Supplementary Information

Fluorescent Sensor Based on 1*H*-Pyrazolo[3,4-*b*]quinoline Derivative for Detecting Zn^{2+} Cations

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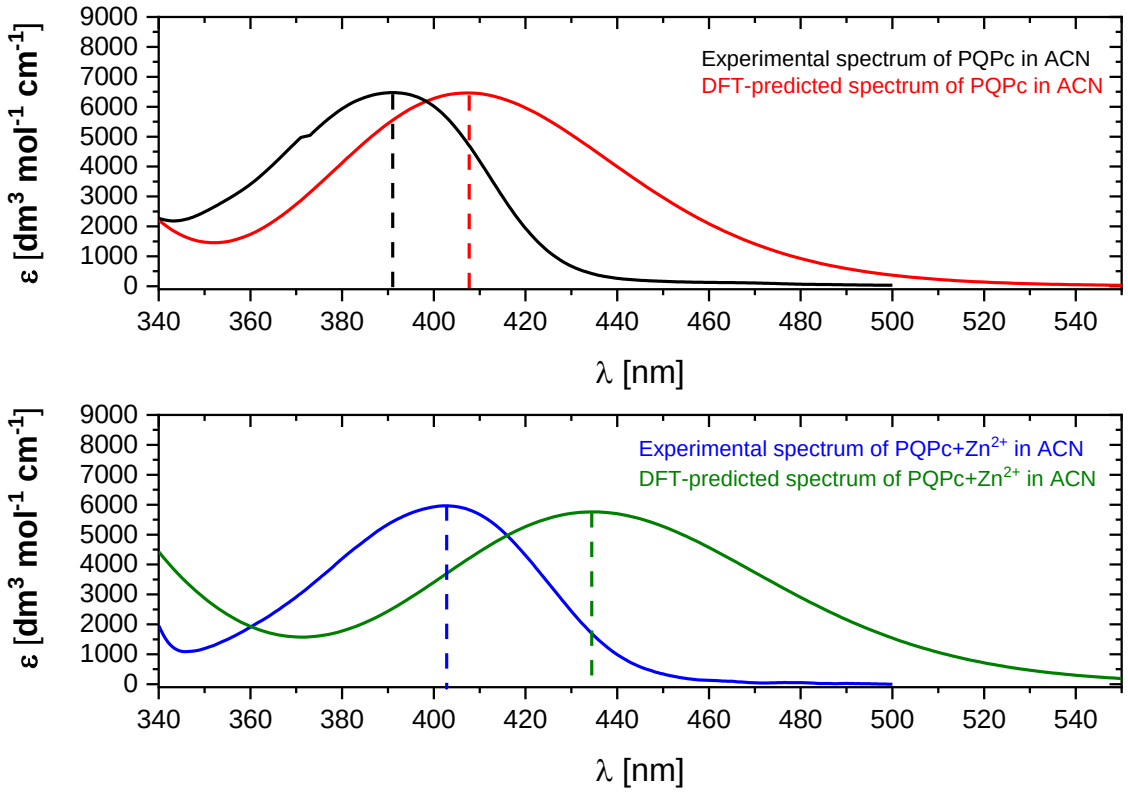


Figure S1. Experimental and DFT-predicted spectra of the PQPc and of the PQPc+Zn^{2+} in acetonitrile.

