Supplementary Information

Pyrene Acetylide Nucleotides in GNA: Probing Duplex Formation and Sensing of Copper(II) Ions

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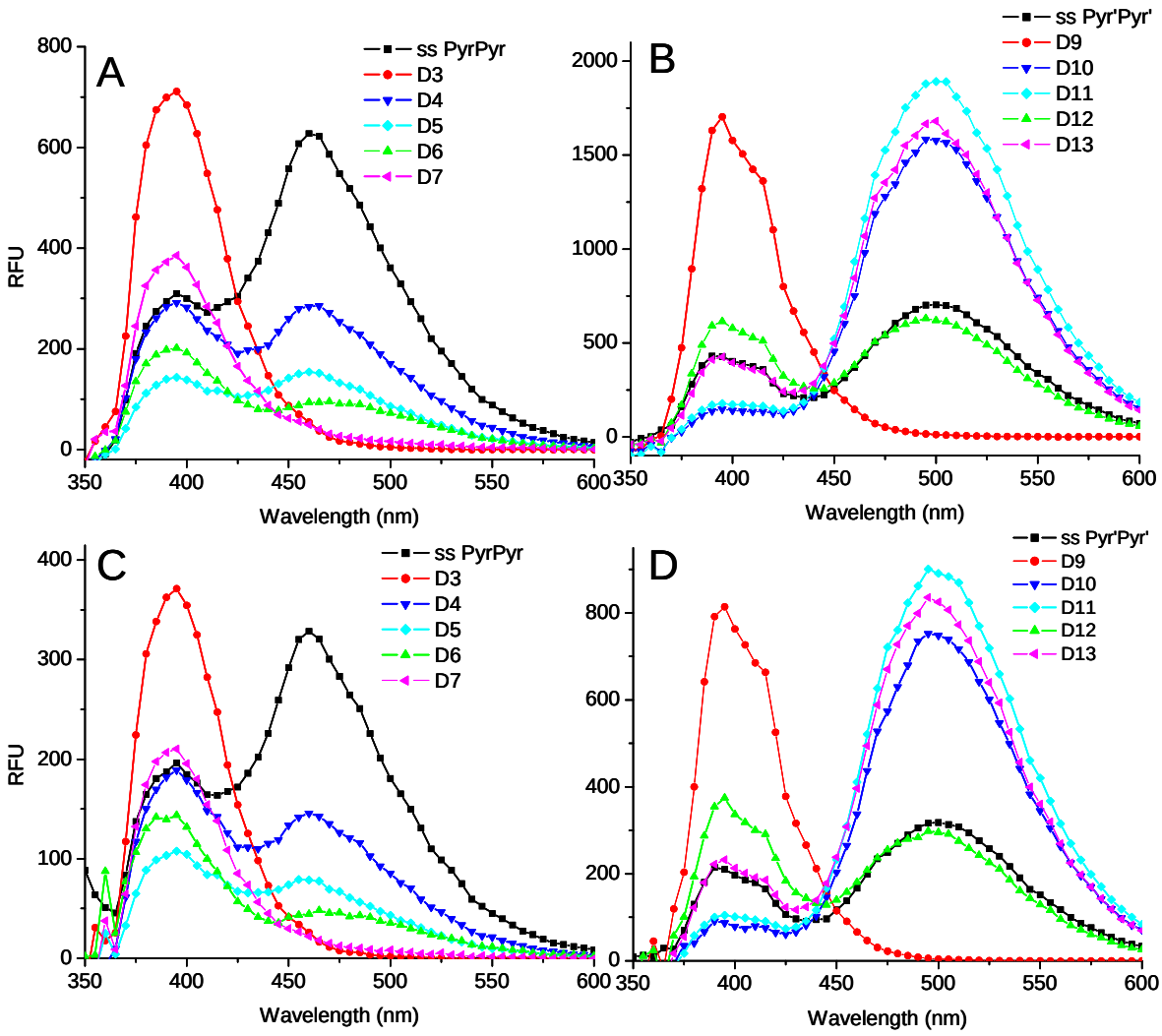


Figure S1: Fluorescence properties of pyrene and pyrene acetylide nucleotides in GNA at different duplex concentrations. Conditions: 10 mM sodium phosphate, 100 mM NaCl, pH 7.0. A) Pyrene containing duplexes at 4 μM of each strand. B) Pyrene acetylide containing duplexes at 4 μM of each strand. C) Pyrene containing duplexes at 2 μM of each strand. D) Pyrene acetylide containing duplexes at 2μM of each stand. See main text for sequence information.

