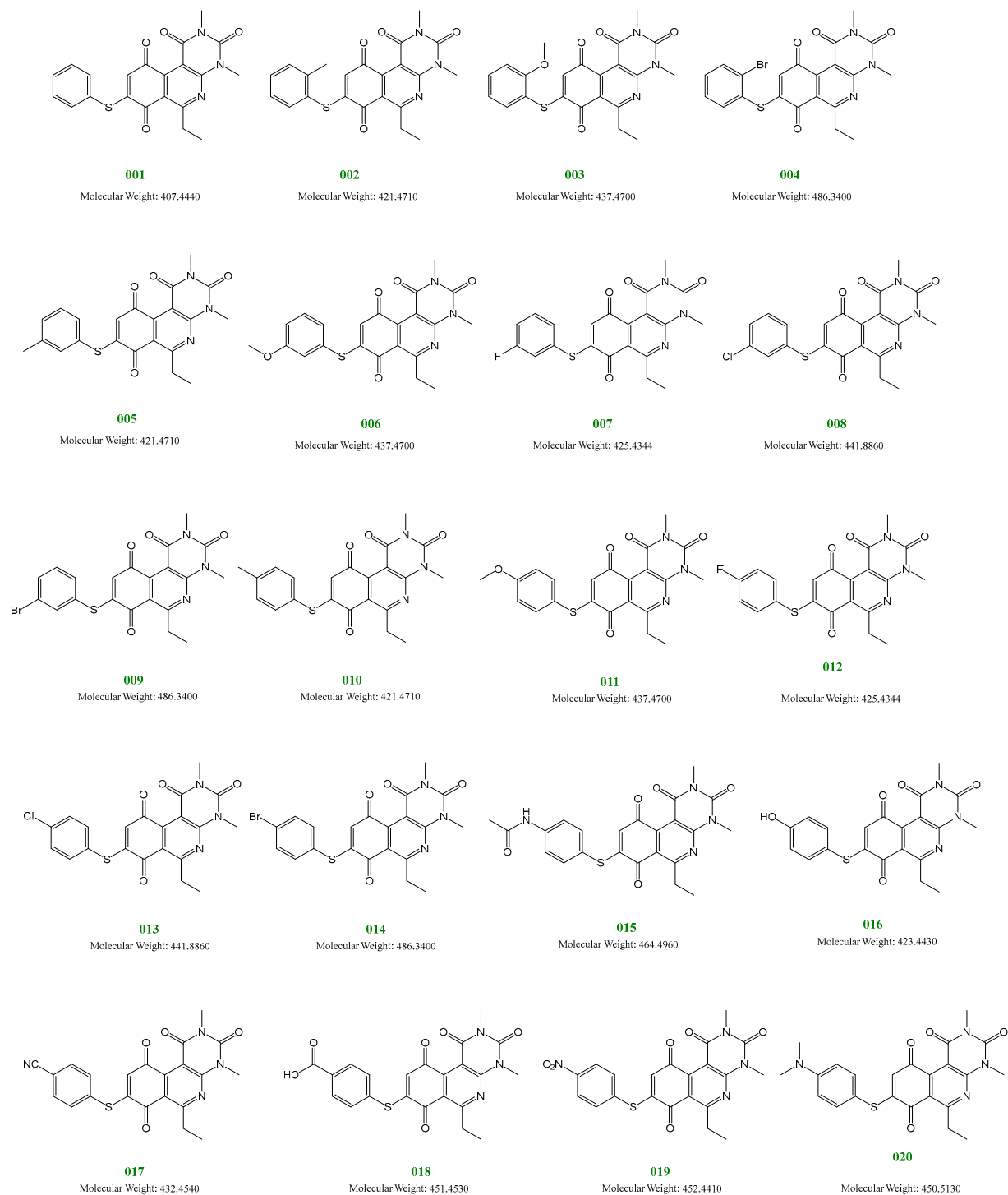


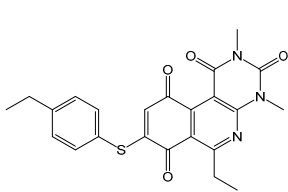
Supplementary Material

**QSAR Studies, Synthesis, and Biological Evaluation of New
Pyrimido-Isoquinolin-Quinone Derivatives against Methicillin-Resistant
*Staphylococcus aureus***

Juan Andrades-Lagos ^{1,2}, Javier Campanini-Salinas ^{2,3,*}, Gianfranco Sabadini ^{4,5},
Victor Andrade ^{6,7,8}, Jaime Mella ^{4,5,*} and David Vásquez-Velásquez ^{2,*}

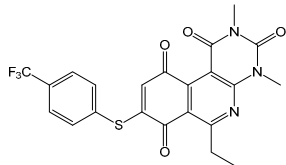
Figure S1. The Chemical structure of the compounds used to construct the QSAR models.





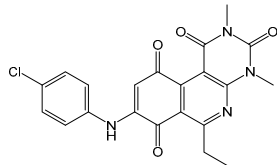
021

Molecular Weight: 435.4980



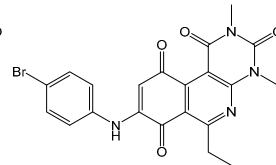
022

Molecular Weight: 475.4422



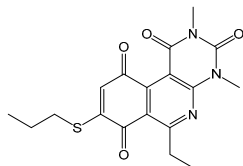
023

Molecular Weight: 424.8410



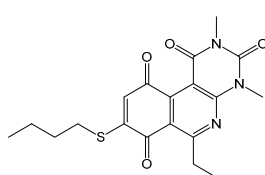
024

Molecular Weight: 469.2950



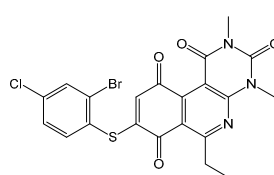
025

Molecular Weight: 373.4270



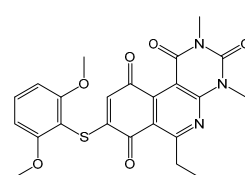
026

Molecular Weight: 387.4540



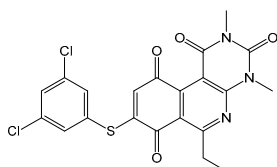
027

Molecular Weight: 520.7820



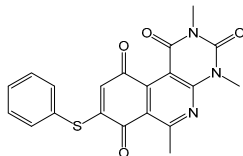
028

Molecular Weight: 467.4960



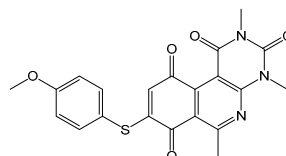
029

Molecular Weight: 476.3280



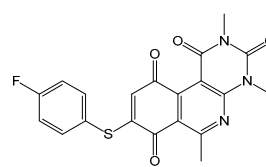
030

Molecular Weight: 393.4170



031

Molecular Weight: 423.4430



032

Molecular Weight: 411.4074

Figure S2. The chemical structure of the new designed and synthesized compounds.

