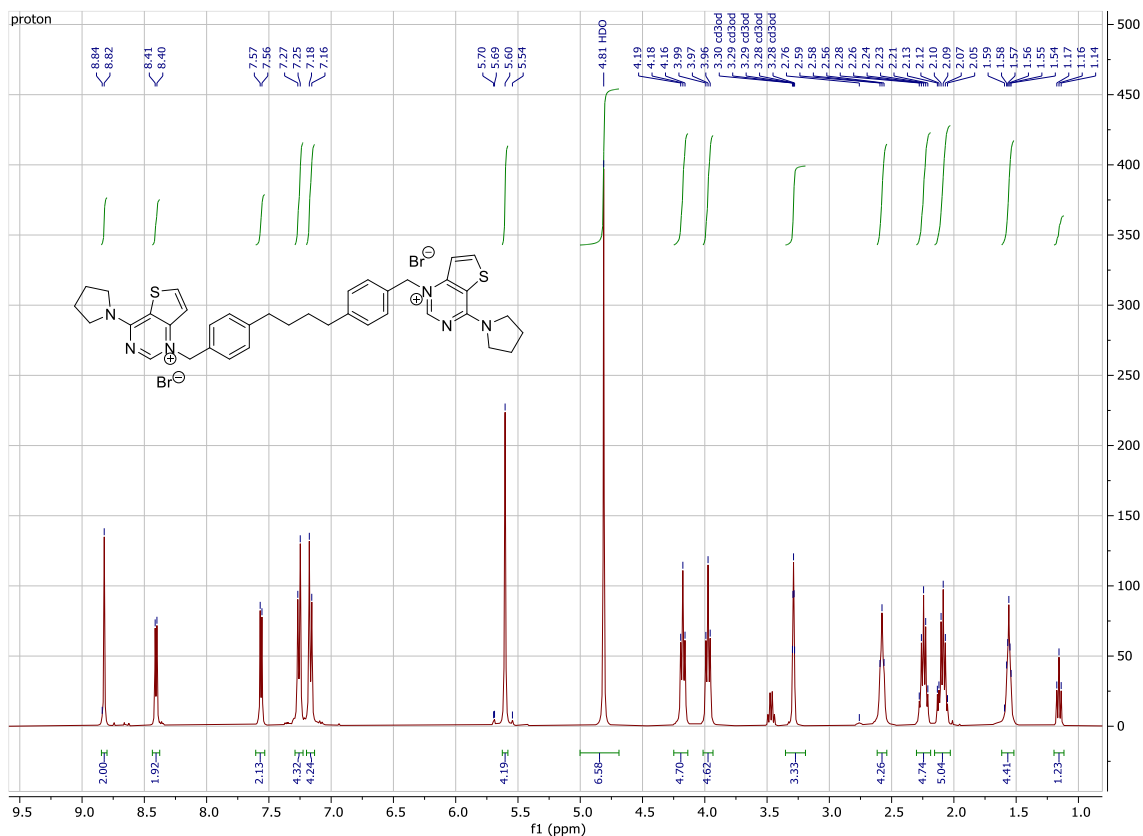
Fg-19



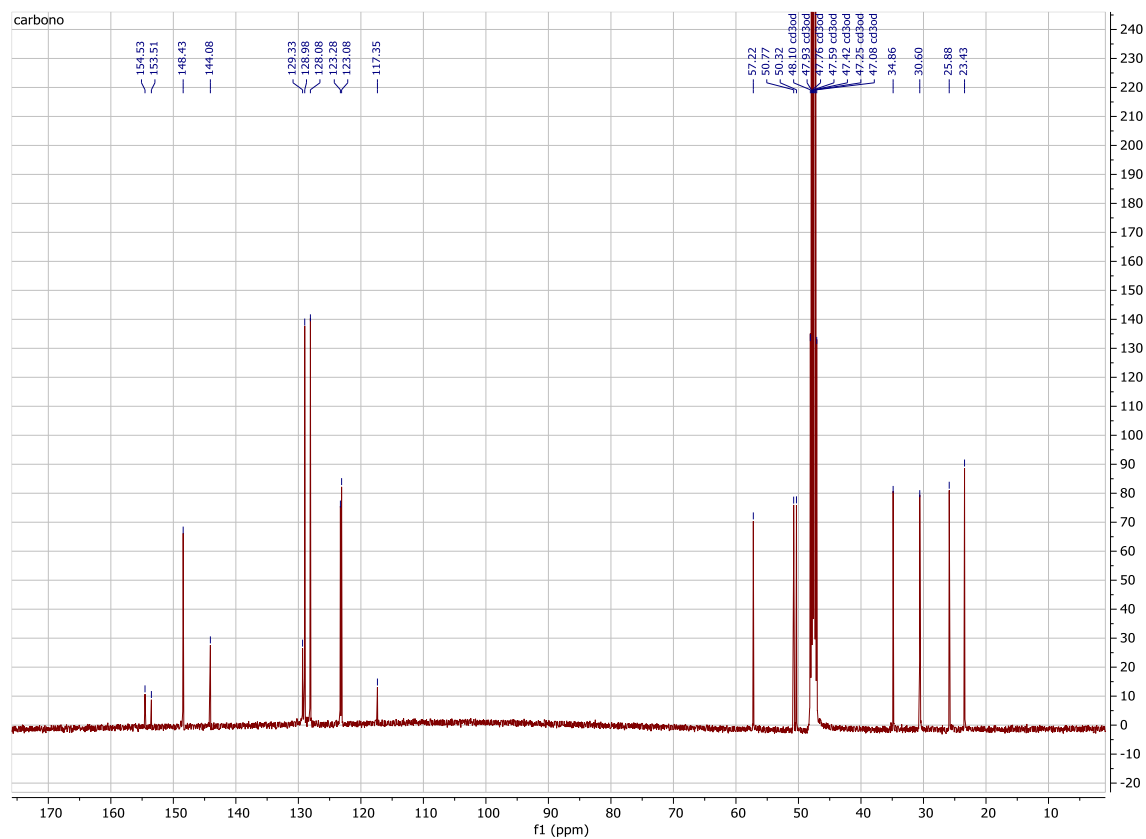
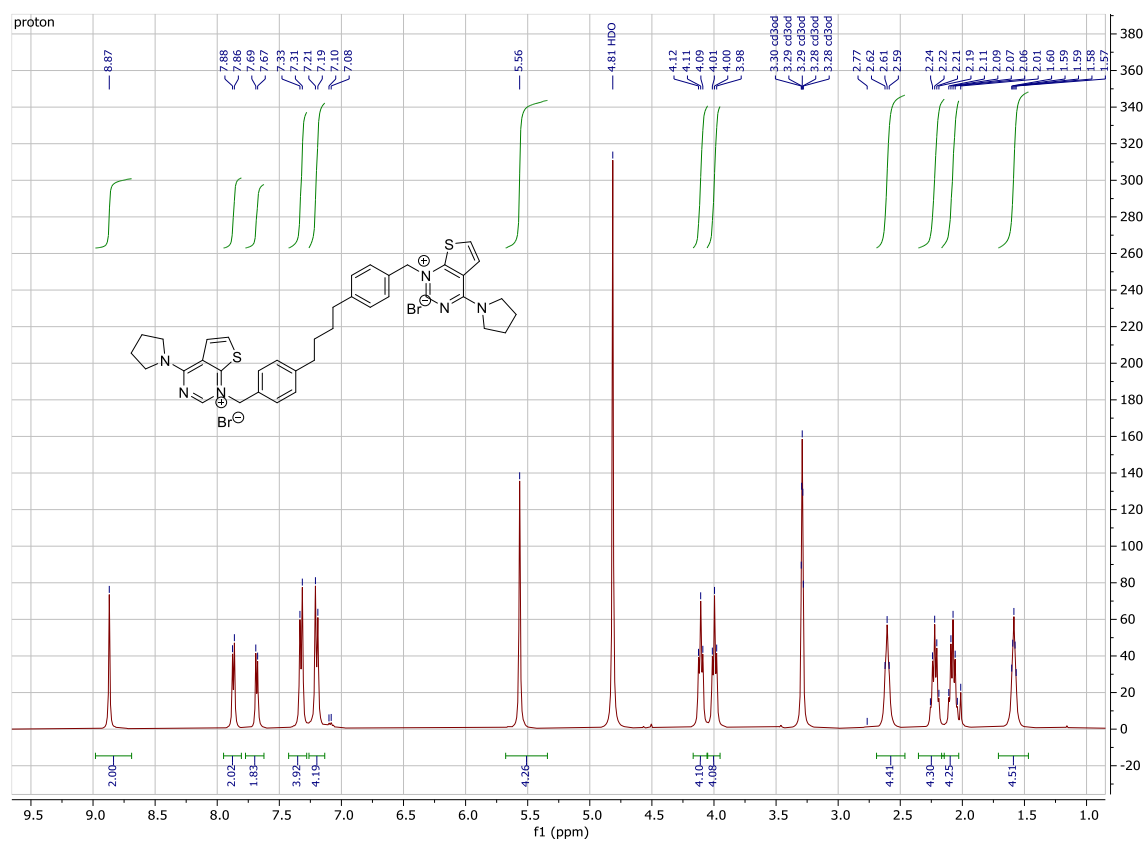
Ff-1



