Supporting Information

Copper-Catalyzed Syntheses of Pyrene-Pyrazole Pharmacophores and Structure Activity Studies for Tubulin Polymerization

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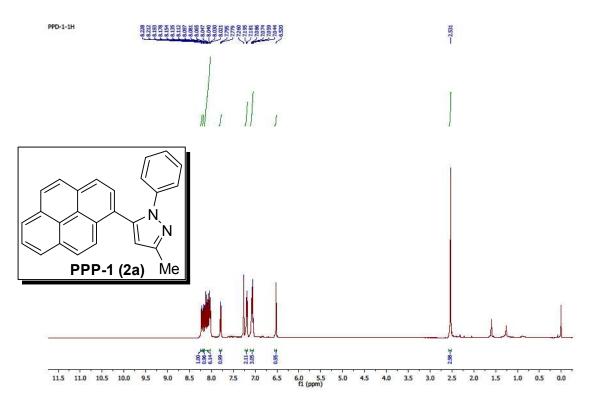


Figure S2. ¹³C NMR Spectra of 2a

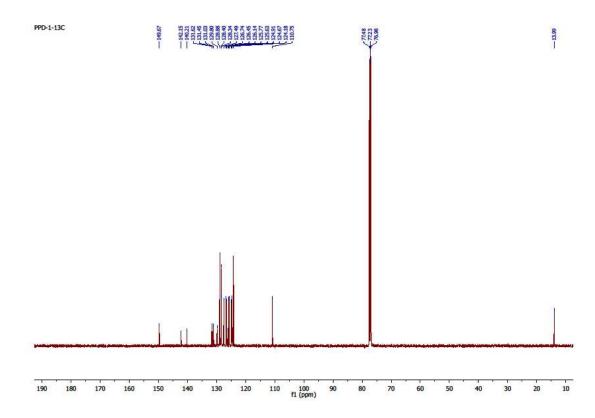
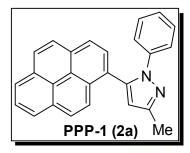


Figure S3. HRMS Spectra of 2a



Elementa	al Composition	Report							Page 1
Single M	ass Analysis								
Tolerance	= 10.0 PPM / D	BE: min = -	-1.5. max = 1	00.0					
	rediction: Off								
	isotope peaks us	ed for i-FIT	= 3						
Monoisotop	ic Mass, Even Elec	ron lons							
112 formula Elements U	(e) evaluated with ' sed:	results with	in limits (up to	50 closest	results for	each mass)			
C: 0-150	H: 0-220 N: 0-3	0:0-5							
DS-1-4th									
Qtor_60615	53 (2.694) AM (Top,4,	Ar, 14000.0,55	8.36,0.70,LS 3);	Cm (63:66)	k.				1: TOF MS ES+
100-3		359.	1536						7.59e+002
*	358.1932	359.0669	359.1933		360.1623		361.150	• 2. CONTRACTORIST	362.1187
-			1		2012 00 00 00 00	360.50		• 2. CONTRACTORIST	362.1187 m/z 362.00
358.0		THIN	16		T				TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT
%- 0		THIN	16	36	T				TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT
*		359.00	359.50	-1.5	T		361.00		TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT



