

Synthesis

K²CO³-Mediated Intramolecular Oxa-Michael Cyclization of α,β -Unsaturated Ketoximes: Synthesis of Densely Arene-Substituted 2-Isoxazolines Bearing One Quaternary Center

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Abstract:

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K₂CO₃-Mediated Intramolecular Oxa-Michael Cyclization of α,β -Unsaturated Ketoximes: Synthesis of Densely Arene-Substituted 2-Isloxazolines Bearing One Quaternary Center

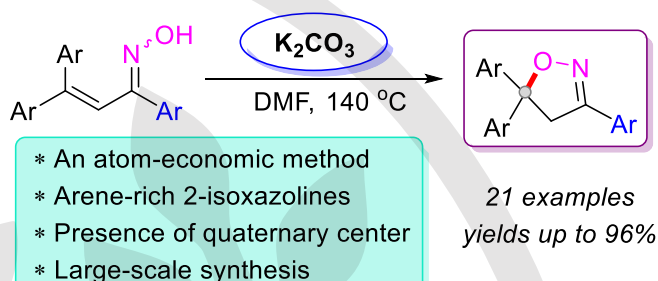
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Abstract An efficient K₂CO₃-mediated intramolecular oxa-Michael cyclization of β,β -diarylated- α,β -unsaturated ketoximes has been described. This methodology features arene-rich 2-isoxazoline derivatives bearing one quaternary center in excellent yields with operationally simple experimental procedure. The deuterium scrambling experiments were carried out to shed light on the reaction pathway. To further demonstrate the synthetic utility of the method, a large-scale synthesis and Ullmann-type C-N bond formation reaction between pyrazole and dibrominated-isoxazoline have been performed.

Key words 2-Isloxazolines. α,β -unsaturated ketoximes. Oxa-Michael cyclization. Ullmann-type amination. Base-mediated reaction

Isloxazoline motifs are an important class of five-membered heterocycles met in kinds of biologically active natural products,¹ pharmaceuticals or drug candidates,² agrochemicals,³ chiral ligands,⁴ and key intermediates in organic and medicinal chemistry.⁵

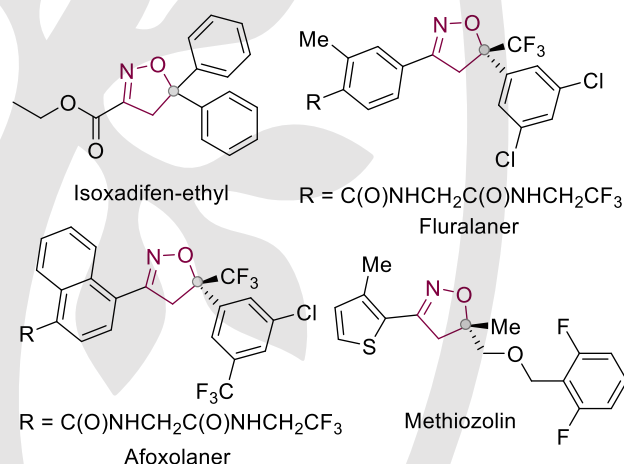


Figure 1 Selected examples of biologically active 2-isoxazoline motifs bearing one quaternary center

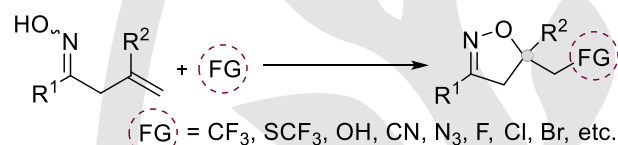
Due to their wide range of pharmaceutical and biological activities, isoxazoline synthesis has been an area of intense research in synthetic organic chemistry.⁶ In particular, 2-isoxazoline bearing one quaternary center has received significant attention in both the pharmaceutical and crop protection industries. For instance, the isoxadifen-ethyl used as a crop safener,⁷ fluralaner and afoxolaner show insecticides as well as acaricides properties,⁸ methiozolin is a selective herbicide⁹ (Figure 1). Besides that, 2-isoxazolines are important precursors which has the ability to undergo various reductive ring opening reactions for the synthesis of useful building blocks including β -amino acids,¹⁰ β -hydroxy ketones,¹¹ β -hydroxy nitriles,¹¹ and γ -amino alcohols.¹²

In this context, a plethora of methods have been reported for the synthesis of 5-substituted-2-isoxazolines. However, there are few strategies are available for the synthesis of 5,5-disubstituted-2-isoxazolines, the scaffolds in which a quaternary center present at 5th position.^{6h-i,10} For example, the traditional path for the isoxazoline synthesis involve [3+2] dipolar cycloaddition of nitrile oxide intermediates to olefins.¹³ Intramolecular oxy-functionalization of β,γ -unsaturated oximes using transition-

metal catalysts such as palladium,¹⁴ copper,¹⁵ cobalt,¹⁶ and gold,¹⁷ is an alternative method (Scheme 1a). To note, only 2-3 examples of 2-isoxazolines bearing a quaternary center have been shown in those reports. However, to the best of our knowledge, synthesis of arene-rich 5,5-diarylated-2-isoxazolines bearing one quaternary center has not been reported starting from α,β -unsaturated ketoximes.