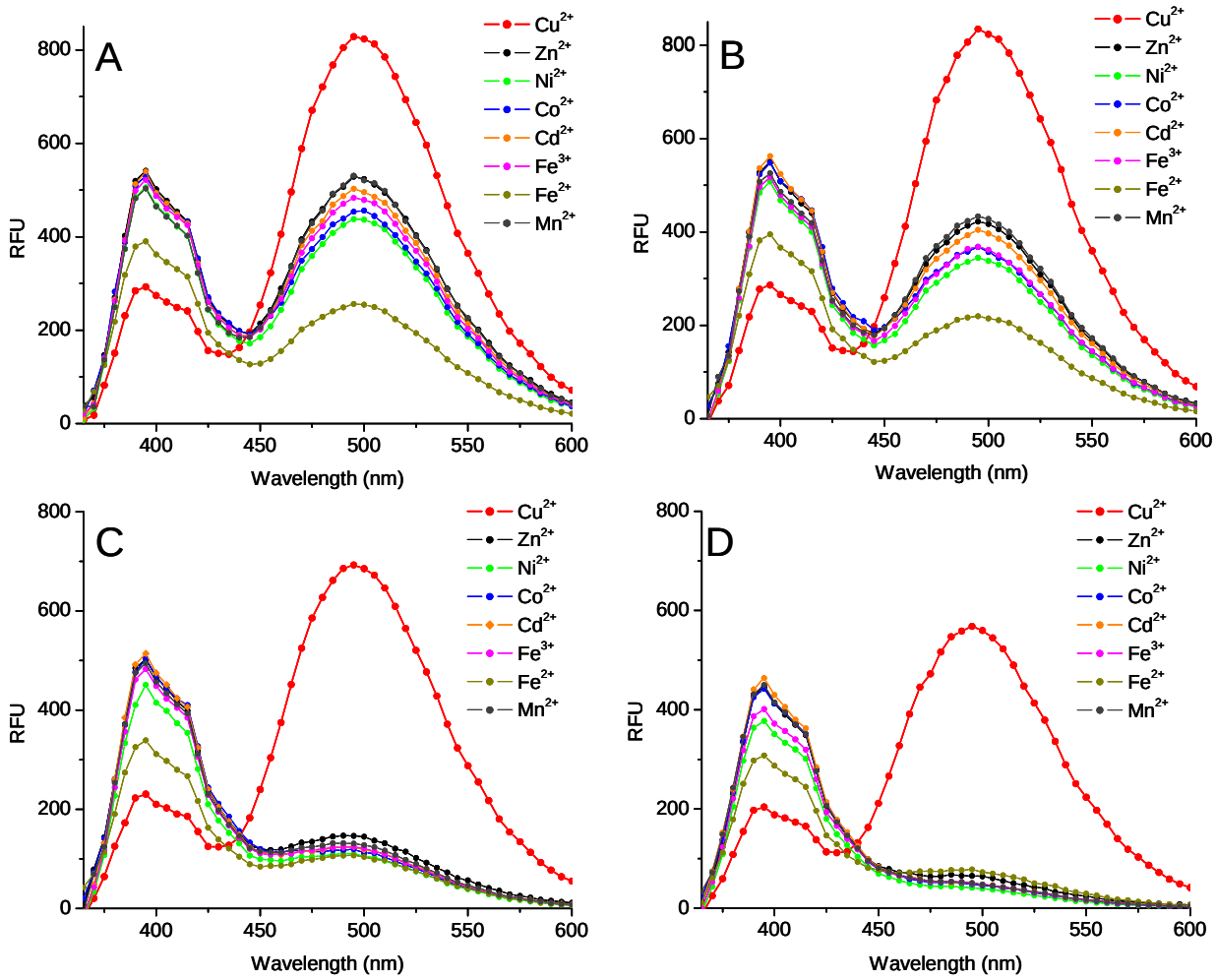
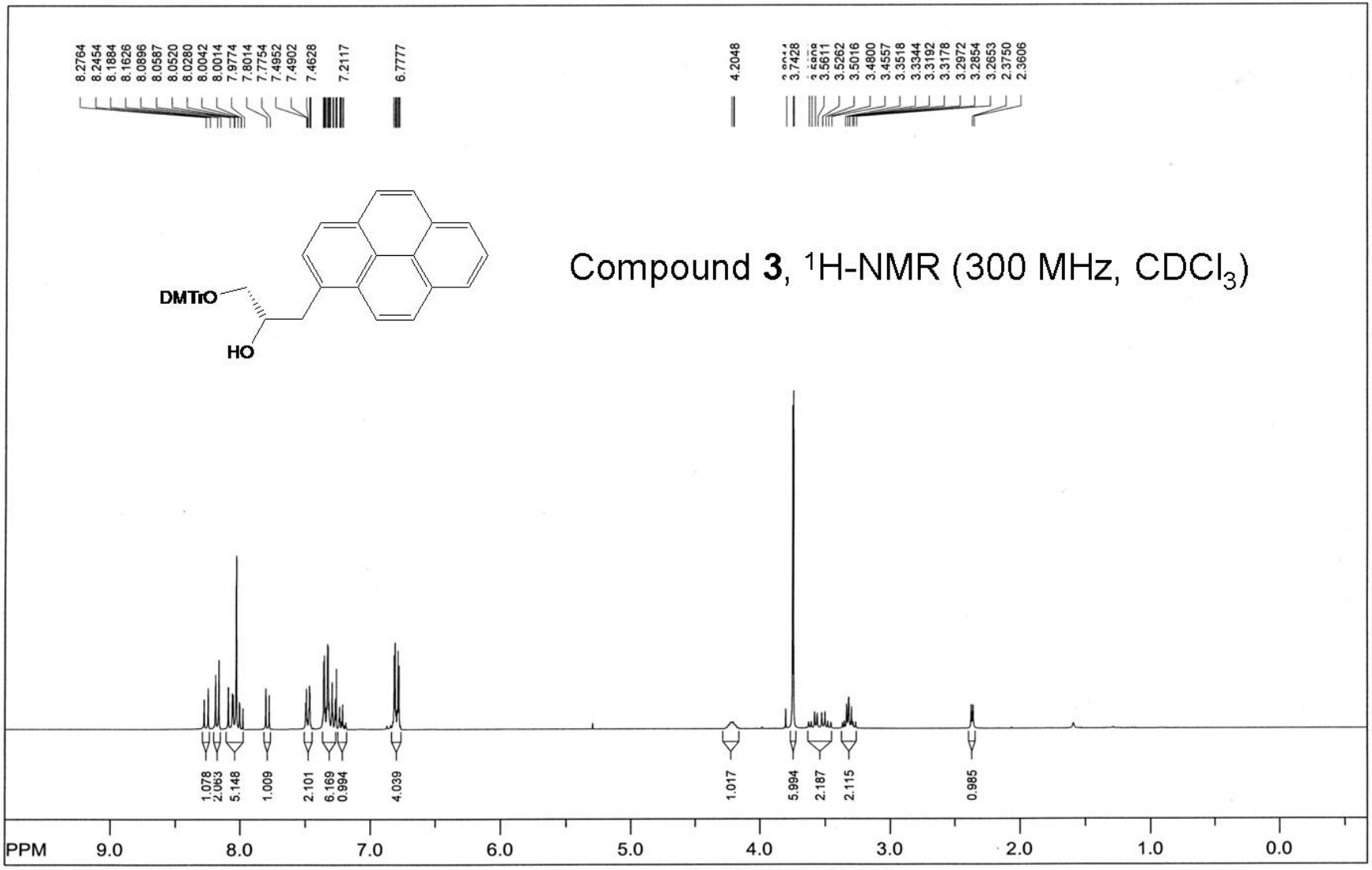


Figure S2: Metal ion-selectivity at different temperatures. Conditions: 10 mM sodium phosphate, 50 mM NaCl, pH 7.0, and 2 μM each strand of duplex D14. A) 25 °C, B) 40 °C, C) 50 °C, D) 60 °C.

Table S1. Maldi-TOF data of used oligonucleotides.