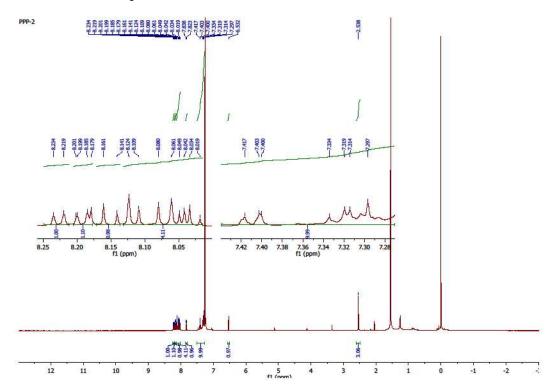
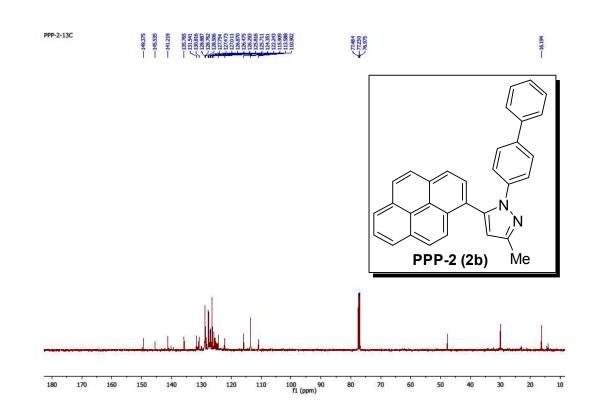


Figure S5. ¹³C NMR Spectra of 2b



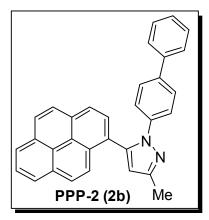


Figure S6. HR MS Spectra of 2b

Elemental Composition Report

435.1857 435.1861

-0.4

-0.9

Page 1

Single Mass Analysis Tolerance = 30.0 PPM / DBE: min = -1.5, max = 100.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 30 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used: C: 0-150 H: 0-220 N: 0-4 PPD-2-P-1 Qtof_61019 63 (2.673) AM (Top,4, Ar, 14000.0,716.46,0.70,LS 3) 1: TOF MS ES+ 2.40e+002 100 435.1857 436.1965 436.2164 436.20 436.40 m/z 434.80 435.00 435.40 435.60 435.80 436.00 435.20 Minimum: Maximum: -1.5 100.0 5.0 30.0 mDa PPM DBE Mass Calc. Mass i-FIT Formula

22.5 n/a

C32 H23 N2



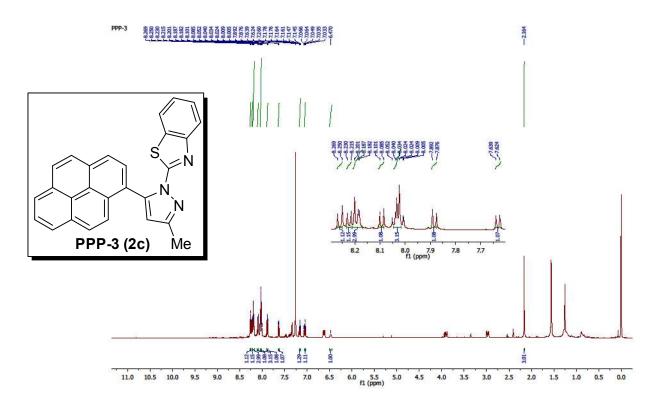


Figure S8. ¹³C NMR Spectra of 2c

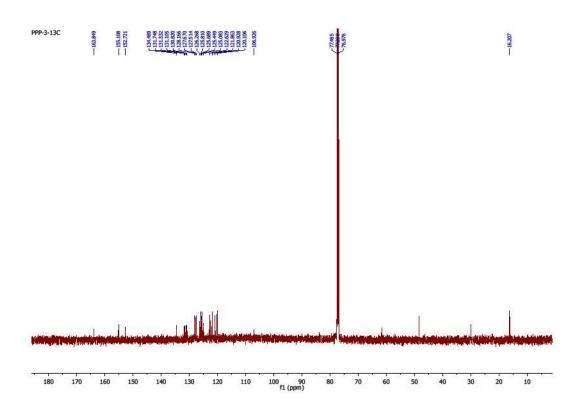


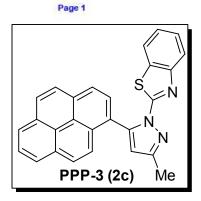
Figure S9. HRMS Spectra of 2c

Elemental Composition Report

Single Mass Analysis Tolerance = 5.0 PPM / DBE: min = -10.0, max = 100.0 Element prediction: Off Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions 79 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass) Elements Used: C: 0-70 H: 0-100 N: 0-5 S: 0-1

