Supplementary Information

Incorporation of Porphyrin Acetylides into Duplexes of the Simplified Nucleic Acid GNA

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Tables of Contents:

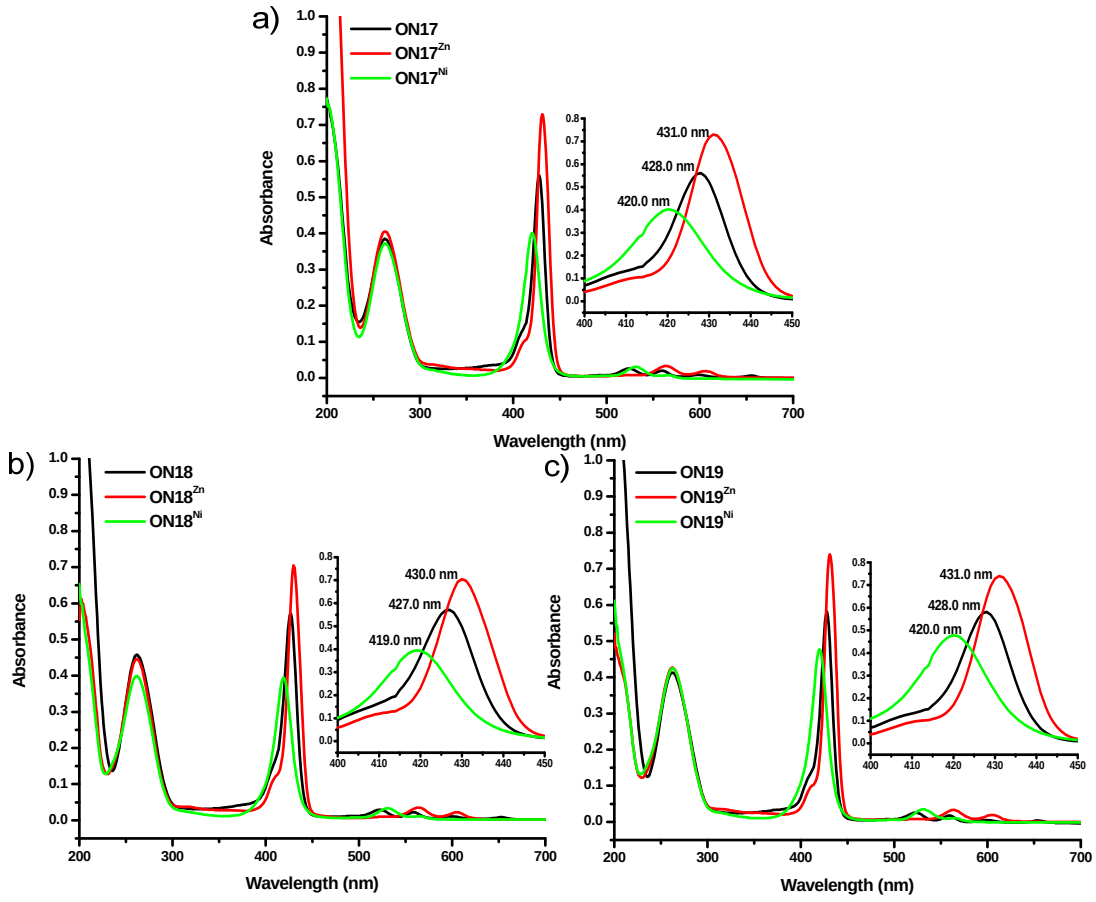


Figure S1: Absorption spectra of GNA single strands with and without metals. a) **ON17**, **ON17^{Zn}** and **ON17^{Ni}**; b) **ON18**, **ON18^{Zn}** and **ON18^{Ni}**; c) **ON19**, **ON19^{Zn}** and **ON19^{Ni}**. The insert shows the expanded porphyrin Soret band region. Conditions: 10 mM sodium phosphate, 100 mM NaCl, pH 7.0, and 2 μM of single strands.

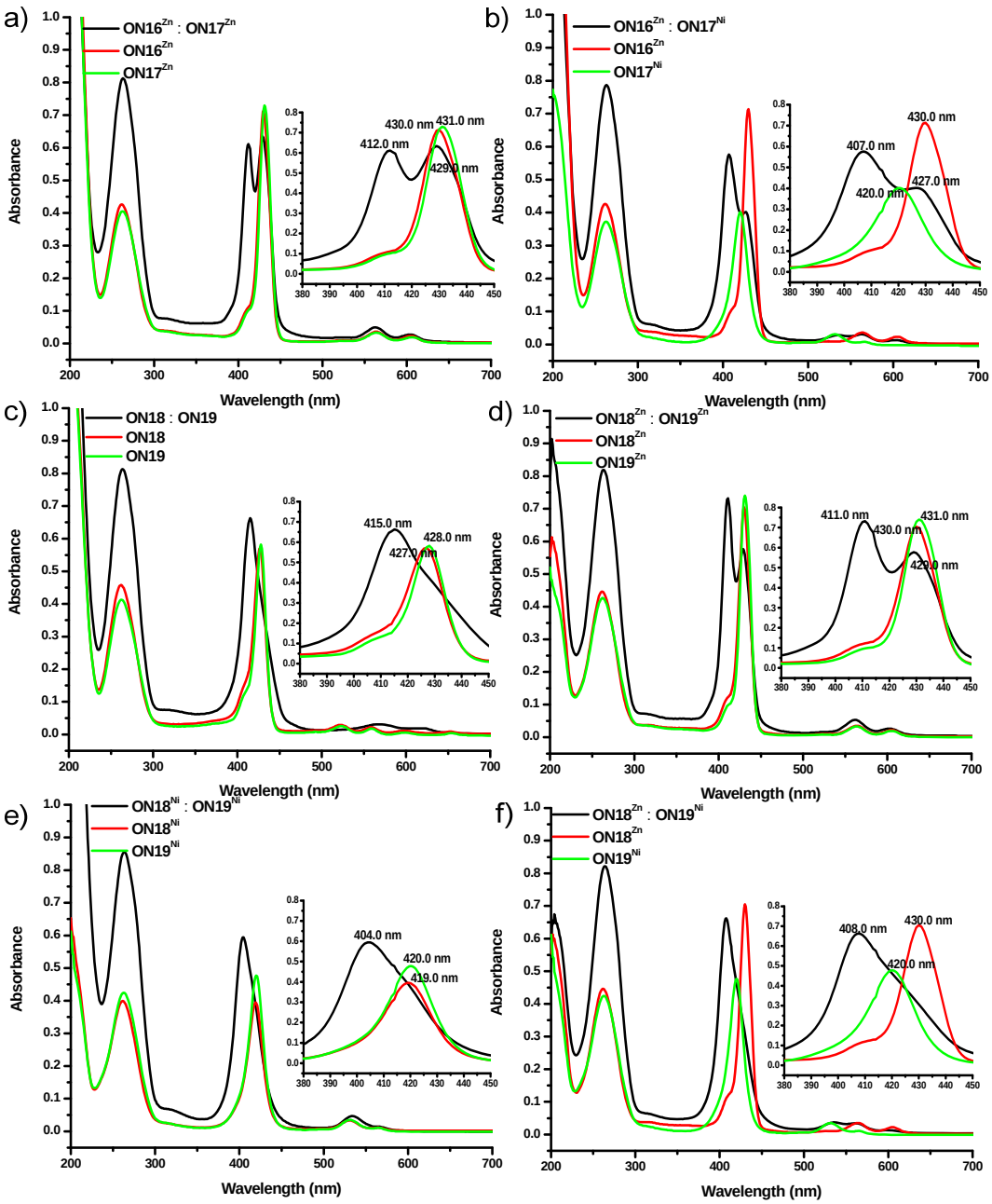


Figure S2: UV–vis spectra of GNA duplexes and their corresponding single strands. a) **ON16^{Zn}**, **ON17^{Zn}** and **ON16^{Zn}**:**ON17^{Zn}**; b) **ON16^{Zn}**, **ON17^{Ni}** and **ON16^{Zn}**:**ON17^{Ni}**, c) **ON18**, **ON19** and **ON18**:**ON19**; d) **ON18^{Zn}**, **ON19^{Zn}** and **ON18^{Zn}**:**ON19^{Zn}**; e) **ON18^{Ni}**, **ON19^{Ni}** and **ON18^{Ni}**:**ON19^{Ni}**; f) **ON18^{Zn}**, **ON19^{Ni}** and **ON18^{Zn}**:**ON19^{Ni}**. The inserts show the expanded porphyrin Soret band regions. Conditions: 10 mM sodium phosphate, 100 mM NaCl, pH 7.0, and 2 μM of each strand.

