Supplementary Information

Rh(I)-Catalyzed [3+2] Annulation Reactions of Cyclopropenones with Amides

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Contents

I. General Information.

^{1}H NMR and ^{13}C NMR spectra were recorded on JEOL ECZS-400YH or JEOL ECS-400 spectrometers in $CDCl_3$ with tetramethylsilane as the internal standard. Data are reported as follows: chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, bs = broad singlet, and m = multiplet), coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4000; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). High resolution mass spectra (HRMS) were obtained on a JEOL JMS-T100LP instrument. Melting points were determined using a Stanford Research Systems apparatus. Column chromatography was performed with SiO_2 (Silicycle SiliaFlash F60 (230-400 mesh)). *E/Z* isomers were separated by Shimadzu Prominence HPLC System, equipped with a Phenomenex Luna Silica (2) (5 μm) column, and some compounds were purified by JAI LC-5060 (GPC) equipped with two JAIGEL-HR columns connected in series.

II. Materials.

Toluene (Kanto Chemical) was purified by passage through activated alumina and under a positive pressure of N_2. Diphenylcyclopropenone (Wako), 2-PhC_6H_4COOH (TCI) were purchased from the commercial suppliers, and used as received. $[Rh(OAc)(cod)]_2$,[1] **1a**,[2] **1b**,[3] **1c**,[4] **1d**,[2] **1e**,[2] **1g**,[5] **1h**,[6] **1i-o**,[7] **1p**,[8] **1q**,[7] **1s**,[9] bis(4-methoxyphenyl)cyclopropenone,[10] bis(4-chlorophenyl)cyclopropenone,[10] diethylcyclopropenone,[11] bicyclo[5.1.0]oct-1(7)-en-8-one,[12] *N*-(quinolin-8-yl)pentanamide,[13] and 4-methyl-*N*-(quinolin-8-yl)benzamide [14] were prepared by the previously reported literature procedure. **1f**,[5] **1r**,[7] **1t**,[9] were prepared from respectively 3-methoxypropanoic acid (Wako), 4-nitrobenzoic acid (TCI) and 2-isopropylbenzoic acid (TCI) according to the literature procedure.

III. General Procedure for the Annulation of Amides with Cyclopropenone

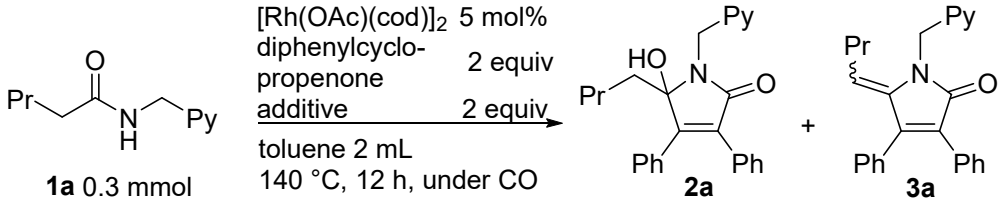
(i) For aliphatic amides.

$[Rh(OAc)(cod)]_2$ (8.1 mg, 0.015 mmol), *N*-(pyridin-2-ylmethyl)pentanamide (**1a**) (57.7 mg, 0.3 mmol), diphenylcyclopropenone (123.7 mg, 0.6 mmol), 2-phenylbenzoic acid (118.8 mg, 0.6 mmol) and toluene (2 mL) were placed in a 50-mL stainless steel autoclave. After charging the autoclave with 10 atm of carbon monoxide three times, it was pressurized to 1 atm. The autoclave was heated in an oil bath at 140 °C for 12 h and was then allowed to cool to room temperature. After filtering the mixture through a celite pad and washing with EtOAc, the filtrate was concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 1/1) and HPLC to afford (*Z*)-5-butylidene-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (**3a-*Z***) (46.2 mg, 41%) as a pale yellow oil and (*E*)-5-butylidene-3,4-diphenyl-*N*-(pyridin-2 -ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (**3a-*E***) (30.0 mg, 30%) as a pale yellow oil.

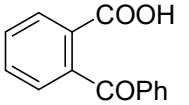
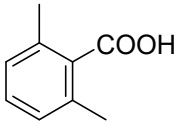
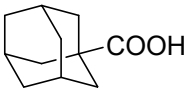
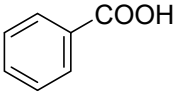
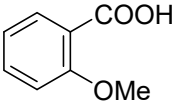
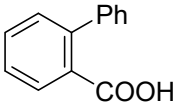
(ii) For aromatic amides.

[Rh(OAc)(cod)]$_2$ (16.2 mg, 0.03 mmol), *N*-(pyridin-2-ylmethyl)benzamide (**1i**) (63.7 mg, 0.3 mmol), Diphenylcyclopropenone (77.3 mg, 0.375 mmol) and toluene (2 mL) were placed in a 50-mL stainless steel autoclave. After charging the autoclave with 10 atm of carbon monoxide three times, it was pressurized to 1 atm. The autoclave was heated in an oil bath at 140 °C for 1 h and was then allowed to cool to room temperature. After filtering the mixture through a celite pad and washing with EtOAc, the filtrate was concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 1/1) to afford 5-hydroxy-3,4,5-triphenyl-*N* -(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (**3i**) (90.4 mg, 72%) as a white solid.

IV. Optimization of Reaction Conditions Using Aliphatic Amides (Table S1)



1a 0.3 mmol **2a** **3a**

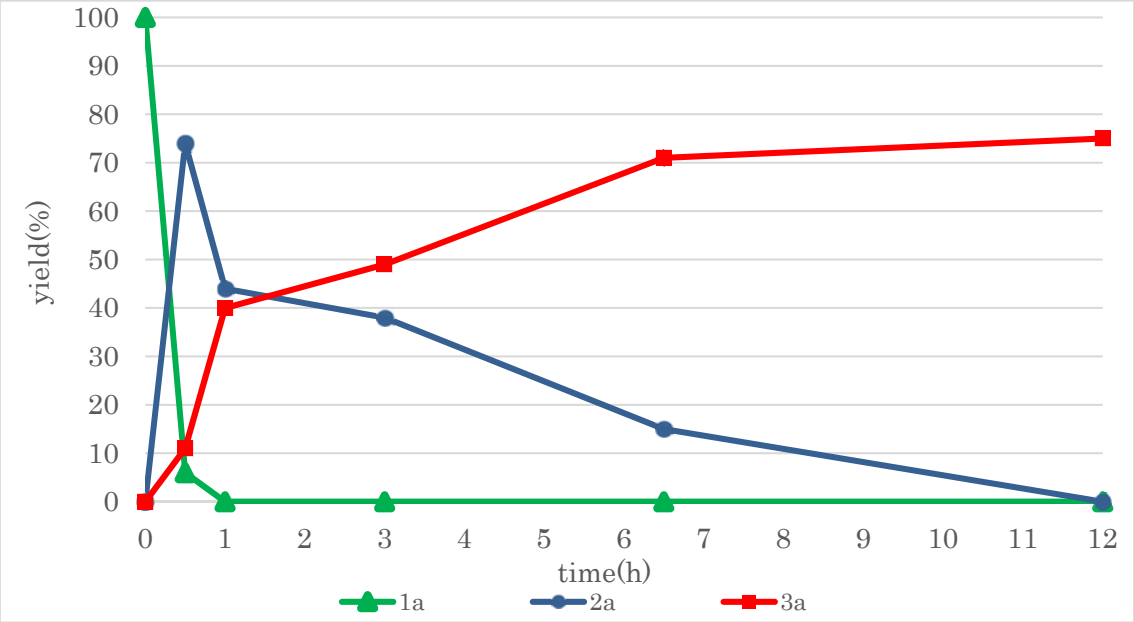
entry	notes	NMR yields (%)			entry	notes	NMR yields (%)		
		2a	**3a**	SM			**2a**	**3a**	SM
1	-	56	18	0	8		5	72	0
2	cat. $Rh(CO)Cl(PPh_3)_2$	0	0	64					
3	Na_2CO_3	85	14	0					
4	PivOH	26	31	0	9		0	75	0
5		13	65	0					
6		10	70	0	10	″ under N_2	0	61	0
					11	″ 130 °C	8	50	17
					12	″ w/o Rh	0	0	83
7		0	62	0	13		0	82	0

The reaction of diphenylcyclopropenone with *N*-(pyridin-2-ylmethyl)pentanamide (**1a**) in the presence of [Rh(OAc)(cod)]$_2$ in toluene at 140 °C under an atmosphere of CO gave a mixture of **2a** in 56% yield and **3a** in 18% yield (entry 1). Using Na_2CO_3 (2 equiv) as an additive gave **2a** as the major product in 85% yield and **3a** in 14% yield (entry 3). In sharp contrast, **3a** was the major product when carboxylic acids were used as additives (entry 4-9). Using 2,6-dimethylbenzoic acid, **3a** was produced as the sole product in the reaction (entry 9). When the reaction was carried out in an atmosphere of N_2,

a slightly lower product yield was obtained compared to the use of a CO atmosphere (entry 10), probably because of the decomposition of diphenylcyclopropenone to diphenylacetylene and CO. No reaction took place when the reaction was carried out in the absence of a rhodium catalyst (entry 12). After screening a series of carboxylic acids, 2-phenylbenzoic acid was found to be the additive of choice (entry 13).

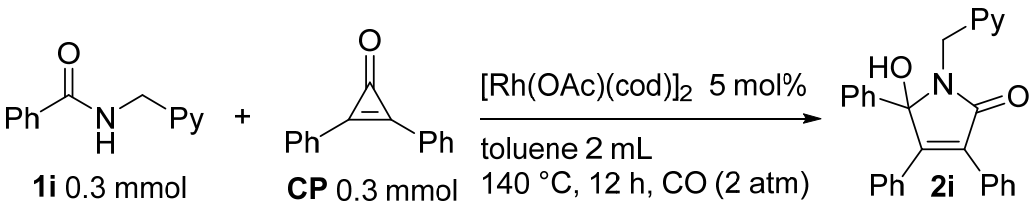
V. Time Course for the Annulation of Aliphatic Amides with Cyclopropenone (Scheme S1)

An examination of the time course for the reaction indicated that **1a** had completely reacted after 1 h and that **2a** was rapidly formed (74% yield after 30 min). During the course of the reaction, the yield of **2a** gradually decreased, the yield of **3a** gradually increased and **2a** had completely disappeared after 12 h.

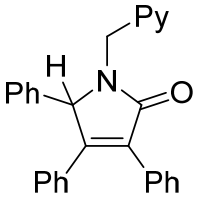


An examination of the time course for the reaction indicated that **1a** had completely reacted after 1 h and that **2a** was rapidly formed (74% yield after 30 min). During the course of the reaction, the yield of **2a** gradually decreased, the yield of **3a** gradually increased and **2a** had completely disappeared after 12 h.

VI. Re-Optimization of Reaction Conditions Using Aromatic Amides (Table S2)



entry	note	NMR yields (%) 2i	SM	
1[a]	120 °C	50	33	
2[a]	140 °C	72	25	
3[a]	160 °C	73	18	
4	under CO	64	23	
5	CO (2 atm)	69	35	
6	CO (3 atm)	44	38	
7	Na_2CO_3 (2 equiv)	43	59	
8	PivOH (1 equiv)	49	39	
9	CP (1.5 equiv), under CO	79	0	20%
10	CP (1.5 equiv), under N_2, 3 h	72	0	16%
11	CP (2 equiv), under CO, 1 h, Na_2CO_3 (2 equiv)	62	0	29%
12	CP (1.3 equiv), under CO, 1 h, 2-PhC_6H_4COOH (1 equiv)	70	12	11%
13[a]	CP (1.25 equiv), CO (1 atm), 1 h	80	0	9%

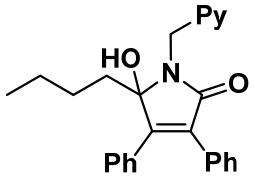


[a] $[Rh(OAc)(cod)]_2$ (10 mol%)

The reaction of *N*-(pyridin-2-ylmethyl) benzamide (**1i**) gave the expected product **2i**. When the reaction was carried out at 120 °C, and a CO pressure of 3 atm, the yield of product was quite low (entry 1-6). The addition of Na_2CO_3 or PivOH had no effect on the reaction (entry 7 and 8). When the amount of cyclopropenone was increased (from 1 equiv to 1.5 equiv), **1i** disappeared and a higher yield of **2i** was obtained, but a reduction product **6** was generated in 21% yield (entry 9). In additional screening (entry 10-13), when the amount of cyclopropenone was reduced to 1.25 equivalents, **2i** was produced in 80% yield. Although no reaction conditions were identified in which the by-product **6** was not formed, **2i** was easily isolated in pure form by silica gel column chromatography.

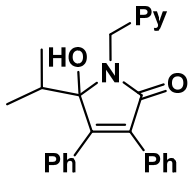
VII. Spectroscopic Data for [3+2] Annulation Products

5-butyl-5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2a)



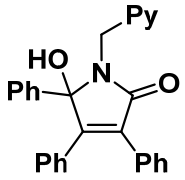
R_f 0.23 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.73 (t, J = 7.0 Hz, 3H), 0.94-1.08 (m, 2H), 1.14 (sep, J = 7.0 Hz, 2H), 1.91 (m, 2H), 4.51 (d, J = 16.0 Hz, 1H), 5.03 (d, J = 16.0 Hz, 1H), 7.17 (dd, J = 6.7, 4.8 Hz, 1H), 7.20-7.23 (m, 3H), 7.28-7.31 (m, 3H), 7.36-7.39 (m, 2 H), 7.45 (d, J = 8.0 Hz, 1H), 7.60-7.63 (m, 2H), 7.66 (dt, J = 7.7, 1.9 Hz, 1H), 8.09 (brs, 1H), 8.42 (dq, J = 4.2, 1.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) 13.89, 22.34, 25.05, 35.47, 44.36, 91.51, 122.67, 122.90, 127.97, 128.03, 128.36, 128.81, 129.20, 129.75, 130.57, 131.00, 132.91, 137.60, 148.30, 154.17, 156.90, 169.92; IR ($CHCl_3$) 2957 w, 2930 w, 2864 w, 1686 m, 1597 w, 1435 w, 1397 w, 1321 w, 1153 w, 1075 w, 1007 w, 908 m, 846 w, 798 w, 728 s, 695 s; HRMS Calcd for $C_{26}H_{27}N_2O_2$ $(M+H)^+$: 399.2067; Found: 399.2058.

5-hydroxy-5-isopropyl-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2g)



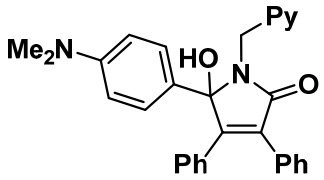
R_f 0.29 (hexane/EtOAc = 1/1). Pale Yellow Solid. Mp = 182, 183 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.75 (d, J = 6.8 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H), 2.17 (sep, J = 6.9 Hz, 1H), 4.64 (d, J = 15.8 Hz, 1H), 5.03 (d, J = 15.8 Hz, 1H), 7.16-7.21 (m, 4H), 7.25-7.31 (m, 5H), 7.43 (d, J = 7.8 Hz, 1H), 7.60-7.63 (m, 2H), 7.67 (td, J = 7.6, 1.4 Hz, 1H), 8.17 (brs, 1H), 8.44 (dq, J = 5.0, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 16.72, 17.00, 35.00, 45.74, 93.40, 122.68, 123.07, 127.88, 128.02, 128.35, 128.76, 129.53, 129.79, 130.96, 131.30, 134.01, 137.64, 148.38, 155.18, 157.20, 170.77; IR ($CHCl_3$) 3057 w, 2966 w, 1688 s, 1598 w, 1573 w, 1437 w, 1392 m, 1301 w, 1152 w, 1065 w, 1006 w, 910 m, 789 w, 757 w, 728 s, 695 s; HRMS Calcd for $C_{25}H_{25}N_2O_2$ $(M+H)^+$: 385.1911; Found: 385.1892.

5-hydroxy-3,4,5-triphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2i)



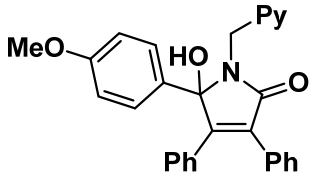
R_f 0.31 (hexane/EtOAc = 1/1). White Solid. Mp = 156, 157 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.03, (d, J = 16.3 Hz, 1H), 5.02 (d, J = 16.3 Hz, 1H), 7.10-7.31 (m, 10H), 7.35 (q, J = 6.7 Hz, 3H), 7.44-7.47 (m, 2H), 7.59 (dd, J = 7.0, 1.6 Hz, 2H), 7.68 (td, J = 7.7, 1.9 Hz, 1H), 8.49 (dq, J = 4.8, 1.0 Hz, 1H), 9.30 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 45.09, 91.64, 122.77, 122.82, 126.76, 128.19, 128.23, 128.47, 128.74, 129.32, 129.35, 129.72, 129.91, 129.92, 131.21, 132.51, 138.00, 139.52, 148.24, 156.33, 156.94, 170.04; IR ($CHCl_3$) 3058 w, 3030 w, 1693 s, 1598 w, 1573 w, 1488 w, 1442 w, 1390 m, 1309 w, 1201 w, 1149 w, 1050 w, 1008 w, 944 w, 910 m, 792 w, 730 s, 695 s; HRMS Calcd for $C_{28}H_{23}N_2O_2$ $(M+H)^+$: 419.1754; Found: 419.1744.

5-(4-(dimethylamino)phenyl)-5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2j)



R_f 0.20 (hexane/EtOAc = 1/1). Yellow Solid. Mp = 202-203 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.95 (s, 6H), 4.06 (d, J = 16.2 Hz, 1H), 5.01 (d, J = 16.2 Hz, 1H), 6.69 (d, J = 8.9 Hz, 2H), 7.12-7.29 (m, 9H), 7.27 (d, J = 7.8 Hz, 1H), 7.41-7.46 (m, 4H), 7.68 (td, J = 7.8, 1.8 Hz, 1H), 9.12 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 40.51, 44.97, 91.84, 112.31, 122.66, 126.18, 127.66, 128.01, 128.12, 128.15, 128.56, 129.33, 129.42, 129.93, 131.46, 132.80, 137.87, 148.23, 150.39, 156.51, 157.21, 169.67; IR ($CHCl_3$) 3057 w, 2881 w, 2850 w, 2806 w, 2245 w, 1691 s, 1610 m, 1521 m, 1441 w, 1391 w, 1356 w, 1225 w, 1164 w, 1065 w, 944 w, 910 m, 823 w, 794 w, 756 w, 730 s, 695 s; HRMS Calcd for $C_{30}H_{28}N_3O_2$ $(M+H)^+$: 462.2176; Found: 462.2157.

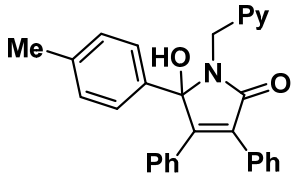
5-hydroxy-5-(4-methoxyphenyl)-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2k)



R_f 0.29 (hexane/EtOAc = 1/1). White Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 3.79 (s, 3H), 4.05 (d, J = 16.2 Hz, 1H), 5.01 (d, J = 16.5 Hz, 1H), 6.87 (d, J = 9.2 Hz, 2H), 7.12-7.27 (m, 9H), 7.39 (d, J = 7.8 Hz, 1H), 7.43-7.46 (m, 2H), 7.49 (d, J = 8.9 Hz, 2H), 7.70 (td, J = 7.8, 1.6 Hz, 1H), 8.49 (dd, J = 5.0, 0.9 Hz, 1H), 9.22 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 44.95, 55.34, 91.54, 114.03, 122.76, 122.78, 128.07, 128.14, 128.16, 128.17, 128.19, 128.67, 129.34, 129.48, 129.89, 131.23, 132.60, 138.02, 148.16, 156.35, 156.96, 159.64, 169.95; IR ($CHCl_3$) 3058 w, 2928 w, 2837

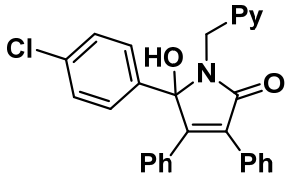
w, 2247 w, 1693 s, 1599 w, 1509 m, 1440 w, 1390 m, 1306 w, 1250 m, 1170 m, 1030 w, 947 w, 911 m, 835 w, 796 w, 730 s, 695 s; HRMS Calcd for $C_{29}H_{25}N_2O_3$ $(M+H)^+$: 449.1860; Found: 449.1887.

5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-5-(*p*-tolyl)-1,5-dihydro-2*H*-pyrrol-2-one (2l)



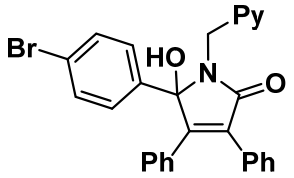
R_f 0.37 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.32 (s, 3H), 4.03 (d, J = 16.5 Hz, 1H), 5.01 (d, J = 16.5 Hz, 1H), 7.11-7.29 (m, 11H), 7.38 (d, J = 8.0 Hz, 1H), 7.44-7.48 (m, 4H), 7.69 (td, J = 7.8, 1.8 Hz, 1H), 9.23 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 21.28, 45.00, 91.66, 122.75, 122.78, 126.66, 128.16, 128.21, 128.69, 128.68, 129.37, 129.47, 129.64, 129.92, 131.27, 132.57, 136.41, 138.00, 138.19, 148.19, 156.30, 156.97, 169.99; IR ($CHCl_3$) 3056 w, 3021 w, 2920 w, 2247 w, 1692 s, 1598 w, 1574 w, 1423 w, 1390 m, 1309 w, 1150 w, 1050 w, 1008 w, 953 w, 909 m, 826 w, 783 w, 728 s, 694 s; HRMS Calcd for $C_{29}H_{25}N_2O_2$ $(M+H)^+$: 433.1911; Found: 433.1899.

5-(4-chlorophenyl)-5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2m)



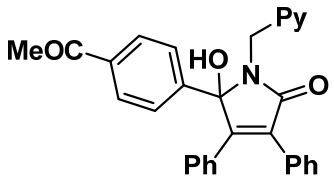
R_f 0.37 (hexane/EtOAc = 1/1). White Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.03 (d, J = 16.3 Hz, 1H), 5.01 (d, J = 16.2 Hz, 1H), 7.12-7.28 (m, 9H), 7.30 (d, J = 8.9 Hz, 2H), 7.39 (d, J = 7.8 Hz, 1H), 7.43-7.48 (m, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.70 (td, J = 7.8, 1.6 Hz, 1H), 8.48 (d, J = 4.4 Hz, 1H), 9.40 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 44.97, 91.22, 122.79, 122.90, 128.23, 128.25, 128.30, 128.85, 128.89, 129.23, 129.73, 129.84, 129.90, 130.93, 132.27, 134.31, 138.08, 138.30, 148.14, 155.92, 156.62, 169.89, 169.89; IR ($CHCl_3$) 3059 w, 2249 w, 1694 s, 1599 w, 1487 w, 1391 m, 1310 w, 1151 w, 1093 w, 1011 w, 907 s, 834 w, 793 w, 726 s, 694 s; HRMS Calcd for $C_{28}H_2ClN_2O_2$ $(M+H)^+$: 453.1364; Found: 453.1368.

5-(4-bromophenyl)-5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2n)



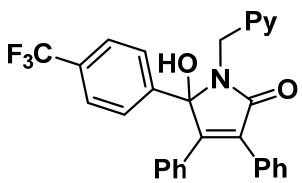
R_f 0.40 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.03 (d, J = 16.3 Hz, 1H), 5.00 (d, J = 16.3 Hz, 1H), 7.12-7.26 (m, 9H), 7.39 (d, J = 7.7 Hz, 1H), 7.42-7.46 (m, 6H), 7.70 (td, J = 8.0, 1.9 Hz, 1H), 8.48 (d, J = 4.5 Hz, 1H), 9.41 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 45.00, 91.27, 122.61, 122.80, 122.91, 128.25, 128.28, 128.32, 128.59, 128.88, 129.24, 129.77, 129.86, 130.93, 131.86, 132.26, 138.07, 138.90, 148.18, 155.87, 156.64, 169.91; IR ($CHCl_3$) 3057 w, 3024 w, 1694 s, 1598 w, 1574 w, 1484 w, 1423 w, 1391 m, 1310 w, 1200 w, 1150 w, 1198 w, 1071 w, 1010 w, 952 w, 909 m, 832 w, 793 w, 729 s, 695 s; HRMS Calcd for $C_{28}H_{22}BrN_2O_2$ $(M+H)^+$: 497.0859; Found: 497.0842.

5-(4-acetylphenyl)-5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2o)



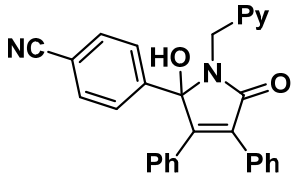
R_f 0.23 (hexane/EtOAc = 1/1). Pale Yellow Solid. Mp = 191-192 °C. ^{1}H NMR ($CDCl_3$, 395.88 MHz) δ 2.56 (s, 3H), 4.02 (d, J = 16.2 Hz, 1H), 5.02 (d, J = 16.2 Hz, 1H), 7.11-7.18 (m, 3H), 7.23-7.27 (m, 6H), 7.39 (d, J = 7.5 Hz, 1H), 7.45-7.47 (m, 2H), 7.68-7.71 (m, 3H), 7.92 (d, J = 8.7 Hz, 2H), 8.49 (d, J = 4.4 Hz, 1H), 9.47 (brs, 1H); ^{13}C NMR ($CDCl_3$, 99.55 MHz) δ 26.76, 45.05, 91.31, 122.77, 122.92, 127.02, 128.23, 128.24, 128.35, 128.73, 128.86, 129.19, 129.82, 129.94, 130.87, 132.18, 137.07, 138.06, 145.07, 148.16, 155.78, 156.53, 169.91, 197.74; IR ($CHCl_3$) 3058 w, 2835 w, 2249 w, 1684 s, 1602 w, 1424 w, 1389 m, 1309 w, 1267 m, 1150 w, 1074 w, 1010 w, 953 w, 909 m, 837 w, 794 w, 727 s, 694 s; HRMS Calcd for $C_{30}H_{25}N_2O_2$ $(M+H)^+$: 461.1860; Found: 461.1827.

5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-5-(4-(trifluoromethyl)phenyl)-1,5-dihydro-2*H*-pyrrol-2-one (2p)



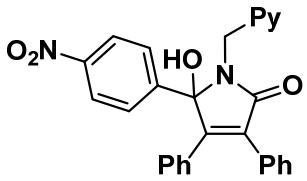
R_f 0.40 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 395.88 MHz) δ 4.01 (d, J = 16.3 Hz, 1H), 5.02 (d, J = 16.3 Hz, 1H), 7.12-7.19 (m, 3H), 7.21-7.7.28 (m, 6H), 7.38 (d, J = 7.7 Hz, 1H), 7.44-7.47 (m, 2H), 7.59 (d, J = 8.1 Hz, 2H), 7.68 (d, J = 7.7, 1.8 Hz, 1H), 7.73 (d, J = 7.7 Hz, 2H), 8.49 (dq, J = 4.1, 0.9 Hz, 1H), 9.51 (brs, 1H); ^{13}C NMR ($CDCl_3$, 99.55 MHz) δ 45.06, 91.20, 122.83, 122.96, 125.45, 125.68 (q, J = 2.0 Hz), 127.21, 128.29 (d, J = 152 Hz), 128.40, 128.94, 129.21, 129.85, 130.01, 130.38, 130.70, 130.85, 132.14, 138.10, 144.03, 148.18, 155.79, 156.51, 169.93; IR ($CHCl_3$) 3060 w, 2923 w, 1696 m, 1599 w, 1574 w, 1485 w, 1389 w, 1323 s, 1165 w, 1124 m, 1067 m, 1016 w, 941 w, 908 m, 866 w, 842 w, 794 w, 729 s, 694 s; HRMS Calcd for $C_{29}H_{22}F_3N_2O_2$ $(M+H)^+$: 487.1628; Found: 487.1642.

4-(2-hydroxy-5-oxo-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-yl)benzonitrile (2q)



R_f 0.26 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.01 (d, J = 16.4 Hz, 1H), 5.01 (d, J = 16.5 Hz, 1H), 7.12-7.26 (m, 9H), 7.39 (d, J = 7.8 Hz, 1H), 7.44-7.46 (m, 2H), 7.61 (d, J = 8.5 Hz, 2H), 7.68-7.72 (m, 3H), 8.48 (d, J = 4.6 Hz, 1H), 9.59 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 44.99, 112.21, 118.59, 122.80, 122.98, 127.51, 128.22, 128.29, 128.43, 128.97, 129.05, 129.74, 129.97, 130.57, 131.93, 132.45, 138.11, 145.33, 148.09, 155.47, 156.23, 169.84; IR ($CHCl_3$) 3059 w, 2763 w, 2229 w, 1696 m, 1600 w, 1487 w, 1423 w, 1388 w, 1310 w, 1202 w, 1150 w, 1051 w, 1010 w, 941 w, 909 m, 840 w, 794 w, 727 s, 694 s; HRMS Calcd for $C_{29}H_{22}N_3O_2$ $(M+H)^+$: 444.1707; Found: 444.1700.

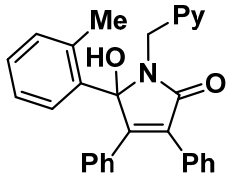
5-hydroxy-5-(4-nitrophenyl)-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2r)



R_f 0.34 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.04 (d, J = 16.2 Hz, 1H), 5.03 (d, J = 16.5 Hz, 1H), 7.13-7.23 (m, 3H), 7.26-7.29 (m, 6H), 7.42 (d, J = 8.0 Hz, 1H), 7.44-7.48 (m, 2H), 7.74 (td, J = 7.8, 1.6 Hz, 1H), 7.77 (d, J = 8.7 Hz, 2H), 8.17 (dd, J = 9.2, 1.2 Hz, 2H), 8.51 (dq, J = 5.0, 0.7 Hz, 1H), 9.67 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 45.10, 91.06, 122.94, 123.13, 123.91, 127.88, 128.32, 128.43, 128.56, 12912, 129.14, 129.83, 130.10, 130.59,

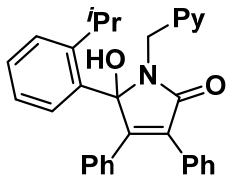
131.96, 138.27, 147.43, 147.98, 148.17, 155.50, 156.25, 169.95; IR ($CHCl_3$) 3061 w, 1697 s, 1599 w, 1520 m, 1487 w, 1424 w, 1388 w, 1347 s, 1312 w, 1199 w, 1151 w, 1100 w, 1051 w, 1011 w, 942 w, 909 m, 871 w, 853 w, 793 w, 728 s, 695 s; HRMS Calcd for $C_{28}H_{22}N_3O_4$ $(M+H)^+$: 464.1605; Found: 464.1598.

5-hydroxy-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-5-(*o*-tolyl)-1,5-dihydro-2*H*-pyrrol-2-one (2s)



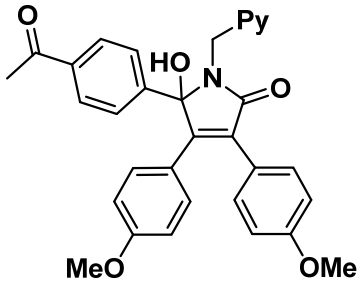
R_f 0.50 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 395.88 MHz) δ 2.27 (s, 3H), 3.99 (d, J = 16.3 Hz, 1H), 4.98 (d, J = 16.3 Hz, 1H), 7.08-7.27 (m, 12H), 7.35 (d, J = 7.8 Hz, 1H), 7.42-7.45 (m, 2H), 7.66 (td, J = 7.8, 1.4 Hz, 1H), 8.18 (dd, J = 7.8, 2.3 Hz, 1H), 8.48 (d, J = 4.6 Hz, 1H), 9.41 (brs, 1H); ^{13}C NMR ($CDCl_3$, 99.54 MHz) δ 20.00, 45.11, 91.12, 122.59, 122.75, 126.37, 128.16, 128.19, 128.24, 128.74, 128.85, 129.01, 129.70, 130.24, 130.48, 131.24, 132.20, 132.47, 135.16, 136.65, 137.92, 148.17, 154.95, 156.71, 170.41; IR ($CHCl_3$) 3060 w, 2247 w, 1692 s, 1598 w, 1574 w, 1482 w, 1439 w, 1389 w, 1311 w, 1203 w, 1130 w, 1041 w, 1008 w, 909 m, 728 s, 694 w; HRMS Calcd for $C_{29}H_{25}N_2O_2$ $(M+H)^+$: 433.1911; Found: 433.1889.

5-hydroxy-5-(2-isopropylphenyl)-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2t)



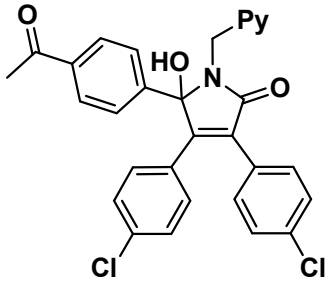
R_f 0.51 (hexane/EtOAc = 1/1). White Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 1.06 (d, J = 6.6 Hz, 3H), 1.19 (t, J = 6.9 Hz, 3H), 3.34 (sept, J = 6.8 Hz, 1H), 4.08 (d, J = 16.3 Hz, 1H), 4.98 (d, J = 16.5, 1H), 7.06-7.43 (m, 15H), 7.68 (td, J = 7.9, 1.8 Hz, 1H), 8.26 (dd, J = 7.8, 0.7 Hz, 1H), 8.48 (dt, J = 4.1, 0.9 Hz, 1H), 9.53 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 24.46, 24.86, 27.88, 45.58, 90.91, 122.62, 122.78, 125.90, 127.13, 128.12, 128.18, 128.37, 128.90, 129.31, 129.45, 129.67, 129.76, 130.10, 131.53, 132.27, 134.64, 137.97, 147.24, 148.13, 156.73, 157.23, 170.41; IR ($CHCl_3$) 3061 w, 2960 w, 2868 w, 2247 w, 1693 s, 1598 w, 1481 w, 1442 w, 1388 m, 1310 w, 1153 w, 1126 w, 1030 w, 957 w, 760 s; HRMS Calcd for $C_{31}H_{29}N_2O_2$ $(M+H)^+$: 461.2224; Found: 461.2228.

5-(4-acetylphenyl)-5-hydroxy-3,4-bis(4-methoxyphenyl)-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2u)



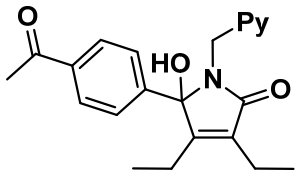
R_f 0.26 (hexane/EtOAc = 1/2). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.57 (s, 3H), 3.71 (s, 3H), 3.78 (s, 3H), 3.98 (d, J = 16.2 Hz, 1H), 4.99 (d, J = 16.5 Hz, 1H), 6.67 (dt, J = 9.2, 2.8 Hz, 2H), 6.83 (dt, J = 8.9, 2.1 Hz, 2H), 7.22-7.26 (m, 3H), 7.39 (d, J = 16.2 Hz, 1H), 7.44 (dt, J = 8.9, 2.0 Hz, 2H), 7.68-7.72 (m, 3H), 7.92 (d, J = 8.7 Hz, 2H), 8.49 (dq, J = 4.8, 0.7 Hz, 1H), 9.43 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 26.78, 44.93, 55.15, 55.27, 91.17, 113.72, 113.79, 122.76, 122.87, 213.55, 124.59, 216.97, 128.25, 128.73, 130.72, 131.17, 136.98, 138.03, 145.68, 148.16, 153.96, 156.66, 159.54, 159.83, 170.32, 197.81; IR ($CHCl_3$) 3072 w, 2931 w, 2838 w, 2249 w, 1685 s, 1604 m, 1572 w, 1507 m, 1423 w, 1389 w, 1295 m, 1250 s, 1178 m, 1150 w, 1029 w, 954 w, 829 w, 732 m; HRMS Calcd for $C_{32}H_{29}N_2O_5$ $(M+H)^+$: 521.2071; Found: 521.2089.

5-(4-acetylphenyl)-3,4-bis(4-chlorophenyl)-5-hydroxy-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2v)



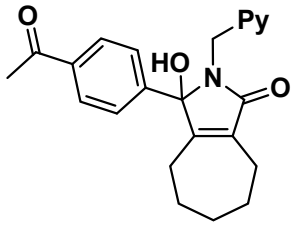
R_f 0.36 (hexane/EtOAc = 1/2). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.58 (s, 3H), 4.02 (d, J = 16.2 Hz, 1H), 5.00 (d, J = 16.5 Hz, 1H), 7.14 (dt, J = 8.9, 2.1 Hz , 2H), 7.20 (dt, J = 8.9, 2.3 Hz, 2H), 7.25-7.29 (m, 3H), 7.38-7.41 (m, 3H), 7.65 (d, J = 8.2 Hz, 2H), 7.74 (td, J = 7.8, 1.6 Hz, 1H), 7.93 (dd, J = 8.7, 1.2 Hz, 2H), 8.51 (dq, J = 5.0, 0.9 Hz, 2H), 9.61 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 26.83, 45.11, 91.29, 122.87, 123.13, 126.97, 128.73, 128.83, 128.90, 129.00, 129.16, 130.42, 130.50, 131.19, 134.69, 135.20, 137.30, 138.30, 144.52, 148.16, 154.98, 156.28, 169.42, 197.70; IR ($CHCl_3$) 3063 w, 2922 w, 2251 w, 1685 m, 1601 w, 1486 w, 1424 w, 1390 w, 1358 w, 1309 w, 1267 w, 1202 w, 1150 w, 1092 w, 1013 w, 954 w, 908 m, 821 w, 727 s; HRMS Calcd for $C_{30}H_{23}Cl_2N_2O_3$ $(M+H)^+$: 529.1080; Found: 529.1075.

5-(4-acetylphenyl)-3,4-diethyl-5-hydroxy-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (2w)



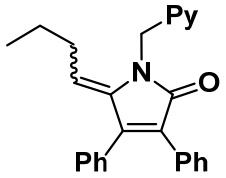
R_f 0.31 (hexane/EtOAc = 1/2). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.86 (t, J = 7.8 Hz, 3H), 1.14 (t, J = 7.5 Hz, 3H), 2.19 (dq, J = 14.2, 7.8 Hz, 1H), 2.29 (dq, J = 14.4, 7.8 Hz, 1H), 2.33 (q, J = 7.6 Hz, 2H), 2.61 (s, 3H), 3.88 (d, J = 16.5 Hz, 1H), 4.94 (d, J = 16.5 Hz, 1H), 7.23 (dd, J = 7.3, 5.0 Hz, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.59 (d, J = 7.1 Hz, 2H), 7.70 (td, J = 7.6, 1.6 Hz, 1H), 7.96 (dd, J = 7.3, 1.2 Hz, 2H), 8.47 (dq, J = 5.0, 0.7 Hz, 1H), 8.90 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.38, 13.50, 17.05, 18.84, 26.83, 44.75, 91.37, 122.66, 122.78, 126.95, 128.72, 131.89, 137.04, 138.02, 145.28, 148.10, 156.88, 159.21, 171.85, 197.83.; IR ($CHCl_3$) 2970 w, 2934 w, 2875 w, 1682 s, 1603 m, 1423 w, 1398 m, 1358 w, 1267 m, 1092 w, 1005 w, 935 w, 842 w, 731 s; HRMS Calcd for $C_{22}H_{25}N_2O_3$ $(M+H)^+$: 365.1860; Found: 365.1863.

3-(4-acetylphenyl)-3-hydroxy-*N*-(pyridin-2-ylmethyl)-3,4,5,6,7,8-hexahydrocyclohepta[c]pyrrol-1(2H)-one (2x)



R_f 0.26 (hexane/EtOAc = 1/2). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 1.37-1.46 (m, 1H), 1.56-1.68 (m, 3H), 1.70-1.75 (m, 2H), 1.95-2.02 (m, 1H), 2.40-2.52 (m, 3H), 2.61 (s, 3H), 3.89 (d, J = 16.2 Hz, 1H), 4.93 (d, J = 16.5 Hz, 1H), 7.23 (dd, J = 7.3, 5.0 Hz, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.59 (d, J = 8.2 Hz, 2H), 7.70 (td, J = 7.8, 1.8 Hz, 1H), 7.96 (dd, J = 7.6, 1.2 Hz, 2H), 8.47 (dq, J = 5.0, 0.9 Hz), 8.97 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 24.68, 26.85, 27.11, 27.16, 27.24, 30.74, 45.00, 91.00, 122.67, 122.82, 126.93, 128.73, 131.98, 137.09, 138.03, 144.97, 148.15, 156.88, 160.65, 171.88, 197.85.; IR ($CHCl_3$) 2924 w, 2851 w, 1681 s, 1603 w, 1425 w, 1401 m, 1360 m, 1267 m, 1161 w, 1009 w, 944 w, 916 w, 843 w, 731 s; HRMS Calcd for $C_{23}H_{25}N_2O3$ $(M+H)^+$: 377.1860; Found: 377.1863.

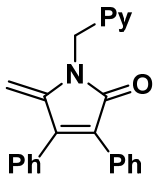
5-butylidene-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3a)



[*Z* isomer] R_f 0.34 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.69 (t, J = 7.3 Hz, 3H), 1.19 (sext, J = 7.6 Hz, 2H), 2.23 (q, J = 7.3 Hz, 2H), 5.09 (t, J = 8.2 Hz, 1H), 5.34 (s, 2H), 7.16-7.26 (m, 7H), 7.36-7.42 (m, 5H), 7.67 (td, J = 7.6, 1.6 Hz, 1H), 8.59 (dq, J = 4.8, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.66, 23.34, 29.17, 47.19, 119.38, 120.77, 122.25, 127.86, 128.04, 128.11, 128.55, 128.59, 129.72, 130.11, 131.11, 132.64, 137.09, 138.41, 145.84, 149.44, 158.20, 169.92; IR ($CHCl_3$) 3056 w, 2959 w, 2929 w, 2871 w, 1685 s, 1647 w, 1591 w, 1572 w, 1438 m, 1407 w, 1374 w, 1352 w, 1235 w, 1166 w, 1118 w, 1071 w, 995 w, 943 w, 914 w, 791 w, 729 m, 695 s; HRMS Calcd for $C_{26}H_{25}N_2O$ $(M+H)^+$: 381.1961; Found: 381.1962.

