Palladium Catalyzed C-H Glycosylation and Retro Diels-Alder Tandem Reaction via Structurally Modified Norbornadiene (smNBDs)

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Table of Contents

S1. General Methods

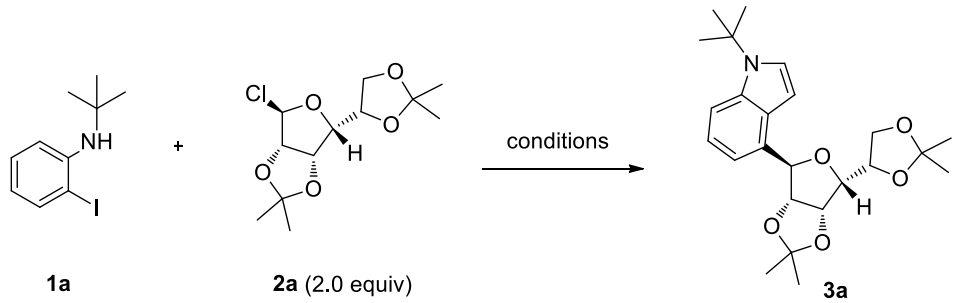
General Procedures. Unless otherwise noted, reactions were performed under an argon atmosphere. Plastic syringes were used to transfer air- and moisture-sensitive reagents. Solvent was freshly distilled/degassed prior to use unless otherwise noted. Analytical TLC was performed with silica gel GF254 plates. For column chromatography, a 200-300 mesh silica gel was employed. Organic solutions were concentrated under reduced pressure using a rotary evaporator. Room temperature (r.t.) is 23-25 ℃.

Materials. Commercial reagents were purchased from Acros, Accela, Adamas, Alfa, Ark, Aladdin, or TCI, and used as received with the following exceptions. Toluene was dried over calcium hydride. Other commercially available reagents and solvents were used without further purification.

Instrumentation. Deuterated solvents were purchased from Cambridge Isotope Laboratories. ^{1}H NMR spectra were recorded on Bruker AVANCE III 400, Agilent Mercury plus 300 BB and INOVA instruments with 400, 300 and 600 MHz frequencies, and ^{13}C NMR spectra were recorded on Bruker AVANCE III 400 and Agilent Mercury plus 300 BB instruments with 101 and 75 MHz frequencies. ^{19}F NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer with a ^{19}F operating frequency of 376 MHz. Chemical shifts (δ) were reported in ppm relative to the residual solvent signal ($CDCl_3$ δ = 7.26 for ^{1}H NMR and δ = 77.0 for ^{13}C NMR). Chemical shifts (ppm) were recorded with tetramethylsilane (TMS) as the internal reference standard. Multiplicities are given as s (singlet), d (doublet), t (triplet), dd (doublet of doublets), ddd (doublet of doublet of doublets), dt (doublet of triplets), td (triplet of doublets) or m (multiplet). HRMS was obtained using a Q-TOF instrument equipped with an ESI source. Data collection for crystal structure was performed at room temperature using Mo Kα radiation on a Bruker APEXII diffractometer.

S2. Optimization of The Reaction Conditions

Table S1 The Screening of the optimal reaction conditions

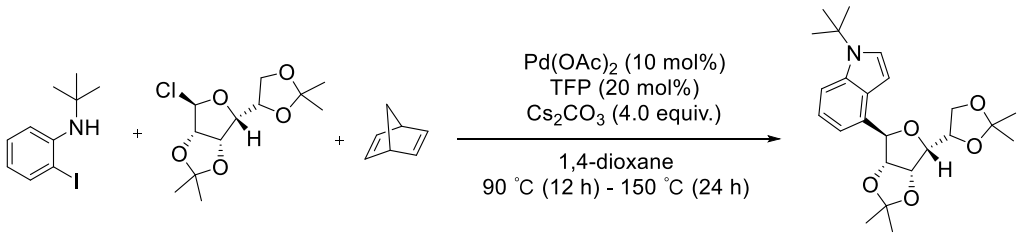


1a **2a** (2.0 equiv) **3a**

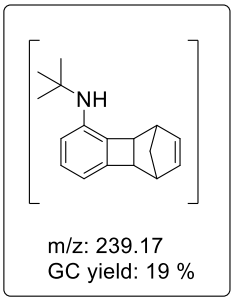
Entries	[M]	Ligand	[N]	Base	Solvent	Temp(^{0}C)	Yield[b](%)
1	$Pd(OAc)_2$	PPh_3	N1	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	trace
2	$Pd(OAc)_2$	PCy_3	N1	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	11
3	$Pd(OAc)_2$	TFP	N1	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	23
4	$Pd(OAc)_2$	TFP	N2	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	19
5	$Pd(OAc)_2$	TFP	N3	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	7
6	$Pd(OAc)_2$	TFP	N4	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	5
7	$Pd(OAc)_2$	TFP	N5	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	24
8	$Pd(OAc)_2$	TFP	N6	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	11
9	$Pd(OAc)_2$	TFP	N7	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	69
10	**$Pd(OAc)_2$**	**TFP**	**N8**	**Cs_2CO_3**	**1,4-Dioxane**	**90^0C (12h) - 150^0C (24h)**	**79**
11	$Pd(OAc)_2$	TFP	N9	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	62
12	$Pd(OAc)_2$	TFP	N10	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	49
13	$Pd(OAc)_2$	TFP	N11	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	trace
14	$Pd(OAc)_2$	TFP	N12	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	trace
15	$Pd(OAc)_2$	TFP	N13	Cs_2CO_3	1,4-Dioxane	90^0C (12h) - 150^0C (24h)	trace
16	$Pd(OAc)_2$	TFP	N8	Cs_2CO_3	THF	90^0C (12h) - 150^0C (24h)	63
17	$Pd(OAc)_2$	TFP	N8	Cs_2CO_3	DME	90^0C (12h) - 150^0C (24h)	trace
18	$Pd(OAc)_2$	TFP	N8	Cs_2CO_3	DCE	90^0C (12h) - 150^0C (24h)	42
19	$Pd(OAc)_2$	TFP	N8	Cs_2CO_3	CH_3CN	90^0C (12h) - 150^0C (24h)	40
20	$Pd(OAc)_2$	TFP	N8	Cs_2CO_3	DMF	90^0C (12h) - 150^0C (24h)	trace

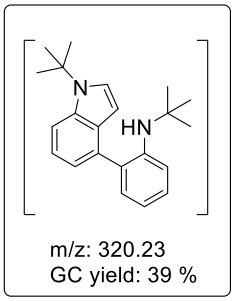
[a] Reaction was performed using *N*-(*tert*-butyl)-2-iodoaniline (0.2 mmol), [b] Isolated yield of product **3a** .

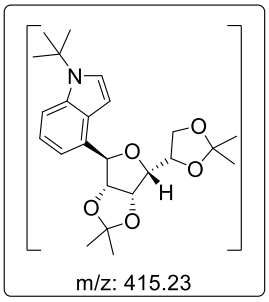
Analysis of by-products of **N1**.

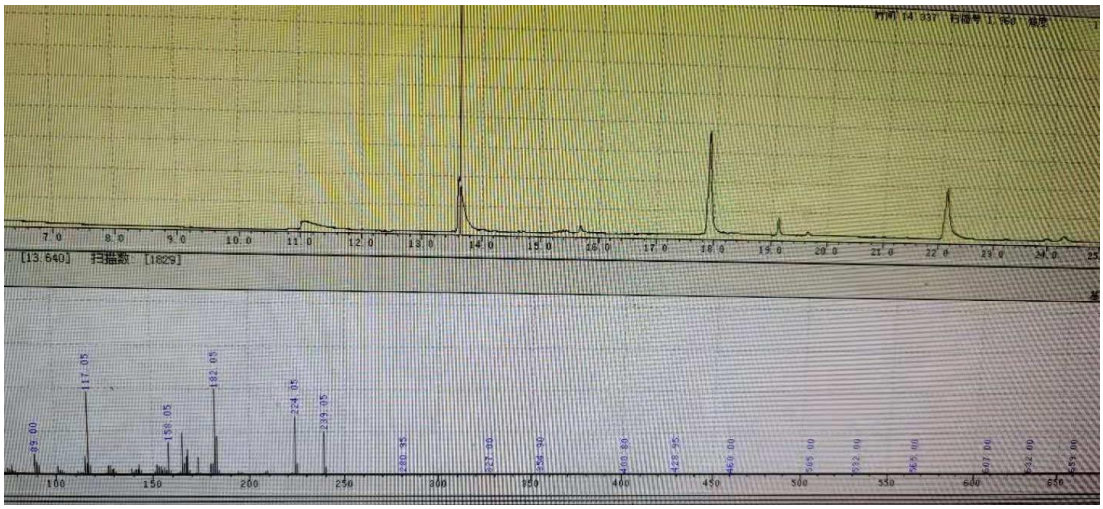


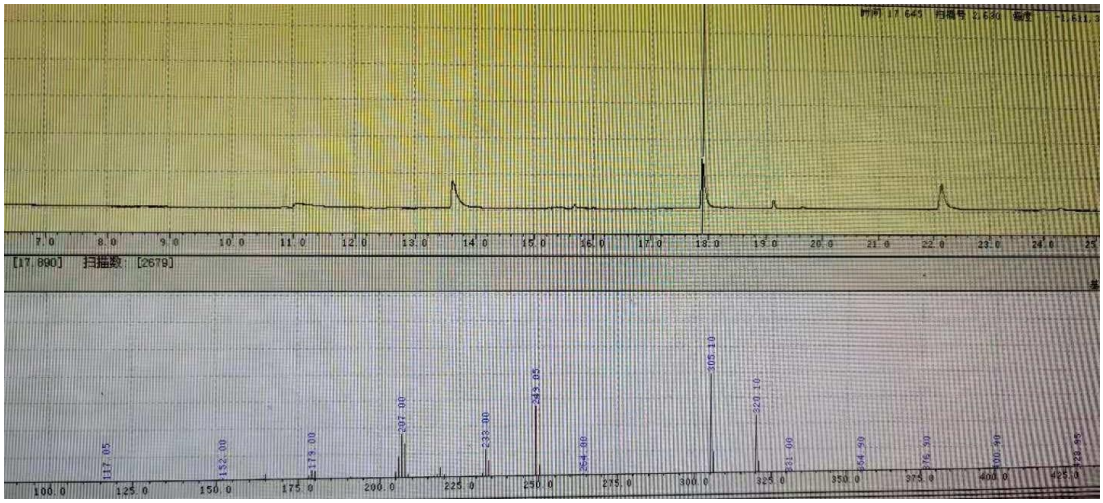
possible byproducts and product (detected by GC-MS)

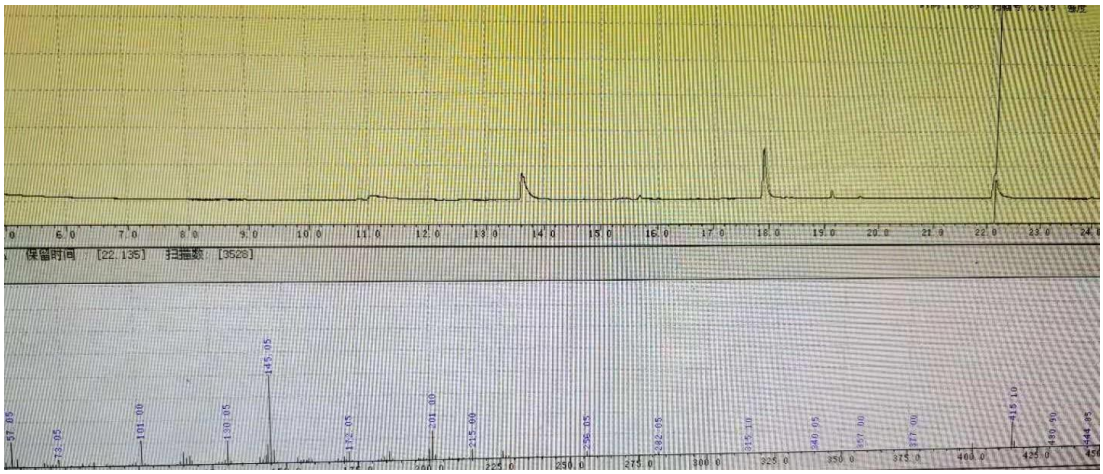








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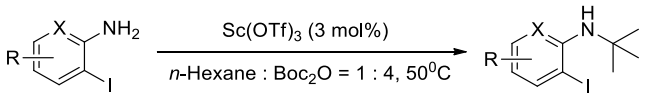
S3. General Procedure

In a 20 mL tube, **1** (0.2 mmol), **2** (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (10 mol%), TFP (20 mol%), Cs_2CO_3 (0.8 mmol, 4.0 equiv.) were added and charged with argon more than three times (The tube was sealed with tipping plug). N8 (0.8 mmol, 4.0 equiv.) were dissolved in 3 mL 1,4-Dioxane, and the mixture was injected into the tube via plastic syringes. Then the white medical adhesive tape was used to reinforce the tipping plug. The resulting light-yellow suspension was stirred vigorously at room temperature for 15 minutes (The time and intensity of stirring at room temperature was important for this reaction) before being placed in a pre-heated oil bath at 90 ℃ stirring at 900~1200 rpm for 12 h, then place it in a preheated oil bath at 150 ℃ stirring at 900~1200 rpm for 24 h. After the reaction was completed, the residue was purified with chromatography column on silica gel or preparative TLC (PTLC) (Petroleum ether/EtOAc = 40:1 - 20:1).

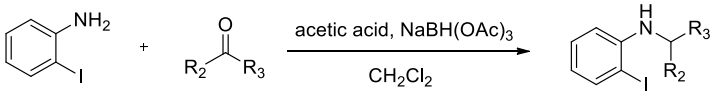
S4. Preparation of Substrates and Product Derivatization.

N-(*tert*-butyl)-2-iodoaniline[1]



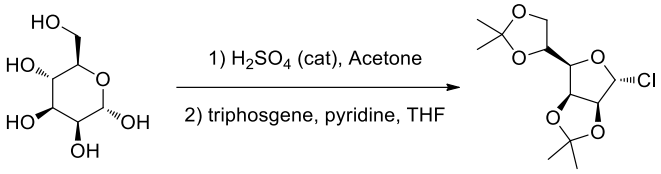
2-Iodoaniline (10 mmol), $Sc(OTf)_3$ (0.15 g, 0.3 mmol) were added to an 100 mL round flask and round flask was charged with argon more than three times. n-Hexane (10 mL) and Boc_2O (40 mL) was added into this round flask. The mixture was stirred at 50 ℃ for 24 h. The reaction needed an open system because a large amount of gas was generated. After the reaction was completed, the residue was purified with chromatography column on silica gel (using petroleum ether as eluant).

N-alkyl-2-iodoaniline[1]



Ketone (15 mmol, 1.5 equiv.), AcOH (1.0 equiv.) were added sequentially to a solution of 2-Iodoaniline (10 mmol) in CH_2Cl_2 (50 mL) and the mixture was stirred at r.t. for 2 h. Then $NaBH(OAc)_3$ (30 mmol, 3 equiv.) was added and stirring at r.t. was continued for further 12 h. The reaction mixture was quenched with aq. 1 N NaOH solution and extracted with CH_2Cl_2. The combined organic extracts were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by flash column chromatography using petroleum ether as eluant.

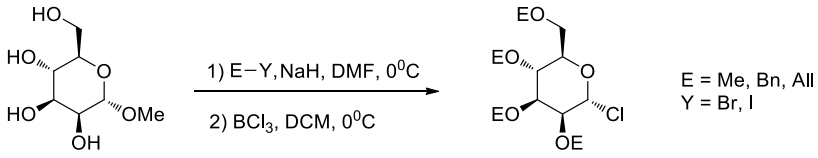
D-mannose Substrate[2]



D-mannose (10 mmol), H_2SO_4 (0.12 mL) were added sequentially in acetone (25 mL) and the mixture was stirred at 0 ℃ for 30 minutes. Afterward the reaction mixture was diluted with EtOAc (50 mL) and washed thoroughly with saturated aq. $NaHCO_3$ solution, water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was used for next step without further purification.

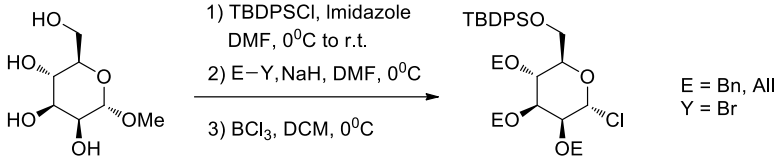
The product got above was dissolved in dry THF (50 mL), triphosgene (1.2 g, 4.0 mmol, 0.4 equiv) was added, and the mixture was stirred at r.t. with exclusion of moisture. Pyridine (1.0 mL) was added in three portions, and the mixture was allowed to stir at r.t. for 2 h while being monitored by TLC. After the reaction was complete, pyridinium hydrochloride

was filtered, the solid was washed with THF (30 mL), and the filtered and concentrated under reduced pressure below 40 ℃. The residue was purified by silica gel flash chromatography to give the desired product.



Methyl α-*D*-mannopyranoside (10 mmol), NaH (1.5 g, 60 mmol, 6.0 equiv.) were added sequentially in CH_2Cl_2 (20 mL) and the mixture was stirred at 0 ℃ for 1 h. Then X-Y (60 mmol, 6.0 equiv.) was added and stirring at 0 ℃. After the complete consumption of Methyl α-*D*-mannopyranoside monitored by TLC analysis, the reaction mixture was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by silica gel flash chromatography to give the desired product.

Boron trichloride (1.5 equiv, 1M in DCM) was slowly to a solution of the product got above (1.0 equiv.) in DCM at 0 ℃. After the complete consumption of starting material monitored by TLC analysis, the reaction mixture was diluted with EtOAc (30 mL) and washed with saturated aq. $NaHCO_3$, water and brine. The resulting residue was purified by silica gel flash chromatography to give corresponding compound.



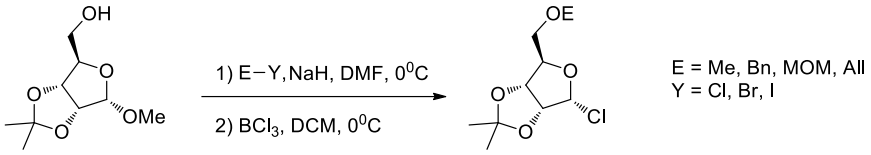
Methyl α-*D*-mannopyranoside (10 mmol), imidazole (2.0 g, 30 mmol, 3.0 equiv) were added sequentially in DMF (20 mL), TBDPSCl (2.86 ml, 11 mmol, 1.1 equiv) was added dropwise over a period of 15 min. The reaction mixture was stirred at 0 ℃ for 17 h, and then the reaction mixture was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure to give the desired product.

The product got above (1.0 equiv.), NaH (1.1 g, 45 mmol, 4,5 equiv.) were added sequentially in CH_2Cl_2 (20 mL) and the mixture was stirred at 0 ℃ for 1 h. Then X-Y (45 mmol, 4.5 equiv.) was added and stirring at 0 ℃. After the complete consumption of starting material monitored by TLC analysis, the reaction mixture was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by silica gel flash chromatography to give the desired product.

Boron trichloride (1.5 equiv, 1M in DCM) was slowly to a solution of the product got above (1.0 equiv.) in DCM at 0 ℃. After the complete consumption of starting material monitored by TLC analysis, the reaction mixture was diluted with

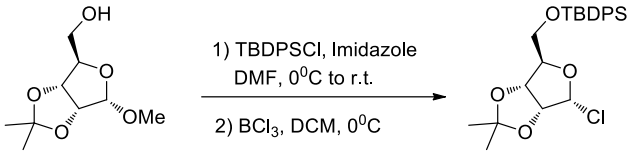
EtOAc (30 mL) and washed with saturated aq. $NaHCO_3$, water and brine. The resulting residue was purified by silica gel flash chromatography to give corresponding compound.

D-ribofuranose Substrate[2]



D-ribofuranoside (10 mmol), NaH (0.36 g, 15 mmol, 1.5 equiv.) were added sequentially in CH_2Cl_2 (20 mL) and the mixture was stirred at 0 ℃ for 1 h. Then X-Y (15 mmol, 1.5 equiv.) was added and stirring at 0 ℃. After the complete consumption of *D*-Ribofuranoside monitored by TLC analysis, the reaction mixture was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by silica gel flash chromatography to give the desired product.

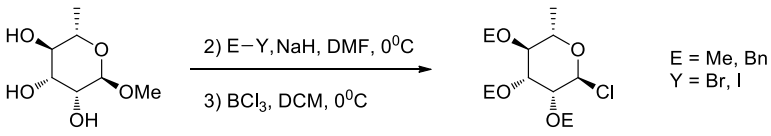
Boron trichloride (1.5 equiv, 1M in DCM) was slowly to a solution of the product got above (1.0 equiv.) in DCM at 0 ℃. After the complete consumption of starting material monitored by TLC analysis, the reaction mixture was diluted with EtOAc (30 mL) and washed with saturated aq. $NaHCO_3$, water and brine. The resulting residue was purified by silica gel flash chromatography to give corresponding compound.



D-ribofuranoside (10 mmol), imidazole (2.0 g, 30 mmol, 3.0 equiv) were added sequentially in DMF (20 mL), TBDPSCl (2.86 ml, 11 mmol, 1.1 equiv) was added dropwise over a period of 15 min. The reaction mixture was stirred at 0 ℃ for 17 h, and then the reaction mixture was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure to give the desired product.

Boron trichloride (1.5 equiv, 1M in DCM) was slowly to a solution of the product got above (1.0 equiv.) in DCM at 0 ℃. After the complete consumption of starting material monitored by TLC analysis, the reaction mixture was diluted with EtOAc (30 mL) and washed with saturated aq. $NaHCO_3$, water and brine. The resulting residue was purified by silica gel flash chromatography to give corresponding compound.

L-rhamonose Substrate[2]

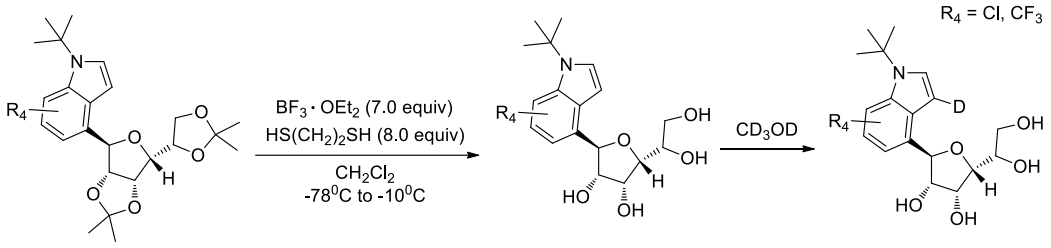


Methyl α-*L*-rhamnoside (10 mmol), NaH (1.1 g, 45 mmol, 4.5 equiv.) were added sequentially in CH_2Cl_2 (20 mL) and the

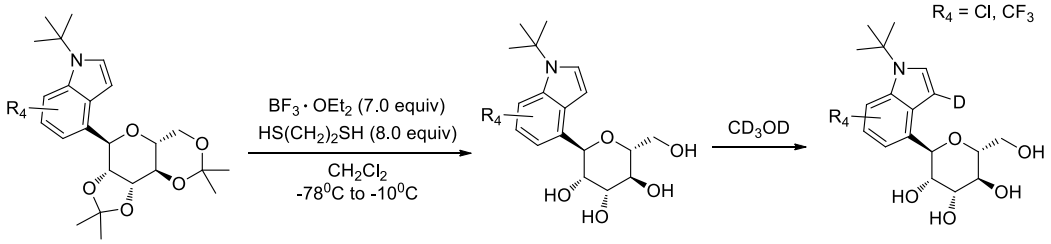
mixture was stirred at 0 ℃ for 1 h. Then X-Y (45 mmol, 4.5 equiv.) was added and stirring at 0 ℃. After the complete consumption of *D*-ribofuranoside monitored by TLC analysis, the reaction mixture was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by silica gel flash chromatography to give the desired product.

Boron trichloride (1.5 equiv, 1M in DCM) was slowly to a solution of the product got above (1.0 equiv.) in DCM at 0 ℃. After the complete consumption of starting material monitored by TLC analysis, the reaction mixture was diluted with EtOAc (30 mL) and washed with saturated aq. $NaHCO_3$, water and brine. The resulting residue was purified by silica gel flash chromatography to give corresponding compound.

Deprotection of Production.[3]



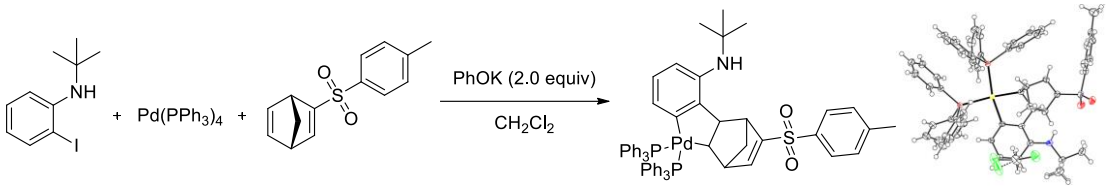
Mannofuranosyl indole (0.2 mmol), 1,2-ethanedithiol (0.14 mL, 1.60 mmol, 8.0 equiv) and boron trifluoride diethyl etherate (0.17 mL, 14.0 mmol, 7.0 equiv) were added sequentially at –78 ℃ in CH_2Cl_2 (3 mL). After the mixture was stirred at –20 ℃ for 16 h, the reaction was quenched with 10% KOH (5 mL). The volatiles were then removed by rotary evaporation. The residue was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by silica gel flash chromatography to give corresponding compound. It is worth noting that in the deprotected product in a deuterated methanol solvent, the hydrogen atom at the indole's C3 position will be replaced by a deuterium atom to generate corresponding deuterated products.



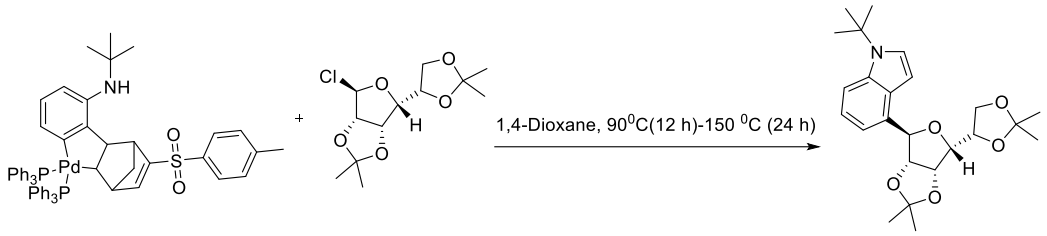
Mannopyranosyl indole (0.2 mmol), 1,2-ethanedithiol (0.14 mL, 1.60 mmol, 8.0 equiv) and boron trifluoride diethyl etherate (0.17 mL, 14.0 mmol, 7.0 equiv) were added sequentially at –78 ℃ in CH_2Cl_2 (3 mL). After the mixture was stirred at –20 ℃ for 16 h, the reaction was quenched with 10% KOH (5 mL). The volatiles were then removed by rotary evaporation. The residue was quenched with EtOAc (50 mL) and washed thoroughly with water and brine. The organic layers dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by silica

gel flash chromatography to give corresponding compound. It is worth noting that in the deprotected product in a deuterated methanol solvent, the hydrogen atom at the indole's C3 position will be replaced by a deuterium atom to generate corresponding deuterated products.

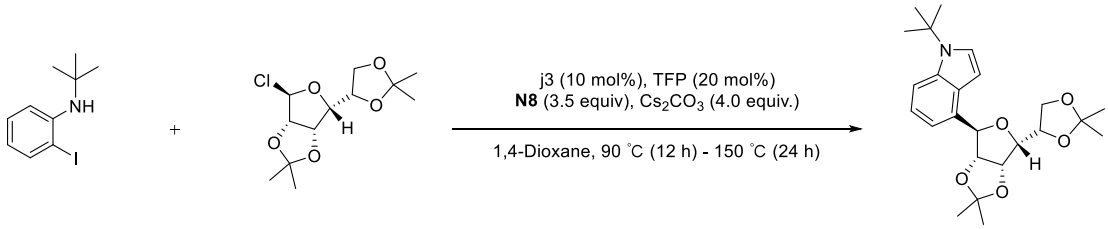
S5. Preparation of intermediate compound.[4]



In an argon-filled glove box, $Pd(PPh_3)_4$ (0.58 g, 0.5 mmol), *N*-(tert-butyl)-2-iodoaniline (0.69 g, 2.5 mmol), N8 (0.62 mg, 2.5 mmol), and PhOK (0.13 g, 1 mmol) were added sequentially in CH_2Cl_2 (15 mL). After the mixture was stirred for 24 h. After cooling to room temperature. the solid was fiitered through Celite in the glove box and the filtrate was concentrated to dryness under reduced pressure. The residue was then dissolved in 15 mL of dry Et_2O and the desired complex slowly precipitated at room temperature as light yellow solid. The solid was collected on a sintered funnel and washed with about 20 mL of diethyl ether, and characterized by single crystal diffraction.



In a 20 mL tube, the intermediate compound (0.2 mmol) and **2** (0.4 mmol, 2.0 equiv.) were added and charged with argon more than three times (The tube was sealed with tipping plug). N8 (0.8 mmol, 4.0 equiv.) 3 mL 1,4-Dioxane was injected into the tube via plastic syringes. The resulting light-yellow suspension was stirred vigorously at room temperature for 15 minutes (The time and intensity of stirring at room temperature was important for this reaction) before being placed in a pre-heated oil bath at 90 ℃ stirring at 900~1200 rpm for 12 h, then place it in a preheated oil bath at 150 ℃ stirring at 900~1200 rpm for 24 h. After the reaction was completed, the residue was purified with chromatography column on silica gel or preparative TLC (PTLC) (Petroleum ether/EtOAc = 40:1 - 20:1).



In a 20 mL tube, **1** (0.2 mmol), **2** (0.4 mmol, 2.0 equiv.), the intermediate compound (10 mol%), TFP (20 mol%), Cs_2CO_3

(0.8 mmol, 4.0 equiv.) were added and charged with argon more than three times (The tube was sealed with tipping plug). N8 (0.8 mmol, 4.0 equiv.) 3 mL 1,4-Dioxane was injected into the tube via plastic syringes. The resulting light-white suspension was stirred vigorously at room temperature for 15 minutes (The time and intensity of stirring at room temperature was important for this reaction) before being placed in a pre-heated oil bath at 90 ℃ stirring at 900~1200 rpm for 12 h, then place it in a preheated oil bath at 150 ℃ stirring at 900~1200 rpm for 24 h. After the reaction was completed, the residue was purified with chromatography column on silica gel or preparative TLC (PTLC) (Petroleum ether/EtOAc = 40:1 - 20:1).

S6. X-ray Crystallographic Information

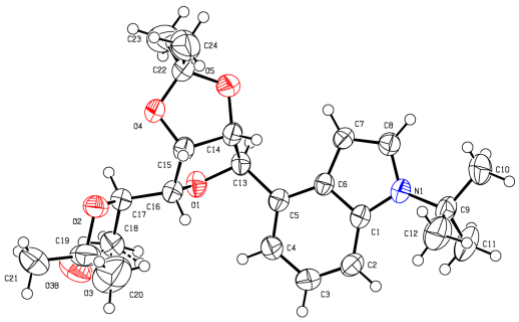


Table S2 Crystal data and structure refinement for compound 3a. (CCDC : 2047890)

Empirical formula	$C_{24}H_{33}NO_5$
Formula weight	415.51
Temperature/K	225(50)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	9.3272(3)
b/Å	10.7693(3)
c/Å	12.3819(3)
α/°	90
β/°	108.361(3)
γ/°	90
Volume/Å^3	1180.42(6)
Z	2
ρ_{calc}g/cm^3	1.169
μ/mm^{-1}	0.656
F(000)	448.0
Crystal size/mm^3	0.07 × 0.04 × 0.03
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.522 to 133.154
Index ranges	-8 ≤ h ≤ 11, -12 ≤ k ≤ 12, -14 ≤ l ≤ 10
Reflections collected	12480
Independent reflections	4124 [R_{int} = 0.0345, R_{sigma} = 0.0306]
Data/restraints/parameters	4124/1/287
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0379, wR_2 = 0.0951
Final R indexes [all data]	R_1 = 0.0405, wR_2 = 0.0991
Largest diff. peak/hole / e Å^{-3}	0.11/-0.17
Flack parameter	0.02(10)

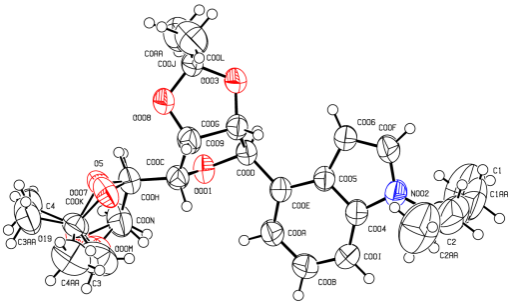


Table S3 Crystal data and structure refinement for compound 3j. (CCDC : 2047891)

Empirical formula	$C_{25}H_{35}NO_5$
Formula weight	429.54
Temperature/K	293.77(10)
Crystal system	monoclinic
Space group	I2
a/Å	11.0067(3)
b/Å	9.2663(2)
c/Å	24.1638(8)
α/°	90
β/°	99.360(3)
γ/°	90
Volume/Å^3	2431.67(13)
Z	4
ρ_{calc}g/cm^3	1.173
μ/mm^{-1}	0.652
F(000)	928.0
Crystal size/mm^3	0.12 ×0.08 ×0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.38 to 133.202
Index ranges	-12 ≤ h ≤ 13, -11 ≤ k ≤ 10, -26 ≤ l ≤ 28
Reflections collected	7101
Independent reflections	3898 [R_{int} = 0.0187, R_{sigma} = 0.0249]
Data/restraints/parameters	3898/25/324
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0426, wR_2 = 0.1053
Final R indexes [all data]	R_1 = 0.0478, wR_2 = 0.1115
Largest diff. peak/hole / e Å^{-3}	0.15/-0.16
Flack parameter	0.09(9)

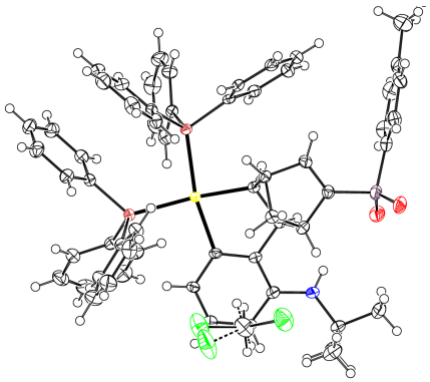


Table S4 Crystal data and structure refinement for intermediate compound. (CCDC : 2067951)

Empirical formula	$C_{61}H_{59}Cl_2NO_2P_2PdS$
Formula weight	1109.39
Temperature/K	149.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.5489(3)
b/Å	13.5596(5)
c/Å	18.1117(6)
α/°	70.689(3)
β/°	89.007(2)
γ/°	77.468(2)
Volume/Å^3	2608.35(15)
Z	2
ρ_{calc}g/cm^3	1.413
μ/mm^{-1}	5.115
F(000)	1148.0
Crystal size/mm^3	0.12 ×0.1 ×0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.18 to 152.114
Index ranges	-10 ≤ h ≤ 14, -17 ≤ k ≤ 17, -22 ≤ l ≤ 22
Reflections collected	25457
Independent reflections	9750[R_{int} =0.0526, R_{sigma} = 0.0616]
Data/restraints/parameters	9750/0/644
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0415, wR_2 = 0.0960
Final R indexes [all data]	R_1 = 0.0523, wR_2 = 0.1002
Largest diff. peak/hole / e Å^{-3}	0.72/-0.91

S7. Computational details

All the calculations were performed using the Gaussian 09 programs[1]. All of the structures were fully optimized with the B3LYP[2-3] method and Ahlrichs' split-valence def2-SVP basis set[4] in 1,4-dioxane solvent employing the Polarizable Continuum Model (PCM)[5]. the temperature is 353.15K. Grimmes's DFT-D3 dispersion correction was used to describe the van der waals interaction.[6] Vibrational frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequency. Transition states connecting relevant minima were further examined by running intrinsic reaction coordinate (IRC) calculations.

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Cartesian Coordinates And Energy

1a

G= -741.584844 Hartree

I	1.37849	-1.83969	0.47352
C	0.66762	-0.95813	-2.35630
C	-0.11101	-0.69817	-3.48759
C	-1.47952	-0.97206	-3.43215
C	-2.06359	-1.49163	-2.27923
C	-1.30815	-1.76782	-1.10956
C	0.08506	-1.47841	-1.20096
H	1.73965	-0.75288	-2.37433
H	0.34979	-0.29044	-4.38954
H	-2.11348	-0.78003	-4.30184
H	-3.13222	-1.69078	-2.28114
H	-1.18220	-2.42292	0.79099
N	-1.84833	-2.27738	0.04220
C	-3.23714	-2.63193	0.37853
C	-3.19331	-3.13094	1.83420
H	-2.82312	-2.34191	2.50880
H	-4.19910	-3.42232	2.16984

H	-2.53403	-4.00912	1.92837
C	-3.76082	-3.77584	-0.51397
H	-3.81887	-3.48939	-1.57275
H	-3.09727	-4.65100	-0.43794
H	-4.77073	-4.07557	-0.19300
C	-4.16771	-1.40370	0.31171
H	-3.78957	-0.60492	0.96816
H	-4.24941	-0.99294	-0.70359
H	-5.18114	-1.67769	0.64428

Cs_2CO_3

G= -304.097467 Hartree

C	-0.33816	0.50314	0.00851
O	0.27821	-0.62130	0.06453
O	-1.66388	0.51146	0.05987
O	0.28621	1.61978	-0.09460
Cs	-1.88158	-2.34133	-0.02773
Cs	-1.83620	3.36384	0.19222

N8

G= -1089.642542 Hartree

C	-1.94947	1.49352	1.20581
C	-0.45806	1.35238	1.58583
C	-0.59794	2.94409	0.00419
C	-2.03037	2.44008	0.26219
H	-2.74963	0.87170	1.60865
H	-2.90784	2.77522	-0.29084
C	-0.03874	2.84854	1.45477
H	1.04881	3.00689	1.51301
H	-0.56118	3.50843	2.16282
C	0.26701	0.79458	0.34314
C	0.18212	1.75360	-0.58779
H	0.68958	-0.20437	0.24031
H	-0.24519	0.83621	2.53020
H	-0.49240	3.89111	-0.53737
S	0.63929	1.74486	-2.28947
O	-0.61560	1.82229	-3.06085
O	1.67516	2.77446	-2.48637
C	1.37592	0.13228	-2.54602
C	2.75453	-0.02220	-2.38414
C	0.55638	-0.94559	-2.89087
C	3.31575	-1.28745	-2.56189
H	3.36996	0.84246	-2.12920
C	1.13531	-2.20285	-3.06378
H	-0.51574	-0.78971	-3.02412
C	2.51931	-2.39480	-2.90239
H	4.39392	-1.41849	-2.43651

H	0.50205	-3.05271	-3.33250
C	3.13885	-3.75129	-3.12432
H	2.44433	-4.56219	-2.85739
H	3.40414	-3.88498	-4.18754
H	4.06175	-3.87606	-2.53836

L

G= -1028.934977 Hartree

P	2.22990	-1.70936	0.30980
C	2.73164	-2.08328	-1.41077
C	2.35914	-3.02501	-2.33750
O	3.64374	-1.23023	-1.96953
C	3.09498	-2.73203	-3.53185
H	1.64700	-3.83022	-2.17322
C	3.86018	-1.63633	-3.24424
H	3.05986	-3.26686	-4.47901
H	4.57642	-1.05436	-3.81972
C	3.52753	-2.58117	1.24440
C	4.27115	-2.15271	2.31639
O	3.92042	-3.84997	0.90359
C	5.16340	-3.22123	2.65407
H	4.18690	-1.18224	2.80161
C	4.90176	-4.22124	1.75950
H	5.90372	-3.24132	3.45123
H	5.32018	-5.21423	1.61027
C	0.85558	-2.90316	0.46288
C	0.76355	-4.24833	0.72711
O	-0.40313	-2.38557	0.30918
C	-0.63228	-4.56867	0.73101
H	1.60414	-4.91810	0.88922
C	-1.28753	-3.39735	0.46702
H	-1.08835	-5.54095	0.90706
H	-2.33901	-3.13749	0.36822

A

G= -2185.865476 Hartree

Pd	1.14358	0.48947	0.04966
P	1.86745	-1.67493	-0.00967
C	2.35252	-2.43997	-1.59453
C	2.15664	-3.67632	-2.15793
O	3.03486	-1.64179	-2.46909
C	2.76299	-3.62934	-3.45544
H	1.64070	-4.51229	-1.69176
C	3.28180	-2.37064	-3.58370
H	2.80570	-4.42619	-4.19537
H	3.82776	-1.86565	-4.37714
C	3.34805	-1.94492	1.00962

C	4.05751	-1.06319	1.78619
O	3.94412	-3.17759	1.05840
C	5.14849	-1.80205	2.34883
H	3.81523	-0.01089	1.91972
C	5.02499	-3.07676	1.86974
H	5.92519	-1.43332	3.01568
H	5.60824	-3.98443	2.00827
C	0.74244	-2.95848	0.62695
C	0.92110	-4.16509	1.25890
O	-0.59499	-2.71631	0.47846
C	-0.38812	-4.68945	1.50811
H	1.88097	-4.61160	1.50534
C	-1.26461	-3.76526	1.00848
H	-0.64407	-5.62780	1.99621
H	-2.34996	-3.71478	0.96342
P	0.72035	2.63289	0.71293
C	-0.90845	3.38233	0.36994
C	-1.32177	4.63002	-0.02606
O	-1.99158	2.55708	0.48539
C	-2.74718	4.56116	-0.15498
H	-0.67597	5.48726	-0.20051
C	-3.09364	3.27937	0.17237
H	-3.42428	5.35918	-0.45331
H	-4.04383	2.75289	0.22319
C	0.86624	2.84195	2.51242
C	1.20797	1.93052	3.48005
O	0.59425	4.04989	3.09877
C	1.14809	2.62400	4.73231
H	1.46158	0.88848	3.29602
C	0.77022	3.90397	4.43466
H	1.35285	2.22302	5.72285
H	0.58841	4.78747	5.04262
C	1.81280	3.95644	0.10167
C	2.25087	5.15384	0.61333
O	2.36181	3.76276	-1.13560
C	3.11743	5.72375	-0.37435
H	1.97498	5.56533	1.58085
C	3.14102	4.83299	-1.41259
H	3.65378	6.66899	-0.31891
H	3.64927	4.82138	-2.37391

B

G= -1898.494647 Hartree

Pd	0.27942	-0.61361	0.50442
P	-1.86760	-0.10089	0.12994
C	-2.05901	1.24966	-1.08927
C	-2.75053	2.43457	-1.10261

O	-1.30350	1.14983	-2.22563
C	-2.39912	3.09585	-2.32556
H	-3.42744	2.78275	-0.32636
C	-1.52296	2.26550	-2.96606
H	-2.75443	4.06093	-2.68135
H	-0.99105	2.32644	-3.91230
C	-2.93216	-1.39427	-0.57277
C	-2.64786	-2.70974	-0.83933
O	-4.21575	-1.11642	-0.96401
C	-3.82956	-3.27276	-1.42181
H	-1.69639	-3.19895	-0.64078
C	-4.74388	-2.25726	-1.47030
H	-3.97875	-4.29524	-1.76257
H	-5.77004	-2.19559	-1.82586
C	-2.90788	0.55460	1.47475
C	-4.26236	0.63473	1.69024
O	-2.24587	1.10322	2.53827
C	-4.43429	1.27157	2.96116
H	-5.03035	0.27773	1.00890
C	-3.17319	1.53329	3.42348
H	-5.37051	1.50172	3.46597
H	-2.79285	1.99707	4.33060
I	2.66470	-2.10193	-1.02559
C	2.36744	-1.36785	1.98501
C	2.58950	-0.61939	3.14650
C	2.89880	0.73726	3.02667
C	2.97183	1.35596	1.77870
C	2.75048	0.64866	0.57193
C	2.43343	-0.75313	0.71093
H	2.19141	-2.44279	2.05118
H	2.52859	-1.10211	4.12383
H	3.09084	1.33460	3.92160
H	3.22959	2.41159	1.72727
H	2.67074	0.56103	-1.41574
N	2.87708	1.22086	-0.67387
C	2.52190	2.60924	-1.05954
C	2.32178	2.56621	-2.58468
H	1.48790	1.89530	-2.84614
H	2.08518	3.56884	-2.96980
H	3.23395	2.20942	-3.08973
C	3.67354	3.58038	-0.74025
H	3.84502	3.68310	0.34034
H	4.60941	3.22753	-1.19996
H	3.44476	4.58319	-1.13434
C	1.20867	3.06970	-0.39975
H	0.39485	2.36857	-0.63198
H	1.29103	3.12866	0.69403

H	0.92761	4.06600	-0.77419

C-ts

G= -1898.491723 Hartree

Pd	0.26128	-0.56883	0.54358
P	-1.89482	-0.06786	0.12292
C	-2.09476	1.35378	-1.00957
C	-2.82959	2.51135	-0.96301
O	-1.31149	1.35544	-2.13167
C	-2.47579	3.26377	-2.13135
H	-3.53742	2.78242	-0.18348
C	-1.55538	2.50919	-2.80260
H	-2.85864	4.23700	-2.43201
H	-1.00280	2.65243	-3.72779
C	-2.90297	-1.34311	-0.68522
C	-2.57267	-2.63126	-1.02294
O	-4.18330	-1.07718	-1.09463
C	-3.72172	-3.18999	-1.67097
H	-1.61241	-3.10491	-0.82867
C	-4.66401	-2.19921	-1.68353
H	-3.83167	-4.19344	-2.07697
H	-5.68177	-2.14442	-2.06348
C	-2.98159	0.46916	1.48274
C	-4.33939	0.46183	1.69132
O	-2.35707	1.00500	2.57519
C	-4.55349	1.02851	2.98892
H	-5.08324	0.09410	0.98918
C	-3.31194	1.34034	3.47230
H	-5.50385	1.18096	3.49671
H	-2.96325	1.78301	4.40238
I	2.37368	-2.21654	-0.74633
C	2.33165	-1.18892	2.23328
C	2.68333	-0.37389	3.31325
C	3.09291	0.93856	3.06453
C	3.14995	1.44445	1.76575
C	2.79796	0.66542	0.63872
C	2.35840	-0.67732	0.91651
H	2.05605	-2.23196	2.39788
H	2.64415	-0.77015	4.33003
H	3.38463	1.58624	3.89527
H	3.49496	2.46476	1.60914
H	2.62130	0.41914	-1.32954
N	2.89399	1.12777	-0.65723
C	2.54922	2.49216	-1.13329
C	2.22893	2.33113	-2.62976
H	1.35692	1.67250	-2.76860
H	1.99530	3.30739	-3.07945

