Supporting Information

Increasing the Dynamic Range of Metal Ion Affinity Changes in Zn^{2+} Photocages Using Multiple Nitrobenzyl Groups

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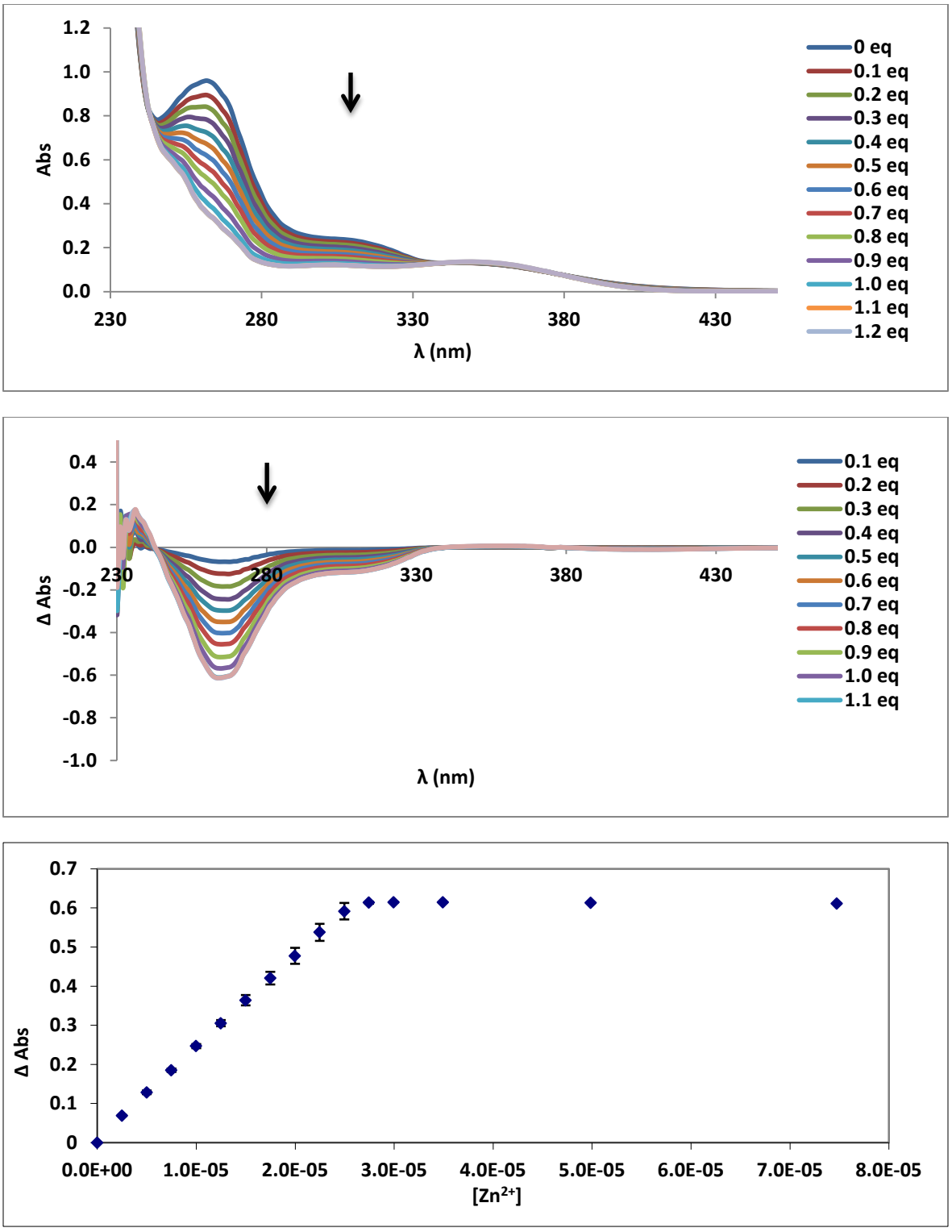


Figure S1 Titration of 25 µM MonoCast with $Zn(ClO_4)_2$ in CH_3CN.

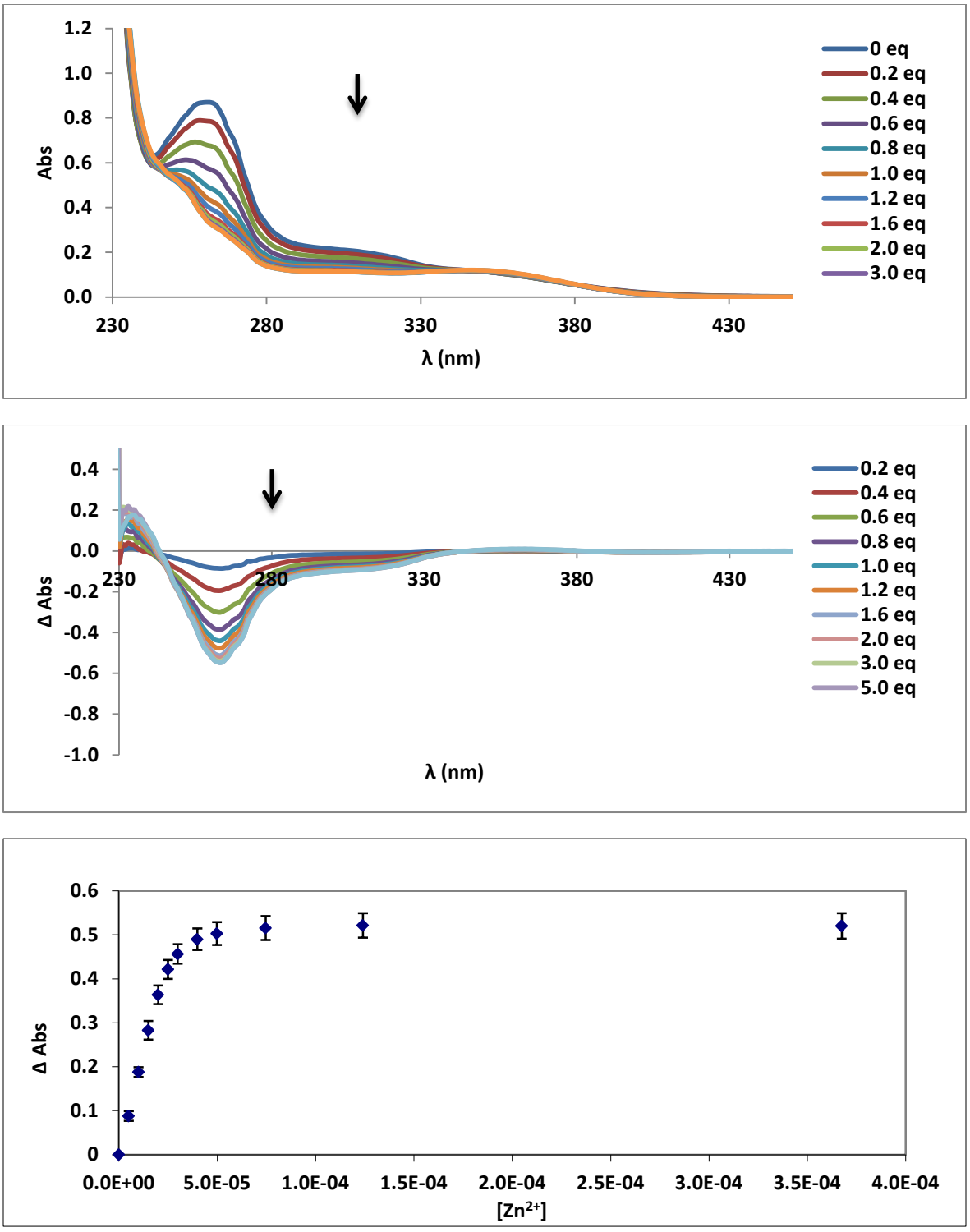


Figure S2 Titration of 25 µM MonoCast with $Zn(ClO_4)_2$ in EtOH.

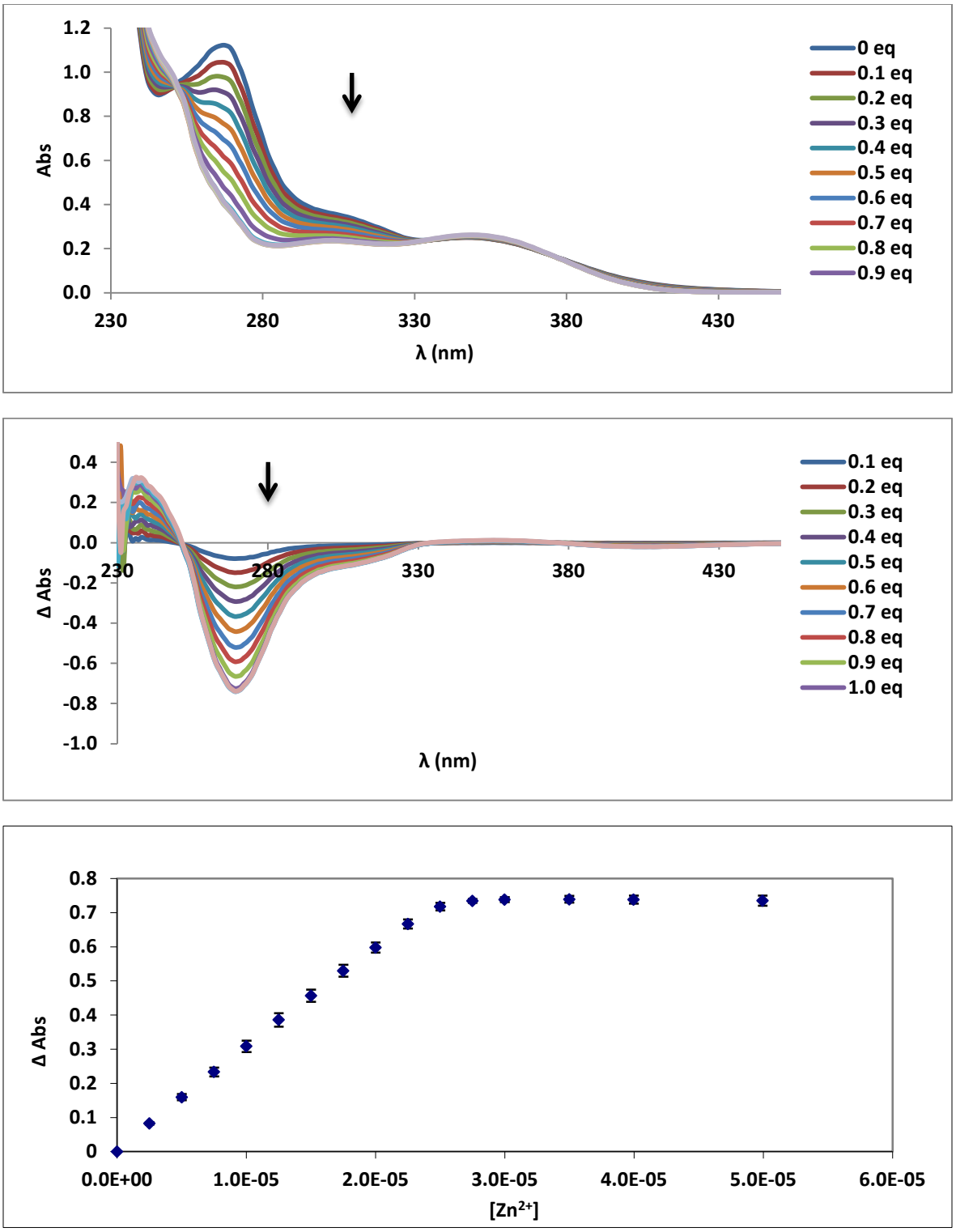


Figure S3 Titration of 25 μM DiCast-1 with $Zn(ClO_4)_2$ in CH_3CN.

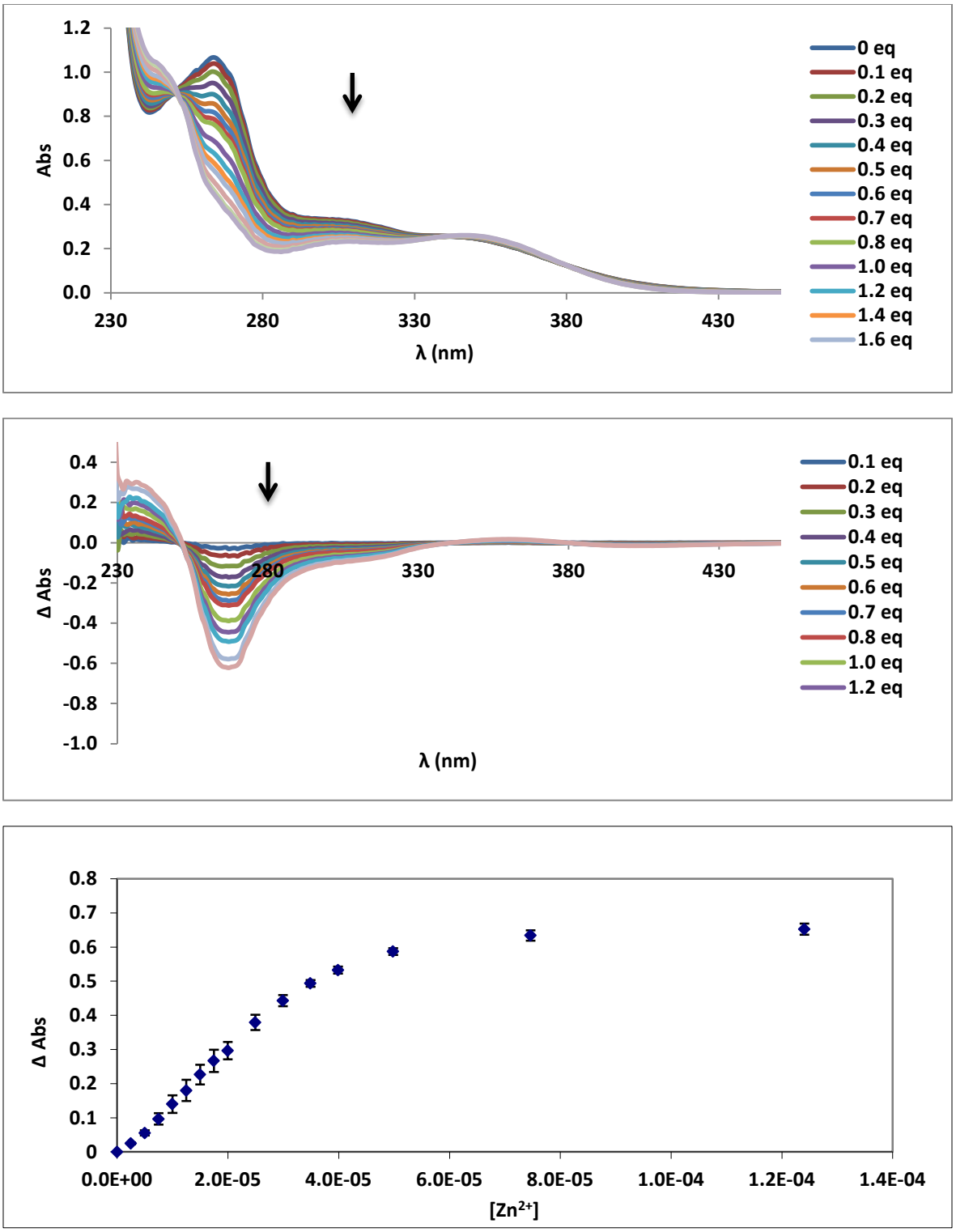


Figure S4 Titration of 25 µM DiCast-1 with $Zn(ClO_4)_2$ in EtOH.

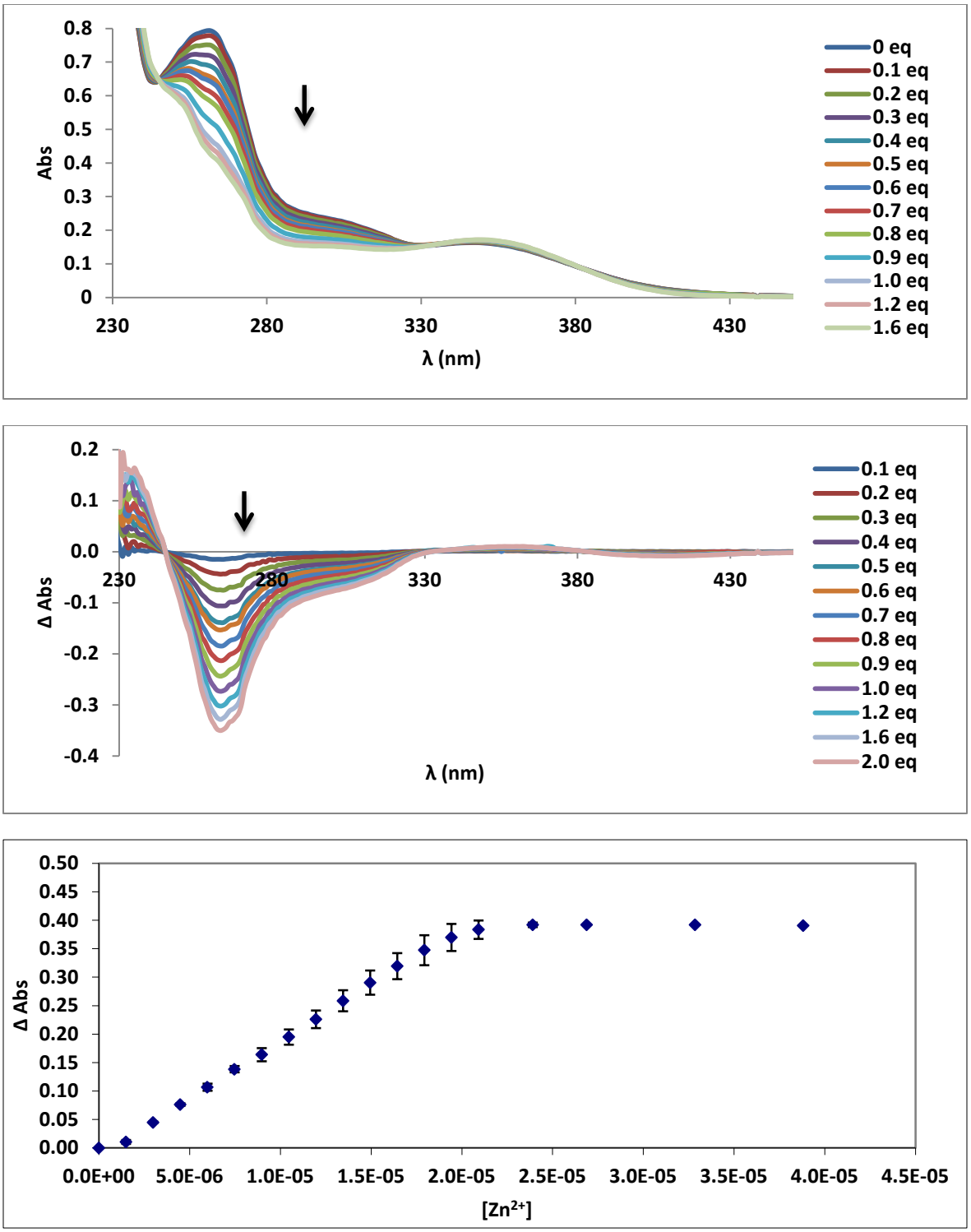


Figure S5 Titration of 15 µM DiCast-2 with $Zn(ClO_4)_2$ in CH_3CN.

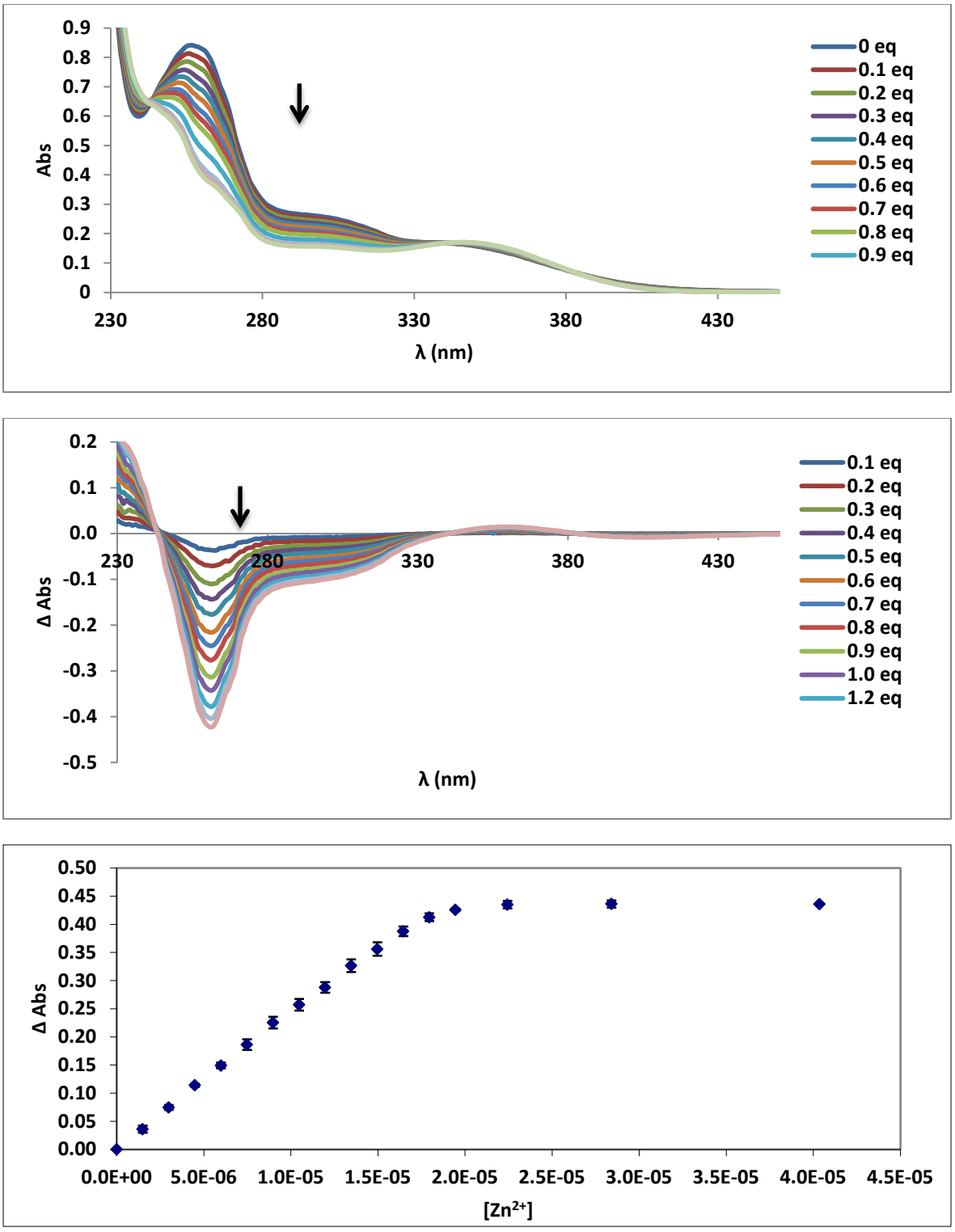


Figure S6 Titration of 15 µM DiCast-2 with $Zn(ClO_4)_2$ in EtOH.

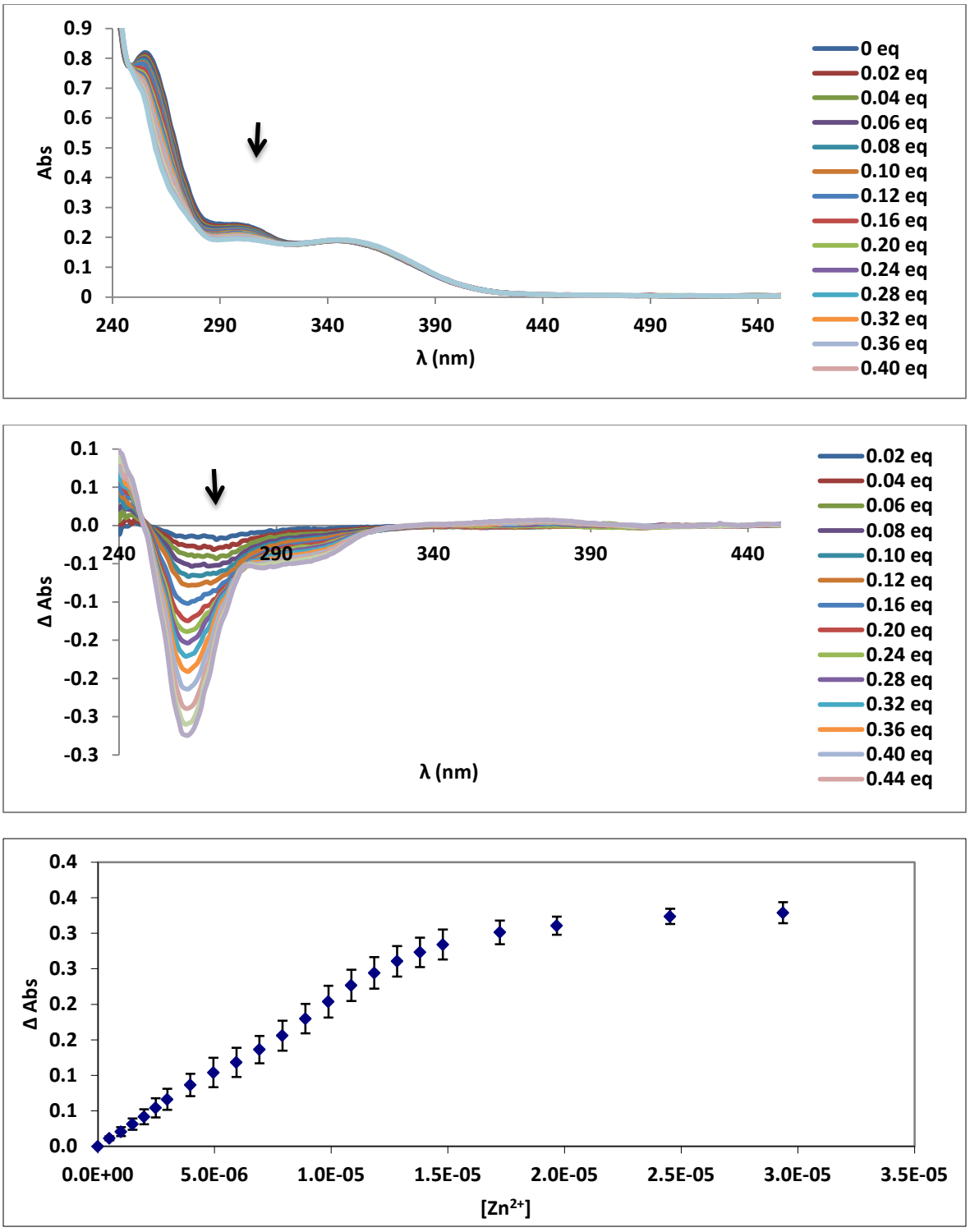


Figure S7 Titration of 25 µM DiCast-3 with $Zn(ClO_4)_2$ in CH_3CN.

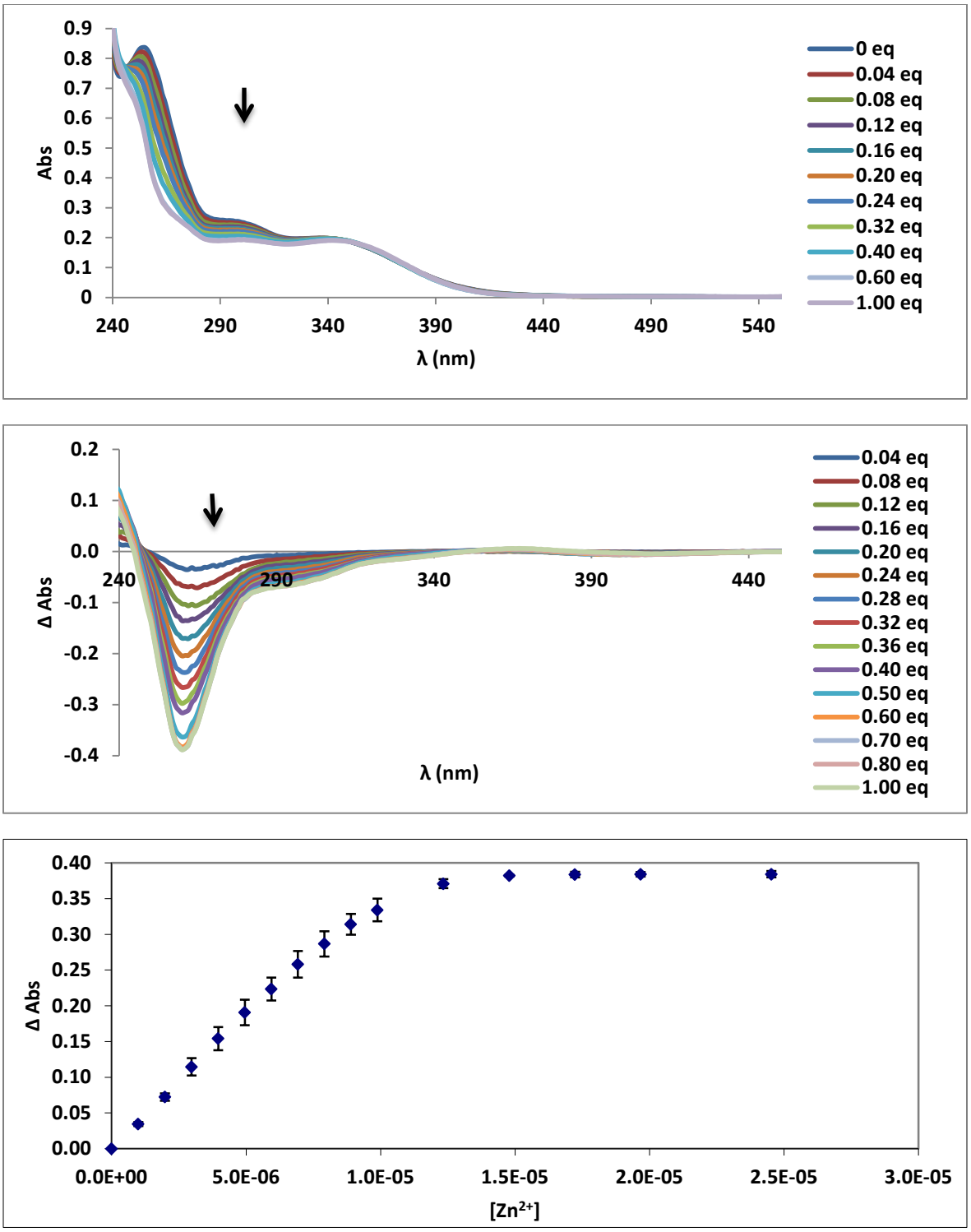
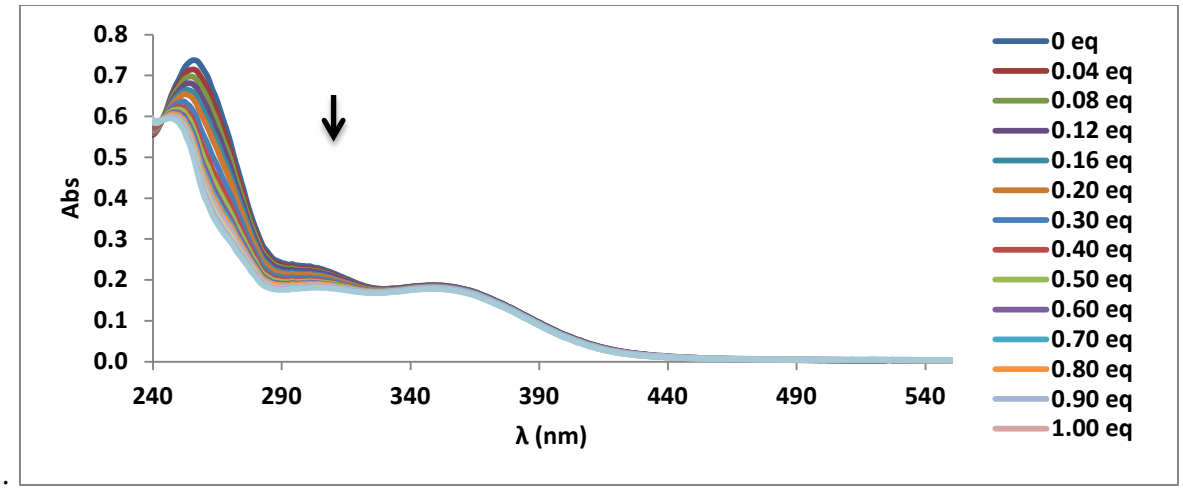


Figure S8 Titration of 25 µM DiCast-3 with $Zn(ClO_4)_2$ in EtOH



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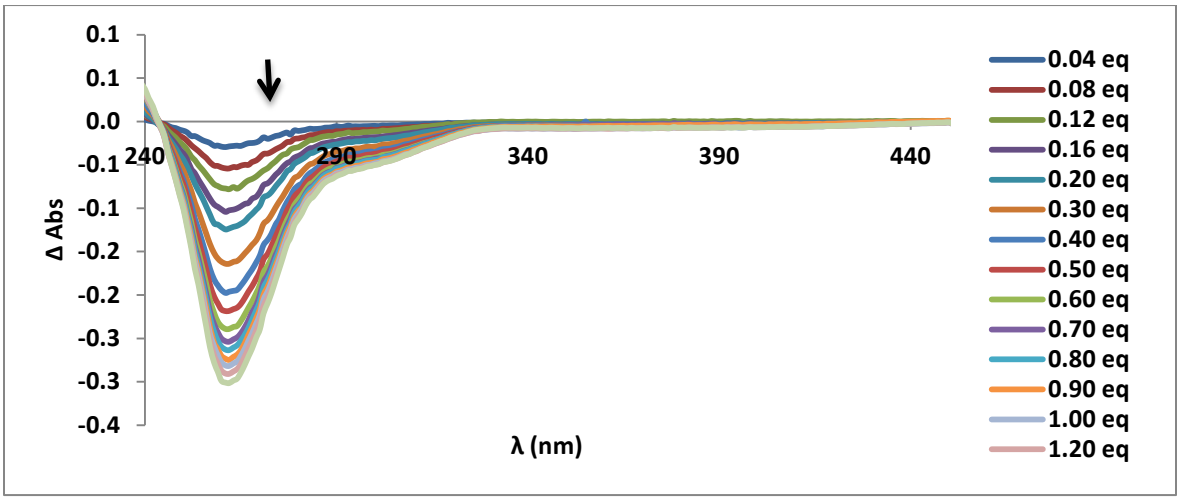


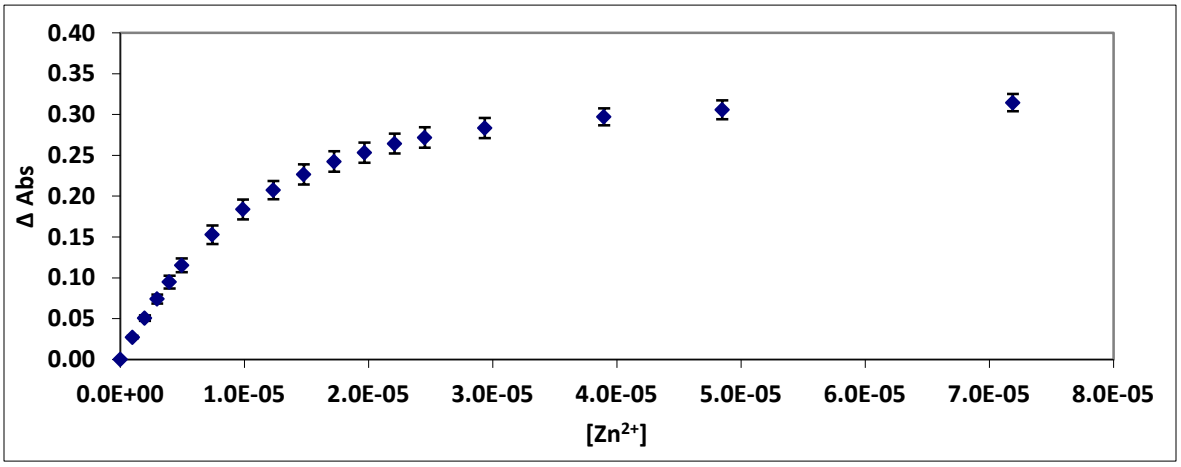


Figure S9 Titration of 25 µM DiCast-3 with $Zn(ClO_4)_2$ in buffer.

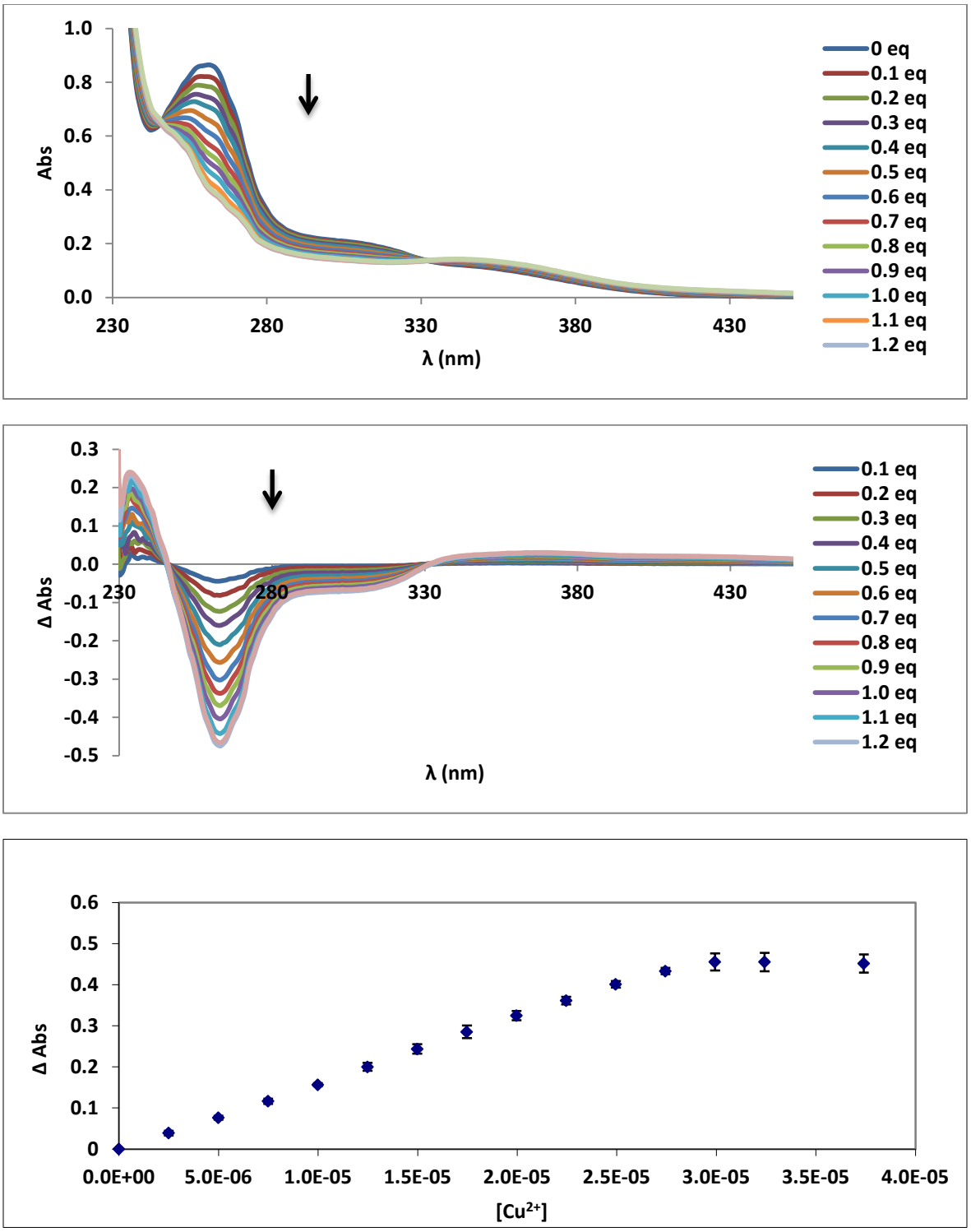


Figure S10 Titration of 25 µM MonoCast with $Cu(ClO_4)_2$ in EtOH.