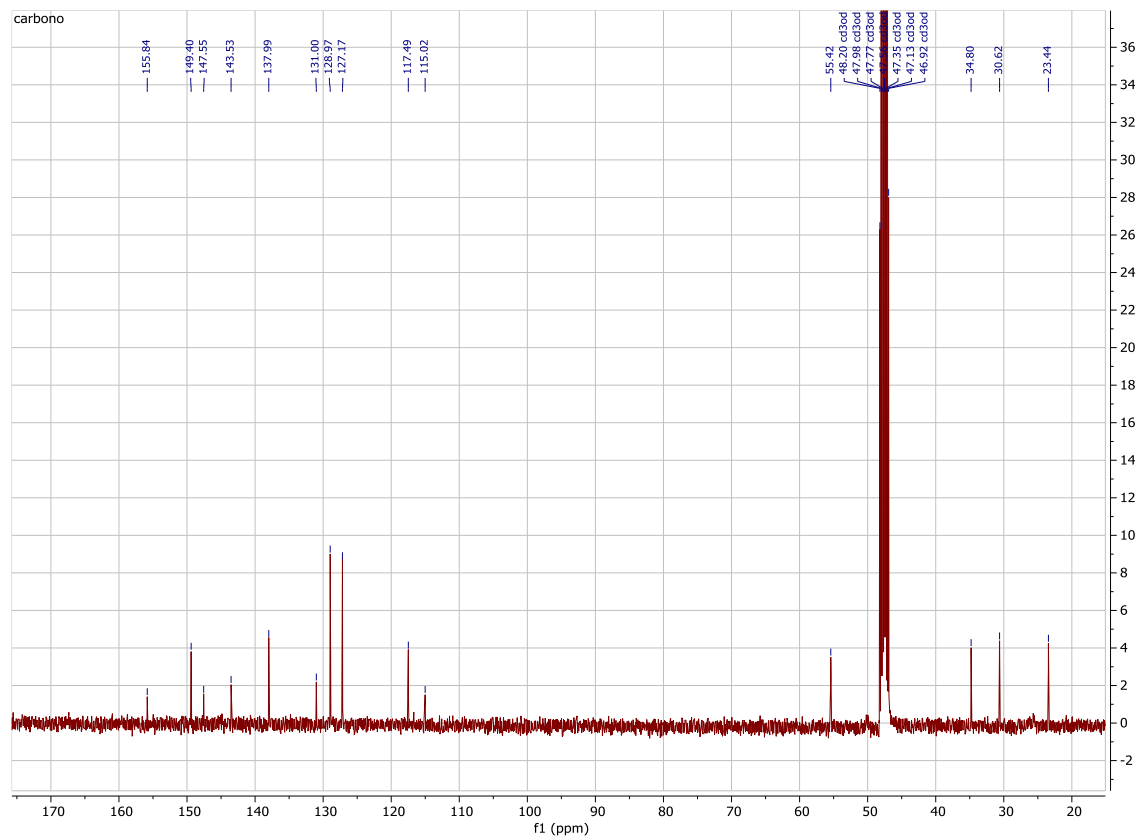
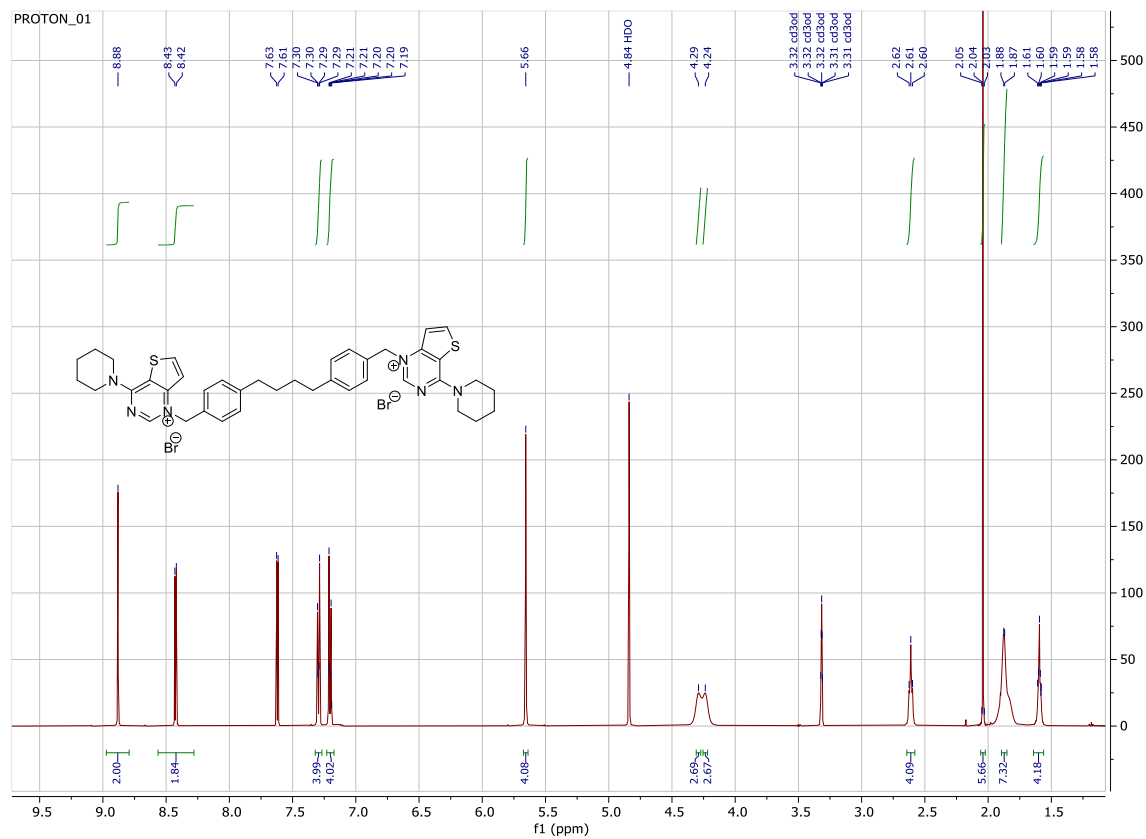
Ff-7



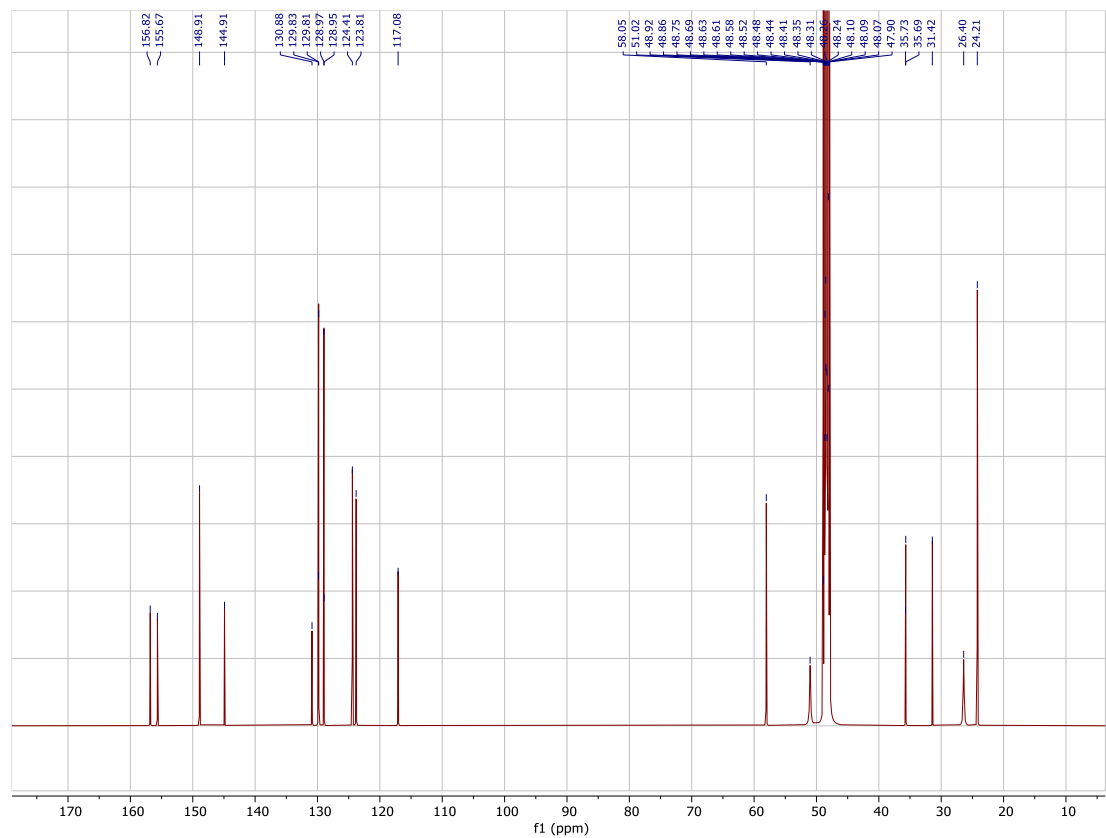
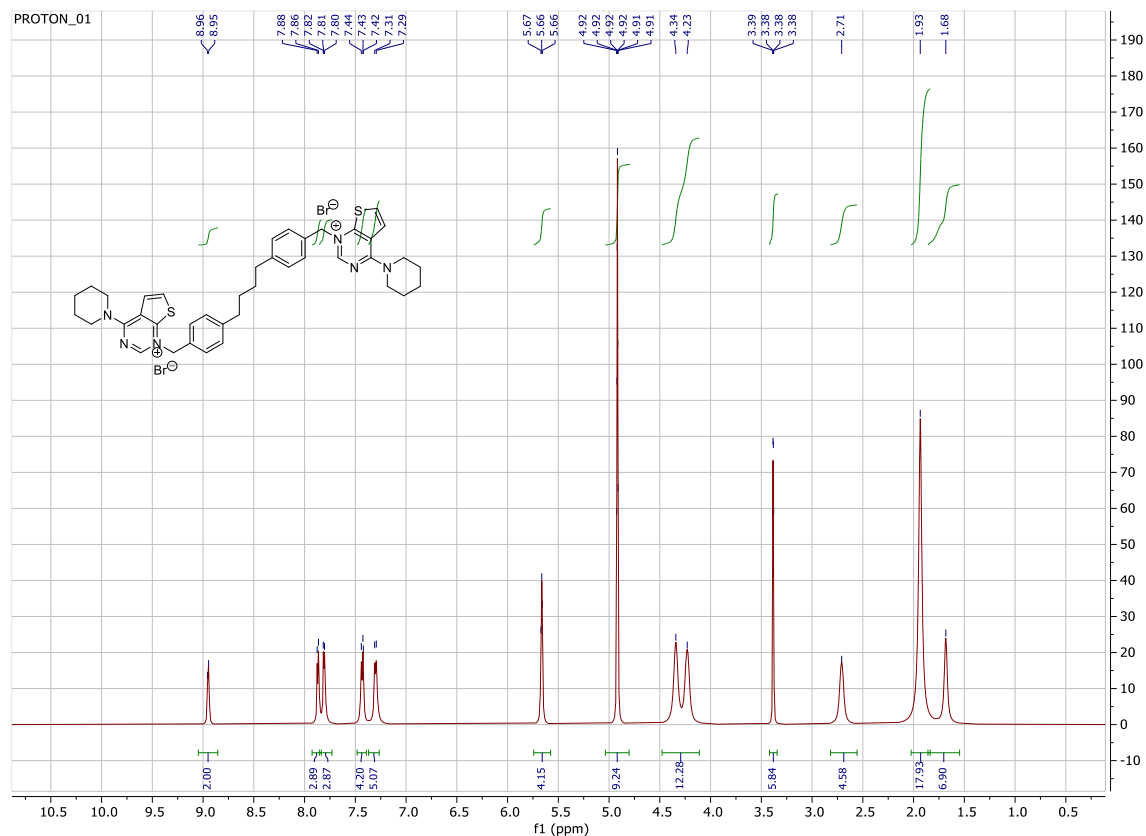
Ff-3