H	3.08783	1.90072	-3.16977
C	3.74932	3.44458	-0.98185
H	4.00745	3.62229	0.07168
H	4.63559	3.02484	-1.48190
H	3.51965	4.42205	-1.43486
C	1.30607	3.05152	-0.41655
H	0.46222	2.35324	-0.51036
H	1.48388	3.21601	0.65504
H	1.01344	4.01364	-0.86424

D

G= -1898.508974 Hartree

Pd	0.26621	-0.38555	0.56617
P	-2.04586	-0.10905	-0.09929
C	-2.19728	1.22853	-1.32270
C	-2.95855	2.36798	-1.39609
O	-1.32247	1.19213	-2.37286
C	-2.52542	3.06606	-2.56978
H	-3.73090	2.66334	-0.68988
C	-1.53497	2.30147	-3.12131
H	-2.90245	4.01191	-2.95320
H	-0.91105	2.41079	-4.00485
C	-3.03389	-1.45866	-0.76957
C	-2.71569	-2.77531	-0.98743
O	-4.32193	-1.22010	-1.17447
C	-3.88211	-3.38163	-1.55509
H	-1.75136	-3.23490	-0.78089
C	-4.81929	-2.38969	-1.64336
H	-4.00386	-4.41801	-1.86274
H	-5.84424	-2.36391	-2.00652
C	-3.07474	0.53386	1.24784
C	-4.41988	0.55344	1.51850
O	-2.39275	1.14355	2.26756
C	-4.56792	1.21805	2.77851
H	-5.19750	0.13865	0.88187
C	-3.30441	1.55402	3.18084
H	-5.49263	1.41735	3.31623
H	-2.91073	2.06170	4.05814
I	1.23643	-2.29367	-0.95238
C	2.35150	-0.83364	2.51525
C	3.42610	-0.40430	3.30442
C	4.28683	0.57944	2.80676
C	4.09004	1.12113	1.53445
C	3.00209	0.72671	0.72881
C	2.10752	-0.22575	1.27834
H	1.69284	-1.62844	2.87796
H	3.60039	-0.85391	4.28529

H	5.14729	0.90250	3.39886
H	4.81110	1.83198	1.12919
H	2.25215	0.58345	-1.10686
N	2.84362	1.22420	-0.58075
C	2.38469	2.61463	-0.84515
C	2.17532	2.69662	-2.36485
H	1.41884	1.96411	-2.69035
H	1.82319	3.69799	-2.65634
H	3.11544	2.48186	-2.89543
C	3.44557	3.63992	-0.41901
H	3.56165	3.67182	0.67405
H	4.42091	3.39745	-0.86812
H	3.14798	4.64751	-0.74964
C	1.05652	2.91892	-0.12426
H	0.26871	2.22057	-0.45209
H	1.17051	2.82469	0.96719
H	0.70645	3.93978	-0.34537

E

G= -2202.696918 Hartree

Pd	0.10344	0.39016	-0.92213
P	-1.51857	1.86109	-0.45493
C	-2.17726	2.66535	-1.94150
C	-2.70352	3.90716	-2.19263
O	-2.15002	1.93396	-3.09468
C	-3.01948	3.93363	-3.58857
H	-2.83517	4.70425	-1.46475
C	-2.66212	2.70796	-4.08044
H	-3.45053	4.75774	-4.15321
H	-2.70615	2.25819	-5.06937
C	-2.93812	1.05462	0.32489
C	-3.19326	-0.28600	0.48606
O	-4.01078	1.78745	0.75757
C	-4.50178	-0.37511	1.06151
H	-2.51354	-1.08551	0.19424
C	-4.94257	0.91282	1.20322
H	-5.04857	-1.27715	1.32908
H	-5.86100	1.34721	1.59184
C	-1.25730	3.30559	0.61032
C	-1.75524	3.66957	1.83788
O	-0.43910	4.28887	0.13709
C	-1.20553	4.96045	2.12551
H	-2.44942	3.09333	2.44331
C	-0.41804	5.28301	1.05467
H	-1.37348	5.56569	3.01367
H	0.20583	6.14039	0.81535
C	1.23220	2.62686	-2.56317

C	2.17448	3.60259	-2.92337
C	3.21767	3.89175	-2.04401
C	3.32034	3.21925	-0.82104
C	2.36960	2.25183	-0.43910
C	1.31499	1.94791	-1.34485
H	0.41102	2.39972	-3.24797
H	2.08708	4.12590	-3.87919
H	3.96661	4.64552	-2.30301
H	4.15234	3.45399	-0.15788
H	1.60744	0.98081	0.87698
N	2.45790	1.53271	0.77142
C	2.85731	2.10146	2.08642
C	2.24410	1.17274	3.14762
H	2.59435	0.13448	3.03768
H	2.51523	1.51195	4.15855
H	1.14292	1.17668	3.07571
C	2.30028	3.52020	2.29447
H	2.67284	4.22955	1.54284
H	1.20392	3.50556	2.22795
H	2.57823	3.89896	3.29062
C	4.38853	2.08724	2.25121
H	4.78173	1.06375	2.14826
H	4.89467	2.72667	1.51474
H	4.66628	2.45099	3.25289
C	0.66670	-2.08494	-0.89923
O	1.05393	-3.25642	-0.75335
O	-0.52429	-1.65615	-0.54339
O	1.45833	-1.13078	-1.35489
Cs	4.06735	-1.46895	-0.07512
Cs	-0.41012	-3.68382	1.83787
I	3.03248	-2.93964	3.41781

F1

G= -3292.314476 Hartree

Pd	0.45187	0.82552	-0.39469
P	-1.45019	2.18840	-0.18938
C	-2.07458	2.95336	-1.71572
C	-1.59331	4.00484	-2.45211
O	-3.19207	2.44386	-2.31200
C	-2.47354	4.14539	-3.57436
H	-0.71500	4.59691	-2.21247
C	-3.42252	3.17286	-3.43589
H	-2.40676	4.87725	-4.37661
H	-4.29421	2.89022	-4.02140
C	-2.90386	1.40908	0.54314
C	-3.06663	0.21132	1.19234
O	-4.07532	2.11741	0.58371

C	-4.42194	0.17914	1.65516
H	-2.29368	-0.54580	1.27751
C	-4.98098	1.36226	1.25532
H	-4.92022	-0.63972	2.16865
H	-5.97558	1.78950	1.36166
C	-1.32803	3.64157	0.90752
C	-1.74170	3.85174	2.19975
O	-0.67078	4.74105	0.45052
C	-1.30033	5.16964	2.54970
H	-2.29910	3.15132	2.81738
C	-0.65426	5.65715	1.44777
H	-1.44601	5.68501	3.49675
H	-0.15017	6.59433	1.22718
C	1.49449	2.88517	-2.18198
C	2.19808	4.01517	-2.62946
C	2.80164	4.84392	-1.68329
C	2.70693	4.55893	-0.31814
C	2.00645	3.42383	0.14503
C	1.39771	2.57736	-0.82488
H	1.00309	2.23764	-2.91548
H	2.26678	4.23556	-3.69762
H	3.35560	5.73143	-2.00208
H	3.17799	5.23372	0.39397
H	1.34793	2.23659	1.60622
N	1.85728	3.10555	1.48589
C	2.73916	3.43388	2.62257
C	2.26562	2.53958	3.78174
H	2.37344	1.47357	3.52518
H	2.86221	2.72836	4.68614
H	1.20669	2.73540	4.01536
C	2.57306	4.90360	3.05915
H	2.93355	5.60907	2.29813
H	1.51298	5.12407	3.24917
H	3.14756	5.09195	3.97998
C	4.21766	3.12560	2.31274
H	4.37744	2.06095	2.08379
H	4.57842	3.70578	1.45145
H	4.85074	3.38029	3.17743
C	2.21126	-0.53366	-0.84754
C	2.19591	-1.99369	-0.33995
C	2.93606	-0.72991	1.36928
C	2.67062	0.23348	0.20005
H	2.28598	-0.28044	-1.90727
H	3.18157	1.18908	0.12380
C	1.82107	-1.77740	1.15410
H	1.97680	-2.67891	1.76464
H	0.80936	-1.38316	1.28902

C	3.69478	-2.33381	-0.15907
C	4.11998	-1.57727	0.86348
H	4.28909	-2.98224	-0.80246
H	1.59928	-2.69530	-0.93162
H	3.06393	-0.28581	2.36187
S	5.73803	-1.24068	1.47715
O	5.97835	0.18902	1.19384
O	5.81321	-1.72677	2.86536
C	6.82703	-2.22263	0.45430
C	7.20415	-3.49599	0.88629
C	7.26956	-1.70307	-0.76575
C	8.03419	-4.26487	0.06909
H	6.85447	-3.86681	1.85148
C	8.09704	-2.48722	-1.56855
H	6.96977	-0.69835	-1.06966
C	8.49244	-3.77635	-1.16673
H	8.33488	-5.26295	0.39868
H	8.44752	-2.09050	-2.52517
C	9.41612	-4.59838	-2.02886
H	9.24321	-4.41057	-3.09941
H	10.46891	-4.34134	-1.81864
H	9.29715	-5.67565	-1.84011
C	-1.38322	-1.07525	-1.41432
O	-1.96533	-2.17665	-1.67740
O	-1.51743	-0.02511	-2.12316
O	-0.64323	-1.01058	-0.31105
Cs	-1.64697	-3.87510	0.63109
Cs	-4.49358	-0.71520	-2.29009
I	-5.49994	-3.48306	0.60997

F2

G= -3292.316948 Hartree

Pd	-0.05087	1.75675	0.46481
P	-2.31284	2.07315	0.22973
C	-2.89623	3.61758	-0.53717
C	-2.27162	4.56049	-1.31143
O	-4.22293	3.93244	-0.41747
C	-3.27577	5.50812	-1.68863
H	-1.21892	4.57510	-1.56595
C	-4.43773	5.07289	-1.11289
H	-3.14458	6.40087	-2.29658
H	-5.45478	5.45802	-1.10115
C	-3.10534	0.84239	-0.84671
C	-2.62498	-0.23875	-1.54284
O	-4.45029	0.97919	-1.08263
C	-3.74445	-0.80782	-2.23504
H	-1.60048	-0.59798	-1.50084

C	-4.82178	-0.02716	-1.91830
H	-3.73675	-1.70720	-2.84811
H	-5.87307	-0.05365	-2.19611
C	-3.31195	2.03016	1.74844
C	-4.64400	1.77433	1.95981
O	-2.69003	2.24785	2.93558
C	-4.83760	1.82492	3.37968
H	-5.38260	1.58410	1.18613
C	-3.61305	2.11646	3.91658
H	-5.76661	1.67637	3.92699
H	-3.25717	2.26591	4.93283
C	-0.10797	4.14398	2.17942
C	0.14304	5.45083	2.63035
C	0.72618	6.36126	1.75332
C	1.06329	5.97601	0.45099
C	0.82746	4.66333	-0.00871
C	0.22115	3.73227	0.88553
H	-0.12718	5.74346	3.64824
H	0.92418	7.38889	2.07094
H	1.51638	6.71462	-0.20707
H	0.80288	3.30652	-1.49564
N	1.17258	4.22564	-1.28511
C	1.67549	4.97468	-2.44747
C	1.80332	3.94839	-3.58746
H	0.83134	3.47344	-3.79945
H	2.14671	4.44000	-4.50948
H	2.52529	3.15779	-3.33130
C	3.07393	5.56762	-2.17375
H	3.06056	6.33848	-1.39265
H	3.77040	4.77941	-1.85143
H	3.47544	6.02801	-3.08987
C	0.70271	6.08746	-2.89805
H	-0.24215	5.65425	-3.25983
H	0.46415	6.78105	-2.08020
H	1.14216	6.67075	-3.72236
C	2.74918	1.98960	0.58882
C	3.54851	1.81757	-0.71497
C	2.51879	-0.13519	-0.31648
C	2.14849	0.80055	0.84696
H	2.80469	2.86350	1.23584
H	1.73260	0.44720	1.79099
C	2.57742	0.87866	-1.48847
H	3.01873	0.45426	-2.40160
H	1.60367	1.33125	-1.71838
C	4.66143	0.77855	-0.40009
C	4.02282	-0.38097	-0.18776
H	5.72938	0.98610	-0.33735

H	3.88334	2.74012	-1.19786
H	1.85732	-0.99051	-0.42196
S	4.55430	-2.00815	0.21597
O	3.87465	-2.37946	1.47500
O	4.29523	-2.84954	-0.97519
C	6.31118	-1.89530	0.49006
C	7.18299	-2.04653	-0.59195
C	6.78081	-1.63371	1.78069
C	8.55443	-1.92239	-0.36914
H	6.78805	-2.26340	-1.58605
C	8.15558	-1.51541	1.98122
H	6.07625	-1.53143	2.60804
C	9.06217	-1.65700	0.91512
H	9.24557	-2.03794	-1.20812
H	8.53410	-1.31187	2.98629
C	10.54732	-1.56172	1.15231
H	10.78175	-0.87711	1.98120
H	10.95705	-2.55138	1.41929
H	11.08079	-1.21816	0.25360
C	-0.95037	-0.94969	1.16125
O	-0.80955	-2.20751	1.29634
O	-1.78419	-0.26715	1.83452
O	-0.22199	-0.34385	0.22859
Cs	0.92805	-3.76430	-0.36021
Cs	-3.83336	-2.36180	1.52071
I	-2.79563	-4.75872	-1.57488
H	-0.58475	3.43495	2.85987

F3

G= -3292.318351 Hartree

Pd	1.15345	0.33985	0.12595
P	-0.35301	2.01123	0.57329
C	-1.89052	2.03235	-0.40402
C	-2.24873	2.74299	-1.52219
O	-2.93233	1.23975	-0.00980
C	-3.60094	2.37058	-1.82111
H	-1.62209	3.46283	-2.04219
C	-3.96916	1.46266	-0.86737
H	-4.22726	2.74142	-2.63012
H	-4.87645	0.88497	-0.69031
C	-0.94462	1.83915	2.26608
C	-0.71310	0.85588	3.19516
O	-1.80417	2.77538	2.78045
C	-1.47681	1.21595	4.35298
H	-0.11221	-0.03542	3.02274
C	-2.11417	2.38769	4.03895
H	-1.53338	0.67951	5.29813

H	-2.78616	3.04205	4.58999
C	0.13598	3.75371	0.49573
C	0.41945	4.67292	1.47107
O	0.34127	4.30200	-0.73783
C	0.82082	5.86531	0.78761
H	0.36358	4.50650	2.54259
C	0.75367	5.58245	-0.54648
H	1.12761	6.80788	1.23546
H	0.96011	6.15834	-1.44399
C	2.60884	1.93609	2.19469
C	3.39682	2.96836	2.72330
C	4.03522	3.83989	1.84236
C	3.90531	3.68129	0.46045
C	3.12395	2.63995	-0.08354
C	2.46040	1.76467	0.82077
H	2.11502	1.24154	2.87553
H	3.50832	3.07806	3.80491
H	4.65074	4.65891	2.22542
H	4.42117	4.37944	-0.19581
H	2.37338	1.63123	-1.64951
N	2.95131	2.43493	-1.44279
C	3.66194	3.01078	-2.58818
C	3.16868	2.24503	-3.82936
H	2.07285	2.32040	-3.92419
H	3.62021	2.66142	-4.74188
H	3.43877	1.17936	-3.77485
C	5.18876	2.81991	-2.46720
H	5.60326	3.34561	-1.59745
H	5.43266	1.75347	-2.34706
H	5.69662	3.19700	-3.36904
C	3.30703	4.50060	-2.77705
H	2.22506	4.60568	-2.94689
H	3.56654	5.10306	-1.89669
H	3.84087	4.91838	-3.64543
C	2.96376	-3.28425	-1.97732
C	1.76901	-2.35389	-1.67608
C	3.60558	-1.05550	-1.82770
C	4.05487	-2.51342	-2.07912
H	2.90184	-4.37177	-2.02167
H	5.08690	-2.82341	-2.23739
C	2.21453	-1.12822	-2.51999
H	1.57903	-0.24346	-2.36678
H	2.29258	-1.35294	-3.59291
C	2.03841	-1.82268	-0.26042
C	3.13626	-1.00419	-0.35306
H	1.60935	-2.24832	0.64849
H	0.76573	-2.76010	-1.82828

H	4.30038	-0.26200	-2.11773
S	4.30782	-0.82042	0.98922
O	5.19916	0.31123	0.69434
O	3.56498	-0.94061	2.25470
C	5.29656	-2.31417	0.82021
C	4.79315	-3.52747	1.29988
C	6.54448	-2.24194	0.20195
C	5.55073	-4.68421	1.13644
H	3.82030	-3.55729	1.79435
C	7.29351	-3.41203	0.04881
H	6.91638	-1.27836	-0.15020
C	6.81009	-4.64767	0.50660
H	5.16252	-5.63726	1.50622
H	8.27273	-3.36208	-0.43479
C	7.62042	-5.90998	0.35691
H	8.47441	-5.76963	-0.32160
H	8.01756	-6.23474	1.33384
H	7.00332	-6.73669	-0.02961
C	-0.98462	-1.70063	0.28435
O	-0.55688	-1.71761	1.47634
O	-1.92335	-2.44722	-0.14914
O	-0.47291	-0.82598	-0.58815
Cs	-3.60672	-1.51436	2.11368
Cs	-2.61037	-1.38590	-2.74308
I	-6.21818	-1.75969	-0.89583

F4

G= -3292.317745 Hartree

Pd	1.16709	0.53435	-0.04048
P	-0.41422	2.16134	-0.63539
C	-0.60610	2.56392	-2.39718
C	0.29025	3.11590	-3.27448
O	-1.79077	2.32975	-3.02855
C	-0.39036	3.21440	-4.53246
H	1.30587	3.42211	-3.03996
C	-1.64756	2.72457	-4.32208
H	0.00741	3.60116	-5.46831
H	-2.52095	2.60564	-4.95884
C	-2.05476	1.84647	0.04361
C	-2.44876	0.97900	1.03038
O	-3.10695	2.63789	-0.32410
C	-3.83320	1.24833	1.27941
H	-1.80728	0.22632	1.47834
C	-4.17587	2.26381	0.43013
H	-4.49623	0.71347	1.95503
H	-5.10544	2.79482	0.23926
C	-0.19312	3.85670	0.02337

C	-0.83728	4.56188	1.00970
O	0.77227	4.63610	-0.53731
C	-0.21556	5.85321	1.05145
H	-1.65816	4.20140	1.62471
C	0.75652	5.83463	0.09054
H	-0.45807	6.68175	1.71345
H	1.49121	6.56015	-0.24839
C	3.13795	2.43438	-1.24174
C	4.04801	3.50425	-1.30162
C	4.29465	4.24093	-0.14431
C	3.65528	3.92083	1.05875
C	2.73697	2.85172	1.13177
C	2.47818	2.11292	-0.05932
H	2.94945	1.83213	-2.13323
H	4.55210	3.74665	-2.24072
H	4.99780	5.07870	-0.16308
H	3.87365	4.51664	1.94332
H	1.37789	1.75708	2.12999
N	2.09051	2.45886	2.29347
C	2.15277	2.98666	3.66050
C	1.20306	2.10416	4.49131
H	1.52203	1.04959	4.47189
H	1.18516	2.43622	5.53971
H	0.17453	2.16203	4.09837
C	1.66059	4.44565	3.74714
H	2.26058	5.12155	3.12357
H	0.62185	4.51600	3.39667
H	1.70753	4.80648	4.78695
C	3.57651	2.86200	4.24265
H	3.90935	1.81261	4.23295
H	4.30924	3.44857	3.67256
H	3.59639	3.21840	5.28436
C	3.94814	-2.06483	2.47736
C	3.06475	-0.80075	2.39116
C	2.02984	-2.41112	1.20893
C	3.32960	-3.02601	1.77784
H	4.92024	-2.10650	2.96911
H	3.67684	-4.03844	1.57385
C	1.67055	-1.48445	2.40284
H	0.83021	-0.80949	2.19226
H	1.49016	-2.04367	3.33201
C	3.15894	-0.37528	0.91446
C	2.48829	-1.34009	0.19758
H	3.92688	0.29580	0.53903
H	3.26643	-0.00590	3.11424
H	1.27568	-3.09578	0.81547
S	2.83393	-1.82568	-1.49815

O	1.84698	-2.85147	-1.86718
O	3.02770	-0.61293	-2.30921
C	4.43120	-2.63050	-1.34852
C	5.58887	-1.84502	-1.31055
C	4.49442	-4.02060	-1.25259
C	6.82254	-2.47176	-1.15584
H	5.51753	-0.75992	-1.41002
C	5.74190	-4.63260	-1.10222
H	3.57634	-4.60851	-1.30156
C	6.92053	-3.87275	-1.04667
H	7.73244	-1.86597	-1.12543
H	5.79903	-5.72184	-1.02929
C	8.26999	-4.52782	-0.89855
H	8.18191	-5.59861	-0.66466
H	8.85201	-4.43314	-1.83098
H	8.86014	-4.04685	-0.10206
C	-1.01558	-1.09798	-1.09865
O	-1.80142	-2.09076	-1.21894
O	-0.96657	-0.14312	-1.93689
O	-0.26772	-1.02869	-0.00127
Cs	-1.96461	-3.33833	1.33330
Cs	-3.88287	-0.37982	-2.48366
I	-5.66524	-2.17443	0.87006

G1-ts

G= -3292.296145 Hartree

Pd	0.55495	0.75124	-0.52104
P	-1.35790	2.16940	-0.41323
C	-2.04652	2.66271	-2.02537
C	-1.44706	3.34078	-3.05321
O	-3.32942	2.34890	-2.35952
C	-2.42980	3.44148	-4.09363
H	-0.42855	3.72213	-3.05355
C	-3.55016	2.82269	-3.61774
H	-2.31588	3.91597	-5.06618
H	-4.54443	2.65572	-4.02534
C	-2.74063	1.53363	0.55275
C	-2.80453	0.41630	1.34669
O	-3.91497	2.23024	0.64681
C	-4.09801	0.42158	1.96179
H	-2.00688	-0.31664	1.42447
C	-4.72362	1.54698	1.49848
H	-4.52250	-0.34158	2.61033
H	-5.70947	1.97376	1.66848
C	-1.19735	3.82137	0.35358
C	-1.70268	4.39896	1.49126
O	-0.40724	4.71765	-0.30186

C	-1.18068	5.73470	1.52845
H	-2.37529	3.92875	2.20404
C	-0.40217	5.86845	0.41334
H	-1.36277	6.49333	2.28678
H	0.20072	6.67781	0.01098
C	2.12924	3.02082	-1.73289
C	2.62944	4.31668	-1.82353
C	2.94085	4.99816	-0.63809
C	2.70361	4.41926	0.60478
C	2.12895	3.12987	0.71225
C	1.87967	2.39884	-0.49374
H	1.95589	2.44673	-2.64878
H	2.80748	4.77754	-2.79776
H	3.37360	6.00149	-0.68107
H	2.93606	4.98839	1.50211
H	1.17603	1.74541	1.79860
N	1.78829	2.54434	1.90890
C	2.05690	2.94728	3.29835
C	1.52544	1.79904	4.17493
H	2.05321	0.85808	3.95443
H	1.67140	2.03143	5.23988
H	0.44657	1.64428	4.00656
C	1.30267	4.23862	3.67660
H	1.62980	5.10204	3.08239
H	0.22476	4.11297	3.50196
H	1.46422	4.47718	4.73970
C	3.56913	3.09977	3.55290
H	4.09358	2.14953	3.37056
H	4.02612	3.86414	2.91032
H	3.74763	3.39070	4.59954
C	2.22096	-0.49699	-0.90143
C	2.47639	-1.57738	0.17390
C	3.64630	0.23718	0.82800
C	3.03372	0.61575	-0.53138
H	2.11081	-0.80149	-1.94689
H	3.68836	1.13052	-1.22918
C	2.57172	-0.69499	1.44374
H	2.95103	-1.23507	2.32271
H	1.62477	-0.19979	1.69004
C	3.96573	-1.93932	0.01762
C	4.65000	-0.85478	0.41439
H	4.36681	-2.85398	-0.41921
H	1.76062	-2.40515	0.17168
H	4.05212	1.05607	1.42706
S	6.35871	-0.44698	0.26083
O	6.42756	0.63394	-0.74281
O	6.89799	-0.21752	1.61204

C	7.10928	-1.92015	-0.42322
C	7.64412	-2.87871	0.44006
C	7.13067	-2.09201	-1.81021
C	8.20261	-4.03646	-0.10374
H	7.62448	-2.70824	1.51797
C	7.69162	-3.25590	-2.33454
H	6.71680	-1.31781	-2.45892
C	8.23549	-4.24418	-1.49367
H	8.62421	-4.79288	0.56355
H	7.71194	-3.40067	-3.41804
C	8.86998	-5.48102	-2.07682
H	8.35776	-5.80161	-2.99669
H	9.92333	-5.28451	-2.34218
H	8.86154	-6.31802	-1.36294
C	-1.50660	-1.15214	-1.34365
O	-2.11709	-2.27171	-1.40263
O	-1.80855	-0.15398	-2.06587
O	-0.55269	-1.02780	-0.42203
Cs	-1.61907	-3.62301	1.07145
Cs	-4.70429	-0.80295	-1.86498
I	-5.49095	-3.19650	1.40534

G2-ts

G= -3292.296216 Hartree

Pd	-0.00462	1.33656	0.31448
P	-2.31689	1.96281	0.16304
C	-2.79957	3.54641	-0.60273
C	-2.13006	4.38231	-1.45893
O	-4.05520	4.04345	-0.37389
C	-3.02854	5.45219	-1.77335
H	-1.10959	4.24915	-1.80203
C	-4.17911	5.18949	-1.08183
H	-2.83794	6.30727	-2.41879
H	-5.13032	5.70937	-0.99198
C	-3.34177	0.80672	-0.78804
C	-3.01782	-0.33403	-1.47858
O	-4.68230	1.06288	-0.92777
C	-4.23427	-0.81268	-2.06950
H	-2.03266	-0.79375	-1.50370
C	-5.20783	0.07458	-1.69973
H	-4.34910	-1.71995	-2.65968
H	-6.27445	0.14275	-1.90214
C	-3.17396	2.09276	1.76096
C	-4.48661	1.96628	2.13741
O	-2.40328	2.34828	2.85258
C	-4.51250	2.14328	3.56029
H	-5.32094	1.77879	1.46679

C	-3.21656	2.37140	3.93491
H	-5.38043	2.11308	4.21649
H	-2.73779	2.56744	4.89109
C	0.56792	3.54830	2.11217
C	0.48050	4.84467	2.61215
C	0.65895	5.91536	1.72705
C	0.90654	5.68688	0.37683
C	0.97608	4.37393	-0.15057
C	0.77749	3.27815	0.74466
H	0.28308	5.01827	3.67230
H	0.60435	6.94527	2.09007
H	1.02255	6.54200	-0.28539
H	1.07779	3.16099	-1.75098
N	1.17478	4.13191	-1.49617
C	1.73214	4.99843	-2.55286
C	2.03168	4.07199	-3.74483
H	1.12162	3.54161	-4.06961
H	2.40430	4.65658	-4.59854
H	2.79659	3.32370	-3.48496
C	3.04838	5.66774	-2.10906
H	2.91151	6.32874	-1.24326
H	3.79759	4.90870	-1.83675
H	3.46055	6.27078	-2.93254
C	0.71320	6.06427	-3.01260
H	-0.18224	5.58622	-3.43723
H	0.38811	6.71312	-2.18820
H	1.15776	6.70399	-3.79085
C	2.46215	1.85630	0.68474
C	3.35378	1.96070	-0.56967
C	2.45745	-0.10048	-0.62877
C	1.89704	0.55522	0.64383
H	2.79147	2.33300	1.60440
H	1.76839	-0.05983	1.53810
C	2.56532	1.09944	-1.59157
H	3.14971	0.87306	-2.49375
H	1.58135	1.48682	-1.88235
C	4.50263	0.95673	-0.26699
C	3.94870	-0.26444	-0.33058
H	5.52163	1.22381	0.01198
H	3.66706	2.96855	-0.85691
H	1.91509	-0.97545	-0.98600
S	4.51937	-1.88779	0.04230
O	3.76210	-2.32199	1.23750
O	4.37770	-2.69222	-1.18978
C	6.24369	-1.72210	0.45769
C	7.20300	-1.84359	-0.55178
C	6.60117	-1.45253	1.78210

C	8.54778	-1.68175	-0.21992
H	6.89398	-2.06768	-1.57431
C	7.95182	-1.29393	2.09173
H	5.83091	-1.37679	2.55175
C	8.94391	-1.40572	1.10118
H	9.30671	-1.77534	-1.00108
H	8.24287	-1.08343	3.12412
C	10.40288	-1.26911	1.45292
H	10.54967	-0.62665	2.33380
H	10.83367	-2.25717	1.69113
H	10.98398	-0.85337	0.61607
C	-1.15279	-1.20545	1.14922
O	-1.04688	-2.45093	1.39691
O	-1.95980	-0.43896	1.75572
O	-0.40589	-0.71725	0.15510
Cs	0.82380	-3.66558	-0.43033
Cs	-4.04148	-2.54793	1.49144
I	-2.89445	-4.64606	-1.84025
H	0.45629	2.70608	2.80110

G3-ts

G= -3292.292364 Hartree

Pd	0.82518	0.17198	-0.00018
P	-0.56353	1.99312	0.48680
C	-2.15099	2.19577	-0.38670
C	-2.54713	3.01962	-1.40901
O	-3.17898	1.35962	-0.04584
C	-3.90910	2.67509	-1.70146
H	-1.93539	3.78738	-1.87574
C	-4.24684	1.67019	-0.83970
H	-4.56143	3.12839	-2.44528
H	-5.14852	1.07550	-0.68288
C	-1.07781	1.88446	2.21595
C	-0.84223	0.91058	3.15487
O	-1.85047	2.87828	2.76267
C	-1.50898	1.33745	4.34992
H	-0.30937	-0.02045	2.96783
C	-2.10058	2.53545	4.04736
H	-1.53637	0.82381	5.30896
H	-2.70210	3.23630	4.62230
C	0.09548	3.68469	0.42242
C	0.47560	4.56350	1.40182
O	0.33630	4.23036	-0.80892
C	0.97291	5.72572	0.72780
H	0.40671	4.39539	2.47252
C	0.85843	5.46927	-0.60786
H	1.36418	6.63358	1.18172

H	1.09311	6.04152	-1.50061
C	2.59111	1.39482	1.93047
C	3.21614	2.47031	2.54822
C	3.88163	3.40964	1.75096
C	3.86142	3.31425	0.36550
C	3.17285	2.26492	-0.28785
C	2.56276	1.24731	0.52336
H	2.11759	0.63355	2.54724
H	3.20594	2.56138	3.63626
H	4.40988	4.24670	2.21562
H	4.34866	4.08960	-0.22076
H	2.29045	1.59496	-1.96083
N	3.03062	2.20732	-1.65176
C	3.73581	2.91671	-2.73130
C	3.34682	2.19307	-4.03366
H	2.25314	2.19739	-4.17443
H	3.79924	2.69638	-4.90049
H	3.69061	1.14763	-4.02513
C	5.26514	2.82976	-2.56384
H	5.62089	3.33534	-1.65725
H	5.59213	1.78062	-2.50828
H	5.76099	3.29865	-3.42748
C	3.27756	4.38594	-2.83393
H	2.19393	4.42604	-3.01889
H	3.48045	4.94482	-1.91065
H	3.79336	4.89479	-3.66356
C	3.20074	-3.03202	-1.76049
C	1.95529	-2.16595	-1.53559
C	3.72333	-0.76591	-1.59484
C	4.25262	-2.20361	-1.81234
H	3.20951	-4.12141	-1.80899
H	5.30420	-2.45861	-1.92424
C	2.38647	-0.93342	-2.37317
H	1.67851	-0.09404	-2.29313
H	2.55763	-1.16707	-3.43324
C	2.06275	-1.56900	-0.11287
C	3.20200	-0.71183	-0.12734
H	1.75150	-2.13313	0.76961
H	0.97860	-2.61021	-1.75155
H	4.40053	0.04603	-1.86759
S	4.47319	-0.82249	1.20896
O	5.39363	0.31680	1.05767
O	3.76296	-1.08884	2.47349
C	5.43185	-2.30860	0.89230
C	4.89511	-3.55478	1.22979
C	6.72105	-2.18997	0.37379
C	5.65692	-4.69860	1.00770

H	3.89334	-3.62016	1.65678
C	7.47395	-3.34767	0.16299
H	7.11877	-1.20137	0.13965
C	6.95532	-4.61632	0.46856
H	5.24132	-5.67759	1.26162
H	8.48528	-3.26274	-0.24344
C	7.77071	-5.86655	0.25865
H	8.66595	-5.67366	-0.35025
H	8.10516	-6.27858	1.22616
H	7.17717	-6.65146	-0.23653
C	-1.28594	-1.80651	0.34950
O	-0.83509	-1.74035	1.52978
O	-2.27089	-2.54039	-0.00194
O	-0.77204	-1.01806	-0.60237
Cs	-3.84623	-1.29781	2.20285
Cs	-3.06784	-1.38431	-2.54692
I	-6.68847	-1.35424	-0.64174

G4-ts

G= -3292.306883 Hartree

Pd	1.09291	0.41080	-0.14753
P	-0.39222	2.16543	-0.68929
C	-0.69480	2.46458	-2.45329
C	0.19622	2.59283	-3.48245
O	-1.97039	2.58050	-2.91604
C	-0.59009	2.79417	-4.66561
H	1.27901	2.53296	-3.40145
C	-1.89481	2.77537	-4.26282
H	-0.22804	2.93131	-5.68247
H	-2.84178	2.89810	-4.78298
C	-1.98235	2.03129	0.14870
C	-2.38831	1.13030	1.10102
O	-2.96063	2.96639	-0.04787
C	-3.69923	1.53510	1.51275
H	-1.81473	0.26281	1.41522
C	-3.99202	2.65383	0.78206
H	-4.34862	1.02292	2.21839
H	-4.85943	3.30810	0.73382
C	0.05259	3.86714	-0.18341
C	-0.48452	4.77477	0.69431
O	1.14329	4.41449	-0.79280
C	0.33888	5.94615	0.61813
H	-1.36882	4.62449	1.30749
C	1.31010	5.66472	-0.30159
H	0.22061	6.87350	1.17472
H	2.15651	6.22279	-0.69252
C	3.44387	2.14343	-0.93985

C	4.28269	3.25581	-0.90745
C	4.35468	4.01011	0.27187
C	3.57384	3.68964	1.38021
C	2.67984	2.59219	1.34768
C	2.65014	1.78641	0.16453
H	3.41507	1.50029	-1.82420
H	4.88439	3.52293	-1.77938
H	5.02518	4.87219	0.33019
H	3.64003	4.31567	2.26766
H	1.13323	1.57951	2.11722
N	1.83800	2.25691	2.38287
C	1.71106	2.78881	3.74857
C	0.64382	1.91616	4.43342
H	0.96212	0.86226	4.47169
H	0.46908	2.25931	5.46355
H	-0.31411	1.97179	3.89007
C	1.22548	4.25202	3.75642
H	1.91113	4.92035	3.21936
H	0.24537	4.32853	3.26696
H	1.13075	4.61632	4.79147
C	3.03516	2.65107	4.52609
H	3.33457	1.59437	4.59836
H	3.85673	3.20353	4.05032
H	2.91609	3.04066	5.54883
C	4.20534	-1.81217	2.28397
C	3.35366	-0.52810	2.19909
C	2.14088	-2.19445	1.28838
C	3.47902	-2.80650	1.75344
H	5.23316	-1.84515	2.64595
H	3.77601	-3.84459	1.60793
C	1.95219	-1.15792	2.42493
H	1.10532	-0.48132	2.25073
H	1.86492	-1.62225	3.41720
C	3.33898	-0.24044	0.68989
C	2.47896	-1.22553	0.13237
H	4.25702	0.08941	0.21454
H	3.66451	0.30785	2.83058
H	1.32331	-2.88130	1.05965
S	2.77956	-1.91267	-1.49507
O	1.83821	-3.03003	-1.68360
O	2.84951	-0.79353	-2.45693
C	4.43309	-2.61505	-1.41437
C	5.54319	-1.78101	-1.58761
C	4.58997	-3.97805	-1.16006
C	6.82209	-2.32372	-1.47549
H	5.40221	-0.72416	-1.82218
C	5.87864	-4.50701	-1.05719

H	3.70738	-4.61025	-1.05005
C	7.01226	-3.69192	-1.20594
H	7.69316	-1.67616	-1.60866
H	6.00551	-5.57480	-0.85946
C	8.40401	-4.26465	-1.11704
H	8.40843	-5.25422	-0.63704
H	8.84040	-4.38080	-2.12410
H	9.07520	-3.60072	-0.54985
C	-1.25517	-1.06424	-1.17408
O	-2.05639	-2.04944	-1.24511
O	-1.30018	-0.07083	-1.95973
O	-0.38048	-1.05751	-0.16736
Cs	-1.85727	-3.36746	1.26940
Cs	-4.21916	-0.14684	-2.14453
I	-5.52616	-1.94122	1.45961

H1

G= -3292.334632 Hartree

Pd	0.10143	0.89699	0.20833
P	-1.92240	2.14000	0.61248
C	-3.43010	1.17541	0.30030
C	-4.03237	0.79381	-0.87085
O	-4.05723	0.57281	1.35394
C	-5.11140	-0.07799	-0.50630
H	-3.73157	1.08946	-1.87377
C	-5.07954	-0.17933	0.85630
H	-5.82383	-0.56165	-1.17180
H	-5.66302	-0.73760	1.58884
C	-2.01788	2.60110	2.35971
C	-1.02962	2.59428	3.31333
O	-3.15492	3.15435	2.88139
C	-1.60008	3.17621	4.49154
H	-0.02237	2.20839	3.17320
C	-2.89239	3.49290	4.16514
H	-1.11376	3.34442	5.45032
H	-3.71033	3.94840	4.71914
C	-2.31671	3.71699	-0.20646
C	-3.28843	4.16331	-1.06688
O	-1.38735	4.69900	-0.01442
C	-2.92465	5.50487	-1.42046
H	-4.16098	3.60453	-1.39468
C	-1.76580	5.77433	-0.74780
H	-3.46251	6.18008	-2.08273
H	-1.12011	6.64693	-0.68776
C	1.24483	2.16667	-1.40688
C	0.80450	3.39525	-1.92087
C	1.76637	4.35506	-2.22347

C	3.12755	4.06718	-2.09347
C	3.59060	2.81290	-1.62567
C	2.60269	1.87004	-1.19596
H	0.52211	1.29780	-1.50547
H	-0.25616	3.57601	-2.09280
H	1.46479	5.33336	-2.60673
H	3.84470	4.82501	-2.39914
H	5.11554	1.46283	-1.52534
N	4.92184	2.45818	-1.57515
C	6.13019	3.28191	-1.76463
C	7.32363	2.37418	-1.41338
H	7.35777	1.49100	-2.06861
H	8.26544	2.93140	-1.52806
H	7.25934	2.00306	-0.37940
C	6.13512	4.48099	-0.79687
H	5.30181	5.17498	-0.97196
H	6.06845	4.12764	0.24371
H	7.07151	5.04901	-0.90940
C	6.28418	3.74661	-3.22877
H	6.29566	2.87506	-3.90155
H	5.46746	4.40810	-3.54963
H	7.23051	4.29537	-3.35903
C	1.81641	-0.26135	0.07303
C	2.32470	-0.62947	1.50223
C	3.93806	0.74090	0.72989
C	2.99264	0.56729	-0.54091
H	1.51751	-1.13950	-0.51556
H	3.54694	-0.03870	-1.27766
C	2.95884	0.71665	1.91442
H	3.47971	0.68185	2.88329
H	2.24482	1.55435	1.90359
C	3.57429	-1.48062	1.29937
C	4.54107	-0.64404	0.88112
H	3.62304	-2.56887	1.35931
H	1.54974	-1.05503	2.14687
H	4.64405	1.57395	0.67996
S	6.11134	-0.97064	0.15771
O	5.99420	-0.58601	-1.27325
O	7.15591	-0.32305	0.97273
C	6.31647	-2.74342	0.24789
C	6.96940	-3.29554	1.35150
C	5.80385	-3.54606	-0.77591
C	7.10045	-4.68327	1.43073
H	7.37099	-2.64180	2.12776
C	5.94395	-4.92938	-0.67796
H	5.31052	-3.08532	-1.63365
C	6.59154	-5.51985	0.42315

H	7.60960	-5.12475	2.29143
H	5.54552	-5.56624	-1.47242
C	6.75661	-7.01638	0.49677
H	5.84569	-7.53676	0.16231
H	7.57864	-7.34725	-0.16124
H	6.99287	-7.35114	1.51737
C	-1.11242	-1.51120	1.22878
O	-1.48557	-2.32755	2.13705
O	-0.62990	-0.33846	1.67779
O	-1.21633	-1.72391	-0.00957
Cs	-3.39862	-3.73773	0.36106
Cs	-2.68614	-0.65422	4.17827
I	-5.82500	-3.01661	3.51121

H2

G= -3292.342244 Hartree

Pd	0.03271	1.36008	0.73022
P	-2.33391	1.92730	0.41802
C	-2.66026	3.35665	-0.67709
C	-1.89020	3.89031	-1.68029
O	-3.86216	4.00808	-0.63336
C	-2.67033	4.92838	-2.28552
H	-0.87882	3.58625	-1.93958
C	-3.85518	4.95373	-1.60238
H	-2.38545	5.57331	-3.11385
H	-4.74979	5.56699	-1.68330
C	-3.23775	0.65564	-0.51580
C	-2.81139	-0.52356	-1.07249
O	-4.55283	0.86629	-0.84478
C	-3.93309	-1.07652	-1.77532
H	-1.81886	-0.94764	-0.94738
C	-4.95929	-0.18976	-1.60115
H	-3.96067	-2.02990	-2.29937
H	-5.99368	-0.16712	-1.93686
C	-3.43329	2.27973	1.82163
C	-4.79387	2.22130	1.99323
O	-2.84000	2.63427	2.99576
C	-5.04173	2.55286	3.36577
H	-5.51637	1.97815	1.21896
C	-3.81419	2.79347	3.92079
H	-6.00416	2.61236	3.87069
H	-3.48787	3.07977	4.91772
C	0.96110	3.21706	1.97614
C	0.02114	4.18224	2.37244
C	-0.29474	5.19757	1.47993
C	0.30814	5.25306	0.22213
C	1.24930	4.29777	-0.21076

C	1.59447	3.23134	0.69807
H	-0.44489	4.11776	3.35537
H	-1.03140	5.95926	1.74700
H	0.00792	6.04533	-0.45709
H	2.45067	3.61375	-1.66872
N	1.79019	4.34800	-1.48264
C	2.01791	5.52563	-2.35366
C	3.02077	5.05341	-3.42191
H	2.62457	4.18614	-3.97436
H	3.21838	5.85726	-4.14573
H	3.98345	4.76859	-2.96614
C	2.63916	6.69970	-1.57329
H	1.97043	7.07757	-0.78816
H	3.57884	6.38492	-1.09288
H	2.86166	7.53374	-2.25673
C	0.72572	5.96329	-3.06973
H	0.29908	5.12234	-3.63713
H	-0.04149	6.32140	-2.37186
H	0.94375	6.78153	-3.77354
C	2.72166	2.16543	0.57957
C	3.52494	1.94122	-0.75574
C	2.34110	0.03209	-0.55852
C	1.97925	0.81260	0.72669
H	3.43665	2.35693	1.39516
H	2.18257	0.23849	1.63860
C	2.49698	1.15154	-1.60966
H	2.91733	0.79182	-2.56005
H	1.55659	1.68888	-1.80195
C	4.52615	0.82990	-0.44022
C	3.81070	-0.30384	-0.35037
H	5.58752	0.96634	-0.23156
H	3.99923	2.83450	-1.18157
H	1.66959	-0.79580	-0.80150
S	4.28539	-1.92140	0.16475
O	3.65593	-2.16865	1.48234
O	3.94994	-2.84978	-0.93768
C	6.05673	-1.85574	0.36118
C	6.87473	-2.15465	-0.73226
C	6.59192	-1.48375	1.59741
C	8.25785	-2.07006	-0.57721
H	6.42743	-2.45240	-1.68225
C	7.97846	-1.40498	1.73099
H	5.92861	-1.26653	2.43660
C	8.83130	-1.69586	0.65159
H	8.90717	-2.30203	-1.42554
H	8.40776	-1.11535	2.69360
C	10.32870	-1.64264	0.81342

H	10.62646	-0.95998	1.62299
H	10.72349	-2.64273	1.06335
H	10.82374	-1.32068	-0.11529
C	-1.19898	-1.04015	1.78139
O	-1.18230	-2.26398	2.11822
O	-2.02550	-0.19196	2.23074
O	-0.31201	-0.67213	0.84363
Cs	0.70999	-3.63596	0.36196
Cs	-4.18956	-2.24713	2.03484
I	-2.96015	-4.85833	-0.84343
H	1.32469	2.51243	2.72854