Representative examples of metal-free approaches using stoichiometric amount of oxidants such as TEMPO/Selectfluor-TBAI/inorganic peroxide $K_2S_2O_8$ to access particularly 5,5-diarylated-2-isoxazoline having one quaternary center have been discussed here (Scheme 1b). In 2013, Chiba and co-workers reported sp^3 C-H bond oxidation with oximes under TEMPO-mediated reaction conditions.¹⁸ Liu and co-workers have demonstrated a selectfluor-Bu₄NI-mediated C-H oxygenation of oximes.¹⁹ Later in 2021, a method for the selective synthesis of 2-isoxazolines bearing quaternary center have been developed by Sureshkumar et al. with the judicious combination of TEMPO and oxidants.²⁰ Herein, we reported an efficient K_2CO_3 -mediated intramolecular oxa-Michael cyclization reaction of β,β -diarylated- α,β -unsaturated ketoximes for the synthesis of densely arene-substituted 2-isoxazolines having a quaternary center (Scheme 1c).

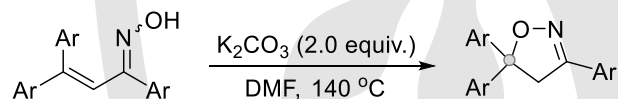
(a) Oxy-functionalization of β,γ -unsaturated oximes



(b) Aliphatic C-H bond oxidation



(c) This work: oxa-Michael cyclization



Scheme 1 Synthetic strategies to 2-isoxazolines bearing quaternary center

Our group recently reported synthesis of densely arene-substituted pyrazolines bearing quaternary center from α,β -unsaturated carbonyl compounds and arylhydrazines via tandem hydrazone and intramolecular aza-Michael reaction.²¹ Encouraged by that result, next, we envisioned to extend this concept to access 2-isoxazolines by reacting α,β -unsaturated carbonyl compounds with hydroxylamine hydrochloride. It has been noticed that the desired cyclized product 2-isoxazolines did not obtained and trace amount of condensation product oximes were noticed. Hence, we decided to focus on intramolecular oxa-Michael reaction beginning with α,β -unsaturated ketoximes under basic medium.

Along this line, we treated 1,3,3-triphenylprop-2-en-1-one oxime (**1a**) with potassium carbonate in DMF at 140 °C (Table 1). To our delight, using K_2CO_3 as a base the desired product **2a** was isolated in 70% yield (Table 1, entry 1). Increasing the loading of K_2CO_3 (2 equiv.) improved the yield of **2a** (entry 2). Inspired by this result, various bases were examined in DMF (entry 3-6). The results turn out that K_2CO_3 was better base than Na_2CO_3 for the reaction (entry 3). Other potassium salts such as K_3PO_4 , KOH and *t*-BuOK gave **2a** in excellent yield (entry 4-6). Screening of polar aprotic solvents like DCE, and CH_3CN the yield of **2a** was decreased to a different extent (entry 7-8). In case of 1,4-dioxane and DMSO, the **2a** was obtained in 72% and 92% yields, respectively (entry 9 and 10). A trace amount of **2a** was

noticed in the presence of protic solvents H_2O and MeOH (entry 11-12).

Table 1 Optimization of Reaction Conditions^a

entry	base (equiv.)	solvent	temp. (°C)	yield ^b (%)
1	K_2CO_3 (1.0)	DMF	140	70
2	K_2CO_3 (2.0)	DMF	140	96
3	Na_2CO_3 (2.0)	DMF	140	24
4	K_3PO_4 (2.0)	DMF	140	90
5	KOH (2.0)	DMF	140	87
6	<i>t</i> -BuOK (2.0)	DMF	140	93
7	K_2CO_3 (2.0)	DCE	140	20
8	K_2CO_3 (2.0)	CH_3CN	140	15
9	K_2CO_3 (2.0)	1,4-dioxane	140	72
10	K_2CO_3 (2.0)	DMSO	140	92
11	K_2CO_3 (2.0)	H_2O	140	trace
12	K_2CO_3 (2.0)	MeOH	140	trace
13	K_2CO_3 (2.0)	DMF	100	10
14	---	DMF	140	trace

^aReactions were carried out using **1a** (0.5 mmol), solvent (2.0 mL) for 3 h.