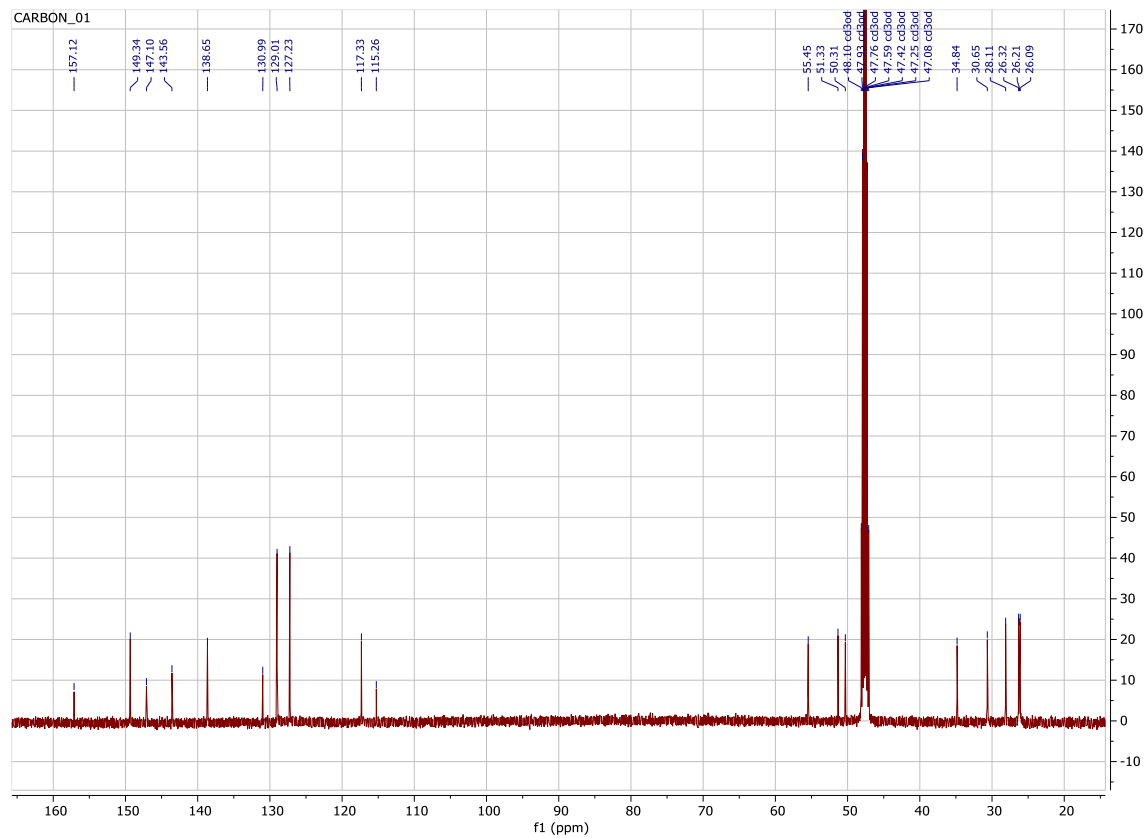
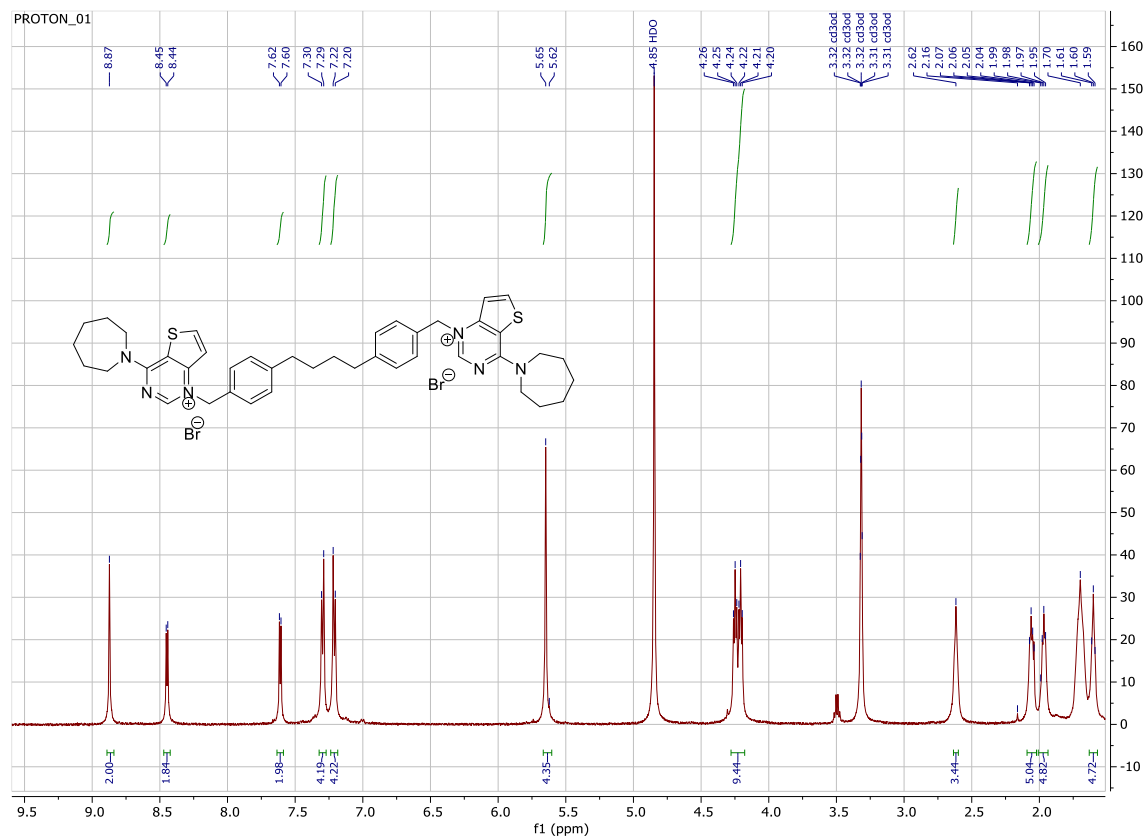
Fa-33