H3

G= -3292.339632 Hartree

Pd	-0.03268	1.22583	-0.90776
P	-1.56688	2.46170	0.45489
C	-0.77713	3.54189	1.68407
C	-1.01423	3.84207	3.00156
O	0.37752	4.15112	1.27677
C	0.06282	4.68808	3.42292
H	-1.85476	3.48816	3.59387
C	0.87336	4.84045	2.33153
H	0.21332	5.12504	4.40797
H	1.79594	5.38829	2.15539
C	-2.62670	3.62912	-0.44320
C	-2.55481	4.98322	-0.64616
O	-3.59153	3.09365	-1.24583
C	-3.53983	5.29207	-1.64241
H	-1.86788	5.66804	-0.15412
C	-4.13203	4.10637	-1.97204
H	-3.76993	6.26889	-2.06241
H	-4.90987	3.82908	-2.67868
C	-2.78993	1.54071	1.42661
C	-3.97055	1.87939	2.04526
O	-2.60995	0.18447	1.51547
C	-4.53290	0.66128	2.54650
H	-4.38513	2.88344	2.11604
C	-3.66042	-0.33517	2.19337
H	-5.46692	0.53599	3.09053
H	-3.67788	-1.41906	2.29365
C	1.11723	0.01229	0.67187
C	0.70464	0.43846	1.94658
C	1.50964	1.32780	2.64741
C	2.75070	1.69577	2.13256
C	3.23280	1.22447	0.89030
C	2.34805	0.42964	0.08606
H	0.56629	-0.80309	0.20449

H	-0.24341	0.08093	2.34773
H	1.19321	1.72236	3.61486
H	3.38759	2.33370	2.73874
H	4.93583	0.71256	-0.04899
N	4.52162	1.47533	0.46655
C	5.51211	2.45107	0.94900
C	6.65340	2.41052	-0.08506
H	6.28613	2.69050	-1.08438
H	7.45685	3.10652	0.19753
H	7.08955	1.39918	-0.14560
C	6.09327	2.07179	2.32897
H	5.33752	2.09904	3.12578
H	6.50722	1.05265	2.29624
H	6.90106	2.76556	2.61052
C	4.91360	3.86875	0.96024
H	4.51778	4.12057	-0.03544
H	4.09442	3.97711	1.68396
H	5.69167	4.60105	1.22443
C	2.56170	0.46293	-4.26784
C	1.78194	1.30189	-3.27199
C	3.69304	0.68614	-2.25889
C	3.69416	0.08046	-3.66068
H	2.19211	0.14675	-5.24514
H	4.45081	-0.60868	-4.03137
C	2.94498	2.00964	-2.53819
H	2.64013	2.55228	-1.63112
H	3.52539	2.67522	-3.19330
C	1.29224	0.30805	-2.17724
C	2.58519	-0.03544	-1.37201
H	0.75250	-0.55068	-2.59512
H	0.96835	1.91561	-3.67202
H	4.68421	0.75789	-1.81283
S	2.92387	-1.88563	-1.28739
O	1.79573	-2.54560	-0.57642
O	3.30193	-2.43401	-2.60329
C	4.35994	-1.93818	-0.21252
C	5.63136	-1.81483	-0.78513
C	4.18967	-1.98448	1.17315
C	6.74171	-1.70855	0.05209
H	5.73921	-1.80151	-1.87120
C	5.31355	-1.87777	1.99450
H	3.18910	-2.08603	1.59544
C	6.60064	-1.72895	1.45220
H	7.73751	-1.60637	-0.38754
H	5.18540	-1.89927	3.07955
C	7.81230	-1.60986	2.34021
H	7.53483	-1.38029	3.37910

H	8.38389	-2.55362	2.34659
H	8.49342	-0.82229	1.98145
C	-2.07343	0.72553	-2.81874
O	-2.96475	0.97382	-3.66866
O	-1.16052	1.66435	-2.57074
O	-2.02618	-0.36464	-2.13245
Cs	-1.08543	-3.03258	-1.75541
Cs	-4.92481	-0.01975	-1.57788
I	-4.46189	-3.60553	0.18221

H4

G= -3292.357158 Hartree

Pd	-1.19228	0.92409	-0.53464
P	0.44903	1.64253	1.06759
C	1.50235	0.35999	1.80916
C	1.32740	-0.46764	2.89371
O	2.60955	-0.03466	1.11832
C	2.39753	-1.42047	2.85383
H	0.52895	-0.40820	3.62864
C	3.14325	-1.11264	1.74977
H	2.58096	-2.23499	3.55116
H	4.01393	-1.55726	1.26853
C	1.60247	2.93617	0.54410
C	1.52836	3.83597	-0.49048
O	2.66324	3.24811	1.35634
C	2.61168	4.75464	-0.29956
H	0.79688	3.80217	-1.29477
C	3.26172	4.34788	0.83454
H	2.87097	5.60586	-0.92589
H	4.13050	4.72168	1.37211
C	-0.28736	2.37340	2.56126
C	0.07258	2.48784	3.88199
O	-1.48978	2.99199	2.36304
C	-0.98359	3.20743	4.52740
H	0.98590	2.10296	4.32887
C	-1.90144	3.48612	3.55111
H	-1.05043	3.48214	5.57809
H	-2.85827	4.00217	3.55061
C	-2.80793	0.10022	0.99533
C	-2.69442	0.13842	2.39154
C	-3.84279	0.38629	3.13486
C	-5.08103	0.52067	2.50111
C	-5.21550	0.43257	1.09623
C	-4.02344	0.28663	0.31833
H	-1.96681	-0.41555	0.45102
H	-1.73118	-0.03069	2.87088
H	-3.79216	0.44598	4.22465

H	-5.96293	0.66494	3.12019
H	-6.39635	0.13241	-0.51138
N	-6.42964	0.47121	0.44012
C	-7.79976	0.57472	0.97147
C	-8.72006	0.55764	-0.26236
H	-8.60644	-0.38367	-0.82542
H	-9.77322	0.64138	0.04276
H	-8.48754	1.39759	-0.93602
C	-8.00612	1.91181	1.70941
H	-7.37691	2.00334	2.60458
H	-7.76814	2.75457	1.04248
H	-9.05520	2.00642	2.02973
C	-8.16186	-0.62350	1.87397
H	-8.03707	-1.56744	1.32071
H	-7.53120	-0.67564	2.77178
H	-9.21046	-0.55229	2.20309
C	-2.66881	0.27850	-1.89697
C	-2.82406	1.32374	-3.05144
C	-4.73869	1.55905	-1.88887
C	-4.06931	0.27719	-1.19382
H	-4.65013	-0.60485	-1.51919
C	-3.52058	2.43337	-2.23086
H	-3.79034	3.30344	-2.84764
H	-2.94291	2.76786	-1.35516
C	-3.97510	0.90126	-3.96028
C	-5.11895	1.07278	-3.27946
H	-3.84907	0.44369	-4.94218
H	-1.87080	1.56765	-3.52584
H	-5.52972	2.02340	-1.29122
S	-2.23423	-1.35756	-2.57683
O	-3.44065	-2.03728	-3.10579
O	-1.09327	-1.16507	-3.51172
C	-1.64701	-2.35258	-1.19467
C	-0.33665	-2.19592	-0.72241
C	-2.53795	-3.23263	-0.57773
C	0.06982	-2.93108	0.38934
H	0.34335	-1.46351	-1.16933
C	-2.11250	-3.95532	0.54090
H	-3.54995	-3.34224	-0.97037
C	-0.80884	-3.81501	1.04273
H	1.08739	-2.80163	0.76487
H	-2.80992	-4.63844	1.03311
C	-0.33978	-4.59198	2.24619
H	-1.17262	-5.08930	2.76459
H	0.38656	-5.36765	1.94985
H	0.17370	-3.93244	2.96417
C	1.03193	1.21636	-2.31147

O	1.69527	1.66880	-3.28578
O	-0.14841	1.77607	-2.05028
O	1.44412	0.27073	-1.55638
Cs	1.77253	-1.48369	-4.09429
Cs	4.25348	1.29598	-1.43902
I	4.93184	-2.48028	-1.68528
H	-6.12456	0.77859	-3.58761

I1-ts

G= -3292.305333 Hartree

Pd	0.33692	0.90500	1.02609
P	-1.61389	2.21111	1.43955
C	-2.95842	2.20760	0.21366
C	-3.42503	3.15100	-0.66548
O	-3.61362	1.02392	0.00473
C	-4.43310	2.50486	-1.45561
H	-3.08545	4.18151	-0.73215
C	-4.51486	1.21882	-1.00290
H	-5.03427	2.94647	-2.24776
H	-5.14348	0.36137	-1.25231
C	-2.49131	1.71709	2.94871
C	-2.13123	0.80705	3.91232
O	-3.70466	2.26397	3.26782
C	-3.18771	0.80139	4.88172
H	-1.22035	0.21128	3.90711
C	-4.11295	1.70511	4.43266
H	-3.24987	0.20890	5.79239
H	-5.07130	2.04448	4.81959
C	-1.36003	3.99315	1.65229
C	-2.16941	5.04300	2.01300
O	-0.08560	4.44866	1.45091
C	-1.33971	6.20784	2.02556
H	-3.23053	4.97343	2.24235
C	-0.08671	5.78057	1.67447
H	-1.63331	7.22812	2.26385
H	0.86546	6.28973	1.54537
C	0.83917	1.45213	-1.10337
C	0.14933	2.43346	-1.84842
C	0.84385	3.21068	-2.77352
C	2.20964	3.00673	-3.00217
C	2.93972	2.03274	-2.28297
C	2.23483	1.30596	-1.27702
H	0.13430	0.30803	-0.96154
H	-0.92777	2.56149	-1.71903
H	0.32005	3.97501	-3.35608
H	2.70347	3.59766	-3.77146
H	4.61275	0.86679	-2.14296

N	4.27370	1.74630	-2.51527
C	5.32285	2.58106	-3.12480
C	6.66427	1.90650	-2.78407
H	6.69891	0.87664	-3.17095
H	7.49583	2.47397	-3.22822
H	6.82590	1.84725	-1.69705
C	5.32089	3.99777	-2.51837
H	4.37927	4.53295	-2.70311
H	5.46899	3.94387	-1.42850
H	6.13881	4.59612	-2.94916
C	5.18162	2.64204	-4.66098
H	5.18800	1.62419	-5.08069
H	4.24742	3.12913	-4.97404
H	6.01811	3.20577	-5.10459
C	2.04435	-0.20208	0.77148
C	2.87054	0.03827	2.07374
C	4.12940	1.00966	0.47728
C	2.95316	0.34965	-0.36490
H	1.71024	-1.23854	0.63646
H	3.38927	-0.47663	-0.95100
C	3.43739	1.44763	1.77831
H	4.15064	1.80080	2.53810
H	2.65876	2.20985	1.61376
C	4.12670	-0.81706	1.91622
C	4.88464	-0.20099	0.99176
H	4.29270	-1.79757	2.36394
H	2.31498	-0.11634	3.00955
H	4.71932	1.76137	-0.05417
S	6.29259	-0.76264	0.09213
O	5.84603	-0.91293	-1.31489
O	7.42509	0.13602	0.38060
C	6.65716	-2.38533	0.74627
C	7.56923	-2.50450	1.79726
C	6.01356	-3.50230	0.20581
C	7.83087	-3.77191	2.31967
H	8.06650	-1.61474	2.18767
C	6.28869	-4.75998	0.74135
H	5.31511	-3.37994	-0.62399
C	7.19862	-4.91599	1.80285
H	8.54270	-3.87556	3.14290
H	5.79001	-5.63995	0.32638
C	7.51306	-6.28595	2.34749
H	6.63622	-6.94960	2.30241
H	8.31303	-6.76170	1.75386
H	7.86145	-6.23904	3.38997
C	-1.05423	-1.48865	-0.15198
O	-1.80346	-2.48653	-0.36366

O	-0.83601	-1.07998	1.06167
O	-0.54993	-0.84399	-1.17968
Cs	-2.62337	-1.69815	-3.14432
Cs	-3.79685	-1.85457	1.74604
I	-6.19269	-2.33549	-1.39899

I2-ts

G= -3292.294386 Hartree

Pd	-0.41519	0.91002	1.14853
P	1.75218	1.62584	1.87423
C	1.84266	3.17072	2.80856
C	0.85708	4.09905	3.04005
O	3.01464	3.59313	3.37103
C	1.46506	5.15216	3.79566
H	-0.17098	4.02964	2.68982
C	2.77287	4.78535	3.96343
H	0.99438	6.06166	4.16291
H	3.61782	5.25296	4.46412
C	2.49221	0.36573	2.94677
C	1.90400	-0.73597	3.52236
O	3.80575	0.42616	3.32186
C	2.92251	-1.38567	4.29294
H	0.86740	-1.04282	3.39439
C	4.05445	-0.63244	4.12591
H	2.82539	-2.28748	4.89419
H	5.07143	-0.72223	4.50124
C	3.07334	1.84790	0.64181
C	4.14888	1.09305	0.25128
O	2.99385	2.97259	-0.13343
C	4.77285	1.80728	-0.82603
H	4.47801	0.14514	0.66598
C	4.03085	2.94044	-1.01349
H	5.66081	1.49199	-1.37002
H	4.11250	3.79090	-1.68635
C	-1.04470	2.30558	-0.48688
C	-0.35791	3.51475	-0.73723
C	-1.05840	4.61650	-1.22031
C	-2.42326	4.52165	-1.51260
C	-3.14416	3.32880	-1.28663
C	-2.44833	2.24222	-0.68072
H	0.71988	3.57138	-0.57670
H	-0.54207	5.56288	-1.40703
H	-2.92201	5.38892	-1.93824
H	-4.74849	2.19244	-1.70787
N	-4.48962	3.16580	-1.60905
C	-5.37022	4.04631	-2.39794
C	-6.70152	3.28363	-2.52773

H	-7.13080	3.07504	-1.53495
H	-7.43027	3.87354	-3.10283
H	-6.55779	2.32469	-3.05386
C	-4.81480	4.31416	-3.81288
H	-3.85036	4.83910	-3.78707
H	-4.66340	3.36352	-4.34851
H	-5.51974	4.92914	-4.39451
C	-5.64795	5.36512	-1.65077
H	-6.03751	5.15519	-0.64292
H	-4.75147	5.98918	-1.54131
H	-6.39760	5.95680	-2.19888
C	-3.14258	0.96955	-0.24365
C	-4.37236	1.17779	0.75177
C	-2.95963	-0.08528	1.97330
C	-2.19928	0.08322	0.62975
H	-3.49813	0.40705	-1.12825
H	-1.92623	-0.87833	0.18096
C	-3.66216	1.28109	2.11524
H	-4.36550	1.31882	2.96036
H	-2.96006	2.12645	2.17436
C	-5.00454	-0.20223	0.85761
C	-4.15659	-0.94701	1.58758
H	-5.88768	-0.54744	0.31861
H	-5.04384	1.99776	0.47952
H	-2.36637	-0.46219	2.81743
S	-4.12308	-2.69308	1.86111
O	-2.80335	-3.16325	1.39181
O	-4.52984	-2.95904	3.25208
C	-5.38136	-3.34173	0.76326
C	-6.67932	-3.52448	1.24232
C	-5.04307	-3.63502	-0.56159
C	-7.65876	-4.00304	0.36876
H	-6.90793	-3.29882	2.28552
C	-6.03365	-4.11234	-1.41789
H	-4.01650	-3.49153	-0.90451
C	-7.35415	-4.30340	-0.96925
H	-8.67843	-4.14937	0.73482
H	-5.77945	-4.34574	-2.45549
C	-8.40413	-4.84713	-1.90467
H	-8.33195	-4.38357	-2.90107
H	-8.27248	-5.93398	-2.04417
H	-9.42051	-4.68234	-1.51808
C	0.61553	-0.86232	-1.06709
O	1.11260	-1.80385	-1.75319
O	0.25893	0.24963	-1.66229
O	0.51803	-0.98404	0.22423
Cs	2.51829	-3.15927	0.54242

Cs	2.69691	-0.01917	-3.49287
I	5.64672	-2.02204	-1.60433
H	-0.37063	1.22962	-0.90030

I3-ts

G= -3292.304100 Hartree

Pd	-0.22023	1.62358	-0.96659
P	-2.00214	2.89525	-0.03001
C	-1.47650	4.05651	1.26256
C	-1.99807	4.43653	2.47425
O	-0.23589	4.60748	1.10555
C	-1.01416	5.27463	3.09168
H	-2.96350	4.13510	2.87438
C	0.03158	5.33851	2.21179
H	-1.07350	5.75837	4.06445
H	0.99578	5.84052	2.23382
C	-2.96750	3.96740	-1.13417
C	-3.43734	5.25379	-1.04141
O	-3.29141	3.44775	-2.35732
C	-4.09508	5.53365	-2.28334
H	-3.32024	5.91254	-0.18381
C	-3.97491	4.39970	-3.03826
H	-4.58877	6.45778	-2.57692
H	-4.30409	4.13095	-4.03930
C	-3.32893	1.98758	0.81761
C	-4.66497	2.23386	1.02946
O	-2.99120	0.79626	1.39547
C	-5.16362	1.12684	1.79233
H	-5.21336	3.10675	0.68086
C	-4.09802	0.28739	1.98978
H	-6.18032	0.96894	2.14668
H	-3.98572	-0.69162	2.45580
C	0.82963	0.89209	0.85065
C	0.34735	1.34312	2.09399
C	1.23748	1.81062	3.05660
C	2.60966	1.80071	2.80769
C	3.14741	1.33661	1.58603
C	2.22682	0.92393	0.57583
H	0.11255	-0.10123	0.27624
H	-0.72209	1.30022	2.30555
H	0.87329	2.16479	4.02513
H	3.28643	2.11750	3.59834
H	4.80294	0.74486	0.58425
N	4.52232	1.23988	1.41382
C	5.58280	2.13550	1.92447
C	6.80111	1.91546	1.00813
H	6.58606	2.22958	-0.02619

H	7.65963	2.50315	1.36489
H	7.09596	0.85401	0.99359
C	5.98980	1.75761	3.36367
H	5.17400	1.91496	4.08221
H	6.27764	0.69589	3.40856
H	6.84633	2.36638	3.69446
C	5.16105	3.61441	1.84211
H	4.88866	3.87588	0.80754
H	4.29511	3.83345	2.48182
H	5.99054	4.26511	2.16003
C	2.87523	0.73869	-3.70746
C	1.92689	1.59947	-2.88544
C	3.73623	1.20261	-1.60948
C	3.95710	0.50978	-2.94950
H	2.64260	0.31369	-4.68500
H	4.81980	-0.10656	-3.19228
C	2.93838	2.44315	-2.07852
H	2.48829	3.01737	-1.25486
H	3.54985	3.10610	-2.70844
C	1.37593	0.64726	-1.78627
C	2.58745	0.44503	-0.81568
H	0.96890	-0.28501	-2.18749
H	1.15226	2.12905	-3.45870
H	4.64566	1.41129	-1.04595
S	2.91257	-1.47910	-0.64419
O	2.46524	-1.89276	0.70937
O	2.34890	-2.18141	-1.82215
C	4.69222	-1.81423	-0.65868
C	5.29718	-2.28653	-1.82815
C	5.41438	-1.72167	0.53326
C	6.65388	-2.60647	-1.81092
H	4.69685	-2.41429	-2.72984
C	6.77497	-2.03977	0.53152
H	4.91734	-1.40877	1.45188
C	7.41897	-2.47604	-0.63719
H	7.12903	-2.97568	-2.72407
H	7.34220	-1.96067	1.46286
C	8.88894	-2.80980	-0.64656
H	9.32652	-2.75808	0.36085
H	9.06284	-3.82256	-1.04496
H	9.44445	-2.11072	-1.29419
C	-1.21113	-1.21281	-1.21139
O	-1.67459	-2.30746	-1.63621
O	-1.51048	-0.09290	-1.79893
O	-0.45975	-1.21382	-0.13598
Cs	-0.10355	-3.98262	0.44581
Cs	-4.40869	-1.20055	-1.38951

I	-4.11851	-3.70088	1.71435

I4-ts

G= -3292.297917 Hartree

Pd	-0.86635	1.40662	-0.65065
P	0.72231	2.54108	0.68269
C	1.83937	1.65974	1.80834
C	1.80869	1.43329	3.16160
O	2.89592	0.99063	1.25728
C	2.91980	0.57511	3.45294
H	1.07791	1.83715	3.85759
C	3.55077	0.34404	2.26250
H	3.22346	0.19466	4.42618
H	4.43107	-0.23021	1.96625
C	1.87876	3.48010	-0.34629
C	1.92664	3.62427	-1.71129
O	2.90045	4.18652	0.22651
C	3.04750	4.47398	-1.98871
H	1.24655	3.15518	-2.41986
C	3.59746	4.77938	-0.77230
H	3.39452	4.81683	-2.96144
H	4.44902	5.38537	-0.47085
C	-0.01042	3.75757	1.80785
C	0.47007	4.58267	2.79517
O	-1.35764	3.95668	1.66477
C	-0.65122	5.32293	3.28601
H	1.50545	4.64386	3.12294
C	-1.73075	4.89761	2.55909
H	-0.65594	6.07127	4.07583
H	-2.78634	5.15848	2.56859
C	-1.86633	0.23254	0.98079
C	-1.49297	0.09635	2.33413
C	-2.46694	-0.07007	3.31508
C	-3.82117	-0.11542	2.97077
C	-4.23644	0.02602	1.63121
C	-3.23739	0.25435	0.63801
H	-0.84552	-0.36335	0.31291
H	-0.43379	0.07108	2.59756
H	-2.18103	-0.18263	4.36541
H	-4.56006	-0.25694	3.75660
H	-5.67455	-0.00551	0.23855
N	-5.57527	-0.01361	1.24487
C	-6.65344	-0.82151	1.86081
C	-7.76311	-0.90001	0.79684
H	-7.40254	-1.42071	-0.10622
H	-8.63101	-1.45487	1.18229
H	-8.09966	0.10872	0.50809

C	-7.22610	-0.12641	3.11030
H	-6.49767	-0.07139	3.93074
H	-7.53803	0.90026	2.86466
H	-8.10234	-0.67907	3.48436
C	-6.18206	-2.25189	2.18831
H	-5.77968	-2.73261	1.28415
H	-5.39122	-2.26091	2.95106
H	-7.02251	-2.85669	2.56363
C	-2.46671	0.69912	-1.77240
C	-2.80706	1.99643	-2.58833
C	-4.37317	1.98211	-0.96711
C	-3.65938	0.56464	-0.77487
H	-4.37455	-0.19978	-1.11932
C	-3.20459	2.89417	-1.38116
H	-3.52662	3.90034	-1.68822
H	-2.42794	2.99692	-0.59226
C	-4.17085	1.84897	-3.26176
C	-5.10207	1.87313	-2.29617
H	-4.30935	1.65865	-4.32389
H	-1.99080	2.33880	-3.23840
H	-4.96741	2.28731	-0.09747
S	-2.24777	-0.77424	-2.86358
O	-3.05306	-0.55729	-4.09016
O	-0.82058	-1.09318	-3.02546
C	-3.02755	-2.13911	-1.97413
C	-2.35100	-2.74939	-0.91520
C	-4.31046	-2.54502	-2.34808
C	-2.99127	-3.77297	-0.21446
H	-1.35030	-2.41041	-0.63606
C	-4.93213	-3.57274	-1.63562
H	-4.80807	-2.04940	-3.18349
C	-4.28563	-4.20032	-0.55711
H	-2.47660	-4.24662	0.62683
H	-5.93819	-3.89252	-1.92128
C	-4.95026	-5.32025	0.20344
H	-6.04149	-5.31558	0.06360
H	-4.57619	-6.30066	-0.13902
H	-4.74135	-5.25101	1.28241
C	1.06553	-0.81529	-0.89157
O	2.00020	-1.59739	-1.21650
O	0.99273	0.37278	-1.40382
O	0.21349	-1.19330	0.04004
Cs	2.17717	-3.18365	1.24108
Cs	4.03588	0.40258	-1.89305
I	6.02441	-2.16887	0.56046
H	-6.17677	1.71539	-2.40692

J1

G= -3292.362826 Hartree

Pd	0.28961	1.12662	0.40793
P	-1.78774	2.25795	0.84230
C	-3.17252	1.26558	0.20117
C	-3.41510	0.85871	-1.08563
O	-4.14887	0.77396	1.02597
C	-4.62934	0.09481	-1.04979
H	-2.79619	1.08547	-1.95191
C	-5.02545	0.06762	0.25904
H	-5.14549	-0.36781	-1.88917
H	-5.83908	-0.42547	0.78879
C	-2.04424	2.35091	2.63541
C	-1.12494	2.19866	3.64491
O	-3.23686	2.76779	3.16382
C	-1.79727	2.53993	4.86296
H	-0.09213	1.88414	3.51123
C	-3.07521	2.87875	4.50350
H	-1.38310	2.54843	5.86919
H	-3.94476	3.21082	5.06669
C	-2.30586	3.92698	0.33226
C	-3.21431	4.41313	-0.57366
O	-1.56755	4.95486	0.84312
C	-3.01735	5.83293	-0.61354
H	-3.93201	3.82371	-1.13886
C	-2.00746	6.10135	0.26733
H	-3.55993	6.55709	-1.21767
H	-1.51304	7.01678	0.58277
C	1.34306	2.40987	-0.72904
C	0.85118	3.62785	-1.23864
C	1.68851	4.44062	-2.00915
C	3.00073	4.06684	-2.30867
C	3.52324	2.84488	-1.83163
C	2.66901	2.03311	-1.03060
H	-0.53446	-0.80368	-0.67313
H	-0.16856	3.95671	-1.04278
H	1.30785	5.39088	-2.39745
H	3.60880	4.71995	-2.93239
H	4.99238	1.43025	-1.85515
N	4.80286	2.38836	-2.12144
C	6.02104	3.16923	-2.39793
C	7.20701	2.20981	-2.19016
H	7.12212	1.32968	-2.84585
H	8.15421	2.72286	-2.41537
H	7.25221	1.83808	-1.15491
C	6.16680	4.34760	-1.41480
H	5.33582	5.06180	-1.49648

H	6.18971	3.97585	-0.37832
H	7.10424	4.89303	-1.60761
C	6.04686	3.67216	-3.85675
H	5.93992	2.82267	-4.54893
H	5.23214	4.37989	-4.06446
H	6.99856	4.18331	-4.07518
C	2.01436	-0.01821	0.27662
C	2.61715	-0.27780	1.70558
C	4.23726	0.91803	0.68609
C	3.15661	0.73940	-0.45991
H	1.75330	-0.96981	-0.21492
H	3.59952	0.10956	-1.24874
C	3.36538	1.05119	1.94942
H	3.96526	1.05508	2.87266
H	2.70444	1.92932	1.92281
C	3.78972	-1.22372	1.46680
C	4.75959	-0.48888	0.88858
H	3.77534	-2.30736	1.59524
H	1.88548	-0.60674	2.45467
H	4.98678	1.69495	0.49976
S	6.21018	-0.99016	0.02576
O	5.95217	-0.76522	-1.41765
O	7.37791	-0.33006	0.64024
C	6.33394	-2.75371	0.30537
C	7.07357	-3.22013	1.39455
C	5.67662	-3.63164	-0.55979
C	7.14549	-4.59509	1.62032
H	7.58639	-2.50890	2.04459
C	5.75937	-5.00319	-0.31754
H	5.11706	-3.23704	-1.40987
C	6.49269	-5.50645	0.77157
H	7.72196	-4.96948	2.47064
H	5.24794	-5.69817	-0.98901
C	6.60756	-6.99162	1.00463
H	5.73868	-7.53416	0.60287
H	7.50571	-7.39232	0.50313
H	6.70032	-7.22703	2.07571
C	-1.18630	-1.55178	0.96538
O	-1.79073	-2.51053	1.47852
O	-0.77663	-0.51643	1.57039
O	-0.99619	-1.62208	-0.39152
Cs	-3.60259	-3.71743	-0.56239
Cs	-3.17500	-1.01079	3.76882
I	-6.16746	-3.11038	2.29333

J2

G= -3292.373937 Hartree

Pd	-0.19528	1.14081	0.17596
P	1.86160	1.88857	1.17505
C	1.83720	3.36348	2.22429
C	0.79331	4.15373	2.63740
O	2.99326	3.77273	2.83481
C	1.34627	5.10663	3.55206
H	-0.23781	4.06147	2.30463
C	2.68324	4.82543	3.62643
H	0.81950	5.90020	4.07777
H	3.50894	5.27467	4.17384
C	2.31746	0.65526	2.44371
C	1.92625	0.56405	3.75496
O	2.98440	-0.48211	2.08497
C	2.38370	-0.71030	4.22767
H	1.37399	1.32105	4.30767
C	3.02180	-1.30398	3.17603
H	2.26808	-1.12692	5.22630
H	3.52782	-2.26219	3.04236
C	3.41887	2.03428	0.24442
C	4.75228	2.01981	0.57575
O	3.29264	2.15136	-1.11468
C	5.47931	2.13548	-0.65438
H	5.15272	1.94653	1.58461
C	4.53458	2.21316	-1.64493
H	6.55935	2.17270	-0.78512
H	4.59206	2.31772	-2.72595
C	-1.23187	2.80379	-0.28174
C	-0.66158	4.08696	-0.39797
C	-1.45137	5.16970	-0.79067
C	-2.80456	5.00832	-1.09704
C	-3.40445	3.73336	-1.03145
C	-2.60000	2.63649	-0.60681
H	0.39537	4.25042	-0.18093
H	-1.00774	6.16765	-0.86643
H	-3.38194	5.87884	-1.39966
H	-4.93048	2.50419	-1.48250
N	-4.74422	3.48754	-1.33553
C	-5.69094	4.33917	-2.07632
C	-6.93450	3.46369	-2.31729
H	-7.35341	3.10910	-1.36191
H	-7.71311	4.03410	-2.84511
H	-6.68464	2.58472	-2.93553
C	-5.13253	4.78811	-3.44317
H	-4.23205	5.40767	-3.33685
H	-4.86378	3.90951	-4.05081
H	-5.88549	5.37339	-3.99486
C	-6.11954	5.55307	-1.22844

H	-6.52839	5.21446	-0.26407
H	-5.28489	6.23402	-1.01692
H	-6.89627	6.12970	-1.75520
C	-3.14756	1.23437	-0.52273
C	-4.19139	0.99974	0.65883
C	-2.47384	-0.35802	1.20544
C	-1.99966	0.25413	-0.15276
H	-3.62142	0.94926	-1.48195
H	-1.83289	-0.53717	-0.89687
C	-3.22968	0.82050	1.85424
H	-3.75091	0.54022	2.78236
H	-2.58769	1.69472	2.02902
C	-4.69392	-0.42423	0.48110
C	-3.66717	-1.22332	0.82856
H	-5.64486	-0.72737	0.04061
H	-4.96067	1.77742	0.73673
H	-1.69687	-0.85068	1.79992
S	-3.48395	-2.96461	0.67896
O	-2.48222	-3.24275	-0.37831
O	-3.18980	-3.50348	2.03015
C	-5.07585	-3.56895	0.14323
C	-6.03466	-3.91418	1.09894
C	-5.34075	-3.66063	-1.22635
C	-7.28534	-4.35579	0.66594
H	-5.79662	-3.84010	2.16153
C	-6.59726	-4.10393	-1.63817
H	-4.56904	-3.39183	-1.94999
C	-7.58664	-4.45867	-0.70346
H	-8.04250	-4.62848	1.40574
H	-6.81470	-4.17933	-2.70692
C	-8.92792	-4.96979	-1.16362
H	-9.24031	-4.49283	-2.10495
H	-8.88235	-6.05717	-1.34843
H	-9.70937	-4.79724	-0.40880
C	1.38999	-1.37089	-0.59757
O	1.81938	-2.53133	-0.67143
O	1.87001	-0.49640	-1.54140
O	0.60415	-0.91647	0.28937
Cs	0.23639	-3.73331	1.65461
Cs	4.75189	-1.88437	-0.46444
I	4.28414	-4.85076	2.04853
H	1.43631	0.37156	-1.42067

J3

G= -3292.370023 Hartree

Pd	0.04507	2.23367	-0.97969
P	-1.85510	2.62928	0.46117

C	-1.81013	3.78853	1.86266
C	-1.85025	3.63972	3.22548
O	-1.52257	5.08828	1.55070
C	-1.57586	4.93340	3.77954
H	-2.03668	2.71289	3.76152
C	-1.38804	5.77079	2.71656
H	-1.52423	5.20191	4.83260
H	-1.16613	6.83137	2.62809
C	-3.38955	3.18987	-0.35856
C	-3.99646	4.41778	-0.42941
O	-4.01818	2.31946	-1.20447
C	-5.06279	4.28906	-1.38029
H	-3.69861	5.30645	0.12107
C	-5.02558	2.99828	-1.82095
H	-5.75976	5.06144	-1.69867
H	-5.61002	2.43905	-2.54740
C	-2.40681	1.10600	1.28785
C	-3.47500	0.77347	2.08918
O	-1.66631	-0.01750	1.04100
C	-3.36950	-0.63158	2.34692
H	-4.23955	1.46114	2.44603
C	-2.24902	-1.05637	1.67866
H	-4.03594	-1.25023	2.94474
H	-1.78954	-2.03274	1.53778
C	1.57981	2.39918	0.30174
C	1.52177	3.17546	1.47139
C	2.64524	3.30315	2.28857
C	3.84108	2.66997	1.96568
C	3.96330	1.89665	0.78973
C	2.80348	1.75763	-0.04189
H	-0.78760	0.02676	-1.29510
H	0.61228	3.70431	1.74635
H	2.58922	3.90558	3.20077
H	4.68989	2.77321	2.63601
H	5.10868	0.48308	-0.12886
N	5.17238	1.30843	0.44525
C	6.53809	1.59264	0.91244
C	7.47108	0.82734	-0.04589
H	7.33818	1.17213	-1.08368
H	8.52324	0.98315	0.23471
H	7.26780	-0.25509	-0.00945
C	6.79444	1.07448	2.34543
H	6.19129	1.60345	3.09541
H	6.53998	0.00663	2.40686
H	7.85433	1.20003	2.61894
C	6.85865	3.09488	0.80234
H	6.70876	3.43879	-0.23262

H	6.22242	3.70746	1.45413
H	7.90733	3.27783	1.08415
C	2.71581	1.45829	-4.32266
C	2.14398	2.45611	-3.32594
C	3.96922	1.52121	-2.37745
C	3.78456	0.88312	-3.74702
H	2.23782	1.17215	-5.26246
H	4.36236	0.03714	-4.11786
C	3.44770	2.95569	-2.67377
H	3.29213	3.56776	-1.77511
H	4.10574	3.48567	-3.37847
C	1.52388	1.55283	-2.20100
C	2.79301	1.09021	-1.40407
H	1.02011	0.70689	-2.68936
H	1.45120	3.20735	-3.72461
H	4.96815	1.45269	-1.94183
S	2.52625	-0.75916	-1.20365
O	1.16876	-0.95399	-0.62182
O	2.79210	-1.47674	-2.48316
C	3.67708	-1.42036	0.00121
C	4.83177	-2.07001	-0.44421
C	3.38209	-1.31070	1.36388
C	5.71544	-2.59817	0.49867
H	5.02486	-2.16413	-1.51416
C	4.28074	-1.83907	2.28865
H	2.46623	-0.81395	1.68559
C	5.45944	-2.48601	1.87569
H	6.61841	-3.11171	0.15812
H	4.06266	-1.74907	3.35586
C	6.44076	-3.01640	2.88904
H	5.93286	-3.36114	3.80219
H	7.03383	-3.84940	2.48351
H	7.14857	-2.22370	3.18891
C	-1.87973	0.71433	-2.79845
O	-2.72225	0.35377	-3.62704
O	-1.38740	1.86060	-2.61377
O	-1.45397	-0.30260	-1.93611
Cs	-0.08746	-2.83690	-3.02760
Cs	-4.51407	-1.00692	-1.46494
I	-2.83562	-4.39549	-0.72586

J4

G= -3292.387502 Hartree

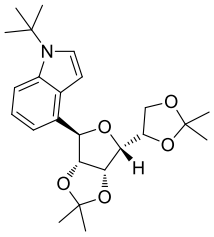
Pd	-0.97714	1.08989	-0.47529
P	0.63802	1.72310	1.16101
C	2.17086	0.85222	0.71836
C	2.34257	-0.44502	0.30782

O	3.39229	1.46307	0.84642
C	3.75908	-0.64369	0.19494
H	1.54772	-1.15412	0.08273
C	4.34478	0.54838	0.52098
H	4.27601	-1.55681	-0.09458
H	5.37267	0.90309	0.51960
C	1.05622	3.47725	1.28455
C	0.35334	4.54633	0.78069
O	2.12083	3.93355	2.01445
C	1.03399	5.72520	1.22481
H	-0.54779	4.47663	0.17413
C	2.09629	5.28569	1.97031
H	0.76311	6.76077	1.02968
H	2.88789	5.79839	2.51271
C	0.50925	1.22661	2.91436
C	0.81951	0.05250	3.55448
O	-0.12941	2.06577	3.77901
C	0.33396	0.18713	4.89716
H	1.33670	-0.79808	3.11714
C	-0.23123	1.42883	4.97379
H	0.40826	-0.54246	5.70092
H	-0.71424	1.98455	5.77360
C	-2.68478	1.23377	0.55418
C	-2.79356	1.85064	1.81320
C	-4.04176	1.94371	2.43250
C	-5.19176	1.42528	1.83528
C	-5.11979	0.80906	0.56901
C	-3.84939	0.74196	-0.07207
H	0.75212	-0.82667	-2.28362
H	-1.92692	2.26724	2.32107
H	-4.12458	2.42938	3.40994
H	-6.14272	1.51323	2.35534
H	-5.96232	-0.26206	-0.90901
N	-6.22321	0.28785	-0.10155
C	-7.51670	-0.14137	0.46024
C	-8.21373	-0.92923	-0.66362
H	-7.62566	-1.81975	-0.94257
H	-9.20826	-1.26953	-0.33962
H	-8.33843	-0.30107	-1.56018
C	-8.39626	1.07384	0.81422
H	-7.96661	1.67876	1.62354
H	-8.51283	1.72408	-0.06622
H	-9.39459	0.74086	1.13973
C	-7.34317	-1.07068	1.67968
H	-6.72698	-1.94086	1.40761
H	-6.84643	-0.56295	2.51752
H	-8.32248	-1.43139	2.03231

C	-2.17790	-0.06621	-1.74951
C	-2.08202	0.37808	-3.25235
C	-4.20709	0.89514	-2.69183
C	-3.69158	0.09754	-1.41544
H	-4.20920	-0.87905	-1.42571
C	-2.94312	1.66277	-3.13213
H	-3.07554	2.16968	-4.09989
H	-2.56614	2.37521	-2.38368
C	-3.01241	-0.48076	-4.10577
C	-4.27594	-0.15174	-3.79155
H	-2.68174	-1.29269	-4.75277
H	-1.05450	0.48867	-3.61300
H	-5.11619	1.47883	-2.49775
S	-1.64899	-1.78313	-1.45976
O	-2.22596	-2.73041	-2.44048
O	-0.14721	-1.80701	-1.33459
C	-2.31223	-2.21704	0.15441
C	-1.72121	-1.74007	1.32605
C	-3.48998	-2.96762	0.19982
C	-2.35348	-1.96034	2.54820
H	-0.79850	-1.16531	1.28281
C	-4.10351	-3.19246	1.43225
H	-3.91590	-3.35783	-0.72609
C	-3.56510	-2.66687	2.61938
H	-1.90556	-1.54924	3.45651
H	-5.02709	-3.77625	1.47251
C	-4.29870	-2.81749	3.92671
H	-4.83501	-3.77707	3.98578
H	-3.61833	-2.74314	4.78812
H	-5.05021	-2.01494	4.02851
C	1.48737	0.95386	-2.69768
O	2.37803	1.54216	-3.35001
O	0.70421	1.50980	-1.87289
O	1.40349	-0.38419	-2.89412
Cs	4.41784	-0.62421	-3.79842
Cs	3.22308	3.84292	-1.66481
I	6.71438	2.13209	-2.21336
H	-5.18939	-0.64409	-4.13256

S8. Characterization Data

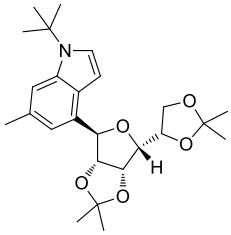
1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3a)



65.6 mg, 79% yield. White crystal.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.32 (d, *J* = 3.4 Hz, 1H), 7.16 (dd, *J* = 8.4, 7.3 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.56 (dd, *J* = 3.4, 0.8 Hz, 1H), 5.53 (s, 1H), 5.15 (dd, *J* = 6.1, 1.2 Hz, 1H), 4.75 (dd, *J* = 6.1, 3.6 Hz, 1H), 4.56-4.53 (m, 1H), 4.30-4.28 (m, 1H), 4.24-4.21 (m, 1H), 4.12 (dd, *J* = 7.8, 3.7 Hz, 1H), 1.74 (s, 9H), 1.63 (s, 3H), 1.45 (s, 3H), 1.41 (s, 3H), 1.39 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.03, 130.34, 127.19, 125.37, 120.40, 114.50, 112.88, 112.70, 109.17, 98.29, 86.79, 84.85, 81.73, 81.07, 73.68, 67.14, 55.92, 29.82, 26.93, 26.33, 25.23, 24.93. **HRMS** (ESI) m/z calculated for $C_{24}H_{33}NO_5Na$ $[M+Na]^+$ 438.2251, found 438.2250.

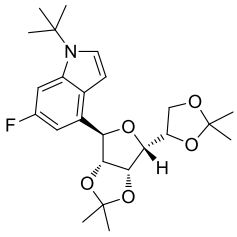
1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-6-methyl-1*H*-indole (3b)



61.9 mg, 72% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H), 7.25 (d, *J* = 3.4 Hz, 1H), 6.85 (s, 1H), 6.50 (d, *J* = 3.3 Hz, 1H), 5.51 (s, 1H), 5.15 (dd, *J* = 6.1, 1.2 Hz, 1H), 4.77 (dd, *J* = 6.1, 3.7 Hz, 1H), 4.57-4.53 (m, 1H), 4.30-4.21 (m, 2H), 4.12 (dd, *J* = 7.8, 3.7 Hz, 1H), 2.51 (s, 3H), 1.73 (s, 9H), 1.63 (s, 3H), 1.46 (s, 3H), 1.41 (s, 3H), 1.39 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.42, 129.95, 129.93, 125.05, 124.78, 116.18, 112.82, 112.63, 109.11, 98.07, 86.73, 84.77, 81.71, 81.01, 73.63, 67.15, 55.74, 29.75, 26.86, 26.28, 25.17, 24.85, 22.40. **HRMS** (ESI) m/z calculated for $C_{25}H_{35}NO_5Na$ $[M+Na]^+$ 452.2407, found 452.2405.

1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-6-fluoro-1*H*-indole (3c)

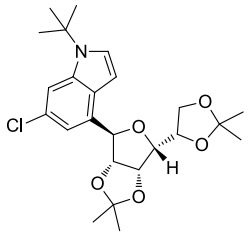


64.2 mg, 74% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.24 (m, 2H), 6.84 (d, *J* = 10.0 Hz, 1H), 6.53 (d, *J* = 3.4 Hz, 1H), 5.48 (s, 1H), 5.09 (d, *J* = 5.9 Hz, 1H), 4.76 (dd, *J* = 6.0, 3.6 Hz, 1H), 4.56-4.51 (m, 1H), 4.28-4.20 (m, 2H), 4.10 (dd, *J* = 7.5, 3.6 Hz, 1H), 1.71 (s, 9H), 1.62 (s, 3H), 1.47 (s, 3H), 1.41 (s, 3H), 1.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.68 (d, *J* = 236.0 Hz), 134.73 (d, *J* = 12.0 Hz), 131.88 (d, *J* = 8.8 Hz), 125.60 (d, *J* = 3.5 Hz), 123.43, 112.92, 109.18, 103.78 (d, *J* = 26.2 Hz), 98.97 (d, *J* = 27.1 Hz), 98.50, 86.80, 84.60 (d, *J* = 1.5 Hz), 81.95, 81.03, 73.61, 67.04, 56.01, 29.63, 26.87, 26.36, 25.22, 24.96. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -120.85. **HRMS** (ESI) m/z calculated for $C_{24}H_{32}FNO_5Na$ $[M+Na]^+$ 456.2157, found 456.2153.

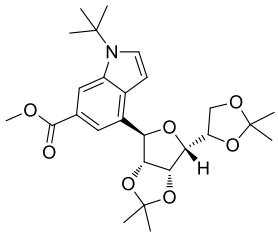
1-(tert-butyl)-6-chloro-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3d)



71.1 mg, 79% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 1.6 Hz, 1H), 7.30 (d, *J* = 3.4 Hz, 1H), 6.99 (t, *J* = 1.4 Hz, 1H), 6.54 (d, *J* = 3.3 Hz, 1H), 5.47 (s, 1H), 5.07 (dd, *J* = 6.0, 1.4 Hz, 1H), 4.77 (dd, *J* = 6.1, 3.7 Hz, 1H), 4.56-4.51 (m, 1H), 4.27-4.20 (m, 2H), 4.09 (dd, *J* = 7.5, 3.7 Hz, 1H), 1.72 (s, 9H), 1.62 (s, 3H), 1.47 (s, 3H), 1.41 (s, 3H), 1.39 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.31, 131.84, 126.53, 126.03, 125.78, 115.28, 112.91, 112.56, 109.16, 98.66, 86.68, 84.52, 81.96, 81.04, 73.59, 67.08, 56.14, 29.78, 26.83, 26.36, 25.22, 24.95. **HRMS** (ESI) m/z calculated for $C_{24}H_{32}ClNO_5Na$ $[M+Na]^+$ 472.1861, found 472.1859.

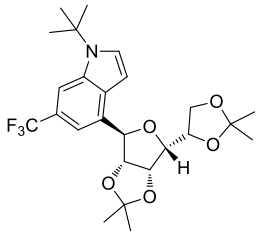
1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole-6-carboxylate (3e)



68.2 mg, 72% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.70 (s, 1H), 7.47 (d, *J* = 3.3 Hz, 1H), 6.63 (d, *J* = 3.3 Hz, 1H), 5.51 (s, 1H), 5.15 (d, *J* = 5.9 Hz, 1H), 4.81 (dd, *J* = 6.1, 3.7 Hz, 1H), 4.54 (q, *J* = 6.0 Hz, 1H), 4.23 (d, *J* = 5.6 Hz, 2H), 4.05 (dd, *J* = 7.8, 3.7 Hz, 1H), 3.95 (s, 3H), 1.78 (s, 9H), 1.63 (s, 3H), 1.45 (s, 3H), 1.41 (s, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 168.17, 134.51, 131.30, 130.05, 128.76, 122.13, 115.73, 115.37, 112.87, 109.22, 99.20, 86.24, 84.43, 81.87, 81.13, 73.57, 67.29, 56.53, 52.06, 30.09, 26.80, 26.40, 25.34, 24.98. **HRMS** (ESI) m/z calculated for $C_{26}H_{35}NO_7Na$ $[M+Na]^+$ 496.2306, found 496.2304.