Minimum: Maxim <mark>um</mark> :		5.0	5.0	-10.0 100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
416.1214	416.1221	-0.7	-1.7	20.5	2743.4	n/a	n/a	C27 H18 N3 S





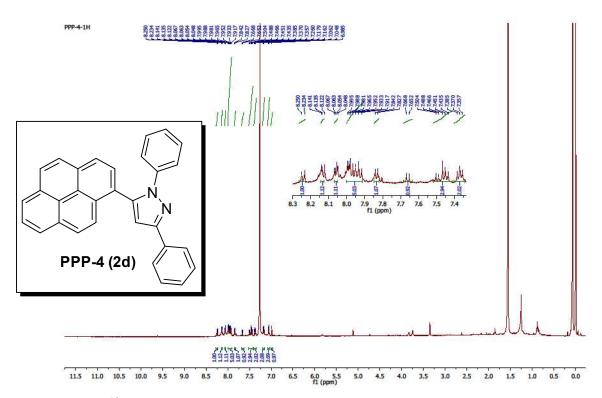


Figure S11. ¹³C NMR Spectra of 2d

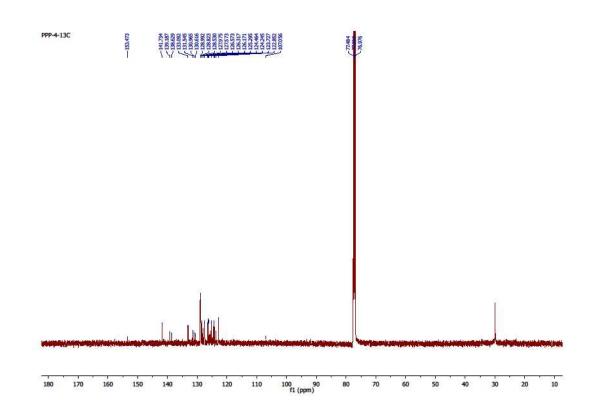
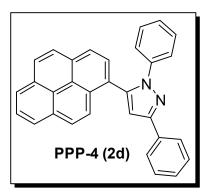


Figure S12. HRMS Spectra of 2d



Elemental	Composition	Report								P	age 1
Single Ma	ss Analysis										
	5.0 PPM / DE	3E: min = -	1.5, max = 1	00.00							
Element pre	ediction: Off										
Number of i	isotope peaks us	ed for i-FIT	r = 3								
194 formula(Elements Us C: 0-200 PPD-4-cr-2	: Mass, Even Elect e) evaluated with 1 ed: H: 0-200 N: 0-5 D (2.538) AM (Top.4,	i O: 0-5	58.36,0.70,LS 3			ach mass)				1: TOF M 3.2	/IS ES+ 14e+003
100- %-				756							
3 /10 3	131 420.2310		ELET OF	XXXX	23.1711	424.1521	an a	425.1658	426.1648	427,1808	
	100 00										
419.00	420.00	421.00	422.00	423	3.00	424.00	43	25.00	426.00	427.00	TT MZ
419.00 Minimum:	420.00	421.00 5.0	422.00 5.0	423 -1.5 100.0	3.00	424.00	4	25.00	426.00	427.00	m/z
419.00 Minimum: Maximum: Mass	420.00 Calc. Mass	421.00	422.00	-1.5	3.00 1-FIT	424.00 Form		25.00	426.00	427.00	++ mz