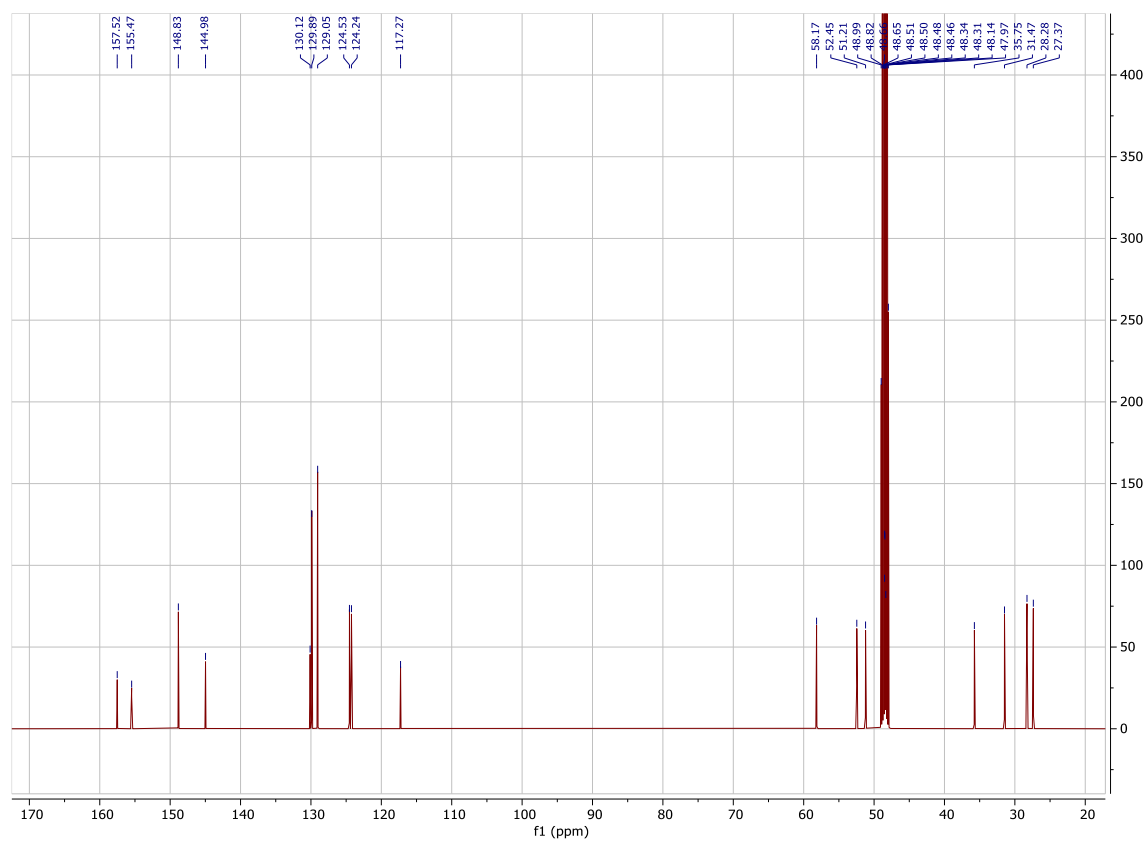
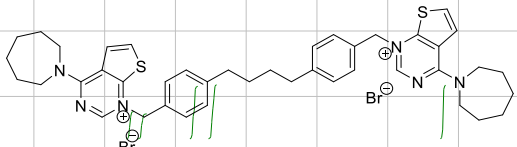


Ff-6

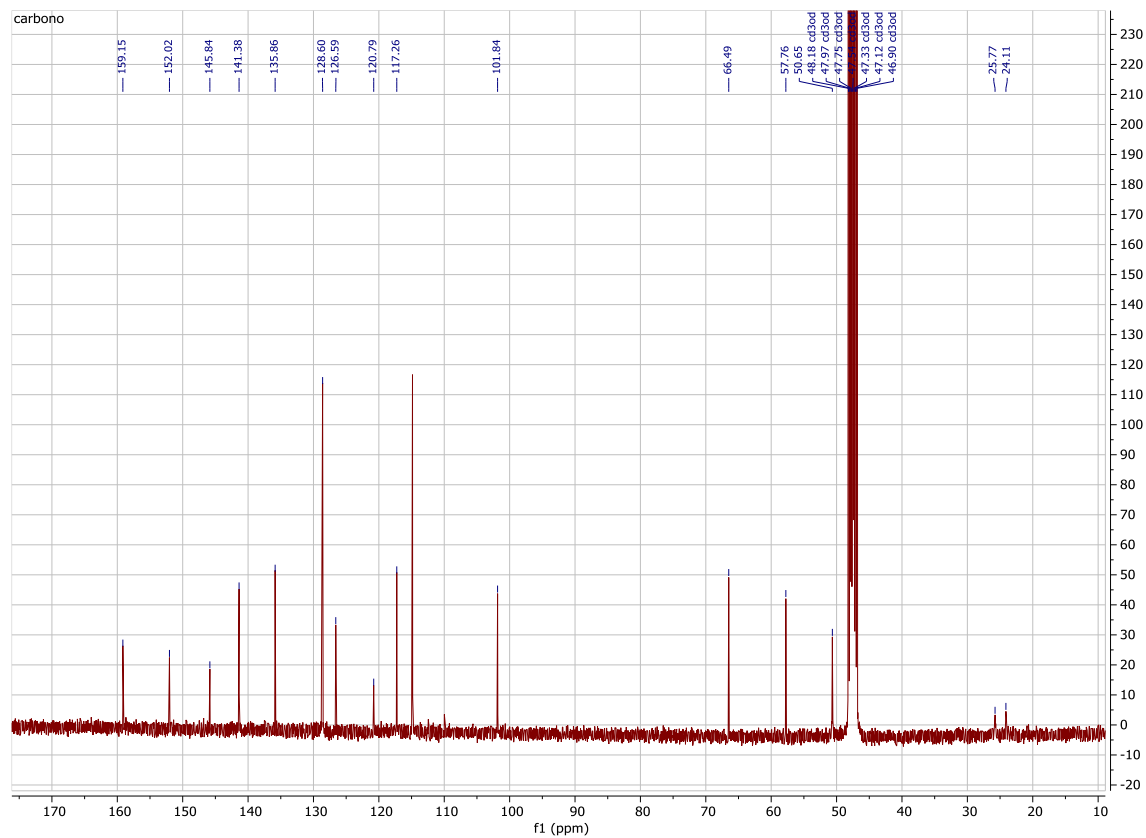
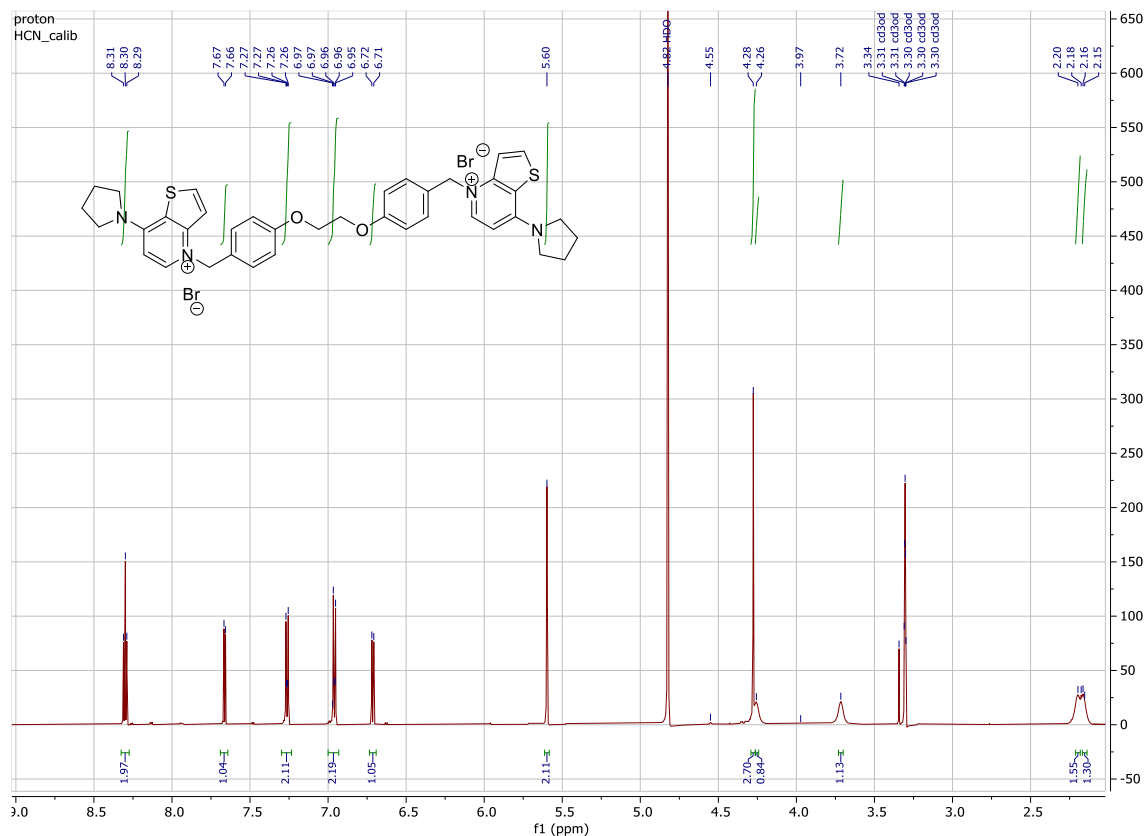