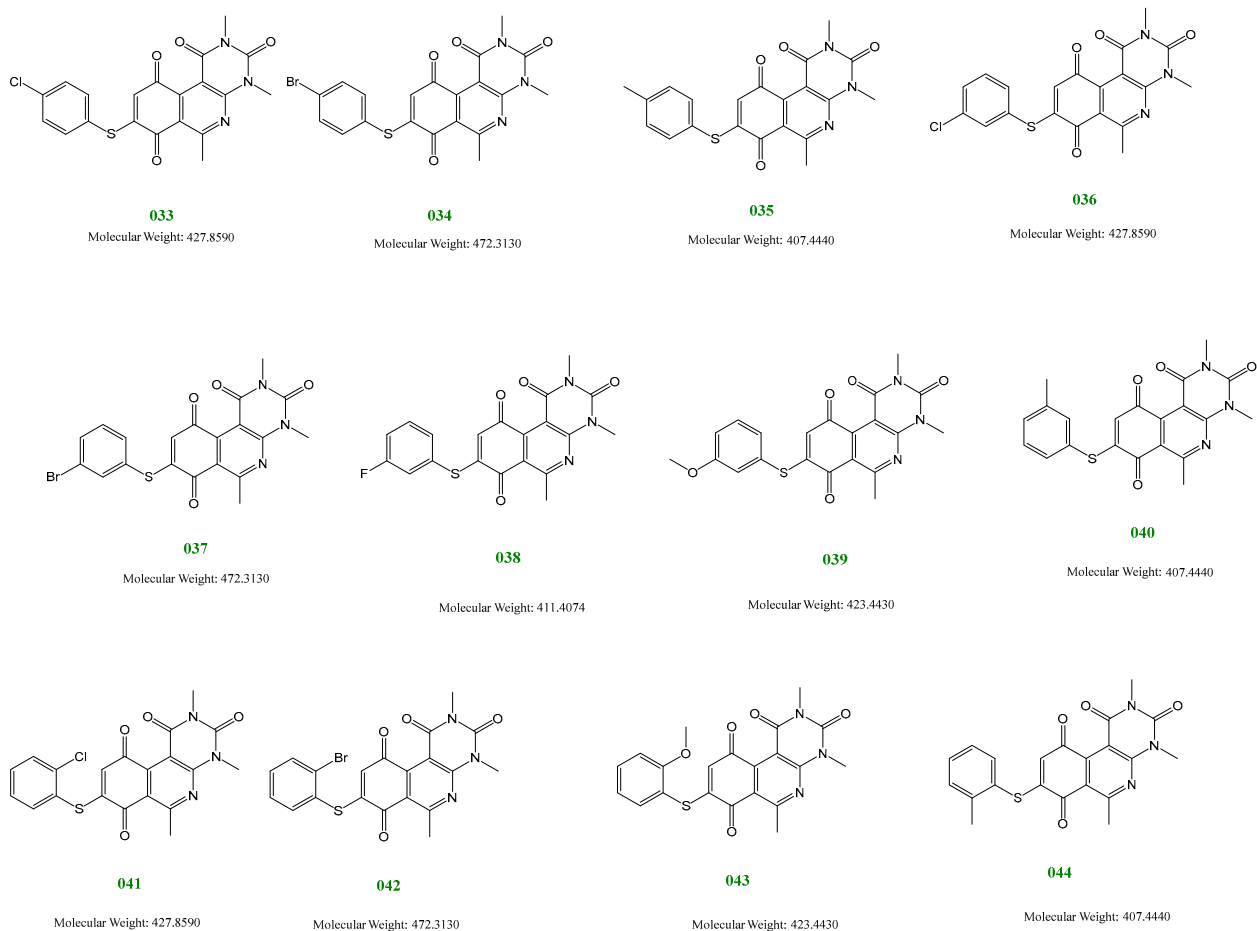


Figure S3. ¹H-NMR compound 33.

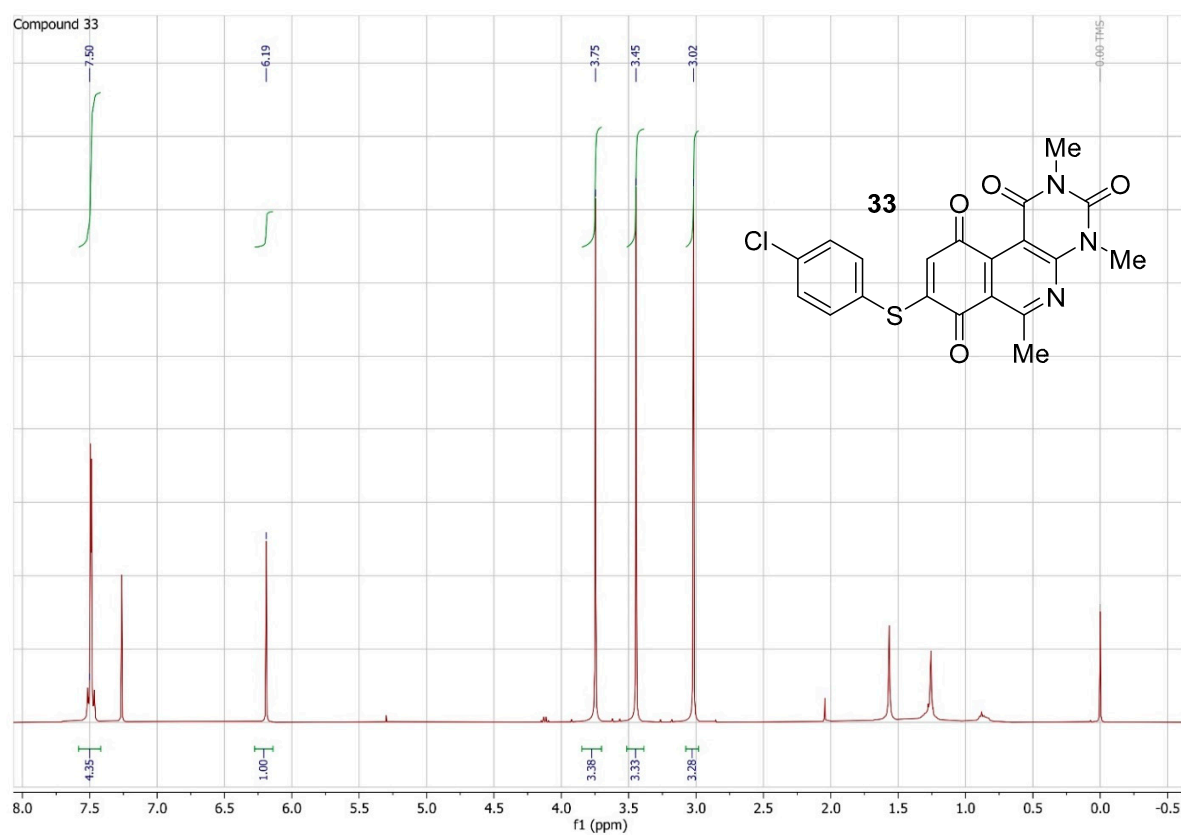


Figure S4. ¹H-NMR compound 34.