^bIsolated yield.

The yield of the product **2a** was hampered upon lowering the temperature (entry 13). In the absence of the base, **2a** was noticed in trace amount. Based upon these results; K_2CO_3 (2 equiv.) as the base in DMF at 140 °C for 3 h (Table 1, entry 2) was established as the optimal reaction condition for intramolecular oxa-Michael cyclization reaction.

To assess the scope of this reaction, a series of α,β -unsaturated ketoximes **1** were subjected to the optimized reaction conditions and the results are summarized in Table 2. At first, we investigated diverse substituents on the arene at olefin side. The α,β -unsaturated ketoximes **1** with electron-donating Me and OMe groups at the *para*-position of the arene afforded the corresponding isoxazoline **2b** and **2c** in 91% and 92% yields, respectively. The arene having electron-withdrawing halo-substituents (*p*-F/*p*-Cl/*p*-Br) were transformed into the products **2d-2f** in good to excellent yields.

Table 2 Diversity of Isoxazolines with Respect to Arene at Olefin Side^{a,b}

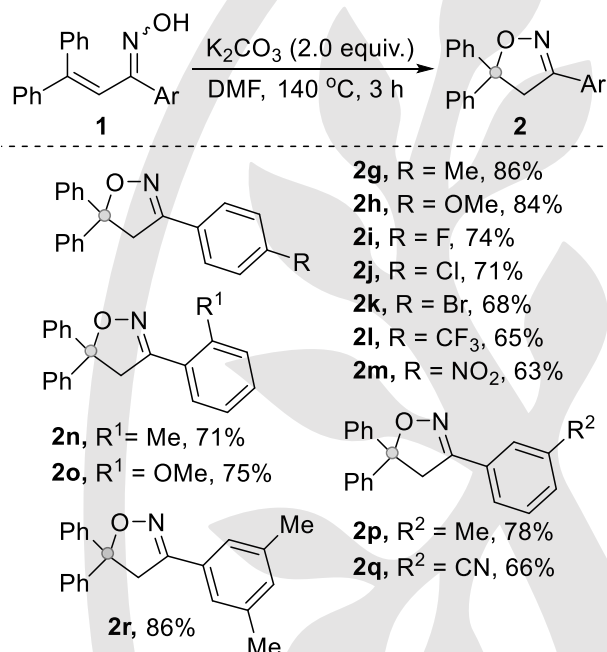
2a , Ar = Ph, 96%
2b , Ar = <i>p</i> -MeC ₆ H ₄ , 91%
2c , Ar = <i>p</i> -OMeC ₆ H ₄ , 92%
2d , Ar = <i>p</i> -FC ₆ H ₄ , 88%
2e , Ar = <i>p</i> -ClC ₆ H ₄ , 84%
2f , Ar = <i>p</i> -BrC ₆ H ₄ , 81%

^aReactions were performed with **1** (0.5 mmol, 1.0 equiv.), K_2CO_3 (1.0 mmol, 2.0 equiv.), in DMF (2.0 mL) at 140 °C for 3 h. ^bIsolated products.

Next, we explored the scope of the arene at the oxime position, and the results are depicted in Table 3. Electron-rich Me and OMe groups at the *para*-position of the arene produced the products

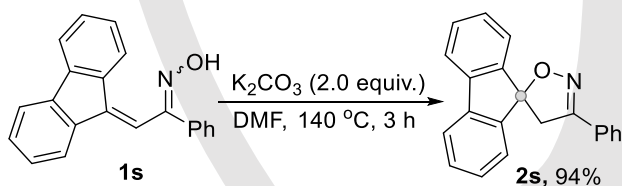
2g-2h in good yields. The halo-substituted (F/Cl/Br) ketoximes gave good yields of arene-rich 2-isoxazolines **2i-2k** up to 74% yield; the labile halo groups would find potential applications in cross-coupling reactions. Moderate yields were found in the case of reaction with ketoxime containing electron-withdrawing *p*-CF₃ (**2l**) and *p*-NO₂ (**2m**) substitution. Furthermore, *ortho*-substituents did not diminish the outcome of the reaction and the corresponding products **2n** and **2o** was isolated in acceptable yields. The structure of **2o** was confirmed by single crystal X-ray analysis (see SI). Quaternary center containing 2-isoxazolines with *meta*-substituents for instance *m*-Me (**2p**), and *m*-CN (**2q**) obtained in good yields. *m*-Xylyl-bearing isoxazoline **2r** was isolated in 86% yield.

Table 3 Diversity of Isoxazolines with Respect to Arene at oxime side^{a,b}



^aReactions were performed with **1** (0.5 mmol, 1.0 equiv.), K₂CO₃ (1.0 mmol, 2.0 equiv.), in DMF (2.0 mL) at 140 °C for 3 h. ^bIsolated products.

