Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for:

Nickel-Catalyzed Intermolecular Carboiodination of Alkynes with Aryl Iodides

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1 Instrumentation and Chemicals

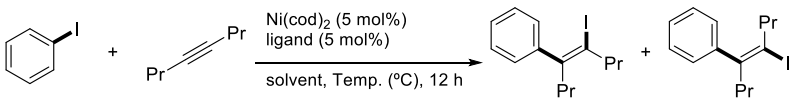
All manipulations of oxygen- and moisture-sensitive materials were conducted in a glove box filled with N_2 or with a standard Schlenk technique under a purified argon atmosphere. Nuclear magnetic resonance spectra were taken on Varian UNITY INOVA 500 (^{1}H, 500 MHz; ^{13}C, 125.7 MHz) spectrometer using tetramethylsilane (^{1}H) as an internal standard. ^{1}H NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, sept = septet, br = broad, m = multiplet), coupling constants (Hz), integration, and identification. GC-MS analyses and High-resolution mass spectra were obtained with a JEOL JMS-700 spectrometer by electron ionization at 70 eV. Infrared spectra (IR) spectra were determined on a SHIMADZU FTIR-8200PC spectrometer. Melting points were determined using a YANAKO MP-500D. EPR spectra were measured with a JEOL JES-FA1000. TLC analyses were performed by means of Merck Kieselgel 60 F_{254} (0.25 mm) Plates. Visualization was accomplished with UV light (254 nm) and/or an aqueous alkaline $KMnO_4$ solution followed by heating. Flash column chromatography was carried out using Kanto Chemical silica gel (spherical, 40–50 mm). Unless otherwise noted, commercially available reagents were used without purification. Toluene was purchased from Wako Pure Chemical Co. stored in the glove box. Bis(1,5-cyclooctadiene)nickel was purchased from Strem Chemicals, Inc. Ligands **L2** and **L8** were synthesized according to the reported methods.[1,2]

[1] **L2**: H. Li, J. Oppenheimer, M. R. Smith III, E. Robert, R. E. Maleczka Jr, *Tetrahedron Lett*. **2016**, *57*, 2231-2232.

[2] **L8**: G. Altenhoff, R. Goddard, C. W. Lehmann, F. Glorius, *J. Am. Chem. Soc*. **2004**, *126*, 15195-15201.

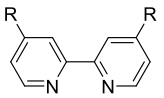
2 Optimization of Reaction Conditions

Table S1. Addtitonal optimization of reaction condition

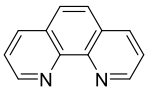


1a **2a** (*Z*)-**3aa** (*E*)-**3aa**

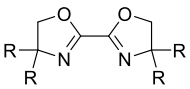
Entry	Ligand	Solvent	Temp. (°C)	Yield (%)	*Z*/*E*
1	**L1**	toluene	50	92	2/1
2	**L2**	toluene	50	60	1/1
3	**L3**	toluene	50	54	1/1
4	**L4**	toluene	50	52	1/1
5	**L5**	toluene	50	7	1/2
6	**L6**	toluene	50	25	2/1
7	**L7**	toluene	50	<5	1/1
8	**L8**	toluene	50	7	1/15
9	**L9**	toluene	50	<5	2/1
10	IPr	toluene	50	<1	–
11	PMe_3	toluene	50	<1	–
12	PCy_3	toluene	50	<1	–
13	dppe	toluene	50	<1	–
14	**L1**	1,4-dioxane	50	35	1/2
15	**L1**	toluene	110	66	1/2
16	**L1**	toluene	25	14	1/1



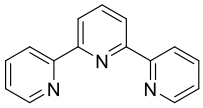
L1: dtbpy (R=*t*Bu)
L2: dCF_3bpy (R=CF_3)
L3: bpy (R=H)
L4: dPhbpy (R=Ph)
L5: dMeObpy (R=OMe)



L6: phen

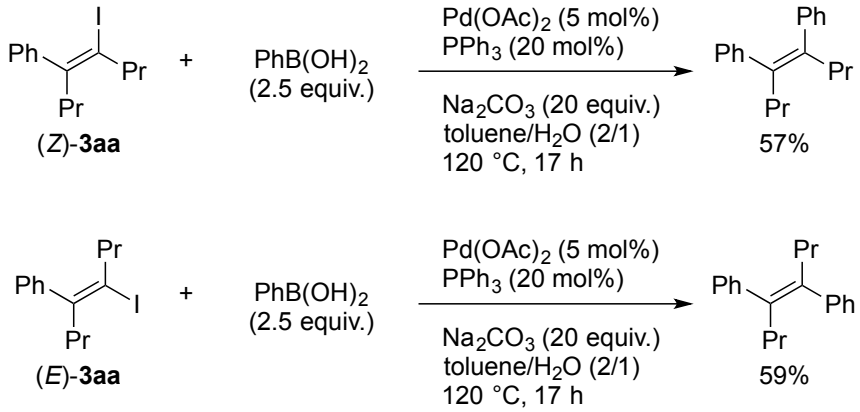


L7: Biox (R=H)
L8: $BioxMe_4$ (R=Me)



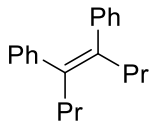
L9: terpy

3 Stereochemical Characterization of Alkenyl Iodide 3aa



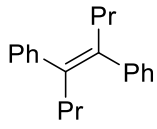
In a 50 mL round-bottom flask, 1 mmol of (*Z*)-**3aa** or (*E*)-**3aa** (50 mM in toluene) was added to a solution of phenylboronic acid (2.5 mmol), palladium(II) acetate (0.05 mmol), triphenylphosphine (0.2 mmol) and Na_2CO_3 (20 mmol) in water (10 mL) under Ar. The mixture was refluxed for 17 h. After cooled to room temperature, the precipitate was washed with water, and the aqueous layer was extracted with ethyl acetate. The organic layer was dried over Na_2SO_4, and evaporated under reduced pressure. The residue was purified by silica gel column chromatography.

(*Z*)-Oct-4-ene-4,5-diyldibenzene: CAS RN [84224-51-1]



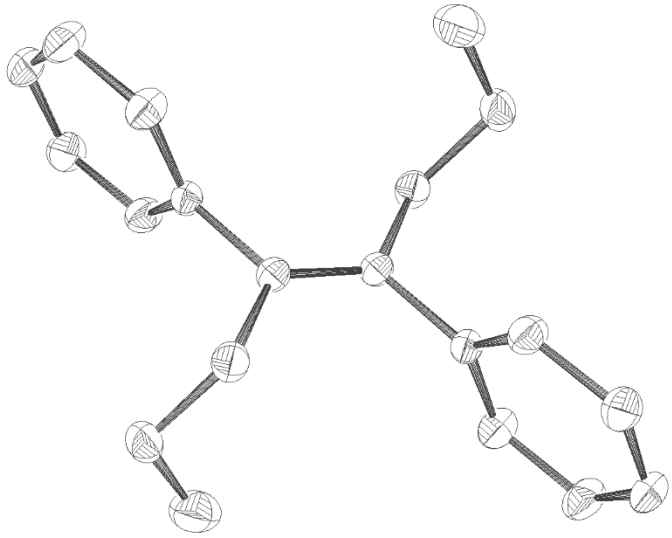
Yield: 57%, white solid. Mp: 39-41 °C. TLC: R_f 0.33 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.06-7.03 (m, 4H; Ar-H), 7.00-6.97 (m, 2H; Ar-H), 6.94-6.91 (m, 4H; Ar-H), 2.54 (dd, *J* =7.5 Hz, 4H; $2CH_2$), 1.39-1.31 (m, 4H; $2CH_2$), 0.91 (t, *J* = 6.5 Hz, 6H; $2CH_3$). ^{13}C NMR ($CDCl_3$) δ 143.8, 138.6, 130.0, 127.5, 125.6, 36.5, 21.8, 14.1. IR (KBr): 2959, 2870, 1441 cm^{-1}. MS *m/z* (%): 265/264 (11/54) $[M]^+$, 91 (100). HRMS (EI) Calcd for $C_{20}H_{24}$: $[M]^+$ (264.1878), found 264.1873.

(*E*)-Oct-4-ene-4,5-diyldibenzene: CAS RN [112068-01-6]



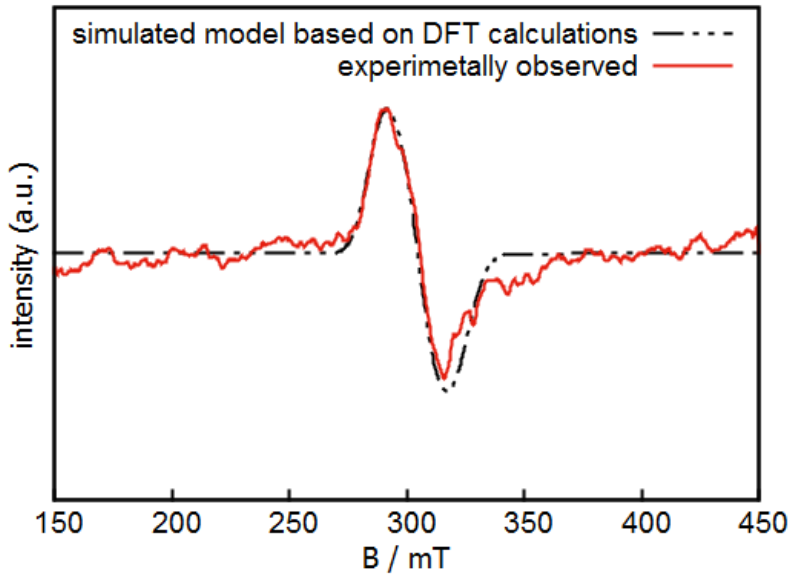
Yield: 59%, white solid. Mp: 88-91 °C. TLC: R_f 0.42 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.37-7.34 (m, 4H; Ar-H), 7.27-7.24 (m, 2H; Ar-H), 7.21-7.19 (m, 4H; Ar-H), 2.11 (dd, *J* =7.5 Hz, 4H; $2CH_2$), 1.21-1.14 (m, 4H; $2CH_2$), 0.69 (t, *J* = 7.5 Hz, 6H; $2CH_3$). ^{13}C NMR ($CDCl_3$) δ 143.2, 138.5, 129.0, 128.1, 126.3, 37.6, 21.6, 14.0. IR (KBr): 2957, 2869, 1440 cm^{-1}. MS *m/z* (%): 265/264 (14/67) $[M]^+$, 91 (100). HRMS (EI) Calcd for $C_{20}H_{24}$: $[M]^+$ (264.1878), found 264.1877.

ORTEP Drawing of (*E*)-Oct-4-ene-4,5-diyldibenzene (CCDC: 1847370)



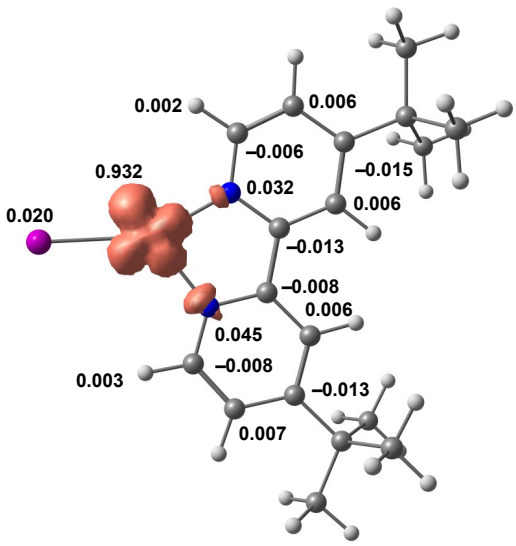
Empirical Formula	$C_{20}H_{24}$
Formula Weight	264.41
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.540 X 0.370 X 0.280 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 11.597(1) Å b = 5.737(5) Å c = 12.14(1) Å β = 94.750(1) ° V = 805(1) Å3
Space Group	$P2_1/n$ (#14)
Z value	2
D_{calc}	1.091 g/cm^3
F_{000}	288.00
μ(MoKα)	0.608 cm^{-1}

4 EPR Spectra of Reaction Mixtures



EPR merged-spectrum of reaction mixtures: standard reaction conditions: $Ni(cod)_2$ (0.025 mmol), dtbpy (0.025 mmol), 4-octyne (0.75 mmol), iodobenzene (0.5 mmol) in toluene (1 mL). EPR experimental parameters (toluene, 77 K): Microwave frequency: 9.092 GHz, power = 0.998 mW, modulation amplitude = 0.1 mT. EPR simulation parameters (isotropic): $g_{1,2,3}$ = 2.025, 2.128, 2.2455; *g*-strain = 0.11, 0.11, 0.11; *A* (Ni, N, N, H, H) = –107, 35, 19, 5, 5 MHz, ; *A*-strain = 2.2, 0.2, 1.3; RMSD of fit = 0.087.

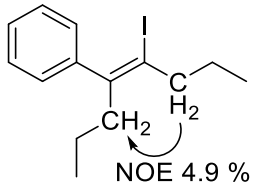
Mulliken Spin Density Plot of Ni(I)I/dtbpy 4



5 Experimental Procedure and Characterization Data for Products

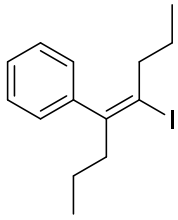
General procedure. To a screw cap vial, an alkyne (0.75 mmol) was added to a solution of bis(1,5-dicyclooctadiene)nickel (0.025 mmol) and 4,4'-di-*tert*-butyl-2,2'-dipyridil (0.025 mmol) in dry toluene (1.0 ml) in a glove box, followed by an aryl iodide (0.5 mmol). The vial was sealed and stirred for 12 h at 50 °C. The reaction mixture was passed through a short silica gel pad, and concentrated in vacuo. The crude product was purified by silica gel column chromatography with given eluent.

(*Z*)-(5-Iodooct-4-en-4-yl)benzene ((*Z*)-3aa).



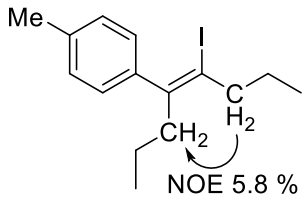
Yield: 42%, colorless oil. TLC: R_f 0.67 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.35-7.32 (m, 2H; Ar-H), 7.29-7.26 (m, 1H; Ar-H), 7.08-7.06 (m, 2H; Ar-H), 2.66 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.45 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.70-1.62 (m, 2H; CH_2), 1.35-1.29 (m, 2H; CH_2), 1.00 (t, *J* = 7.5 Hz, 3H; CH_3), 0.89 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 147.8, 147.5, 128.5, 128.2, 127.0, 106.5, 43.1, 36.9, 23.2, 21.6, 13.9, 13.2. IR (neat): 2959, 2971, 1456, 1113 cm^{-1}. MS *m/z* (%): 315/314 (9/50) $[M]^+$, 105 (55), 91 (100); HRMS (APCI) Calcd for $C_{14}H_{20}I^+$: $[M+H]^+$ (315.0604), found 315.0594.

(*E*)-(5-Iodooct-4-en-4-yl)benzene ((*E*)-3aa).



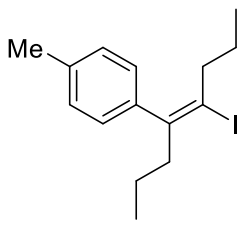
Yield: 39%, colorless oil. TLC: R_f 0.47 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.34-7.31 (m, 2H; Ar-H), 7.27-7.24 (m, 1H; Ar-H), 7.07-7.05 (m, 2H; Ar-H), 2.53 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.24 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.51-1.47 (m, 2H; CH_2), 1.36-1.31 (m, 2H; CH_2), 0.90 (t, *J* = 7.5 Hz, 3H; CH_3), 0.75 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.4, 140.9, 128.4, 128.3, 127.0, 108.5, 47.1, 43.8, 23.6, 20.6, 13.9, 13.0. IR (neat): 2959, 2971, 1457, 1112 cm^{-1}. MS *m/z* (%): 315/314 (7/45) $[M]^+$, 105 (52), 91 (100); HRMS (APCI) Calcd for $C_{14}H_{20}I^+$: $[M+H]^+$ (315.0604), found 315.0598.

(*Z*)-1-(5-Iodooct-4-en-4-yl)-4-methylbenzene ((*Z*)-3ba).



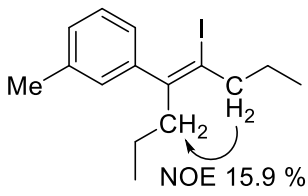
Yield: 45%, colorless oil. TLC: R_f 0.55 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.16-7.14 (m, 2H; Ar-H), 6.98-6.96 (m, 2H; Ar-H), 2.65 (dd, *J* = 7.0 Hz, 2H; CH_2), 2.43 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.36 (s, 3H; CH_3), 1.68-1.63 (m, 2H; CH_2), 1.34-1.30 (m, 2H; CH_2), 0.99 (t, *J* = 7.5 Hz, 3H; CH_3), 0.87 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 147.4, 144.9, 136.7, 128.9, 128.3, 106.4, 43.2, 36.9, 23.2, 21.6, 21.4, 13.9, 13.2. IR (neat): 2960, 1507, 1457, 1113 cm^{-1}. MS *m/z* (%):329/328 (5/43) $[M]^+$, 105 (100). HRMS (APCI) Calcd for $C_{15}H_{22}I^+$: $[M+H]^+$ (329.0761), found 329.0751.

(*E*)-1-(5-Iodooct-4-en-4-yl)-4-methylbenzene ((*E*)-3ba).



Yield: 36%, colorless oil. TLC: R_f 0.69 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.14-7.12 (m, 2H; Ar-H), 6.96-6.94 (m, 2H; Ar-H), 2.52 (dd, *J* = 7.0 Hz, 2H; CH_2), 2.35 (s, 3H; CH_3), 2.26 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.49-1.46 (m, 2H; CH_2), 1.37-1.29 (m, 2H; CH_2), 0.89 (t, *J* = 7.0 Hz, 3H; CH_3), 0.76 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.3, 137.9, 136.6, 129.1, 128.1, 108.3, 47.2, 43.8, 23.6, 21.3, 20.7, 13.9, 13.0. IR (neat): 2960, 1507, 1457 cm^{-1}. MS *m/z* (%):329/328 (6/38) $[M]^+$, 105 (100). HRMS (APCI) Calcd for $C_{15}H_{22}I^+$: $[M+H]^+$ (329.0761), found 329.0753.

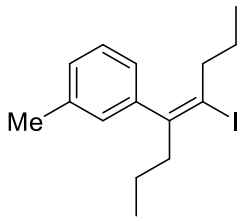
(*Z*)-1-(5-Iodooct-4-en-4-yl)-3-methylbenzene ((*Z*)-3ca).



Yield: 49%, colorless oil. TLC: R_f 0.72 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.22 (t, *J* = 7.5 Hz, 1H; Ar-H), 7.10-7.07 (m, 1H; Ar-H), 6.88-6.85 (m, 2H; Ar-H), 2.65 (dd, *J* = 7.0 Hz, 2H; CH_2), 2.43 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.35 (s, 3H; CH_3), 1.69-1.62 (m, 2H; CH_2), 1.36-1.29 (m, 2H; CH_2), 1.00 (t, *J* = 7.5 Hz, 3H; CH_3), 0.87 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ147.8, 147.6, 137.8, 129.0, 128.1, 127.8,

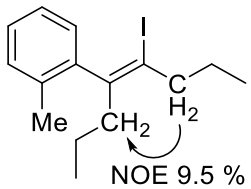
125.6, 106.3, 43.1, 36.9, 23.2, 21.7, 21.6, 13.9, 13.2. IR (neat): 2960, 1560, 1457 cm^{-1}. MS *m/z* (%): 329/328 (6/40) $[M]^+$, 105 (100). HRMS (APCI) Calcd for $C_{15}H_{22}I^+$: $[M+H]^+$ (329.0761), found 329.0755.

(*E*)-1-(5-Iodooct-4-en-4-yl)-3-methylbenzene ((*E*)-3ca).



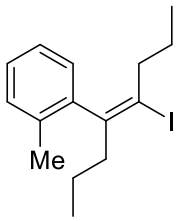
Yield: 22%, colorless oil. TLC: R_f 0.86 (hexane). ^1H NMR ($CDCl_3$) δ 7.20 (t, *J* = 7.5 Hz, 1H; Ar-H), 7.08-7.06 (m, 1H; Ar-H), 6.88-6.84 (m, 2H; Ar-H), 2.52 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.35 (s, 3H; CH_3), 2.25 (dd, *J* = 7.0 Hz, 2H; CH_2), 1.52-1.46 (m, 2H; CH_2), 1.38-1.31 (m, 2H; CH_2), 0.90 (t, *J* = 7.5 Hz, 3H; CH_3), 0.76 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.5, 140.9, 138.0, 128.9, 128.2, 127.7, 125.4, 108.3, 47.1, 43.8, 23.6, 21.6, 20.7, 13.9, 13.0. IR (neat): 2960, 1559, 1507, 1457 cm^{-1}. MS *m/z* (%): 329/328 (6/42) $[M]^+$, 105 (100). HRMS (APCI) Calcd for $C_{15}H_{22}I^+$: $[M+H]^+$ (329.0761), found 329.0757.

(*Z*)-1-(5-Iodooct-4-en-4-yl)-2-methylbenzene ((*Z*)-3da).



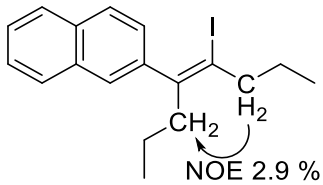
Yield: 59%, colorless oil. TLC: R_f 0.66 (hexane). ^1H NMR ($CDCl_3$) δ 7.20-7.15 (m, 2H; Ar-H), 6.90-6.89 (m, 2H; Ar-H), 2.75-2.18 (m, 2H; CH_2), 2.63-2.52 (m, 2H; CH_2), 2.21 (s, 3H; CH_3), 1.70-1.63 (m, 2H; CH_2), 1.59-1.31 (m, 2H; CH_2), 1.01 (t, *J* = 7.0 Hz, 3H; CH_3), 0.89 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 147.3, 146.9, 134.7, 130.3, 128.6, 127.2, 125.7, 107.8, 42.6, 36.3, 23.2, 21.5, 19.4, 14.2, 13.2. IR (neat): 2960, 1560, 1507, 1457 cm^{-1}. MS *m/z* (%): 329/328 (7/48) $[M]^+$, 105 (100). HRMS (APCI) Calcd for $C_{15}H_{22}I^+$: $[M+H]^+$ (329.0761), found 329.0751.

(*E*)-1-(5-Iodooct-4-en-4-yl)-2-methylbenzene ((*E*)-3da).



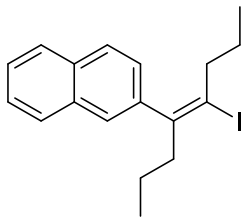
Yield: 32%, colorless oil. TLC: R_f 0.87 (hexane). ^1H NMR ($CDCl_3$) δ 7.19-7.11 (m, 2H; Ar-H), 6.92-6.91 (m, 2H; Ar-H), 2.56-2.27 (m, 2H; CH_2), 2.18-2.11 (m, 2H; CH_2), 2.18 (s, 3H; CH_3), 1.49-1.44 (m, 2H; CH_2), 1.39-1.33 (m, 2H; CH_2), 0.91 (t, *J* = 7.0 Hz, 3H; CH_3), 0.73 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ145.6, 140.2, 135.1, 130.3, 128.9, 127.2, 125.6, 108.1, 46.2, 43.5, 23.2, 20.5, 19.6, 14.2, 13.1. IR (neat): 2960, 1559, 1507, 1457 cm^{-1}. MS *m/z* (%): 329/328 (6/42) $[M]^+$, 105 (100). HRMS (APCI) Calcd for $C_{15}H_{22}I^+$: $[M+H]^+$ (329.0761), found 329.0754.

(*Z*)-2-(5-Iodooct-4-en-4-yl)naphthalene ((*Z*)-3ea).



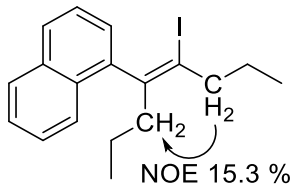
Yield: 53%, colorless oil. TLC: R_f 0.54 (hexane). ^1H NMR ($CDCl_3$) δ 7.85-7.82 (m, 3H; Ar-H), 7.54-7.45 (m, 3H; Ar-H), 7.24-7.22 (m, 1H; Ar-H), 2.72 (t, *J* = 7.5 Hz, 2H; CH_2), 2.54 (t, *J* = 7.5 Hz, 2H; CH_2), 1.74-1.66 (m, 2H; CH_2), 1.37-1.33 (m, 2H; CH_2), 1.04 (t, *J* = 7.5 Hz, 3H; CH_3), 0.88 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 147.4, 145.2, 133.5, 143.6, 128.2, 127.9, 127.8, 127.2, 127.0, 126.1, 106.8, 43.2, 37.0, 23.2, 21.7, 13.9, 13.2. IR (neat): 2958, 2870, 1597, 1457, 1107 cm^{-1}. MS *m/z* (%): 365/364 (12/63) $[M]^+$, 141 (100). HRMS (APCI) Calcd for $C_{18}H_{22}I^+$: $[M+H]^+$ (365.0761), found 365.0753.

(*E*)-2-(5-Iodooct-4-en-4-yl)naphthalene ((*E*)-3ea).



Yield: 25%, colorless oil. TLC: R_f 0.68 (hexane). ^1H NMR ($CDCl_3$) δ 7.85-7.80 (m, 3H; Ar-H), 7.52-7.46 (m, 3H; Ar-H), 7.22-7.20 (m, 1H; Ar-H), 2.62 (t, *J* = 8.0 Hz, 2H; CH_2), 2.30 (t, *J* = 7.5 Hz, 2H; CH_2), 1.54-1.48 (m, 2H; CH_2), 1.42-1.35 (m, 2H; CH_2), 0.91 (t, *J* = 7.5 Hz, 3H; CH_3), 0.74 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.3, 138.4, 133.4, 132.5, 128.1, 128.0, 127.9, 126.9, 126.8, 126.4, 126.1, 108.9, 47.1, 43.9, 23.6, 20.7, 13.9, 13.0. IR (neat): 2958, 2869, 1596, 1456, 1113 cm^{-1}. MS *m/z* (%): 365/364 (10/57) $[M]^+$, 141 (100). HRMS (APCI) found Calcd for $C_{18}H_{22}I^+$: $[M+H]^+$ (365.0761), 365.0754.

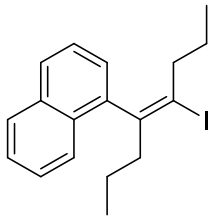
(*Z*)-1-(5-Iodooct-4-en-4-yl)naphthalene ((*Z*)-3fa).



Yield: 48%, colorless oil. TLC: R_f 0.51 (hexane). ^1H NMR ($CDCl_3$) δ 7.88-7.78 (m, 3H; Ar-H), 7.49-7.45 (m, 3H; Ar-H), 7.15-7.14 (m, 1H; Ar-H), 2.88-2.37 (m, 2H; CH_2), 2.77-2.66 (m, 2H; CH_2), 1.79-1.73 (m, 2H; CH_2), 1.45-1.32 (m, 2H; CH_2), 1.10 (t, *J* = 7.5 Hz, 3H; CH_3), 0.88 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 145.9, 145.3, 134.0, 130.4, 128.7, 127.4, 126.2, 125.9, 125.5, 125.5, 108.9, 42.9,

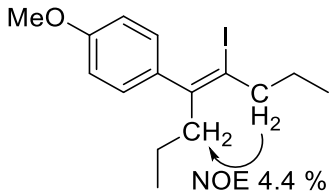
37.1, 23.4, 22.1, 14.1, 13.4. IR (neat): 2959, 2360, 1456, 1130 cm^{-1}. MS *m/z* (%): 365/364 (6/43) $[M]^+$, 165 (100), 153 (71). HRMS (APCI) Calcd for $C_{18}H_{22}I^+$: $[M+H]^+$ (365.0761), found 365.0757.

(*E*)-1-(5-Iodooct-4-en-4-yl)naphthalene ((*E*)-3fa).



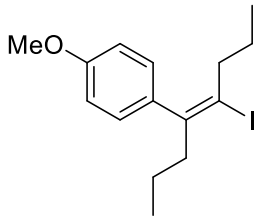
Yield: 19%, colorless oil. TLC: R_f 0.77 (hexane). ^1H NMR ($CDCl_3$) δ 7.87-7.76 (m, 3H; Ar-H), 7.49-7.42 (m, 3H; Ar-H), 7.14-7.13 (m, 1H; Ar-H), 2.74-2.44 (m, 2H; CH_2), 2.15-2.06 (m, 2H; CH_2), 1.46-1.41 (m, 2H; CH_2), 1.40-1.35 (m, 2H; CH_2), 0.89 (t, *J* = 7.5 Hz, 3H; CH_3), 0.65 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 144.5, 138.4, 134.0, 131.2, 128.5, 127.6, 126.3, 126.1, 125.8, 125.8, 125.4, 109.4, 46.9, 44.0, 23.4, 21.0, 14.1, 13.0. IR (neat): 2958, 2360, 1458, 1113 cm^{-1}. MS *m/z* (%): 365/364 (6/33) $[M]^+$, 165 (100), 153 (77). HRMS (APCI) Calcd for $C_{18}H_{22}I^+$: $[M+H]^+$ (365.0761), found 365.0756.

(*Z*)-1-(5-Iodooct-4-en-4-yl)-4-methoxybenzene ((*Z*)-3ga).



Yield: 47%, colorless oil. TLC: R_f 0.37 (hexane/ethyl acetate = 20/1). ^1H NMR ($CDCl_3$) δ 7.01-6.99 (m, 2H; Ar-H), 6.88-6.86 (m, 2H; Ar-H), 3.82, (s, 3H; OCH_3), 2.65 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.43 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.67 (m, 2H; CH_2), 1.34-1.29 (m, 2H; CH_2), 0.99 (t, *J* = 7.5 Hz, 3H; CH_3), 0.86 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 158.6, 147.1, 140.3, 129.6, 113.6, 106.8, 55.4, 43.3, 36.9, 23.2, 21.6, 13.9, 13.2. IR (neat): 2958, 1605, 1507, 1245 cm^{-1}. MS *m/z* (%): 345/344 (9/58) $[M]^+$, 121 (100). HRMS (APCI) Calcd for $C_{15}H_{22}IO^+$: $[M+H]^+$ (345.0710), found 345.0706.

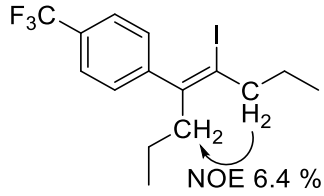
(*E*)-1-(5-Iodooct-4-en-4-yl)-4-methoxybenzene ((*E*)-3ga).



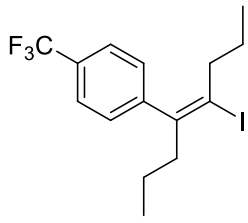
Yield: 23%, colorless oil. TLC: R_f 0.47 (hexane/ethyl acetate = 20/1). ^1H NMR ($CDCl_3$) δ 7.01-6.99 (m, 2H; Ar-H), 6.87-6.85 (m, 2H; Ar-H), 3.81, (s, 3H; OCH_3), 2.52 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.27 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.53-1.47 (m, 2H; CH_2), 1.35-1.31 (m, 2H; CH_2), 0.89 (t, *J* = 7.0 Hz, 3H; CH_3), 0.76 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 158.6, 146.0, 133.0, 129.3, 113.8, 108.4, 55.4, 47.2, 43.8, 23.6, 20.7, 13.9, 13.0. IR (neat): 2958, 1605, 1507, 1245 cm^{-1}. MS *m/z* (%): 345/344 (11/62) $[M]^+$, 121 (100). HRMS (APCI) Calcd for $C_{15}H_{22}IO^+$: $[M+H]^+$ (345.0710), found 345.0704.

(*Z*)-1-(5-Iodooct-4-en-4-yl)-4-(trifluoromethyl)benzene ((*Z*)-3ha).

Yield: 53%, colorless oil. TLC: R_f 0.59 (hexane). ^1H NMR ($CDCl_3$) δ 7.61-7.59 (m, 2H; Ar-H), 7.20-7.18 (m, 2H; Ar-H), 2.67 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.45 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.70-1.63 (m, 2H; CH_2), 1.33-1.27 (m, 2H; CH_2), 1.00 (t, *J* = 7.5 Hz, 3H; CH_3), 0.88 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 151.2, 146.4, 129.3 (d, *J* = 32.2 Hz), 129.0, 128.3 (q, *J* = 271.6 Hz), 125.4 (q, *J* = 3.4 Hz), 107.0, 43.1, 36.8, 23.2, 21.5, 13.9, 13.2. ^{19}F ($CDCl_3$) d -62.9. IR (neat): 2962, 1325, 1126 cm^{-1}. MS *m/z* (%): 383/382 (10/61) $[M]^+$, 185 (55), 173 (100), 159 (80). HRMS (EI) Calcd for $C_{15}H_{18}F_3I$: $[M]^+$ (382.0405), found 382.0397.

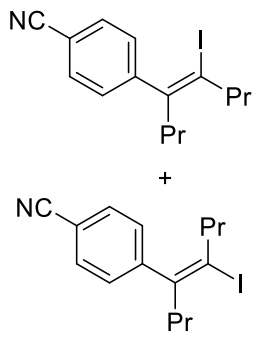


(*E*)-1-(5-Iodooct-4-en-4-yl)-4-(trifluoromethyl)benzene ((*E*)-3ha).



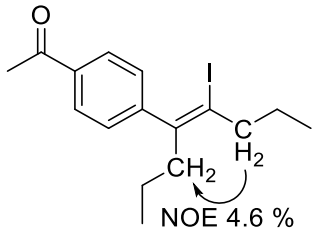
Yield: 8%, colorless oil. TLC: R_f 0.66 (hexane). ^1H NMR ($CDCl_3$) δ 7.60-7.58 (m, 2H; Ar-H), 7.20-7.18 (m, 2H; Ar-H), 2.54 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.22 (dd, *J* = 7.0 Hz, 2H; CH_2), 1.52-1.48 (m, 2H; CH_2), 1.35-1.30 (m, 2H; CH_2), 0.91 (t, *J* = 7.5 Hz, 3H; CH_3), 0.76 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 145.2, 144.8, 129.4 (q, *J* = 32.7 Hz), 128.7, 125.5 (q, *J* = 272.0 Hz), 109.2, 47.0, 43.8, 23.6, 20.6, 13.8, 12.9. IR (neat): 2962, 1325, 1126 cm^{-1}. MS *m/z* (%): 383/382 (8/58) $[M]^+$, 185 (58), 173 (100), 159 (77). HRMS (EI) Calcd for $C_{15}H_{18}F_3I$: $[M]^+$ (382.0405), found 382.0406.

(*Z*)-4-(5-Iodooct-4-en-4-yl)benzonitrile ((*Z*)-3ia) and (*E*)-4-(5-Iodooct-4-en-4-yl)benzonitrile ((*E*)-3ia) (19 : 1 mixture).



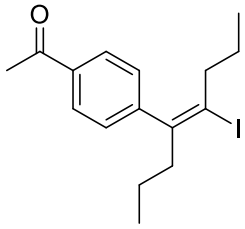
Yield: 60%, yellow oil. TLC: R_f 0.28 (hexane/ethyl acetate = 20/1). ^{1}H NMR ($CDCl_3$) δ 7.65-7.63 (m, 2H; Ar-H), 7.19-7.17 (m, 2H; Ar-H), 2.66 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.52 (dd, *J* = 8.0 Hz, 0.1H; CH_2), 2.44 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.20 (dd, *J* = 7.0 Hz, 0.1H; CH_2), 1.69-1.61 (m, 2H; CH_2), 1.51-1.45 (m, 0.1H; CH_2), 1.32-1.25 (m, 2H; CH_2), 0.99 (t, *J* = 7.0 Hz, 3H; CH_3), 0.87 (t, *J* = 7.0 Hz, 3H; CH_3), 0.75 (t, *J* = 7.5 Hz, 0.15H; CH_3). ^{13}C NMR ($CDCl_3$) δ152.2, 146.0, 144.7, 132.4, 132.3, 129.5, 129.1, 119.1, 118.9, 111.1, 111.0, 109.5, 107.4, 46.8, 43.8, 43.0, 36.6, 23.5, 23.1, 21.5, 20.6, 13.9, 13.8, 13.2, 12.9. IR (neat): 2960, 2229, 1601, 1456, 1270, 1132 cm^{-1}. MS *m/z* (%): 340/339 (12/70) $[M]^+$, 142 (77), 130(100), 116 (85). HRMS (EI) Calcd for $C_{15}H_{18}IN$: $[M]^+$ (339.0484), found 339.0480.

(*Z*)-1-(4-(5-Iodooct-4-cn-4-yl)phenyl)ethan-1-one ((*Z*)-3ja): CAS RN [935762-72-4].



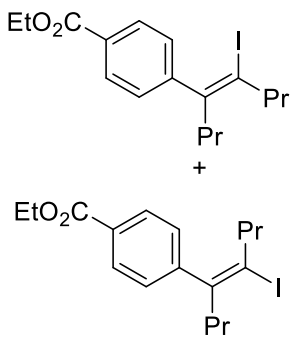
Yield: 87%, yellow oil. TLC: R_f 0.37 (hexane/THF = 10/1). ^{1}H NMR ($CDCl_3$) δ 7.96-7.94 (m, 2H; Ar-H), 7.18-7.17 (m, 2H; Ar-H), 2.67 (dd, *J* = 7.0 Hz, 2H; CH_2), 2.61 (s, 3H; $C(O)CH_3$), 2.46 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.70-1.62 (m, 2H; CH_2), 1.34-1.27 (m, 2H; CH_2), 1.00 (t, *J* = 7.5 Hz, 3H; CH_3), 0.87 (t, *J* = 7.5 Hz, 3H; CH_3) . ^{13}C NMR ($CDCl_3$) δ 197.8, 152.5, 146.7, 135.9, 128.9, 128.9, 128.6, 106.7, 43.1, 36.8, 26.8, 23.1, 21.6, 13.9, 13.2; IR (neat): 2959, 1692, 1602, 1265 cm^{-1}. MS *m/z* (%): 357/356 (4/15) $[M]^+$, 43 (100). HRMS (APCI) Calcd for $C_{16}H_{22}IO^+$: $[M+H]^+$ (357.0710), found 357.0710.

(*E*)-1-(4-(5-Iodooct-4-en-4-yl)phenyl)ethan-1-one ((*E*)-3ja).



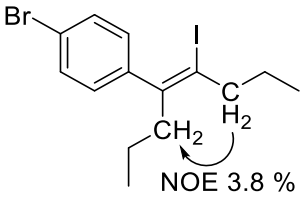
Yield: 11%, yellow oil. TLC: R_f 0.37 (hexane/THF = 20/1). ^{1}H NMR ($CDCl_3$) δ 7.94-7.92 (m, 2H; Ar-H), 7.18-7.16 (m, 2H; Ar-H), 2.61 (s, 3H; $C(O)CH_3$), 2.54 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.23 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.53-1.46 (m, 2H; CH_2), 1.36-1.29 (m, 2H; CH_2), 0.90 (t, *J* = 7.5 Hz, 3H; CH_3), 0.75 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 197.8, 146.2, 145.5, 136.0, 128.6, 128.6, 108.9, 46.9, 43.9, 26.7, 23.6, 20.7, 13.8, 12.9. IR (neat): 2959, 1693, 1602, 1265 cm^{-1}. MS *m/z* (%): 357/356(3/13) $[M]^+$, 43 (100); HRMS (APCI) Calcd for $C_{16}H_{22}IO^+$: $[M+H]^+$ (357.0710), found 357.0704.

(*Z*)-Ethyl-4-(5-iodooct-4-en-4-yl)phenyl propionate ((*Z*)-3ka) and (*E*)-Ethyl-4-(5-iodooct-4-en-4-yl)phenyl propionate ((*E*)-3ka) (8.8 : 1 mixture).



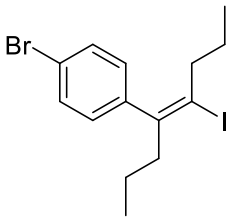
Yield: 88%, yellow oil. TLC: R_f 0.42 (hexane/ethyl acetate = 20/1). ^{1}H NMR ($CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 2H; Ar-H), 7.14 (d, *J* = 8.0 Hz, 2H; Ar-H), 4.37 (q, *J* = 7.0 Hz, 2H; CO_2CH_2), 2.66 (dd, *J* = 7.0 Hz, 2H; CH_2), 2.53 (dd, *J* = 8.0 Hz, 0.22H; CH_2), 2.45 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.22 (dd, *J* = 7.0 Hz, 0.22H; CH_2), 1.68-1.63 (m, 2H; CH_2), 1.52-1.47 (m, 2H; CH_2), 1.39 (t, *J* = 7.0 Hz, 3H; CH_3), 1.32-1.27 (m, 2H; CH_2), 1.00 (t, *J* = 7.0 Hz, 3H; CH_3), 0.87 (t, *J* = 7.0 Hz, 3H; CH_3), 0.75 (t, *J* = 7.0 Hz, 0.34H; CH_3). ^{13}C NMR ($CDCl_3$) δ 166.6, 152.2, 146.7, 145.8, 145.6, 129.7, 129.2, 128.6, 128.3, 108.8, 106.7, 61.1, 46.9, 43.8, 43.0, 36.7, 23.5, 23.1, 21.5, 20.6, 14.6, 13.9, 13.2, 12.9. IR (neat): 2962, 1715, 1607, 1279, 1110 cm^{-1}. MS *m/z* (%): 387/386 (10/82) $[M]^+$, 342/341 (3/22) $[M\text{-}OEt]^+$, 129 (80), 119 (100). HRMS (APCI) Calcd for $C_{17}H_{24}IO_2^+$: $[M+H]^+$ (387.0815), found 387.0808.

(*Z*)-1-Bromo-4-(5-iodooct-4-en-4-yl)benzene ((*Z*)-3la).



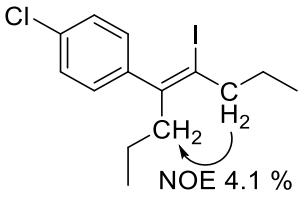
Yield: 68%, colorless oil. TLC: R_f 0.62 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.48-7.45 (m, 2H; Ar-H), 6.96-6.94 (m, 2H; Ar-H), 2.65 (dd, *J* = 7.0 Hz, 2H; CH_2), 2.42 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.69-1.61 (m, 2H; CH_2), 1.31-1.28 (m, 2H; CH_2), 0.99 (t, *J* = 7.5 Hz, 3H; CH_3), 0.87 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.5, 146.4, 131.5, 130.3, 121.1, 107.0, 43.1, 36.8, 23.1, 21.5, 13.9, 13.2. IR (neat): 2960, 1493, 1113, 1070, 1010 cm^{-1}. MS *m/z* (%):395/394/393/392 (8/68/6/70) $[M]^+$, 157 (85), 129 (100). HRMS (APCI) Calcd for $C_{14}H_{19}BrI^+$: $[M+H]^+$ (392.9709), found 392.9702.

(*E*)-1-Bromo-4-(5-iodooct-4-en-4-yl)benzene ((*E*)-3la).



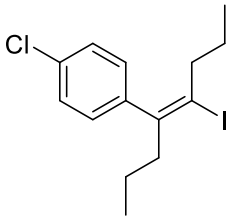
Yield: 15%, colorless oil. TLC: R_f 0.68 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.46-7.45 (m, 2H; Ar-H), 7.00-6.91 (m, 2H; Ar-H), 2.50 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.23 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.57-1.45 (m, 2H; CH_2), 1.34-1.29 (m, 2H; CH_2), 0.90 (t, *J* = 7.0 Hz, 3H; CH_3), 0.76 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ145.2, 139.8, 131.7, 130.0, 121.1, 108.9, 46.9, 43.8, 23.6, 20.6, 13.8, 13.0. IR (neat): 2959, 1495, 1113, 1070, 1012 cm^{-1}. MS *m/z* (%): 395/394/393/392 (8/60/8/60) $[M]^+$, 157 (87), 129 (100). HRMS (APCI) Calcd for $C_{14}H_{19}BrI^+$: $[M+H]^+$ (392.9709), found 392.9702.

(*Z*)-1-chloro-4-(5-iodooct-4-en-4-yl)benzene ((*Z*)-3ma).



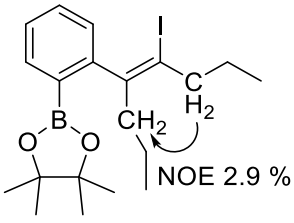
Yield: 53%, colorless oil. TLC: R_f 0.68 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.32-7.30 (m, 2H; Ar-H), 7.02-7.00 (m, 2H; Ar-H), 2.65 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.42 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.68-1.61 (m, 2H; CH_2), 1.34-1.26 (m, 2H; CH_2), 0.99 (t, *J* = 7.5 Hz, 3H; CH_3), 0.87 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.4, 146.1, 132.9, 129.9, 128.6, 107.0, 43.2, 36.8, 23.1, 21.5, 13.9, 13.2. IR (neat): 2959, 1495, 1113, 1014 cm^{-1}. MS *m/z* (%): 351/350/349/348 (2/16/6/50) $[M]^+$, 125 (100). HRMS (APCI) Calcd for $C_{14}H_{19}ClI^+$: $[M+H]^+$ (349.0214), found 349.0208.