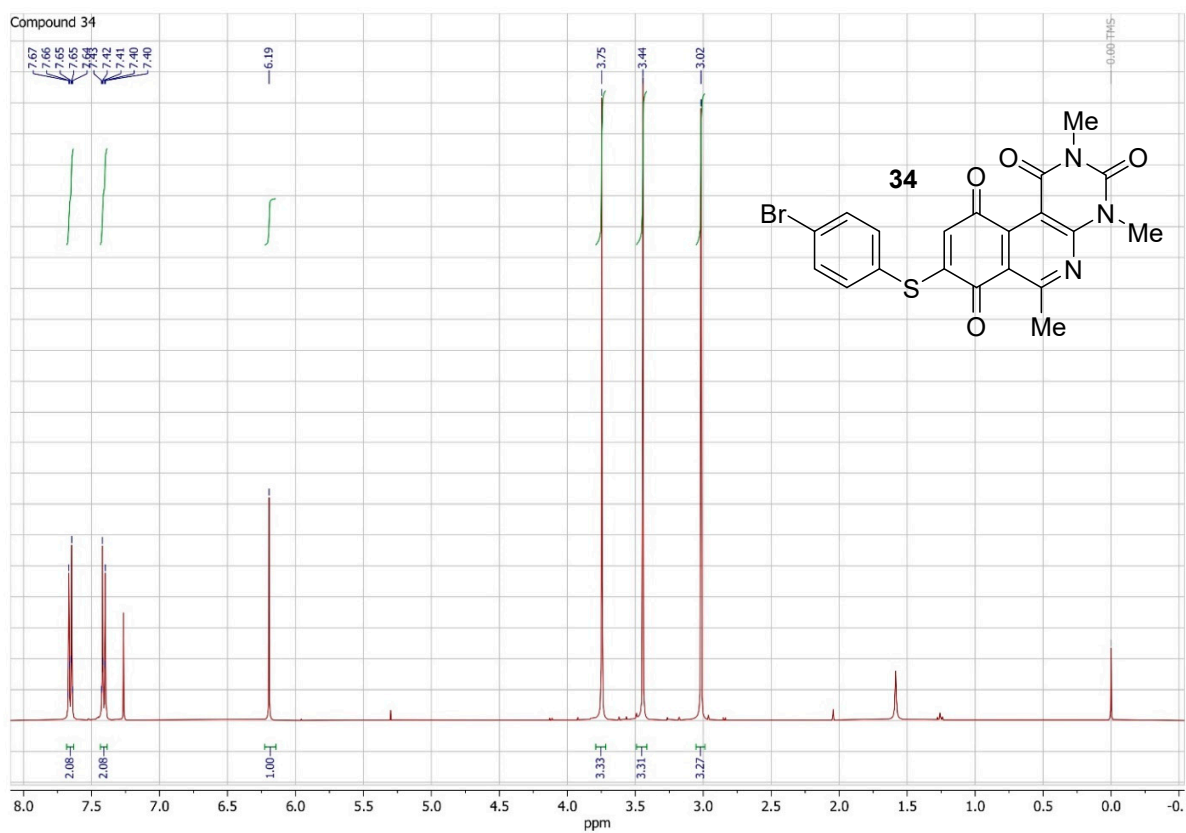


Figure S5. ¹H-NMR compound 35.

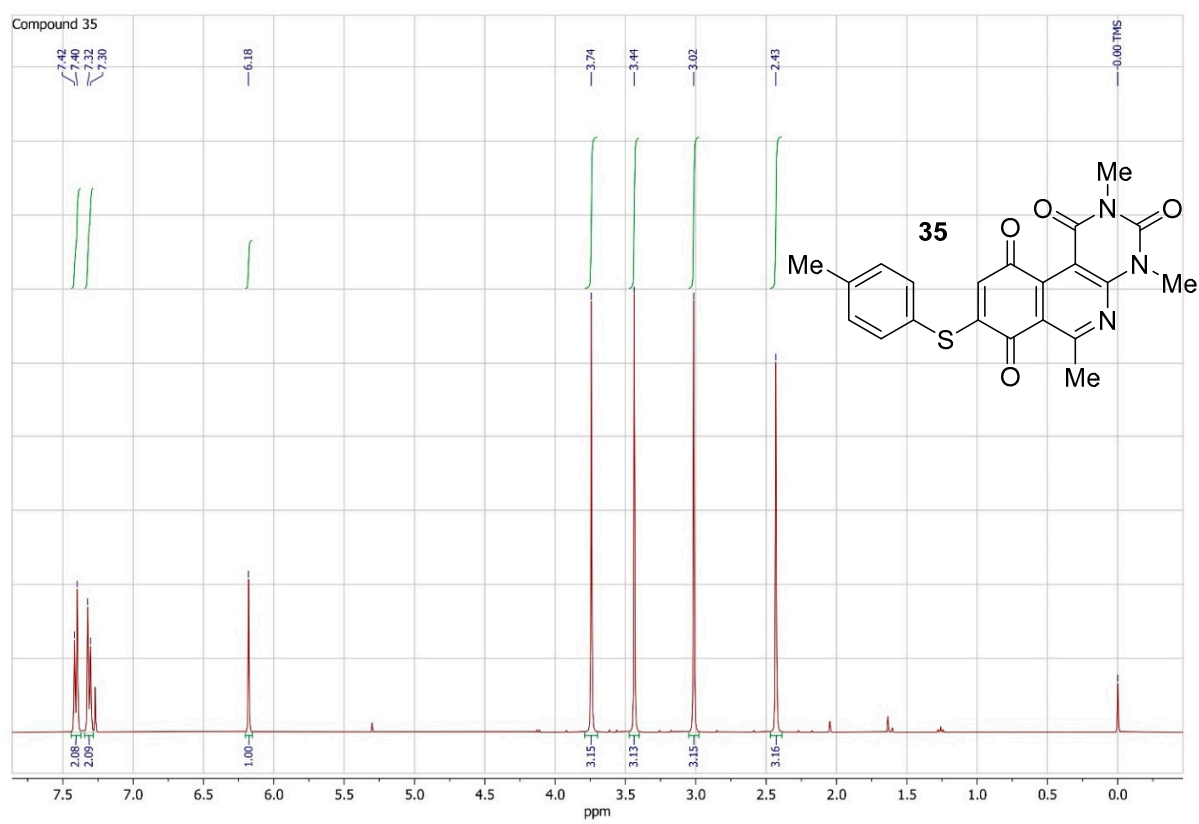


Figure S6. ¹H-NMR compound 36.