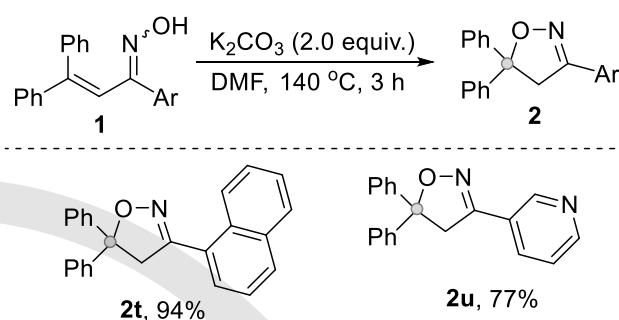
To our delight, the rigid 9-fluorenyl ketoxime **1s** was tolerated under the standard reaction conditions to provide spirocyclic isoxazoline product **2s** in 94% yield (Scheme 2).



Scheme 2 Synthesis of the Spirocyclic 2-Isoxazoline Compound

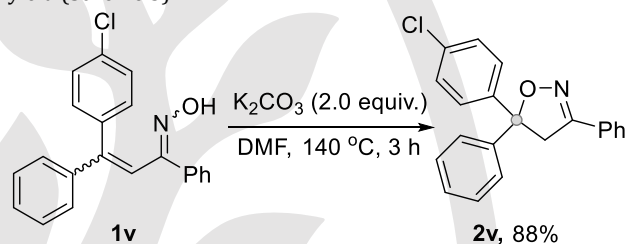
In addition, ketoxime containing naphthyl ring **1t** gave the π -extended *N*-heterocyclic compound **2t** in excellent yield. Heterocycle pyridyl group incorporated ketoxime **1u** reacted well to furnish the product **2u** in good yield.

Table 4 Synthesis of π -conjugated and pyridyl group bearing 2-isoxazolines^{a,b}



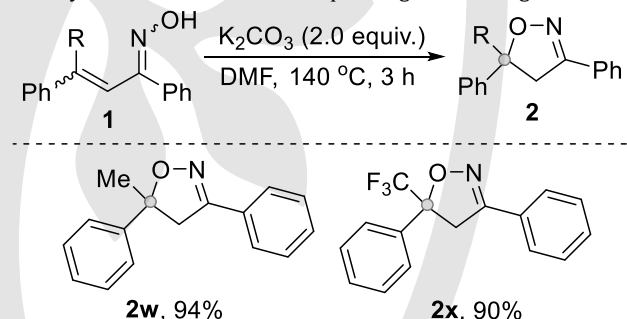
^aReactions were performed with **1** (0.5 mmol, 1.0 equiv.), K₂CO₃ (1.0 mmol, 2.0 equiv.), in DMF (2.0 mL) at 140 °C for 3 h. ^bIsolated products.

To further explore the versatility of the reaction, we focused on the possibility of chiral center containing 2-isoxazoline by taking unsymmetrical arenes at olefin side **1v**. The reaction proceeded well under the optimized reaction conditions to give 5-(4-chlorophenyl)-3,5-diphenyl-4,5-dihydroisoxazole (**2v**) in 88% yield (Scheme 3).



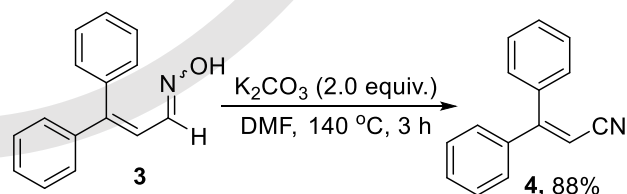
Scheme 3 Reaction with unsymmetrical arenes at olefin side

It is worthy to note that the reaction of methyl/phenyl substituted (at olefin side)- α,β -unsaturated ketoxime **1w** afforded the 2-isoxazoline **2w** in excellent yield (Scheme 4). To our delight, the core structure of Fluralaner (Figure 1) **2x** has been synthesized from the corresponding CF₃-bearing ketoxime.