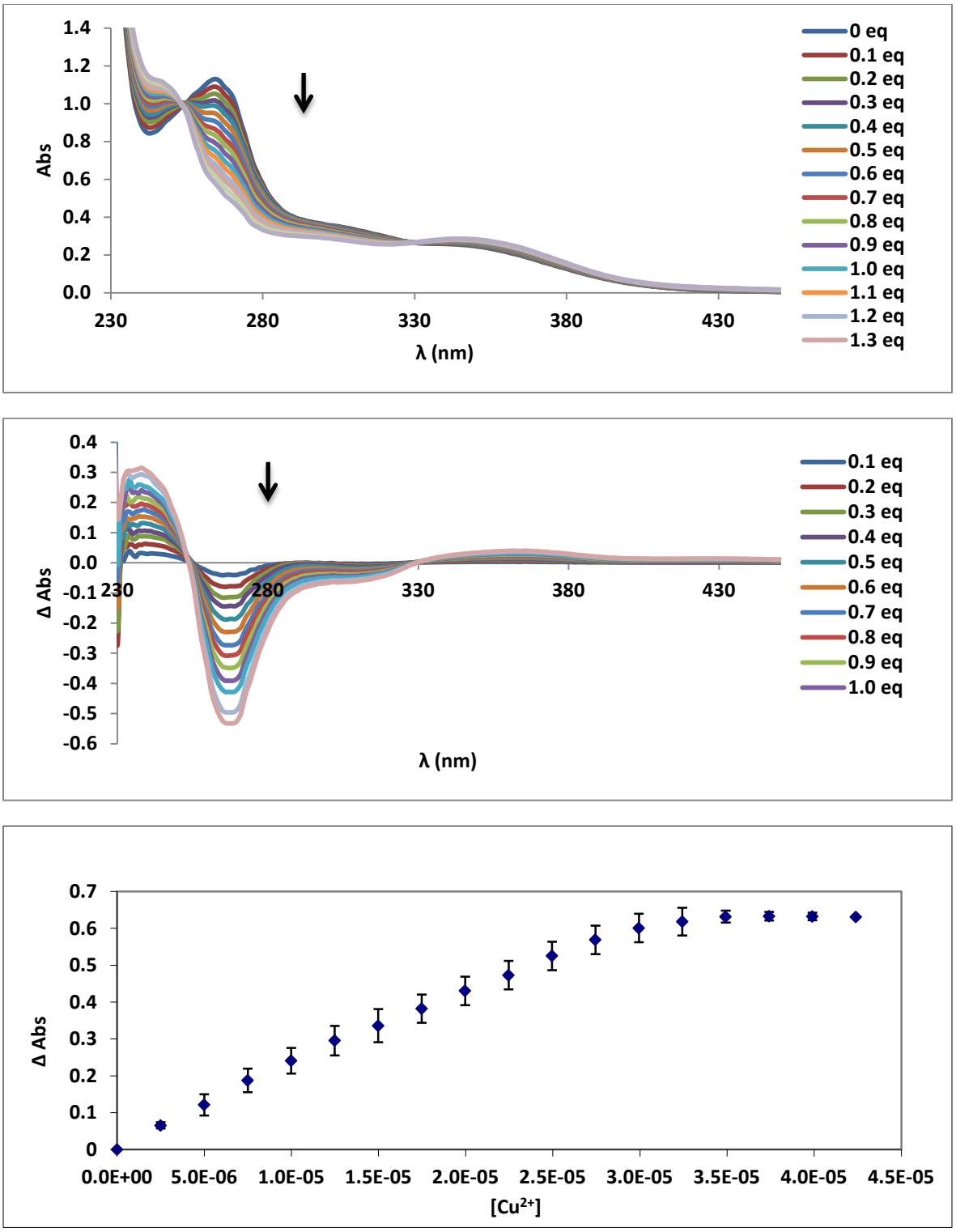


Figure S11 Titration of 25 µM DiCast-1 with $Cu(ClO_4)_2$ in EtOH.

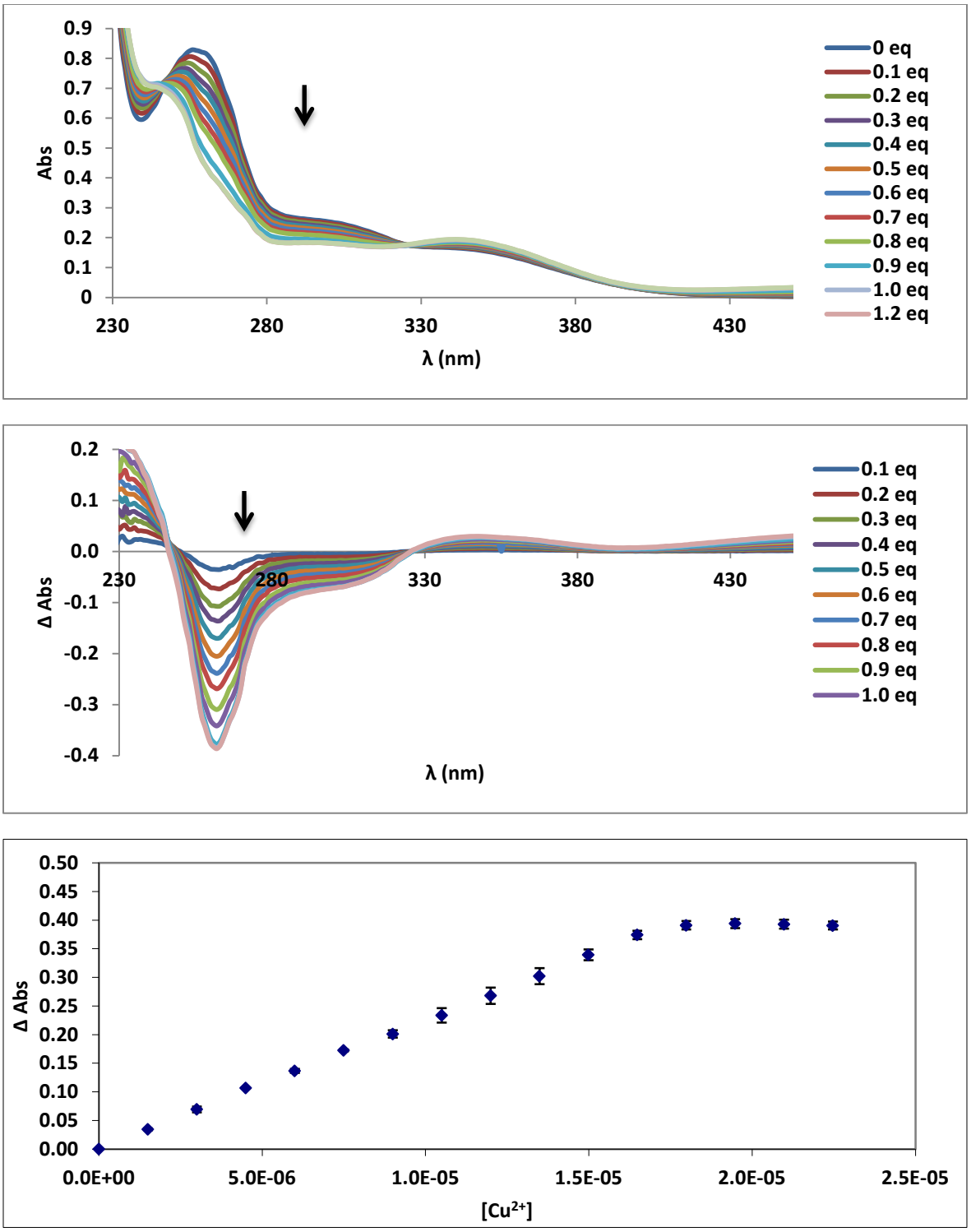


Figure S12 Titration of 15 µM DiCast-2 with $Cu(ClO_4)_2$ in EtOH.

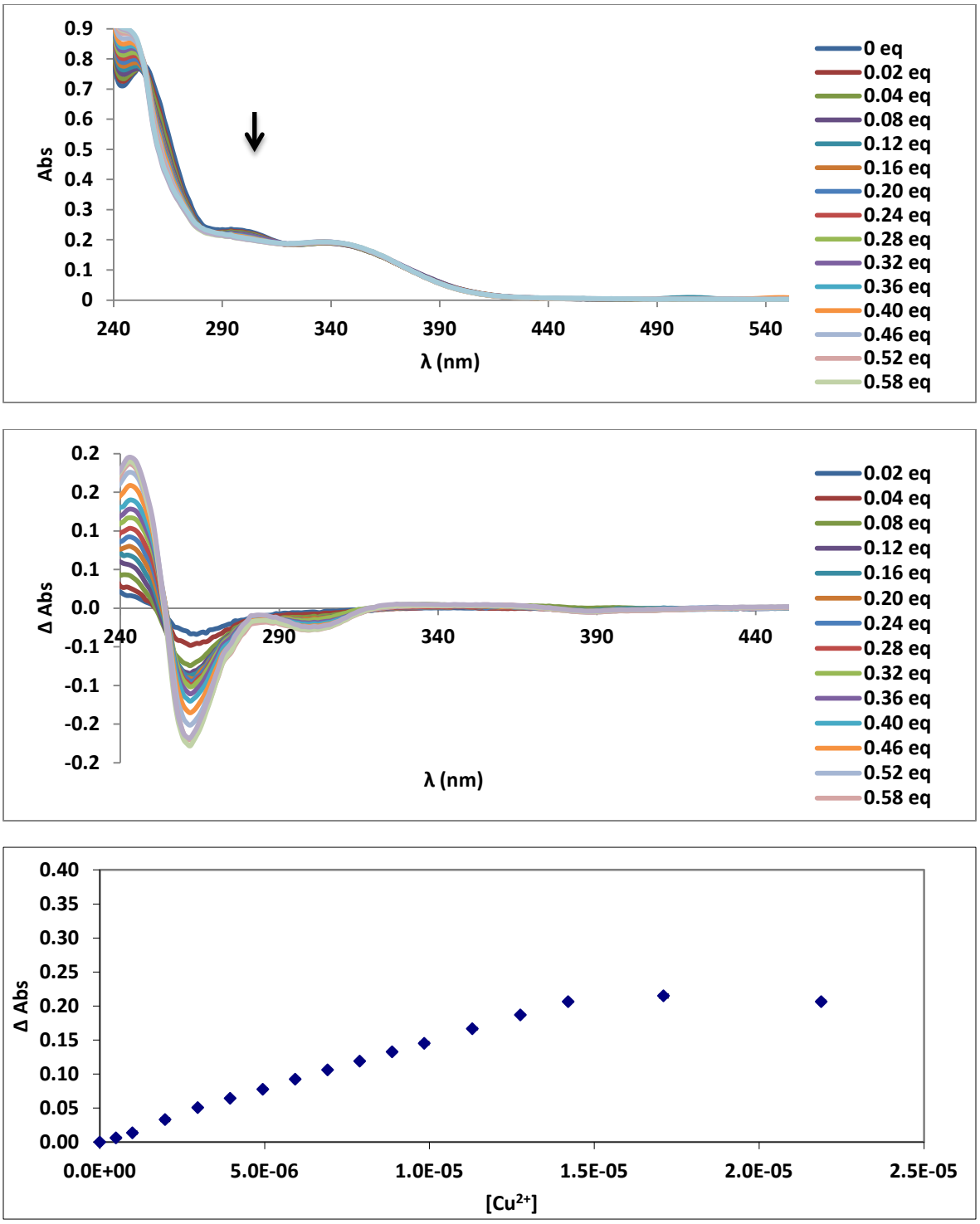
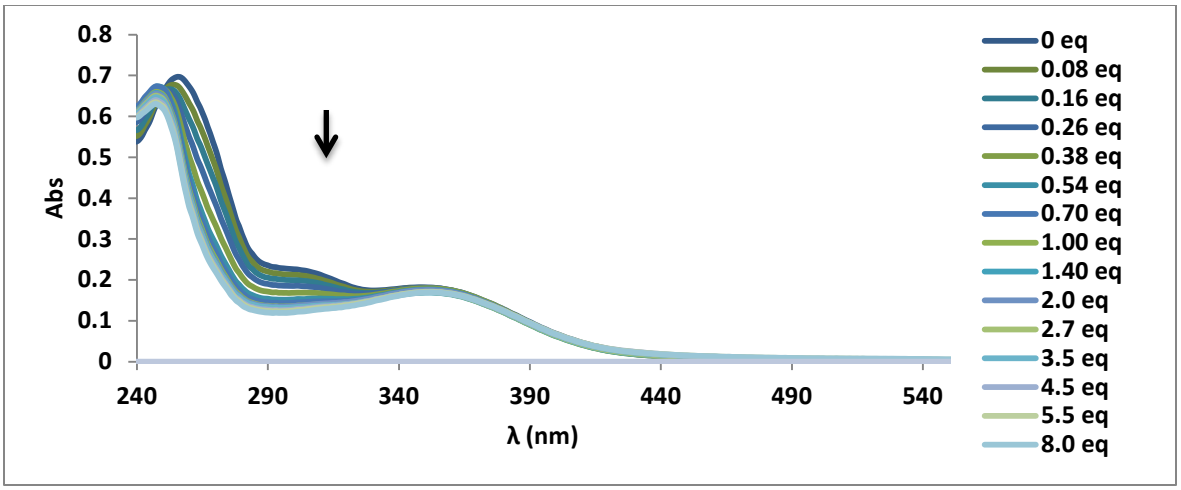
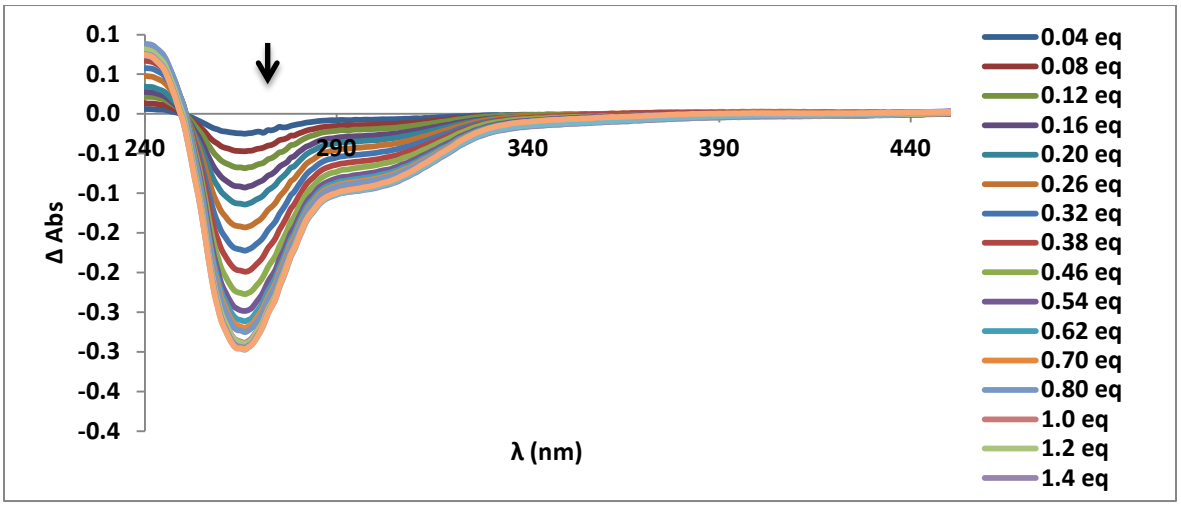


Figure S13 Titration of 25 µM DiCast-3 with $Cu(ClO_4)_2$ in EtOH.





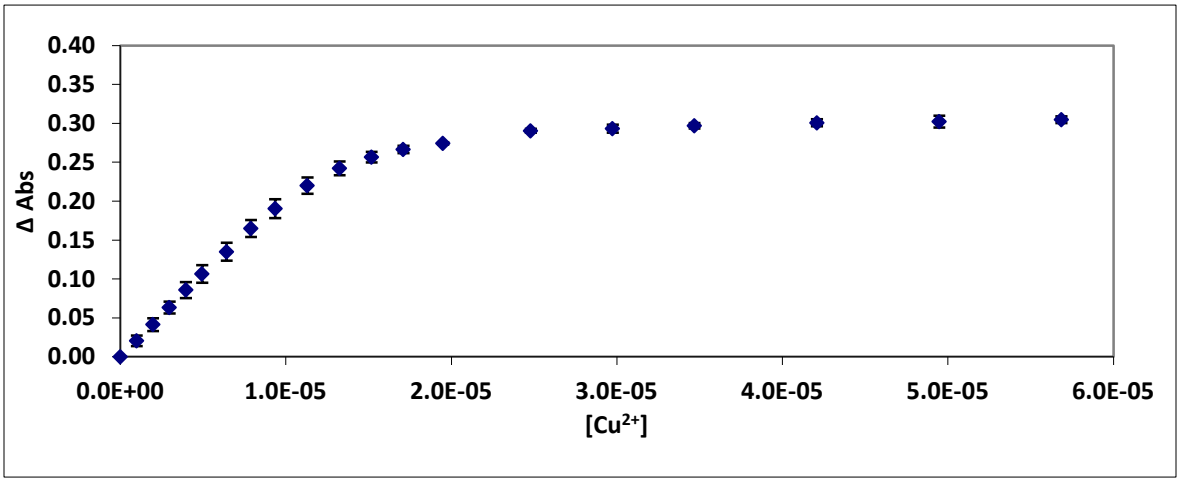


Figure S14 Titration of 25 µM DiCast-3 with $Cu(ClO_4)_2$ in buffer.

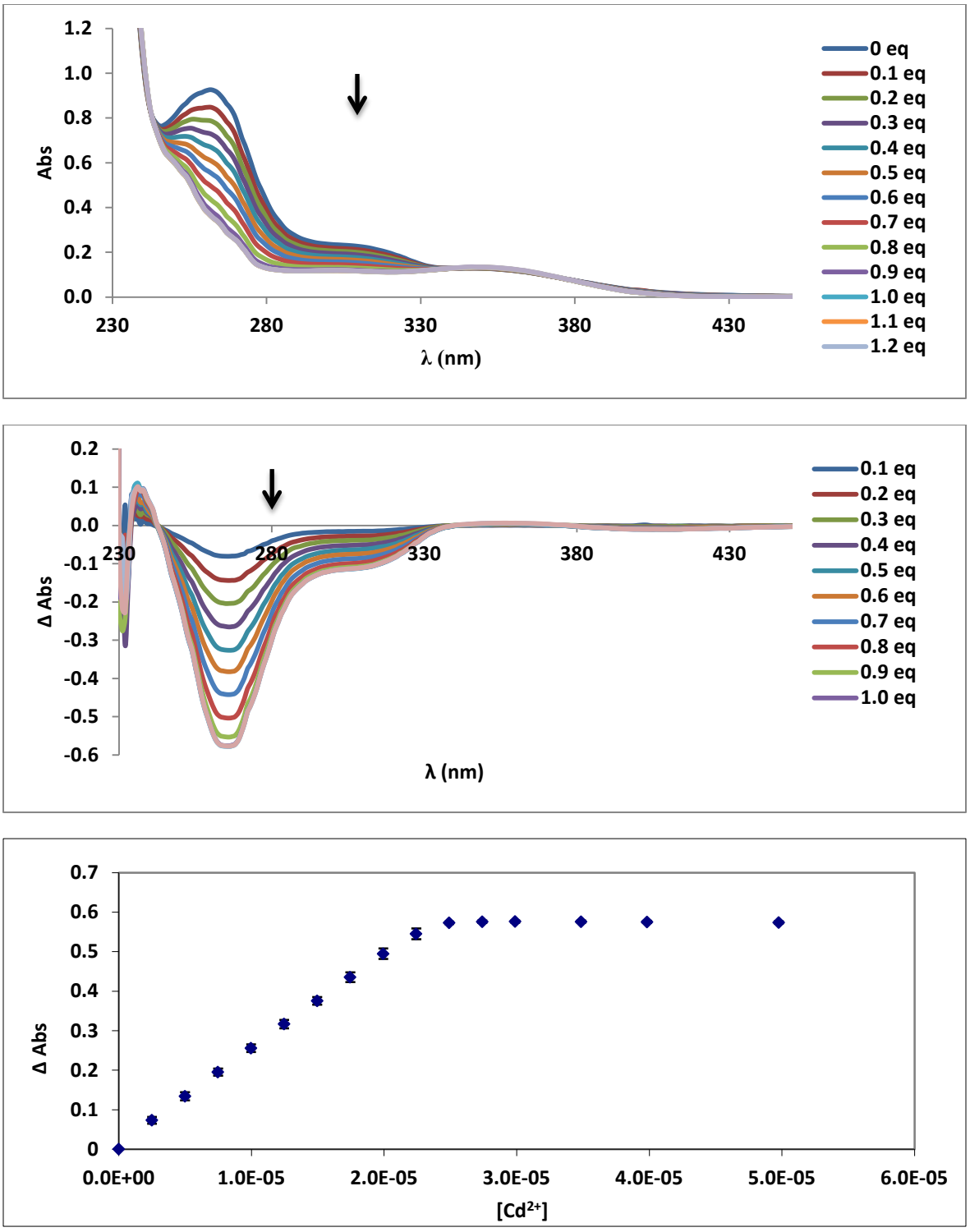


Figure S15 Titration of 25 µM MonoCast with $Cd(ClO_4)_2$ in CH_3CN.

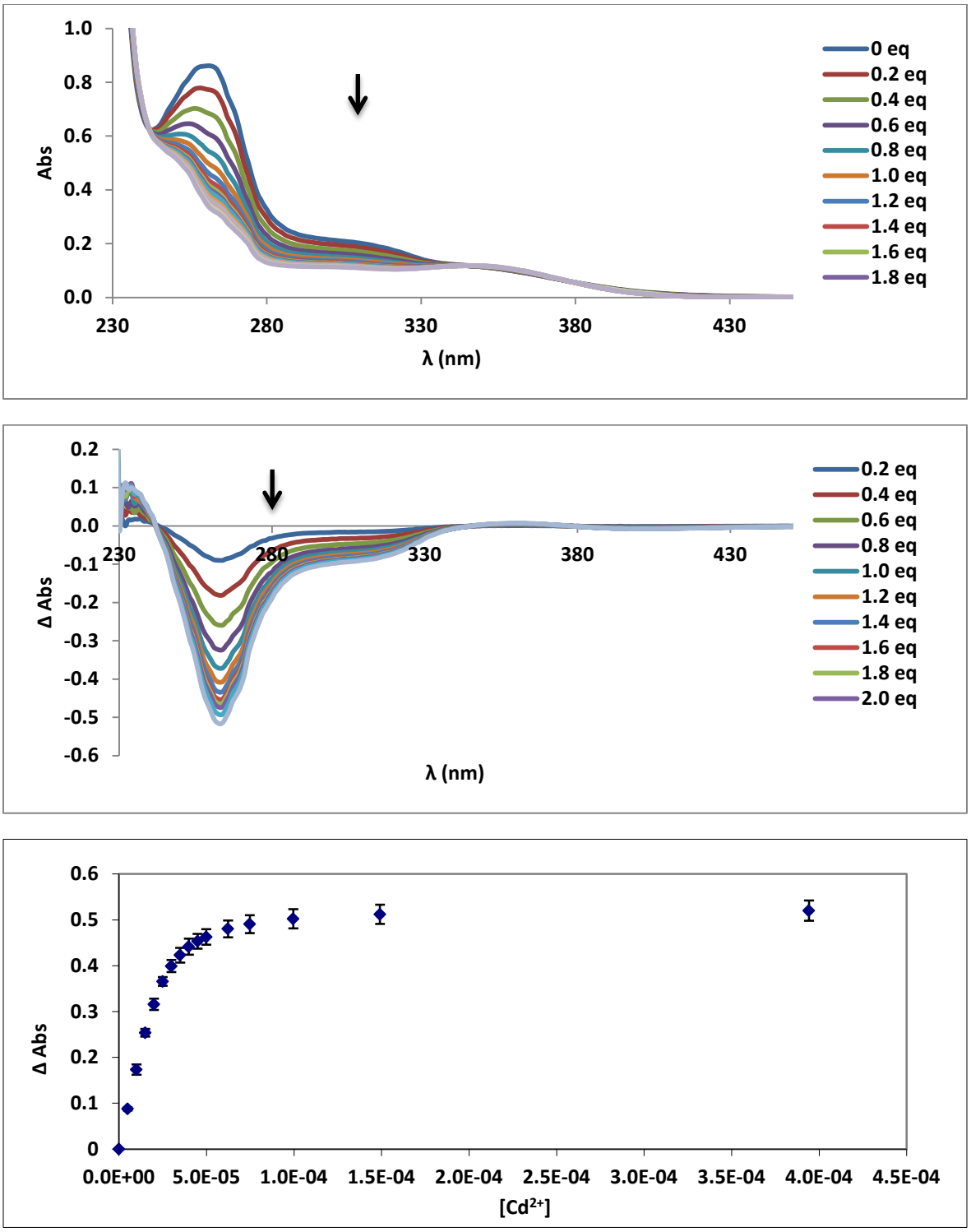
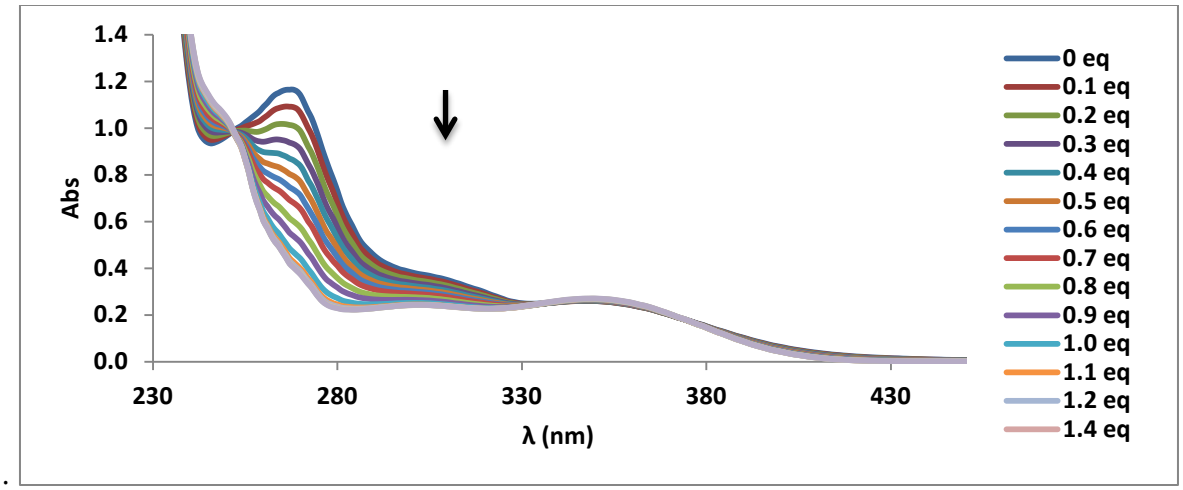


Figure S16 Titration of 25 µM MonoCast with $Cd(ClO_4)_2$ in EtOH



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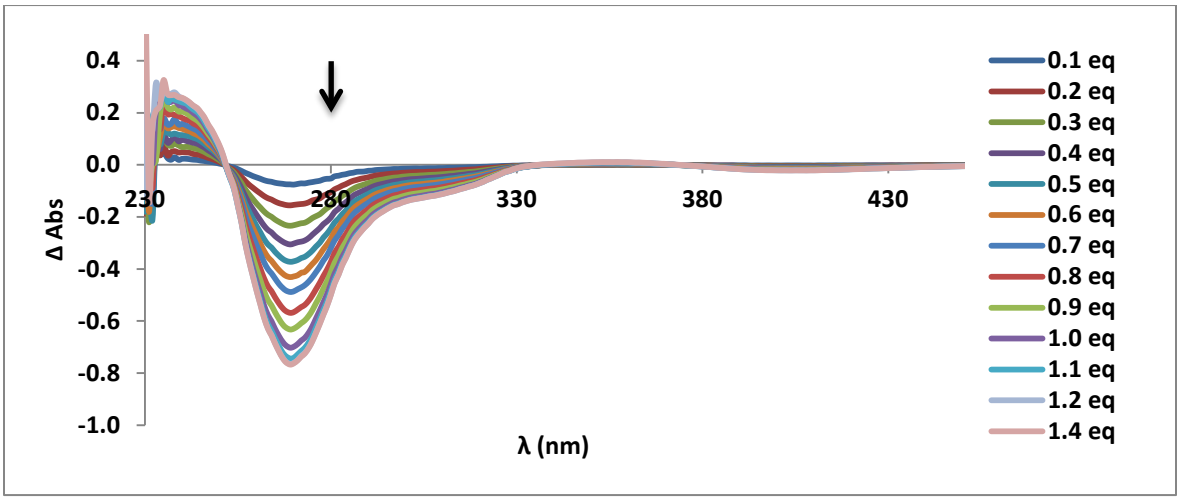

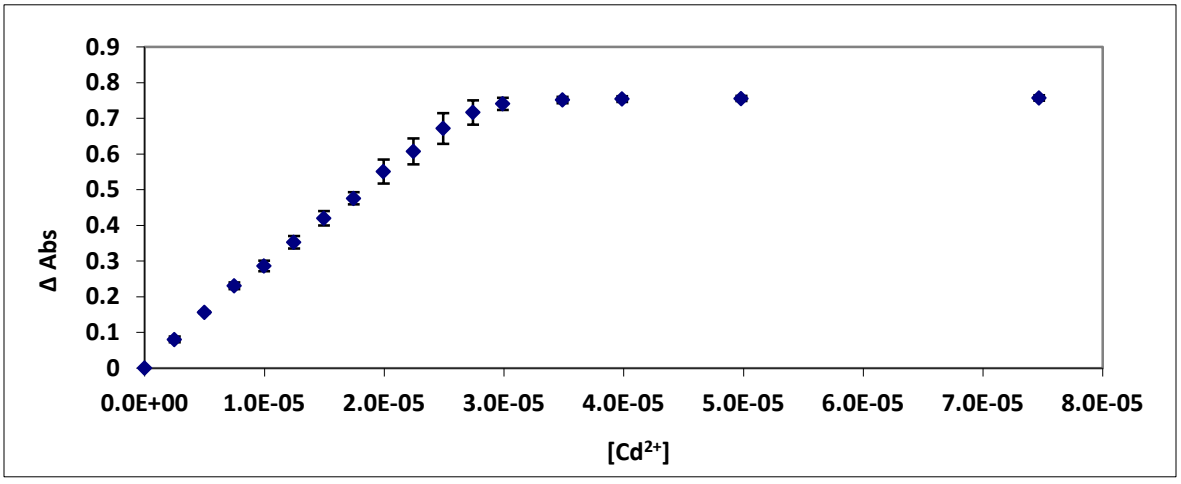

Figure S17 Titration of 25 μM DiCast-1 with $Cd(ClO_4)_2$ in CH_3CN

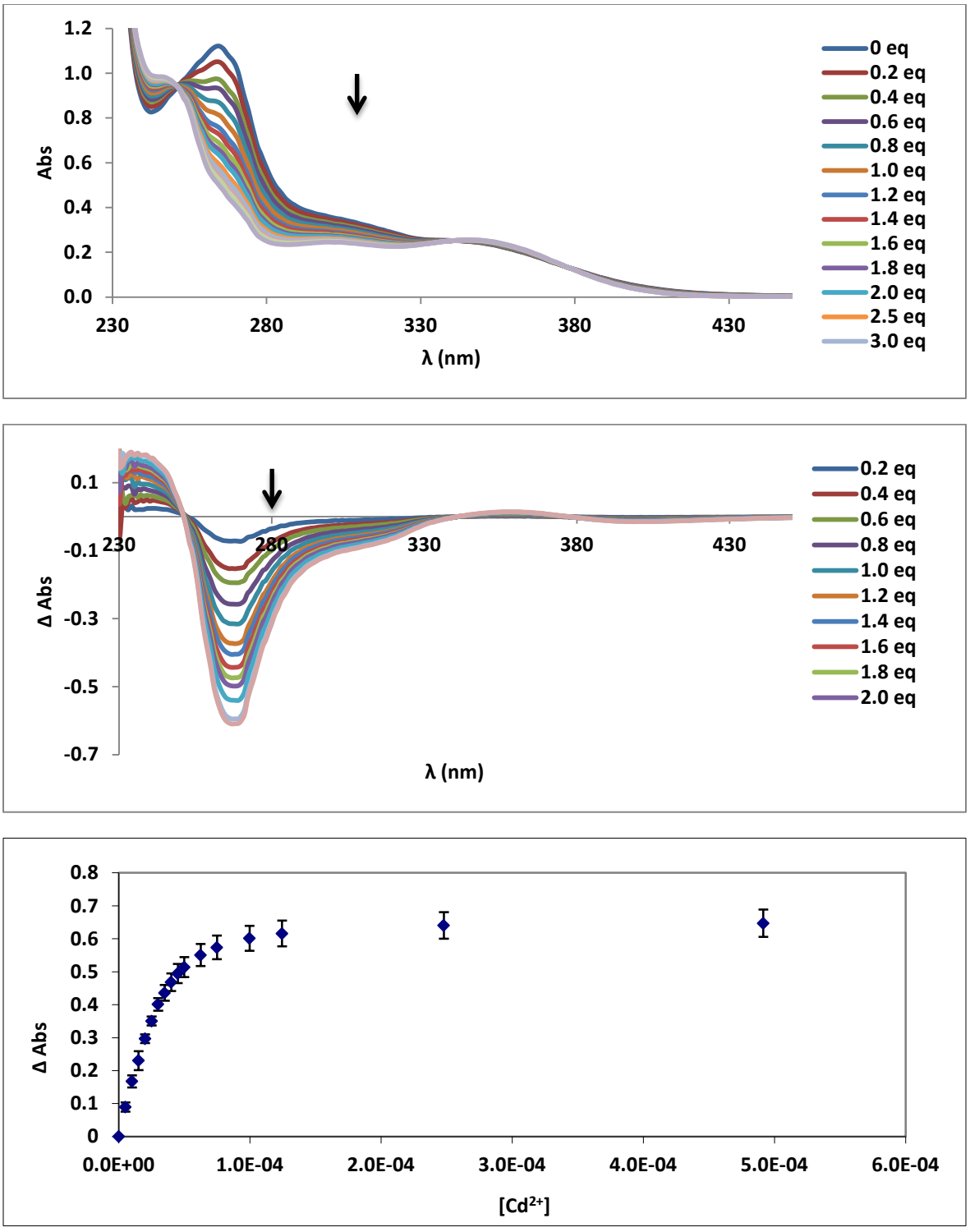

Figure S18 Titration of 25 µM DiCast-1 with $Cd(ClO_4)_2$ in EtOH.

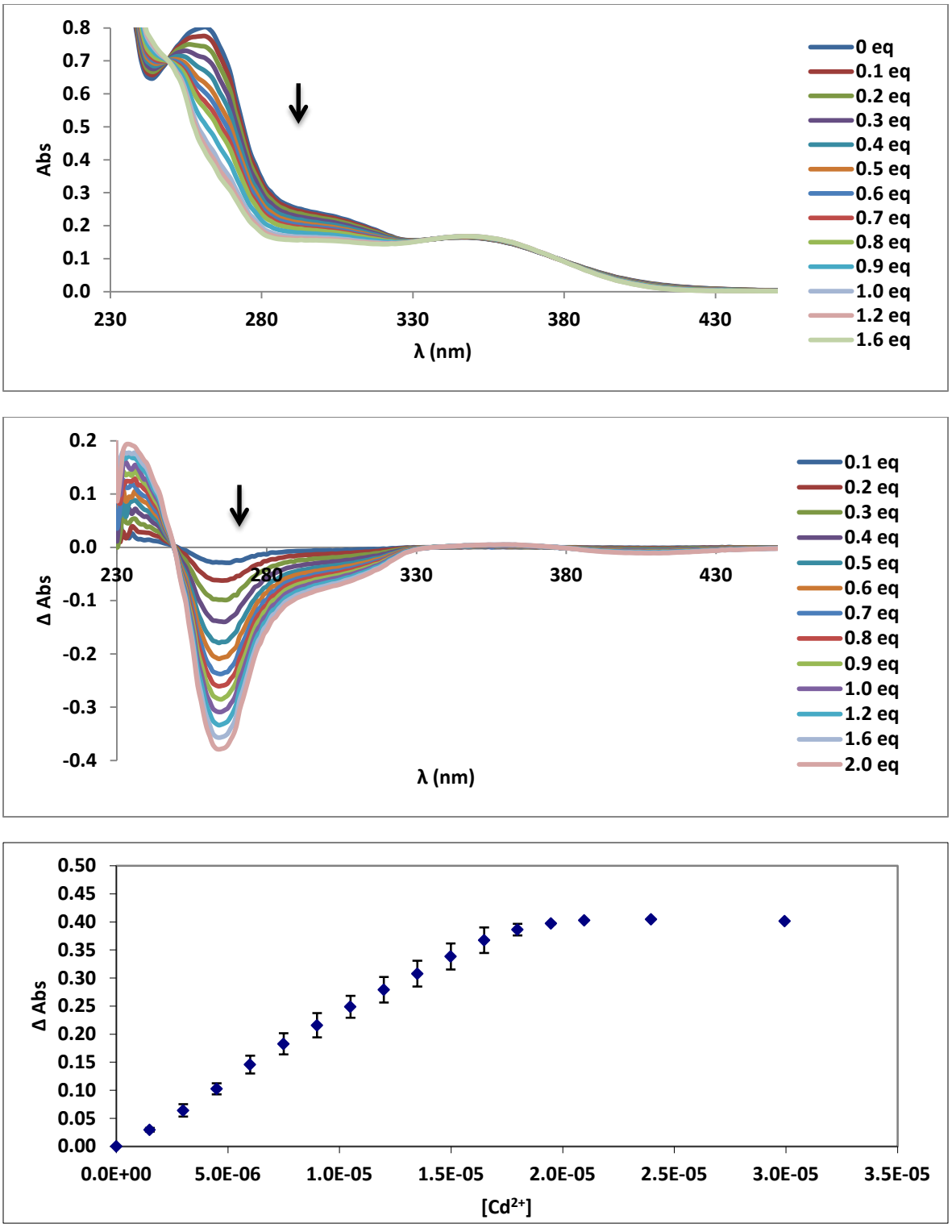

Figure S19 Titration of 15 µM DiCast-2 with $Cd(ClO_4)_2$ in CH_3CN.

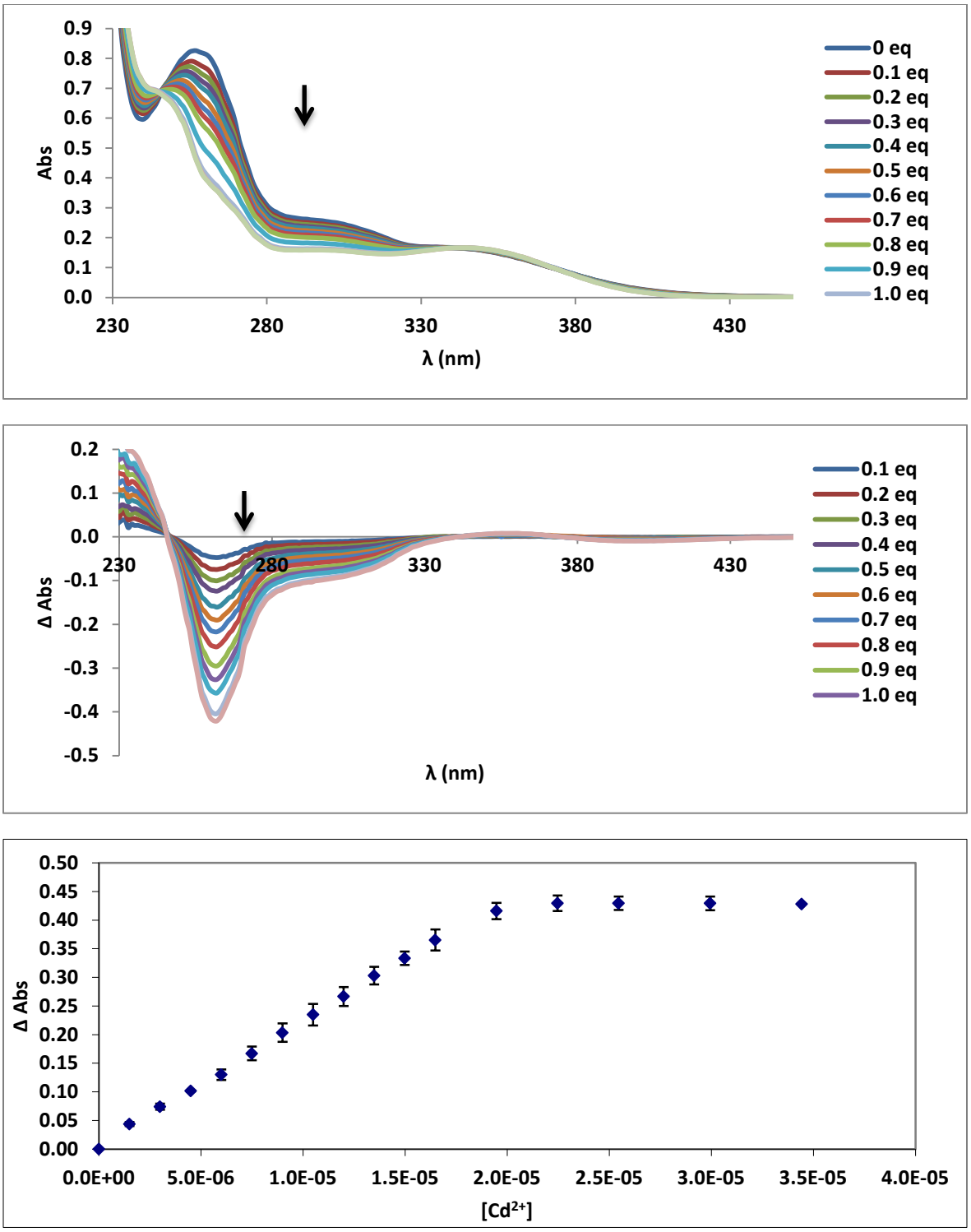

Figure S20 Titration of 15 µM DiCast-2 with $Cd(ClO_4)_2$ in EtOH.