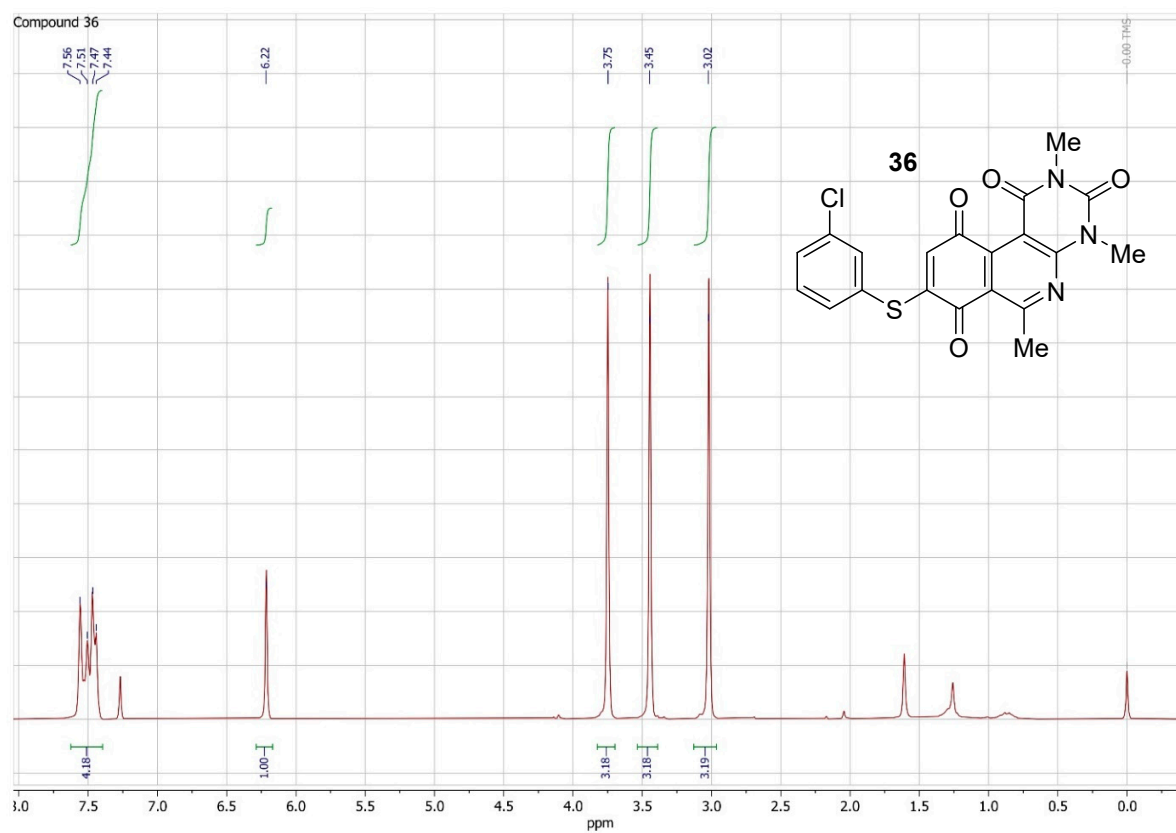


Figure S7. ¹H-NMR compound 37.

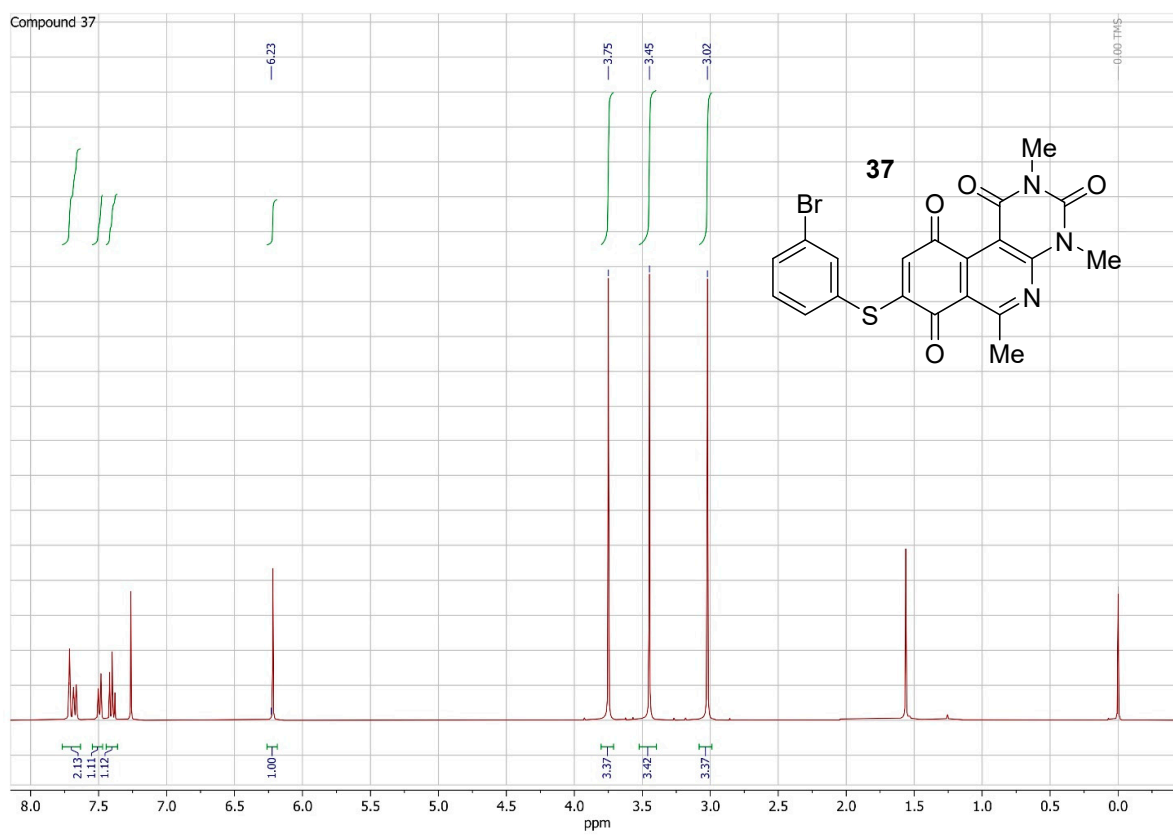


Figure S8. ¹H-NMR compound 38.