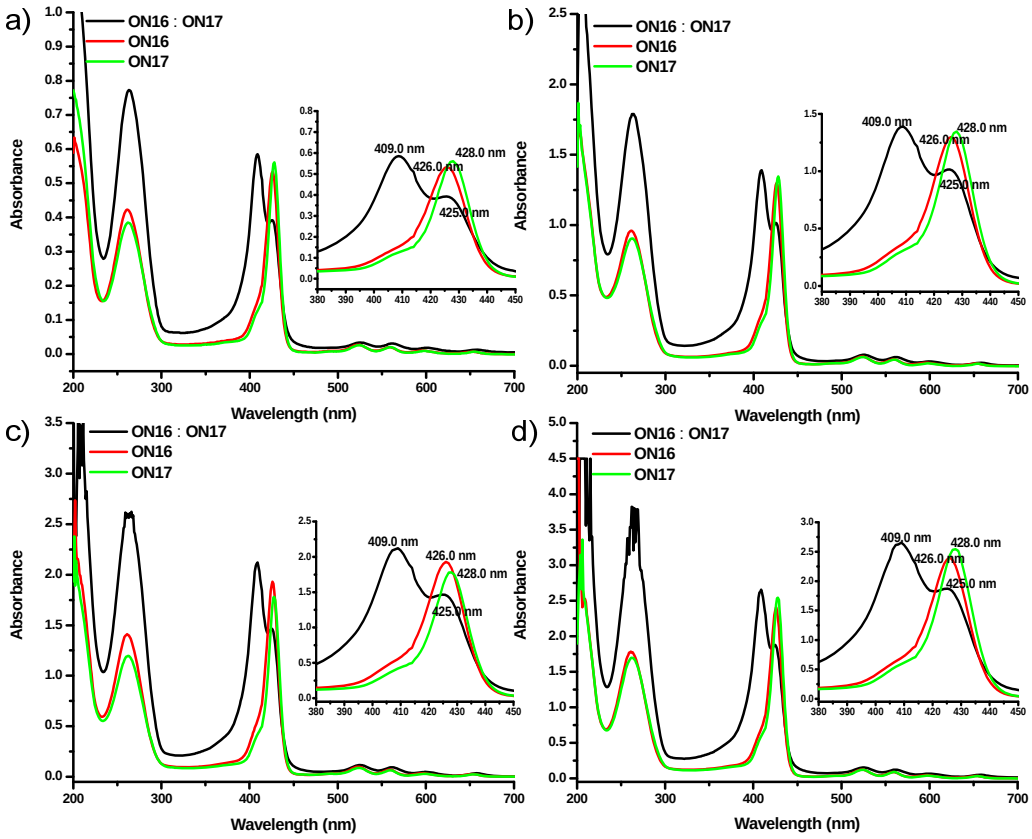


Figure S3: Concentration-dependent UV-vis spectra of single strands **ON16**, **ON17** and their duplex **ON16:ON17**. a) 2 μM of each strand; b) 4 μM of each strand; c) 6 μM of each strand; d) 8 μM of each strand. The inserts show the expanded porphyrin Soret band regions. Conditions: 10 mM sodium phosphate, 100 mM NaCl, pH 7.0.

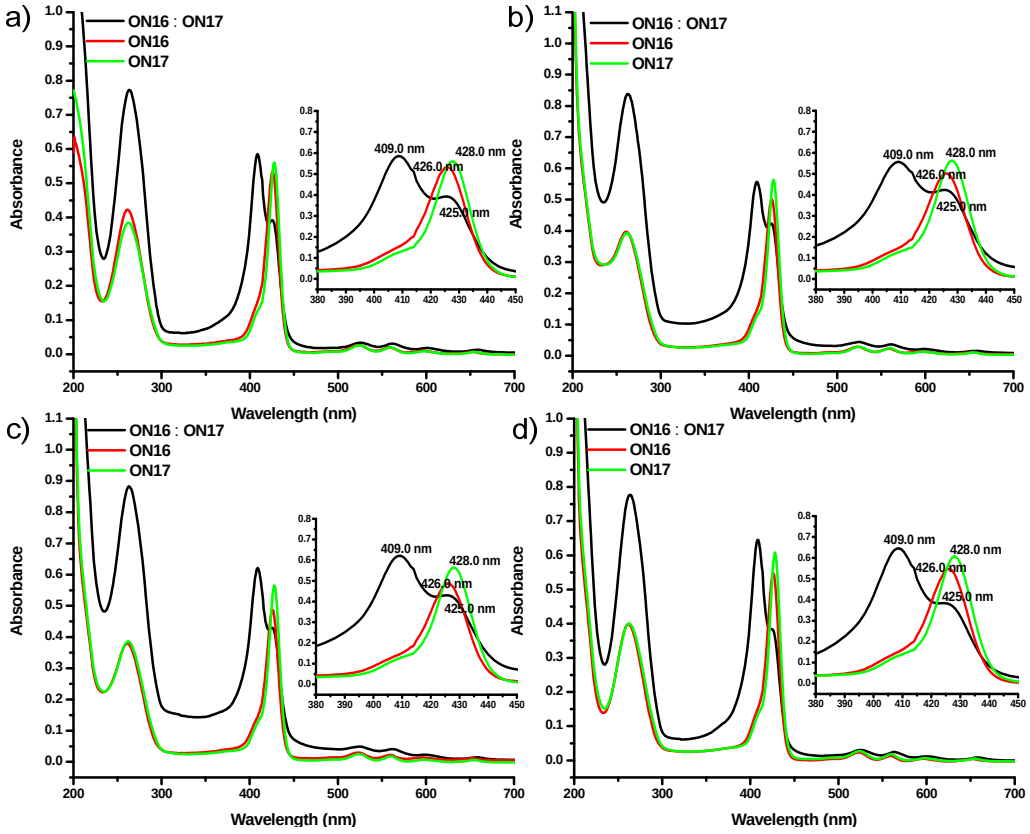


Figure S4: Salt concentration-dependent UV-vis spectra of single strands **ON16**, **ON17** and their duplex **ON16:ON17**. a) 100 mM NaCl; b) 200 mM NaCl; c) 400 mM NaCl; d) 800 mM NaCl. The inserts show the expanded porphyrin Soret band regions. Conditions: 10 mM sodium phosphate, pH 7.0, 2 μM of each strand.

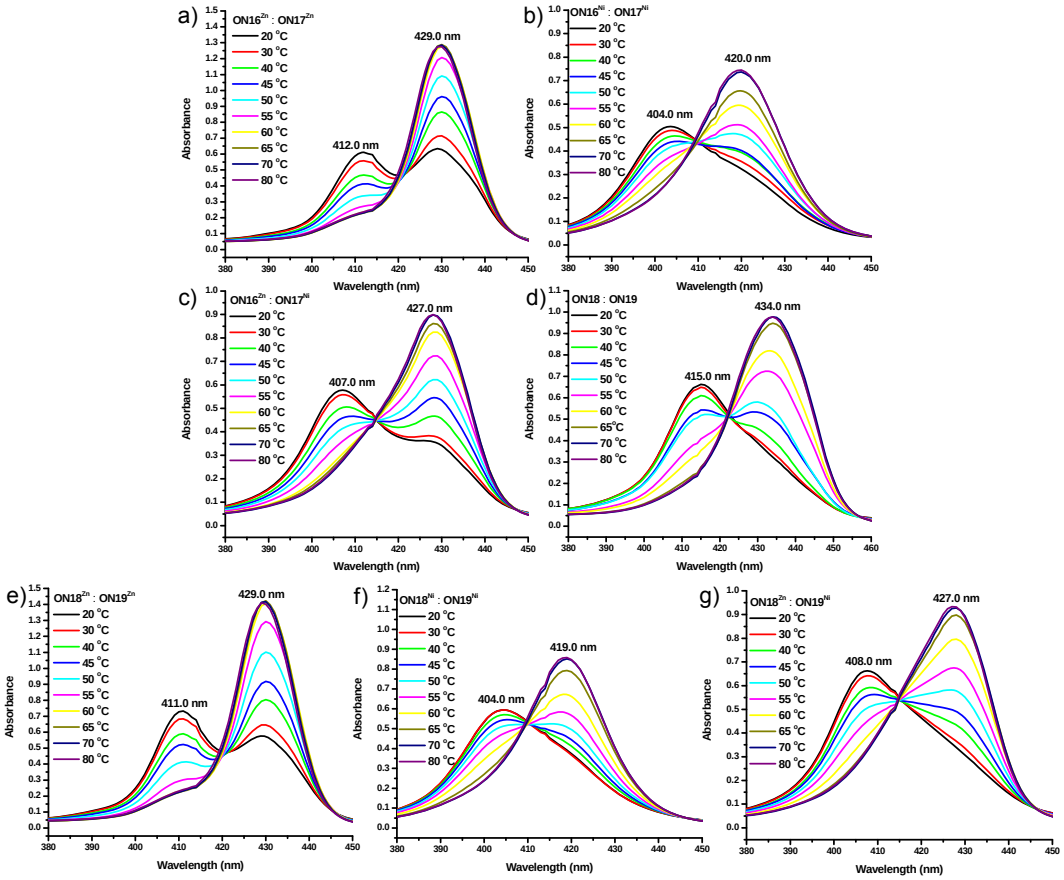


Figure S5: Temperature-dependent UV-vis spectra of duplexes. a) **ON16^{Zn}**:**ON17^{Zn}**; b) **ON16^{Ni}**:**ON17^{Ni}**; c) **ON16^{Zn}**:**ON17^{Ni}**; d) **ON18**:**ON19**; e) **ON18^{Zn}**:**ON19^{Zn}**; f) **ON18^{Ni}**:**ON19^{Ni}**; g) **ON18^{Zn}**:**ON19^{Ni}** at Soret band region. Conditions: 10 mM sodium phosphate, 100 mM NaCl, pH 7.0, 2 μM of each strand.