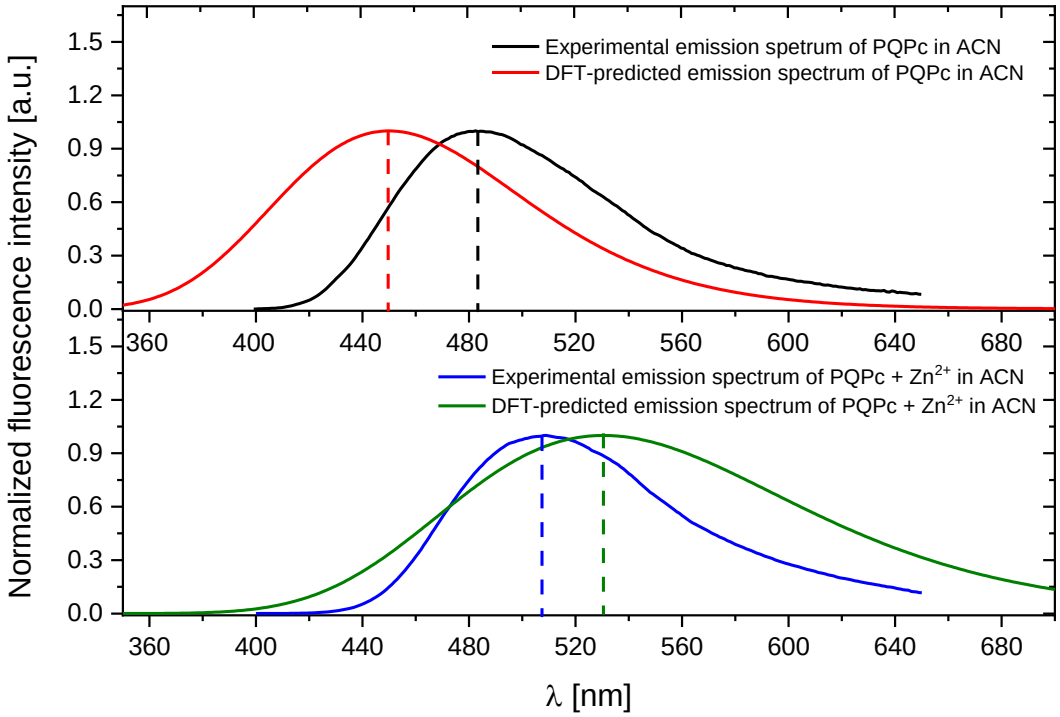


Figure S2. Experimental and DFT-predicted emission spectra of the PQPc and of the PQPc+Zn^{2+} in acetonitrile.

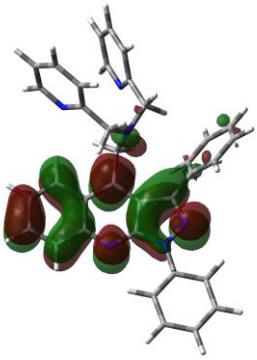
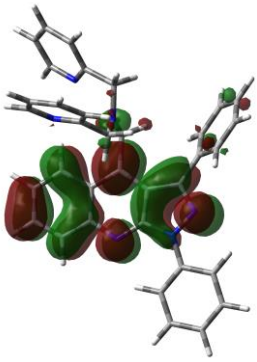
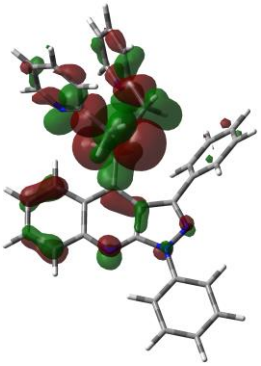
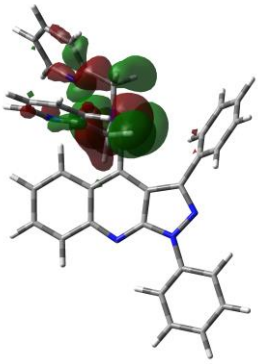
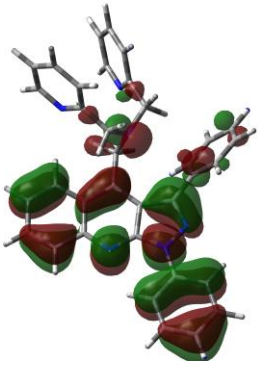
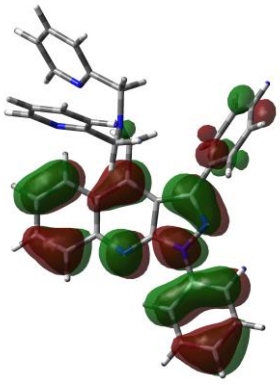
	Ground state geometry	Excited state geometry
LUMO		
HOMO		
HOMO-1		

Figure S3. Comparison of the HOMO-1, HOMO, and LUMO orbitals calculated for the PQPc complex in the ground-state geometry with the same type of orbitals in the excited-state geometry.

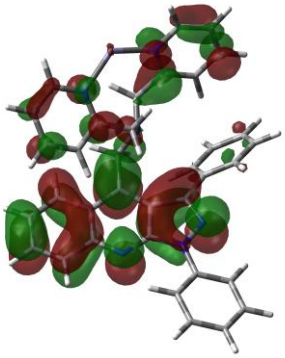
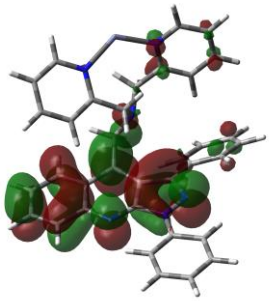
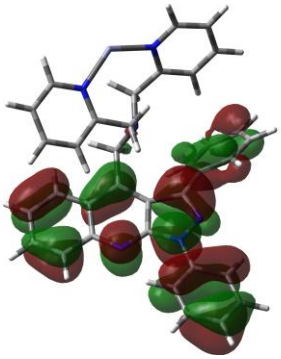
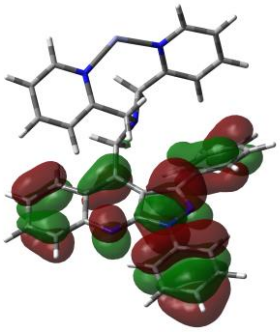
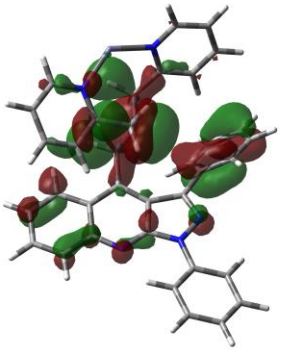
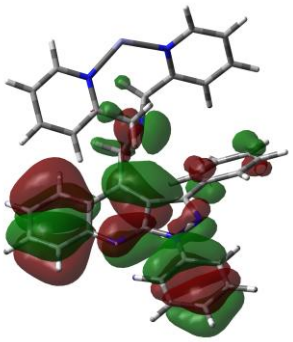
	Ground state geometry	Excited state geometry
LUMO		
HOMO		
HOMO-1		

Figure S4. Comparison of the HOMO-1, HOMO, and LUMO orbitals calculated for the PQPc+Zn^{2+} complex in the ground-state geometry with the same type of orbitals in the excited-state geometry.