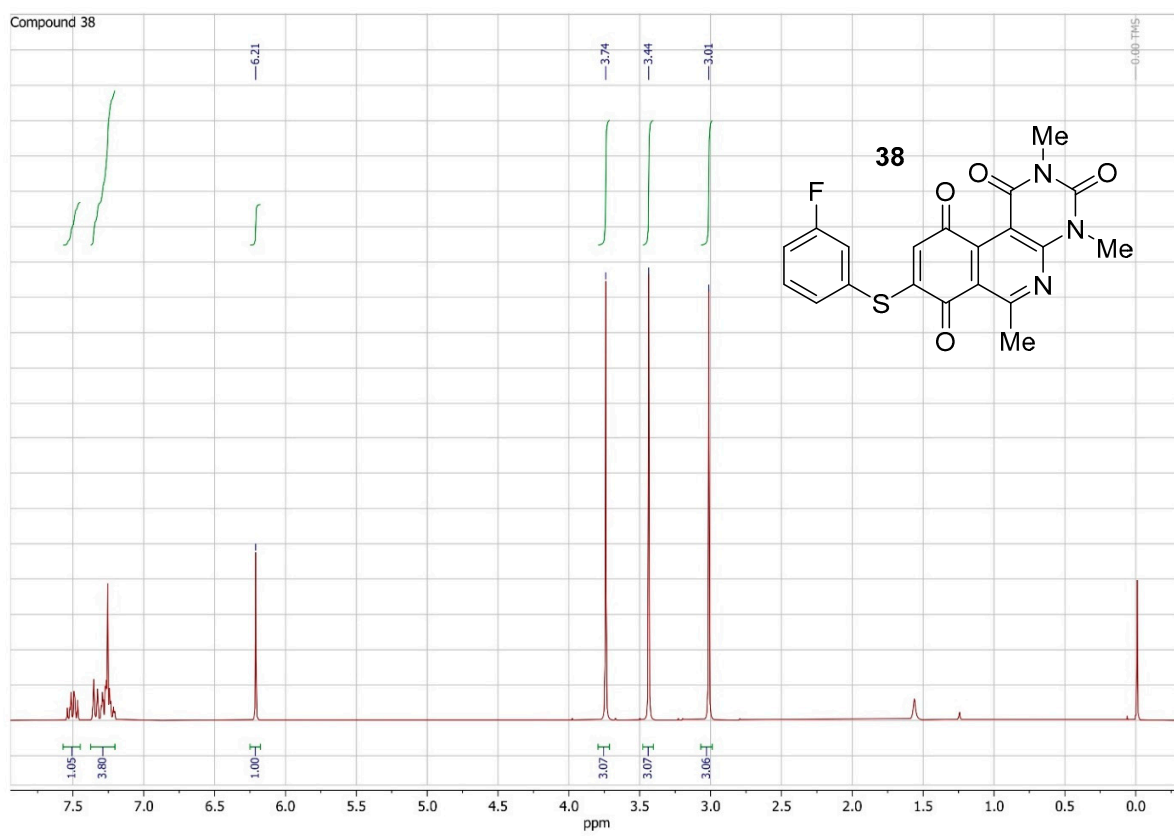


Figure S9. ¹H-NMR compound 39.

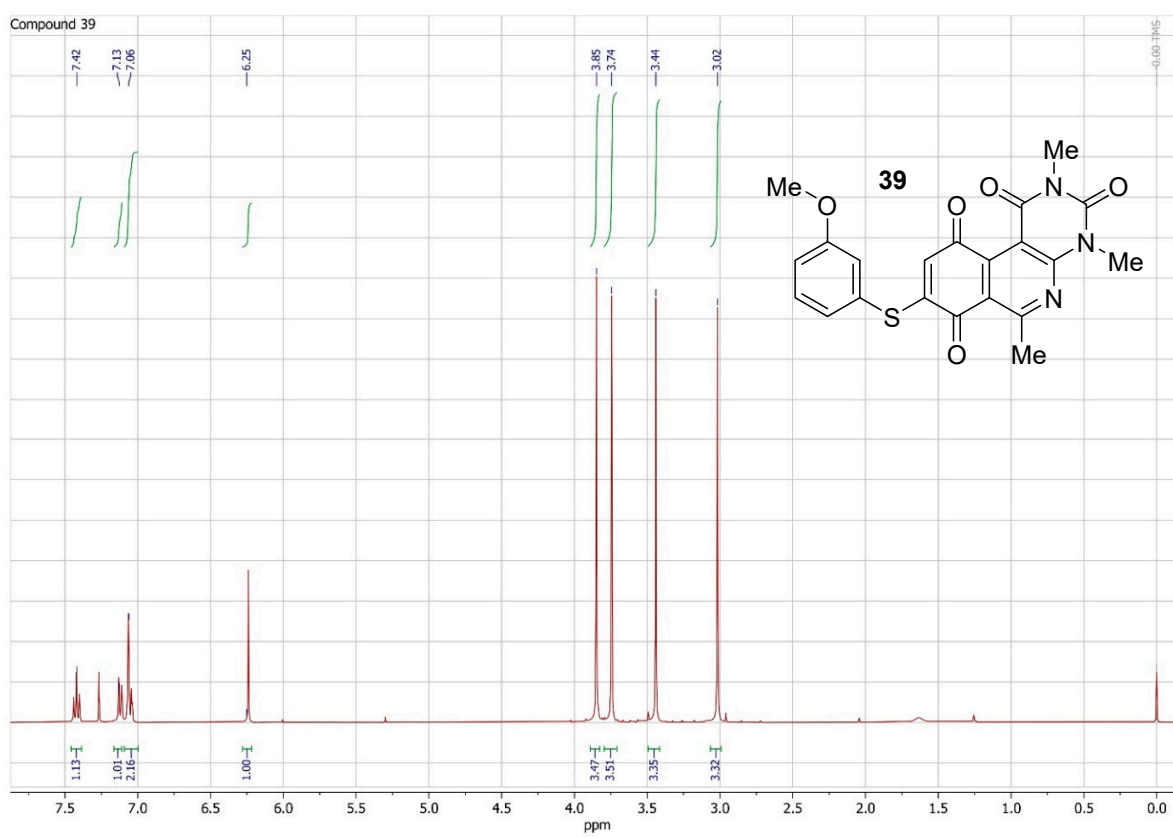


Figure S10. ¹H-NMR compound 40.