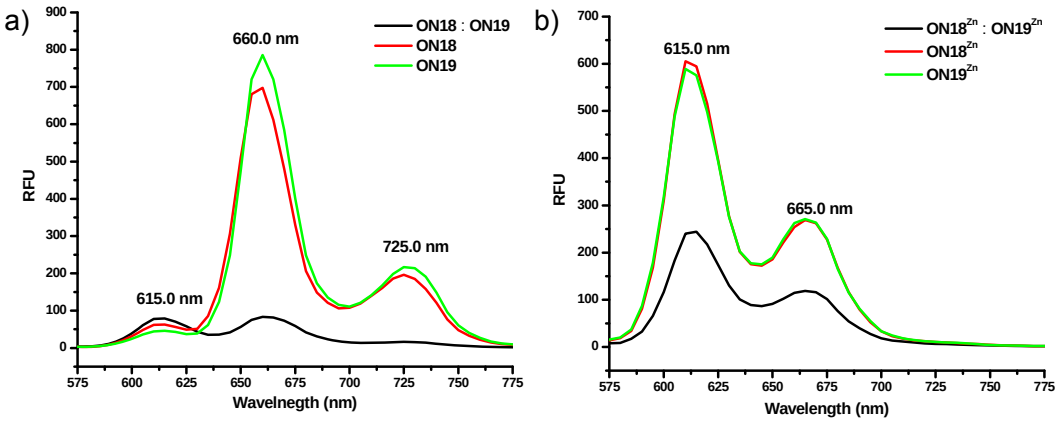
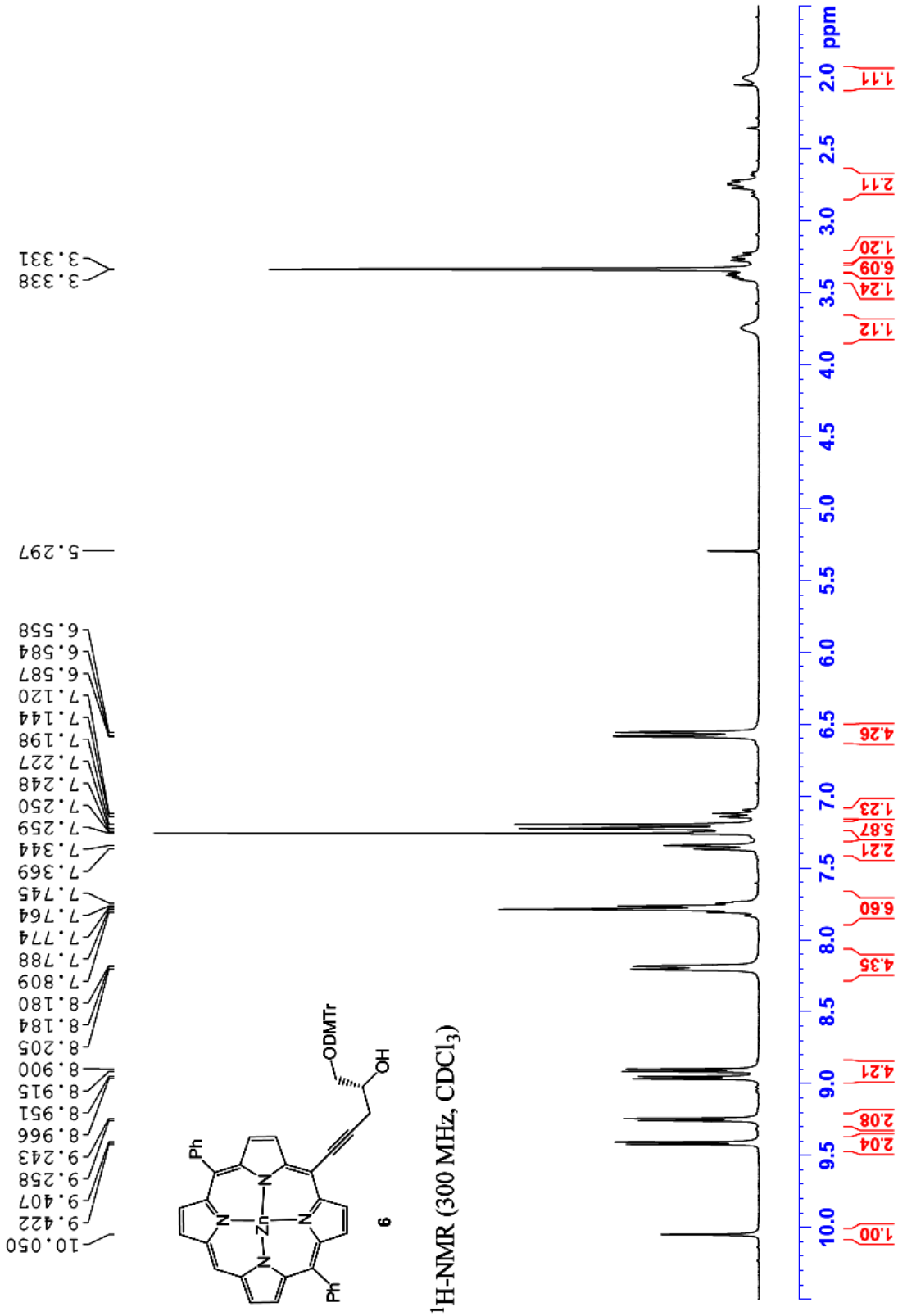


Figure S6: Fluorescence spectra of a) **ON18**, **ON19** and **ON18**:**ON19**; b) **ON18**^{Zn}, **ON19**^{Zn} and **ON18**^{Zn}:**ON19**^{Zn}. Conditions: 10 mM sodium phosphate, 100 mM NaCl, pH 7.0, and 2 μM of each strand.

Table S1. Maldi-TOF data of used oligonucleotides.