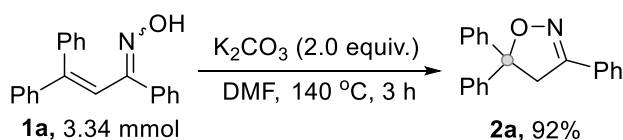
Scheme 4 Synthesis of the 5-methyl-2-isoxazoline **2w** and Fluralaner core **2x**

Motivated by good performance of the reaction with α,β -unsaturated ketoximes, we next turned our attention to examine the intramolecular oxa-Michael cyclization reaction with α,β -unsaturated aldoxime **3**. To note, the reaction profile was completely changed and conjugated nitrile **4** was obtained instead of cyclized product 2-isoxazoline (Scheme 5).²²

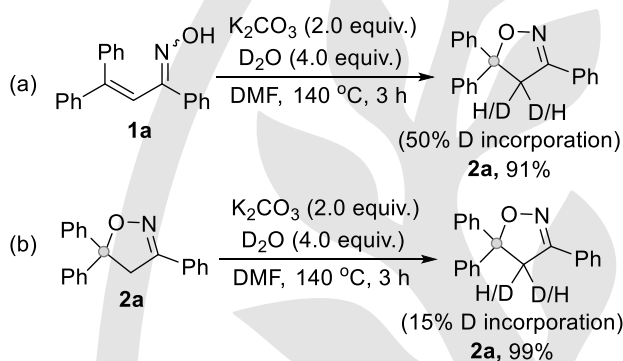


Scheme 5 Reaction with aldoxime of 3,3-diphenylacrylaldehyde (**3**)

To further demonstrate the practical utility of this reaction, we performed a large-scale synthesis. The reaction was scaled-up to 3.34 mmol of **1a** and the target compound **2a** was obtained in excellent yield without compromising the yield (Scheme 6).

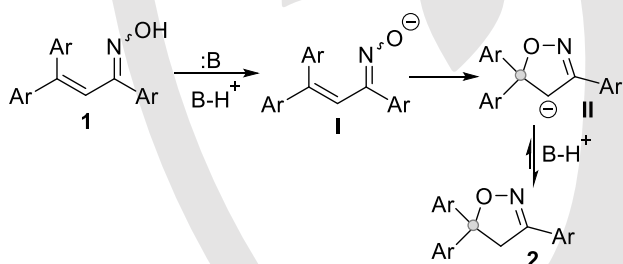
Scheme 6 Large-Scale Synthesis of **2a**

To shed light on the reaction mechanism of intramolecular oxa-Michael cyclization, several control experiments were conducted (Scheme 7). When the reaction of **1a** was performed under the optimized condition in the presence of D_2O (4.0 equiv.), the 50% D incorporation has been seen in the product **2a**, suggesting the involvement of a carbanion intermediate in the reaction (Scheme 7a). Deuterium scrambling was happened at 4th position of **2a**, indicating acidic nature of the methylene group (Scheme 7b).



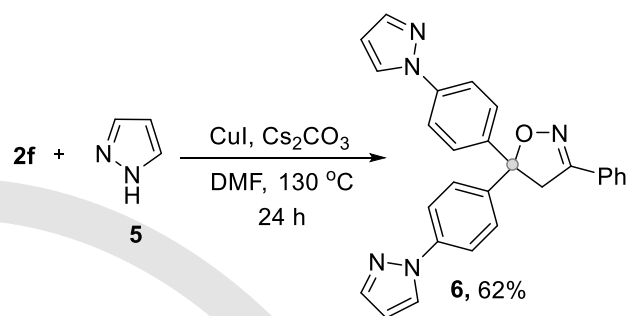
Scheme 7 The Deuterium Scrambling Experiments

Based on the above-mentioned results and the literature reports,^{18,23} a plausible reaction mechanism for the intramolecular oxa-Michael cyclization reaction was illustrated in Scheme 8. Initially, an intramolecular nucleophilic attack of the O-anionic center of the oxime **I** (probably generated by the deprotonation of **1** by the K_2CO_3) to the β -carbon of the α,β -unsaturated ketoximes provides the corresponding carbanion species **II**. Subsequently, abstraction of proton by the C-4 position of **II** would afford desired 2-isoxazoline **2**.



Scheme 8 Plausible Reaction Mechanism

Finally, we wish to demonstrate the synthetic versatility of dibrominated isoxazoline product **2f**. For that we chosen Ullmann-type amination reaction with pyrazole (Scheme 9).²⁴ Gratifyingly, the dual C-N bonded product **6** was afforded in 62% yield.

Scheme 9 Ullmann-Type Amination Reaction of Isoxazoline Compound **2f**

In conclusion, we have demonstrated an efficient approach to access arene-rich 2-isoxazolines bearing quaternary center from β,β -diarylated- α,β -unsaturated ketoximes. The protocol features wide substrate scope with reasonable yields. Deuterium scrambling experiments were carried out to understand the reaction path and the nature of the 2-isoxazolines. Further studies on the synthesis of chiral 2-isoxazoline and related *N*-heterocyclic compounds are in progress in our laboratory.