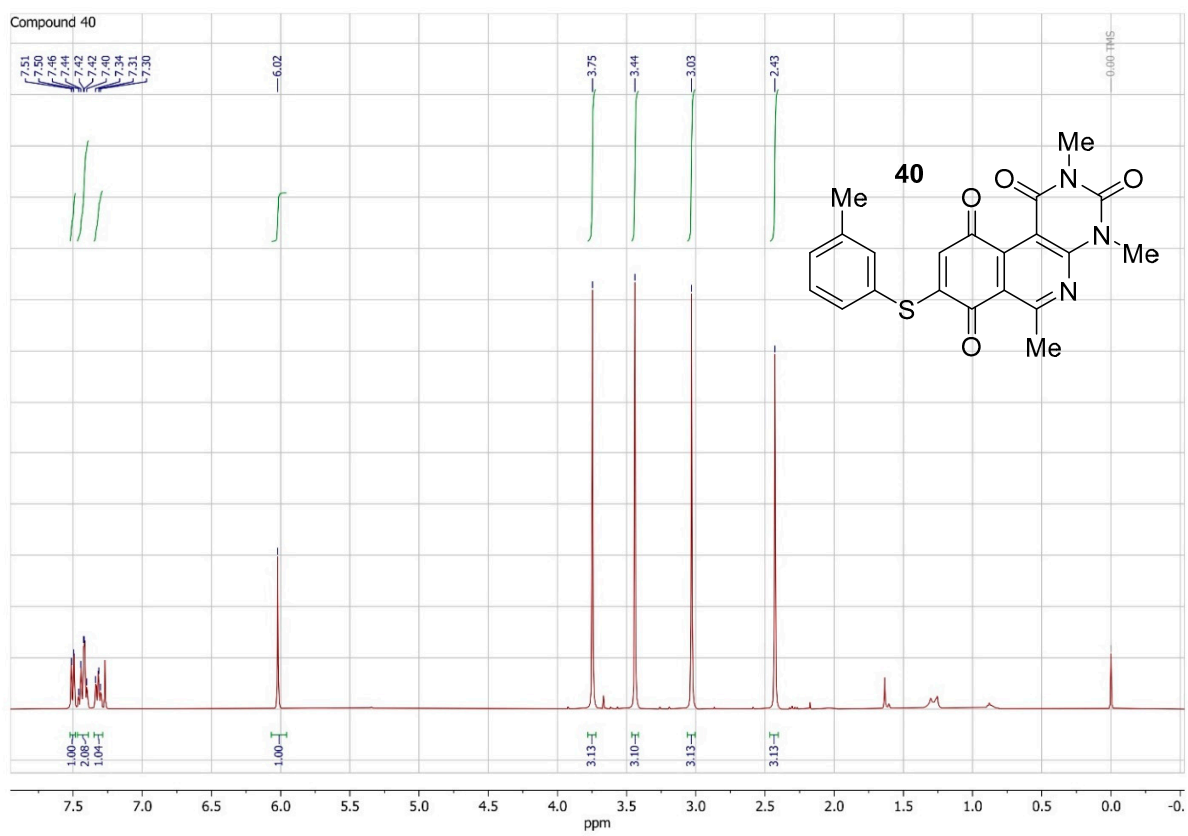


Figure S11. ¹H-NMR compound 41.

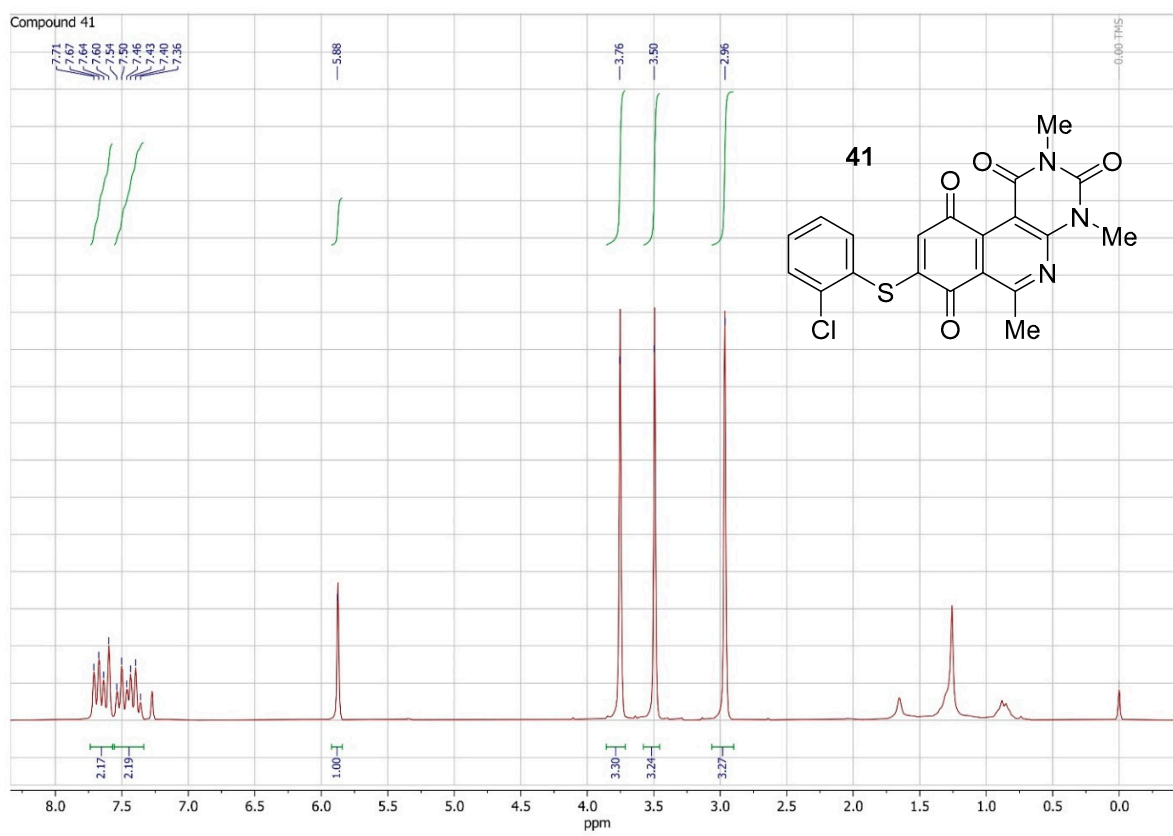


Figure S12. ^1H -NMR compound 42.

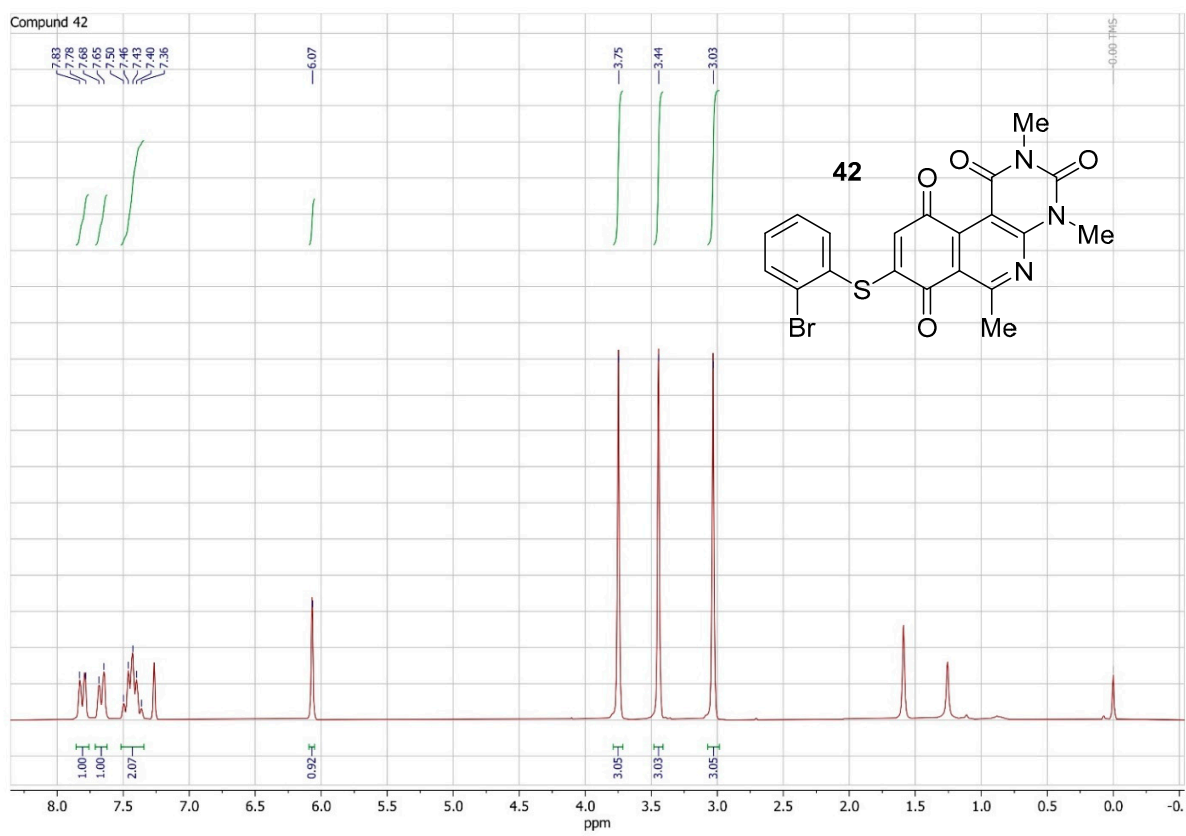


Figure S13. ^1H -NMR compound 43.