Name	Oligonucleotides	M_{calcd}	M_{found}
ON 1	3'-TAAAAATAATAATATT-2'	4222.7($C_{128}H_{167}N_{62}O_{74}P_{15}$)	4223.3
ON 2	3'-AATATTATTATTTTTA-2'	4186.6($C_{128}H_{171}N_{50}O_{82}P_{15}$)	4185.5
ON 3	3'-TAAAAATATAATATT-2'	3951.5($C_{120}H_{157}N_{57}O_{70}P_{14}$)	3949.3
ON 4	3'-AATATTATATTTTTA-2'	3924.5($C_{120}H_{160}N_{48}O_{76}P_{14}$)	3923.2
ON 5	3'-AATATTATAATTTTTA-2'	4195.7($C_{128}H_{170}N_{53}O_{80}P_{15}$)	4195.0
ON 6	3'-TAAAAATPATAATATT-2'	4574.1($C_{157}H_{184}N_{61}O_{74}P_{15}$)	4574.3
ON 6^{Zn}	3'-TAAAAATP^{Zn}ATAATATT-2'	4637.5($C_{157}H_{182}N_{61}O_{74}P_{15}Zn_1$)	4638.3
ON 6^{Ni}	3'-TAAAAATP^{Ni}ATAATATT-2'	4630.8($C_{157}H_{182}N_{61}Ni_1O_{74}P_{15}$)	4630.5
ON 7	3'-AATATTATHATTTTTA-2'	4048.5($C_{122}H_{165}N_{48}O_{80}P_{15}$)	4048.2