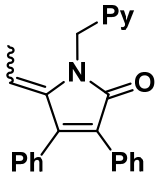
[*E* isomer] R_f 0.26 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.54 (t, J = 7.4 Hz, 3H), 1.12 (sext, J = 7.3 Hz, 2H), 1.60 (q, J = 7.1 Hz, 2H), 5.13 (s, 2H), 5.59 (t, J = 8.4 Hz, 1H), 7.18-7.22 (m, 4H), 7.25-7.28 (m, 4H), 7.35-7.40 (m, 5H), 7.67 (td, J = 7.8, 1.8 Hz, 1H), 8.56 (dq, J = 4.8, 0.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.49, 23.49, 28.83, 45.37, 119.75, 121.92, 122.43, 127.98, 128.01, 128.44, 128.73, 129.24, 129.78, 131.00, 131.98, 134.80, 137.11, 137.52, 142.72, 149.18, 157.75, 167.92; IR ($CHCl_3$) 3056 w, 2958 w, 2926 w, 2869 w, 1685 s, 1593 w, 1475 w, 1438 w, 1415 w, 1379 w, 1333 w, 1226 w, 1172 w, 1089 w, 996 w, 947 w, 914 w, 750 m, 695 m; HRMS Calcd for $C_{26}H_{25}N_2O$ $(M+H)^+$: 381.1961; Found: 381.1942.

5-methylene-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3b)



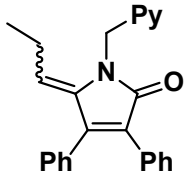
R_f 0.29 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.78 (d, J = 2.0 Hz, 1H), 5.10 (d, J = 2.3 Hz, 1H), 5.10 (s, 2H), 7.18 (ddd, J = 7.3, 4.8, 0.9 Hz, 1H), 7.22-7.27 (m, 5H), 7.29 (d, J = 8.0 Hz, 1H), 7.34-7.37 (m, 3H), 7.42-7.46 (m, 2H), 7.65 (td, J = 7.6, 1.6 Hz, 1H), 8.56 (dd, J = 4.8, 0.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 45.63, 97.90, 121.82, 122.49, 128.12, 128.27, 128.65, 128.74, 129.69, 129.77, 130.29, 130.57, 131.77, 137.06, 143.13, 145.26, 149.23, 157.10, 168.70; IR ($CHCl_3$) 3056 w, 2926 w, 1691 s, 1628 m, 1593 w, 1475 w, 1440 m, 1399 m, 1374 w, 1319 w, 1286 w, 1228 w, 1181 w, 1084 w, 1031 w, 996 w, 913 w, 856 w, 798 w, 765 w, 730 m, 696 s; HRMS Calcd for $C_{23}H_{19}N_2O$ $(M+H)^+$: 339.1492; Found: 339.1489.

5-ethylidene-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3c)



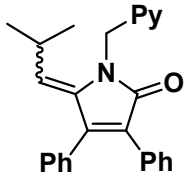
[*Z* isomer] R_f 0.34 (hexane/EtOAc = 1/1). Yellow Pale Solid. Mp = 151-153 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 1.84 (d, J = 8.0 Hz, 3H), 5.21 (q, J = 8.2 Hz, 2H), 5.36 (s, 2H), 7.18-7.7.26 (m, 7H), 7.37-7.43 (m, 5H), 7.68 (td, J = 7.6, 1.6 Hz, 1H), 8.59 (dd, J = 3.9, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.16, 47.11, 113.14, 120.82, 122.28, 127.87, 128.05, 128.56, 128.59, 128.64, 129.71, 130.09, 131.07, 132.63, 137.14, 139.58, 145.63, 149.49, 158.31, 169.95; IR ($CHCl_3$) 3056 w, 2931 w, 2246 w, 1684 s, 1592 w, 1475 w, 1435 m, 1374 w, 1353 w, 1234 w, 1166 w, 1071 w, 995 w, 942 w, 911 w, 789 m, 752 w, 728 s, 695 s; HRMS Calcd for $C_{24}H_{21}N_2O$ $(M+H)^+$: 353.1648; Found: 353.1635.
[*E* isomer] R_f 0.29 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 1.34 (d, J = 8.0 Hz, 3H), 5.11 (s, 2H), 5.68 (q, J = 8.0 Hz, 1H), 7.19-7.22 (m, 4H), 7.25-7.30 (m, 3H), 7.35-7.40 (m, 5H), 7.68 (td, J = 7.5, 1.6 Hz, 1H), 8.56 (dd, J = 4.17, 0.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.43, 45.36, 113.52, 122.03, 122.49, 128.00, 128.03, 128.47, 128.89, 129.29, 129.79, 130.95, 131.98, 134.76, 137.20, 138.03, 142.67, 149.20, 157.73, 167.98; IR ($CHCl_3$) 3056 w, 2925 s, 2856 w, 1684 s, 1592 w, 1476 w, 1439 w, 1415 w, 1377 w, 1312 w, 1174 w, 996 w, 945 w, 914 w, 822 w, 751 w, 730 w, 695 w; HRMS Calcd for $C_{24}H_{21}N_2O$ $(M+H)^+$: 353.1648; Found: 353.1628.

3,4-diphenyl-5-propylidene-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3d)



[*Z* isomer] R_f 0.24 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.80 (t, J = 7.7 Hz, 3H), 2.28 (quin, J = 7.3 Hz, 2H), 5.09 (t, J = 8.2 Hz, 1H), 5.33 (s, 2H), 7.17-7.26 (m, 7H), 7.36-7.42 (m, 5H), 7.67 (td, J = 7.8, 1.8 Hz, 1H), 8.59 (dq, J = 4.6, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 14.57, 20.73, 47.16, 120.73, 122.23, 127.84, 128.03, 128.18, 128.54, 128.57, 128.59, 129.70, 130.10, 131.09, 132.59, 137.07, 137.87, 145.86, 149.46, 158.15, 169.87; IR ($CHCl_3$) 3056 w, 3016 w, 2966 w, 2931 w, 2873 w, 1685 s, 1646 w, 1591 w, 1436 m, 1407 w, 1374 w, 1233 w, 1168 w, 1119 w, 1072 w, 1030 w, 995 w, 944 w, 913 w, 794 w, 752 w, 728 m, 695 m; HRMS Calcd for $C_{25}H_{23}N_2O$ $(M+H)^+$: 367.1805; Found: 367.1791.
[*E* isomer] R_f 0.19 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.73 (t, J = 7.5 Hz, 3H), 1.66 (quin, J = 7.3 Hz, 2H), 5.12 (s, 2H), 5.57 (t, J = 8.2 Hz, 1H), 7.18-7.21 (m, 4H), 7.25-7.29 (m, 3H), 7.34-7.39 (m, 5H), 7.67 (td, J = 7.8, 1.8 Hz, 1H), 8.57 (dq, J = 4.8, 0.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 14.73, 20.52, 45.31, 121.10, 121.91, 122.43, 127.96, 127.99, 128.47, 128.73, 129.13, 129.75, 130.94, 132.01, 134.74, 136.96, 137.14, 142.67, 149.13, 157.67, 167.95; IR ($CHCl_3$) 3056 w, 3014 w, 2965 w, 2931 w, 2872 w, 1681 s, 1638 w, 1592 w, 1476 w, 1438 w, 1415 m, 1380 w, 1336 w, 1223 w, 1173 w, 1089 w, 1030 w, 996 w, 946 w, 914 w, 853 w, 795w, 751 w, 729 m, 695 m; HRMS Calcd for $C_{25}H_{23}N_2O$ $(M+H)^+$: 367.1805; Found: 367.1791.

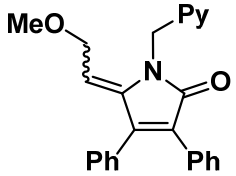
5-(2-methylpropylidene)-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3e)



[*Z* isomer] R_f 0.34 (hexane/EtOAc = 1/1). Yellow Solid. Mp = 150-152 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.76 (d, J = 6.4 Hz, 6H), 2.85-2.98 (m, 1H), 4.92 (d, J = 11.2 Hz, 1H), 5.33 (s, 2H), 7.15-7.25 (m, 7H), 7.36-7.41 (m, 5H), 7.67 (td, J = 7.8, 1.8 Hz, 1H), 8.60 (dq, J = 4.8, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 23.37, 26.68, 47.21, 120.74, 122.24, 126.38, 127.86, 128.05, 128.30, 128.55, 128.59, 129.73, 130.20, 131.14, 132.60, 135.99, 137.04, 146.22, 149.47, 158.12, 169.80; IR ($CHCl_3$) 2964 w, 2927 w, 1686 s, 1647 w, 1591 w, 1439 m, 1408 m, 1373 w, 1233 w, 1166 w, 1072 w, 968 w, 943 w, 912 w, 792 w, 753 m, 727 s, 696 s; HRMS Calcd for $C_{26}H_{25}N_2O$ $(M+H)^+$: 381.1961; Found: 381.1974.

[*E* isomer] R_f 0.26 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.69 (d, J = 6.4 Hz, 6H), 1.97-2.07 (m, 1H), 5.13 (s, 2H), 5.38 (d, J = 11.0 Hz, 1H), 7.18-7.21 (m, 4H), 7.25-7.28 (m, 2H), 7.34-7.39 (m, 6H), 7.69 (td, J = 7.8, 1.8 Hz, 1H), 8.57 (dq, J = 4.1, 0.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 23.36, 25.83, 45.35, 121.84, 122.39, 126.97, 127.97, 128.01, 128.50, 128.67, 129.07, 129.76, 130.99, 132.15, 134.87, 135.69, 137.06, 142.72, 149.14, 157.73, 167.88; IR ($CHCl_3$) 3056 w, 2964 w, 2928 w, 2868 w, 1684 s, 1639 w, 1593 w, 1439 w, 1415 w, 1380 w, 1340 w, 1287 w, 1224 w, 1173 w, 1086 w, 995 w, 946 w, 913 w, 863 w, 751 w, 731 m, 695 w; HRMS Calcd for $C_{26}H_{25}N_2O$ $(M+H)^+$: 381.1961; Found: 381.1961.

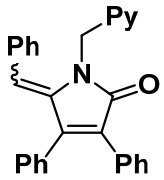
5-(2-methoxyethylidene)-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3f)



[*Z* isomer] R_f 0.29 (hexane/EtOAc = 1/2). Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 3.18 (s, 3H), 4.12 (d, J = 7.1 Hz, 2H), 5.24 (t, J = 7.1 Hz, 1H), 5.27 (s, 2H), 7.19-7.26 (m, 7H), 7.36-7.39 (m, 3H), 7.40-7.43 (m. 2H), 7.68 (td, J = 7.8, 1.8 Hz, 1H), 8.60 (dq, J = 4.8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 47.02, 58.33, 67.30, 113.12, 120.94, 122.43, 128.10, 128.17, 128.71, 128.74, 129.15, 129.71, 130.00, 130.69, 132.05, 137.18, 140.26, 145.64, 149.54, 157.86, 169.90; IR ($CHCl_3$) 3057 w, 2927 w, 2819 w, 1697 s, 1594 w, 1440 m, 1409 w, 1191 w, 1159 w, 1084 w, 943 w, 755 w, 729 w, 696 m; HRMS Calcd for $C_{25}H_{23}N_2O_2$ $(M+H)^+$: 383.1754; Found: 383.1773.

[*E* isomer] R_f 0.23 (hexane/EtOAc = 1/2). Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.95 (s, 3H), 3.43 (d, J = 7.3 Hz, 2H), 5.13 (s, 2H), 5.68 (t, J = 7.4 Hz, 1H), 7.18-7.23 (m, 4H), 7.26-7.29 (m, 3H), 7.36-7.41 (m, 5H), 7.67 (td, J = 7.8, 1.8 Hz, 1H), 8.57 (dq, J = 5.0, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 45.39, 57.90, 66.79, 113.50, 121.78, 122.53, 128.06, 128.35, 128.82, 128.92, 129.17, 129.78, 130.53, 132.72, 134.15, 137.14, 139.71, 142.22, 149.39, 157.16, 168.23; IR ($CHCl_3$) 3056 w, 2925 w, 2818 w, 1690 s, 1641 w, 1592 w, 1476 w, 1438 w, 1412 w, 1376 w, 1330 w, 1238 w, 1188 w, 1087 m, 996 w, 944 w, 914 w, 780 w, 752 w, 729 w, 695 m; HRMS Calcd for $C_{25}H_{23}N_2O_2$ $(M+H)^+$: 383.1754; Found: 383.1746.

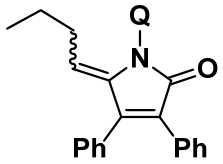
5-benzylidene-3,4-diphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3h)



[*Z* isomer] R_f 0.40 (hexane/EtOAc = 1/1). Pale Yellow Solid. Mp = 142-143 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.96 (s, 2H), 6.18 (s, 1H), 6.79 (d, J = 7.8 Hz, 1H), 6.95 (dt, J = 7.1, 0.9 Hz, 2H), 7.05 (dd, J = 6.6, 5.0 Hz, 1H), 7.09-7.26 (m, 5H), 7.35-7.53 (m, 8H), 8.35 (dq, J = 3.9, 0.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 47.50, 115.86, 120.33, 121.57, 127.73, 127.93, 128.09, 128.40, 128.70, 128.75, 129.10, 129.16, 129.80, 130.15, 130.89, 132.39, 134.54, 136.25, 139.47, 146.23, 149.12, 156.93, 170.97; IR ($CHCl_3$) 3056 w, 2927 w, 2361 w, 2248 w, 1693 s, 1633 w, 1592 w, 1573 w, 1487w, 1441 w, 1402 w, 1370 w, 1331 w, 1236 w, 1208 w, 1160 w, 1076 w, 1028 w, 996 w, 944 w, 913 w, 792 w, 750 w, 727 m, 696 m; HRMS Calcd for $C_{29}H_{23}N_2O$ $(M+H)^+$: 415.1805; Found: 415.1789.

[*E* isomer] R_f 0.26 (hexane/EtOAc = 1/1). Pale Yellow Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 5.24 (s, 2H), 6.72 (d, J = 8.0 Hz, 2H), 6.79-6.83 (m, 3H), 6.86-6.94 (m, 4H), 7.01 (tt, J = 6.4, 1.4 Hz, 1H), 7.20-7.30 (m, 7H), 7.38 (d, J = 8.0 Hz, 1H), 7.71 (td, J = 7.6, 1.6 Hz, 1H), 8.59 (dq, J = 4.1, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 45.79, 116.91, 122.05, 122.61, 126.79, 127.21, 127.73, 127.99, 128.03, 128.13, 129.72, 129.95, 130.29, 130.78, 132.82, 133.04, 133.97, 137.22, 138.40, 142.63, 149.36, 157.43, 168.29; IR ($CHCl_3$) 3055 w, 2926 w, 1687 s, 1624 w, 1592 w, 1476 w, 1440 w, 1409 w, 1377 w, 1334 w, 1212 w, 1163 w, 1076 w, 1028 w, 996 w, 947 w, 913 w, 842 w, 795 w, 754 m, 730 m, 696 m; HRMS Calcd for $C_{29}H_{23}N_2O$ $(M+H)^+$: 415.1805; Found: 415.1782.

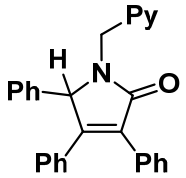
5-butylidene-3,4-diphenyl-*N*-(quinolin-8-yl)-1,5-dihydro-2*H*-pyrrol-2-one (5)



[isomer 1] R_f 0.34 (hexane/EtOAc = 1/1). White Amorphous. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.39 (t, J = 7.3 Hz, 3H), 0.85-1.05 (m, 2H), 1.21 (sextd, J = 8.0, 1.6 Hz, 1H), 1.39 (sextd, J = 8.4, 1.6 Hz, 1H), 5.14 (t, J = 8.0 Hz, 1H), 7.18-7.23 (m, 3H), 7.37-7.39 (m, 5H), 7.43 (q, J = 4.1 Hz, 1H), 7.46-7.48 (m, 2H), 7.64 (dd, J = 8.2, 7.3 Hz, 1H), 7.81 (dd, J = 7.3, 1.4 Hz, 1H), 7.92 (dd, J = 8.2, 1.4 Hz, 1H), 8.21 (dd, J = 8.2, 1.6 Hz, 1H), 8.98 (dd, J = 4.1, 1.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.58, 22.69, 28.85, 118.68, 121.81, 126.28, 127.63, 127.86, 128.24, 128.43, 128.50, 128.51, 129.02, 129.28, 129.94, 130.29, 130.74, 131.37, 132.86, 135.71, 136.29, 140.06, 145.77, 151.23, 169.93; IR ($CHCl_3$) 3055 w, 2959 w, 2929 w, 2870 w, 2245 w, 1688 m, 1647 w, 1596 w, 1500 w, 1474 w, 1406 w, 1371 w, 1259 w, 1212 w, 1176 w, 1121 w, 1074 w, 1029 w, 908 m, 829 w, 802 w, 789 w, 726 s, 694 m; HRMS Calcd for $C_{29}H_{25}N_2O$ $(M+H)^+$: 417.1961; Found: 417.1930.

[isomer 2] R_f 0.23 (hexane/EtOAc = 1/1). Pale Yellow Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 0.54 (t, J = 7.4 Hz, 3H), 1.07 (sext, J = 7.6 Hz, 2H), 1.62 (qd, J = 7.3, 1.6 Hz, 2H), 5.04 (t, J = 8.5 Hz, 1H), 7.17-7.21 (m, 3H), 7.40-7.48 (m, 8H), 7.68 (dd, J = 8.0, 7.3 Hz, 1H), 7.79 (dd, J = 7.3, 1.6 Hz, 1H), 7.94 (dd, J = 8.2, 1.6 Hz, 1H), 8.214(dd, J = 8.5, 1.8 Hz, 1H), 8.98 (dd, J = 4.1, 1.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 13.60, 23.42, 28.90, 119.81, 121.79, 126.48, 127.83, 127.91, 128.36, 128.68, 128.73, 129.13, 129.47, 129.51, 129.55, 129.59, 129.68, 129.98, 130.08, 131.68, 133.40, 135.09, 136.37, 140.17, 151.19; IR ($CHCl_3$) 3055 w, 2958 w, 2927 w, 2869 w, 1689 s, 1596 w, 1499 w, 1475 w, 1443 w, 1428 w, 1406 w, 1372 w, 1216 w, 1143 w, 1100 w, 1071 w, 1029 w, 911 w, 806 w, 729 m, 695 m; HRMS Calcd for $C_{29}H_{25}N_2O$ $(M+H)^+$: 417.1961; Found: 417.1947.

3,4,5-triphenyl-*N*-(pyridin-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (6)



R_f 0.17 (hexane/EtOAc = 1/1). Colorless Oil. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 4.00 (d, J = 15.3 Hz, 1H), 5.22 (d, J = 15.3 Hz, 1H), 5.57 (s, 1H), 7.04-7.34 (m, 15H), 7.50 (dq, J = 7.6, 1.6 Hz, 2H), 7.63 (td, J = 7.8, 1.8 Hz, 1H), 8.56 (d, J = 4.3 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 46.15, 66.80, 122.46, 122.98, 128.24, 128.35, 128.43, 128.68, 128.71, 128.77, 129.06, 129.07, 129.89, 131.55, 132.07, 132.92, 135.25, 136.96, 149.44, 153.20, 157.39, 170.44; IR ($CHCl_3$) 3059 w, 2924 w, 2242 w, 1680 s, 1590 w, 1492 w, 1431 w, 1403 m, 1351 w, 1316 w, 1206 w, 1073 w, 996 w, 944 w, 912 m, 840 w, 782 w, 730 s, 696 s; HRMS Calcd for $C_{28}H_{23}N_2O$ $(M+H)^+$: 403.1805; Found: 403.17995.

VIII. X-ray structure and data of compound 3h-*Z*

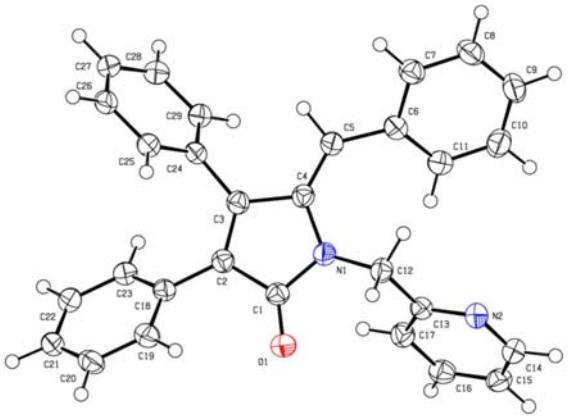


Figure S1. The structure of **3h-*Z*** was determined by the X-ray diffraction.

CCDC-1898257 contains the supplementary crystallographic data of compound **3h-*Z***. X-Ray crystallographic structure analysis of *Z*-5-benzylidene-3,4-diphenyl-N-(pyridin-2-ylmethyl) -1,5-dihydro-2H-pyrrol-2-one (**3h-*Z***) was performed on Rigaku R-AXIS RAPID imaging plate diffractometer with graphite monochromated Cu-Kα radiation. The data were collected at a temperature of -150 ± 1 °C to a maximum 2θ value of 148.6°. A total of 2428 oscillation images were collected. A sweep of data was done using ω scans from -12.0 to 14.0° in 0.50° step, at χ = -33.0° and φ = 26.0°. The structure was solved by direct methods (SIR92)[15] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically and all hydrogen atoms were placed using riding model. The crystal data are mentioned below:

Crystal Data:

Empirical Formula	$C_{29}H_{22}N_2O$
Formula Weight	414.51
Crystal Color, Habit	pale yellow, prism
Crystal Dimensions	0.600 × 0.250 × 0.250 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.8127(3) Å
	b = 9.8576(3) Å
	c = 12.3569(4) Å
	α = 95.274(3) °
	β = 96.148(3) °
	γ = 115.124(3) °
	V = 1063.36(7) $Å^3$

Space Group	P-1 (#2)
Z value	2
D_{calc}	1.294 g/cm^3
F_{000}	436.00
μ(CuKa)	6.158 cm^{-1}

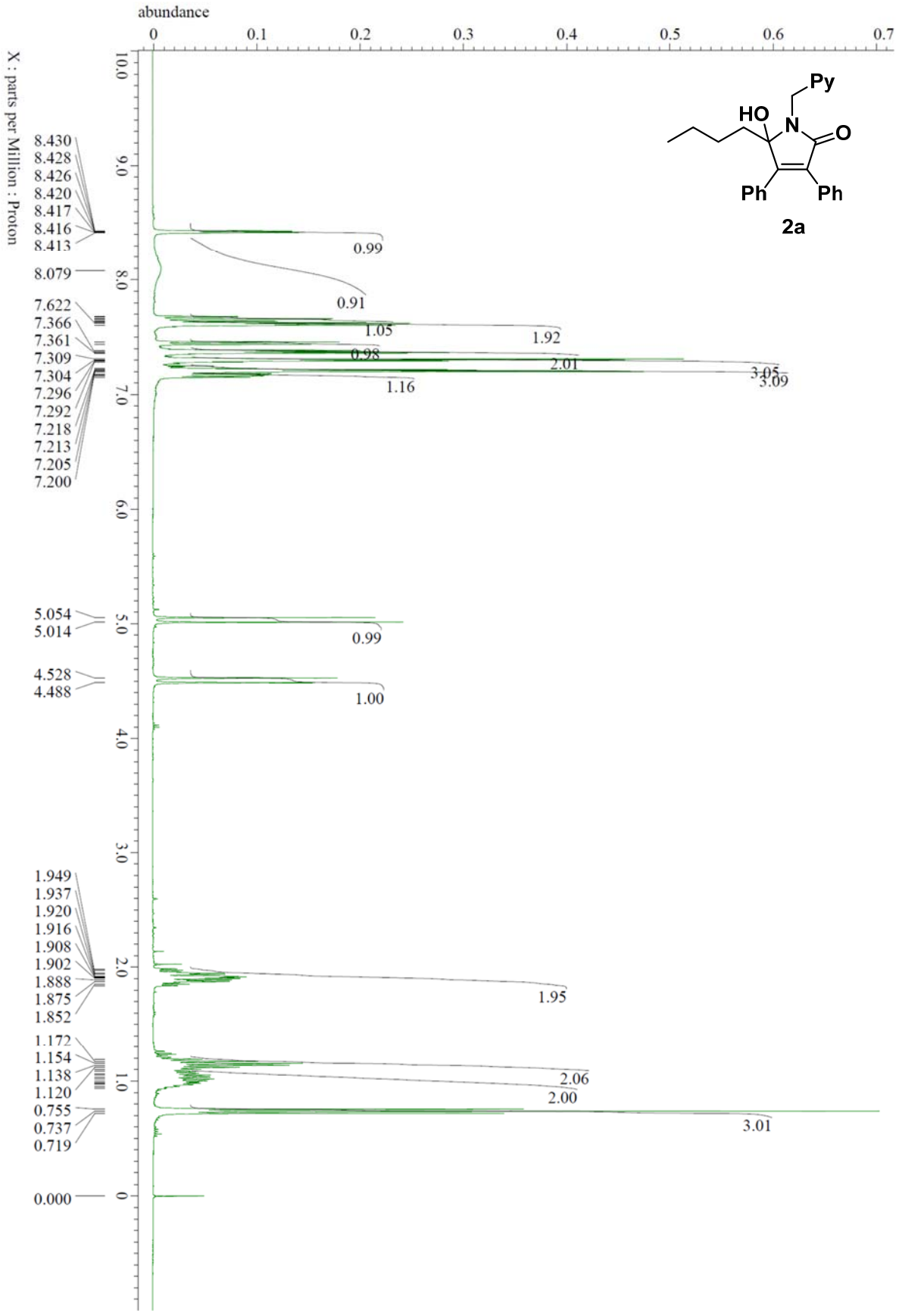
Table S3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C1	1.225(2)	N1	C1	1.389(2)
N1	C4	1.406(2)	N1	C12	1.4624(19)
N2	C13	1.3438(19)	N2	C14	1.332(2)
C1	C2	1.474(2)	C2	C3	1.359(2)
C2	C18	1.474(2)	C3	C4	1.476(2)
C3	C24	1.481(2)	C4	C5	1.349(3)
C5	C6	1.476(2)	C6	C7	1.401(2)
C6	C11	1.398(2)	C7	C8	1.388(3)
C8	C9	1.380(3)	C9	C10	1.392(3)
C10	C11	1.386(3)	C12	C13	1.512(2)
C13	C17	1.3861(17)	C14	C15	1.3866(19)
C15	C16	1.383(2)	C16	C17	1.387(2)
C18	C19	1.405(3)	C18	C23	1.388(2)
C19	C20	1.391(3)	C20	C21	1.382(2)
C21	C22	1.388(3)	C22	C23	1.385(2)
C24	C25	1.401(2)	C24	C29	1.390(3)
C25	C26	1.382(2)	C26	C27	1.386(3)
C27	C28	1.390(3)	C28	C29	1.390(2)

Table S4. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	N1	C4	110.37(13)	C1	N1	C12	118.26(15)
C4	N1	C12	127.87(13)	C13	N2	C14	117.56(11)
O1	C1	N1	123.56(14)	O1	C1	C2	129.60(16)
N1	C1	C2	106.80(14)	C1	C2	C3	107.91(14)
C1	C2	C18	122.75(15)	C3	C2	C18	129.33(15)
C2	C3	C4	109.03(14)	C2	C3	C24	125.96(15)
C4	C3	C24	124.92(15)	N1	C4	C3	105.62(14)
N1	C4	C5	130.97(14)	C3	C4	C5	123.39(15)
C4	C5	C6	132.40(15)	C5	C6	C7	117.66(14)
C5	C6	C11	123.90(14)	C7	C6	C11	118.16(16)
C6	C7	C8	121.05(16)	C7	C8	C9	120.09(17)
C8	C9	C10	119.60(19)	C9	C10	C11	120.54(17)
C6	C11	C10	120.52(16)	N1	C12	C13	114.83(10)
N2	C13	C12	113.01(11)	N2	C13	C17	123.07(14)
C12	C13	C17	123.86(13)	N2	C14	C15	123.44(14)
C14	C15	C16	118.44(15)	C15	C16	C17	119.04(12)
C13	C17	C16	118.43(14)	C2	C18	C19	120.52(14)
C2	C18	C23	120.69(17)	C19	C18	C23	118.79(15)
C18	C19	C20	119.96(15)	C19	C20	C21	120.4(2)
C20	C21	C22	120.03(17)	C21	C22	C23	119.82(16)
C18	C23	C22	121.03(19)	C3	C24	C25	118.24(16)
C3	C24	C29	122.70(15)	C25	C24	C29	118.98(15)
C24	C25	C26	120.29(18)	C25	C26	C27	120.63(17)
C26	C27	C28	119.36(16)	C27	C28	C29	120.34(19)
C24	C29	C28	120.36(17)				