Figure S13. ¹H NMR Spectra of 2e

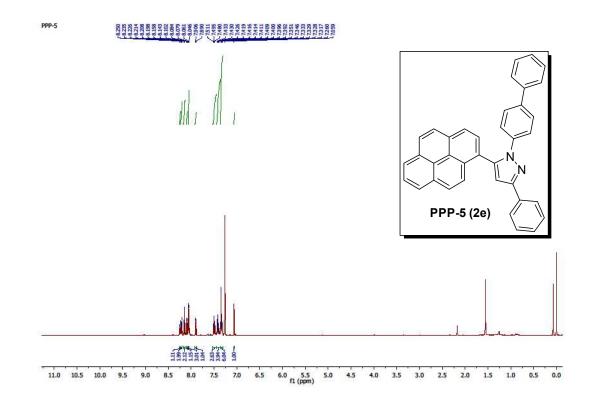


Figure S14. ¹³C NMR Spectra of 2e

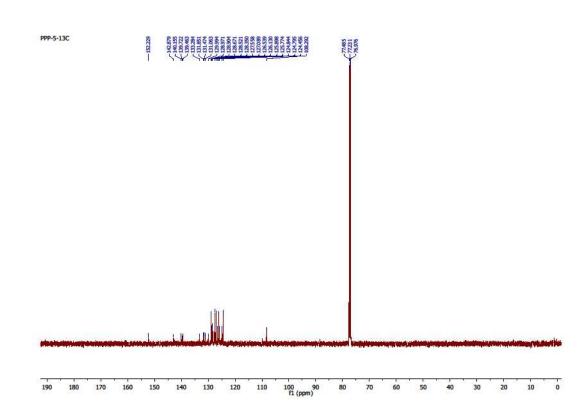
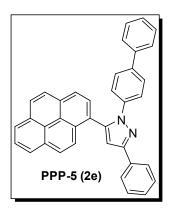


Figure S15. HRMS Spectra of 2e



Elemental Composition Report

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 500 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass) Elements Used: C: 0-150 H: 0-220 N: 0-5 O: 0-6 Na: 0-1 PPD-5-N Qtof_61267 85 (3.646) AM (Top.4, Ar,14000.0,716.46,0.70,LS 3); Cm (84:89)

1: TOF MS ES+ 1.34e+003

Page 1

100-					497.3	2036						1.040.100
*	493.34			496.4	4217	498.1989 497.2461	499.2036	500.3	2137	501.2163	umo es	502.6387 m/z
4	193.0	494.0	495.0	496.0	497.0	496.0	499.0	500.0		501.0	502.0	503.0
Minimum					-1.5							
Maximum	-		5.0	10.0	100.0	R.						
Mass	Cal	.c. Mass	mDa	PPM	DBE	i-FIT	Formula					
497.203		.2052	-1.6	-3.2	14.5	57.2	C28 H30		05	Na		
	491	2018 2076 1994	1.8 -4.0 4.2	3.6 -8.0 8.4	26.5 17.5 23.5	18.8 45.2 26.5	C37 H25 C30 H29 C35 H26	N2	O5 Na			