Name	Oligonucleotides	M_{calcd}	M_{found}
D1	3'-TAAAAATAATAATATT-2'	4222.7 ($C_{128}H_{167}N_{62}O_{74}P_{15}$)	4223.3
	2'-ATTTTTATTATTATAA-3'	4186.6 ($C_{128}H_{171}N_{50}O_{82}P_{15}$)	4185.5
D2	3'-TAAAAATHATAATATT-2'	4075.5 ($C_{122}H_{162}N_{57}O_{74}P_{15}$)	4076.0
	2'-ATTTTTAPyrTATTATAA-3'	4262.8 ($C_{139}H_{175}N_{48}O_{80}P_{15}$)	4261.8
D3	3'-TAAAAATMeATAATATT-2'	4089.6 ($C_{123}H_{164}N_{57}O_{74}P_{15}$)	4090.3
	2'-ATTTTTAPyrTATTATAA-3'	4262.8 ($C_{139}H_{175}N_{48}O_{80}P_{15}$)	4261.8
D4	3'-TAAAAATMeMeTAATATT-2'	3956.5 ($C_{118}H_{161}N_{52}O_{74}P_{15}$)	3956.5
	2'-ATTTTTAPyrPyrATTATAA-3'	4338.9 ($C_{150}H_{179}N_{46}O_{78}P_{15}$)	4339.1