VIII. Copies of ^{1}H and ^{13}C NMR Spectra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7.0
6.0
5.0
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2.0
1.0
0
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8.426
8.420
8.417
8.416
8.413
8.079
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7.292
7.218
7.213
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1.05
1.92
0.98
2.01
3.05
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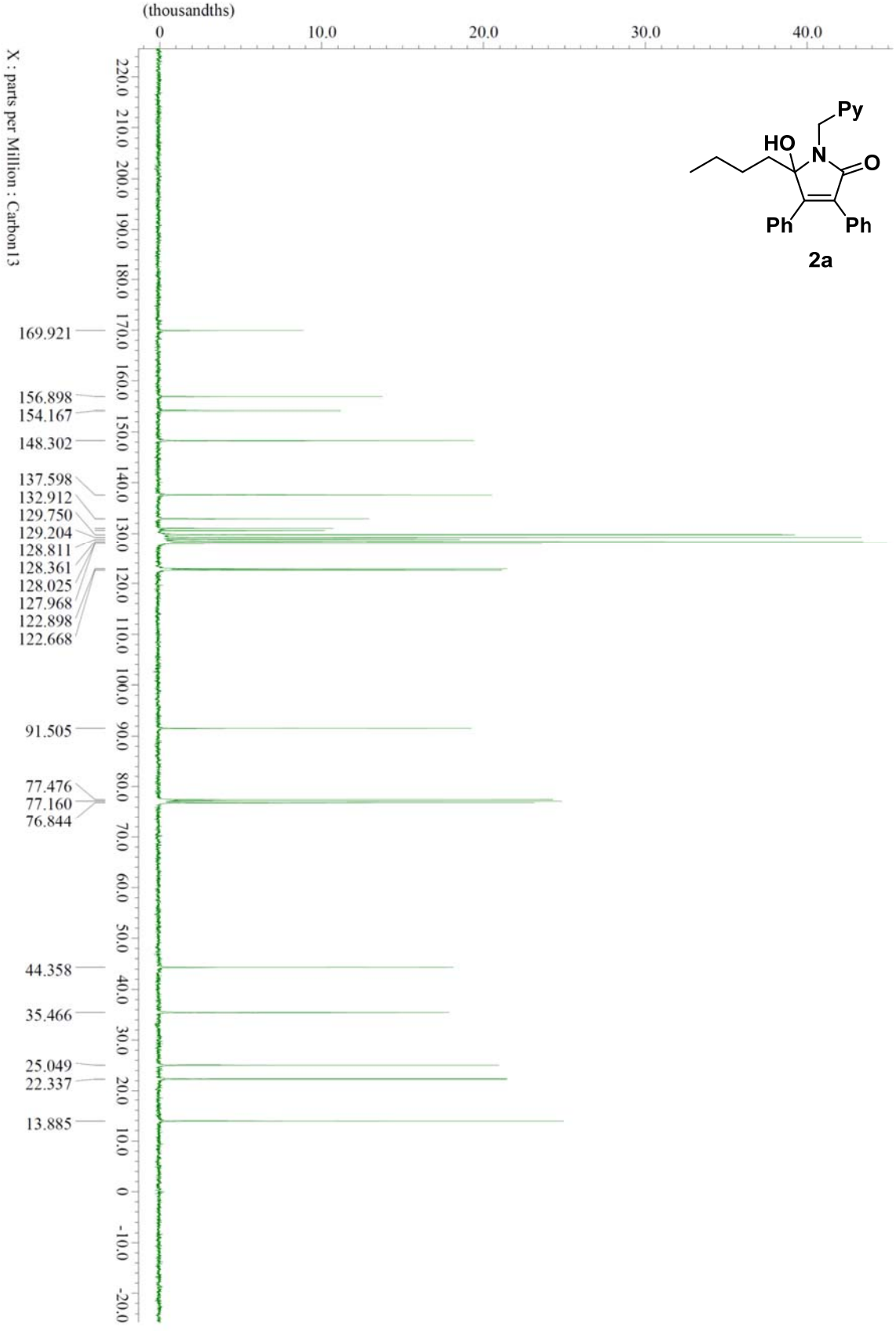
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-10.0
-20.0
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154.167
148.302
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132.912
129.750
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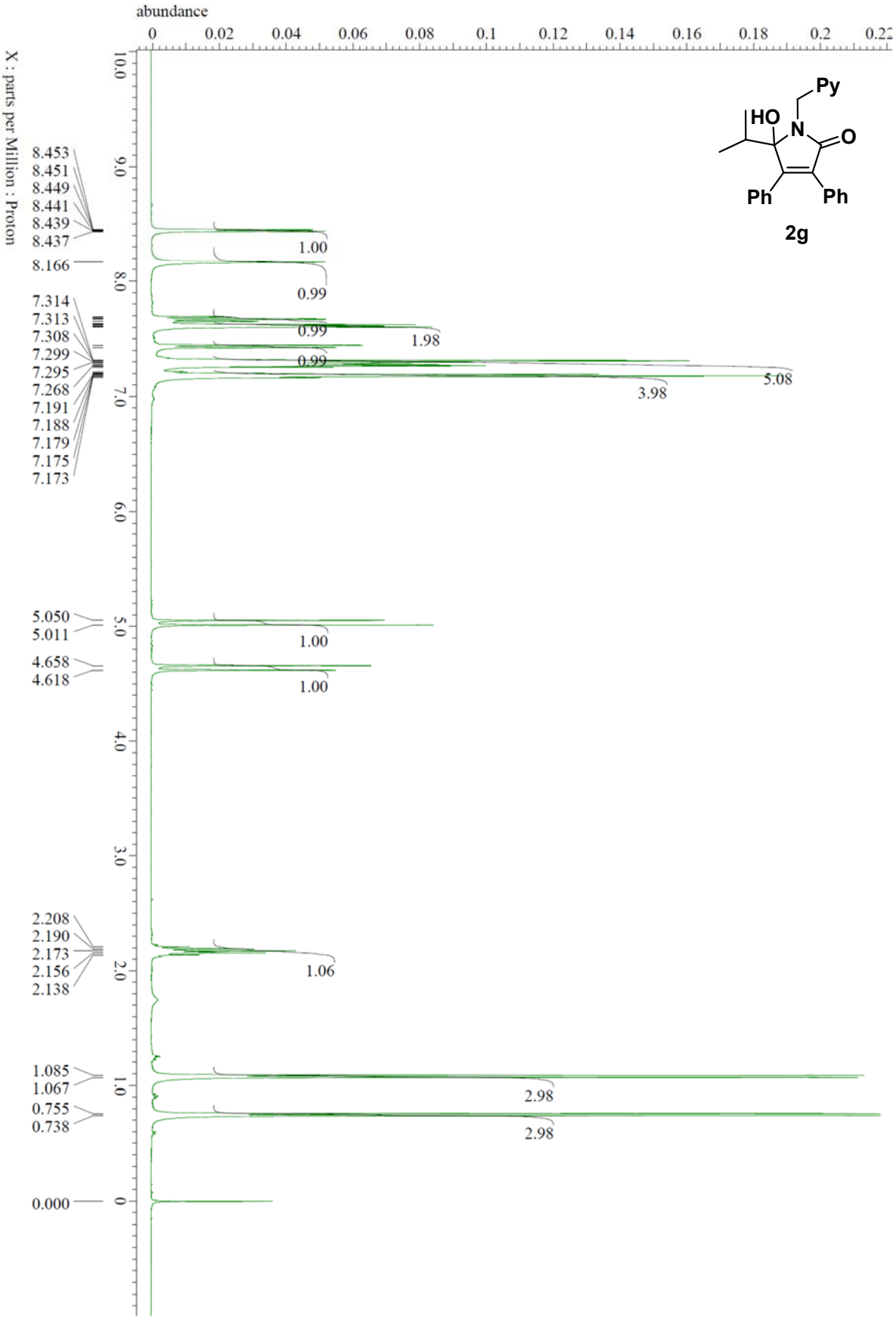
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O
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7.313
7.308
7.299
7.295
7.268
7.191
7.188
7.179
7.175
7.173
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2.190
2.173
2.156
2.138
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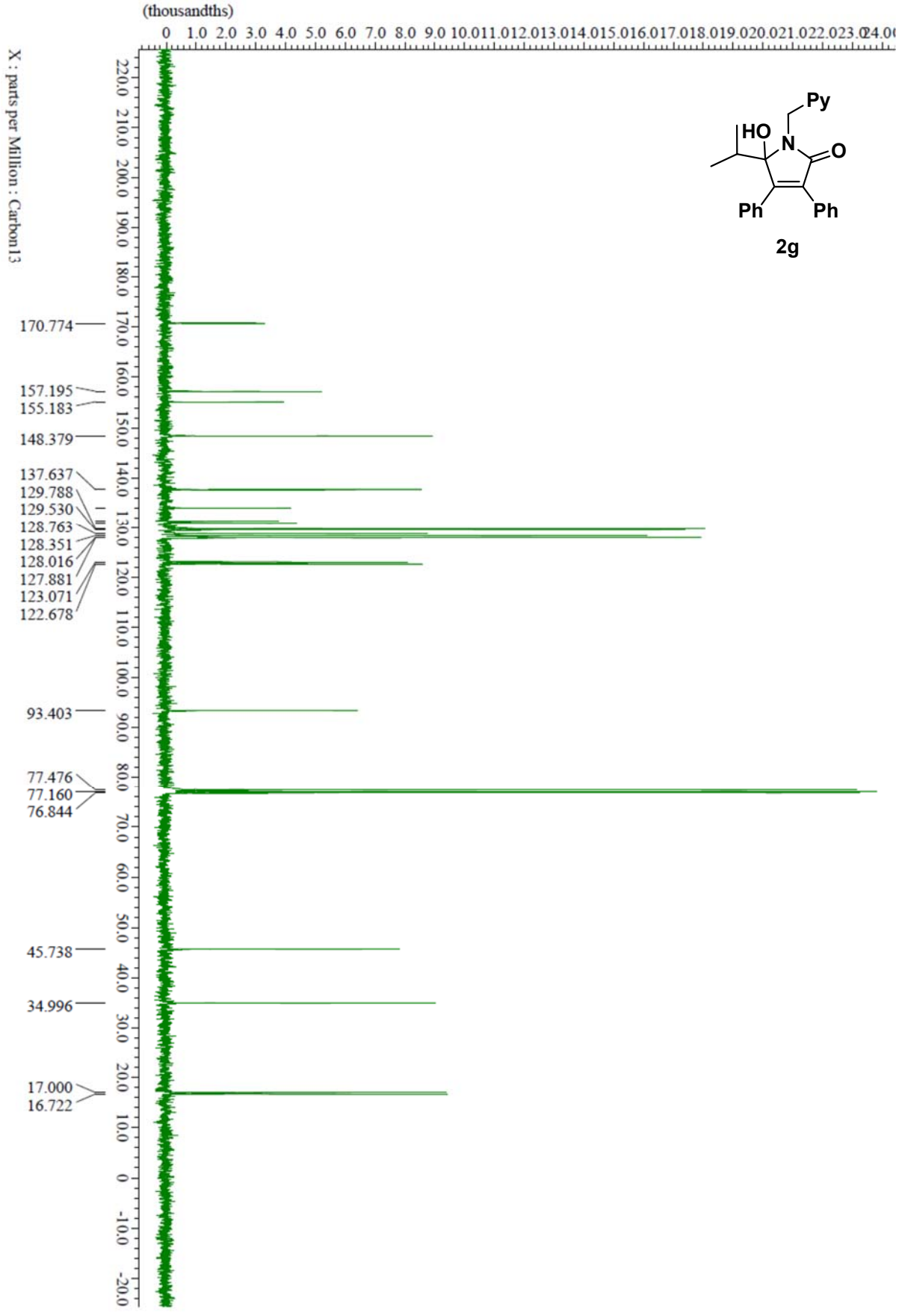
2.98
2.98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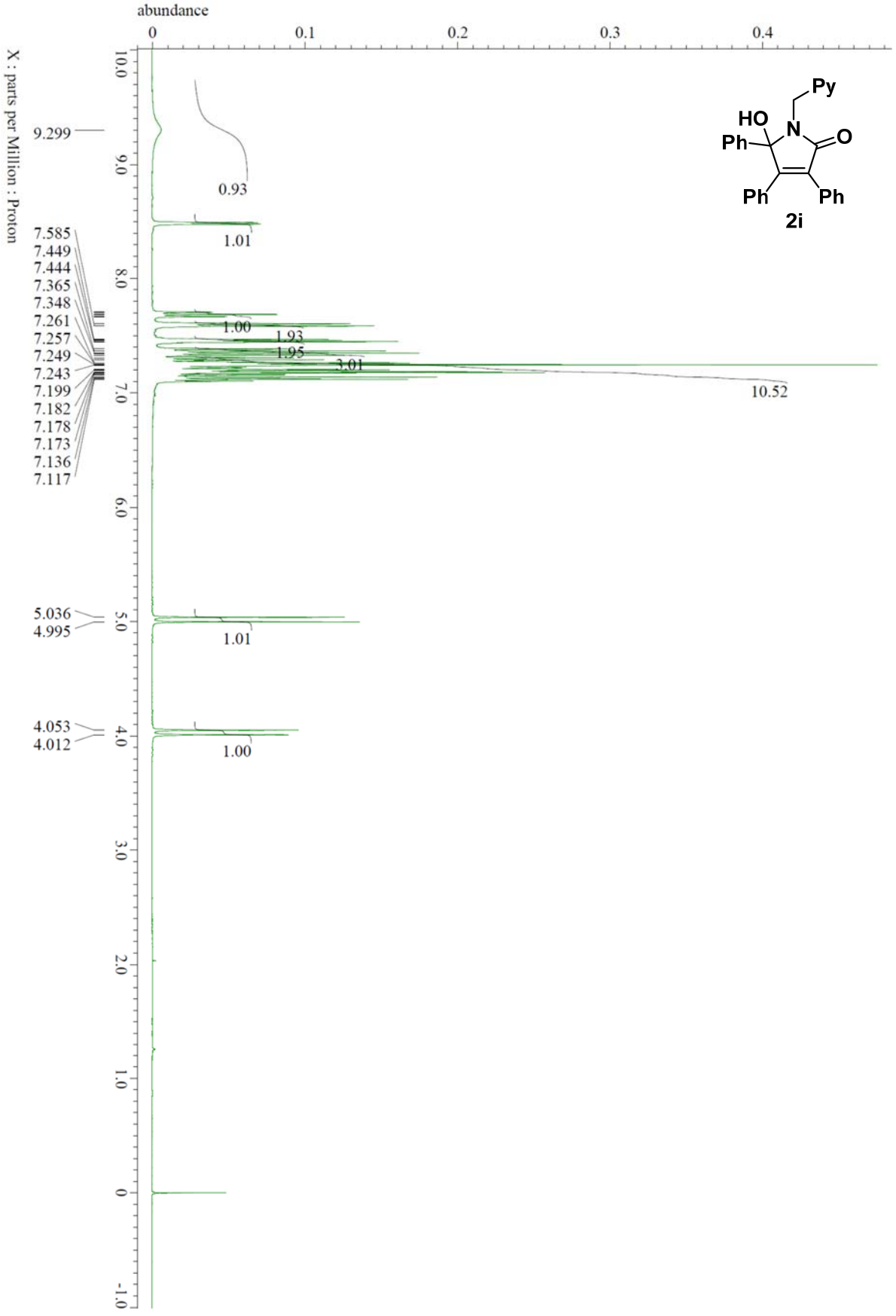
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7.117
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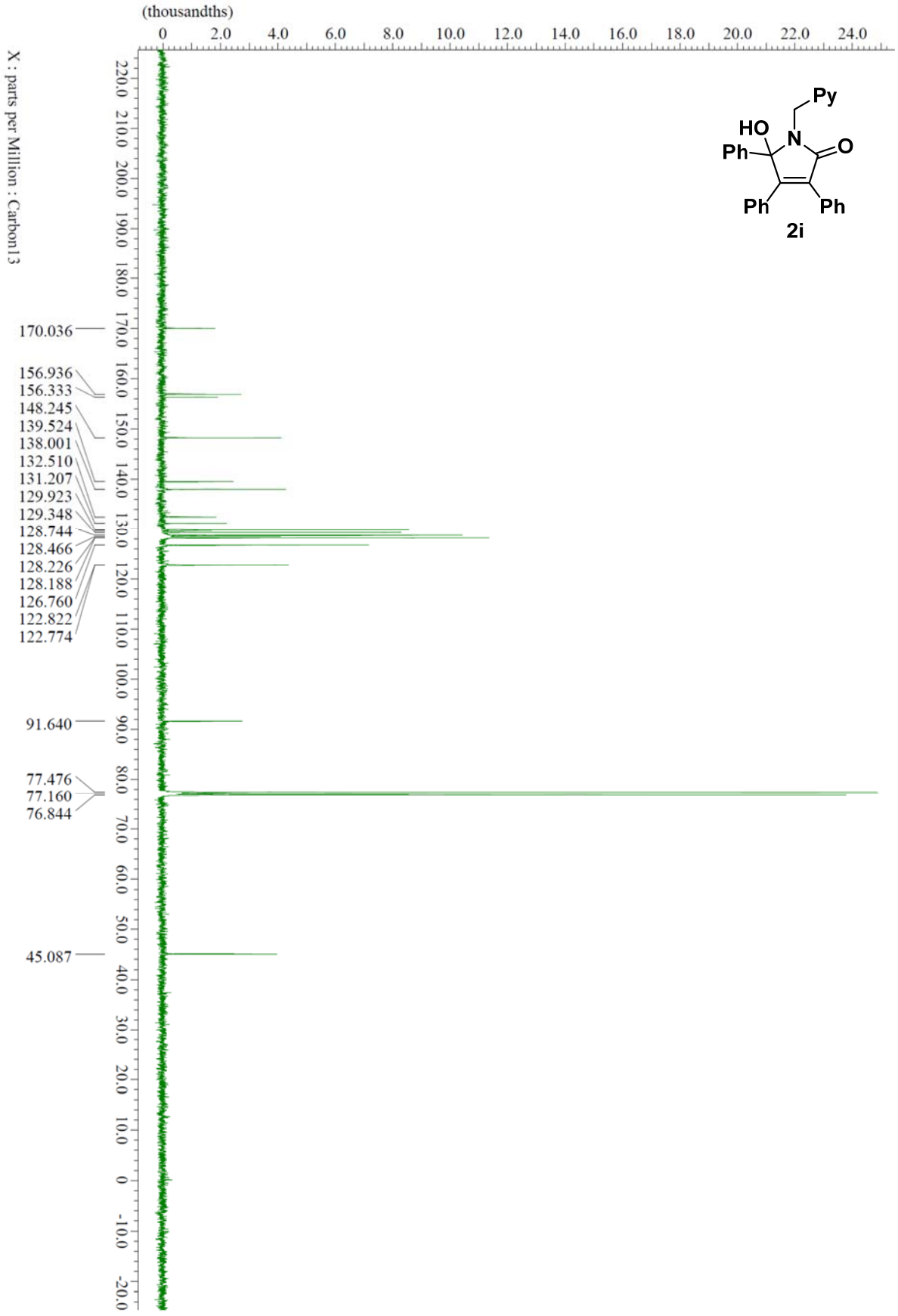
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156.333
148.245
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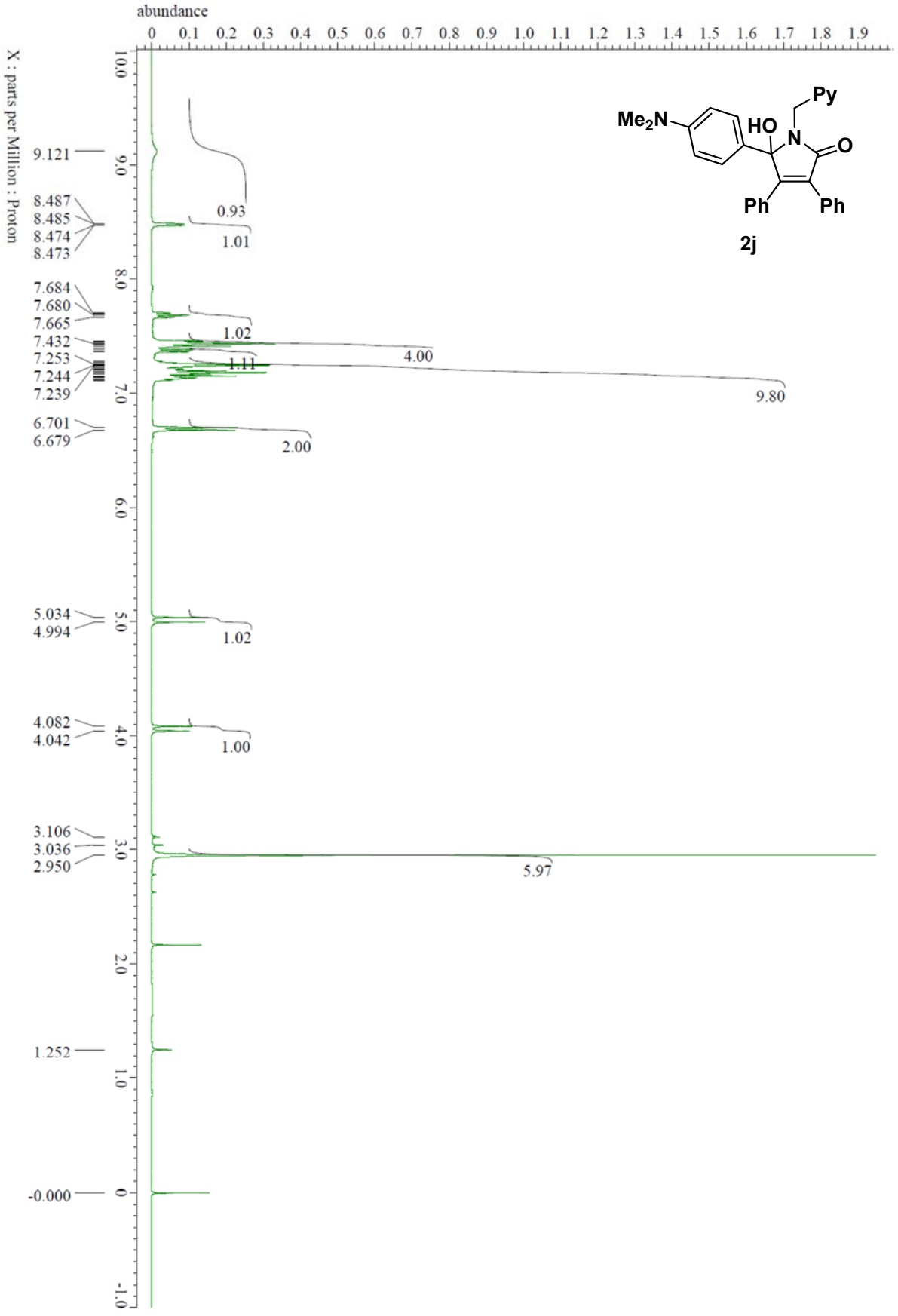
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1.02
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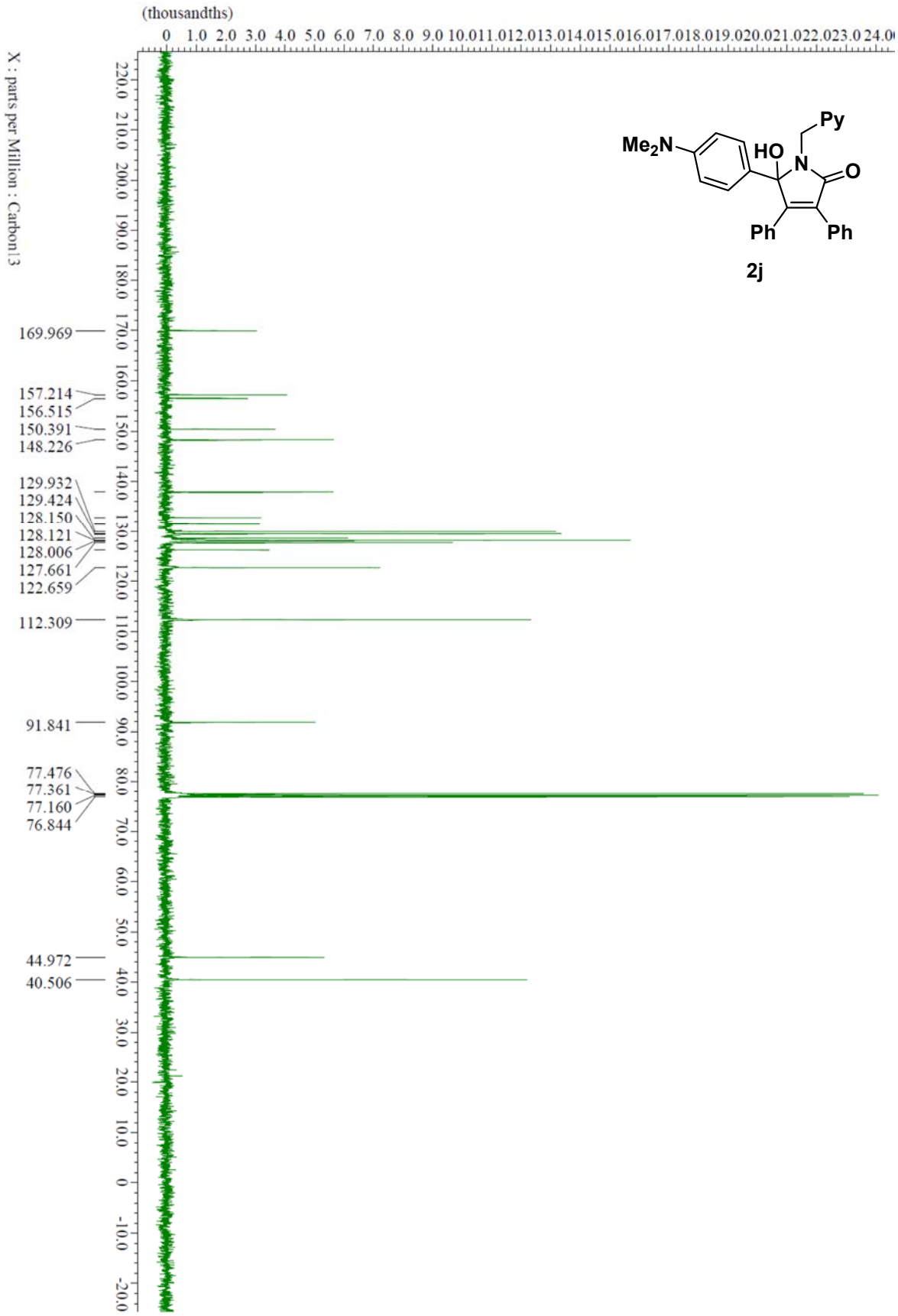
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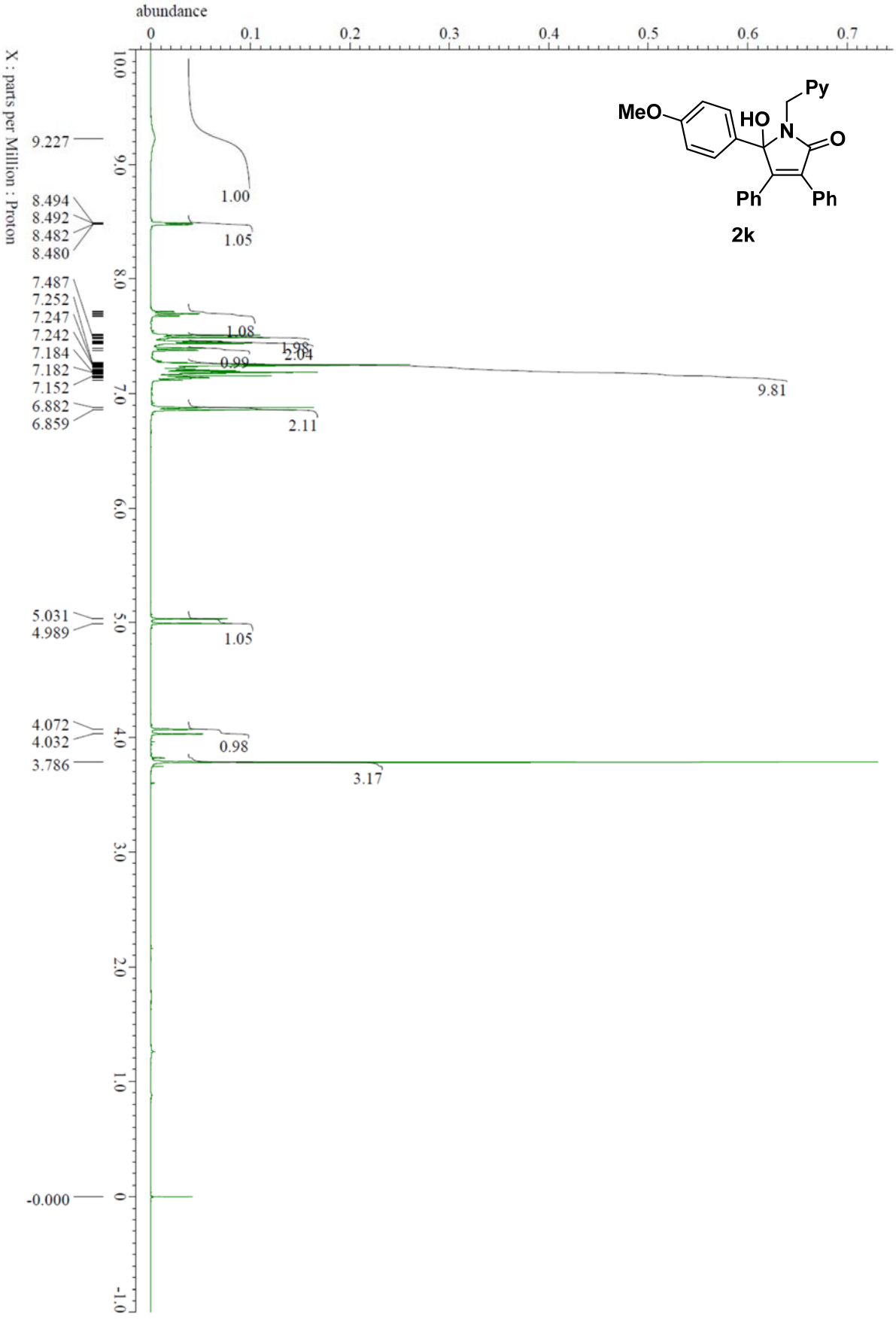
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7.247
7.242
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7.182
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1.08
1.98
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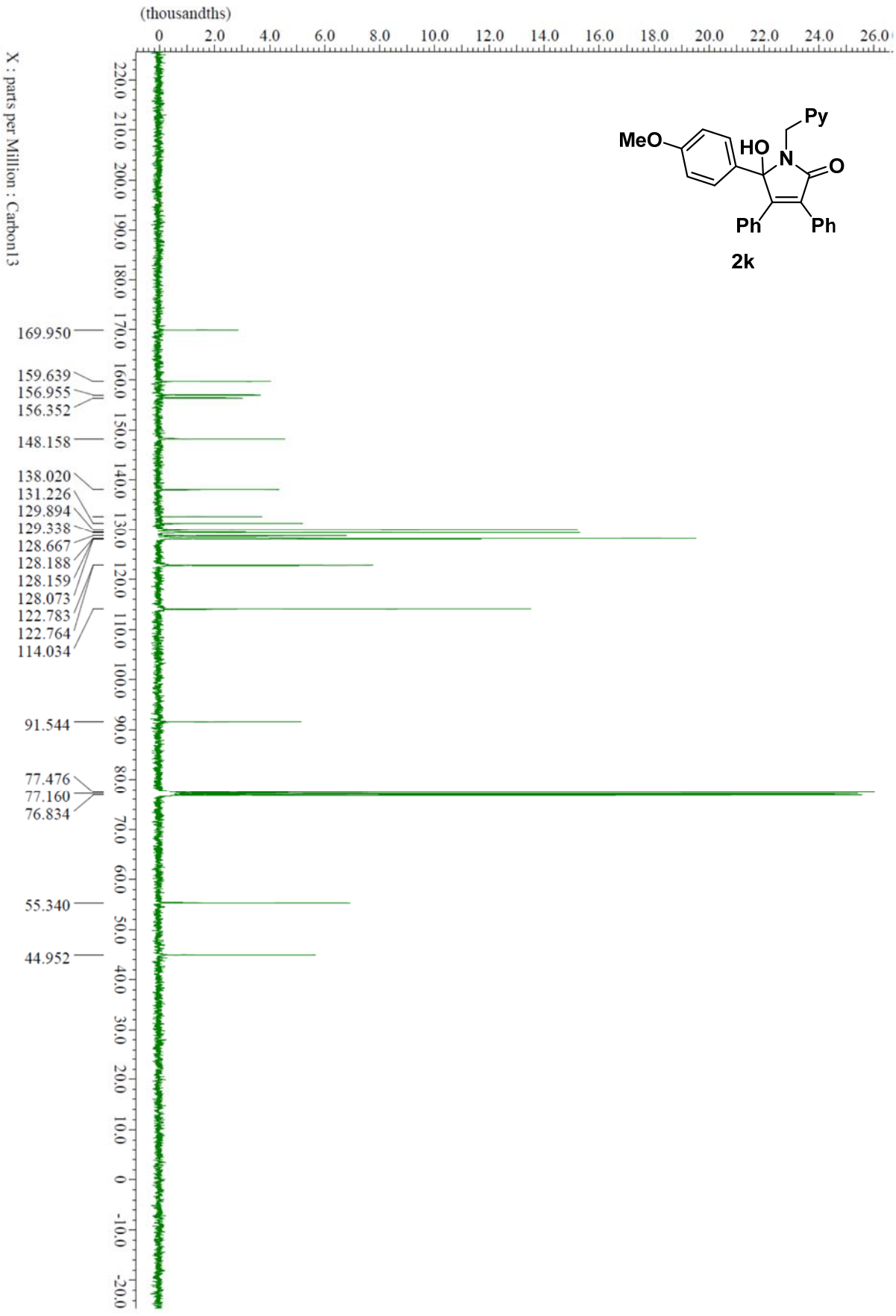
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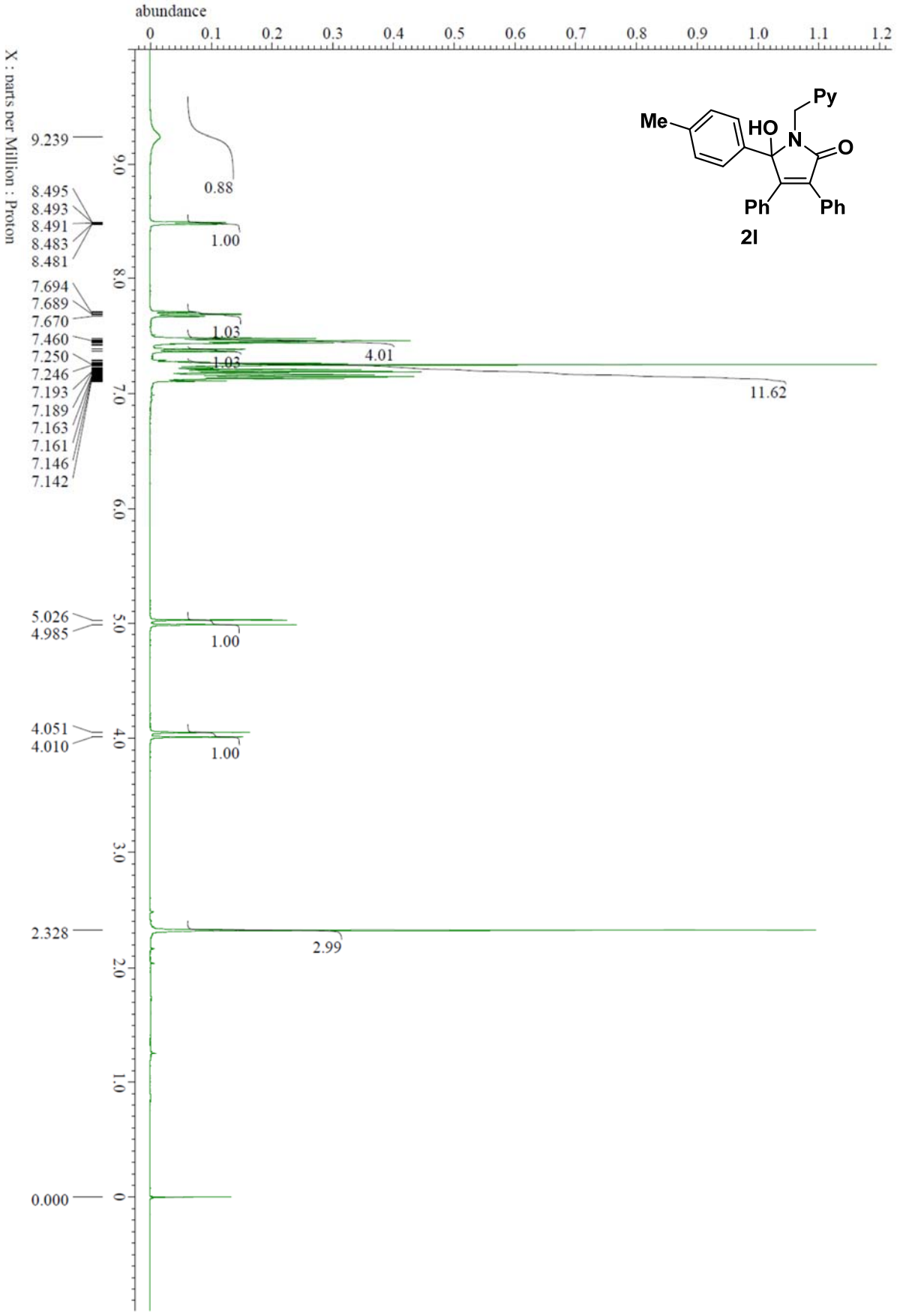
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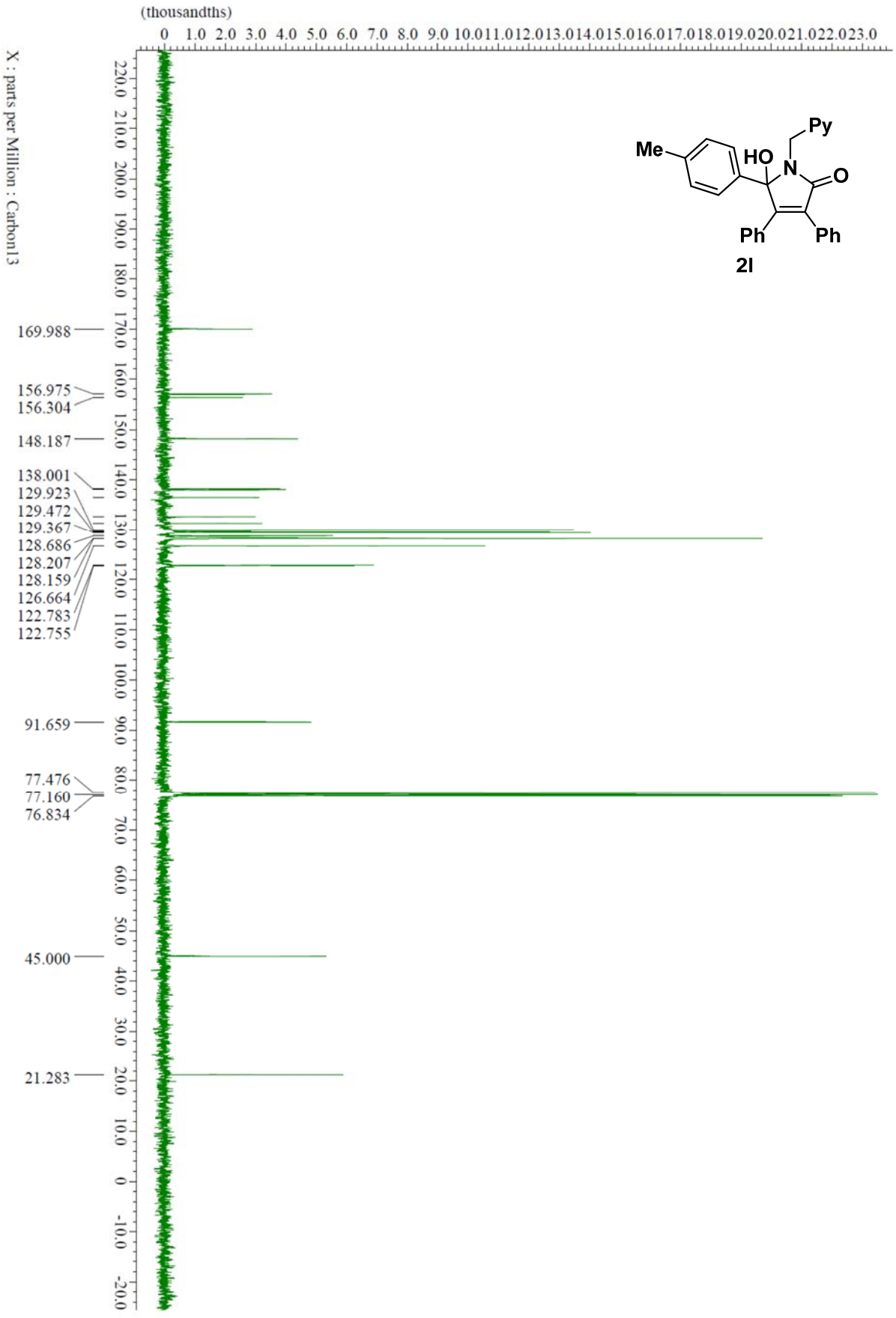
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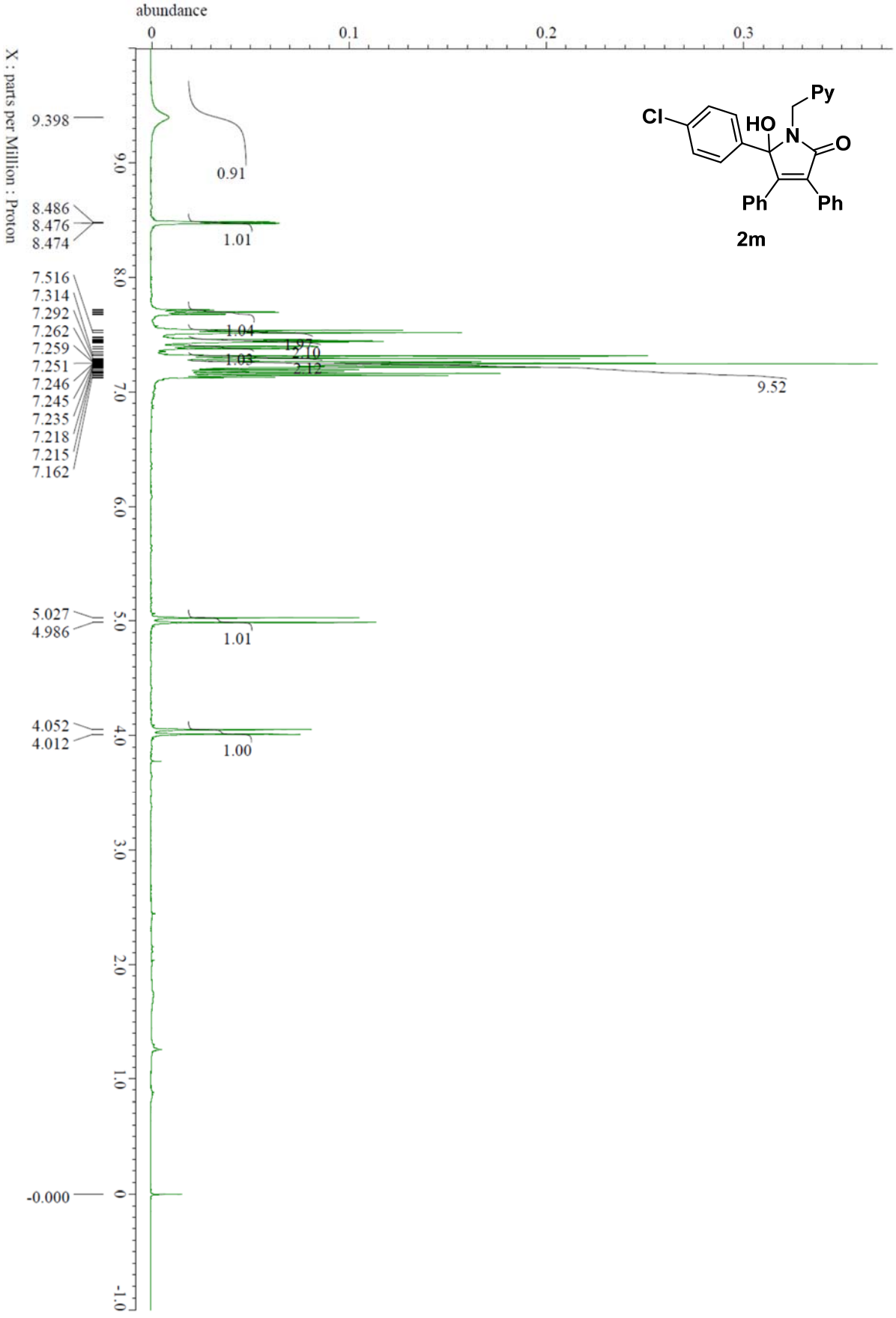
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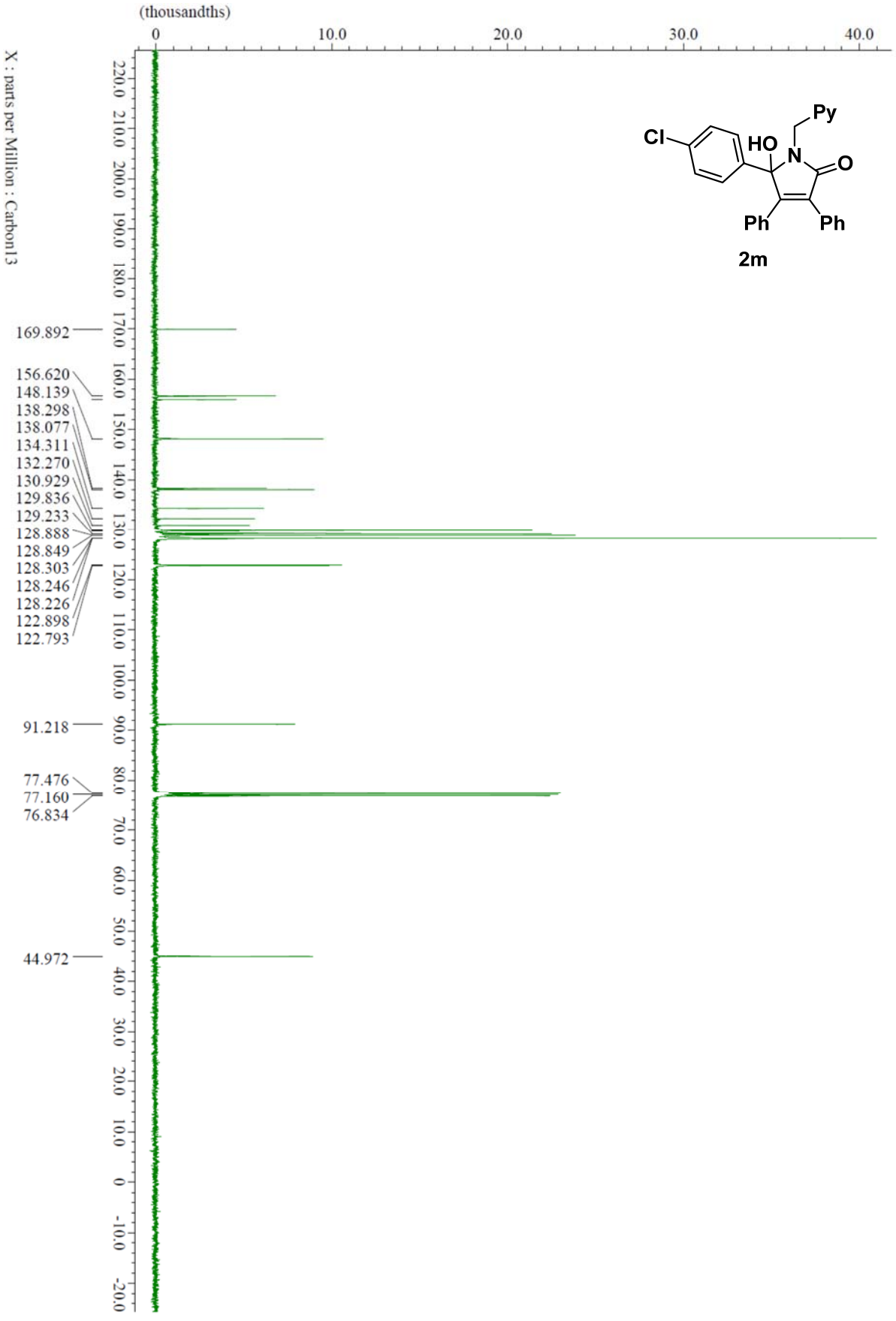
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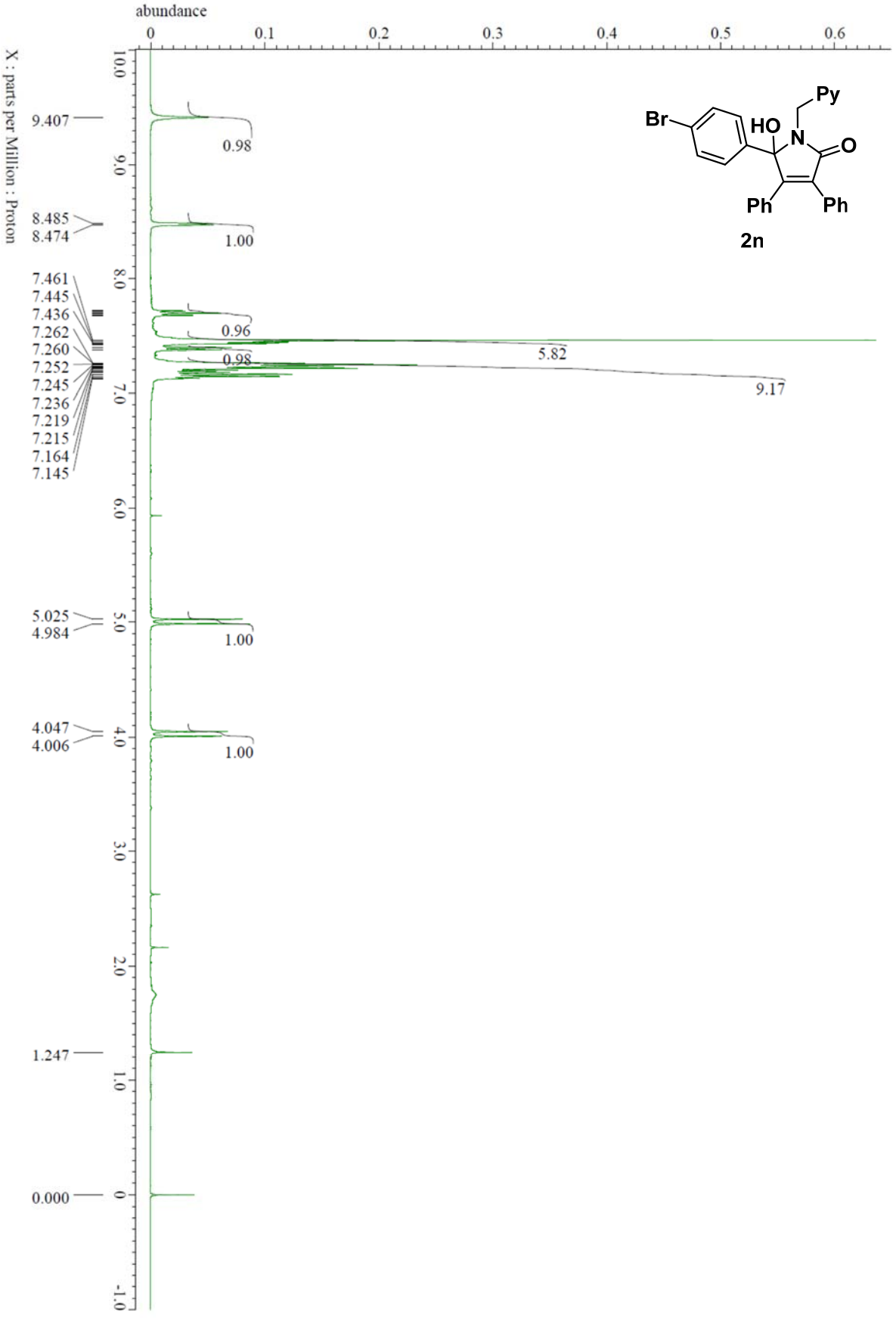
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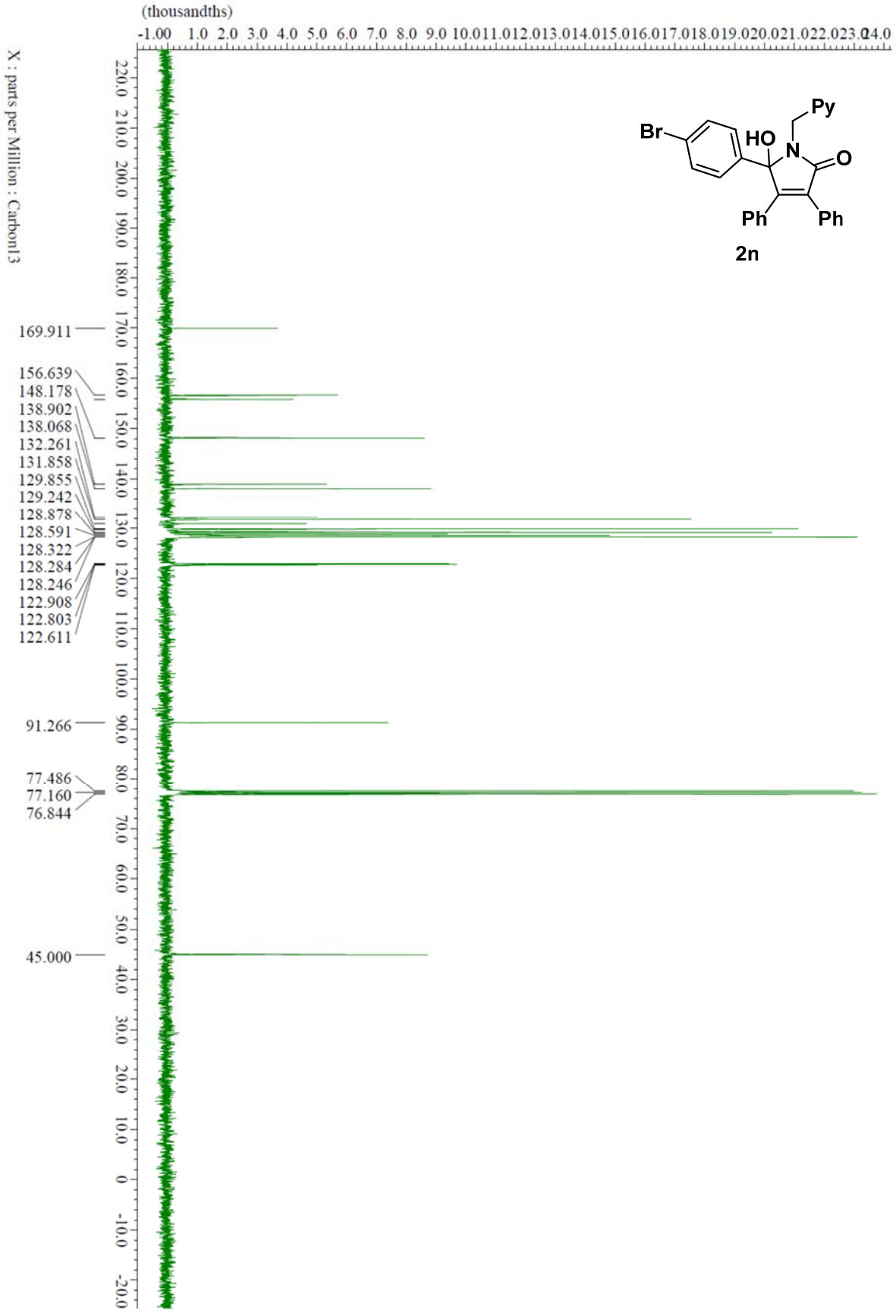
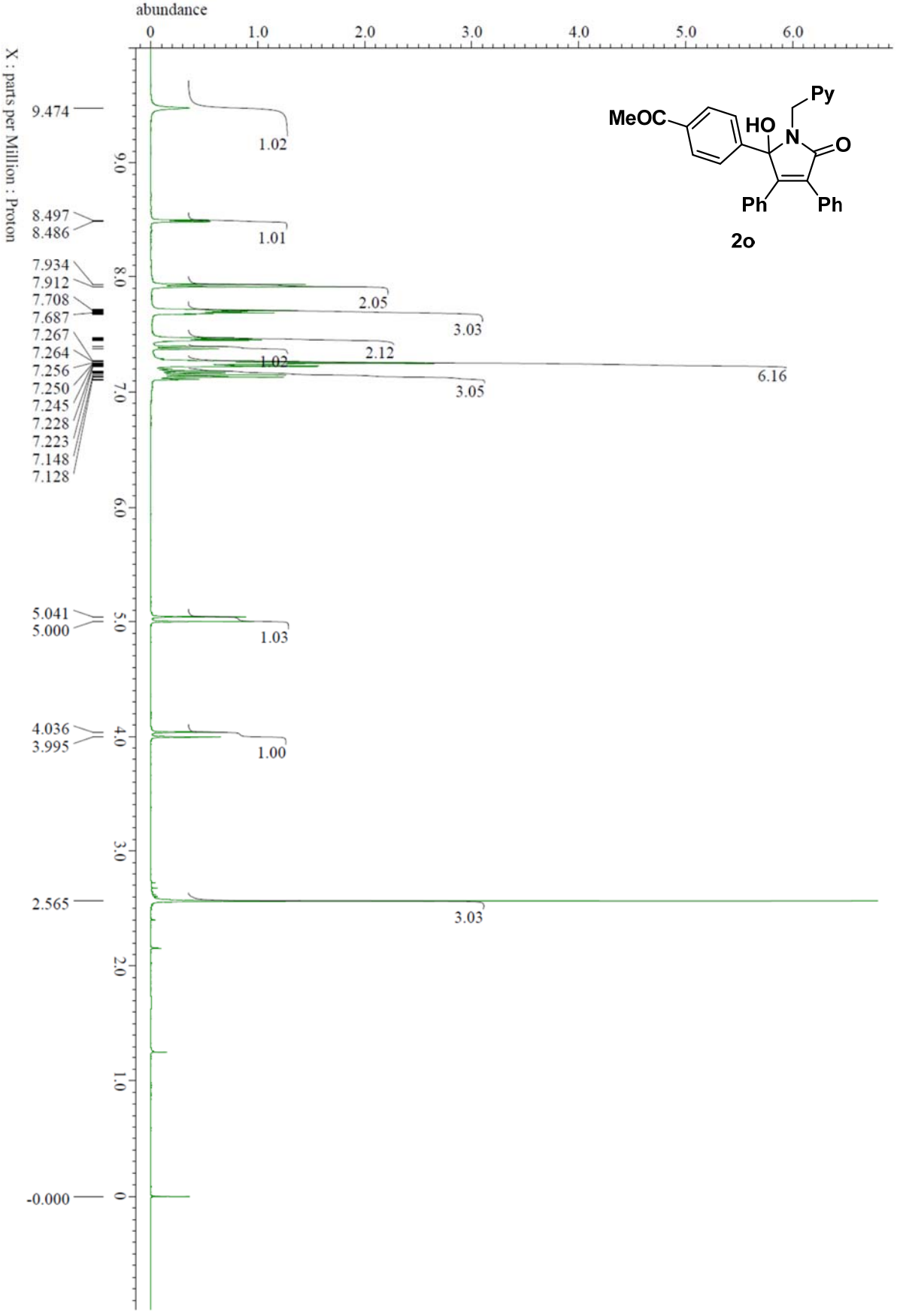
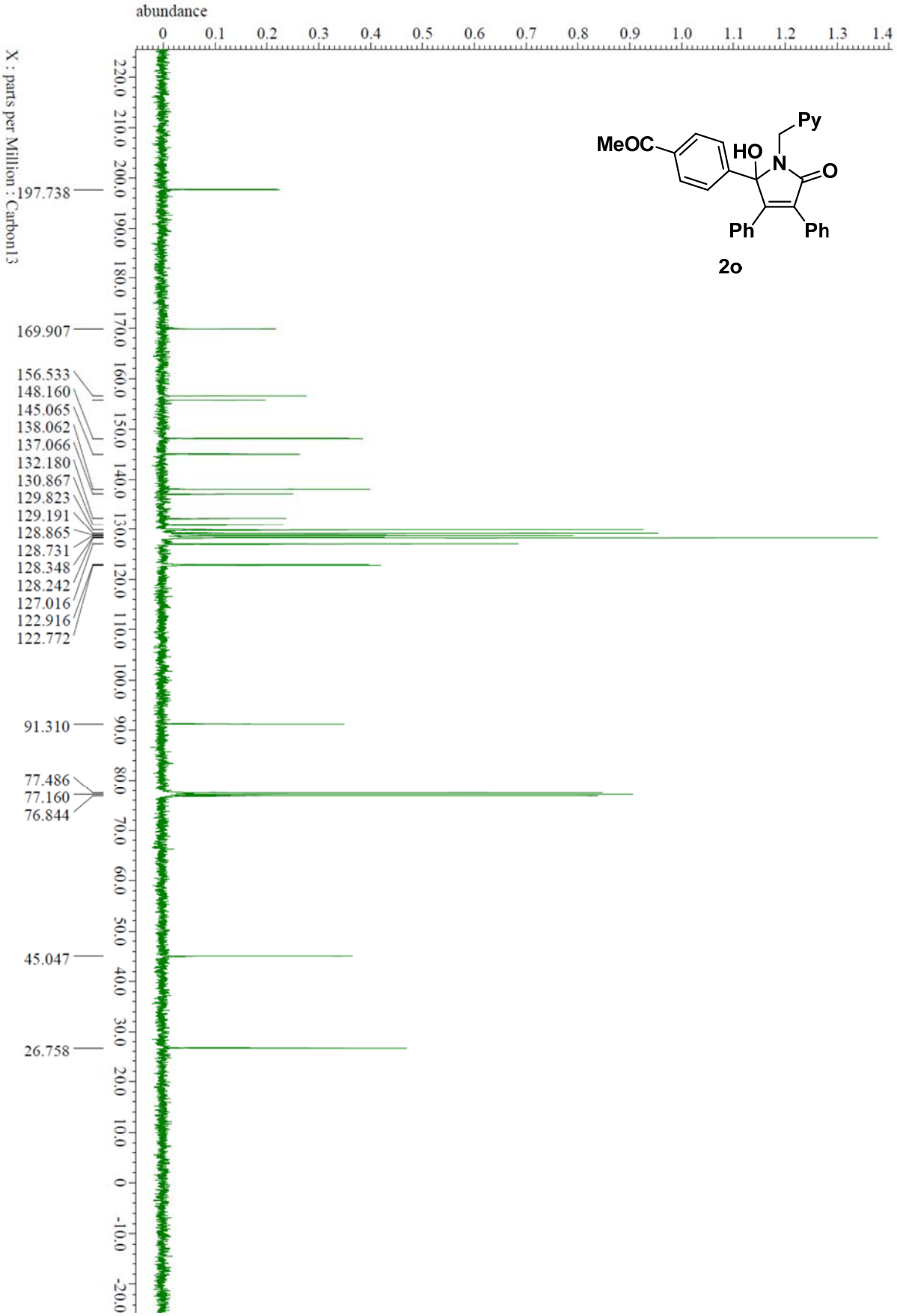
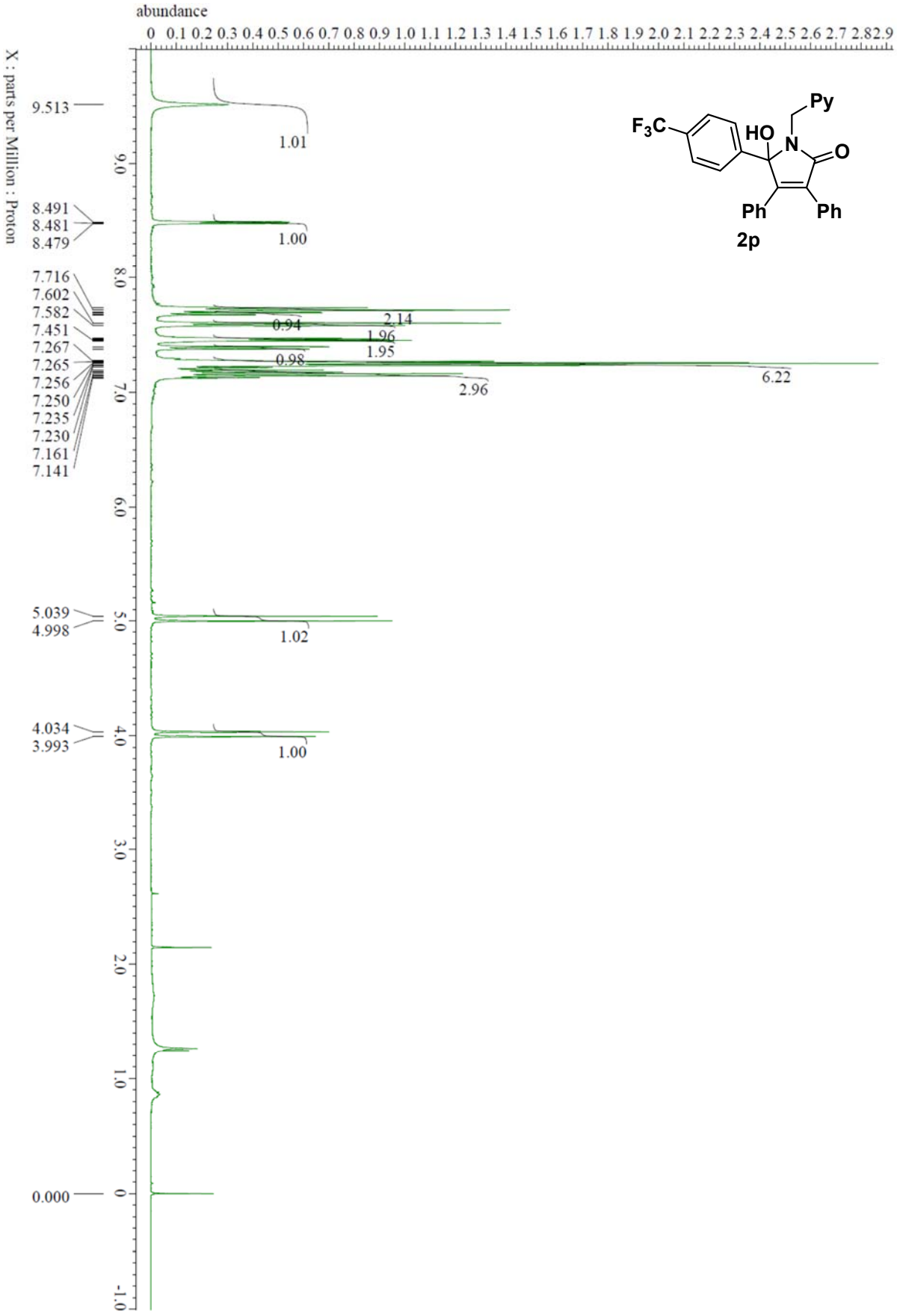
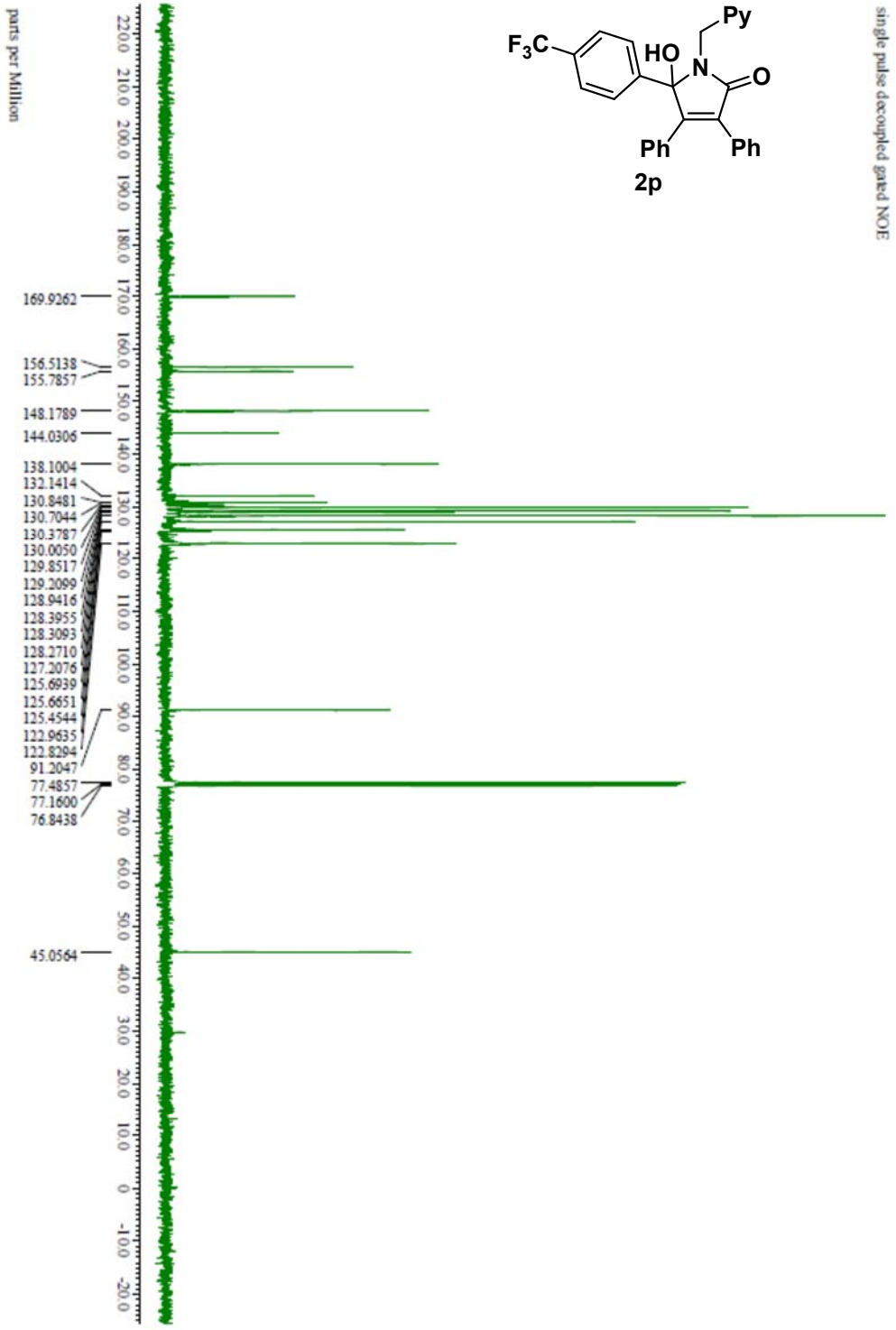
1.00
1.00

