

Supporting Information

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

Dinabandhu Sar,^{§,⊥,#} Indrajit Srivastava,^{§,⊥,#} Santosh K. Misra,^{⊥,#} Fatemeh Ostadhossein,^{⊥,#} Parinaz Fathi,^{⊥,#} and Dipanjan Pan^{*,⊥,#,§,@}

[⊥]Department of Bioengineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA.

[#]Mills Breast Cancer Institute and Carle Foundation Hospital, 502 North Busey, Urbana, Illinois 61801, USA.

[§]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA.

[@]Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA.

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Figure S1. ^1H NMR Spectra of **2a**

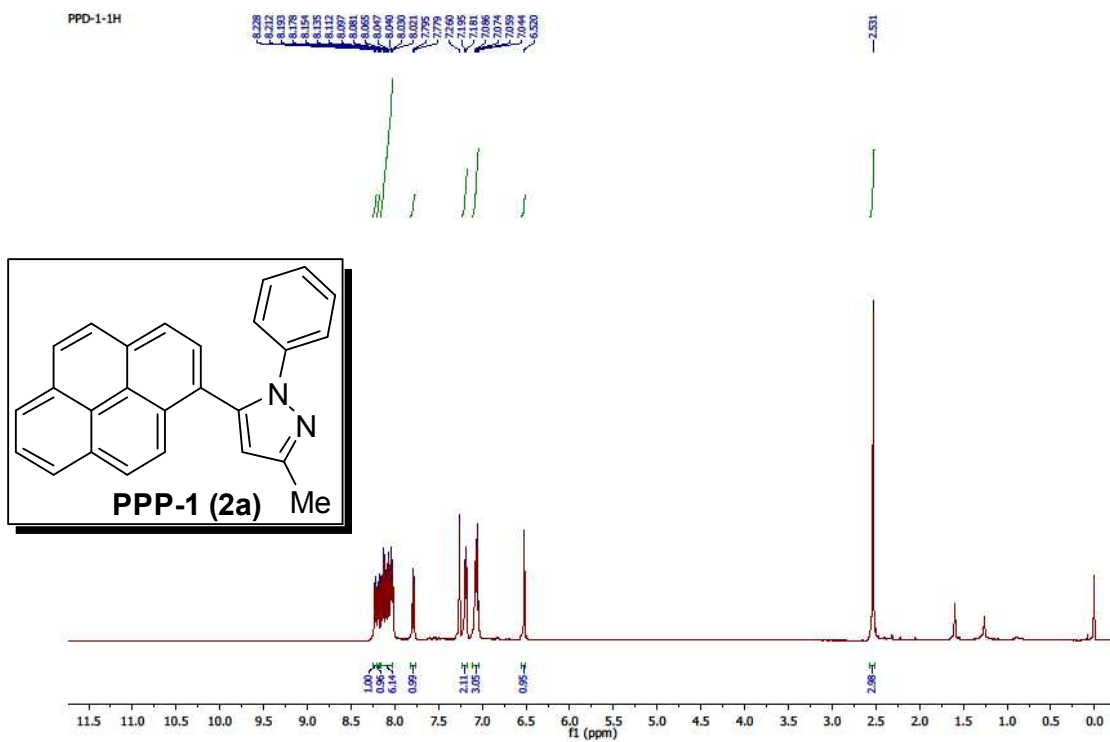


Figure S2. ^{13}C NMR Spectra of **2a**

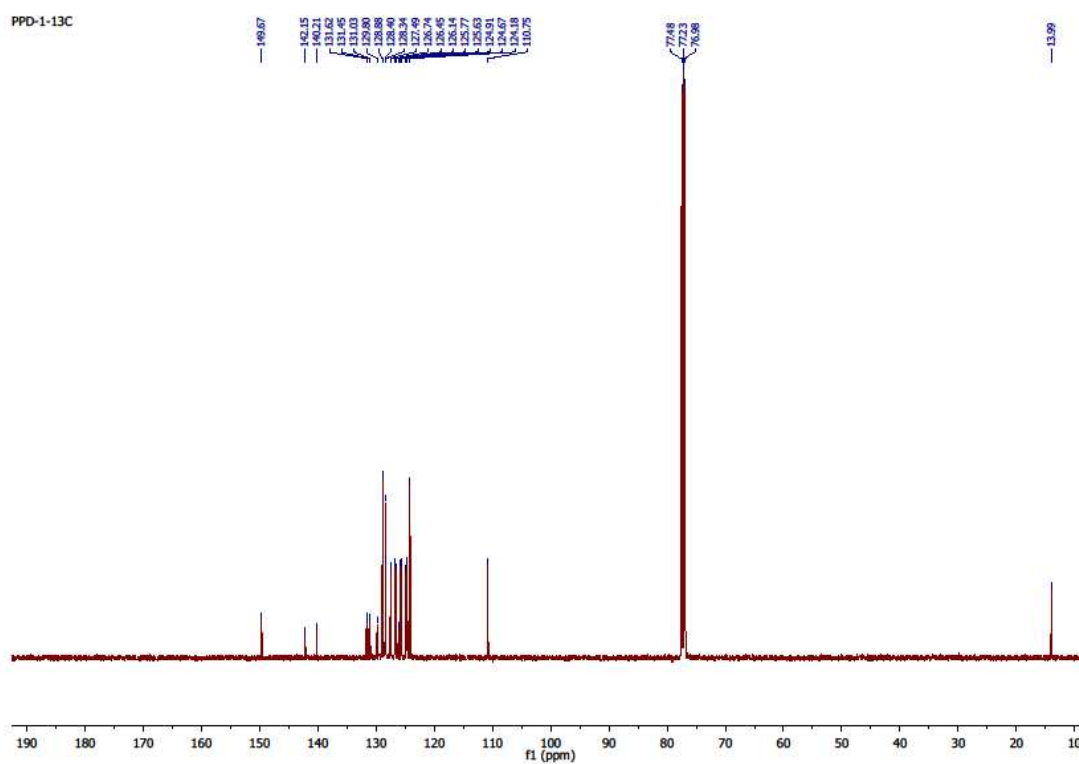
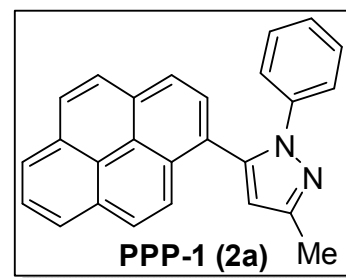


Figure S3. HRMS Spectra of 2a



Elemental Composition Report

Page 1

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

112 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

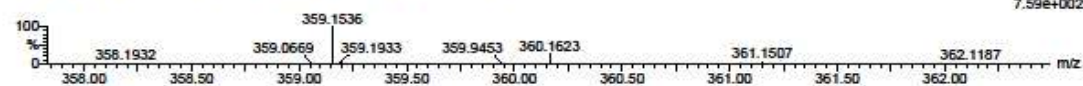
Elements Used:

C: 0-150 H: 0-220 N: 0-3 O: 0-5

DS-1-4th

Qtof_60615 63 (2.694) AM (Top,4, Ar, 14000.0,558.36,0.70,LS 3); Cm (63:66)

1: TOF MS ES+
7.59e+002



Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
359.1536	359.1548	-1.2	-3.3	18.5	3.2	C26 H19 N2