(*E*)-1-Chloro-4-(5-iodooct-4-en-4-yl)benzene ((*E*)-3ma).



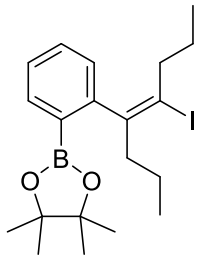
Yield: 7%, colorless oil. TLC: R_f 0.78 (hexane). ^{1}H NMR ($CDCl_3$) δ 7.32-7.29 (m, 2H; Ar-H), 7.01-6.98 (m, 2H; Ar-H), 2.51 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.24 (dd, *J* = 7.0 Hz, 2H; CH_2), 1.54-1.45 (m, 2H; CH_2), 1.34-1.28 (m, 2H; CH_2), 0.90 (t, *J* = 7.0 Hz, 3H; CH_3), 0.76 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 145.2, 139.2, 133.0, 129.6, 128.7, 108.9, 47.0, 43.8, 23.6, 20.6, 13.8, 13.0. IR (neat): 2959, 1499, 1092, 1016 cm^{-1}. MS *m/z* (%): 351/350/349/348 (2/14/6/42) $[M]^+$, 125 (100). HRMS (APCI) Calcd for $C_{14}H_{19}ClI^+$: $[M+H]^+$ (349.0214), found 349.0209.

(*Z*)-2-(2-(5-Iodooct-4-en-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane ((*Z*)-3na).



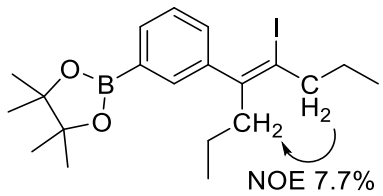
Yield: 31%, colorless oil. TLC: R_f 0.40 (hexane/ethyl acetate = 40/1). ^{1}H NMR ($CDCl_3$) δ 7.84-7.83 (m, 1H; Ar-H), 7.42-7.39 (m, 1H; Ar-H), 7.28-7.25 (m, 1H; Ar-H), 6.96-6.95 (m, 1H; Ar-H), 2.75-2.57 (m, 2H; CH_2), 2.56-2.28 (m, 2H; CH_2), 1.72-1.64 (m, 2H; CH_2), 1.47-1.29 (m, 2H; CH_2), 1.30 (s, 12H; $4CH_3$), 1.03 (t, *J* = 7.5 Hz, 3H; CH_3), 0.88 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 154.2, 148.4, 136.0, 130.7, 128.8, 126.3, 105.9, 83.5, 43.2, 37.4, 25.1, 25.0, 22.8, 21.5, 14.3, 13.6. IR (neat): 2958, 1462, 1368, 1303, 1134 cm^{-1}. MS *m/z* (%): 441/440 (1/4) $[M]^+$, 314/313 (18/93) $[M-I]^+$, 185 (90), 83 (100). HRMS (APCI) Calcd for $C_{20}H_{31}BIO_2^+$: $[M+H]^+$ (441.1456), found 441.1446.

(*E*)-2-(2-(5-Iodooct-4-en-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane and an uncharacterized isomer ((*E*)-3na) (1 : 0.22 mixture).



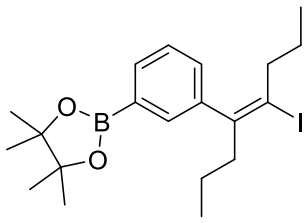
Yield: 11%, colorless oil. TLC: R_f 0.42 (hexane/ethyl acetate = 40/1). ^{1}H NMR ($CDCl_3$) δ 7.78-7.76 (m, 1H; Ar-H), 7.74-7.73 (m,0.21H), 7.38-7.35 (m,0.21H), 7.25-7.24 (m, 0.21H), 7.38-7.35 (m, 0.21H), 7.25-7.24 (m, 0.21H), 7.23-7.20(m, 1H; Ar-H), 7.08-7.06 (m, 1H; Ar-H), 6.97-6.96 (m, 0.21H), 6.89-6.86 (m, 1H; Ar-H), 2.62-2.35 (m, 0.42H), 2.55-2.23 (m, 2H; CH_2), 2.26-2.10 (m, 2H; CH_2), 2.20-2,10 (m, 0.42H), 1.53-1.45 (m, 2H; CH_2), 1.43-1.34 (m, 2H; CH_2), 1.30 (s, 2.52H), 1.31-1.24 (m, 0.42H), 1.00 (t, *J* = 7.0 Hz, 3H; CH_3), 0.97 (s, 6H), 0.93 (s, 6H), 0.89 (t, *J* = 7.5 Hz, 3H; CH_3), 0.89 (t, *J* = 7.5 Hz, 0.63H; CH_3), 0.70 (t, *J* = 7.5 Hz, 0.63H; CH_3). ^{13}C NMR ($CDCl_3$) δ 153.7, 149.4, 147.3, 146.9, 138.6, 135.5, 130.5, 130.4, 128.6, 127.8, 127.1, 126.2, 107.9, 100.2, 83.7, 82.8, 47.7, 43.8, 35.5, 32.8, 25.1, 25.0, 24.9, 24.6, 24.5, 23.2, 23.2, 21.2, 20.5, 14.6, 14.6, 14.3, 13.1, 1.2. IR (neat): 2959, 1484, 1352, 1314, 1146 cm^{-1}. MS *m/z* (%): 441/440 (20/92) $[M]^+$, 384/383 (9/57) $[M-I]^+$, 213 (98), 157 (96, 143 (100). HRMS (APCI) Calcd for $C_{20}H_{31}BIO_2^+$: $[M+H]^+$ (441.1456), found 441.1454.

(*Z*)-2-(3-(5-Iodooct-4-en-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane ((*Z*)-3oa).



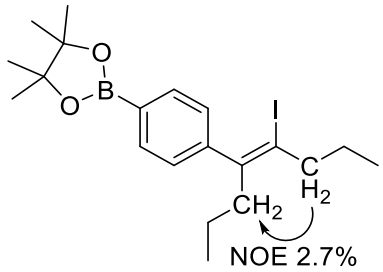
Yield: 62%, pink oil. TLC: R_f 0.23 (hexane/ethyl acetate = 40/1). ^{1}H NMR ($CDCl_3$) δ 7.74-7.72 (m, 1H; Ar-H), 7.50 (s, 1H; Ar-H), 7.33 (t, *J* = 7.5 Hz, 2H; Ar-H), 7.19-7.17 (m, 1H; Ar-H), 2.66 (t, *J* = 7 Hz, 2H; CH_2), 2.46 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.69-1.62 (m, 2H; CH_2), 1.35 (s, 12H;4CH_3), 1.33-1.30 (m, 2H; CH_2), 1.00 (t, *J* = 7.0 Hz, 3H; CH_3), 0.87 (t, *J* = 7.0 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 147.5, 147.1, 134.2, 133.6, 131.9, 127.5, 106.4, 84.0, 43.2, 36.9, 31.8, 25.1, 23.2, 21.6, 14.0, 13.3. IR (neat): 2960, 1358, 1313, 1145 cm^{-1}. MS *m/z* (%): 441/440 (11/60) $[M]^+$, 101 (100), 83 (98). HRMS (APCI) Calcd for $C_{20}H_{31}BIO_2^+$: $[M+H]^+$ (441.1456), found 441.1455.

(*E*)-2-(3-(5-Iodooct-4-en-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane ((*E*)-3oa).



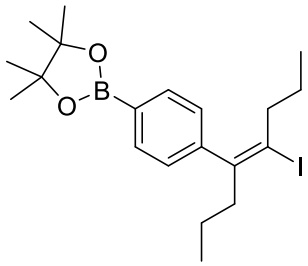
Yield: 22%, colorless oil. TLC: R_f 0.28 (hexane/ethyl acetate = 40/1). ^{1}H NMR ($CDCl_3$) δ 7.71-7.69 (m, 1H; Ar-H), 7.51 (s, 1H; Ar-H), 7.34-7.31 (m, 1H; Ar-H), 7.15-7.14 (m, 1H; Ar-H), 2.54 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.23 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.53-1.46 (m, 2H; CH_2), 1.38-1.32 (m, 2H; CH_2), 1.35 (s, 12H; 4CH_3), 0.90 (t, *J* = 7.5 Hz, 3H; CH_3) , 0.75 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.3, 140.2, 134.4, 133.4, 131.2, 127.8, 108.5, 84.0, 47.1, 43.9, 25.1, 23.6, 20.6, 13.9, 12.9. IR (neat): 2959, 1358, 1314, 1145 cm^{-1}. MS *m/z* (%): 441/440 (17/73) $[M]^+$, 101 (100), 83 (96). HRMS (APCI) Calcd for $C_{20}H_{31}BIO_2^+$: $[M+H]^+$ (441.1456), found 441.1454.

(*Z*)-2-(4-(5-Iodooct-4-en-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane ((*Z*)-3pa).



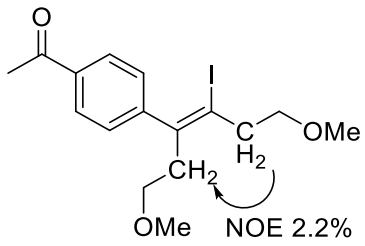
Yield: 70%, colorless oil. TLC: R_f 0.41 (hexane/ethyl acetate = 40/1). ^{1}H NMR ($CDCl_3$) δ 7.80-7.78 (m, 2H; Ar-H), 7.09-7.08 (m, 2H; Ar-H), 2.66 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.43 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.69-1.62 (m, 2H; CH_2), 1.32-1.26 (m, 2H; CH_2), 1.34 (s, 12H; 4CH_3), 1.00 (t, *J* = 7.5 Hz, 3H; CH_3), 0.85 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 150.6, 147.5, 134.8, 127.8, 106.1, 83.9, 43.1, 36.8, 25.1, 23.2, 21.5, 13.9, 13.2. IR (neat): 2962, 1609, 1361, 1144 cm^{-1}. MS *m/z* (%): 441/440 (14/81) $[M]^+$, 101 (100), 83 (92). HRMS (APCI) Calcd for $C_{20}H_{31}BIO_2^+$: $[M+H]^+$ (441.1456), found 441.1447.

(*E*)-2-(4-(5-Iodooct-4-en-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane ((*E*)-3pa).



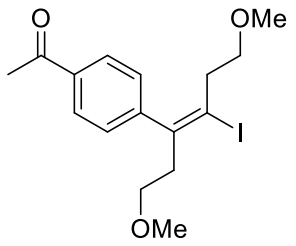
Yield: 26%, white solid. Mp. 77 °C (hexane/ethyl acetate), TLC: R_f 0.44 (hexane/ethyl acetate = 40/1). ^{1}H NMR ($CDCl_3$) δ 7.78-7.76 (m, 2H; Ar-H), 7.09-7.07 (m, 2H; Ar-H), 2.52 (dd, *J* = 7.5 Hz, 2H; CH_2), 2.24 (dd, *J* = 7.5 Hz, 2H; CH_2), 1.52-1.44 (m, 2H; CH_2), 1.35 (s, 12H; $4CH_3$), 1.34-1.29 (m, 2H; CH_2), 0.89 (t, *J* = 7.5 Hz, 3H; CH_3), 0.72 (t, *J* = 7.5 Hz, 3H; CH_3). ^{13}C NMR ($CDCl_3$) δ 146.3, 144.0, 134.9, 127.7, 108.5, 84.0, 47.0, 43.9, 25.1, 23.6, 20.6, 13.9, 12.9. IR (neat): 2959, 1608, 1359, 1145 cm^{-1}. MS *m/z* (%): 441/440 (13/70) $[M]^+$, 101 (100), 83 (96). HRMS (APCI) Calcd for $C_{20}H_{31}BIO_2^+$: $[M+H]^+$ (441.1456), found 441.1456.

(*Z*)-1-(4-(4-Iodo-1,6-dimethoxyhex-3-en-3-yl)phenyl)ethan-1-one ((*Z*)-3jb).



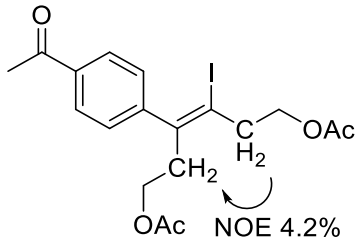
Yield: 43%, colorless oil. TLC: R_f 0.08 (hexane/ethyl acetate =10/1). ^{1}H NMR ($CDCl_3$) δ 7.96-7.95 (m, 2H; Ar-H), 7.20-7.18 (m, 2H; Ar-H), 3.61 (t, *J* = 7.0 Hz, 2H; CH_2), 3.40 (s, 3H; OCH_3), 3.27 (t, *J* = 7.5 Hz, 2H; CH_2), 3.24 (s, 3H; OCH_3), 3.02 (t, *J* = 7.0 Hz, 2H; CH_2), 2.78 (t, *J* = 7.0 Hz, 2H; CH_2), 2.61 (s, 3H;$C(O)CH_3$). ^{13}C NMR ($CDCl_3$) δ 197.8, 151.8, 145.3, 136.2, 128.8, 102.6, 71.6, 70.1, 59.1, 58.7, 41.8, 34.9, 26.7. IR (neat): 2925, 2875, 1683, 1603, 1265, 1116 cm^{-1}. MS *m/z* (%): 262/261 (8/46) $[M-I]^+$, 45 (100). HRMS (APCI) Calcd for $C_{16}H_{22}IO_3^+$: $[M+H]^+$ (389.0608), found 389.0604.

(*E*)-1-(4-(4-Iodo-1,6-dimethoxyhex-3-en-3-yl)phenyl)ethan-1-one ((*E*)-3jb).



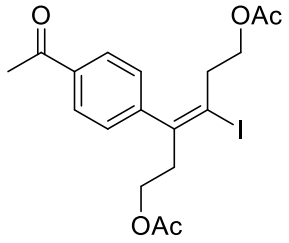
Yield: 10%, colorless oil. TLC: R_f 0.10 (hexane/ethyl acetate =10/1). ^{1}H NMR ($CDCl_3$) δ 7.94-7.92 (m, 2H; Ar-H), 7.25-7.23 (m, 2H; Ar-H), 3.46 (t, *J* = 7.0 Hz, 2H; CH_2), 3.32 (t, *J* = 7.5 Hz, 2H; CH_2), 3.25 (s, 3H; OCH_3), 3.24 (s, 3H; OCH_3), 2.88 (t, *J* = 7.0 Hz, 2H; CH_2), 2.60 (s, 3H; $C(O)CH_3$). ^{13}C NMR ($CDCl_3$) δ 197.7, 145.1, 144.4, 136.3, 128.7, 128.6, 105.0, 71.9, 69.7, 58.9, 58.7, 44.8, 42.1. IR (neat): 2925, 2875, 1683, 1602, 1265, 1116 cm^{-1}. MS *m/z* (%): 262/261 (10/52) $[M-I]^+$, 45 (100). HRMS (APCI) Calcd for $C_{16}H_{22}IO_3^+$: $[M+H]^+$ (389.0608), found 389.0605.

(*Z*)-3-(4-Acetylphenyl)-4-iodohex-3-ene-1,6-diyl diacetate ((*Z*)-3jc).



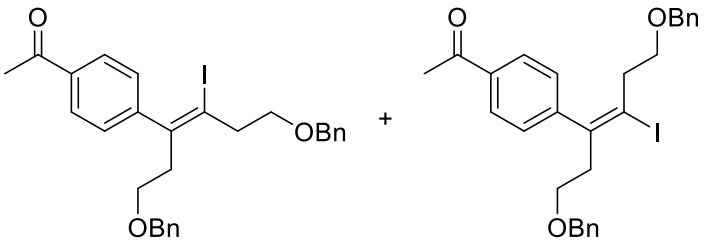
Yield: 74%, colorless oil. TLC: R_f 0.25 (hexane/ethyl acetate =2/1). ^{1}H NMR ($CDCl_3$) δ 7.98-7.96 (m, 2H; Ar-H), 7.19-7.17 (m, 2H; Ar-H), 4.31 (t, *J* = 7.0 Hz, 2H; OCH_2), 4.00 (t, *J* = 6.5 Hz, 2H; OCH_2), 3.10 (t, *J* = 7.0 Hz, 2H; CH_2), 2.86 (t, *J* = 6.5 Hz, 2H; CH_2), 2.62 (s, 3H; $C(O)CH_3$), 2.11 (s, 3H; $OC(O)CH_3$), 2.00 (s, 3H; $OC(O)CH_3$). ^{13}C NMR ($CDCl_3$) δ 197.7, 171.1, 170.9, 150.9, 145.1, 136.4, 128.8, 128.6, 101.9, 63.1, 40.7, 33.5, 26.8, 21.1, 21.0. IR (neat): 2959, 1738, 1683, 1603, 1385, 1362, 1266, 1042 cm^{-1}. MS *m/z* (%): 318/317 (4/30) $[M-I]^+$, 43 (100). HRMS (APCI) Calcd for $C_{18}H_{22}IO_5^+$: $[M+H]^+$ (445.0506), found 445.0496.

(*E*)-3-(4-Acetylphenyl)-4-iodohex-3-ene-1,6-diyl diacetate ((*E*)-3jc).



Yield: 25%, colorless oil. TLC: R_f 0.29 (hexane/ethyl acetate =2/1). ^{1}H NMR ($CDCl_3$) δ 7.96-7.94 (m, 2H; Ar-H), 7.24-7.21 (m, 2H; Ar-H), 4.14 (t, *J* = 6.5 Hz, 2H; OCH_2), 4.05 (t, *J* = 6.5 Hz, 2H; OCH_2), 2.95 (t, *J* = 6.5 Hz, 2H; CH_2), 2.61 (s, 3H; $C(O)CH_3$), 2.01 (s, 3H; $OC(O)CH_3$), 1.98 (s, 3H; $OC(O)CH_3$). ^{13}C NMR ($CDCl_3$) δ 197.6, 171.0, 170.8, 144.6, 144.5, 136.5, 128.8, 128.6, 104.2, 63.4, 61.3, 43.9, 41.2, 26.8, 21.1, 21.0. IR (neat): 2958, 1738, 1683, 1602, 1384, 1363, 1265, 1043 cm^{-1}. MS *m/z* (%): 318/317 (3/18) $[M-I]^+$, 43 (100). HRMS (APCI) Calcd for $C_{18}H_{22}IO_5^+$: $[M+H]^+$ (445.0506), found 445.0504.

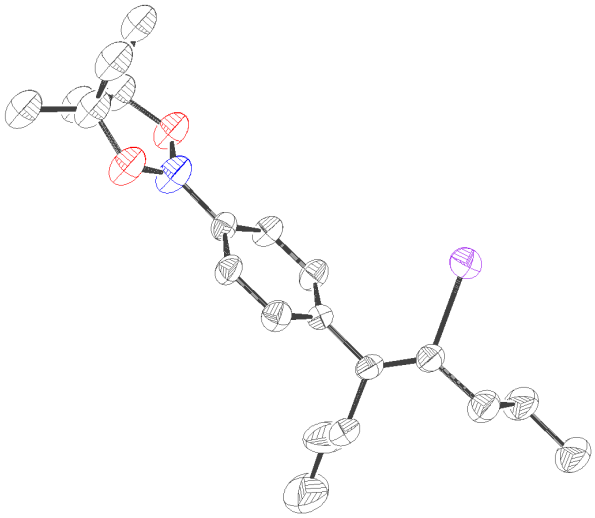
(*Z*)-1-(4-(1,6-Bis(benzyloxy)-4-iodohex-3-en-3-yl)phenyl)ethan-1-one ((*Z*)-3jd) and (*E*)-1-(4-(1,6-Bis(benzyloxy)-4-iodohex-3-en-3-yl)phenyl)ethan-1-one ((*E*)-3jd) (6.1 : 1 mixture).



Yield: 90%, colorless oil. TLC: R_f 0.74 (hexane/ethyl acetate =3/1). ^{1}H NMR ($CDCl_3$) δ 7.94-7.92 (m, 2H; Ar-H), 7.88-7.86 (m, 0.33H; Ar-H), 7.37-7.24 (m, 10H; Ph-H), 7.37-7.24 (m, 1.6H; Ph-H), 7.15-7.13 (m, 2H; Ar-H), 7.21-7.20 (m, 0.33H; Ar-H), 4.54 (s, 2H; Ph-CH_2), 4.43 (s, 0.33H; Ph-CH_2), 4.42 (s, 0.33H; Ph-CH_2), 4.35 (s, 2H; Ph-CH_2), 3.71 (t, *J* = 7.0 Hz, 2H; CH_2), 3.57 (t, *J* = 7.0 Hz, 0.33H; CH_2), 3.44 (t, *J* = 7.0 Hz, 0.33H; CH_2), 3.36 (t, *J* = 7.5 Hz, 2H; CH_2), 3.08 (t, *J* = 7.0 Hz, 2H; CH_2), 2.94 (t, *J* = 7.5 Hz, 0.33H; CH_2), 2.83 (t, *J* = 7.5 Hz, 2H; CH_2), 2.62 (s, 3H; C(O)CH_3), 2.61 (t, *J* = 7.0 Hz, 0.33H; CH_2), 2.60 (s, 0.49H; C(O)CH_3). ^{13}C NMR ($CDCl_3$) δ 198.1, 152.0, 145.4, 145.2, 144.5, 138.7, 138.6, 138.5, 138.4, 136.2, 136.1, 128.9, 128.8, 128.7, 128.7, 128.0, 128.0, 127.9, 127.9, 127.8, 105.4, 103.0, 73.5, 73.2, 73.1, 69.5, 69.2, 69.0, 67.8, 67.5, 45.1, 42.5, 42.2, 35.2, 27.0, 20.5. IR (neat): 2858, 1682, 1601, 1453, 1358, 1265, 1104 cm^{-1}. MS *m/z* (%):413 (13), 307 (42), 91 (100). HRMS (ESI) Calcd for $C_{28}H_{30}IO_3^+$: $[M+H]^+$ (541.1228), found 541.1234.

6 X-ray Single Crystal Analysis of (*Z*)-3pa

ORTEP Drawing of (*Z*)-3pa (CCDC: 1847371)



Empirical Formula	$C_{20}H_{30}BIO_2$
Formula Weight	440.17
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.440 X 0.410 X 0.220 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 13.66(2) Å b = 10.672(8) Å c = 15.64(2) Å β = 105.433(7) ° V = 2198(4) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.330 g/cm^3
F_{000}	896.00
μ(MoKα)	14.655 cm^{-1}

7 Computational Details

General Methods. Calculations were performed on Gaussian 09 E.01.[3] For all calculations M06 was used. Geometry optimization and frequency calculations were carried out using 6-31G(d) (H, C, N) and Lanl2dz (I) and f polarization function added Lanl2dz(f)[4] (Ni) basis sets. Single-point calculations were performed with 6-311+G(2d,p) (H, C, N) and SDD (I) and 2f polarization functions added SDD(2f)[5] (Ni). Solvation effects of toluene were added all calculations using CPCM. EPR parameter calculations were performed with ORCA 4.0.1.2.[6,7] Single-point calculations were carried out at the B3LYP level with Alrichs' all-electron Gaussian triple-ζ basis sets def2-TZVP for all atoms.[8,9] The EPR spectra were simulated using EasySpin for MATLAB with calculated *g*-value and *A*-value.[10]

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Cartesian coordinates for **Ni(I)I/dtbpy 4**

C	-0.210714	1.321534	1.911155	C	0.455218	5.351061	4.703014
C	1.912814	2.041294	2.449087	H	-0.827891	5.715172	2.297951
C	1.416073	3.113620	3.178949	H	-2.254273	4.715258	2.645552
C	0.038176	3.301444	3.281589	H	-1.900349	6.128691	3.654372
C	-0.773535	2.370483	2.623653	H	-0.896555	3.256776	5.864524
C	-0.990065	0.294157	1.187602	H	-1.941244	4.690072	5.740065
C	-0.867508	-1.603661	-0.115010	H	-2.294581	3.250405	4.768811
C	-2.250089	-1.690033	-0.206164	H	-0.046385	6.160343	5.249228
C	-3.046238	-0.738610	0.430135	H	1.080791	4.805813	5.422768
C	-2.376048	0.265764	1.136659	H	1.111069	5.815693	3.954230
H	2.984343	1.868341	2.350721	C	-4.567479	-0.755728	0.384351
H	2.118758	3.788816	3.658357	C	-5.110844	-0.879801	1.812735
H	-1.855882	2.470019	2.671726	C	-5.066283	0.550008	-0.245834
H	-0.225960	-2.335531	-0.603841	C	-5.103253	-1.924113	-0.439014
H	-2.685148	-2.505017	-0.777111	H	-4.764511	-1.807932	2.287092
H	-2.947255	1.034853	1.652372	H	-4.803425	-0.039429	2.448390
N	1.125851	1.164472	1.829030	H	-6.209130	-0.896937	1.792803
N	-0.241867	-0.640385	0.561790	H	-4.684346	0.665122	-1.269192
Ni	1.722877	-0.416997	0.753221	H	-6.163950	0.545738	-0.290674
I	4.103412	-1.076050	0.335885	H	-4.761500	1.432833	0.330778
C	-0.593398	4.447356	4.059807	H	-6.200465	-1.893491	-0.444528
C	-1.442908	5.294538	3.104942	H	-4.766798	-1.878042	-1.483745
C	-1.482648	3.871709	5.168299	H	-4.802884	-2.893817	-0.019245

Cartesian coordinates for **O1**

C	-0.978701	3.057946	0.528915	I	1.749426	0.578854	2.056917
C	1.078293	4.016355	0.046274	C	2.060889	-0.481370	-0.917977
C	0.626020	5.282224	0.391936	C	1.372794	-1.795340	-0.940147
C	-0.688465	5.417949	0.822060	H	1.015948	-2.069102	0.063597
C	-1.502736	4.296093	0.893367	H	0.510403	-1.785013	-1.621718
C	-1.738779	1.794965	0.567137	H	2.045962	-2.597740	-1.274609
C	-1.662815	-0.490428	0.219196	C	3.878526	1.207423	-1.088363
C	-2.993163	-0.644324	0.583699	C	3.693955	2.151699	-2.102536
C	-3.711333	0.486035	0.950663	C	4.664856	1.554848	0.016698
C	-3.077934	1.720218	0.943388	C	4.251980	3.424580	-1.999371
H	2.100243	3.844970	-0.299272	H	3.106003	1.881100	-2.978539
H	1.293257	6.136666	0.324838	C	5.217780	2.825308	0.123894
H	-1.080088	6.392751	1.103272	H	4.828131	0.818907	0.803886
H	-2.530556	4.390060	1.232297	C	5.009122	3.766221	-0.883122
H	-1.059701	-1.344964	-0.079199	H	4.098464	4.146706	-2.799934
H	-3.448091	-1.630622	0.575147	H	5.818048	3.081606	0.995321
H	-4.756778	0.410388	1.240154	H	5.446829	4.759924	-0.801265
H	-3.625306	2.615166	1.225813	C	4.348252	-1.182510	-1.677689
N	0.292198	2.942144	0.114065	H	4.745424	-0.887624	-2.659877
N	-1.052416	0.693452	0.209377	H	5.202470	-1.205395	-0.984834
Ni	0.944646	1.058440	-0.367800	H	3.950990	-2.198794	-1.761428
C	3.325256	-0.175580	-1.208208	I	0.154247	1.256713	-2.853375

Cartesian coordinates for **O2**

C	-0.996171	3.083461	0.505507	C	-1.769730	-0.456474	0.271086
C	1.061503	3.997978	-0.038396	C	-3.111569	-0.567553	0.606059
C	0.642699	5.276511	0.306699	C	-3.804901	0.590568	0.934762
C	-0.656615	5.440813	0.770054	C	-3.138721	1.807360	0.915700
C	-1.488515	4.333990	0.873378	H	2.071345	3.806012	-0.407661
C	-1.788091	1.838097	0.573641	H	1.323761	6.117898	0.214979

H	-1.022899	6.424848	1.053711
H	-2.503783	4.449102	1.242961
H	-1.185146	-1.329620	-0.015325
H	-3.596415	-1.539528	0.599870
H	-4.859463	0.549971	1.197272
H	-3.671707	2.723421	1.154747
N	0.261019	2.937205	0.056489
N	-1.124989	0.709557	0.262232
Ni	0.839138	0.967081	-0.338013
C	3.309623	-0.079382	-0.996208
I	1.850171	0.357685	1.971000
C	2.192572	-0.522063	-0.389766
C	1.619360	-1.898233	-0.480243
H	0.839497	-2.064623	0.270152
H	1.164894	-2.042412	-1.472764
H	2.384960	-2.671780	-0.325448
C	3.895580	1.284712	-0.871057
C	3.737724	2.201936	-1.917334
C	4.689608	1.641435	0.222912
C	4.335112	3.457927	-1.854439
H	3.122941	1.929074	-2.776241
C	5.283108	2.897807	0.286539
H	4.843530	0.923456	1.027277
C	5.105764	3.810571	-0.749982
H	4.197025	4.161509	-2.673981
H	5.895901	3.160950	1.147083
H	5.575882	4.791356	-0.700845
C	3.992583	-0.934655	-2.032493
H	3.784332	-0.541145	-3.039346
H	5.082564	-0.901542	-1.894407
H	3.666170	-1.978889	-2.010023
I	0.103900	0.846510	-2.947492

Cartesian coordinates for **O3**

C	-0.898824	2.847066	0.471015
C	1.083673	3.873127	-0.134299
C	0.742750	5.043850	0.529143
C	-0.471061	5.091766	1.201715
C	-1.304380	3.982811	1.168370
C	-1.730288	1.630529	0.365875
C	-1.847368	-0.528629	-0.456152
C	-3.147834	-0.692082	-0.000140
C	-3.747616	0.369168	0.667069
C	-3.035975	1.546424	0.848532
H	2.035027	3.779587	-0.657569
H	1.423393	5.890480	0.521041
H	-0.770785	5.984320	1.746168
H	-2.257930	4.004280	1.688358
H	-1.334963	-1.318359	-1.005981
H	-3.675554	-1.625507	-0.174607
H	-4.767619	0.286912	1.035422
H	-3.502514	2.390208	1.349347
N	0.292767	2.798070	-0.156589
N	-1.154915	0.595106	-0.268169
Ni	0.771514	0.951981	-0.976655
C	2.827054	0.396595	-0.727560
I	2.049042	1.122646	2.228889
C	2.038754	0.039701	0.367796
C	1.515248	-1.354381	0.603619
H	0.612304	-1.340267	1.224594
H	1.263343	-1.856626	-0.339715
H	2.266696	-1.971617	1.119131
C	3.736888	1.578389	-0.797463
C	3.687161	2.435141	-1.904550
C	4.736916	1.782010	0.157556
C	4.571885	3.500669	-2.019857
H	2.924319	2.269077	-2.668023
C	5.626016	2.846700	0.040583
H	4.828455	1.092828	0.995900
C	5.539492	3.716109	-1.041406
H	4.505624	4.164292	-2.880358
H	6.395387	2.989731	0.797571
H	6.233465	4.550072	-1.130565
C	3.185372	-0.646037	-1.770474
H	2.414530	-1.406634	-1.925040
H	3.369364	-0.167032	-2.738092
H	4.115370	-1.152490	-1.465462
I	0.239370	0.970918	-3.556322

Cartesian coordinates for **E1**

C	-1.180274	2.066716	-0.063525
C	0.773642	3.017470	-0.848722
C	0.337050	4.296656	-0.528841
C	-0.908368	4.444160	0.064256
C	-1.679548	3.313842	0.299190
C	-1.932569	0.812523	0.098124
C	-1.908453	-1.479150	-0.227730
C	-3.226293	-1.601089	0.187613
C	-3.902290	-0.461387	0.599709
C	-3.248690	0.760953	0.547881
H	1.750487	2.843561	-1.298997
H	0.972388	5.152546	-0.738784
H	-1.281231	5.427469	0.341597
H	-2.656912	3.408374	0.763831
H	-1.327598	-2.349789	-0.521349
H	-3.701574	-2.577877	0.192048
H	-4.931148	-0.517757	0.947266
H	-3.765840	1.668434	0.846065
N	0.040740	1.924929	-0.621109
N	-1.264867	-0.306168	-0.260066
Ni	0.620687	-0.024556	-0.696574
C	0.988760	-2.323340	0.836053
I	2.987053	0.319665	-1.506564
C	1.038615	-1.834718	-0.419961
C	1.223470	-2.707478	-1.627397
H	0.895552	-2.204689	-2.546202
H	2.283198	-2.967220	-1.776492
H	0.663948	-3.653760	-1.544718
C	0.642747	-1.453456	1.982920
C	1.191719	-0.172728	2.144876

C	-0.320038	-1.870113	2.913803	H	-1.517985	-1.371359	4.627490
C	0.761111	0.671748	3.163657	H	-0.559507	0.914509	4.854025
H	1.982184	0.153803	1.468575	C	1.110166	-3.804497	1.117428
C	-0.755392	-1.026513	3.929979	H	1.447870	-3.990784	2.145091
H	-0.759825	-2.863852	2.816977	H	0.148507	-4.332658	0.993162
C	-0.222782	0.254451	4.056148	H	1.826491	-4.286546	0.441444
H	1.209196	1.659866	3.266373				

Cartesian coordinates for **E2**

C	-2.207240	2.492160	0.753245	I	1.825765	1.301070	-1.221299
C	-0.524244	3.049504	2.243923	C	1.022475	-0.757941	0.482881
C	-1.186268	4.203663	2.637805	C	1.320950	-1.956992	-0.320264
C	-2.418195	4.491115	2.062218	H	0.849403	-1.947642	-1.309302
C	-2.932154	3.628594	1.104587	H	2.404179	-2.092209	-0.453618
C	-2.629842	1.548439	-0.297895	H	0.962577	-2.835450	0.241273
C	-2.001689	-0.286199	-1.556400	C	2.219798	0.434569	2.443314
C	-3.180324	-0.256702	-2.287815	C	3.488350	0.575078	1.865522
C	-4.118779	0.724145	-1.986954	C	1.987769	1.071668	3.671960
C	-3.840607	1.640498	-0.983131	C	4.469932	1.350796	2.471003
H	0.446710	2.779551	2.661212	H	3.706221	0.062794	0.929904
H	-0.738773	4.859735	3.379294	C	2.968703	1.848055	4.278583
H	-2.969747	5.384501	2.346029	H	1.015688	0.961036	4.155090
H	-3.882362	3.849887	0.625839	C	4.215531	1.996841	3.677337
H	-1.231390	-1.030696	-1.753925	H	5.447114	1.441499	1.998772
H	-3.354070	-0.987163	-3.073187	H	2.757595	2.336966	5.228839
H	-5.058409	0.779248	-2.531914	H	4.986186	2.602514	4.150909
H	-4.561317	2.416607	-0.739045	C	0.580094	-1.450418	2.809546
N	-1.024121	2.203904	1.336988	H	1.368745	-2.052325	3.287523
N	-1.733437	0.583794	-0.580962	H	0.012246	-0.955900	3.609035
Ni	-0.092095	0.579589	0.651811	H	-0.119000	-2.127320	2.302569
C	1.168645	-0.424299	1.845589				

Cartesian coordinates for **E3**

C	-2.760935	1.159385	0.521853	I	2.124144	-1.529596	-1.465417
C	-1.535540	1.223957	2.485960	C	0.640254	-1.999326	0.095930
C	-2.442203	2.090304	3.081999	C	0.128600	-3.397713	-0.137756
C	-3.553603	2.491373	2.350671	H	-0.286581	-3.513686	-1.147551
C	-3.715032	2.022125	1.053679	H	0.918049	-4.157982	-0.016190
C	-2.818583	0.609463	-0.846610	H	-0.674280	-3.634219	0.573465
C	-1.762188	-0.776785	-2.371352	C	2.003034	-0.550620	1.725341
C	-2.704174	-0.497064	-3.352699	C	3.137639	-1.103340	2.334599
C	-3.742241	0.373678	-3.045459	C	2.024048	0.817212	1.435451
C	-3.799646	0.937860	-1.777533	C	4.252167	-0.325746	2.627059
H	-0.644304	0.881371	3.010135	H	3.152361	-2.169524	2.563750
H	-2.275164	2.438154	4.097705	C	3.136631	1.601592	1.725605
H	-4.289434	3.165228	2.783470	H	1.150503	1.261476	0.954453
H	-4.578287	2.325637	0.466952	C	4.256833	1.033459	2.323502
H	-0.919878	-1.442658	-2.560184	H	5.124766	-0.784413	3.090809
H	-2.618585	-0.954125	-4.334689	H	3.126783	2.663384	1.482141
H	-4.499626	0.618220	-3.786711	H	5.128774	1.644577	2.551573
H	-4.598785	1.629707	-1.523849	C	0.360152	-2.236180	2.610341
N	-1.687959	0.762987	1.240541	H	1.036615	-3.074547	2.850324
N	-1.817886	-0.245785	-1.147066	H	0.310898	-1.597513	3.503466
Ni	-0.570467	-0.609800	0.350358	H	-0.639821	-2.660869	2.460093
C	0.829351	-1.425812	1.409401				

Cartesian coordinates for **O1**

C	-1.695500	1.950659	0.960979
C	0.172284	3.104245	0.229225
C	-0.355882	4.320975	0.640886
C	-1.601597	4.327260	1.253051
C	-2.283769	3.128660	1.412376
C	-2.357151	0.635497	1.032852
C	-2.169200	-1.626910	0.566012
C	-3.477820	-1.869151	0.953297
C	-4.238835	-0.802517	1.414692
C	-3.675390	0.464077	1.449728
H	1.150284	3.036836	-0.247301
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H	-2.045452	5.257373	1.600380
H	-3.261704	3.117886	1.885167
H	-1.523699	-2.427040	0.207511
H	-3.885208	-2.873937	0.888931
H	-5.268343	-0.950775	1.731892
H	-4.265344	1.313107	1.782389
N	-0.474239	1.950491	0.393402
N	-1.619604	-0.412386	0.621067
Ni	0.253536	0.039241	0.030331
C	0.842172	-2.188859	1.549081
I	2.693182	0.580816	-0.417654
C	0.943554	-1.756505	0.279666
C	1.329603	-2.599553	-0.888915
H	1.451942	-2.018116	-1.806342
H	2.274750	-3.130252	-0.695470
H	0.556063	-3.359818	-1.088394
C	0.388817	-1.327780	2.666072
C	0.876621	-0.028670	2.858853
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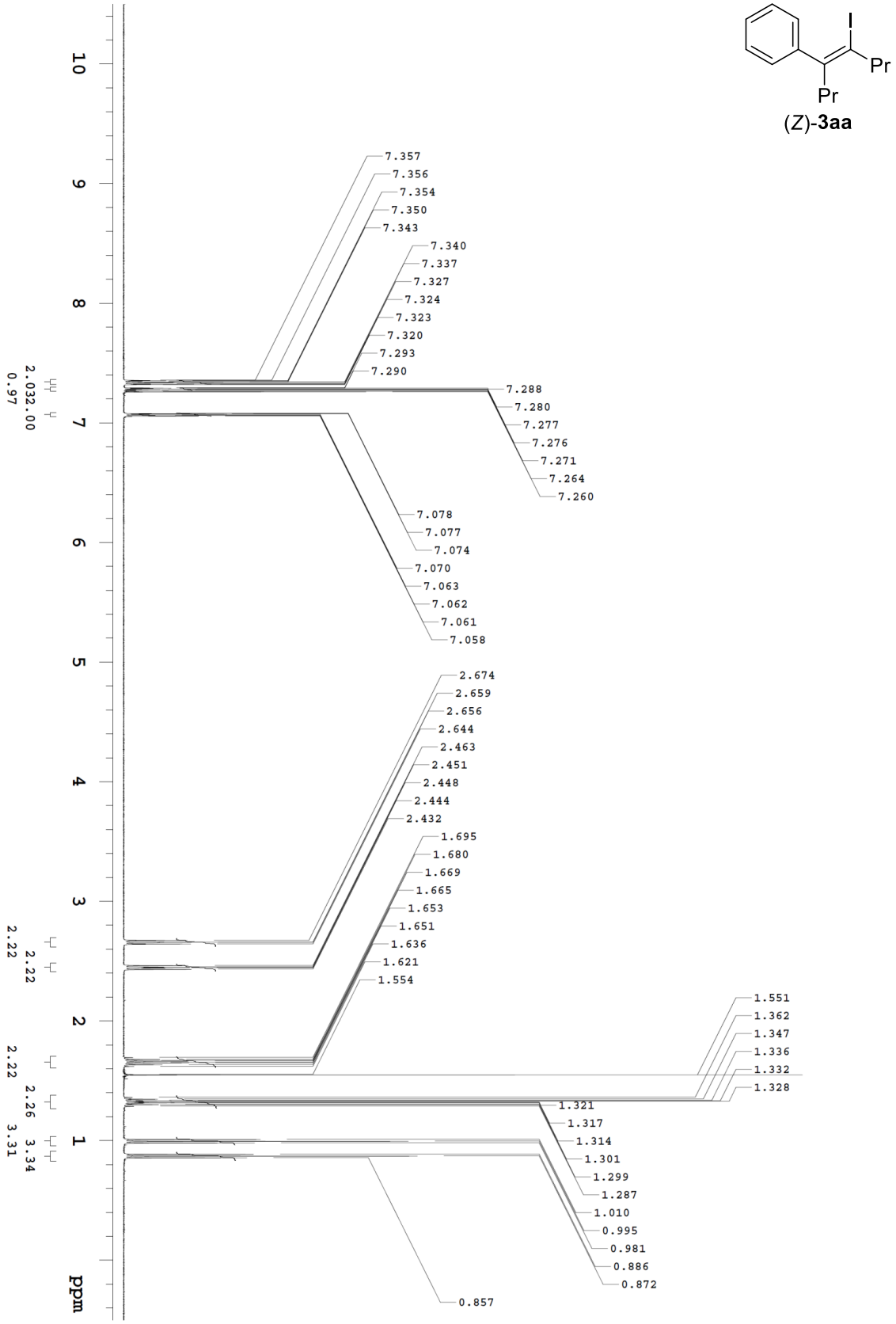
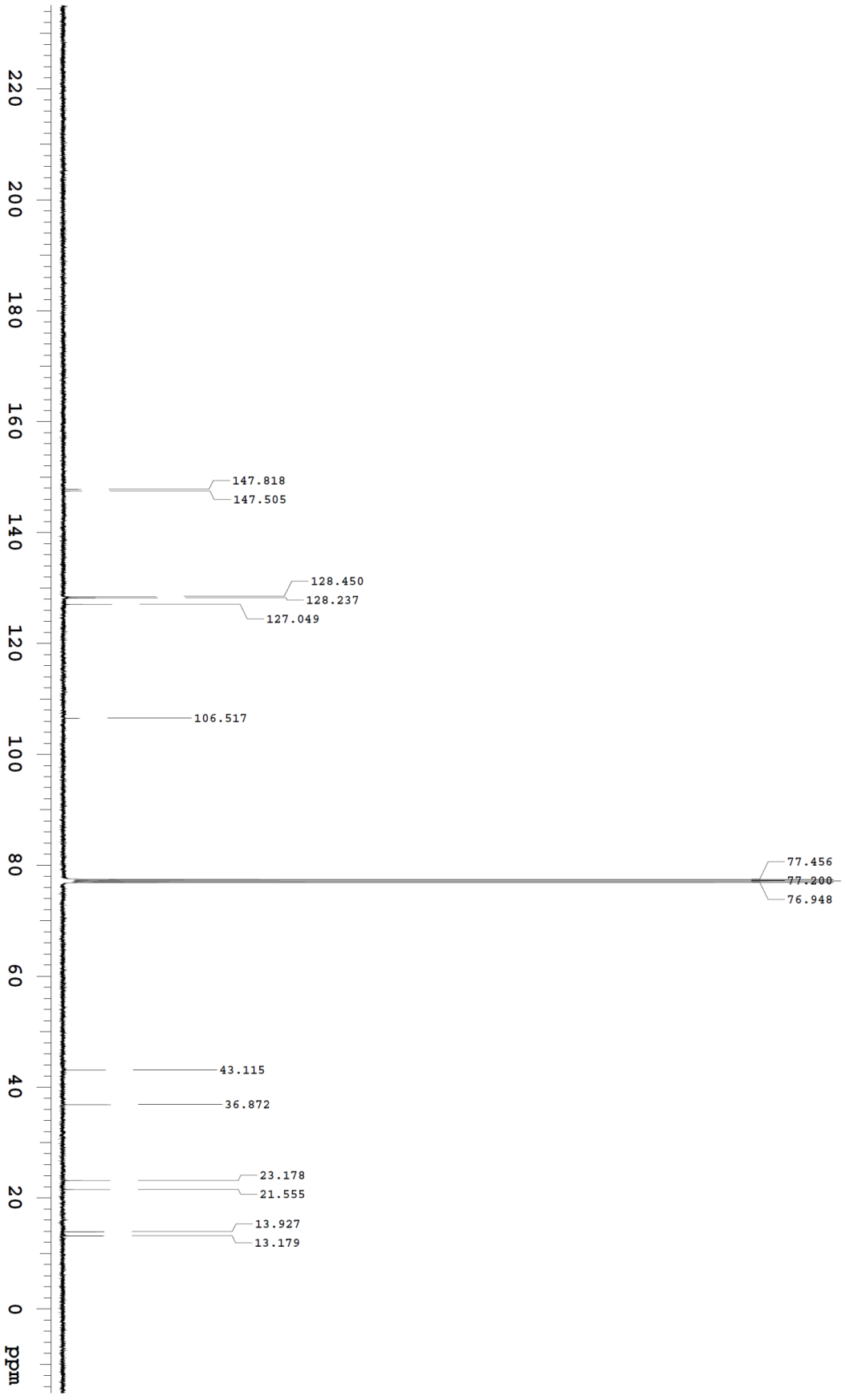
8. NMR Spectra of Products