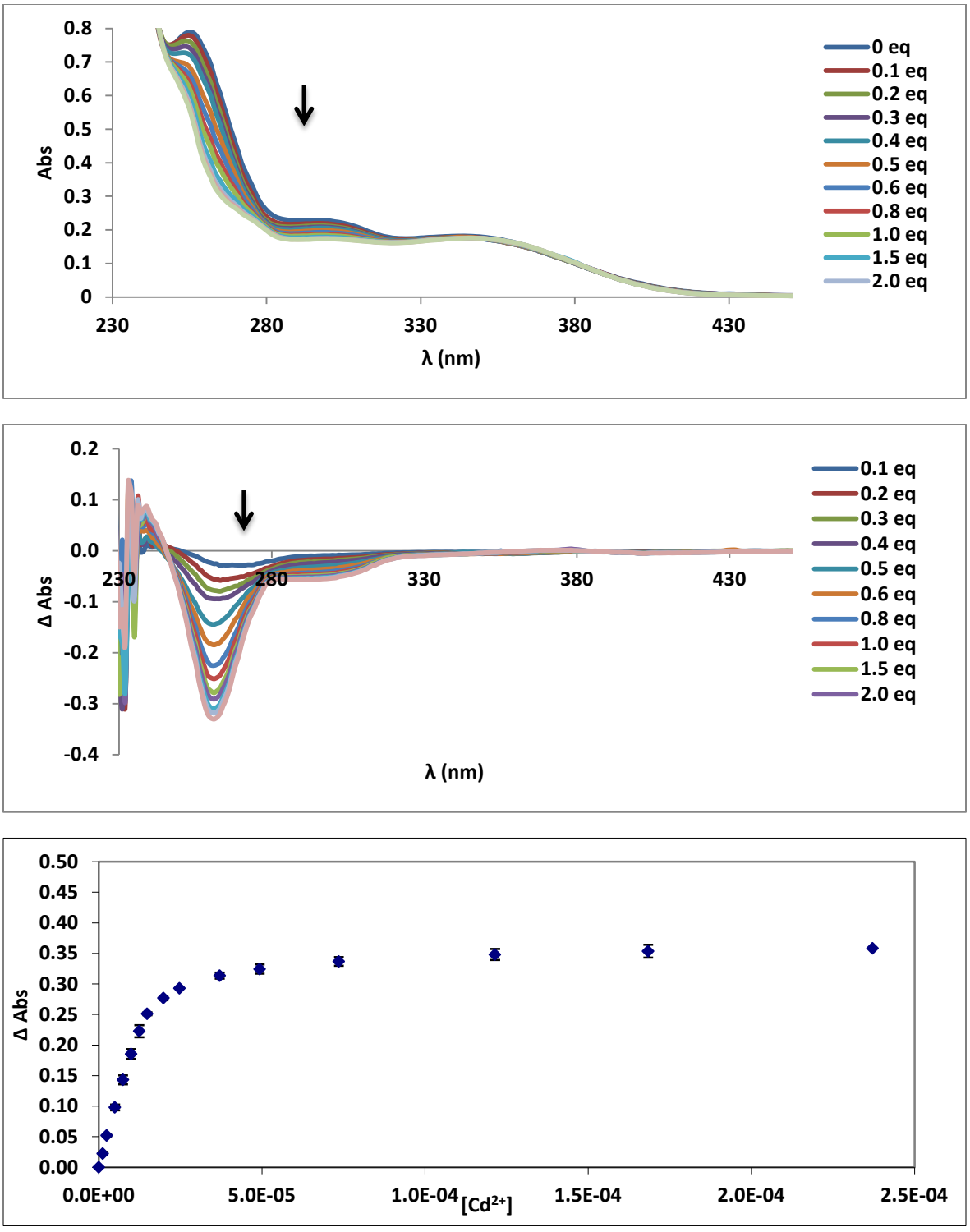

Figure S21 Titration of 25 μM DiCast-3 with $Cd(ClO_4)_2$ in CH_3CN.

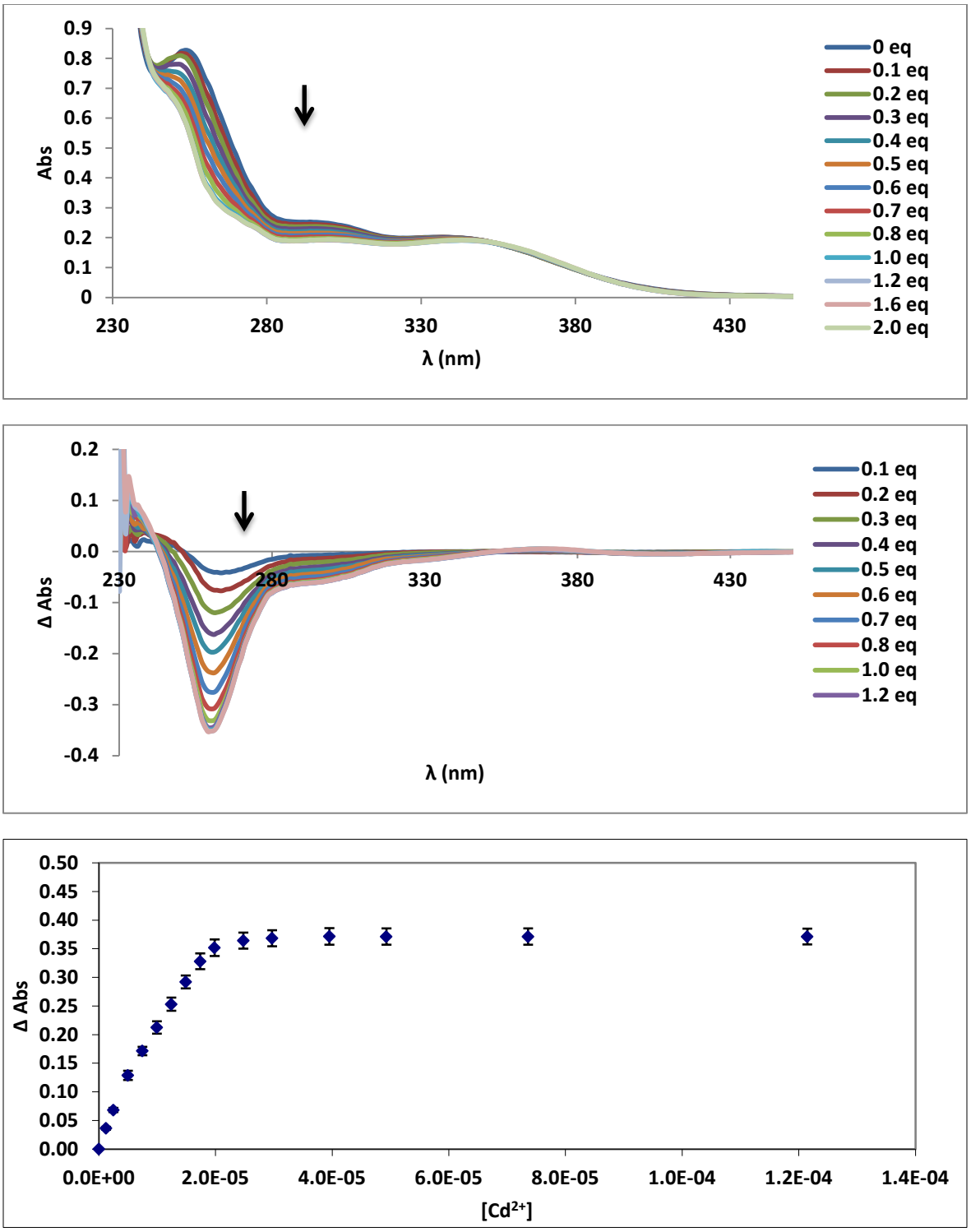

Figure S22 Titration of 25 µM DiCast-3 with $Cd(ClO_4)_2$ in EtOH.

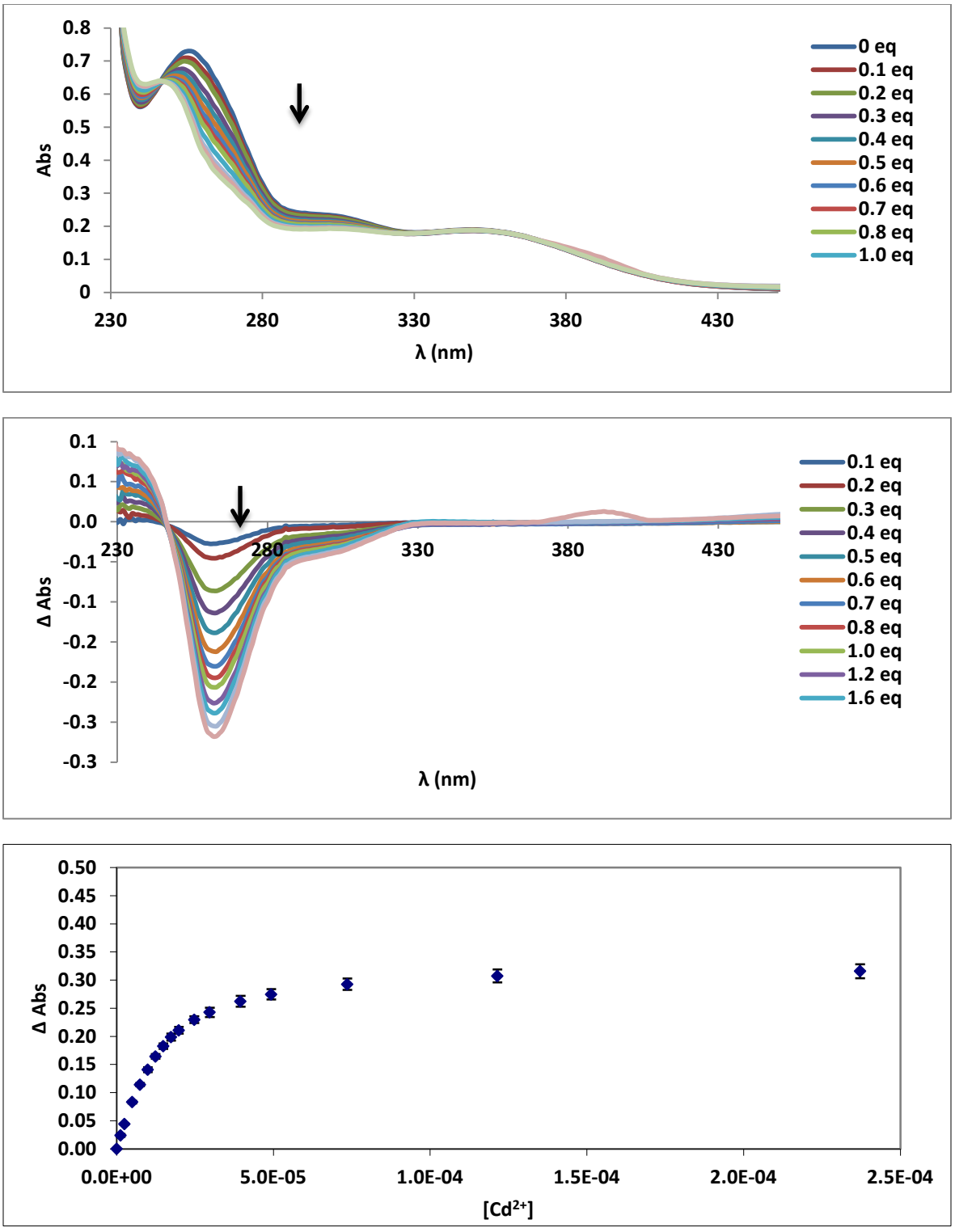

Figure S23 Titration of 25 µM DiCast-3 with $Cd(ClO_4)_2$ in buffer.

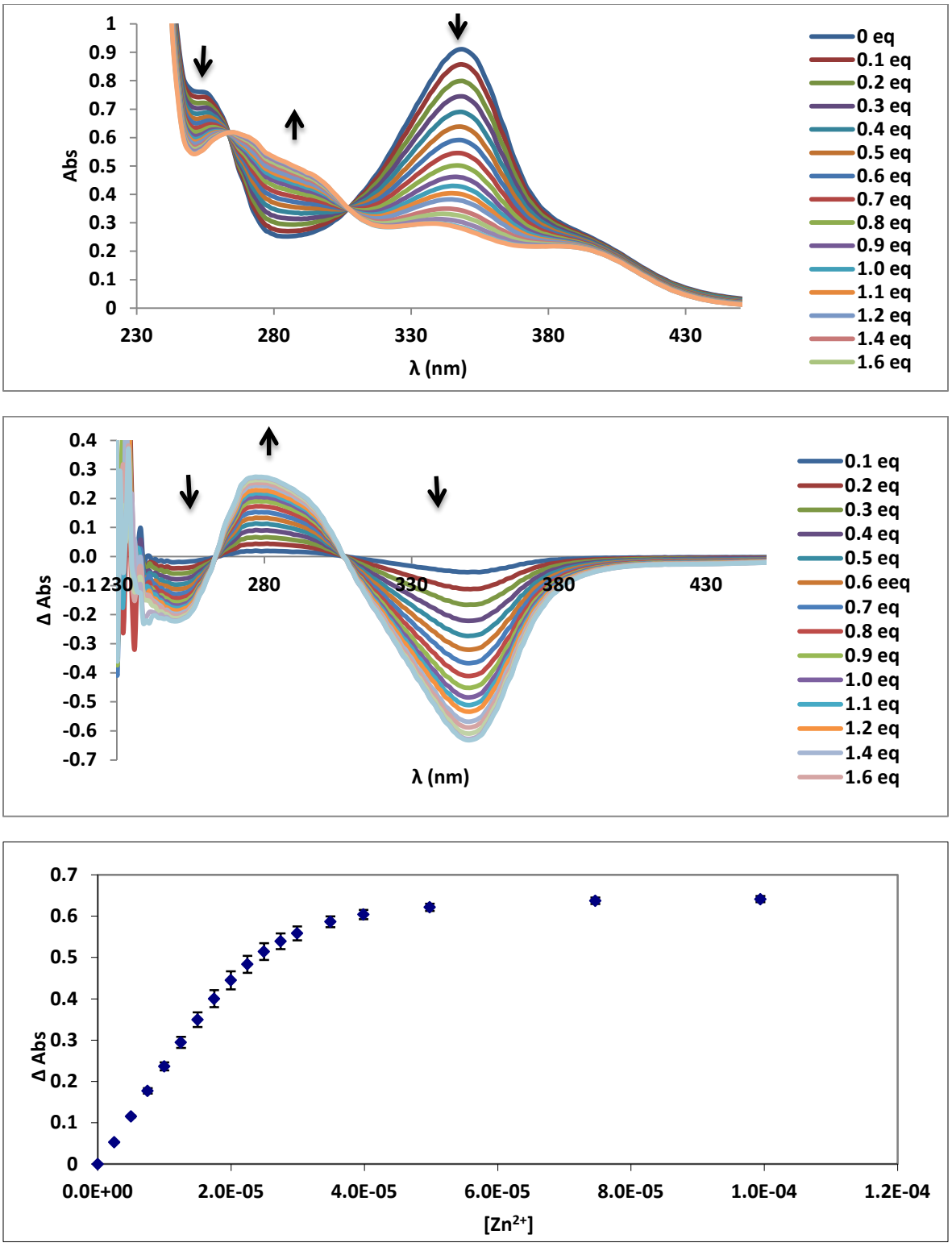

Figure S24 Titration of 25 µM MonoUnc with $Zn(ClO_4)_2$ in CH_3CN.

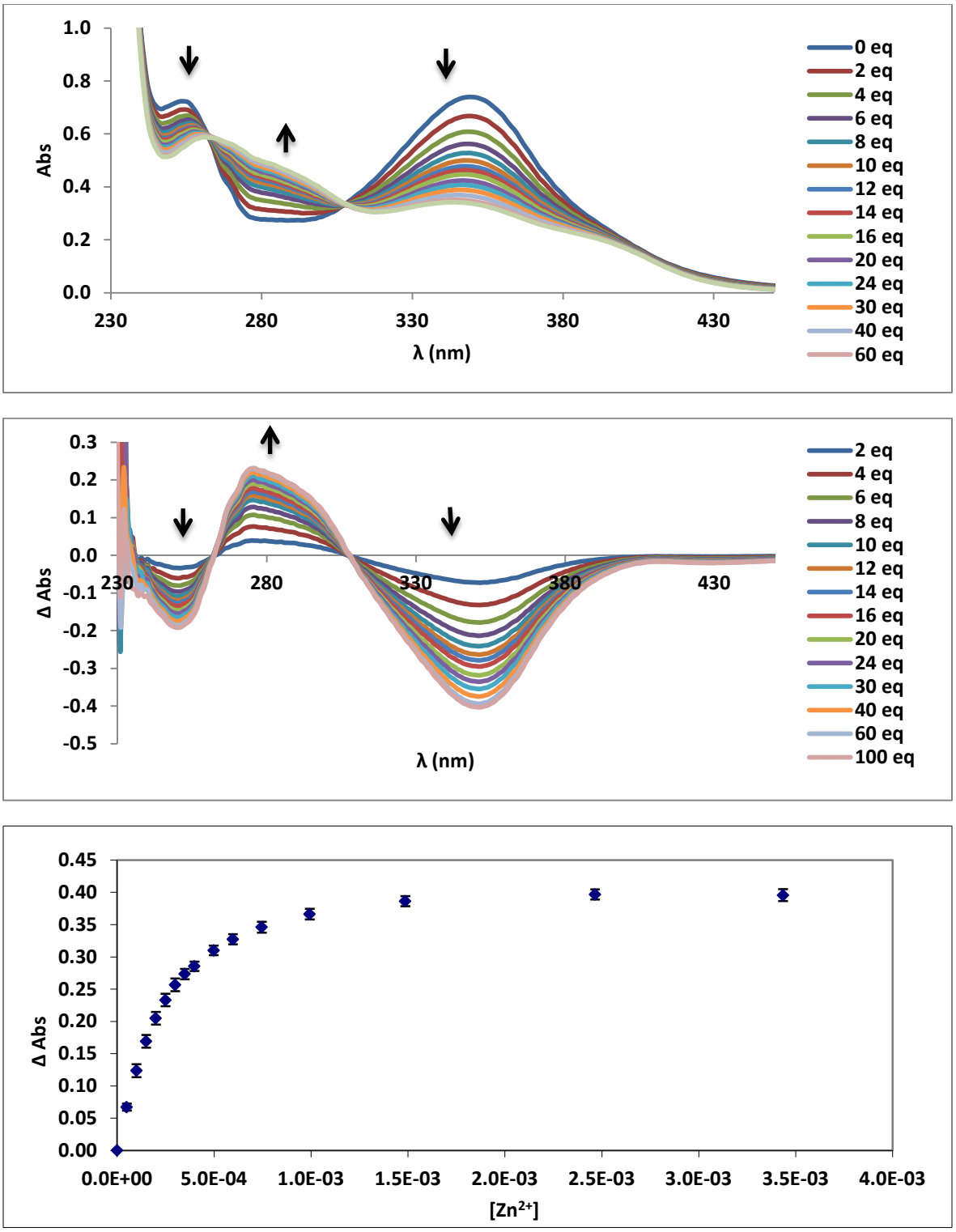

Figure S25 Titration of 25 µM MonoUnc with $Zn(ClO_4)_2$ in EtOH.

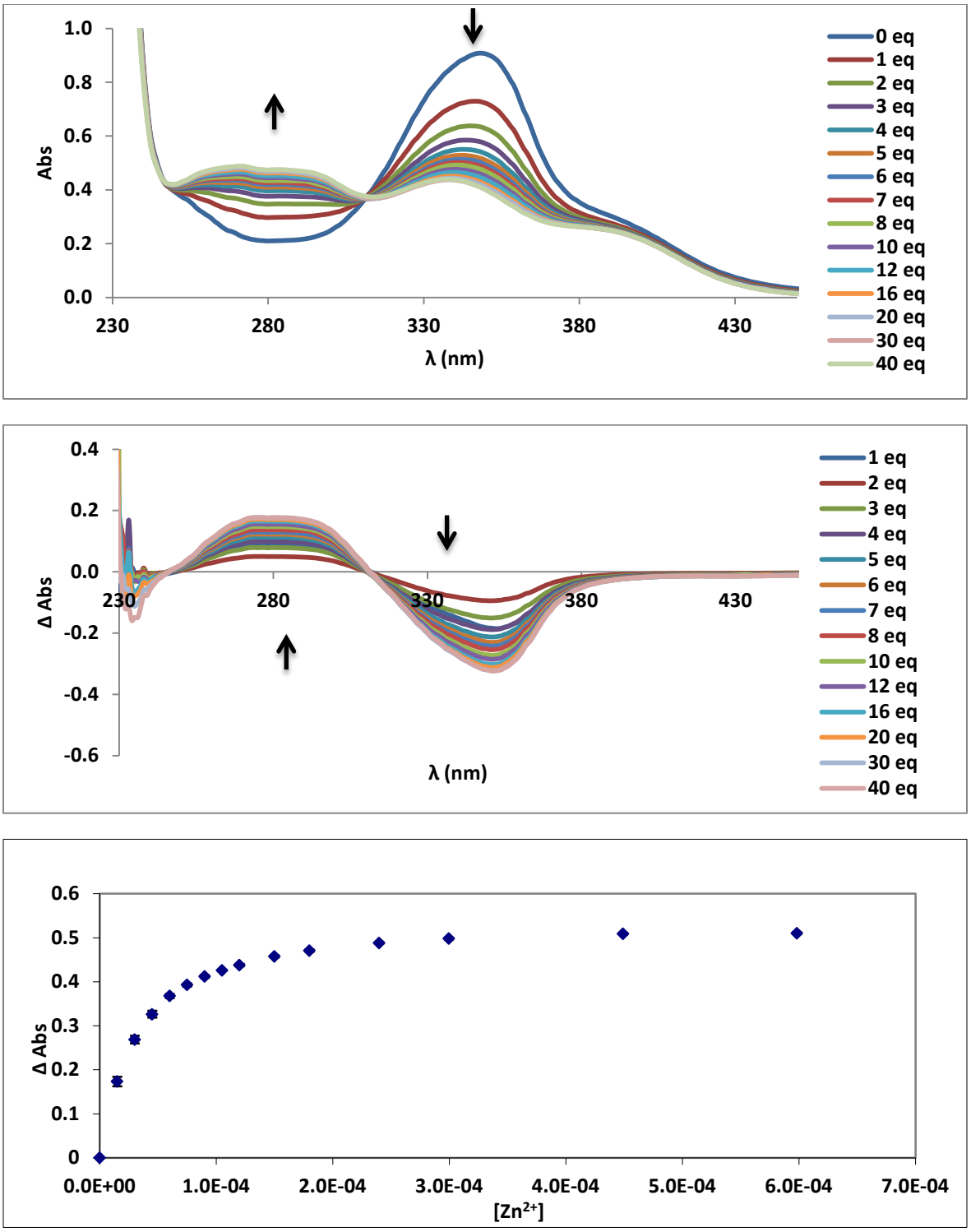

Figure S26 Titration of 15 μM DiUnc-1 with $Zn(ClO_4)_2$ in CH_3CN.

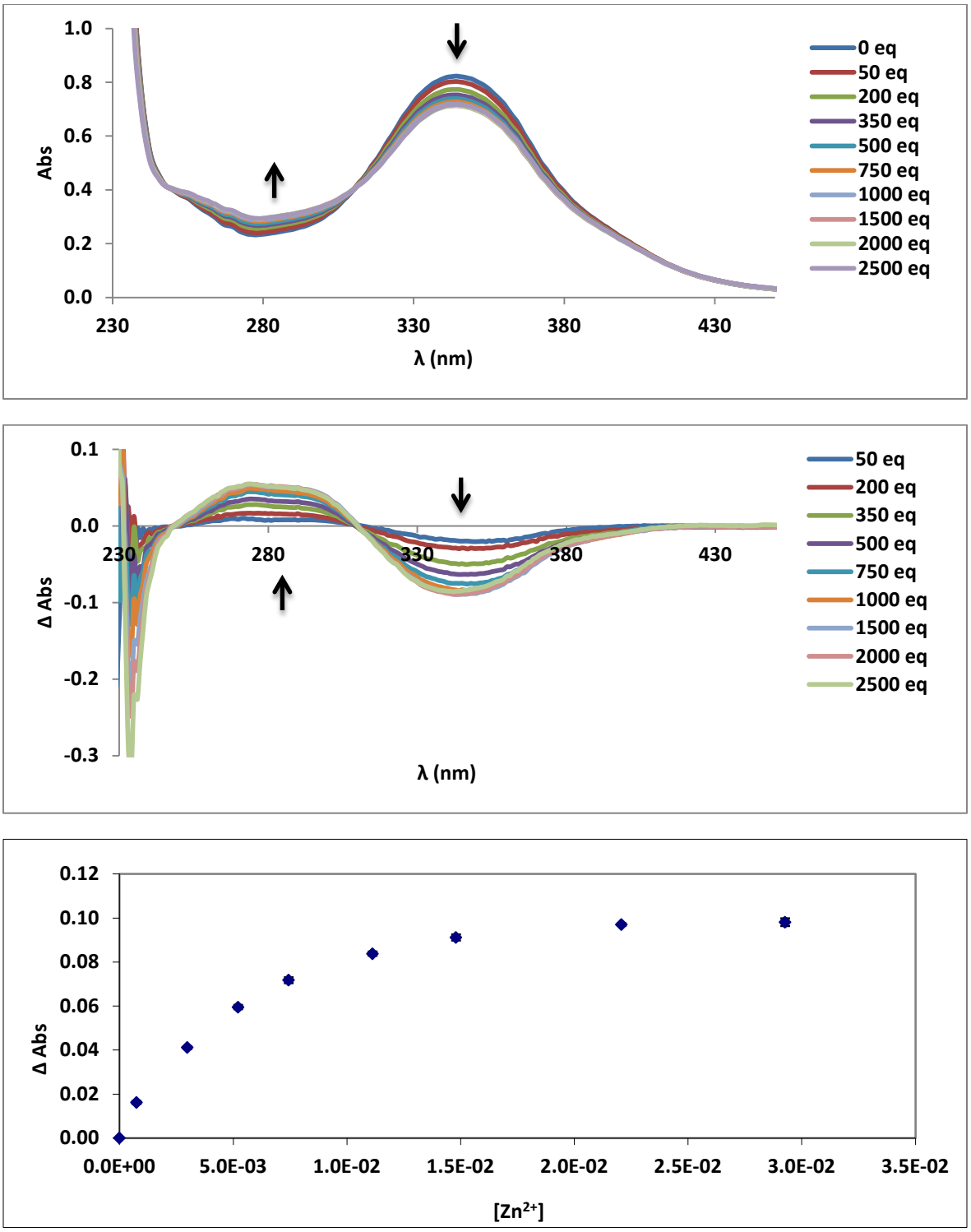

Figure S27 Titration of 15 µM DiUnc-1 with $Zn(ClO_4)_2$ in EtOH.

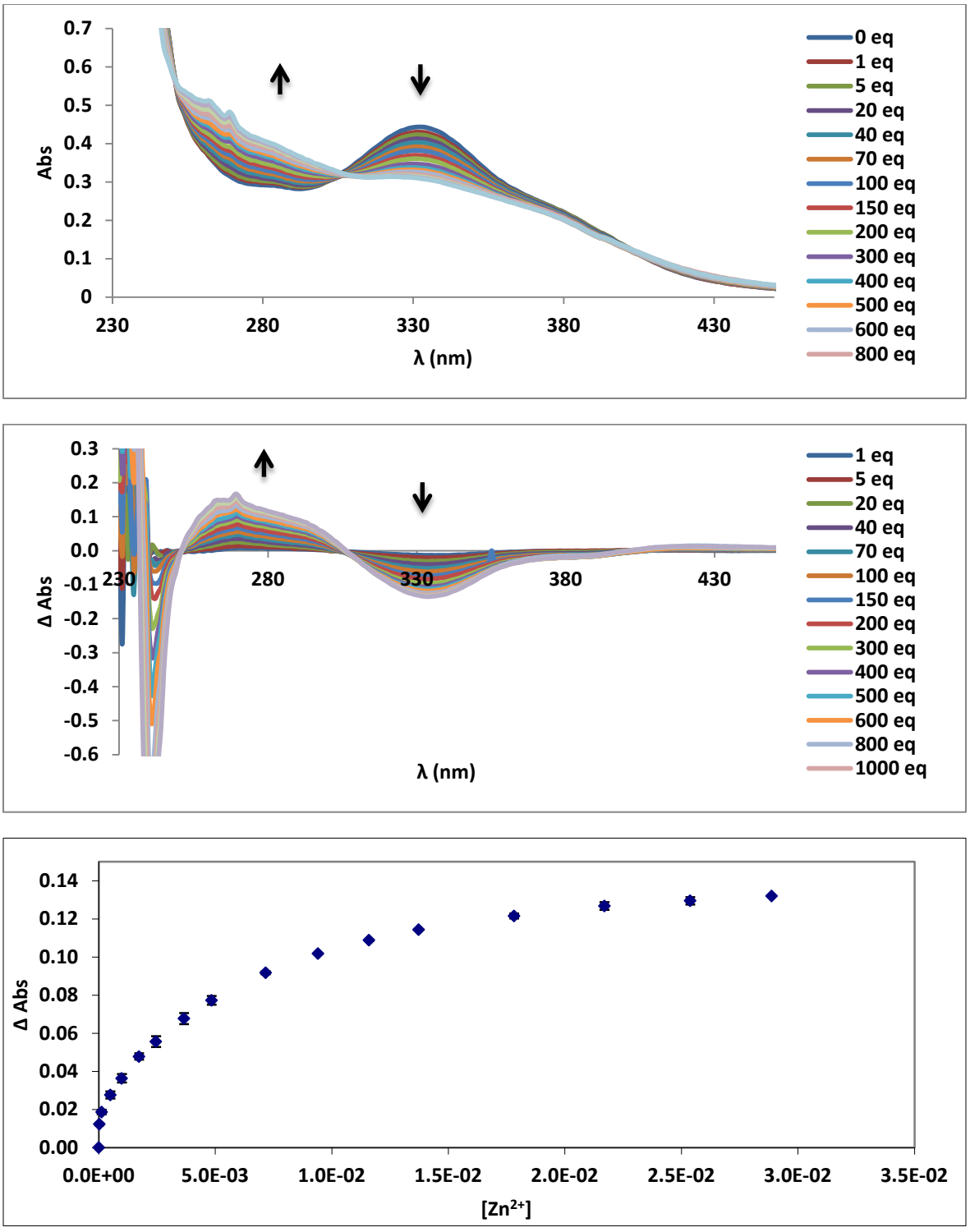

Figure S28 Titration of 25 µM DiUnc-2 with $Zn(ClO_4)_2$ in CH_3CN.

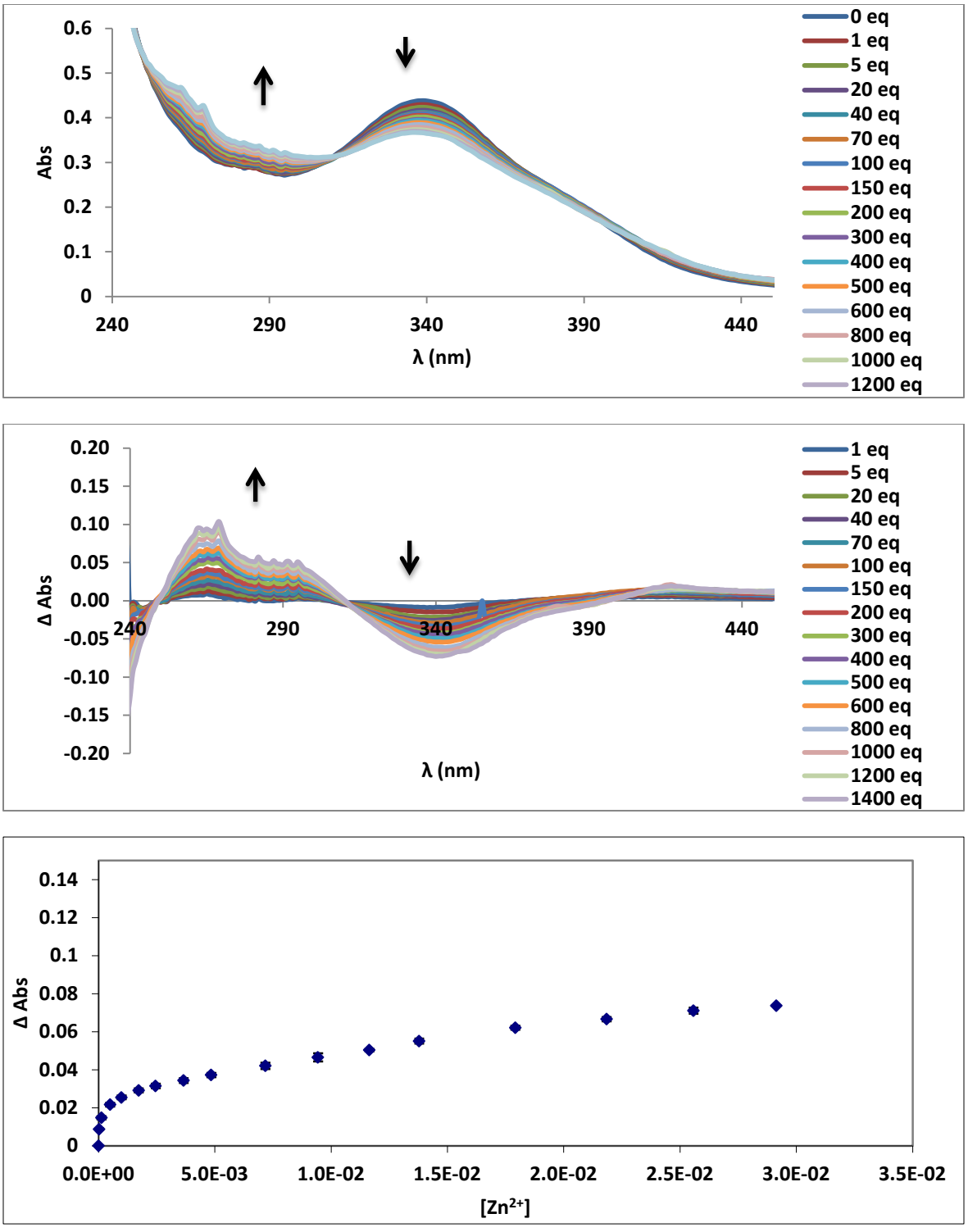

Figure S29 Titration of 25 µM DiUnc-2 with $Zn(ClO_4)_2$ in EtOH

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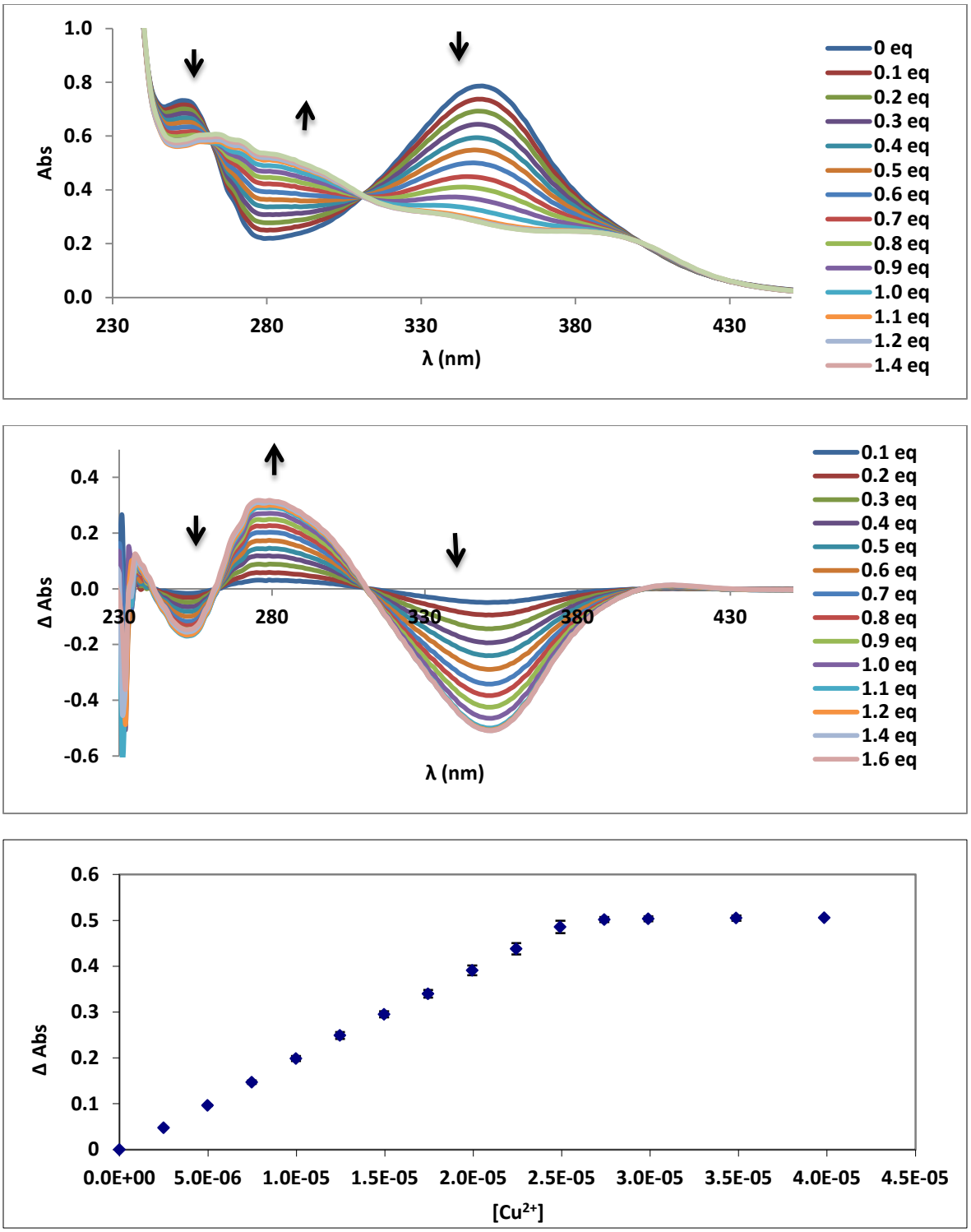