Figure S4. ^1H NMR Spectra of **2b**

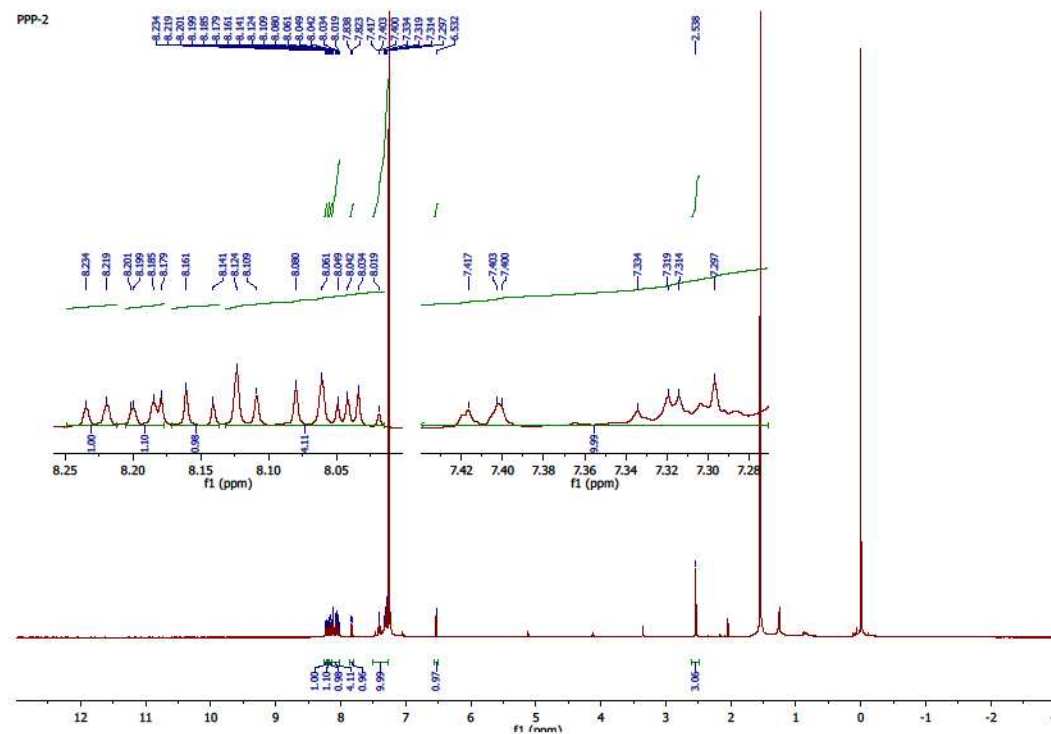


Figure S5. ^{13}C NMR Spectra of **2b**

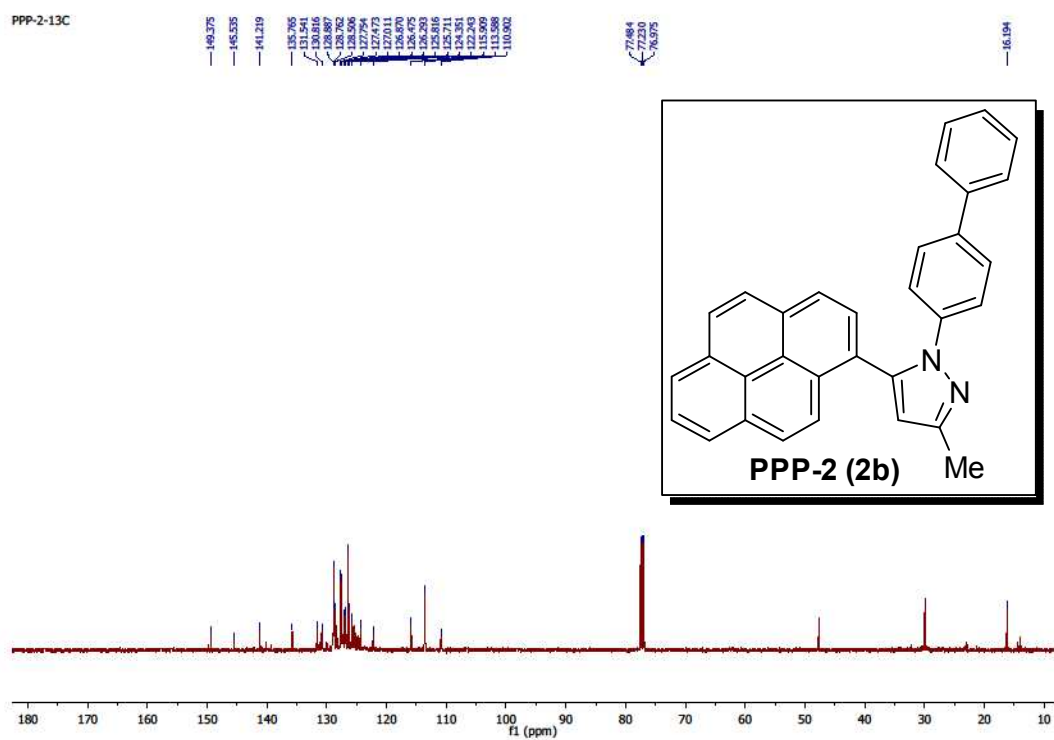
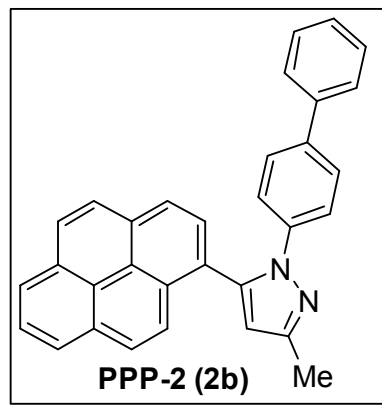


Figure S6. HR MS Spectra of 2b



Elemental Composition Report

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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)

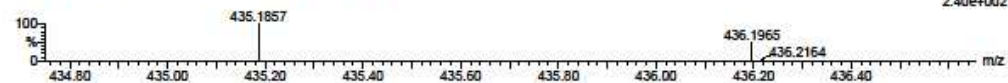
Elements Used:

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



Minimum:				-1.5		
Maximum:		5.0	30.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
435.1857	435.1861	-0.4	-0.9	22.5	n/a	C32 H23 N2