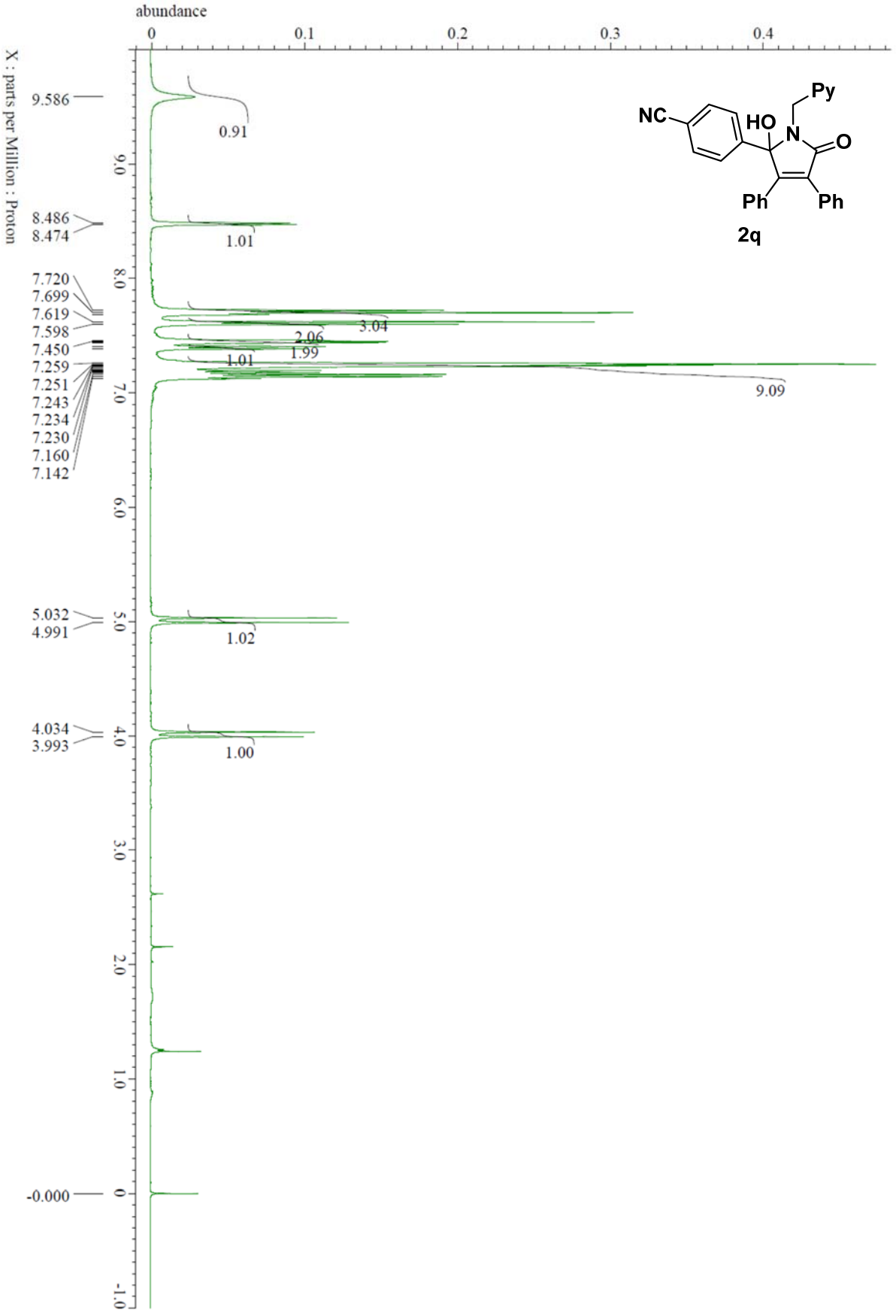

(thousandths)
X : parts per Million : Carbon13
Br
HO
N
O
Py
Ph
Ph
2n
169.911
156.639
148.178
138.902
138.068
132.261
131.858
129.855
129.242
128.878
128.591
128.322
128.284
128.246
122.908
122.803
122.611
91.266
77.486
77.160
76.844
45.000

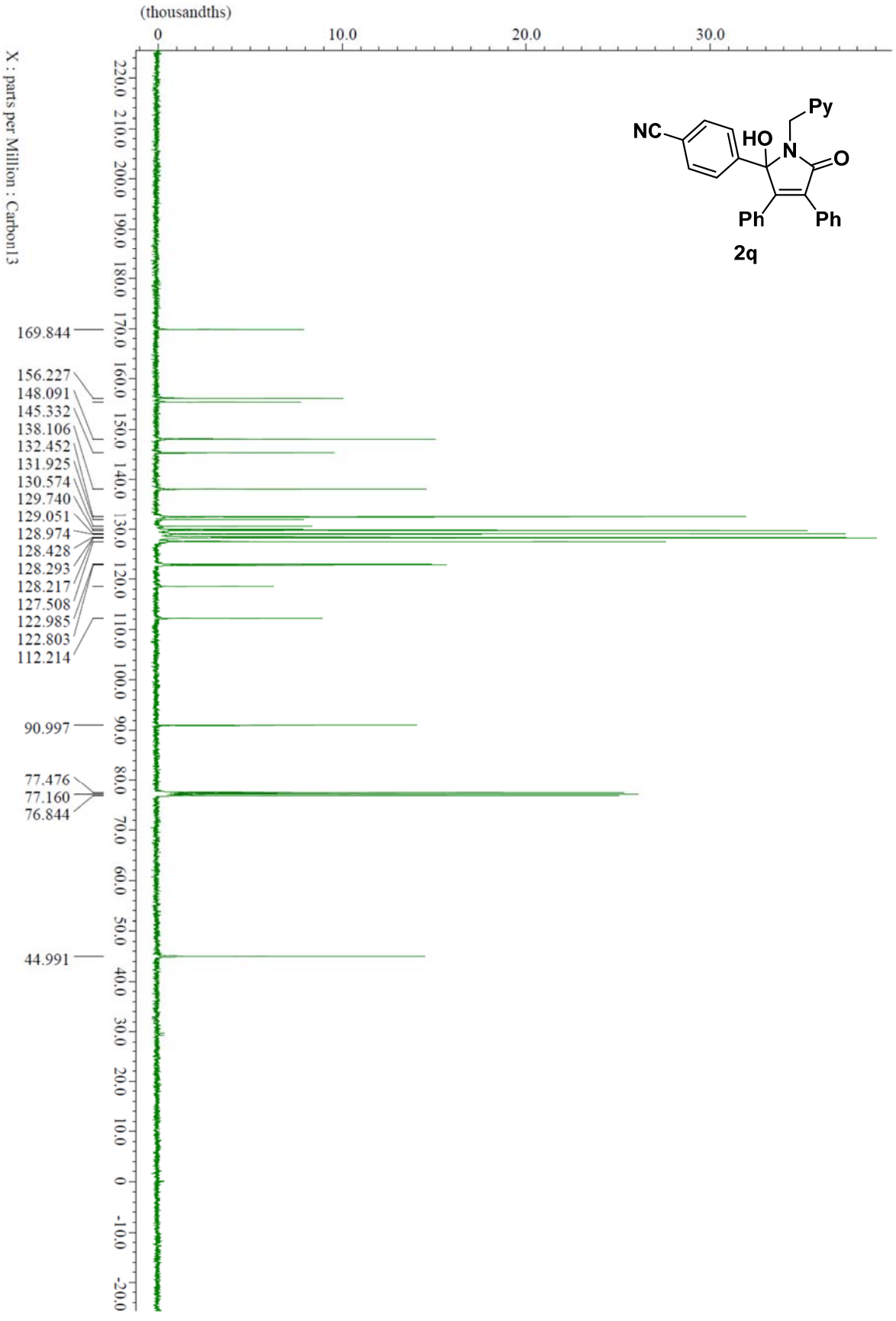

abundance
X : parts per Million : Proton
MeOC
HO
N
O
Py
Ph
Ph
2o
9.474
8.497
8.486
7.934
7.912
7.708
7.687
7.267
7.264
7.256
7.250
7.245
7.228
7.223
7.148
7.128
5.041
5.000
4.036
3.995
2.565
-0.000
1.02
1.01
2.05
3.03
1.02
2.12
6.16
3.05
1.03
1.00
3.03

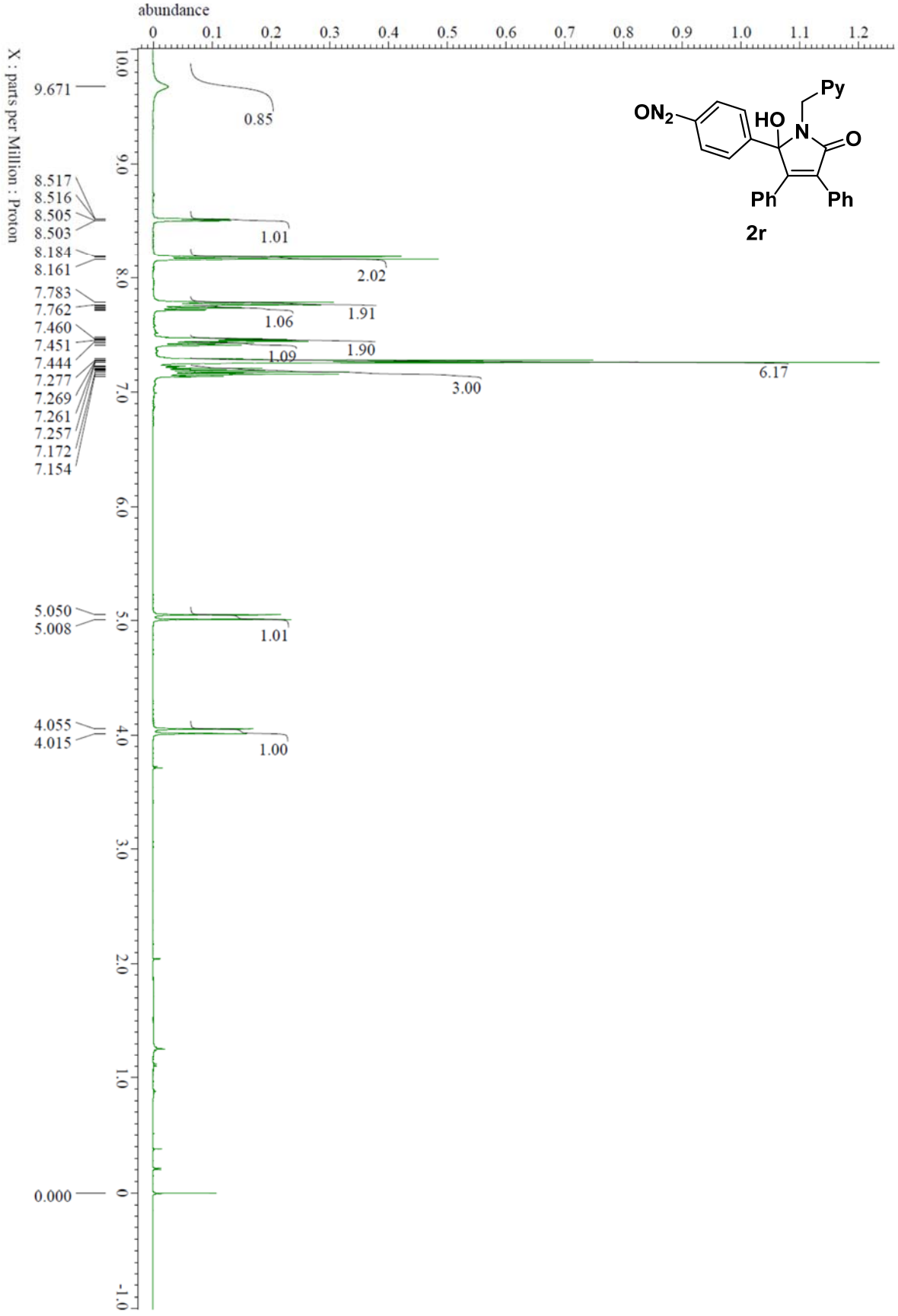

abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
197.738
169.907
156.533
148.160
145.065
138.062
137.066
132.180
130.867
129.823
129.191
128.865
128.731
128.348
128.242
127.016
122.916
122.772
91.310
77.486
77.160
76.844
45.047
26.758
MeOC
HO
N
O
Py
Ph
Ph
2o

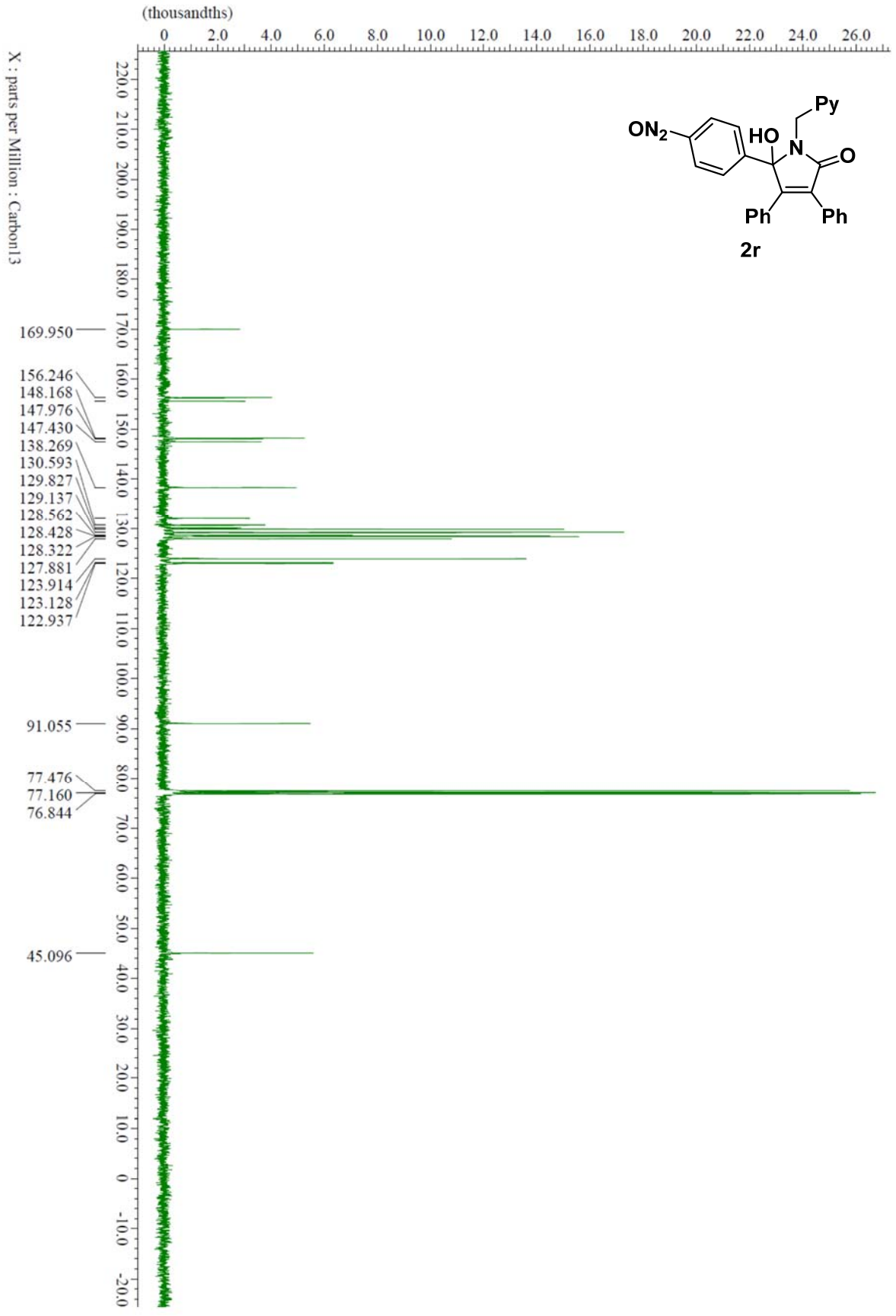

abundance
X : parts per Million : Proton
9.513
8.491
8.481
8.479
7.716
7.602
7.582
7.451
7.267
7.265
7.256
7.250
7.235
7.230
7.161
7.141
5.039
4.998
4.034
3.993
0.000
1.01
1.00
0.94
2.14
1.96
1.95
0.98
6.22
2.96
1.02
1.00
F3C
HO
N
O
Py
Ph
Ph
2p

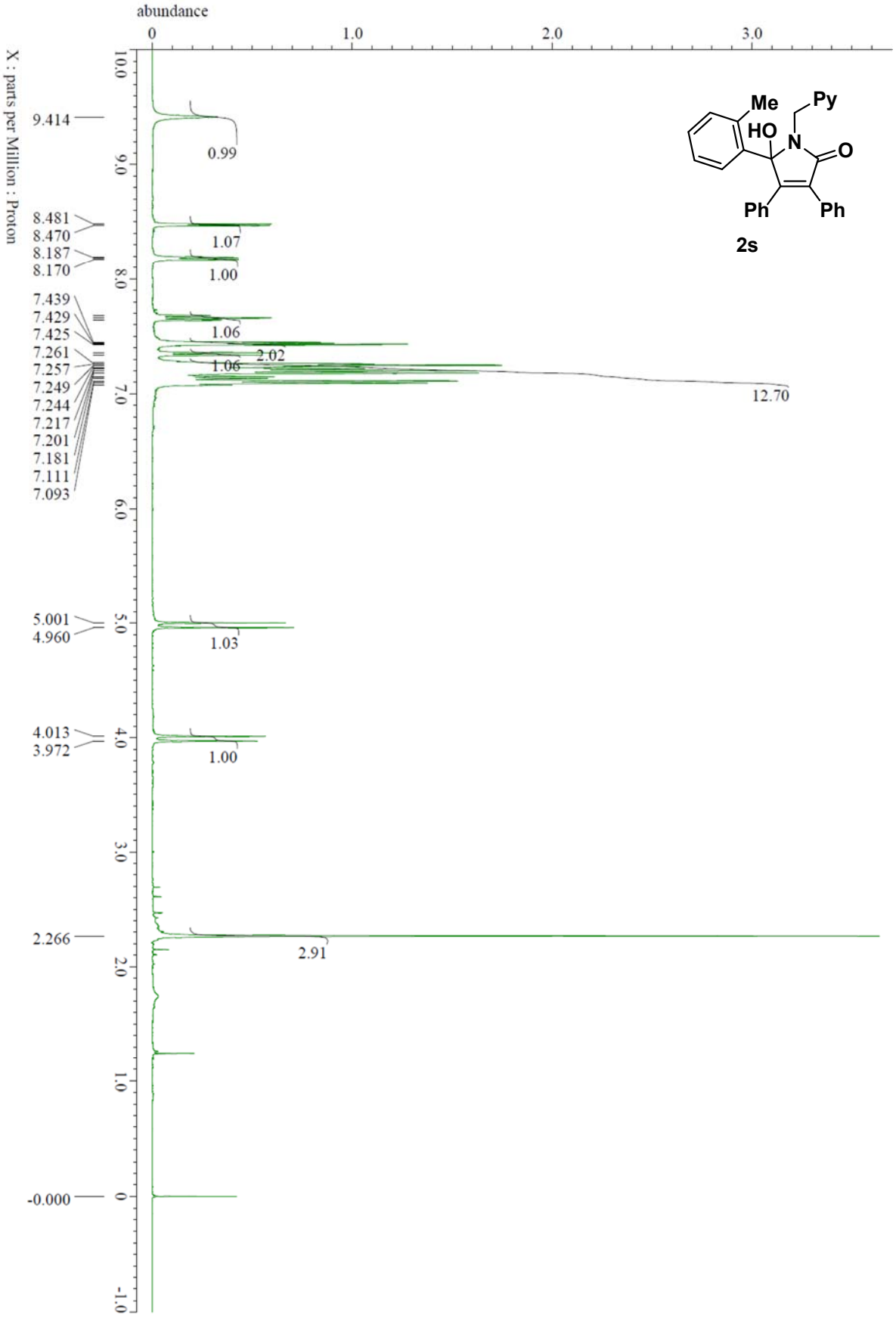

parts per Million
single pulse decoupled gated NOE
169.9262
156.5138
155.7857
148.1789
144.0306
138.1004
132.1414
130.8481
130.7044
130.3787
130.0050
129.8517
129.2099
128.9416
128.3955
128.3093
128.2710
127.2076
125.6939
125.6651
125.4544
122.9635
122.8294
91.2047
77.4857
77.1600
76.8438
45.0564
F3C
HO
N
O
Py
Ph
Ph
2p

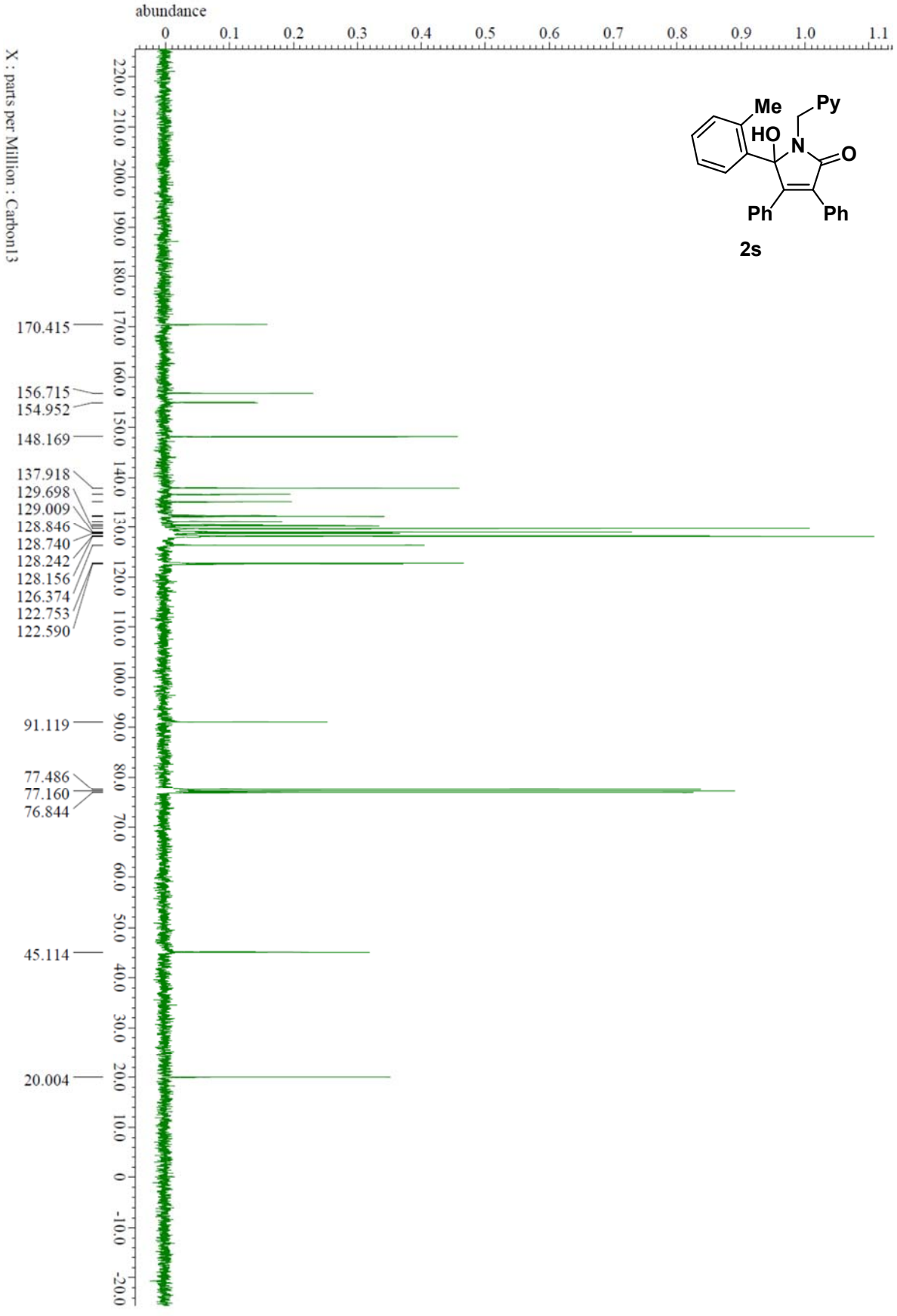

abundance
0
0.1
0.2
0.3
0.4
X : parts per Million : Proton
9.586
8.486
8.474
7.720
7.699
7.619
7.598
7.450
7.259
7.251
7.243
7.234
7.230
7.160
7.142
5.032
4.991
4.034
3.993
-0.000
0.91
1.01
3.04
2.06
1.99
1.01
9.09
1.02
1.00
NC
HO
N
O
Py
Ph
Ph
2q

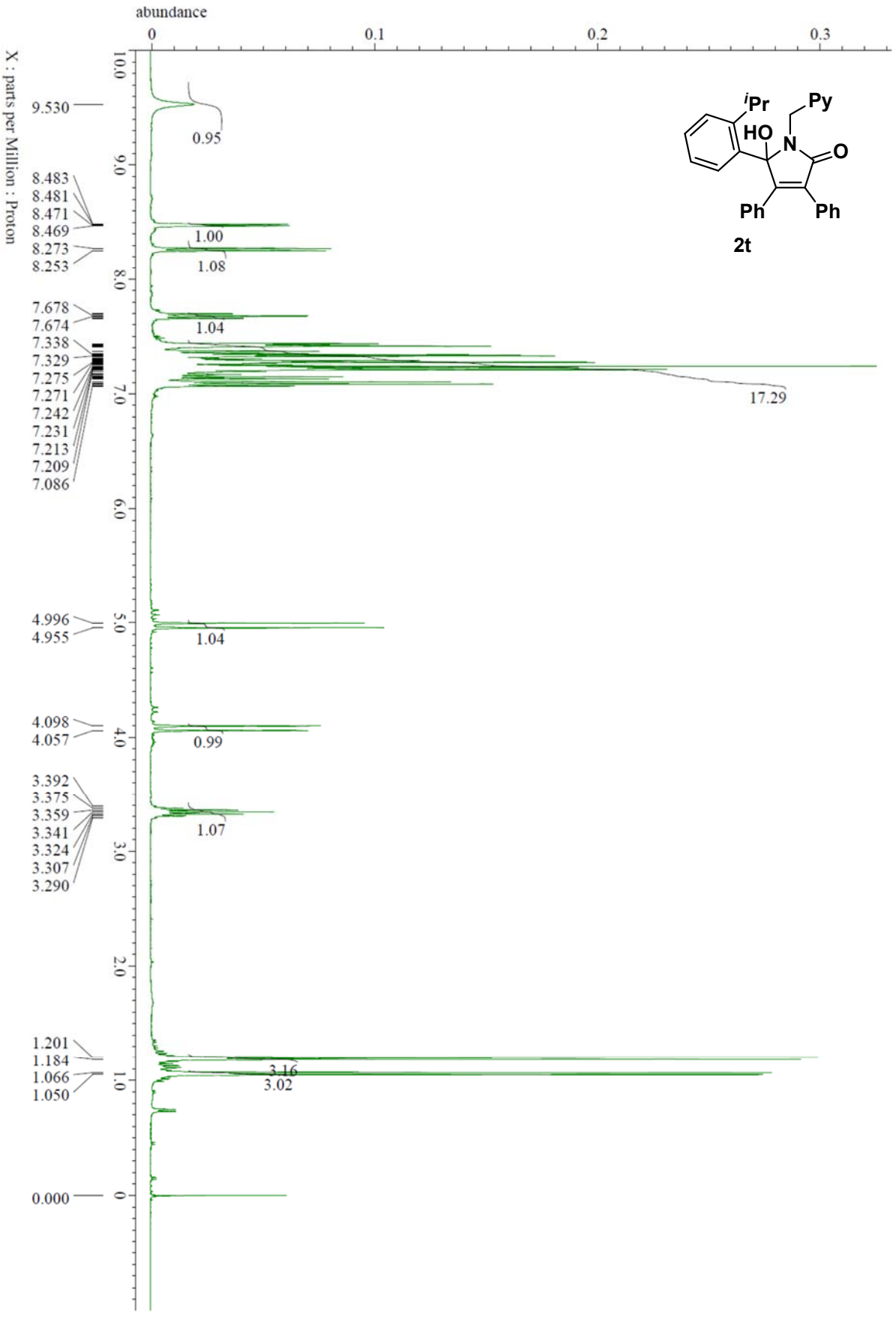

(thousandths)
0
10.0
20.0
30.0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
169.844
156.227
148.091
145.332
138.106
132.452
131.925
130.574
129.740
129.051
128.974
128.428
128.293
128.217
127.508
122.985
122.803
112.214
90.997
77.476
77.160
76.844
44.991
NC
HO
N
O
Py
Ph
Ph
2q