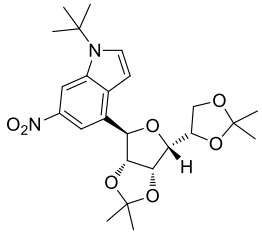
1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-6-(trifluoromethyl)-1*H*-indole (3f)



68.7 mg, 71% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.45 (d, *J* = 3.4 Hz, 1H), 7.25 (s, 1H), 6.63 (dd, *J* = 3.4, 0.9 Hz, 1H), 5.52 (s, 1H), 5.10 (dd, *J* = 6.0, 1.4 Hz, 1H), 4.79 (dd, *J* = 6.0, 3.6 Hz, 1H), 4.57-4.52 (m, 1H), 4.26-4.21 (m, 2H), 4.08 (dd, *J* = 7.5, 3.6 Hz, 1H), 1.76 (s, 9H), 1.64 (s, 3H), 1.46 (s, 3H), 1.42 (s, 3H), 1.40 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 133.99, 131.35, 129.64, 128.10, 125.22 (q, *J* = 271.5 Hz), 122.55 (q, *J* = 31.6 Hz), 113.01, 111.20 (q, *J* = 3.4 Hz), 110.16 (q, *J* = 4.5 Hz), 109.22, 98.96, 86.55, 84.56, 82.01, 81.06, 73.55, 67.13, 56.48, 29.95, 26.76, 26.40, 25.30, 24.99. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -60.34. **HRMS** (ESI) m/z calculated for $C_{25}H_{32}F_3NO_5Na$ $[M+Na]^+$ 506.2125, found 506.2124.

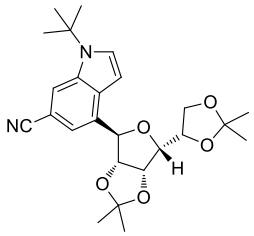
1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-6-nitro-1*H*-indole (3g)



60.8 mg, 66% yield. Light yellow crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 1.9 Hz, 1H), 7.93 (t, *J* = 1.5 Hz, 1H), 7.58 (d, *J* = 3.3 Hz, 1H), 6.69 (d, *J* = 3.3 Hz, 1H), 5.49 (s, 1H), 5.09 (dd, *J* = 6.0, 1.5 Hz, 1H), 4.82 (dd, *J* = 5.9, 3.7 Hz, 1H), 4.56-4.52 (m, 1H), 4.24 (d, *J* = 5.7 Hz, 2H), 4.07 (dd, *J* = 7.5, 3.6 Hz, 1H), 1.80 (s, 9H), 1.64 (s, 3H), 1.46 (s, 3H), 1.42-1.41 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.13, 133.49, 132.24, 131.18, 113.20, 110.30, 109.72, 109.28, 99.97, 86.28, 84.29, 82.14, 81.12, 73.51, 67.16, 57.10, 30.13, 26.80, 26.46, 25.30, 25.03. **HRMS** (ESI) m/z calculated for $C_{24}H_{32}N_2O_7Na$ $[M+Na]^+$ 483.2102, found 483.2100.

1-(tert-butyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole-6-carbonitrile (3h)

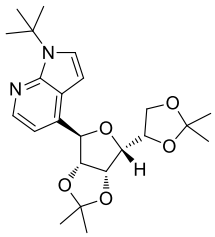


68.7 mg, 78% yield. Light yellow crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.51 (d, *J* = 3.3 Hz, 1H), 7.24 (s, 1H), 6.64 (d, *J* = 3.3 Hz, 1H), 5.47 (s, 1H), 5.04 (dd, *J* = 6.0, 1.6 Hz, 1H), 4.78 (dd, *J* = 6.0, 3.6 Hz, 1H), 4.53 (q, *J* = 6.1 Hz, 1H),

4.26-4.19 (m, 2H), 4.08 (dd, *J* = 7.3, 3.6 Hz, 1H), 1.76 (s, 9H), 1.63 (s, 3H), 1.48 (s, 3H), 1.42-1.39 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 133.81, 132.09, 130.50, 129.29, 120.94, 117.80, 117.00, 113.11, 109.20, 103.05, 99.56, 86.47, 84.39, 82.06, 81.05, 73.56, 66.93, 56.77, 29.95, 26.83, 26.39, 25.21, 24.96. **HRMS** (ESI) m/z calculated for $C_{25}H_{32}N_2O_5Na$ $[M+Na]^+$ 463.2203, found 463.2200.

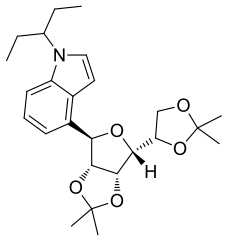
1-(*tert*-butyl)-4-((3a*R*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (3i)



50.8 mg, 61% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 4.8 Hz, 1H), 7.38 (d, *J* = 3.7 Hz, 1H), 7.00-6.99 (m, 1H), 6.52 (d, *J* = 3.7 Hz, 1H), 5.48 (s, 1H), 5.13-5.12 (m, 1H), 4.74 (dd, *J* = 6.0, 3.6 Hz, 1H), 4.56-4.52 (m, 1H), 4.31-4.20 (m, 2H), 4.06 (dd, *J* = 7.4, 3.6 Hz, 1H), 1.81 (s, 9H), 1.62 (s, 3H), 1.46 (s, 3H), 1.41-1.39 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 148.13, 141.84, 139.05, 125.65, 118.85, 113.07, 110.84, 109.20, 96.62, 86.65, 84.30, 81.90, 80.98, 73.60, 66.97, 56.60, 29.36, 26.90, 26.34, 25.23, 24.97. **HRMS** (ESI) m/z calculated for $C_{23}H_{32}N_2O_5Na$ $[M+Na]^+$ 439.2203, found 439.2202.

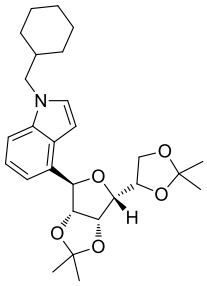
4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(pentan-3-yl)-1*H*-indole (3j)



58.4 mg, 68% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.3 Hz, 1H), 7.18-7.14 (m, 2H), 7.03 (d, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 3.2 Hz, 1H), 5.54 (s, 1H), 5.16 (d, *J* = 6.0 Hz, 1H), 4.77 (dd, *J* = 6.1, 3.6 Hz, 1H), 4.58-4.53 (m, 1H), 4.31-4.28 (m, 1H), 4.24-4.21 (m, 1H), 4.15-4.12 (m, 2H), 1.93-1.83 (m, 4H), 1.63 (s, 3H), 1.45 (s, 3H), 1.41-1.40 (m, 6H), 0.77 (td, *J* = 7.4, 1.9 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.01, 130.37, 125.29, 124.53, 120.87, 114.75, 112.74, 109.19, 109.17, 99.72, 86.89, 84.98, 81.79, 81.15, 73.73, 67.17, 59.82, 28.51, 28.49, 26.92, 26.39, 25.28, 25.05, 10.92, 10.89. **HRMS** (ESI) m/z calculated for $C_{25}H_{32}N_2O_5Na$ $[M+Na]^+$ 452.2407, found 452.2405.

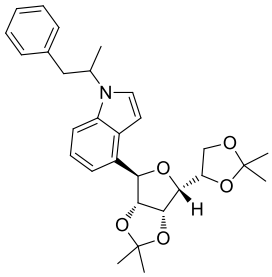
1-(cyclohexylmethyl)-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3k)



59.2 mg, 65% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.3 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 1H), 7.10 (d, *J* = 3.2 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.59 (d, *J* = 3.1 Hz, 1H), 5.53 (s, 1H), 5.16 (d, *J* = 5.9 Hz, 1H), 4.76 (dd, *J* = 6.1, 3.6 Hz, 1H), 4.57-4.53 (m, 1H), 4.30-4.27 (m, 1H), 4.24-4.20 (m, 1H), 4.12 (dd, *J* = 7.7, 3.6 Hz, 1H), 4.99-3.89 (m, 2H), 1.88-1.81 (m, 1H), 1.73-1.63 (m, 8H), 1.45 (s, 3H), 1.40 (d, *J* = 6.5 Hz, 6H), 1.24-1.13 (m, 3H), 1.04-0.95 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.46, 130.37, 128.69, 125.41, 121.05, 114.78, 112.75, 109.24, 109.17, 99.00, 86.81, 84.91, 81.74, 81.11, 73.69, 67.14, 53.12, 38.82, 31.06, 26.92, 26.36, 26.26, 25.70, 25.67, 25.25, 25.00. **HRMS** (ESI) m/z calculated for $C_{27}H_{37}NO_5Na$ $[M+Na]^+$ 478.2564, found 478.2561.

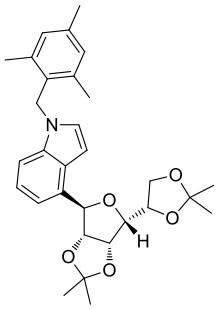
4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(1-phenylpropan-2-yl)-1*H*-indole (3l)



62.1 mg, 65% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.15 (m, 6H), 7.07-7.01 (m, 3H), 6.63 (t, *J* = 3.7 Hz, 1H), 5.53 (d, *J* = 3.7 Hz, 1H), 5.17-5.13 (m, 1H), 4.79-4.71 (m, 2H), 4.56-4.53 (m, 1H), 4.30-4.20 (m, 2H), 4.13-4.09 (m, 1H), 3.20-3.15 (m, 1H), 3.05-3.02 (m, 1H), 1.63 (s, 3H), 1.53 (dd, *J* = 6.8, 2.2 Hz, 3H), 1.46 (s, 3H), 1.41-1.39 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.92, 137.86, 135.91, 135.82, 130.49, 130.43, 129.11, 128.44, 128.40, 126.61, 125.60, 125.43, 124.43, 124.25, 121.09, 115.04, 114.97, 112.77, 109.19, 109.10, 109.03, 99.78, 99.72, 86.81, 84.91, 81.76, 81.15, 81.12, 73.69, 67.16, 53.17, 53.08, 43.46, 43.40, 26.94, 26.38, 25.26, 25.07, 25.02, 20.10, 19.99. **HRMS** (ESI) m/z calculated for $C_{29}H_{35}NO_5Na$ $[M+Na]^+$ 500.2407, found 500.2405.

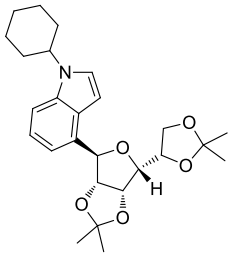
4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(2,4,6-trimethylbenzyl)-1*H*-indole (3m)



66.9 mg, 68% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.2 Hz, 1H), 7.24 (t, *J* = 7.7 Hz, 1H), 7.09 (d, *J* = 7.2 Hz, 1H), 6.94 (s, 2H), 6.65 (d, *J* = 3.3 Hz, 1H), 6.51 (d, *J* = 3.3 Hz, 1H), 5.52 (s, 1H), 5.20 (s, 2H), 5.15 (d, *J* = 6.0 Hz, 1H), 4.75 (dd, *J* = 6.1, 3.6 Hz, 1H), 4.57-4.52 (m, 1H), 4.30-4.20 (m, 2H), 4.12 (dd, *J* = 7.8, 3.7 Hz, 1H), 2.32 (s, 3H), 2.21 (s, 6H), 1.61 (s, 3H), 1.45 (s, 3H), 1.41 (s, 3H), 1.37 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.12, 138.00, 136.59, 130.41, 129.36, 128.66, 126.06, 125.82, 121.20, 115.23, 112.72, 109.15, 108.83, 99.30, 86.76, 84.84, 81.71, 81.08, 73.69, 67.12, 43.81, 26.92, 26.32, 25.24, 24.93, 20.99, 19.58. **HRMS** (ESI) m/z calculated for $C_{30}H_{37}NO_5Na$ $[M+Na]^+$ 514.2564, found 514.2563.

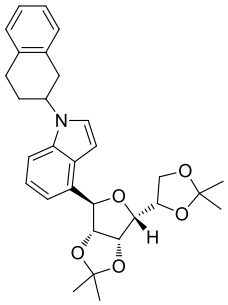
1-cyclohexyl-4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3n)



61.8 mg, 70% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.3 Hz, 1H), 7.27-7.25 (m, 1H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.62 (d, *J* = 3.3 Hz, 1H), 5.53 (s, 1H), 5.16 (d, *J* = 5.9 Hz, 1H), 4.75 (dd, *J* = 6.1, 3.6 Hz, 1H), 4.57-4.52 (m, 1H), 4.30-4.19 (m, 3H), 4.11 (dd, *J* = 7.8, 3.7 Hz, 1H), 2.15-2.12 (m, 2H), 1.97-1.92 (m, 2H), 1.82-1.70 (m, 4H), 1.63 (s, 3H), 1.56-1.48 (m, 2H), 1.45 (s, 3H), 1.41-1.39 (m, 6H), 1.35-1.24 (m, *J* = 12.7, 6.4 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.71, 130.36, 125.36, 124.19, 120.93, 114.92, 112.73, 109.17, 109.03, 99.37, 86.76, 84.91, 81.73, 81.10, 73.69, 67.15, 55.25, 33.63, 33.49, 26.93, 26.34, 25.93, 25.59, 25.25, 24.97. **HRMS** (ESI) m/z calculated for $C_{26}H_{35}NO_5Na$ $[M+Na]^+$ 264.2407, found 264.2406.

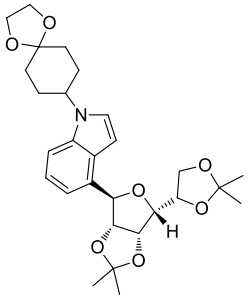
4-((3a*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(1,2,3,4-tetrahydronaphthalen-2-yl)-1*H*-indole (3o)



60.7 mg, 62% yield. Light yellow crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.3 Hz, 1H), 7.24-7.16 (m, 5H), 7.15-7.06 (m, 2H), 6.65 (t, *J* = 3.6 Hz, 1H), 5.55 (s, 1H), 5.17 (d, *J* = 6.0 Hz, 1H), 4.81-4.75 (m, 2H), 4.58-4.53 (m, 1H), 4.31-4.20 (m, 2H), 4.13-4.10 (m, 1H), 3.38-3.31 (m, 1H), 3.24-3.11 (m, 1H), 3.10-2.91 (m, 2H), 2.35-2.28 (m, 2H), 1.63 (s, 3H), 1.46 (s, 3H), 1.41-1.39 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.92, 135.30, 135.27, 134.24, 130.54, 129.09, 128.88, 126.42, 126.40, 126.16, 126.12, 125.53, 124.43, 124.29, 121.25, 121.24, 115.19, 112.76, 109.17, 109.03, 109.00, 99.93, 99.87, 86.74, 84.85, 81.72, 81.09, 73.67, 67.12, 51.82, 51.71, 36.27, 35.98, 29.45, 29.43, 28.68, 28.43, 26.93, 26.34, 25.23, 24.96. **HRMS** (ESI) m/z calculated for $C_{30}H_{35}NO_5Na$ $[M+Na]^+$ 512.2407, found 512.2406.

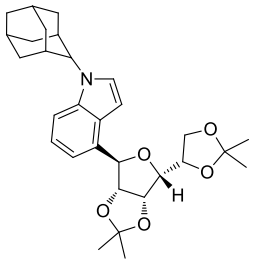
4-((3a*R*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(1,4-dioxaspiro[4.5]decan-8-yl)-1*H*-indole (3p)



63.9 mg, 64% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.3 Hz, 1H), 7.28 (d, *J* = 3.3 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 3.2 Hz, 1H), 5.53 (s, 1H), 5.16-5.15 (m, 1H), 4.75 (dd, *J* = 6.1, 3.6 Hz, 1H), 4.57-4.52 (m, 1H), 4.34-4.27 (m, 2H), 4.24-4.20 (m, 1H), 4.11 (dd, *J* = 7.8, 3.7 Hz, 1H), 4.01 (s, 4H), 2.15-2.08 (m, 4H), 1.96-1.91 (m, 2H), 1.85-1.77 (m, 2H), 1.63 (s, 3H), 1.45 (s, 3H), 1.41-1.39 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.77, 130.43, 125.40, 124.30, 121.08, 115.02, 112.74, 109.15, 108.95, 107.62, 99.62, 86.73, 84.87, 81.70, 81.07, 73.65, 67.11, 64.50, 64.39, 53.97, 34.08, 34.06, 30.25, 30.13, 26.90, 26.32, 25.21, 24.96. **HRMS** (ESI) m/z calculated for $C_{28}H_{37}NO_7$ $[M+Na]^+$ 522.2462 found 522.2460.

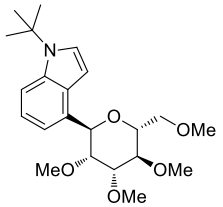
1-((1*R*,3*R*,5*R*,7*R*)-adamantan-2-yl)-4-((3a*R*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3p)



56.2 mg, 57% yield. White crystal.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 3.3 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.61 (d, *J* = 3.2 Hz, 1H), 5.54 (s, 1H), 5.18 (d, *J* = 6.1 Hz, 1H), 4.76 (dd, *J* = 6.0, 3.6 Hz, 1H), 4.57-4.53 (m, 2H), 4.31-4.20 (m, 2H), 4.12 (dd, *J* = 7.8, 3.6 Hz, 1H), 2.54 (s, 2H), 2.15 (d, *J* = 13.3 Hz, 1H), 2.04-1.96 (m, 7H), 1.83 (s, 2H), 1.78-1.65 (m, 2H), 1.63 (s, 3H), 1.45 (s, 3H), 1.41-1.39 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.51, 130.25, 126.10, 125.59, 120.84, 115.02, 112.72, 110.20, 109.16, 98.79, 86.80, 84.89, 81.72, 81.09, 73.69, 67.14, 61.01, 38.50, 38.27, 37.58, 32.50, 32.33, 32.16, 32.12, 27.72, 27.23, 26.92, 26.34, 25.24, 24.96. **HRMS** (ESI) m/z calculated for $C_{30}H_{39}NO_5Na$ $[M+Na]^+$ 516.2720, found 516.2718.

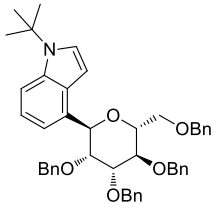
1-(*tert*-butyl)-4-((2*R*,3*R*,4*R*,5*R*,6*R*)-3,4,5-trimethoxy-6-(methoxymethyl)tetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3r)



59.6 mg, 79% yield. Light yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.29 (d, *J* = 3.4 Hz, 1H), 7.10 (dd, *J* = 8.4, 7.3 Hz, 1H), 7.00 (d, *J* = 7.4 Hz, 1H), 6.84 (dd, *J* = 3.4, 0.9 Hz, 1H), 5.42 (d, *J* = 4.1 Hz, 1H), 4.30 (dd, *J* = 4.2, 3.2 Hz, 1H), 3.79-3.78 (m, 1H), 3.70 (t, *J* = 7.4 Hz, 1H), 3.65-3.60 (m, 2H), 3.59 (s, 3H), 3.56-3.54 (m, 1H), 3.50 (s, 3H), 3.38-3.37 (m, 6H), 1.72 (s, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.31, 130.13, 128.99, 125.04, 120.01, 117.17, 113.29, 100.23, 80.37, 77.00, 76.46, 73.37, 73.06, 71.32, 59.45, 59.06, 58.15, 57.89, 55.67, 29.77. **HRMS** (ESI) m/z calculated for $C_{22}H_{33}NO_5Na$ $[M+Na]^+$ 414.2251, found 414.2248.

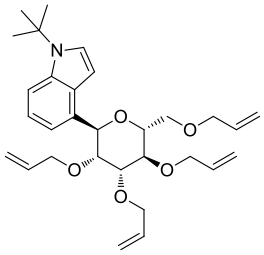
1-(*tert*-butyl)-4-((2*R*,3*R*,4*R*,5*R*,6*R*)-3,4,5-tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3s)



112.6 mg, 81% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.5 Hz, 1H), 7.34-7.17 (m, 21H), 6.97 (t, *J* = 7.9 Hz, 1H), 6.81 (d, *J* = 3.4 Hz, 1H), 6.67 (d, *J* = 7.3 Hz, 1H), 5.44 (d, *J* = 4.3 Hz, 1H), 4.75 (d, *J* = 11.2 Hz, 1H), 4.67-4.62 (m, 3H), 4.58-4.43 (m, 5H), 4.11 (t, *J* = 7.2 Hz, 1H), 3.99 (dd, *J* = 7.5, 3.0 Hz, 1H), 3.86-3.77 (m, 2H), 3.73-3.69 (m, 1H), 1.70 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.58, 138.52, 135.29, 130.27, 128.88, 128.31, 128.23, 128.17, 128.13, 127.98, 127.72, 127.69, 127.57, 127.42, 127.35, 127.31, 124.95, 120.03, 117.34, 113.17, 100.51, 78.20, 75.50, 74.97, 74.24, 73.89, 73.70, 73.19, 72.47, 71.85, 69.20, 55.63, 29.80. **HRMS** (ESI) m/z calculated for $C_{46}H_{49}NO_5Na$ $[M+Na]^+$ 718.3503, found 718.3500.

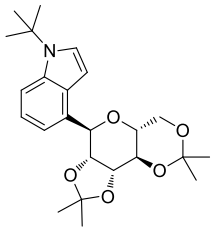
1-(*tert*-butyl)-4-((2*R*,3*R*,4*R*,5*R*,6*R*)-3,4,5-tris(allyloxy)-6-((allyloxy)methyl)tetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3t)



84.2 mg, 85% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 1H), 7.27 (d, *J* = 3.3 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.97 (d, *J* = 7.3 Hz, 1H), 6.87 (d, *J* = 3.2 Hz, 1H), 6.04-5.82 (m, 4H), 5.39-5.33 (m, 2H), 5.28-5.26 (m, 1H), 5.25-5.09 (m, 6H), 4.46 (dd, *J* = 4.1, 2.4 Hz, 1H), 4.29-4.20 (m, 3H), 4.15-3.91 (m, 7H), 3.71 (d, *J* = 4.2 Hz, 2H), 3.57 (q, *J* = 4.9 Hz, 1H), 1.71 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.27, 135.26, 135.23, 135.12, 134.98, 130.20, 128.88, 124.92, 119.90, 117.25, 117.04, 116.82, 116.47, 116.17, 113.18, 100.48, 78.42, 75.22, 74.63, 74.47, 73.56, 72.66, 72.18, 71.40, 71.28, 69.06, 55.59, 29.74. **HRMS** (ESI) m/z calculated for $C_{30}H_{41}NO_5Na$ $[M+Na]^+$ 518.2877, found 518.2874.

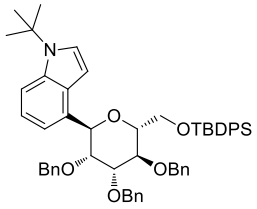
1-(*tert*-butyl)-4-((3a*R*,4*R*,5a*R*,9a*R*,9b*R*)-2,2,8,8-tetramethylhexahydro-[1,3]dioxolo[4',5':4,5]pyrano[3,2-*d*][1,3]dioxin-4-yl)-1*H*-indole (3u)



43.2 mg, 52% yield. Light yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 3.4 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.57 (d, *J* = 3.3 Hz, 1H), 5.42 (d, *J* = 4.5 Hz, 1H), 4.86-4.84 (m, 1H), 4.42 (t, *J* = 6.9 Hz, 1H), 4.14 (dd, *J* = 10.6, 7.5 Hz, 1H), 3.83-3.81 (m, 2H), 3.54-3.50 (m, 1H), 1.73 (s, 9H), 1.61 (s, 3H), 1.56 (s, 3H), 1.42 (s, 3H), 1.38 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.38, 129.74, 129.01, 125.48, 120.15, 117.54, 113.91, 109.23, 99.45, 98.76, 76.13, 76.04, 75.14, 73.21, 64.26, 62.80, 55.86, 29.83, 29.06, 27.91, 25.56, 18.97. **HRMS** (ESI) m/z calculated for $C_{24}H_{33}NO_5Na$ $[M+Na]^+$ 438.2251, found 438.2249.

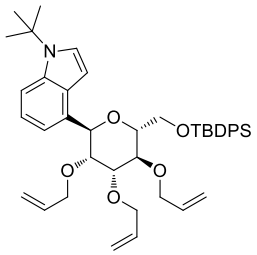
1-(*tert*-butyl)-4-((2*R*,3*R*,4*R*,5*R*,6*R*)-3,4,5-tris(benzyloxy)-6-(((*tert*-butyldiphenylsilyl)oxy)methyl)tetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3v)



138.3 mg, 82% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 6.5 Hz, 2H), 7.69-7.66 (m, 2H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.42-7.20 (m, 21H), 7.10 (d, *J* = 3.4 Hz, 1H), 6.95 (t, *J* = 7.9 Hz, 1H), 6.70 (d, *J* = 3.3 Hz, 1H), 6.66 (d, *J* = 7.3 Hz, 1H), 5.37 (d, *J* = 4.6 Hz, 1H), 4.81-4.65 (m, 4H), 4.56-4.42 (m, 3H), 4.28 (t, *J* = 6.9 Hz, 1H), 4.09-4.02 (m, 2H), 3.93 (dd, *J* = 10.6, 4.6 Hz, 1H), 3.60 (q, *J* = 5.0 Hz, 1H), 1.66 (s, 9H), 1.06 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.69, 138.64, 135.88, 135.57, 135.21, 134.75, 133.81, 133.53, 130.57, 129.60, 129.45, 129.43, 128.83, 128.33, 128.27, 128.08, 127.73, 127.67, 127.58, 127.50, 127.41, 127.22, 124.92, 119.93, 117.42, 113.09, 100.49, 77.86, 75.56, 75.14, 74.96, 73.95, 73.70, 72.50, 71.88, 62.89, 55.55, 29.77, 26.83, 26.53, 19.27. **HRMS** (ESI) m/z calculated for $C_{55}H_{61}NO_5SiNa$ $[M+Na]^+$ 866.4211, found 866.4210.

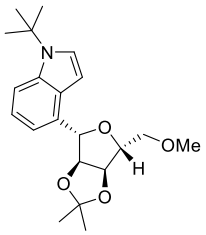
1-(*tert*-butyl)-4-((2*R*,3*R*,4*R*,5*R*,6*R*)-3,4,5-tris(allyloxy)-6-(((*tert*-butyldiphenylsilyl)oxy)methyl)tetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3w)



90.1 mg, 65% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 6.1 Hz, 2H), 7.69-7.67 (m, 2H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.43-7.38 (m, 6H), 7.14 (d, *J* = 3.4 Hz, 1H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.3 Hz, 1H), 6.76 (d, *J* = 3.3 Hz, 1H), 6.03-5.94 (m, 1H), 5.92-5.76 (m, 2H), 5.37-5.29 (m, 2H), 5.24-5.04 (m, 5H), 4.44 (dd, *J* = 4.8, 3.1 Hz, 1H), 4.29-4.20 (m, 3H), 4.16-4.12 (m, 1H), 4.06-4.02 (m, 2H), 3.97-3.93 (m, 3H), 3.89 (dd, *J* = 10.5, 4.9 Hz, 1H), 3.59 (q, *J* = 5.2 Hz, 1H), 1.68 (s, 9H), 1.06 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.87, 135.57, 135.45, 135.33, 135.30, 135.20, 133.92, 133.65, 130.76, 129.41, 128.91, 127.55, 127.47, 124.93, 119.91, 117.48, 116.95, 116.70, 116.31, 113.13, 100.58, 78.18, 75.20, 75.03, 74.81, 74.22, 72.47, 71.60, 71.15, 63.02, 55.58, 29.80, 26.85, 19.29. **HRMS** (ESI) m/z calculated for $C_{43}H_{55}NO_5SiNa$ $[M+Na]^+$ 716.3742, found 716.3740.

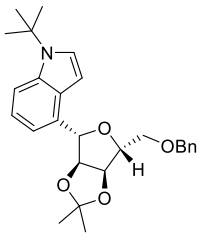
1-(*tert*-butyl)-4-((3a*S*,4*S*,6*R*,6a*R*)-6-(methoxymethyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3x)



50.3 mg, 70% yield. Light yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.2 Hz, 1H), 7.29 (d, *J* = 3.4 Hz, 1H), 7.18-7.12 (m, 2H), 6.63 (dt, *J* = 3.4, 0.9 Hz, 1H), 5.27 (d, *J* = 4.6 Hz, 1H), 4.77-4.75 (m, 1H), 4.70 (dd, *J* = 6.9, 4.9 Hz, 1H), 4.26 (q, *J* = 4.9 Hz, 1H), 3.72-3.67 (m, 2H), 3.46 (d, *J* = 0.6 Hz, 3H), 1.72 (s, 9H), 1.66 (s, 3H), 1.34 (d, *J* = 0.9 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.05, 131.42, 127.44, 125.16, 120.42, 115.78, 114.75, 113.08, 98.59, 86.32, 85.45, 83.14, 82.06, 72.86, 59.49, 55.75, 29.80, 27.52, 25.49. **HRMS** (ESI) m/z calculated for $C_{21}H_{29}NO_4Na$ $[M+Na]^+$ 382.1989, found 382.1988.

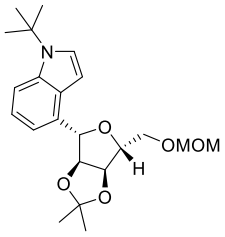
4-((3a*S*,4*S*,6*R*,6a*R*)-6-((benzyloxy)methyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(tert-butyl)-1*H*-indole (3y)



54.8 mg, 63% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.3 Hz, 1H), 7.39 – 7.10 (m, 8H), 6.65 (d, *J* = 3.4 Hz, 1H), 5.28 (d, *J* = 3.3 Hz, 1H), 4.78-4.74 (m, 2H), 4.64 (d, *J* = 3.5 Hz, 2H), 4.31 (q, *J* = 4.2 Hz, 1H), 3.78 (d, *J* = 4.4 Hz, 2H), 1.71 (s, 9H), 1.66 (s, 3H), 1.33 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.12, 135.03, 131.50, 128.28, 127.73, 127.52, 127.40, 125.10, 120.39, 115.81, 114.59, 113.05, 98.73, 86.35, 85.53, 83.39, 81.89, 73.53, 70.21, 55.70, 29.77, 27.54, 25.51. **HRMS** (ESI) m/z calculated for $C_{27}H_{33}NO_4Na$ $[M+Na]^+$ 458.2302, found 458.2299.

1-(*tert*-butyl)-4-((3a*S*,4*S*,6*R*,6a*R*)-6-((methoxymethoxy)methyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3z)

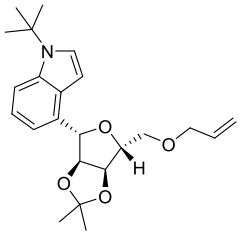


59.2 mg, 76% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 3.4 Hz, 1H), 7.18-7.11 (m, 2H), 6.63 (d, *J* = 3.3 Hz, 1H), 5.29 (d, *J* = 4.5 Hz, 1H), 4.78-4.70 (m, 4H), 4.29 (q, *J* = 4.8 Hz, 1H), 3.84 (d, *J* = 4.8 Hz, 2H), 3.41 (s, 3H), 1.72 (s, 9H), 1.67 (s, 3H), 1.34 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ

135.02, 131.41, 127.39, 125.11, 120.41, 115.62, 114.72, 113.05, 98.58, 96.75, 86.38, 85.35, 83.12, 82.04, 67.75, 55.73, 55.31, 29.77, 27.51, 25.48. **HRMS** (ESI) m/z calculated for $C_{22}H_{31}NO_5Na$ $[M+Na]^+$ 412.2094, found 412.2092.

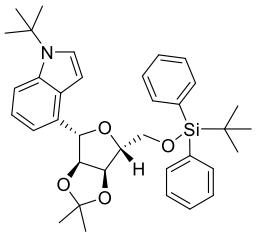
4-((3a*S*,4*S*,6*R*,6a*R*)-6-((allyloxy)methyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1-(tert-butyl)-1*H*-indole (3aa)



55.5 mg, 72% yield. Light yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.29 (dd, *J* = 3.4, 1.7 Hz, 1H), 7.18-7.11 (m, 2H), 6.66-6.65 (m, 1H), 5.97-5.93 (m, 1H), 5.33-5.21 (m, 2H), 5.20 (dt, *J* = 10.4, 1.5 Hz, 1H), 4.78-4.73 (m, 2H), 4.29-4.27 (m, 1H), 4.12-4.10 (m, 2H), 3.76-3.74 (m, 2H), 1.72 (s, 9H), 1.66 (s, 3H), 1.34 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.01, 134.62, 131.46, 127.40, 125.05, 120.36, 117.02, 115.79, 114.56, 113.01, 98.67, 86.30, 85.47, 83.32, 81.89, 72.48, 70.11, 55.66, 29.74, 27.52, 25.49. **HRMS** (ESI) m/z calculated for $C_{23}H_{31}NO_4Na$ $[M+Na]^+$ 408.2145, found 408.2144.

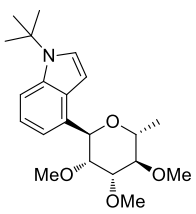
1-(*tert*-butyl)-4-((3a*S*,4*S*,6*R*,6a*R*)-6-(((*tert*-butyldiphenylsilyl)oxy)methyl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)-1*H*-indole (3ab)



82.3 mg, 71% yield. Light yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75-7.71 (m, 4H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.42-7.35 (m, 6H), 7.25-7.23 (m, 2H), 7.11-7.09 (m, 1H), 6.67 (d, *J* = 3.2 Hz, 1H), 5.32 (d, *J* = 4.8 Hz, 1H), 4.83 (dd, *J* = 6.7, 4.5 Hz, 1H), 4.71 (dd, *J* = 6.7, 4.9 Hz, 1H), 4.24 (q, *J* = 4.1 Hz, 1H), 4.01-3.92 (m, 2H), 1.72 (s, 9H), 1.66 (s, 3H), 1.34 (s, 3H), 1.09 (s, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 135.72, 135.70, 134.99, 133.40, 133.32, 131.89, 129.66, 129.61, 127.69, 127.67, 127.51, 125.07, 120.49, 115.49, 114.34, 112.87, 98.85, 86.57, 84.96, 84.50, 81.44, 63.99, 55.74, 29.83, 27.67, 26.88, 25.62, 19.30. **HRMS** (ESI) m/z calculated for $C_{36}H_{45}NO_4SiNa$ $[M+Na]^+$ 606.3010, found 606.3008.

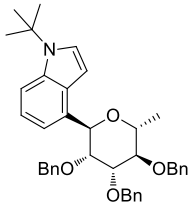
1-(*tert*-butyl)-4-((2*R*,3*R*,4*S*,5*R*,6*R*)-3,4,5-trimethoxy-6-methyltetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3ac)



50.6 mg, 70% yield. Light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.4 Hz, 1H), 7.29 (d, *J* = 3.4 Hz, 1H), 7.10 (t, *J* = 7.9 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.83 (d, *J* = 3.4 Hz, 1H), 5.43 (d, *J* = 3.3 Hz, 1H), 4.36 (t, *J* = 3.3 Hz, 1H), 3.74 (dd, *J* = 8.1, 3.3 Hz, 1H), 3.59 (s, 3H), 3.51 (s, 3H), 3.48 (s, 3H), 3.42-3.40 (m, 1H), 3.30 (t, *J* = 7.9 Hz, 1H), 1.73 (s, 9H), 1.31 (d, *J* = 6.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.28, 130.18, 129.07, 125.05, 119.97, 116.72, 113.26, 100.27, 82.19, 80.98, 77.20, 73.27, 69.80, 60.05, 58.34, 57.72, 55.68, 29.76, 17.74. **HRMS** (ESI) m/z calculated for $C_{21}H_{31}NO_4Na$ $[M+Na]^+$ 384.2145, found 384.2143.

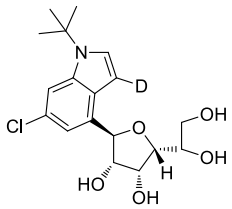
1-(*tert*-butyl)-4-((2*R*,3*R*,4*S*,5*R*,6*R*)-3,4,5-tris(benzyloxy)-6-methyltetrahydro-2*H*-pyran-2-yl)-1*H*-indole (3ad)



93.1 mg, 79% yield. Light yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 1H), 7.36-7.22 (m, 16H), 6.95-6.93 (m, 1H), 6.78 (dd, *J* = 3.3, 0.8 Hz, 1H), 6.56 (d, *J* = 7.3 Hz, 1H), 5.43 (d, *J* = 3.5 Hz, 1H), 4.85 (d, *J* = 11.1 Hz, 1H), 4.73-4.62 (m, 5H), 4.46 (t, *J* = 3.3 Hz, 1H), 3.95 (dd, *J* = 8.1, 3.0 Hz, 1H), 3.72 (t, *J* = 7.9 Hz, 1H), 3.53-3.48 (m, 1H), 1.69 (s, 9H), 1.36 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 138.64, 138.59, 138.48, 135.22, 130.25, 128.88, 128.29, 128.22, 128.18, 128.04, 128.00, 127.68, 127.55, 127.42, 127.41, 124.92, 119.96, 116.80, 113.06, 100.39, 80.96, 78.90, 74.90, 74.41, 74.38, 72.41, 72.00, 70.30, 55.59, 29.75, 17.99. **HRMS** (ESI) m/z calculated for $C_{39}H_{43}NO_4Na$ $[M+Na]^+$ 612.3084, found 612.3083.

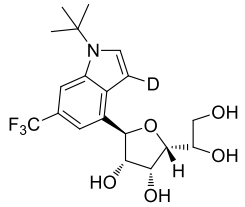
(2*R*,3*S*,4*R*,5*R*)-2-(1-(tert-butyl)-6-chloro-1*H*-indol-4-yl)-5-((*R*)-1,2-dihydroxyethyl)tetrahydrofuran-3,4-diol (4a')



61.4 mg, 83% yield. White crystal.

^{1}H NMR (600 MHz, CD_3OD) δ 7.60 (s, 1H), 7.33 (d, *J* = 6.9 Hz, 1H), 7.11 (s, 1H), 5.14 (d, *J* = 8.1 Hz, 1H), 4.34 (t, *J* = 3.9 Hz, 1H), 4.24-4.20 (m, 2H), 4.08 (d, *J* = 7.0 Hz, 1H), 3.86 (d, *J* = 11.4 Hz, 1H), 3.71-3.68 (m, 1H), 1.65 (s, 9H). **^{13}C NMR** (151 MHz, CD_3OD) 136.43, 135.53, 127.84, 127.10, 126.81, 117.06, 113.09, 100.08, 82.71, 81.34, 79.88, 73.57, 71.58, 64.63, 56.77, 29.73. **HRMS** (ESI) m/z calculated for $C_{18}H_{23}DClNO_5Na$ $[M+Na]^+$ 393.1313, found 393.1302.

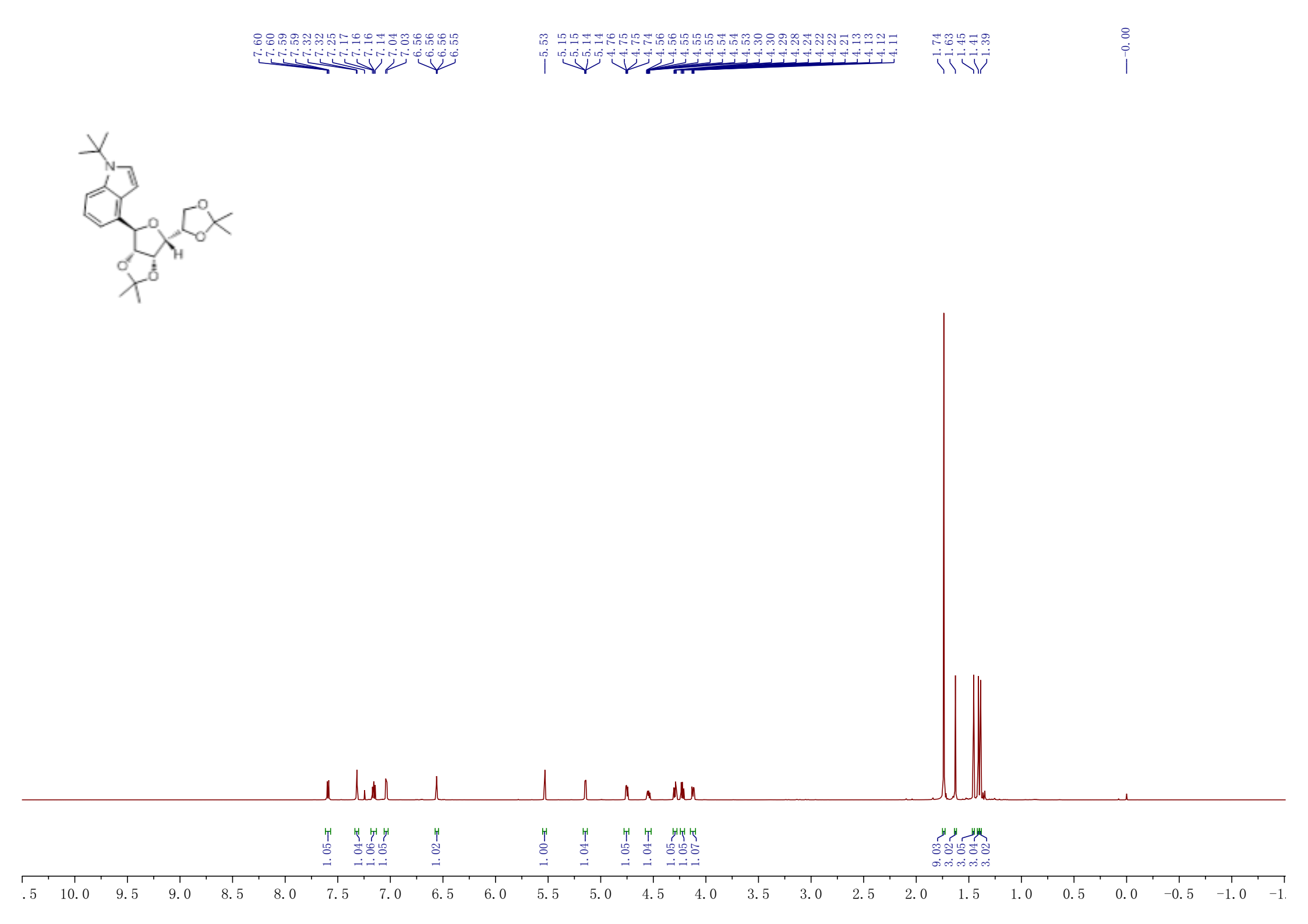
(2*R*,3*S*,4*R*,5*R*)-2-(1-(tert-butyl)-6-(trifluoromethyl)-1*H*-indol-4-yl)-5-((*R*)-1,2-dihydroxyethyl)tetrahydrofuran-3,4-diol (4b')



63.9 mg, 79% yield. White crystal.

^{1}H NMR (600 MHz, CD_3OD) δ 7.87 (s, 1H), 7.55 (d, *J* = 1.3 Hz, 1H), 7.36 (d, *J* = 1.3 Hz, 1H), 5.22 (d, *J* = 8.1 Hz, 1H), 4.39 (t, *J* = 3.9 Hz, 1H), 4.30-4.26 (m, 2H), 4.11 (s, 1H), 3.90-3.87 (m, 1H), 3.72 (dd, *J* = 12.0, 5.9 Hz, 1H), 1.72 (s, 9H). **^{13}C NMR** (151 MHz, CD_3OD) δ 135.04, 131.65, 129.15, 126.63 (q, *J* = 270.7 Hz), 122.99 (q, *J* = 31.2 Hz), 113.01, 110.59, 100.19, 82.85, 81.28, 79.73, 73.70, 71.74, 64.41, 57.17, 49.64, 29.82. ^{19}F NMR (376 MHz, CD_3OD) δ -61.54. **HRMS** (ESI) m/z calculated for $C_{19}H_{23}DF_3NO_5Na$ $[M+Na]^+$ 427.1577, found 427.1576.