Figure S30 Titration of 25 µM MonoUnc with $Cu(ClO_4)_2$ in EtOH

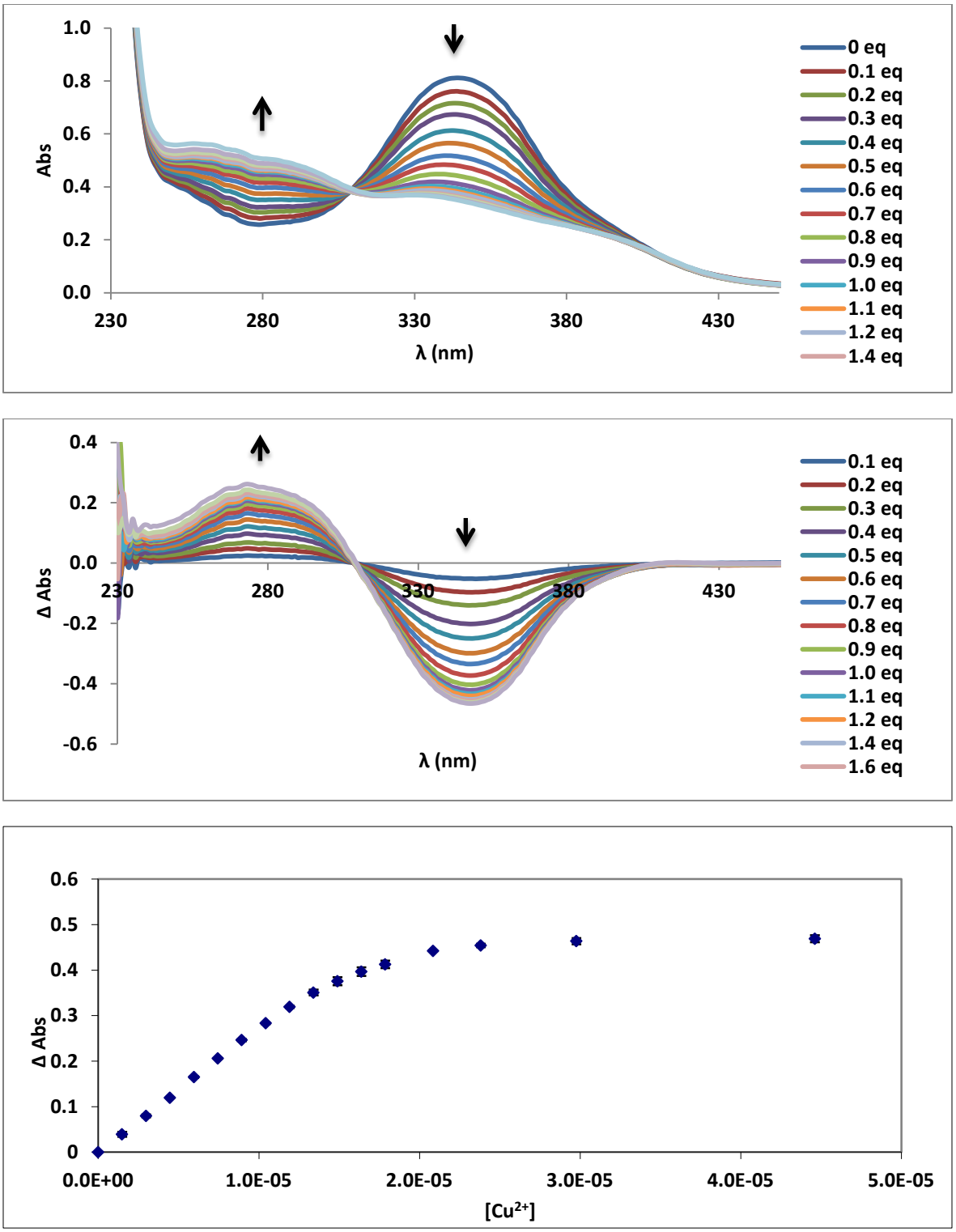


Figure S31 Titration of 15 µM DiUnc-1 with $Cu(ClO_4)_2$ in EtOH

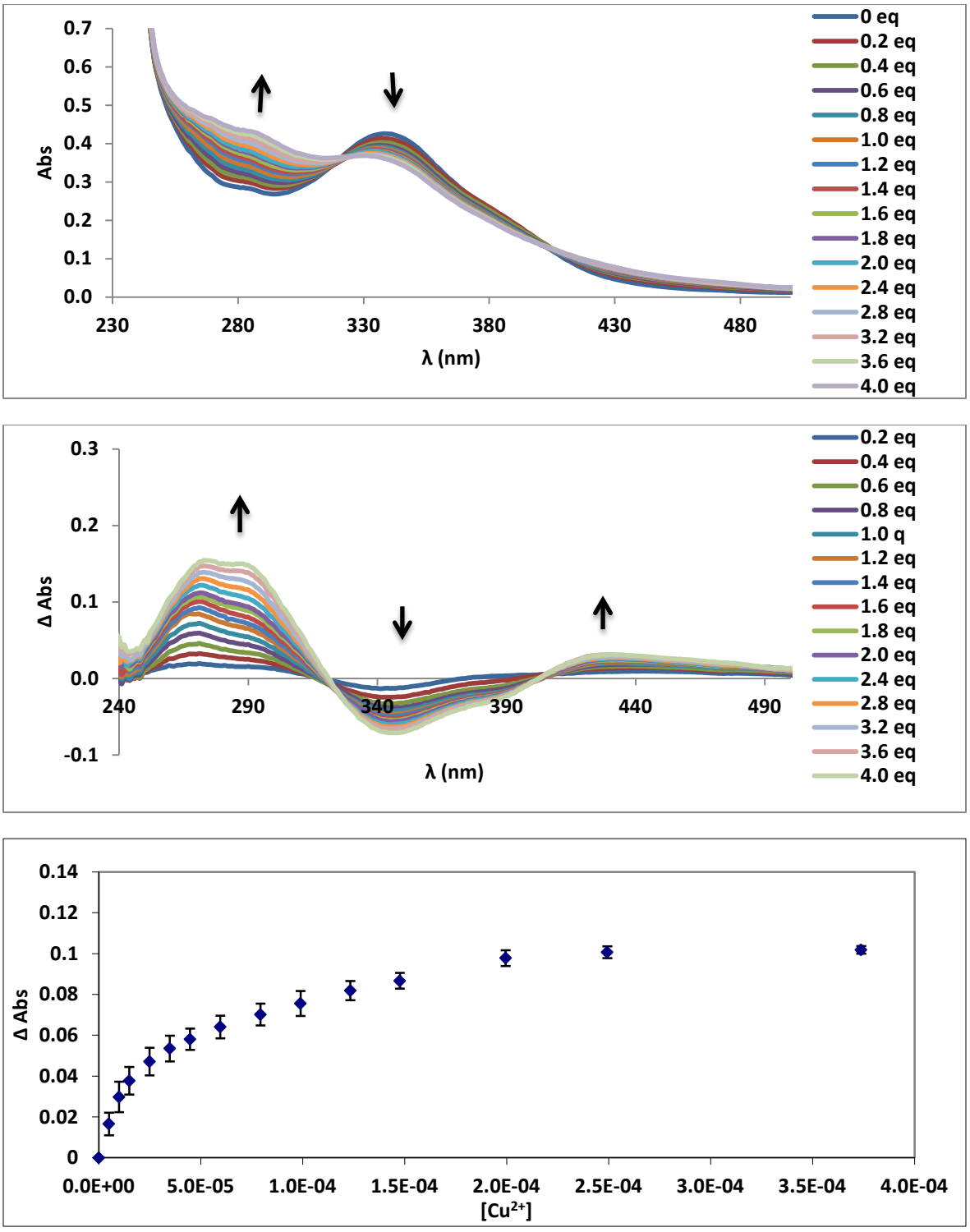


Figure S32 Titration of 25 µM DiUnc-2 with $Cu(ClO_4)_2$ in EtOH

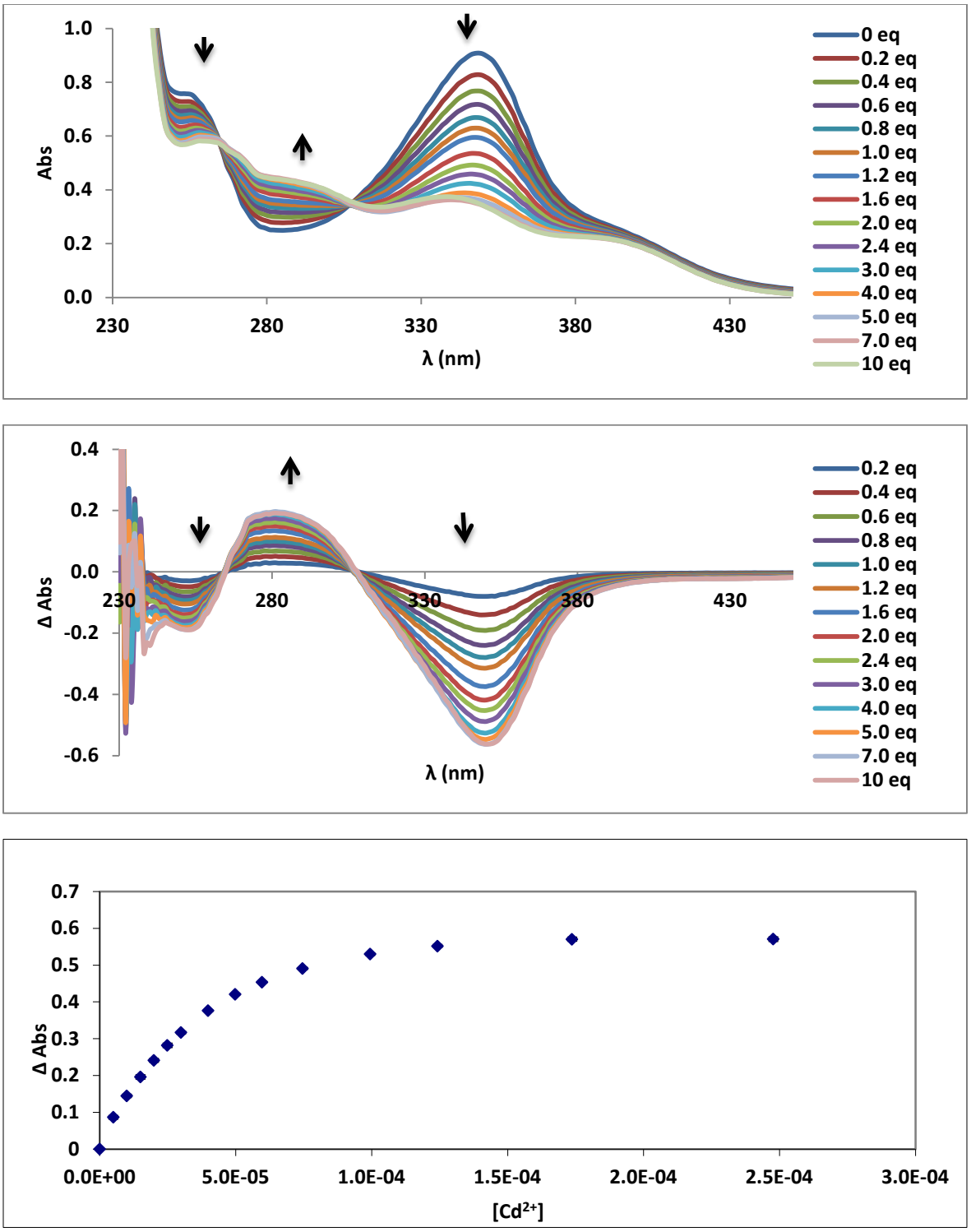
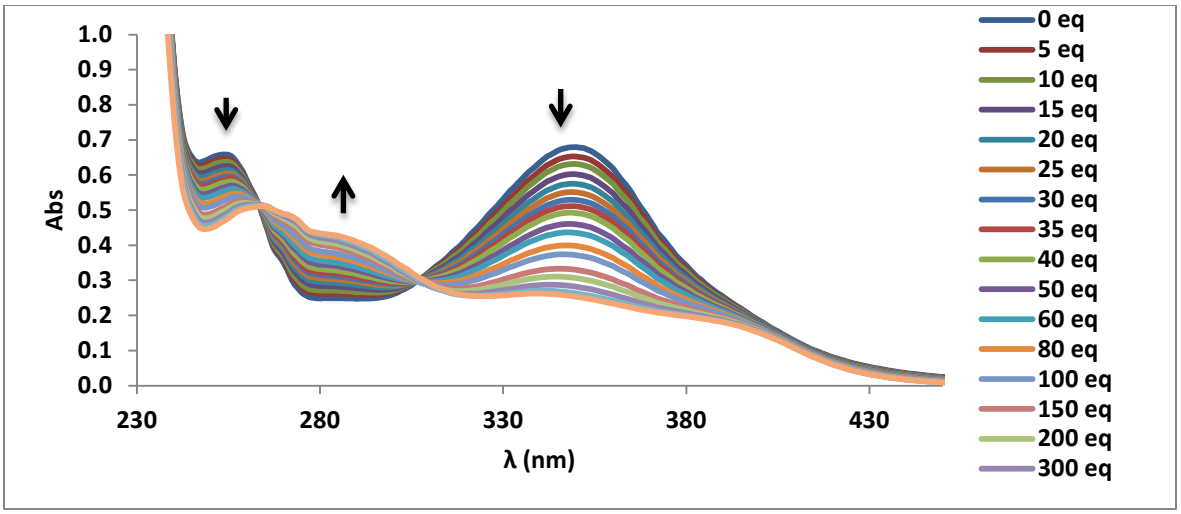
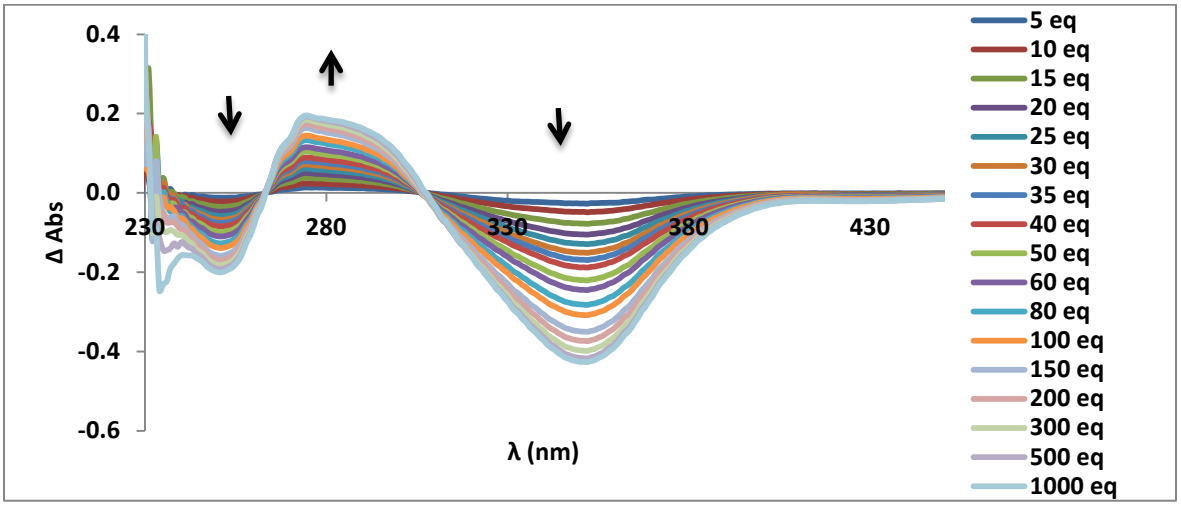


Figure S33 Titration of 25 µM MonoUnc with $Cd(ClO_4)_2$ in CH_3CN.





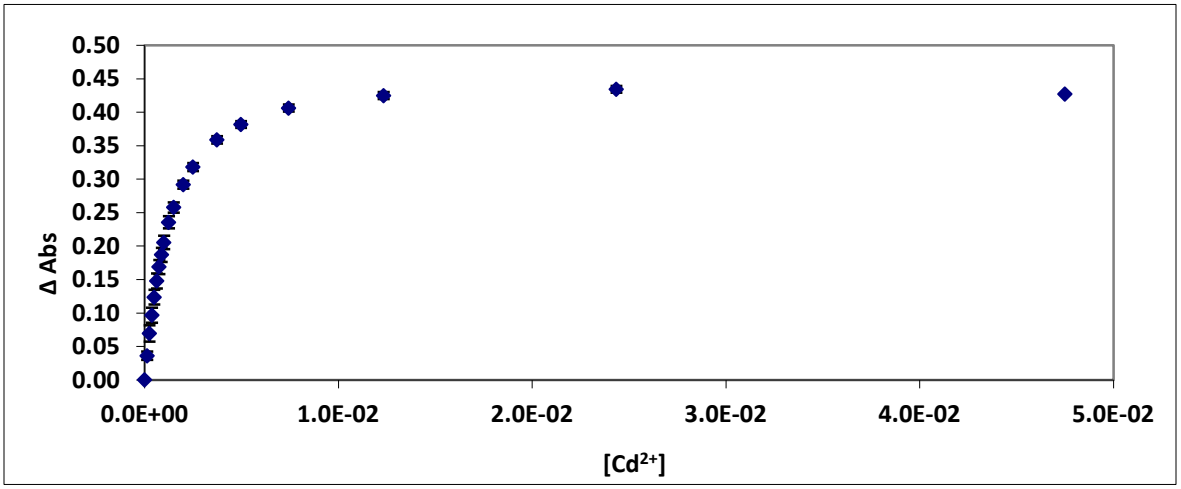


Figure S34 Titration of 25 µM MonoUnc with $Cd(ClO_4)_2$ in EtOH

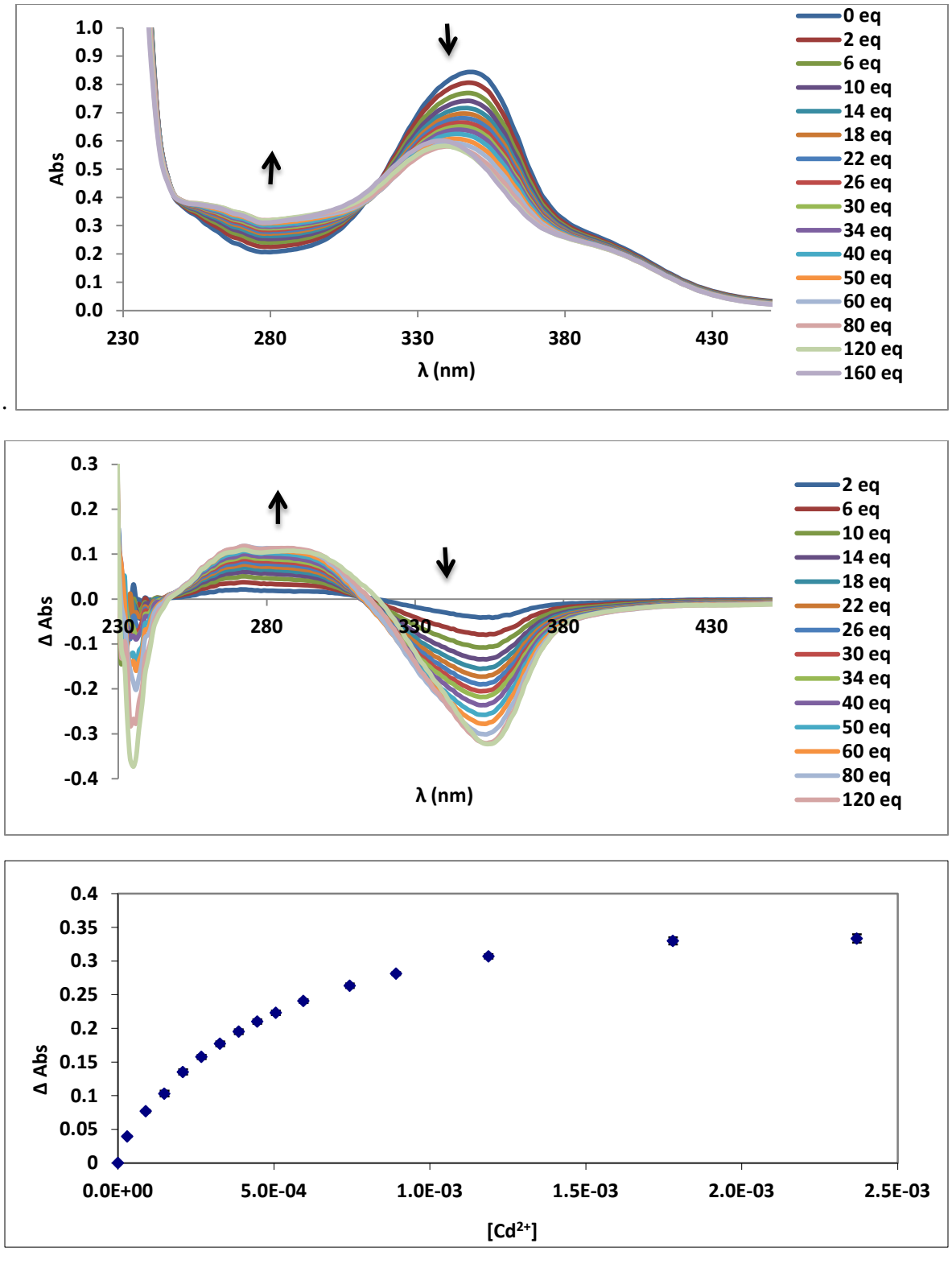


Figure S35 Titration of 15 µM DiUnc-1 with $Cd(ClO_4)_2$ in CH_3CN.

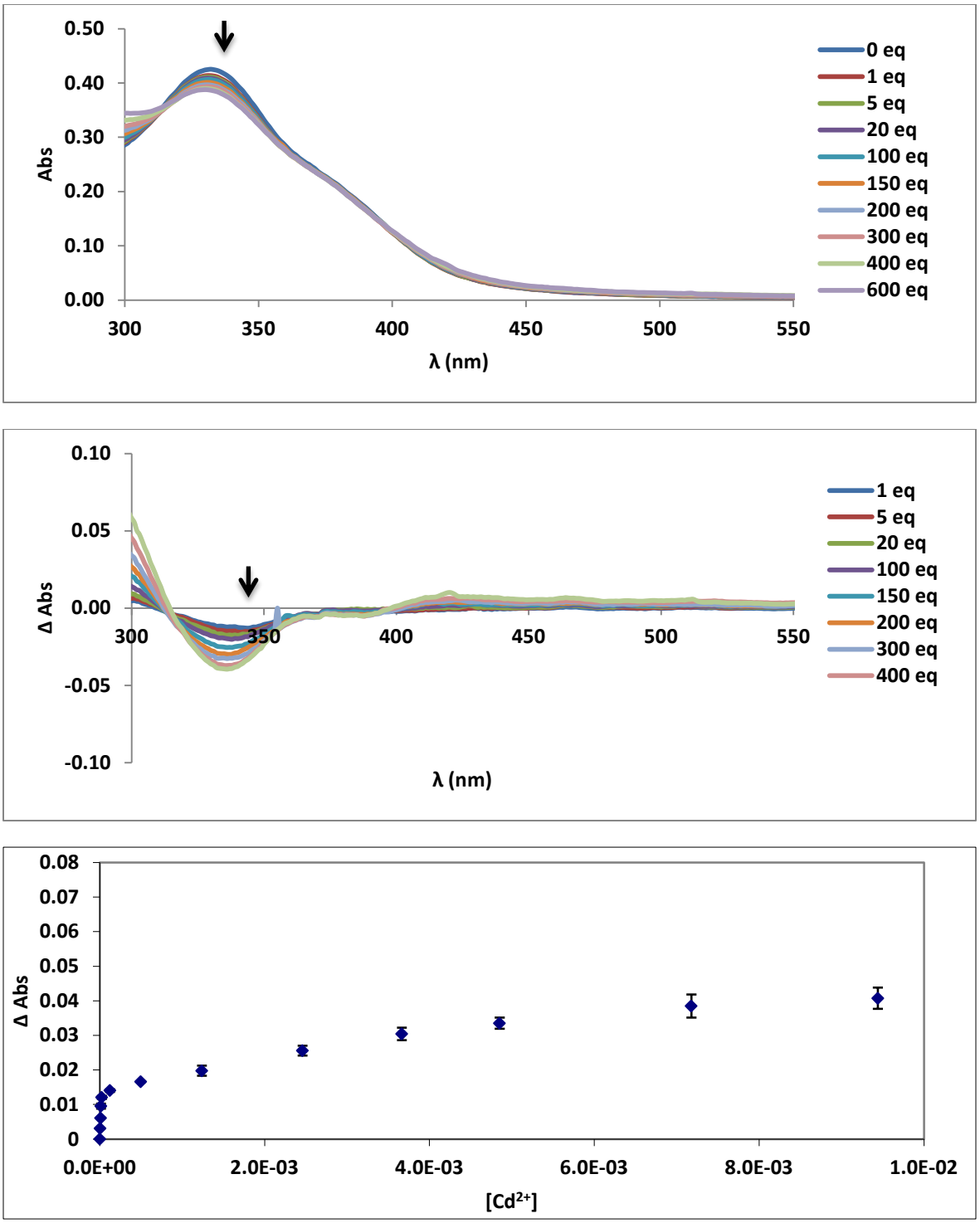


Figure S36 Titration of 25 µM DiUnc-2 with $Cd(ClO_4)_2$ in CH_3CN.

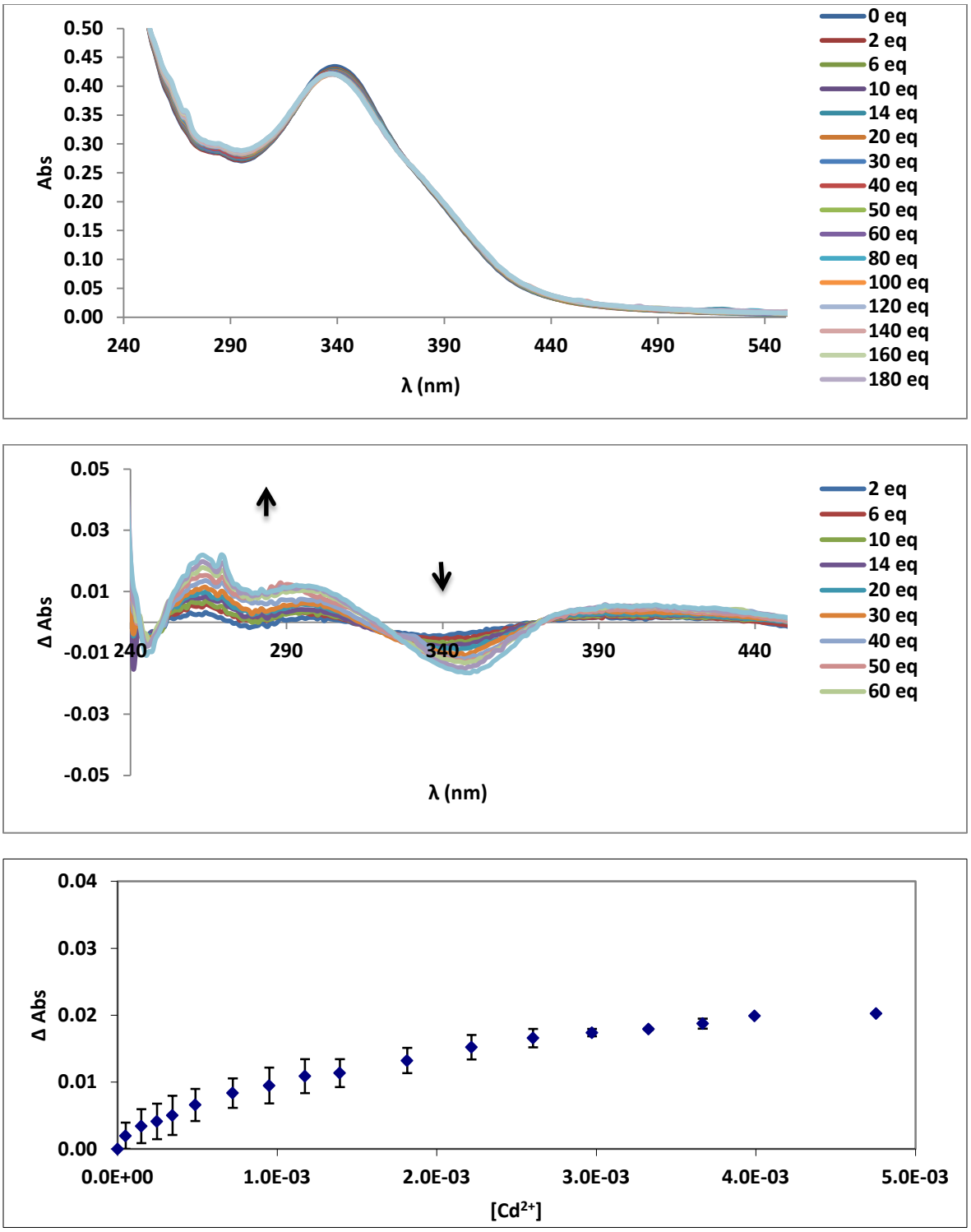


Figure S37 Titration of 25 µM DiUnc-2 with $Cd(ClO_4)_2$ in EtOH.

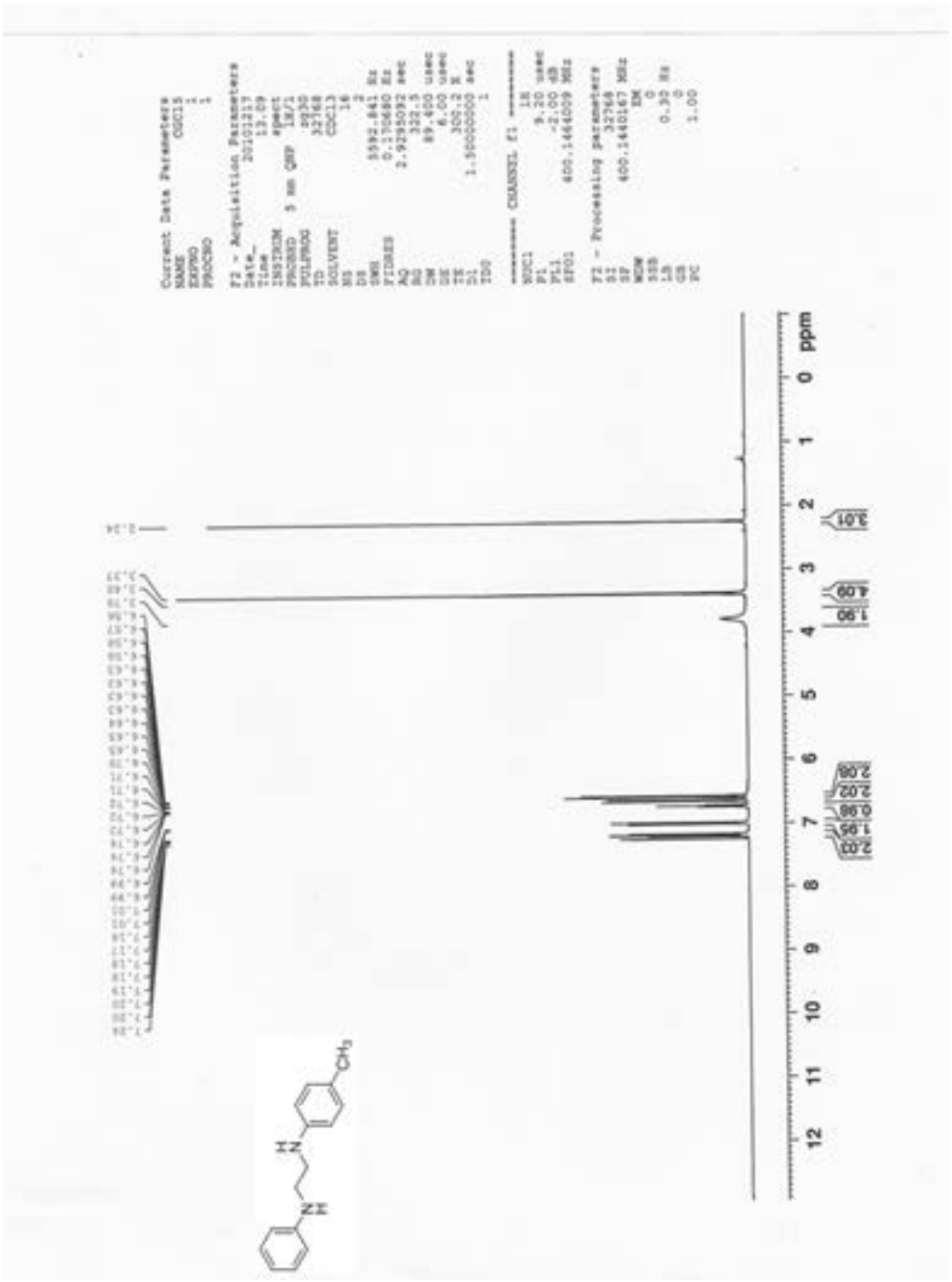


Figure S38 ^{1}H of compound **9**.

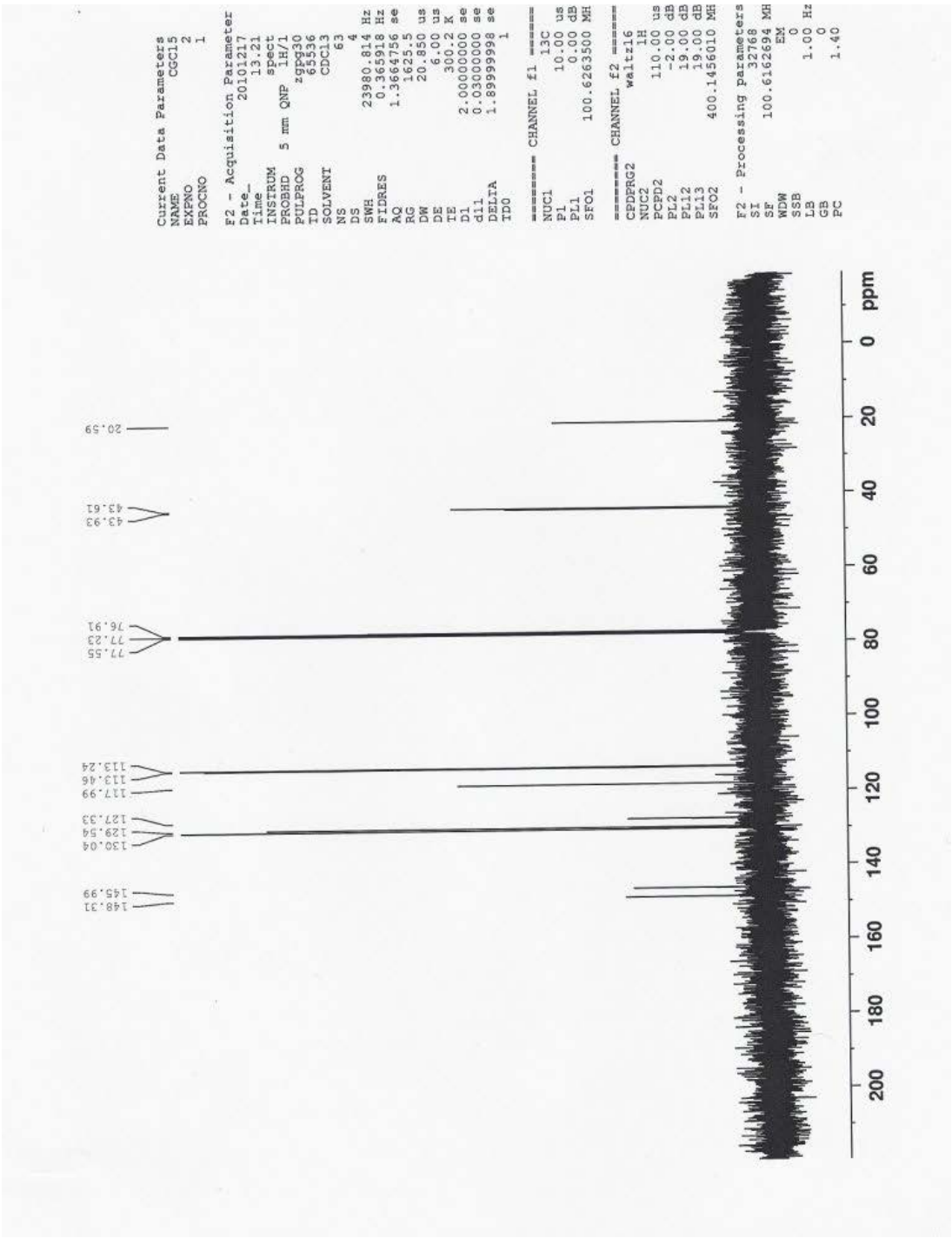


Figure S39 ^{13}C NMR of compound **9**.

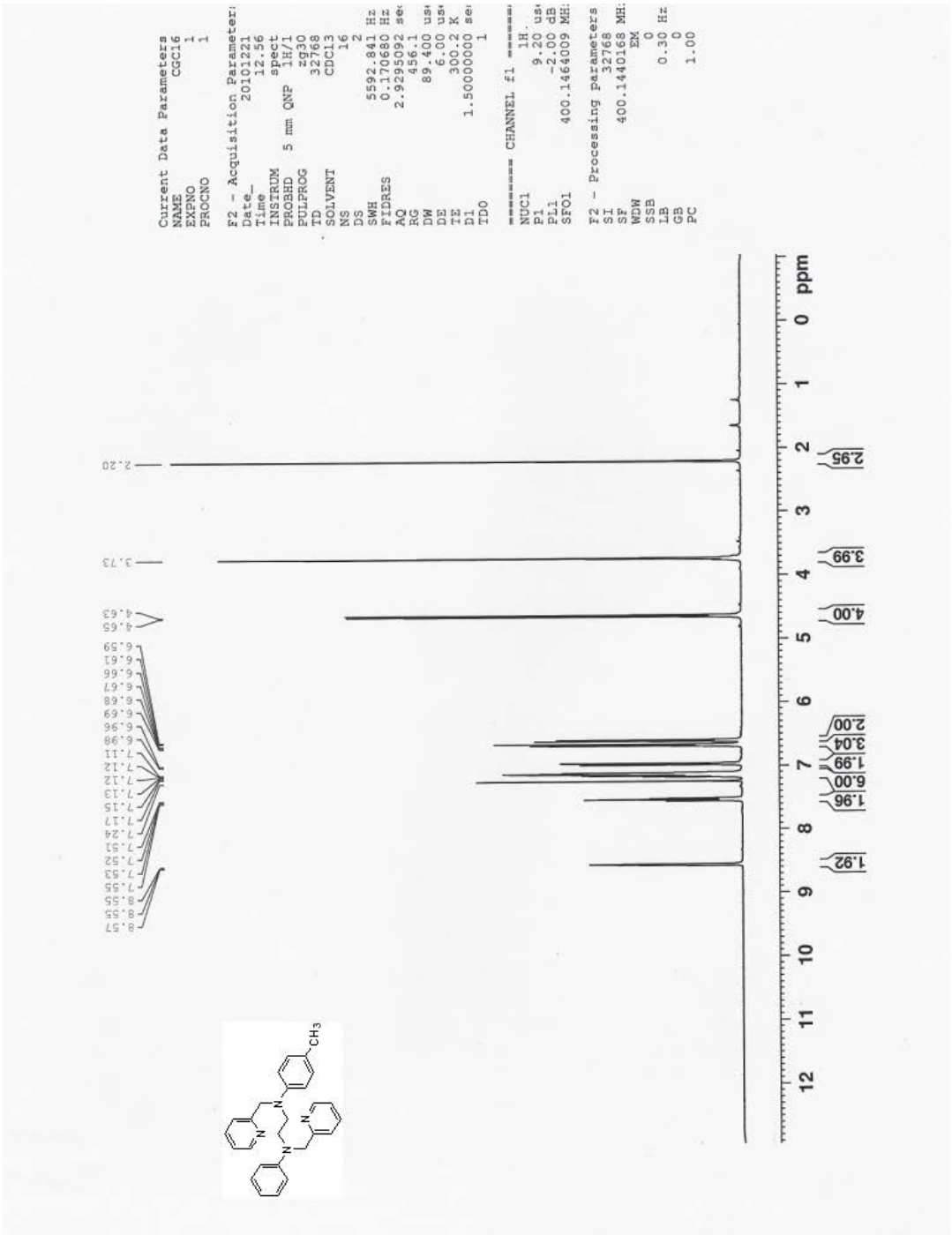


Figure S40 ^{1}H of compound **10**.

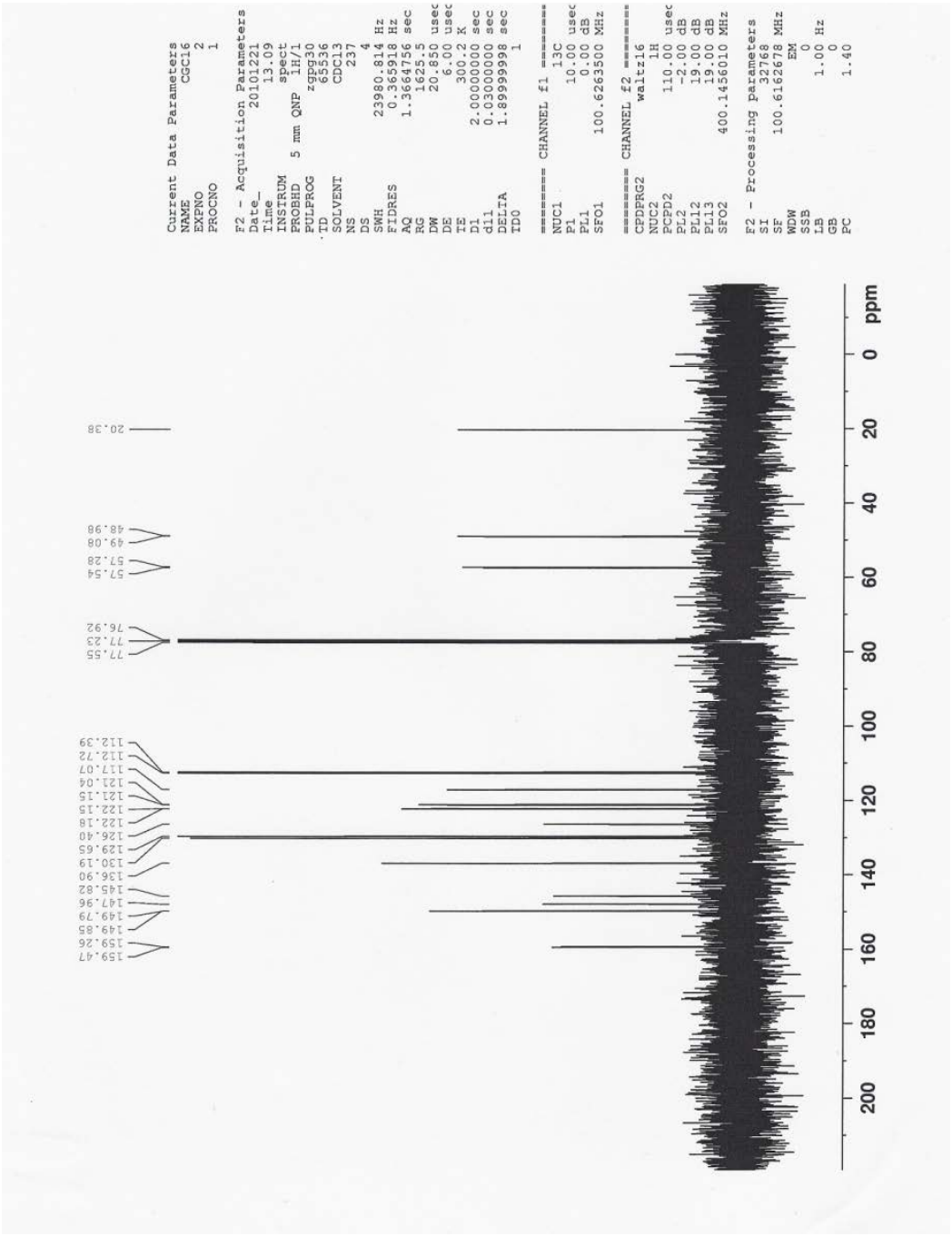


Figure S41 ^{13}C NMR of compound **10**.