Figure S7. ^1H NMR Spectra of 2c

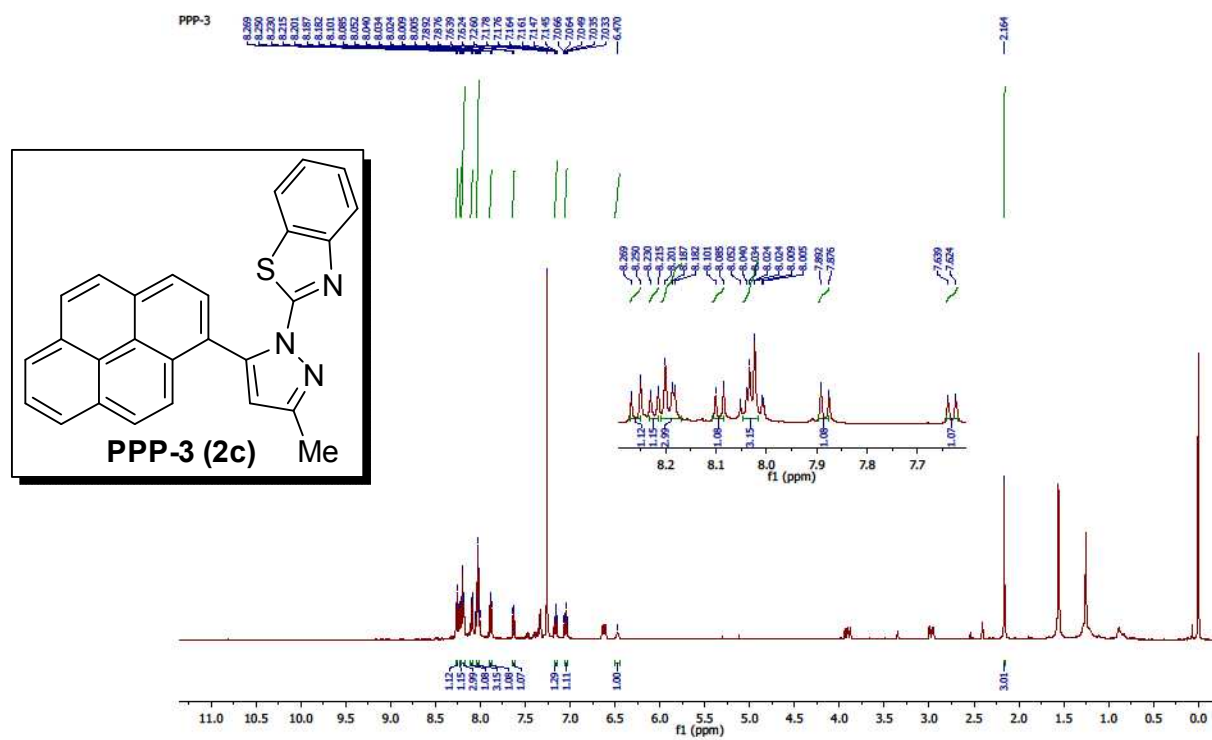


Figure S8. ^{13}C NMR Spectra of **2c**

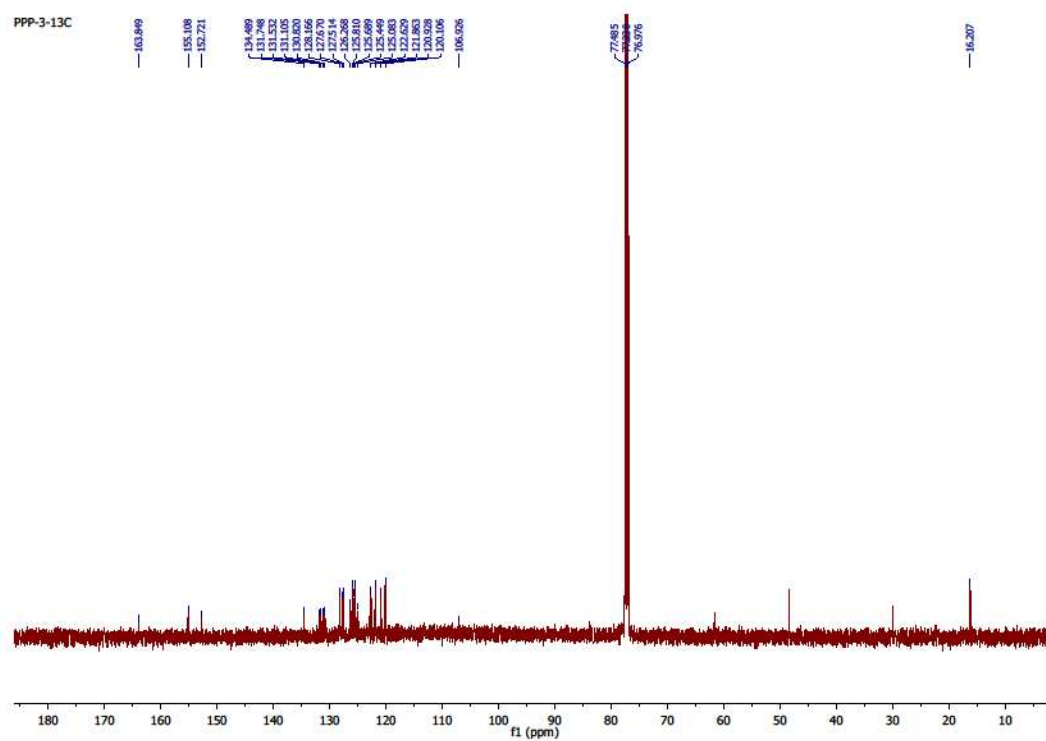


Figure S9. HRMS Spectra of 2c

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:										
Maximum:		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	2742.4	n/a	n/a	C27 H18 N2 S		

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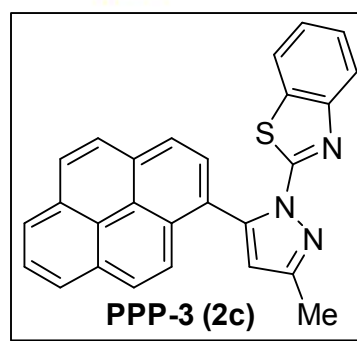