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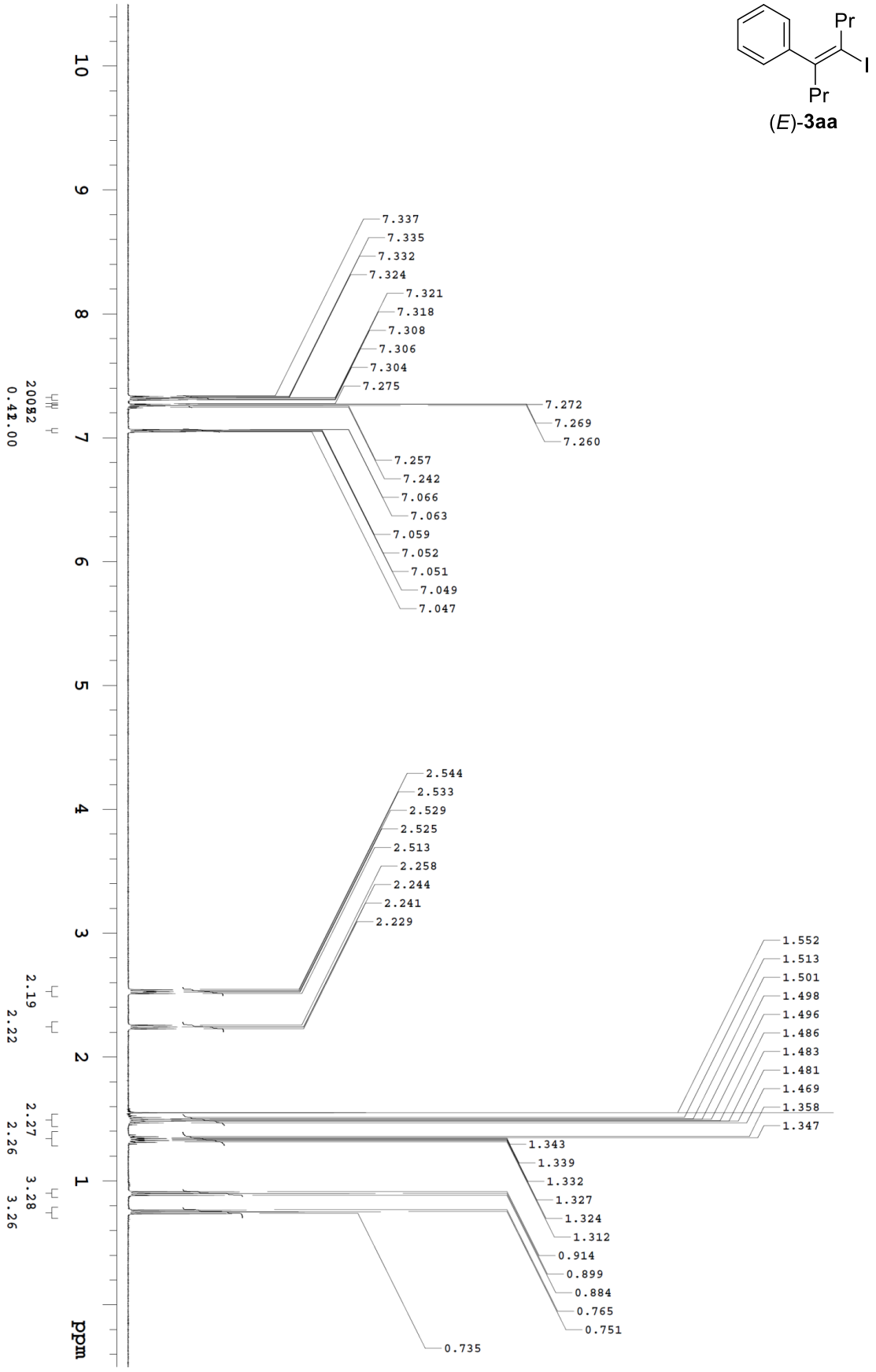
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7.051
7.049
7.047
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2.258
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2.241
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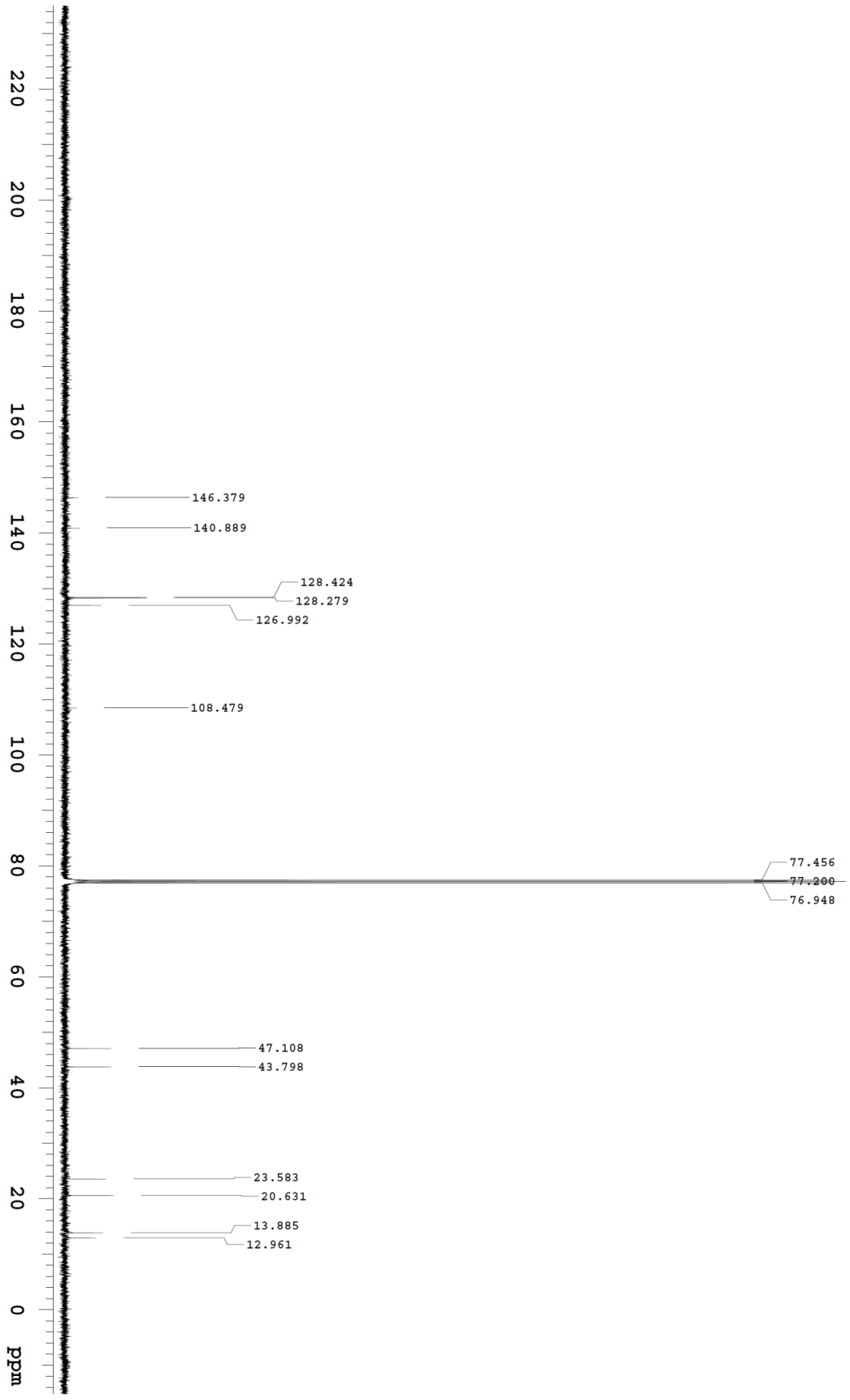
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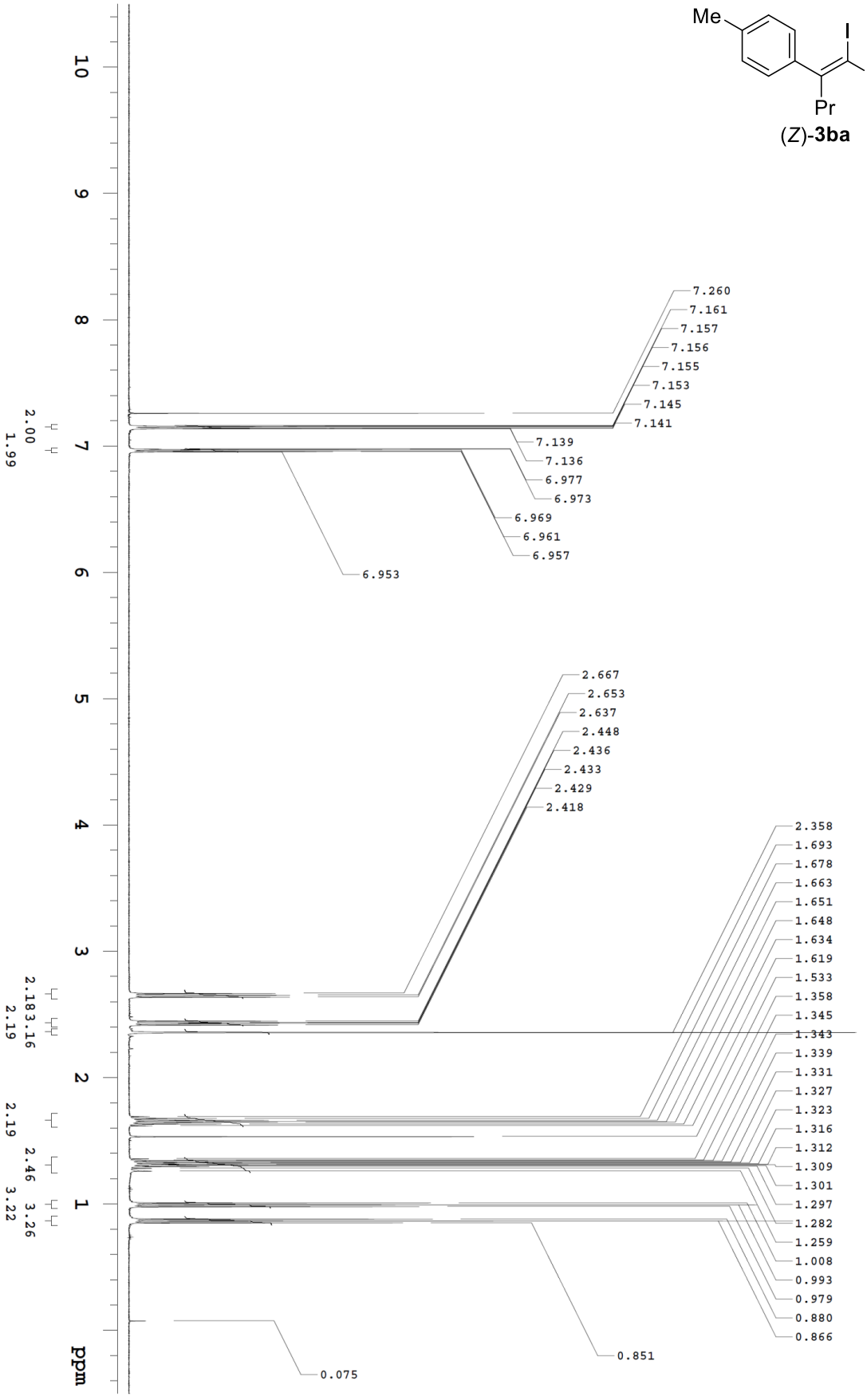
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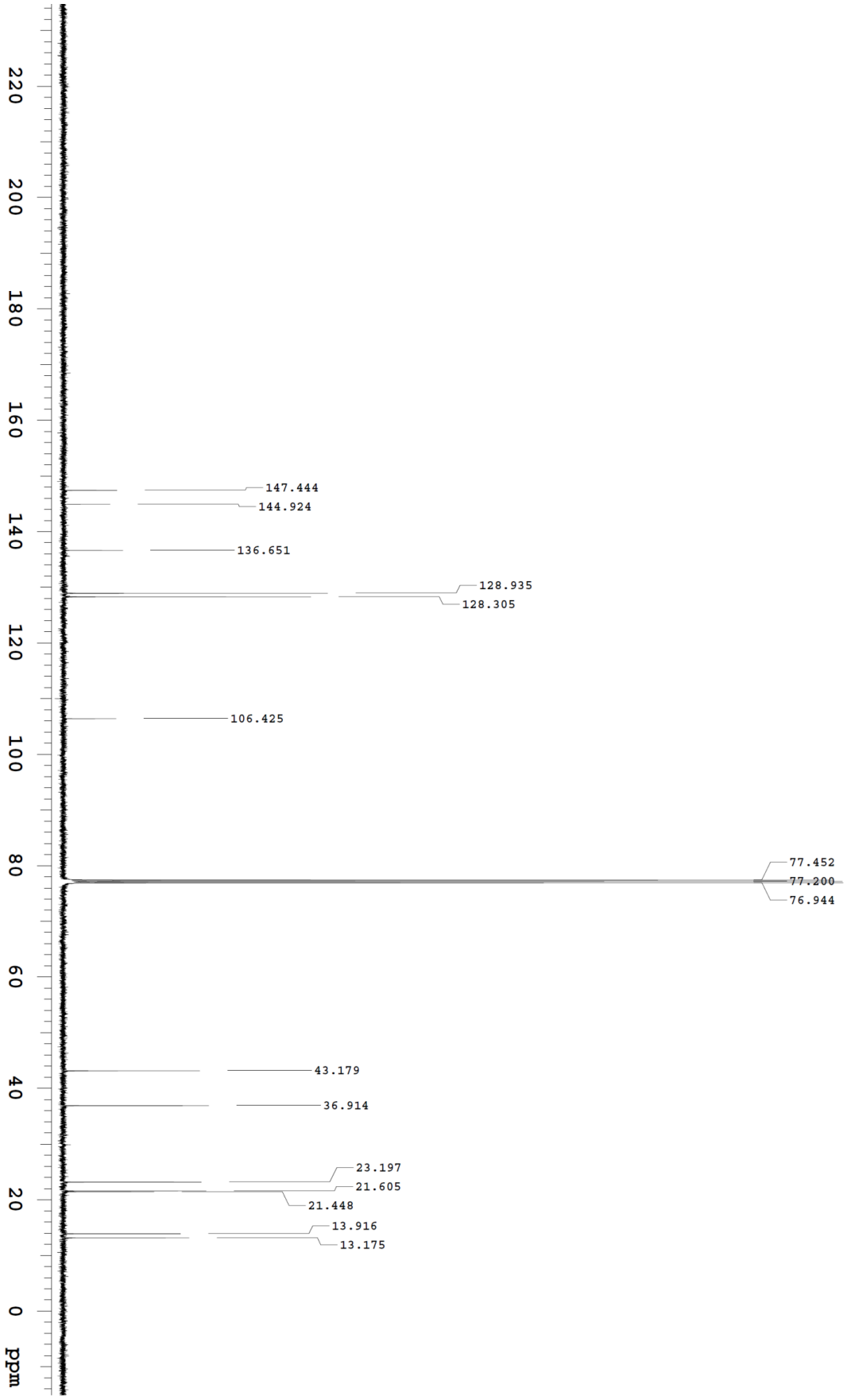
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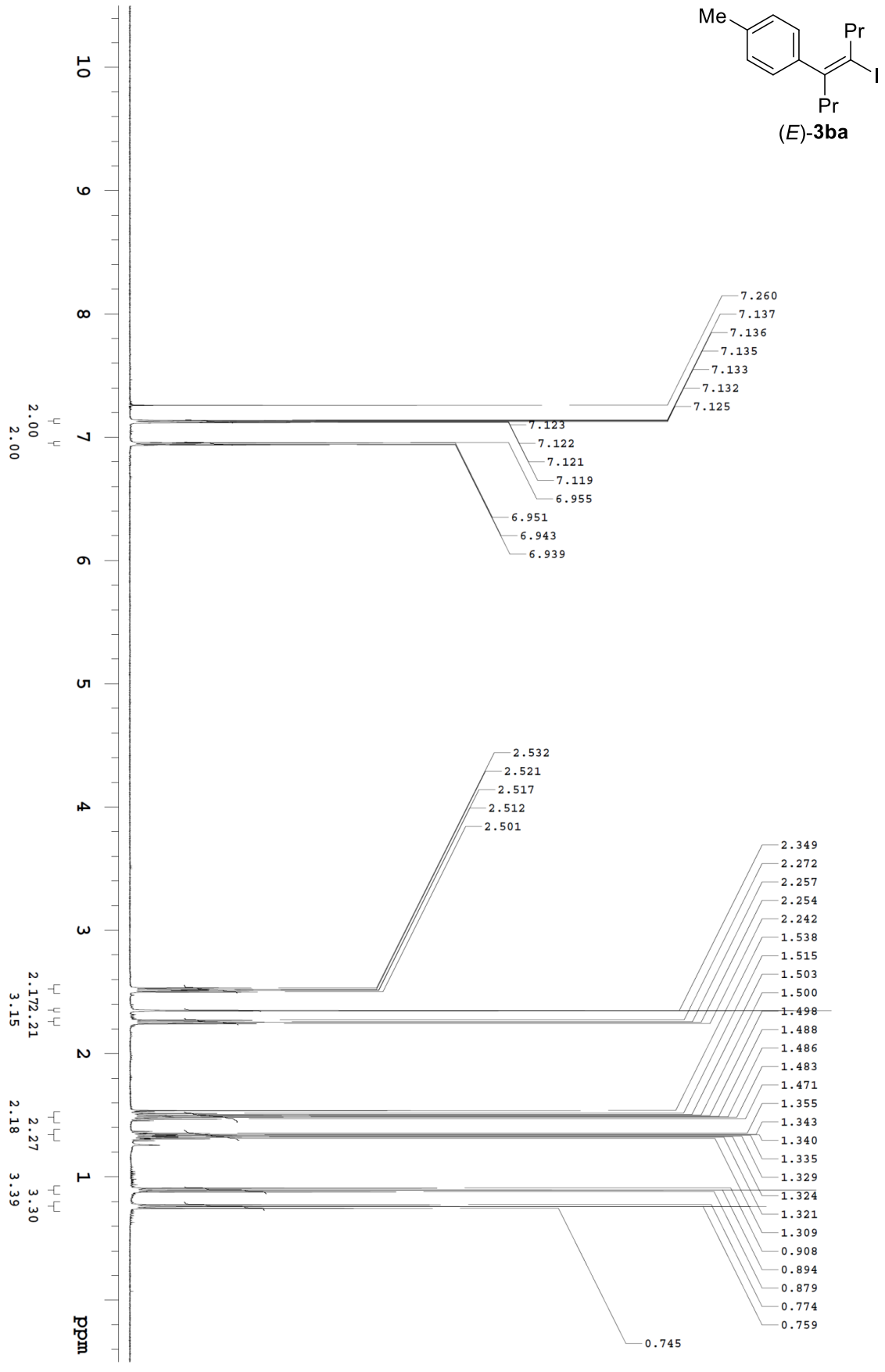
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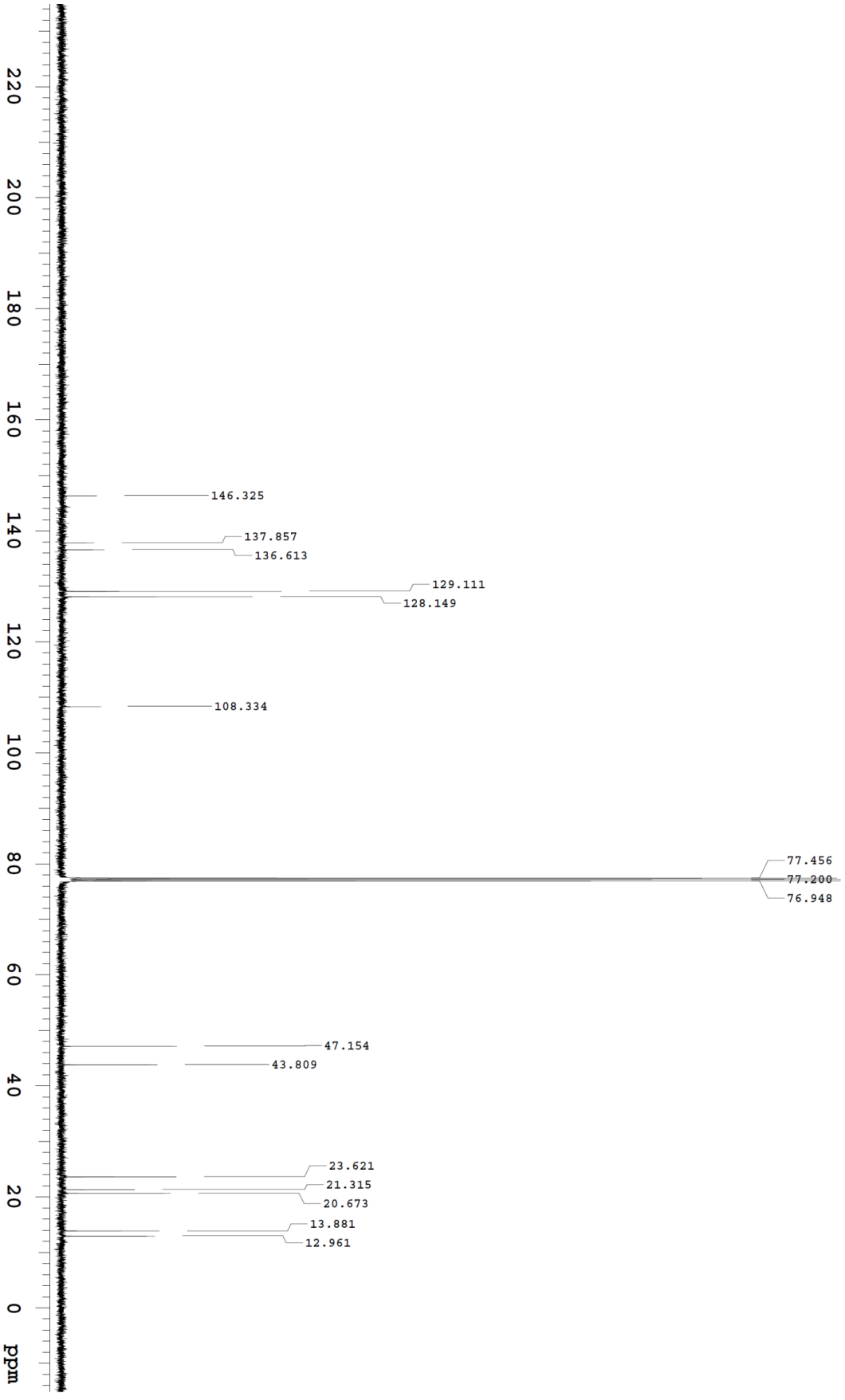
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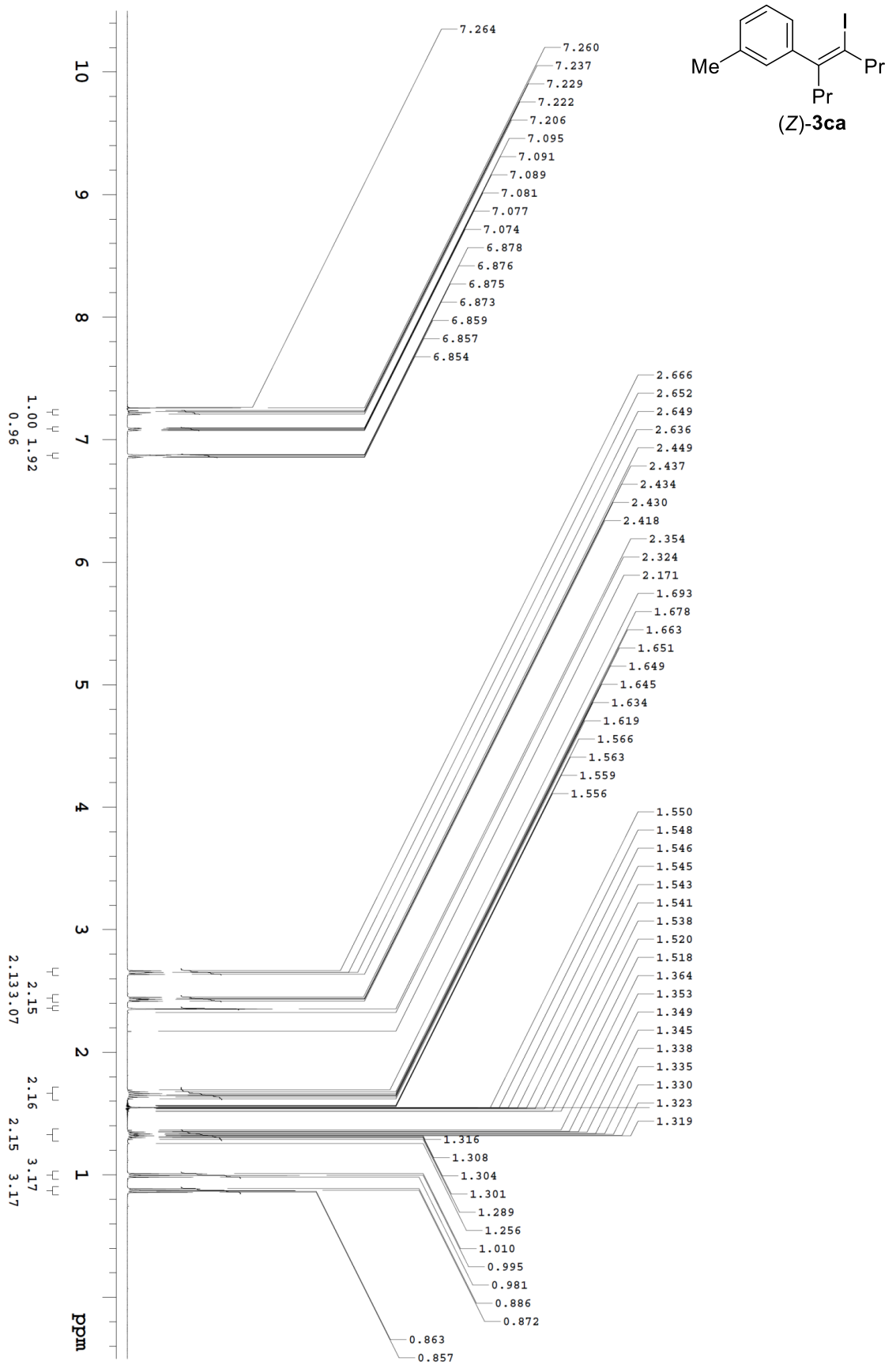
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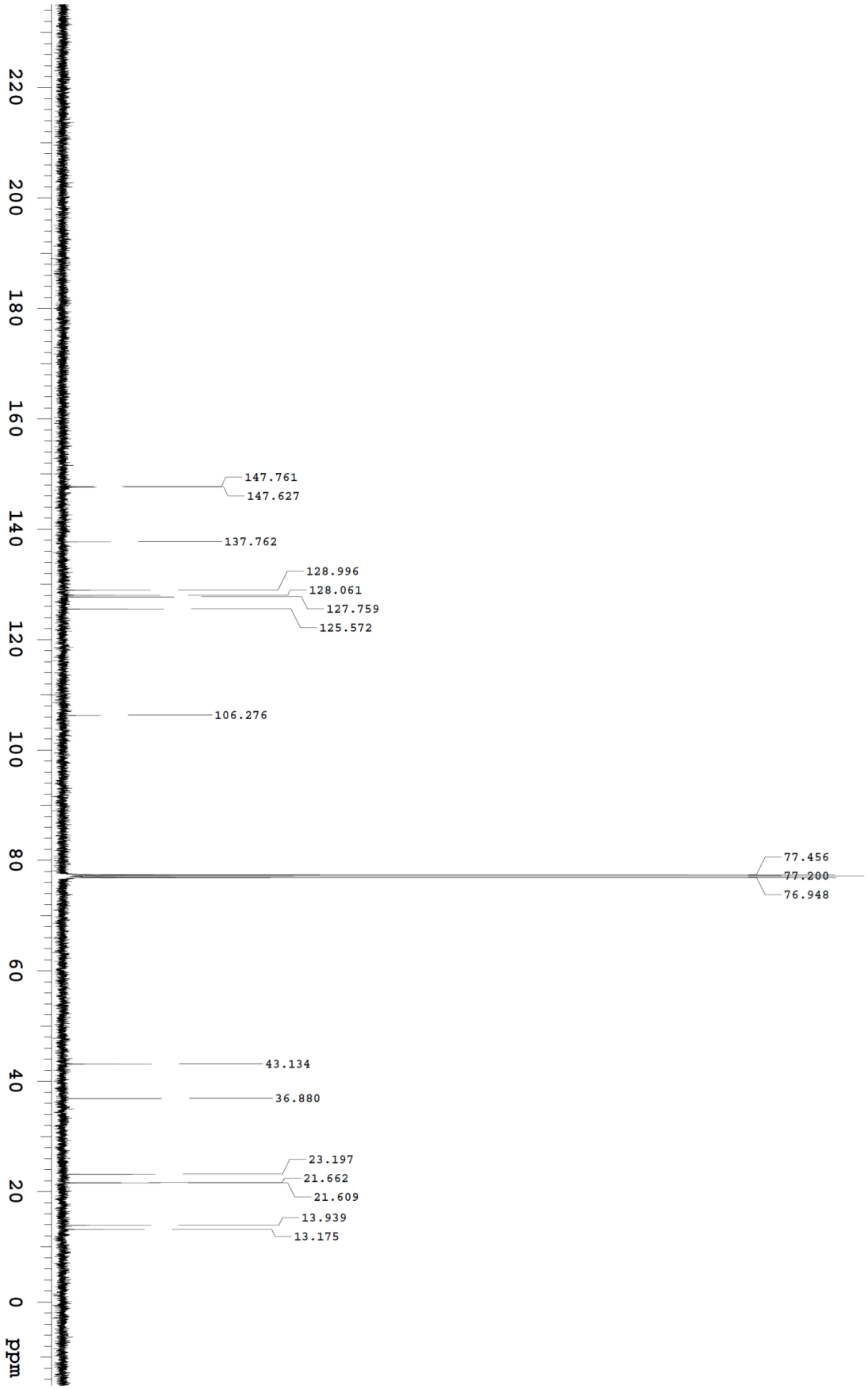
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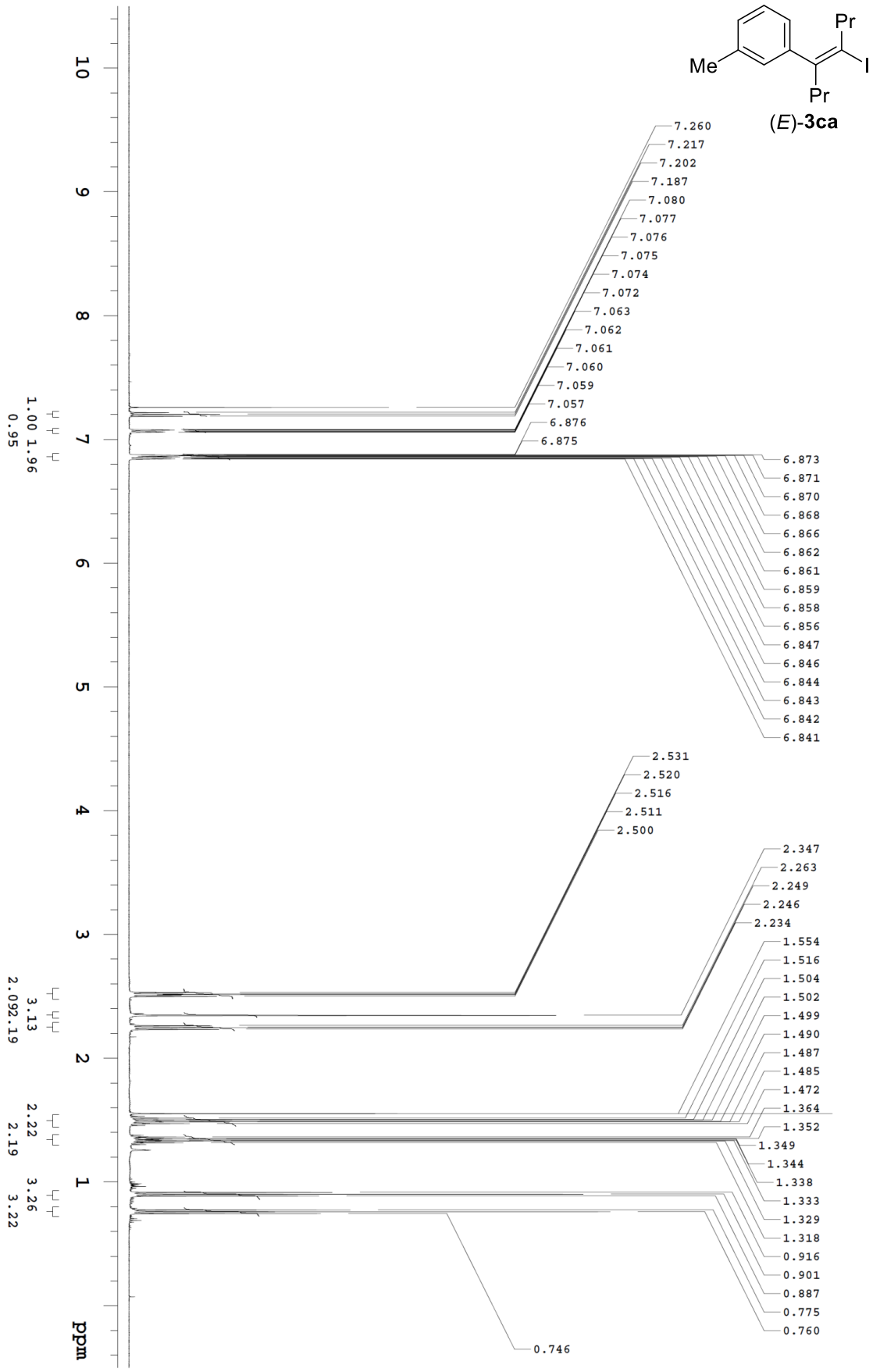
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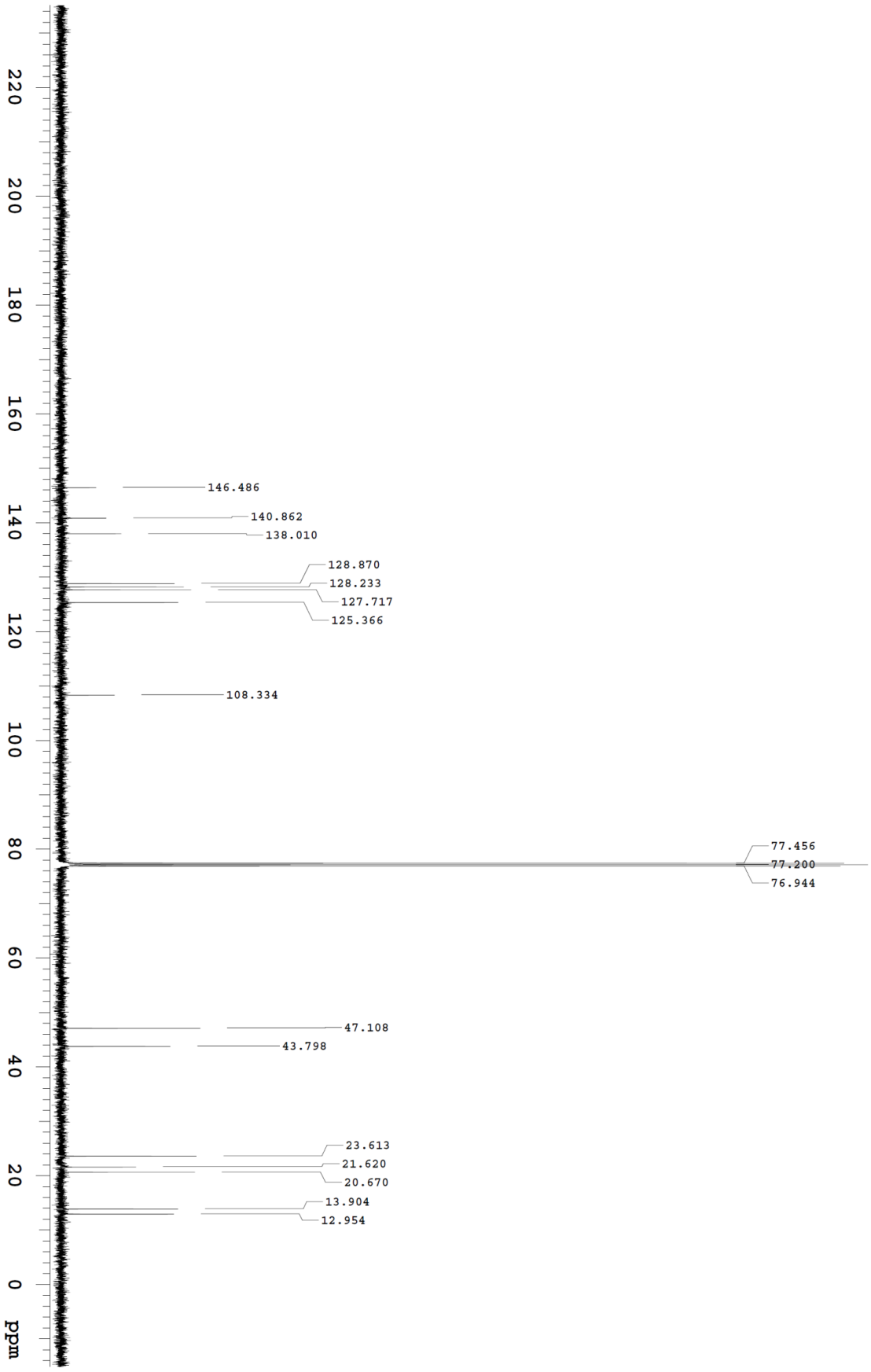
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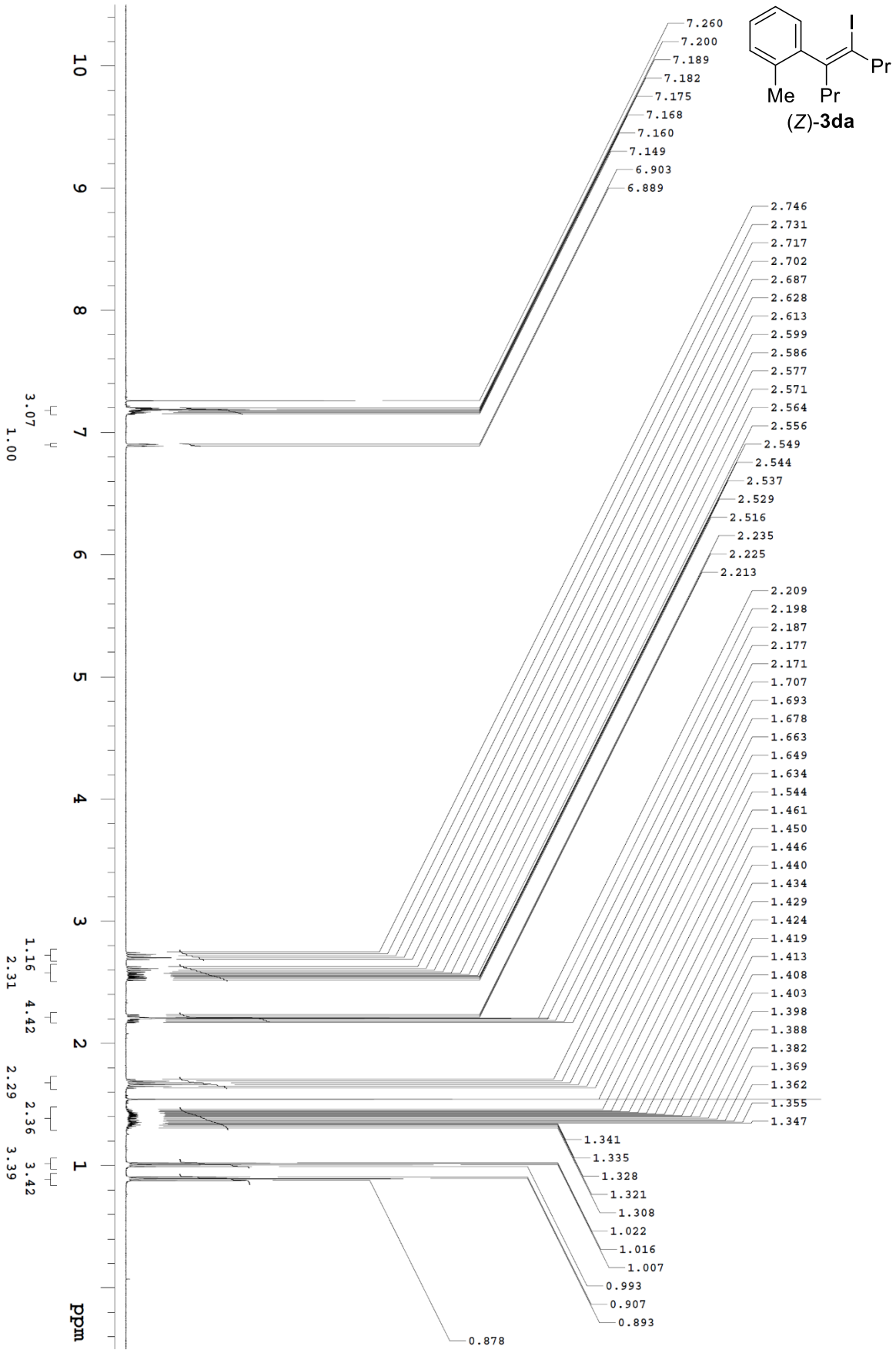
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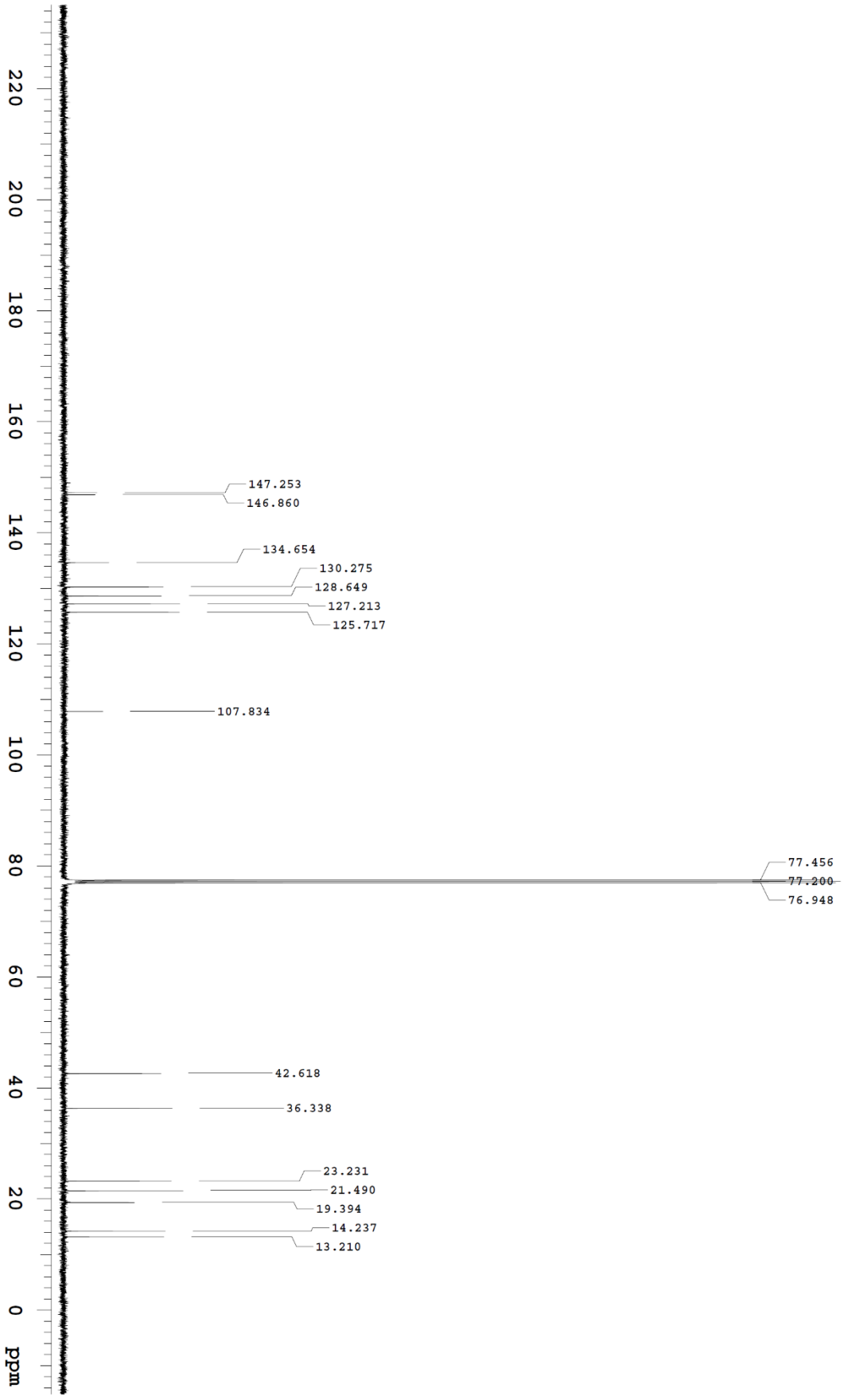
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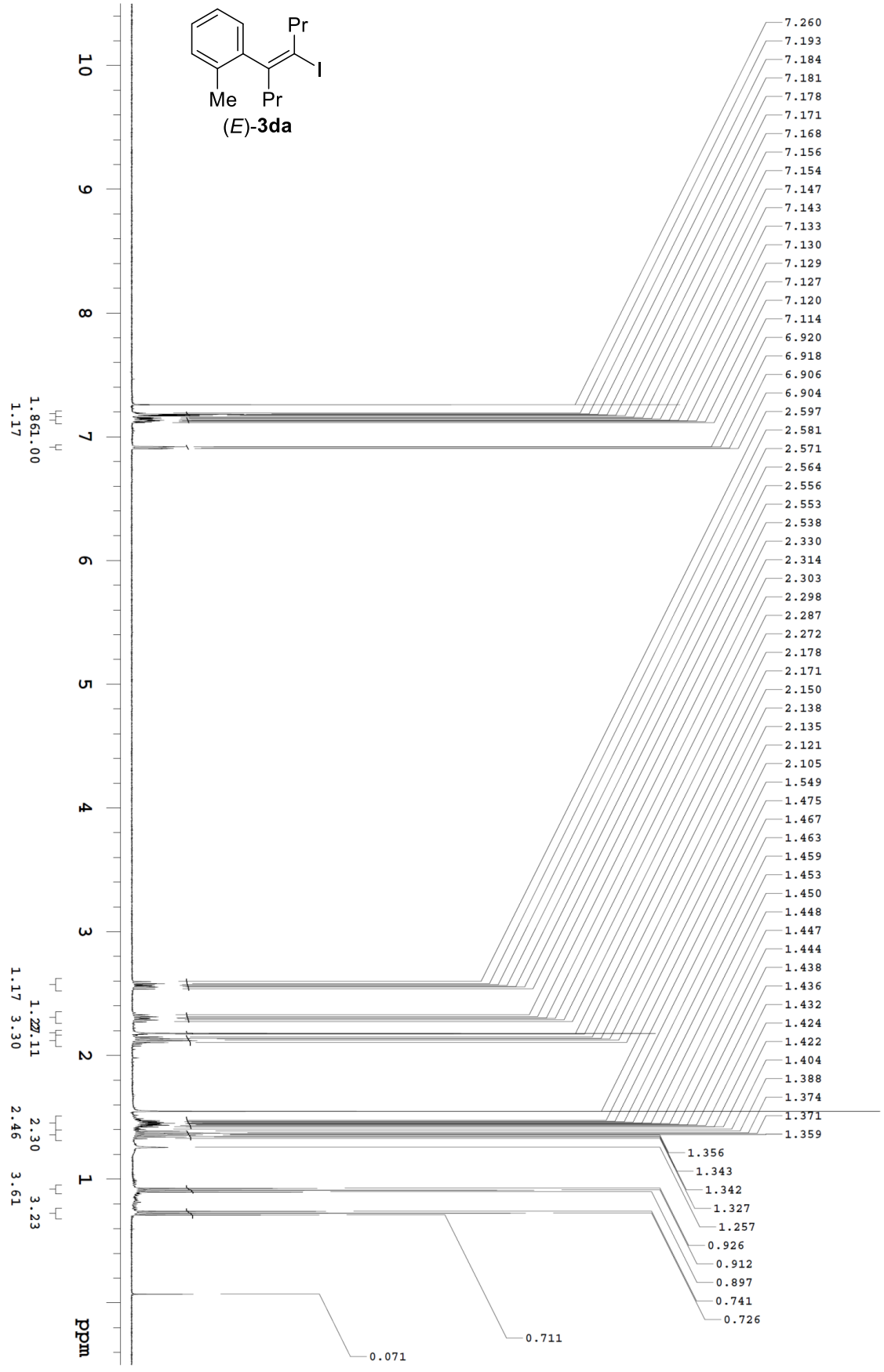
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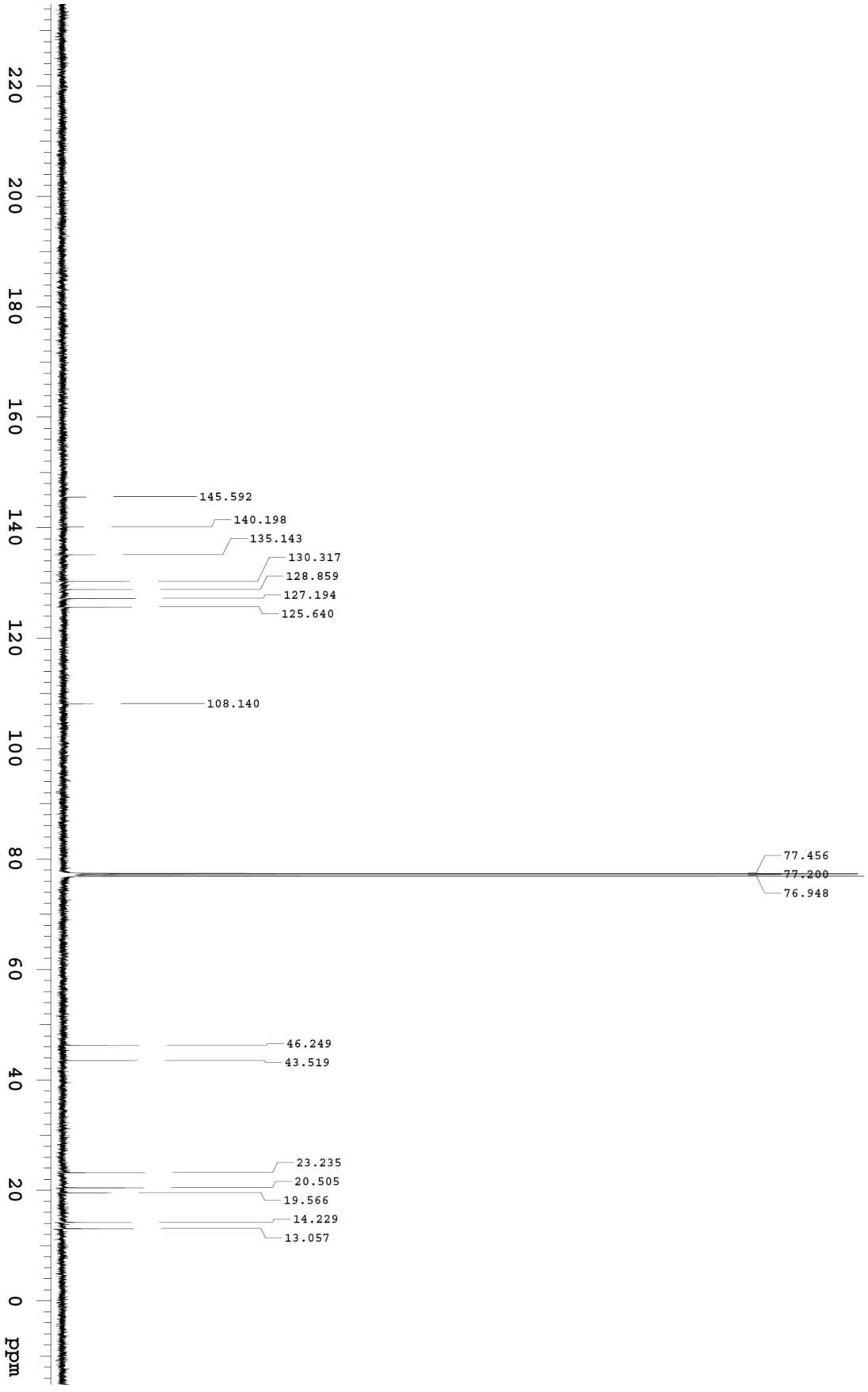
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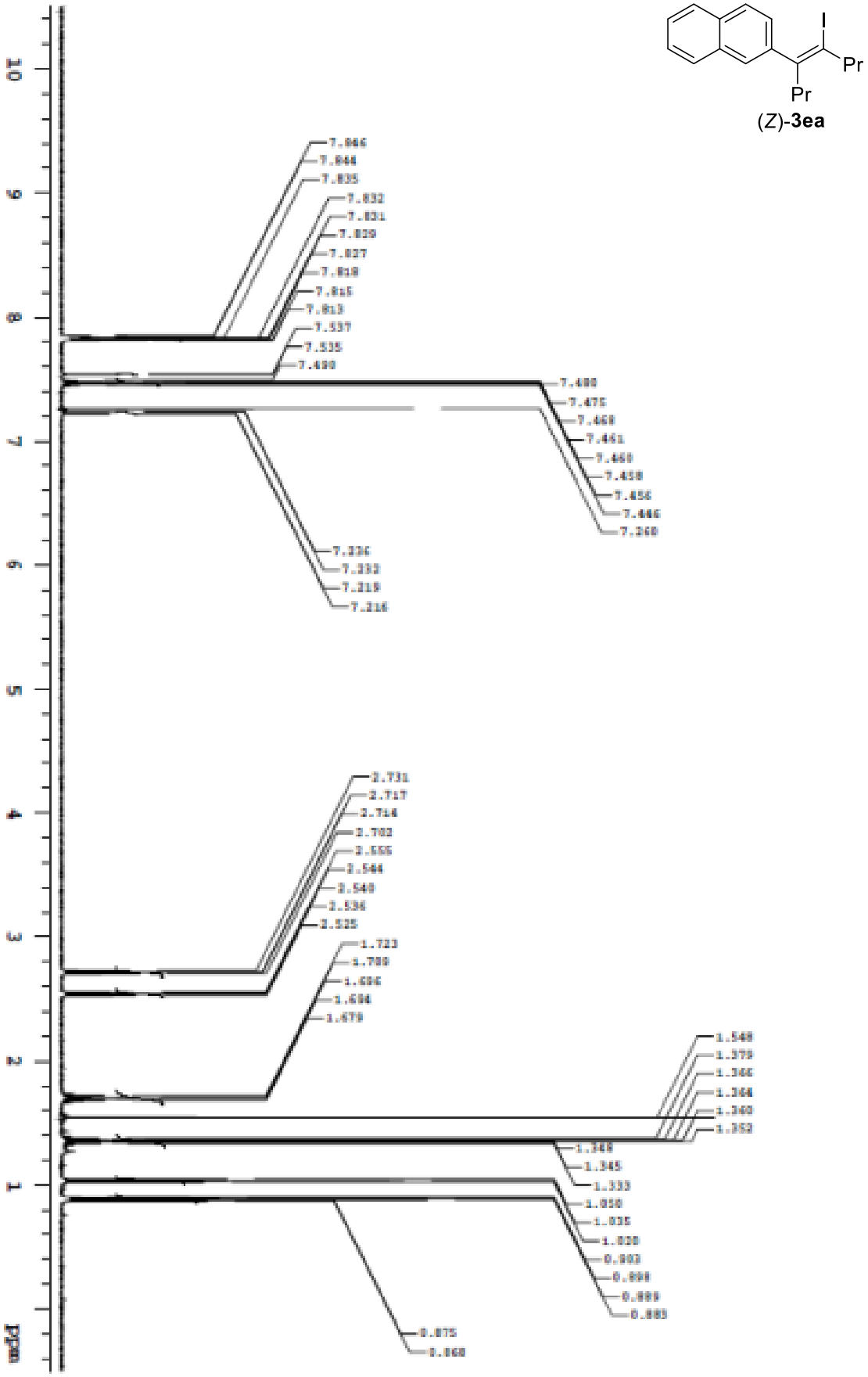
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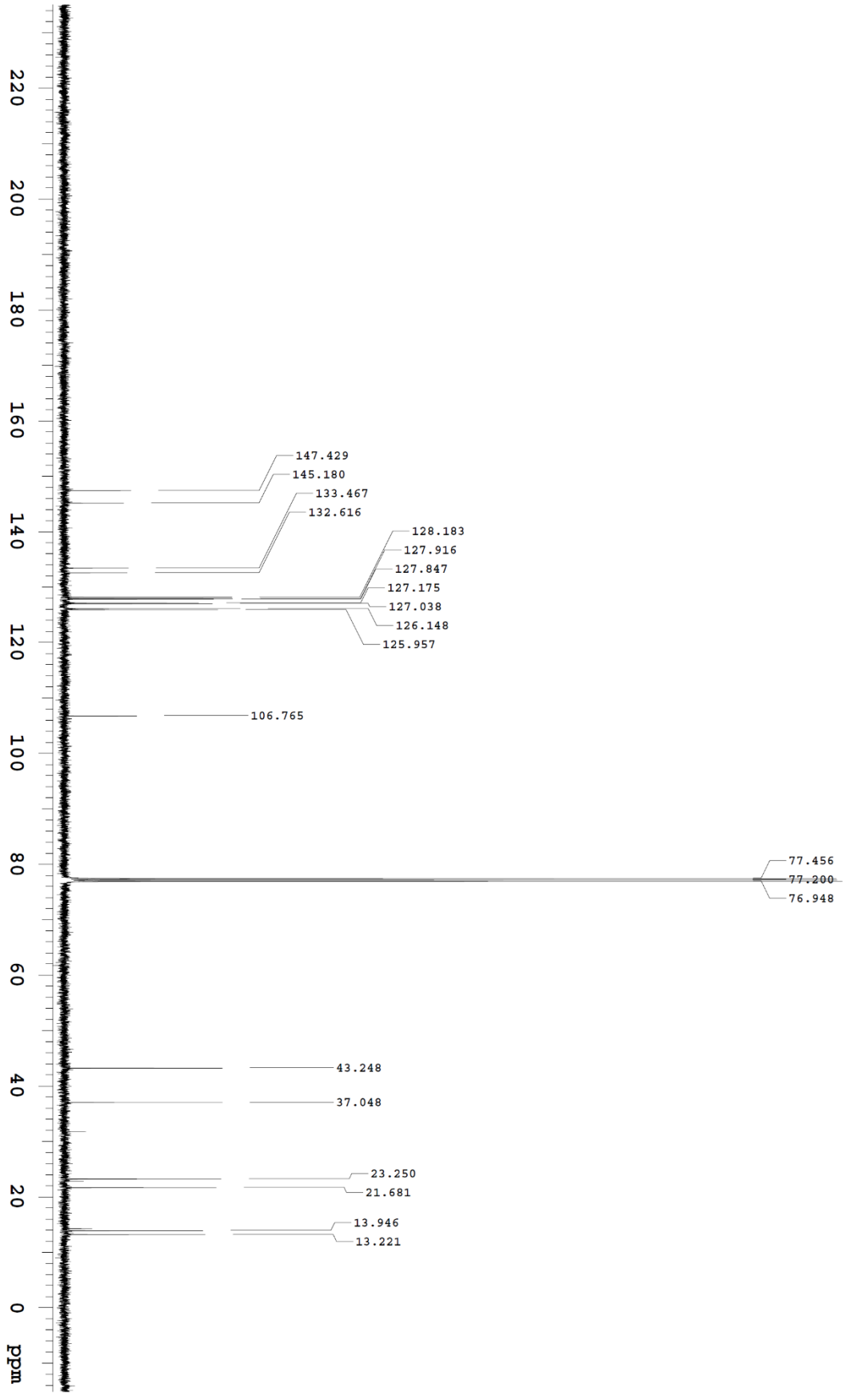
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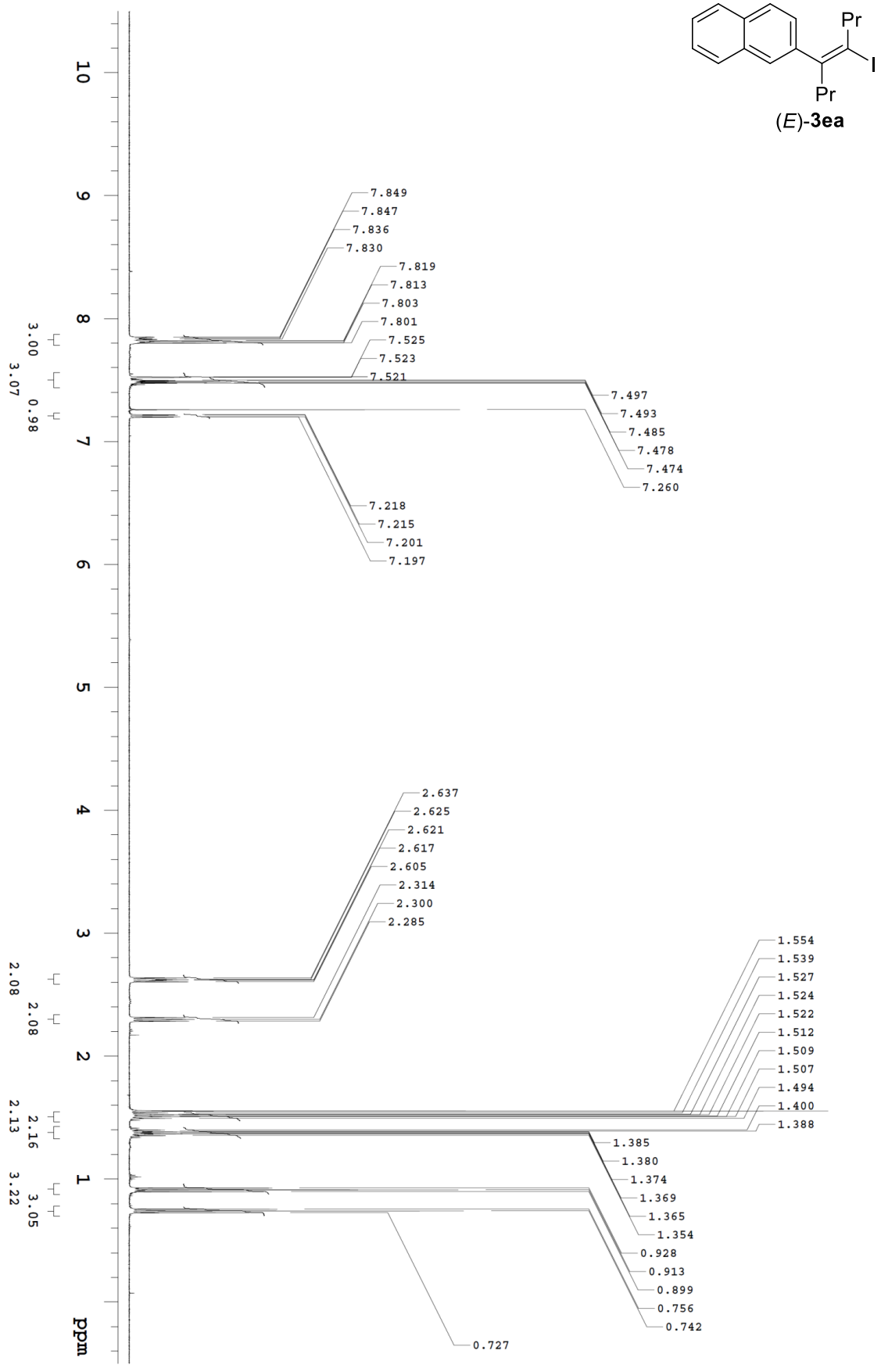
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7.521
7.497
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7.478
7.474
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7.218
7.215
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1.522
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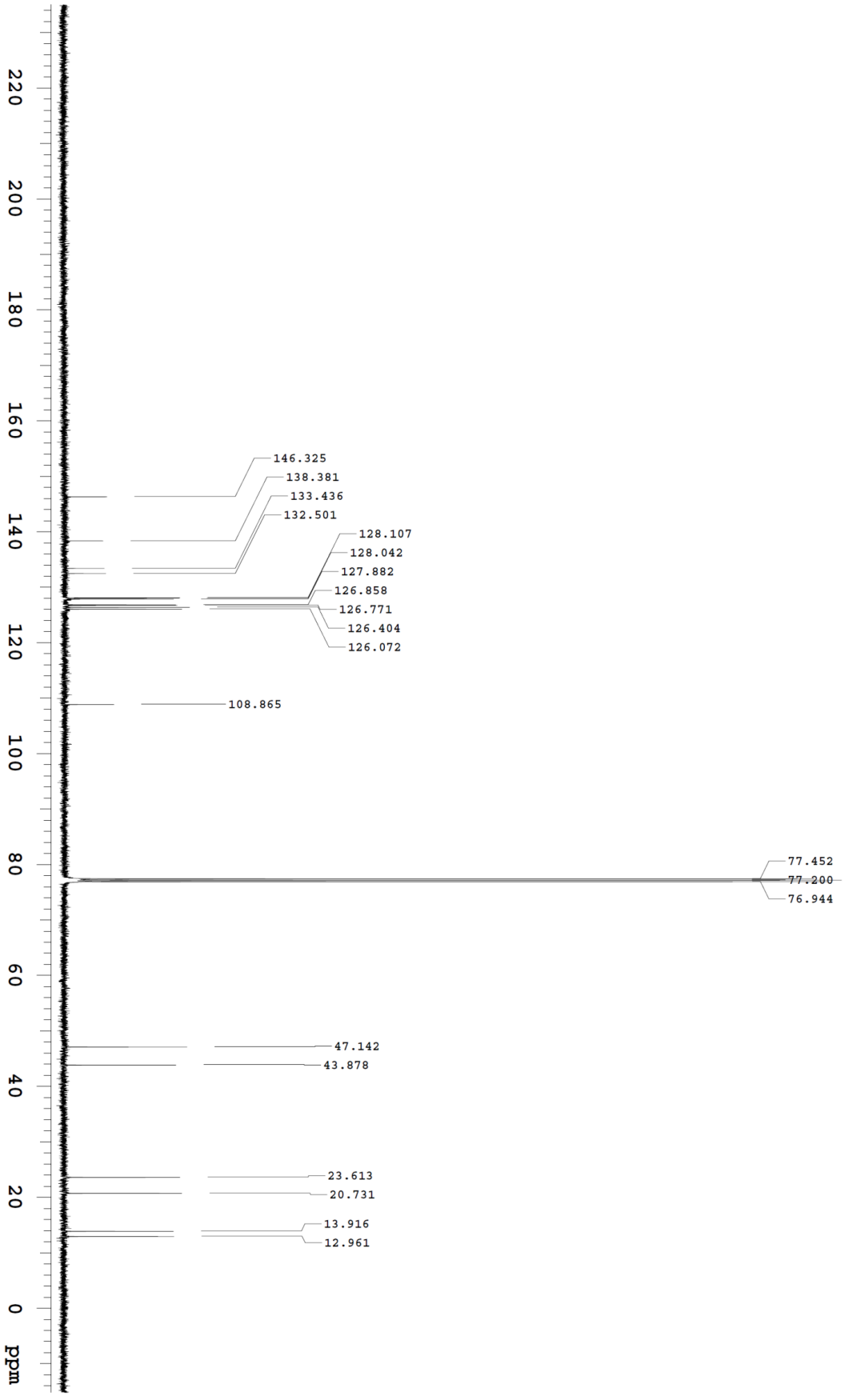
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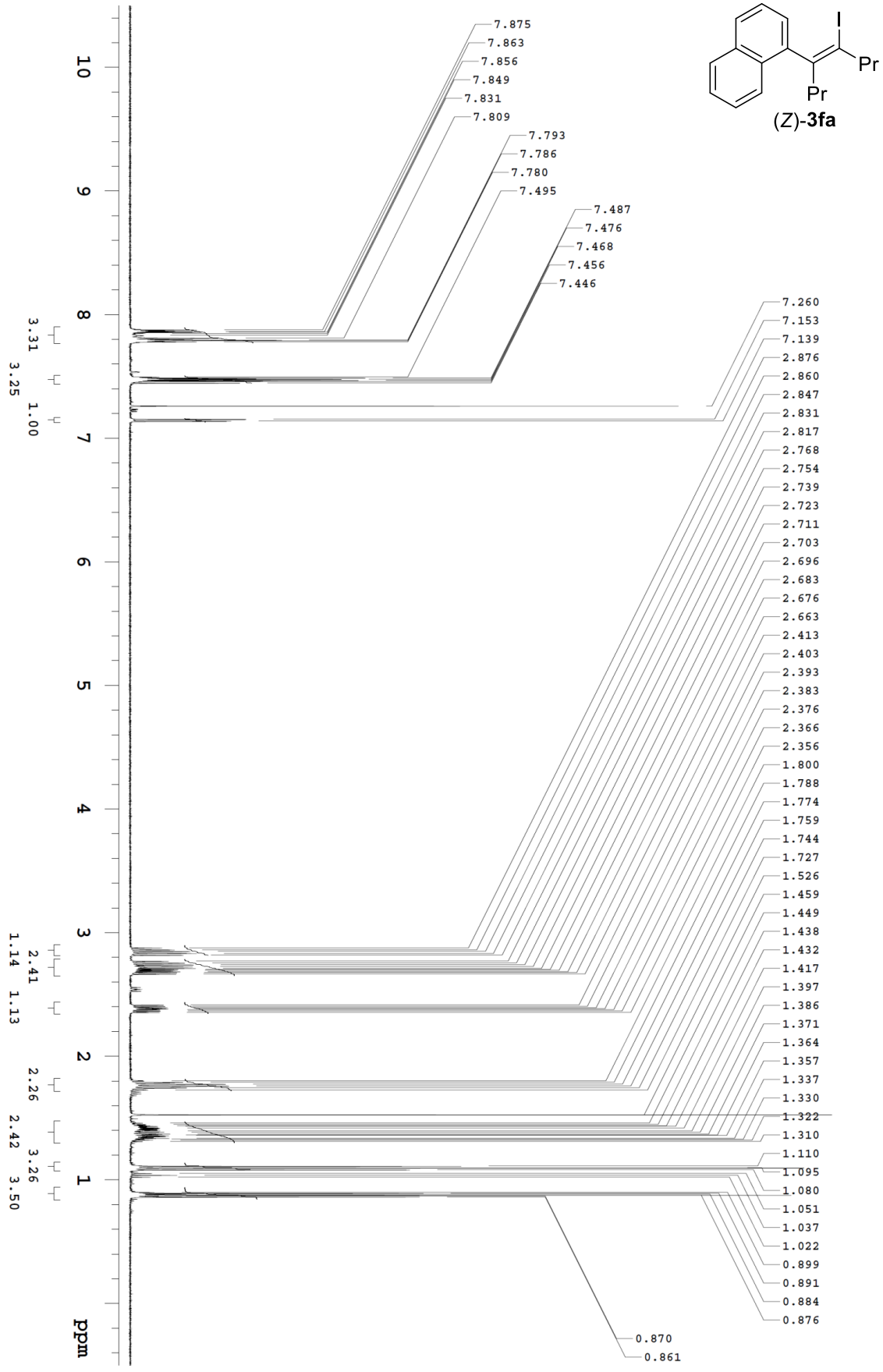
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7.487
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7.468
7.456
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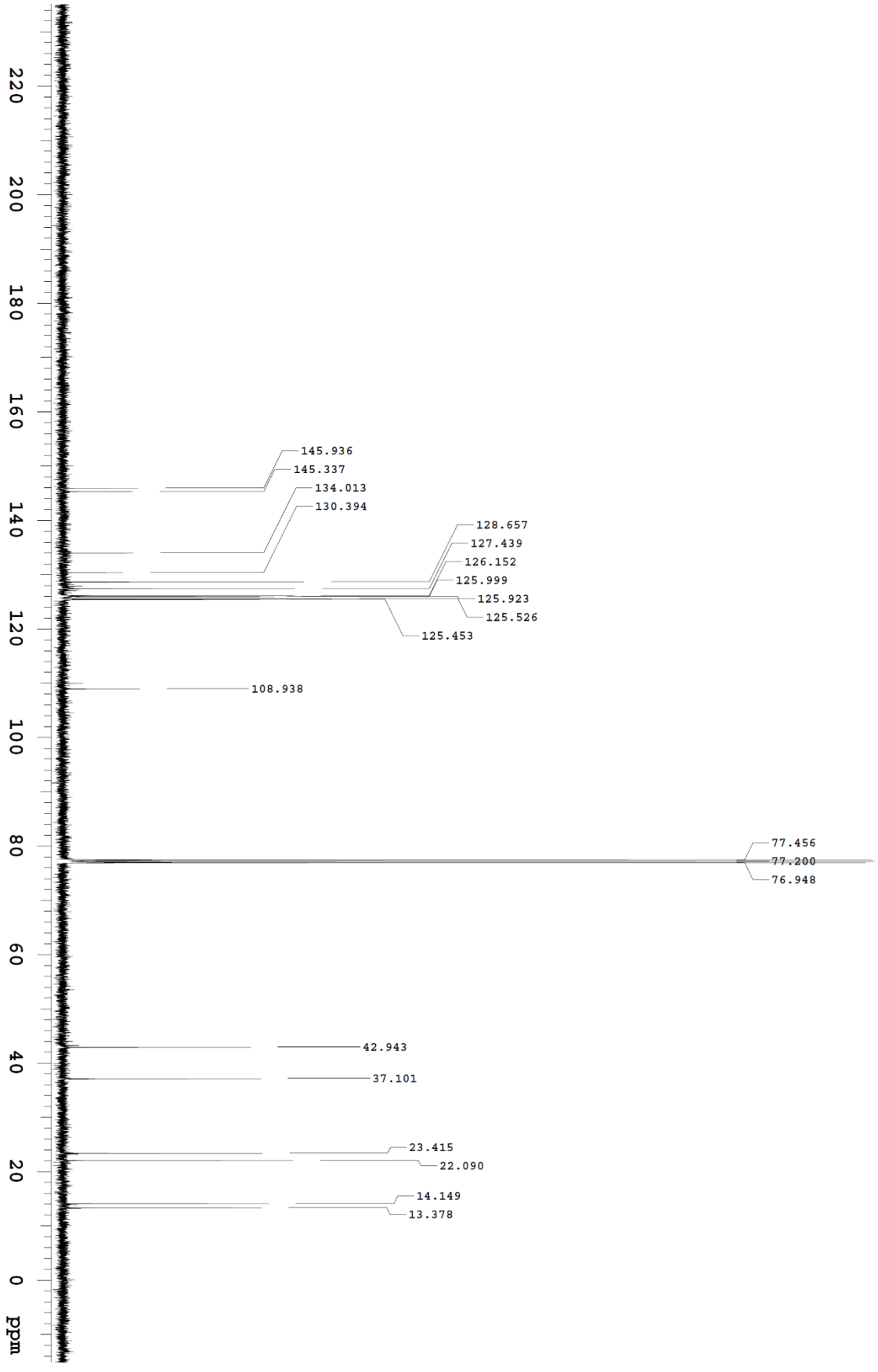
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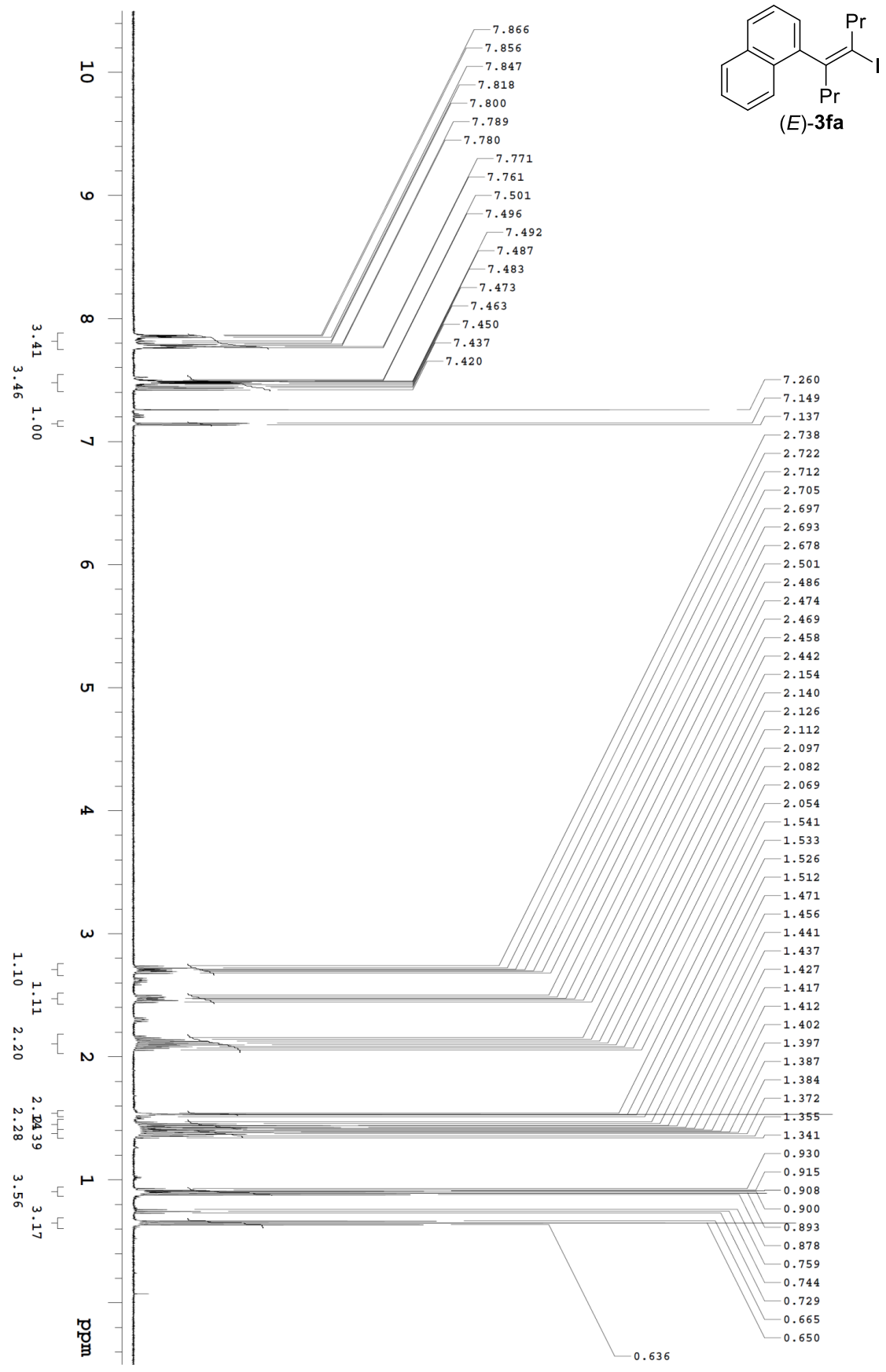
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7.492
7.487
7.483
7.473
7.463
7.450
7.437
7.420
7.260
7.149
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2.722
2.712
2.705
2.697
2.693
2.678
2.501
2.486
2.474
2.469
2.458
2.442
2.154
2.140
2.126
2.112
2.097
2.082
2.069
2.054
1.541
1.533
1.526
1.512
1.471
1.456
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1.402
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1.372
1.355
1.341
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0.908
0.900
0.893
0.878
0.759
0.744
0.729
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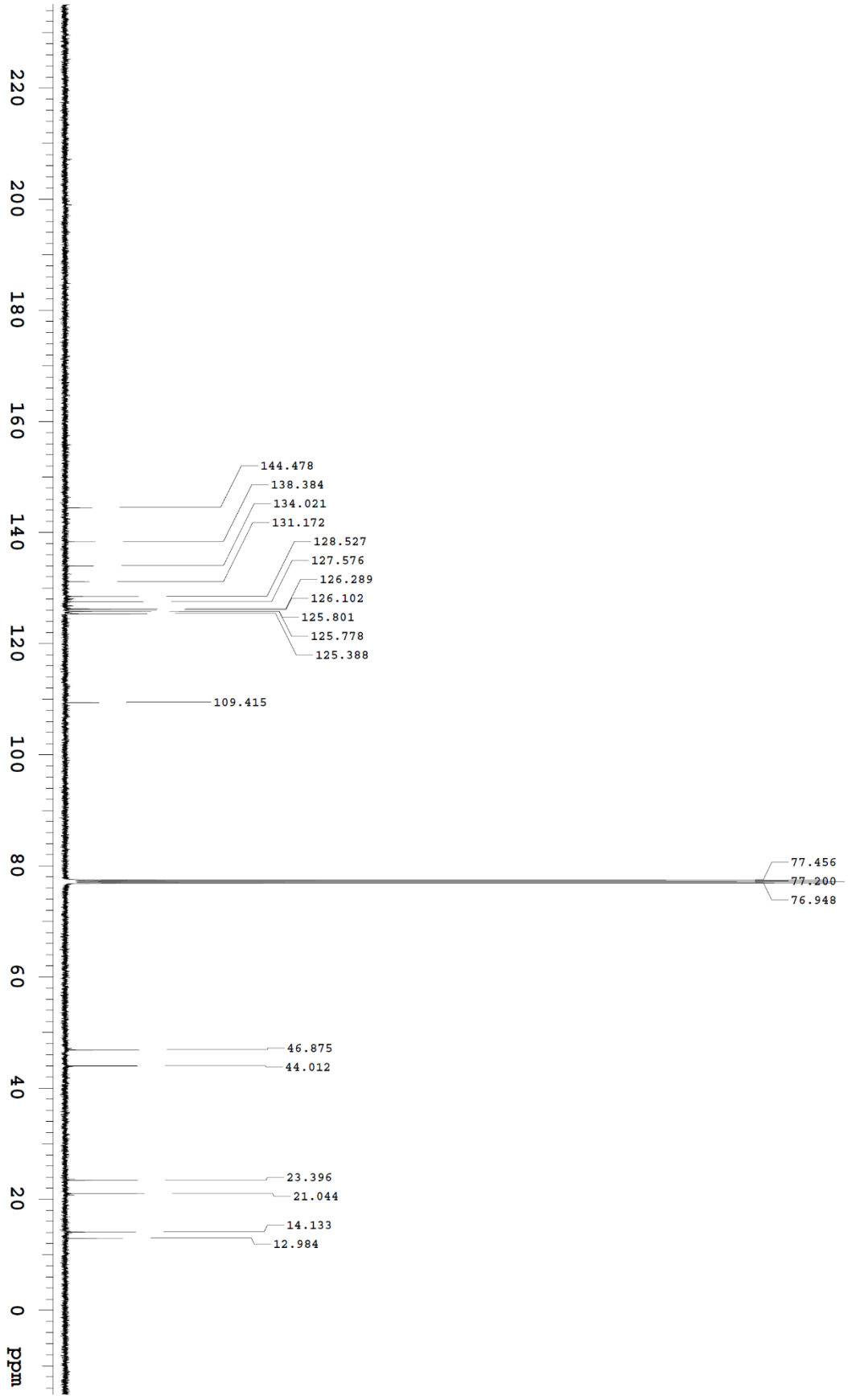
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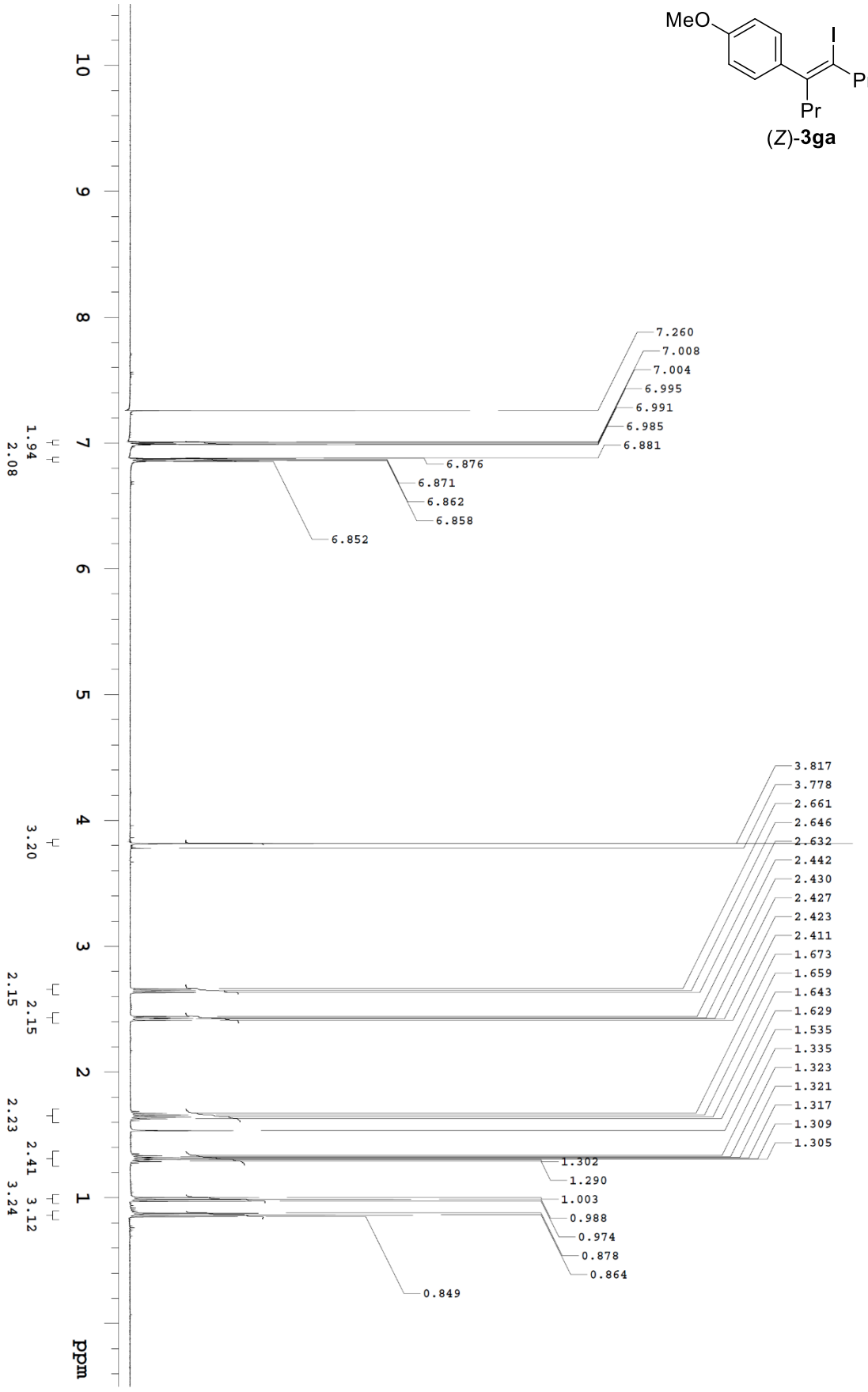
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6.871
6.862
6.858
6.852
3.817
3.778
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2.646
2.632
2.442
2.430
2.427
2.423
2.411
1.673
1.659
1.643
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1.335
1.323
1.321
1.317
1.309
1.305
1.302
1.290
1.003
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0.974
0.878
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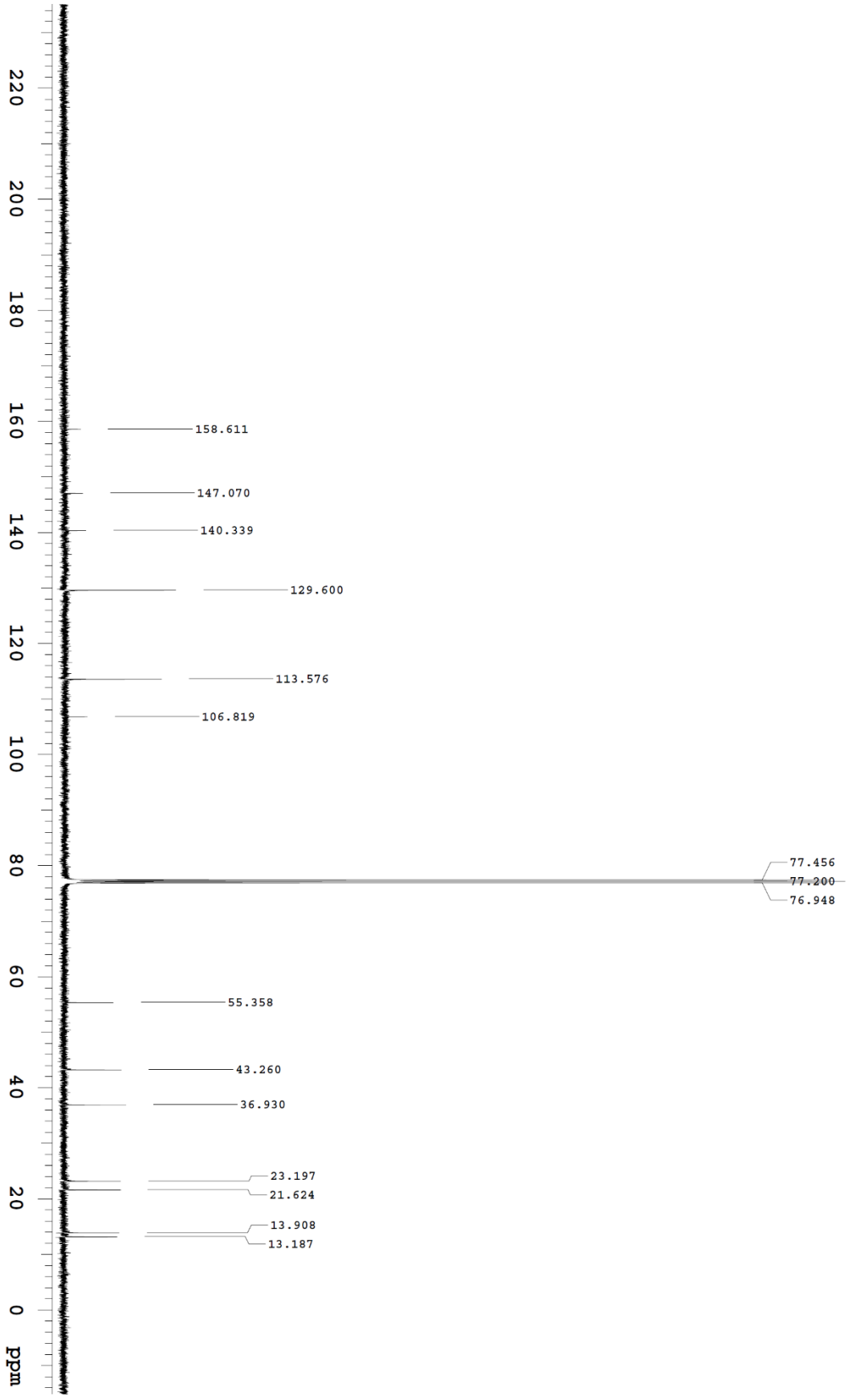
2.23
2.41
3.24
3.12
ppm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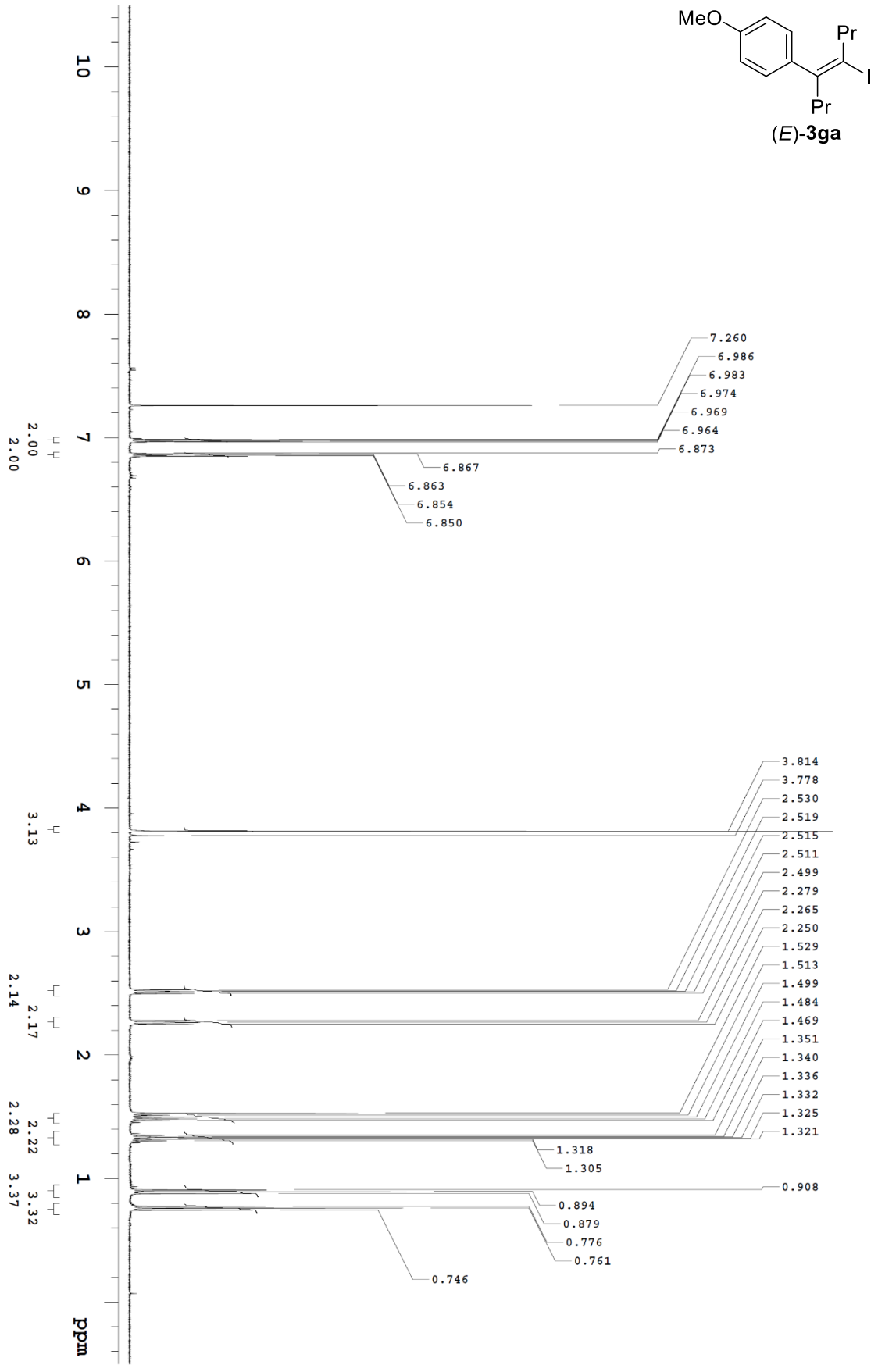
13.187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6.854
6.850
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2.515
2.511
2.499
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1.499
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1.321
1.318
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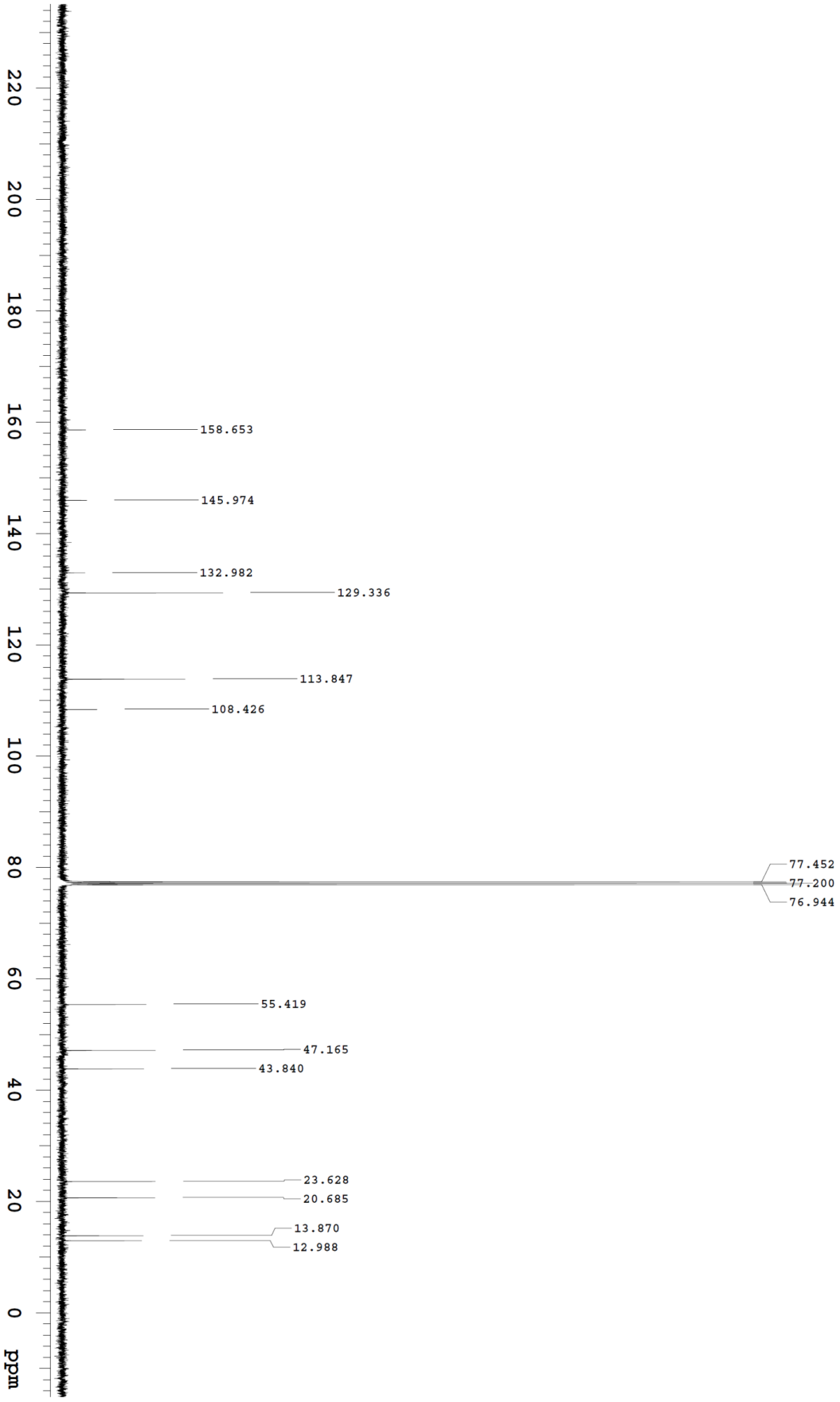
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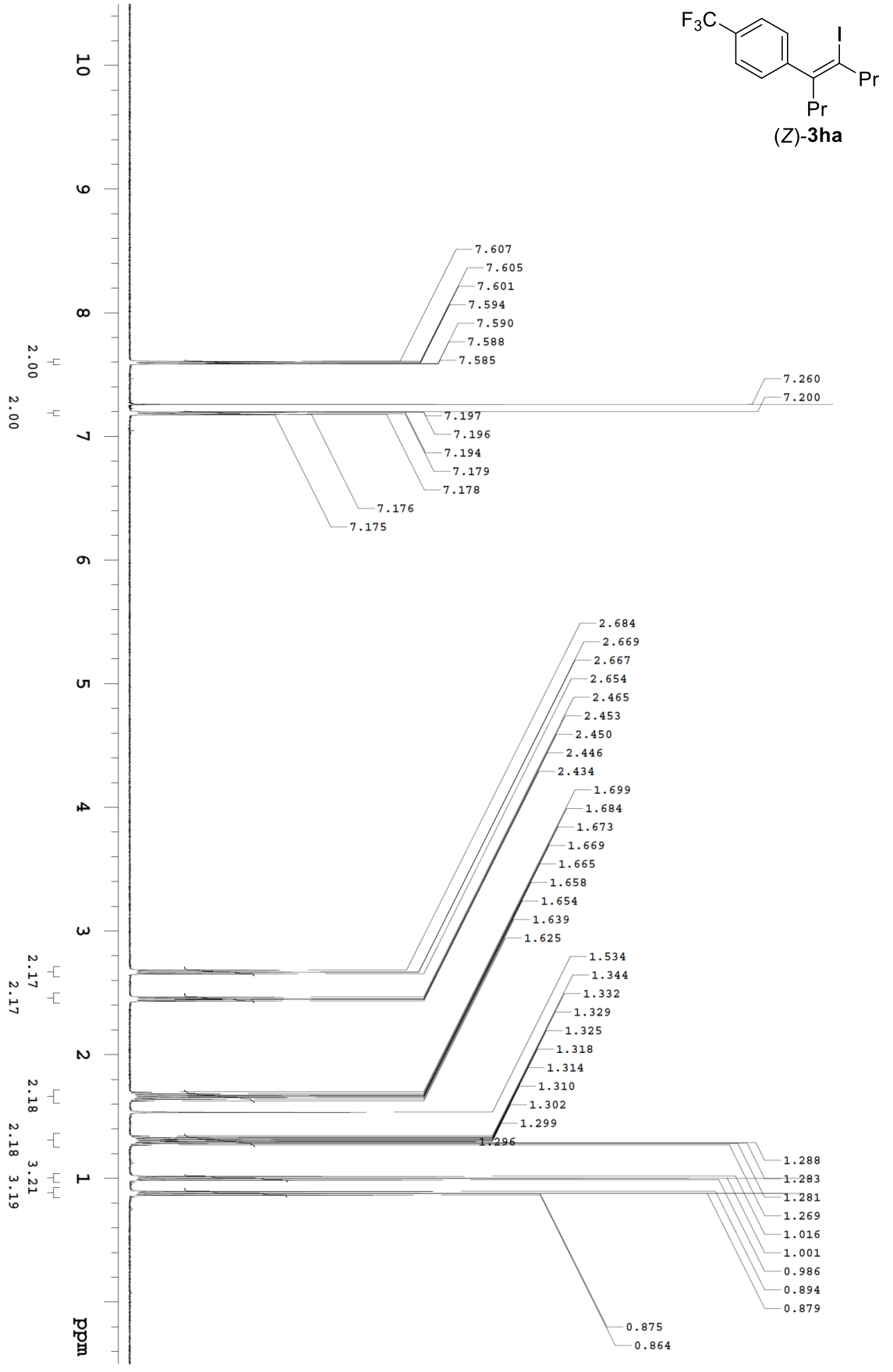
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7.196
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7.179
7.178
7.176
7.175
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2.669
2.667
2.654
2.465
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2.446
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1.684
1.673
1.669
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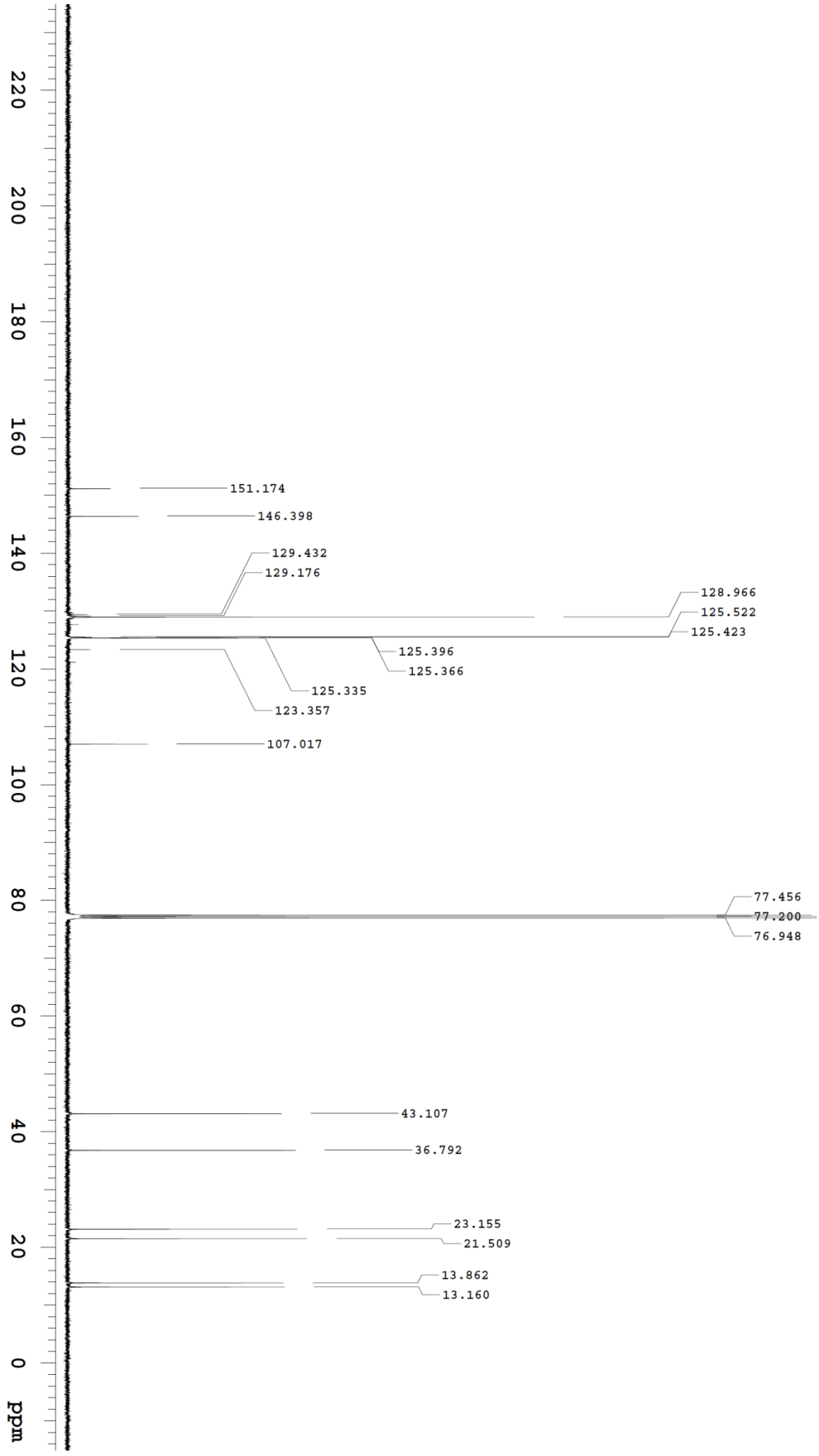
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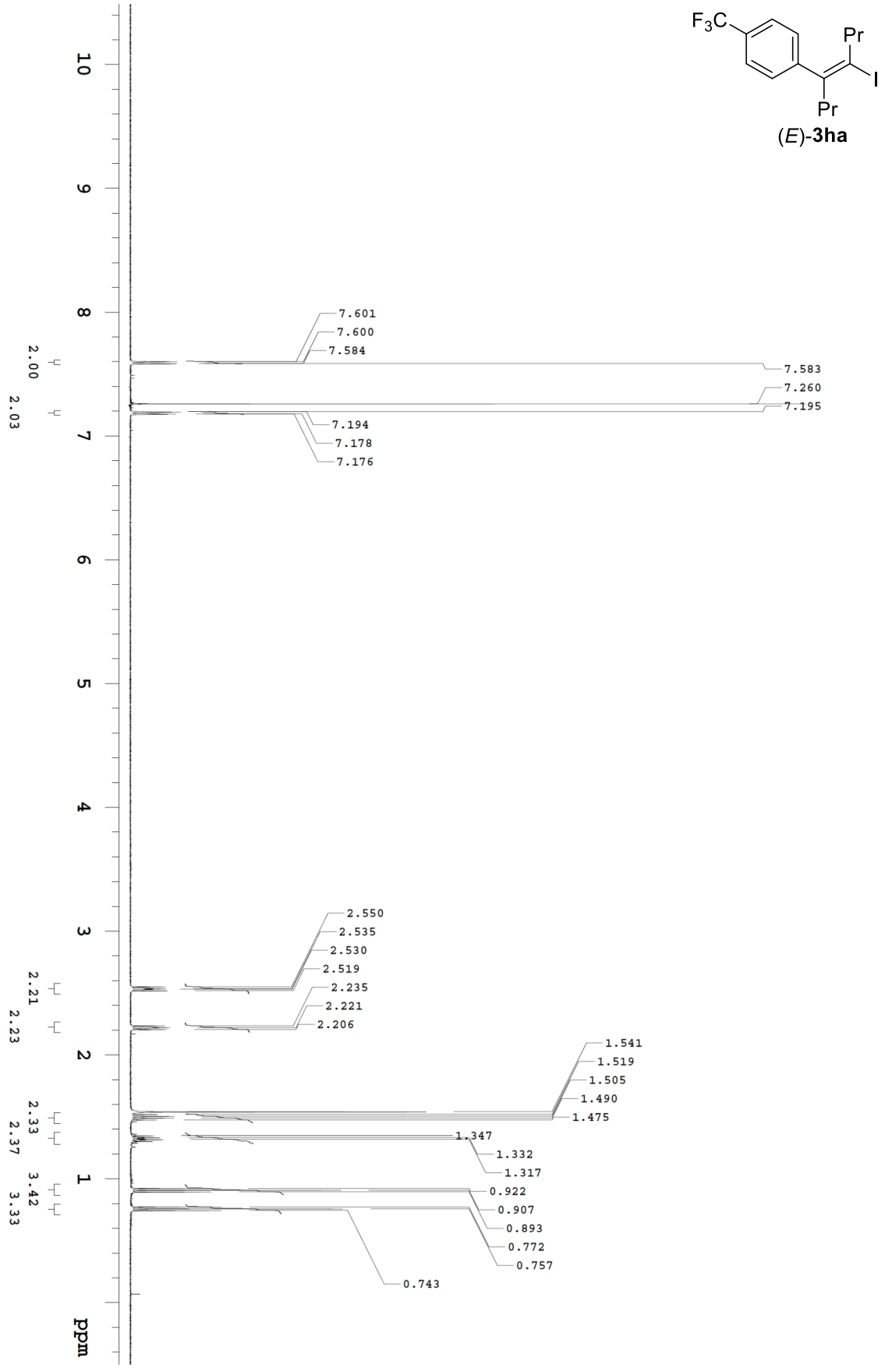
F3C
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Pr
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7.176
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2.535
2.530
2.519
2.235
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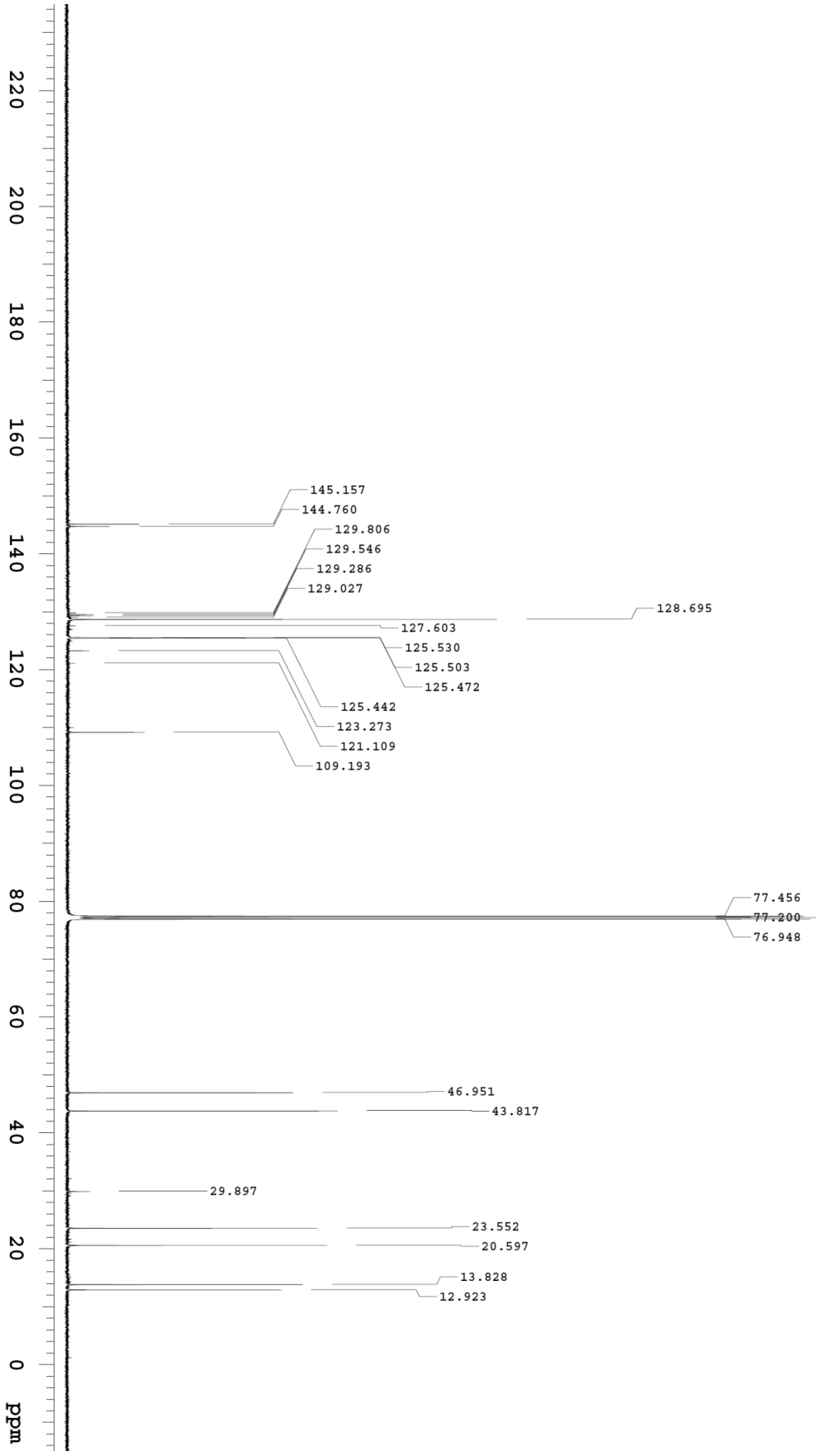
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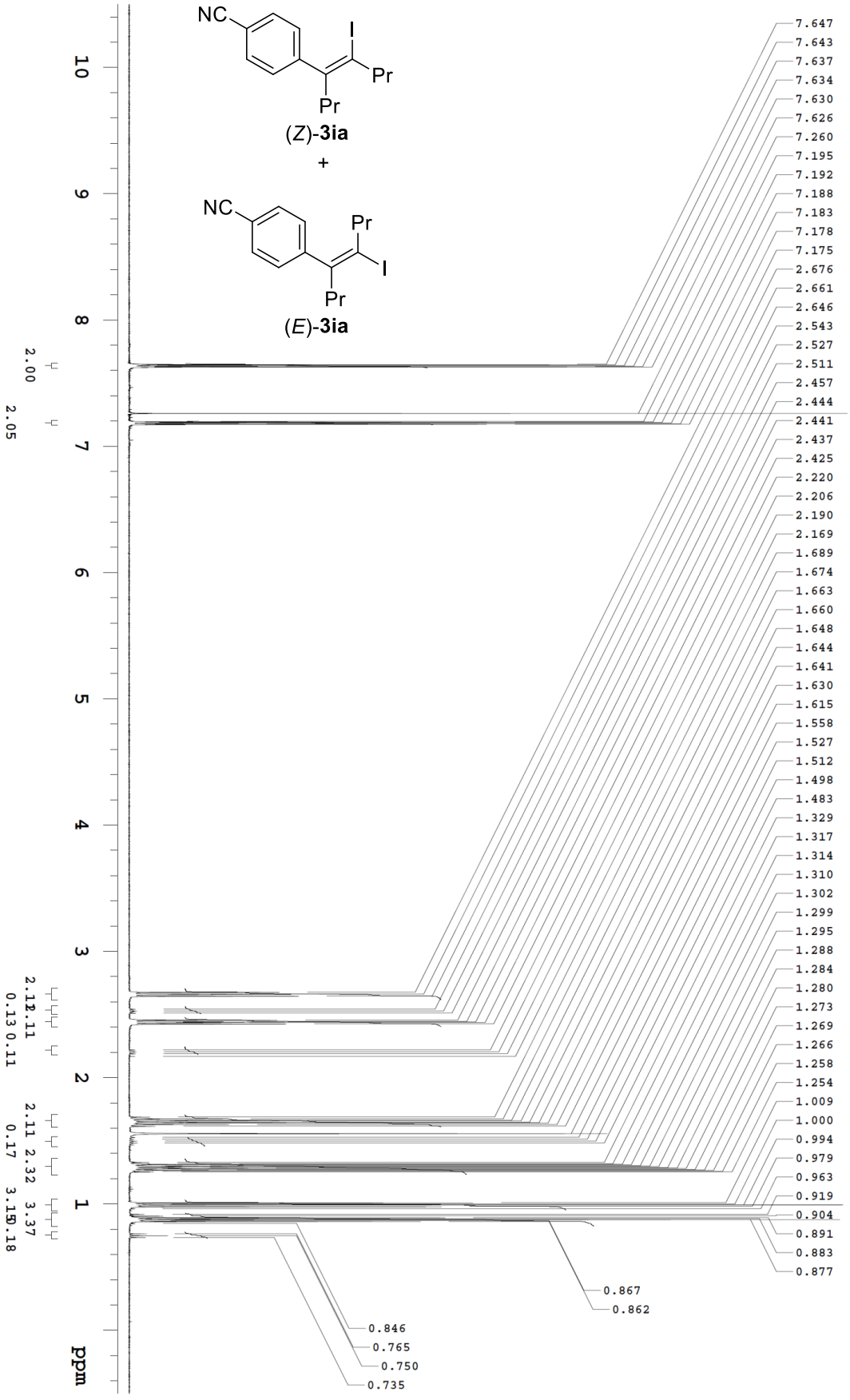
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+
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Pr
I
Pr
(E)-3ia
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0.11
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7
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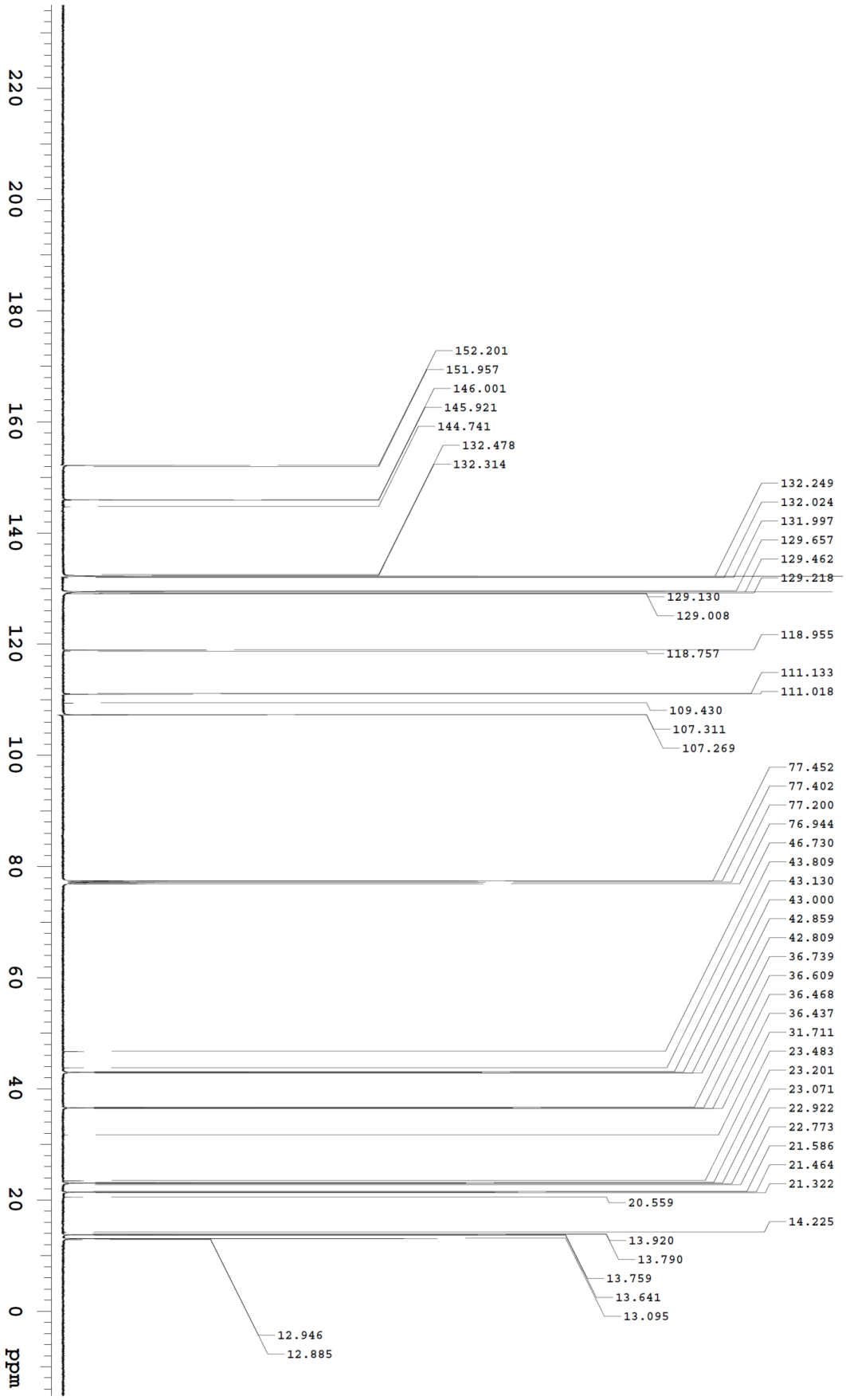
ppm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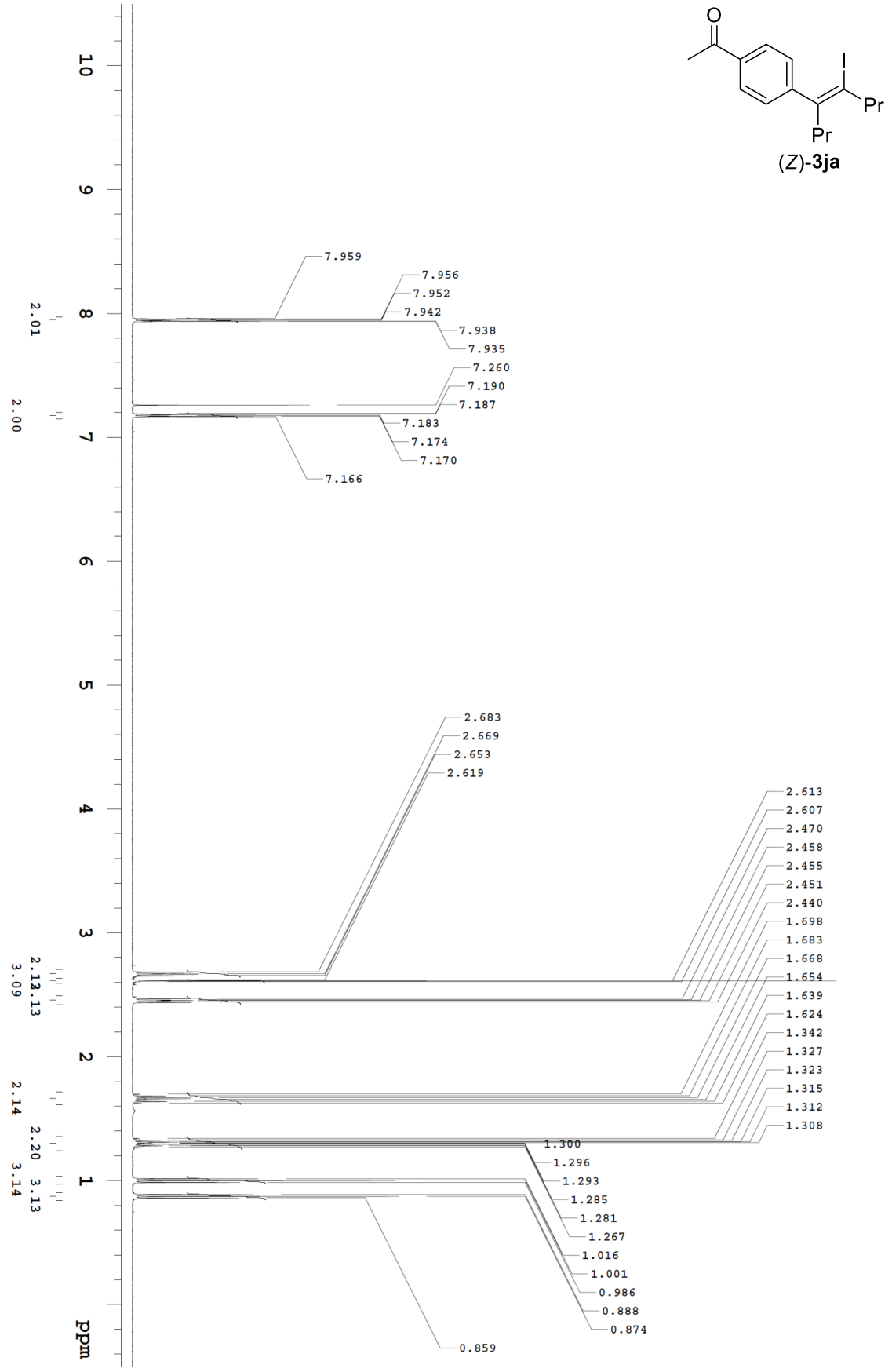
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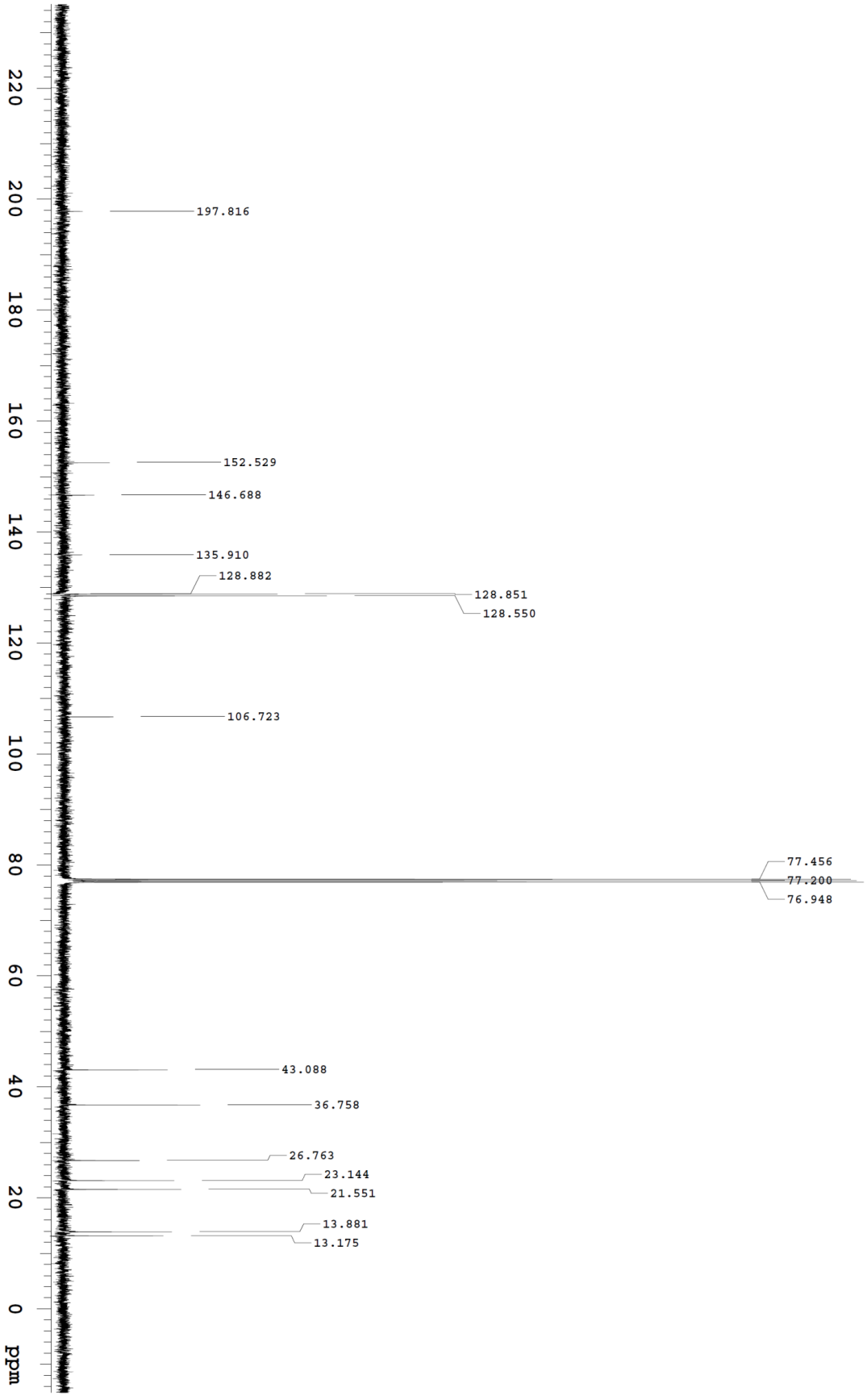
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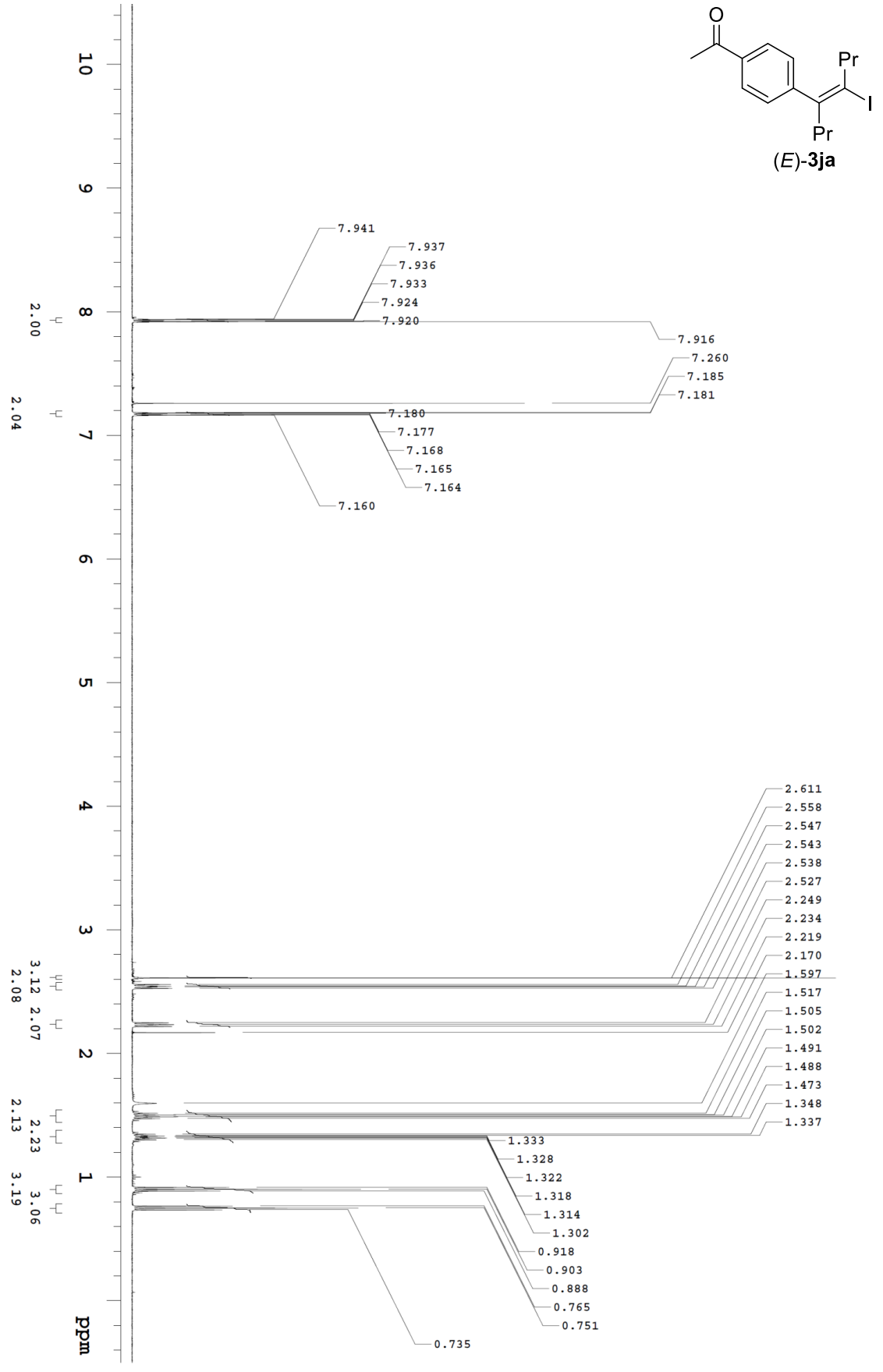
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7.180
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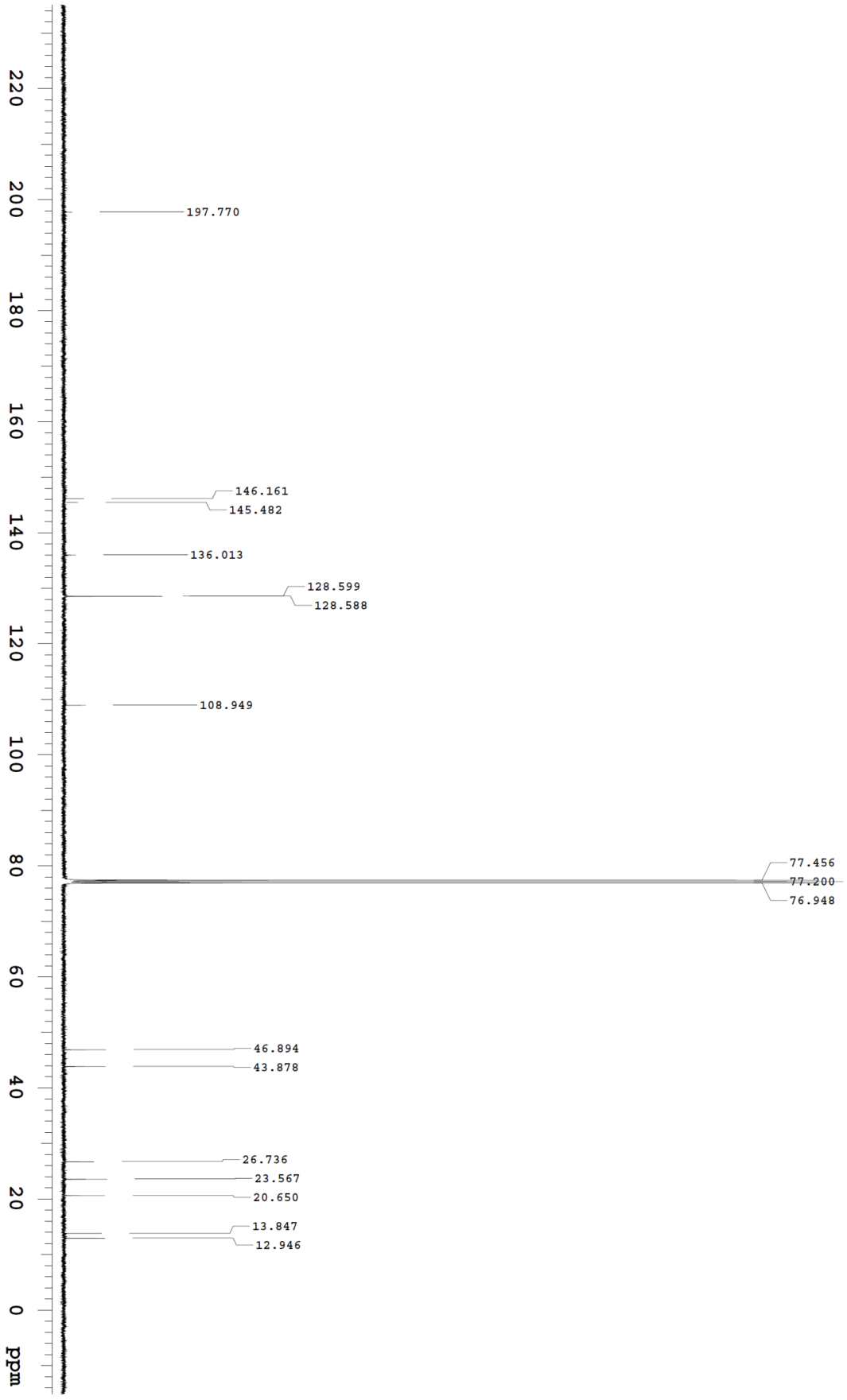
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76.948
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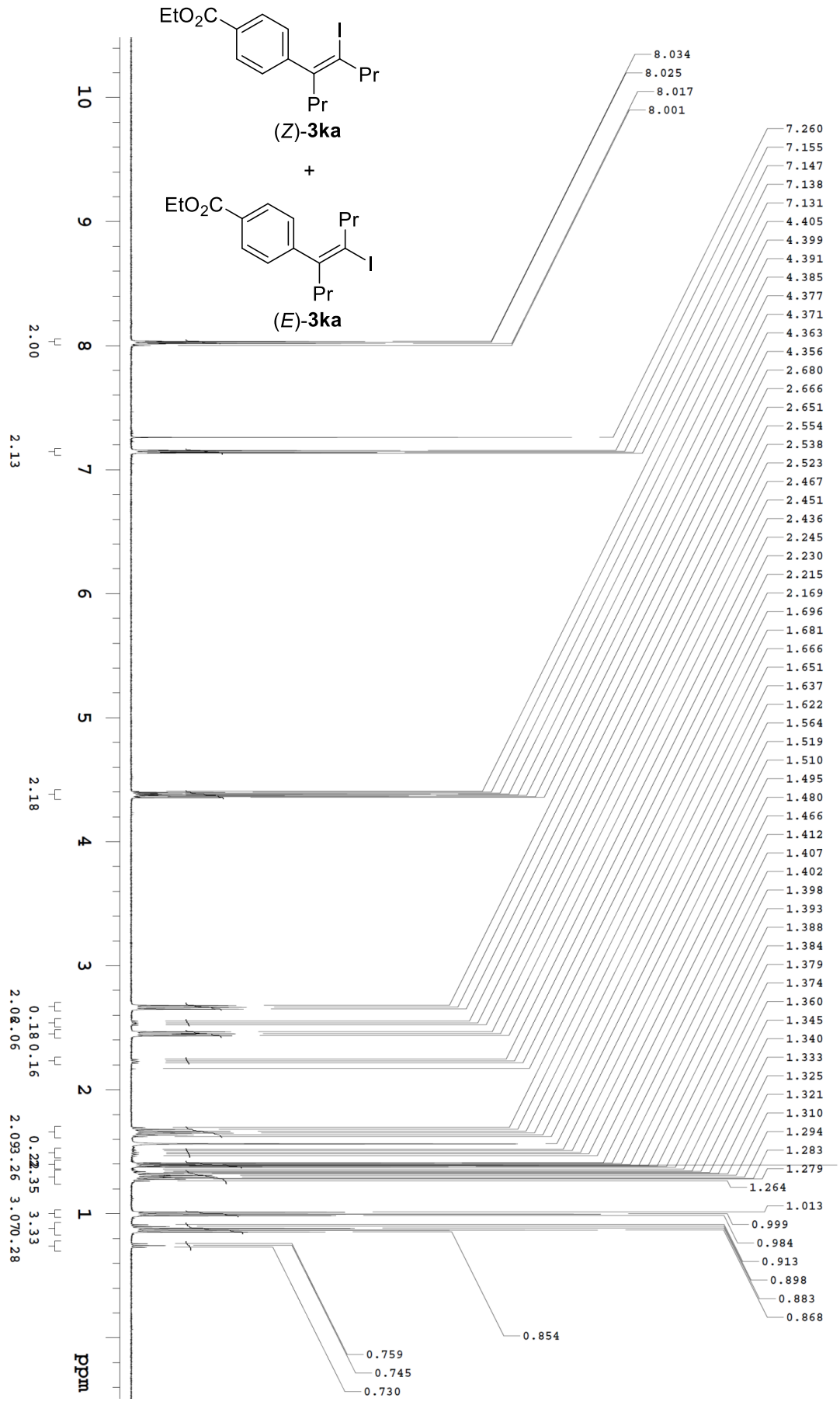
23.567
20.650
13.847
12.946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Pr
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+
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I
Pr
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7.138
7.131
4.405
4.399
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4.385
4.377
4.371
4.363
4.356
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2.554
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2.451
2.436
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2.230
2.215
2.169
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1.681
1.666
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1.637
1.622
1.564
1.519
1.510
1.495
1.480
1.466
1.412
1.407
1.402
1.398
1.393
1.388
1.384
1.379
1.374
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1.340
1.333
1.325
1.321
1.310
1.294
1.283
1.279
1.264
1.013
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0.984
0.913
0.898
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2.13
2.18
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0.16
2.06
2.08
0.22
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7
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3
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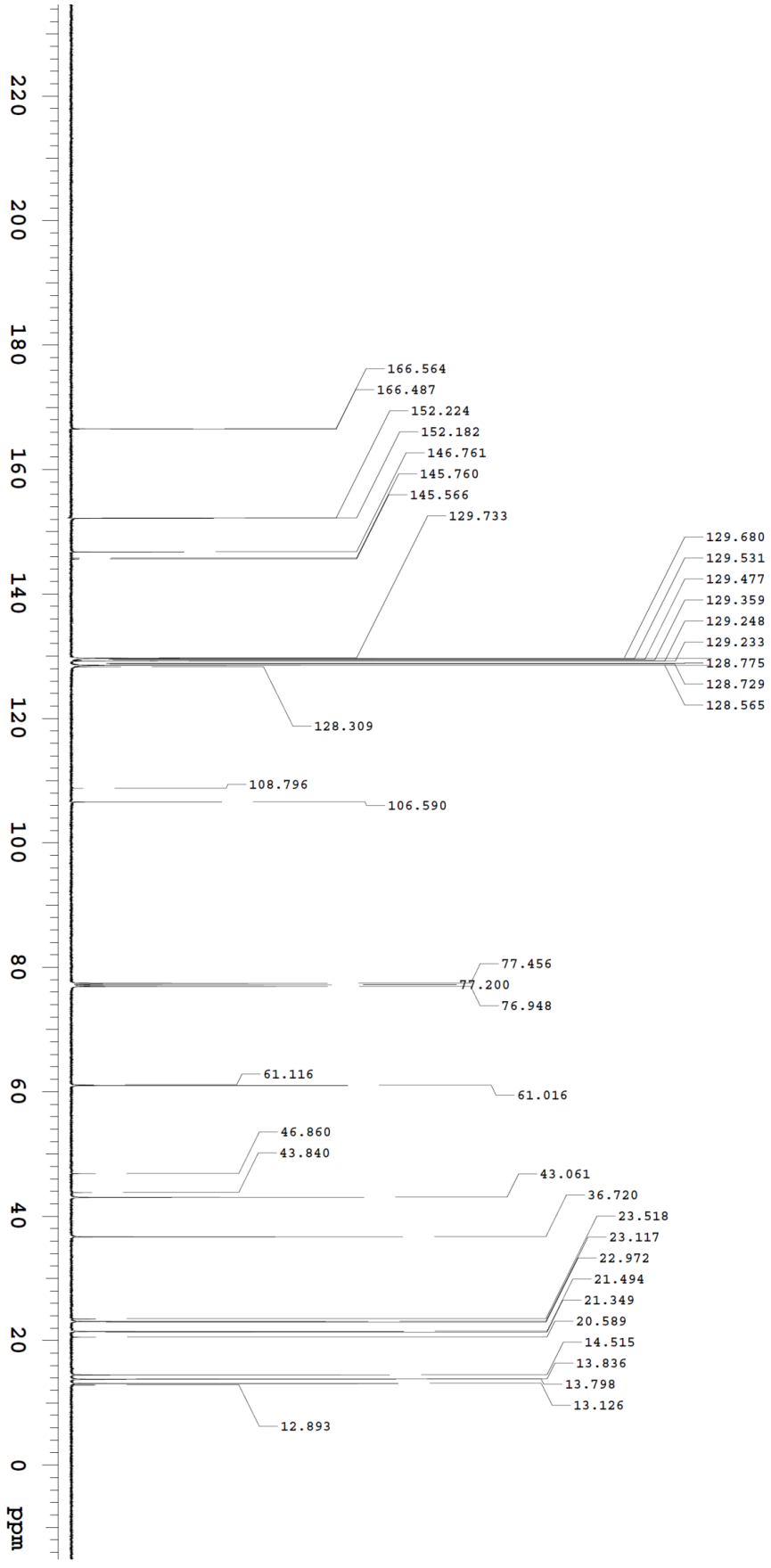
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129.477
129.359
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128.775
128.729
128.565
128.309
108.796
106.590
77.456
77.200
76.948
61.116
61.016
46.860
43.840
43.061
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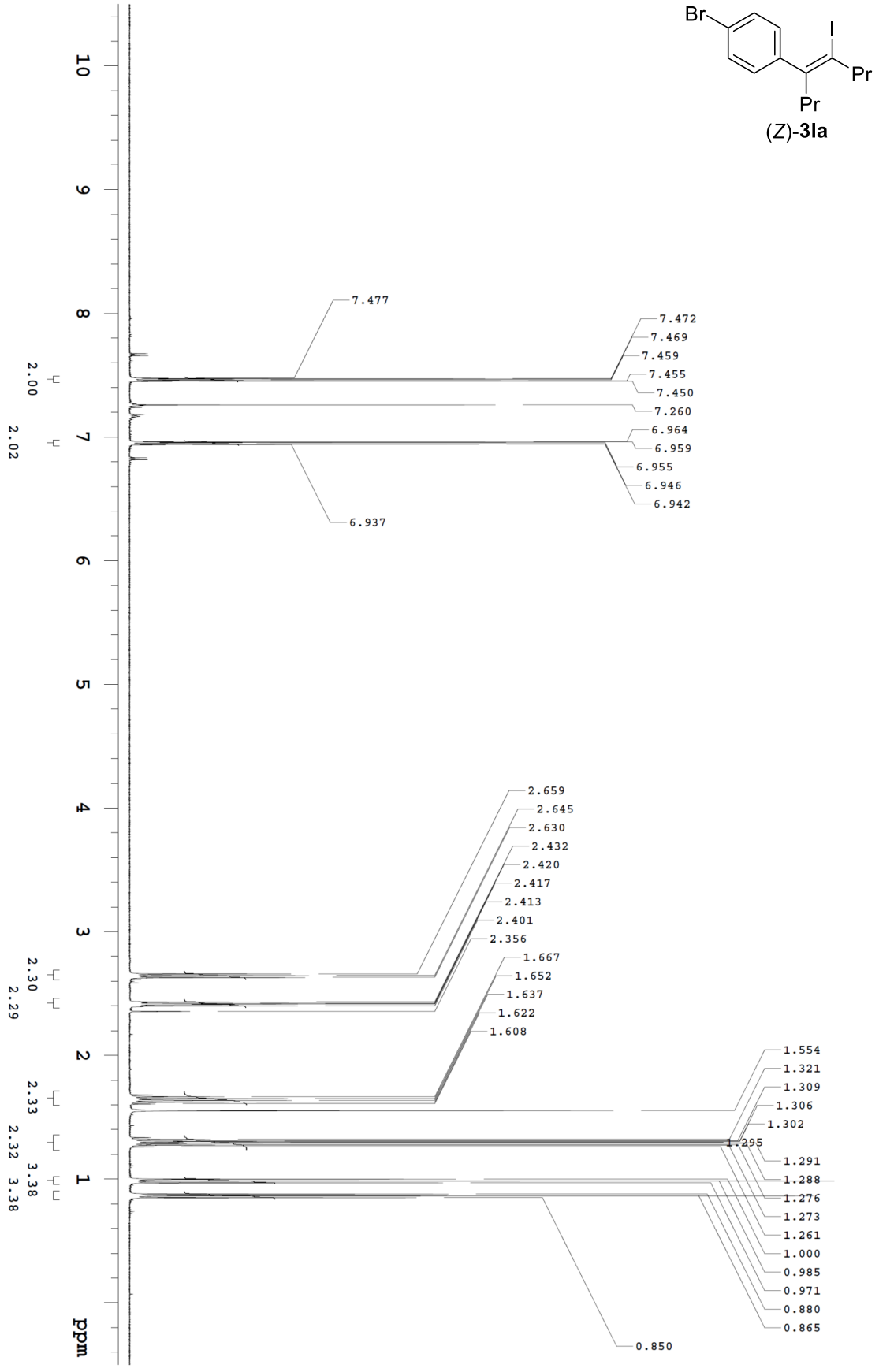
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7.260
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6.959
6.955
6.946
6.942
6.937
2.659
2.645
2.630
2.432
2.420
2.417
2.413
2.401
2.356
1.667
1.652
1.637
1.622
1.608
1.554
1.321
1.309
1.306
1.302
1.295
1.291
1.288
1.276
1.273
1.261
1.000
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0.971
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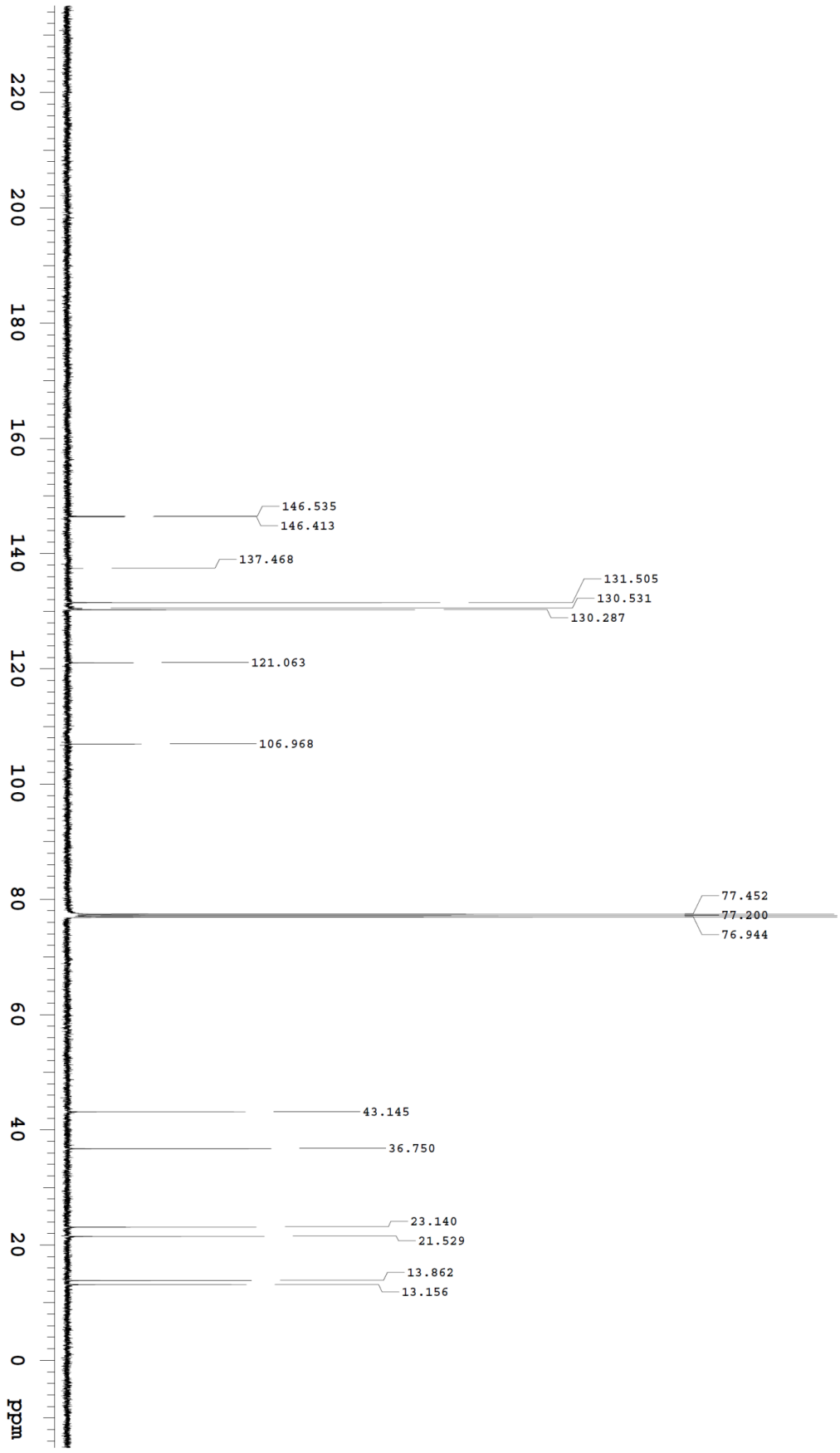
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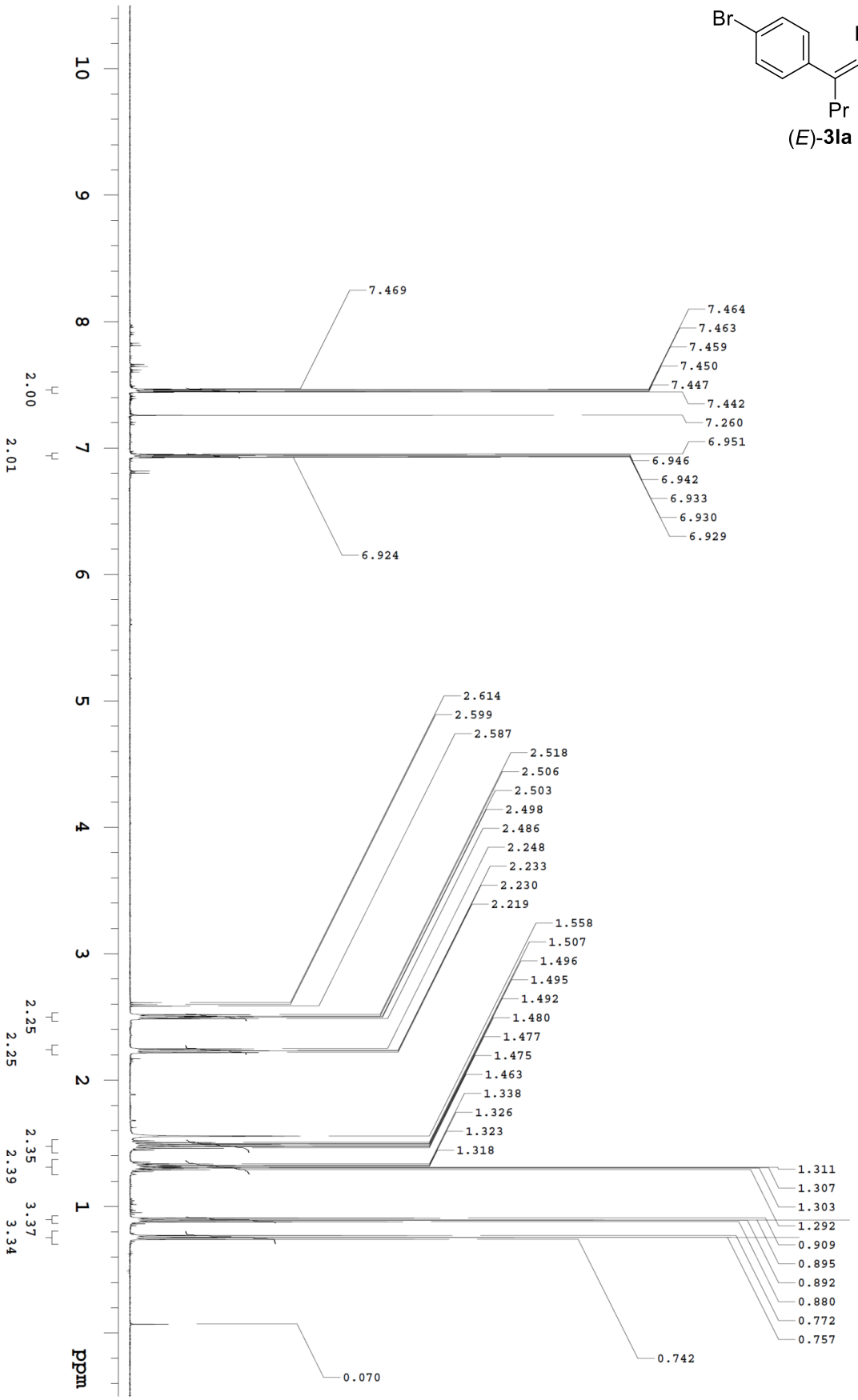
13.156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Pr
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6.946
6.942
6.933
6.930
6.929
6.924
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2.599
2.587
2.518
2.506
2.503
2.498
2.486
2.248
2.233
2.230
2.219
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1.507
1.496
1.495
1.492
1.480
1.477
1.475
1.463
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1.323
1.318
1.311
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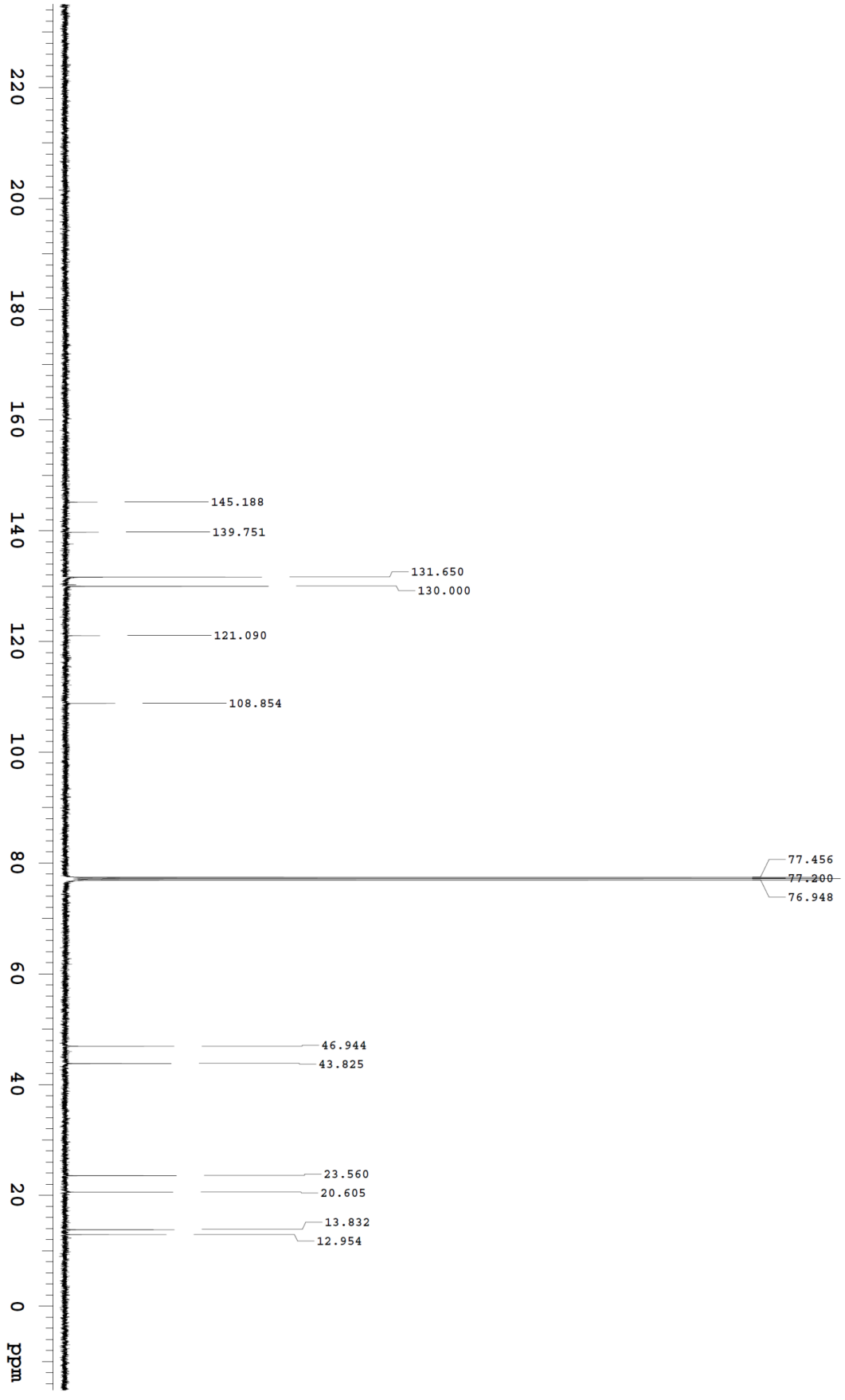
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43.825
23.560
20.605
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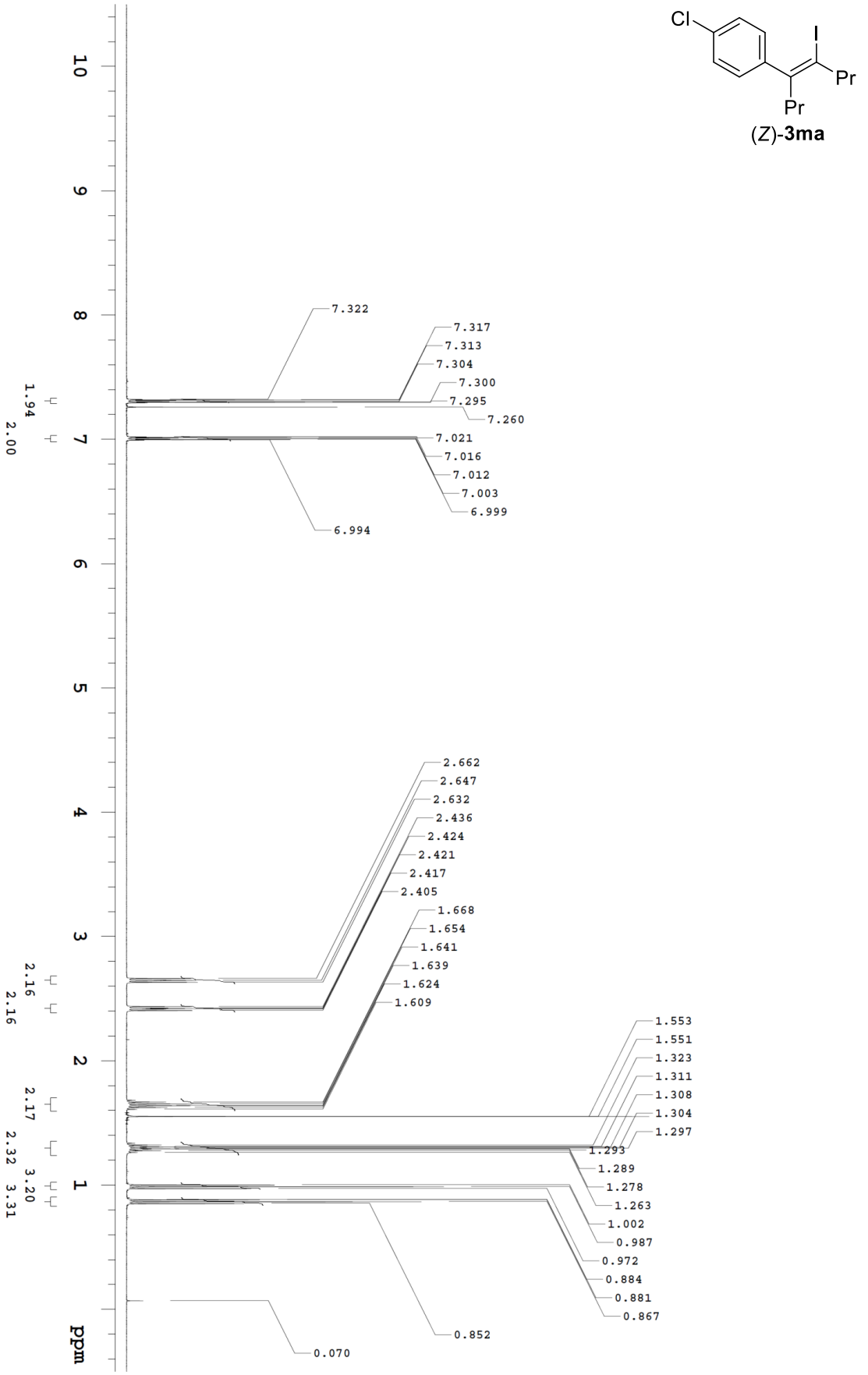
12.954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7.260
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7.016
7.012
7.003
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6.994
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2.647
2.632
2.436
2.424
2.421
2.417
2.405
1.668
1.654
1.641
1.639
1.624
1.609
1.553
1.551
1.323
1.311
1.308
1.304
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1.293
1.289
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0.972
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0.881
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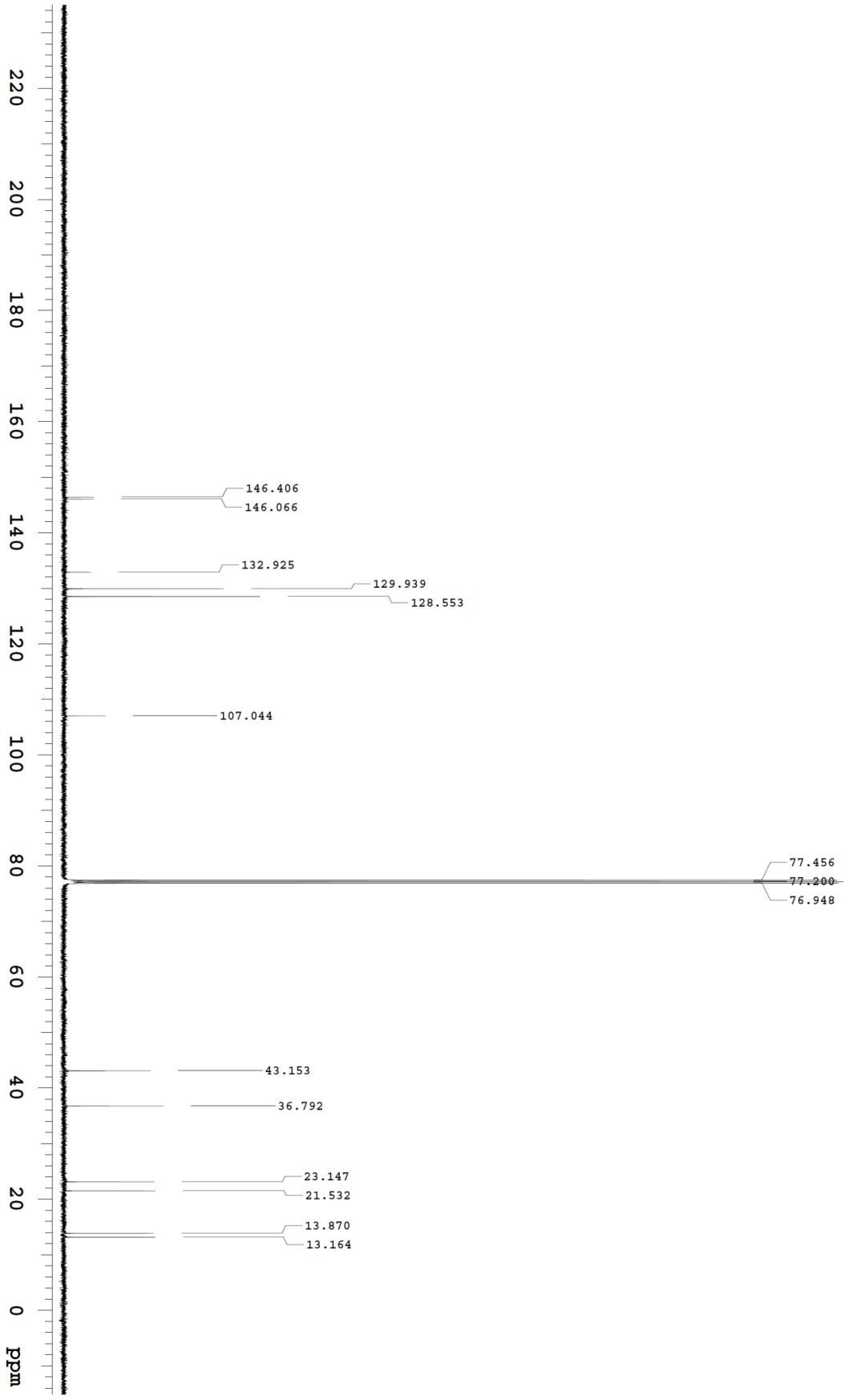
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20
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77.200
76.948
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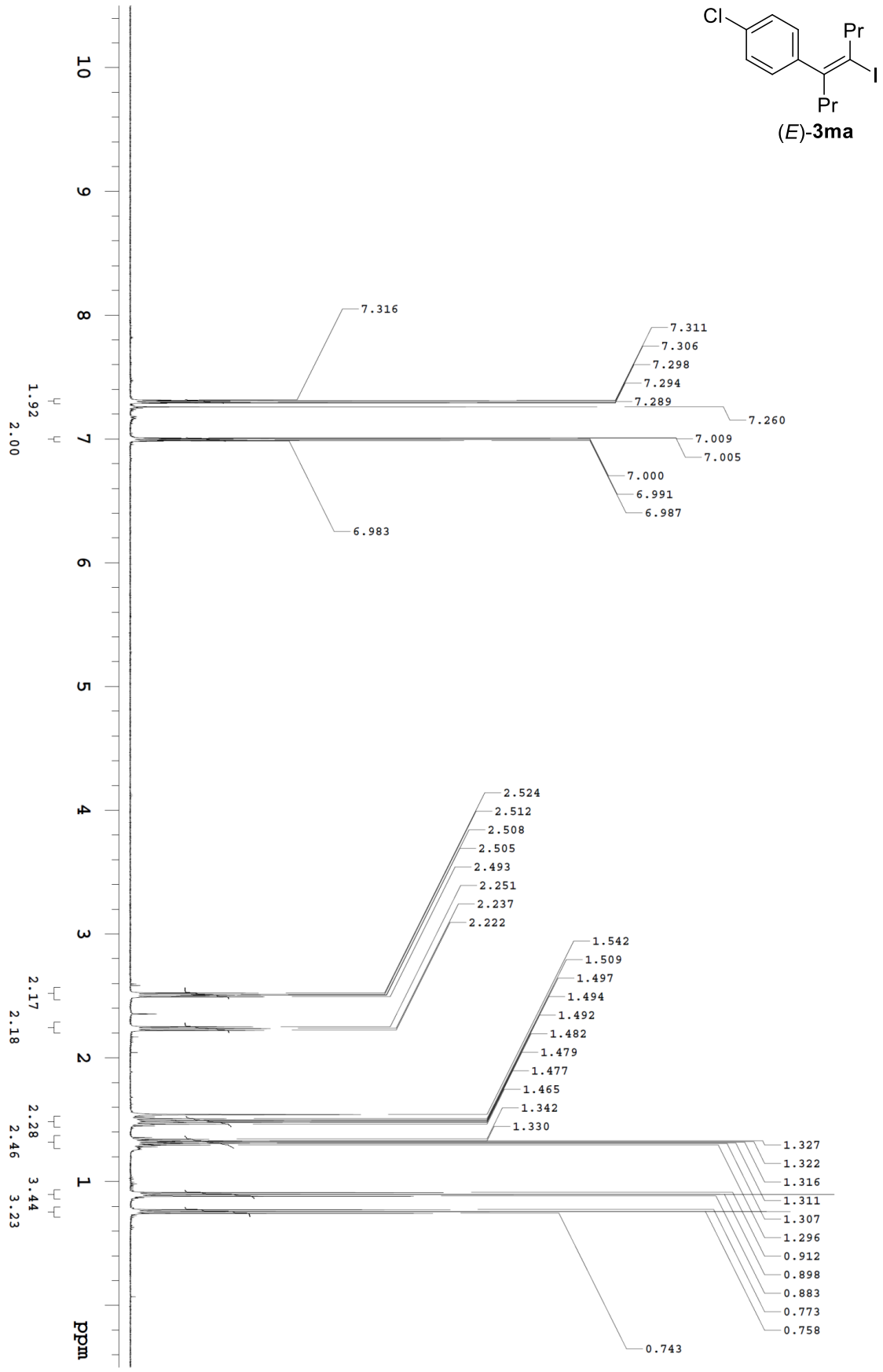
13.164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Pr
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7.005
7.000
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6.987
6.983
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2.512
2.508
2.505
2.493
2.251
2.237
2.222
1.542
1.509
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1.494
1.492
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1.479
1.477
1.465
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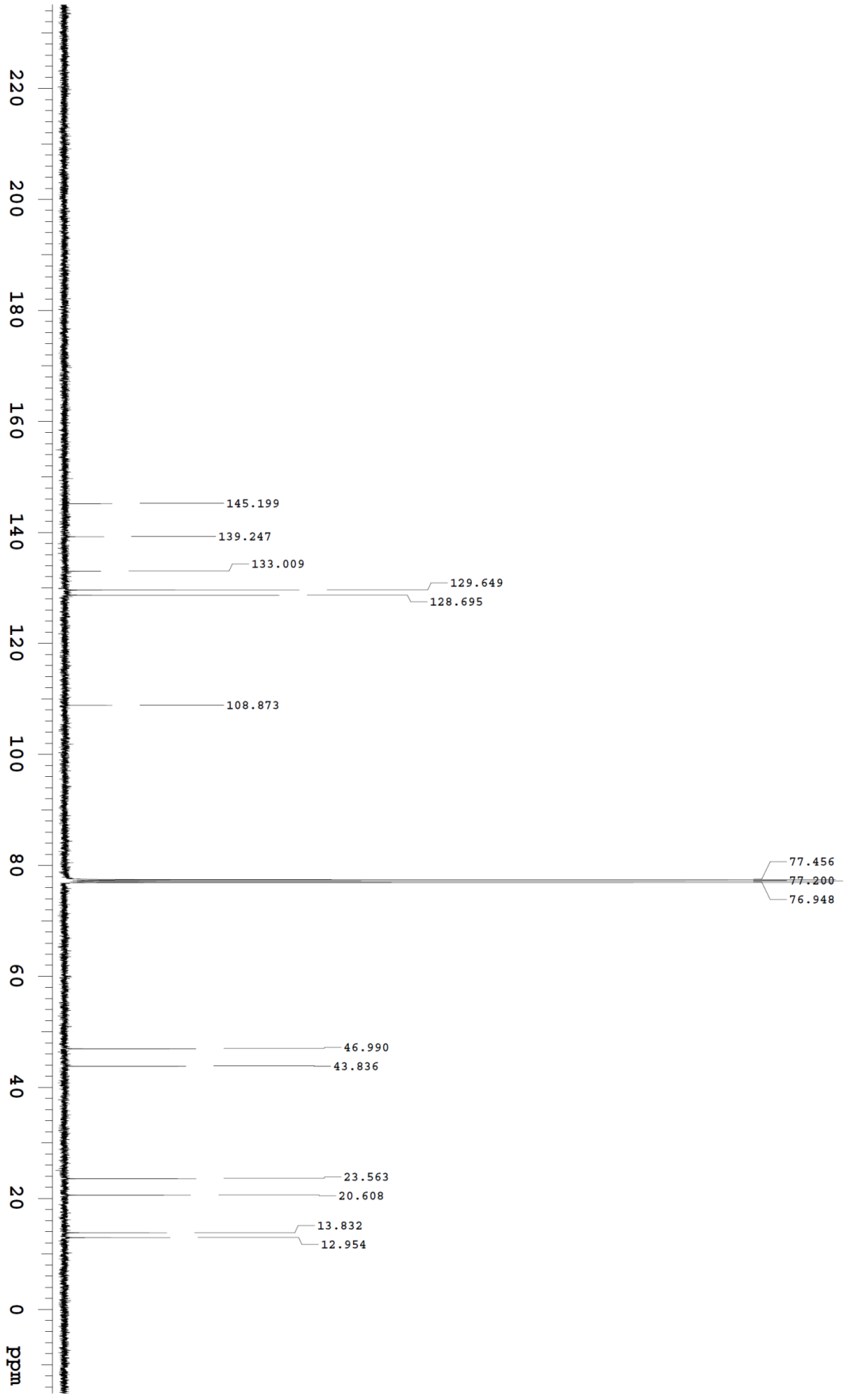
ppm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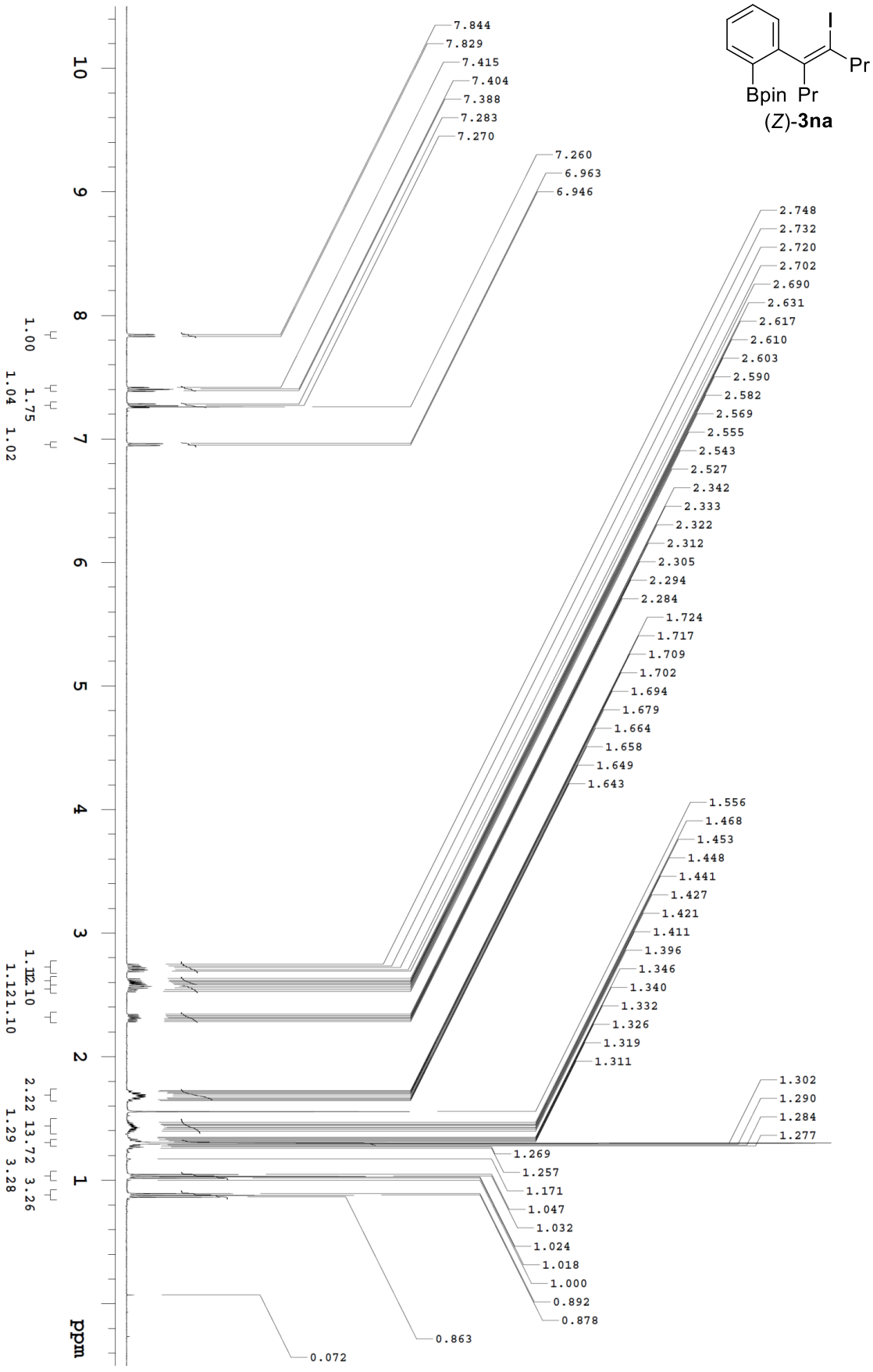
12.954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2.720
2.702
2.690
2.631
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2.610
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2.582
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2.555
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2.527
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2.322
2.312
2.305
2.294
2.284
1.724
1.717
1.709
1.702
1.694
1.679
1.664
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1.453
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1.441
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1.411
1.396
1.346
1.340
1.332
1.326
1.319
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1.277
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0.072
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3.26
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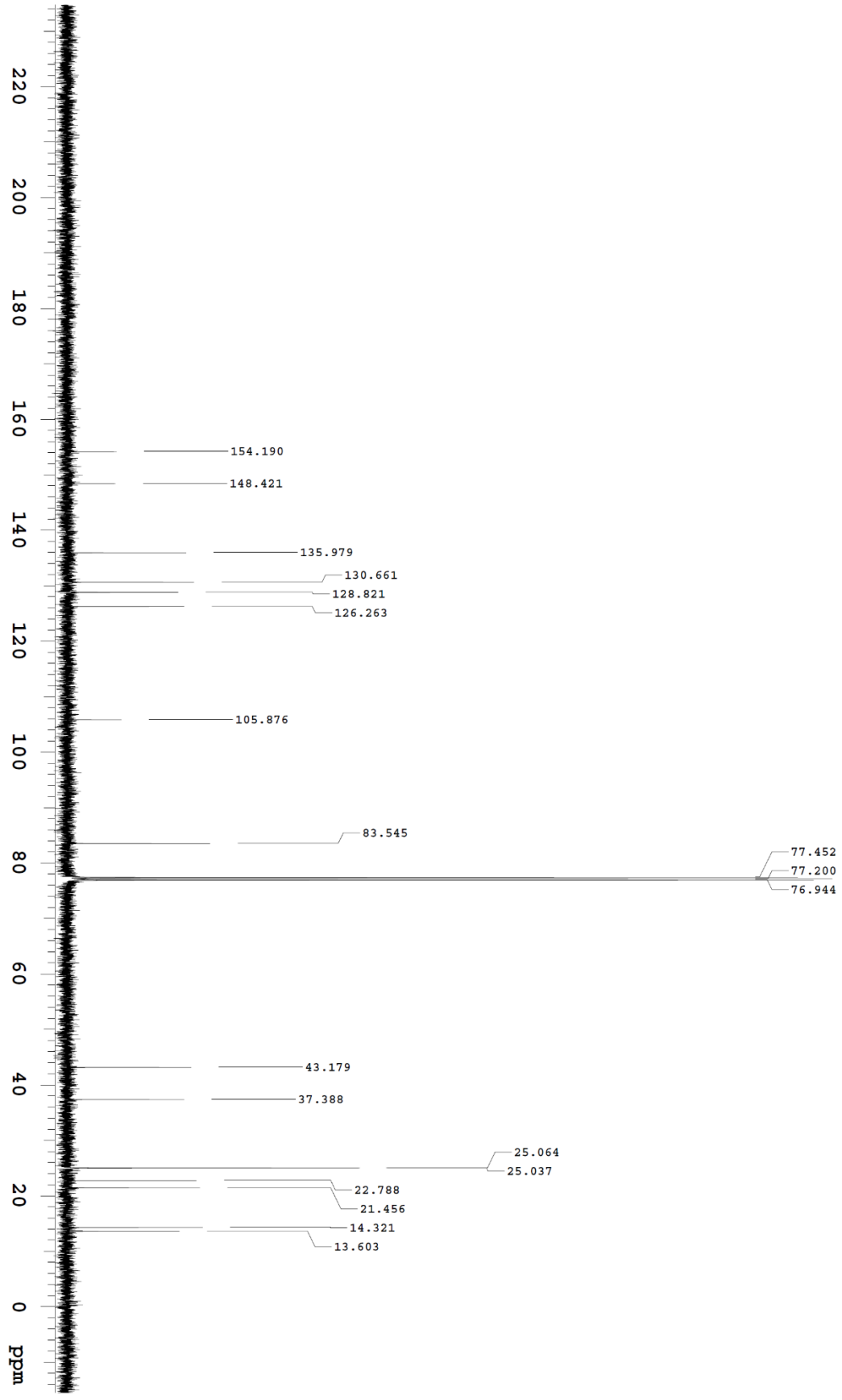
Pr
Pr
I
(Z)-3na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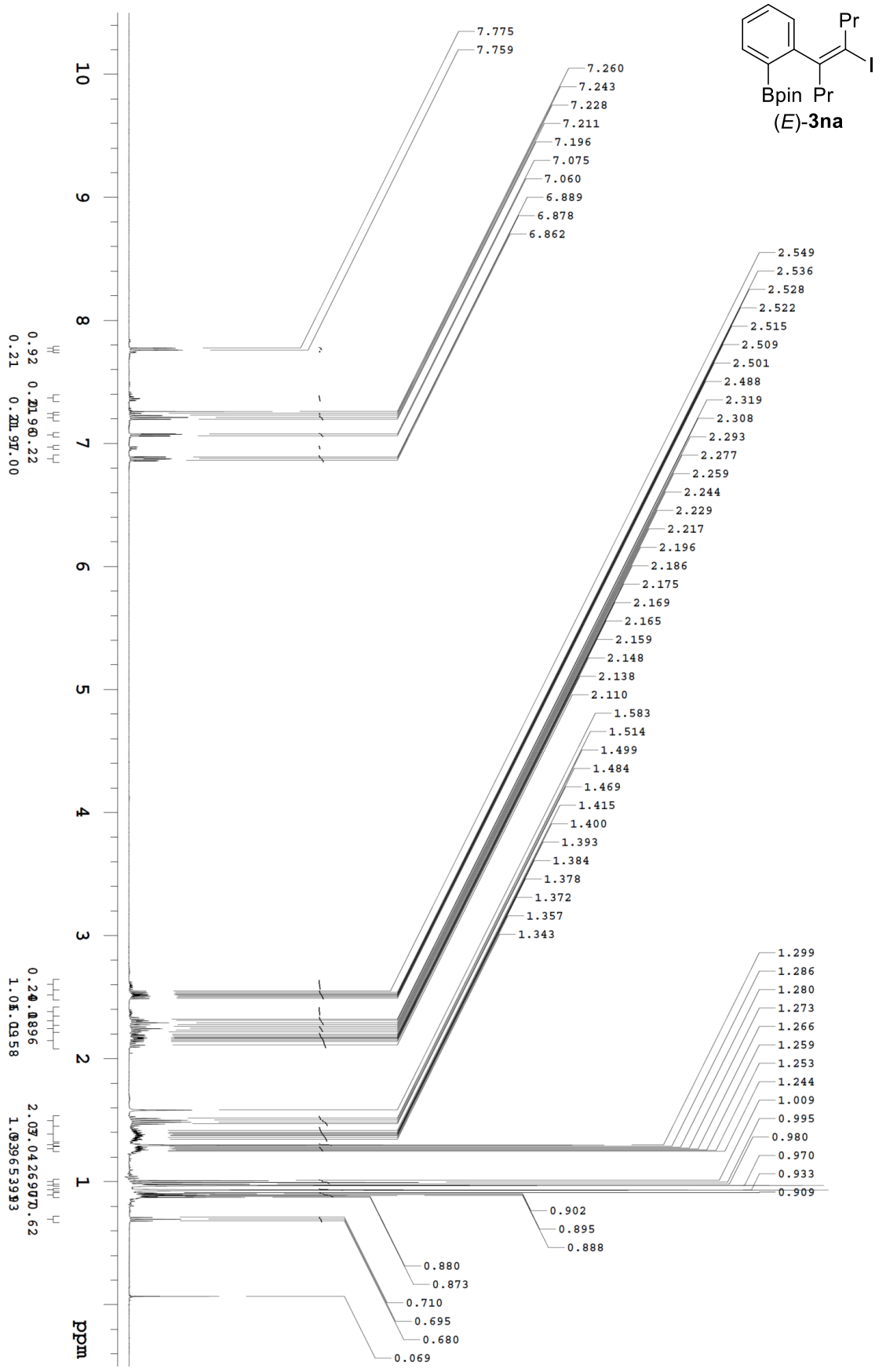
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Bpin Pr
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6.889
6.878
6.862
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2.515
2.509
2.501
2.488
2.319
2.308
2.293
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2.159
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1.280
1.273
1.266
1.259
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1.244
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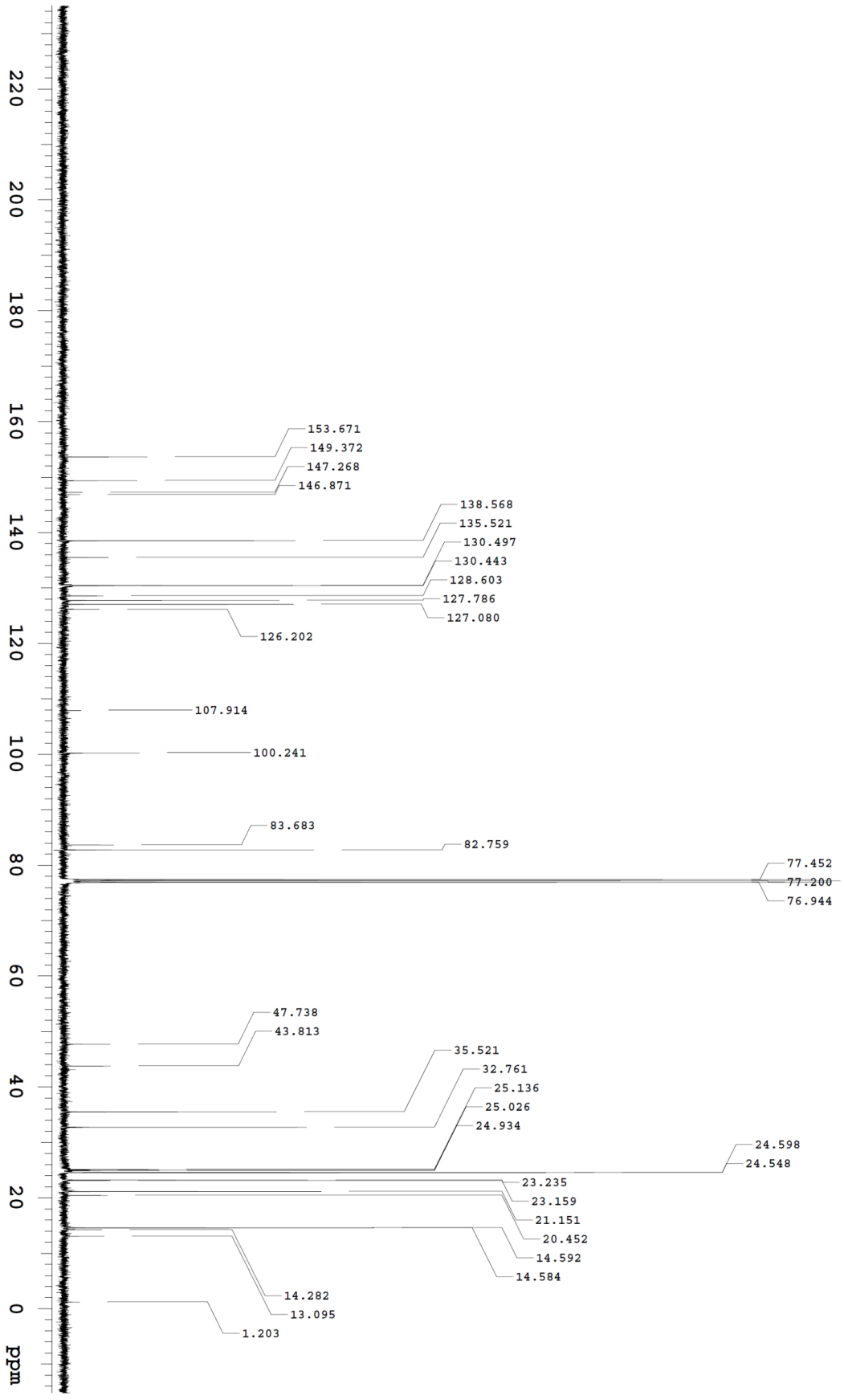
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126.202
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100.241
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82.759
77.452
77.200
76.944
47.738
43.813
35.521
32.761
25.136
25.026
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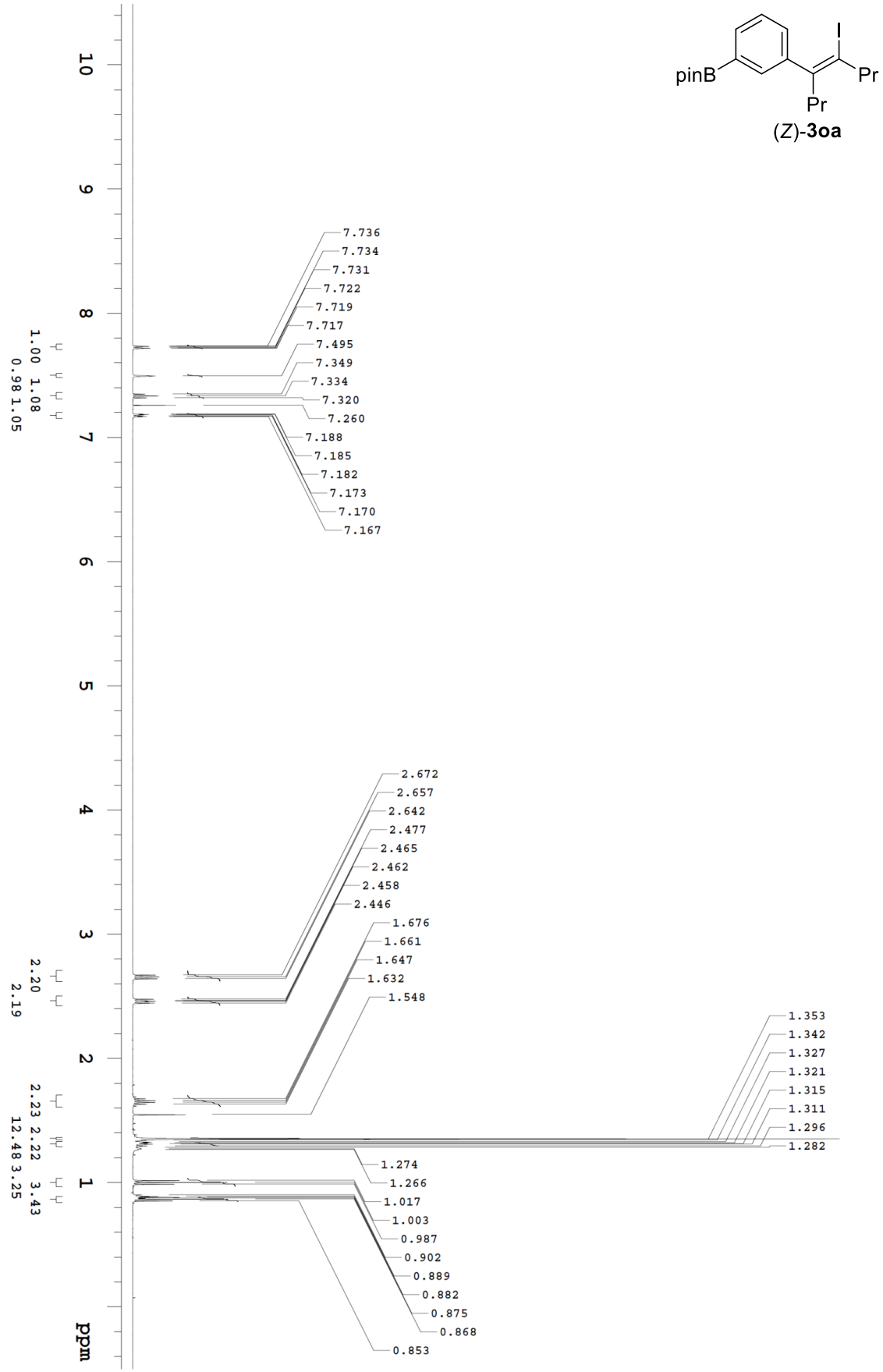
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Pr
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7.334
7.320
7.260
7.188
7.185
7.182
7.173
7.170
7.167
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1.274
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1.003
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0.902
0.889
0.882
0.875
0.868
0.853
1.00 1.08 0.98 1.05
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7
6
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3
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1
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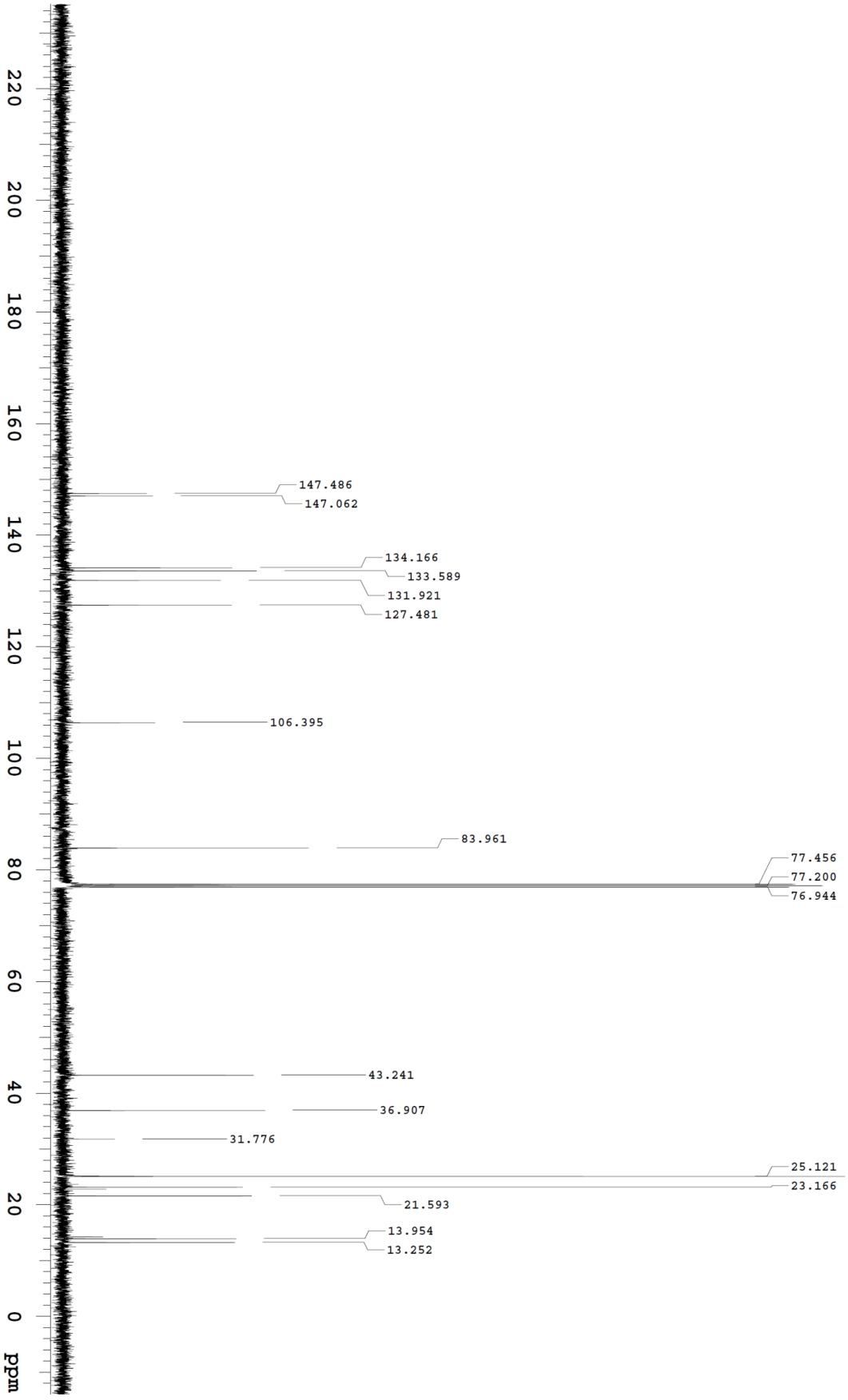
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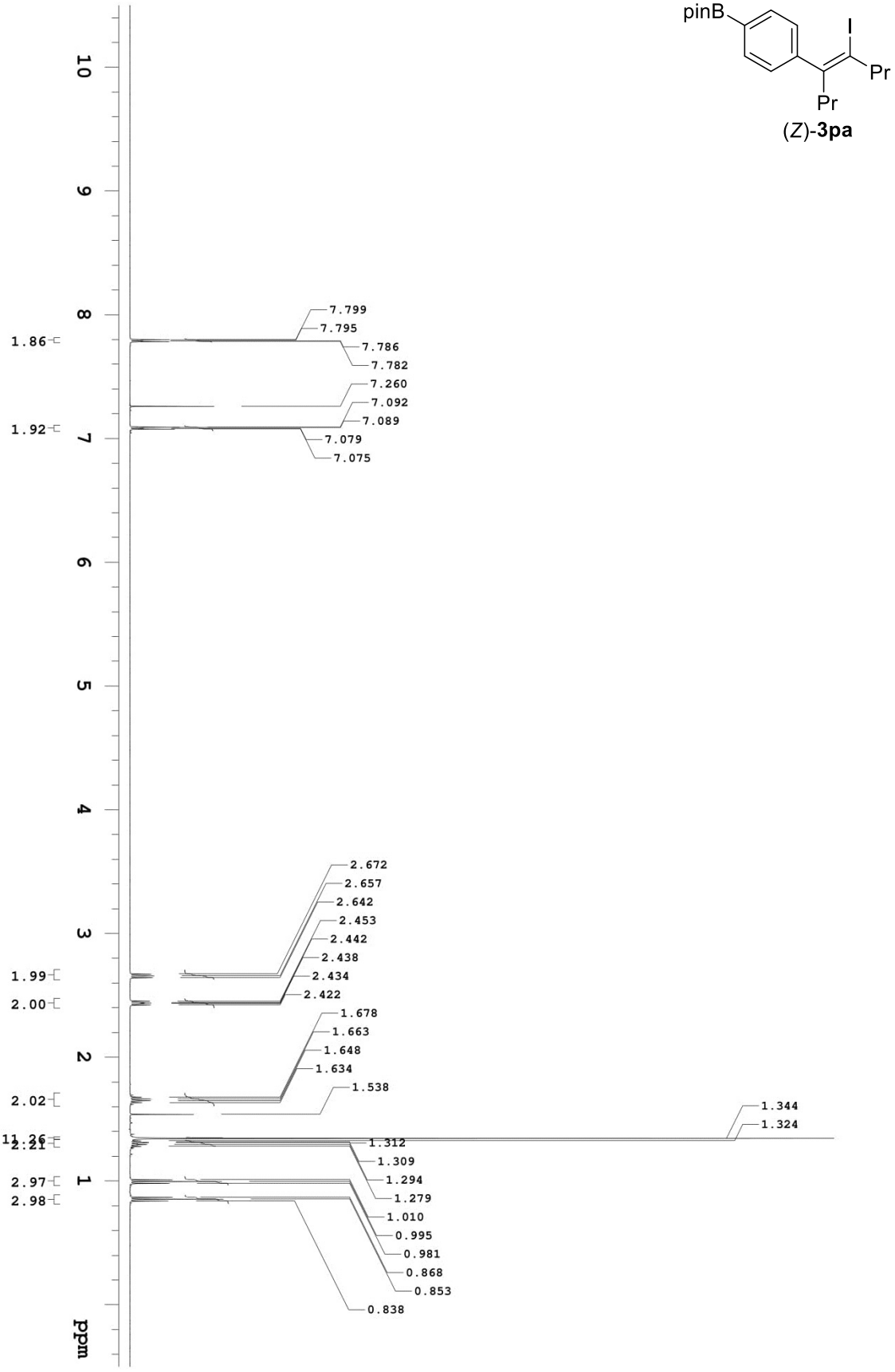
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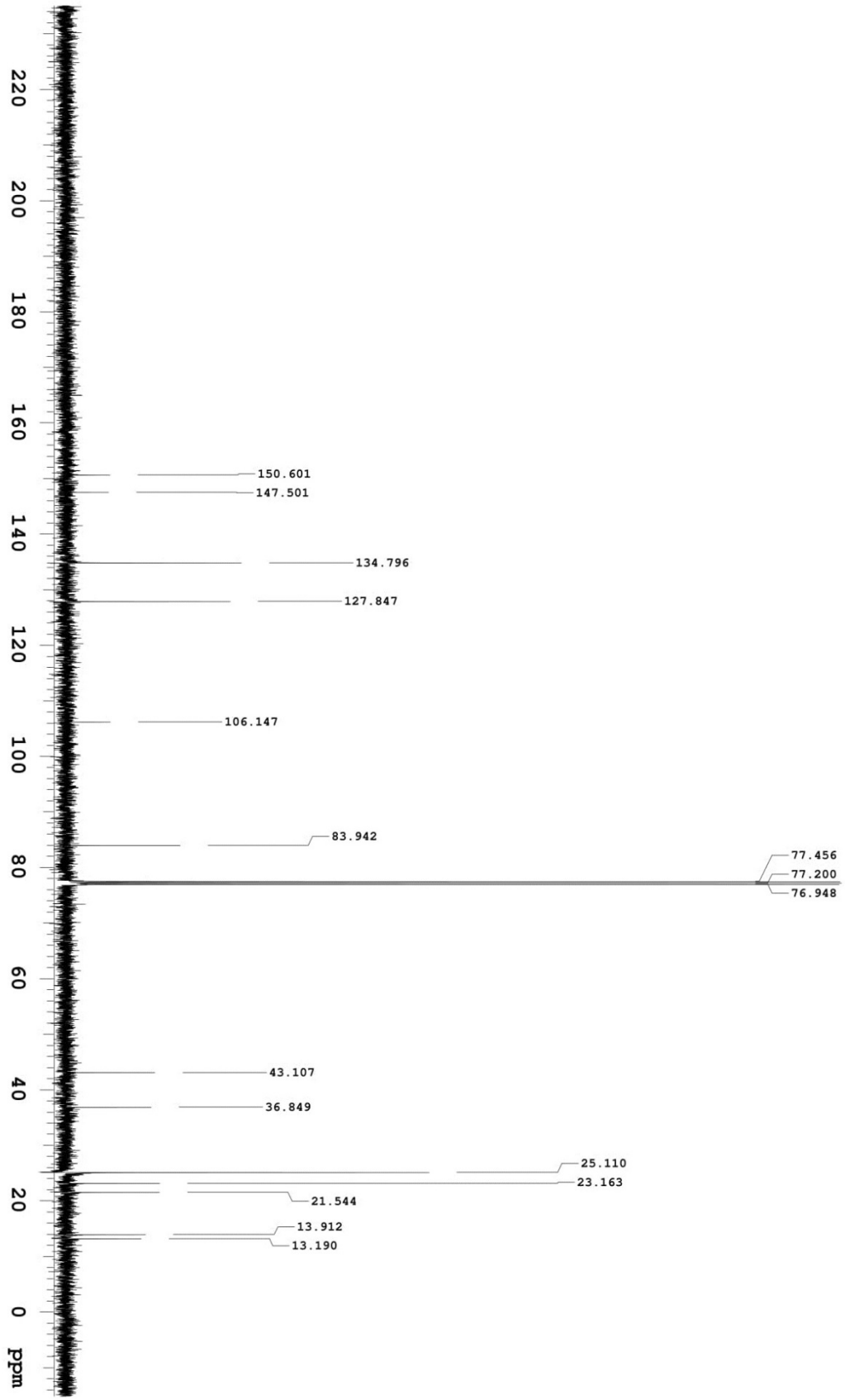
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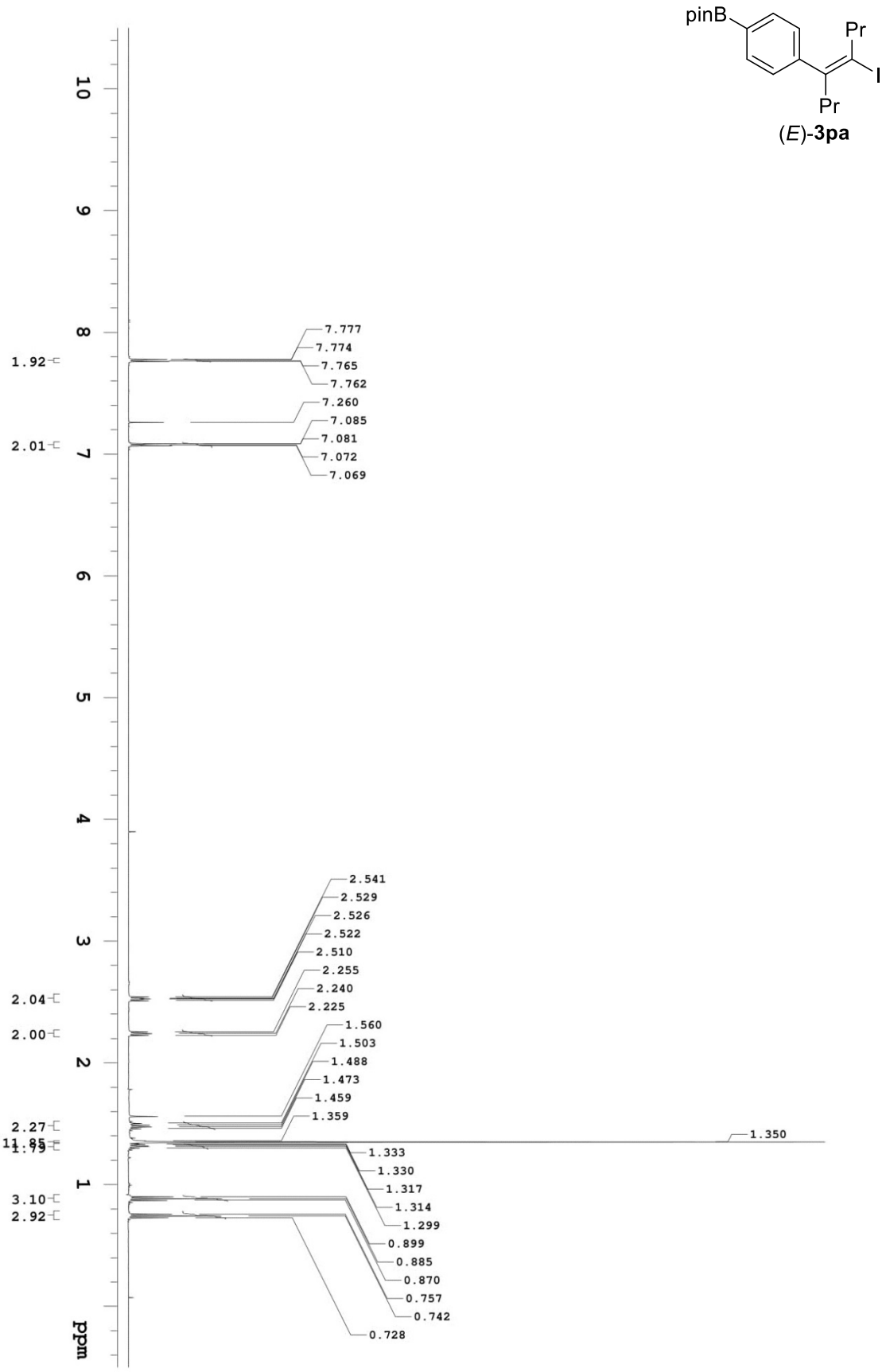
13.190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Pr
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Pr
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7.069
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2.522
2.510
2.255
2.240
2.225
1.560
1.503
1.488
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1.459
1.359
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1.330
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1.314
1.299
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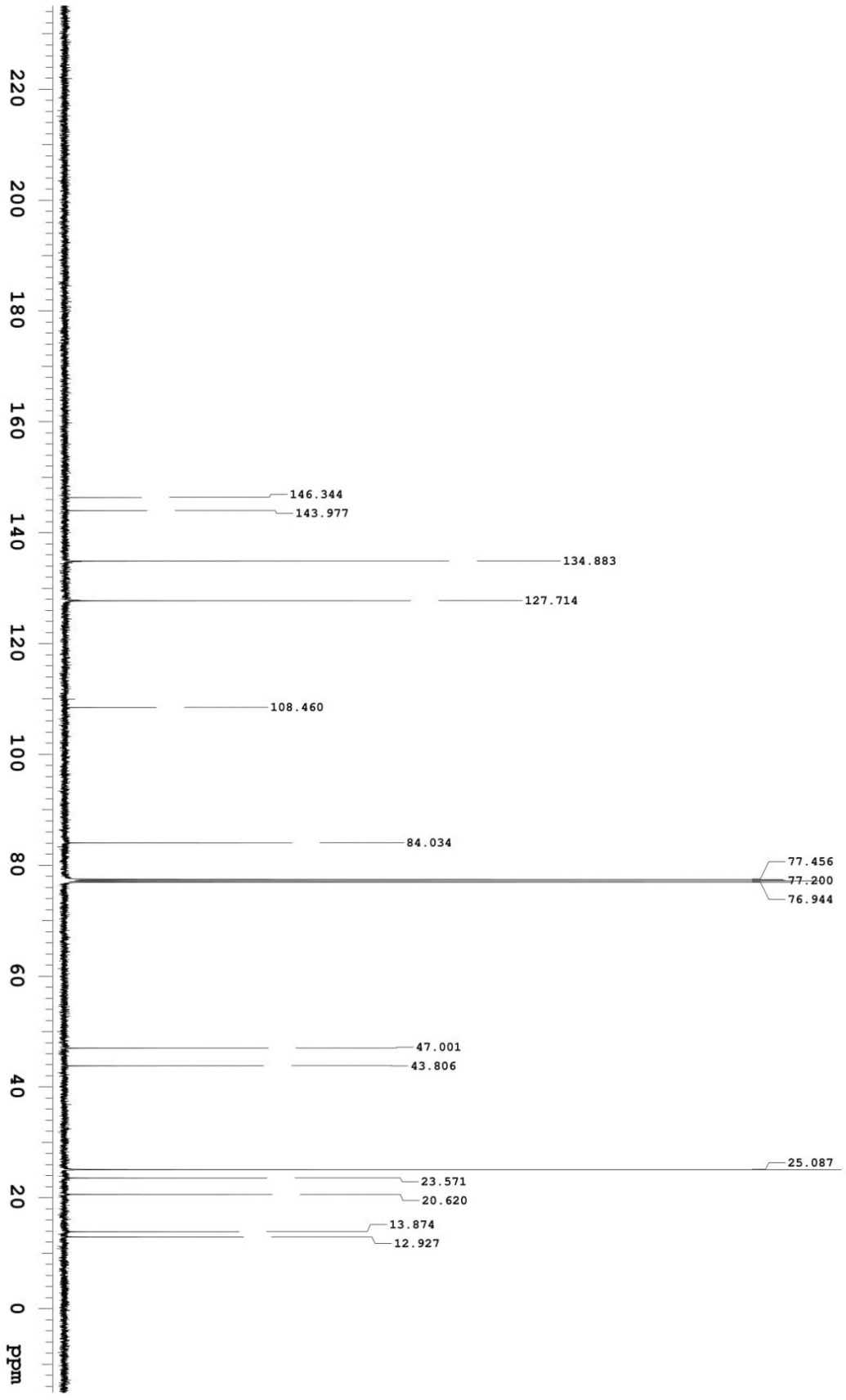
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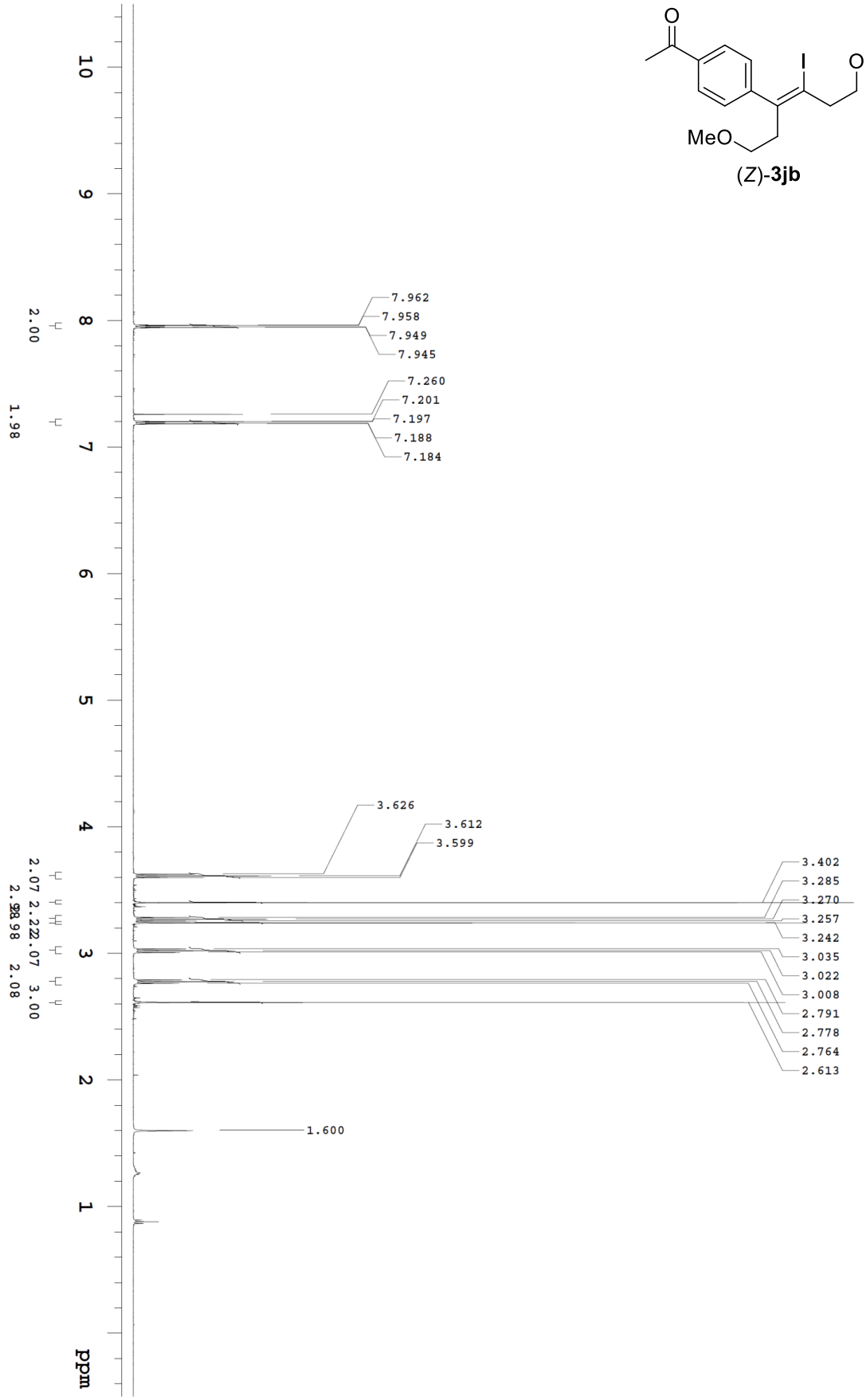
O
I
OMe
MeO
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7.184
3.626
3.612
3.599
3.402
3.285
3.270
3.257
3.242
3.035
3.022
3.008
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3.00
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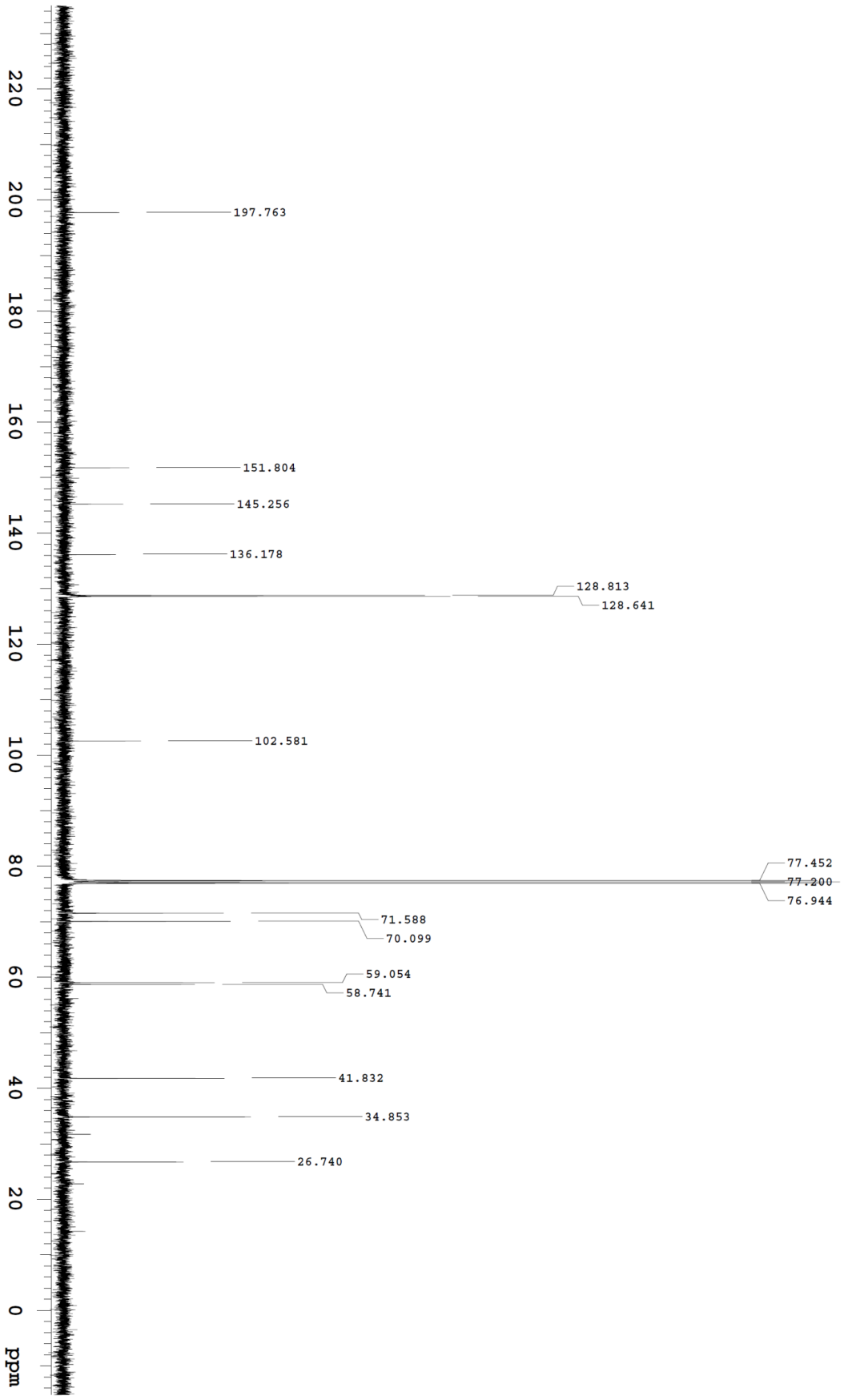
ppm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76.944
71.588
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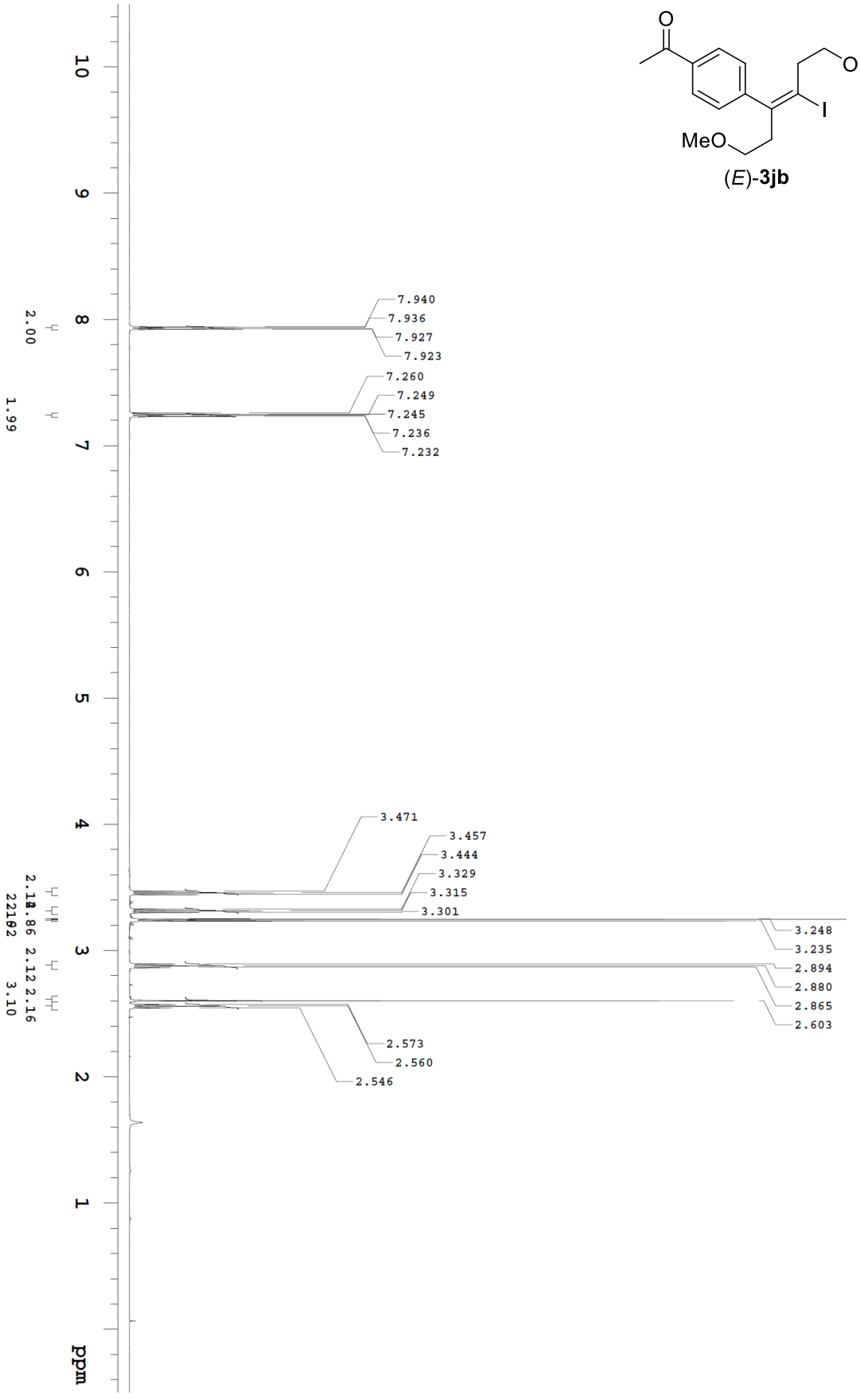
34.853
26.740