^1H and ^{13}C NMR spectra were recorded at $25\text{ }^\circ\text{C}$ on a Bruker Avance III 500 MHz spectrometer operating at 500 MHz for ^1H , 125 MHz for ^{13}C NMR experiments. Chemical shifts were calibrated to the residual proton and carbon resonance of the solvent, CDCl_3 (^1H δ 7.26; ^{13}C δ 77.0) / $\text{DMSO}-d_6$ (^1H δ 2.50; ^{13}C δ 39.52). The following abbreviations were used to illuminate the diversities: δ = chemical shifts, J = coupling constant, s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, m = multiplet. Chemical shifts are given in ppm relative to the internal standard of tetramethylsilane (TMS). High-resolution mass spectra (HRMS) were obtained by using a TOF analyzer in ESI mode. X-ray data were taken at 273K with a Bruker APEX-II CCD single crystal diffractometer by using graphite monochromated Mo-K α radiation (0.71073 Å). Data integration was done using SAINT.^{25a} Intensities for absorption were corrected using SADABS.^{25b} Structure solution and refinement were carried out using Bruker SHELX-TL.^{25c-d} TLC analysis was performed with pre-coated TLC plates (0.2 mm, Silica gel 60 F-254, Merck). Column chromatography was done using silica gel (100-200 mesh) as an adsorbent. Unless otherwise stated, all reagents and starting materials obtained from commercial suppliers were used without further purification. Benzophenone, Ethynylmagnesium bromide (0.5 M in THF), *n*-BuLi (1.6 M in hexane), Phenylacetylene, Hydroxylamine hydrochloride, Aryl halides, CuI, $\text{PdCl}_2(\text{PPh}_3)_2$, K_2CO_3 were purchased from Sigma-Aldrich, TCI, Avra and CDH India. DMF was vacuum distilled over 4Å molecular sieves and stored under nitrogen. All the reactions were performed in an oven-dried glass pressure tube (capacity 15 mL) procured from the Sigma-Aldrich India (catalogue No. Z181099) under an atmosphere of N_2 . Reactions were monitored by thin-layer chromatography (TLC). The products were purified by column chromatography on silica gel using petroleum ether and ethyl acetate as the eluent.

General procedure for the synthesis of α,β -unsaturated ketoximes (**1a** as representative):¹⁸

A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 1,3,3-triphenylprop-2-en-1-one (142 mg, 0.5 mmol) in EtOH (3 mL) was added hydroxylamine hydrochloride (52 mg, 0.75 mmol) and pyridine (101 μL , 1.25 mmol) under the argon atmosphere.

The reaction mixture was stirred at 60 °C in an oil bath and upon completion the reaction (monitored by TLC) mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by silica gel column chromatography to provide the desired product 1,3,3-triphenylprop-2-en-1-one oxime (**1a**).

General procedure for the synthesis of isoxazolines (2a as representative):

A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 1,3,3-triphenylprop-2-en-1-one oxime (**1a**, 150 mg, 0.5 mmol), K₂CO₃ (138 mg, 1.0 mmol) in DMF (2.0 mL) was stirred at 140 °C in an oil bath for 3 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 98:2) to provide 3,5,5-triphenyl-4,5-dihydroisoxazole (**2a**).

Compounds **2a**,¹⁸ **2g-h**,¹⁸ **2k-l**,¹⁸ **2w**,²⁰ **2x**,²⁶ **427** are previously reported and showed the identical spectra according to the literature.

3,5,5-Triphenyl-4,5-dihydroisoxazole (2a)¹⁸

Yield: 96% (144 mg), White solid; mp 143-144 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.73 – 7.67 (m, 2H), 7.51 – 7.45 (m, 4H), 7.42 – 7.32 (m, 7H), 7.31 – 7.26 (m, 2H), 4.00 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.2, 144.1, 130.1, 129.6, 128.7, 128.4, 127.6, 126.7, 126.1, 92.0, 48.2 ppm.

3-Phenyl-5,5-di-*p*-tolyl-4,5-dihydroisoxazole (2b)

Yield: 91% (149 mg), White solid; mp 107-108 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.70 (dd, *J* = 6.4, 2.8 Hz, 2H), 7.45 – 7.33 (m, 7H), 7.16 (d, *J* = 8.0 Hz, 4H), 3.96 (s, 2H), 2.34 (s, 6H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.2, 141.3, 137.3, 130.0, 129.7, 129.0, 128.6, 126.6, 126.0, 91.9, 48.1, 21.0 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₃H₂₂NO⁺: 328.1696; found: 328.1697.