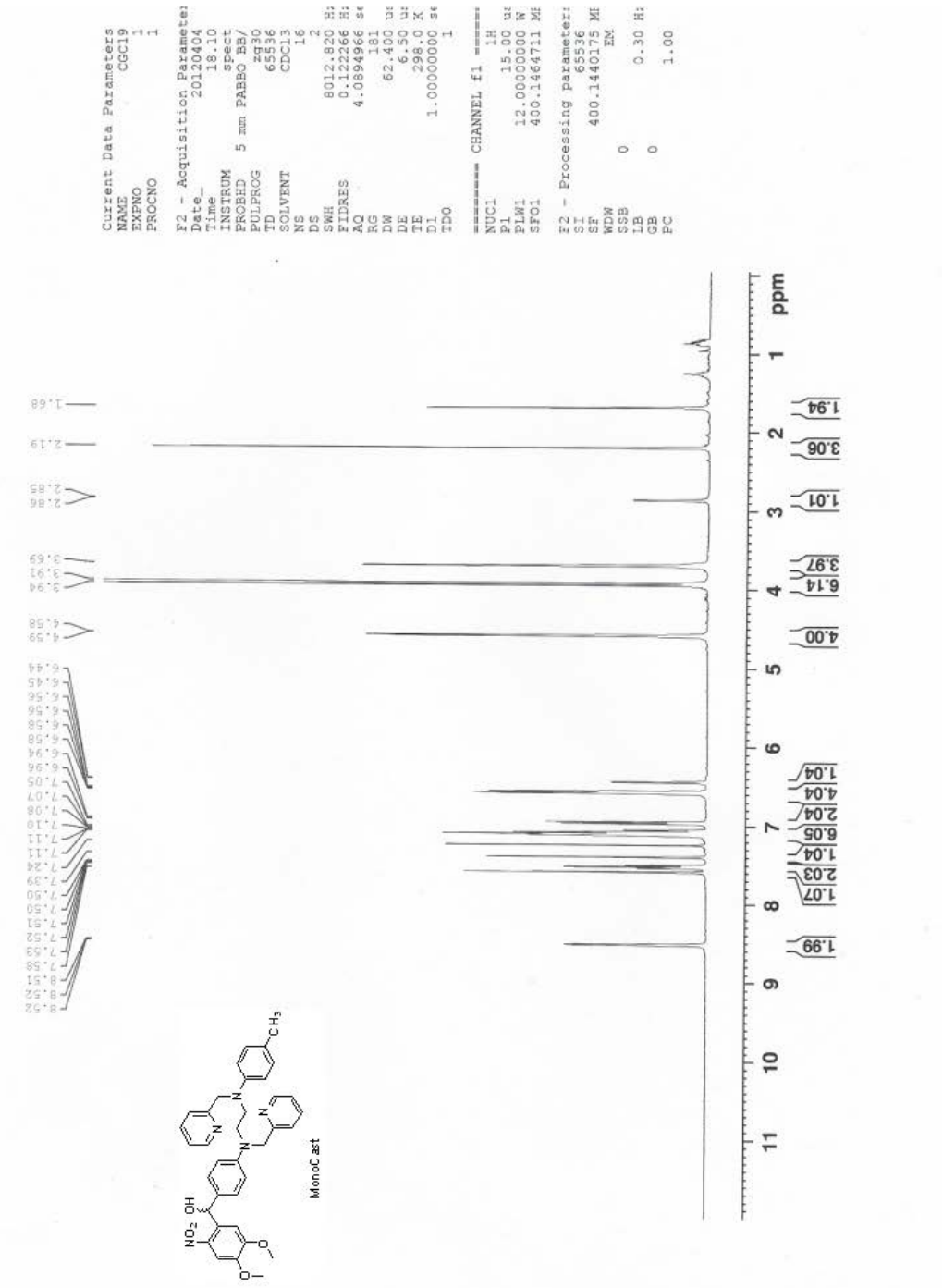


Figure S42 ^{1}H of compound MonoCast, **3**.

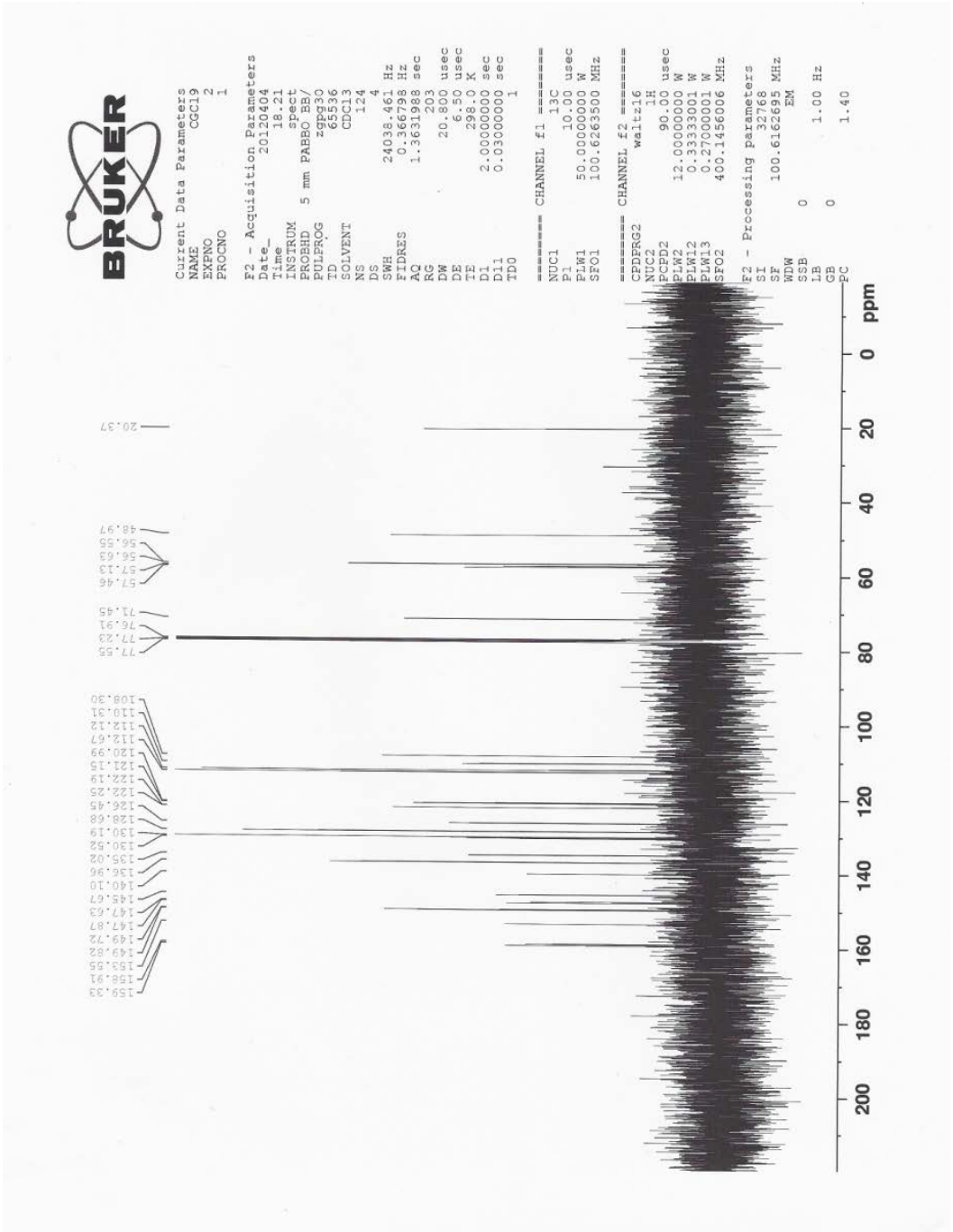


Figure S43 ^{13}C NMR of compound MonoCast, **3**.

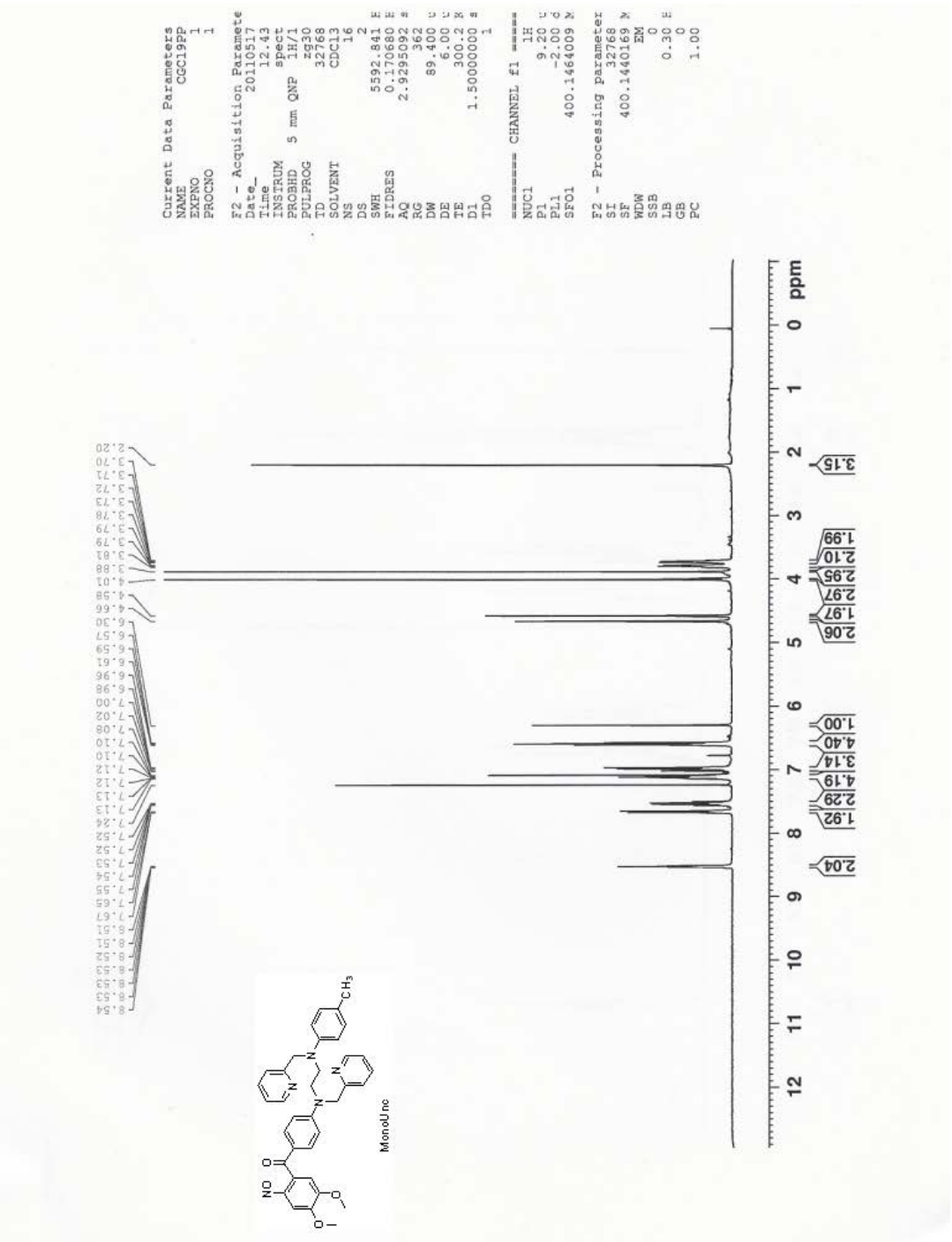


Figure S44 ^{1}H of compound MonoUnc, **12**.

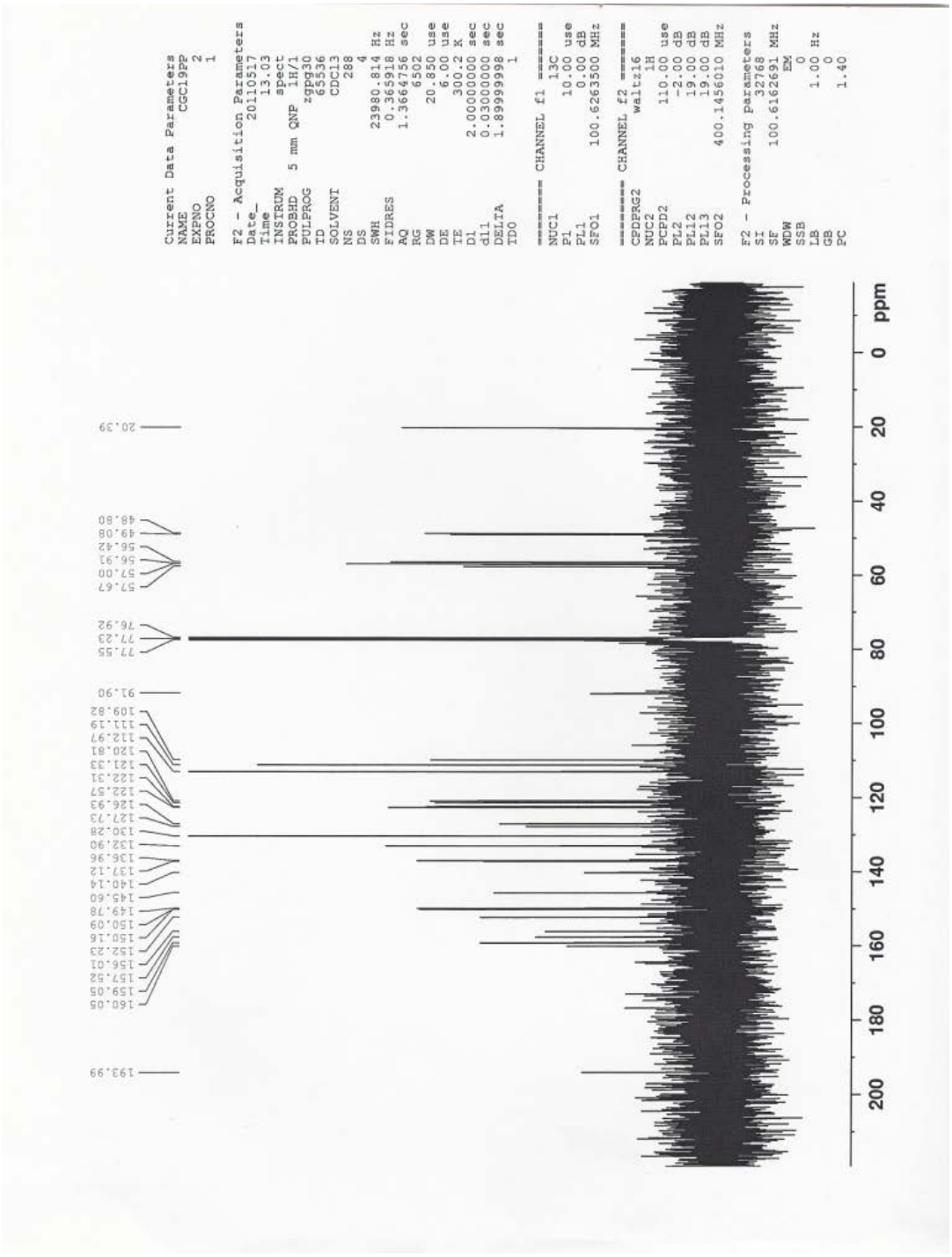


Figure S45 ^{13}C NMR of compound MonoUnc, **12**.

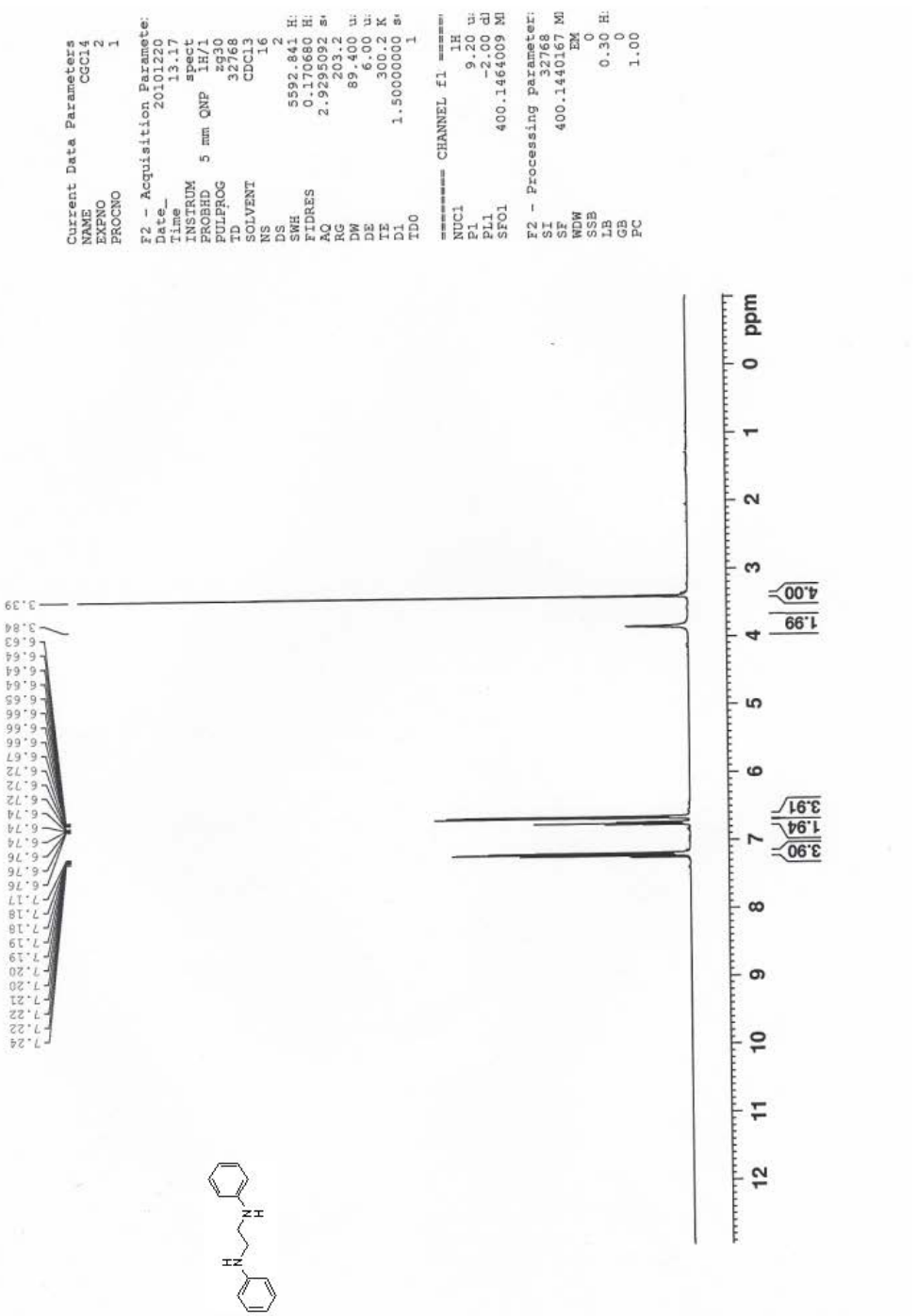


Figure S46 ^{1}H of compound **13**.

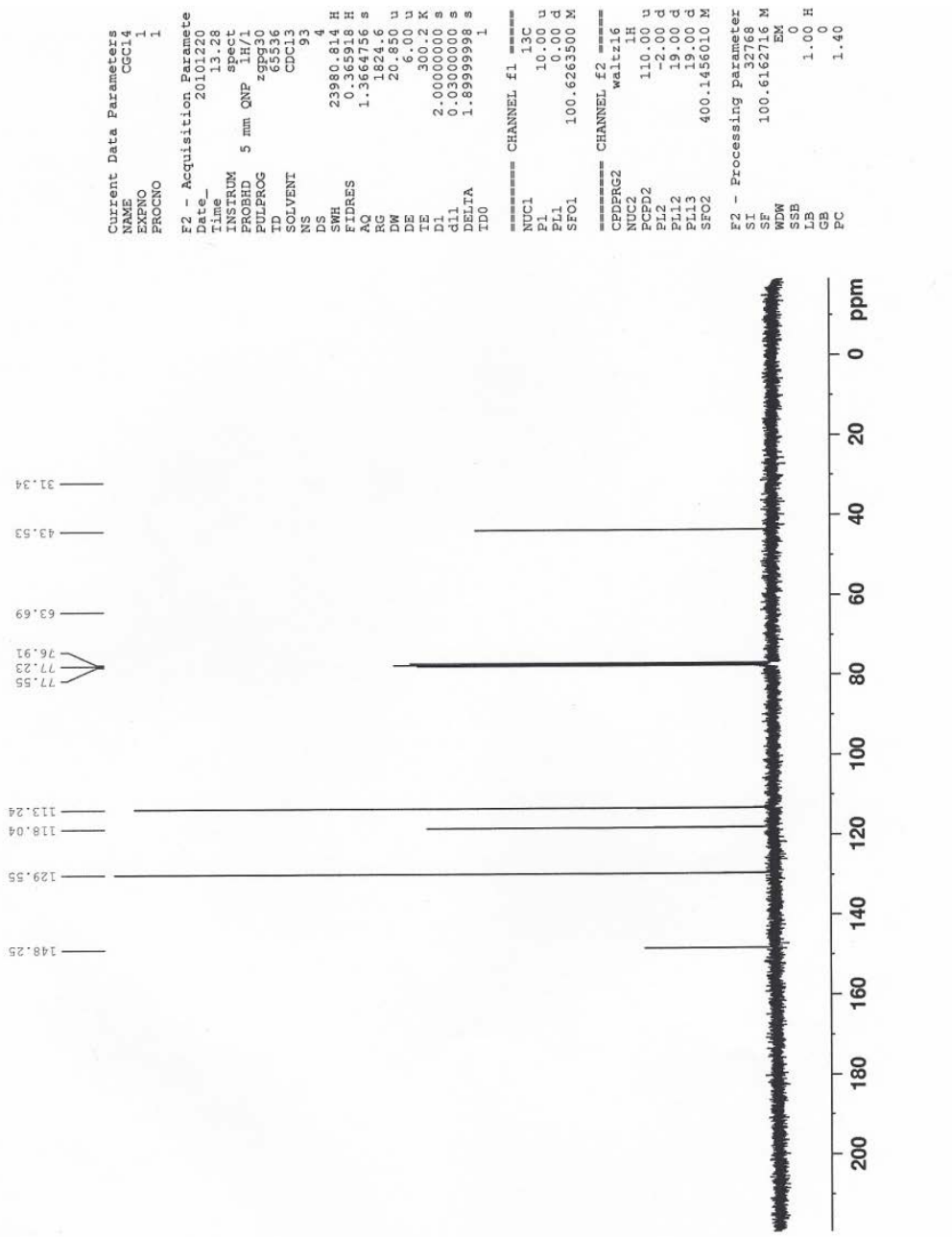


Figure S47 ^{13}C NMR of compound **13**.

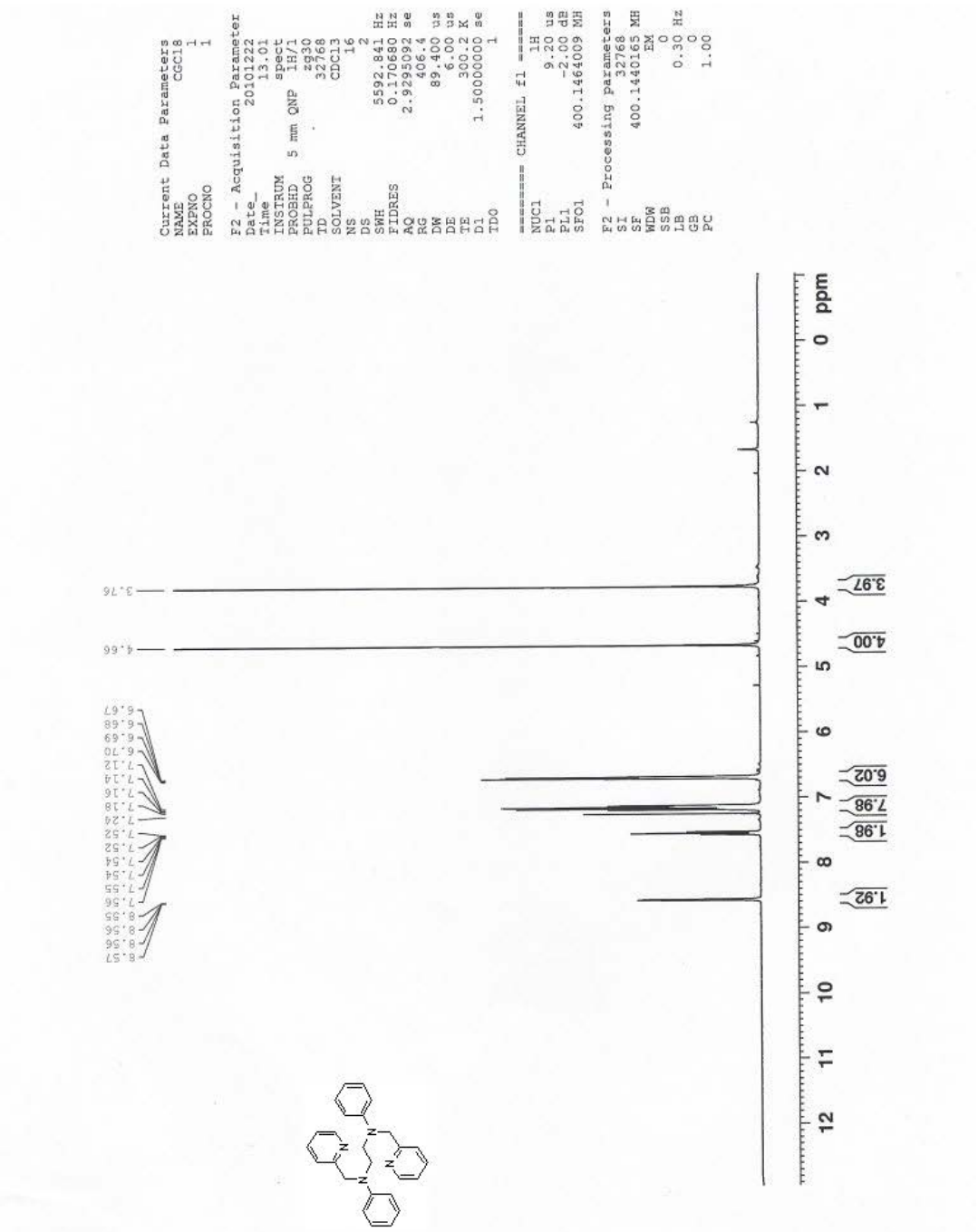


Figure S48 ^{1}H and of compound **14**.

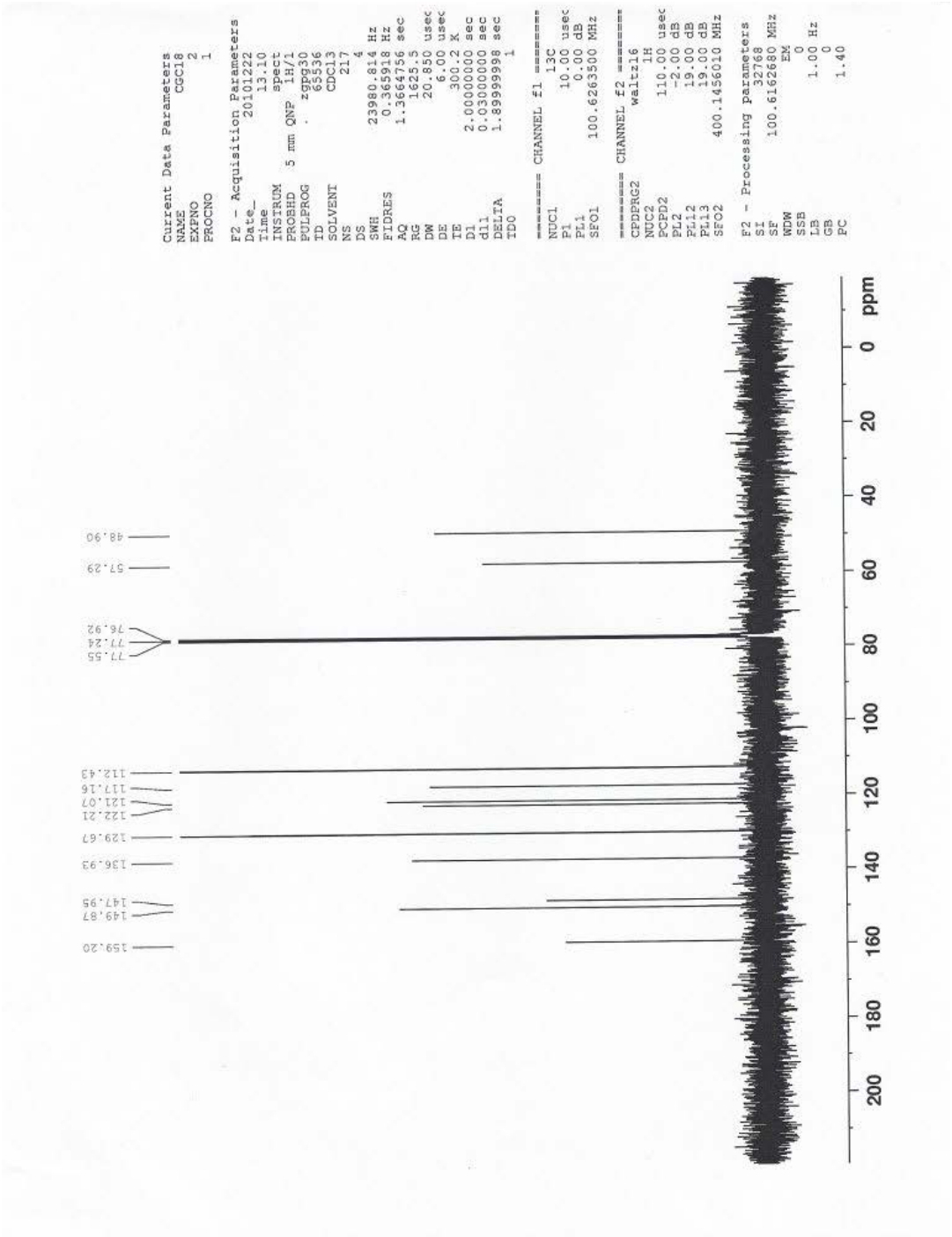


Figure S49 ^{13}C NMR of compound **14**.

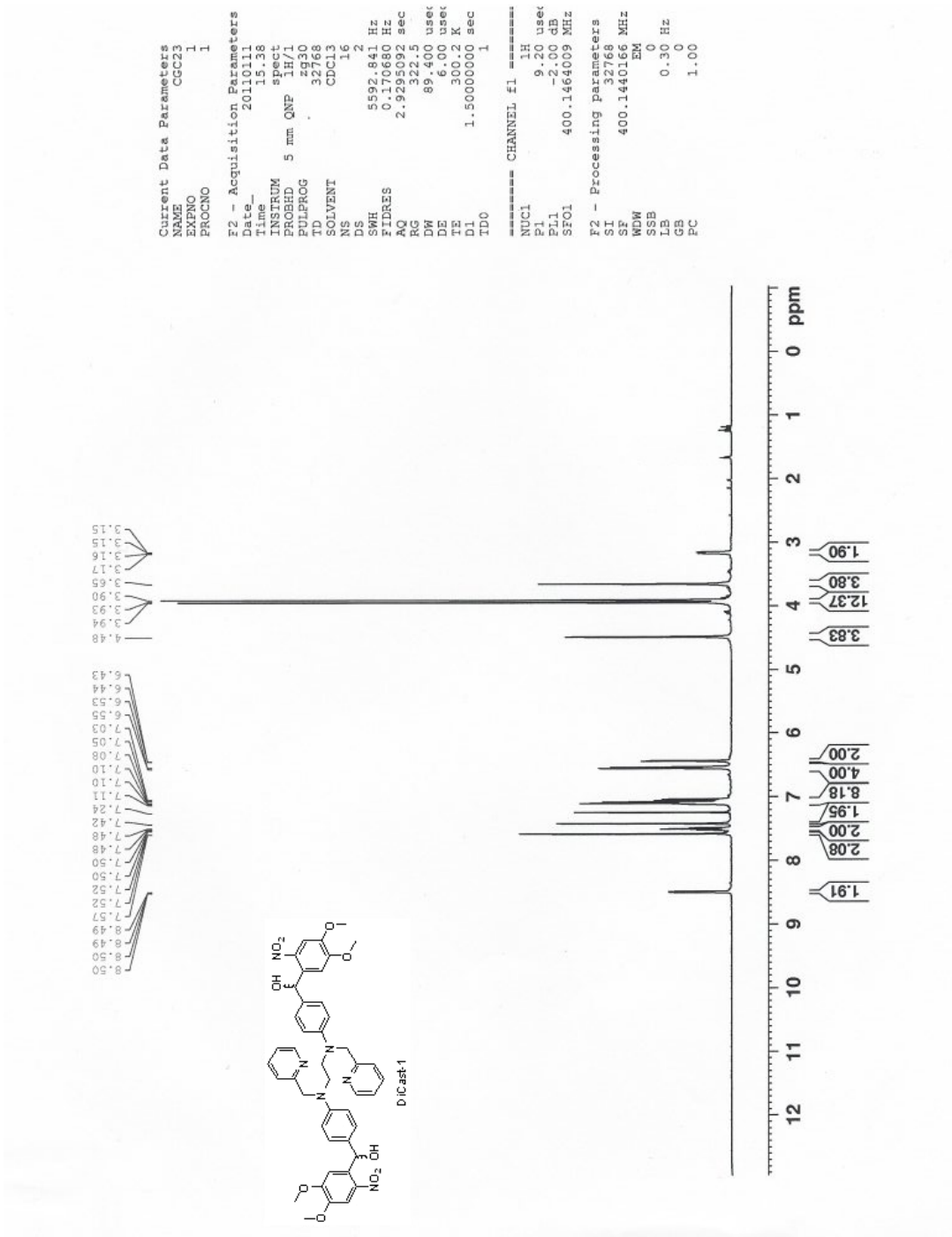


Figure S50 ^{1}H of compound DiCast-1, **4**.

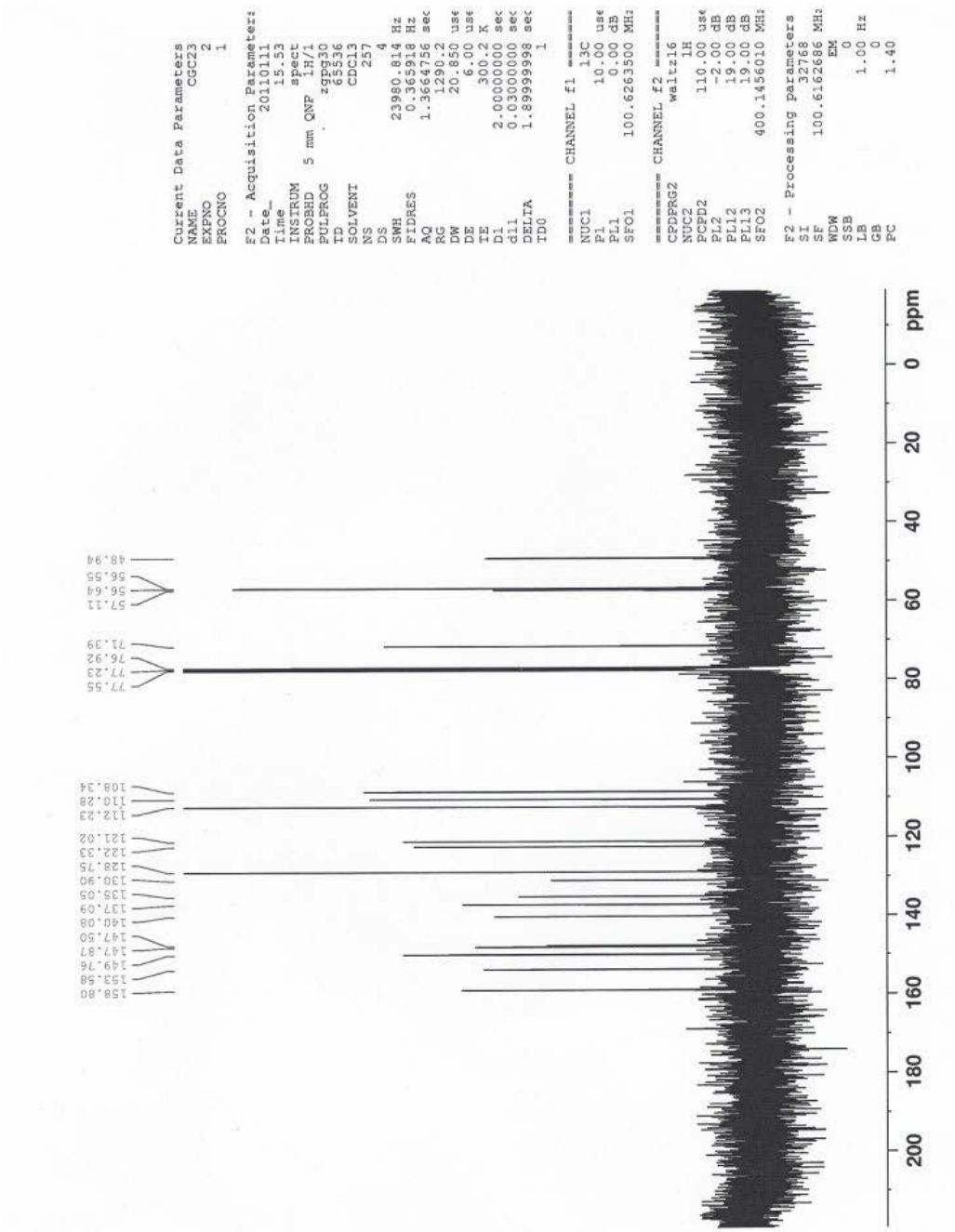


Figure S51 ^{13}C NMR of compound DiCast-1, **4**.

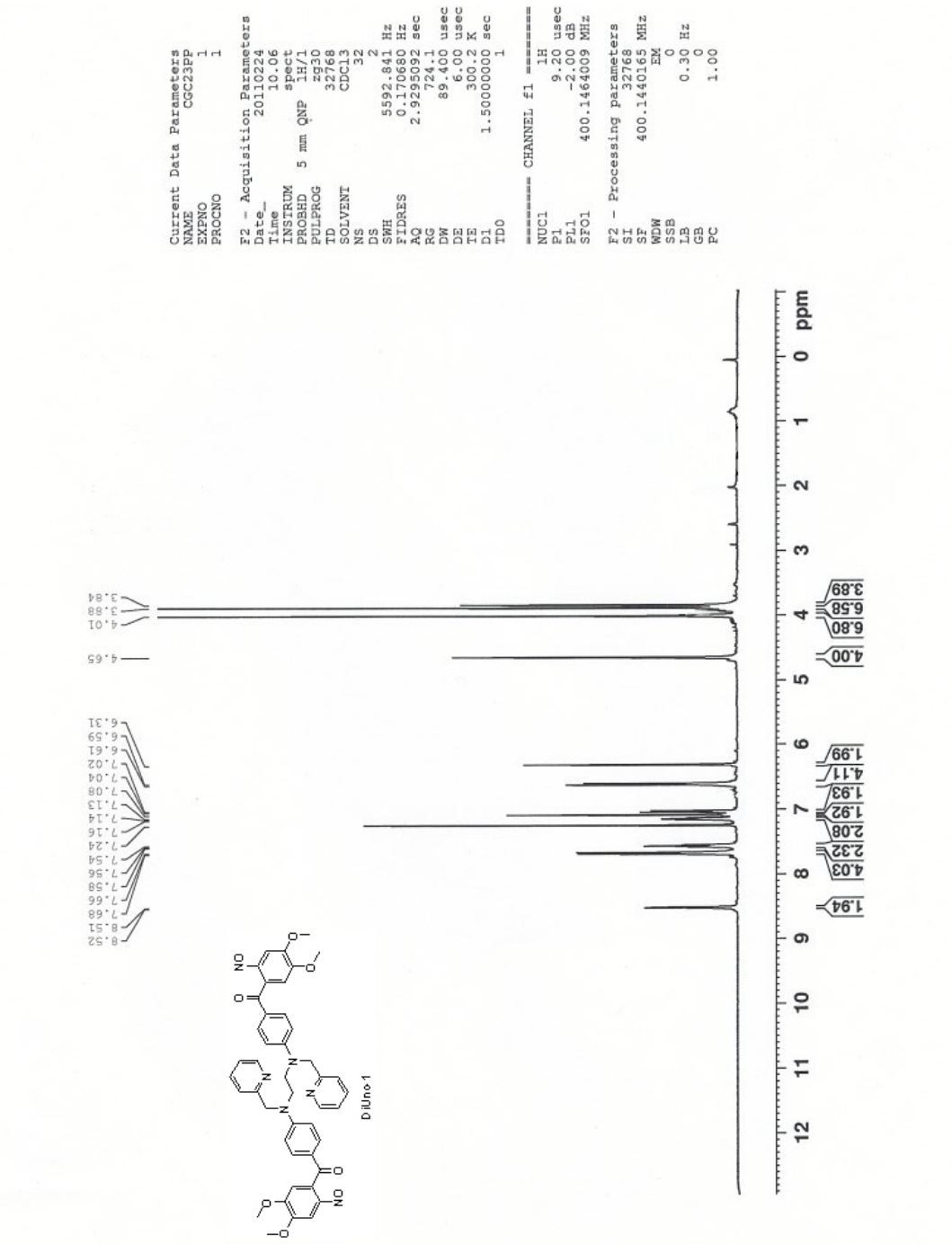


Figure S52 ^{1}H of compound DiUnc-1, **15**.