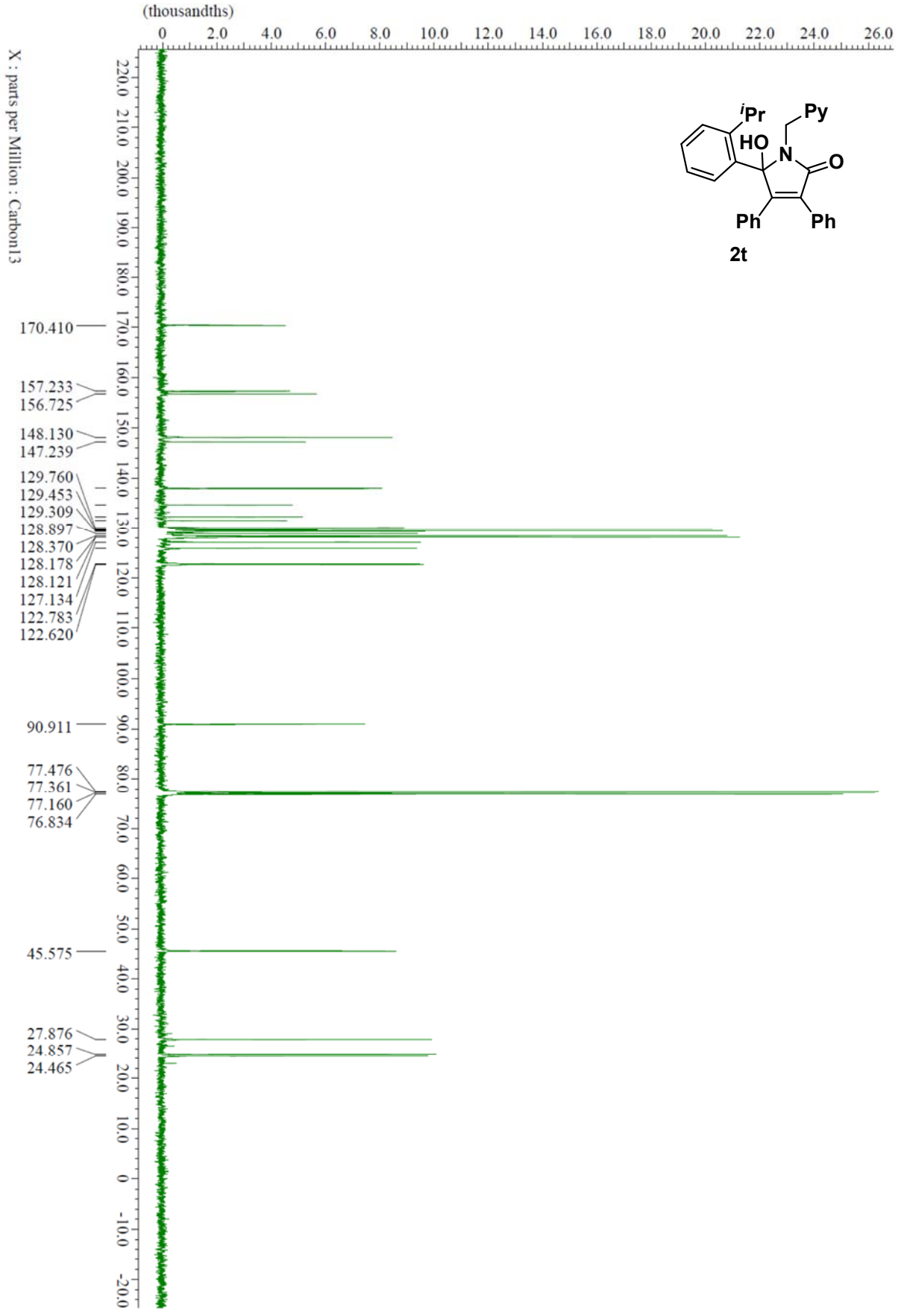

abundance
X : parts per Million : Proton
9.671
8.517
8.516
8.505
8.503
8.184
8.161
7.783
7.762
7.460
7.451
7.444
7.277
7.269
7.261
7.257
7.172
7.154
5.050
5.008
4.055
4.015
0.000
0.85
1.01
2.02
1.06
1.91
1.09
1.90
6.17
3.00
1.01
1.00
ON2
HO
N
O
Py
Ph
Ph
2r

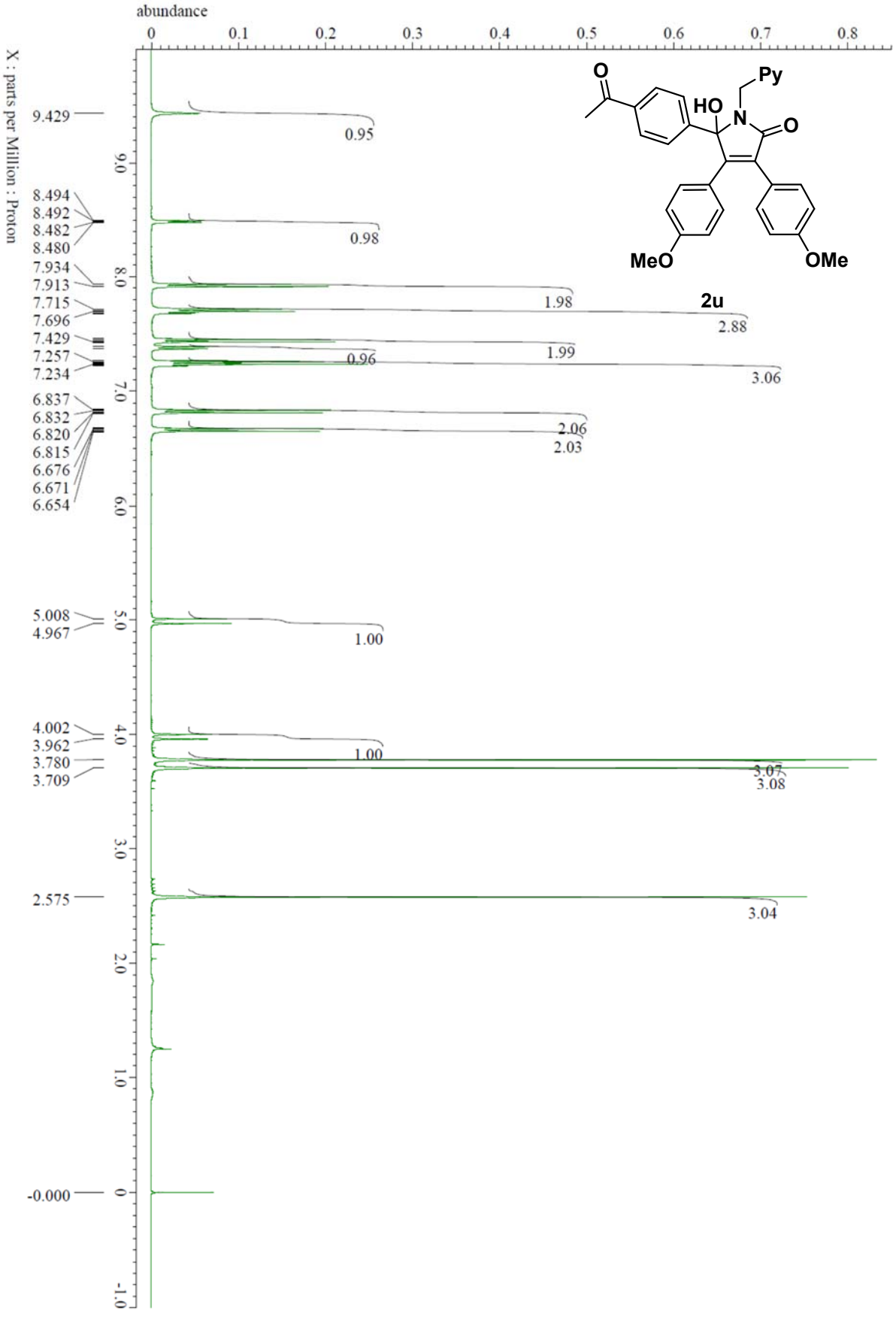

(thousandths)
X : parts per Million : Carbon13
169.950
156.246
148.168
147.976
147.430
138.269
130.593
129.827
129.137
128.562
128.428
128.322
127.881
123.914
123.128
122.937
91.055
77.476
77.160
76.844
45.096
ON2
HO
N
O
Py
Ph
Ph
2r

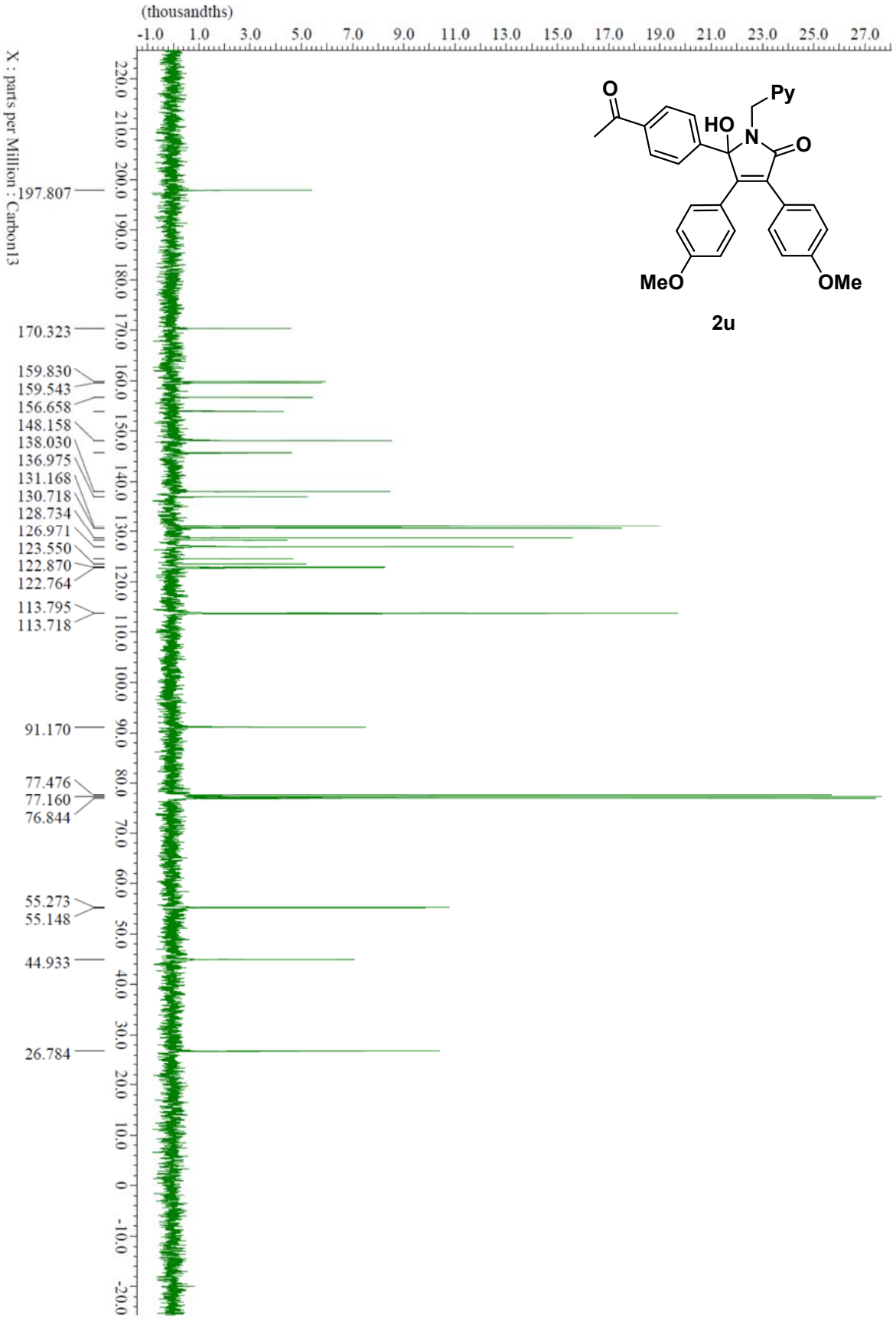

abundance
0
1.0
2.0
3.0
X : parts per Million : Proton
9.414
8.481
8.470
8.187
8.170
7.439
7.429
7.425
7.261
7.257
7.249
7.244
7.217
7.201
7.181
7.111
7.093
5.001
4.960
4.013
3.972
2.266
-0.000
0.99
1.07
1.00
1.06
2.02
1.06
12.70
1.03
1.00
2.91
Me
Py
HO
N
O
Ph
Ph
2s

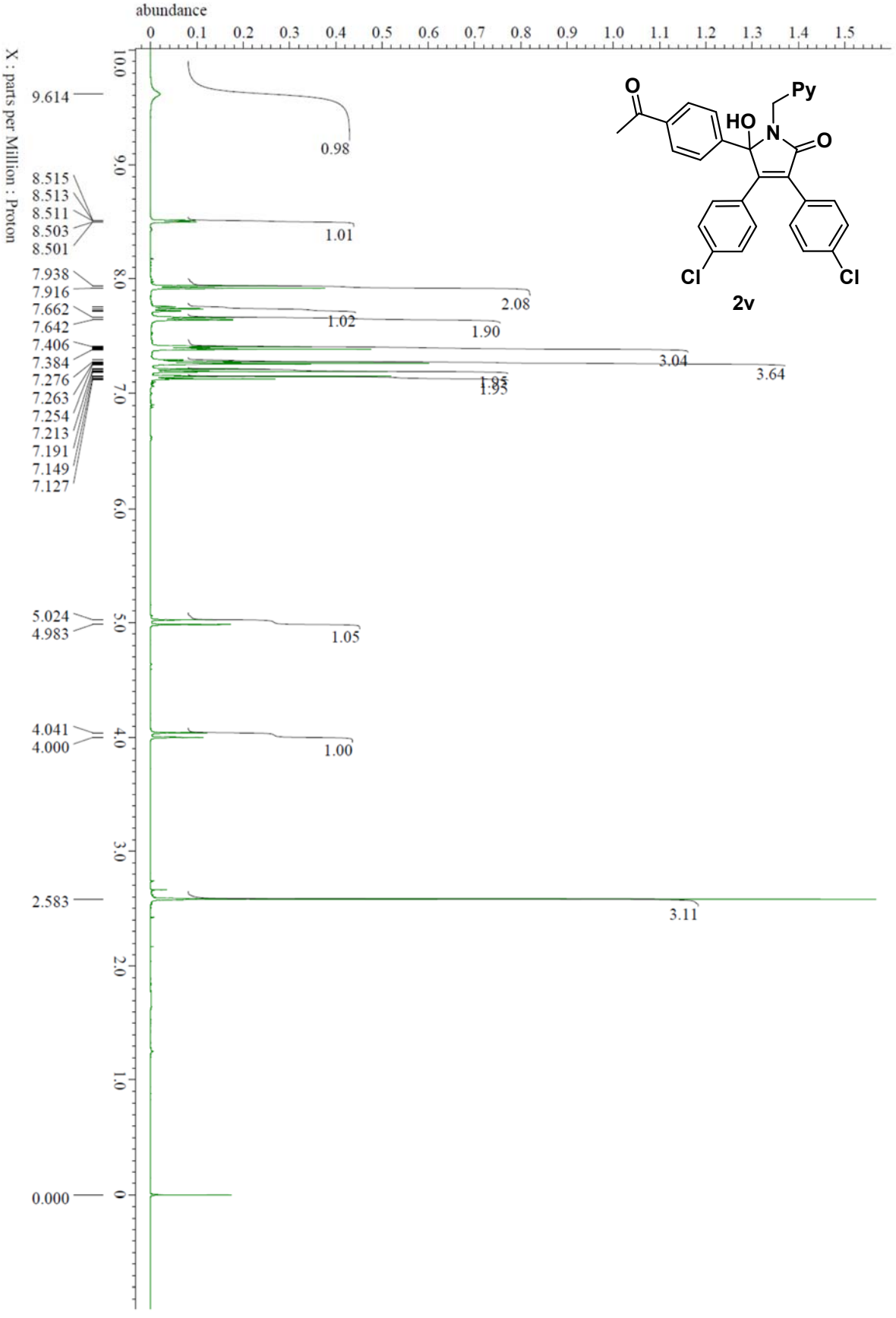

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
X : parts per Million : Carbon13
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
170.415
156.715
154.952
148.169
137.918
129.698
129.009
128.846
128.740
128.242
128.156
126.374
122.753
122.590
91.119
77.486
77.160
76.844
45.114
20.004
Me
Py
HO
N
O
Ph
Ph
2s

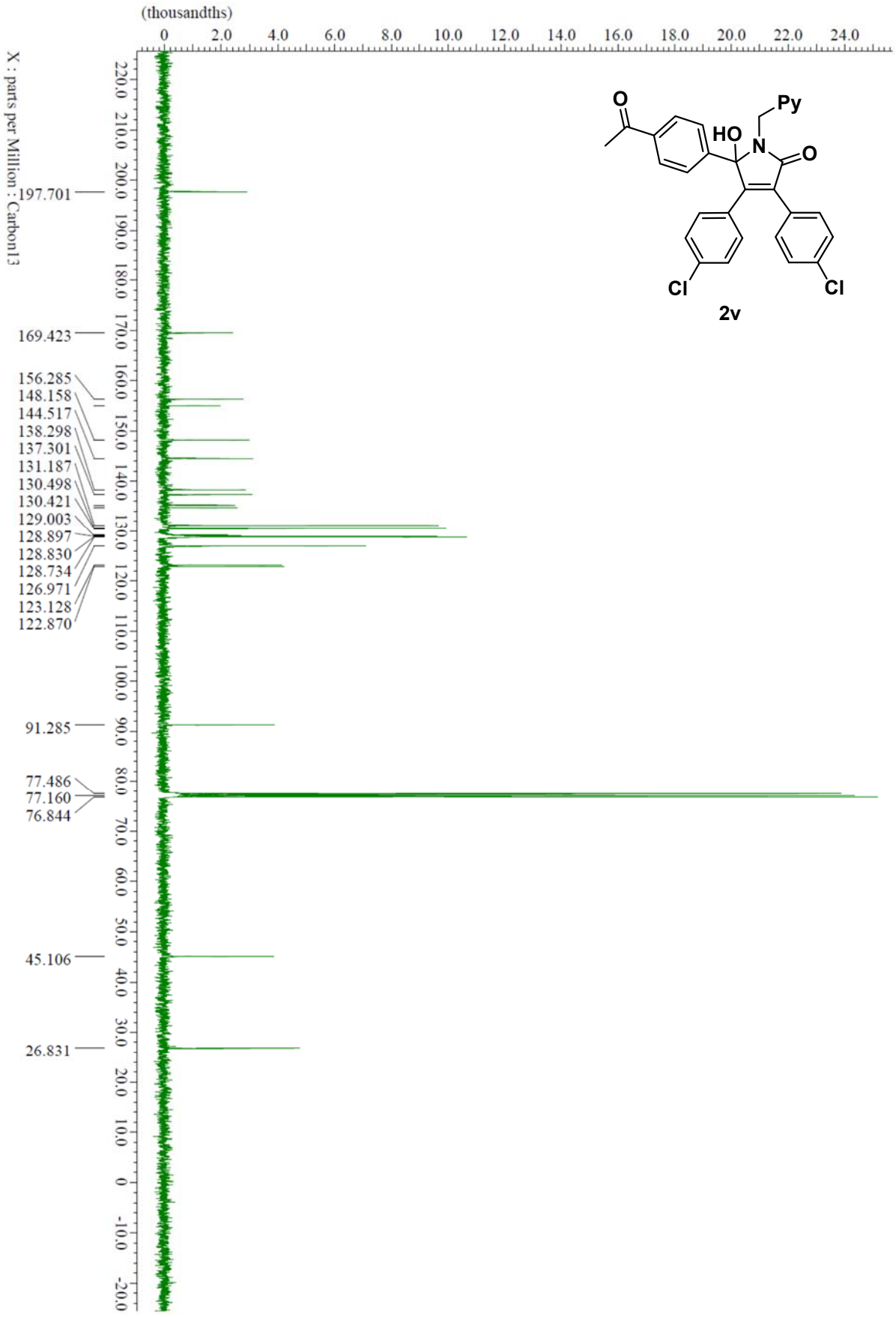

abundance
0
0.1
0.2
0.3
X : parts per Million : Proton
9.530
8.483
8.481
8.471
8.469
8.273
8.253
7.678
7.674
7.338
7.329
7.275
7.271
7.242
7.231
7.213
7.209
7.086
4.996
4.955
4.098
4.057
3.392
3.375
3.359
3.341
3.324
3.307
3.290
1.201
1.184
1.066
1.050
0.000
0.95
1.00
1.08
1.04
17.29
1.04
0.99
1.07
3.16
3.02
iPr
Py
HO
N
O
Ph
Ph
2t

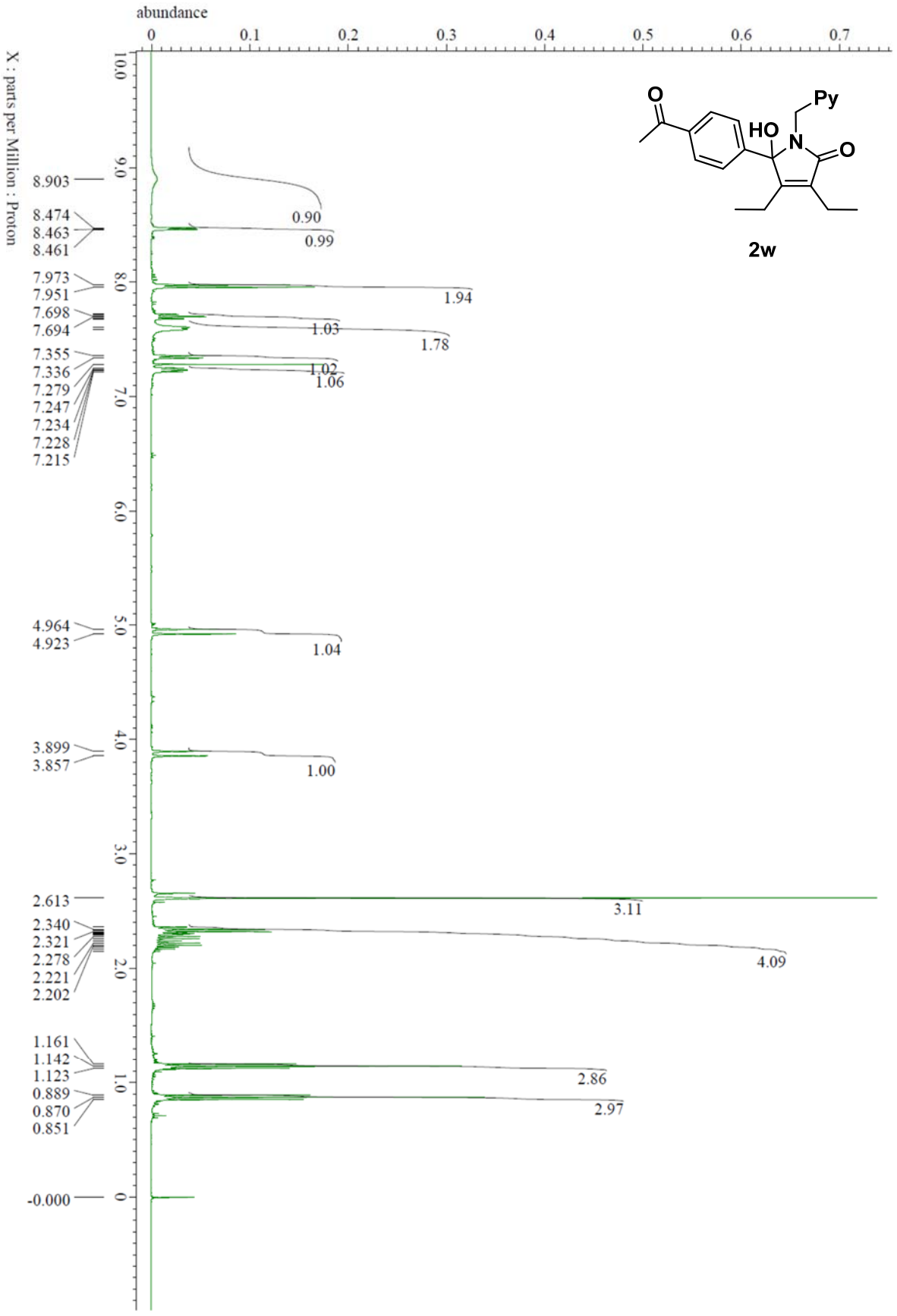

(thousandths)
X : parts per Million : Carbon13
170.410
157.233
156.725
148.130
147.239
129.760
129.453
129.309
128.897
128.370
128.178
128.121
127.134
122.783
122.620
90.911
77.476
77.361
77.160
76.834
45.575
27.876
24.857
24.465
iPr
Py
HO
N
O
Ph
Ph
2t

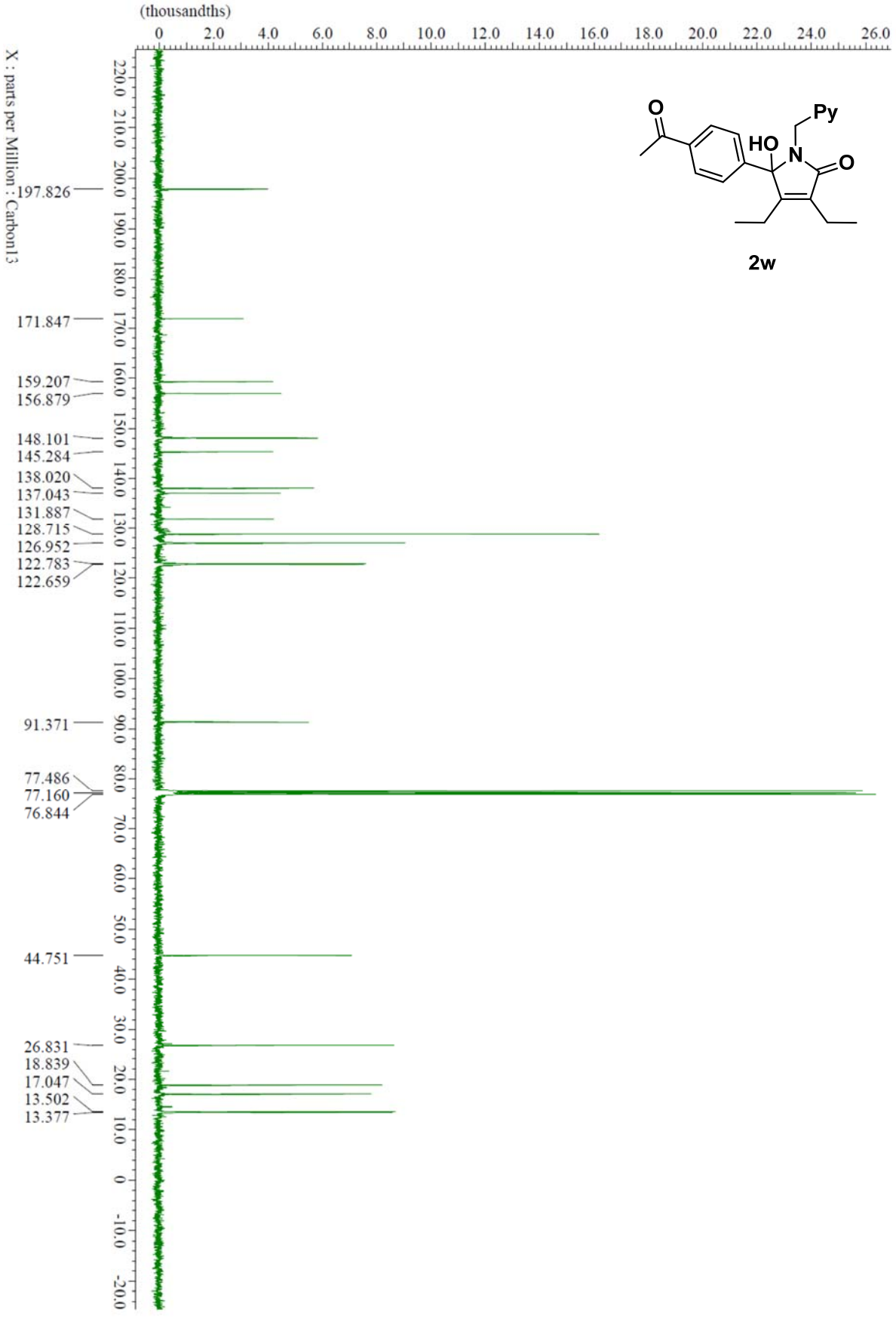

abundance
X : parts per Million : Proton
2u
MeO
OMe
HO
N
Py
9.429
8.494
8.492
8.482
8.480
7.934
7.913
7.715
7.696
7.429
7.257
7.234
6.837
6.832
6.820
6.815
6.676
6.671
6.654
5.008
4.967
4.002
3.962
3.780
3.709
2.575
-0.000
0.95
0.98
1.98
2.88
0.96
1.99
3.06
2.06
2.03
1.00
1.00
3.07
3.08
3.04

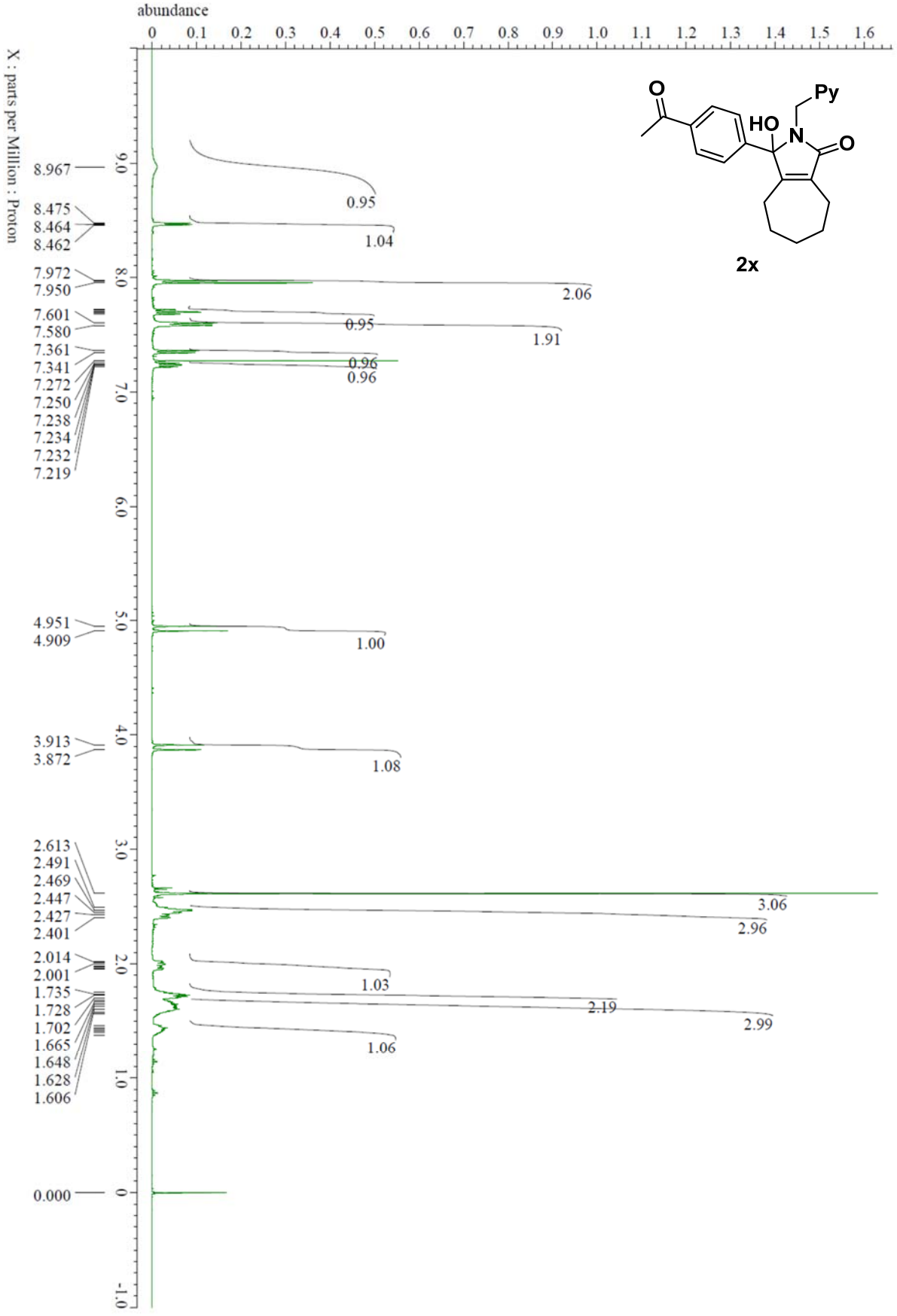

(thousandths)
-1.0 1.0 3.0 5.0 7.0 9.0 11.0 13.0 15.0 17.0 19.0 21.0 23.0 25.0 27.0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
197.807
170.323
159.830
159.543
156.658
148.158
138.030
136.975
131.168
130.718
128.734
126.971
123.550
122.870
122.764
113.795
113.718
91.170
77.476
77.160
76.844
55.273
55.148
44.933
26.784
O
Py
HO
N
O
MeO
OMe
2u

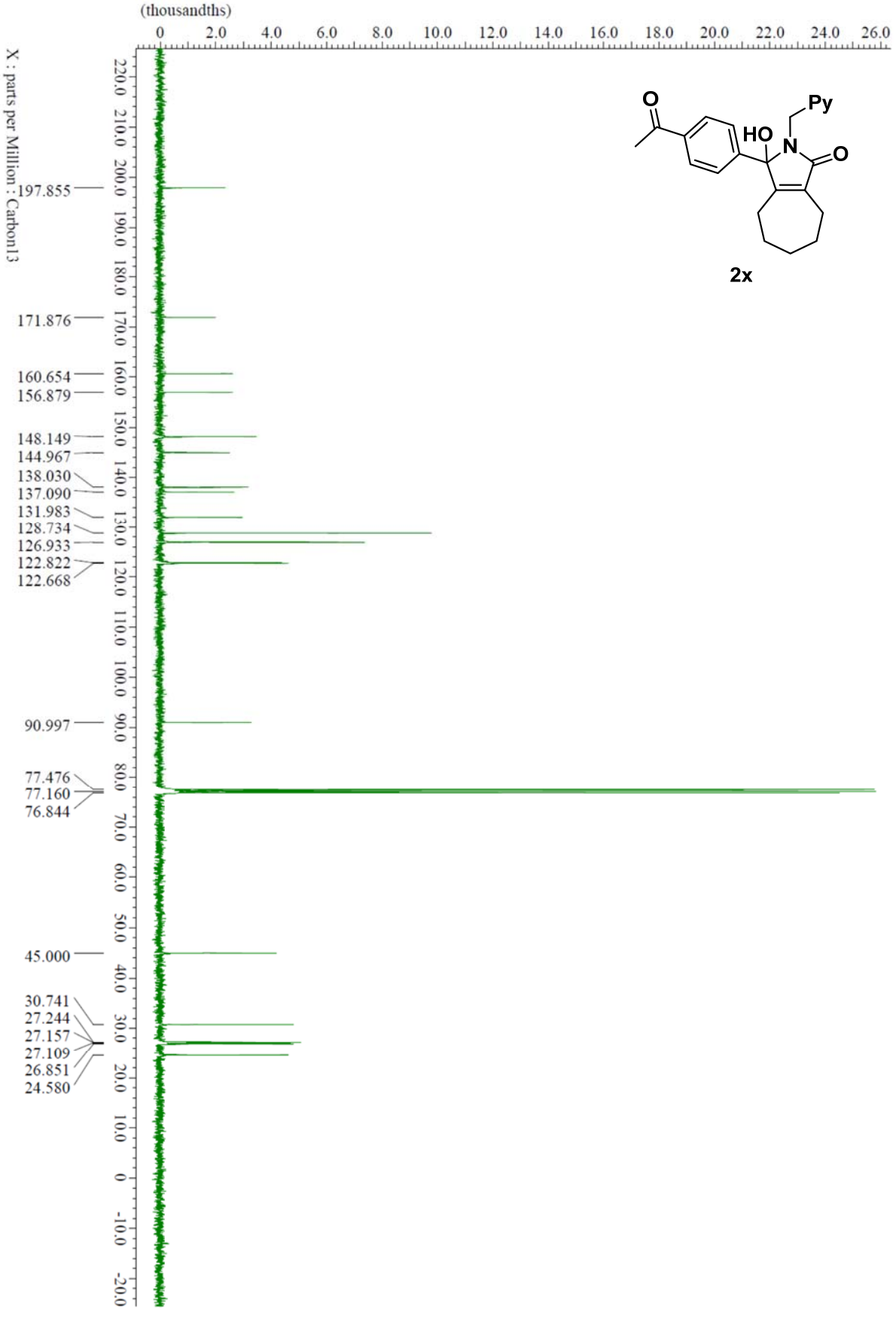

abundance
X : parts per Million : Proton
2v
9.614
8.515
8.513
8.511
8.503
8.501
7.938
7.916
7.662
7.642
7.406
7.384
7.276
7.263
7.254
7.213
7.191
7.149
7.127
5.024
4.983
4.041
4.000
2.583
0.000
0.98
1.01
2.08
1.02
1.90
3.04
3.64
1.95
1.05
1.00
3.11

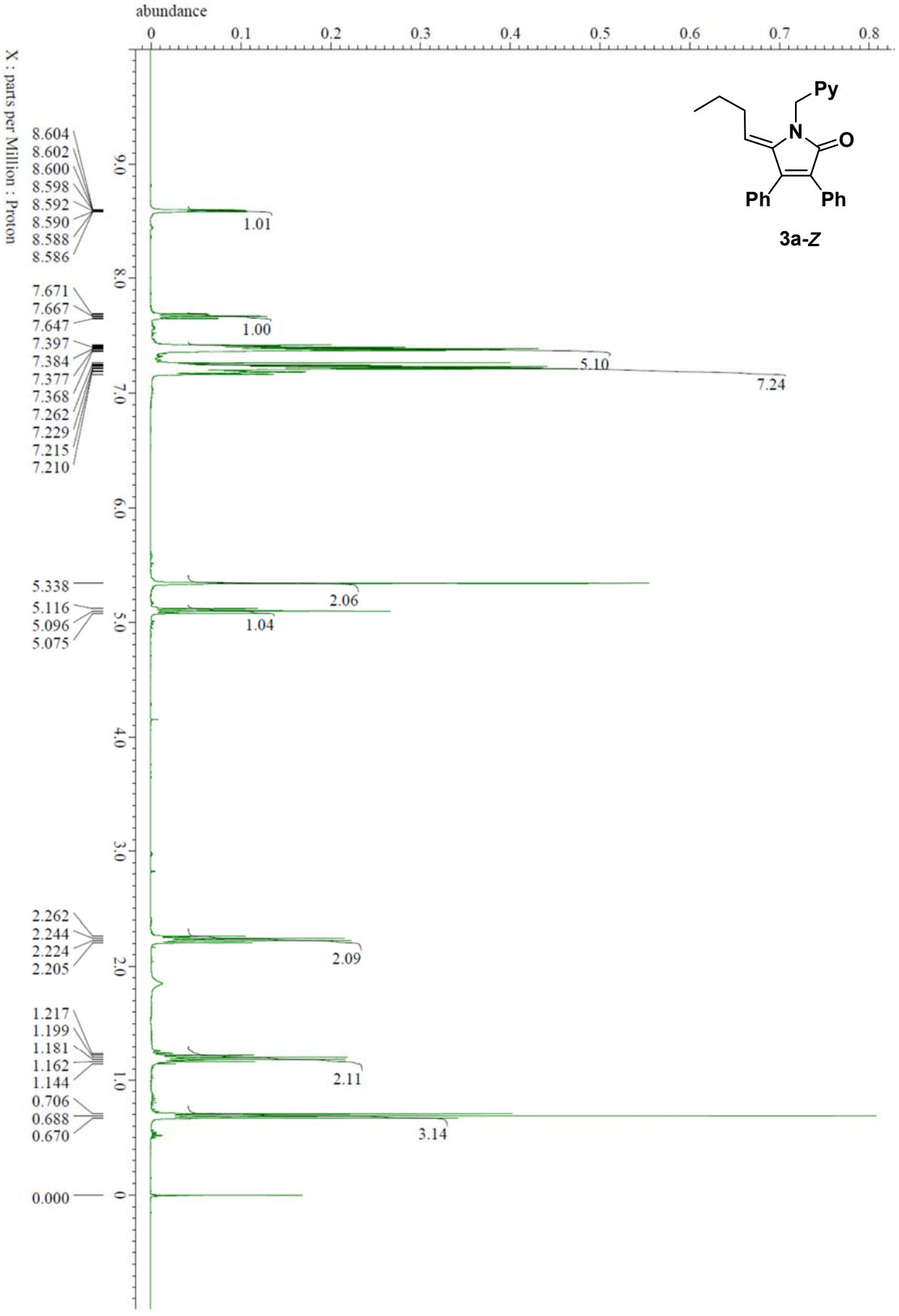

(thousandths)
X : parts per Million : Carbon13
197.701
169.423
156.285
148.158
144.517
138.298
137.301
131.187
130.498
130.421
129.003
128.897
128.830
128.734
126.971
123.128
122.870
91.285
77.486
77.160
76.844
45.106
26.831
O
Py
HO
N
O
Cl
Cl
2v