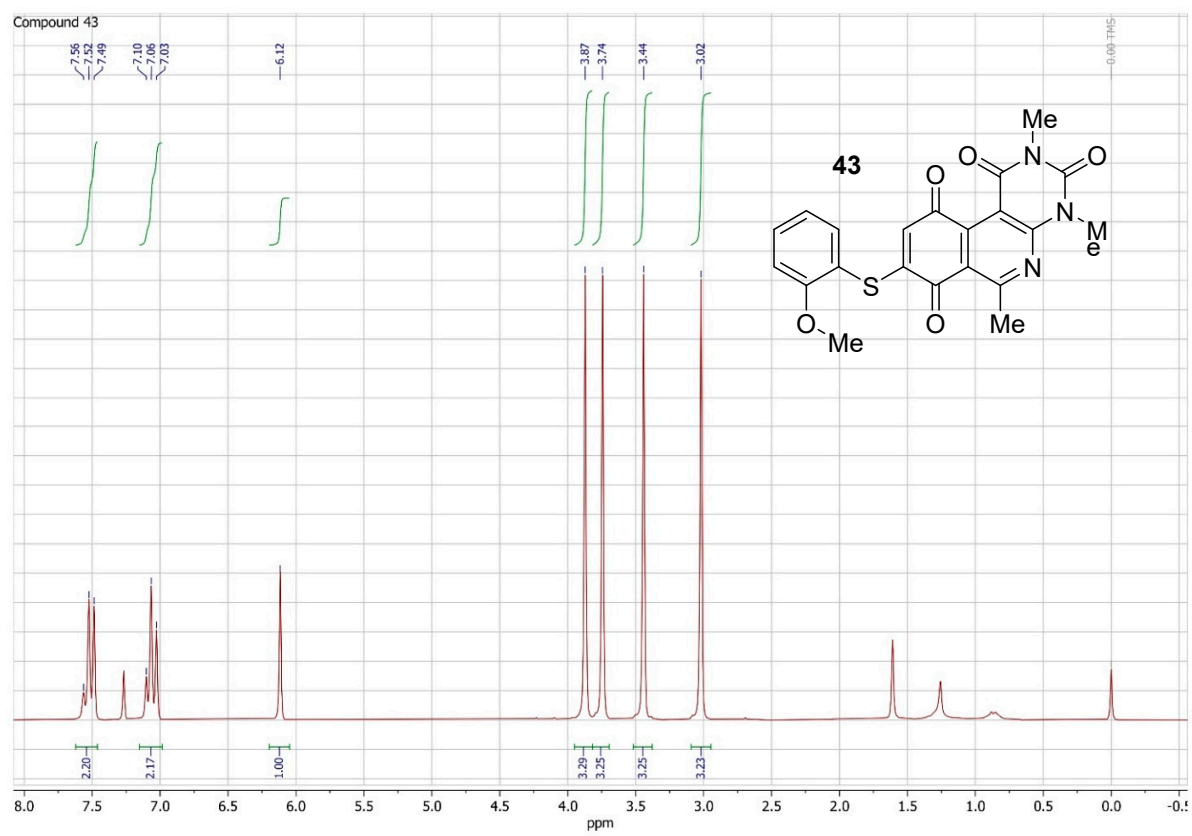


Figure S14. ^1H -NMR compound 44.

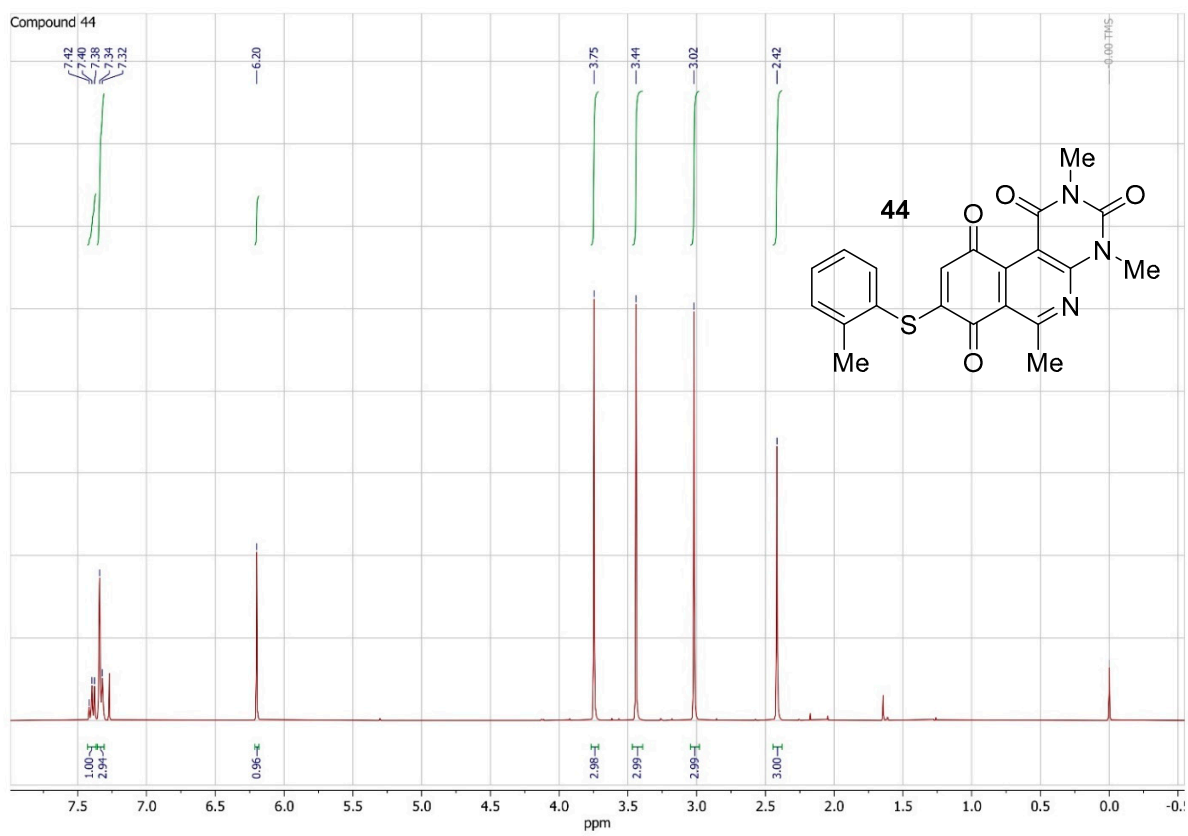


Figure S15. ^1H -NMR compound 45.