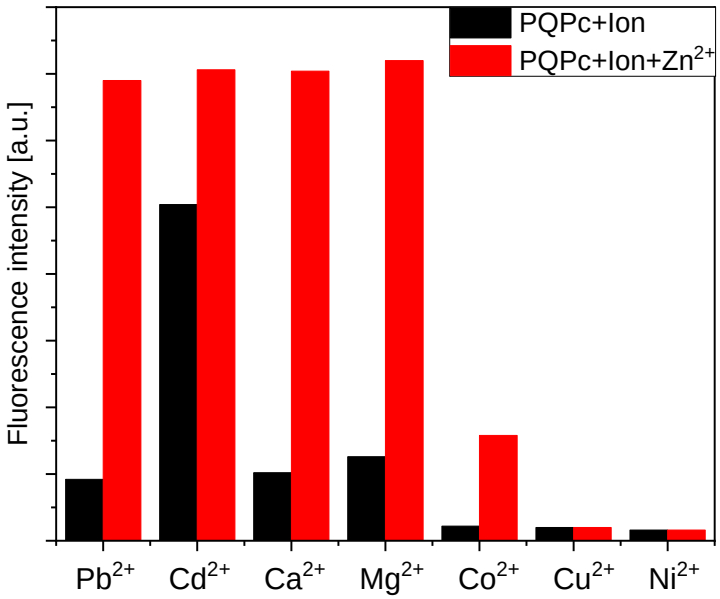


Figure S5. The diagram of selectivity of PQPc toward Zn^{2+} ion in the presence of other cation.

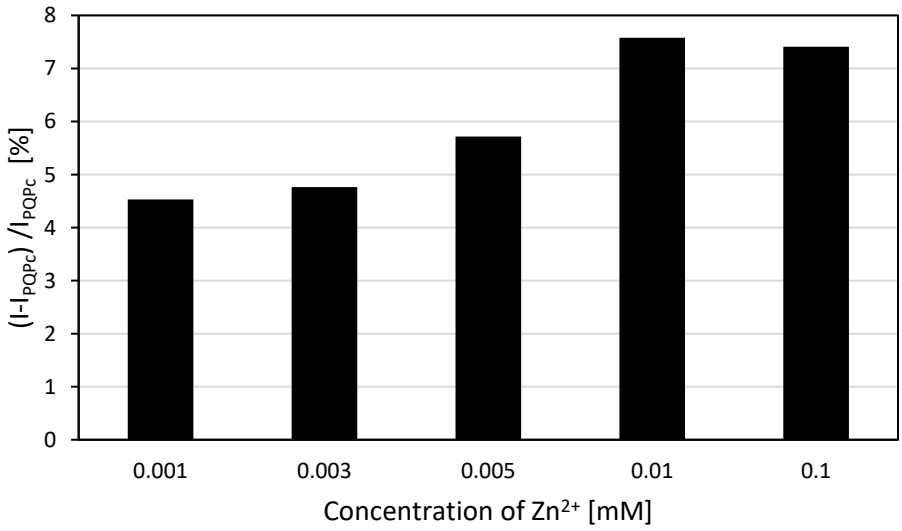


Figure S6. Fluorescence enhancement of PQPc in cells treated with zinc(II) ions (λ_{ex}=380 nm, λ_{em}=495 nm).