497.2036

Figure S16. ¹H NMR Spectra of 2f

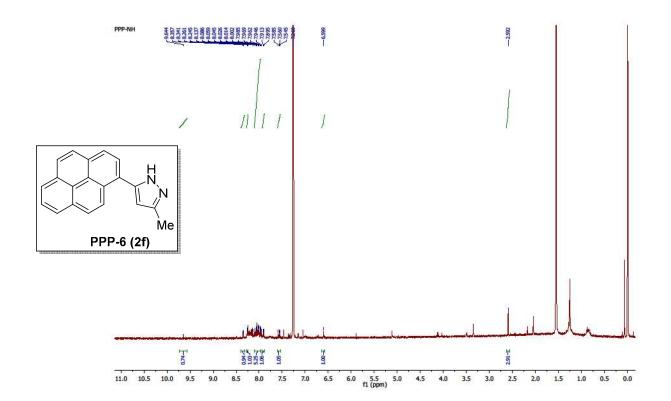


Figure S17. ¹³C NMR Spectra of 2f

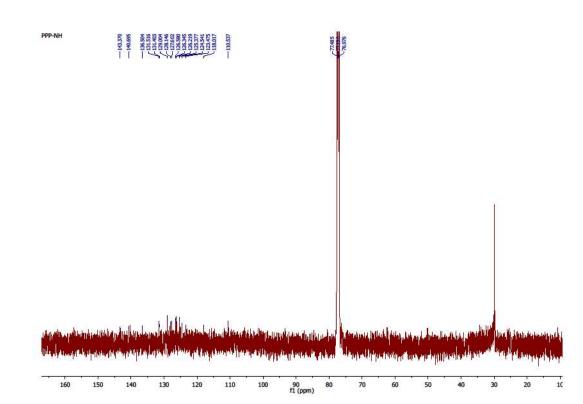
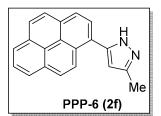


Figure S18. HRMS Spectra of 2f



Elemental	Composition	Report									P	age 1
Single Ma	ss Analysis											
	10.0 PPM / D	BE: min = -	1.5, max = 1	00.0								
Element pre	ediction: Off											
Number of i	sotope peaks us	ed for i-FIT	= 3									
	Mass, Even Elect		i limits (un to	50 closest re	sults for an	(arem do						
Elements Us		Tesuits within	rinning (up to	ou orosesere	cours for car	an massy						
C: 0-200	H: 0-200 N: 0-6	0:0-5	Na: 0-1									
PPD-NH												
Qtor_61689 61	(2.606) AM (Top,5,)	Ar,14000.0,716	5.46,0.70,LS 3);	; Cm (58:65)							1: TOF 1	
	I (2.606) AM (Top,5,)	Ar,14000.0,716	5.46,0.70,LS 3);		13.1239							MS ES+ 06e+003
100	1 (2.605) AM (Top,5,)	Ar,14000.0,716	5.46,0.70,LS 3)		5 283.1591			284.12	24			06e+003
100		Ar,14000.0,716	5.46,0.70,LS 3) 282.50	28	5 283.1591	53.50		284.12	24	284.50	1.1	
100 %281.	1416			28	5 283.1591				24	284.50	285.1420	06e+003
100 281.00 Minimum:	1416	282.00	282.50	28 283.072 283.0 283.0	5 283.1591		284		24	284.50	285.1420	06e+003
100 % 281. 281.00 Minimum: Maximum:	1416 281.50	282.00 5.0	282.50 10.0	283.0725 283.0725 283.0 -1.5 100.0	5 283.1591 00 21	83.50	284		24	284.50	285.1420	06e+003

Figure S19. ¹H NMR Spectra of 2g

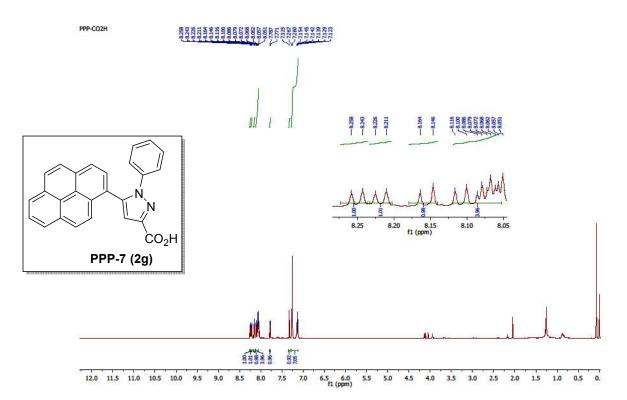


Figure S20. ¹³C NMR Spectra of 2g

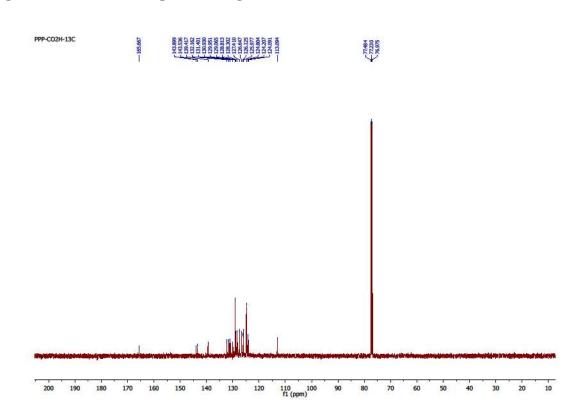
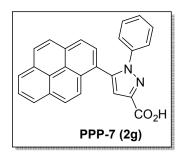