D5	3'-TAAAAATPyrPyrTAATATT-2'	4356.9 ($C_{150}H_{177}N_{52}O_{74}P_{15}$)	4356.0
	2'-ATTTTTAMeMeATTATAA-3'	3938.4 ($C_{118}H_{163}N_{46}O_{78}P_{15}$)	3938.1
D6	3'-TAAAAATMePyrTAATATT-2'	4156.7 ($C_{134}H_{169}N_{52}O_{74}P_{15}$)	4155.9
	2'-ATTTTTAPyrMeATTATAA-3'	4138.7 ($C_{134}H_{171}N_{46}O_{78}P_{15}$)	4137.5
D7	3'-TAAAAATPyrMeTAATATT-2'	4156.7 ($C_{134}H_{169}N_{52}O_{74}P_{15}$)	4156.5
	2'-ATTTTTAMePyrATTATAA-3'	4138.7 ($C_{134}H_{171}N_{46}O_{78}P_{15}$)	4137.7
D8	3'-TAAAAATPyr'ATAATATT-2'	4313.8 ($C_{141}H_{172}N_{57}O_{74}P_{15}$)	4313.9
	2'-ATTTTTAMeTATTATAA-3'	4062.5 ($C_{123}H_{167}N_{48}O_{80}P_{15}$)	4062.8
D9	3'-TAAAAATPyr'ATAATATT-2'	4313.8 ($C_{141}H_{172}N_{57}O_{74}P_{15}$)	4313.9
	2'-ATTTTTAHTATTATAA-3'	4048.5 ($C_{122}H_{165}N_{48}O_{80}P_{15}$)	4048.2
D10	3'-TAAAAATHHTAATATT-2'	3928.4 ($C_{116}H_{157}N_{52}O_{74}P_{15}$)	3928.2
	2'-ATTTTTAPyr'Pyr'ATTATAA-3'	4386.9 ($C_{154}H_{179}N_{46}O_{78}P_{15}$)	4387.1
D11	3'-TAAAAATPyr'Pyr'TAATATT-2'	4404.9 ($C_{154}H_{177}N_{52}O_{74}P_{15}$)	4405.2
	2'-ATTTTTAHHATTATAA-3'	3910.3 ($C_{116}H_{159}N_{46}O_{78}P_{15}$)	3910.0
D12	3'-TAAAAATHPyr'TAATATT-2'	4166.7 ($C_{135}H_{167}N_{52}O_{74}P_{15}$)	4165.4