Figure S10. ^1H NMR Spectra of **2d**

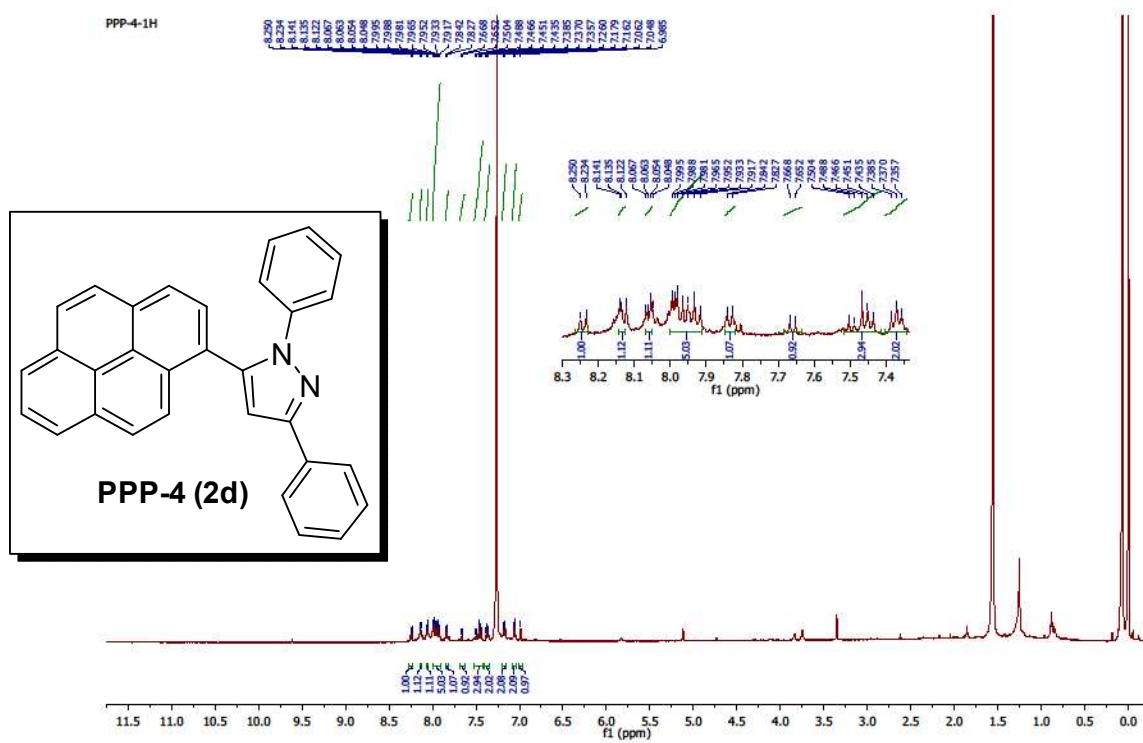


Figure S11. ^{13}C NMR Spectra of **2d**

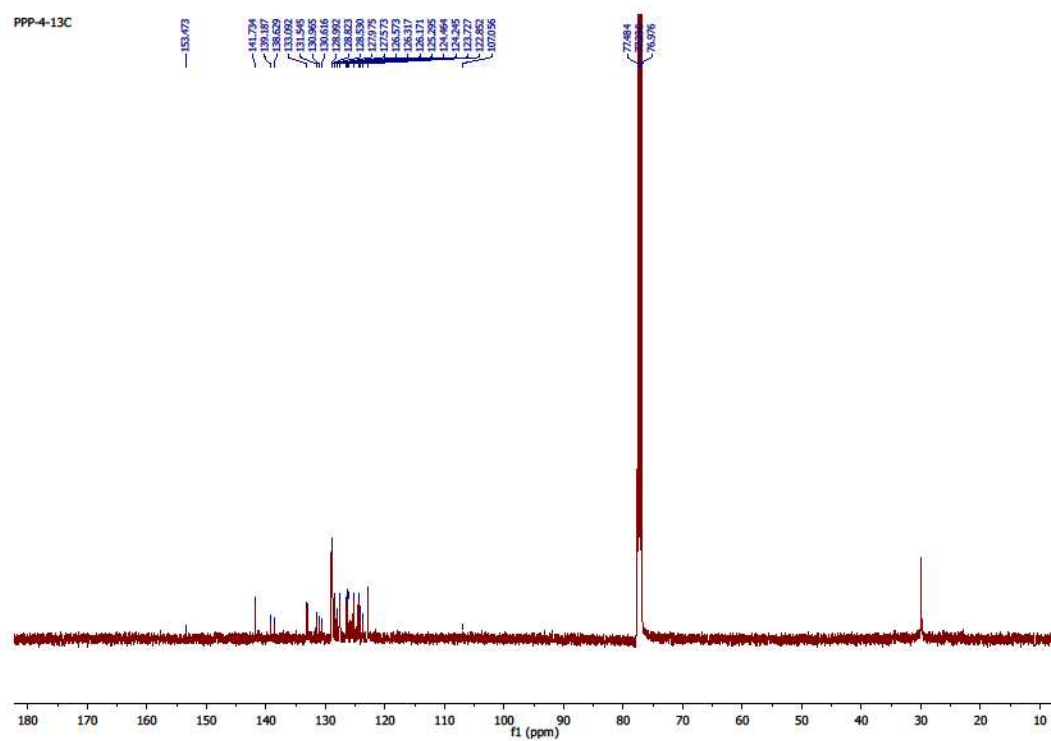
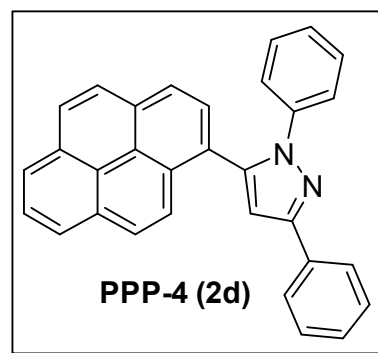


Figure S12. HRMS Spectra of 2d



Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 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

194 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

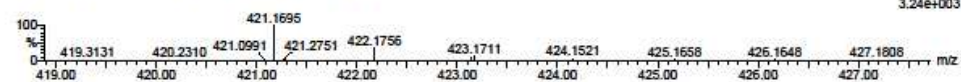
Elements Used:

C: 0-200 H: 0-200 N: 0-5 O: 0-5

PPD-4-gr-2

Qtof_62589 60 (2.538) AM (Top,4, Ar,14000.0,558.36,0.70,LS 3); Cm (58:61)

1: TOF MS ES+
3.24e+003



Minimum: -1.5
Maximum: 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
421.1695	421.1705	-1.0	-2.4	22.5	33.8	C31 H21 N2