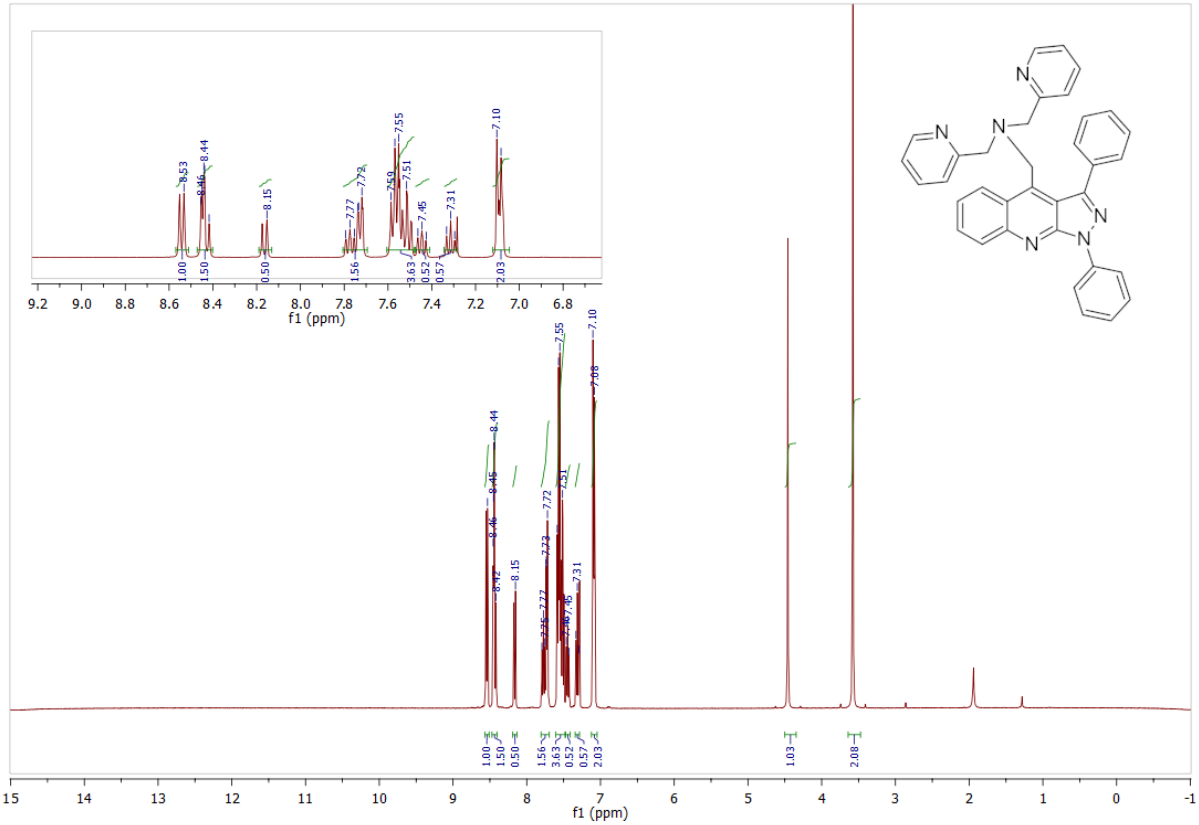


Figure S7. ^{1}H NMR recorded for the investigated sensor.

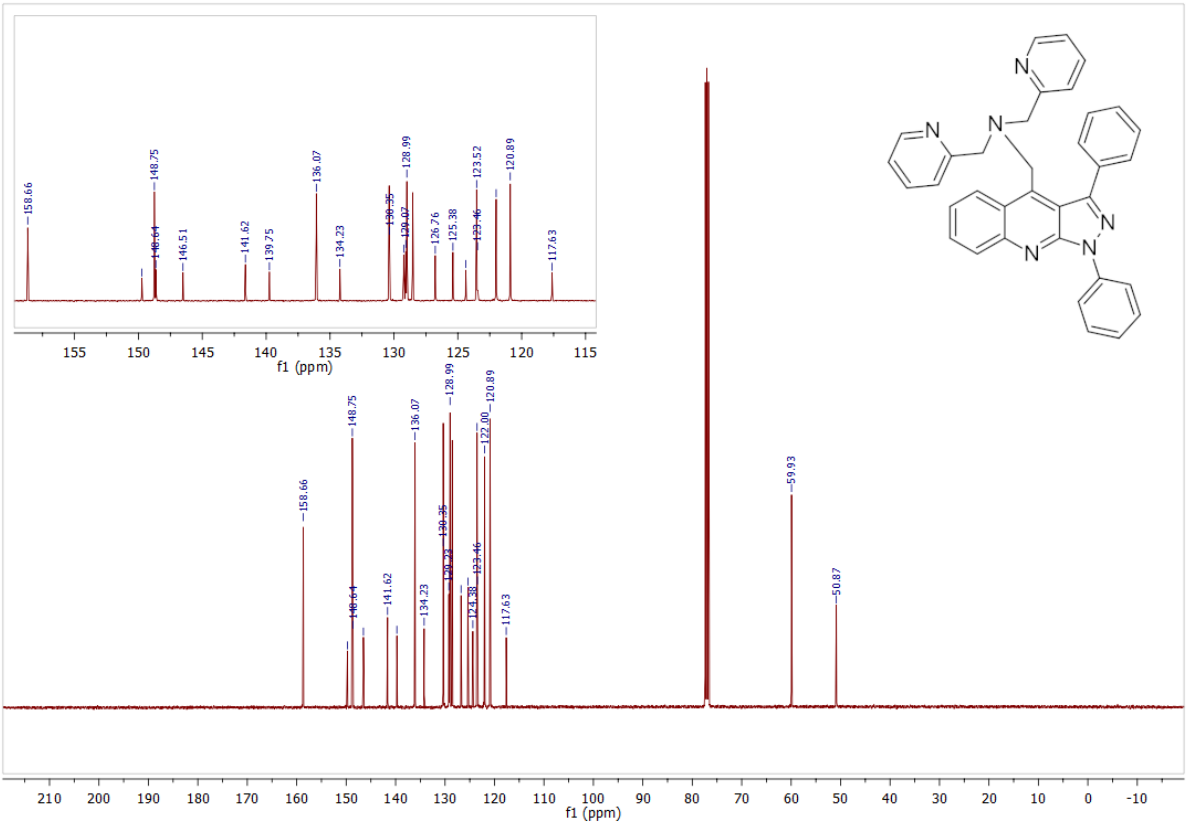


Figure S8. ^{13}C NMR recorded for the investigated sensor.