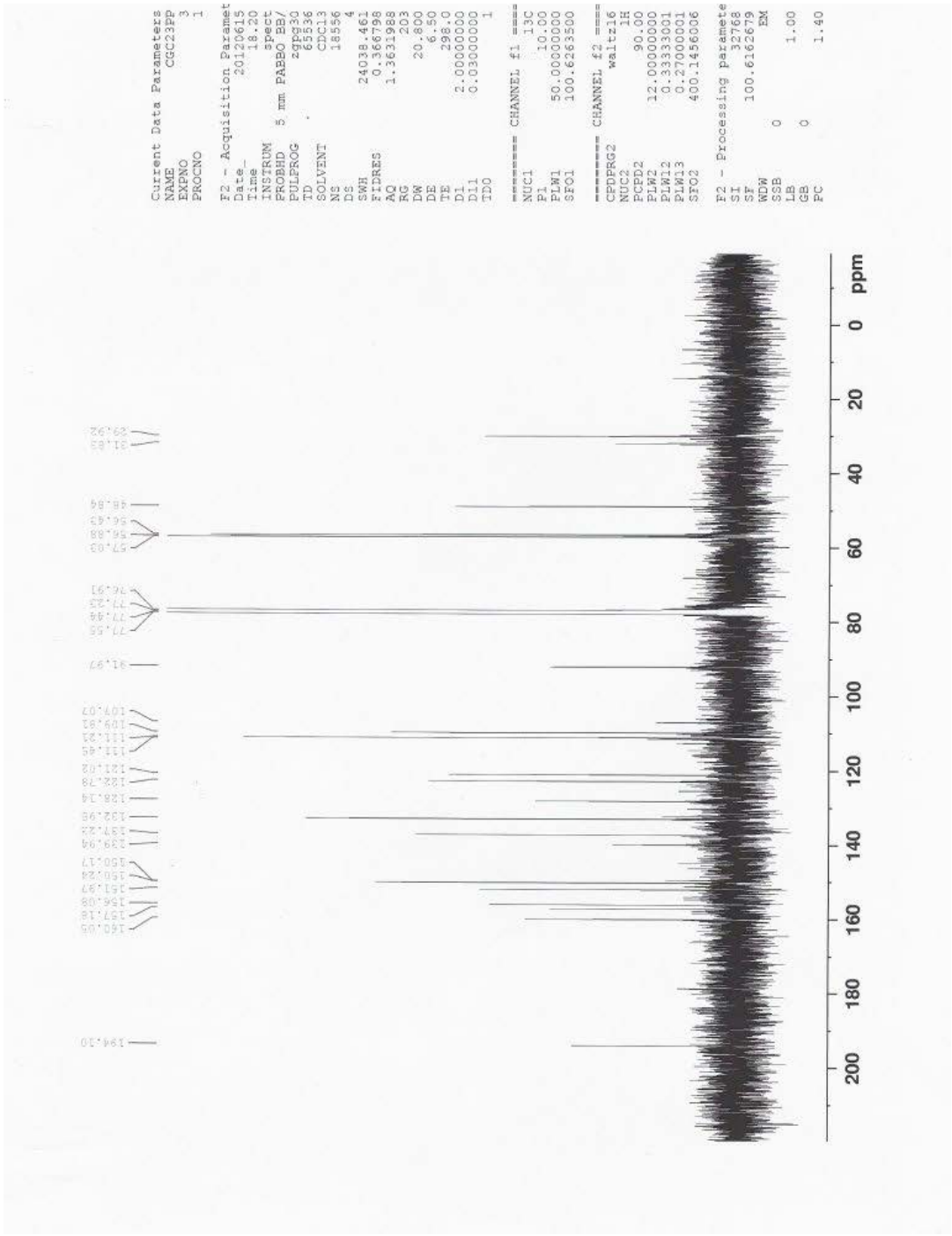


Figure S53 ^{13}C NMR of compound DiUnc-1, **15**.

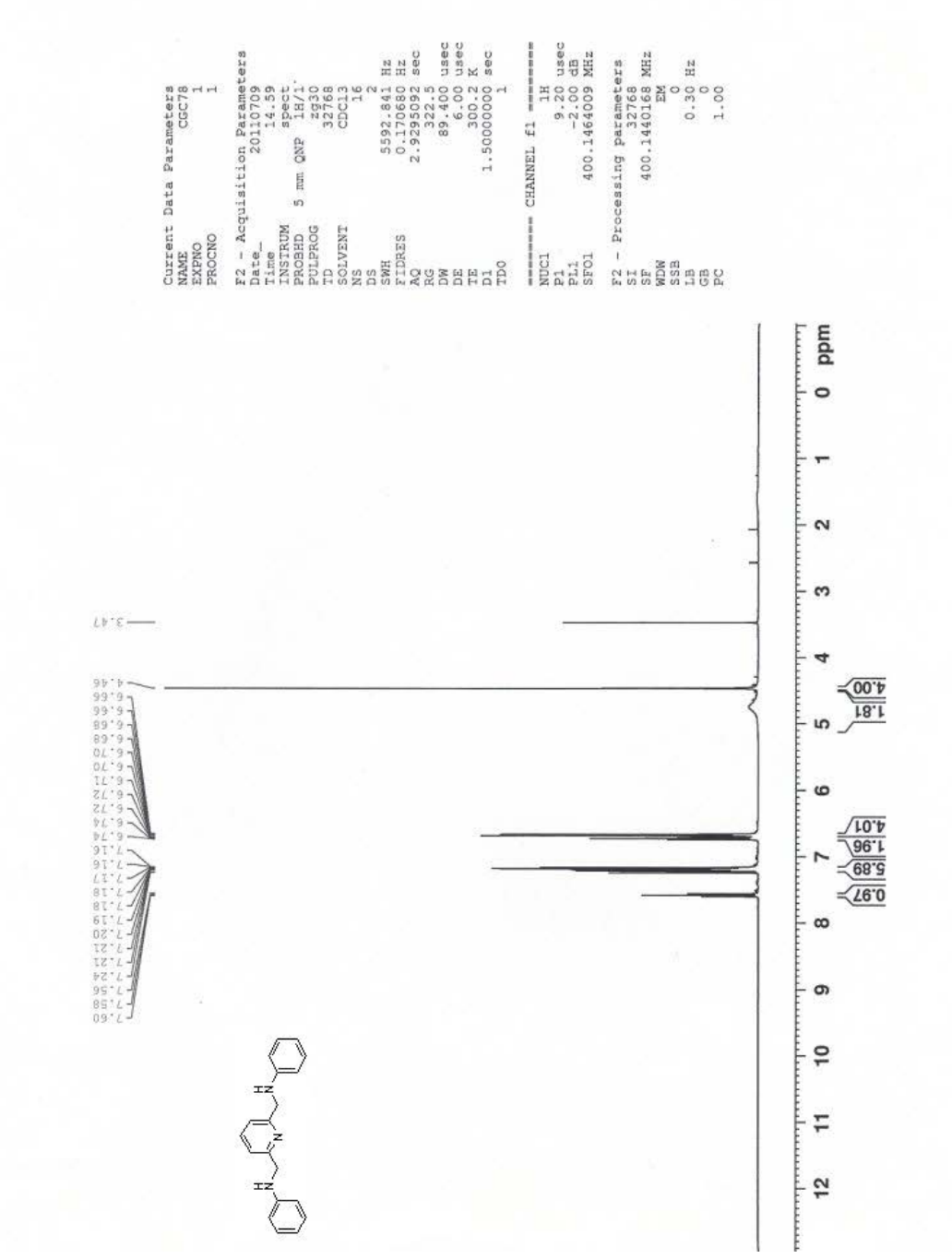


Figure S54 ^{1}H of compound **17**.

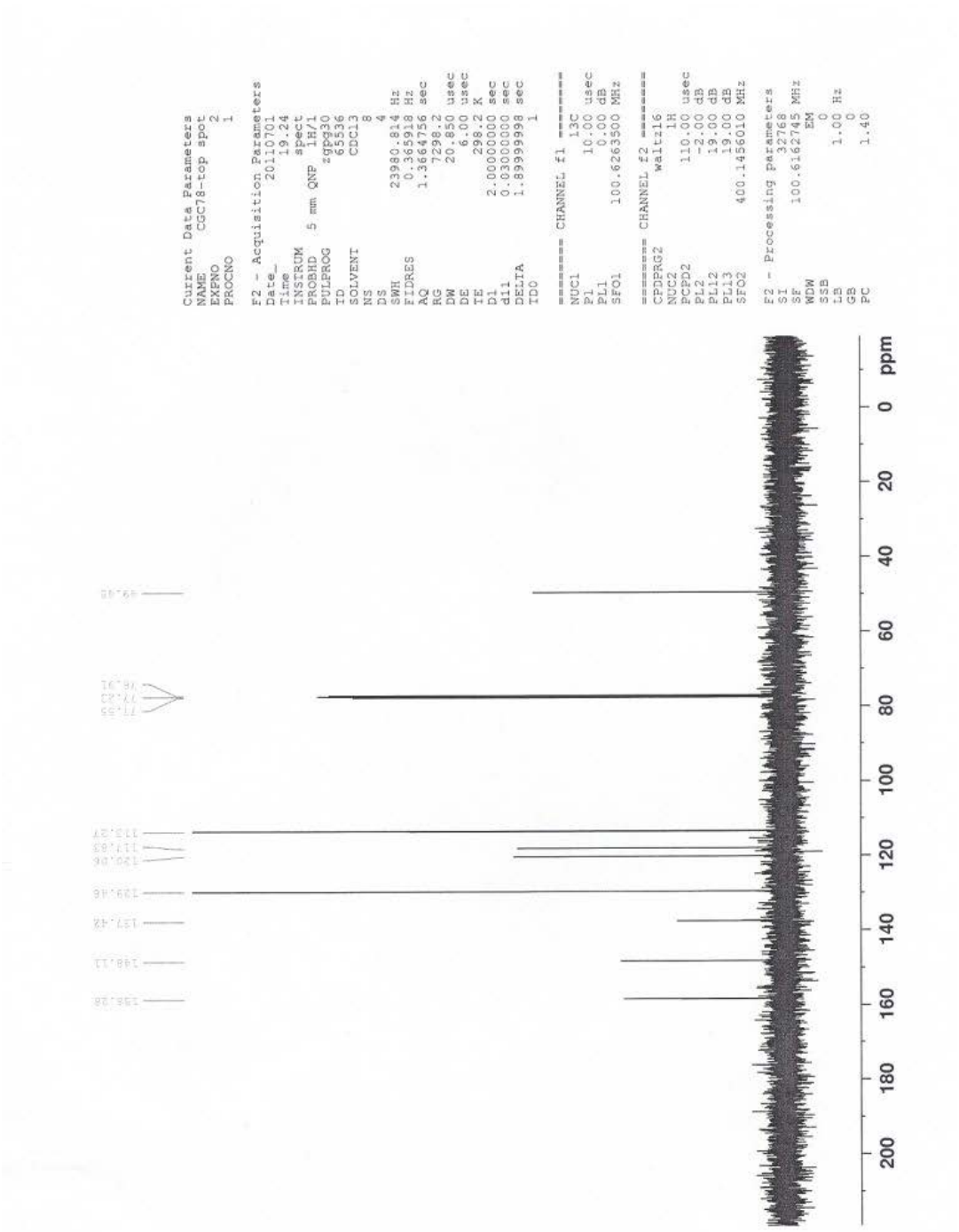


Figure S55 ^{13}C NMR of compound **17**.

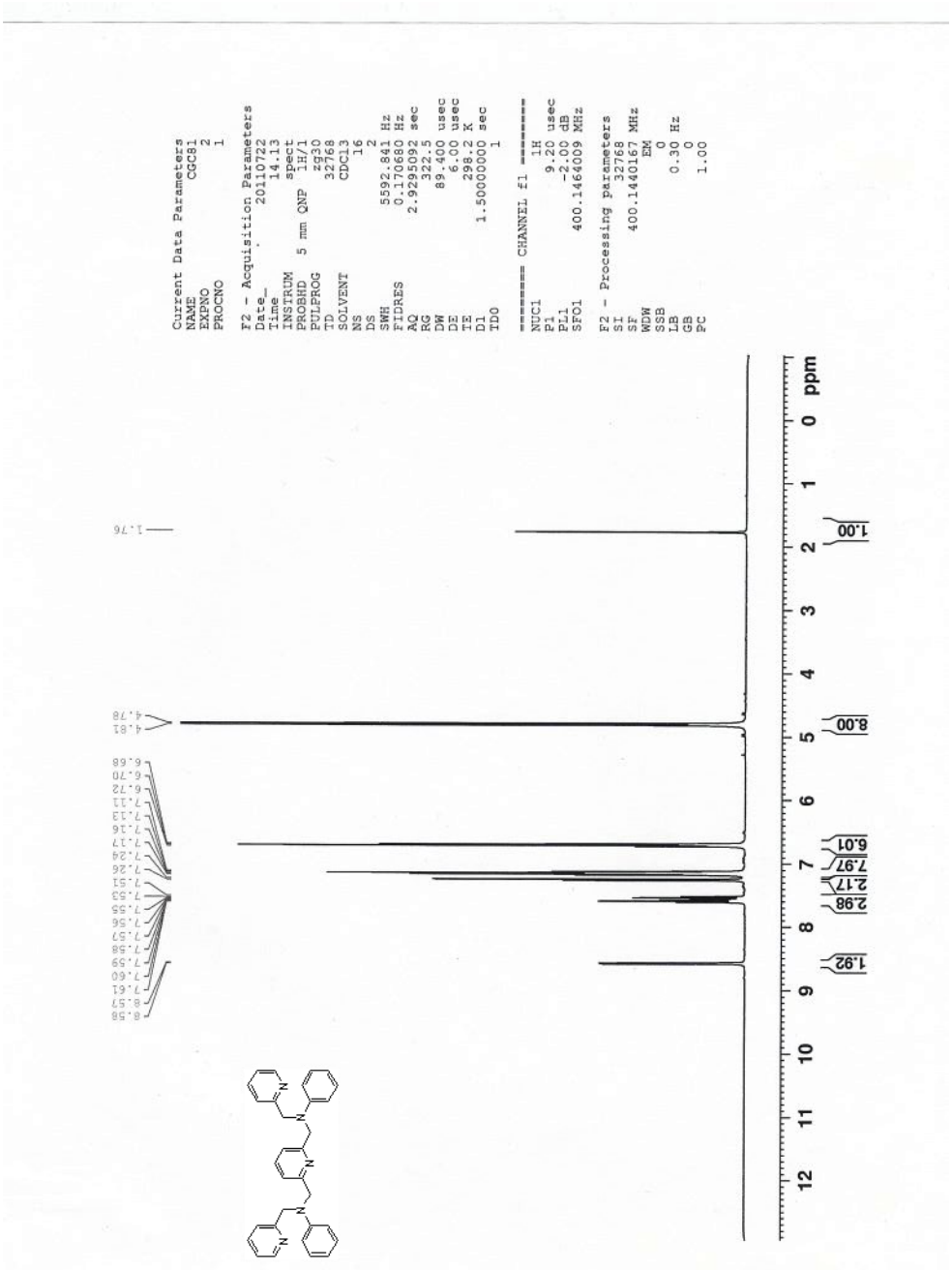


Figure S56 ^{1}H of compound **18**.

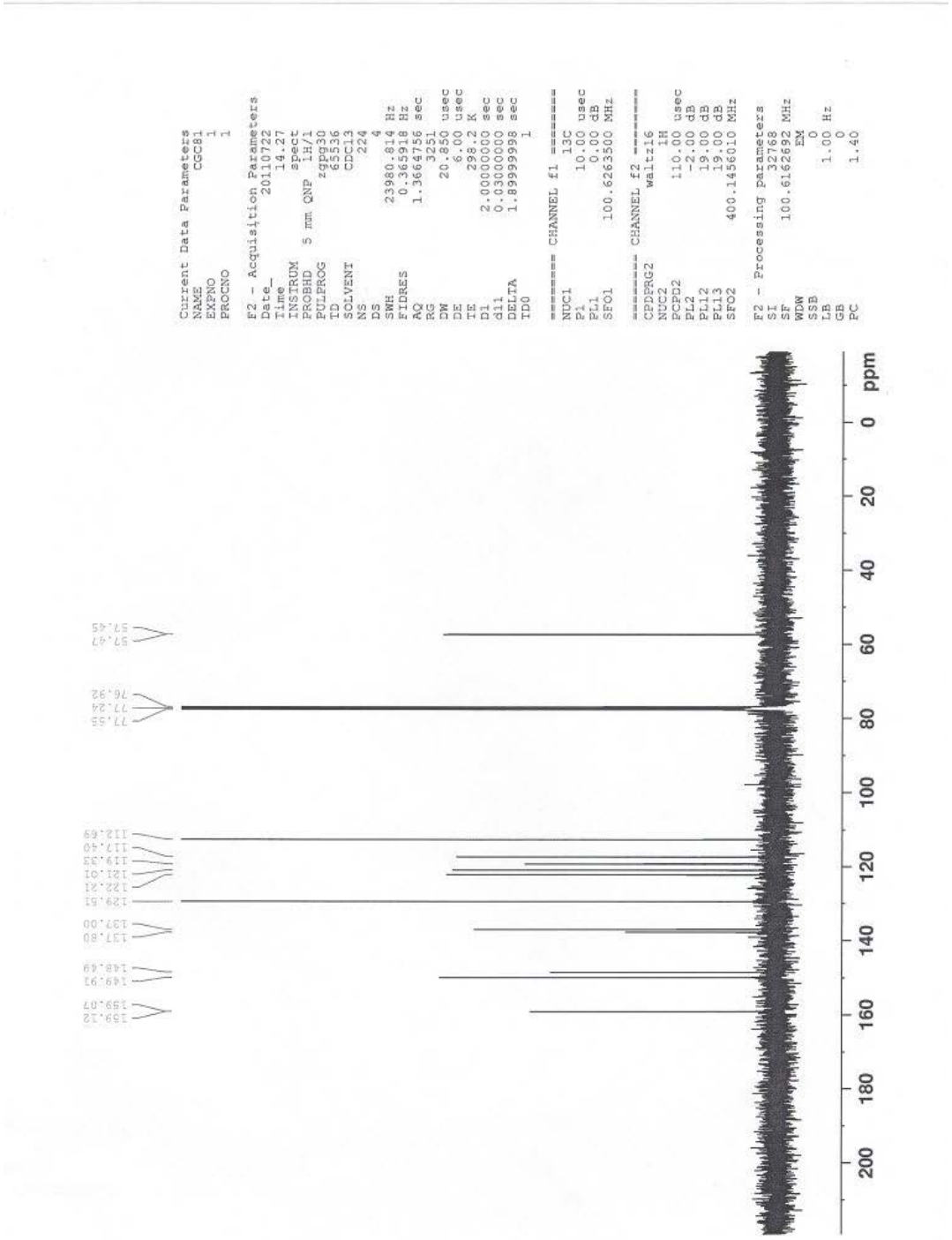


Figure S57 ^{13}C NMR of compound **18**.

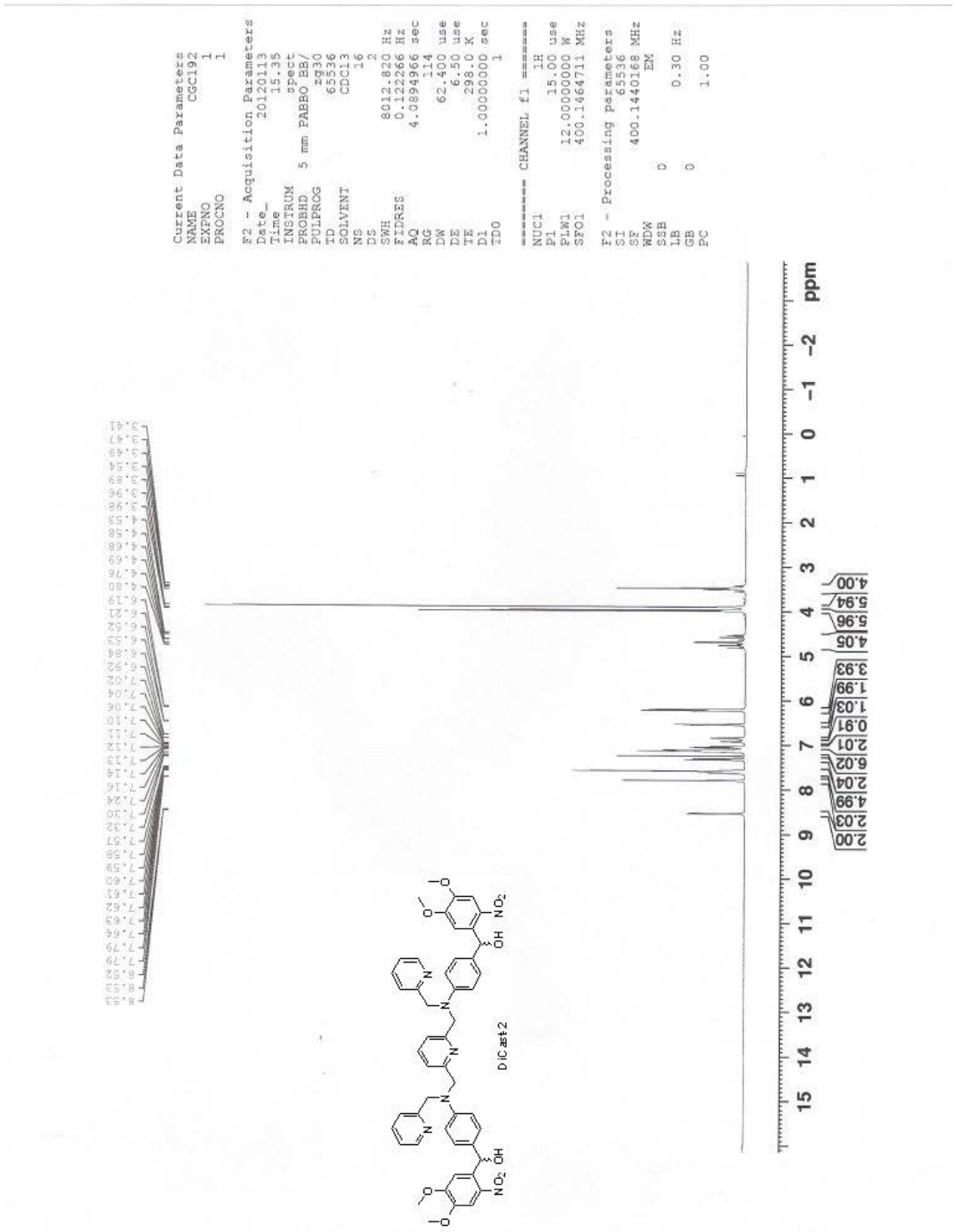


Figure S58 ^{1}H of compound DiCast-2, **5**.

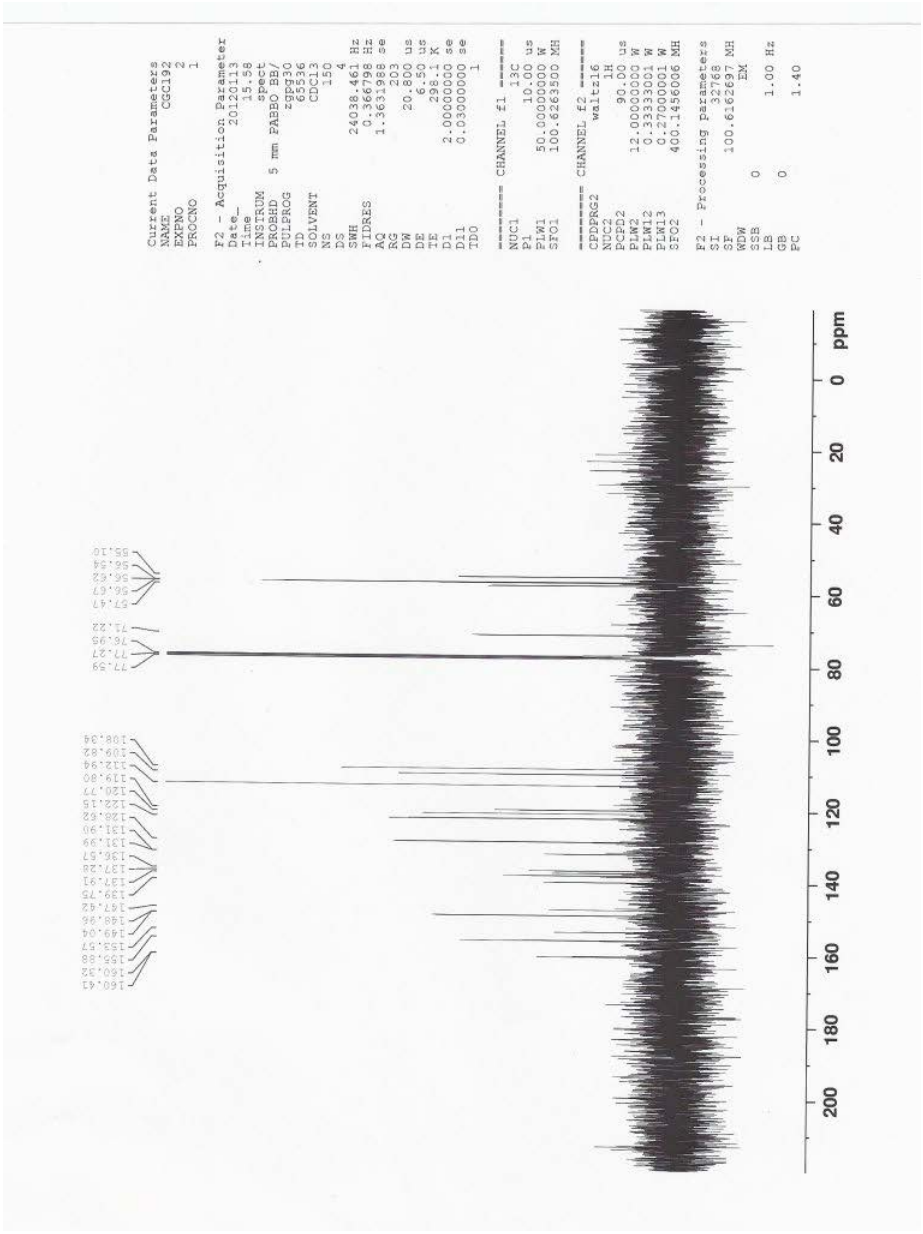


Figure S59 ^{13}C NMR of compound DiCast-2, **5**.

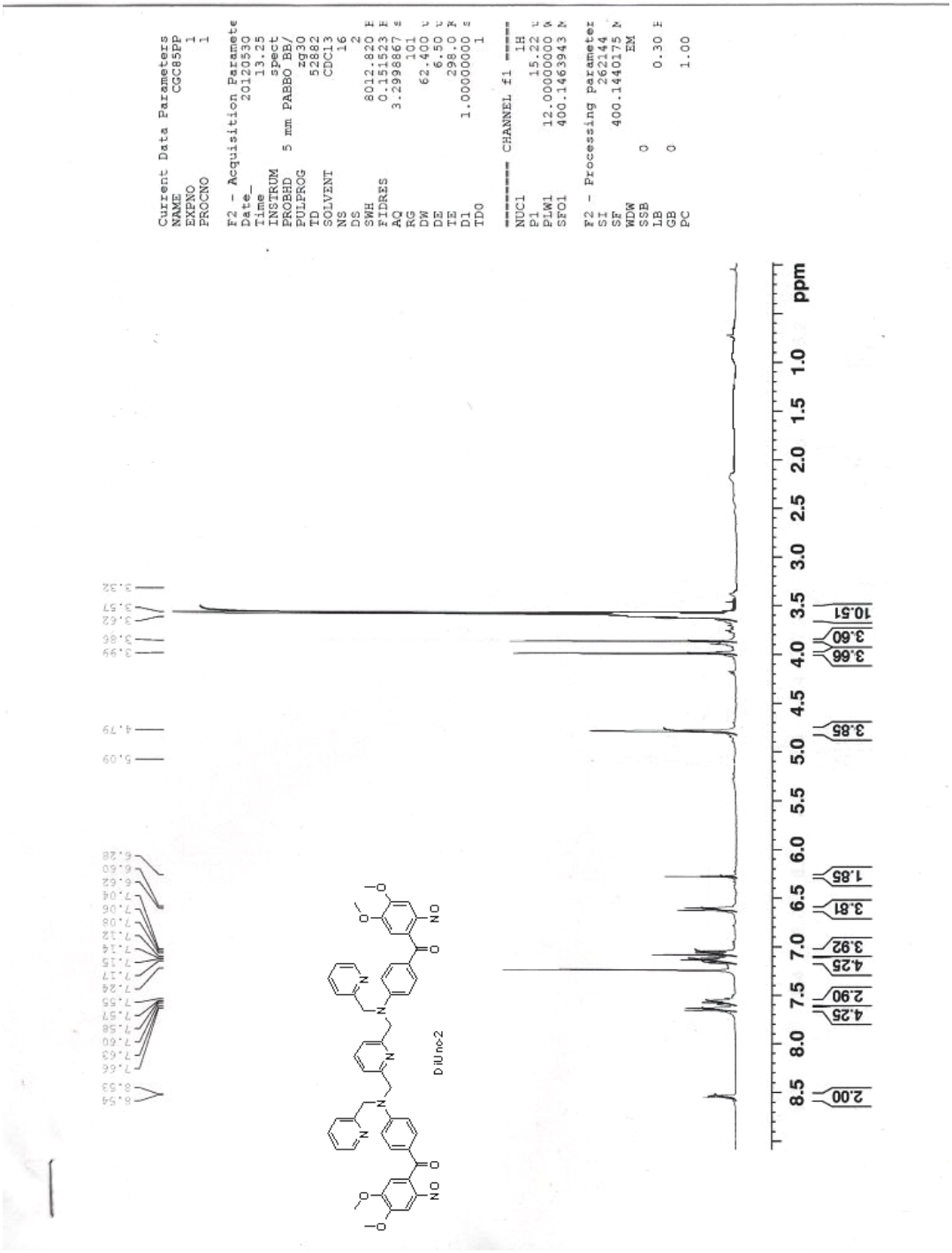


Figure S60 ^{1}H of compound DiUnc-2, **19**.

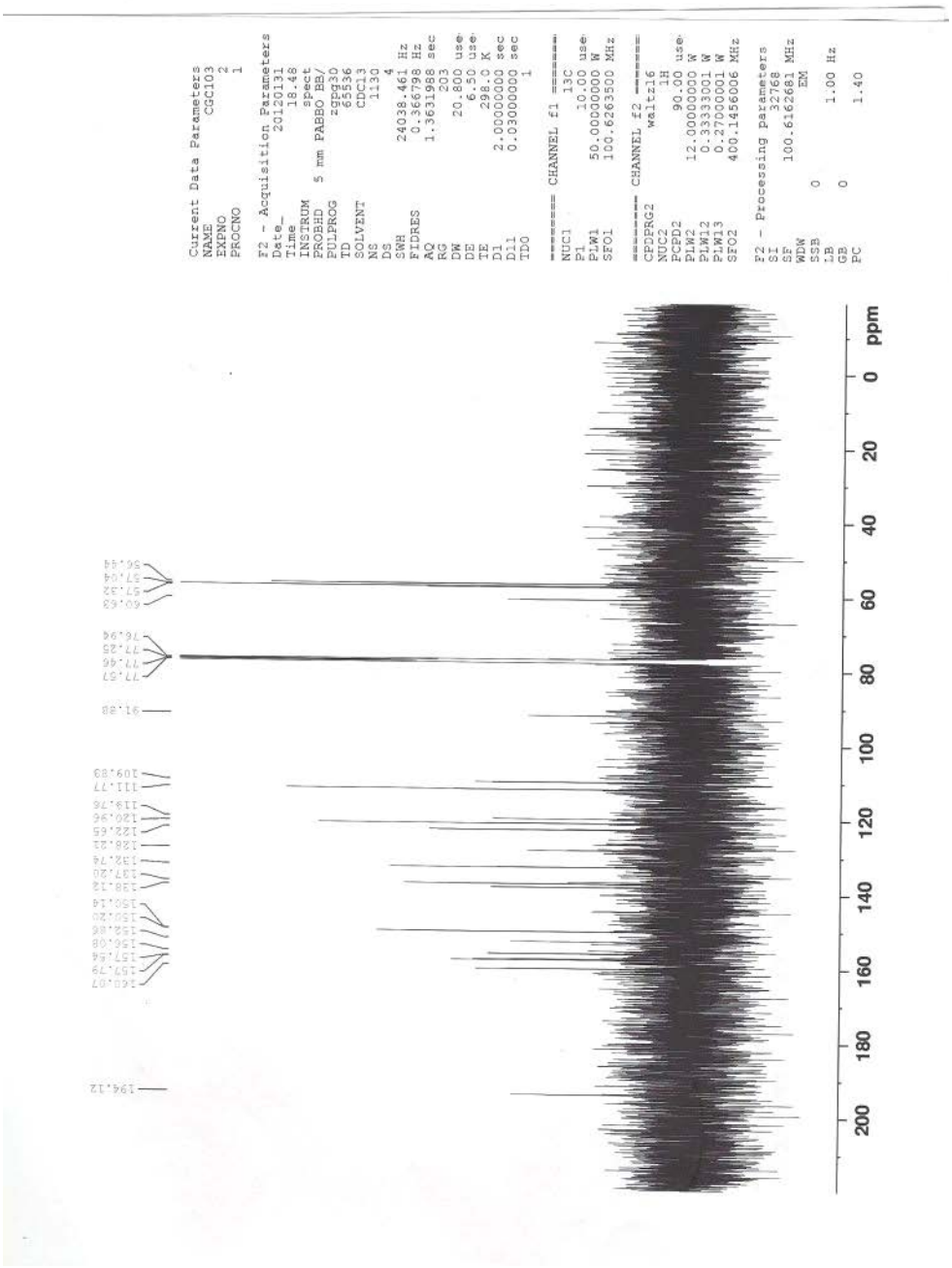


Figure S61 ^{13}C NMR of compound DiUnc-2, **19**.

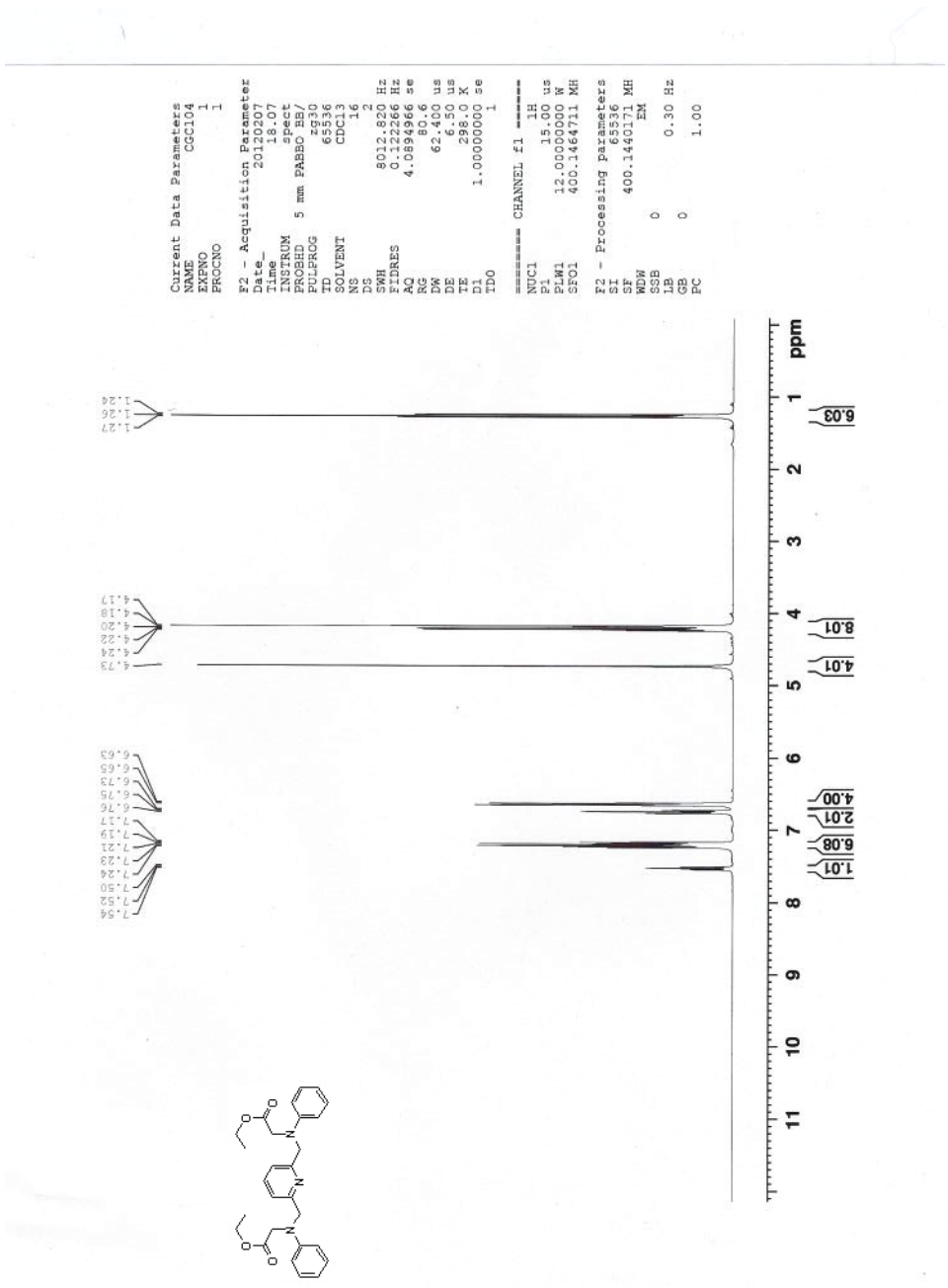


Figure S62 ^{1}H of compound **20**.

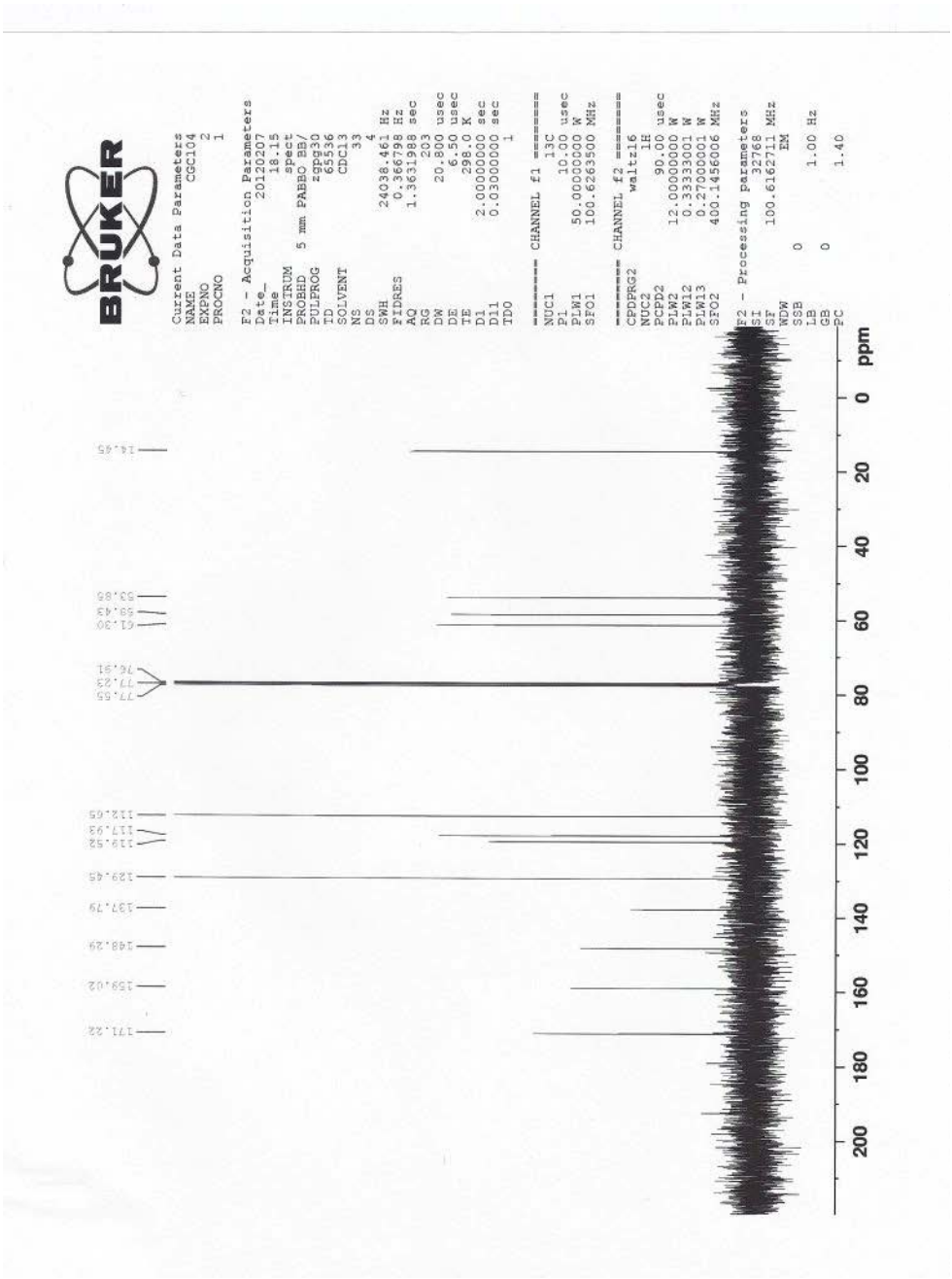


Figure S63 ^{13}C NMR of compound **20**.