ON 8	3'-TAAAAATTAATATT-2'	3680.3($C_{112}H_{147}N_{52}O_{66}P_{13}$)	3678.2
ON 9	3'-AATATTAATTTTTA-2'	3662.3($C_{112}H_{149}N_{46}O_{70}P_{13}$)	3661.2
ON 10	3'-TAAAAATPHTAATATT-2'	4427.0($C_{151}H_{179}N_{56}O_{74}P_{15}$)	4434.2
ON 10^{Zn}	3'-TAAAAATP^{Zn}HTAATATT-2'	4490.4($C_{151}H_{177}N_{56}O_{74}P_{15}Zn_1$)	4498.1
ON 11	3'-AATATTA PHATTTTTA-2'	4408.9($C_{151}H_{181}N_{50}O_{78}P_{15}$)	4416.9
ON 11^{Zn}	3'-AATATTA P^{Zn} ATTTTTA-2'	4472.3($C_{151}H_{179}N_{50}O_{78}P_{15}Zn_1$)	4479.6
ON 12	3'-TTATAAAAATAATAATATTAAT-2'	5822.7($C_{176}H_{230}N_{83}O_{104}P_{21}$)	5821.5
ON 13	3'-ATTAATATTATTATTTTTATAA-2'	5786.6($C_{176}H_{234}N_{71}O_{112}P_{21}$)	5784.0
ON 14	3'-TTATAAAAATTAATATTAAT-2'	5280.3($C_{160}H_{210}N_{73}O_{96}P_{19}$)	5277.6
ON 15	3'-ATTAATATTAATTTTTATAA-2'	5262.3($C_{160}H_{212}N_{67}O_{100}$P19)	5260.5