5,5-Bis(4-methoxyphenyl)-3-phenyl-4,5-dihydroisoxazole (2c)

Yield: 92% (165 mg), Yellow solid; mp 90-91 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.74 – 7.63 (m, 2H), 7.38 (dd, *J* = 9.9, 6.0 Hz, 7H), 6.88 (d, *J* = 8.7 Hz, 4H), 3.93 (s, 2H), 3.79 (s, 6H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 159.0, 156.2, 136.3, 132.2, 130.0, 128.6, 127.4, 126.6, 113.6, 91.6, 55.2, 48.3 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₃H₂₂NO₃⁺: 360.1594; found: 360.1596.

5,5-Bis(4-fluorophenyl)-3-phenyl-4,5-dihydroisoxazole (2d)

Yield: 88% (147 mg), White solid; mp 105-106 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.75 – 7.64 (m, 2H), 7.42 (dd, *J* = 8.6, 5.3 Hz, 7H), 7.04 (t, *J* = 8.6 Hz, 4H), 3.95 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 162.2 (d, *J*_{C-F} = 250.0 Hz), 156.3, 139.6 (d, *J*_{C-F} = 3.7 Hz), 130.3, 129.3, 128.8, 127.9 (d, *J*_{C-F} = 7.5 Hz), 126.7, 115.3 (d, *J*_{C-F} = 21.2 Hz), 91.1, 48.4 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆F₂NO⁺: 336.1194; found: 336.1190.

5,5-Bis(4-chlorophenyl)-3-phenyl-4,5-dihydroisoxazole (2e)

Yield: 84% (155 mg), White solid; mp 100-101 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.74 – 7.63 (m, 2H), 7.46 – 7.36 (m, 7H), 7.32 (d, *J* = 8.5 Hz, 4H), 3.94 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.3, 142.0, 133.9, 130.4, 129.1, 128.8, 128.7, 127.5, 126.7, 91.0, 48.1 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆Cl₂NO⁺: 368.0603; found: 368.0606.

5,5-Bis(4-bromophenyl)-3-phenyl-4,5-dihydroisoxazole (2f)

Yield: 81% (185 mg), White solid; mp 118-119 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.67 (d, *J* = 5.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 4H), 7.40 (d, *J* = 5.7 Hz, 3H), 7.32 (d, *J* = 8.3 Hz, 4H), 3.92 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.3, 142.5, 131.7, 130.4, 129.1, 128.8, 127.8, 126.7, 122.1, 91.1, 48.0 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆Br₂NO⁺: 457.9573; found: 457.9571.

5,5-Diphenyl-3-(*p*-tolyl)-4,5-dihydroisoxazole (2g)¹⁸

Yield: 86% (135 mg), White solid; mp 129-130 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.60 (d, *J* = 8.1 Hz, 2H), 7.49 (d, *J* = 7.7 Hz, 4H), 7.36 (t, *J* = 7.6 Hz, 4H), 7.28 (dd, *J* = 12.8, 5.5 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 3.99 (s, 2H), 2.38 (s, 3H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.2, 144.1, 140.3, 129.3, 128.4, 127.6, 126.7, 126.6, 126.1, 91.7, 48.3, 21.4 ppm.

3-(4-Methoxyphenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2h)¹⁸

Yield: 84% (138 mg), Yellow solid; mp 143-144 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.65 (d, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 7.7 Hz, 4H), 7.35 (t, *J* = 7.6 Hz, 4H), 7.28 (dd, *J* = 12.5, 5.3 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 3.98 (s, 2H), 3.82 (s, 3H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 161.0, 155.8, 144.2, 128.3, 128.2, 127.5, 126.1, 122.1, 114.1, 91.6, 55.3, 48.4 ppm.

3-(4-Fluorophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2i)

Yield: 74% (117 mg), White solid; mp 121-122 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.72 – 7.64 (m, 2H), 7.49 – 7.42 (m, 4H), 7.38 – 7.32 (m, 4H), 7.27 (t, *J* = 7.3 Hz, 2H), 7.07 (t, *J* = 8.7 Hz, 2H), 3.96 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 163.8 (d, *J*_{C-F} = 248.7 Hz), 155.2, 143.9, 128.6, 128.6, 128.4, 127.7, 126.0, 115.8 (d, *J*_{C-F} = 21.2 Hz), 92.1, 48.3 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇FN⁺: 318.1289; found: 318.1287.

3-(4-Chlorophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2j)

Yield: 71% (119 mg), White solid; mp 139-140 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.63 (d, *J* = 8.5 Hz, 2H), 7.46 (d, *J* = 7.6 Hz, 4H), 7.36 (dd, *J* = 12.1, 4.9 Hz, 6H), 7.28 (t, *J* = 7.3 Hz, 2H), 3.96 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.3, 143.9, 136.1, 129.0, 128.5, 128.1, 127.9, 127.7, 126.0, 92.3, 48.0 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇ClNO⁺: 334.0993 found: 334.0991.