	2'-ATTTTTAPyr'HTTATAA-3'	4148.7 ($C_{135}H_{169}N_{46}O_{78}P_{15}$)	4147.1
D13	3'-TAAAAATPyr'HTAATATT-2'	4166.7 ($C_{135}H_{167}N_{52}O_{74}P_{15}$)	4166.5
	2'-ATTTTTAHPyr'ATTATAA-3'	4148.7 ($C_{135}H_{169}N_{46}O_{78}P_{15}$)	4148.3
D14	3'-TATAPyr'HTAATMTAAA-2'	3894.5 ($C_{128}H_{158}N_{46}O_{70}P_{14}$)	3893.3
	2'-ATATHPyr'ATTAMATTT-3'	3876.5 ($C_{128}H_{160}N_{40}O_{74}P_{14}$)	3875.6



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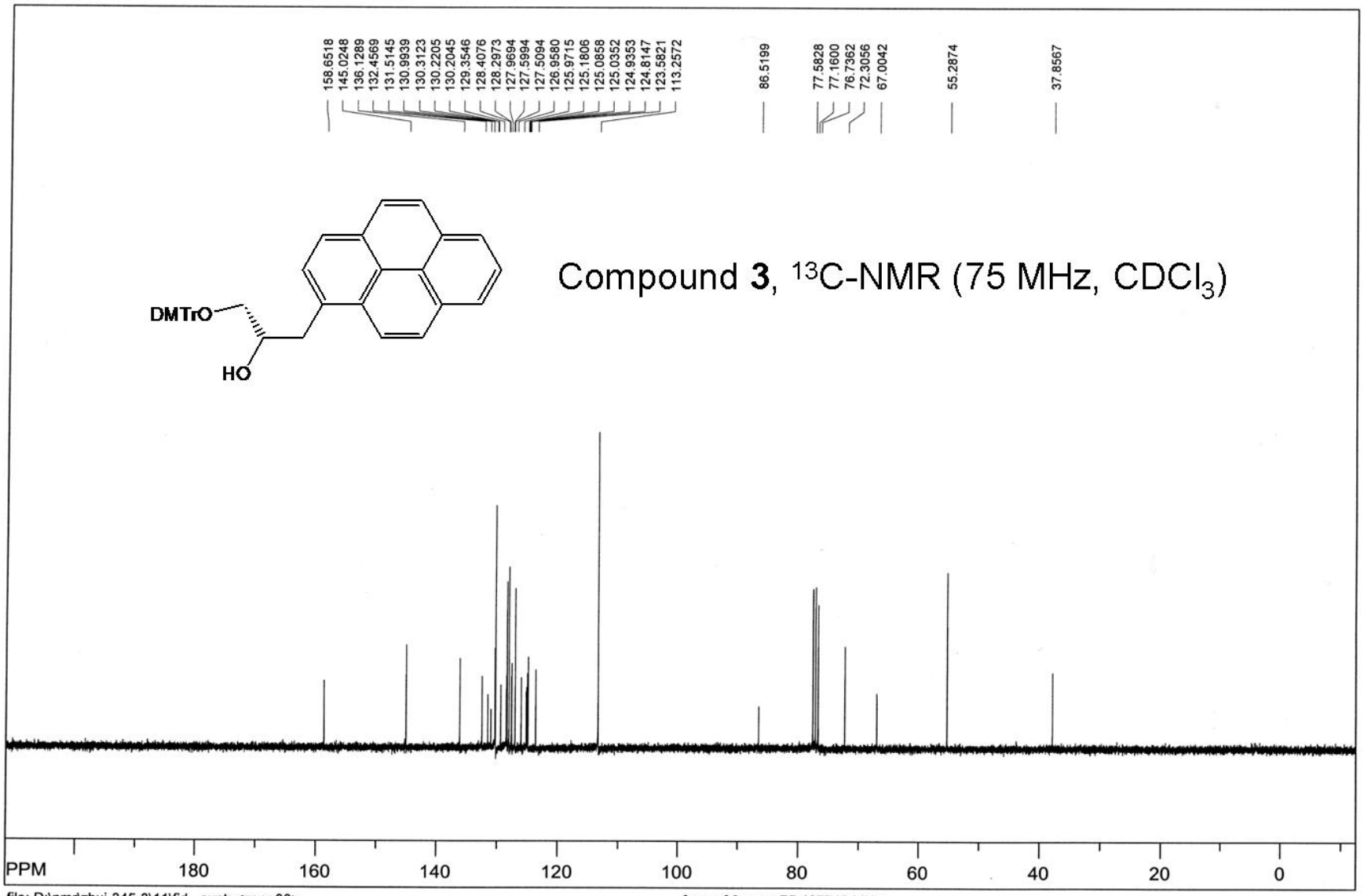

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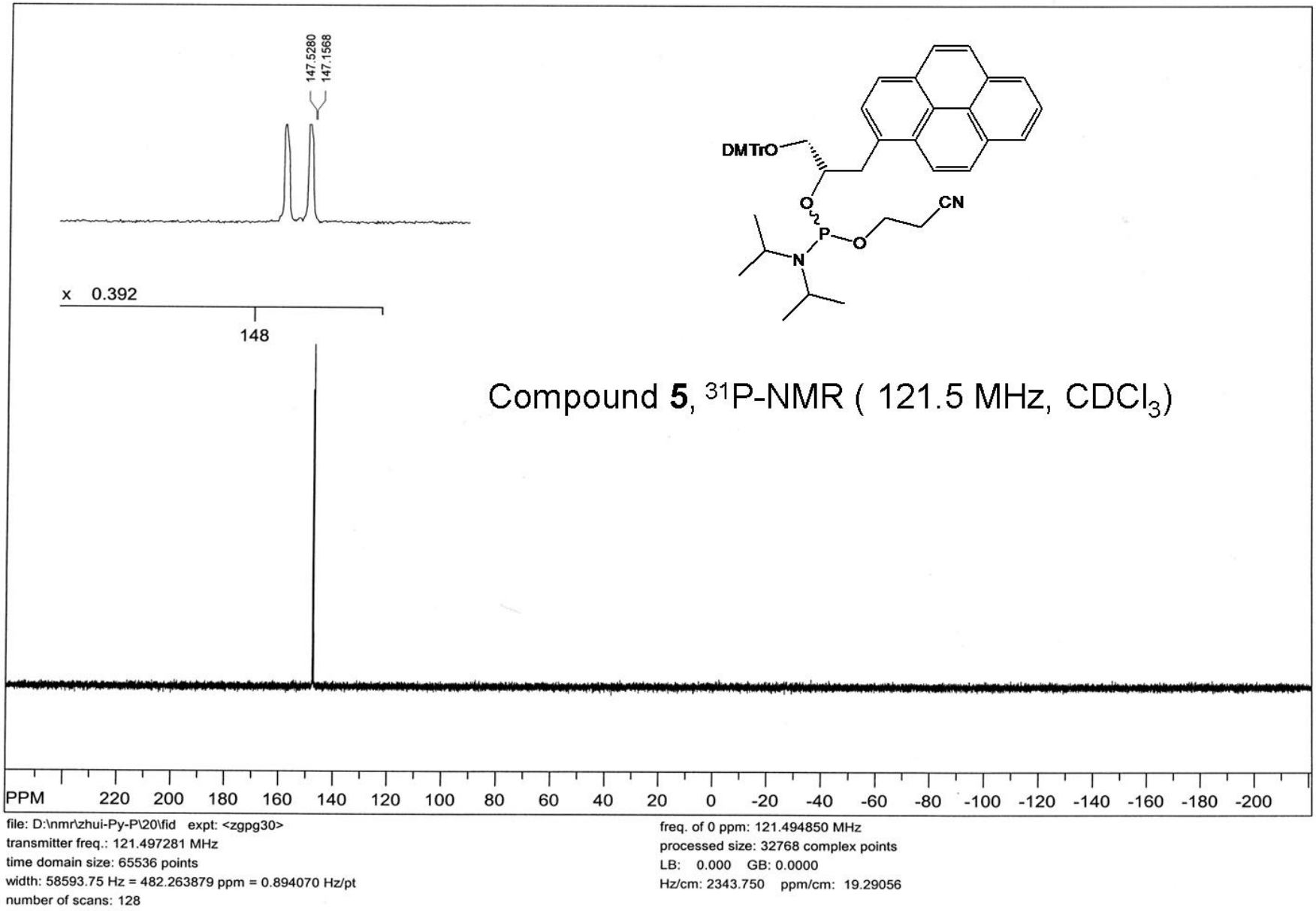
147.5280
147.1568
x 0.392
148
DMTrO
O
P
O
N
CN