O
OMe
I
MeO
(E)-3jb
7.940
7.936
7.927
7.923
7.260
7.249
7.245
7.236
7.232
3.471
3.457
3.444
3.329
3.315
3.301
3.248
3.235
2.894
2.880
2.865
2.603
2.573
2.560
2.546
2.00
1.99
2.18
2.86
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2.21
2.02
3.10
10
9
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7
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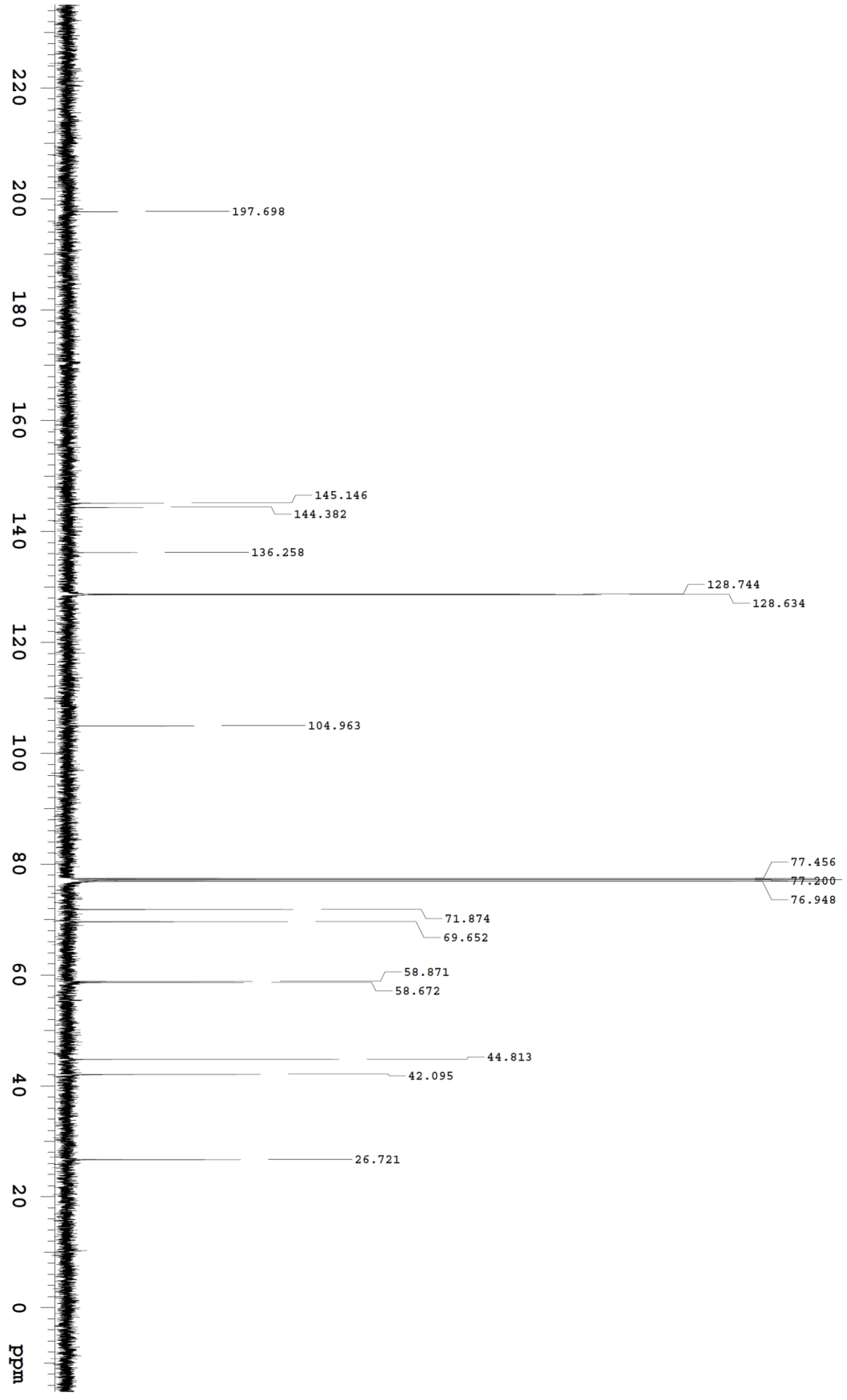
5
4
3
2
1
ppm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140
120
100
80
60
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20
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128.744
128.634
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77.200
76.948
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69.652
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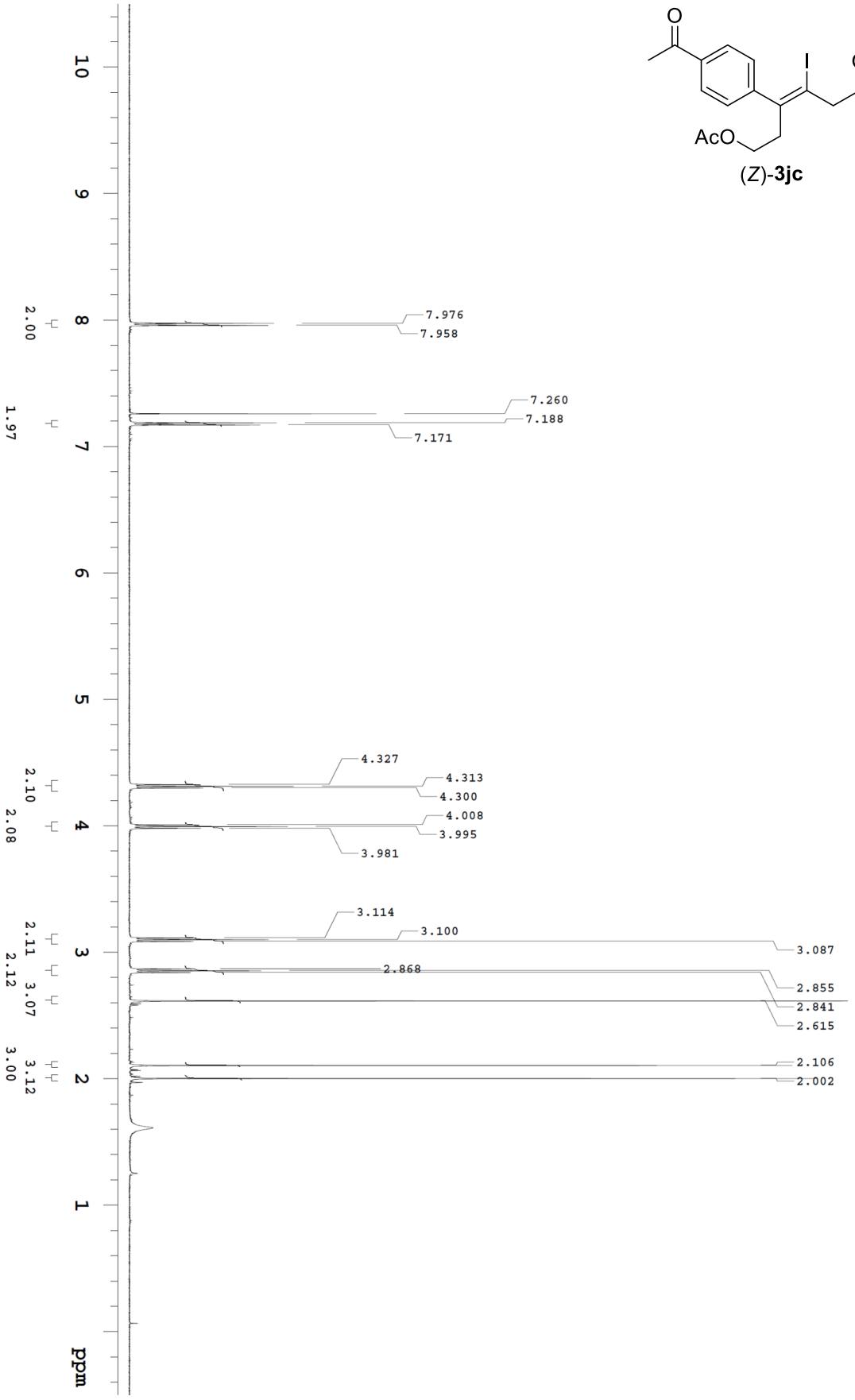
42.095
26.721