Fa-29

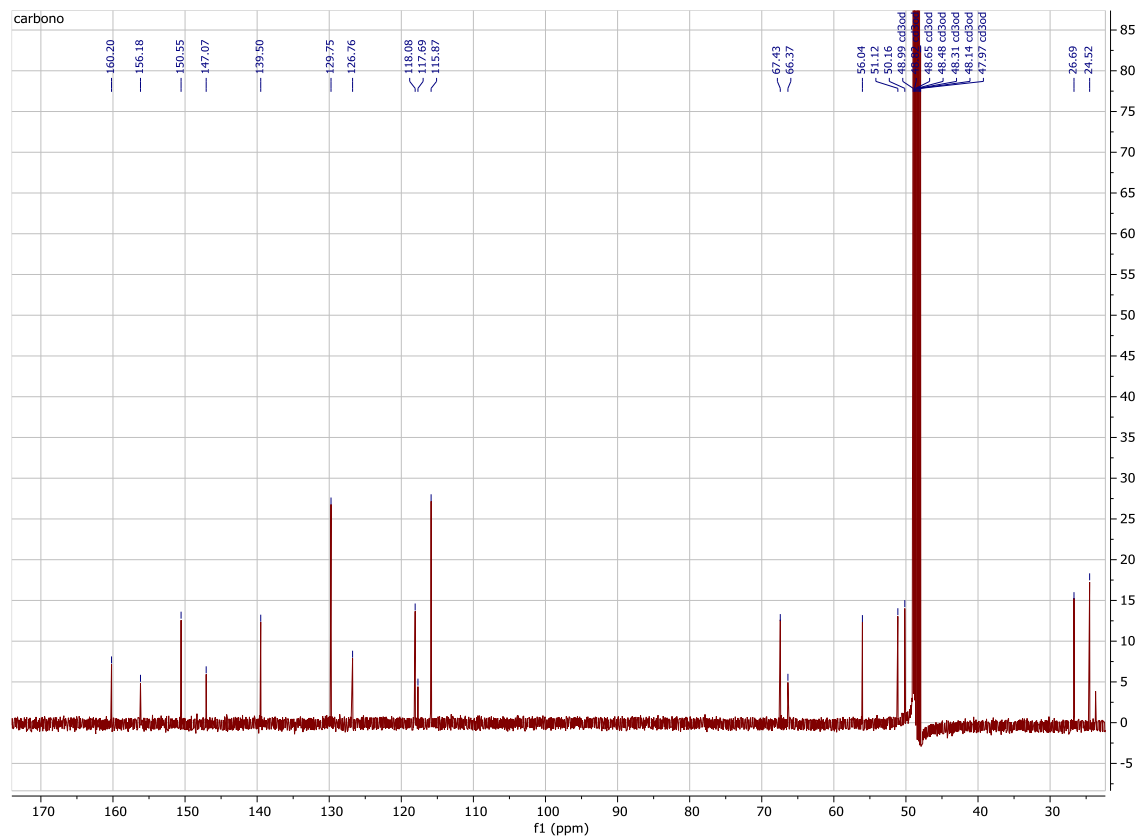
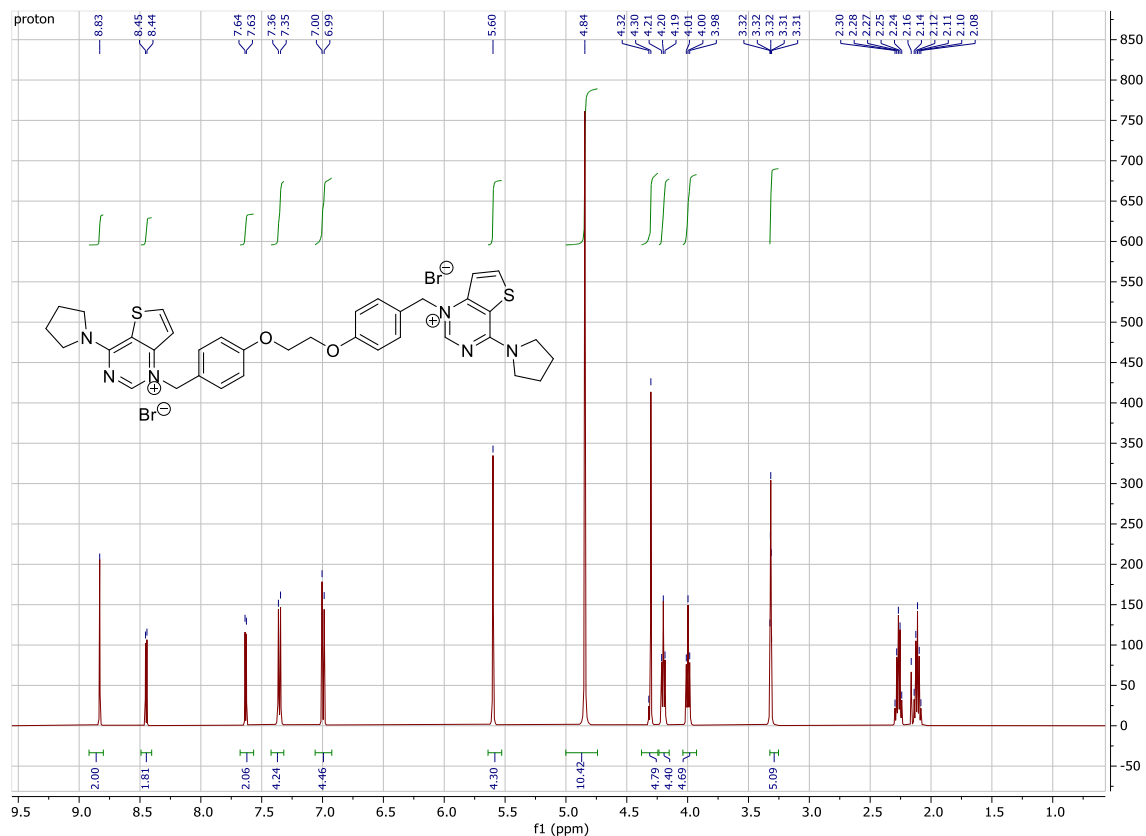