S9. NMR Spectroscopic Date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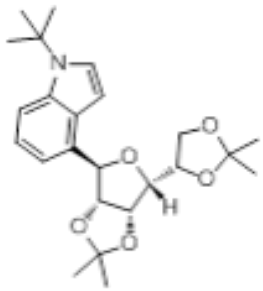

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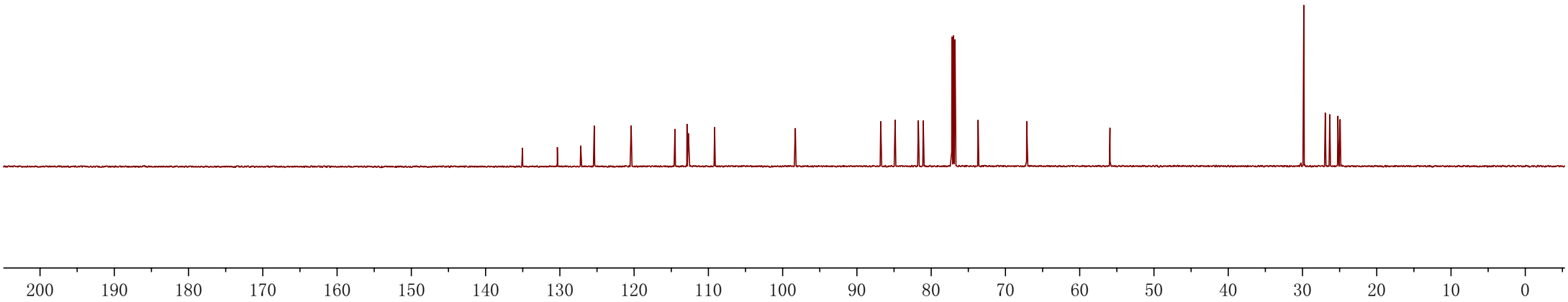

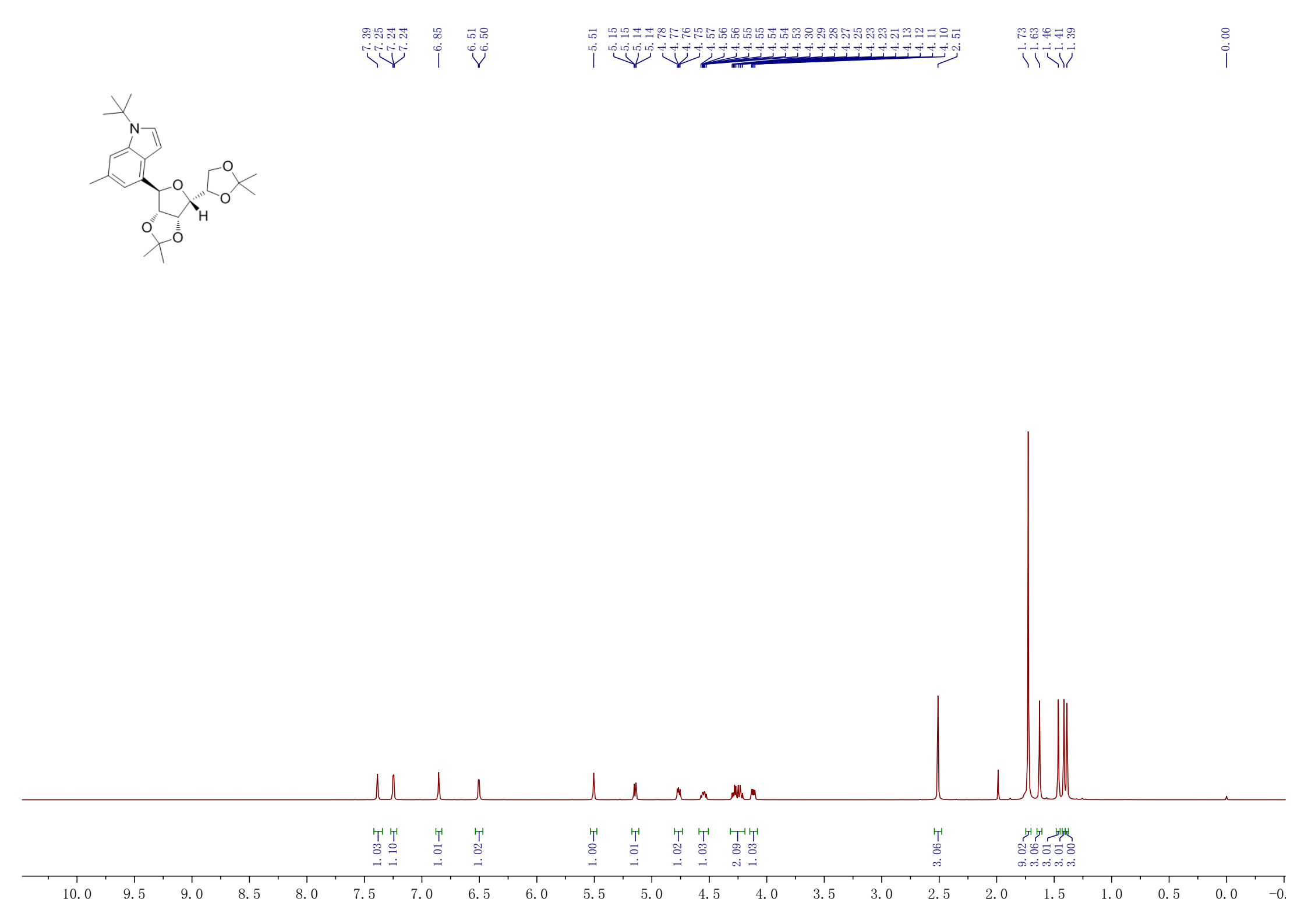
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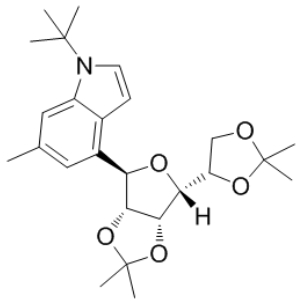

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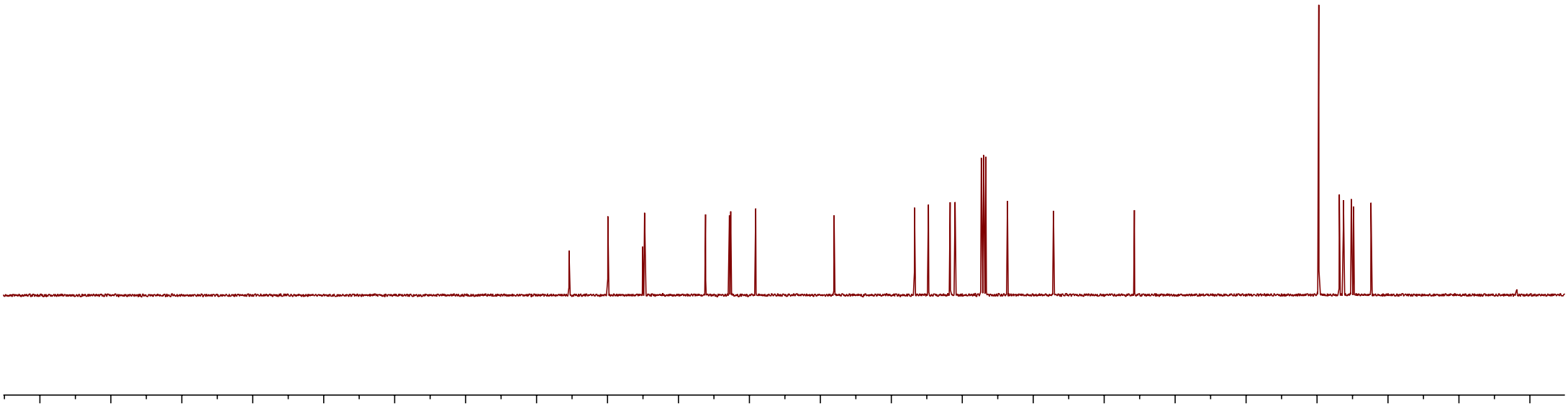

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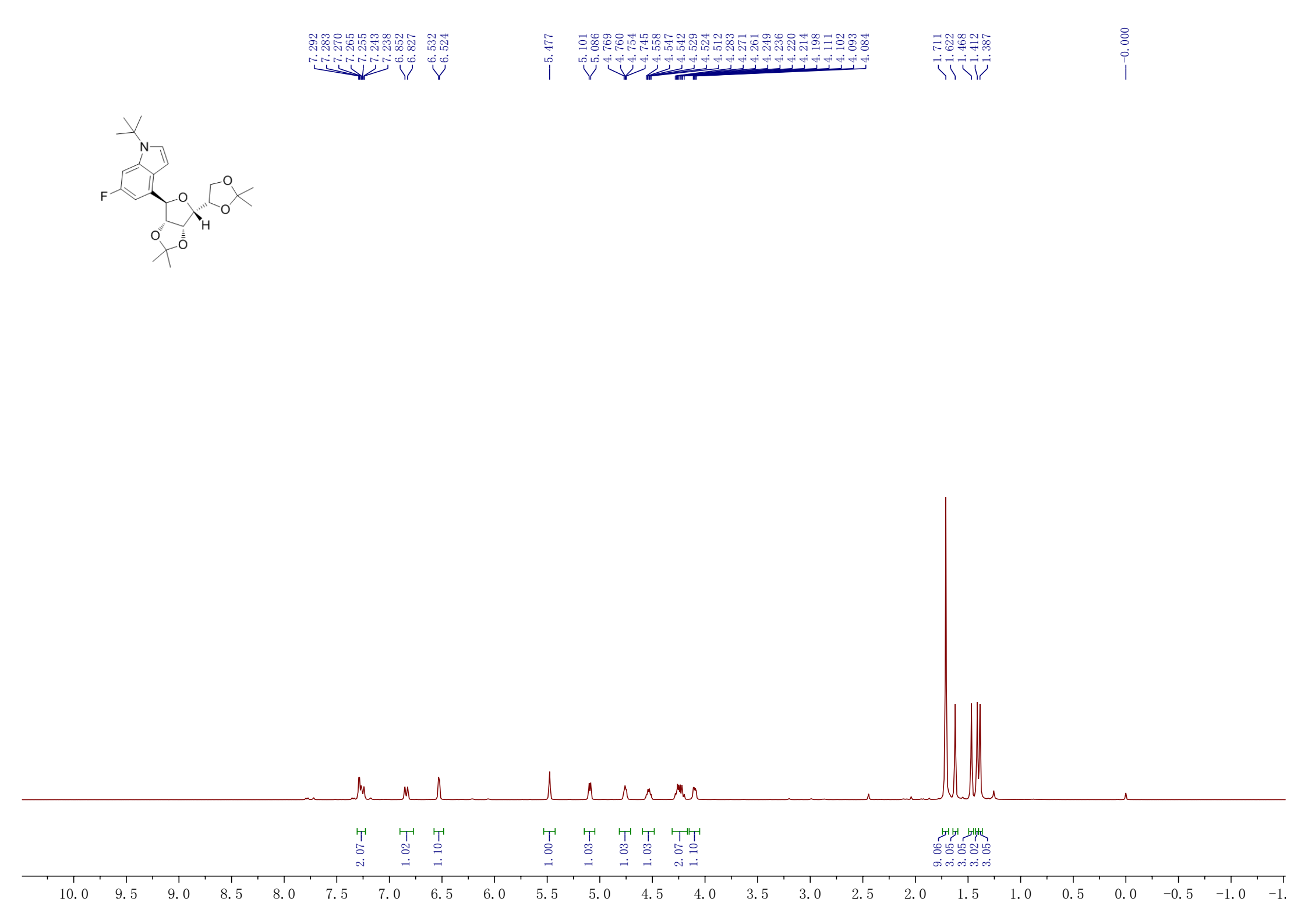
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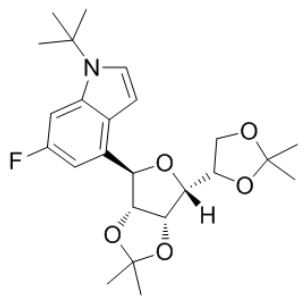

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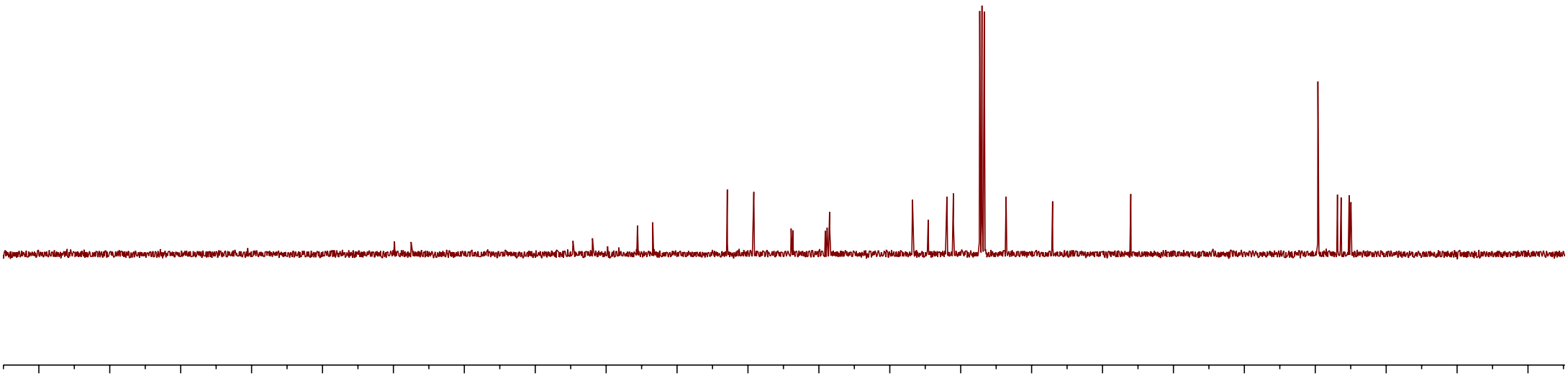

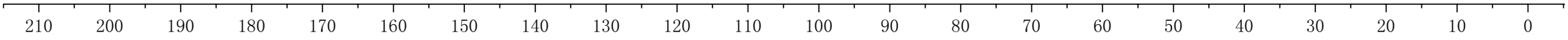

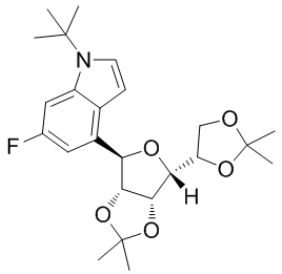

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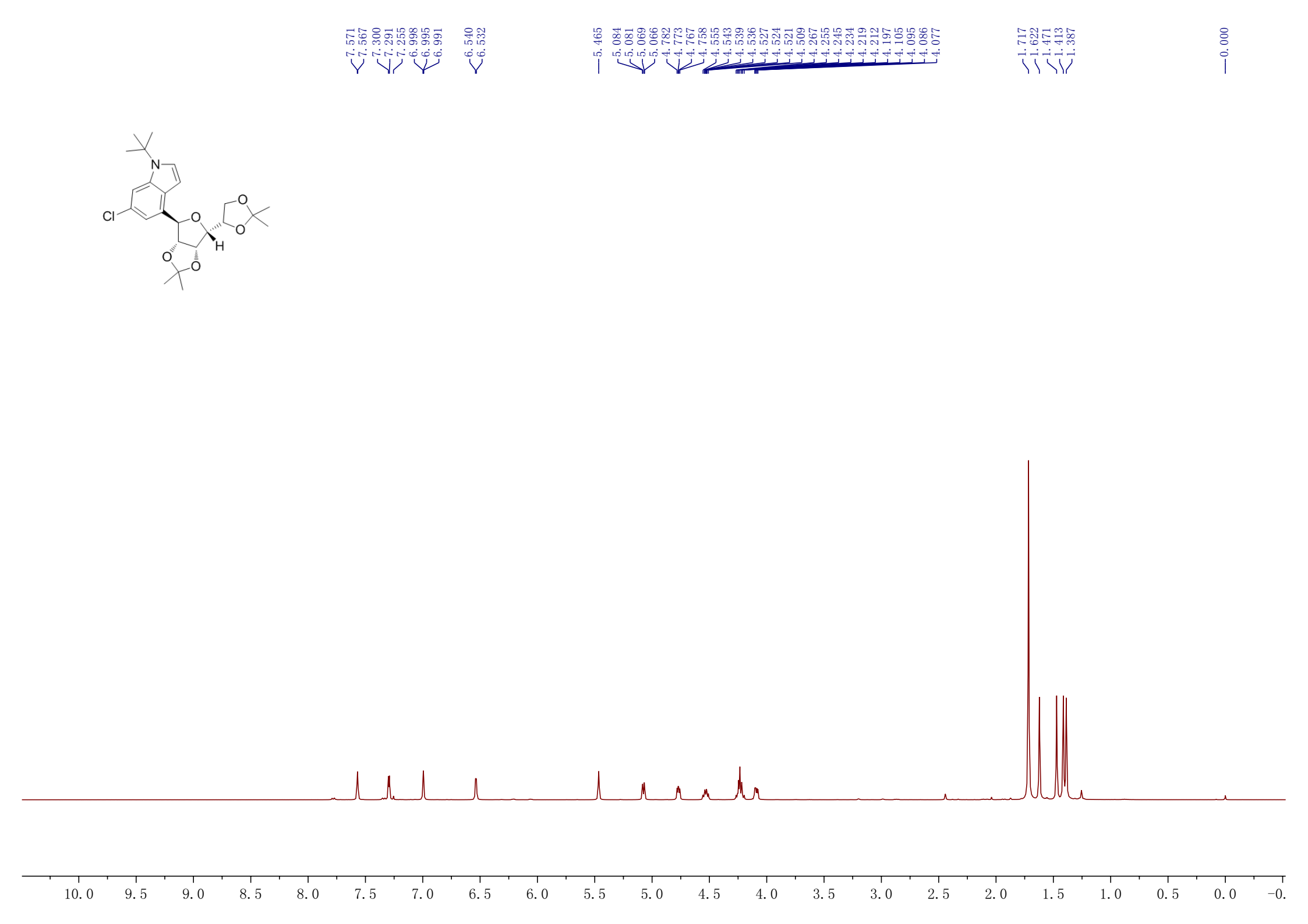
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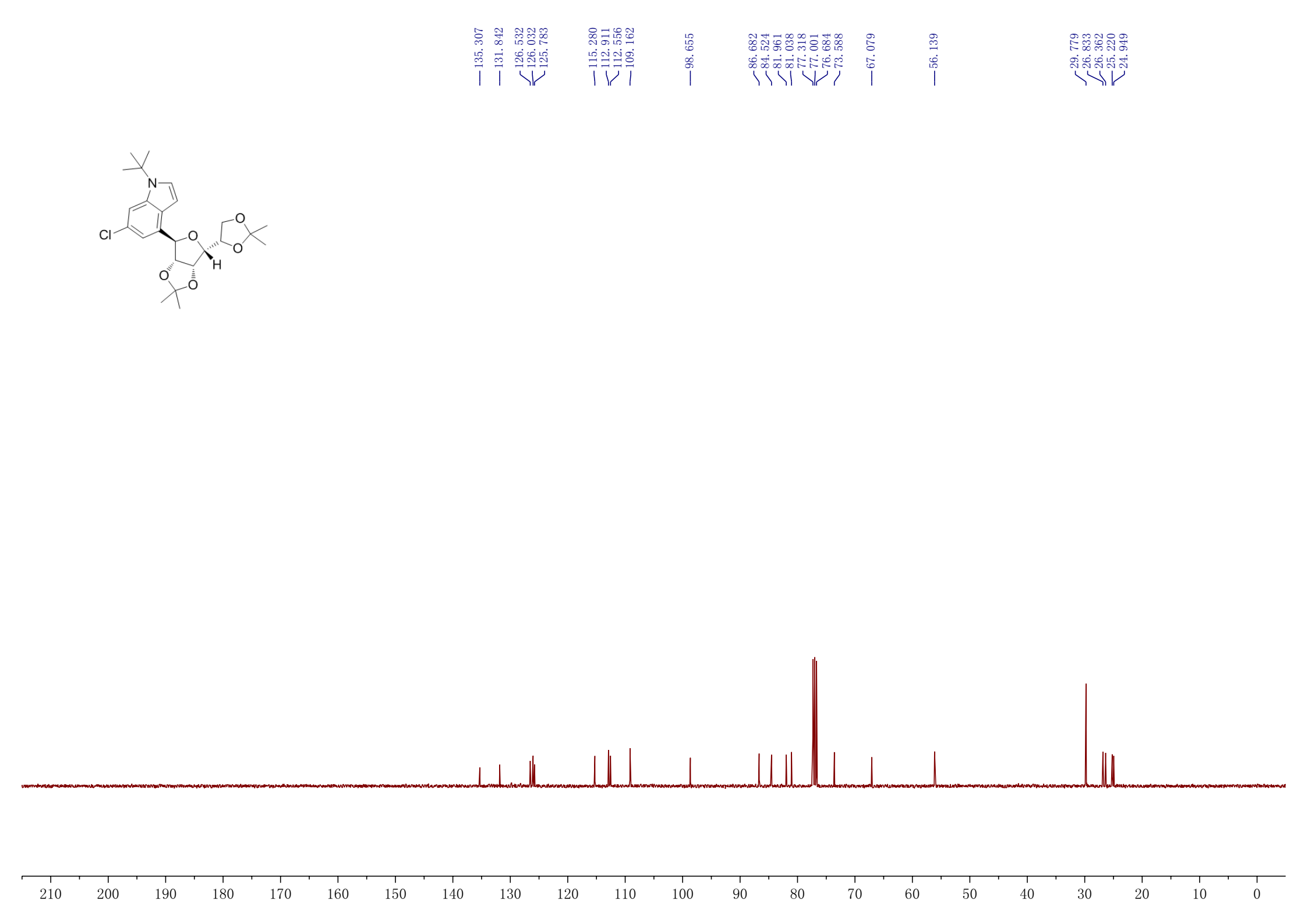
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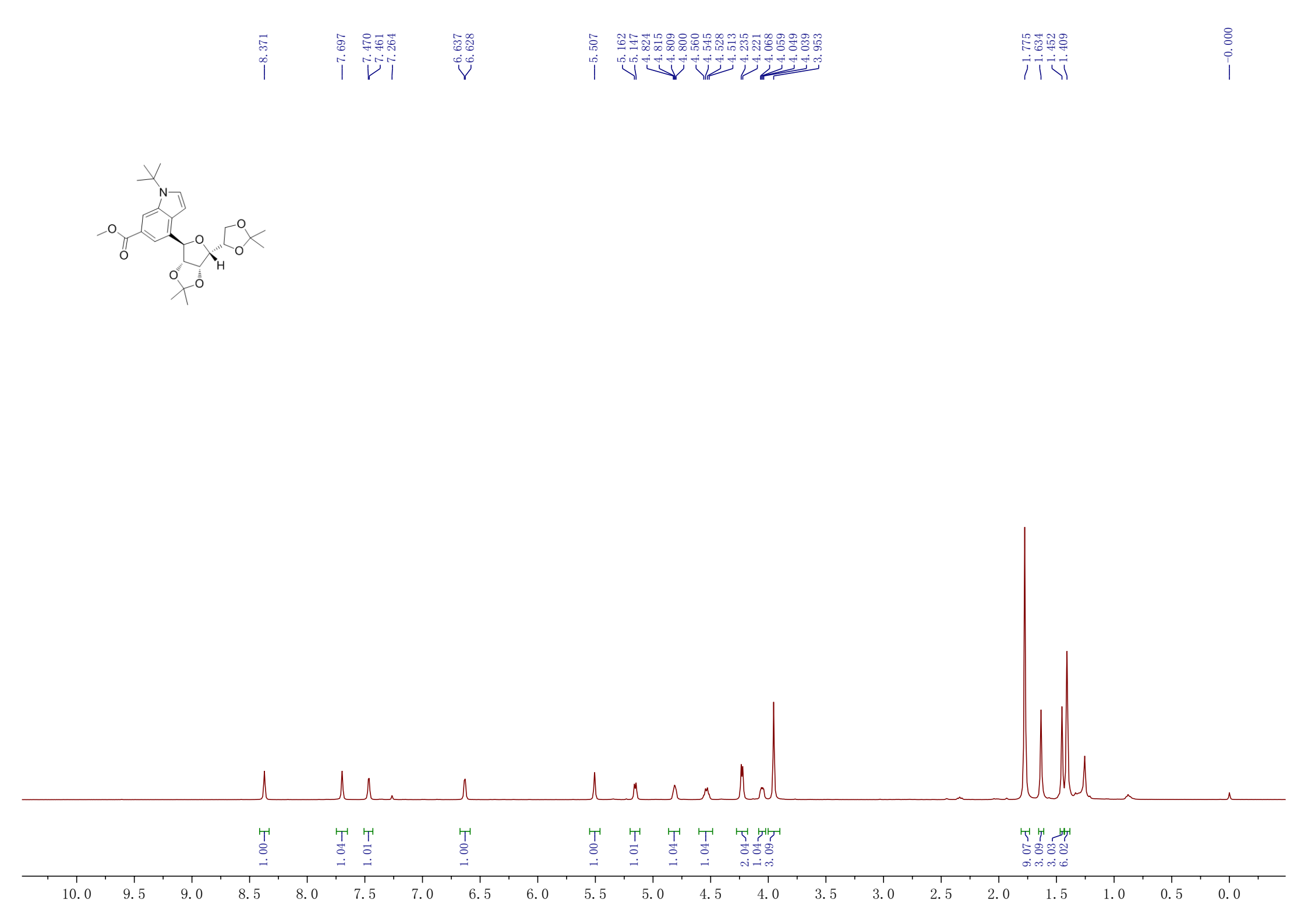
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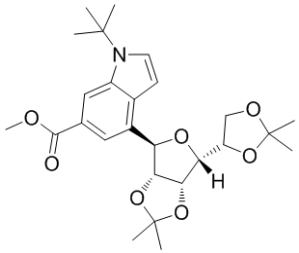

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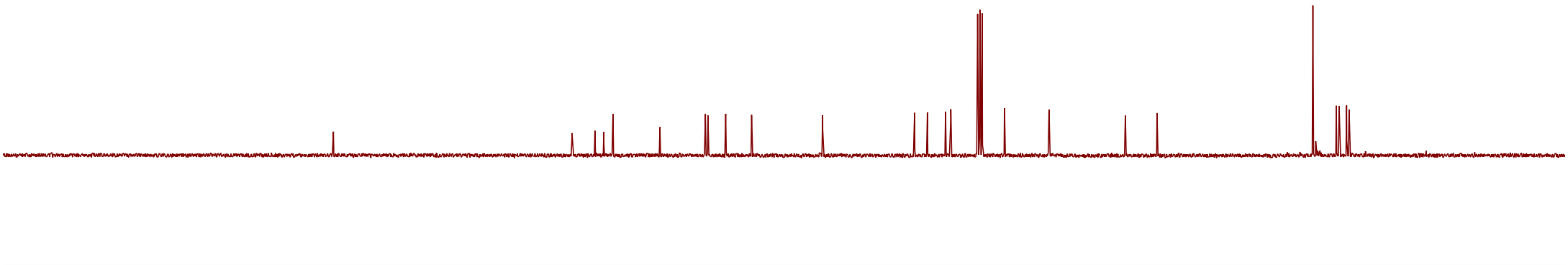

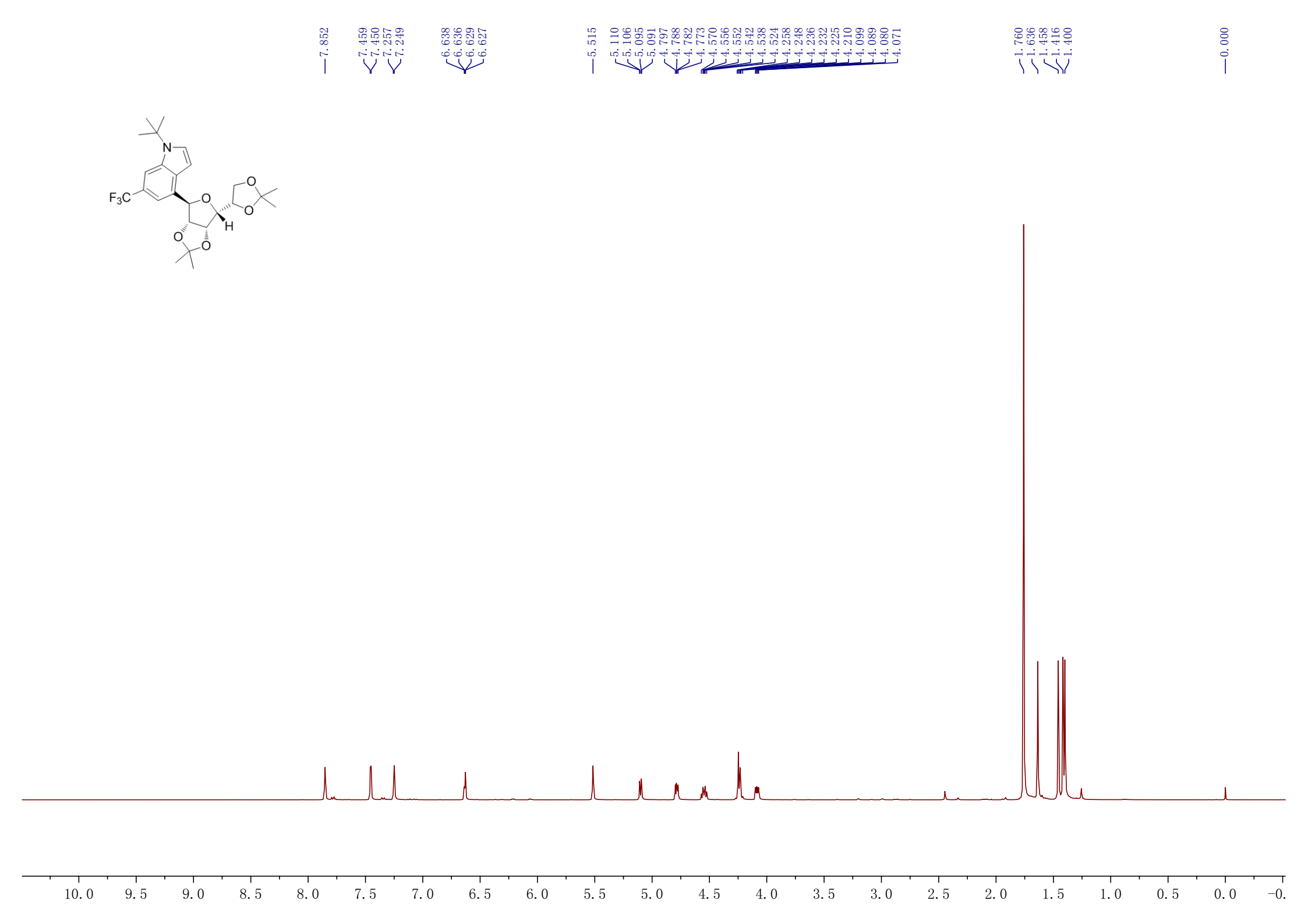
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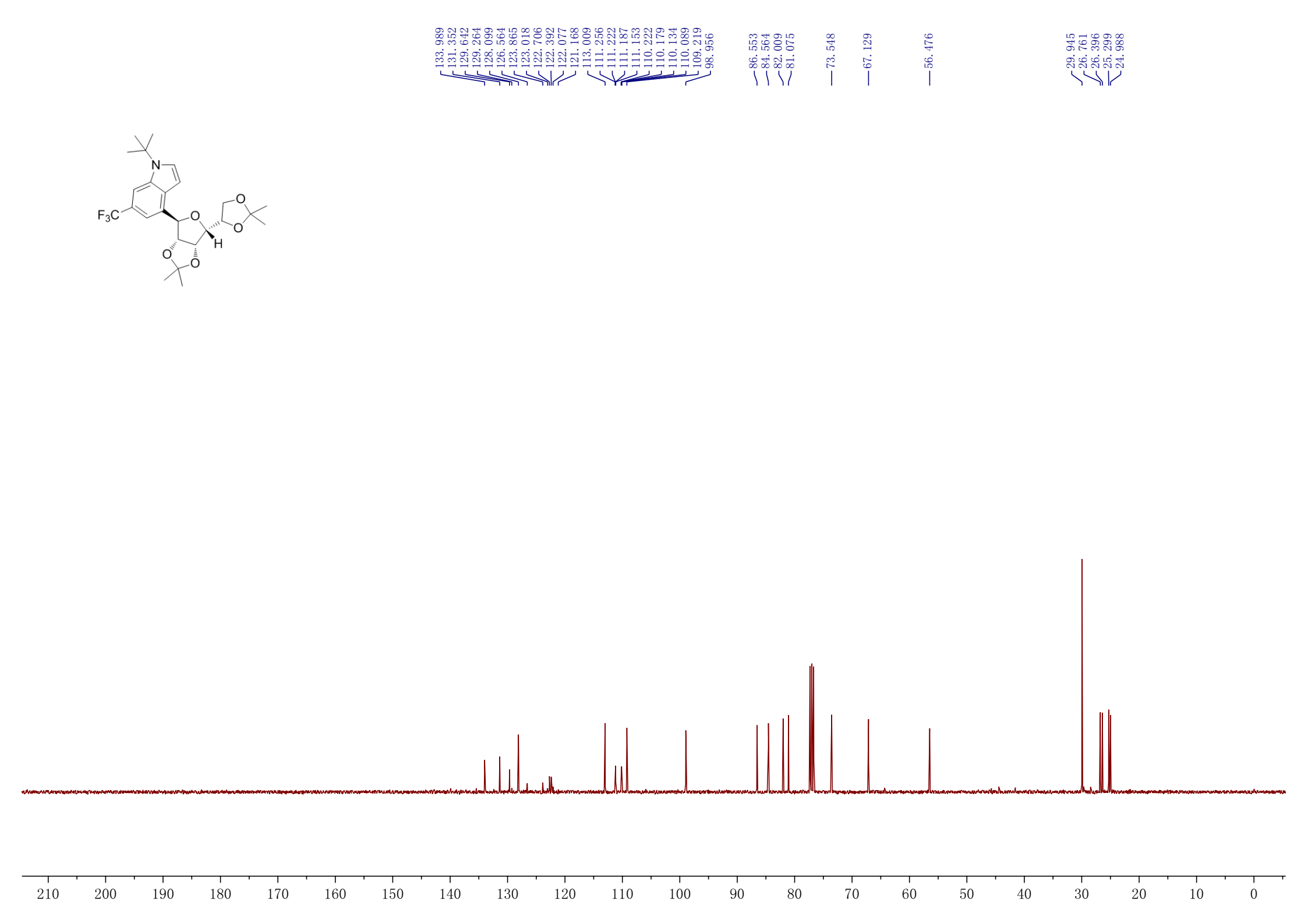
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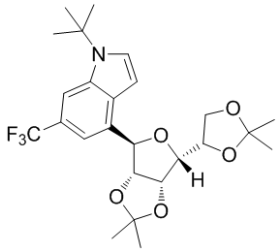
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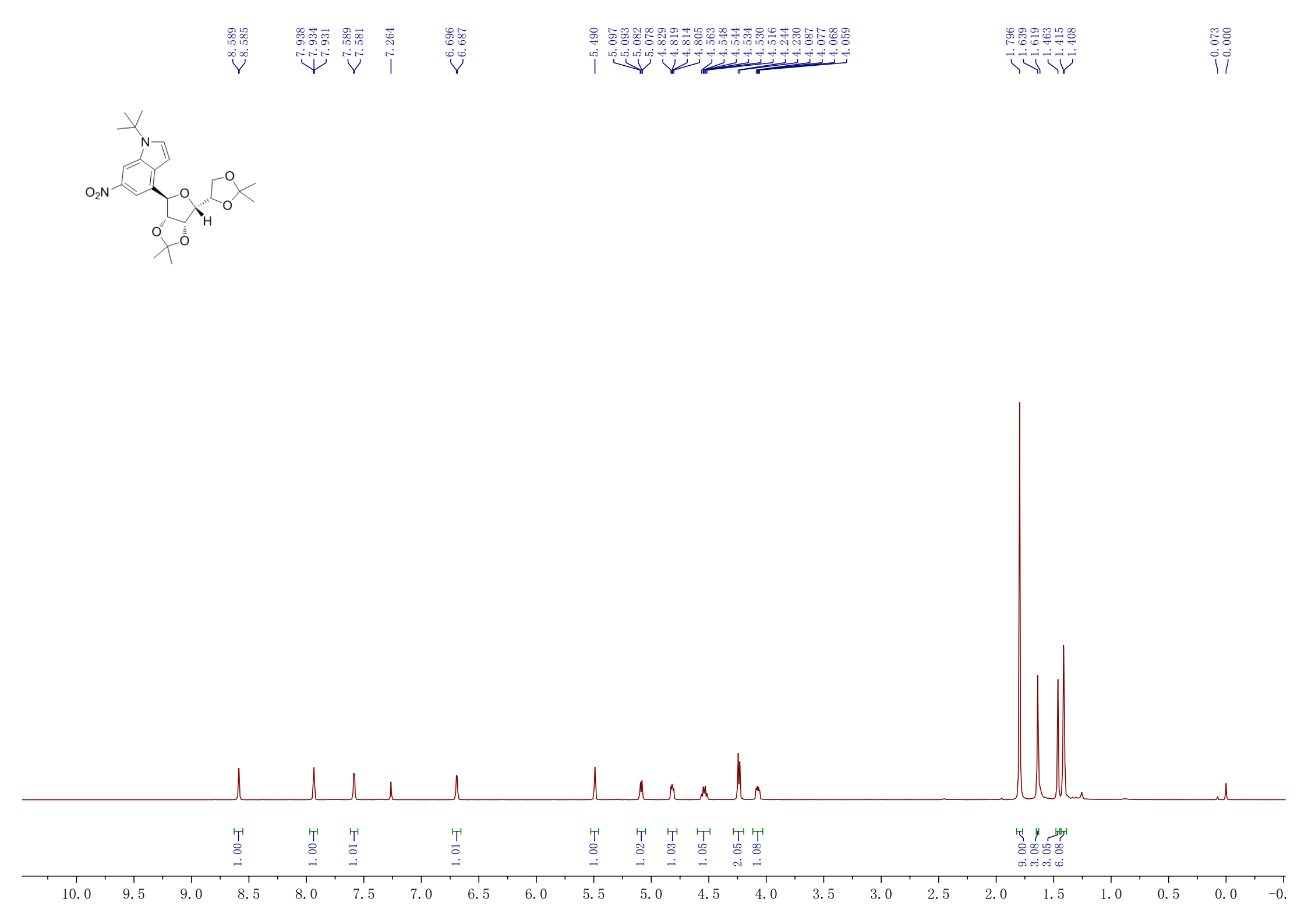
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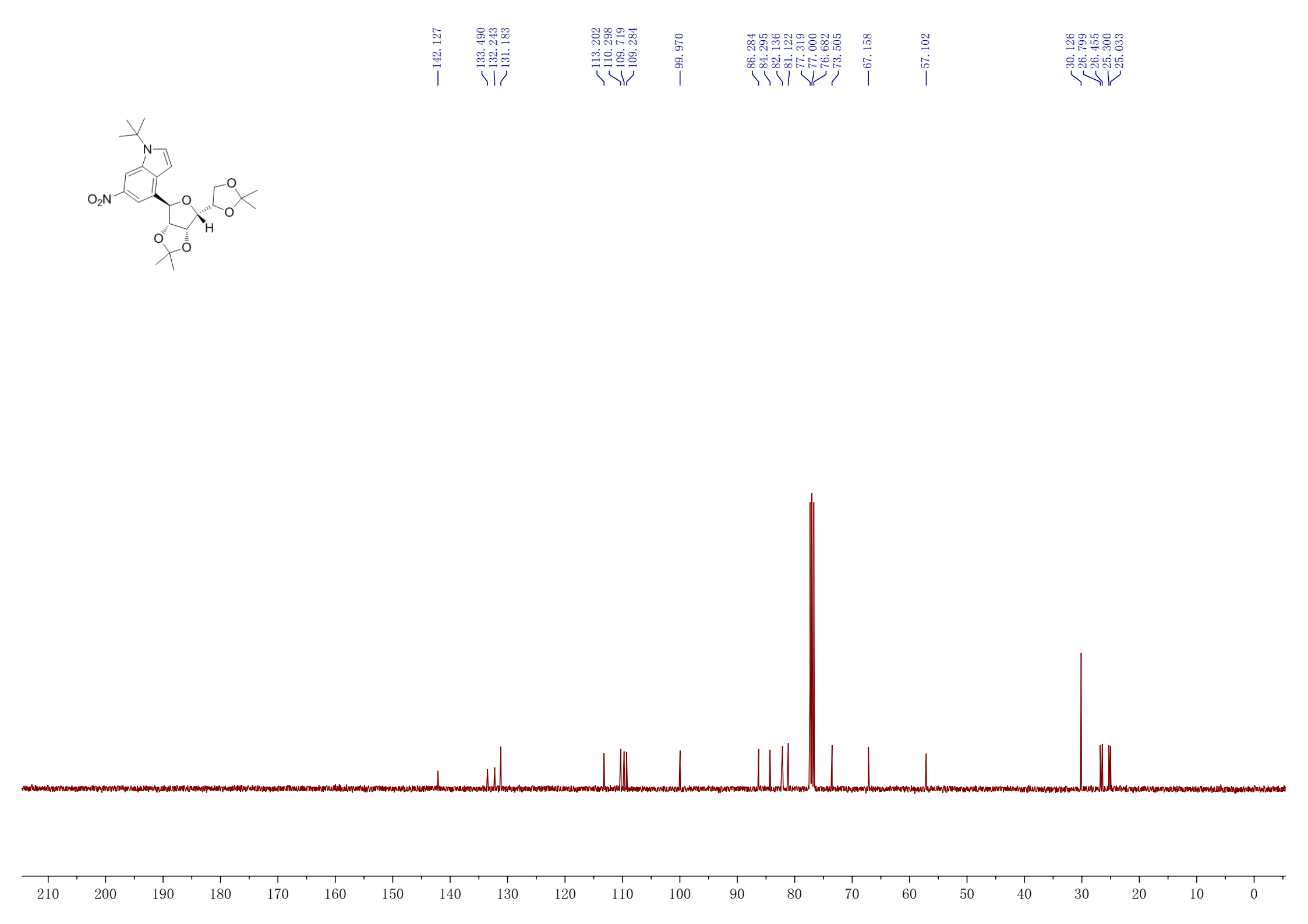
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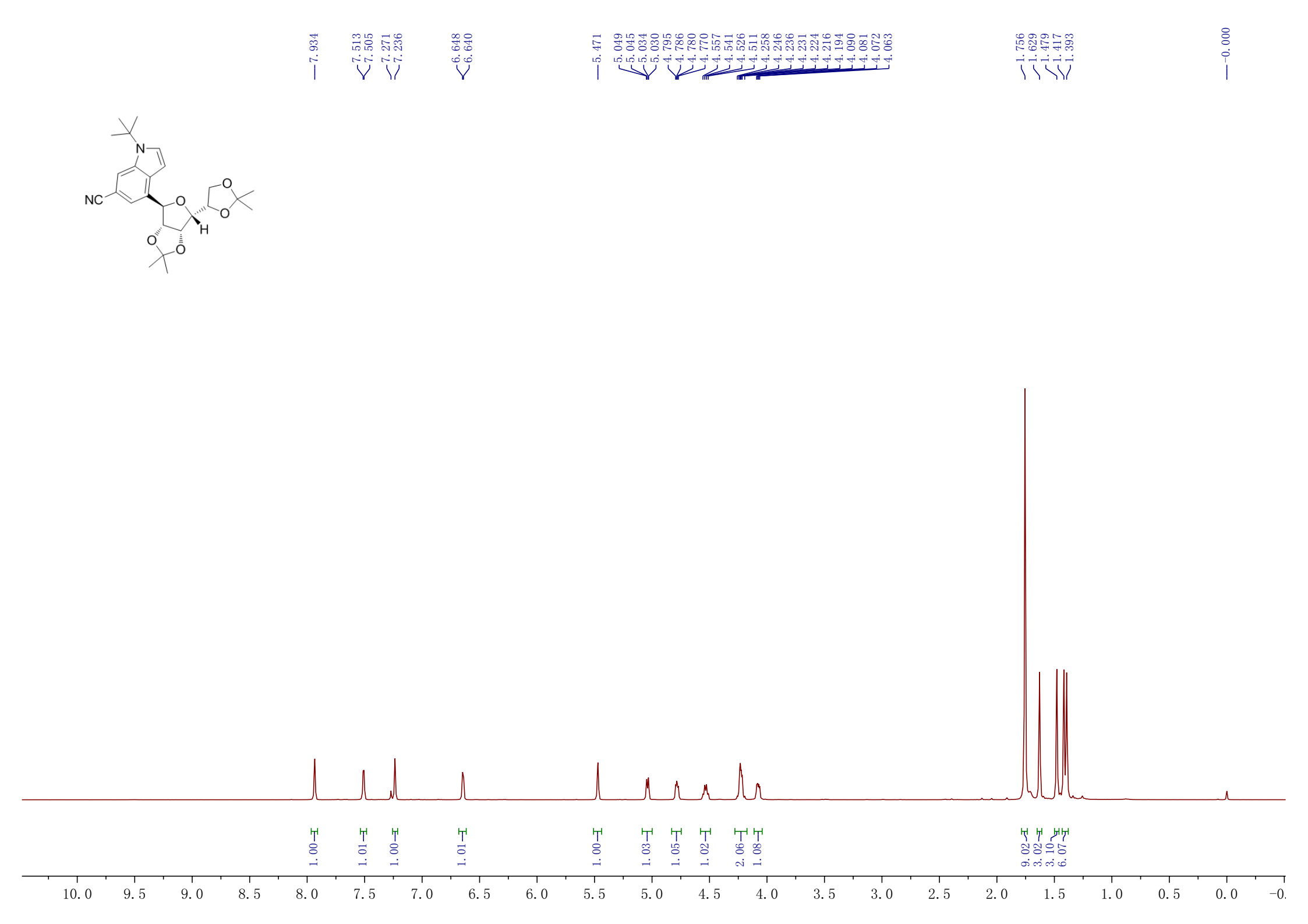
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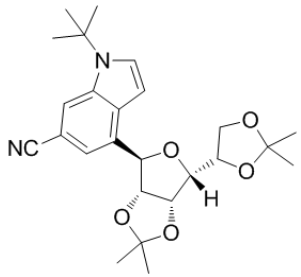

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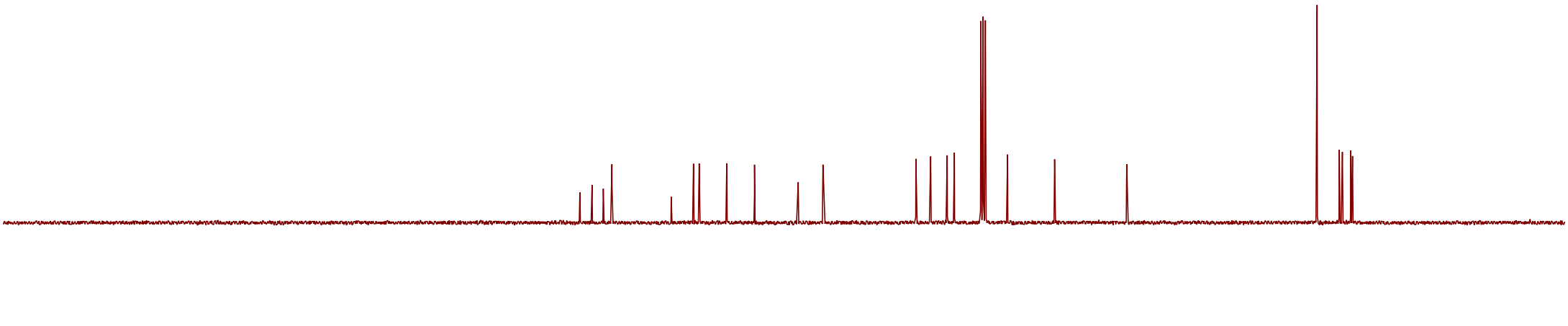