ON 16	3'-TTATAAAAATPHTAATATTAAT-2'	6027.0($C_{199}H_{242}N_{77}O_{104}P_{21}$)	6025.8
ON 16^{Zn}	3'-TTATAAAAATP^{Zn}HTAATATTAAT-2'	6090.3($C_{199}H_{240}N_{77}O_{104}P_{21}Zn_1$)	6088.3
ON 16^{Ni}	3'-TTATAAAAATP^{Ni}HTAATATTAAT-2'	6083.6($C_{199}H_{240}N_{77}Ni_1O_{104}P_{21}$)	6082.2
ON 17	3'-ATTAATATTAPHATTTTTATAA-2'	6008.9($C_{199}H_{244}N_{71}O_{108}P_{21}$)	6006.6
ON 17^{Zn}	3'-ATTAATATTAP^{Zn}HATTTTTATAA-2'	6072.3($C_{199}H_{242}N_{71}O_{108}P_{21}Zn_1$)	6072.4
ON 17^{Ni}	3'-ATTAATATTAP^{Ni}HATTTTTATAA-2'	6065.6($C_{199}H_{242}N_{71}Ni_1O_{108}P_{21}$)	6068.0
ON 18	3'-TTATAAAAATHPTAATATTAAT-2'	6027.0($C_{199}H_{242}N_{77}O_{104}P_{21}$)	6027.1
ON 18^{Zn}	3'-TTATAAAAATHP^{Zn}TAATATTAAT-2'	6090.3($C_{199}H_{240}N_{77}O_{104}P_{21}Zn_1$)	6089.2