O
I
OAc
AcO
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4.300
4.008
3.995
3.981
3.114
3.100
3.087
2.868
2.855
2.841
2.615
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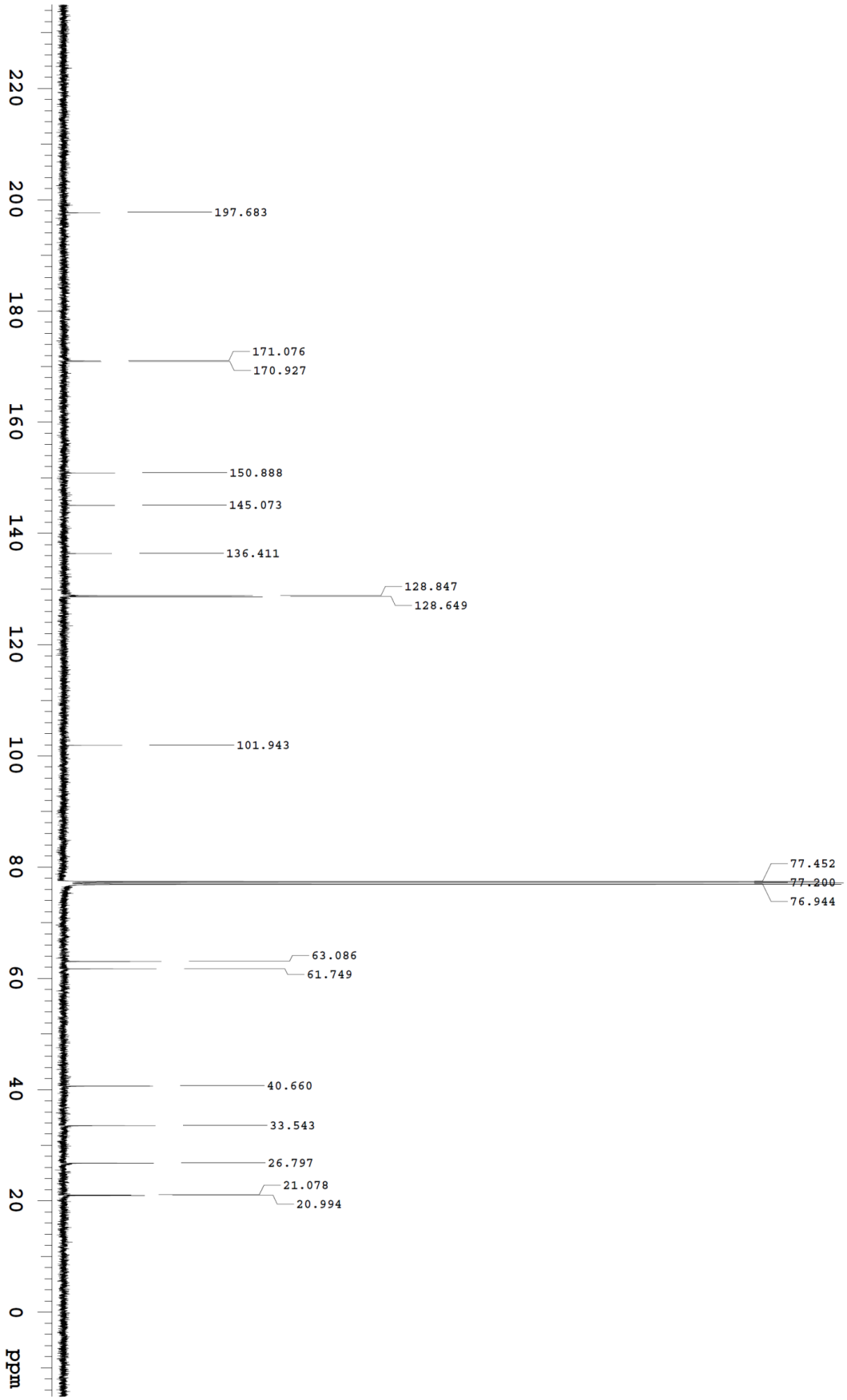
2.00
1.97
2.10
2.08
2.11
2.12
3.07
3.00
3.12
ppm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200
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80
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20
0
ppm
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170.927
150.888
145.073
136.411
128.847
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101.943
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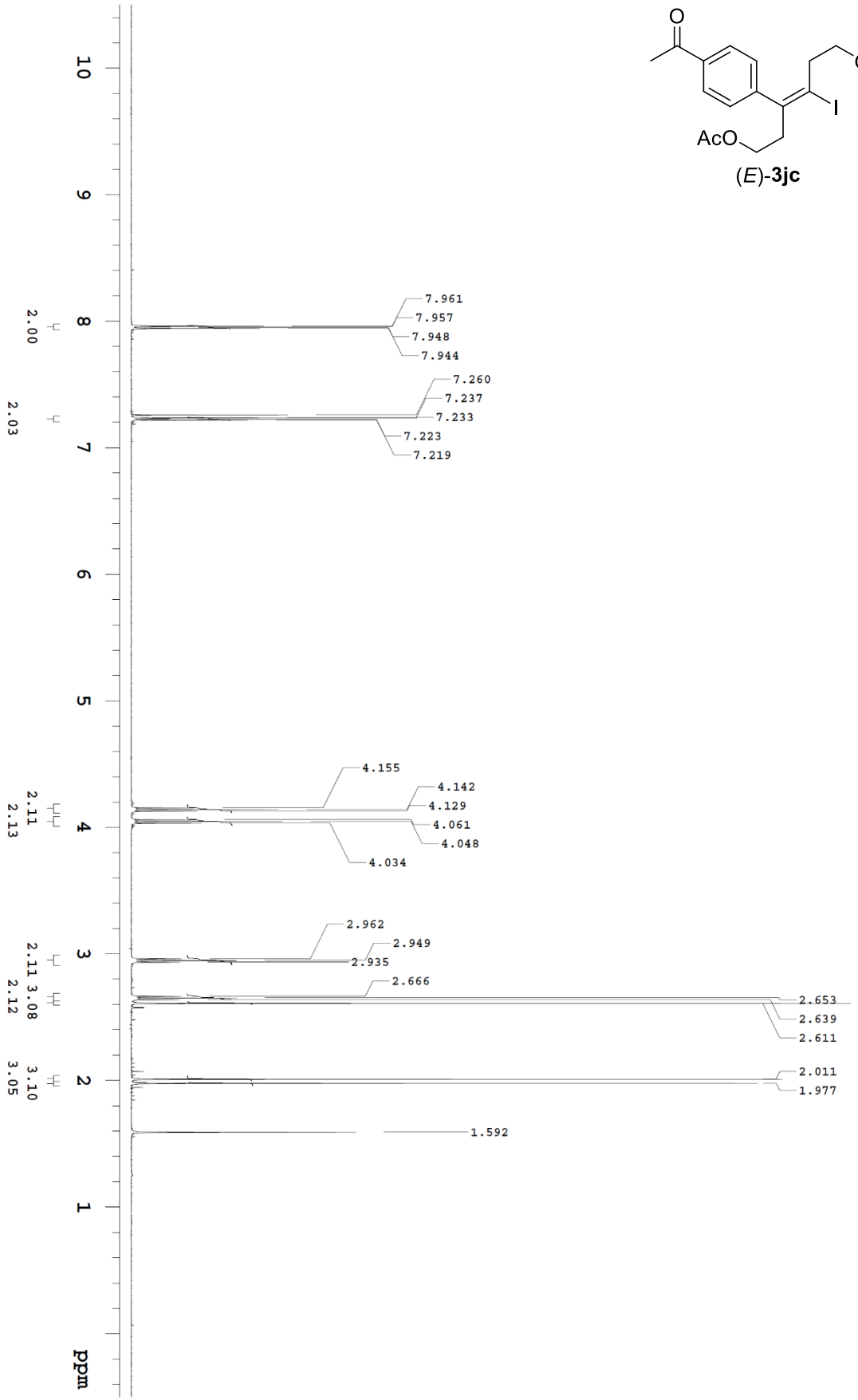
77.200
76.944
63.086
61.749
40.660
33.543
26.797
21.078
20.994