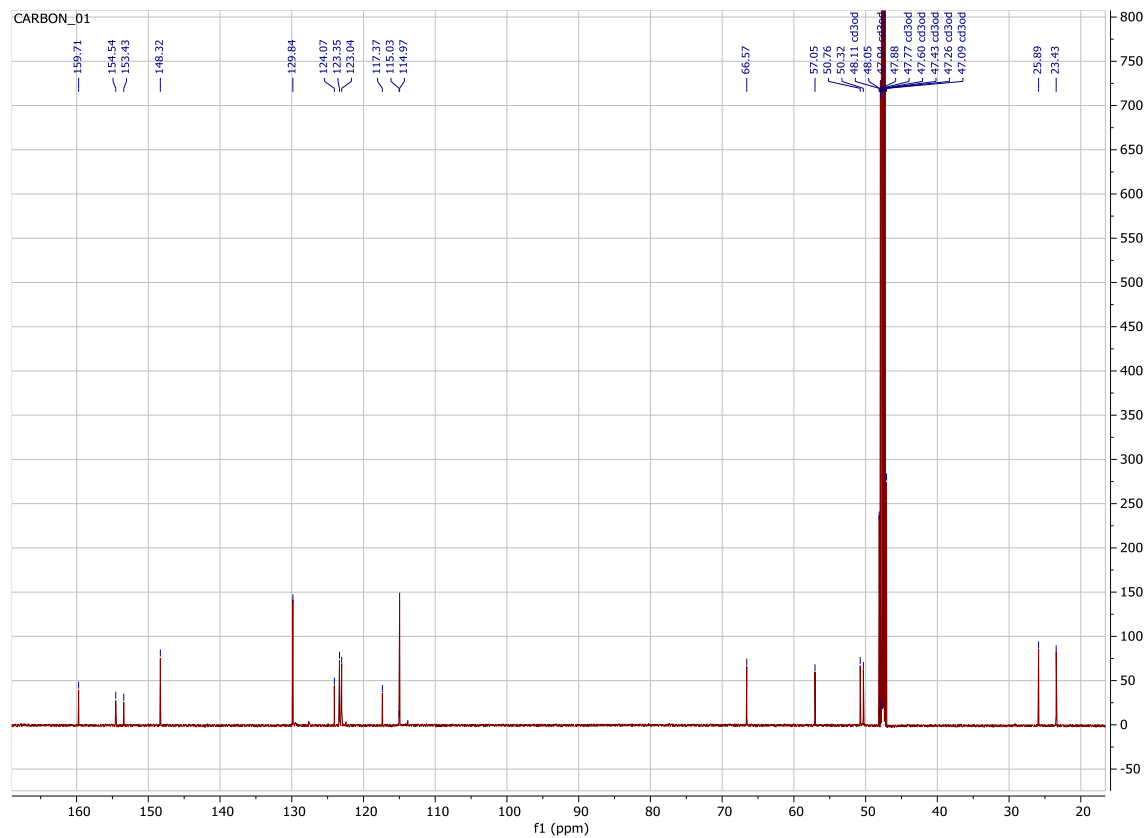
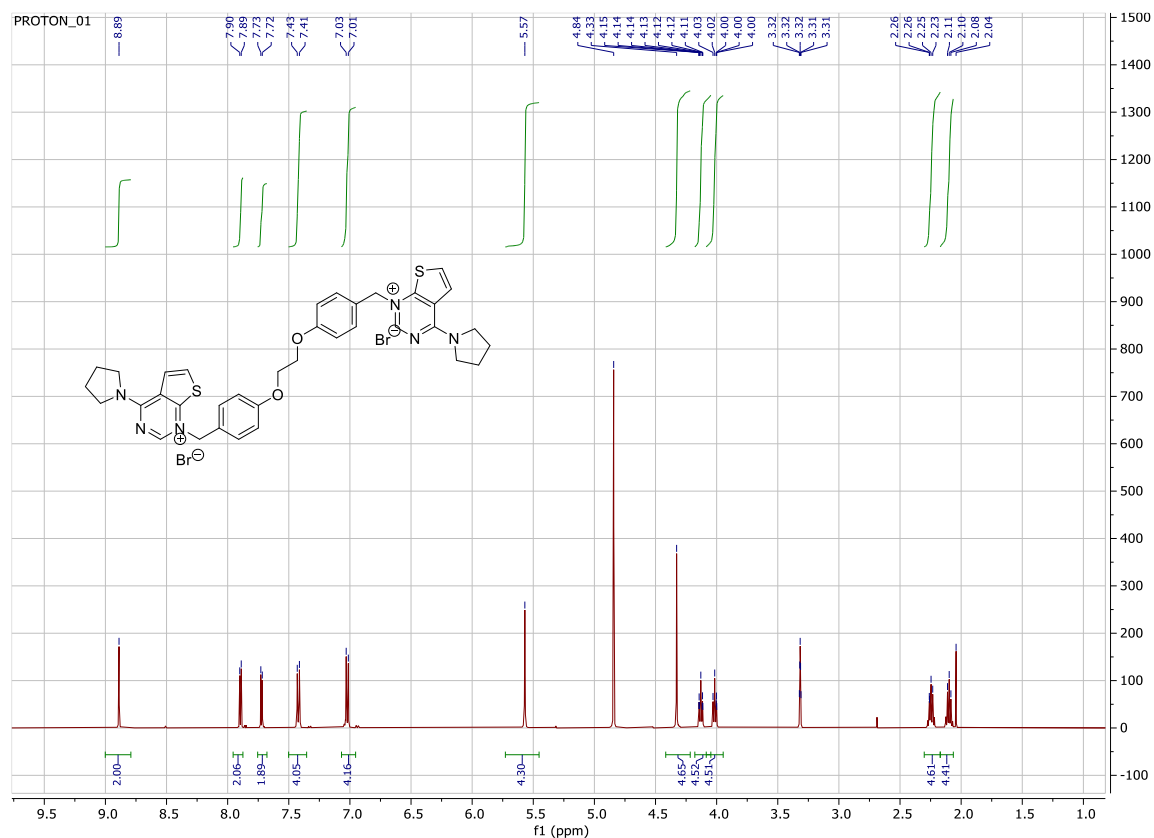
Ff-2



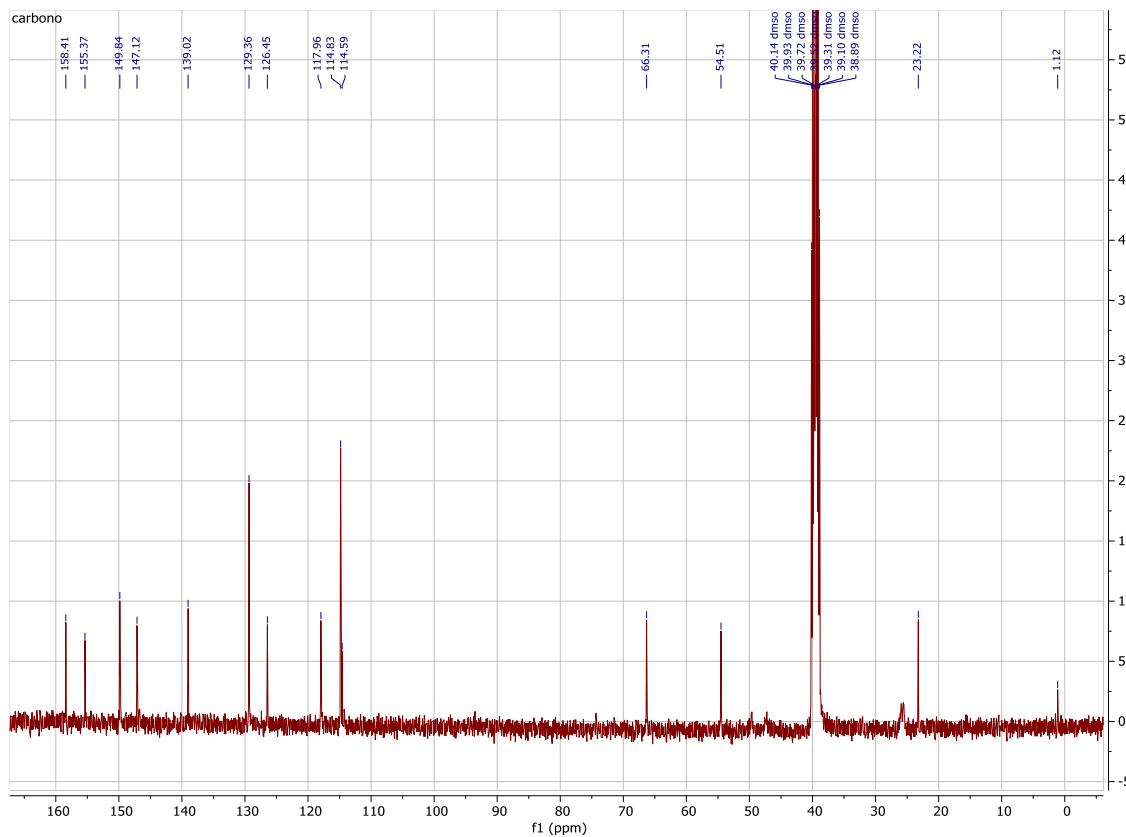
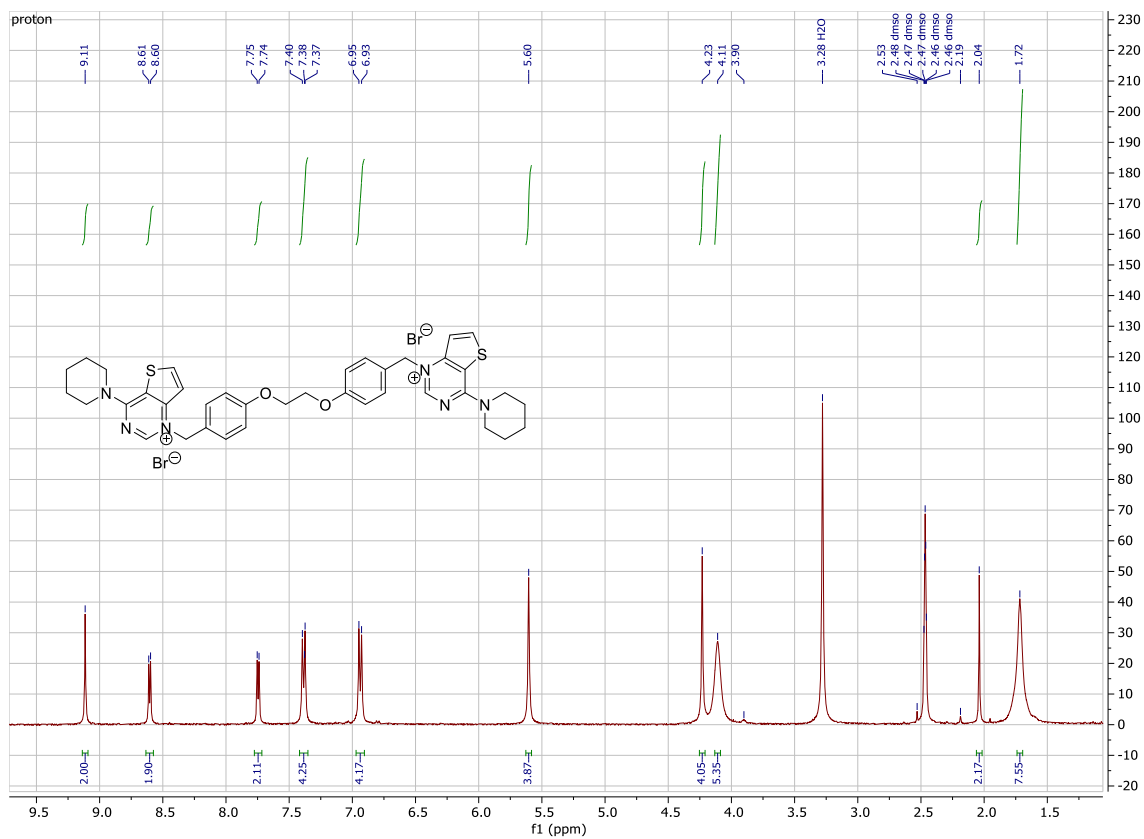
Ff-8