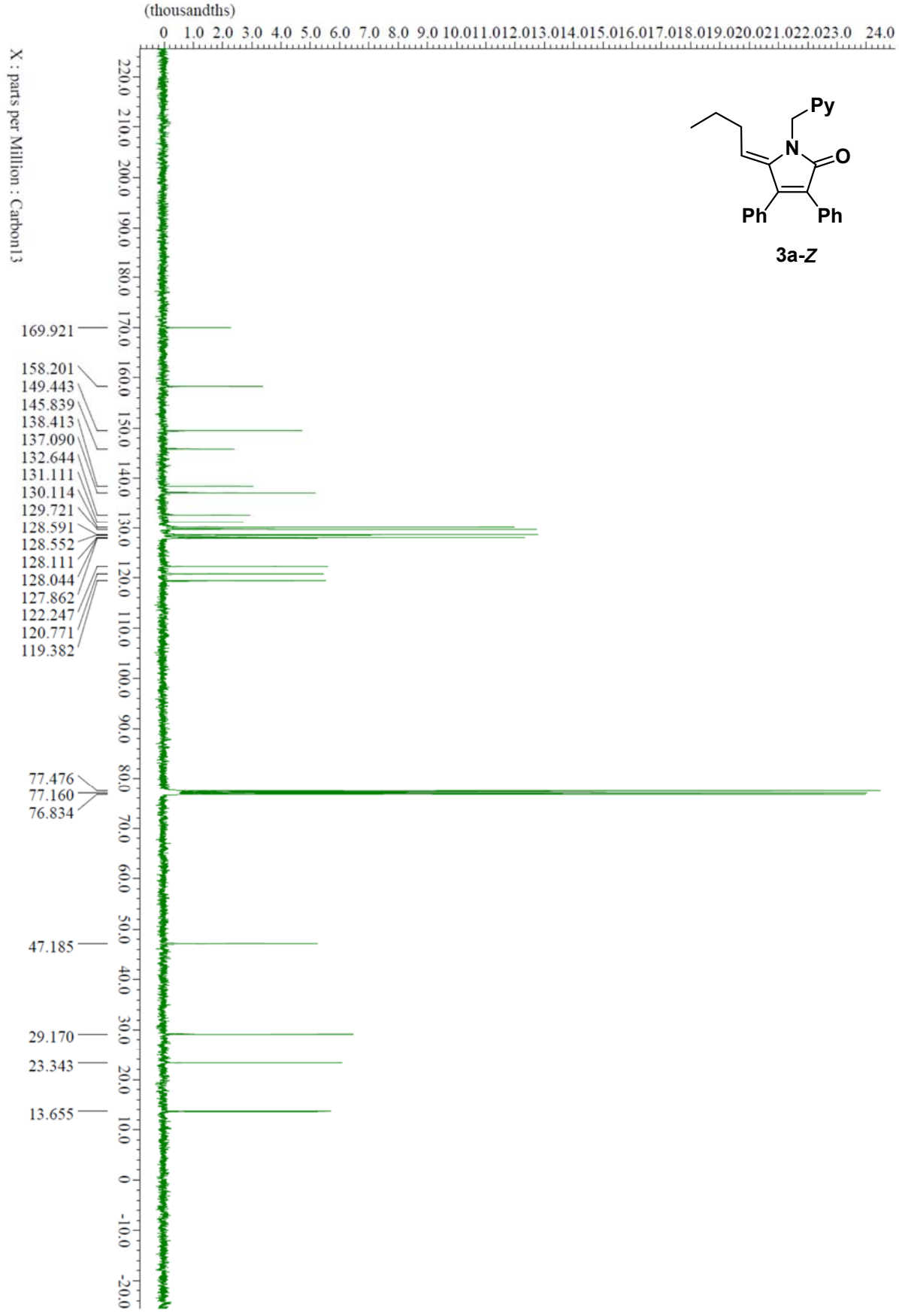

abundance
X : parts per Million : Proton
2w
8.903
8.474
8.463
8.461
7.973
7.951
7.698
7.694
7.355
7.336
7.279
7.247
7.234
7.228
7.215
4.964
4.923
3.899
3.857
2.613
2.340
2.321
2.278
2.221
2.202
1.161
1.142
1.123
0.889
0.870
0.851
-0.000
0.90
0.99
1.94
1.03
1.78
1.02
1.06
1.04
1.00
3.11
4.09
2.86
2.97


(thousandths)
X : parts per Million : Carbon13
197.826
171.847
159.207
156.879
148.101
145.284
138.020
137.043
131.887
128.715
126.952
122.783
122.659
91.371
77.486
77.160
76.844
44.751
26.831
18.839
17.047
13.502
13.377
O
Py
HO
N
O
2w


abundance
X : parts per Million : Proton
2x
8.967
8.475
8.464
8.462
7.972
7.950
7.601
7.580
7.361
7.341
7.272
7.250
7.238
7.234
7.232
7.219
4.951
4.909
3.913
3.872
2.613
2.491
2.469
2.447
2.427
2.401
2.014
2.001
1.735
1.728
1.702
1.665
1.648
1.628
1.606
0.000
0.95
1.04
2.06
0.95
1.91
0.96
0.96
1.00
1.08
3.06
2.96
1.03
2.19
2.99
1.06


(thousandths)
0 2.0 4.0 6.0 8.0 10.0 12.0 14.0 16.0 18.0 20.0 22.0 24.0 26.0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
197.855
171.876
160.654
156.879
148.149
144.967
138.030
137.090
131.983
128.734
126.933
122.822
122.668
90.997
77.476
77.160
76.844
45.000
30.741
27.244
27.157
27.109
26.851
24.580
O
Py
HO
N
O
2x


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.604
8.602
8.600
8.598
8.592
8.590
8.588
8.586
7.671
7.667
7.647
7.397
7.384
7.377
7.368
7.262
7.229
7.215
7.210
5.338
5.116
5.096
5.075
2.262
2.244
2.224
2.205
1.217
1.199
1.181
1.162
1.144
0.706
0.688
0.670
0.000
1.01
1.00
5.10
7.24
2.06
1.04
2.09
2.11
3.14
Py
N
O
Ph
Ph
3a-Z


(thousandths)
X : parts per Million : Carbon13
Py
N
O
Ph
Ph
3a-Z
169.921
158.201
149.443
145.839
138.413
137.090
132.644
131.111
130.114
129.721
128.591
128.552
128.111
128.044
127.862
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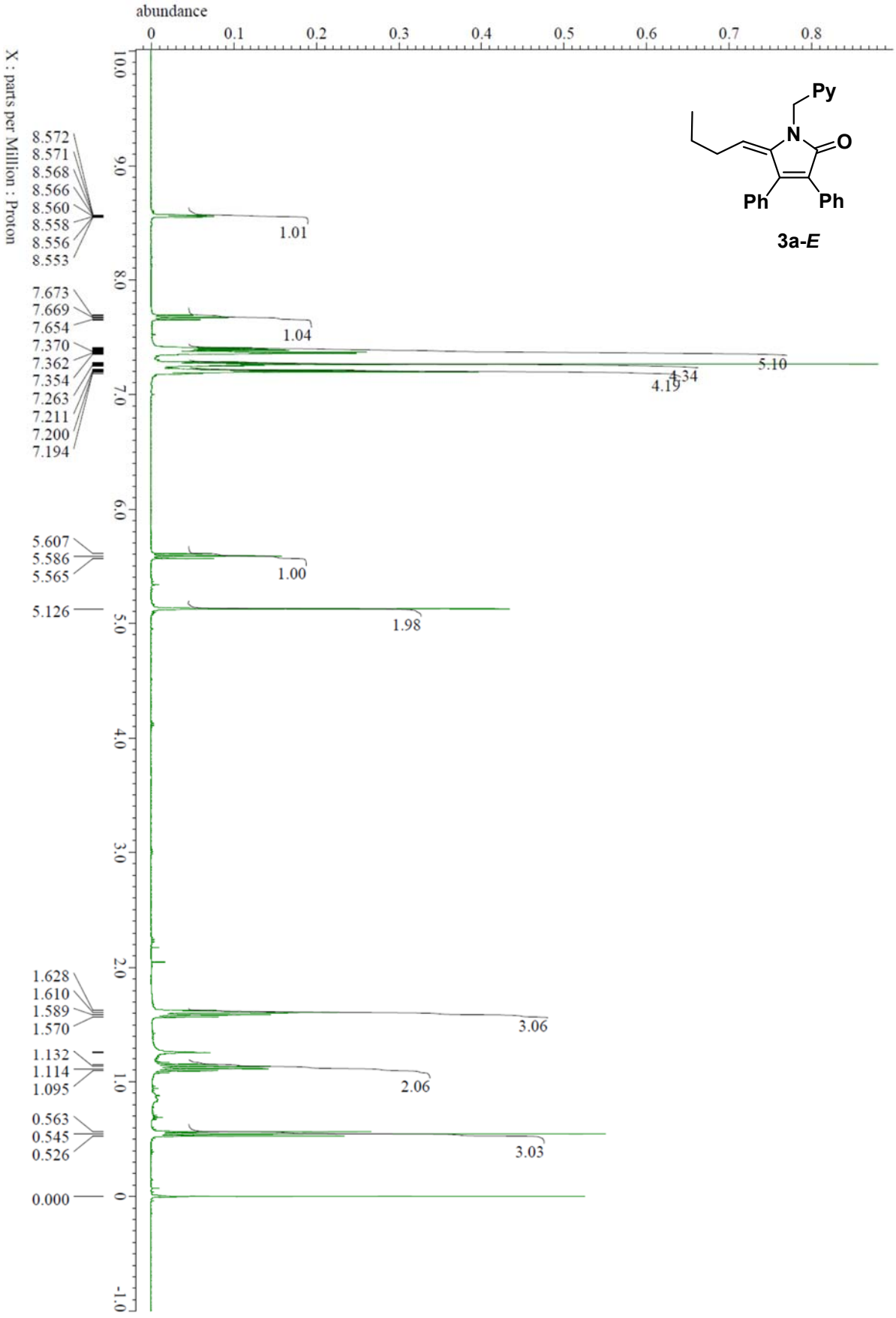
120.771
119.382
77.476
77.160
76.834
47.185
29.170
23.343
13.655


abundance
X : parts per Million : Proton
Py
N
O
Ph
Ph
3a-E
8.572
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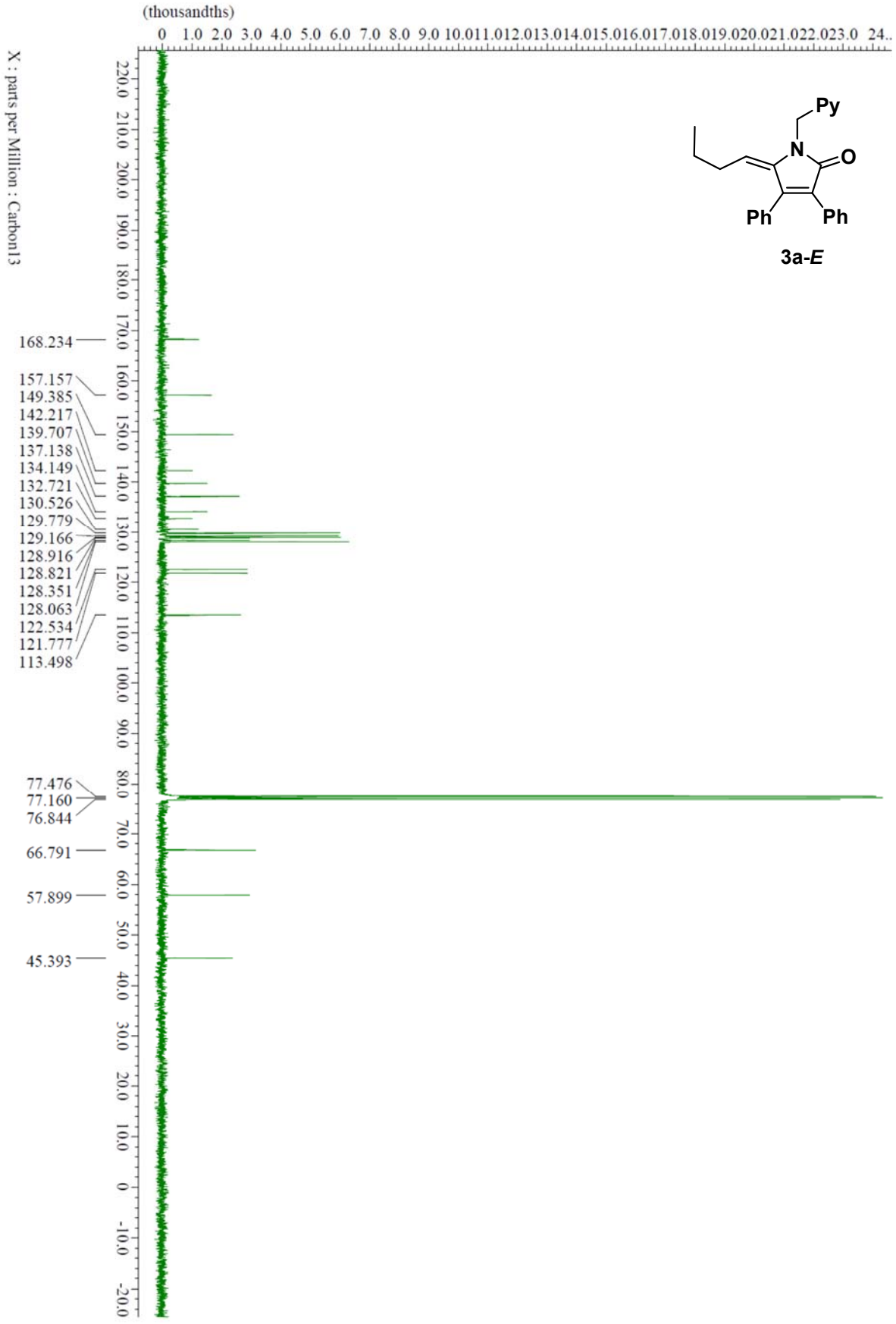
8.568
8.566
8.560
8.558
8.556
8.553
7.673
7.669
7.654
7.370
7.362
7.354
7.263
7.211
7.200
7.194
5.607
5.586
5.565
5.126
1.628
1.610
1.589
1.570
1.132
1.114
1.095
0.563
0.545
0.526
0.000
1.01
1.04
5.10
4.34
4.19
1.00
1.98
3.06
2.06
3.03


(thousandths)
X : parts per Million : Carbon13
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149.385
142.217
139.707
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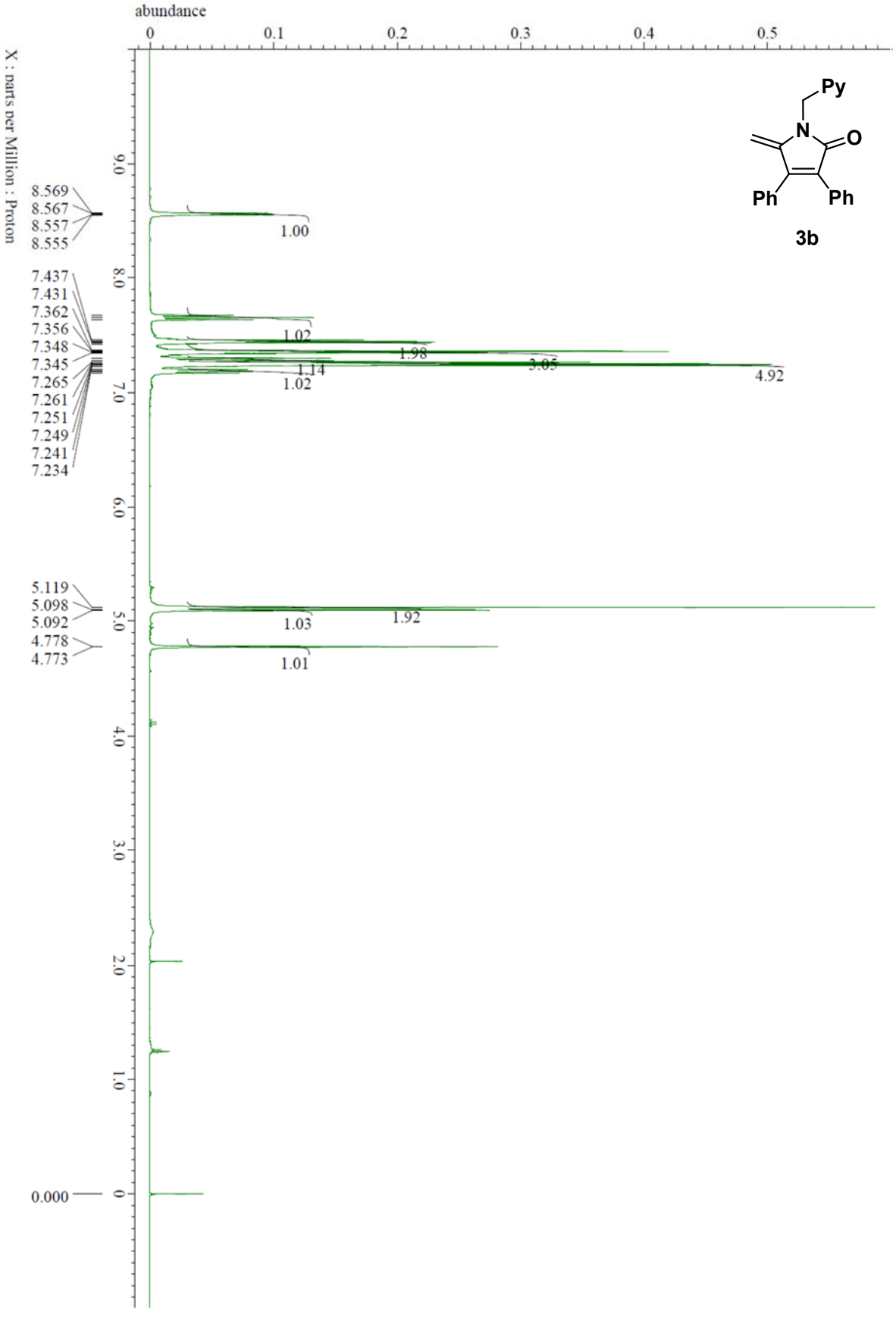
134.149
132.721
130.526
129.779
129.166
128.916
128.821
128.351
128.063
122.534
121.777
113.498
77.476
77.160
76.844
66.791
57.899
45.393
Py
N
O
Ph
Ph

3a-*E*


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : Proton
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.569
8.567
8.557
8.555
7.437
7.431
7.362
7.356
7.348
7.345
7.265
7.261
7.251
7.249
7.241
7.234
5.119
5.098
5.092
4.778
4.773
0.000
1.00
1.02
1.98
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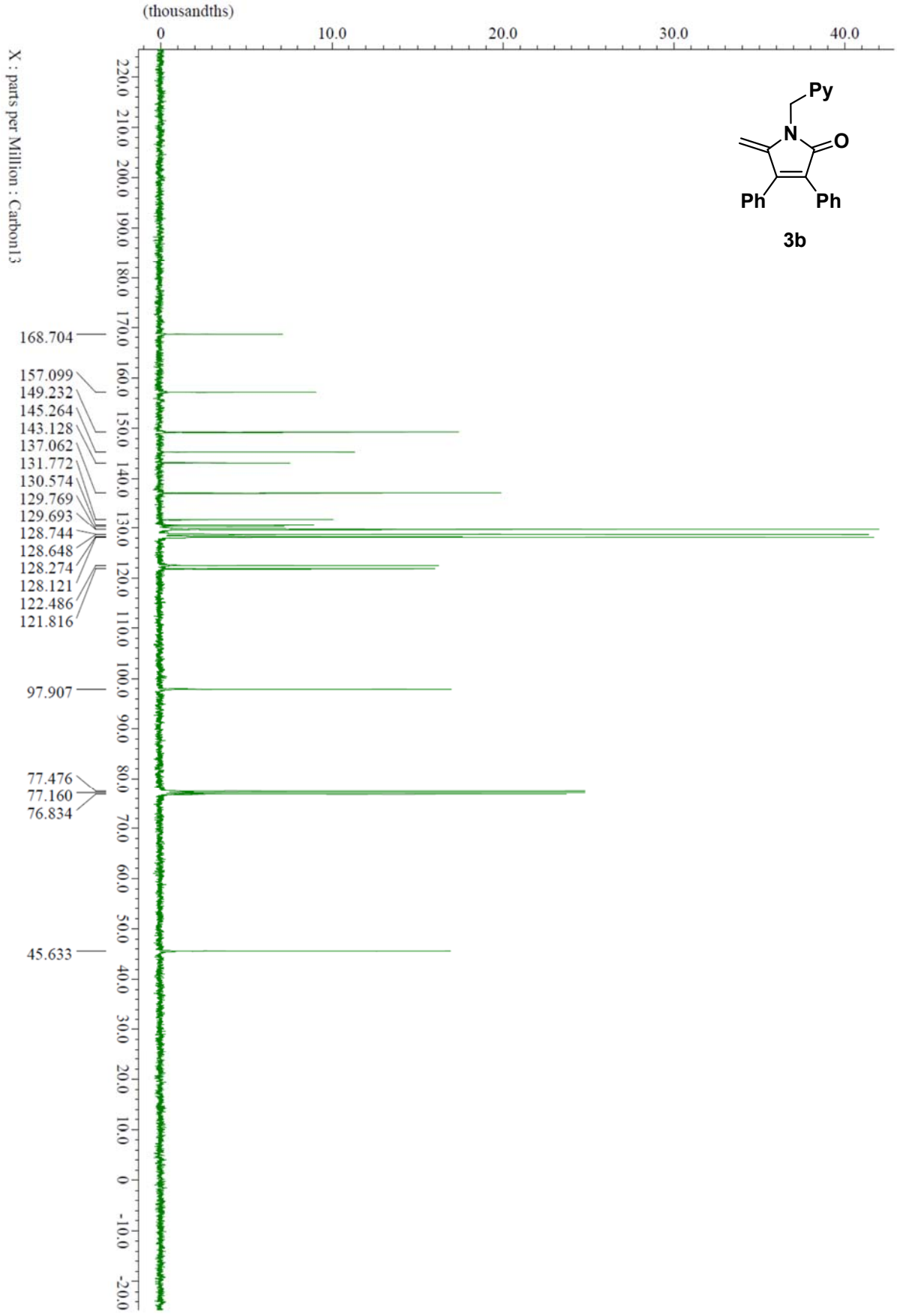
1.14
1.02
4.92
1.03
1.92
1.01
Py
N
O
Ph
Ph
3b


(thousandths)
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30.0
40.0
X : parts per Million : Carbon13
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200.0
190.0
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170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
168.704
157.099
149.232
145.264
143.128
137.062
131.772
130.574
129.769
129.693
128.744
128.648
128.274
128.121
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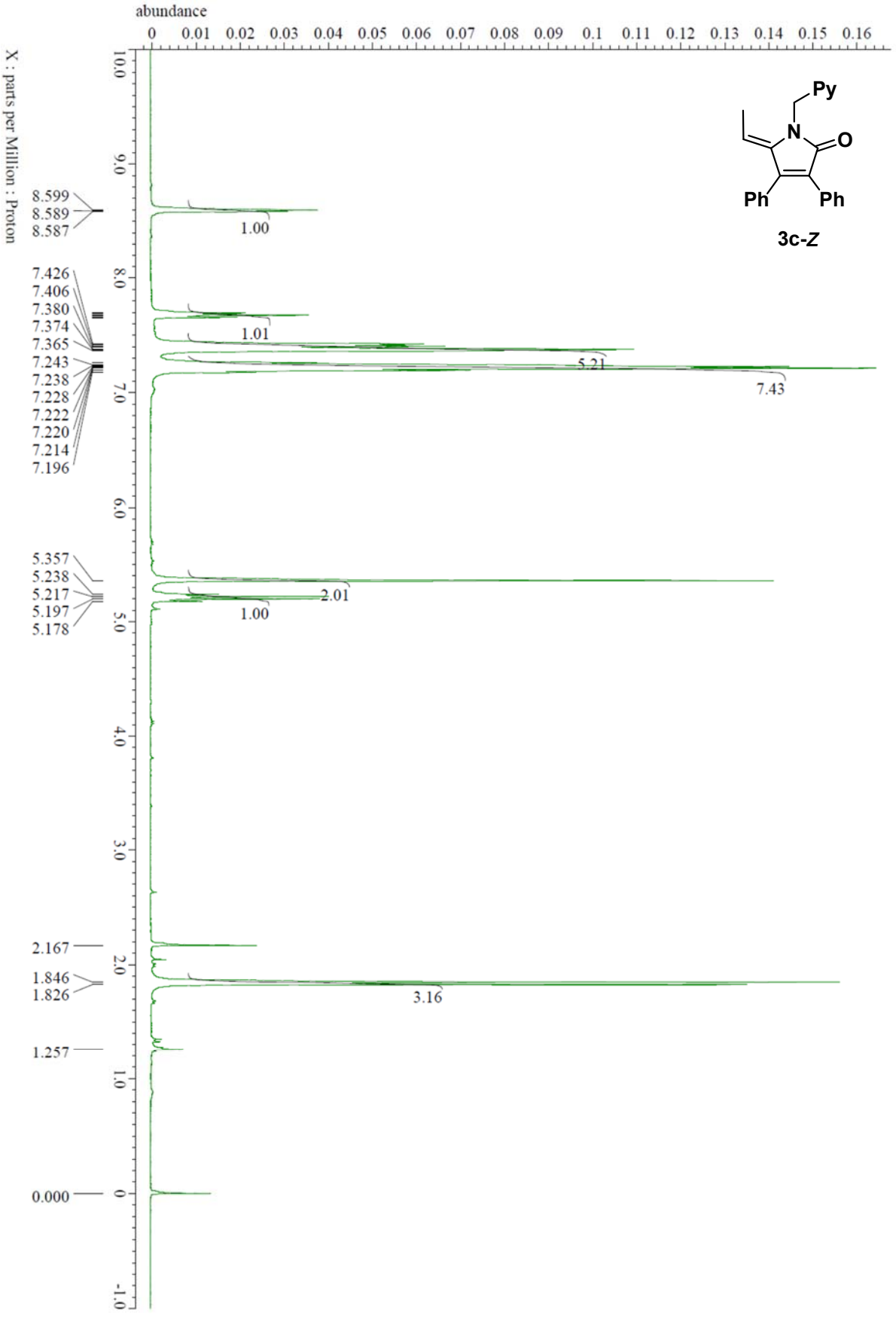
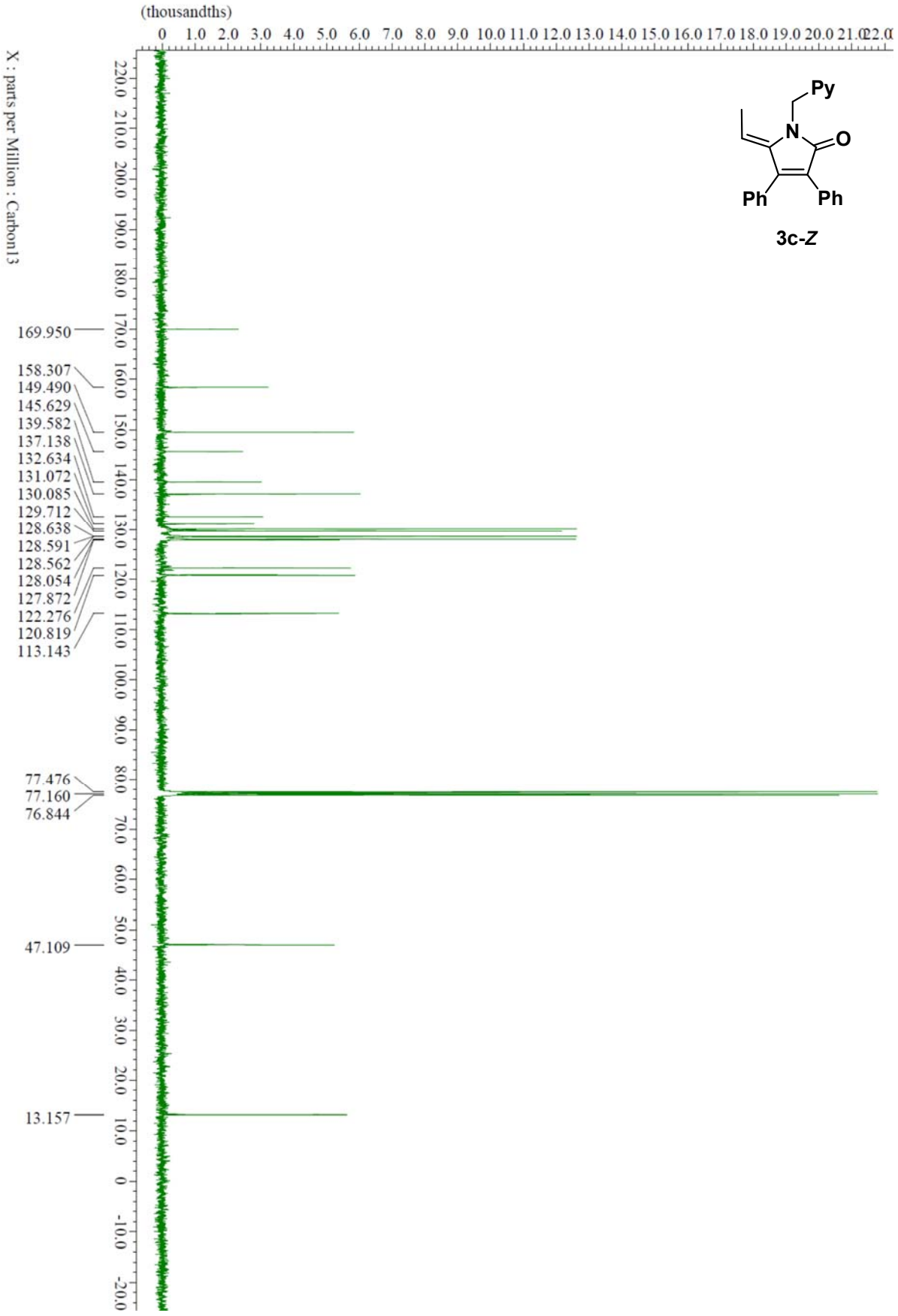
121.816
97.907
77.476
77.160
76.834
45.633
Py
N
O
Ph
Ph
3b


abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16
X : parts per Million : Proton
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0
8.599
8.589
8.587
7.426
7.406
7.380
7.374
7.365
7.243
7.238
7.228
7.222
7.220
7.214
7.196
5.357
5.238
5.217
5.197
5.178
2.167
1.846
1.826
1.257
0.000
1.00
1.01
5.21
7.43
2.01
1.00
3.16
Py
N
O
Ph
Ph
3c-Z


(thousandths)
X : parts per Million : Carbon13
Py
N
O
Ph
Ph
3c-Z
169.950
158.307
149.490
145.629
139.582
137.138
132.634
131.072
130.085
129.712
128.638
128.591
128.562
128.054
127.872
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120.819
113.143
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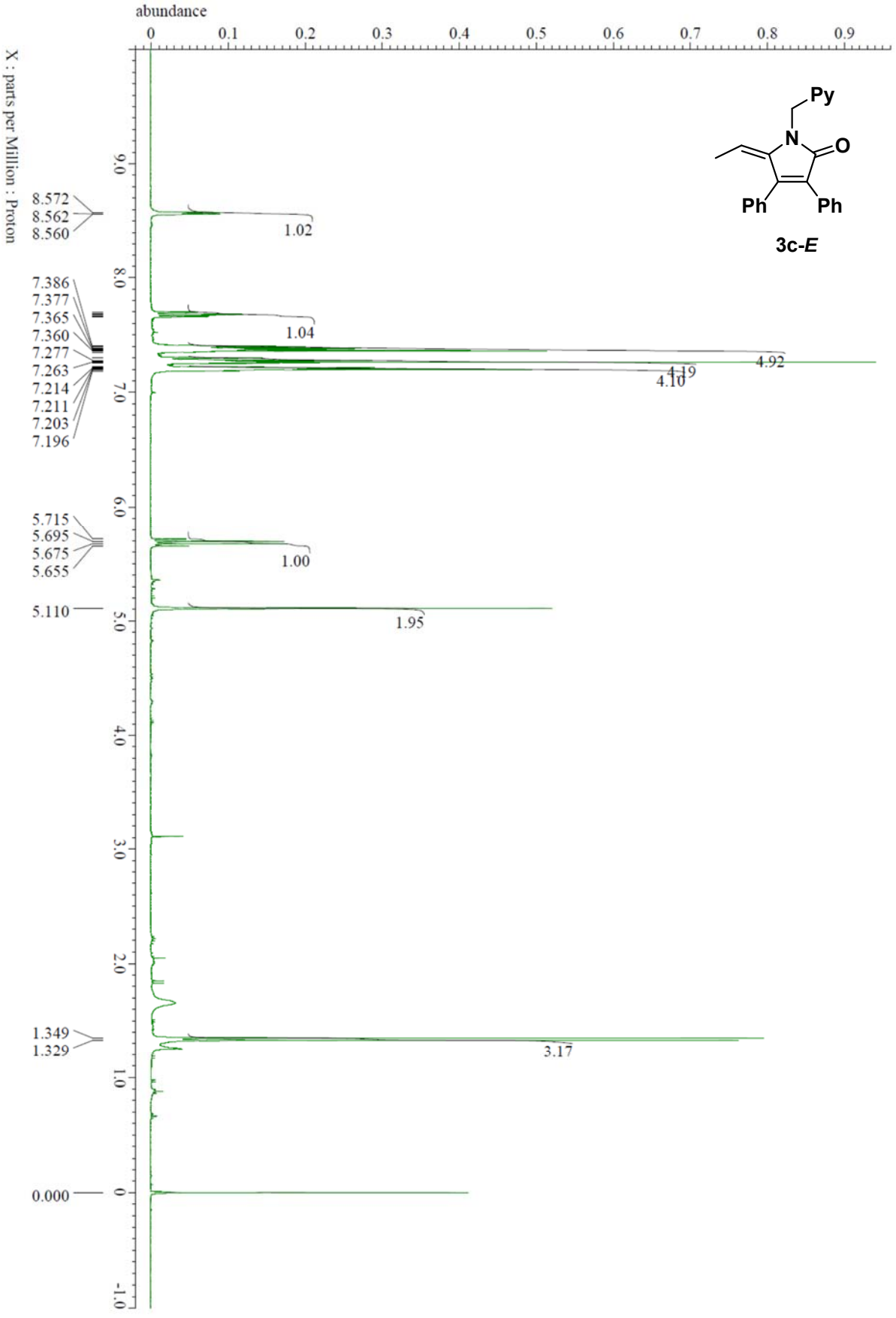
77.160
76.844
47.109
13.157


abundance
X : parts per Million : Proton
Py
N
O
Ph
Ph
3c-E
8.572
8.562
8.560
7.386
7.377
7.365
7.360
7.277
7.263
7.214
7.211
7.203
7.196
5.715
5.695
5.675
5.655
5.110
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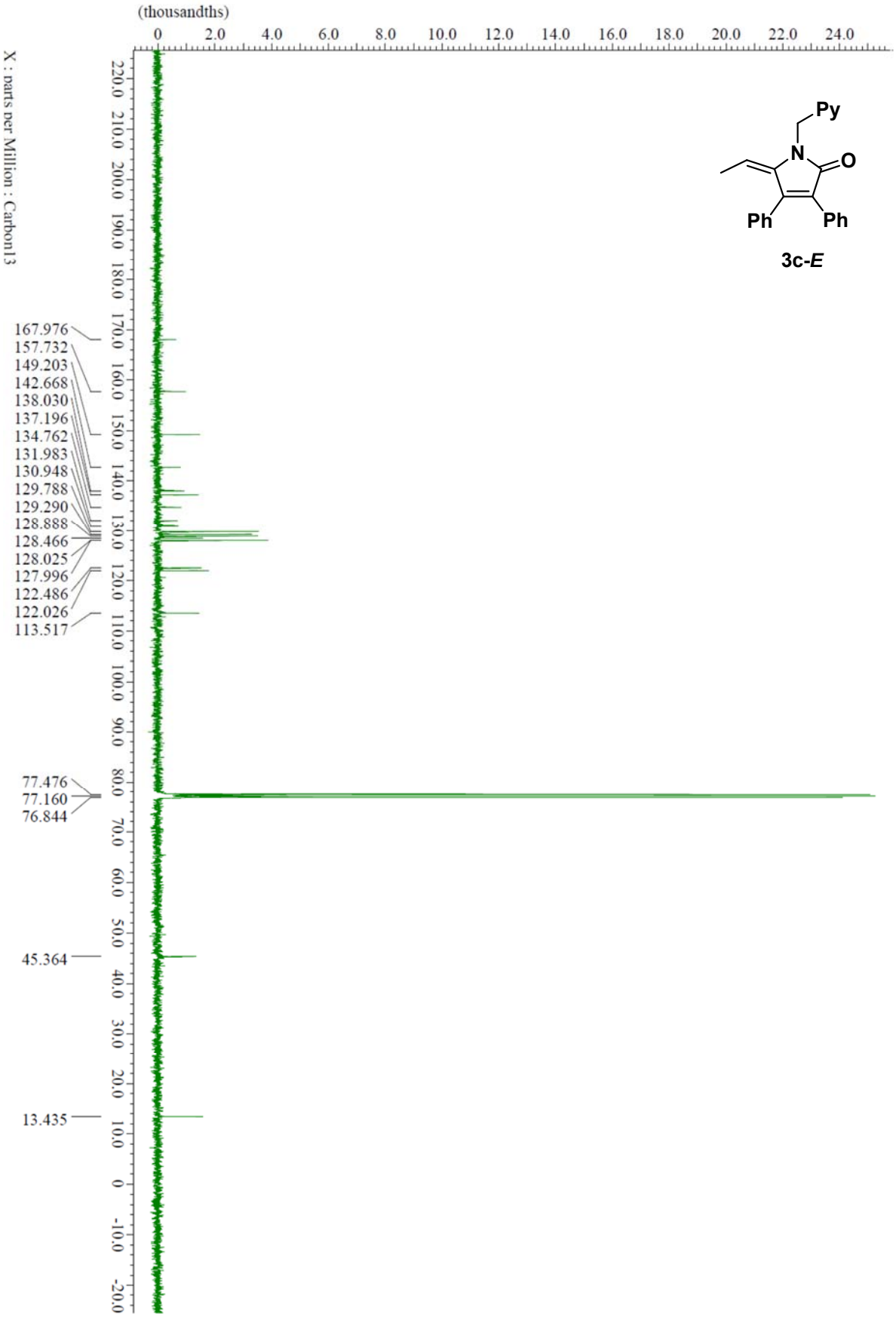
1.329
0.000
1.02
1.04
4.92
4.19
4.10
1.00
1.95
3.17


(thousandths)
0 2.0 4.0 6.0 8.0 10.0 12.0 14.0 16.0 18.0 20.0 22.0 24.0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
167.976
157.732
149.203
142.668
138.030
137.196
134.762
131.983
130.948
129.788
129.290
128.888
128.466
128.025
127.996
122.486
122.026
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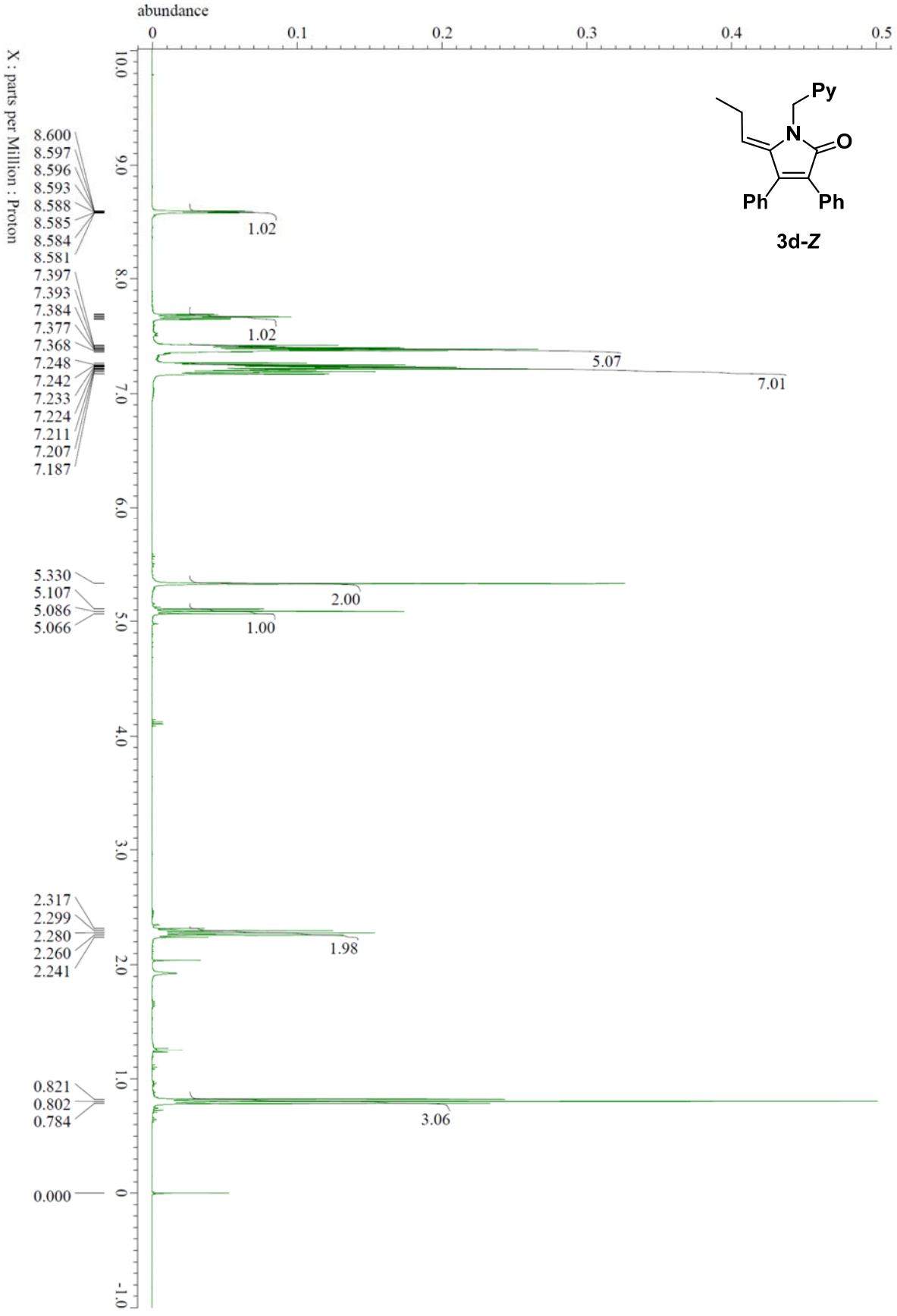
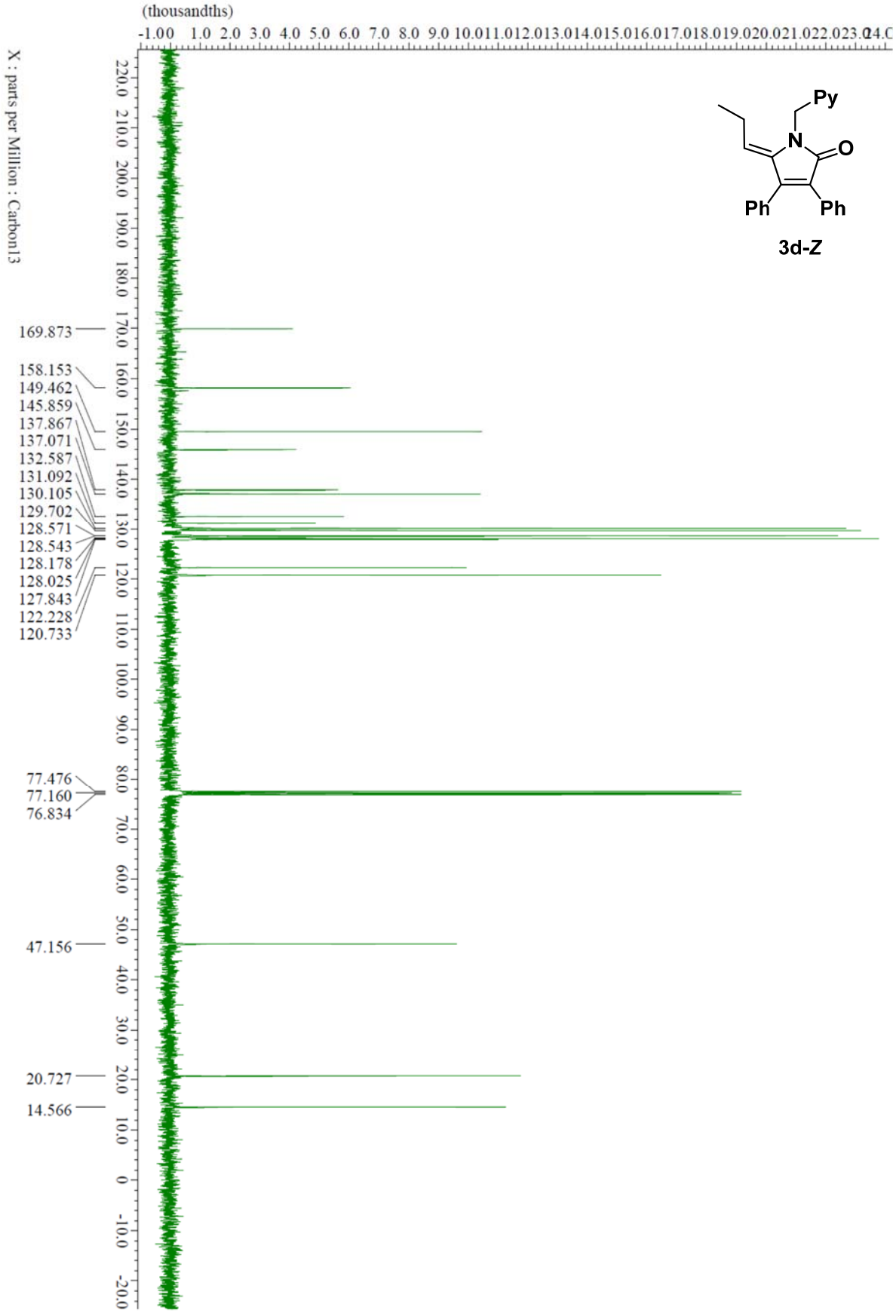
77.476
77.160
76.844
45.364
13.435
Py
N
O
Ph
Ph
3c-E