Figure S13. ^1H NMR Spectra of **2e**

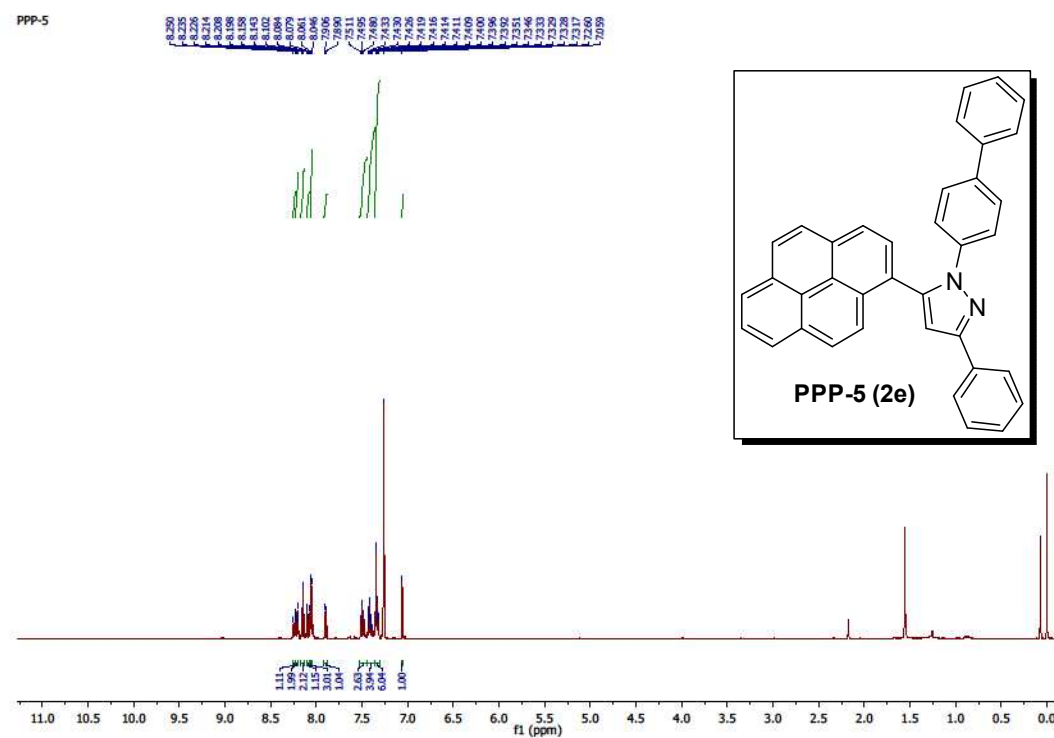


Figure S14. ^{13}C NMR Spectra of **2e**

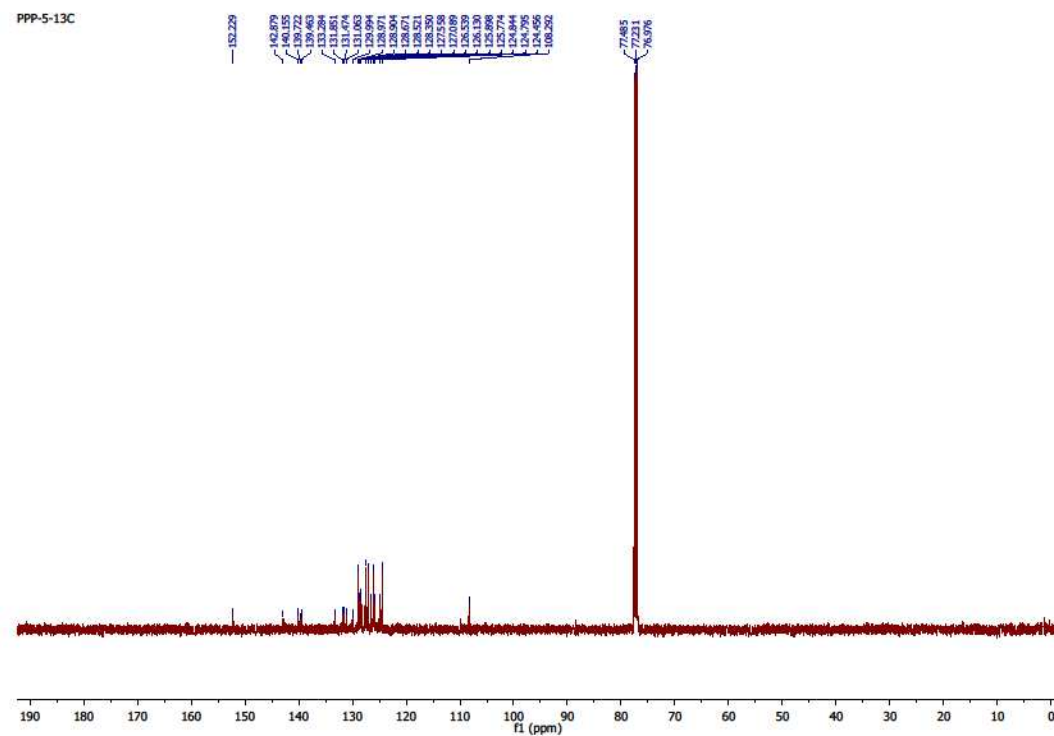
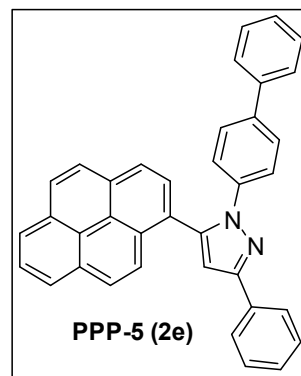


Figure S15. HRMS Spectra of 2e



Elemental Composition Report

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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: 0-8 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

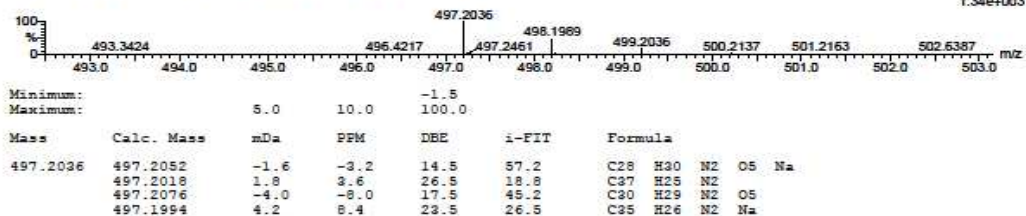


Figure S16. ^1H NMR Spectra of **2f**

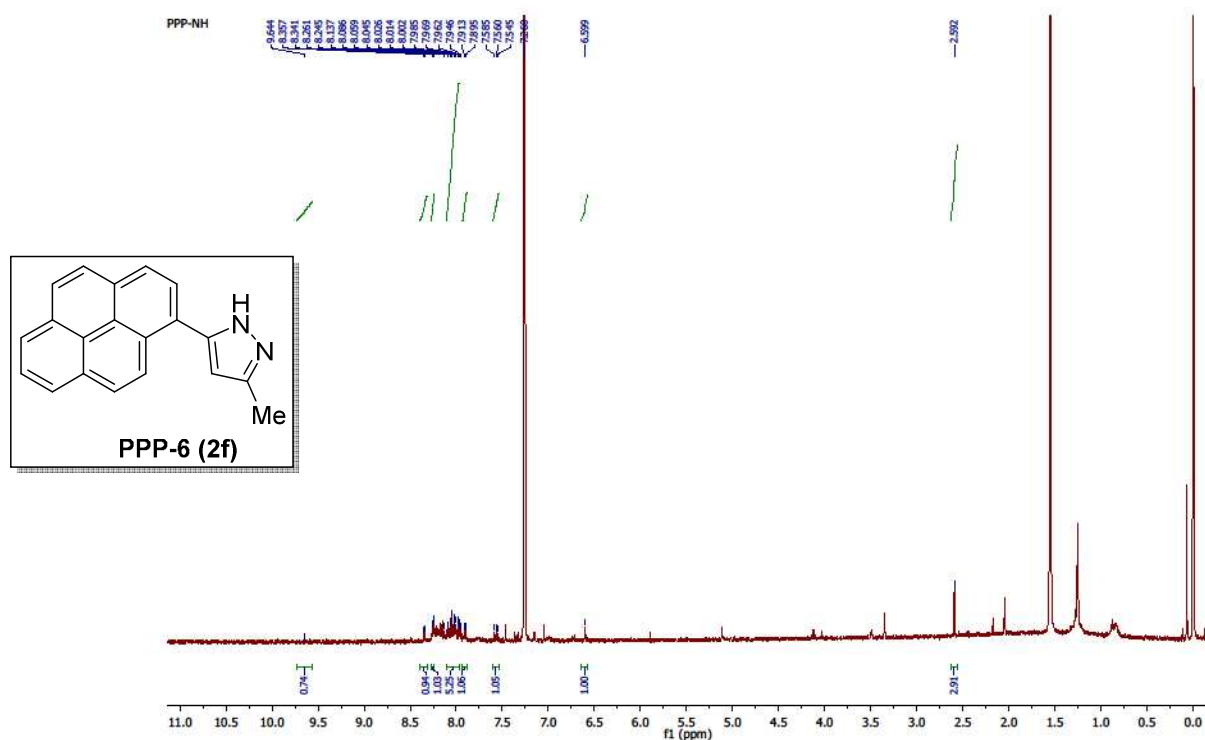


Figure S17. ^{13}C NMR Spectra of **2f**

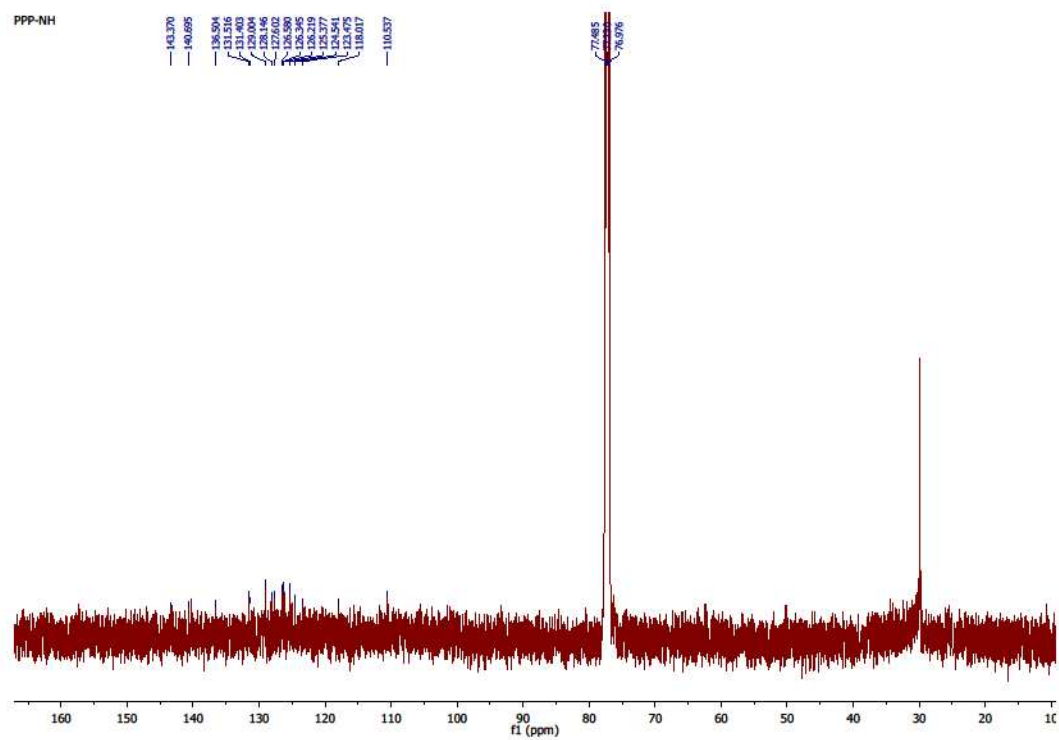
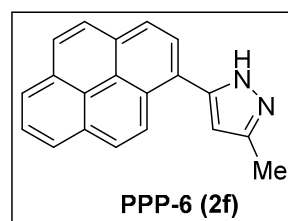