O
OAc
I
AcO
(E)-3jc
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7.957
7.948
7.944
7.260
7.237
7.233
7.223
7.219
4.155
4.142
4.129
4.061
4.048
4.034
2.962
2.949
2.935
2.666
2.653
2.639
2.611
2.011
1.977
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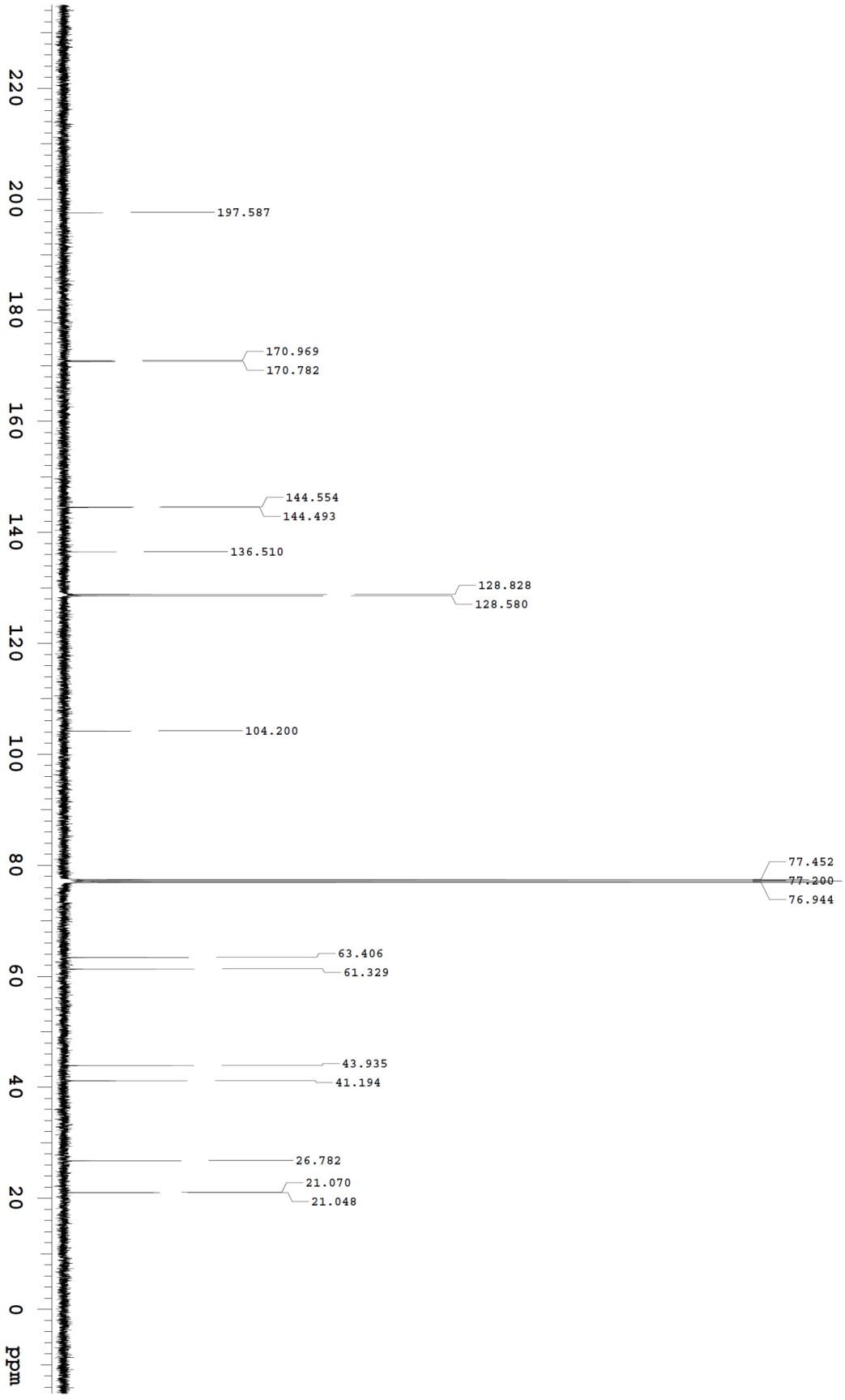
2.00
2.03
2.11
2.13
2.11
3.08
2.12
3.10
3.05
ppm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200
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80
60
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20
0
ppm
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170.782
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136.510
128.828
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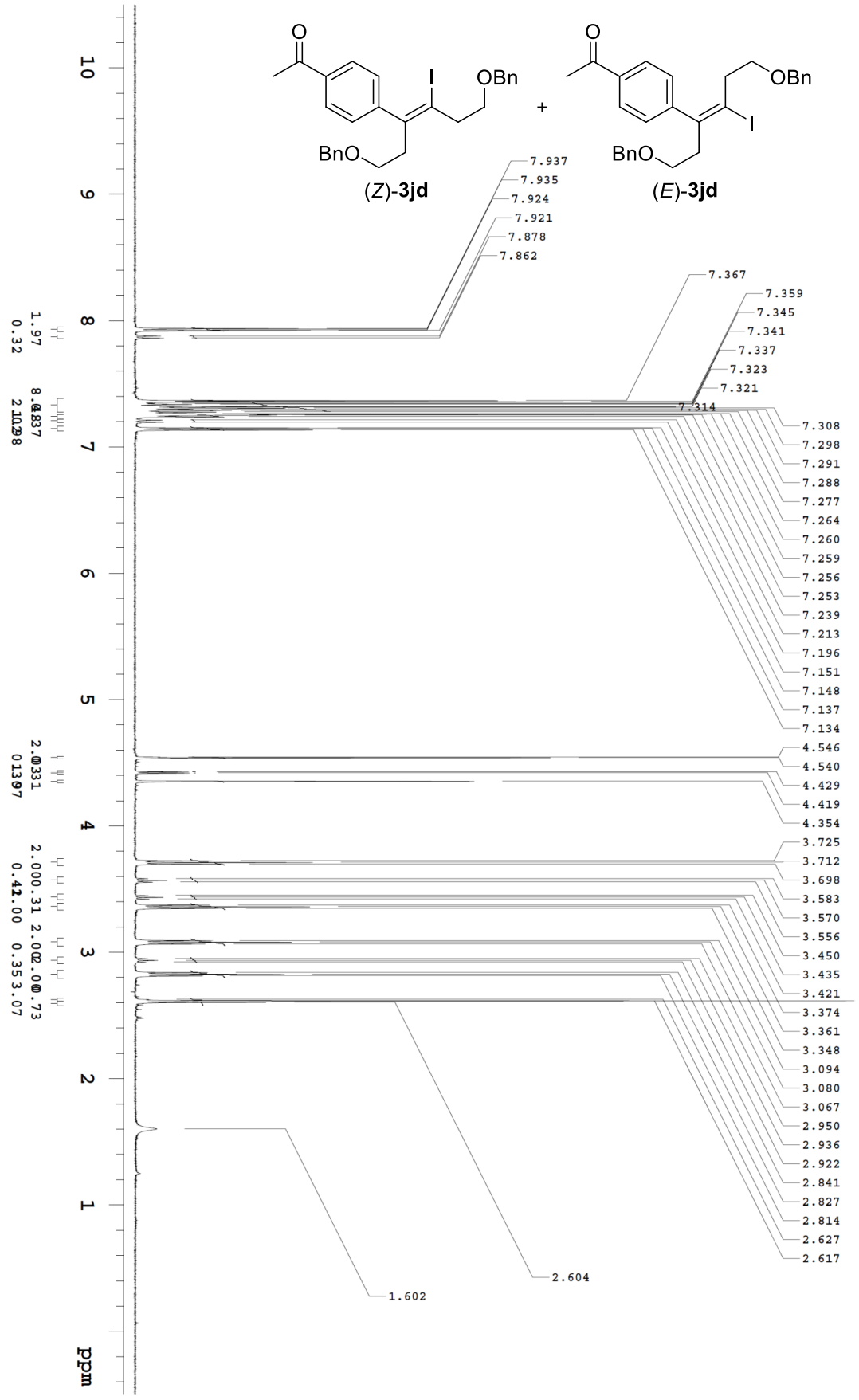
77.452
77.200
76.944
63.406
61.329
43.935
41.194
26.782
21.070
21.048