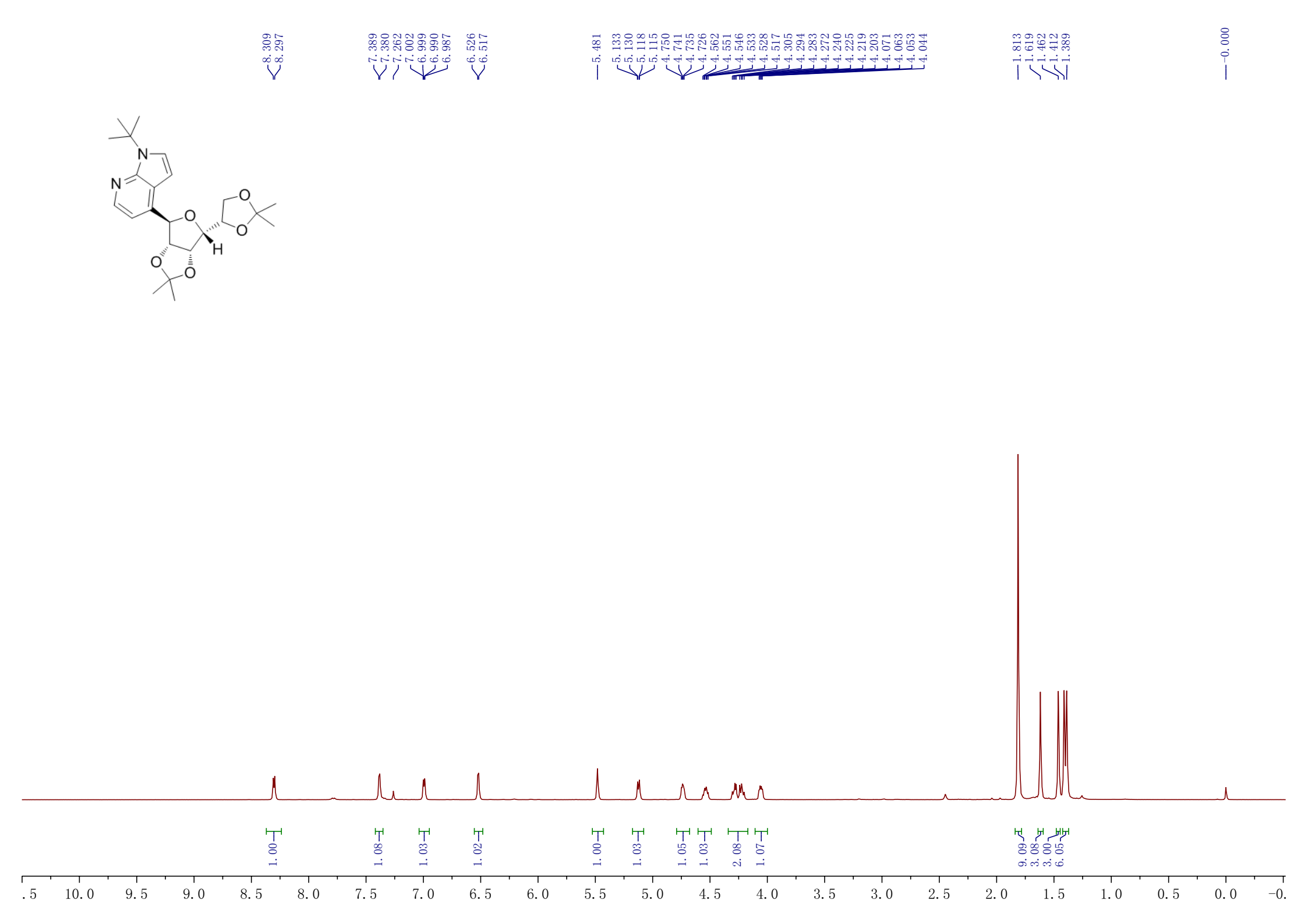
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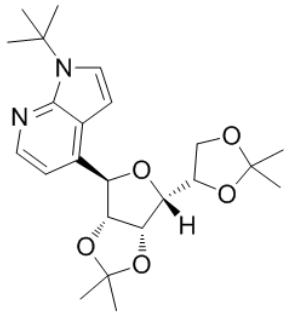

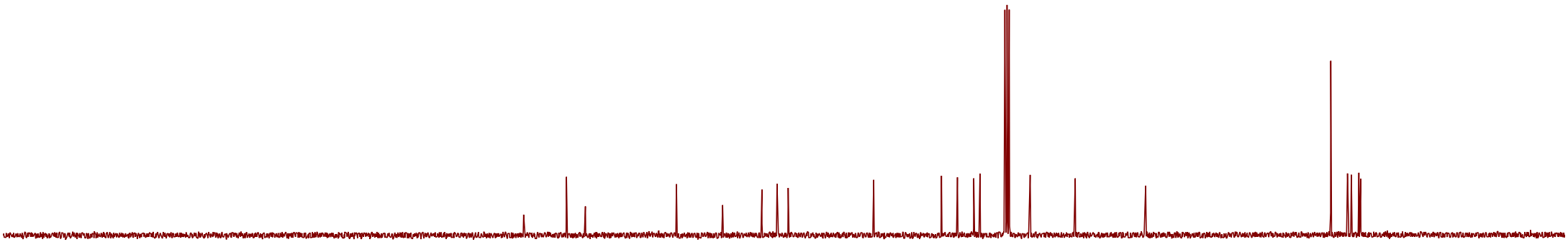

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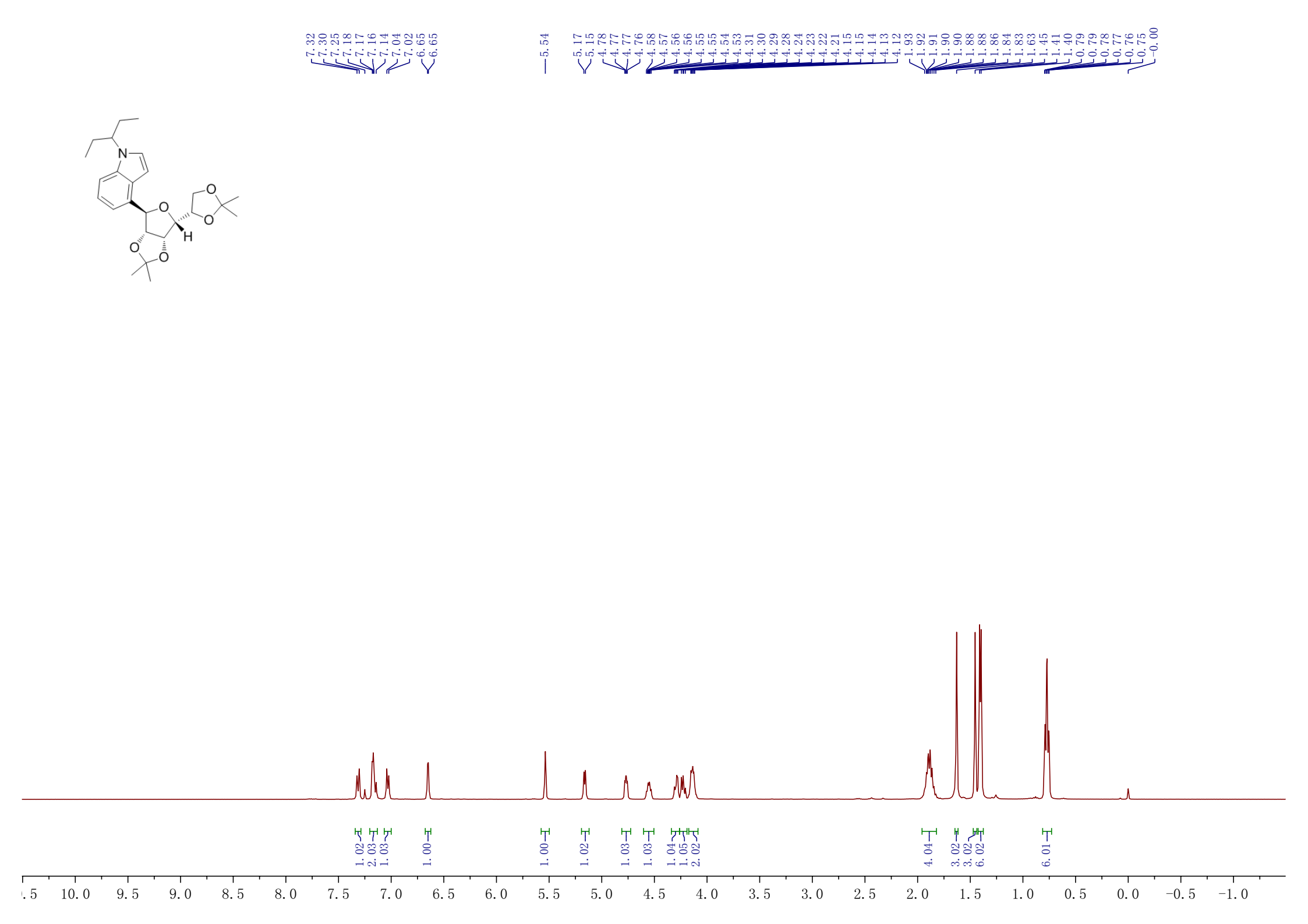
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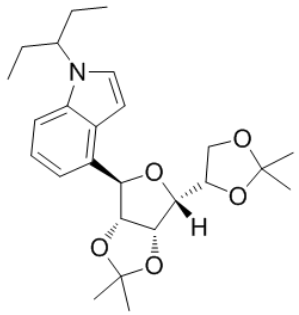

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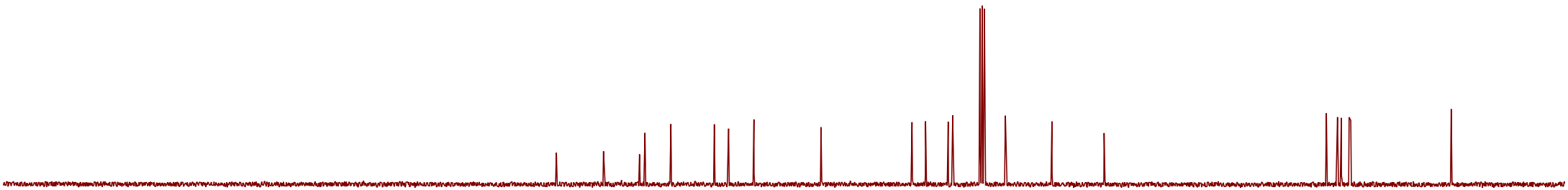

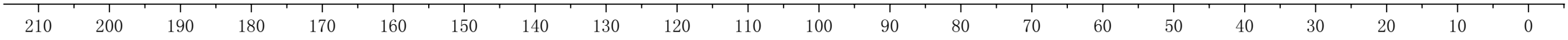

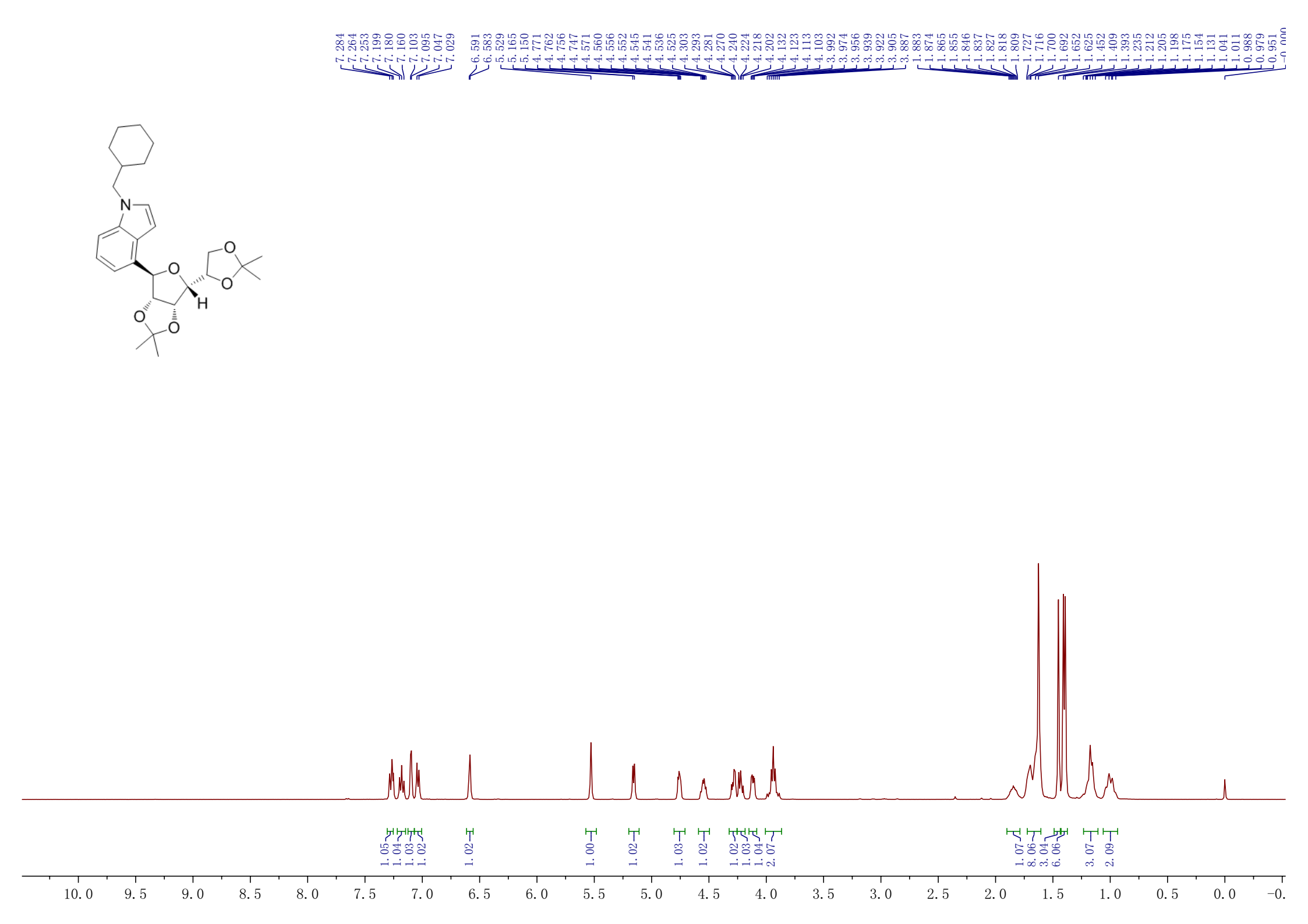
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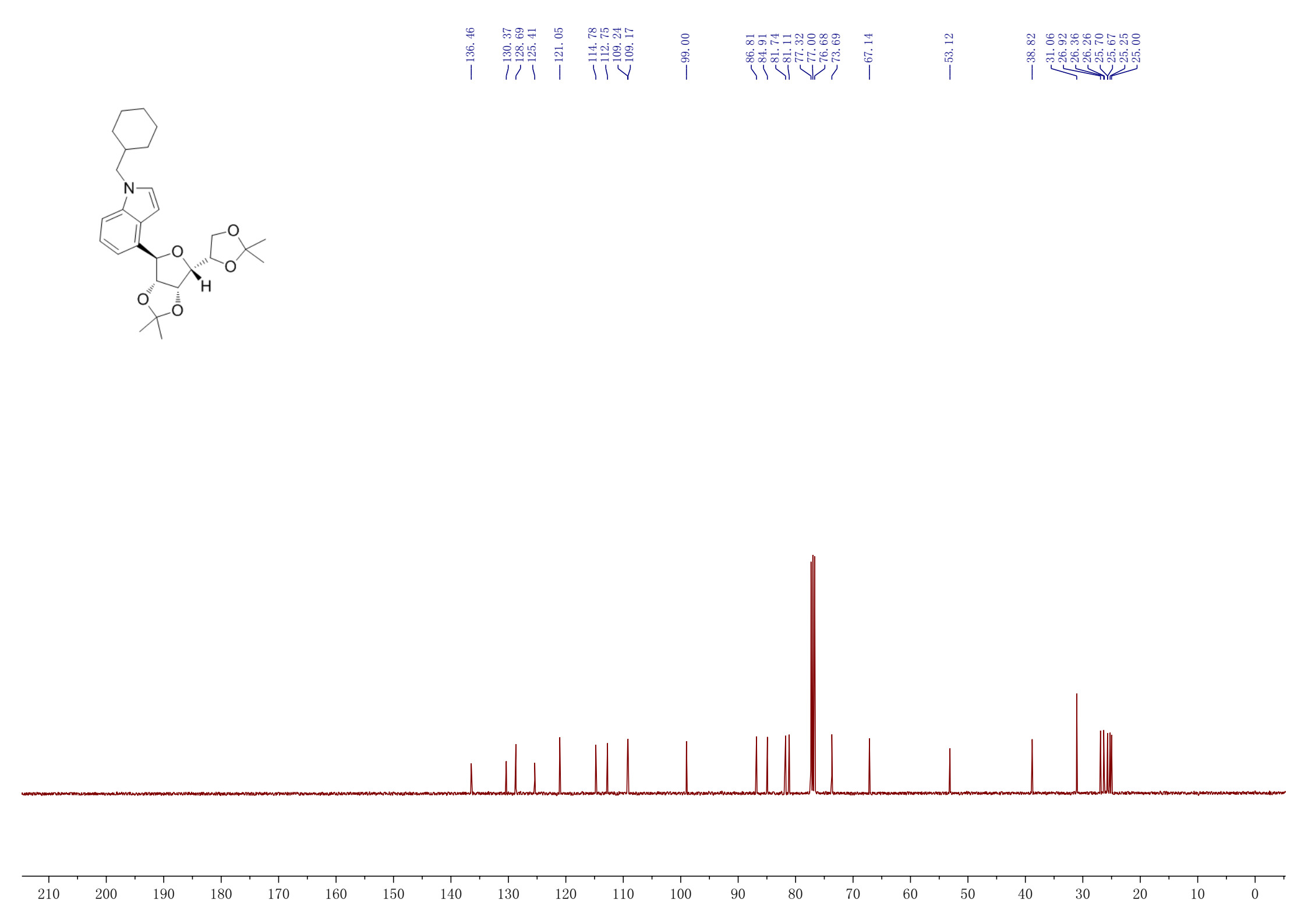
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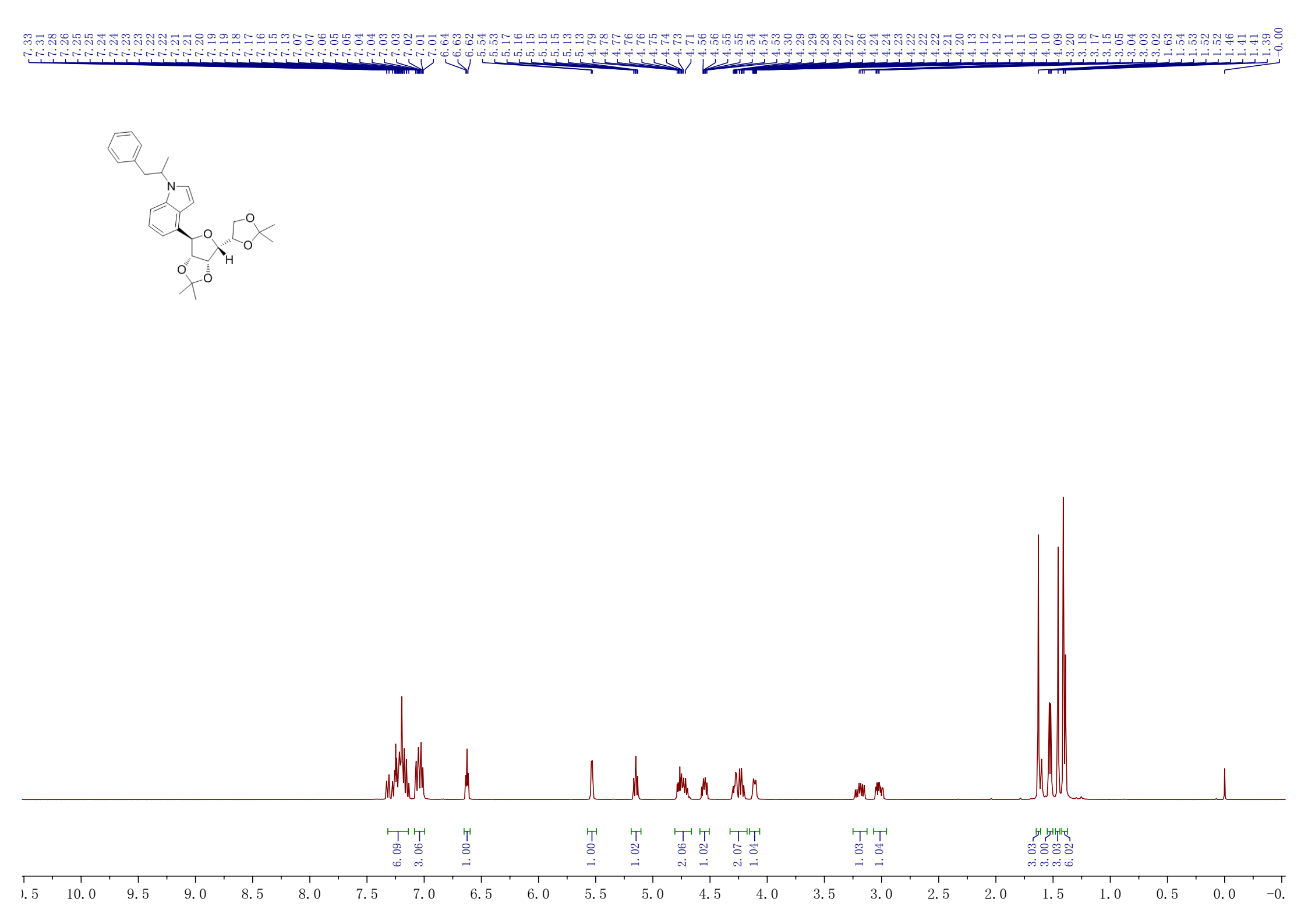
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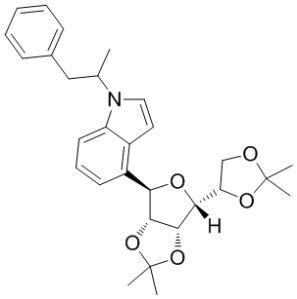

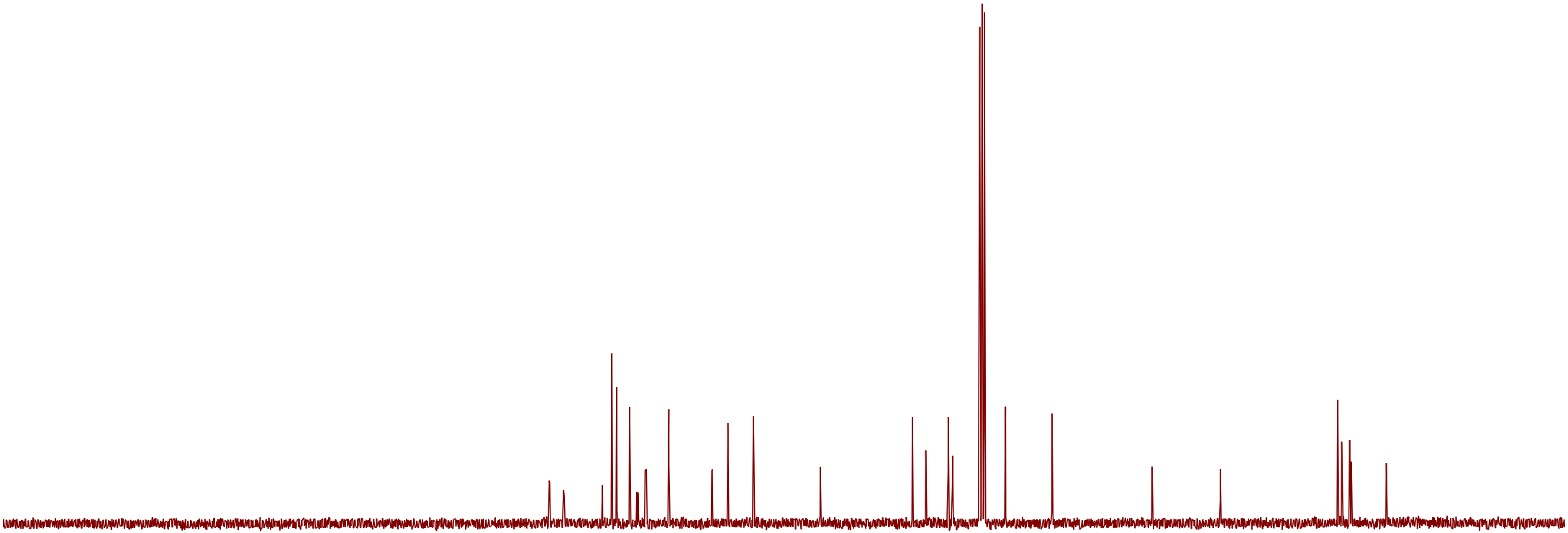

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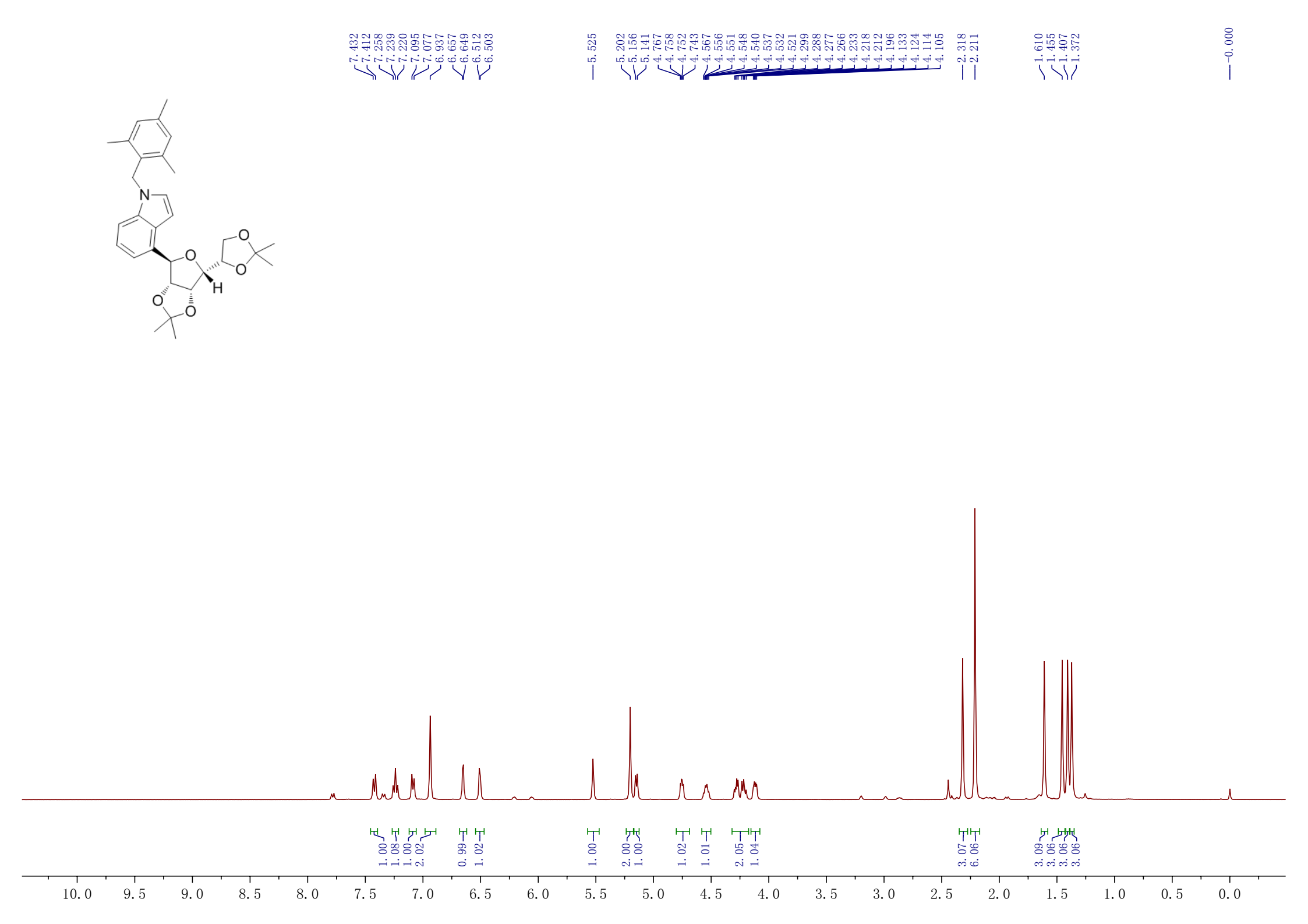
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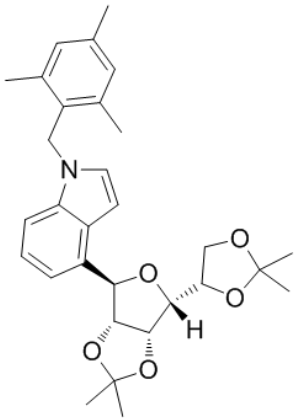

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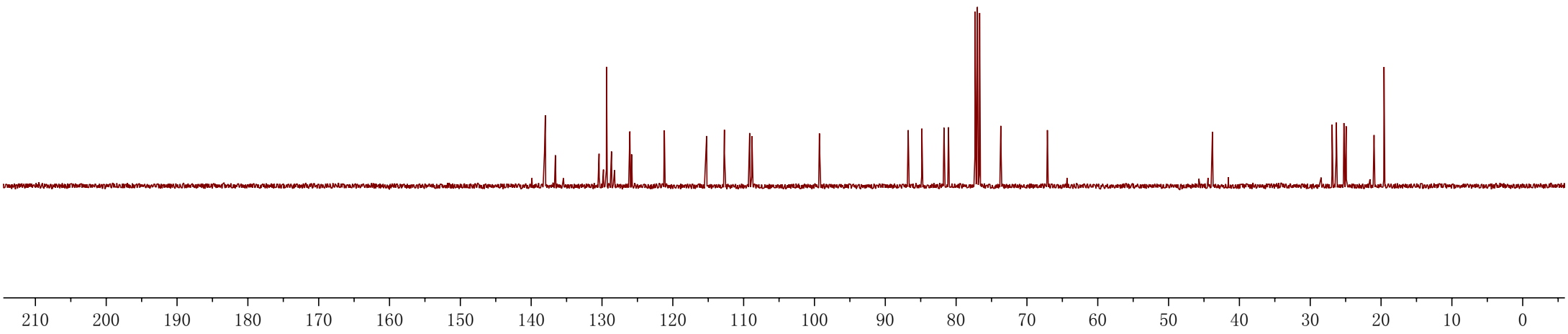

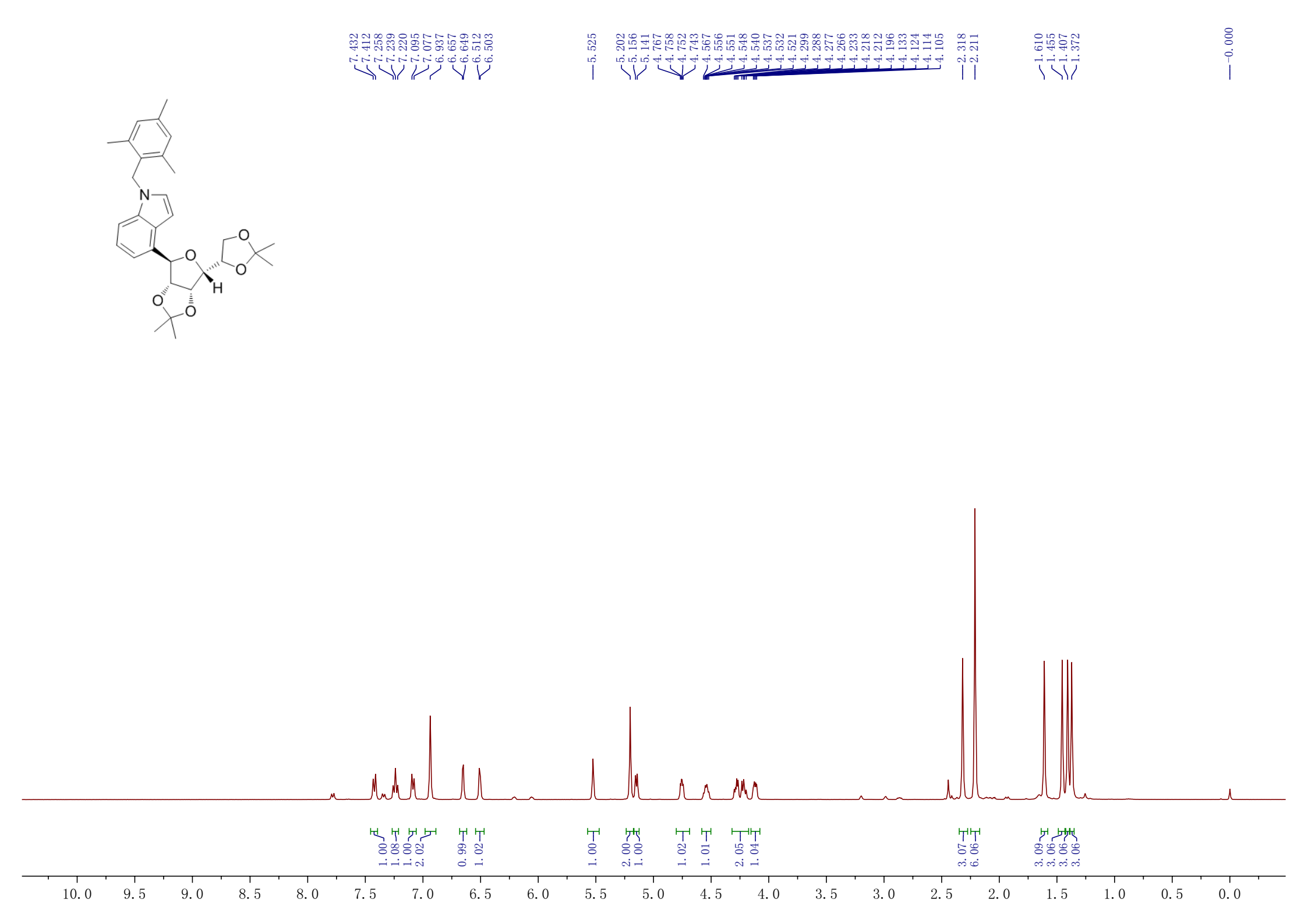
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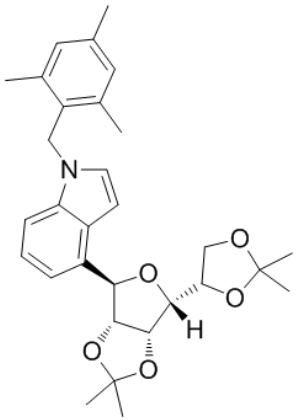

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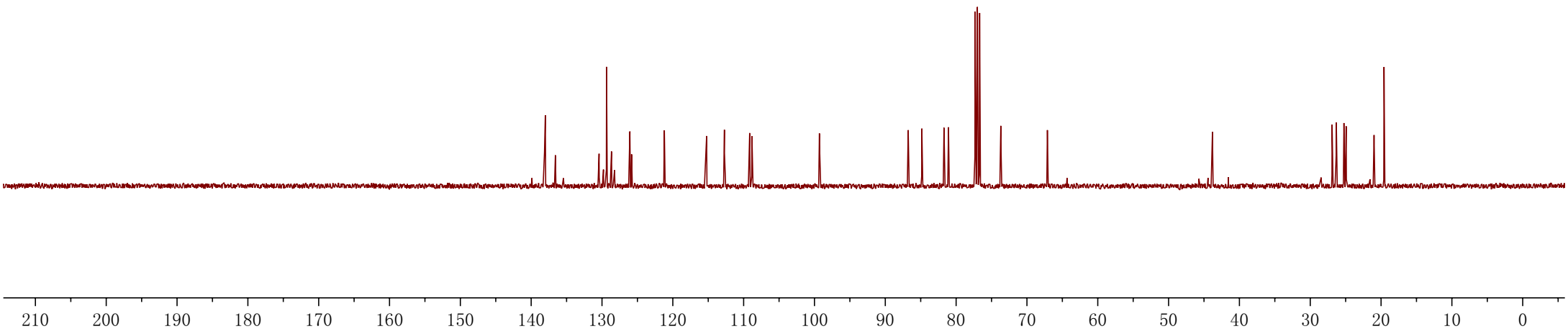

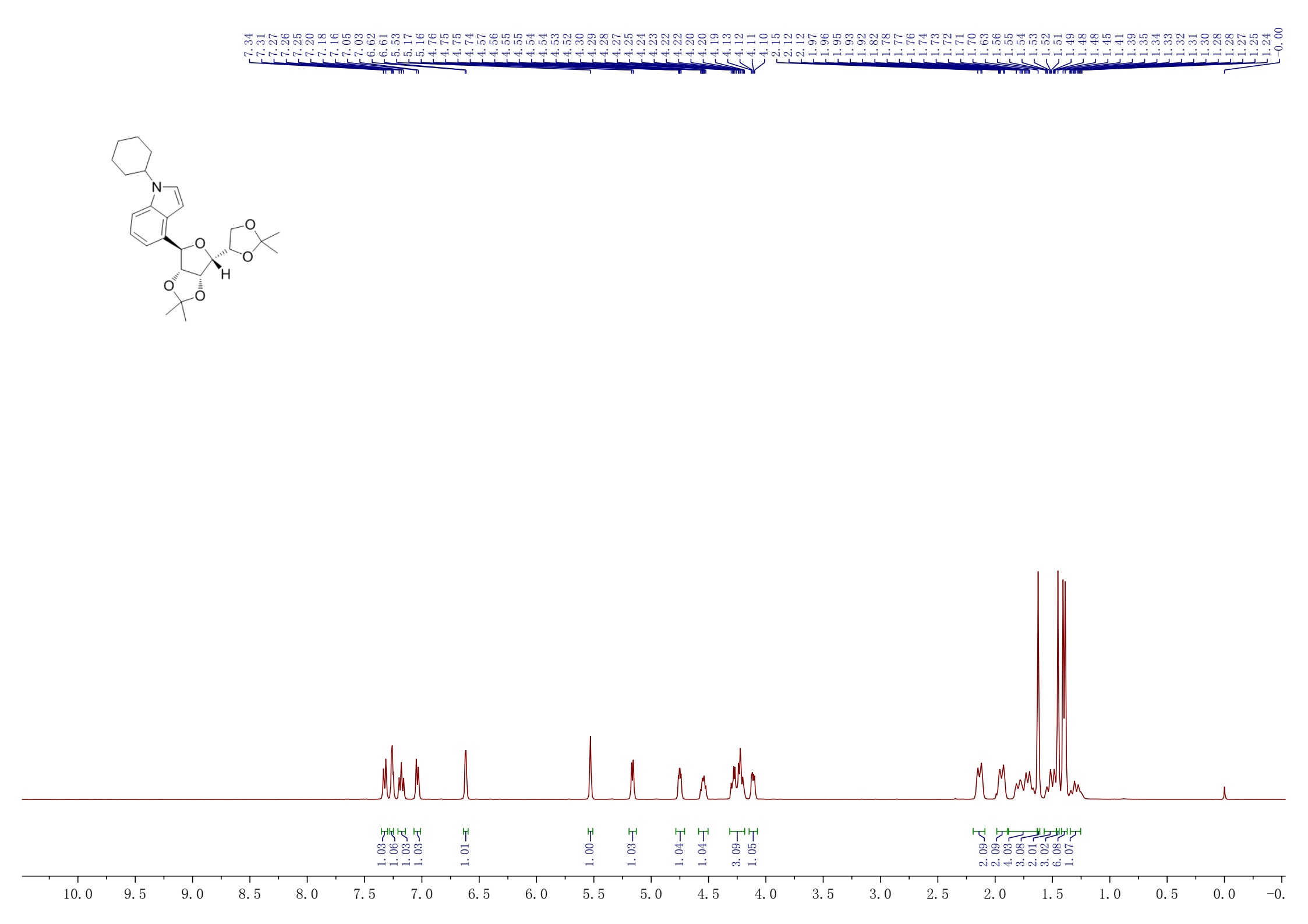
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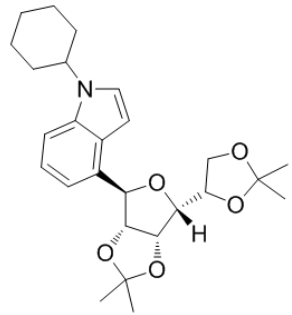

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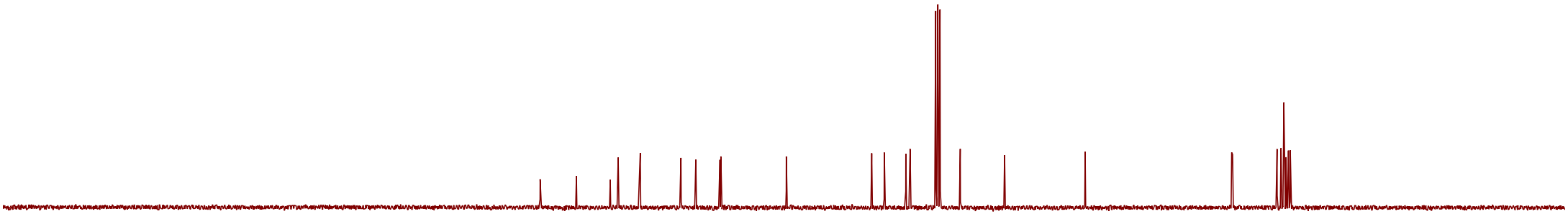

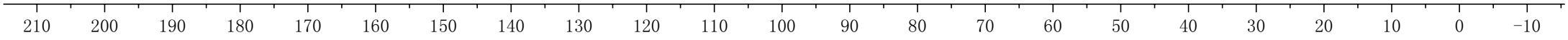

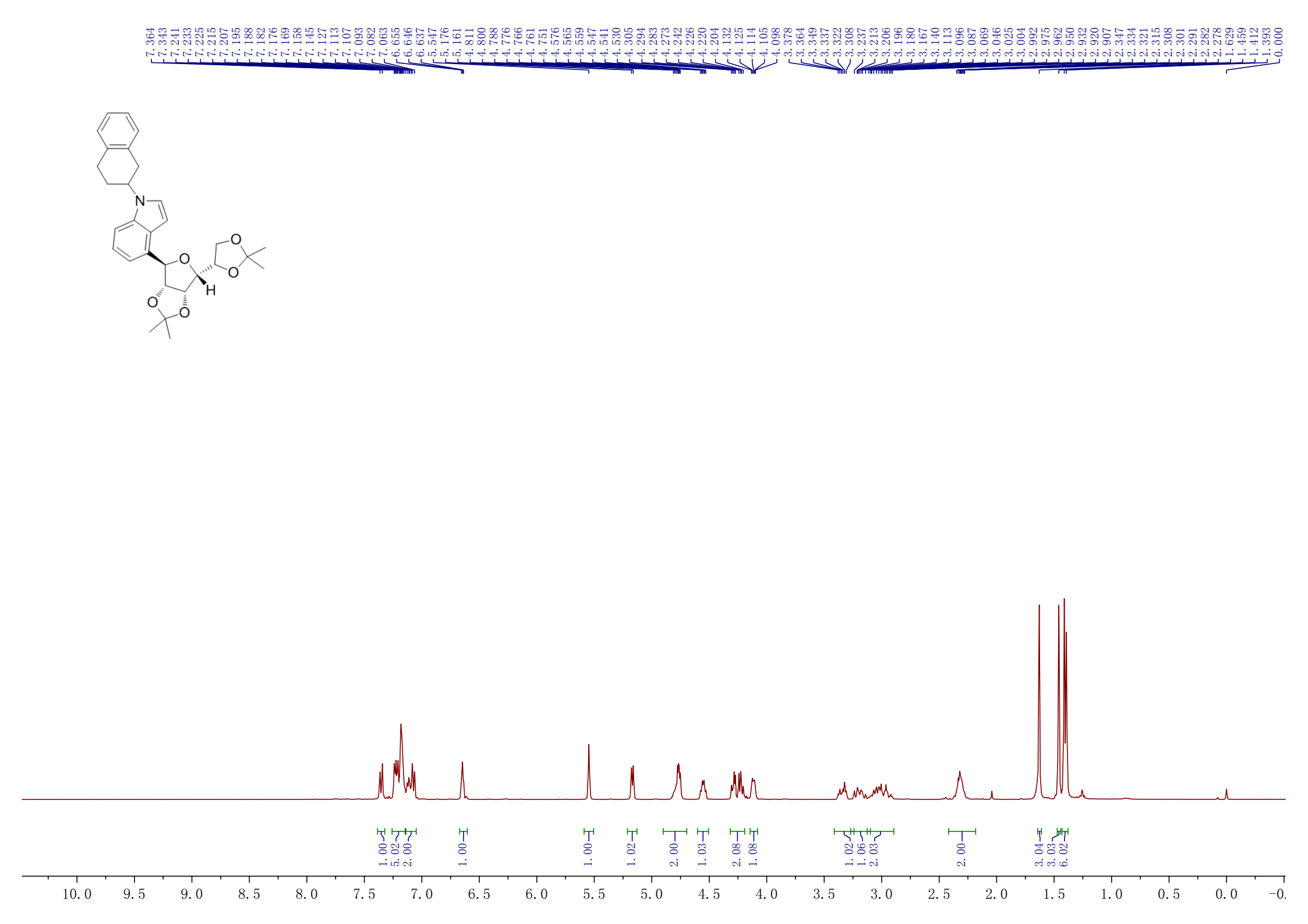
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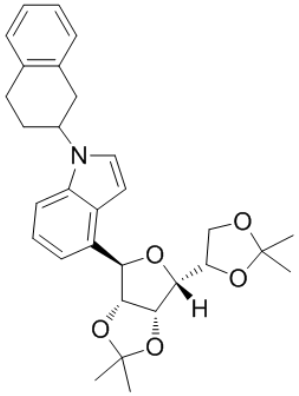