Figure S18. HRMS Spectra of **2f**



Elemental Composition Report

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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

291 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

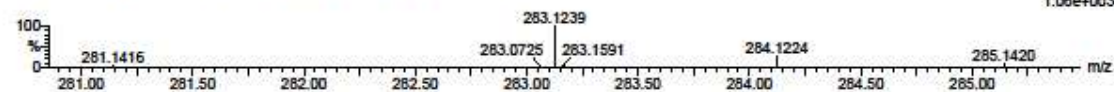
Elements Used:

C: 0-200 H: 0-200 N: 0-6 O: 0-5 Na: 0-1

PPD-NH

Qtof_61689 61 (2.606) AM (Top, S, Ar, 14000.0, 716.46, 0.70, LS 3); Cm (58:65)

1: TOF MS ES+
1.06e+003



Minimum: -1.5
Maximum: 100.0

Mass	Calc. Mass	mDa	PFM	DBE	i-FIT	Formula
283.1239	283.1235	0.4	1.4	14.5	12.5	C20 H15 N2
	283.1211	2.8	9.9	11.5	18.1	C18 H16 N2 Na

Figure S19. ^1H NMR Spectra of **2g**

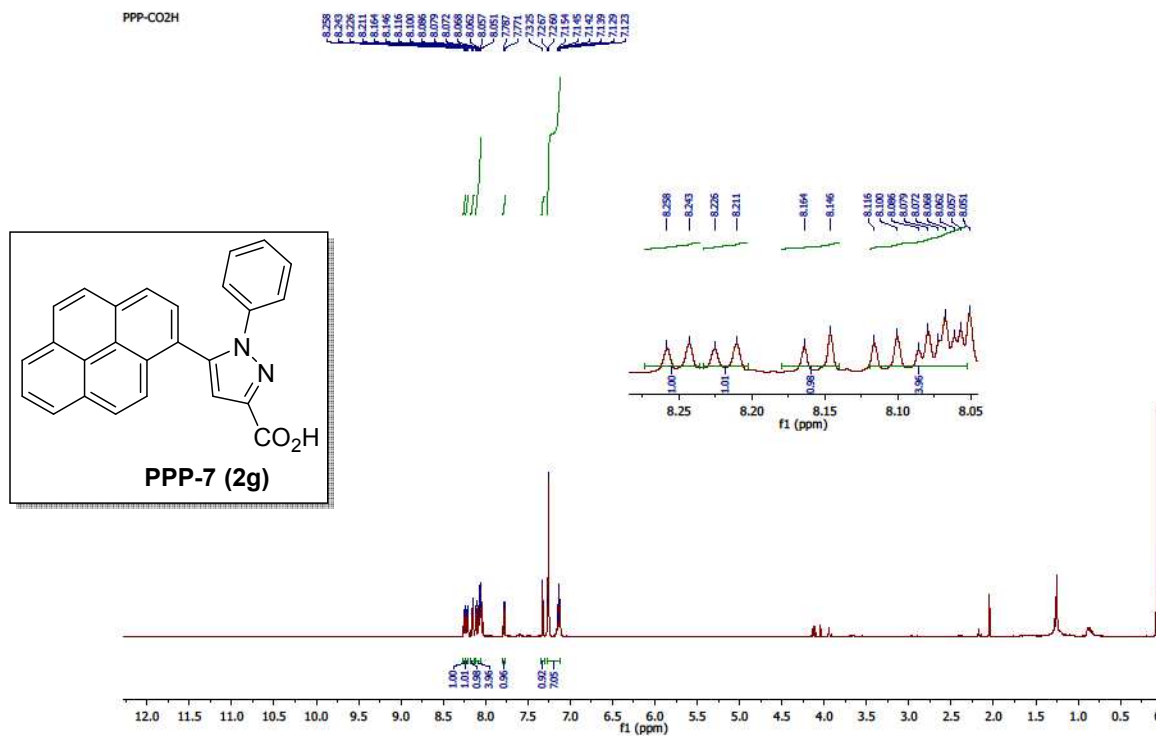


Figure S20. ^{13}C NMR Spectra of **2g**

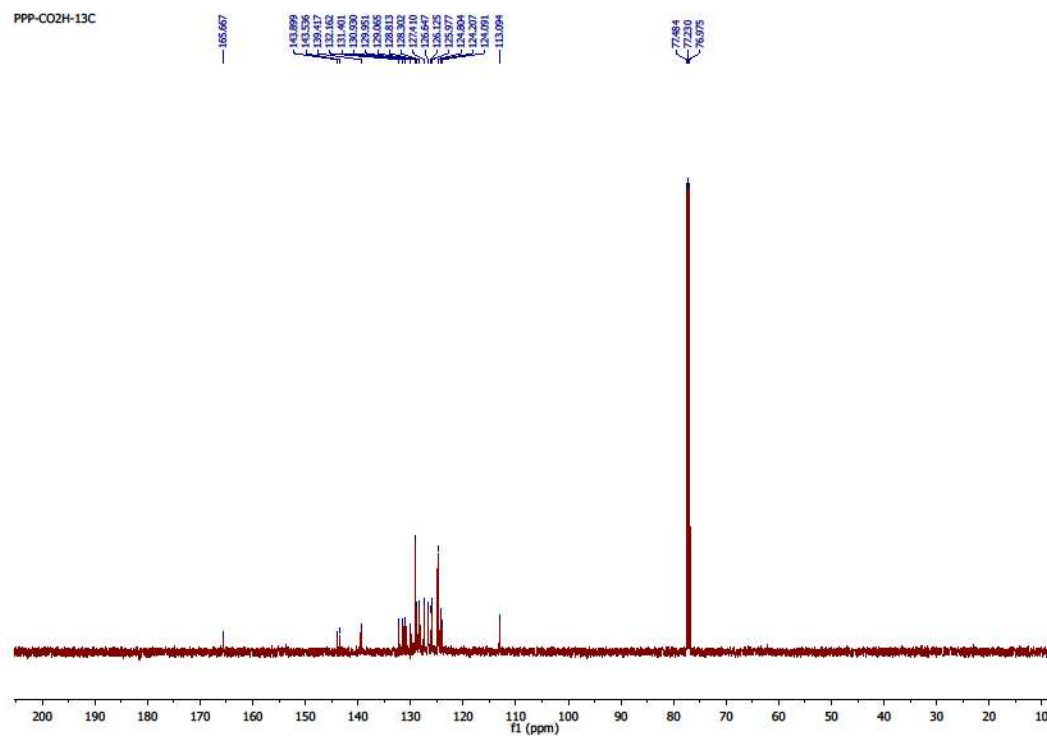
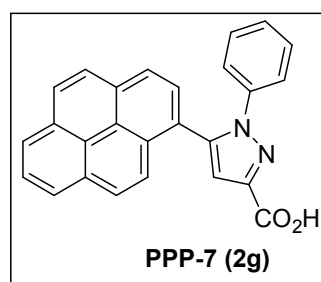