Optimized (B3LYP/cc-pVDZ) ground-state geometries of PQPc in vacuum.

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Optimized (B3LYP/cc-pVDZ) ground-state geometries of PQPc in ACN.

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Optimized (B3LYP/cc-pVDZ) excited-state geometries of PQPc in ACN.

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6	No	Show	6	C	-0.8096580	-2.2768730	-1.8448600
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19	No	Show	19	C	0.7979530	4.8227670	1.5352040
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25	No	Show	25	C	5.8834430	0.7464840	1.1489530
26	No	Show	26	C	-0.9035880	0.6099360	-1.0916510
27	No	Show	27	N	-1.8396930	0.5707600	0.0384760
28	No	Show	28	C	-1.5041630	-0.0579590	1.3052850
29	No	Show	29	C	-3.0607980	1.3594810	-0.0779390
30	No	Show	30	C	-2.6559200	-0.8174270	1.9306500
31	No	Show	31	C	-4.1593900	0.7042650	-0.9231240
32	No	Show	32	C	-2.9823610	-0.6450780	3.2799710
33	No	Show	33	C	-4.0019520	-1.4306810	3.8238100
34	No	Show	34	C	-4.6591860	-2.3427170	2.9975420
35	No	Show	35	C	-4.2670380	-2.4286130	1.6579430
36	No	Show	36	N	-3.2834070	-1.6914480	1.1252460
37	No	Show	37	N	-3.8068750	0.2030860	-2.1101060
38	No	Show	38	C	-4.7678710	-0.3112290	-2.8922430
39	No	Show	39	C	-6.1162080	-0.3310780	-2.5308760
40	No	Show	40	C	-6.4773680	0.2017000	-1.2919570
41	No	Show	41	C	-5.4814270	0.7251250	-0.4653240
42	No	Show	42	H	-1.6713280	-4.0974640	-2.6093790
43	No	Show	43	H	0.4726450	-5.3869090	-2.4481920
44	No	Show	44	H	2.5165350	-4.2598160	-1.5427100
45	No	Show	45	H	-1.7613620	-1.7479590	-1.9057180
46	No	Show	46	H	0.8444230	3.0766930	-1.9330360
47	No	Show	47	H	-0.2402940	5.2901880	-1.6792370
48	No	Show	48	H	-0.2667630	6.4285200	0.5437230
49	No	Show	49	H	0.8029570	5.3189020	2.5087370
50	No	Show	50	H	1.8565030	3.0793930	2.2557870
51	No	Show	51	H	4.8530870	-2.2202820	-0.1799420
52	No	Show	52	H	7.1893370	-2.8388360	0.4281740
53	No	Show	53	H	8.7005760	-1.1616560	1.5031110
54	No	Show	54	H	7.8363020	1.1430430	1.9561470

55	No	Show	55	H	5.5032290	1.7474490	1.3416020
56	No	Show	56	H	-1.5362520	0.3499900	-1.9616360
57	No	Show	57	H	-0.6791830	1.6808400	-1.2255840
58	No	Show	58	H	-1.1532100	0.7465930	1.9751750
59	No	Show	59	H	-0.6520450	-0.7233550	1.1171710
60	No	Show	60	H	-3.4405950	1.5706880	0.9269210
61	No	Show	61	H	-2.7804470	2.3117050	-0.5519050
62	No	Show	62	H	-2.4491860	0.0840420	3.8923000
63	No	Show	63	H	-4.2788620	-1.3263120	4.8745760
64	No	Show	64	H	-5.4616380	-2.9768800	3.3774410
65	No	Show	65	H	-4.7658420	-3.1273120	0.9794850
66	No	Show	66	H	-4.4407380	-0.7208590	-3.8520190
67	No	Show	67	H	-6.8606800	-0.7552830	-3.2060620
68	No	Show	68	H	-7.5197540	0.2062900	-0.9678280
69	No	Show	69	H	-5.7256710	1.1403970	0.5133340

Optimized (B3LYP/cc-pVDZ) ground-state geometries of PQPc+Zn^{2+} in vacuum.