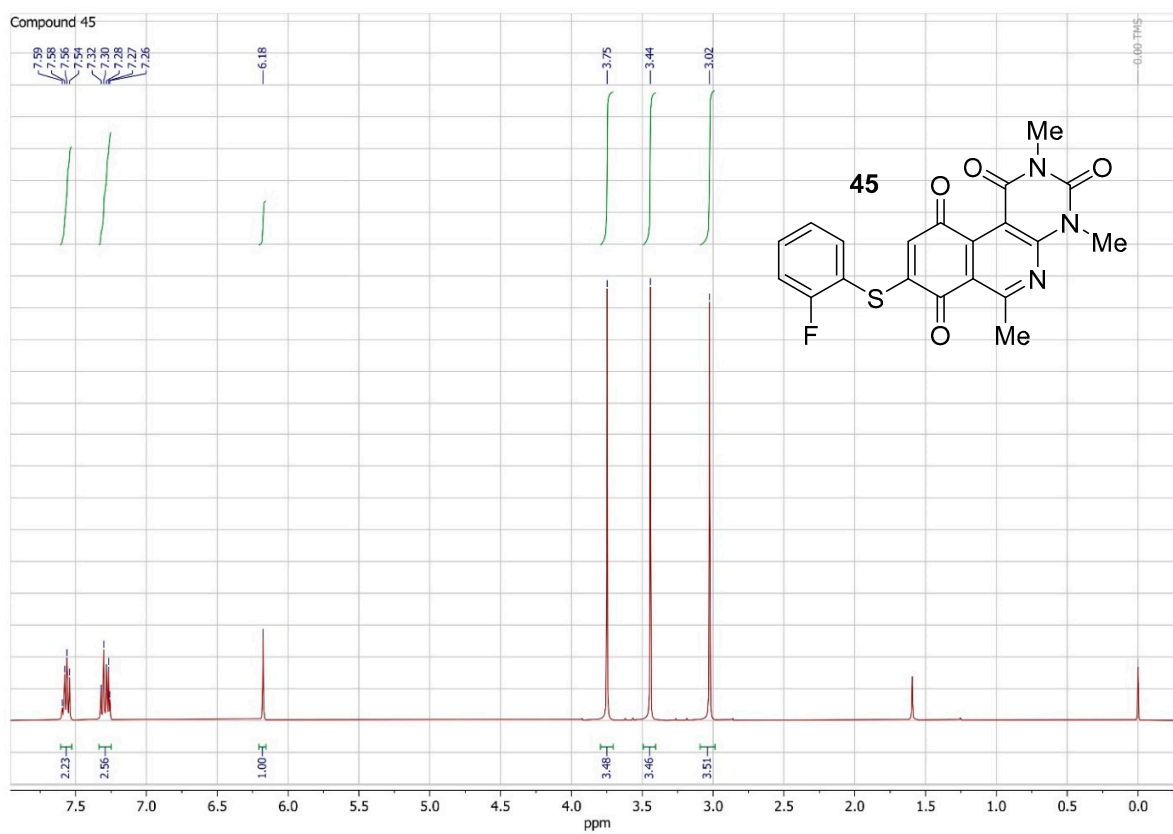


Table S1. The sequential search of the best CoMFA and CoMSIA models.

Model	q ²	N	SEP	SEE	r ²	F	Field Contributions				
							S	E	H	D	A
CoMFA-S	0.66	5	0.286	0.123	0.938	48.017	1				
CoMFA-E	0.541	2	0.305	0.212	0.779	33.54		1			
CoMFA-SE	0.619	3	0.286	0.14	0.909	59.703	0.659	0.341			
CoMSIA-S	0.591	5	0.314	0.219	0.801	12.857	1				
CoMSIA-E	0.482	2	0.324	0.217	0.769	31.585		1			
CoMSIA-H	0.237	1	0.383	0.31	0.502	20.169			1		
CoMSIA-D	0.416	3	0.354	0.303	0.572	8.03				1	
CoMSIA-A	0.275	5	0.275	0.303	0.618	5.17					1
CoMSIA-SE	0.468	2	0.329	0.226	0.748	28.158	0.418	0.582			
CoMSIA-SEH	0.526	13	0.457	0.021	0.999	651.809	0.132	0.34	0.528		
CoMSIA-SEHD	0.551	3	0.31	0.23	0.754	18.364	0.065	0.136	0.251	0.549	
CoMSIA-SEHA	0.534	14	0.506	0.025	0.999	431.371	0.113	0.252	0.518		0.117
CoMSIA-SED	0.515	4	0.331	0.227	0.773	14.492	0.188	0.302		0.41	
CoMSIA-SEA	0.596	5	0.312	0.159	0.895	27.276	0.269	0.504			0.227
CoMSIA-SEDA	0.52	5	0.34	0.223	0.794	12.332	0.175	0.353		0.275	0.197
CoMSIA-SH	0.393	2	0.351	0.243	0.71	23.247	0.271		0.729		
CoMSIA-SD	0.56	7	0.348	0.227	0.813	8.716	0.653			0.347	
CoMSIA-SA	0.397	5	0.381	0.218	0.802	12.956	0.55				0.45
CoMSIA-SHD	0.512	3	0.323	0.254	0.698	13.84	0.077		0.273	0.65	
CoMSIA-SHA	0.467	14	0.542	0.061	0.993	73.68	0.217		0.556		0.228
CoMSIA-SDA	0.494	8	0.387	0.227	0.827	0.827	0.576			0.258	0.166
CoMSIA-SHDA	0.507	15	0.562	0.066	0.993	58.439	0.203		0.532	0.131	0.134
CoMSIA-EH	0.505	15	0.564	0.021	0.999	596.284		0.4	0.6		
CoMSIA-ED	0.499	5	0.347	0.224	0.791	12.139		0.58		0.42	
CoMSIA-EA	0.574	4	0.311	0.187	0.846	23.398		0.688			0.312
CoMSIA-EHD	0.535	3	0.315	0.239	0.733	16.434		0.148	0.262	0.591	
CoMSIA-EHA	0.526	16	0.604	0.024	0.999	412.994		0.288	0.576		0.136
CoMSIA-EDA	0.502	5	0.346	0.23	0.781	11.386		0.465		0.286	0.249
CoMSIA-EHDA	0.568	5	0.568	0.136	0.924	38.632		0.224	0.37	0.241	0.164
CoMSIA-HD	0.477	3	0.335	0.268	0.664	11.862			0.273	0.727	
CoMSIA-HA	0.443	14	0.443	0.075	0.99	48.305			0.764		0.236
CoMSIA-HDA	0.454	2	0.333	0.279	0.615	15.186			0.117	0.749	0.133
CoMSIA-DA	0.439	3	0.347	0.298	0.586	8.502				0.842	0.158
CoMSIA-ALL	0.571	5	0.321	0.137	0.922	37.606	0.088	0.192	0.341	0.239	0.139