Figure S21. HRMS Spectra of 2g



Elemental Composition Report

Page 1

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

479 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

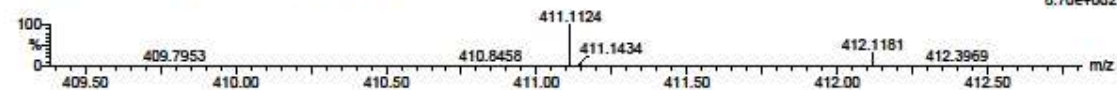
Elements Used:

C: 0-200 H: 0-200 N: 0-6 O: 0-6 Na: 0-1

PPD-C-1

Qtof_61716a 59 (2.505) AM (Top,5, Ar,14000.0,558.36,0.70,LS 3); Cm (57:59)

1: TOF MS ES+
8.70e+002



Minimum:

Maximum: 5.0 10.0 -1.5 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula			
411.1124	411.1134	-1.0	-2.4	22.5	n/a	C28	H15	N2	O2
	411.1109	1.5	3.6	19.5	n/a	C26	H16	N2	O2 Na
	411.1150	-2.6	-6.3	23.5	n/a	C31	H16	Na	
	411.1093	3.1	7.5	18.5	n/a	C23	H15	N4	O4

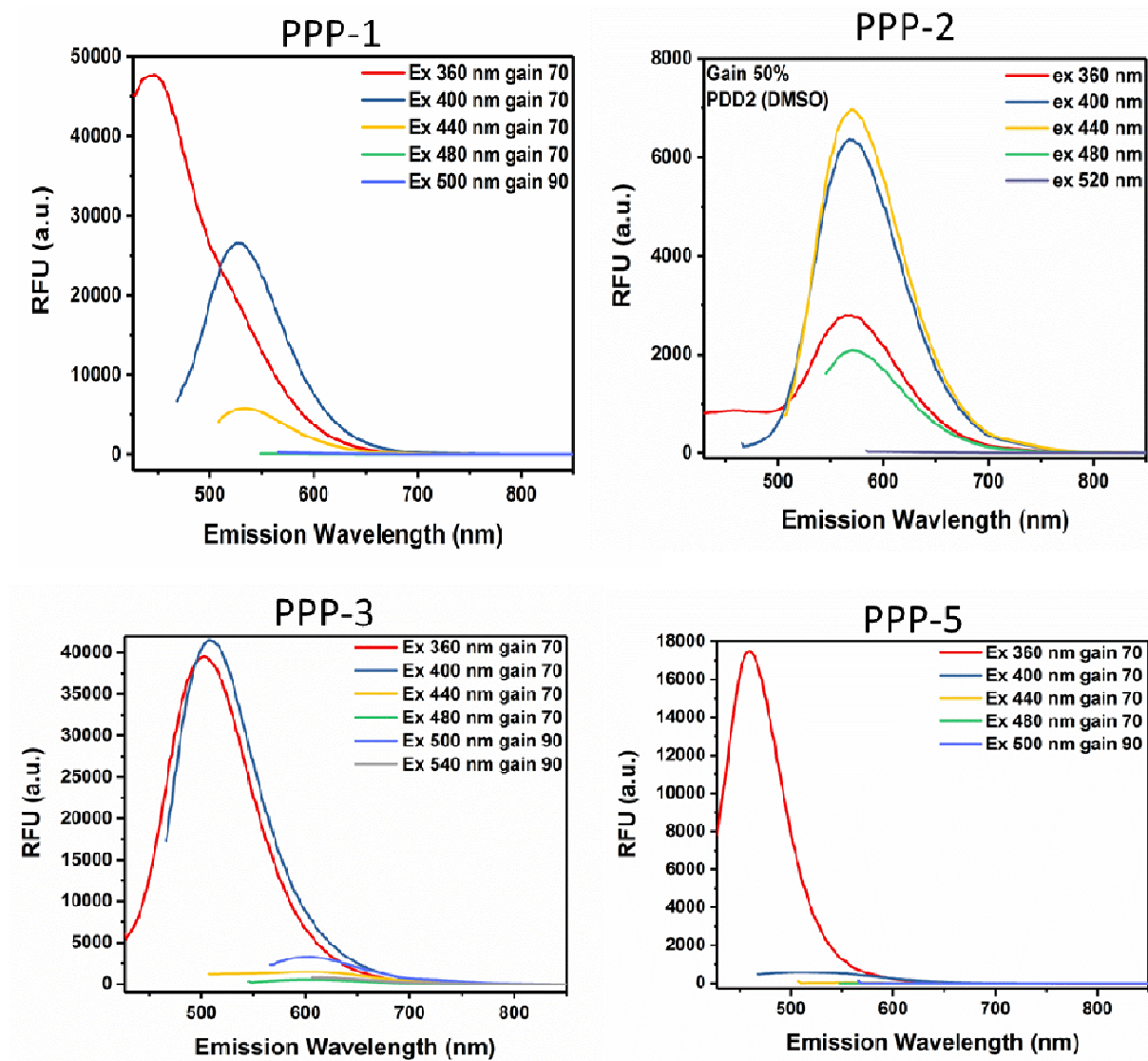


Figure S22. Fluorescence spectra of representative PPP agents (2a-c, e) at different excitation ranging from 360-540 nm.

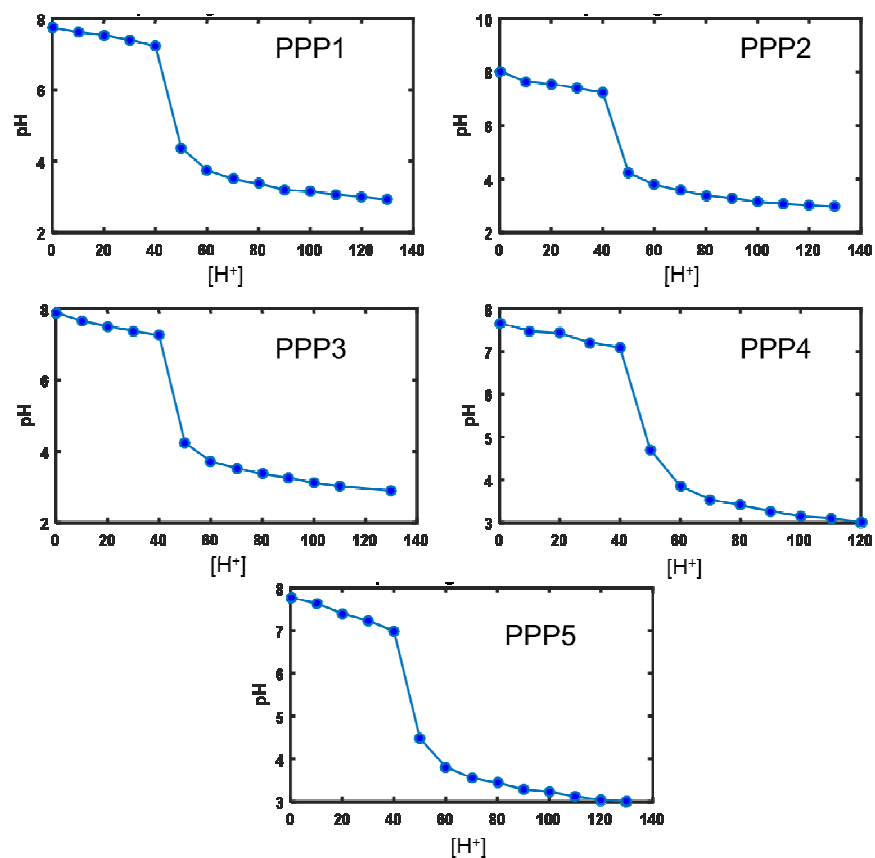


Figure S23. pH response of PPP agents (2a-e) with varying concentration of hydronium ion within pH ranging from 3-7.77 confirming similar overall trend across all the molecules.