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	0.8963610	4.6288840	2.0783640
2	No	Show	2	C	2.1401800	4.9884150	1.4922920
3	No	Show	3	C	2.9010510	4.0340030	0.8612520
4	No	Show	4	C	2.4648870	2.6768040	0.7899210
5	No	Show	5	C	1.1825000	2.3030060	1.3570790
6	No	Show	6	C	0.4289320	3.3352280	2.0036520
7	No	Show	7	N	3.2849000	1.7970530	0.1666820
8	No	Show	8	C	2.9005710	0.5401590	0.1950830
9	No	Show	9	C	1.6886060	0.0151200	0.7696960
10	No	Show	10	C	0.7570830	0.9387570	1.2630820
11	No	Show	11	N	3.5913550	-0.5404260	-0.3363880
12	No	Show	12	N	2.9343920	-1.6897450	-0.0723200
13	No	Show	13	C	1.8150290	-1.4191800	0.5869150
14	No	Show	14	C	1.0485510	-2.5732750	1.1006140
15	No	Show	15	C	4.8639070	-0.5956560	-0.9802990
16	No	Show	16	C	0.5136330	-2.5840510	2.4034670
17	No	Show	17	C	-0.0843120	-3.7380710	2.9224350
18	No	Show	18	C	-0.1409850	-4.9076310	2.1563570
19	No	Show	19	C	0.4049900	-4.9138240	0.8658700
20	No	Show	20	C	0.9889020	-3.7588960	0.3402750
21	No	Show	21	C	5.4328390	0.5542630	-1.5537770
22	No	Show	22	C	6.6739900	0.4550030	-2.1820850
23	No	Show	23	C	7.3467850	-0.7697800	-2.2477130
24	No	Show	24	C	6.7687270	-1.9095940	-1.6748210
25	No	Show	25	C	5.5321860	-1.8318230	-1.0400220
26	No	Show	26	C	-0.6539740	0.5303720	1.6342200
27	No	Show	27	N	-1.3945360	-0.0884570	0.5029720
28	No	Show	28	C	-1.4405160	0.6645320	-0.7564530
29	No	Show	29	C	-2.6023420	-0.7572150	0.9271670
30	No	Show	30	C	-2.1359730	2.0308010	-0.7877940
31	No	Show	31	C	-3.1179670	-1.8309790	-0.0192440
32	No	Show	32	C	-1.4004700	3.2144500	-0.8521920
33	No	Show	33	C	-2.0476980	4.4509080	-0.9211120
34	No	Show	34	C	-3.4437280	4.4959570	-0.9152000
35	No	Show	35	C	-4.1425460	3.3001560	-0.8534900
36	No	Show	36	N	-3.5075870	2.0995630	-0.7982040
37	No	Show	37	N	-4.1653500	-1.4965710	-0.8264220
38	No	Show	38	C	-4.7304070	-2.4099490	-1.6542920
39	No	Show	39	C	-4.2566380	-3.7131210	-1.7073400
40	No	Show	40	C	-3.1682640	-4.0680750	-0.9032420
41	No	Show	41	C	-2.5912370	-3.1183500	-0.0550510
42	No	Show	42	H	0.3149680	5.3833650	2.6122390
43	No	Show	43	H	2.4959020	6.0179260	1.5623720
44	No	Show	44	H	3.8693410	4.2699100	0.4179600
45	No	Show	45	H	-0.5123120	3.0972680	2.4995490
46	No	Show	46	H	0.6459490	-1.7159140	3.0523710
47	No	Show	47	H	-0.4640380	-3.7367360	3.9465070
48	No	Show	48	H	-0.5790530	-5.8164040	2.5741550

49	No	Show	49	H	0.3966680	-5.8317090	0.2733370
50	No	Show	50	H	1.4363790	-3.7717420	-0.6545600
51	No	Show	51	H	4.9150740	1.5079320	-1.4989660
52	No	Show	52	H	7.1178150	1.3469590	-2.6278850
53	No	Show	53	H	8.3182360	-0.8363870	-2.7406390
54	No	Show	54	H	7.2898940	-2.8676810	-1.7155570
55	No	Show	55	H	5.0792460	-2.7106880	-0.5851760
56	No	Show	56	H	-1.2118960	1.3888850	2.0423720
57	No	Show	57	H	-0.6292770	-0.2331240	2.4233560
58	No	Show	58	H	-1.8890550	0.0150530	-1.5294640
59	No	Show	59	H	-0.4033300	0.8268110	-1.0793720
60	No	Show	60	H	-2.3988180	-1.2341080	1.8977040
61	No	Show	61	H	-3.4674130	-0.0572520	1.1662980
62	No	Show	62	H	-0.3121900	3.1610720	-0.8538230
63	No	Show	63	H	-1.4631220	5.3709750	-0.9818290
64	No	Show	64	H	-3.9896020	5.4387070	-0.9665310
65	No	Show	65	H	-5.2341490	3.2817160	-0.8567300
66	No	Show	66	H	-5.5673570	-2.0742840	-2.2687360
67	No	Show	67	H	-4.7342870	-4.4330620	-2.3730710
68	No	Show	68	H	-2.7734350	-5.0857180	-0.9273090
69	No	Show	69	H	-1.7462700	-3.3748550	0.5840630
70	No	Show	70	Zn	-4.4820670	0.4186350	-0.7236180

Optimized (B3LYP/cc-pVDZ) ground-state geometries of PQPc+Zn^{2+} in ACN.