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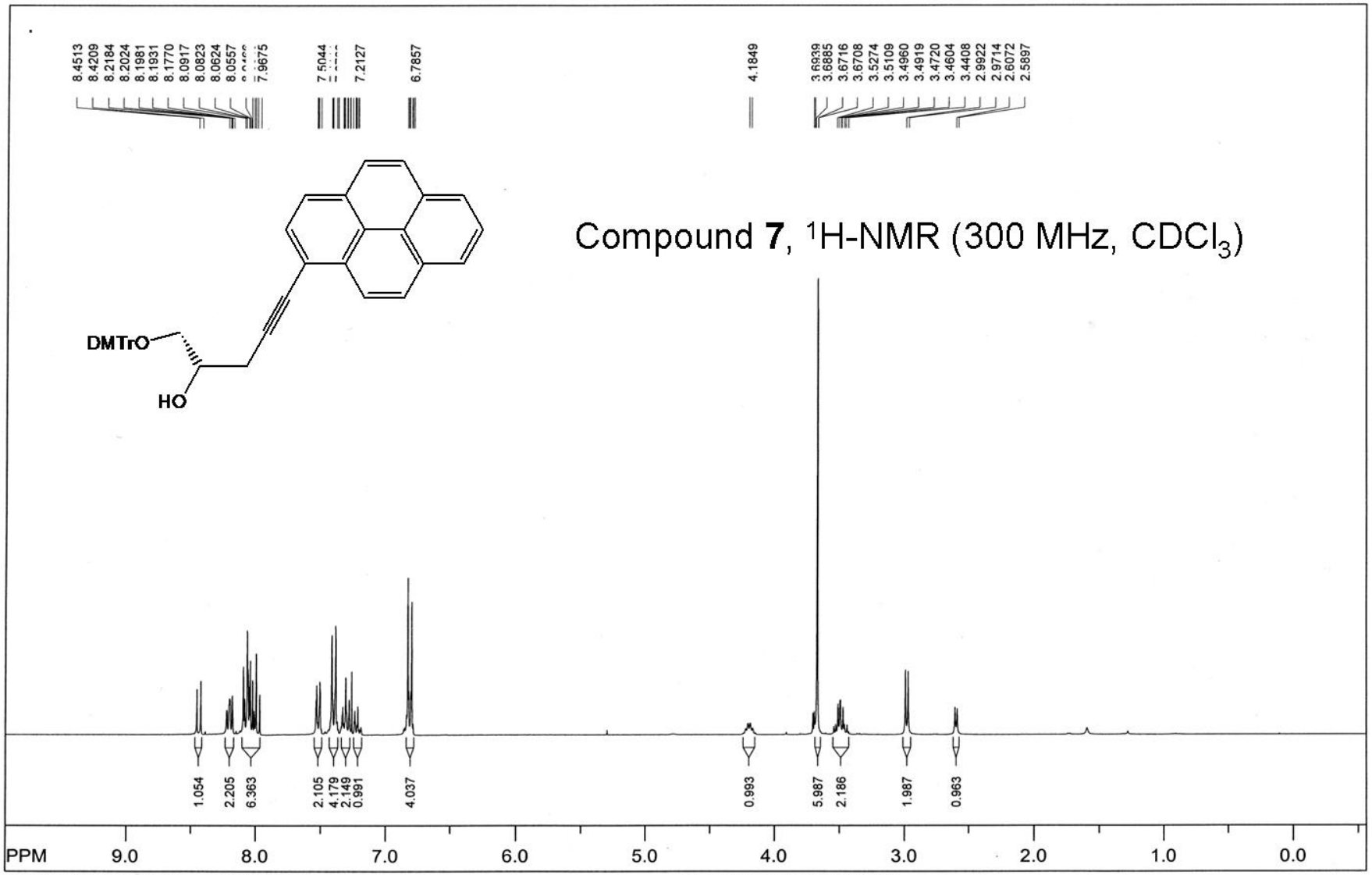

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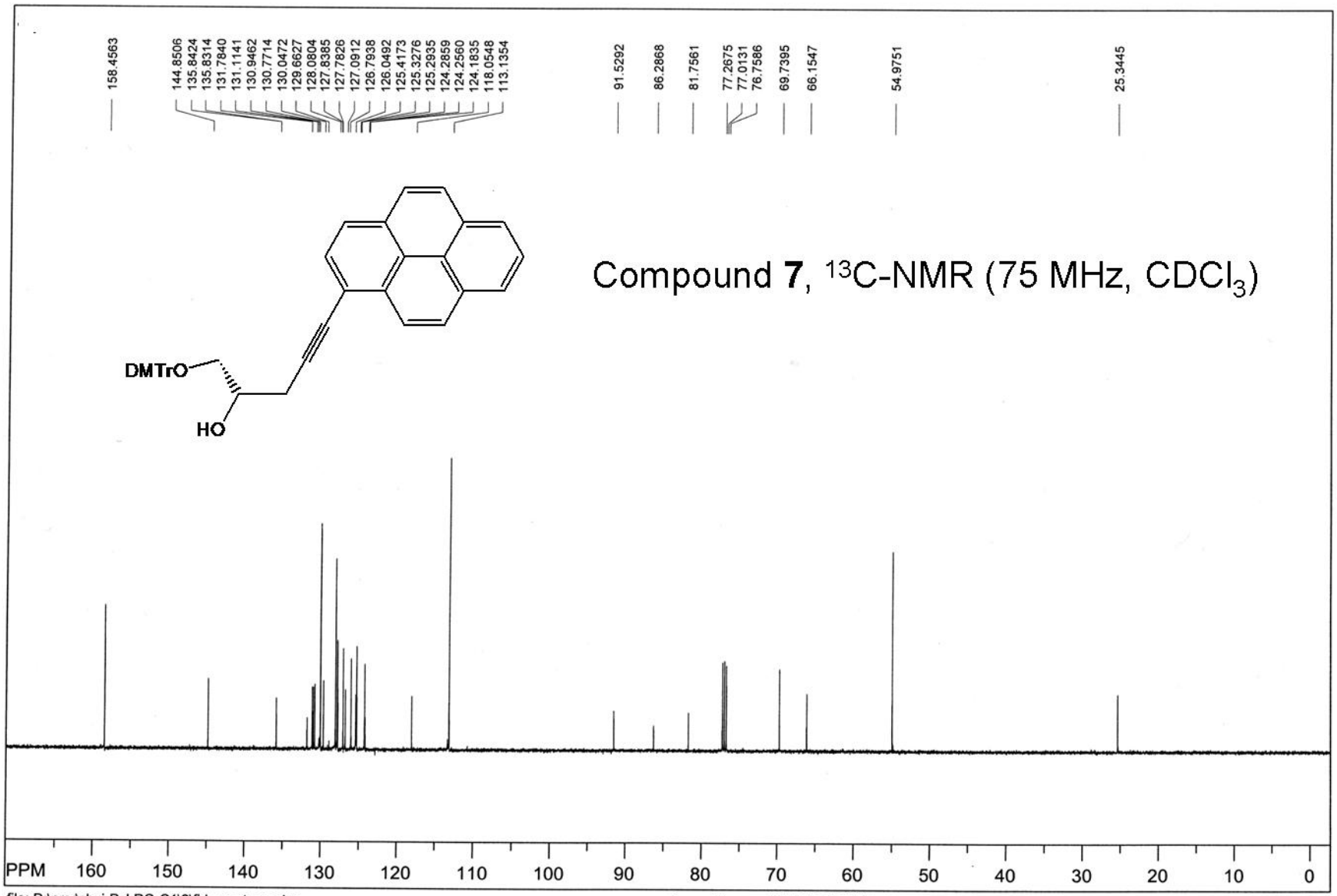

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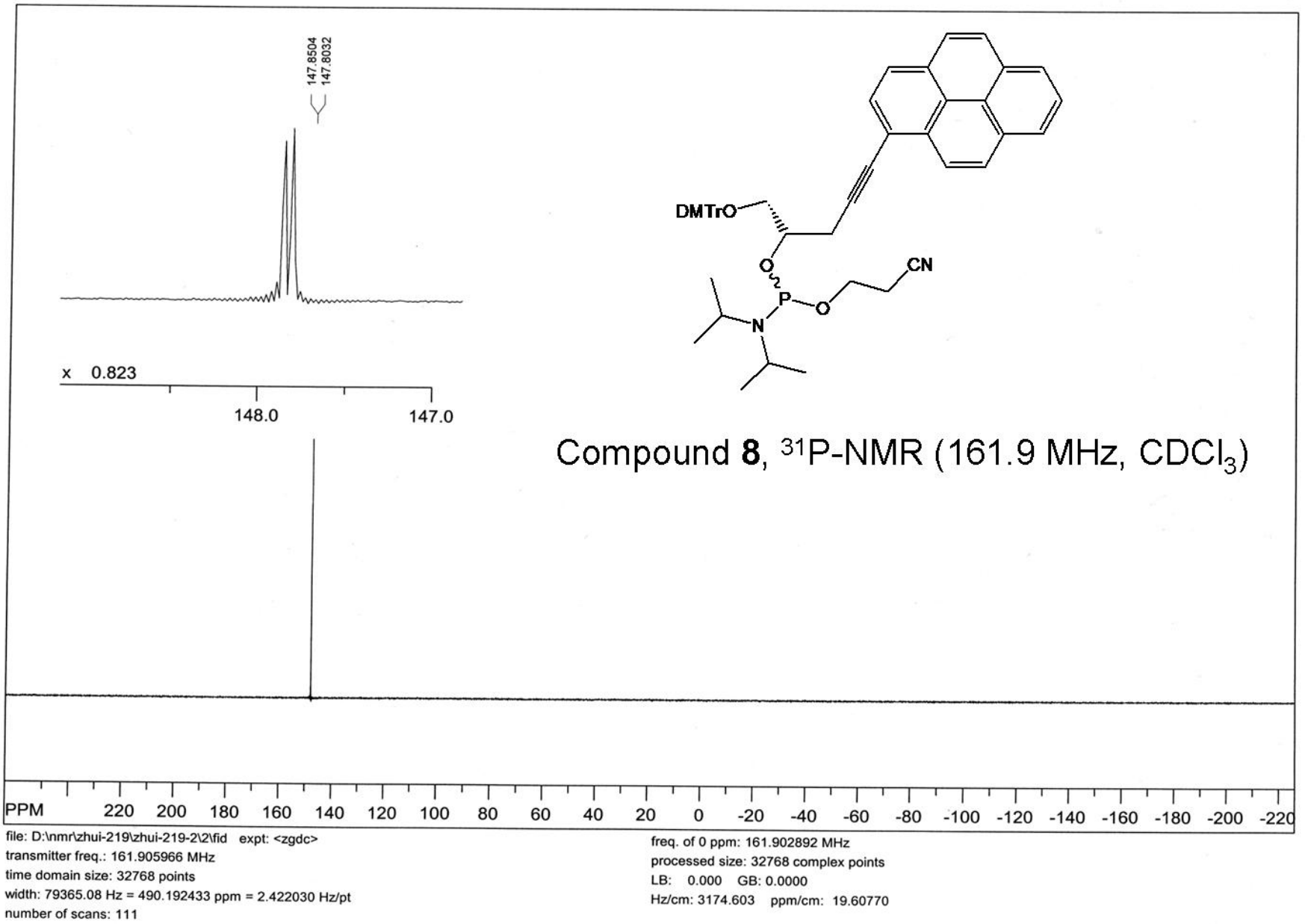
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147.8032
x 0.823
148.0
147.0
DMTrO
O
P
N
O
CN
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PPM
220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220
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processed size: 32768 complex points
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