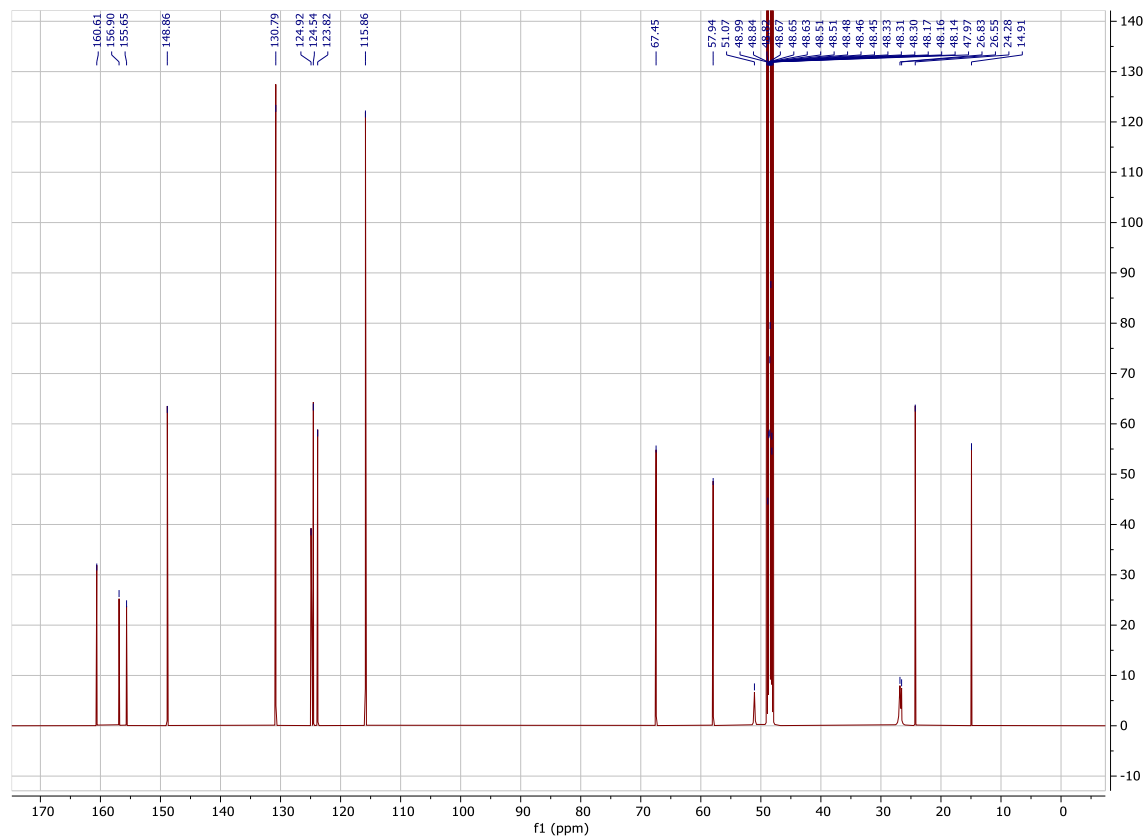
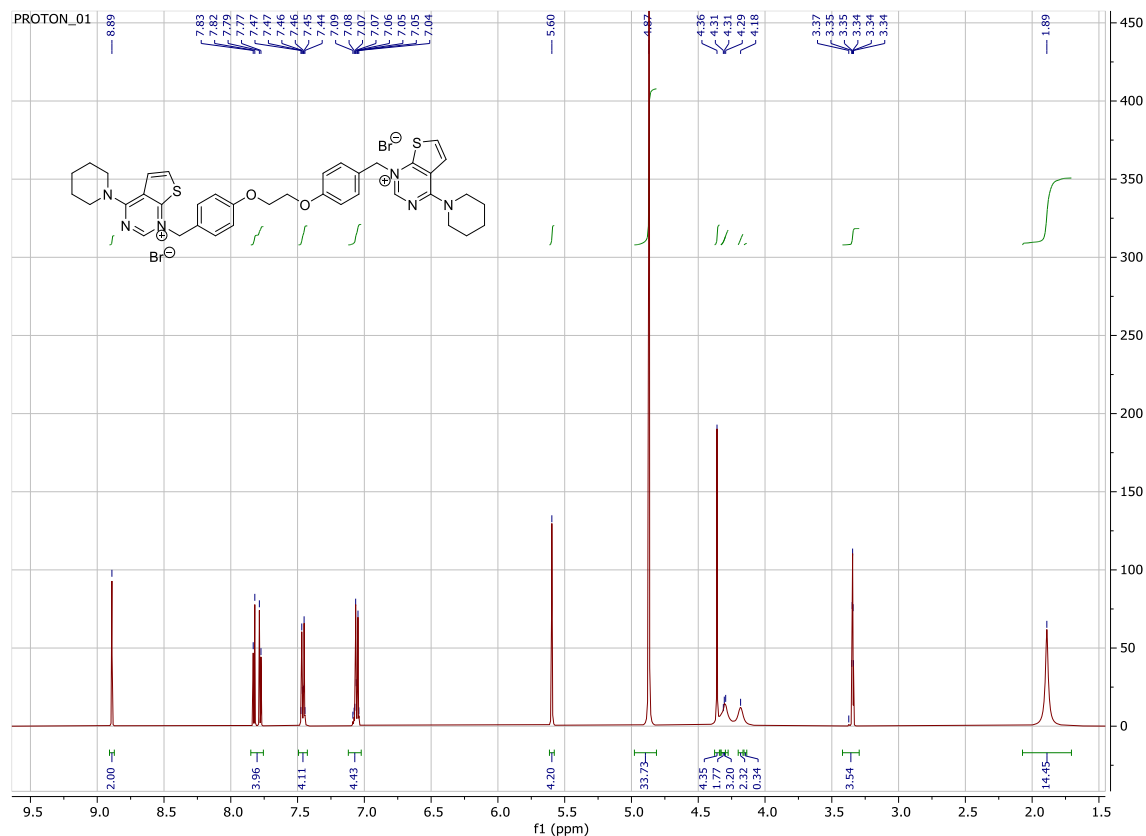
Ff-4