(Z)-3jd
(E)-3jd
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7.924
7.921
7.878
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7.367
7.359
7.345
7.341
7.337
7.323
7.321
7.314
7.308
7.298
7.291
7.288
7.277
7.264
7.260
7.259
7.256
7.253
7.239
7.213
7.196
7.151
7.148
7.137
7.134
4.546
4.540
4.429
4.419
4.354
3.725
3.712
3.698
3.583
3.570
3.556
3.450
3.435
3.421
3.374
3.361
3.348
3.094
3.080
3.067
2.950
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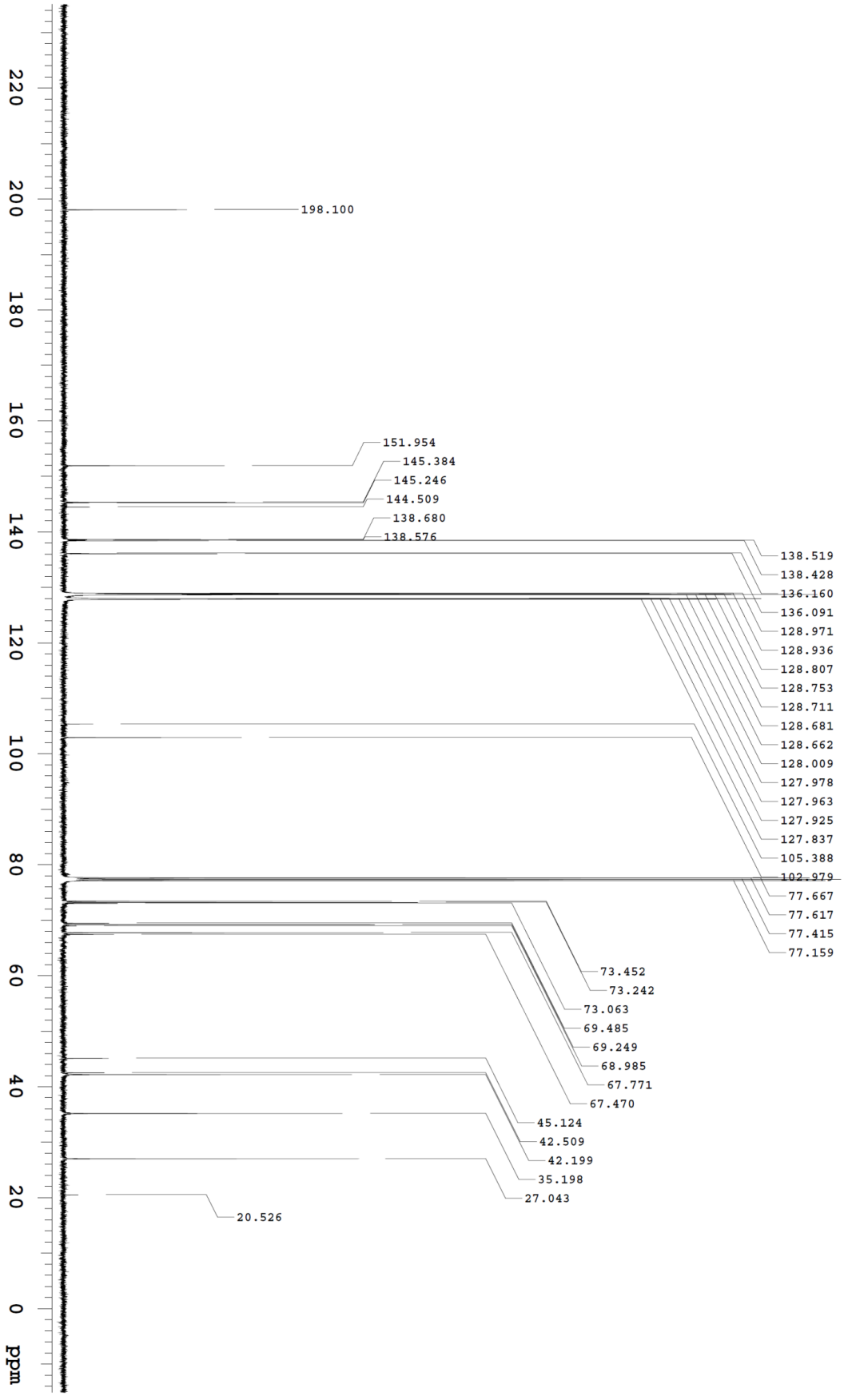
2.922
2.841
2.827
2.814
2.627
2.617
2.604
1.602
ppm