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	1.1961960	4.4727480	2.3217990
2	No	Show	2	C	2.4797950	4.7752590	1.7928040
3	No	Show	3	C	3.1930200	3.8076340	1.1270540
4	No	Show	4	C	2.6692940	2.4905550	0.9613520
5	No	Show	5	C	1.3547890	2.1742610	1.4808130
6	No	Show	6	C	0.6510510	3.2194880	2.1628270
7	No	Show	7	N	3.4404060	1.5982890	0.2883980
8	No	Show	8	C	2.9596750	0.3732370	0.2303740
9	No	Show	9	C	1.7089870	-0.0962610	0.7633330
10	No	Show	10	C	0.8307980	0.8526990	1.3009050
11	No	Show	11	N	3.5744440	-0.7174200	-0.3623750
12	No	Show	12	N	2.8356980	-1.8434590	-0.1604590
13	No	Show	13	C	1.7365450	-1.5250690	0.5016980
14	No	Show	14	C	0.8840160	-2.6430500	0.9642290
15	No	Show	15	C	4.8357260	-0.8224220	-1.0152670
16	No	Show	16	C	0.4302140	-2.7048090	2.2939700
17	No	Show	17	C	-0.2393120	-3.8384210	2.7652780
18	No	Show	18	C	-0.4575090	-4.9312680	1.9188090
19	No	Show	19	C	-0.0080400	-4.8789640	0.5936660
20	No	Show	20	C	0.6558850	-3.7454310	0.1199370
21	No	Show	21	C	5.5114670	0.3192440	-1.4762200
22	No	Show	22	C	6.7425790	0.1752090	-2.1225600
23	No	Show	23	C	7.3059040	-1.0881040	-2.3227160
24	No	Show	24	C	6.6231570	-2.2201250	-1.8641890

25	No	Show	25	C	5.3962850	-2.0960900	-1.2107670
26	No	Show	26	C	-0.6106070	0.5333690	1.6491060
27	No	Show	27	N	-1.3712960	-0.1253970	0.5655020
28	No	Show	28	C	-1.3649230	0.5393930	-0.7491840
29	No	Show	29	C	-2.6989040	-0.5036310	1.0604860
30	No	Show	30	C	-1.8642330	1.9812830	-0.8610870
31	No	Show	31	C	-3.3985020	-1.5407130	0.2049480
32	No	Show	32	C	-0.9417390	3.0275390	-0.9467140
33	No	Show	33	C	-1.3694640	4.3502500	-1.0524540
34	No	Show	34	C	-2.7375070	4.6158390	-1.0683520
35	No	Show	35	C	-3.6173590	3.5450160	-1.0028290
36	No	Show	36	N	-3.2001180	2.2573980	-0.9110280
37	No	Show	37	N	-4.3662150	-1.1378420	-0.6577550
38	No	Show	38	C	-5.0400670	-2.0455210	-1.4029610
39	No	Show	39	C	-4.7721100	-3.4046320	-1.3198650
40	No	Show	40	C	-3.7676830	-3.8344830	-0.4499150
41	No	Show	41	C	-3.0791800	-2.8939800	0.3152640
42	No	Show	42	H	0.6385760	5.2400400	2.8620290
43	No	Show	43	H	2.8978510	5.7757600	1.9210010
44	No	Show	44	H	4.1831790	4.0076370	0.7144810
45	No	Show	45	H	-0.3289990	3.0228100	2.5942880
46	No	Show	46	H	0.6465480	-1.8849810	2.9812320
47	No	Show	47	H	-0.5732550	-3.8743540	3.8044510
48	No	Show	48	H	-0.9719380	-5.8200090	2.2904020
49	No	Show	49	H	-0.1732660	-5.7272020	-0.0742690
50	No	Show	50	H	1.0152010	-3.7096710	-0.9095780
51	No	Show	51	H	5.0798720	1.3039690	-1.3176150
52	No	Show	52	H	7.2614840	1.0690270	-2.4760410
53	No	Show	53	H	8.2671320	-1.1905860	-2.8302510
54	No	Show	54	H	7.0494330	-3.2150630	-2.0103930
55	No	Show	55	H	4.8637500	-2.9743770	-0.8509610
56	No	Show	56	H	-1.1247690	1.4464870	1.9897640
57	No	Show	57	H	-0.6314640	-0.1613600	2.5026250
58	No	Show	58	H	-1.9324420	-0.0981290	-1.4423660
59	No	Show	59	H	-0.3311360	0.5325800	-1.1189740
60	No	Show	60	H	-2.5586100	-0.9464220	2.0569840
61	No	Show	61	H	-3.3658750	0.3694150	1.2255350
62	No	Show	62	H	0.1217440	2.7951790	-0.9386360
63	No	Show	63	H	-0.6414150	5.1596920	-1.1236680
64	No	Show	64	H	-3.1281070	5.6301130	-1.1452590
65	No	Show	65	H	-4.6952400	3.7087560	-1.0354450
66	No	Show	66	H	-5.8032910	-1.6514370	-2.0745660
67	No	Show	67	H	-5.3401700	-4.1056450	-1.9308500
68	No	Show	68	H	-3.5254800	-4.8948420	-0.3623260
69	No	Show	69	H	-2.2969460	-3.2012730	1.0073620
70	No	Show	70	Zn	-4.6060760	0.8177540	-0.9875460

Optimized (B3LYP/cc-pVDZ) excited-state geometries of PQPc+Zn^{2+} in ACN.