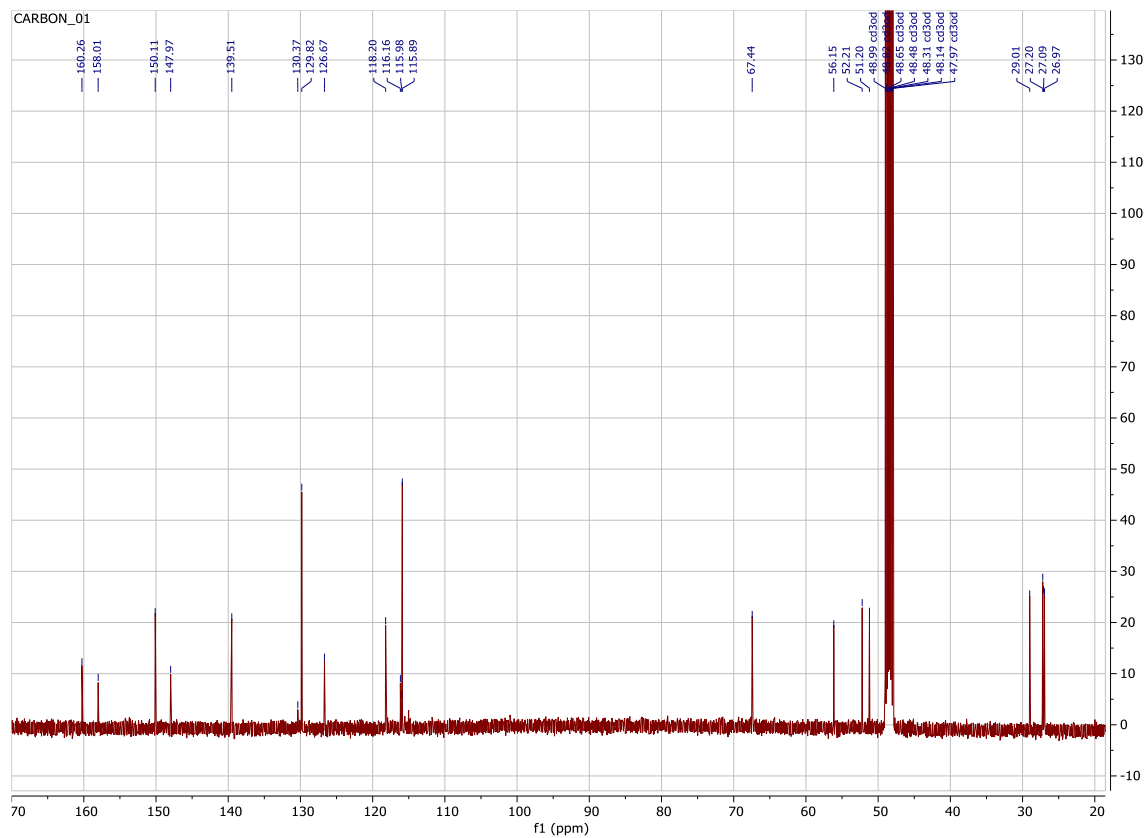
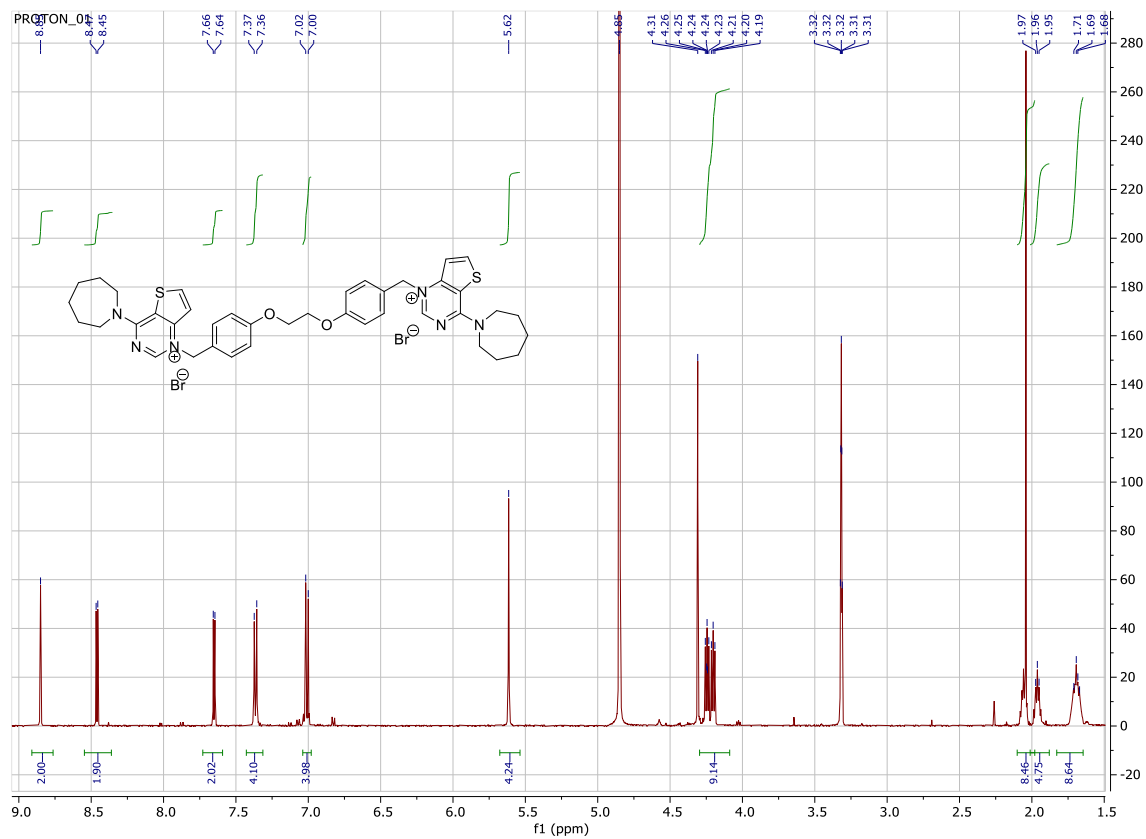
Fa-28



Ff-5



Ff-34



Ff-36

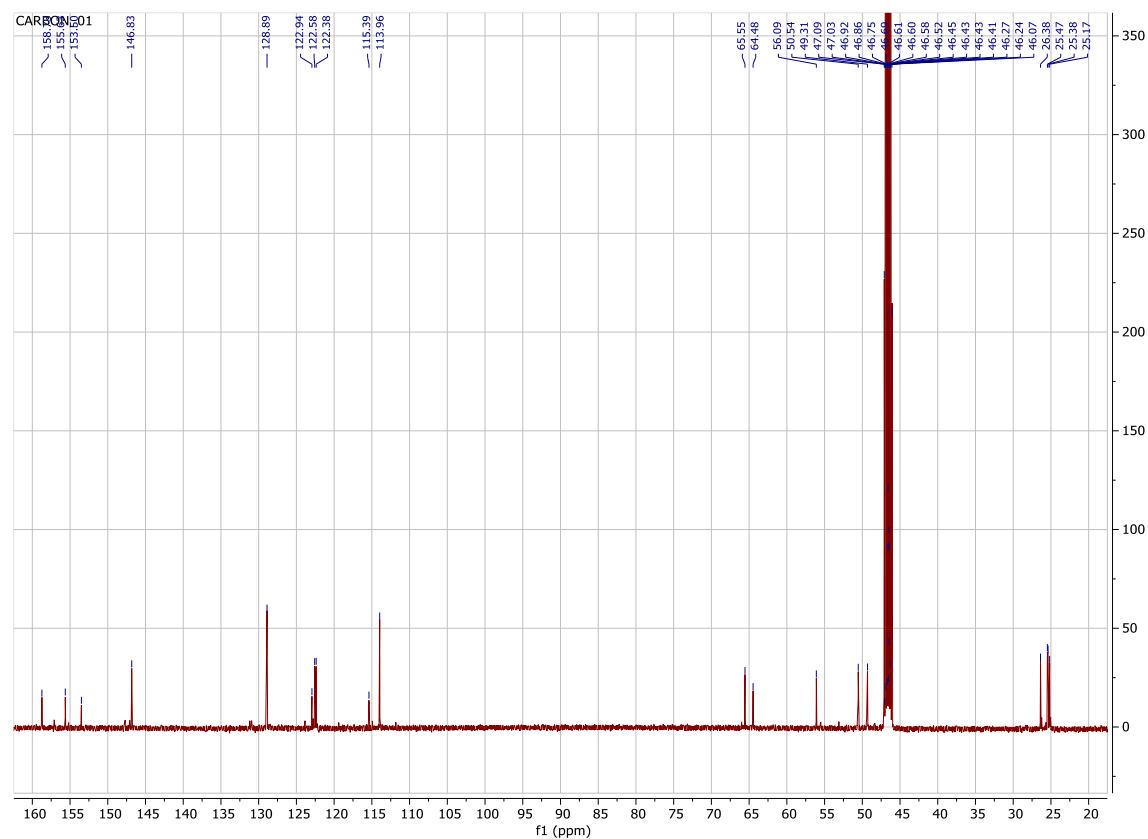
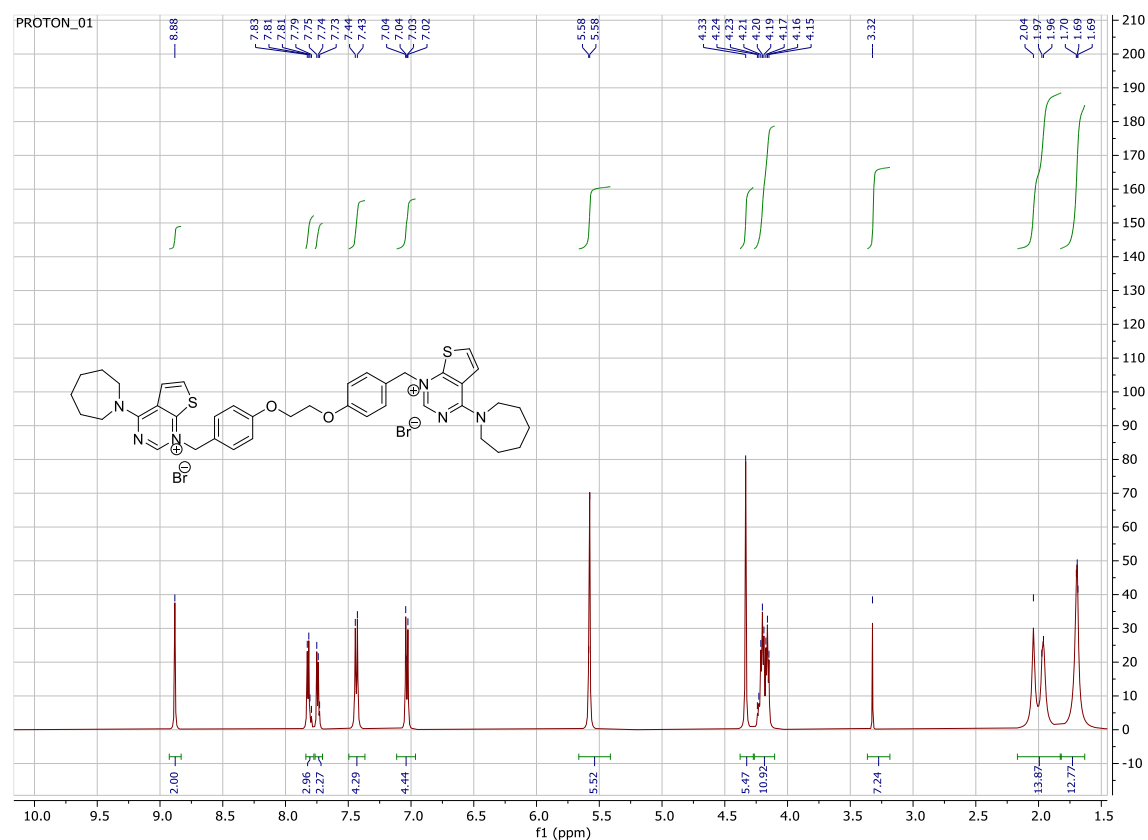


Figure S3. Spectra.