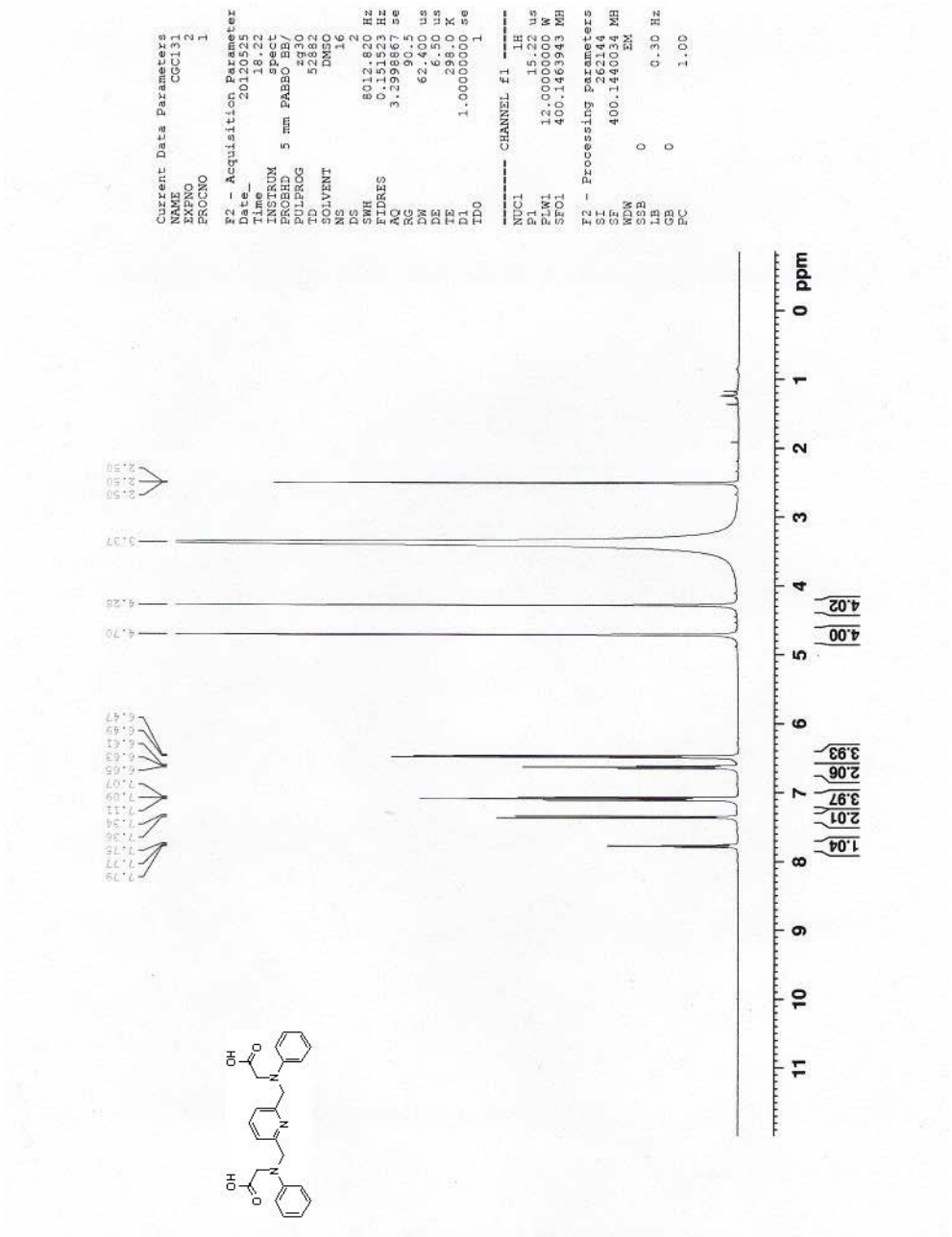


Figure S64 ^{1}H of compound **23**.

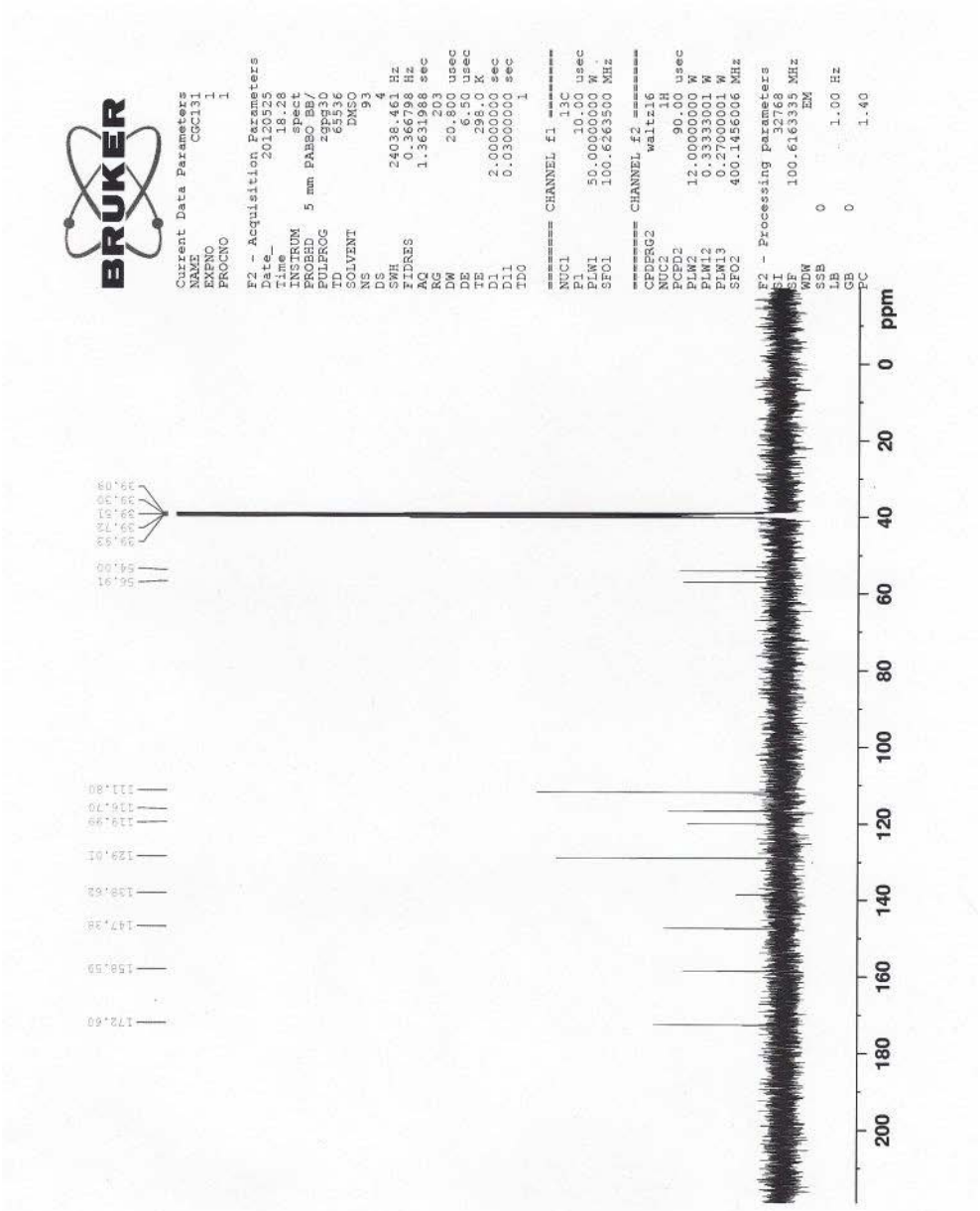


Figure S65 ^{13}C NMR of compound **23**.

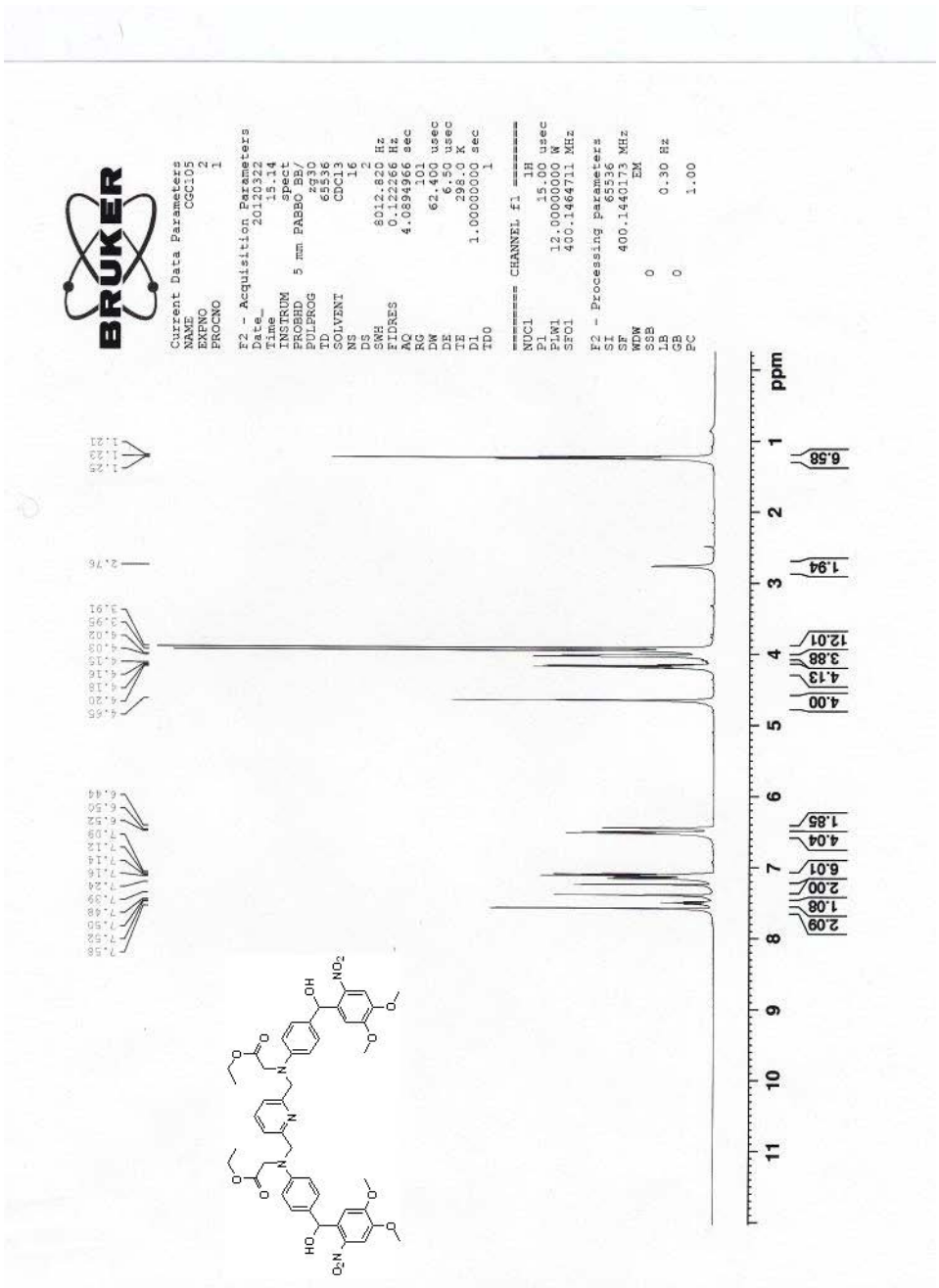


Figure S66 ^{1}H of compound **21**.

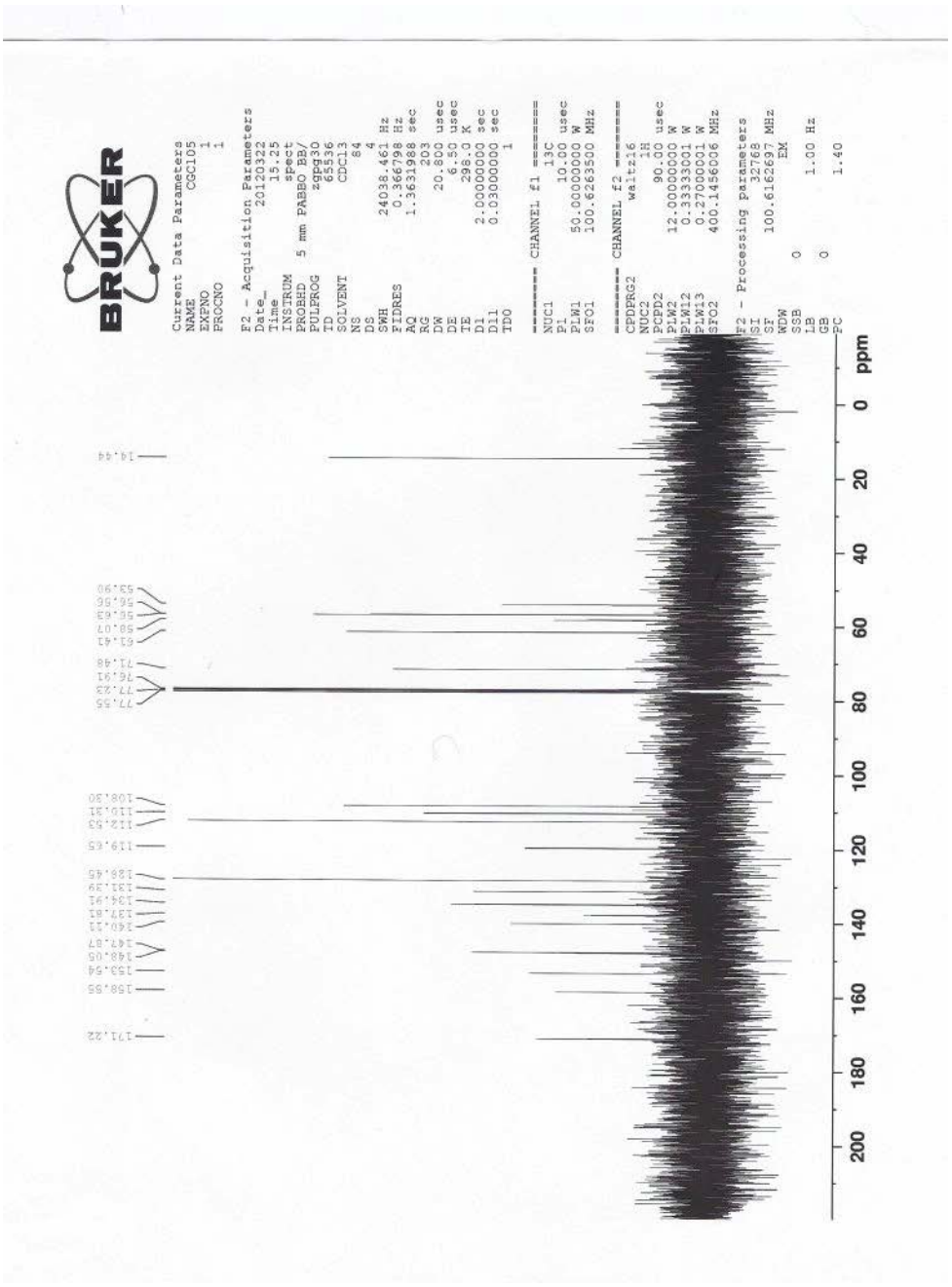


Figure S67 ^{13}C NMR of compound **21**.

Figure S68 ^{1}H of compound DiCast-3, **6**.

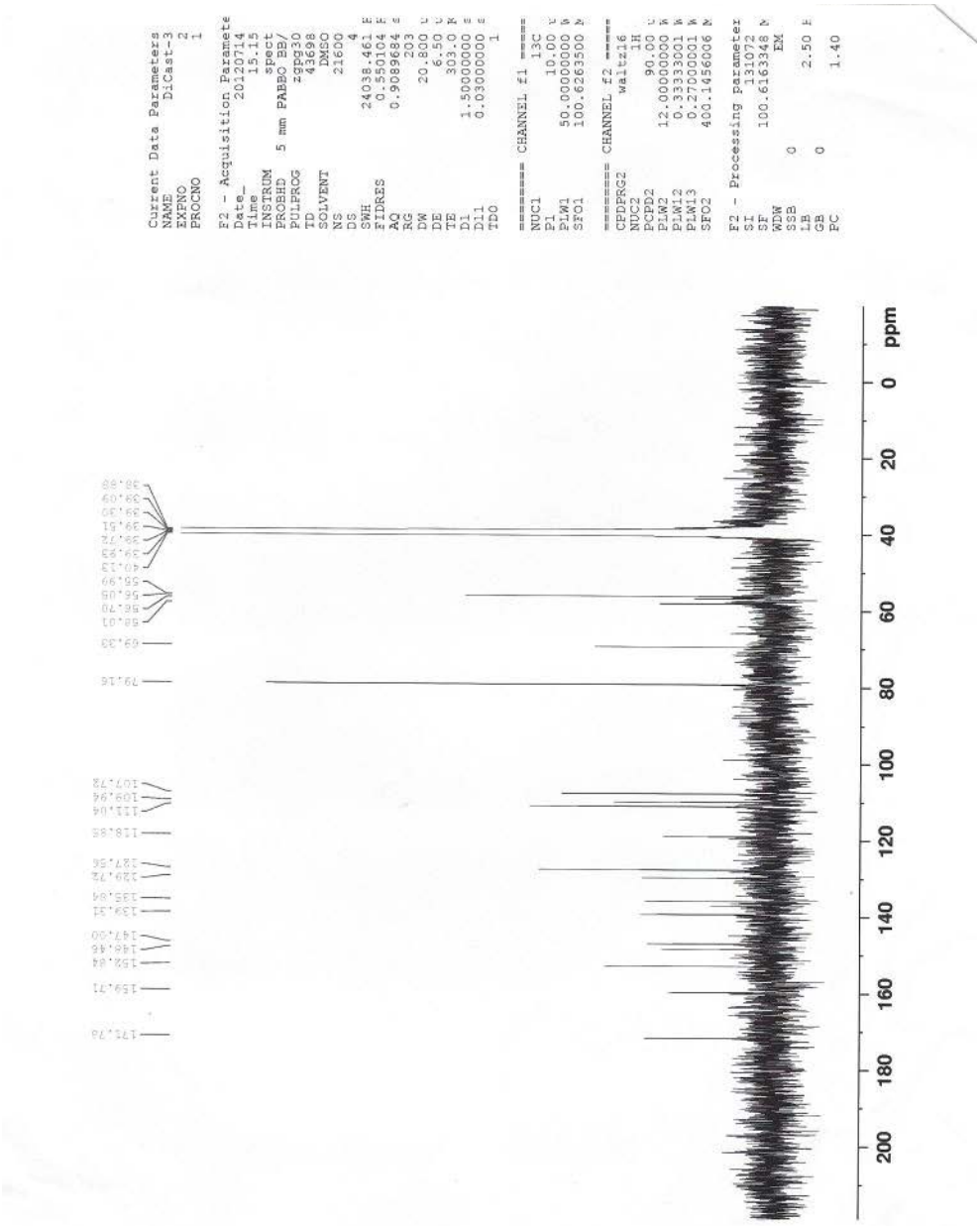


Figure S69 ^{13}C NMR of compound DiCast-3, **6**.

Table S1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for [Zn(**18**)][Zn(NO_3)$_4$]

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.72895 (6)	0.15577 (4)	0.19264 (2)	0.0464 (2)
N1	0.8008 (4)	0.0130 (3)	0.20808 (19)	0.0522 (10)
N2	0.6693 (5)	0.2935 (3)	0.2168 (2)	0.0567 (11)
C1	0.9324 (7)	0.3391 (6)	0.0694 (4)	0.090 (3)
H3	0.9701	0.3787	0.0451	0.108*
N3	0.8233 (4)	0.2259 (3)	0.13958 (19)	0.0504 (10)
C2	0.7319 (5)	0.2152 (4)	0.3154 (2)	0.0517 (12)
N4	0.7649 (4)	0.1489 (3)	0.28304 (18)	0.0462 (10)
C3	0.8855 (5)	−0.0125 (3)	0.1678 (2)	0.0520 (12)
C4	0.8165 (5)	0.0742 (4)	0.3110 (2)	0.0523 (12)
C5	0.6643 (7)	0.2940 (4)	0.2820 (3)	0.0716 (18)
H31A	0.5716	0.2947	0.2860	0.086*
H31B	0.7064	0.3488	0.3008	0.086*
N5	0.5839 (4)	0.0935 (3)	0.13444 (19)	0.0520 (10)
C6	0.5453 (5)	0.3175 (4)	0.1776 (2)	0.0544 (13)
C7	0.4039 (7)	−0.0051 (7)	0.0560 (4)	0.094 (3)
H15	0.3409	−0.0394	0.0291	0.112*
C8	0.3139 (7)	0.2922 (6)	0.1483 (4)	0.093 (2)
H11	0.2370	0.2632	0.1545	0.111*
C9	0.8631 (7)	0.0058 (4)	0.2731 (3)	0.0690 (17)
H25A	0.9593	0.0114	0.2778	0.083*
H25B	0.8446	−0.0536	0.2878	0.083*
C10	0.5023 (6)	0.1326 (5)	0.0880 (3)	0.0655 (16)
H13	0.5080	0.1947	0.0825	0.079*
C11	0.7499 (6)	0.2099 (5)	0.3771 (3)	0.0652 (16)
H29	0.7294	0.2590	0.3998	0.078*
C12	0.9281 (7)	0.2500 (6)	0.0566 (3)	0.087 (2)
H4	0.9635	0.2270	0.0244	0.104*
C13	0.4161 (7)	0.3915 (5)	0.0921 (3)	0.081 (2)
H9	0.4102	0.4311	0.0590	0.097*
C14	0.4323 (7)	0.2752 (5)	0.1863 (3)	0.0764 (18)
H12	0.4371	0.2344	0.2187	0.092*
C15	0.5778 (5)	0.0059 (4)	0.1423 (3)	0.0550 (13)
C16	1.0528 (7)	−0.0509 (6)	0.0907 (4)	0.093 (2)
H22	1.1098	−0.0640	0.0642	0.112*
C17	0.4886 (7)	−0.0451 (5)	0.1028 (4)	0.081 (2)
H16	0.4861	−0.1074	0.1081	0.097*
C18	0.8309 (6)	0.0653 (5)	0.3723 (3)	0.0692 (16)
H27	0.8640	0.0116	0.3915	0.083*
C19	0.8698 (6)	0.1950 (5)	0.0927 (3)	0.0666 (16)
H5	0.8628	0.1335	0.0838	0.080*
C20	0.5376 (6)	0.3764 (4)	0.1303 (3)	0.0649 (15)

H8	0.6138	0.4062	0.1239	0.078*
C21	0.9321 (7)	−0.0898 (5)	0.0825 (3)	0.087 (2)
H21	0.9056	−0.1303	0.0500	0.104*
C22	0.8473 (6)	−0.0711 (4)	0.1208 (3)	0.0658 (16)
H20	0.7636	−0.0985	0.1146	0.079*
C23	0.7845 (6)	0.3422 (4)	0.2069 (3)	0.0661 (16)
H6A	0.8569	0.3342	0.2426	0.079*
H6B	0.7631	0.4061	0.2034	0.079*
C24	1.0904 (6)	0.0066 (5)	0.1371 (4)	0.085 (2)
H23	1.1743	0.0337	0.1431	0.102*
C25	0.8838 (6)	0.3708 (5)	0.1159 (3)	0.077 (2)
H2	0.8861	0.4325	0.1241	0.092*
C26	0.4104 (7)	0.0843 (7)	0.0483 (3)	0.089 (2)
H14	0.3523	0.1128	0.0159	0.107*
C27	0.6716 (6)	−0.0317 (4)	0.1962 (3)	0.0617 (15)
H18A	0.6326	−0.0259	0.2324	0.074*
H18B	0.6842	−0.0955	0.1894	0.074*
C28	0.8310 (5)	0.3135 (4)	0.1512 (3)	0.0579 (14)
C29	1.0078 (6)	0.0262 (4)	0.1758 (3)	0.0696 (16)
H24	1.0354	0.0667	0.2081	0.084*
C30	0.7976 (7)	0.1332 (5)	0.4058 (3)	0.0773 (19)
H28	0.8075	0.1275	0.4484	0.093*
N6	0.1299 (5)	0.2552 (4)	0.7825 (3)	0.0691 (13)
N7	0.3924 (5)	0.4363 (3)	0.7797 (2)	0.0653 (13)
O1	0.4089 (6)	0.4819 (5)	0.7384 (3)	0.117 (2)
O2	0.2911 (5)	0.4431 (3)	0.7991 (3)	0.1014 (18)
O3	0.0638 (5)	0.3141 (4)	0.7976 (3)	0.1101 (18)
O4	0.2481 (4)	0.2476 (3)	0.8102 (2)	0.0749 (12)
O5	0.0882 (5)	0.2036 (4)	0.7420 (3)	0.1131 (19)
O6	0.6038 (6)	0.2589 (6)	0.9903 (3)	0.148 (3)
N8	0.5191 (7)	0.2980 (7)	0.9562 (3)	0.096 (2)
O7	0.4414 (6)	0.2547 (4)	0.9165 (3)	0.116 (2)
O8	0.4711 (6)	0.3832 (4)	0.8055 (4)	0.138 (3)
C31	0.3059 (7)	0.3505 (6)	0.1014 (4)	0.091 (2)
H10	0.2237	0.3624	0.0754	0.109*
Zn2	0.31212 (7)	0.34496 (4)	0.86933 (3)	0.0639 (2)
O9	0.2128 (6)	0.4287 (4)	0.9095 (3)	0.1099 (19)
O10	0.1002 (6)	0.4376 (5)	0.9776 (2)	0.115 (2)
N9	0.1589 (6)	0.3901 (5)	0.9465 (3)	0.0889 (18)
O11	0.1689 (7)	0.3103 (5)	0.9507 (3)	0.120 (2)
O12	0.4999 (8)	0.3789 (6)	0.9527 (4)	0.139 (3)

Table S2: Atomic displacement parameters (Å^2) for [Zn(**18**)][Zn(NO_3)$_4$]

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0563 (4)	0.0426 (3)	0.0413 (3)	0.0025 (3)	0.0124 (3)	−0.0012 (2)
N1	0.054 (3)	0.049 (2)	0.054 (3)	0.009 (2)	0.012 (2)	0.0016 (19)
N2	0.061 (3)	0.051 (3)	0.056 (3)	0.012 (2)	0.008 (2)	−0.005 (2)
C1	0.061 (4)	0.123 (7)	0.079 (5)	−0.027 (4)	−0.003 (4)	0.047 (5)
N3	0.045 (2)	0.057 (3)	0.050 (2)	0.0039 (19)	0.010 (2)	0.008 (2)
C2	0.042 (3)	0.063 (3)	0.048 (3)	0.000 (2)	0.007 (2)	−0.012 (2)
N4	0.041 (2)	0.057 (3)	0.042 (2)	0.0015 (19)	0.0096 (18)	−0.0037 (19)
C3	0.049 (3)	0.049 (3)	0.061 (3)	0.005 (2)	0.017 (3)	0.000 (2)
C4	0.048 (3)	0.060 (3)	0.050 (3)	0.002 (2)	0.013 (2)	0.007 (2)
C5	0.088 (5)	0.073 (4)	0.053 (3)	0.030 (3)	0.012 (3)	−0.010 (3)
N5	0.051 (3)	0.059 (3)	0.048 (2)	0.002 (2)	0.015 (2)	−0.004 (2)
C6	0.053 (3)	0.056 (3)	0.052 (3)	0.013 (3)	0.008 (3)	−0.008 (2)
C7	0.056 (4)	0.148 (8)	0.083 (5)	−0.032 (5)	0.025 (4)	−0.053 (5)
C8	0.060 (4)	0.119 (6)	0.103 (6)	0.006 (4)	0.027 (4)	−0.011 (5)
C9	0.087 (4)	0.060 (3)	0.060 (4)	0.023 (3)	0.015 (3)	0.017 (3)
C10	0.064 (4)	0.083 (4)	0.051 (3)	0.005 (3)	0.017 (3)	−0.008 (3)
C11	0.057 (3)	0.086 (4)	0.051 (3)	0.001 (3)	0.009 (3)	−0.016 (3)
C12	0.061 (4)	0.140 (8)	0.059 (4)	0.001 (4)	0.013 (3)	0.024 (4)
C13	0.080 (5)	0.096 (5)	0.063 (4)	0.033 (4)	0.007 (3)	0.008 (4)
C14	0.075 (5)	0.088 (5)	0.072 (4)	0.014 (4)	0.029 (4)	−0.001 (3)
C15	0.052 (3)	0.058 (3)	0.065 (3)	−0.007 (3)	0.035 (3)	−0.013 (3)
C16	0.068 (5)	0.124 (7)	0.099 (6)	0.000 (4)	0.043 (4)	−0.022 (5)
C17	0.077 (5)	0.081 (5)	0.097 (5)	−0.030 (4)	0.048 (4)	−0.035 (4)
C18	0.067 (4)	0.082 (4)	0.054 (4)	0.001 (3)	0.004 (3)	0.013 (3)
C19	0.057 (4)	0.087 (4)	0.056 (3)	0.004 (3)	0.011 (3)	0.010 (3)
C20	0.065 (4)	0.063 (3)	0.065 (4)	0.014 (3)	0.010 (3)	0.002 (3)
C21	0.075 (5)	0.104 (5)	0.088 (5)	−0.005 (4)	0.033 (4)	−0.034 (4)
C22	0.059 (4)	0.069 (4)	0.079 (4)	−0.004 (3)	0.035 (3)	−0.015 (3)
C23	0.060 (4)	0.052 (3)	0.077 (4)	0.008 (3)	−0.006 (3)	−0.005 (3)
C24	0.048 (4)	0.098 (5)	0.109 (6)	−0.002 (3)	0.018 (4)	−0.003 (5)
C25	0.059 (4)	0.076 (4)	0.083 (5)	−0.022 (3)	−0.017 (4)	0.037 (4)
C26	0.068 (4)	0.133 (7)	0.061 (4)	−0.003 (5)	0.005 (3)	−0.028 (4)
C27	0.073 (4)	0.046 (3)	0.075 (4)	−0.001 (3)	0.038 (3)	0.003 (3)
C28	0.040 (3)	0.057 (3)	0.068 (4)	−0.003 (2)	−0.011 (3)	0.014 (3)
C29	0.060 (4)	0.075 (4)	0.072 (4)	0.001 (3)	0.010 (3)	−0.009 (3)
C30	0.082 (5)	0.106 (5)	0.040 (3)	0.003 (4)	0.005 (3)	−0.002 (3)
N6	0.053 (3)	0.066 (3)	0.087 (4)	−0.001 (3)	0.010 (3)	0.009 (3)
N7	0.063 (3)	0.066 (3)	0.071 (3)	−0.003 (3)	0.023 (3)	−0.013 (3)
O1	0.115 (4)	0.162 (6)	0.087 (4)	−0.039 (4)	0.048 (3)	0.017 (4)
O2	0.097 (4)	0.059 (3)	0.176 (5)	0.013 (2)	0.092 (4)	0.011 (3)
O3	0.073 (3)	0.104 (4)	0.158 (5)	0.023 (3)	0.034 (3)	0.005 (4)
O4	0.051 (2)	0.058 (2)	0.106 (3)	0.0032 (19)	−0.004 (2)	−0.002 (2)

O5	0.084 (4)	0.130 (5)	0.114 (4)	−0.019 (3)	−0.005 (3)	−0.036 (4)
O6	0.089 (4)	0.268 (10)	0.081 (4)	0.010 (5)	0.007 (3)	0.053 (5)
N8	0.083 (5)	0.137 (7)	0.073 (4)	0.003 (5)	0.030 (4)	0.004 (5)
O7	0.108 (4)	0.096 (4)	0.128 (5)	0.013 (3)	−0.016 (4)	−0.006 (4)
O8	0.077 (4)	0.096 (4)	0.215 (7)	0.016 (3)	−0.028 (4)	−0.001 (5)
C31	0.054 (4)	0.132 (7)	0.086 (5)	0.023 (4)	0.011 (4)	−0.014 (5)
Zn2	0.0693 (5)	0.0544 (4)	0.0717 (5)	−0.0018 (3)	0.0231 (4)	−0.0002 (3)
O9	0.150 (5)	0.088 (4)	0.111 (4)	0.029 (3)	0.072 (4)	0.015 (3)
O10	0.104 (4)	0.165 (6)	0.086 (4)	0.040 (4)	0.041 (3)	0.011 (4)
N9	0.083 (4)	0.113 (6)	0.068 (4)	0.013 (4)	0.011 (3)	0.011 (4)
O11	0.158 (6)	0.095 (4)	0.100 (4)	−0.021 (4)	0.013 (4)	0.018 (3)
O12	0.160 (7)	0.119 (6)	0.154 (6)	−0.021 (5)	0.070 (5)	−0.026 (5)

Table S3: Geometric parameters (Å, º) for $[Zn(\mathbf{18})][Zn(NO_3)_4]$

Zn1—N4	2.002 (4)	C13—H9	0.9500
Zn1—N3	2.006 (4)	C14—H12	0.9500
Zn1—N5	2.018 (4)	C15—C17	1.382 (9)
Zn1—N2	2.271 (4)	C15—C27	1.506 (8)
Zn1—N1	2.285 (4)	C16—C24	1.355 (10)
N1—C3	1.447 (7)	C16—C21	1.367 (10)
N1—C27	1.481 (7)	C16—H22	0.9500
N1—C9	1.482 (7)	C17—H16	0.9500
N2—C6	1.453 (7)	C18—C30	1.364 (9)
N2—C23	1.467 (8)	C18—H27	0.9500
N2—C5	1.485 (7)	C19—H5	0.9500
C1—C25	1.348 (11)	C20—H8	0.9500
C1—C12	1.374 (11)	C21—C22	1.391 (8)
C1—H3	0.9500	C21—H21	0.9500
N3—C19	1.340 (7)	C22—H20	0.9500
N3—C28	1.348 (7)	C23—C28	1.504 (9)
C2—N4	1.328 (6)	C23—H6A	0.9900
C2—C11	1.370 (7)	C23—H6B	0.9900
C2—C5	1.504 (8)	C24—C29	1.383 (9)
N4—C4	1.349 (6)	C24—H23	0.9500
C3—C22	1.376 (8)	C25—C28	1.369 (8)
C3—C29	1.380 (8)	C25—H2	0.9500
C4—C18	1.369 (8)	C26—H14	0.9500
C4—C9	1.488 (8)	C27—H18A	0.9900
C5—H31A	0.9900	C27—H18B	0.9900
C5—H31B	0.9900	C29—H24	0.9500
N5—C15	1.337 (7)	C30—H28	0.9500
N5—C10	1.342 (7)	N6—O5	1.211 (7)
C6—C20	1.381 (8)	N6—O3	1.218 (7)
C6—C14	1.390 (9)	N6—O4	1.265 (6)
C7—C26	1.365 (12)	N7—O1	1.202 (7)
C7—C17	1.368 (11)	N7—O8	1.206 (7)
C7—H15	0.9500	N7—O2	1.230 (6)
C8—C31	1.367 (11)	O2—Zn2	2.149 (5)
C8—C14	1.374 (10)	O4—Zn2	2.006 (4)
C8—H11	0.9500	O6—N8	1.199 (9)
C9—H25A	0.9900	N8—O12	1.237 (10)
C9—H25B	0.9900	N8—O7	1.260 (9)
C10—C26	1.378 (9)	O7—Zn2	2.053 (6)
C10—H13	0.9500	O8—Zn2	2.484 (8)
C11—C30	1.369 (9)	C31—H10	0.9500
C11—H29	0.9500	Zn2—O9	1.973 (5)
C12—C19	1.391 (9)	Zn2—O12	2.470 (8)
C12—H4	0.9500	O9—N9	1.245 (8)

C13—C31	1.359 (11)	O10—N9	1.251 (8)
C13—C20	1.394 (9)	N9—O11	1.211 (9)
N4—Zn1—N3	128.87 (17)	C7—C17—C15	119.4 (7)
N4—Zn1—N5	126.58 (17)	C7—C17—H16	120.3
N3—Zn1—N5	104.54 (17)	C15—C17—H16	120.3
N4—Zn1—N2	78.66 (17)	C30—C18—C4	120.1 (6)
N3—Zn1—N2	81.59 (18)	C30—C18—H27	120.0
N5—Zn1—N2	112.23 (17)	C4—C18—H27	120.0
N4—Zn1—N1	79.04 (16)	N3—C19—C12	122.0 (7)
N3—Zn1—N1	113.80 (17)	N3—C19—H5	119.0
N5—Zn1—N1	80.60 (17)	C12—C19—H5	119.0
N2—Zn1—N1	157.68 (16)	C6—C20—C13	118.8 (6)
C3—N1—C27	114.7 (4)	C6—C20—H8	120.6
C3—N1—C9	113.9 (4)	C13—C20—H8	120.6
C27—N1—C9	109.8 (5)	C16—C21—C22	121.0 (7)
C3—N1—Zn1	112.3 (3)	C16—C21—H21	119.5
C27—N1—Zn1	98.4 (3)	C22—C21—H21	119.5
C9—N1—Zn1	106.4 (3)	C3—C22—C21	119.6 (6)
C6—N2—C23	115.7 (5)	C3—C22—H20	120.2
C6—N2—C5	113.1 (4)	C21—C22—H20	120.2
C23—N2—C5	110.4 (5)	N2—C23—C28	113.7 (5)
C6—N2—Zn1	109.6 (3)	N2—C23—H6A	108.8
C23—N2—Zn1	98.5 (3)	C28—C23—H6A	108.8
C5—N2—Zn1	108.2 (3)	N2—C23—H6B	108.8
C25—C1—C12	120.7 (7)	C28—C23—H6B	108.8
C25—C1—H3	119.7	H6A—C23—H6B	107.7
C12—C1—H3	119.7	C16—C24—C29	120.6 (6)
C19—N3—C28	118.8 (5)	C16—C24—H23	119.7
C19—N3—Zn1	126.4 (4)	C29—C24—H23	119.7
C28—N3—Zn1	114.7 (4)	C1—C25—C28	119.6 (7)
N4—C2—C11	121.4 (5)	C1—C25—H2	120.2
N4—C2—C5	117.9 (5)	C28—C25—H2	120.2
C11—C2—C5	120.5 (5)	C7—C26—C10	119.1 (8)
C2—N4—C4	119.7 (4)	C7—C26—H14	120.4
C2—N4—Zn1	120.6 (4)	C10—C26—H14	120.4
C4—N4—Zn1	119.5 (3)	N1—C27—C15	112.7 (4)
C22—C3—C29	118.9 (5)	N1—C27—H18A	109.0
C22—C3—N1	122.8 (5)	C15—C27—H18A	109.0
C29—C3—N1	118.3 (5)	N1—C27—H18B	109.0
N4—C4—C18	120.4 (5)	C15—C27—H18B	109.0
N4—C4—C9	117.2 (4)	H18A—C27—H18B	107.8
C18—C4—C9	122.3 (5)	N3—C28—C25	121.4 (6)
N2—C5—C2	112.6 (4)	N3—C28—C23	115.5 (5)
N2—C5—H31A	109.1	C25—C28—C23	123.0 (6)
C2—C5—H31A	109.1	C3—C29—C24	120.6 (6)
N2—C5—H31B	109.1	C3—C29—H24	119.7

C2—C5—H31B	109.1	C24—C29—H24	119.7
H31A—C5—H31B	107.8	C18—C30—C11	118.9 (6)
C15—N5—C10	120.0 (5)	C18—C30—H28	120.6
C15—N5—Zn1	115.1 (4)	C11—C30—H28	120.6
C10—N5—Zn1	124.8 (4)	O5—N6—O3	123.2 (6)
C20—C6—C14	119.6 (6)	O5—N6—O4	118.3 (6)
C20—C6—N2	122.3 (5)	O3—N6—O4	118.6 (6)
C14—C6—N2	118.1 (5)	O1—N7—O8	124.2 (7)
C26—C7—C17	119.7 (7)	O1—N7—O2	120.2 (6)
C26—C7—H15	120.2	O8—N7—O2	115.6 (7)
C17—C7—H15	120.2	N7—O2—Zn2	104.1 (4)
C31—C8—C14	120.4 (7)	N6—O4—Zn2	114.6 (4)
C31—C8—H11	119.8	O6—N8—O12	128.0 (10)
C14—C8—H11	119.8	O6—N8—O7	118.7 (10)
N1—C9—C4	113.1 (4)	O12—N8—O7	113.3 (8)
N1—C9—H25A	109.0	N8—O7—Zn2	106.2 (5)
C4—C9—H25A	109.0	N7—O8—Zn2	88.1 (5)
N1—C9—H25B	109.0	C13—C31—C8	119.8 (7)
C4—C9—H25B	109.0	C13—C31—H10	120.1
H25A—C9—H25B	107.8	C8—C31—H10	120.1
N5—C10—C26	121.1 (7)	O9—Zn2—O4	130.1 (2)
N5—C10—H13	119.4	O9—Zn2—O7	122.5 (3)
C26—C10—H13	119.4	O4—Zn2—O7	87.1 (2)
C30—C11—C2	119.4 (6)	O9—Zn2—O2	85.2 (2)
C30—C11—H29	120.3	O4—Zn2—O2	92.6 (2)
C2—C11—H29	120.3	O7—Zn2—O2	142.8 (2)
C1—C12—C19	117.5 (7)	O9—Zn2—O12	85.7 (3)
C1—C12—H4	121.3	O4—Zn2—O12	139.5 (2)
C19—C12—H4	121.3	O7—Zn2—O12	54.0 (3)
C31—C13—C20	121.2 (7)	O2—Zn2—O12	111.2 (3)
C31—C13—H9	119.4	O9—Zn2—O8	126.7 (2)
C20—C13—H9	119.4	O4—Zn2—O8	87.3 (2)
C8—C14—C6	120.2 (7)	O7—Zn2—O8	90.7 (3)
C8—C14—H12	119.9	O2—Zn2—O8	52.23 (18)
C6—C14—H12	119.9	O12—Zn2—O8	82.9 (2)
N5—C15—C17	120.7 (6)	N9—O9—Zn2	111.3 (5)
N5—C15—C27	116.1 (5)	O11—N9—O9	118.3 (7)
C17—C15—C27	123.2 (6)	O11—N9—O10	124.8 (8)
C24—C16—C21	119.4 (7)	O9—N9—O10	116.9 (8)
C24—C16—H22	120.3	N8—O12—Zn2	86.4 (5)
C21—C16—H22	120.3		