Row	Highlight	Display	Tag	Symbol	X	Y	Z

1	No	Show	1	C	1.3285900	4.4307290	2.5618540
2	No	Show	2	C	2.5753130	4.7248610	1.9989920
3	No	Show	3	C	3.2413780	3.7414410	1.2612340
4	No	Show	4	C	2.6873400	2.4603460	1.0694170
5	No	Show	5	C	1.3860590	2.1504260	1.6234030
6	No	Show	6	C	0.7502510	3.1710970	2.3776210
7	No	Show	7	N	3.4246040	1.5486840	0.3301240
8	No	Show	8	C	2.9004890	0.3427510	0.2799620
9	No	Show	9	C	1.6842200	-0.1241280	0.8291800
10	No	Show	10	C	0.7998140	0.8470300	1.3898030
11	No	Show	11	N	3.4943570	-0.7807900	-0.3702040
12	No	Show	12	N	2.7620460	-1.9113100	-0.1751830
13	No	Show	13	C	1.7038430	-1.5472240	0.5808010
14	No	Show	14	C	0.8976850	-2.6345040	1.1294420
15	No	Show	15	C	4.6609480	-0.8575750	-1.1168540
16	No	Show	16	C	0.3200990	-2.5401130	2.4144960
17	No	Show	17	C	-0.3345960	-3.6343960	2.9788330
18	No	Show	18	C	-0.4341050	-4.8398930	2.2705820
19	No	Show	19	C	0.1358540	-4.9468990	0.9937820
20	No	Show	20	C	0.8045670	-3.8623720	0.4322480
21	No	Show	21	C	5.4842770	0.2816110	-1.3237080
22	No	Show	22	C	6.6462410	0.1528190	-2.0725820
23	No	Show	23	C	7.0112770	-1.0840120	-2.6255790
24	No	Show	24	C	6.1948800	-2.2108490	-2.4229970
25	No	Show	25	C	5.0306010	-2.1111010	-1.6794810
26	No	Show	26	C	-0.6651210	0.6051100	1.6395030
27	No	Show	27	N	-1.3714850	-0.0796990	0.5245310
28	No	Show	28	C	-1.2916170	0.5841980	-0.7881460
29	No	Show	29	C	-2.7281640	-0.4520420	0.9301780
30	No	Show	30	C	-1.8480060	2.0027360	-0.9056460
31	No	Show	31	C	-3.3211590	-1.5337060	0.0543450
32	No	Show	32	C	-0.9661870	3.0856880	-0.8248710
33	No	Show	33	C	-1.4308410	4.3956990	-0.9189270
34	No	Show	34	C	-2.7968570	4.6118450	-1.0950800
35	No	Show	35	C	-3.6332400	3.5083680	-1.1789950
36	No	Show	36	N	-3.1822030	2.2308470	-1.0912770
37	No	Show	37	N	-4.2168540	-1.1930910	-0.9073270
38	No	Show	38	C	-4.7689570	-2.1513780	-1.6918080
39	No	Show	39	C	-4.4490300	-3.4930350	-1.5518690
40	No	Show	40	C	-3.5185510	-3.8585820	-0.5750670
41	No	Show	41	C	-2.9534020	-2.8702630	0.2270590
42	No	Show	42	H	0.8002930	5.1812250	3.1540790
43	No	Show	43	H	3.0296010	5.7079810	2.1374610
44	No	Show	44	H	4.2170240	3.9409360	0.8131740
45	No	Show	45	H	-0.2105030	2.9697430	2.8521200
46	No	Show	46	H	0.4382790	-1.6243470	2.9927140
47	No	Show	47	H	-0.7583140	-3.5527060	3.9816150
48	No	Show	48	H	-0.9483040	-5.6947130	2.7145150
49	No	Show	49	H	0.0621160	-5.8845520	0.4393050
50	No	Show	50	H	1.2580050	-3.9449940	-0.5556030
51	No	Show	51	H	5.1836900	1.2308270	-0.8886470

52	No	Show	52	H	7.2783490	1.0279820	-2.2307790
53	No	Show	53	H	7.9272050	-1.1720710	-3.2121800
54	No	Show	54	H	6.4783950	-3.1736180	-2.8509160
55	No	Show	55	H	4.3927230	-2.9740570	-1.5071520
56	No	Show	56	H	-1.1558640	1.5655060	1.8791570
57	No	Show	57	H	-0.8349850	-0.0377050	2.5201500
58	No	Show	58	H	-1.7627460	-0.0711320	-1.5367890
59	No	Show	59	H	-0.2297150	0.6371390	-1.0616800
60	No	Show	60	H	-2.6643930	-0.8522910	1.9525580
61	No	Show	61	H	-3.4160060	0.4177310	1.0012640
62	No	Show	62	H	0.0956440	2.8869640	-0.6884400
63	No	Show	63	H	-0.7344000	5.2334650	-0.8577750
64	No	Show	64	H	-3.2178310	5.6137510	-1.1748930
65	No	Show	65	H	-4.7060310	3.6381070	-1.3272850
66	No	Show	66	H	-5.4803930	-1.8141520	-2.4460050
67	No	Show	67	H	-4.9204360	-4.2305790	-2.2009190
68	No	Show	68	H	-3.2394030	-4.9044030	-0.4373370
69	No	Show	69	H	-2.2280010	-3.1233710	0.9982790
70	No	Show	70	Zn	-4.5609070	0.7394980	-1.2945170