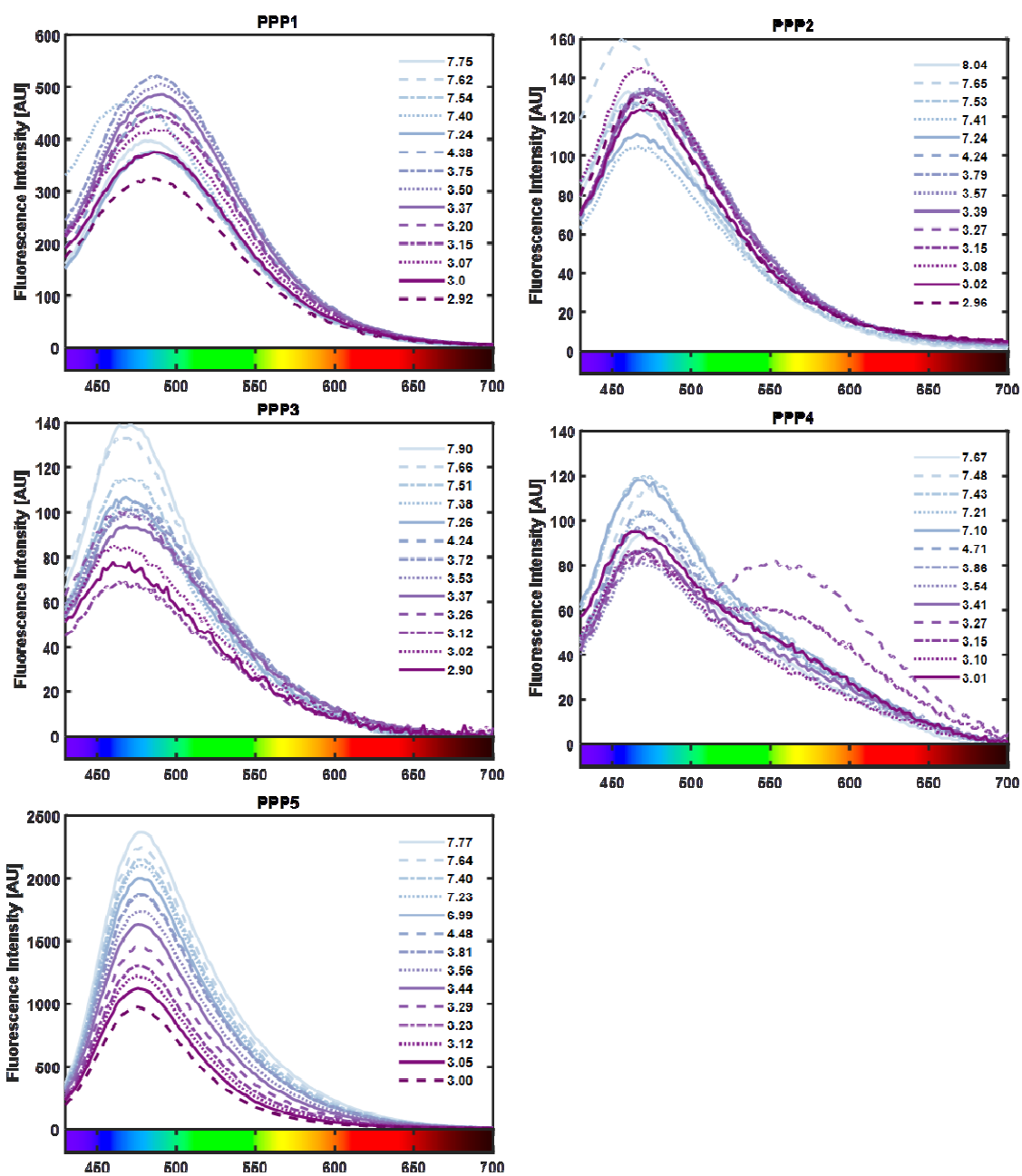


Figure S24. Overlaid fluorescence spectra of PPP agents (2a-e) at different pH ranging from 3-7.77, observing the emission from 400-700nm.

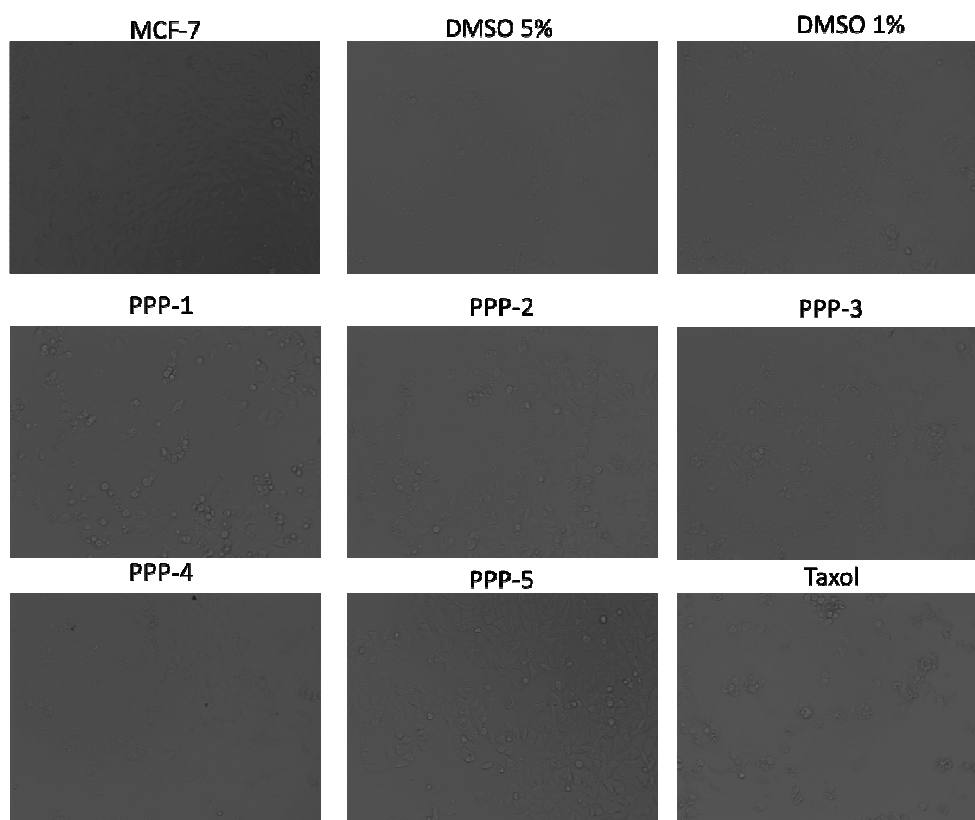


Figure S25. Bright field images of MCF-7 cell treated with PPPs and controls.