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
8.600
8.597
8.596
8.593
8.588
8.585
8.584
8.581
7.397
7.393
7.384
7.377
7.368
7.248
7.242
7.233
7.224
7.211
7.207
7.187
5.330
5.107
5.086
5.066
2.317
2.299
2.280
2.260
2.241
0.821
0.802
0.784
0.000
1.02
1.02
5.07
7.01
2.00
1.00
1.98
3.06
Py
N
O
Ph
Ph
3d-Z


(thousandths)
X : parts per Million : Carbon13
Py
N
O
Ph
Ph
3d-Z
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145.859
137.867
137.071
132.587
131.092
130.105
129.702
128.571
128.543
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128.025
127.843
122.228
120.733
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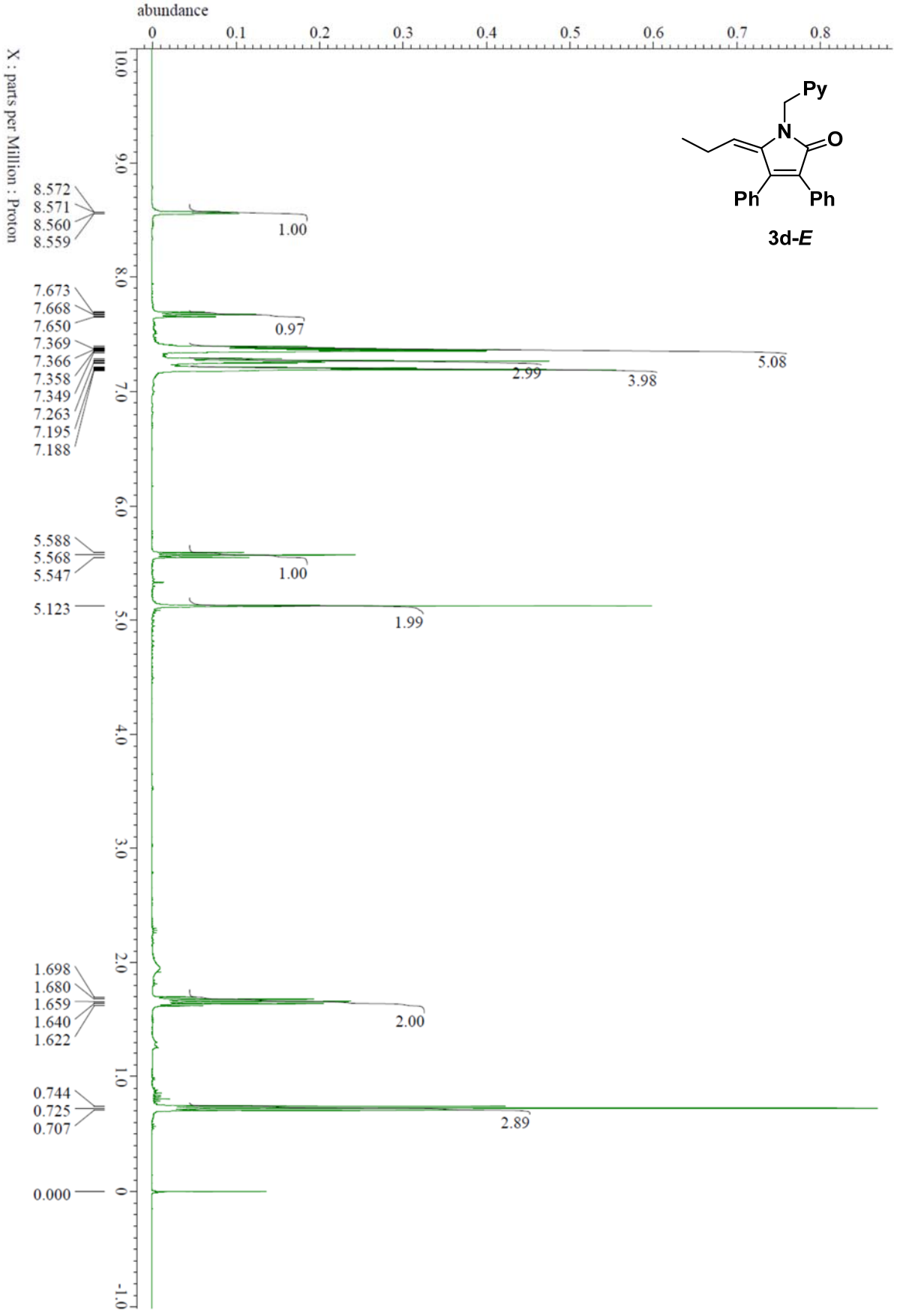
77.160
76.834
47.156
20.727
14.566


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
8.572
8.571
8.560
8.559
1.00
7.673
7.668
7.650
7.369
7.366
7.358
7.349
7.263
7.195
7.188
0.97
2.99
3.98
5.08
5.588
5.568
5.547
1.00
5.123
1.99
1.698
1.680
1.659
1.640
1.622
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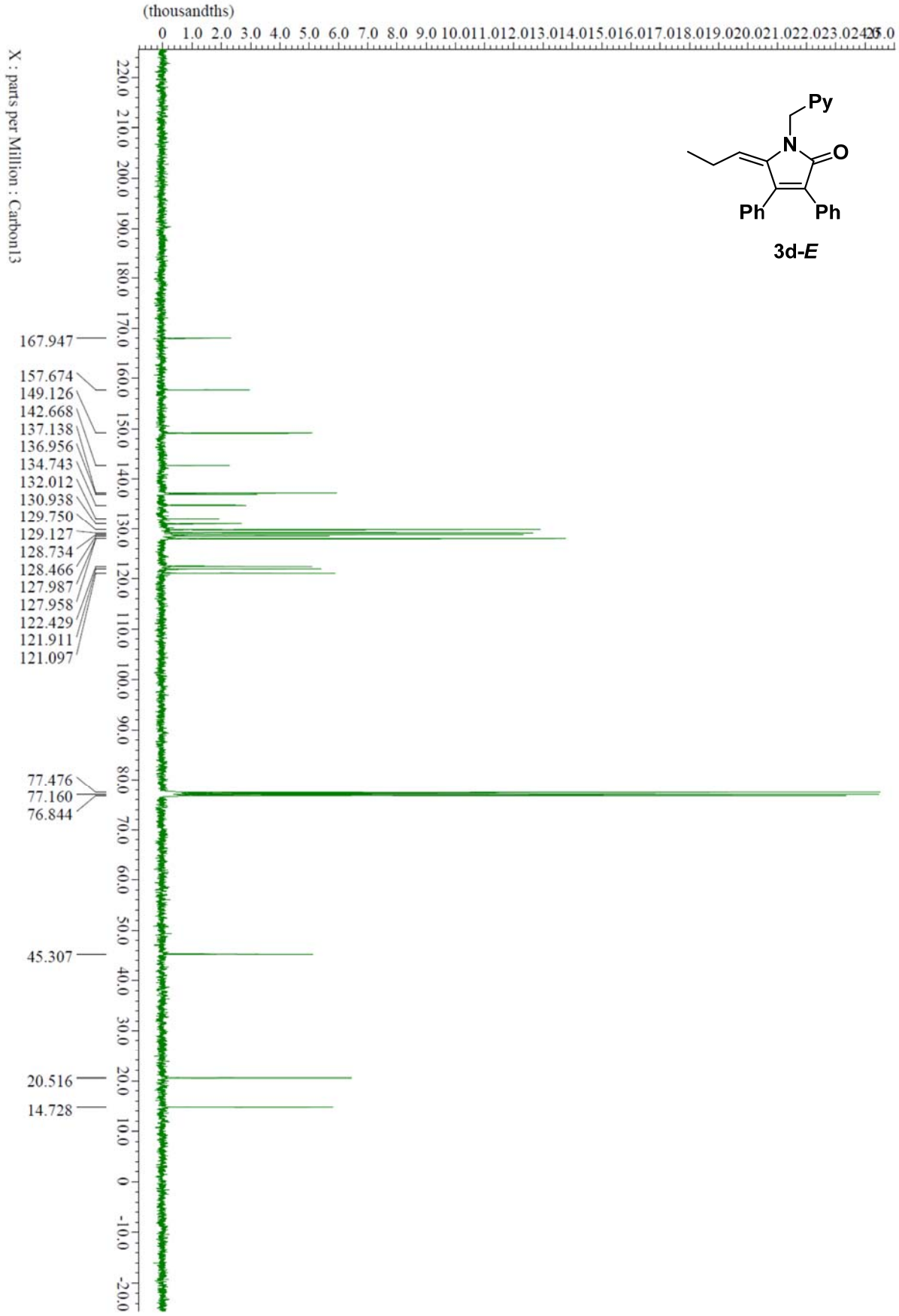
0.744
0.725
0.707
2.89
0.000
Py
N
O
Ph
Ph
3d-E


(thousandths)
X : parts per Million : Carbon13
Py
N
O
Ph
Ph
3d-E
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149.126
142.668
137.138
136.956
134.743
132.012
130.938
129.750
129.127
128.734
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127.987
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122.429
121.911
121.097
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77.160
76.844
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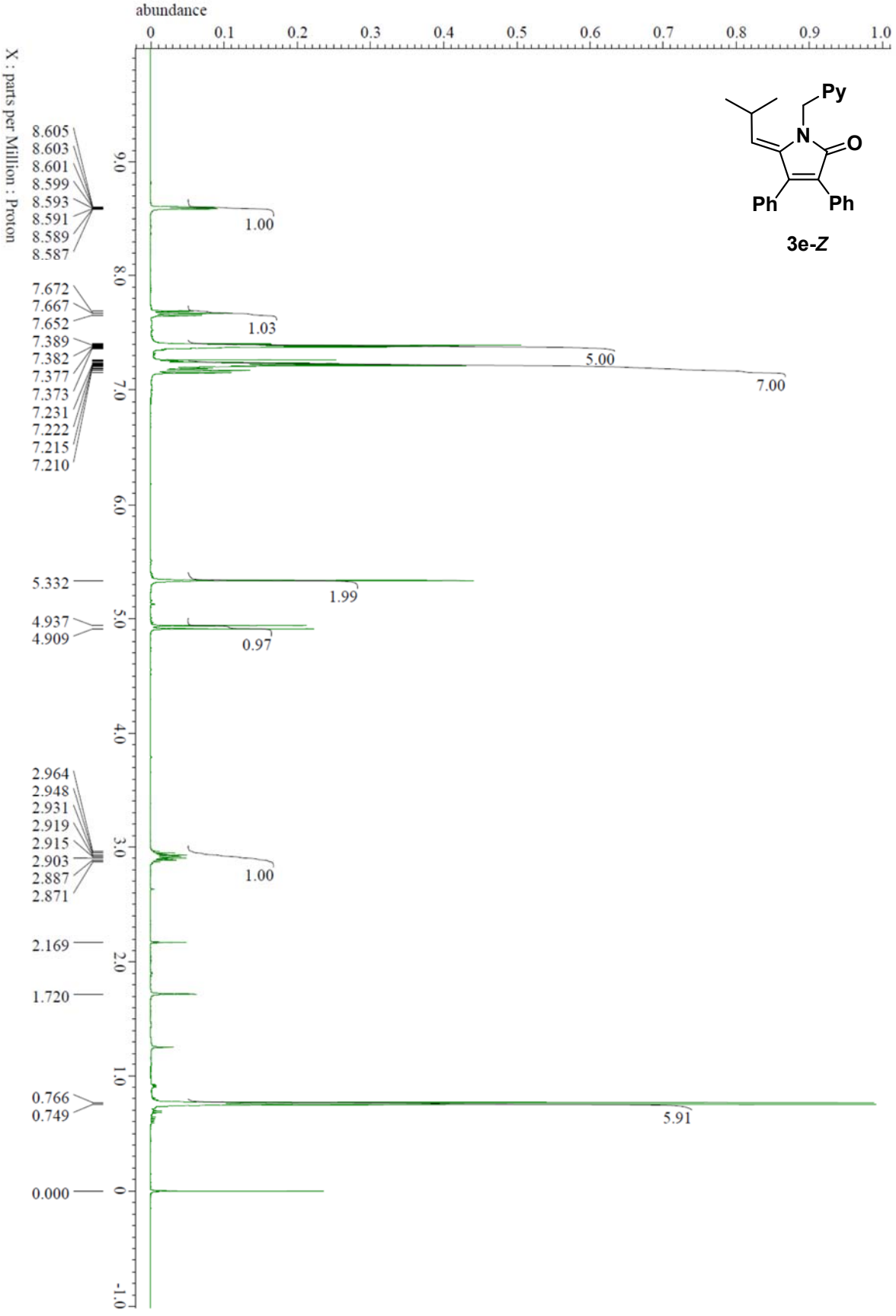
20.516
14.728


abundance
X : parts per Million : Proton
Py
N
O
Ph
Ph
3e-Z
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8.601
8.599
8.593
8.591
8.589
8.587
7.672
7.667
7.652
7.389
7.382
7.377
7.373
7.231
7.222
7.215
7.210
5.332
4.937
4.909
2.964
2.948
2.931
2.919
2.915
2.903
2.887
2.871
2.169
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0.000
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1.03
5.00
7.00
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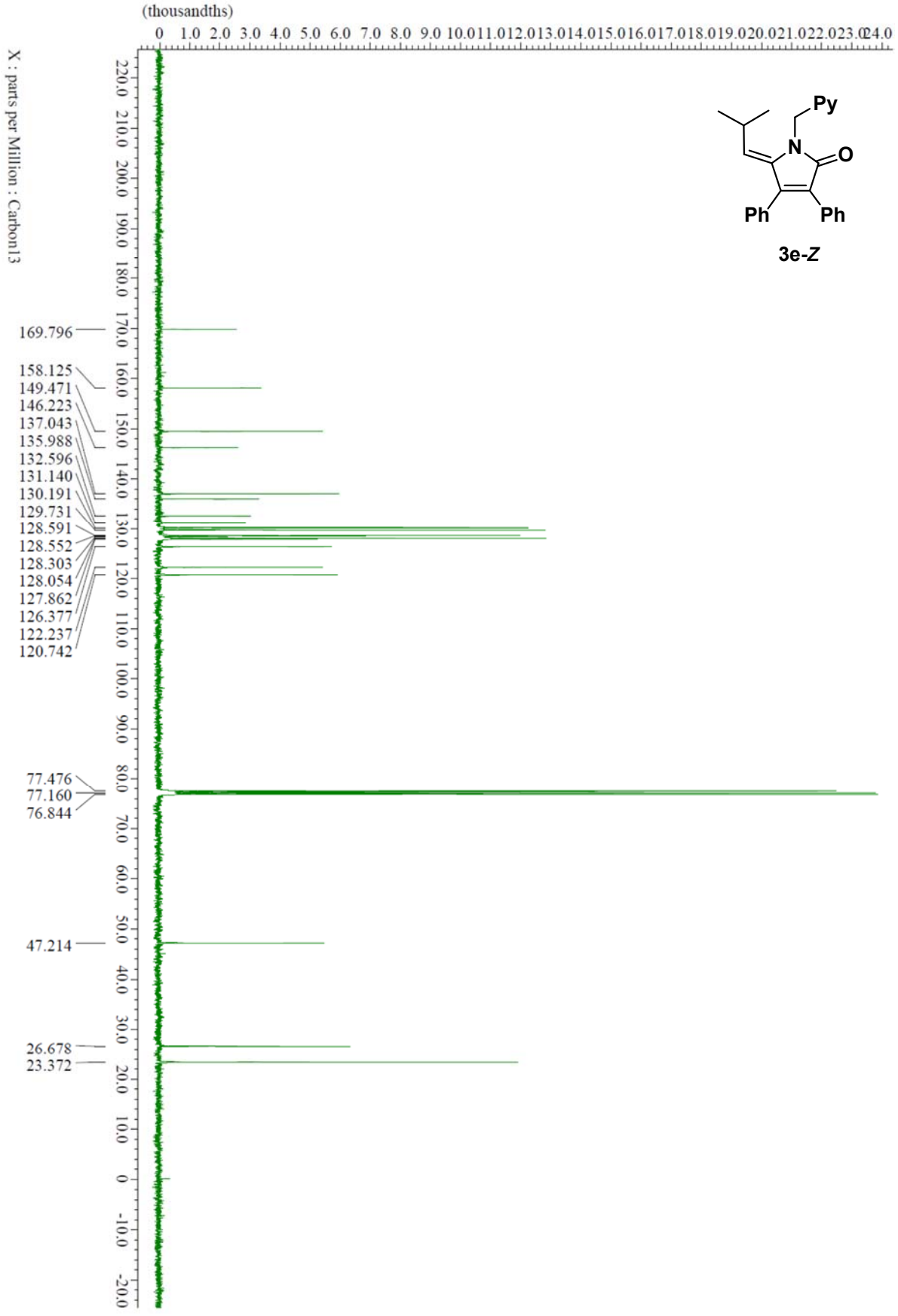
0.97
1.00
5.91


(thousandths)
X : parts per Million : Carbon13
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131.140
130.191
129.731
128.591
128.552
128.303
128.054
127.862
126.377
122.237
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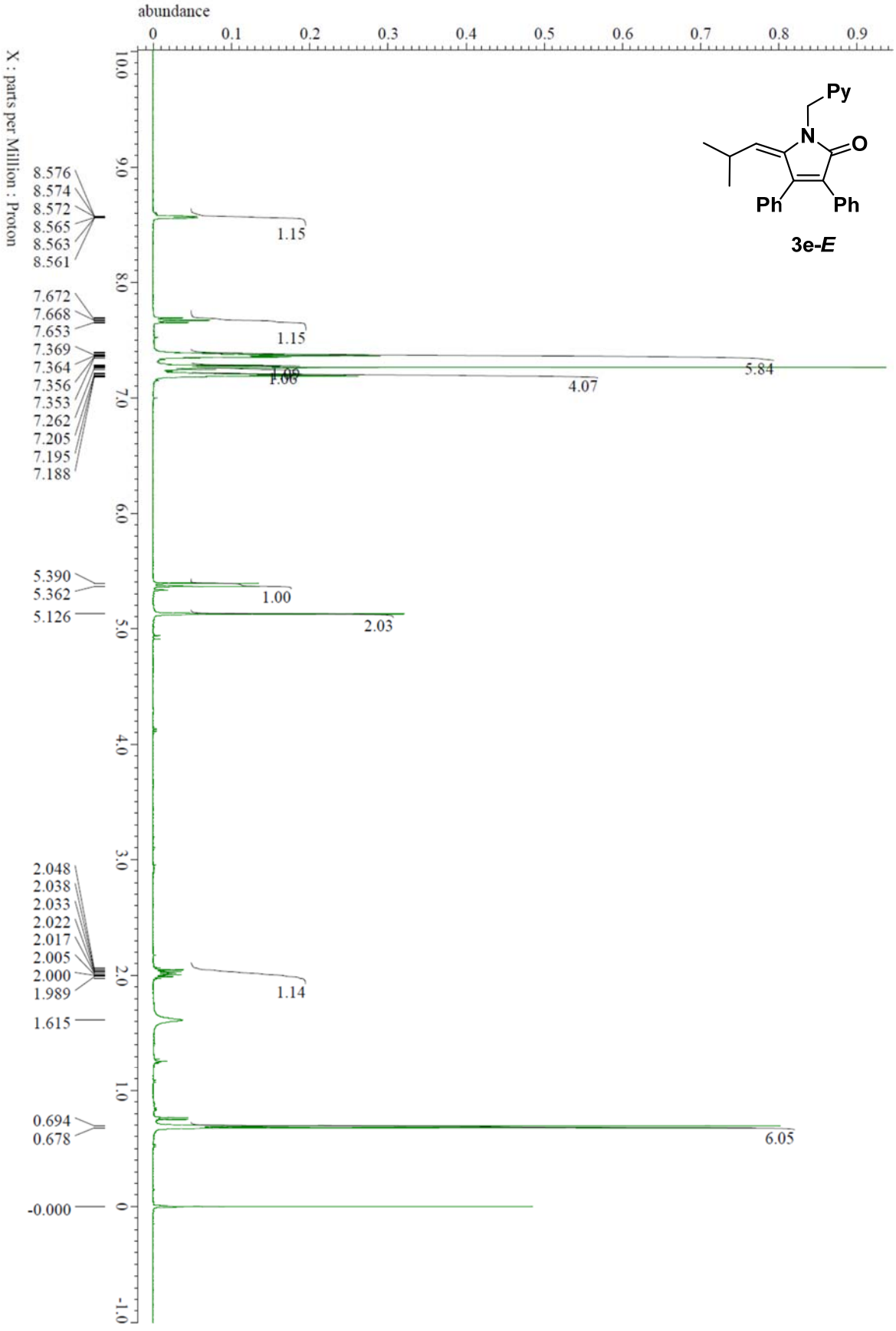
77.476
77.160
76.844
47.214
26.678
23.372
Py
N
O
Ph
Ph

3e-*Z*


abundance
X : parts per Million : Proton
Py
N
O
Ph
Ph
3e-E
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8.565
8.563
8.561
7.672
7.668
7.653
7.369
7.364
7.356
7.353
7.262
7.205
7.195
7.188
5.390
5.362
5.126
2.048
2.038
2.033
2.022
2.017
2.005
2.000
1.989
1.615
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0.678
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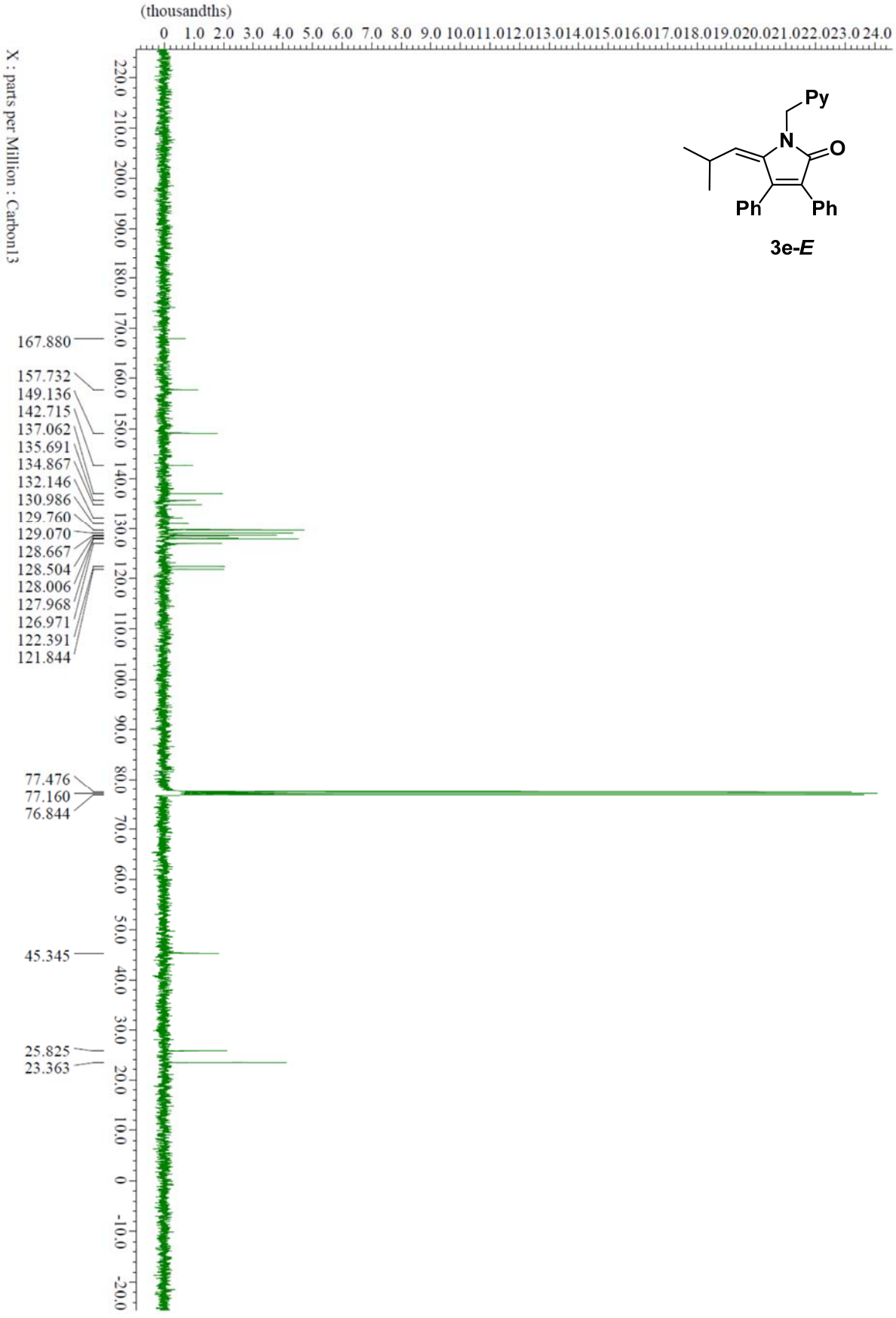
1.15
1.06
4.07
5.84
1.00
2.03
1.14
6.05


(thousandths)
X : parts per Million : Carbon13
Py
N
O
Ph
Ph
3e-E
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137.062
135.691
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128.667
128.504
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126.971
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121.844
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76.844
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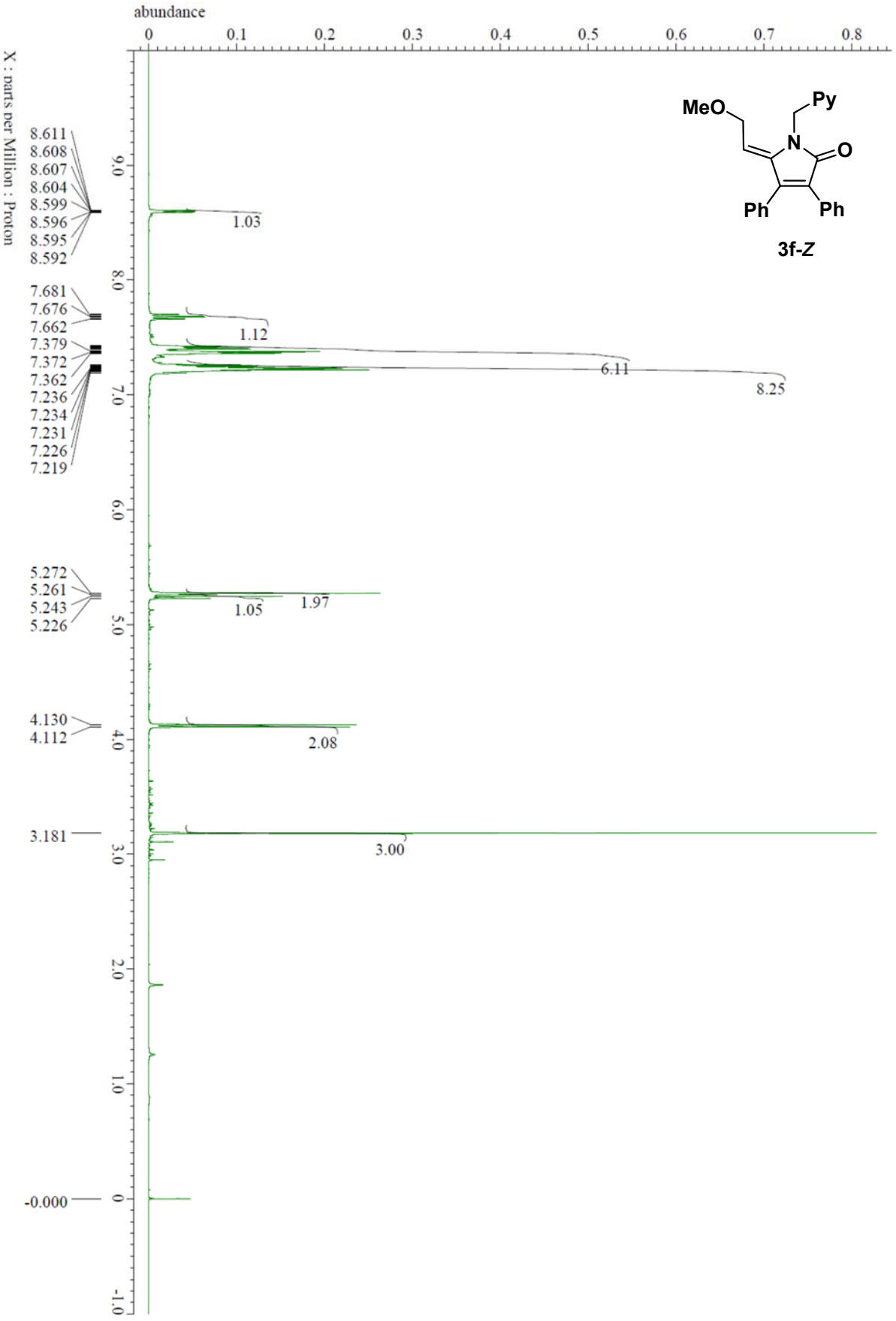
23.363


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : Proton
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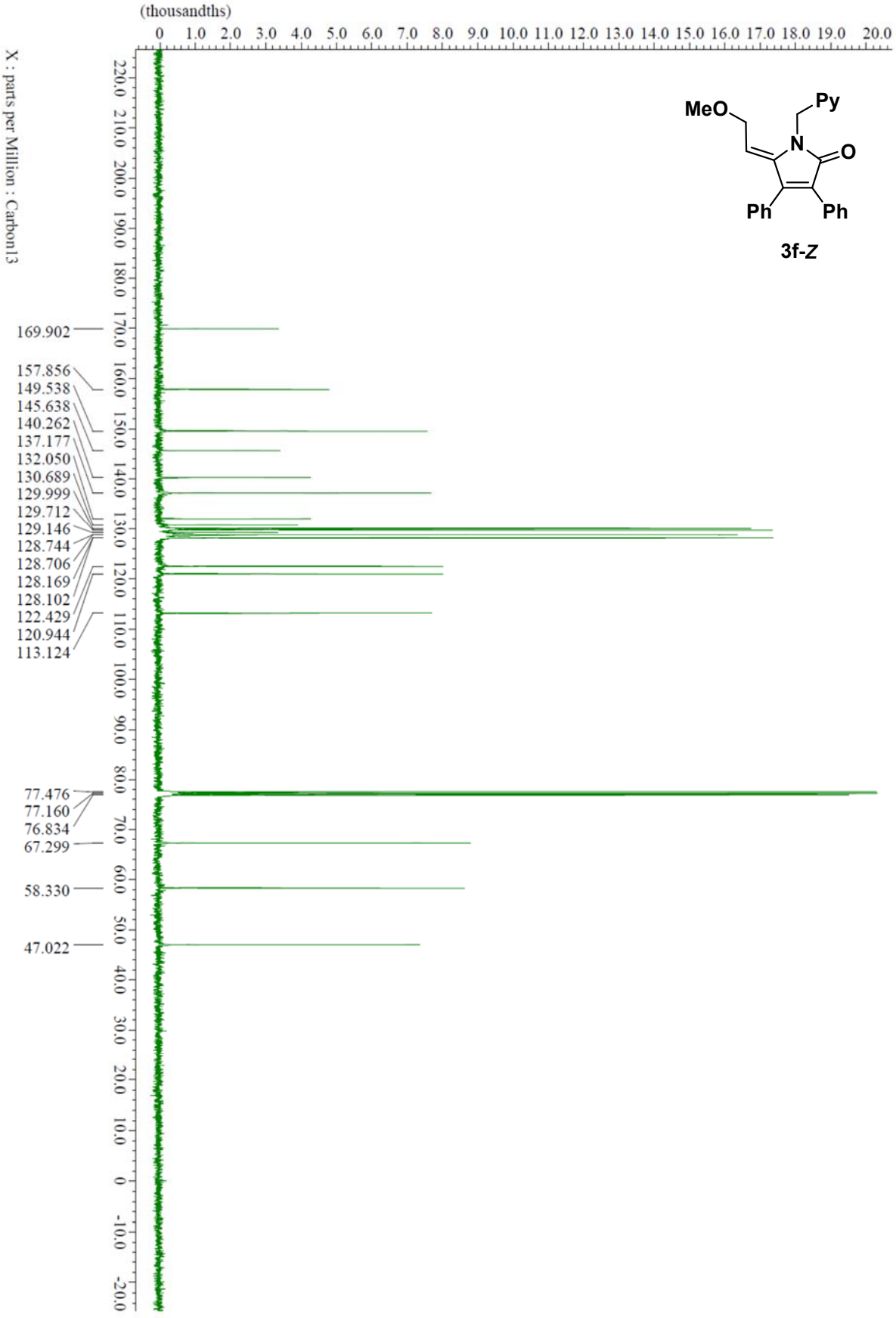
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
8.611
8.608
8.607
8.604
8.599
8.596
8.595
8.592
7.681
7.676
7.662
7.379
7.372
7.362
7.236
7.234
7.231
7.226
7.219
5.272
5.261
5.243
5.226
4.130
4.112
3.181
-0.000
1.03
1.12
6.11
8.25
1.05
1.97
2.08
3.00
MeO
Py
N
O
Ph
Ph
3f-Z


(thousandths)
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MeO
Py
N
O
Ph
Ph
3f-Z
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140.262
137.177
132.050
130.689
129.999
129.712
129.146
128.744
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113.124
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77.160
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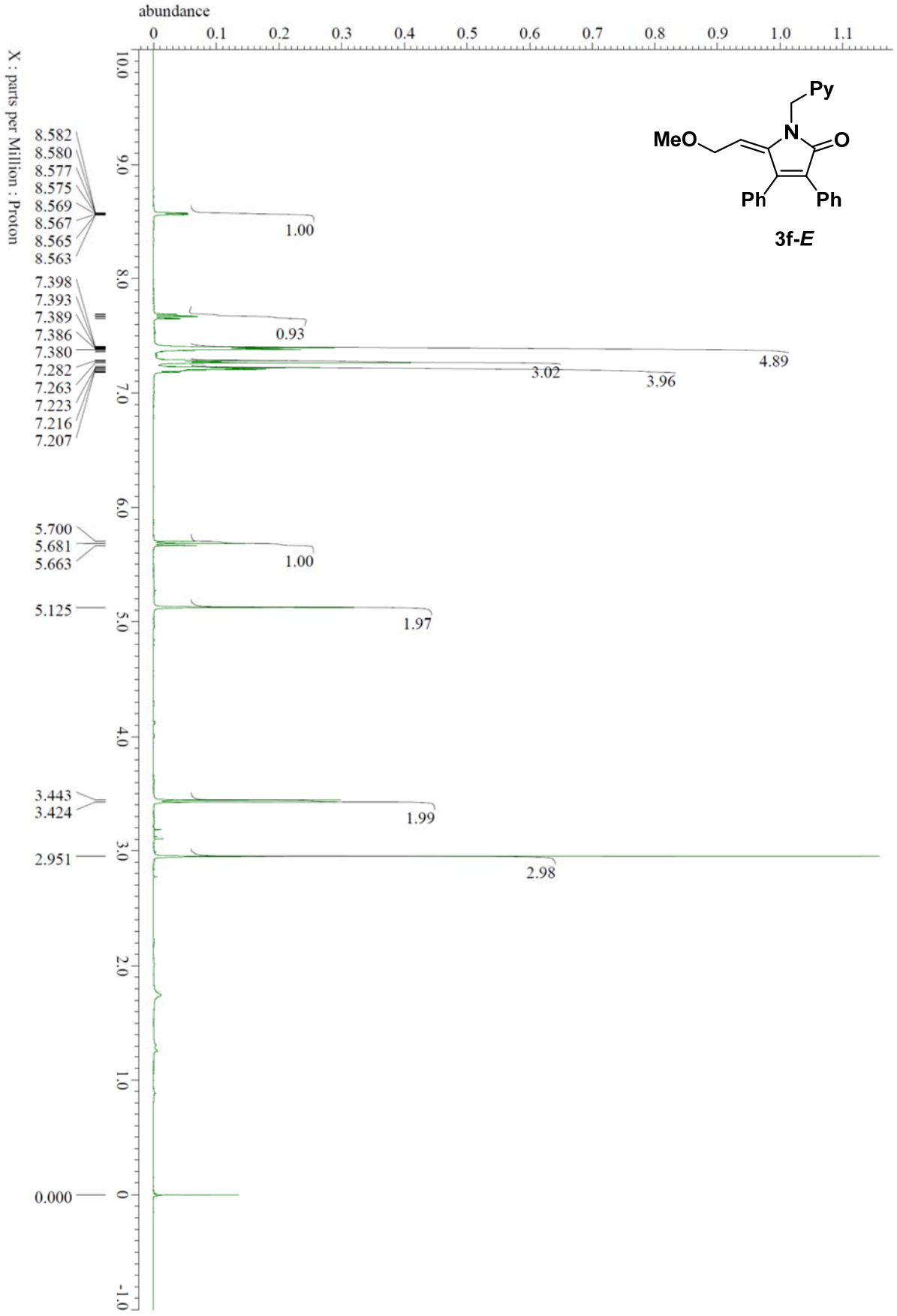
67.299
58.330
47.022


abundance
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0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
8.582
8.580
8.577
8.575
8.569
8.567
8.565
8.563
7.398
7.393
7.389
7.386
7.380
7.282
7.263
7.223
7.216
7.207
5.700
5.681
5.663
5.125
3.443
3.424
2.951
0.000
1.00
0.93
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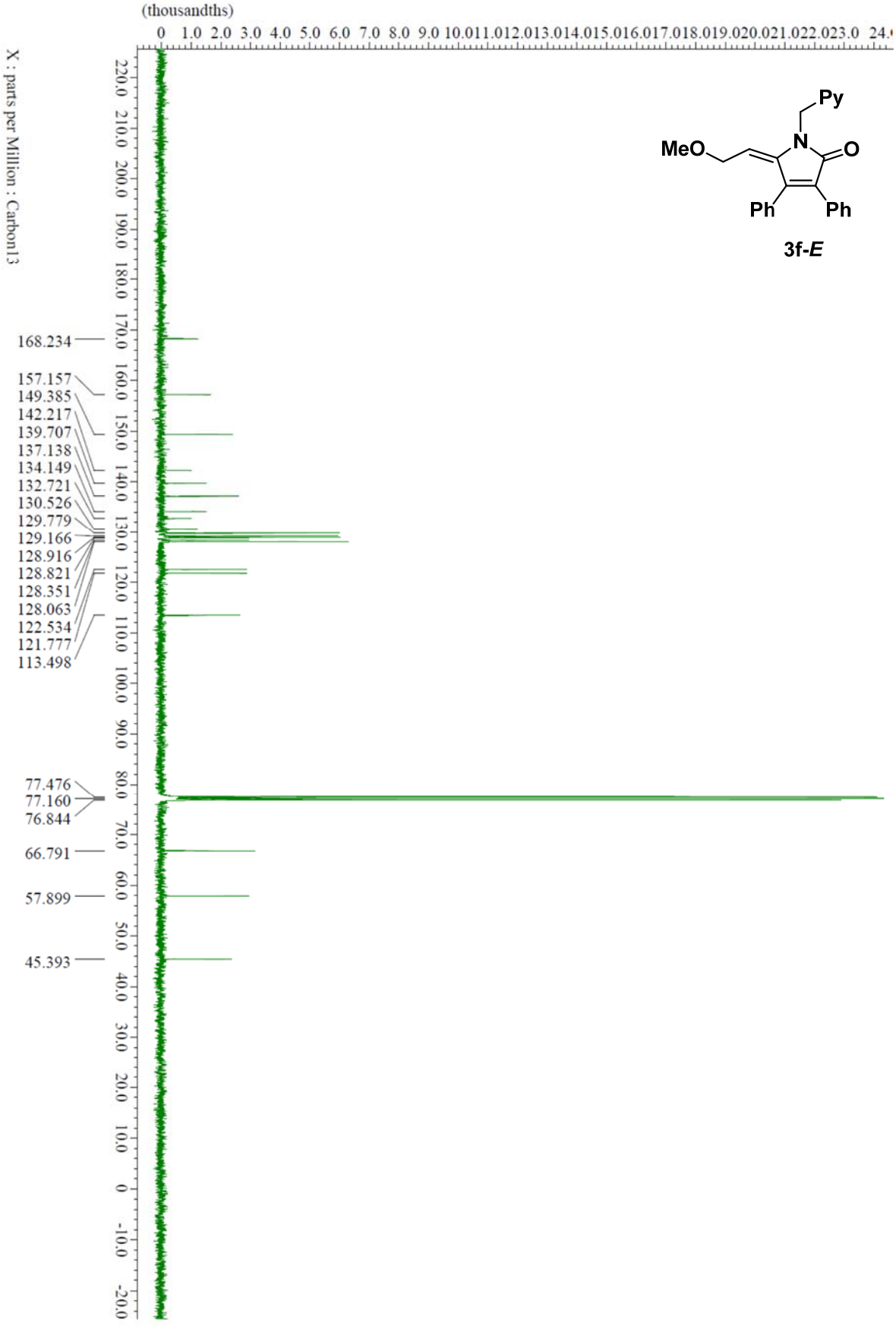
1.00
1.97
1.99
2.98
Py
N
O
MeO
Ph
Ph
3f-E