ON 18^{Ni}	3'-TTATAAAAATHP^{Ni}TAATATTAAT-2'	6083.6($C_{199}H_{240}N_{77}Ni_1O_{104}P_{21}$)	6082.4
ON 19	3'-ATTAATATTAHPATTTTTATAA-2'	6008.9($C_{199}H_{244}N_{71}O_{108}P_{21}$)	6006.7
ON 19^{Zn}	3'-ATTAATATTAHP^{Zn}ATTTTTATAA-2'	6072.3($C_{199}H_{242}N_{71}O_{108}P_{21}Zn_1$)	6072.4
ON 19^{Ni}	3'-ATTAATATTAHP^{Ni}ATTTTTATAA-2'	6065.6($C_{199}H_{242}N_{71}Ni_1O_{108}P_{21}$)	6064.8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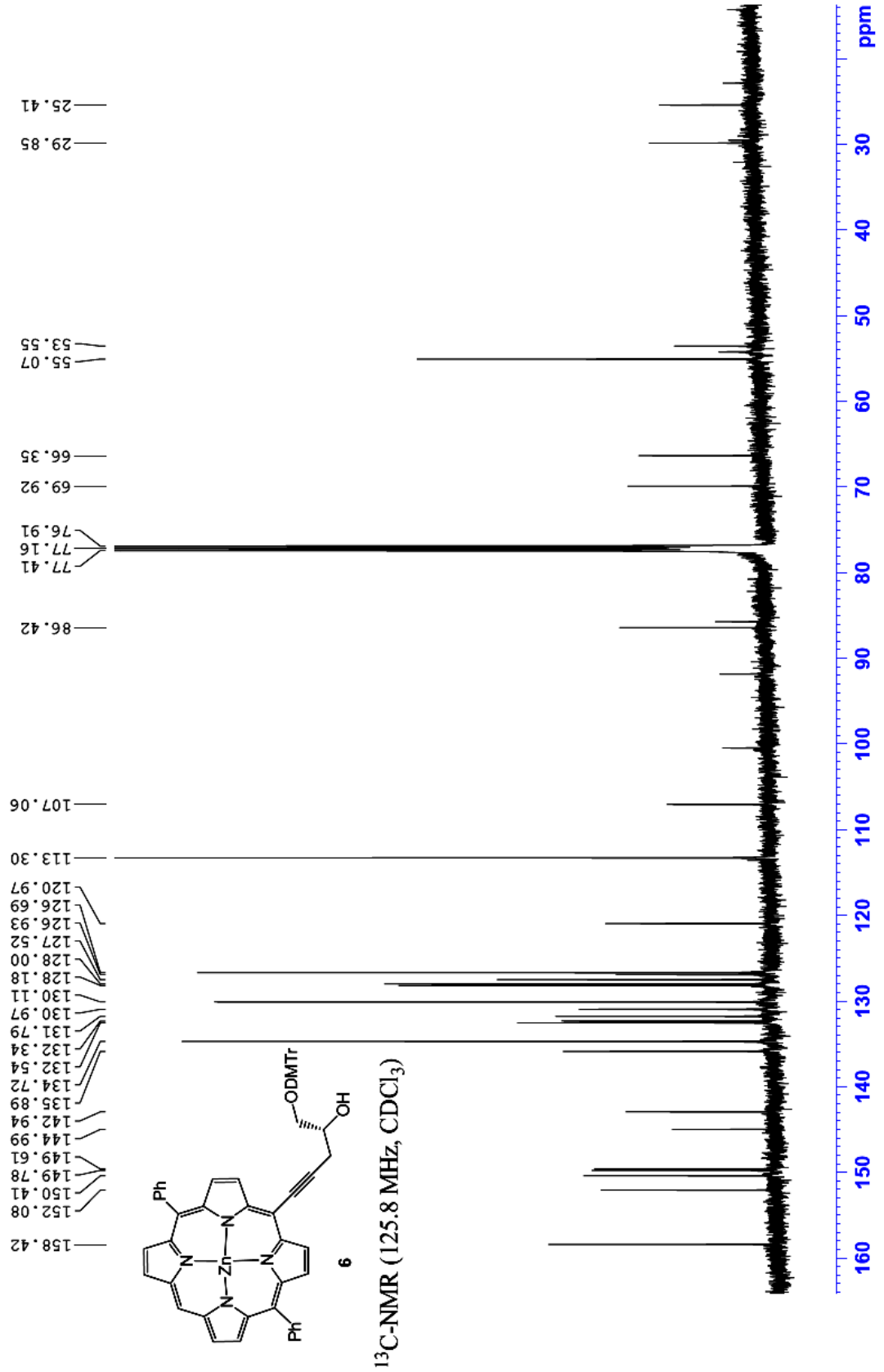
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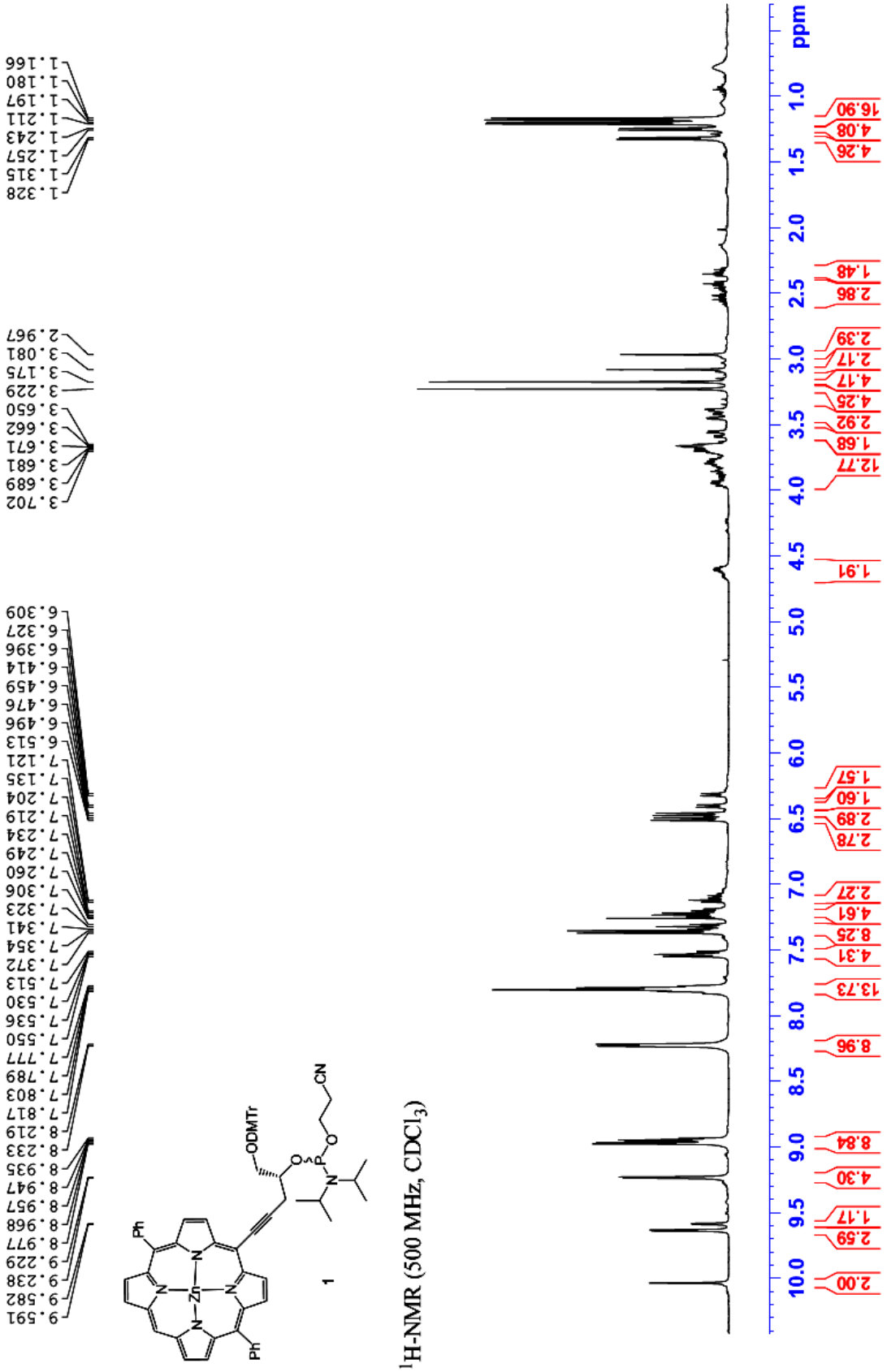
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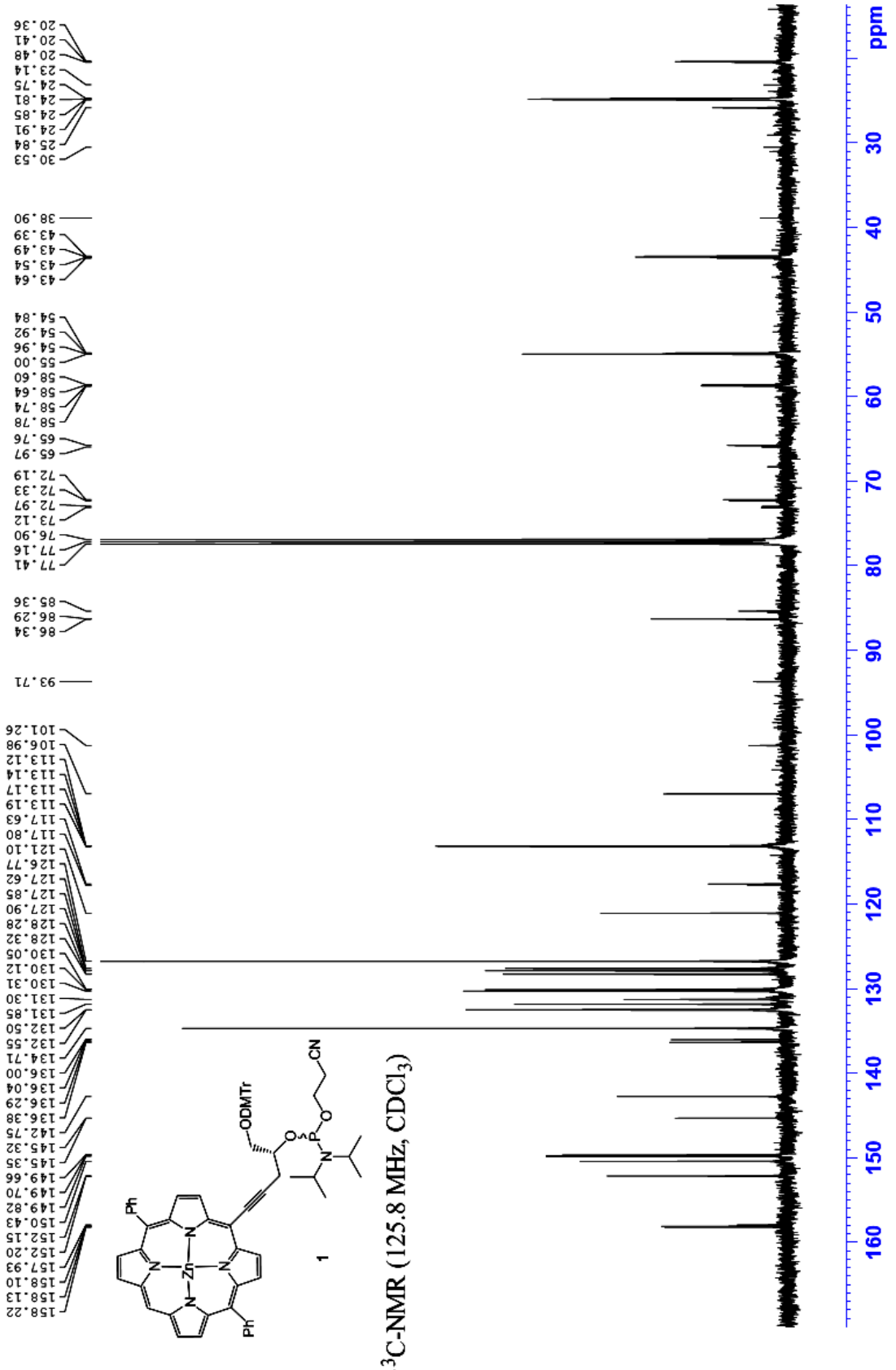
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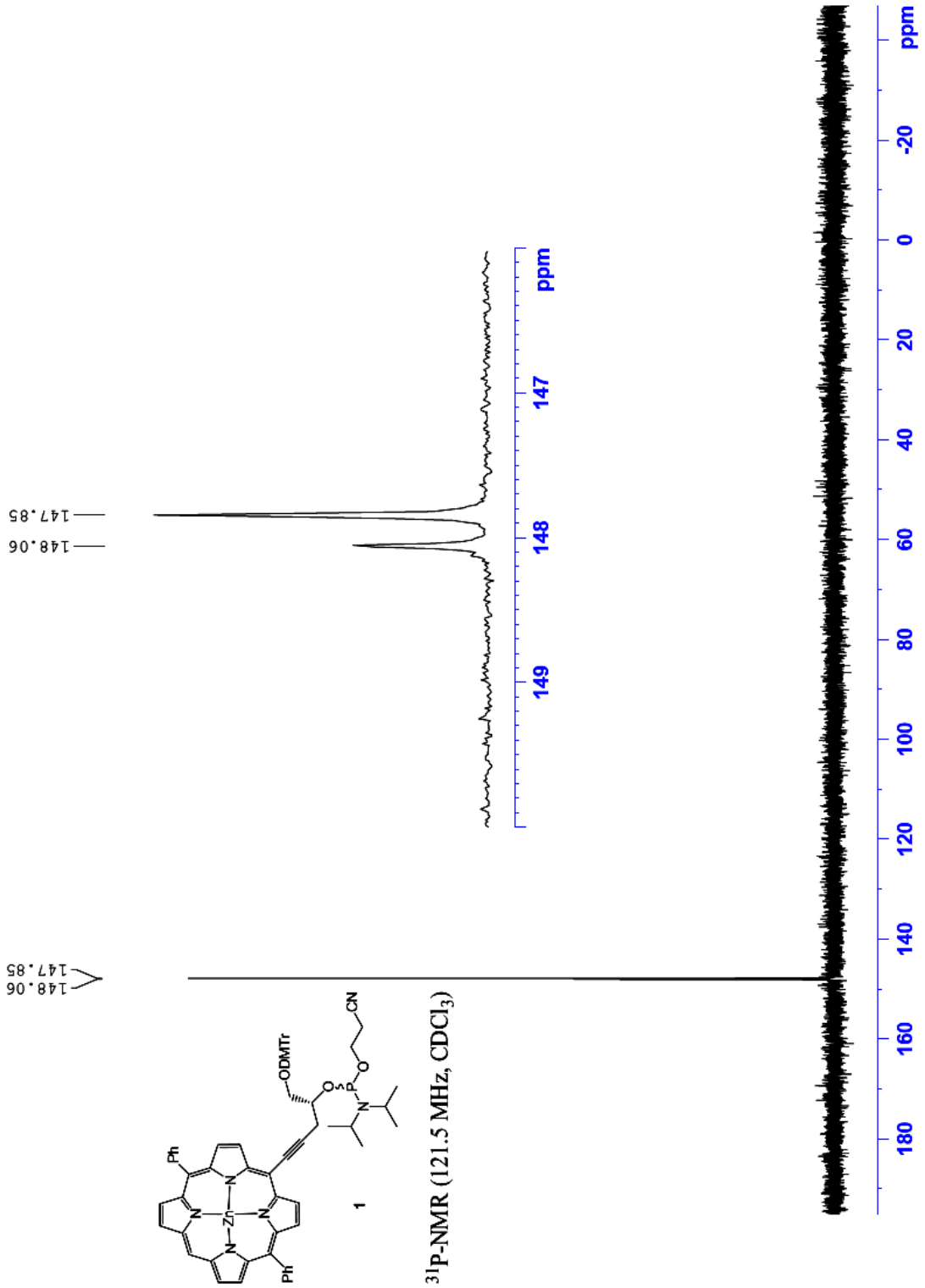
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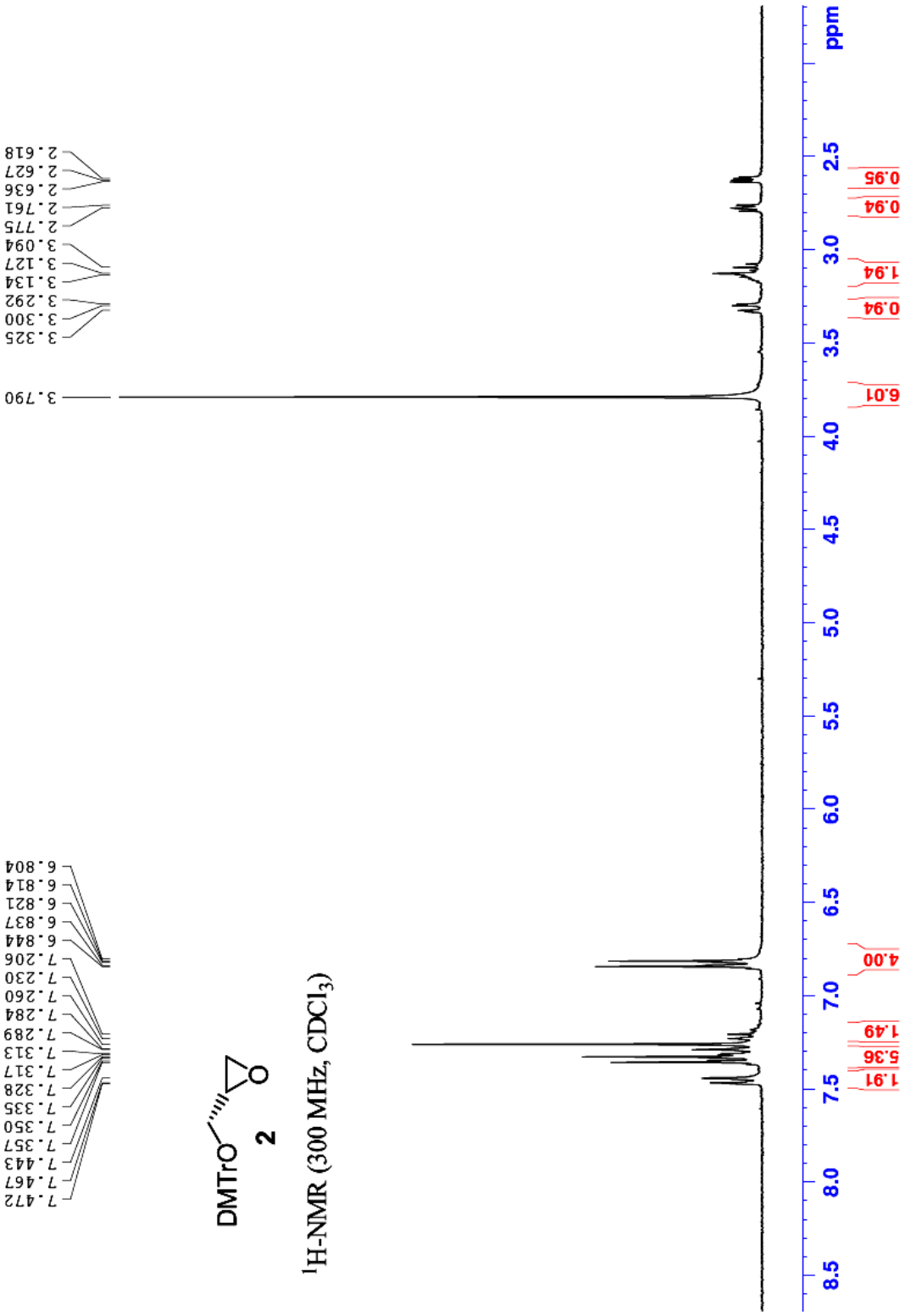