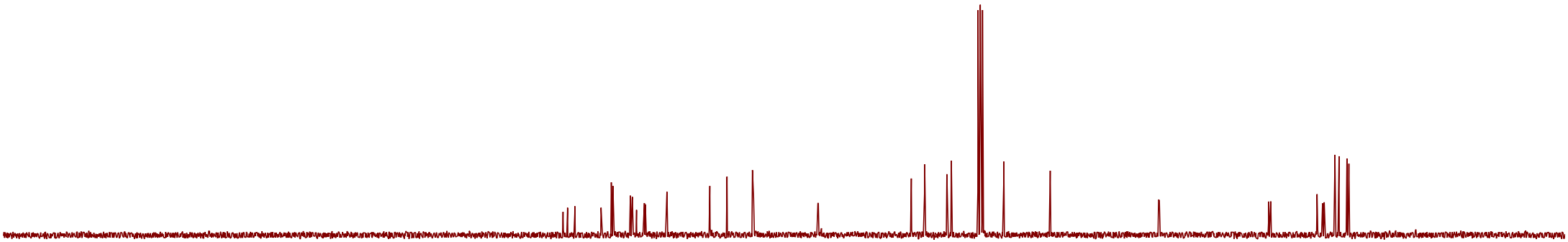

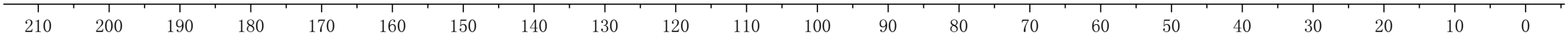

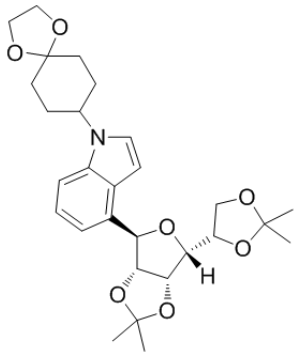

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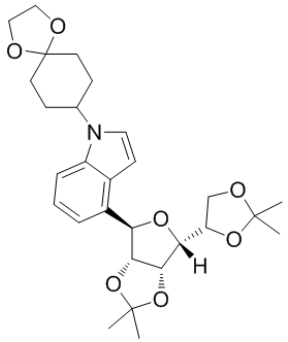

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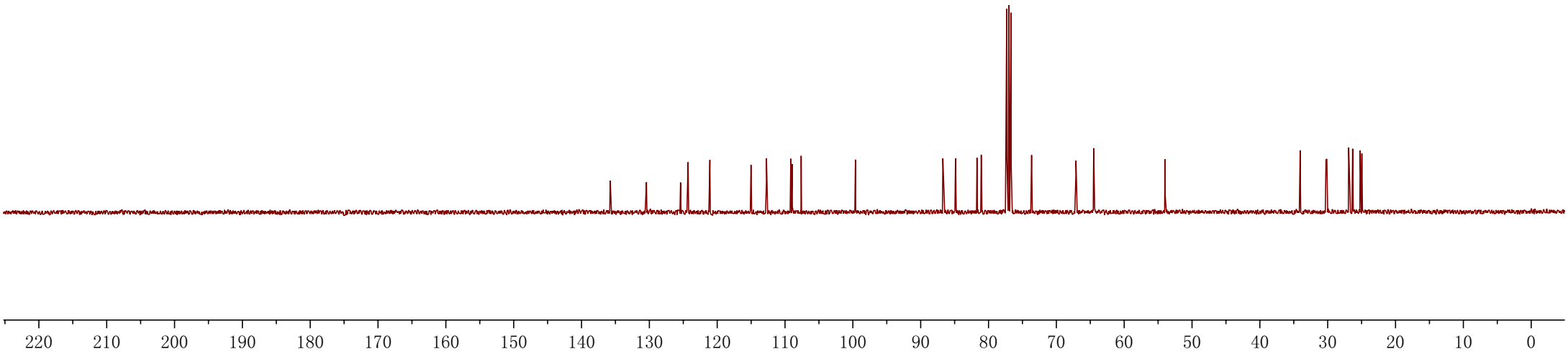

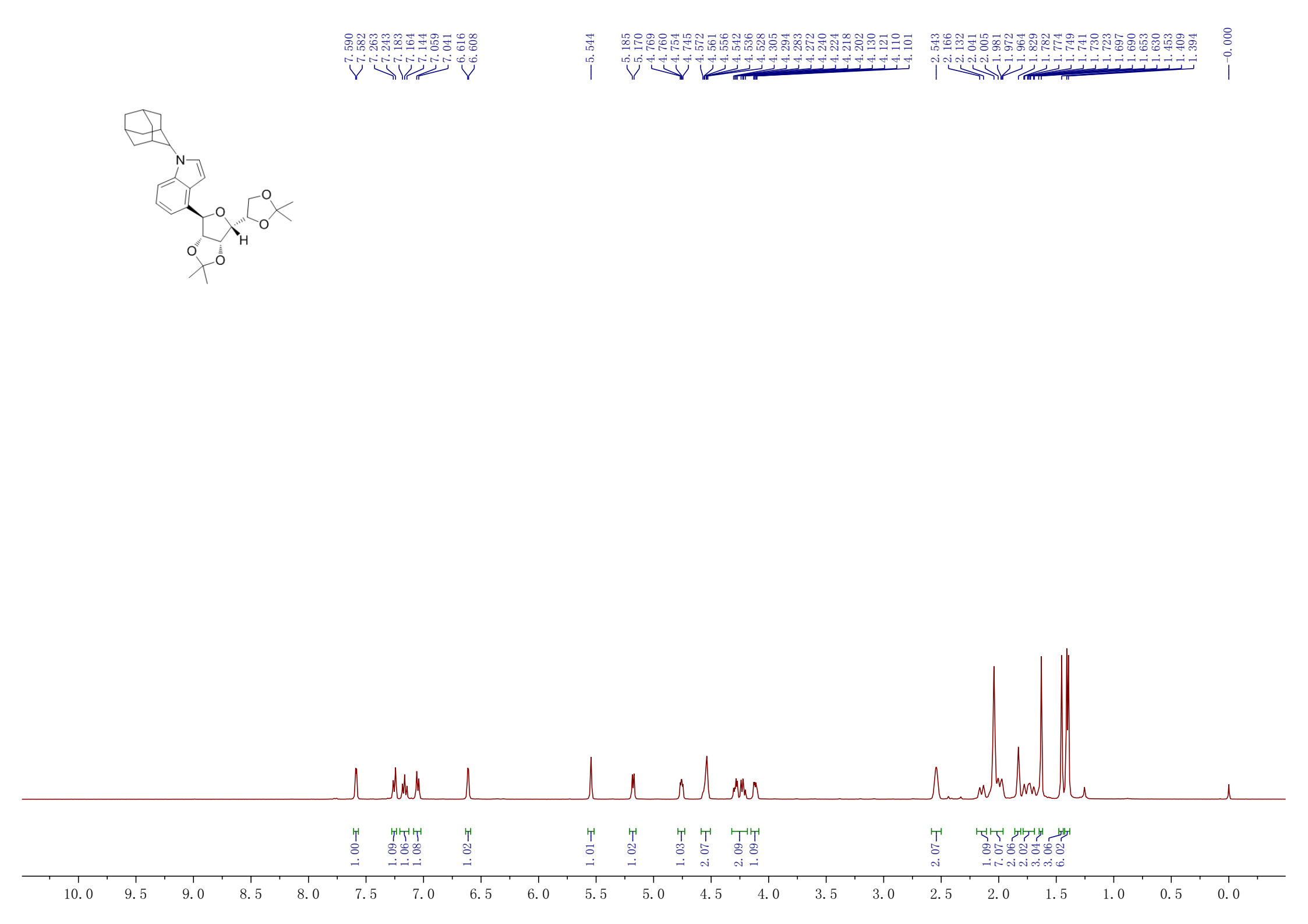
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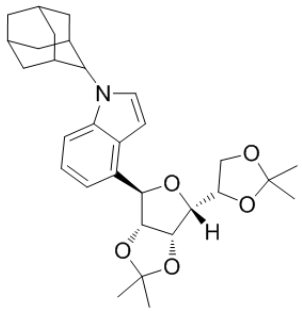

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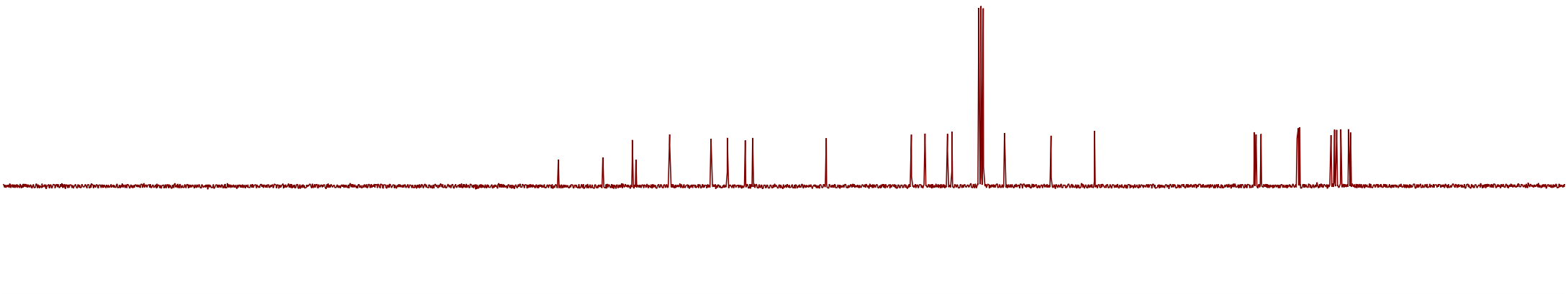

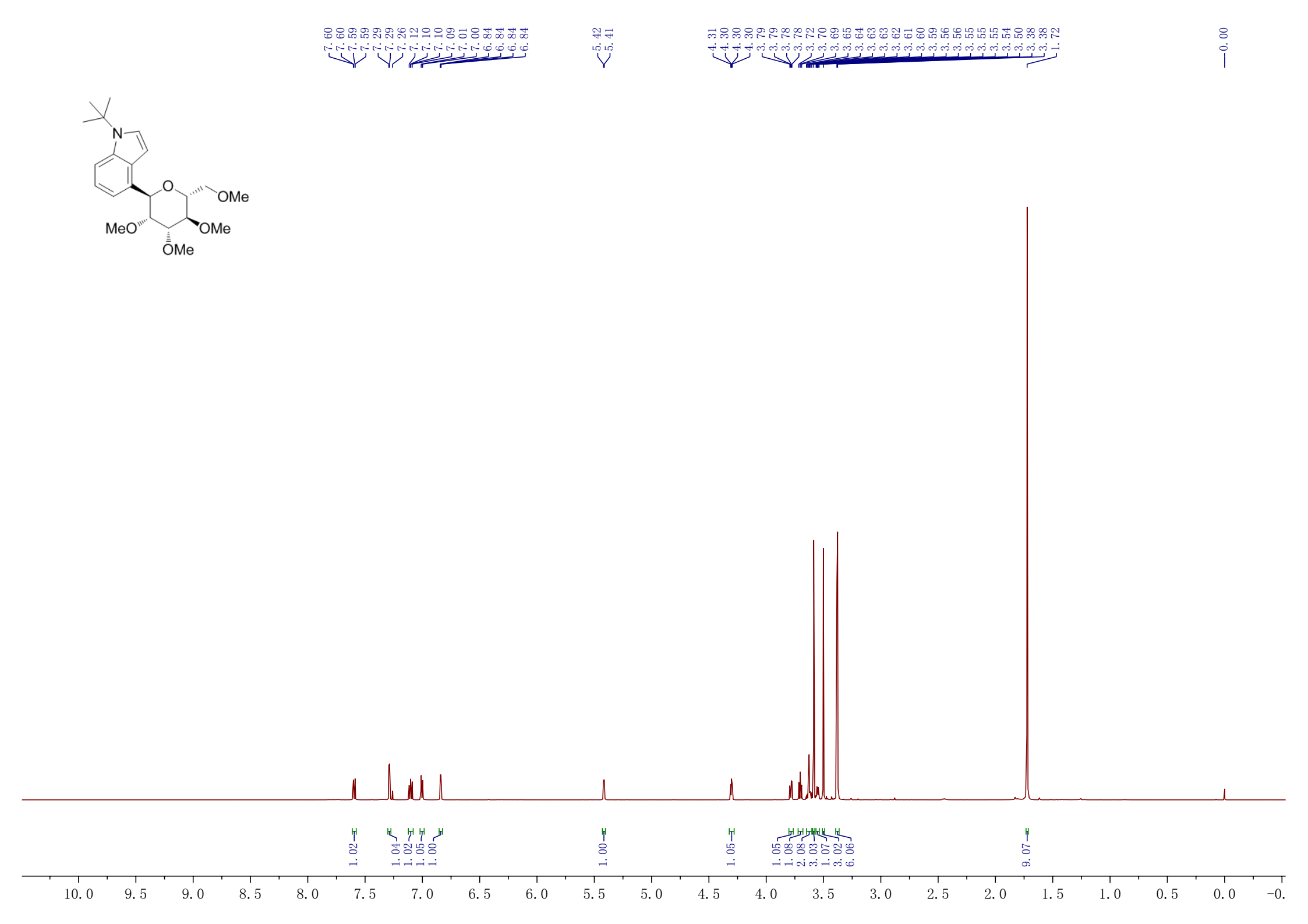
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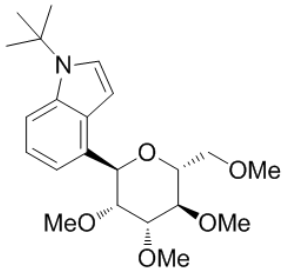

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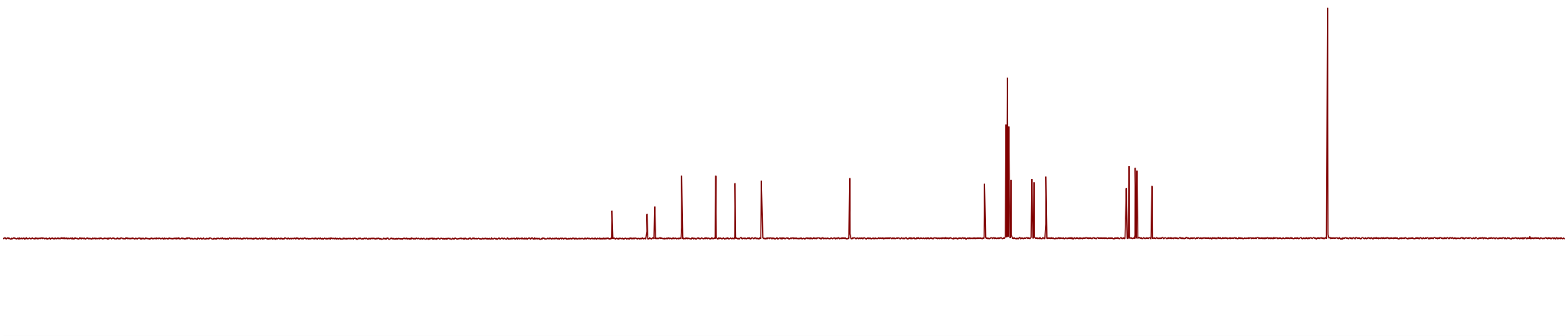

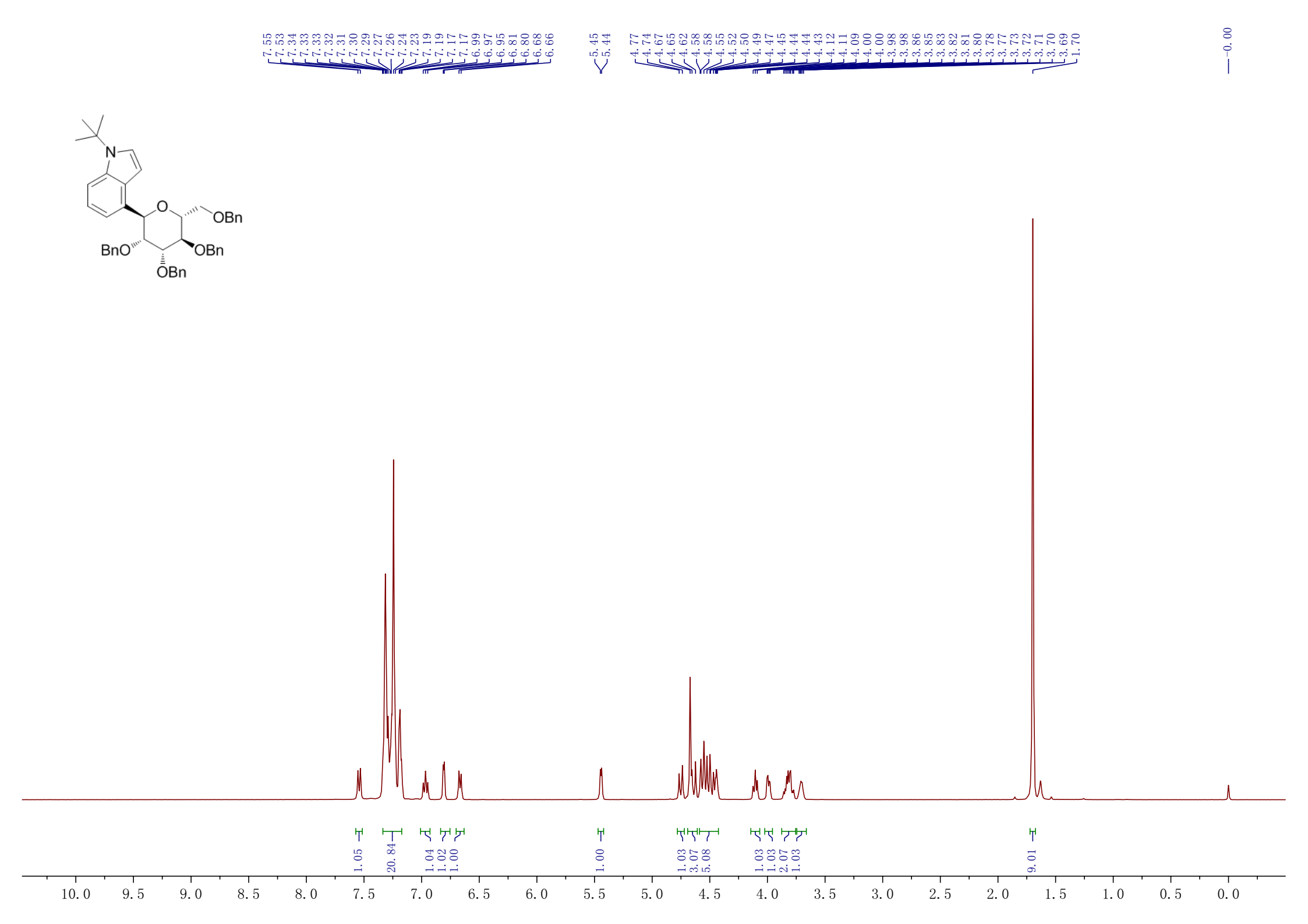
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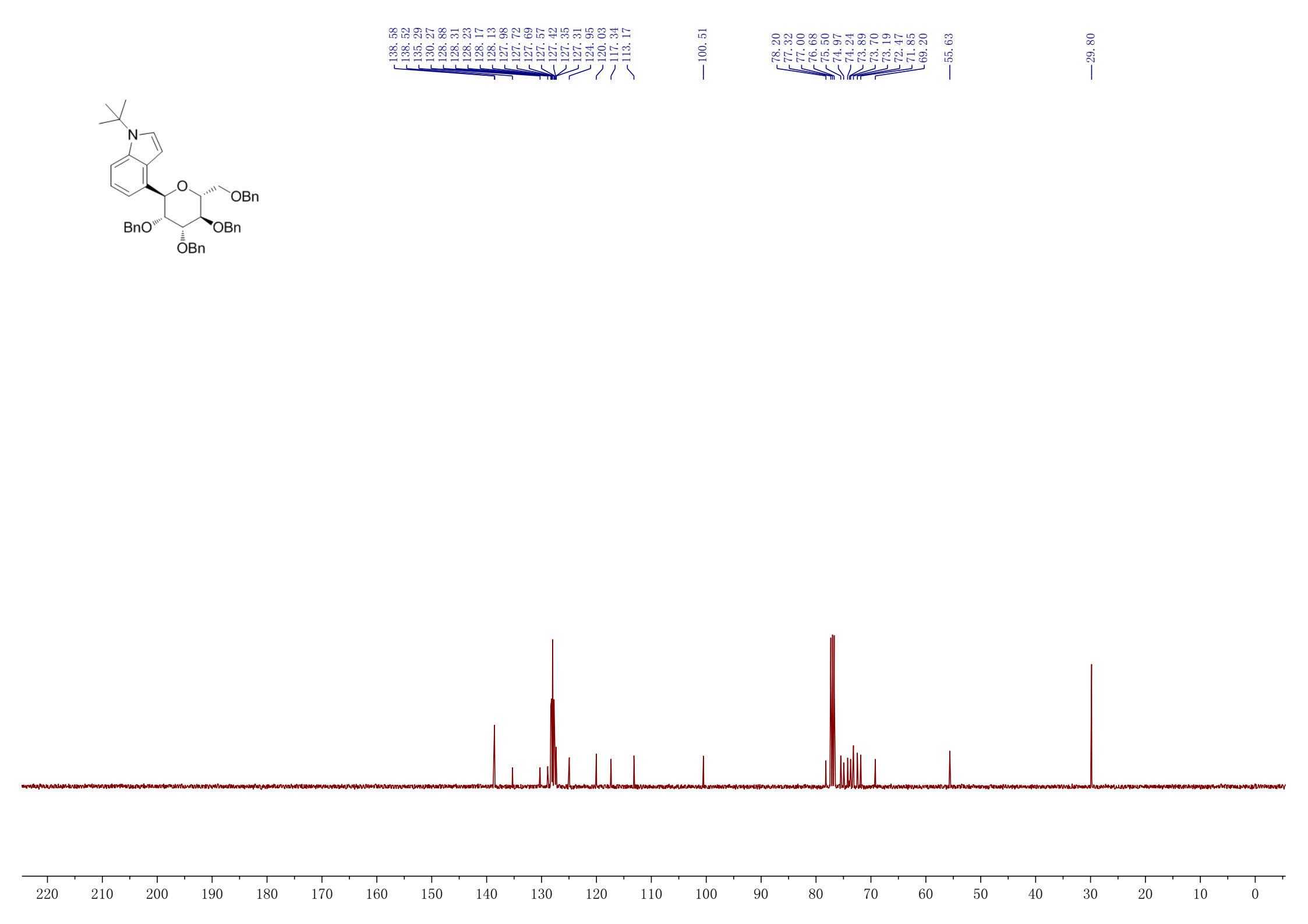
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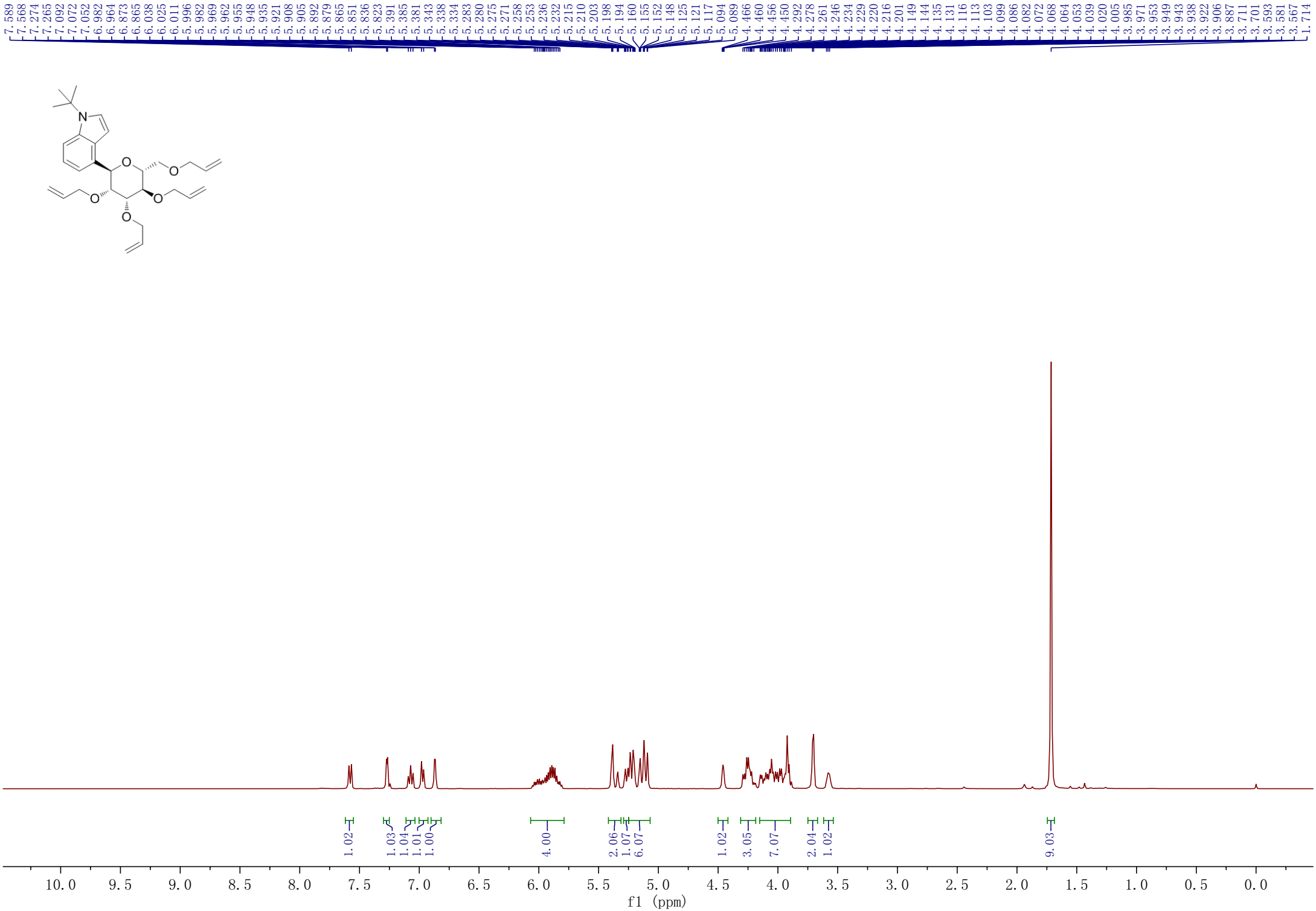
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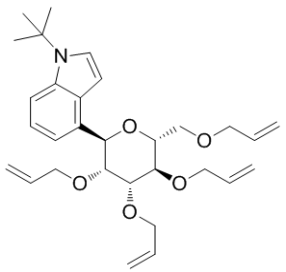

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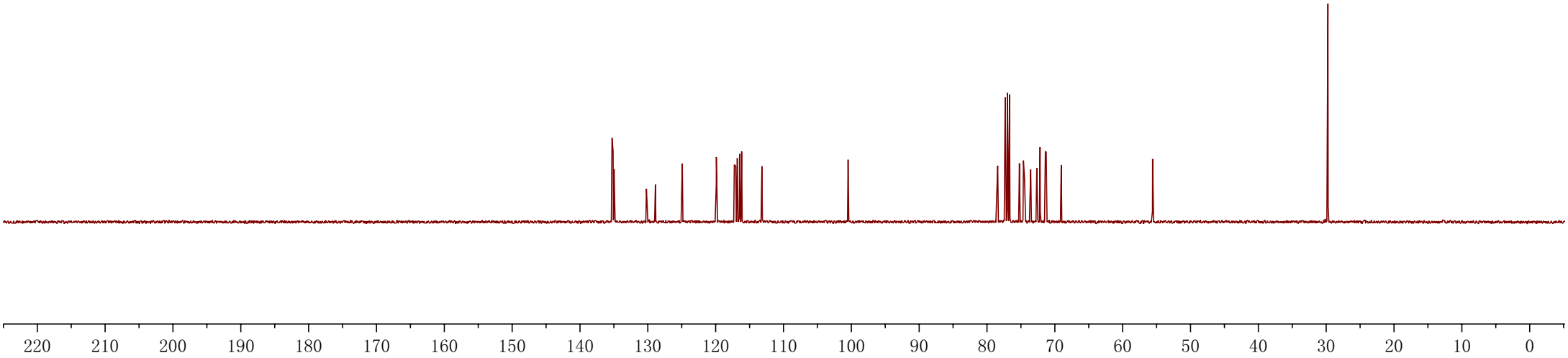

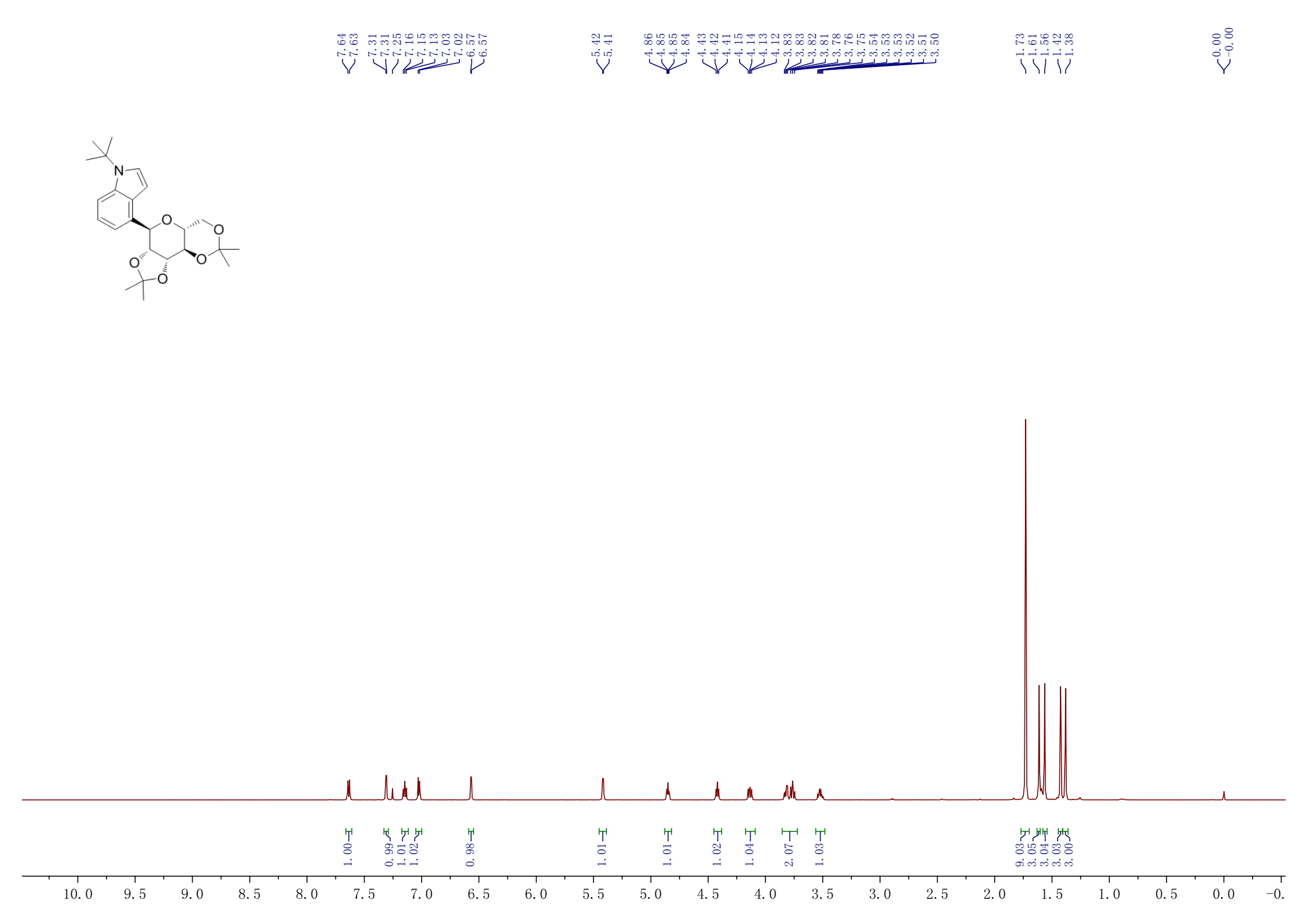
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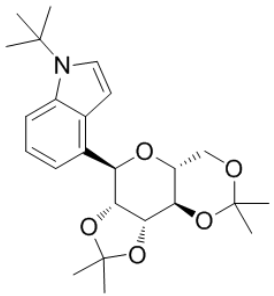

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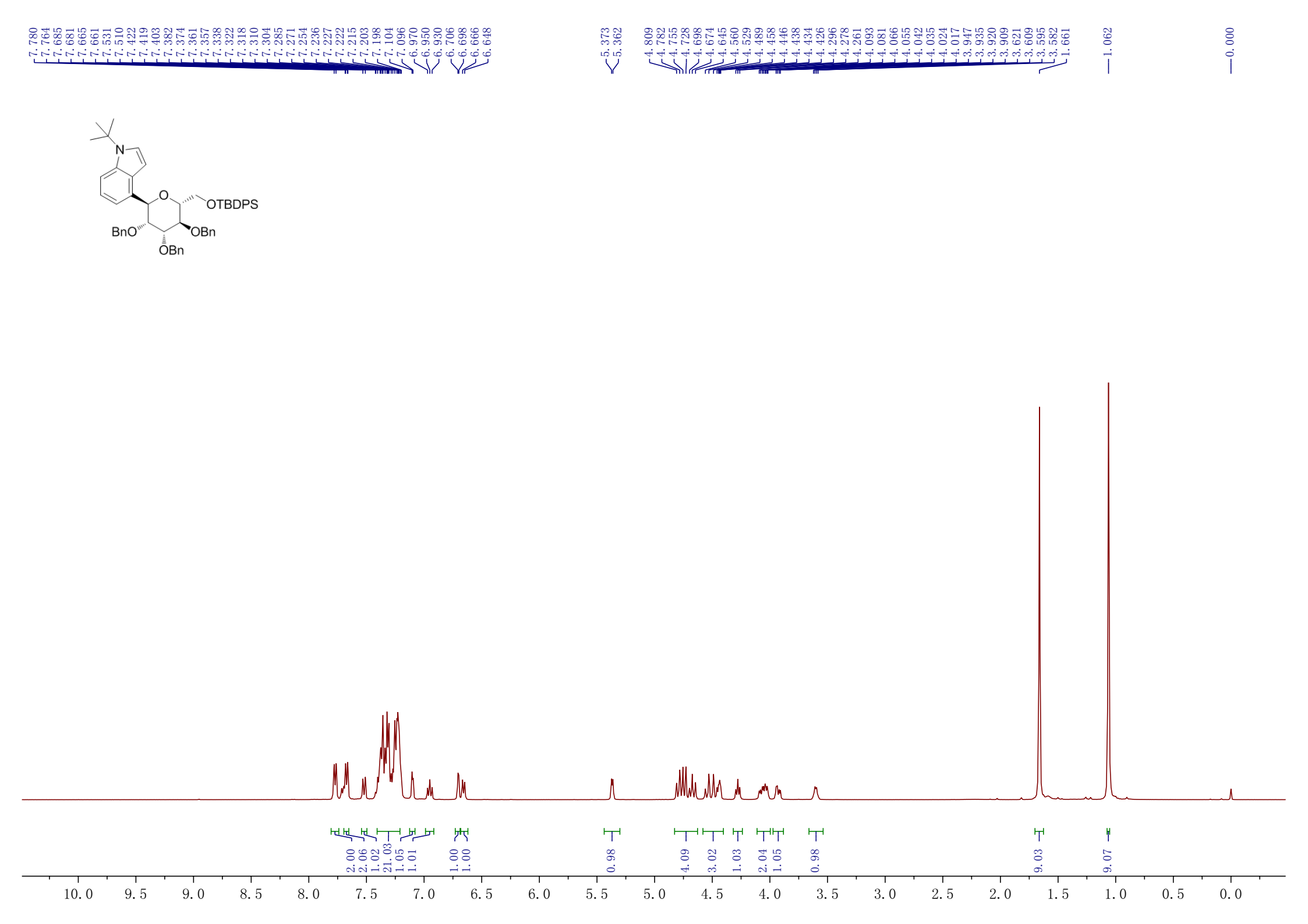
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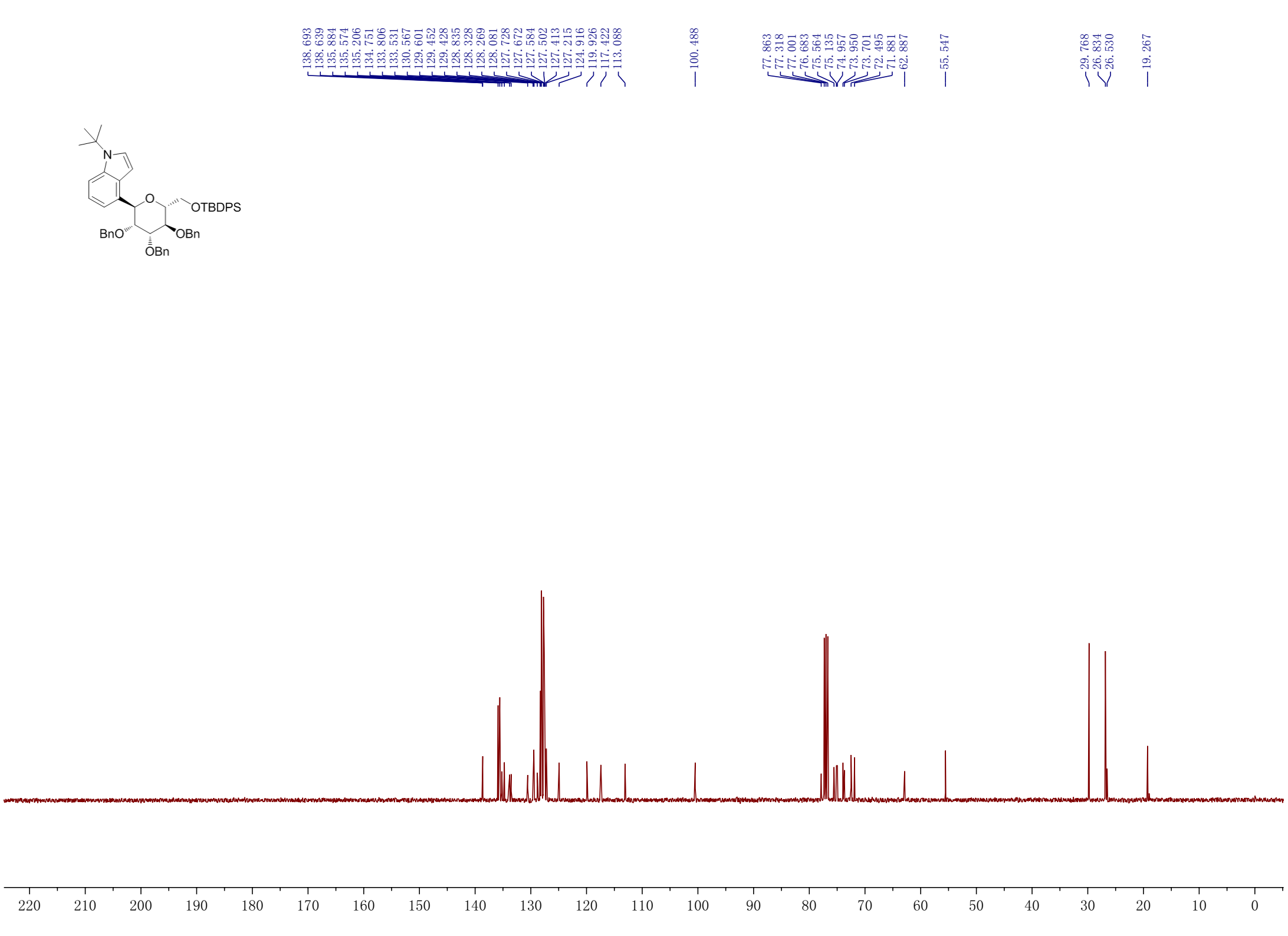
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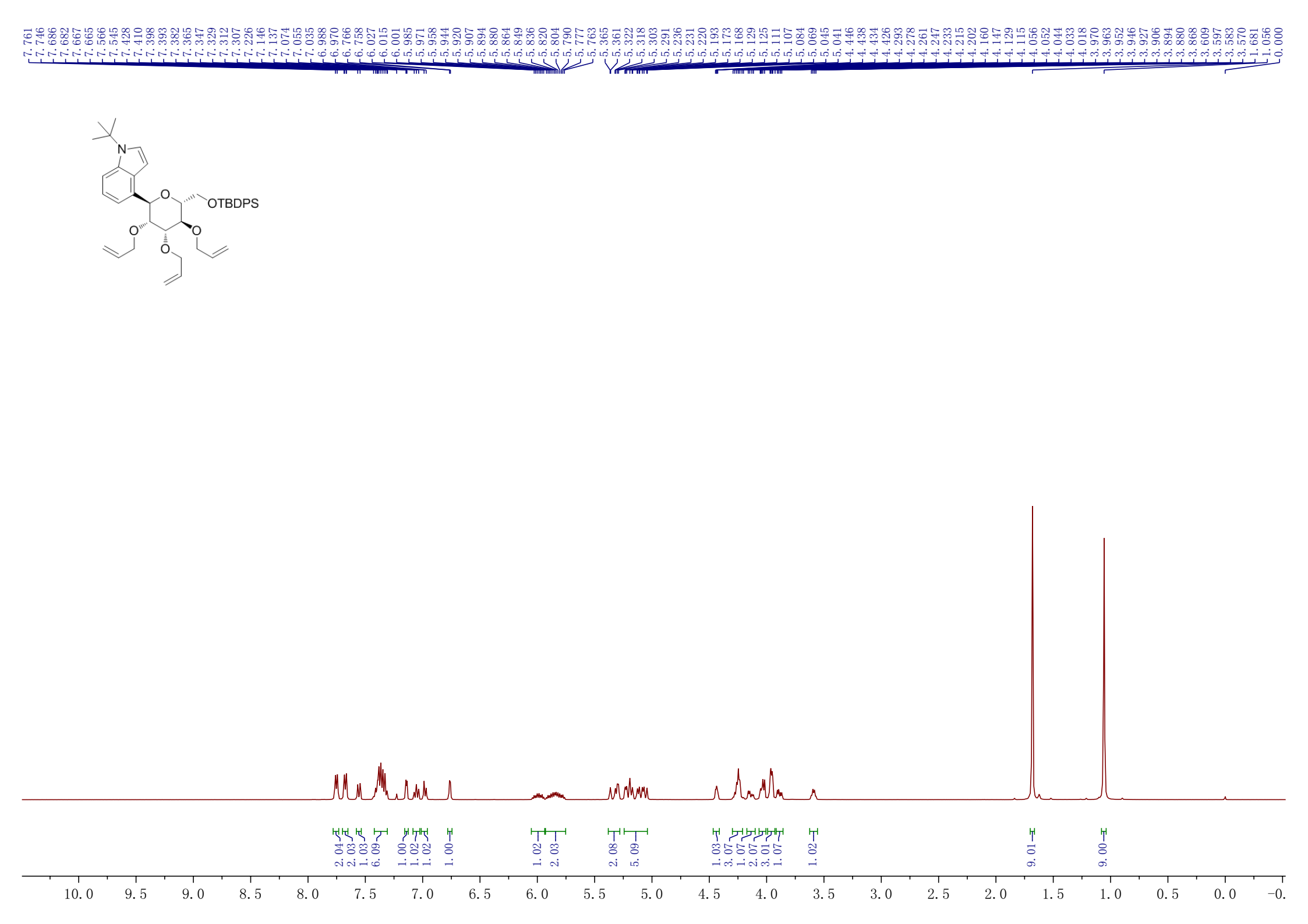
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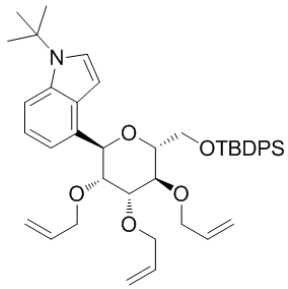

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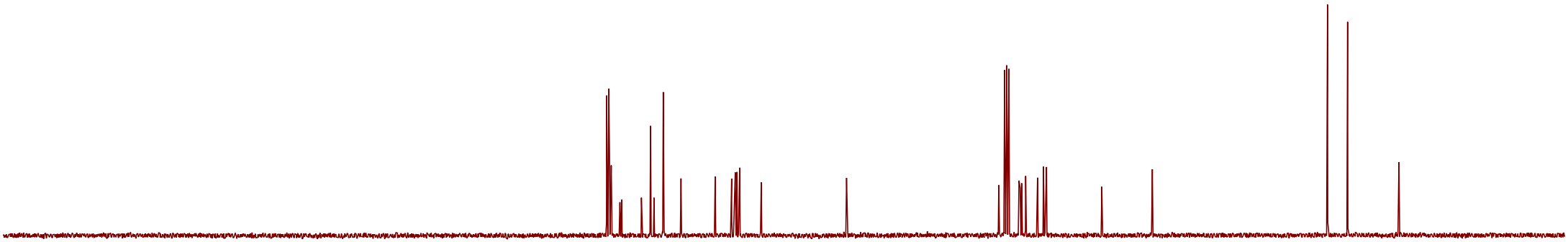