(thousandths)
X : parts per Million : Carbon13
Py
N
O
MeO
Ph
Ph
3f-E
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139.707
137.138
134.149
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129.779
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128.916
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121.777
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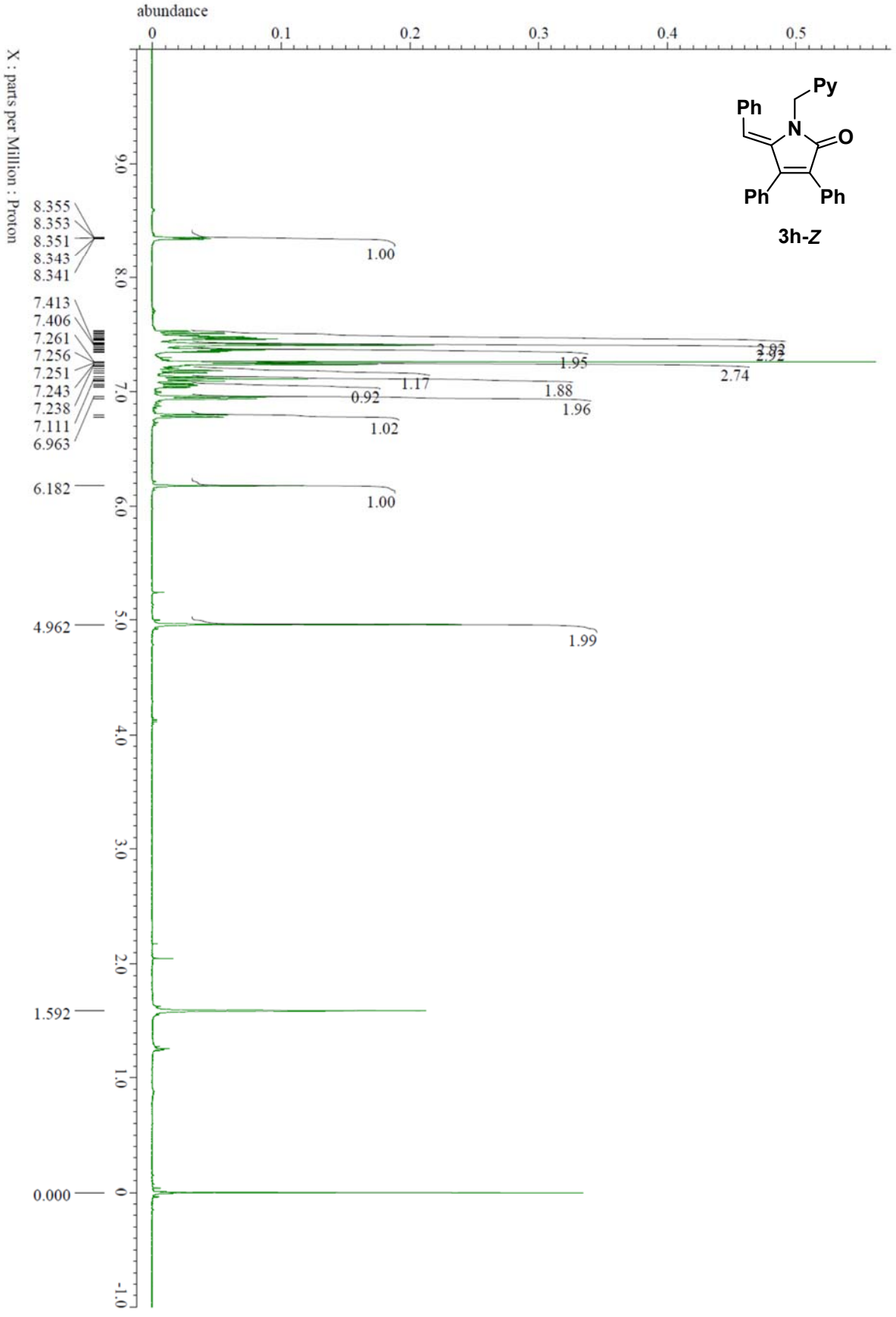
45.393


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : Proton
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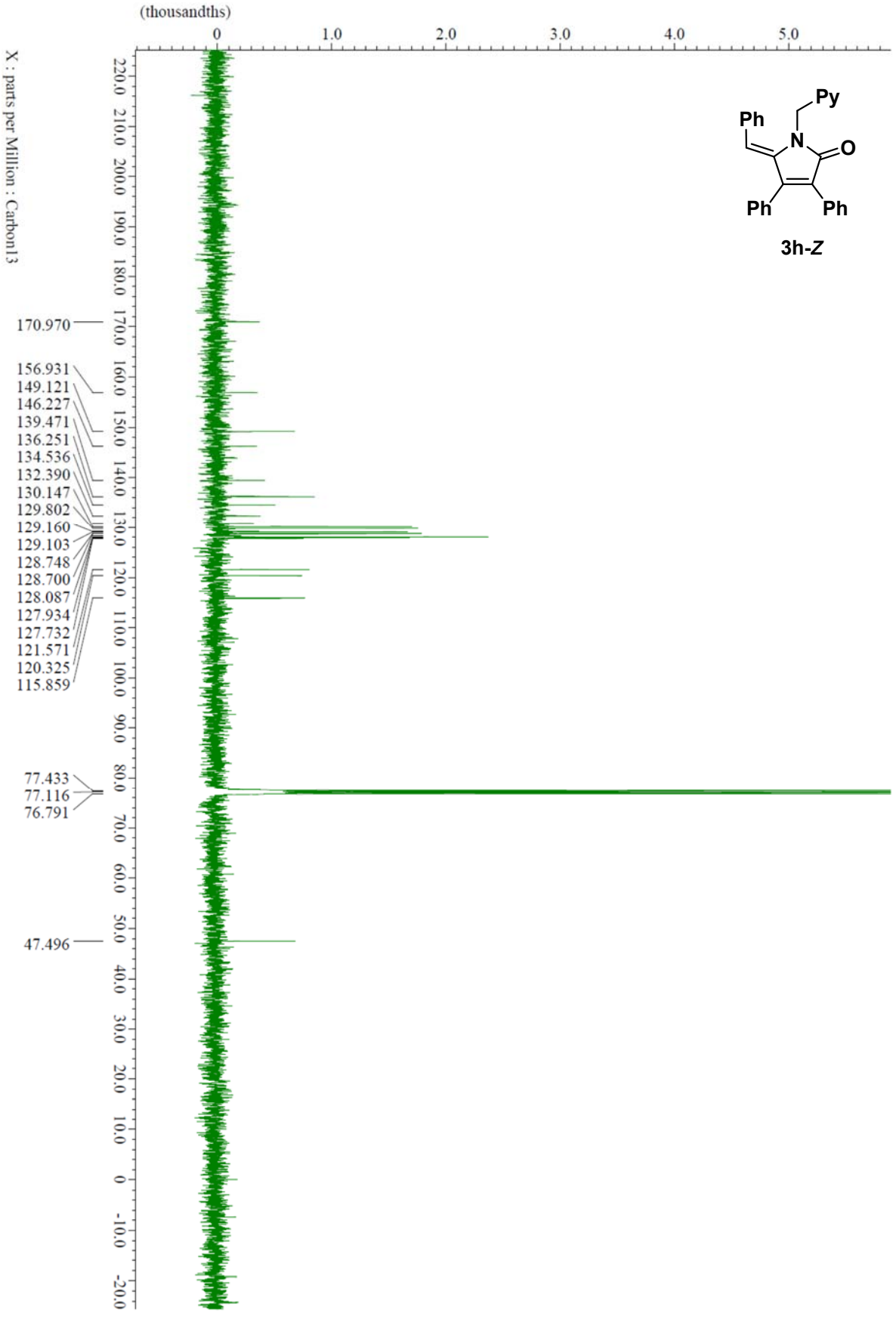
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
8.355
8.353
8.351
8.343
8.341
7.413
7.406
7.261
7.256
7.251
7.243
7.238
7.111
6.963
6.182
4.962
1.592
0.000
1.00
1.95
2.74
1.17
0.92
1.88
1.96
1.02
1.00
1.99
Py
Ph
N
O
Ph
Ph
3h-Z


(thousandths)
0
1.0
2.0
3.0
4.0
5.0
X : parts per Million : Carbon13
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210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
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80.0
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10.0
0
-10.0
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170.970
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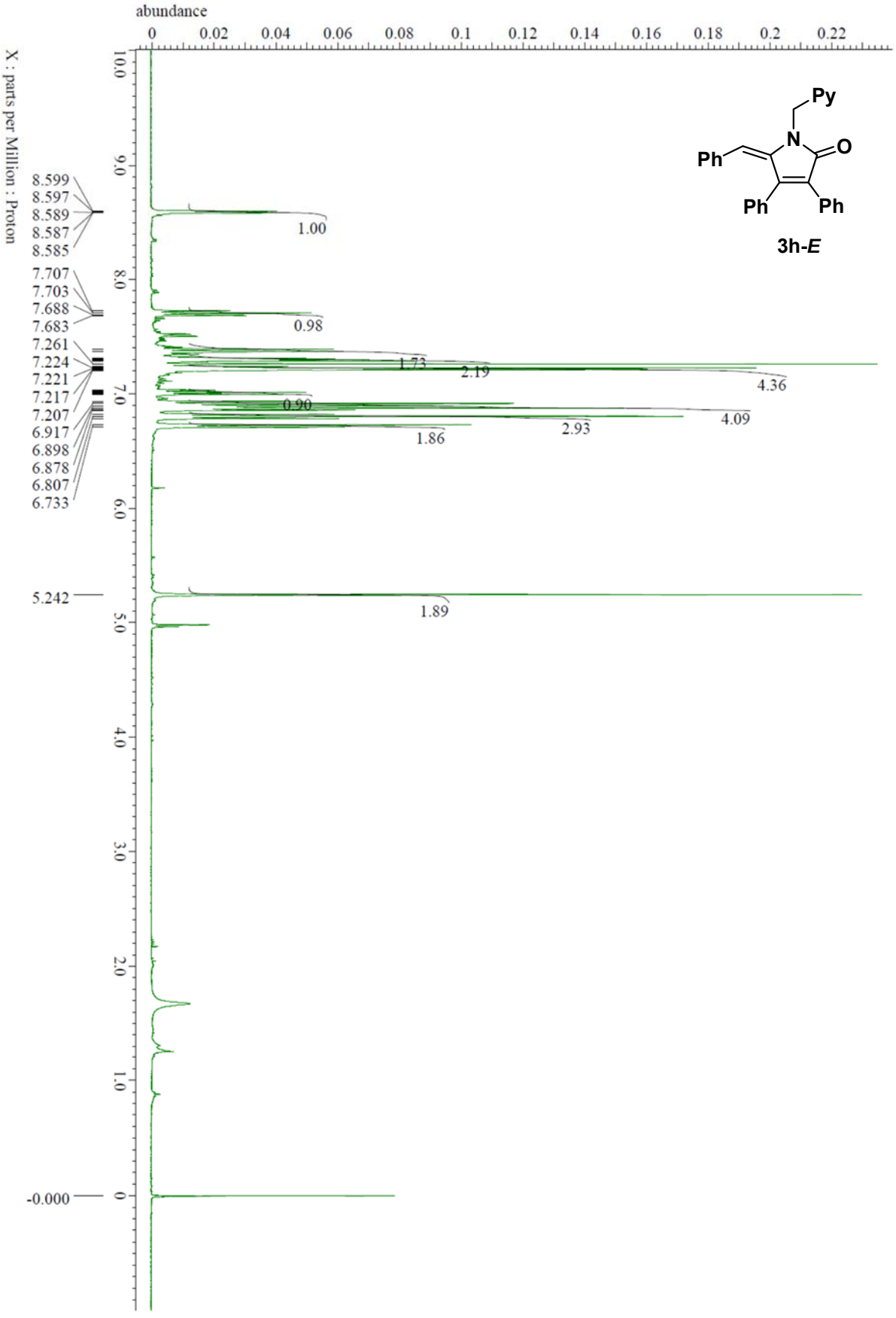
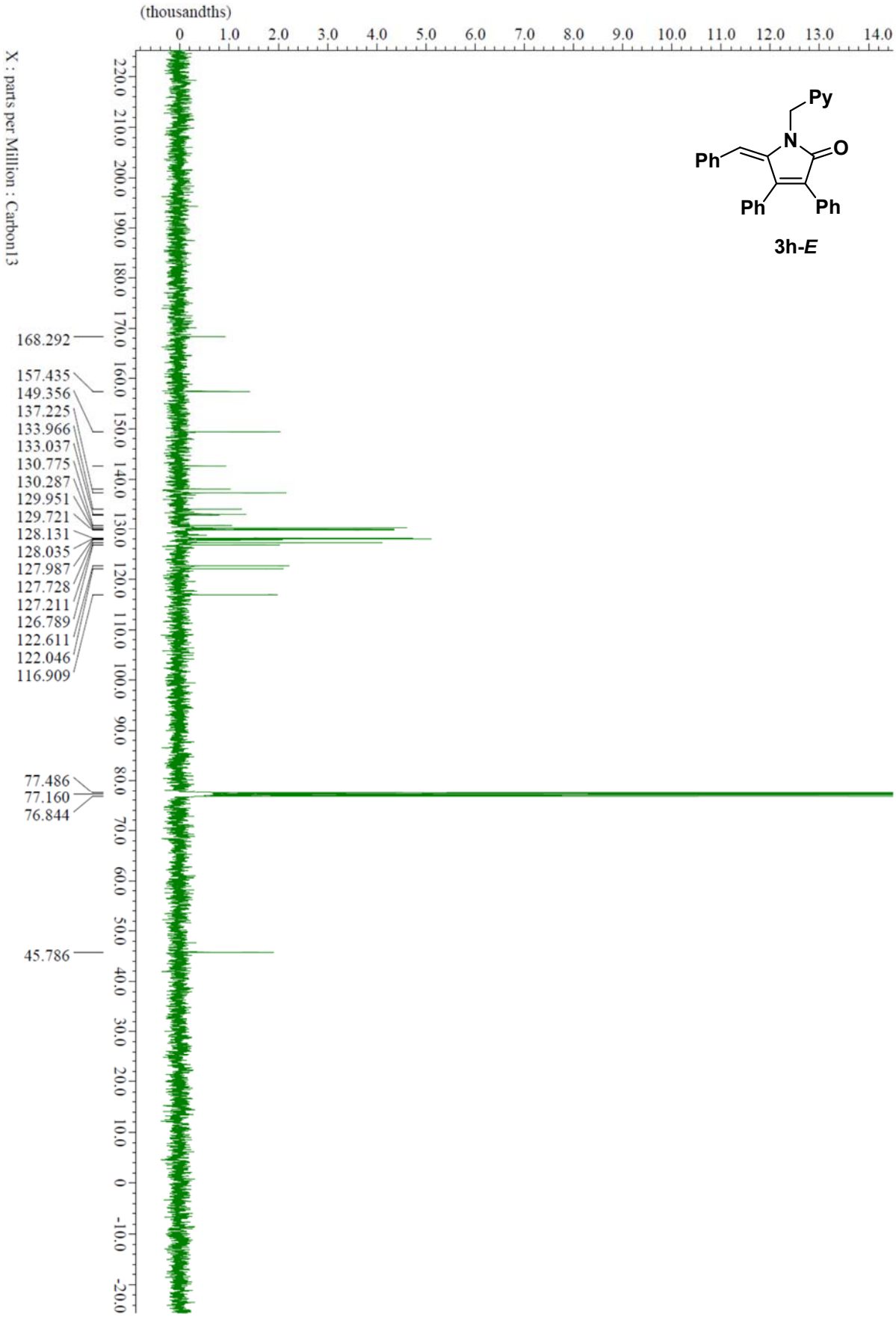
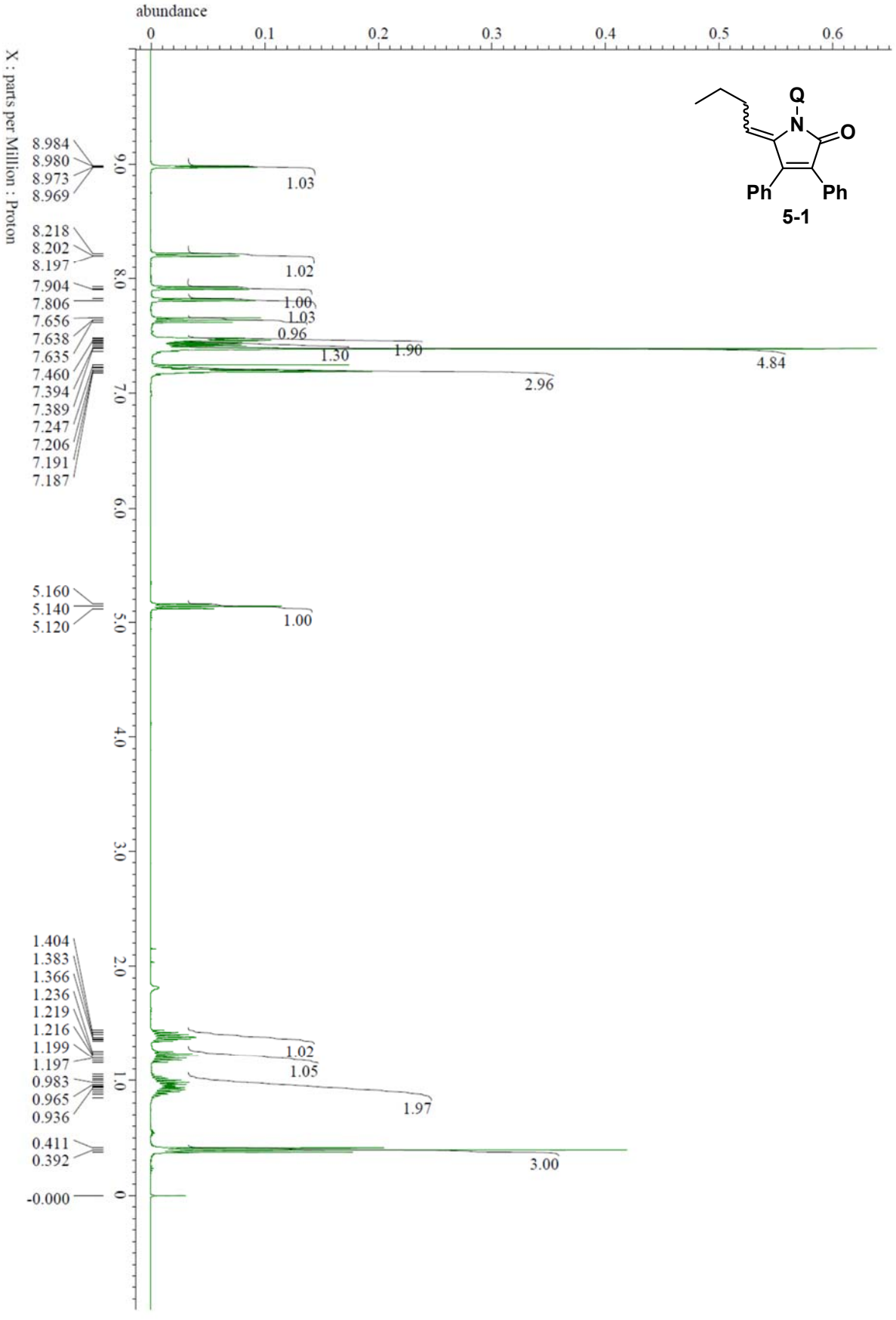
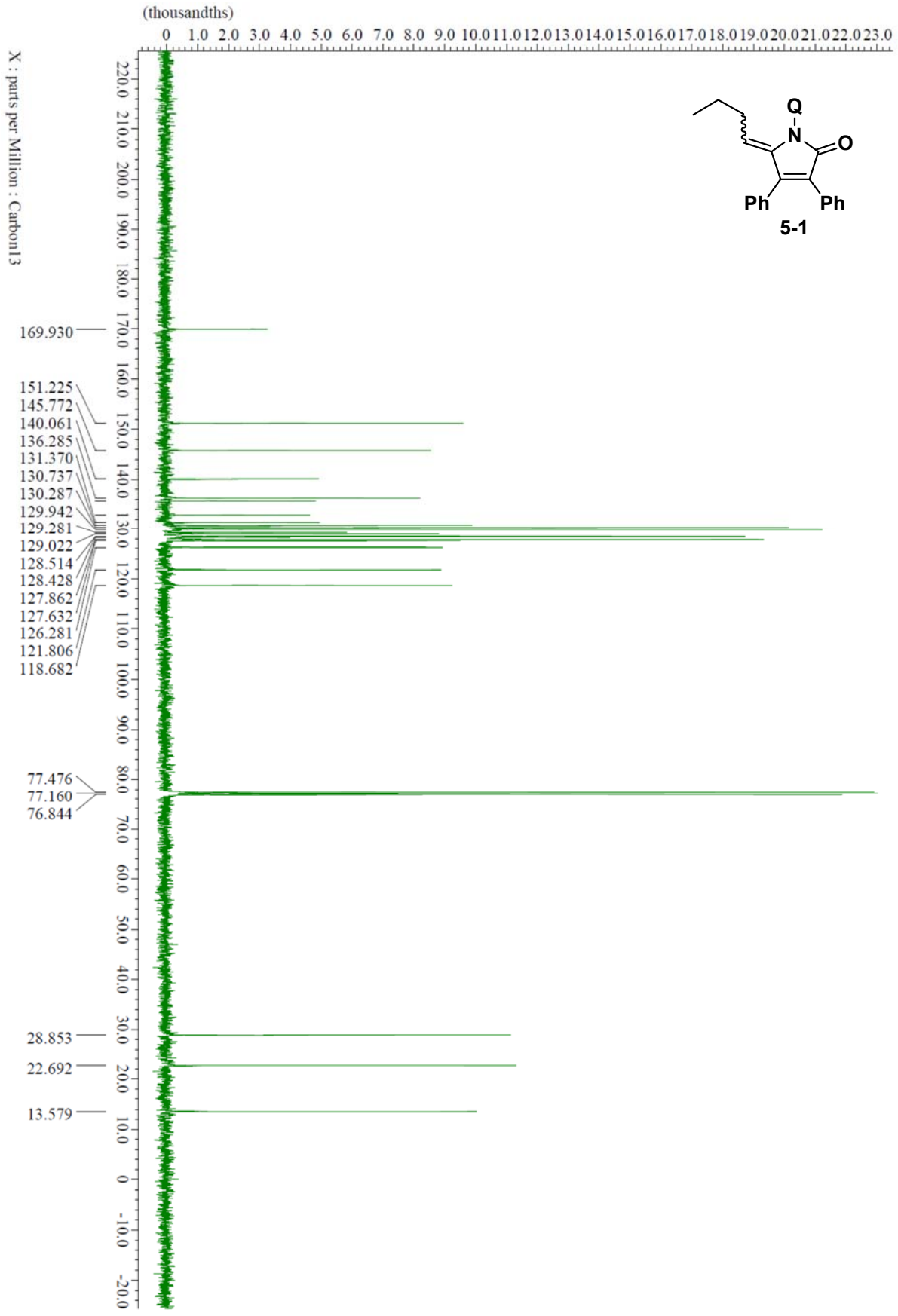
128.748
128.700
128.087
127.934
127.732
121.571
120.325
115.859
77.433
77.116
76.791
47.496
Py
Ph
N
O
Ph
Ph
3h-Z

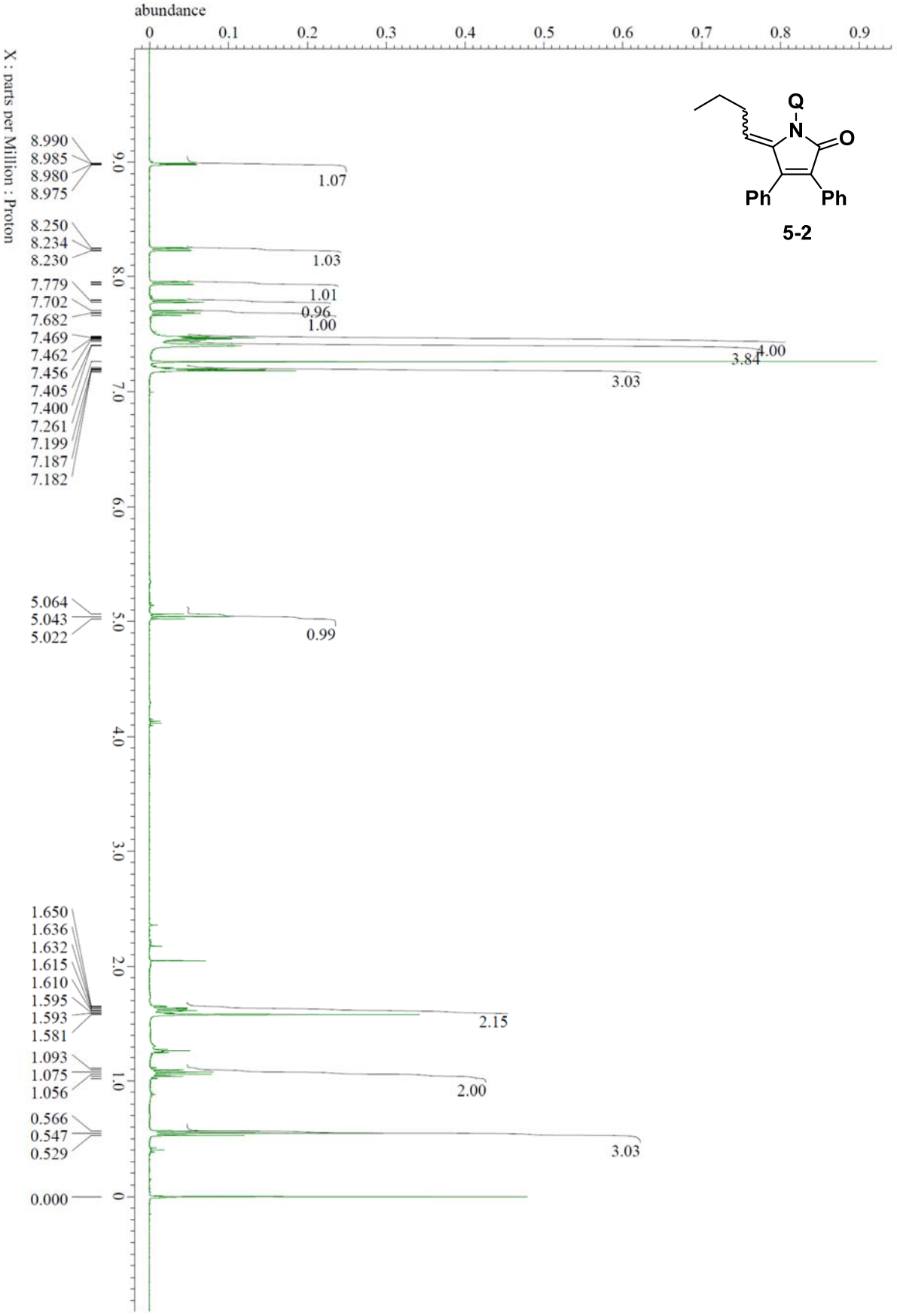

abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.599
8.597
8.589
8.587
8.585
7.707
7.703
7.688
7.683
7.261
7.224
7.221
7.217
7.207
6.917
6.898
6.878
6.807
6.733
5.242
-0.000
1.00
0.98
1.73
2.19
4.36
0.90
4.09
2.93
1.86
1.89
Py
N
O
Ph
Ph
Ph
3h-E

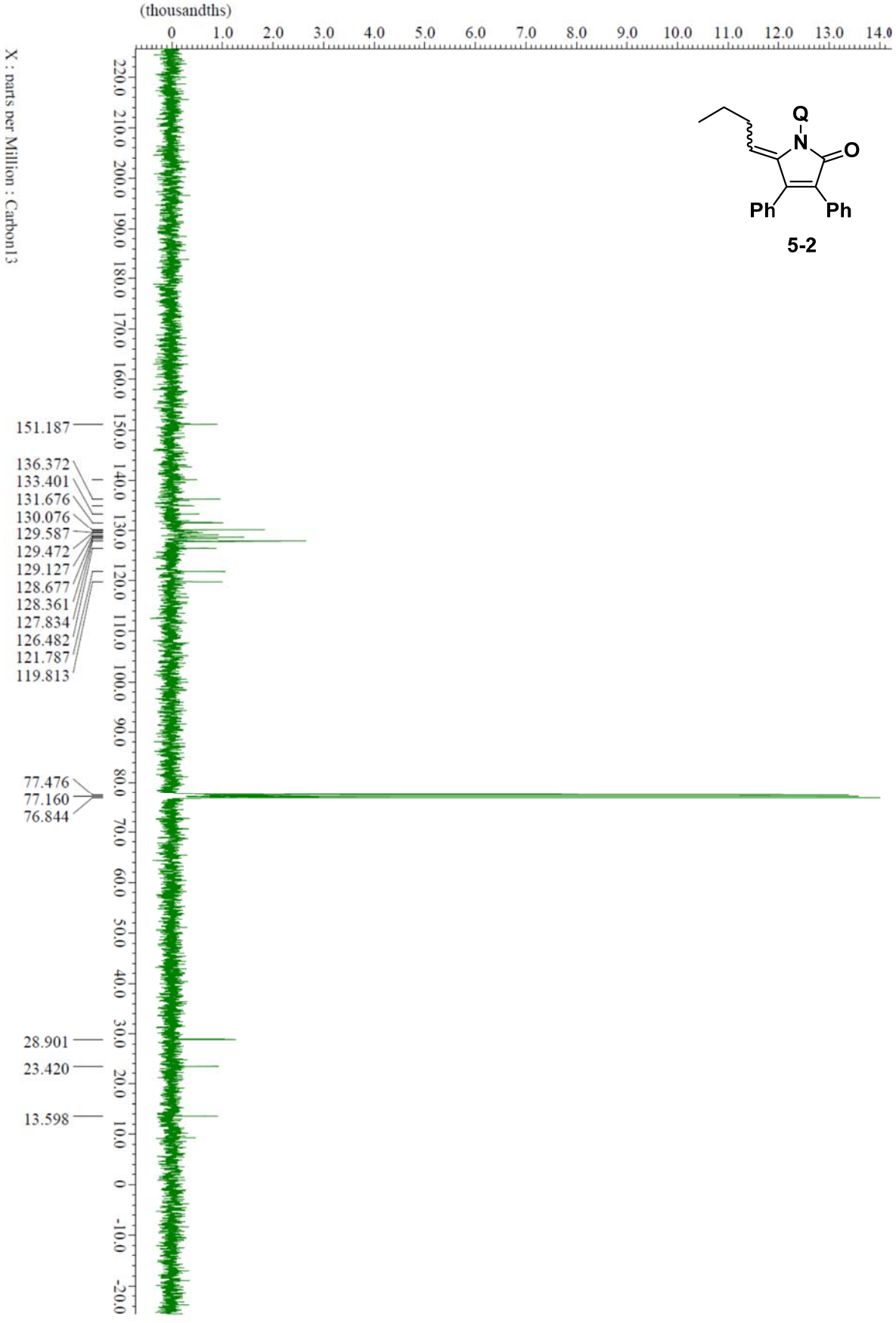

(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
168.292
157.435
149.356
137.225
133.966
133.037
130.775
130.287
129.951
129.721
128.131
128.035
127.987
127.728
127.211
126.789
122.611
122.046
116.909
77.486
77.160
76.844
45.786
Py
N
O
Ph
Ph
Ph

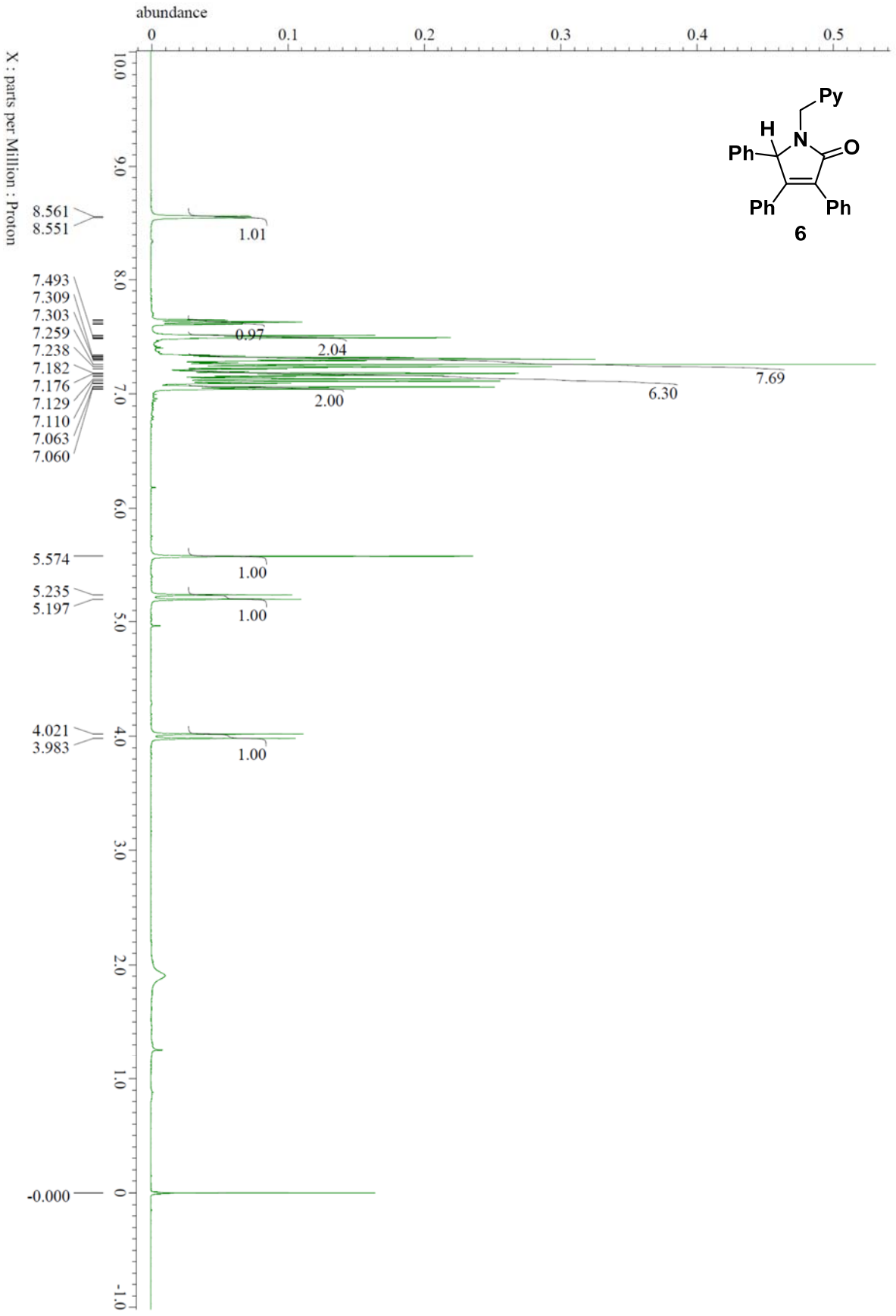
3h-*E*

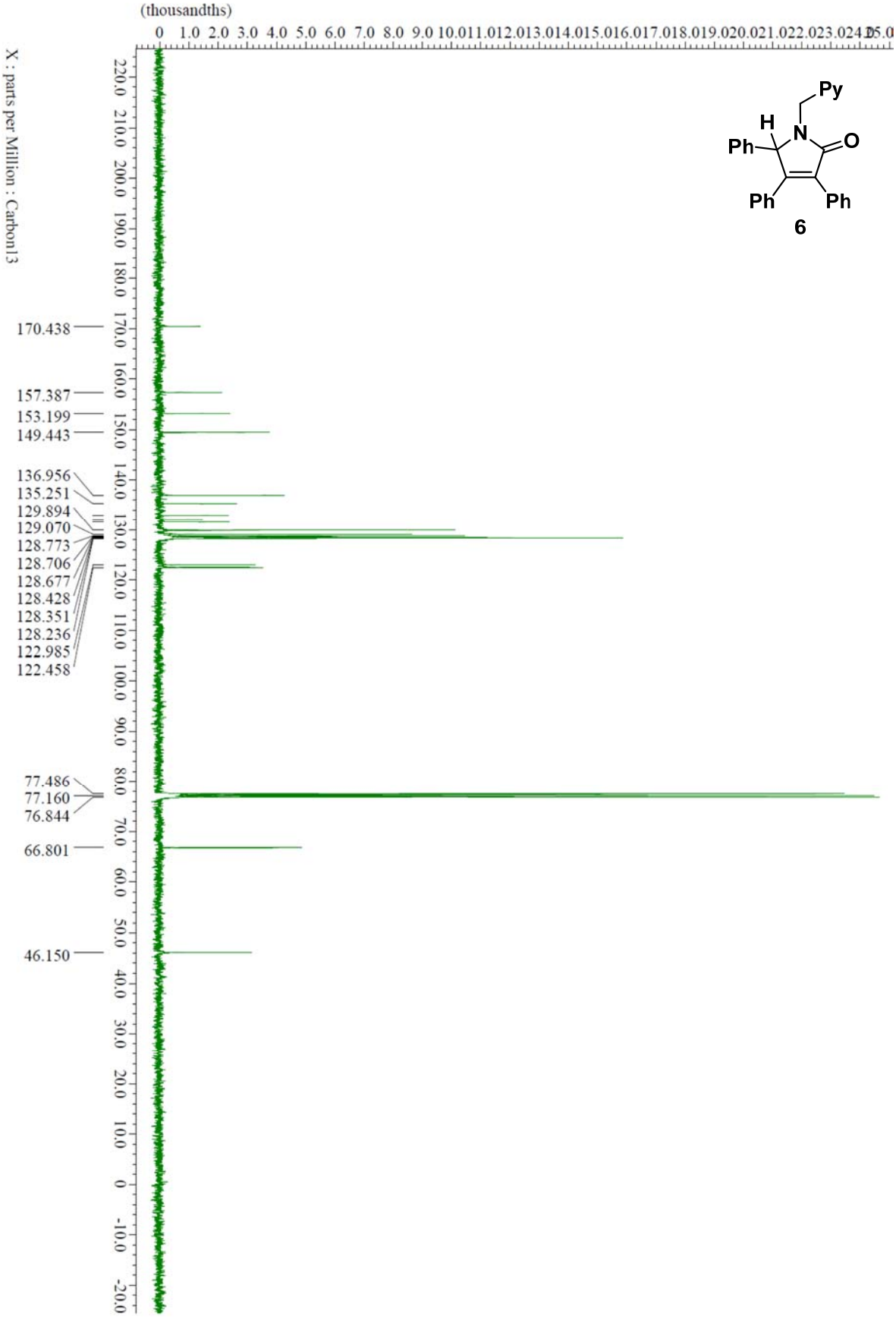

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.984
8.980
8.973
8.969
8.218
8.202
8.197
7.904
7.806
7.656
7.638
7.635
7.460
7.394
7.389
7.247
7.206
7.191
7.187
5.160
5.140
5.120
1.404
1.383
1.366
1.236
1.219
1.216
1.199
1.197
0.983
0.965
0.936
0.411
0.392
-0.000
1.03
1.02
1.00
1.03
0.96
1.30
1.90
4.84
2.96
1.00
1.02
1.05
1.97
3.00
Q
N
O
Ph
Ph
5-1


(thousandths)
X : parts per Million : Carbon13
169.930
151.225
145.772
140.061
136.285
131.370
130.737
130.287
129.942
129.281
129.022
128.514
128.428
127.862
127.632
126.281
121.806
118.682
77.476
77.160
76.844
28.853
22.692
13.579
Q
N
O
Ph
Ph
5-1


abundance
X : parts per Million : Proton
Q
N
O
Ph
Ph
5-2


(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
151.187
136.372
133.401
131.676
130.076
129.587
129.472
129.127
128.677
128.361
127.834
126.482
121.787
119.813
77.476
77.160
76.844
28.901
23.420
13.598
Q
N
O
Ph
Ph
5-2


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
8.561
8.551
7.493
7.309
7.303
7.259
7.238
7.182
7.176
7.129
7.110
7.063
7.060
5.574
5.235
5.197
4.021
3.983
-0.000
1.01
0.97
2.04
2.00
7.69
6.30
1.00
1.00
1.00
Py
H
N
O
Ph
Ph
Ph
6


(thousandths)
X : parts per Million : Carbon13
170.438
157.387
153.199
149.443
136.956
135.251
129.894
129.070
128.773
128.706
128.677
128.428
128.351
128.236
122.985
122.458
77.486
77.160
76.844
66.801
46.150
Py
H
N
O
Ph
Ph
Ph
6

IX. References

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