Figure S21. HRMS Spectra of 2g



Elementa	al Composition	Report										Page '
Single M	ass Analysis											
	= 10.0 PPM / D rediction: Off	BE: min = -	-1.5, max =	100.0								
	isotope peaks us	ed for i-FIT	= 3									
Monoisotop	ic Mass, Even Elect	ron lons										
179 formula Tements U	(e) evaluated with 4	results with	in limits (up t	to 50 closest r	results for eac	h mass)						
	H: 0-200 N: 0-6	O: 0-6	Na: 0-1									
	59 (2.505) AM (Top,5	Ar,14000.0,5	58.36,0.70,LS	3); Cm (57:59)							
Qtor_61718a	59 (2.505) AM (Top,5	Ar,14000.0,5	58. <mark>3</mark> 6,0.70,LS	3); Cm (57:59) 411.1124							
Qtor_61718a	59 (2.505) AM (Top,5	, Ar,14000.0,5	58. <mark>3</mark> 6,0.70,LS	3); Cm (57:59 410.8458		6				412.118	8	.70e+00
Qtor_61718a	409.7953		58.36,0.70,LS 410.50	410.8458	411.1124	411.5			41:	412.118	8	MS ES- .70e+00
Calor_61718a	409.7953			410.8458	411.1124		,		412		8 1 412.3969	.70e+00
Qtor_61718a	409.7953			410.8458 41	411.1124				41:		8 1 412.3969	.70e+00
Qtbr_61718a 100- %- 409.5 410.5 410.5 410.5	409.7953		410.50	410.8458 41 -1.5	411.1124		5		412		8 1 412.3969	.70e+00
Qubr_61718a	409.7953 0 410.0 Calc. Mass 411.1134	0 5.0 mDa -1.0	410.50 10.0 PPM -2.4	410.8458 41 -1.5 100.0 DBE 22.5	411.1124 411.143 1.00 i.FIT n/a	411.50 Form C28	ula H15	, N2	02	200	8 1 412.3969	.70e+00
100 *	409.7953 0 410.0 Calc. Mass	0 5.0 nDa	410.50 10.0 PPM	410.8458 41 -1.5 100.0 DBE	411.1124 411.143 1.00	411.50 Form	ula	N2 N2 N2			8 1 412.3969	.70e+00

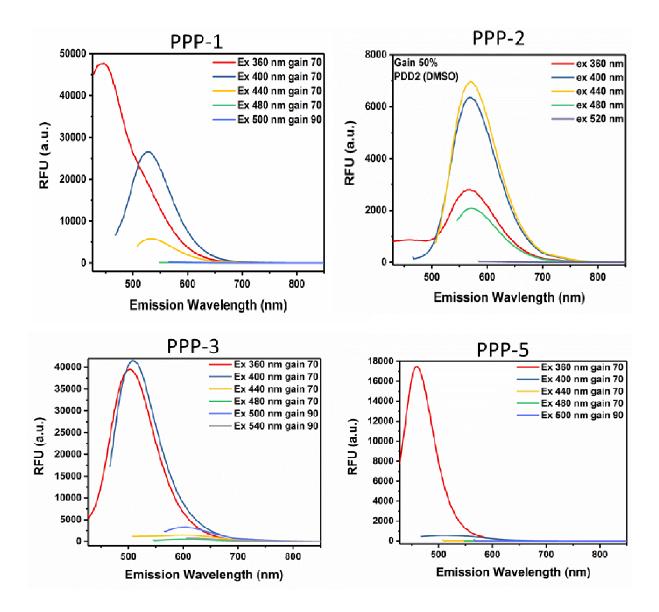


Figure S22. Fluorescence spectra of representative PPP agents (2a-c, e) at different excitation ranging from 360-540 nm.