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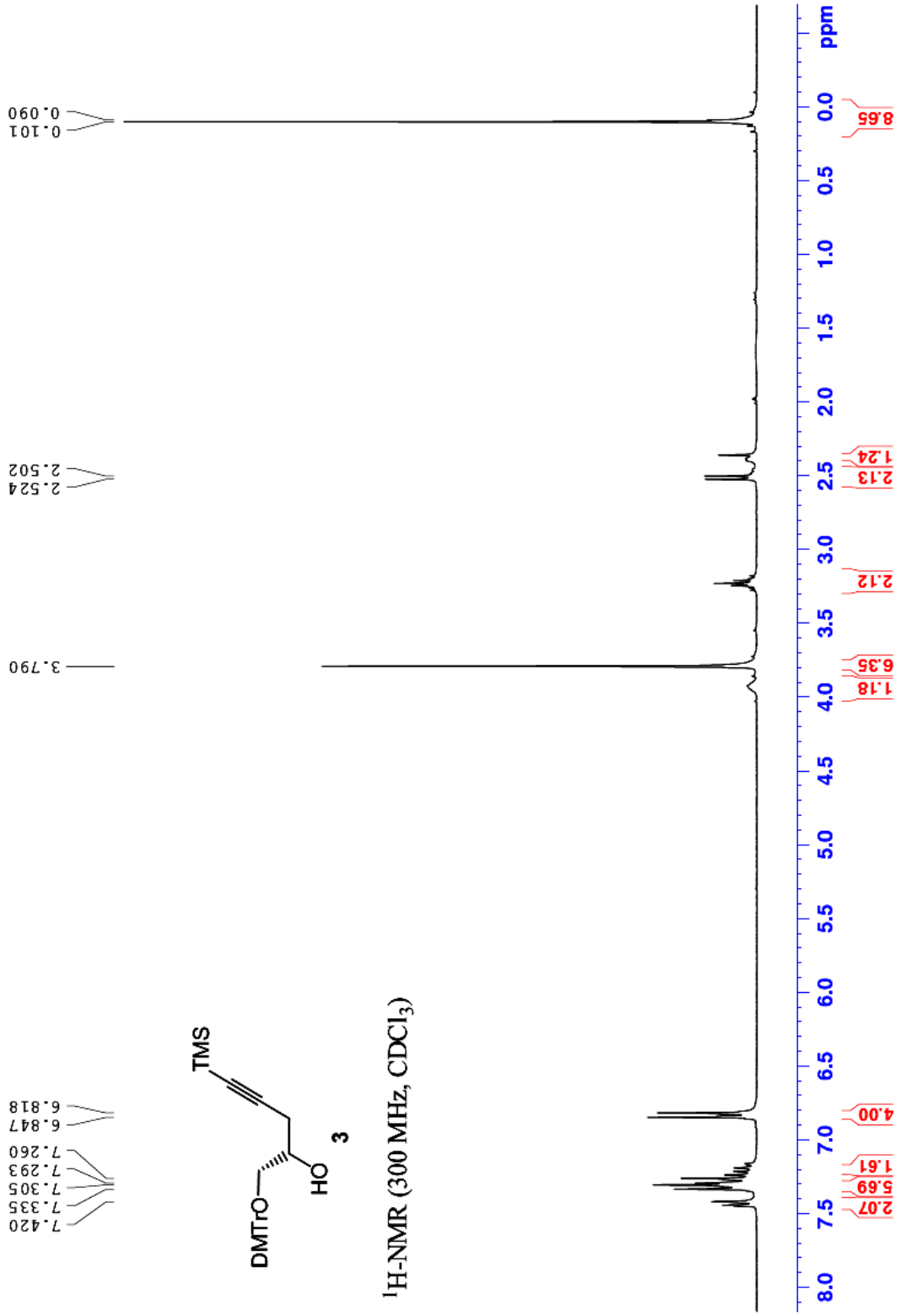
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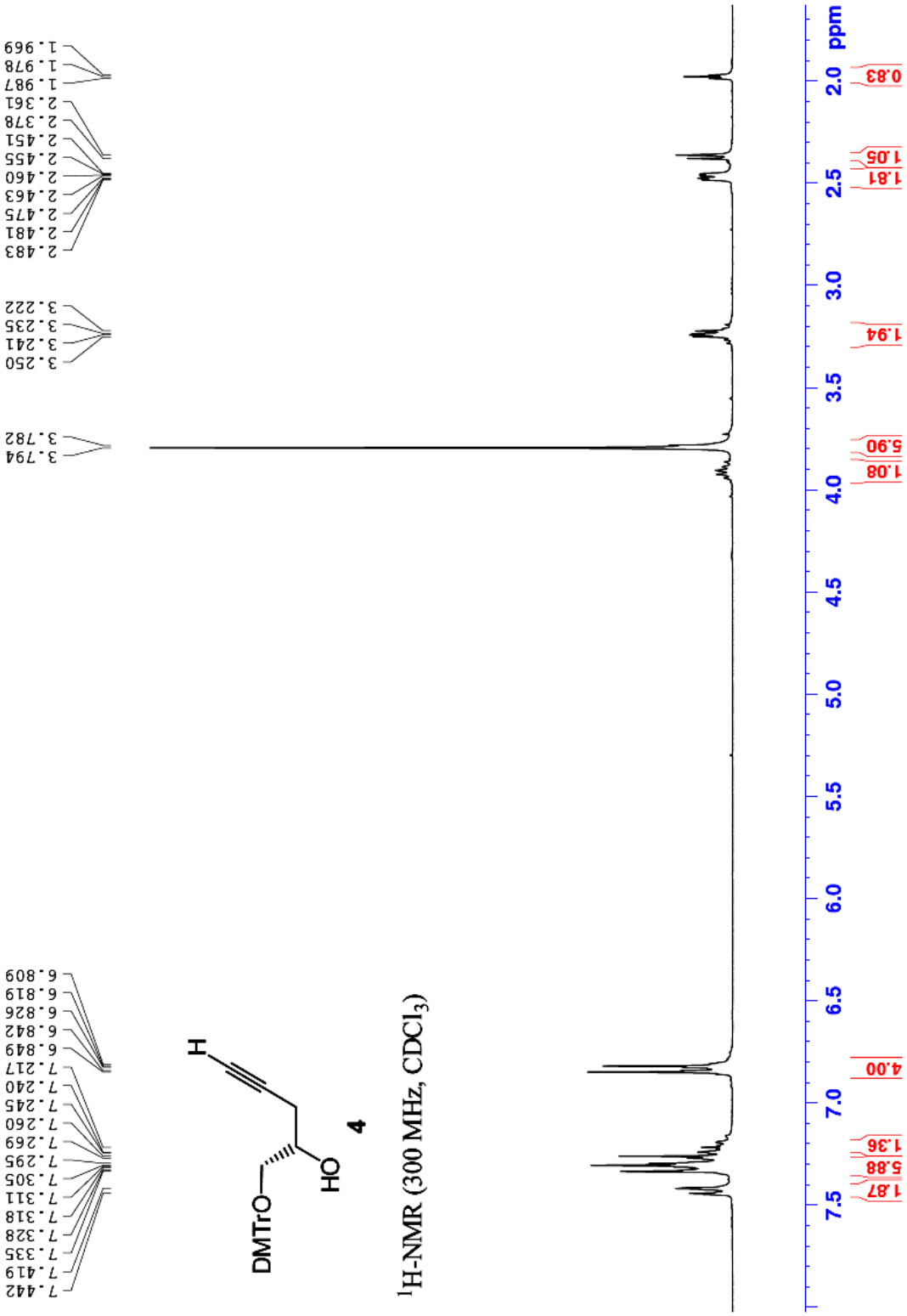
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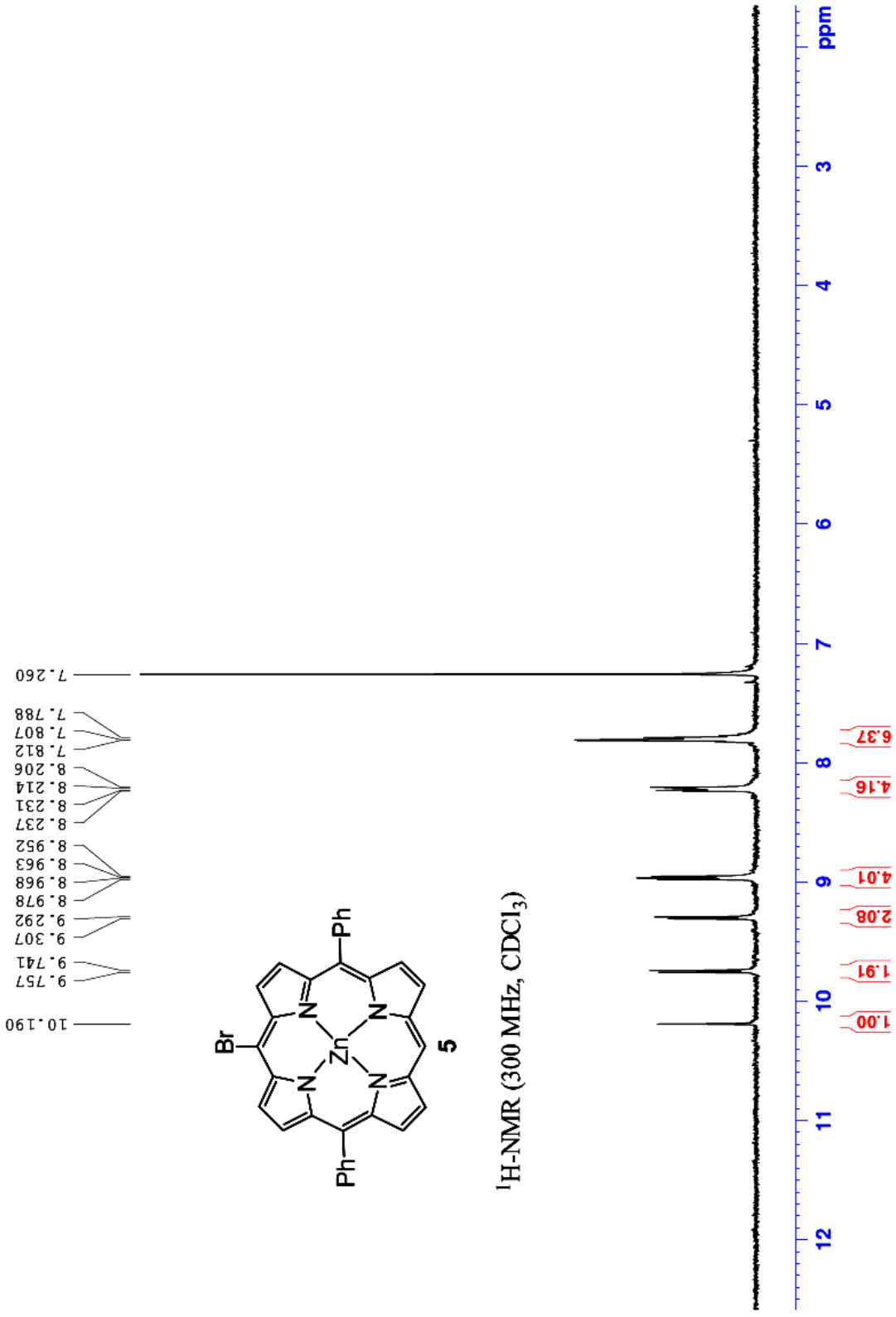
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Ph
Ph
Zn
N
N
N
N
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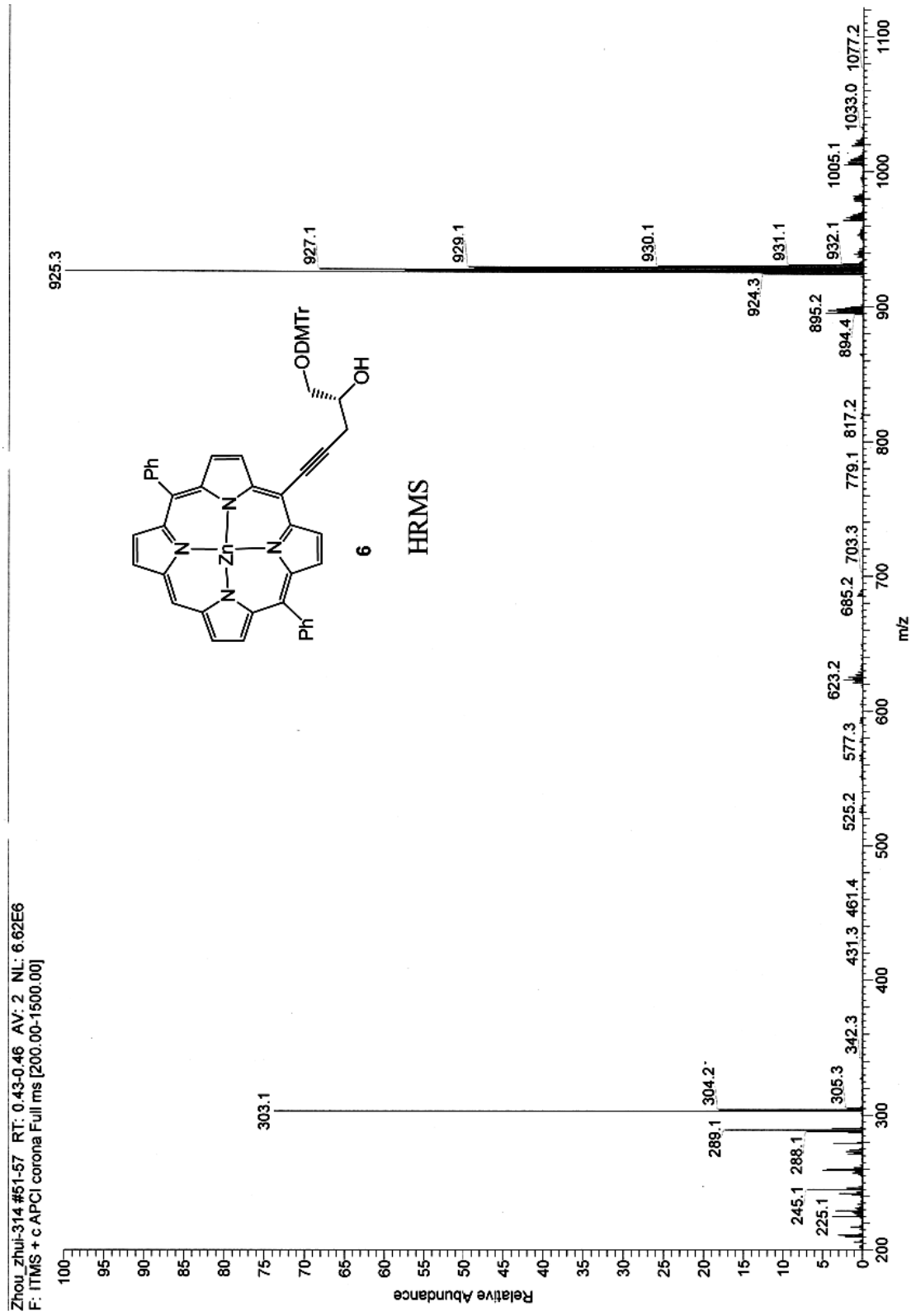
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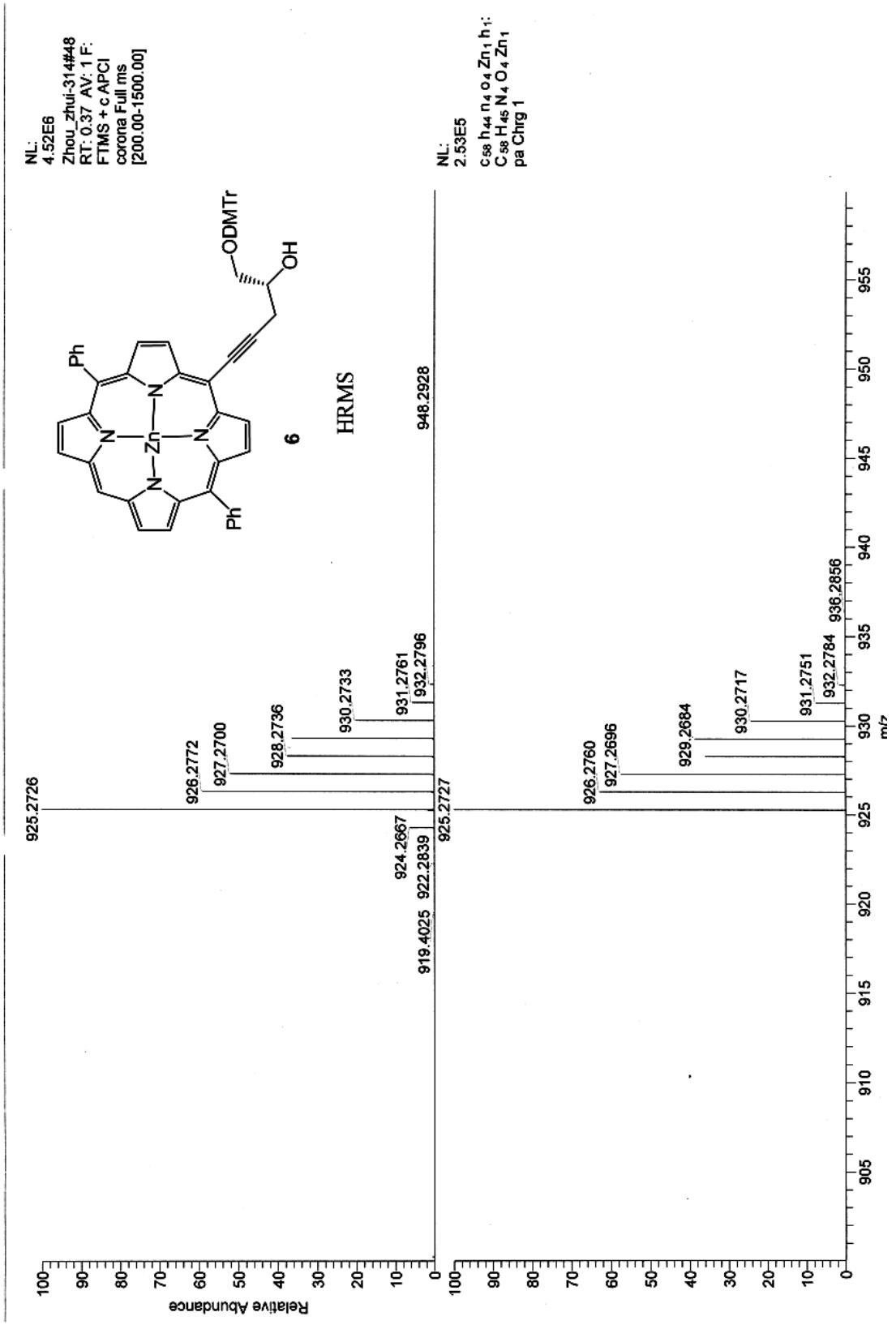
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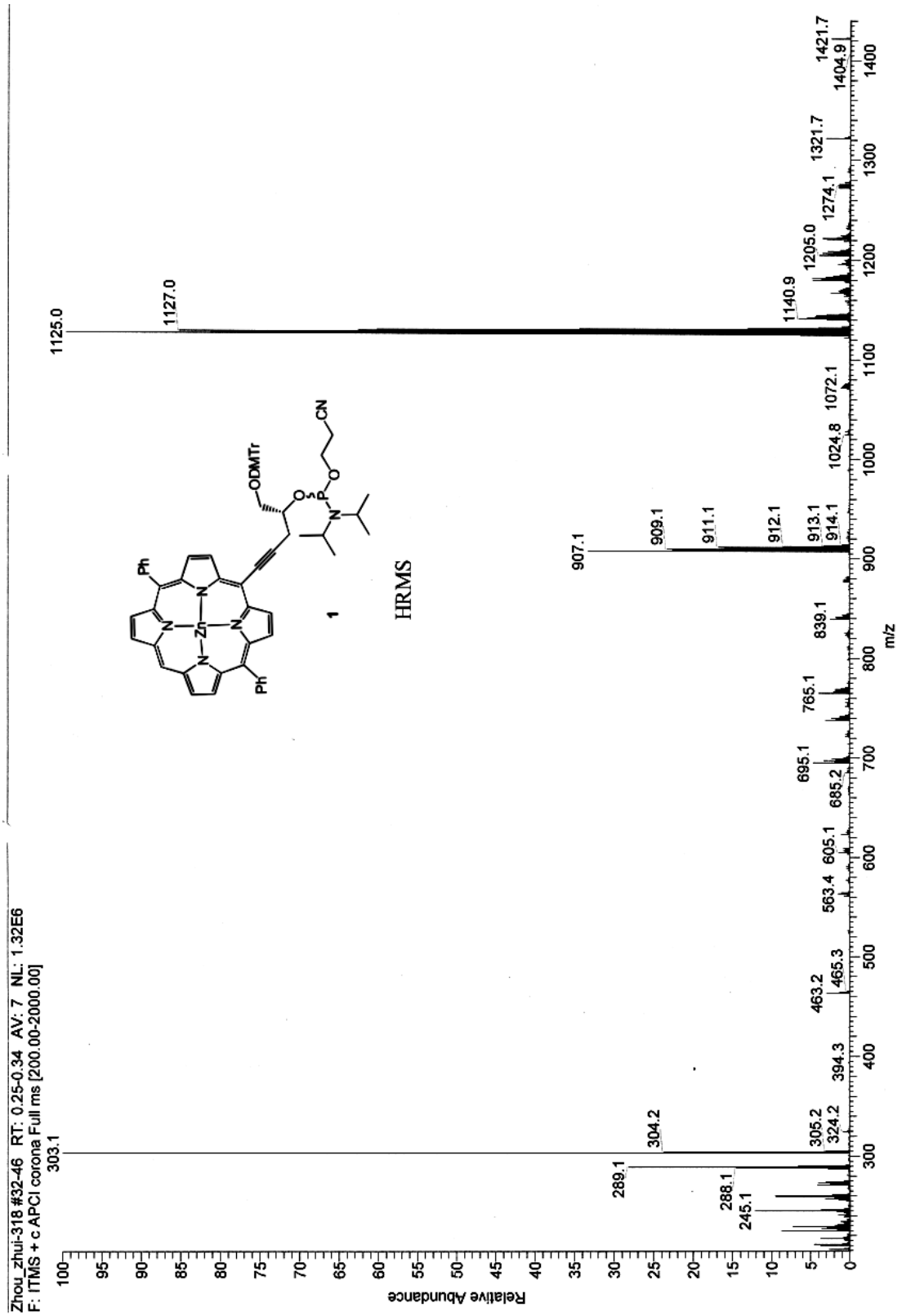
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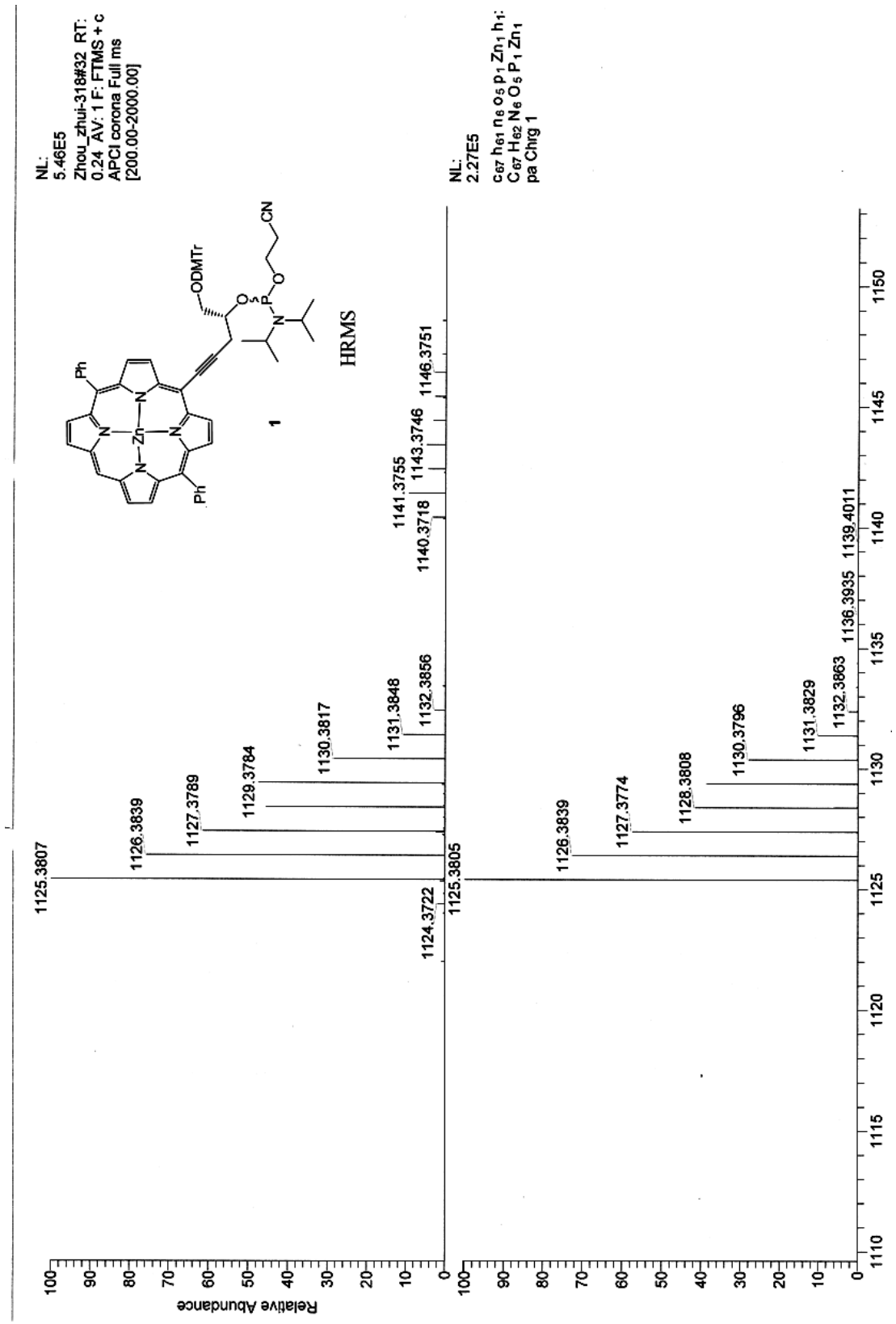
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