Table S4: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for [Zn_3K(**23**)$_2$(H_2O)Cl_3]

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5740 (2)	0.0877 (3)	0.2030 (3)	0.0156 (10)
C2	0.5889 (2)	0.1712 (3)	0.2473 (3)	0.0173 (10)
H2A	0.6261	0.1906	0.2213	0.021*
H2B	0.5568	0.2085	0.2249	0.021*
C3	0.6242 (2)	0.2402 (3)	0.4095 (3)	0.0133 (9)
C4	0.6005 (2)	0.3168 (3)	0.3868 (4)	0.0191 (10)
H4	0.5664	0.3223	0.3406	0.023*
C5	0.6278 (2)	0.3846 (3)	0.4328 (4)	0.0212 (11)
H5	0.6118	0.4354	0.4171	0.025*
C6	0.6786 (2)	0.3777 (3)	0.5016 (4)	0.0209 (11)
H6	0.6972	0.4232	0.5317	0.025*
C7	0.7013 (2)	0.3009 (3)	0.5251 (4)	0.0225 (11)
H7	0.7352	0.2952	0.5719	0.027*
C8	0.6743 (2)	0.2330 (3)	0.4800 (4)	0.0181 (10)
H8	0.6900	0.1822	0.4970	0.022*
C9	0.53554 (19)	0.1546 (3)	0.4023 (3)	0.0134 (9)
H9A	0.5111	0.1218	0.3527	0.016*
H9B	0.5154	0.2060	0.4086	0.016*
C10	0.5410 (2)	0.1131 (3)	0.5065 (3)	0.0145 (9)
C11	0.5013 (2)	0.1294 (3)	0.5813 (4)	0.0188 (10)
H11	0.4715	0.1685	0.5696	0.023*
C12	0.5067 (2)	0.0868 (3)	0.6735 (4)	0.0198 (10)
H12	0.4797	0.0956	0.7240	0.024*
C13	0.5524 (2)	0.0311 (3)	0.6902 (3)	0.0167 (10)
H13	0.5567	0.0021	0.7522	0.020*
C14	0.5926 (2)	0.0184 (3)	0.6127 (3)	0.0133 (9)
C15	0.6449 (2)	−0.0381 (3)	0.6318 (3)	0.0163 (10)
H15A	0.6567	−0.0400	0.7060	0.020*
H15B	0.6323	−0.0919	0.6099	0.020*
C16	0.7352 (2)	0.0463 (3)	0.6242 (3)	0.0134 (9)
C17	0.7128 (2)	0.1002 (3)	0.6968 (4)	0.0183 (10)
H17	0.6742	0.0923	0.7184	0.022*
C18	0.7470 (2)	0.1647 (3)	0.7367 (4)	0.0204 (10)
H18	0.7310	0.1994	0.7841	0.025*
C19	0.8047 (2)	0.1780 (3)	0.7070 (4)	0.0236 (11)
H19	0.8271	0.2222	0.7324	0.028*
C20	0.8288 (2)	0.1242 (3)	0.6386 (4)	0.0215 (11)
H20	0.8679	0.1318	0.6192	0.026*
C21	0.7946 (2)	0.0586 (3)	0.5988 (4)	0.0195 (10)
H21	0.8118	0.0225	0.5545	0.023*
C22	0.7270 (2)	−0.0846 (3)	0.5340 (4)	0.0154 (9)
H22A	0.7374	−0.1224	0.5901	0.018*

H22B	0.7642	−0.0678	0.5057	0.018*
C23	0.6871 (2)	−0.1267 (3)	0.4494 (3)	0.0136 (9)
C24	0.7586 (2)	0.0477 (3)	0.3200 (3)	0.0130 (9)
C25	0.8235 (2)	0.0811 (3)	0.3360 (3)	0.0159 (10)
H25A	0.8220	0.1395	0.3401	0.019*
H25B	0.8425	0.0611	0.4014	0.019*
C26	0.9249 (2)	0.0586 (3)	0.2729 (4)	0.0175 (10)
C27	0.9529 (2)	0.0763 (4)	0.3700 (4)	0.0305 (13)
H27	0.9296	0.0902	0.4243	0.037*
C28	1.0154 (2)	0.0738 (4)	0.3875 (5)	0.0382 (15)
H28	1.0334	0.0853	0.4535	0.046*
C29	1.0506 (2)	0.0545 (4)	0.3093 (5)	0.0350 (14)
H29	1.0925	0.0539	0.3211	0.042*
C30	1.0233 (3)	0.0359 (4)	0.2125 (5)	0.0477 (18)
H30	1.0469	0.0221	0.1587	0.057*
C31	0.9611 (2)	0.0377 (4)	0.1946 (5)	0.0389 (15)
H31	0.9434	0.0247	0.1288	0.047*
C32	0.8382 (2)	0.0949 (3)	0.1517 (3)	0.0158 (10)
H32A	0.8653	0.1386	0.1370	0.019*
H32B	0.7987	0.1182	0.1592	0.019*
C33	0.8335 (2)	0.0381 (3)	0.0603 (3)	0.0137 (9)
C34	0.8309 (2)	0.0673 (3)	−0.0407 (4)	0.0187 (10)
H34	0.8321	0.1226	−0.0530	0.022*
C35	0.8264 (2)	0.0139 (3)	−0.1227 (4)	0.0203 (11)
H35	0.8237	0.0326	−0.1911	0.024*
C36	0.8259 (2)	−0.0689 (3)	−0.1020 (4)	0.0183 (10)
H36	0.8242	−0.1060	−0.1562	0.022*
C37	0.82796 (19)	−0.0946 (3)	0.0001 (3)	0.0153 (10)
C38	0.8250 (2)	−0.1821 (3)	0.0297 (3)	0.0152 (9)
H38A	0.7832	−0.1977	0.0340	0.018*
H38B	0.8416	−0.2148	−0.0236	0.018*
C39	0.9245 (2)	−0.1992 (3)	0.1266 (4)	0.0188 (10)
C40	0.9520 (2)	−0.1878 (4)	0.0352 (5)	0.0344 (13)
H40	0.9286	−0.1798	−0.0270	0.041*
C41	1.0143 (3)	−0.1883 (4)	0.0359 (6)	0.0491 (18)
H41	1.0323	−0.1795	−0.0259	0.059*
C42	1.0498 (3)	−0.2013 (4)	0.1256 (6)	0.0462 (18)
H42	1.0916	−0.2036	0.1247	0.055*
C43	1.0229 (3)	−0.2112 (4)	0.2186 (5)	0.0377 (14)
H43	1.0468	−0.2189	0.2805	0.045*
C44	0.9607 (2)	−0.2096 (3)	0.2190 (5)	0.0313 (13)
H44	0.9429	−0.2156	0.2815	0.038*
C45	0.8339 (2)	−0.2654 (3)	0.1847 (4)	0.0184 (10)
H45A	0.8618	−0.2810	0.2431	0.022*
H45B	0.8292	−0.3110	0.1375	0.022*
C46	0.7726 (2)	−0.2446 (3)	0.2244 (3)	0.0135 (9)

N1	0.59578 (16)	0.1679 (2)	0.3630 (3)	0.0127 (8)
N2	0.58552 (16)	0.0580 (2)	0.5214 (3)	0.0123 (8)
N3	0.69759 (17)	−0.0142 (2)	0.5759 (3)	0.0118 (8)
N4	0.85990 (17)	0.0574 (2)	0.2505 (3)	0.0159 (8)
N5	0.83138 (16)	−0.0414 (2)	0.0796 (3)	0.0119 (8)
N6	0.85917 (17)	−0.1970 (2)	0.1305 (3)	0.0157 (8)
O1	0.69746 (15)	−0.20142 (18)	0.4418 (2)	0.0174 (7)
O2	0.64880 (14)	−0.08724 (18)	0.3933 (2)	0.0136 (6)
O3	0.59529 (14)	0.02735 (19)	0.2561 (2)	0.0155 (7)
O4	0.54337 (16)	0.0824 (2)	0.1194 (3)	0.0244 (8)
O5	0.72171 (14)	0.07995 (19)	0.3743 (2)	0.0162 (7)
O6	0.74823 (14)	−0.00970 (18)	0.2570 (2)	0.0154 (7)
O7	0.75429 (13)	−0.17312 (18)	0.2194 (2)	0.0148 (7)
O8	0.74484 (14)	−0.30284 (19)	0.2606 (2)	0.0163 (7)
O9	0.52851 (17)	−0.0842 (2)	0.0803 (3)	0.0238 (8)
Cl1	0.67309 (5)	−0.09698 (7)	−0.06496 (9)	0.0195 (2)
Cl2	0.86402 (5)	−0.11590 (7)	0.38815 (9)	0.0201 (3)
Cl3	0.58975 (5)	−0.26577 (7)	0.23638 (10)	0.0228 (3)
Zn1	0.63882 (2)	0.03867 (3)	0.39748 (4)	0.01148 (13)
Zn2	0.82115 (2)	−0.08384 (3)	0.22795 (4)	0.01275 (13)
Zn3	0.67184 (2)	−0.28810 (3)	0.34298 (4)	0.01309 (13)
K1	0.64340 (4)	−0.10316 (6)	0.16817 (7)	0.0156 (2)
H98	0.534 (3)	−0.030 (4)	0.083 (5)	0.037 (17)*
H99	0.515 (3)	−0.093 (4)	0.025 (5)	0.034 (19)*

Table S5: Atomic displacement parameters (Å^2) for $[Zn_3K(\mathbf{23})_2(H_2O)Cl_3]$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.013 (2)	0.021 (2)	0.013 (2)	0.0018 (19)	0.0021 (18)	0.0000 (19)
C2	0.022 (2)	0.018 (2)	0.011 (2)	0.002 (2)	−0.0033 (19)	0.0018 (19)
C3	0.015 (2)	0.014 (2)	0.011 (2)	−0.0002 (18)	0.0033 (18)	−0.0004 (18)
C4	0.019 (2)	0.016 (2)	0.022 (2)	0.0036 (19)	−0.005 (2)	0.0001 (19)
C5	0.022 (3)	0.013 (2)	0.028 (3)	0.008 (2)	−0.002 (2)	0.004 (2)
C6	0.023 (3)	0.012 (2)	0.027 (3)	−0.005 (2)	0.000 (2)	−0.003 (2)
C7	0.019 (3)	0.021 (3)	0.026 (3)	0.001 (2)	−0.006 (2)	0.001 (2)
C8	0.019 (2)	0.014 (2)	0.021 (2)	0.0015 (19)	0.000 (2)	0.0009 (19)
C9	0.011 (2)	0.012 (2)	0.017 (2)	−0.0015 (17)	0.0001 (18)	−0.0064 (18)
C10	0.014 (2)	0.015 (2)	0.015 (2)	−0.0032 (18)	−0.0005 (18)	−0.0076 (18)
C11	0.011 (2)	0.020 (2)	0.025 (3)	−0.0021 (19)	0.0024 (19)	−0.008 (2)
C12	0.016 (2)	0.024 (3)	0.021 (2)	−0.006 (2)	0.009 (2)	−0.006 (2)
C13	0.019 (2)	0.020 (2)	0.011 (2)	−0.007 (2)	0.0034 (18)	−0.0060 (19)
C14	0.016 (2)	0.013 (2)	0.011 (2)	−0.0056 (18)	−0.0001 (18)	−0.0025 (17)
C15	0.022 (2)	0.016 (2)	0.011 (2)	−0.0035 (19)	0.0024 (18)	0.0024 (18)
C16	0.020 (2)	0.009 (2)	0.011 (2)	0.0010 (18)	−0.0034 (18)	0.0033 (17)
C17	0.019 (2)	0.019 (2)	0.017 (2)	0.004 (2)	−0.0008 (19)	0.0001 (19)
C18	0.027 (3)	0.015 (2)	0.018 (2)	0.004 (2)	−0.006 (2)	−0.0058 (19)
C19	0.035 (3)	0.015 (2)	0.019 (3)	−0.008 (2)	−0.008 (2)	0.000 (2)
C20	0.023 (3)	0.030 (3)	0.012 (2)	−0.006 (2)	0.0000 (19)	0.003 (2)
C21	0.028 (3)	0.018 (2)	0.012 (2)	−0.003 (2)	0.001 (2)	−0.0021 (19)
C22	0.015 (2)	0.013 (2)	0.017 (2)	0.0022 (18)	−0.0038 (18)	0.0004 (18)
C23	0.015 (2)	0.016 (2)	0.010 (2)	−0.0008 (19)	0.0043 (18)	−0.0009 (18)
C24	0.018 (2)	0.014 (2)	0.007 (2)	0.0015 (18)	0.0022 (18)	0.0004 (17)
C25	0.015 (2)	0.019 (2)	0.014 (2)	0.0021 (19)	0.0033 (18)	0.0005 (18)
C26	0.012 (2)	0.017 (2)	0.022 (2)	−0.0033 (19)	−0.0024 (19)	0.0012 (19)
C27	0.020 (3)	0.050 (4)	0.022 (3)	−0.004 (2)	0.004 (2)	0.003 (2)
C28	0.018 (3)	0.059 (4)	0.035 (3)	−0.007 (3)	−0.011 (2)	0.009 (3)
C29	0.012 (3)	0.040 (3)	0.053 (4)	0.000 (2)	−0.001 (2)	−0.005 (3)
C30	0.022 (3)	0.070 (5)	0.053 (4)	−0.002 (3)	0.011 (3)	−0.025 (4)
C31	0.020 (3)	0.062 (4)	0.035 (3)	−0.004 (3)	0.003 (2)	−0.015 (3)
C32	0.013 (2)	0.015 (2)	0.019 (2)	−0.0036 (18)	0.0031 (19)	0.0035 (19)
C33	0.013 (2)	0.013 (2)	0.015 (2)	0.0029 (18)	0.0021 (18)	0.0036 (18)
C34	0.023 (3)	0.015 (2)	0.018 (2)	0.002 (2)	0.002 (2)	0.0041 (19)
C35	0.016 (2)	0.032 (3)	0.013 (2)	0.002 (2)	−0.0007 (19)	0.007 (2)
C36	0.015 (2)	0.024 (3)	0.016 (2)	−0.003 (2)	0.0004 (18)	−0.004 (2)
C37	0.008 (2)	0.022 (2)	0.015 (2)	−0.0042 (18)	−0.0019 (17)	0.0000 (19)
C38	0.014 (2)	0.017 (2)	0.015 (2)	0.0014 (18)	0.0028 (18)	−0.0046 (18)
C39	0.017 (2)	0.010 (2)	0.029 (3)	−0.0019 (19)	0.003 (2)	0.001 (2)
C40	0.022 (3)	0.045 (4)	0.036 (3)	0.004 (3)	0.003 (2)	0.009 (3)
C41	0.031 (3)	0.064 (5)	0.056 (4)	0.008 (3)	0.022 (3)	0.023 (4)
C42	0.013 (3)	0.049 (4)	0.077 (5)	0.001 (3)	0.006 (3)	0.032 (4)

C43	0.022 (3)	0.040 (3)	0.050 (4)	−0.004 (3)	−0.004 (3)	0.012 (3)
C44	0.024 (3)	0.029 (3)	0.041 (3)	−0.002 (2)	0.002 (2)	−0.001 (3)
C45	0.017 (2)	0.013 (2)	0.026 (3)	−0.0031 (19)	0.007 (2)	0.0006 (19)
C46	0.014 (2)	0.012 (2)	0.014 (2)	−0.0014 (18)	−0.0036 (18)	−0.0010 (18)
N1	0.0129 (19)	0.0141 (19)	0.0103 (18)	0.0000 (15)	−0.0034 (15)	−0.0002 (15)
N2	0.0086 (18)	0.0128 (19)	0.0158 (19)	−0.0038 (15)	0.0024 (15)	−0.0011 (15)
N3	0.0163 (19)	0.0104 (18)	0.0085 (17)	−0.0017 (15)	0.0006 (15)	−0.0037 (14)
N4	0.0128 (19)	0.020 (2)	0.0148 (19)	−0.0001 (16)	0.0023 (15)	−0.0020 (16)
N5	0.0098 (18)	0.0146 (19)	0.0110 (18)	−0.0005 (15)	−0.0007 (14)	−0.0022 (15)
N6	0.0125 (19)	0.015 (2)	0.020 (2)	0.0002 (16)	0.0021 (16)	0.0038 (16)
O1	0.0227 (18)	0.0129 (16)	0.0163 (16)	−0.0003 (13)	−0.0012 (13)	−0.0016 (13)
O2	0.0152 (16)	0.0129 (16)	0.0125 (15)	−0.0008 (13)	0.0006 (13)	−0.0011 (13)
O3	0.0165 (16)	0.0165 (17)	0.0130 (15)	0.0005 (13)	−0.0011 (13)	−0.0017 (13)
O4	0.031 (2)	0.0239 (19)	0.0167 (18)	0.0000 (15)	−0.0060 (15)	0.0024 (14)
O5	0.0126 (16)	0.0190 (17)	0.0172 (16)	−0.0010 (13)	0.0025 (13)	−0.0018 (13)
O6	0.0148 (16)	0.0131 (16)	0.0183 (16)	−0.0021 (13)	0.0020 (13)	−0.0014 (13)
O7	0.0126 (16)	0.0123 (16)	0.0195 (17)	−0.0009 (13)	0.0018 (13)	0.0011 (13)
O8	0.0169 (17)	0.0158 (16)	0.0165 (16)	−0.0024 (13)	0.0038 (13)	0.0001 (13)
O9	0.028 (2)	0.025 (2)	0.017 (2)	−0.0026 (16)	−0.0074 (16)	0.0012 (16)
Cl1	0.0258 (6)	0.0145 (5)	0.0188 (6)	0.0027 (5)	0.0048 (5)	−0.0022 (4)
Cl2	0.0209 (6)	0.0227 (6)	0.0162 (6)	0.0000 (5)	−0.0028 (5)	0.0019 (5)
Cl3	0.0173 (6)	0.0202 (6)	0.0294 (7)	−0.0022 (5)	−0.0074 (5)	−0.0006 (5)
Zn1	0.0112 (3)	0.0131 (3)	0.0101 (2)	−0.0003 (2)	0.00063 (19)	−0.0010 (2)
Zn2	0.0122 (3)	0.0130 (3)	0.0130 (3)	−0.0005 (2)	0.0011 (2)	0.0005 (2)
Zn3	0.0136 (3)	0.0113 (3)	0.0143 (3)	−0.0012 (2)	0.0007 (2)	−0.0007 (2)
K1	0.0153 (5)	0.0183 (5)	0.0131 (5)	0.0019 (4)	0.0011 (4)	−0.0013 (4)

Table S6: Geometric parameters (Å, º) for $[Zn_3K(\mathbf{23})_2(H_2O)Cl_3]$

C1—O4	1.229 (6)	C30—C31	1.380 (8)
C1—O3	1.280 (6)	C30—H30	0.9300
C1—C2	1.524 (6)	C31—H31	0.9300
C2—N1	1.486 (6)	C32—N4	1.463 (6)
C2—H2A	0.9700	C32—C33	1.505 (6)
C2—H2B	0.9700	C32—H32A	0.9700
C3—C8	1.385 (7)	C32—H32B	0.9700
C3—C4	1.395 (6)	C33—N5	1.342 (6)
C3—N1	1.460 (6)	C33—C34	1.385 (6)
C4—C5	1.388 (7)	C34—C35	1.375 (7)
C4—H4	0.9300	C34—H34	0.9300
C5—C6	1.381 (7)	C35—C36	1.398 (7)
C5—H5	0.9300	C35—H35	0.9300
C6—C7	1.393 (7)	C36—C37	1.378 (7)
C6—H6	0.9300	C36—H36	0.9300
C7—C8	1.380 (7)	C37—N5	1.349 (6)
C7—H7	0.9300	C37—C38	1.502 (6)
C8—H8	0.9300	C38—N6	1.470 (6)
C9—N1	1.483 (5)	C38—H38A	0.9700
C9—C10	1.503 (6)	C38—H38B	0.9700
C9—H9A	0.9700	C39—C40	1.380 (7)
C9—H9B	0.9700	C39—C44	1.392 (8)
C10—N2	1.347 (6)	C39—N6	1.456 (6)
C10—C11	1.383 (6)	C40—C41	1.380 (8)
C11—C12	1.378 (7)	C40—H40	0.9300
C11—H11	0.9300	C41—C42	1.362 (9)
C12—C13	1.376 (7)	C41—H41	0.9300
C12—H12	0.9300	C42—C43	1.388 (9)
C13—C14	1.407 (6)	C42—H42	0.9300
C13—H13	0.9300	C43—C44	1.382 (8)
C14—N2	1.344 (6)	C43—H43	0.9300
C14—C15	1.496 (6)	C44—H44	0.9300
C15—N3	1.476 (6)	C45—N6	1.465 (6)
C15—H15A	0.9700	C45—C46	1.531 (6)
C15—H15B	0.9700	C45—H45A	0.9700
C16—C21	1.398 (7)	C45—H45B	0.9700
C16—C17	1.413 (6)	C46—O7	1.252 (5)
C16—N3	1.415 (6)	C46—O8	1.255 (5)
C17—C18	1.385 (7)	N1—Zn1	2.372 (4)
C17—H17	0.9300	N2—Zn1	2.085 (4)
C18—C19	1.383 (7)	N4—Zn2	2.503 (4)
C18—H18	0.9300	N5—Zn2	2.065 (4)
C19—C20	1.389 (7)	N6—Zn2	2.444 (4)

C19—H19	0.9300	O1—Zn3	1.972 (3)
C20—C21	1.399 (7)	O2—Zn1	2.100 (3)
C20—H20	0.9300	O2—K1	2.903 (3)
C21—H21	0.9300	O3—Zn1	2.000 (3)
C22—N3	1.462 (6)	O3—K1	2.701 (3)
C22—C23	1.518 (6)	O5—Zn1	2.007 (3)
C22—H22A	0.9700	O6—Zn2	2.089 (3)
C22—H22B	0.9700	O6—K1	2.949 (3)
C23—O2	1.254 (5)	O7—Zn2	2.092 (3)
C23—O1	1.265 (5)	O7—K1	2.752 (3)
C24—O5	1.239 (5)	O8—Zn3	2.021 (3)
C24—O6	1.259 (5)	O9—K1	2.723 (4)
C24—C25	1.542 (6)	O9—H98	0.90 (7)
C25—N4	1.470 (6)	O9—H99	0.76 (7)
C25—H25A	0.9700	Cl1—Zn3^{i}	2.2425 (12)
C25—H25B	0.9700	Cl1—K1	3.1255 (15)
C26—C27	1.383 (7)	Cl2—Zn2	2.2641 (12)
C26—C31	1.383 (7)	Cl3—Zn3	2.2223 (13)
C26—N4	1.448 (6)	Cl3—K1	3.1018 (16)
C27—C28	1.387 (7)	Zn1—K1	3.7814 (11)
C27—H27	0.9300	Zn2—K1	3.9708 (12)
C28—C29	1.360 (8)	Zn3—Cl1^{ii}	2.2425 (12)
C28—H28	0.9300	Zn3—K1	3.8252 (12)
C29—C30	1.376 (9)	K1—H98	2.86 (6)
C29—H29	0.9300		
O4—C1—O3	124.5 (4)	C46—C45—H45A	109.3
O4—C1—C2	118.7 (4)	N6—C45—H45B	109.3
O3—C1—C2	116.8 (4)	C46—C45—H45B	109.3
N1—C2—C1	110.1 (4)	H45A—C45—H45B	108.0
N1—C2—H2A	109.6	O7—C46—O8	125.5 (4)
C1—C2—H2A	109.6	O7—C46—C45	119.3 (4)
N1—C2—H2B	109.6	O8—C46—C45	115.2 (4)
C1—C2—H2B	109.6	C3—N1—C9	110.7 (3)
H2A—C2—H2B	108.2	C3—N1—C2	112.7 (3)
C8—C3—C4	119.0 (4)	C9—N1—C2	108.9 (3)
C8—C3—N1	119.7 (4)	C3—N1—Zn1	120.7 (3)
C4—C3—N1	121.3 (4)	C9—N1—Zn1	99.3 (2)
C5—C4—C3	120.3 (4)	C2—N1—Zn1	103.2 (3)
C5—C4—H4	119.9	C14—N2—C10	119.3 (4)
C3—C4—H4	119.9	C14—N2—Zn1	124.0 (3)
C6—C5—C4	120.8 (4)	C10—N2—Zn1	116.7 (3)
C6—C5—H5	119.6	C16—N3—C22	117.6 (4)
C4—C5—H5	119.6	C16—N3—C15	116.0 (3)
C5—C6—C7	118.5 (4)	C22—N3—C15	111.1 (3)
C5—C6—H6	120.7	C26—N4—C32	114.9 (4)
C7—C6—H6	120.7	C26—N4—C25	116.5 (4)

C8—C7—C6	121.1 (5)	C32—N4—C25	112.0 (4)
C8—C7—H7	119.4	C26—N4—Zn2	111.3 (3)
C6—C7—H7	119.4	C32—N4—Zn2	102.2 (3)
C7—C8—C3	120.2 (4)	C25—N4—Zn2	97.6 (3)
C7—C8—H8	119.9	C33—N5—C37	120.1 (4)
C3—C8—H8	119.9	C33—N5—Zn2	120.9 (3)
N1—C9—C10	111.2 (4)	C37—N5—Zn2	118.4 (3)
N1—C9—H9A	109.4	C39—N6—C45	114.7 (4)
C10—C9—H9A	109.4	C39—N6—C38	114.7 (4)
N1—C9—H9B	109.4	C45—N6—C38	111.1 (4)
C10—C9—H9B	109.4	C39—N6—Zn2	115.0 (3)
H9A—C9—H9B	108.0	C45—N6—Zn2	100.9 (3)
N2—C10—C11	122.2 (4)	C38—N6—Zn2	98.6 (2)
N2—C10—C9	116.3 (4)	C23—O1—Zn3	135.9 (3)
C11—C10—C9	121.4 (4)	C23—O2—Zn1	124.9 (3)
C12—C11—C10	118.9 (4)	C23—O2—K1	119.9 (3)
C12—C11—H11	120.5	Zn1—O2—K1	96.87 (11)
C10—C11—H11	120.5	C1—O3—Zn1	122.9 (3)
C13—C12—C11	119.4 (4)	C1—O3—K1	122.9 (3)
C13—C12—H12	120.3	Zn1—O3—K1	106.15 (13)
C11—C12—H12	120.3	C24—O5—Zn1	126.2 (3)
C12—C13—C14	119.4 (4)	C24—O6—Zn2	117.1 (3)
C12—C13—H13	120.3	C24—O6—K1	138.1 (3)
C14—C13—H13	120.3	Zn2—O6—K1	102.69 (11)
N2—C14—C13	120.7 (4)	C46—O7—Zn2	116.2 (3)
N2—C14—C15	119.0 (4)	C46—O7—K1	133.7 (3)
C13—C14—C15	120.2 (4)	Zn2—O7—K1	109.35 (12)
N3—C15—C14	112.7 (4)	C46—O8—Zn3	122.6 (3)
N3—C15—H15A	109.1	K1—O9—H98	89 (4)
C14—C15—H15A	109.1	K1—O9—H99	130 (5)
N3—C15—H15B	109.1	H98—O9—H99	105 (6)
C14—C15—H15B	109.1	$Zn3^{i}$—Cl1—K1	119.01 (5)
H15A—C15—H15B	107.8	Zn3—Cl3—K1	90.30 (4)
C21—C16—C17	116.7 (4)	O3—Zn1—O5	106.15 (13)
C21—C16—N3	122.4 (4)	O3—Zn1—N2	116.66 (13)
C17—C16—N3	120.9 (4)	O5—Zn1—N2	130.08 (13)
C18—C17—C16	121.5 (4)	O3—Zn1—O2	85.86 (12)
C18—C17—H17	119.3	O5—Zn1—O2	103.60 (12)
C16—C17—H17	119.3	N2—Zn1—O2	103.86 (13)
C19—C18—C17	120.8 (5)	O3—Zn1—N1	75.93 (12)
C19—C18—H18	119.6	O5—Zn1—N1	91.40 (13)
C17—C18—H18	119.6	N2—Zn1—N1	76.10 (13)
C18—C19—C20	119.0 (4)	O2—Zn1—N1	159.11 (12)
C18—C19—H19	120.5	O3—Zn1—K1	43.31 (9)
C20—C19—H19	120.5	O5—Zn1—K1	90.78 (9)
C19—C20—C21	120.4 (5)	N2—Zn1—K1	138.17 (10)

C19—C20—H20	119.8	O2—Zn1—K1	49.67 (8)
C21—C20—H20	119.8	N1—Zn1—K1	116.81 (9)
C16—C21—C20	121.5 (4)	N5—Zn2—O6	96.29 (13)
C16—C21—H21	119.2	N5—Zn2—O7	108.79 (13)
C20—C21—H21	119.2	O6—Zn2—O7	82.50 (12)
N3—C22—C23	112.3 (4)	N5—Zn2—Cl2	148.55 (10)
N3—C22—H22A	109.1	O6—Zn2—Cl2	104.46 (9)
C23—C22—H22A	109.1	O7—Zn2—Cl2	97.28 (9)
N3—C22—H22B	109.1	N5—Zn2—N6	73.67 (13)
C23—C22—H22B	109.1	O6—Zn2—N6	147.94 (12)
H22A—C22—H22B	107.9	O7—Zn2—N6	72.68 (12)
O2—C23—O1	125.8 (4)	Cl2—Zn2—N6	98.63 (10)
O2—C23—C22	120.2 (4)	N5—Zn2—N4	74.13 (13)
O1—C23—C22	114.0 (4)	O6—Zn2—N4	72.11 (12)
O5—C24—O6	126.5 (4)	O7—Zn2—N4	154.60 (12)
O5—C24—C25	114.9 (4)	Cl2—Zn2—N4	89.91 (9)
O6—C24—C25	118.5 (4)	N6—Zn2—N4	130.39 (12)
N4—C25—C24	111.6 (4)	N5—Zn2—K1	91.68 (10)
N4—C25—H25A	109.3	O6—Zn2—K1	46.43 (8)
C24—C25—H25A	109.3	O7—Zn2—K1	40.84 (8)
N4—C25—H25B	109.3	Cl2—Zn2—K1	119.74 (4)
C24—C25—H25B	109.3	N6—Zn2—K1	102.53 (9)
H25A—C25—H25B	108.0	N4—Zn2—K1	115.13 (9)
C27—C26—C31	117.8 (5)	O1—Zn3—O8	102.99 (13)
C27—C26—N4	123.5 (4)	O1—Zn3—Cl3	117.18 (10)
C31—C26—N4	118.6 (4)	O8—Zn3—Cl3	110.36 (10)
C26—C27—C28	120.8 (5)	O1—Zn3—Cl1^{ii}	106.69 (10)
C26—C27—H27	119.6	O8—Zn3—Cl1^{ii}	101.42 (10)
C28—C27—H27	119.6	Cl3—Zn3—Cl1^{ii}	116.28 (5)
C29—C28—C27	120.8 (5)	O1—Zn3—K1	79.69 (9)
C29—C28—H28	119.6	O8—Zn3—K1	83.66 (9)
C27—C28—H28	119.6	Cl3—Zn3—K1	54.18 (4)
C28—C29—C30	119.0 (5)	Cl1^{ii}—Zn3—K1	170.45 (4)
C28—C29—H29	120.5	O3—K1—O9	72.12 (11)
C30—C29—H29	120.5	O3—K1—O7	127.81 (10)
C29—C30—C31	120.6 (6)	O9—K1—O7	159.64 (12)
C29—C30—H30	119.7	O3—K1—O2	59.67 (9)
C31—C30—H30	119.7	O9—K1—O2	111.50 (11)
C30—C31—C26	121.0 (5)	O7—K1—O2	80.48 (9)
C30—C31—H31	119.5	O3—K1—O6	75.09 (9)
C26—C31—H31	119.5	O9—K1—O6	141.59 (11)
N4—C32—C33	114.3 (4)	O7—K1—O6	57.72 (9)
N4—C32—H32A	108.7	O2—K1—O6	66.21 (9)
C33—C32—H32A	108.7	O3—K1—Cl3	113.83 (8)
N4—C32—H32B	108.7	O9—K1—Cl3	81.39 (9)
C33—C32—H32B	108.7	O7—K1—Cl3	85.54 (7)

H32A—C32—H32B	107.6	O2—K1—Cl3	77.44 (7)
N5—C33—C34	121.2 (4)	O6—K1—Cl3	130.96 (7)
N5—C33—C32	118.1 (4)	O3—K1—Cl1	119.79 (8)
C34—C33—C32	120.7 (4)	O9—K1—Cl1	81.94 (9)
C35—C34—C33	119.4 (4)	O7—K1—Cl1	89.46 (7)
C35—C34—H34	120.3	O2—K1—Cl1	163.87 (7)
C33—C34—H34	120.3	O6—K1—Cl1	97.76 (7)
C34—C35—C36	119.1 (4)	Cl3—K1—Cl1	114.55 (4)
C34—C35—H35	120.5	O3—K1—Zn1	30.54 (7)
C36—C35—H35	120.5	O9—K1—Zn1	99.75 (9)
C37—C36—C35	119.1 (4)	O7—K1—Zn1	98.89 (7)
C37—C36—H36	120.5	O2—K1—Zn1	33.46 (6)
C35—C36—H36	120.5	O6—K1—Zn1	55.95 (6)
N5—C37—C36	121.1 (4)	Cl3—K1—Zn1	106.52 (4)
N5—C37—C38	116.0 (4)	Cl1—K1—Zn1	138.60 (4)
C36—C37—C38	122.9 (4)	O3—K1—Zn3	116.59 (7)
N6—C38—C37	110.9 (4)	O9—K1—Zn3	116.22 (9)
N6—C38—H38A	109.5	O7—K1—Zn3	54.50 (6)
C37—C38—H38A	109.5	O2—K1—Zn3	59.59 (6)
N6—C38—H38B	109.5	O6—K1—Zn3	96.02 (7)
C37—C38—H38B	109.5	Cl3—K1—Zn3	35.52 (3)
H38A—C38—H38B	108.0	Cl1—K1—Zn3	123.62 (4)
C40—C39—C44	118.8 (5)	Zn1—K1—Zn3	93.01 (3)
C40—C39—N6	122.4 (5)	O3—K1—Zn2	105.90 (7)
C44—C39—N6	118.7 (4)	O9—K1—Zn2	162.47 (9)
C41—C40—C39	120.3 (6)	O7—K1—Zn2	29.81 (6)
C41—C40—H40	119.8	O2—K1—Zn2	80.69 (6)
C39—C40—H40	119.8	O6—K1—Zn2	30.89 (6)
C42—C41—C40	121.1 (6)	Cl3—K1—Zn2	114.40 (4)
C42—C41—H41	119.5	Cl1—K1—Zn2	84.32 (3)
C40—C41—H41	119.5	Zn1—K1—Zn2	83.51 (2)
C41—C42—C43	119.4 (5)	Zn3—K1—Zn2	80.56 (2)
C41—C42—H42	120.3	O3—K1—H98	57.9 (13)
C43—C42—H42	120.3	O9—K1—H98	18.3 (13)
C44—C43—C42	120.0 (6)	O7—K1—H98	171.2 (12)
C44—C43—H43	120.0	O2—K1—H98	108.1 (12)
C42—C43—H43	120.0	O6—K1—H98	123.3 (14)
C43—C44—C39	120.4 (5)	Cl3—K1—H98	98.1 (13)
C43—C44—H44	119.8	Cl1—K1—H98	81.7 (12)
C39—C44—H44	119.8	Zn1—K1—H98	87.8 (13)
N6—C45—C46	111.6 (4)	Zn3—K1—H98	131.3 (13)
N6—C45—H45A	109.3	Zn2—K1—H98	147.5 (13)

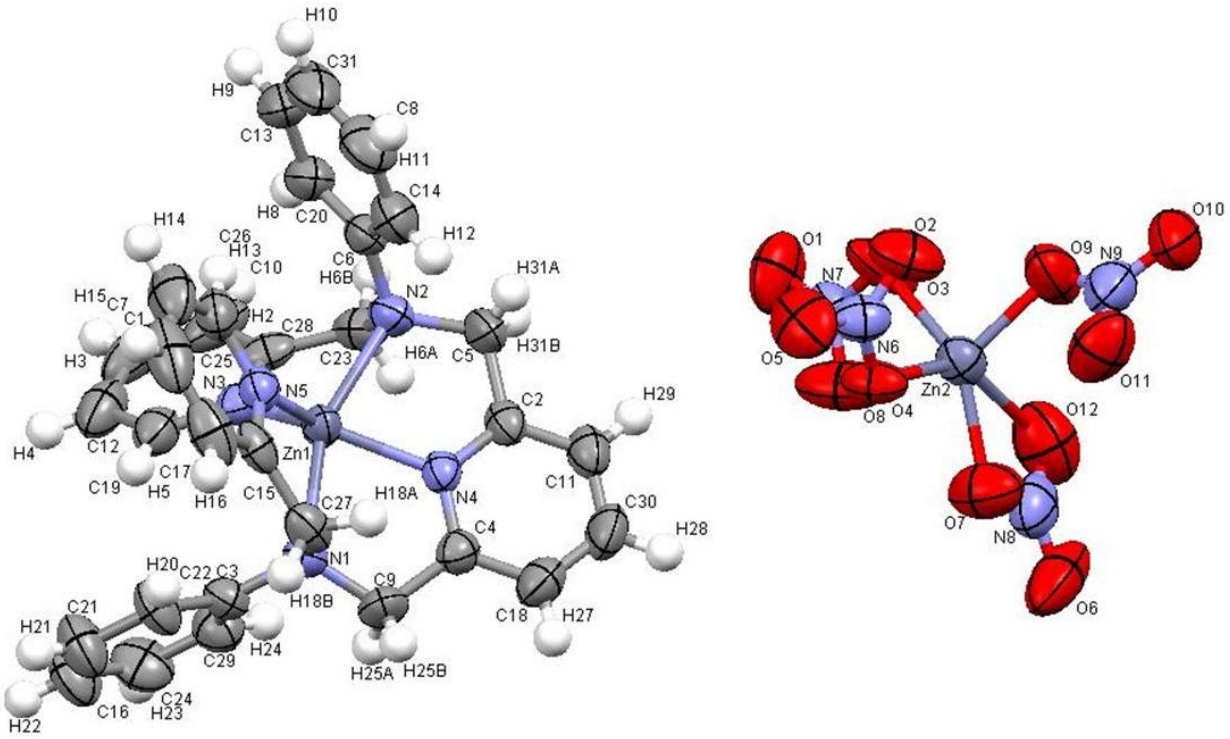


Figure S70: Perspective view of [Zn(**18**)][Zn(NO_3)$_4$] with complete labeling

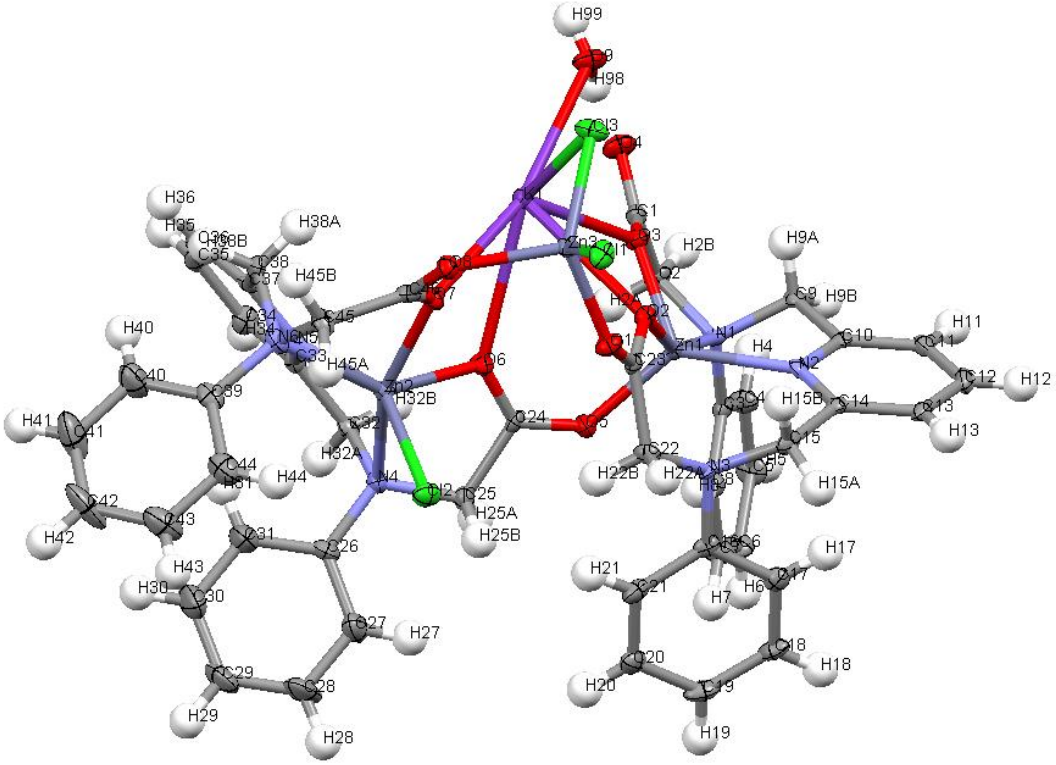


Figure S71: Perspective view of $[Zn_3K(\mathbf{23})_2(H_2O)Cl_3]$with complete labeling