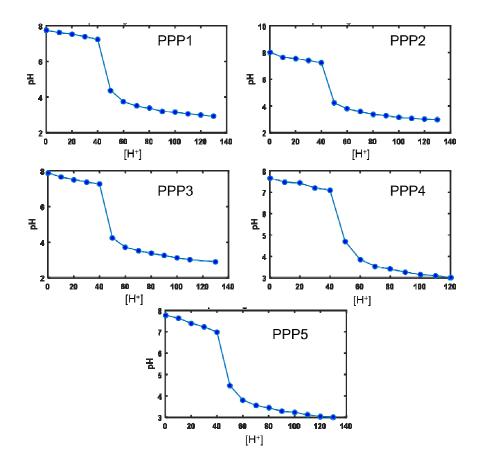


Figure S23. pH response of PPP agents (2a-e) with varying concentration of hydronium ion within pH ranging from 3-7.77 confirming similar overall trend across all the molecules.

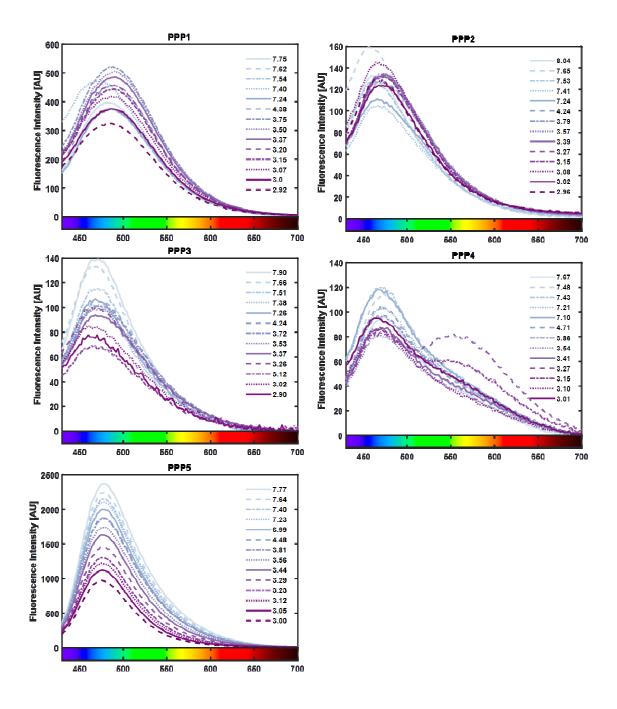


Figure S24. Overlaid fluorescence spectra of PPP agents (2a-e) at different pH ranging from 3-7.77, observing the emission from 400-700nm.

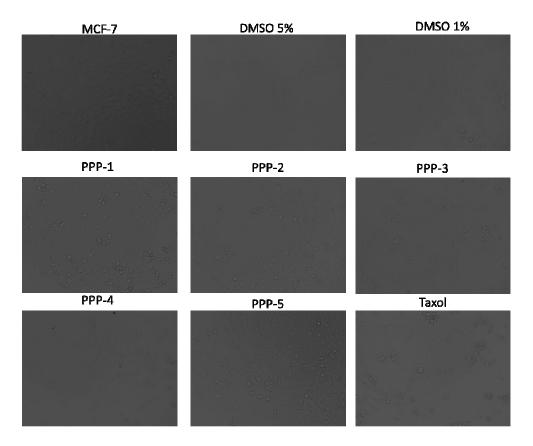


Figure S25. Bright field images of MCF-7 cell treated with PPPs and controls.