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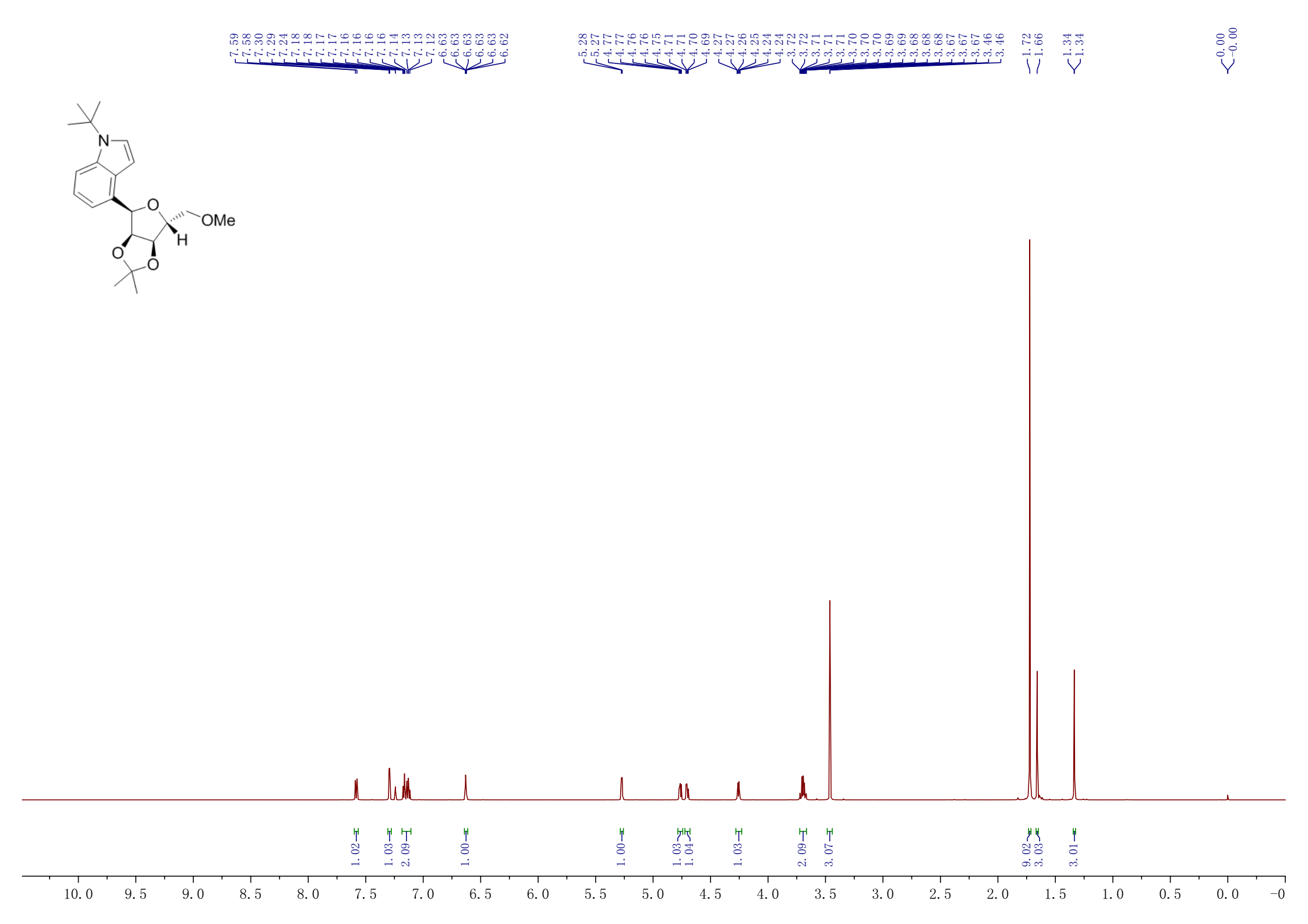
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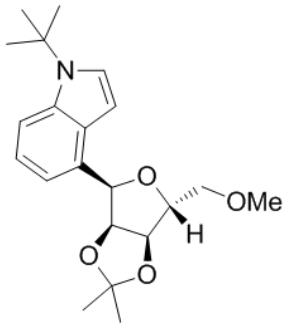

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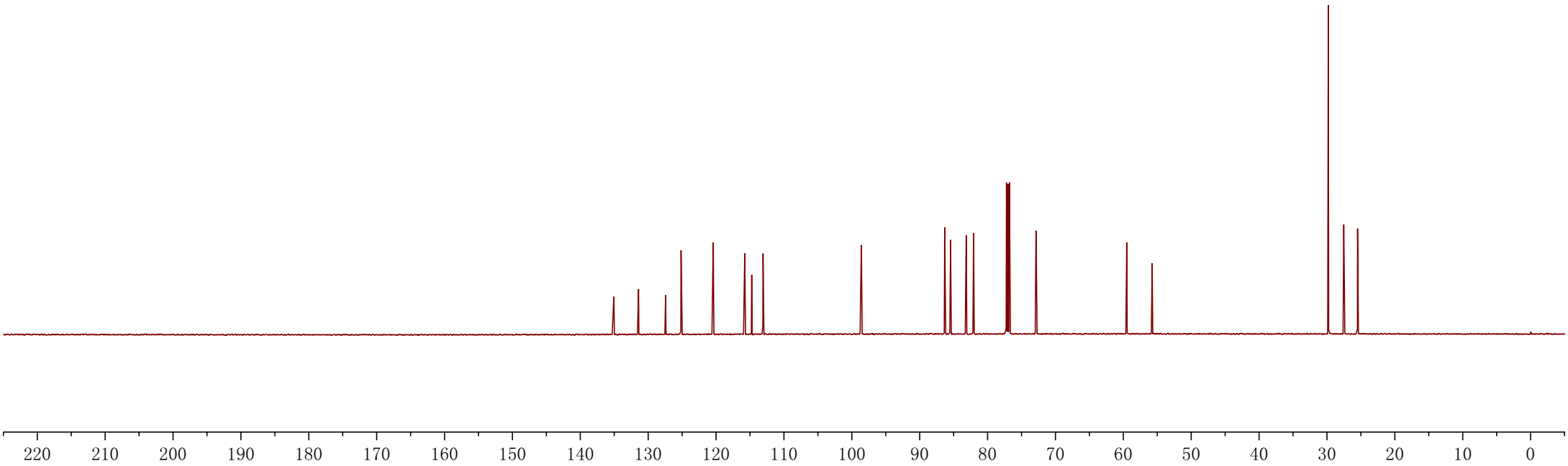

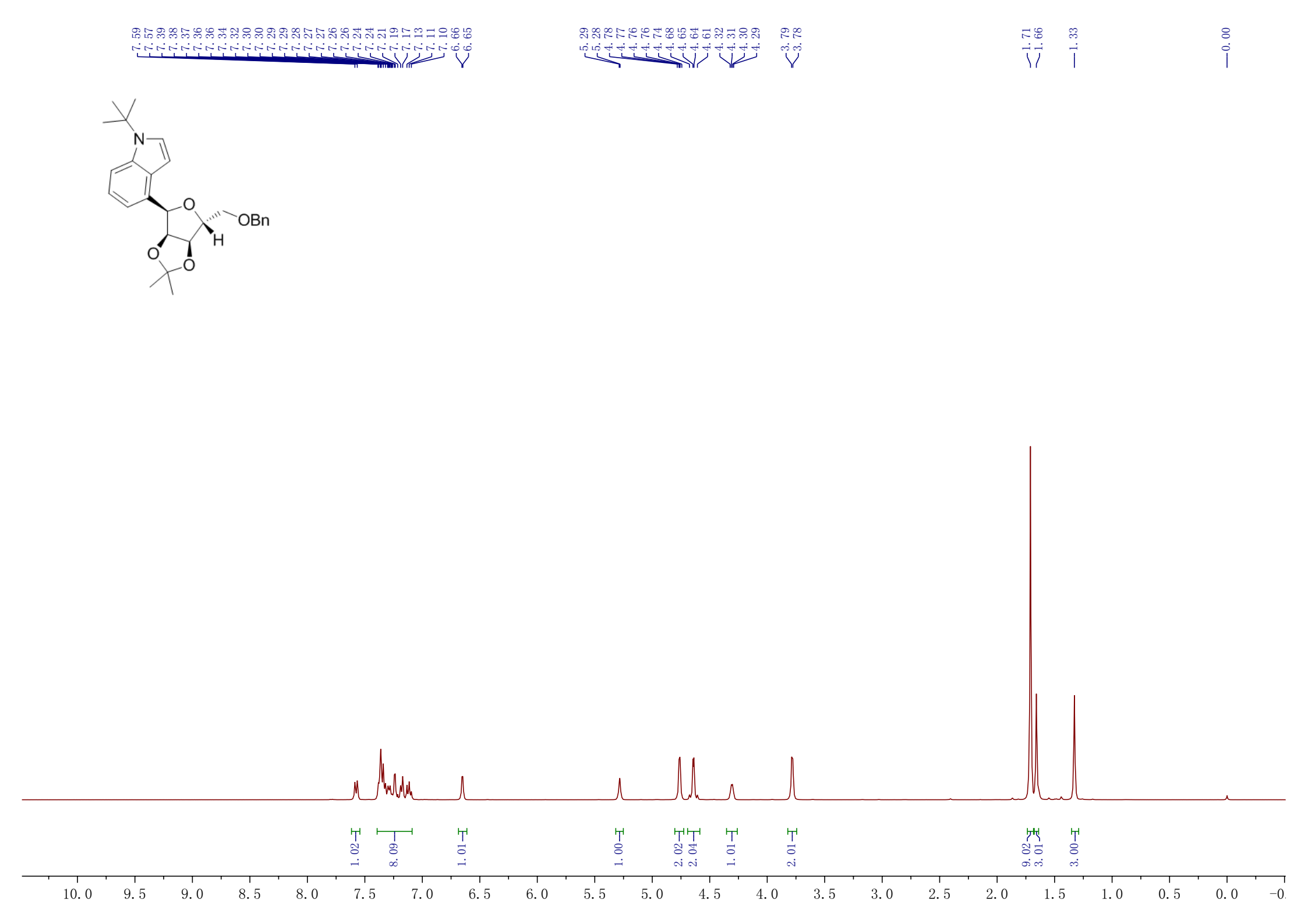
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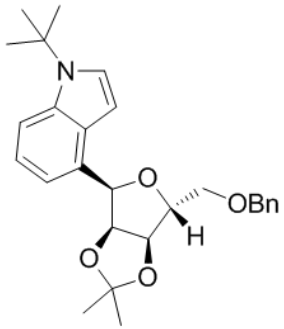

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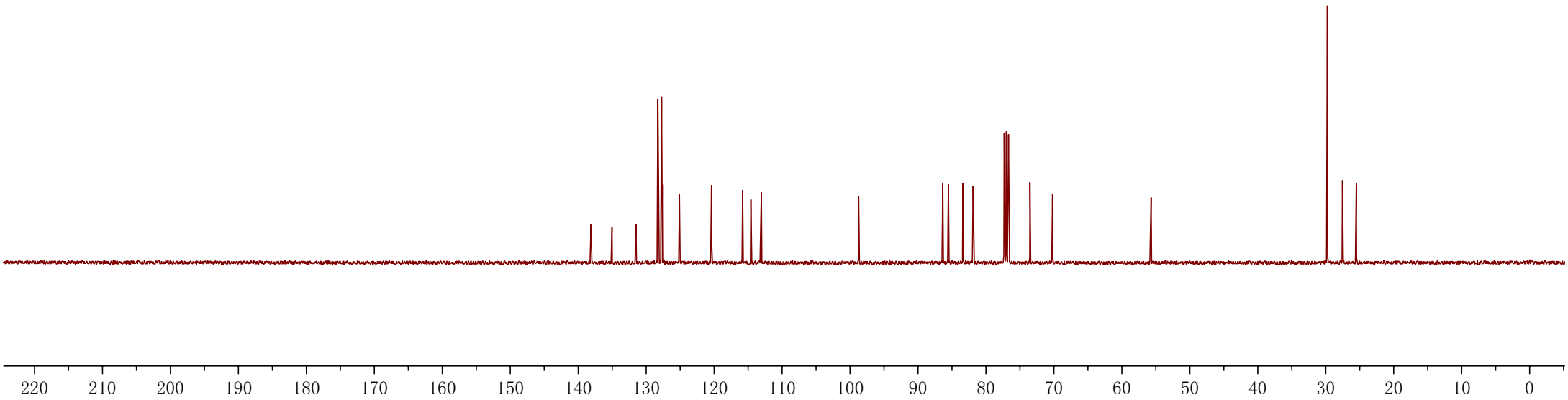

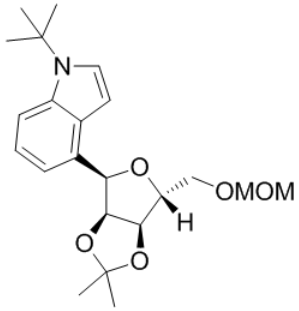

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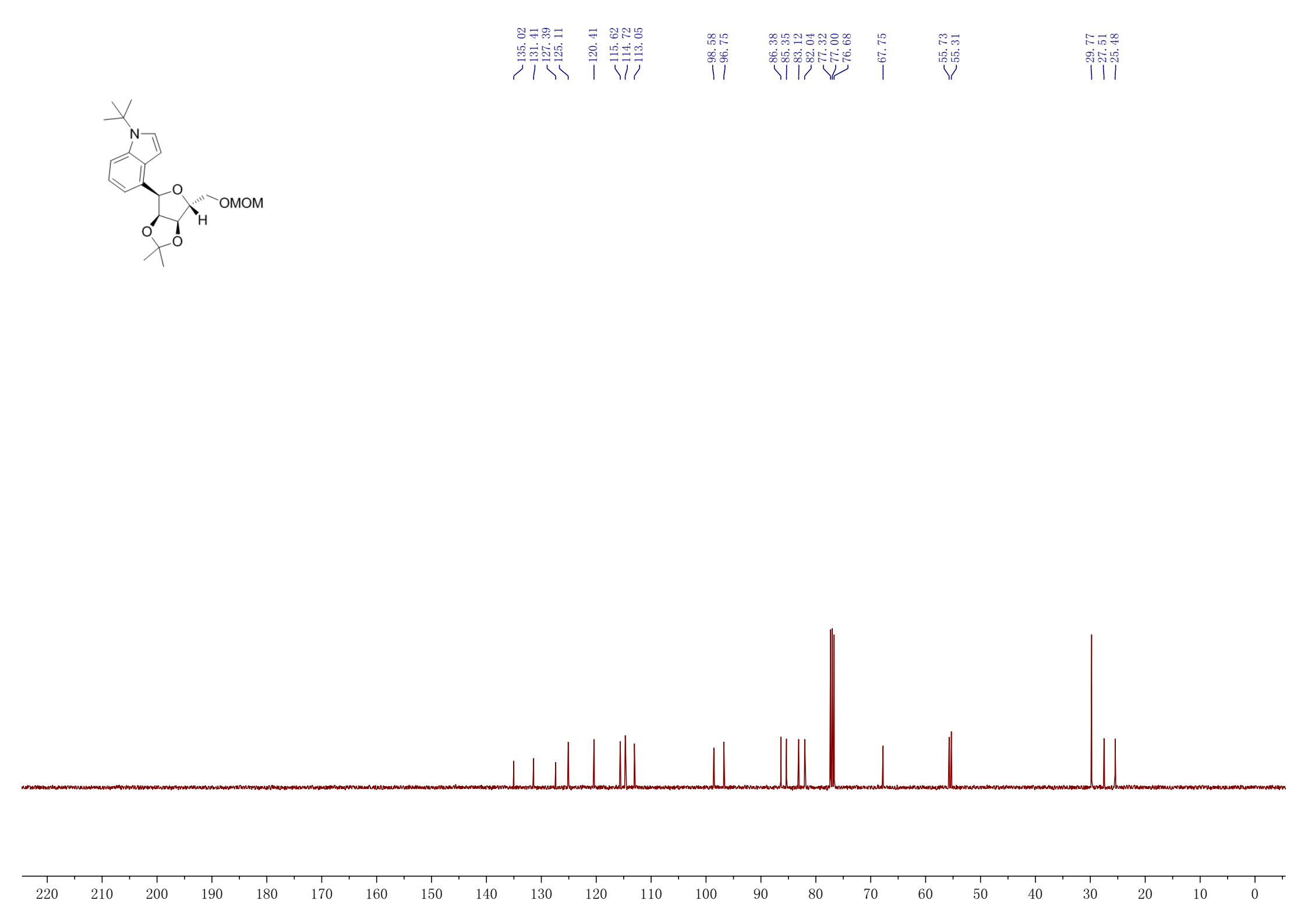
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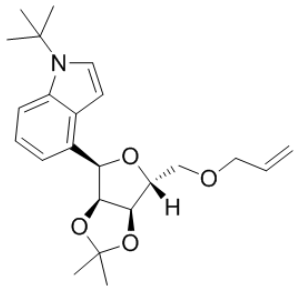
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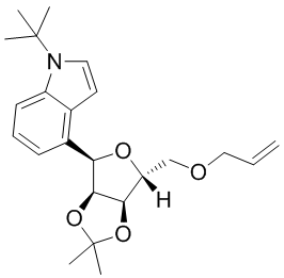

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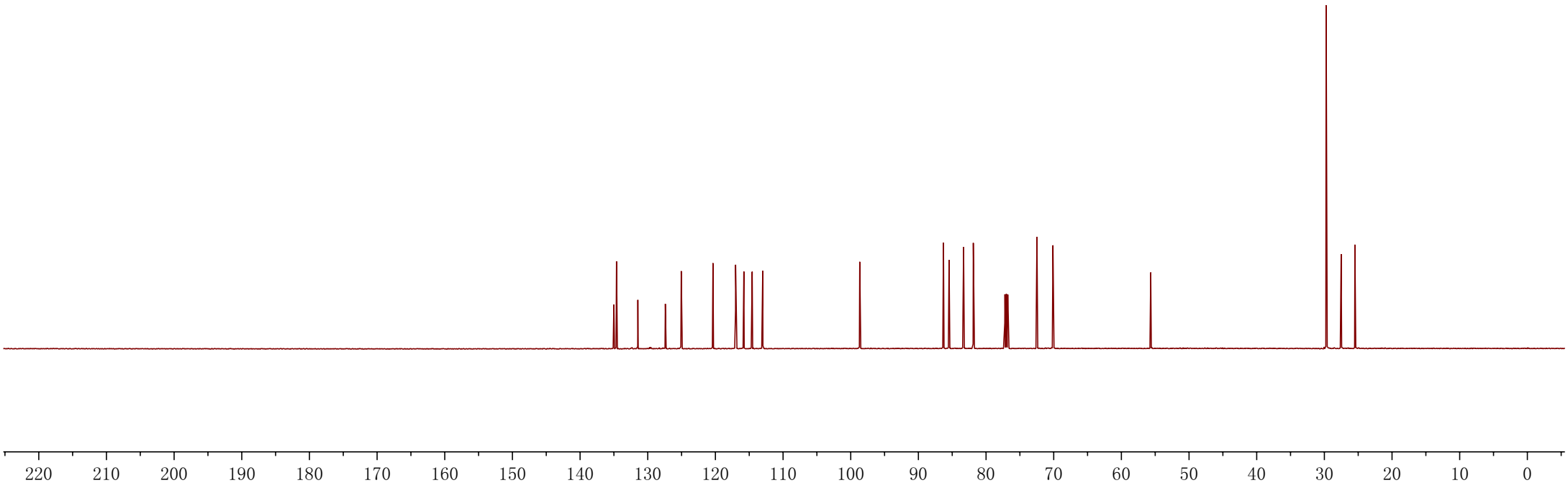

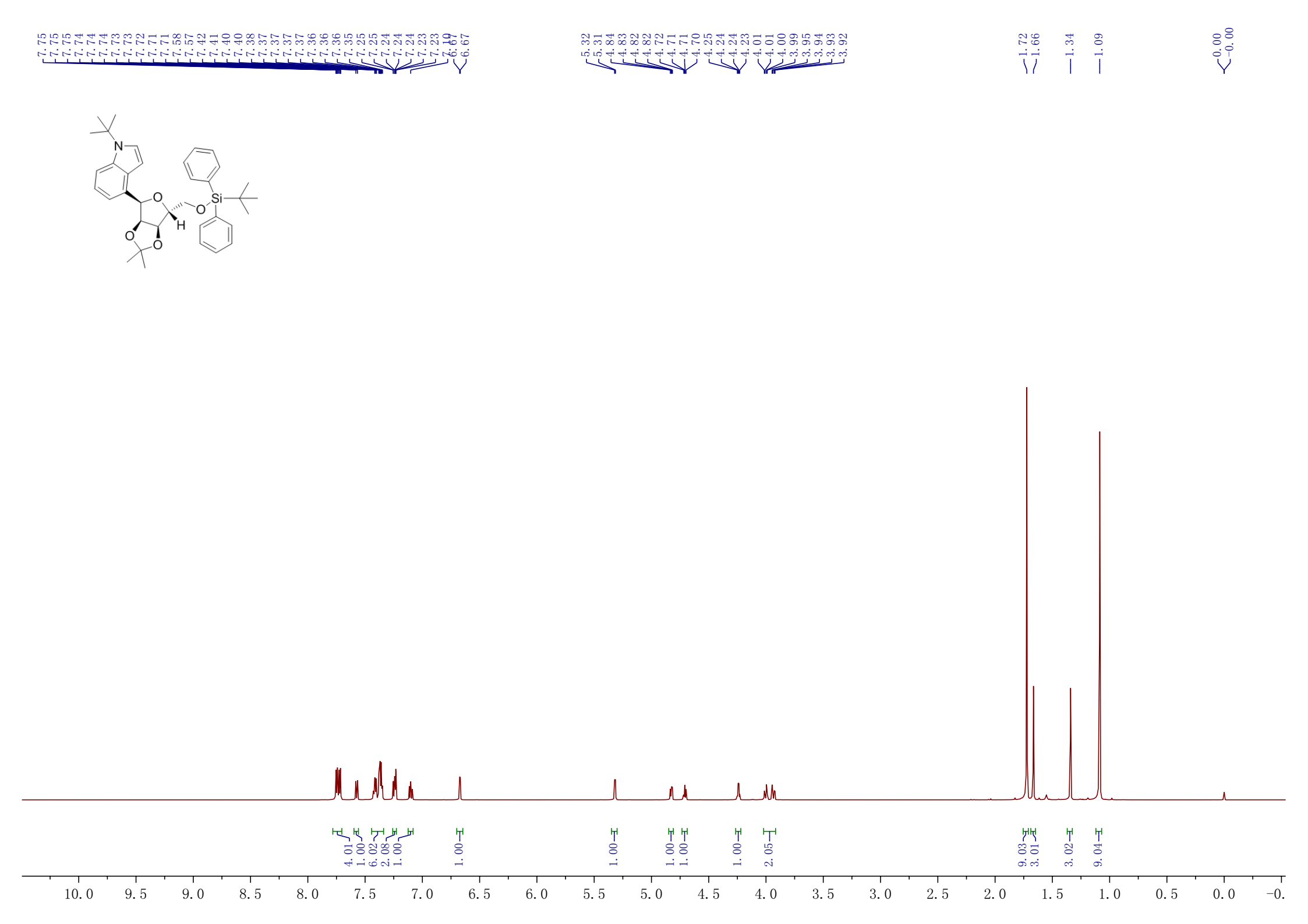
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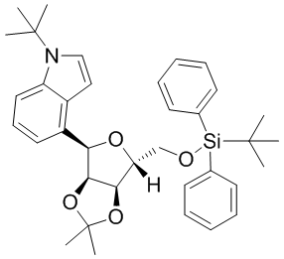

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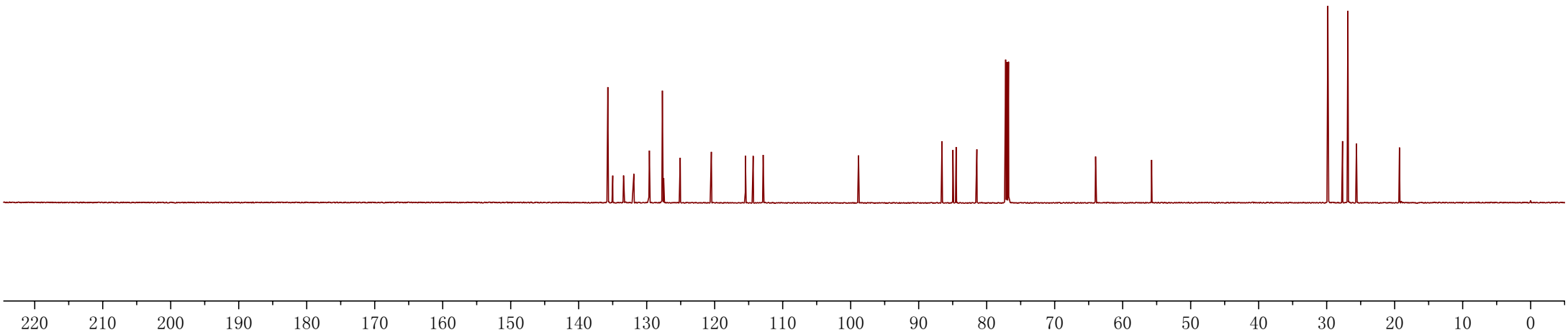

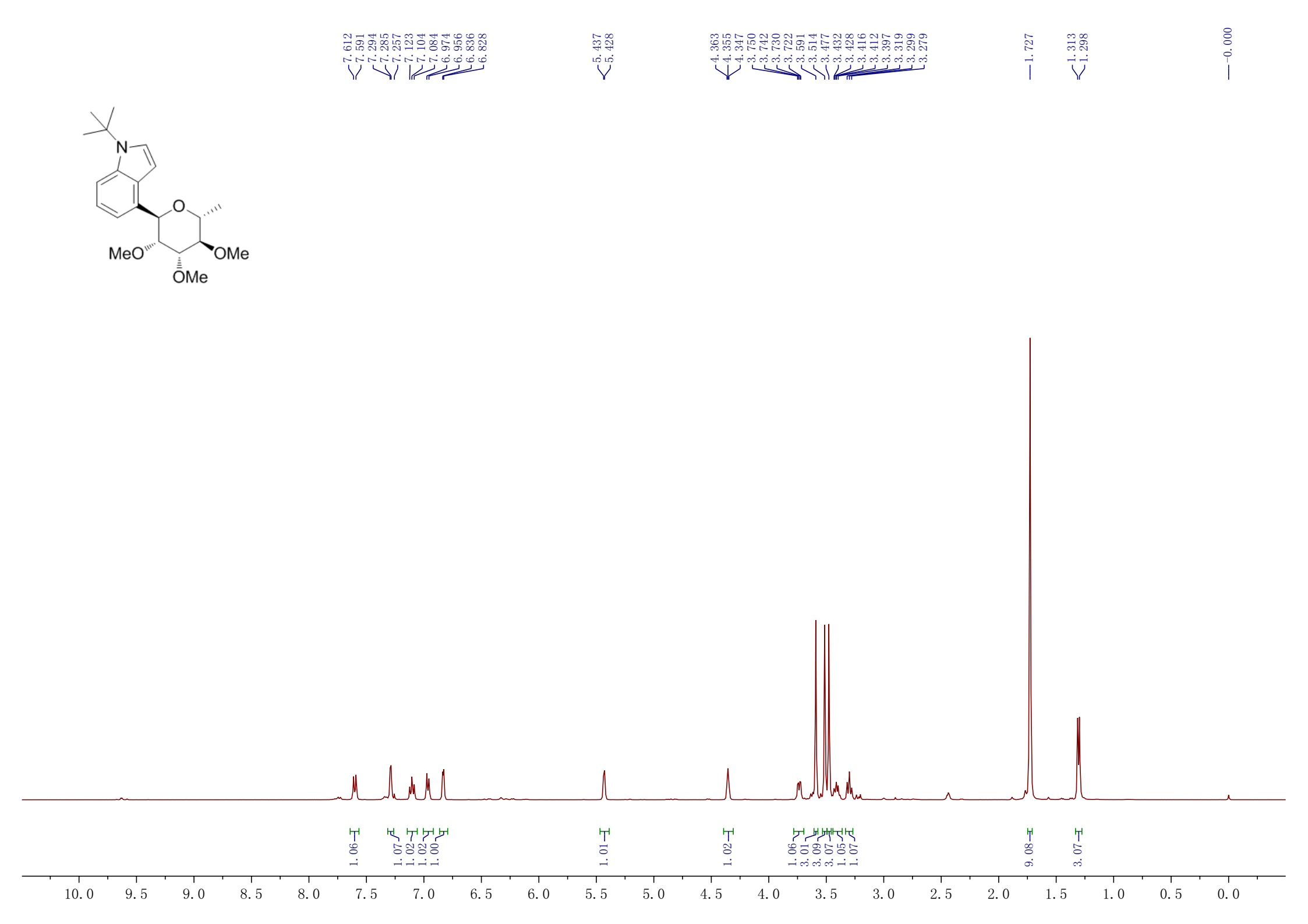
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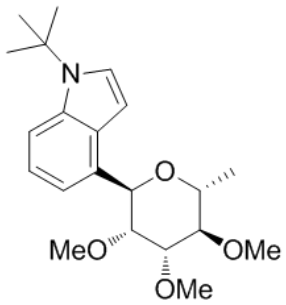

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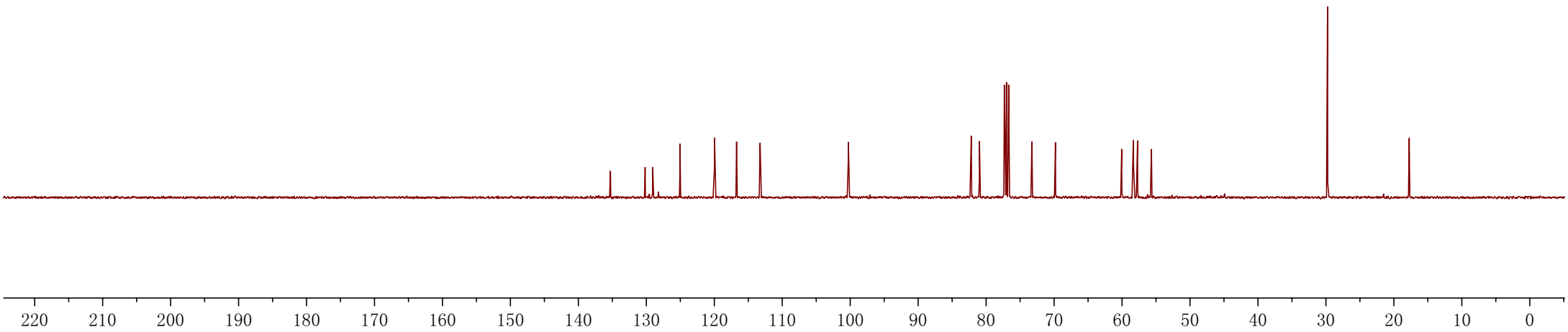

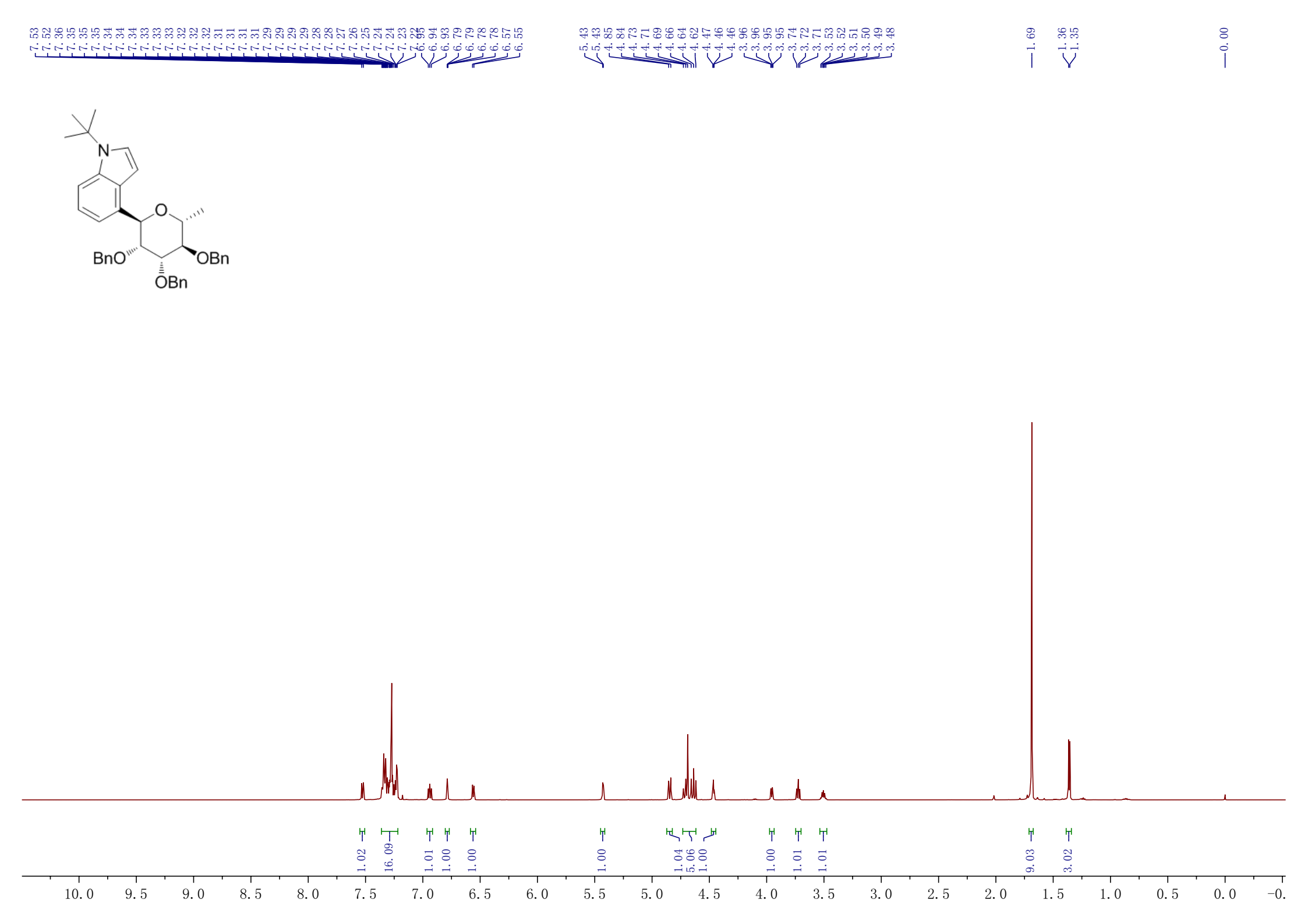
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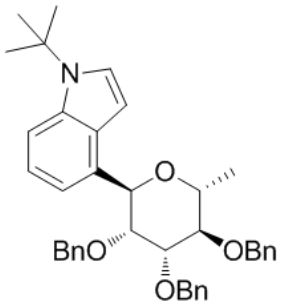

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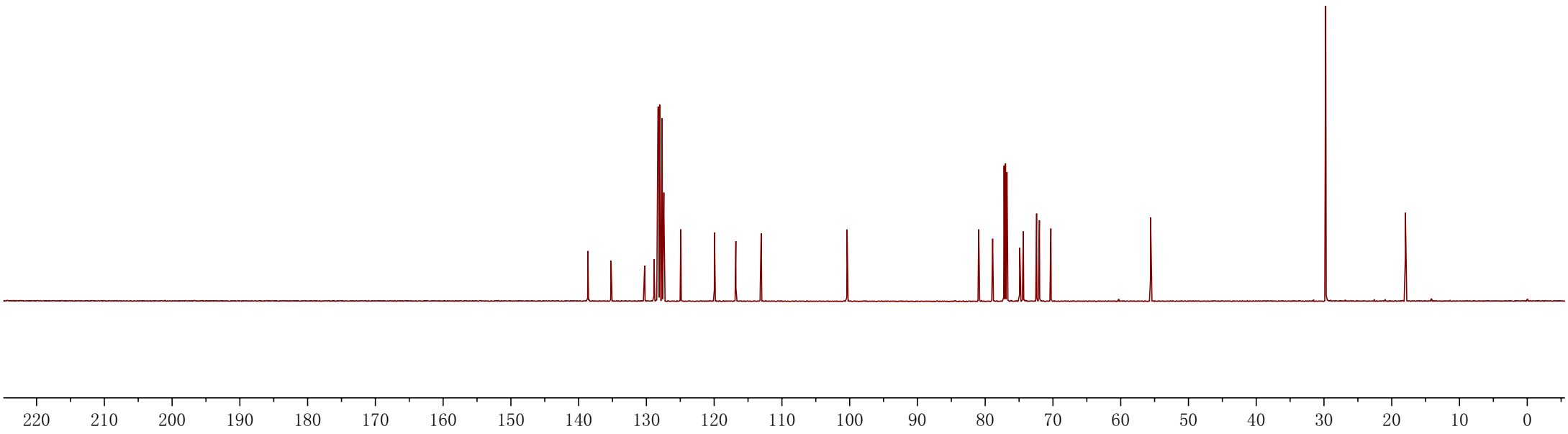

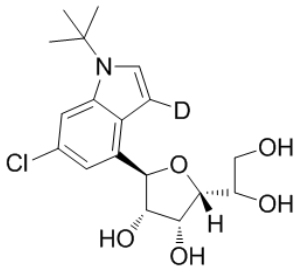

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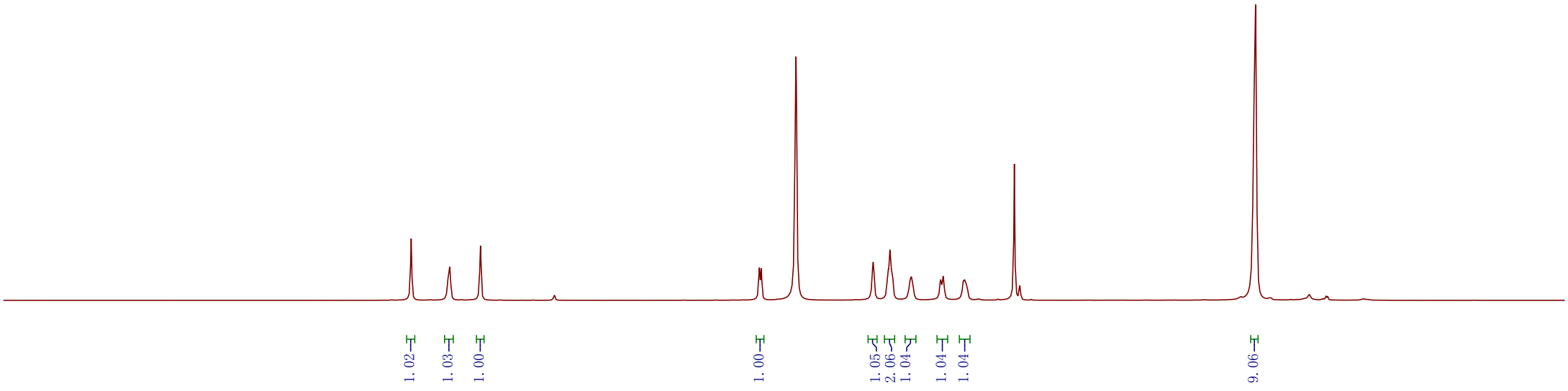

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1.04
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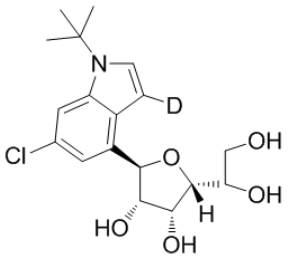

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100.08
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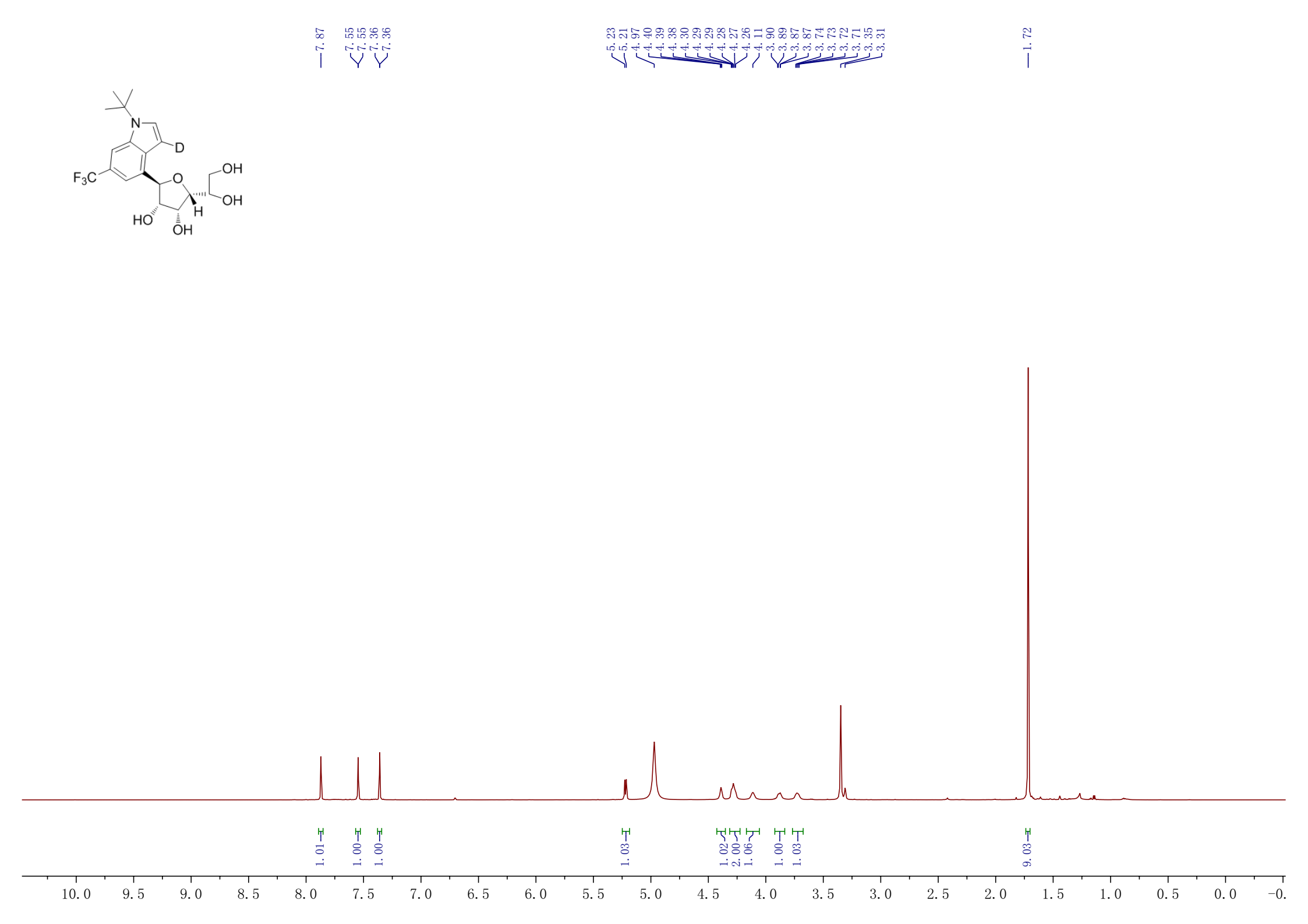
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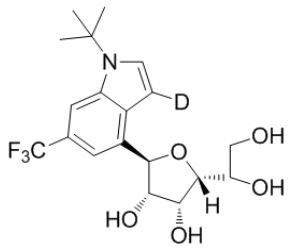

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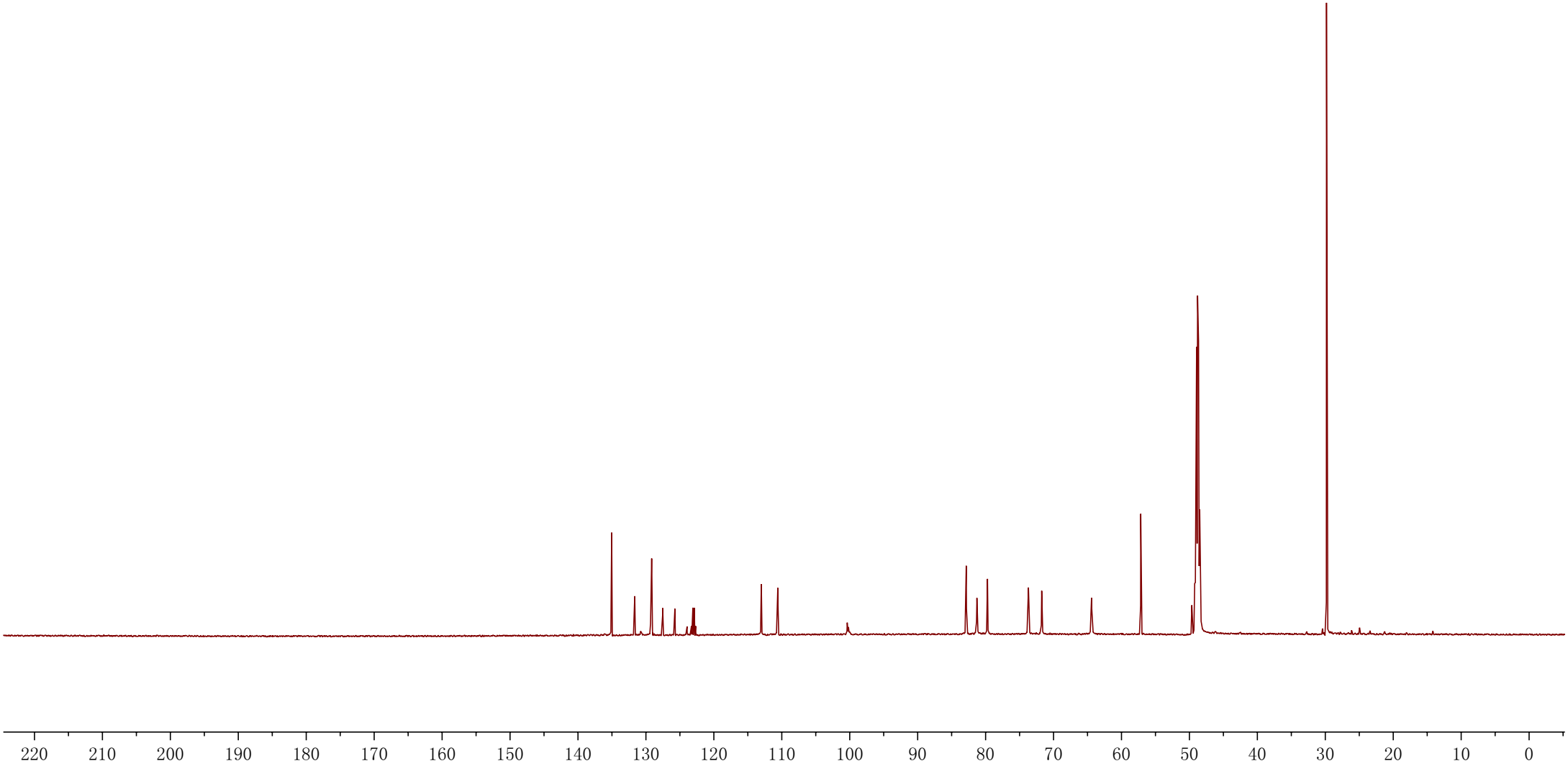

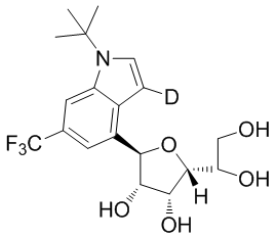

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S10. Reference

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