220
200
180
160
140
120
100
80
60
40
20
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ppm
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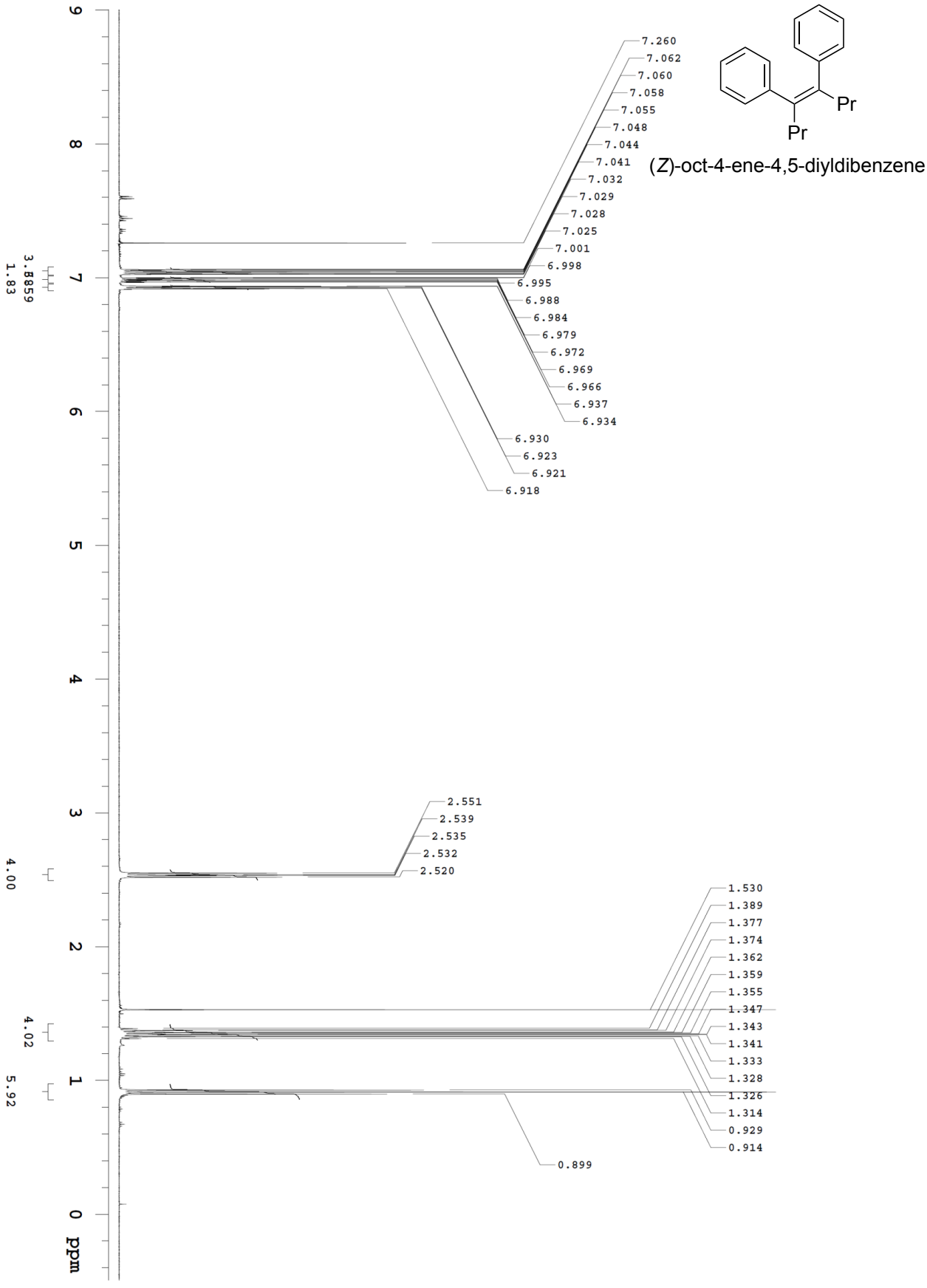
145.246
144.509
138.680
138.576
138.519
138.428
136.160
136.091
128.971
128.936
128.807
128.753
128.711
128.681
128.662
128.009
127.978
127.963
127.925
127.837
105.388
102.979
77.667
77.617
77.415
77.159
73.452
73.242
73.063
69.485
69.249
68.985
67.771
67.470
45.124
42.509
42.199
35.198
27.043
20.526


7.260
7.062
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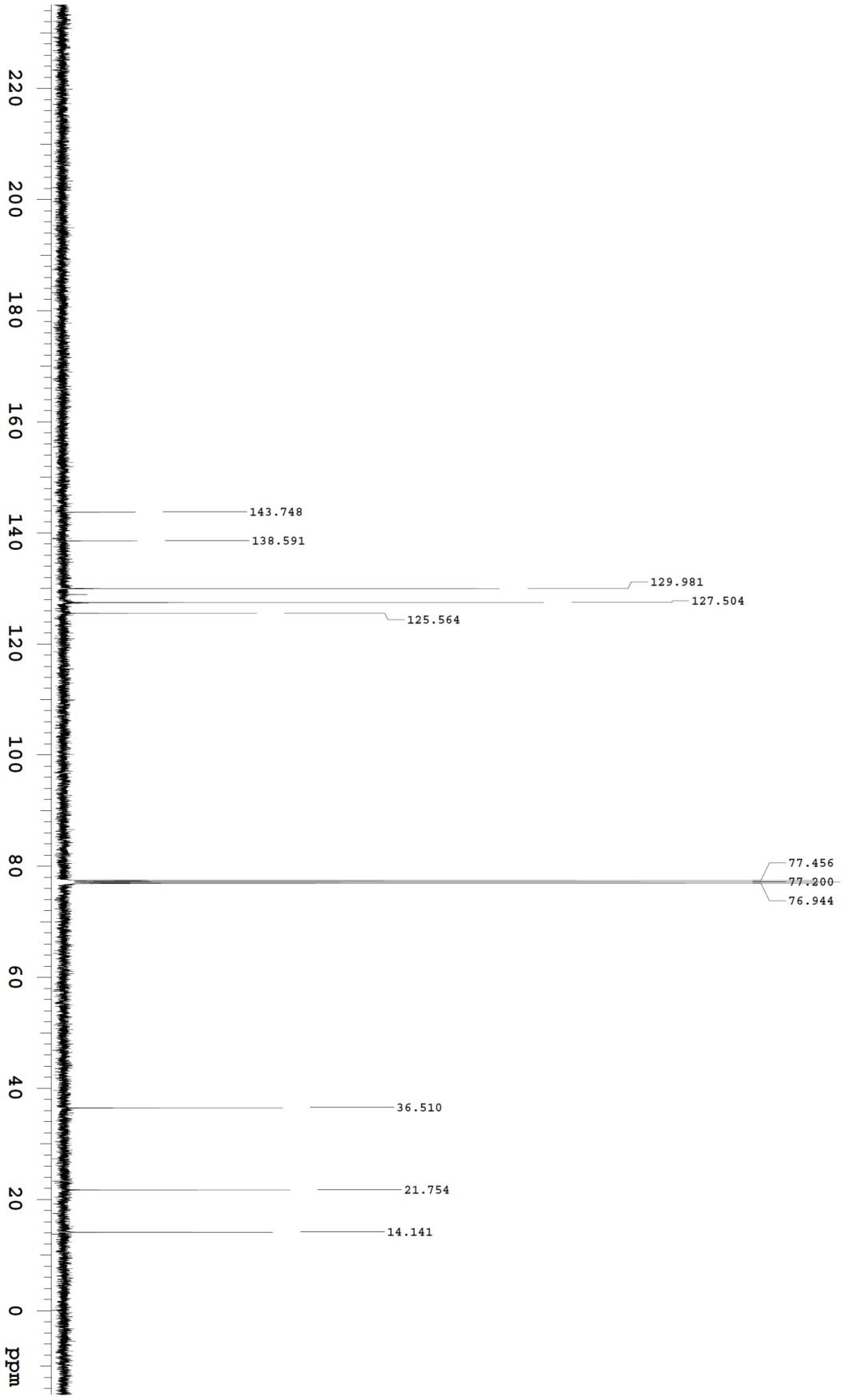
7.058
7.055
7.048
7.044
7.041
7.032
7.029
7.028
7.025
7.001
6.998
6.995
6.988
6.984
6.979
6.972
6.969
6.966
6.937
6.934
6.930
6.923
6.921
6.918
3.8859
1.83
4.00
4.02
5.92
2.551
2.539
2.535
2.532
2.520
1.530
1.389
1.377
1.374
1.362
1.359
1.355
1.347
1.343
1.341
1.333
1.328
1.326
1.314
0.929
0.914
0.899
Pr
Pr
(Z)-oct-4-ene-4,5-diyldibenzene
9
8
7
6
5
4
3
2
1
0
ppm


220
200
180
160
140
120
100
80
60
40
20
0
ppm
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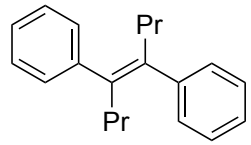
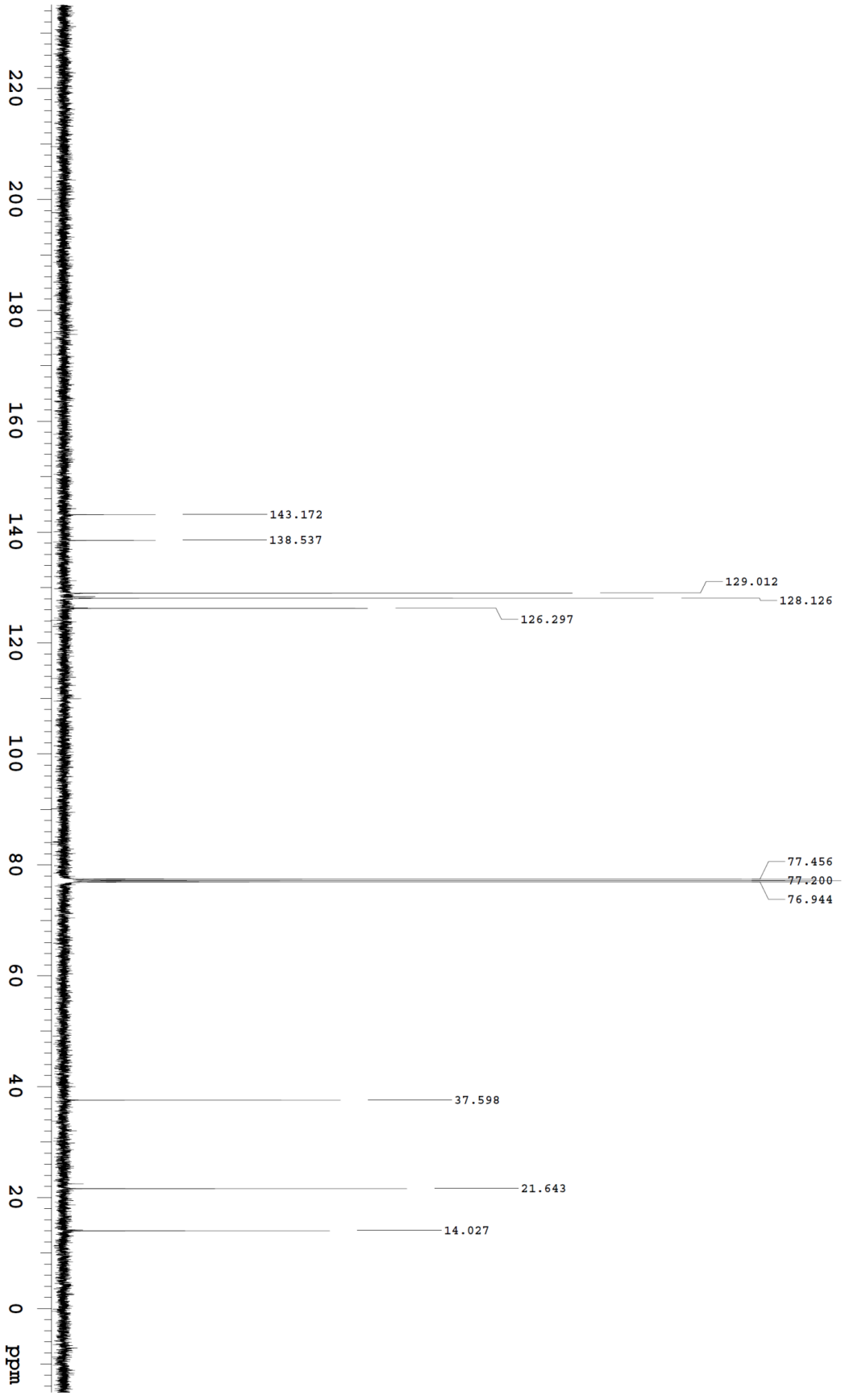
129.981
127.504
125.564
77.456
77.200
76.944
36.510
21.754
14.141



(*E*)-oct-4-ene-4,5-diyldibenzene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140
120
100
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60
40
20
0
ppm
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138.537
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128.126
126.297
77.456
77.200
76.944
37.598
21.643
14.027