3-(4-Bromophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2k)¹⁸

Yield: 68% (129 mg), White solid; mp 170-171 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.51 (dd, *J* = 13.3, 8.2 Hz, 6H), 7.37 (t, *J* = 7.5 Hz, 4H), 7.30 (t, *J* = 7.1 Hz, 2H), 3.98 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.4, 143.8, 131.8, 128.4, 128.0, 127.7, 126.0 (2C), 124.3, 92.3, 47.9 ppm.

5,5-Diphenyl-3-(4-(trifluoromethyl)phenyl)-4,5-dihydroisoxazole (2l)¹⁸

Yield: 65% (119 mg), White solid; mp 134-135 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.52 – 7.44 (m, 4H), 7.40 – 7.33 (m, 4H), 7.33 – 7.27 (m, 2H), 4.00 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.2, 143.7, 133.0, 131.8 (q, *J*_{C-F} = 32.6 Hz), 128.5, 127.8, 126.9, 126.0, 125.7 (q, *J*_{C-F} = 4.0 Hz), 123.8 (q, *J*_{C-F} = 270.6 Hz), 92.7, 47.8 ppm.

3-(4-Nitrophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2m)

Yield: 63% (108 mg), Yellow solid; mp 139-140 °C.

¹H NMR (500 MHz, CDCl₃) δ 8.25 (d, *J* = 8.8 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 4H), 7.37 (t, *J* = 7.6 Hz, 4H), 7.30 (t, *J* = 7.3 Hz, 2H), 4.02 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 154.7, 148.4, 143.4, 135.6, 128.5, 127.9, 127.3, 125.9, 124.0, 93.3, 47.6 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇N₂O₃⁺: 345.1234 found: 345.1226.

5,5-Diphenyl-3-(*o*-tolyl)-4,5-dihydroisoxazole (2n)

Yield: 71% (111 mg), White solid; mp 93-94 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.49 (d, *J* = 7.8 Hz, 4H), 7.35 (dd, *J* = 15.8, 7.9 Hz, 5H), 7.27 (dd, *J* = 12.6, 4.7 Hz, 4H), 7.21 (t, *J* = 7.1 Hz, 1H), 4.03 (s, 2H), 2.53 (s, 3H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.3, 144.0, 138.0, 131.5, 129.4, 128.7, 128.7, 128.4, 127.6, 126.1, 125.7, 90.9, 50.5, 22.7 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₂₀NO⁺: 314.1539 found: 314.1541.

3-(2-Methoxyphenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2o)

Yield: 75% (123 mg), White solid; mp 151-152 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.76 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.52 – 7.46 (m, 4H), 7.34 (ddd, *J* = 10.0, 6.1, 2.6 Hz, 5H), 7.27 (ddd, *J* = 7.7, 4.1, 1.4 Hz, 2H), 6.95 (td, *J* = 7.6, 1.0 Hz, 1H), 6.91 (d, *J* = 8.3 Hz, 1H), 4.09 (s, 2H), 3.83 (s, 3H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.5, 144.3, 131.3, 129.4, 128.4, 128.3, 127.4, 126.5, 126.2, 120.8, 111.4, 91.6, 55.5, 50.6 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₂₀NO₂⁺: 330.1489 found: 330.1490.

5,5-Diphenyl-3-(*m*-tolyl)-4,5-dihydroisoxazole (2p)

Yield: 78% (122 mg), White solid; mp 118-119 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.54 (s, 1H), 7.48 (dd, *J* = 8.2, 0.9 Hz, 5H), 7.35 (dd, *J* = 10.4, 4.8 Hz, 4H), 7.30 – 7.25 (m, 3H), 7.21 (d, *J* = 7.6 Hz, 1H), 3.99 (s, 2H), 2.37 (s, 3H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.4, 144.1, 138.4, 130.9, 129.4, 128.6, 128.4, 127.6, 127.2, 126.1, 123.8, 91.9, 48.3, 21.3 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₂₀NO⁺: 314.1539 found: 314.1539.

3-(5,5-Diphenyl-4,5-dihydroisoxazol-3-yl)benzonitrile (2q)

Yield: 66% (107 mg), White solid; mp 141-142 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.96 (d, *J* = 7.9 Hz, 1H), 7.93 (s, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.47 (d, *J* = 7.6 Hz, 4H), 7.37 (t, *J* = 7.5 Hz, 4H), 7.30 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 154.5, 143.4, 133.1, 130.9, 130.5, 130.0, 129.6, 128.5, 127.8, 125.9, 118.0, 113.0, 92.8, 47.5 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₁₇N₂O⁺: 325.1335 found: 325.1338.

3-(3,5-Dimethylphenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2r)

Yield: 86% (141 mg), White solid; mp 133-134 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.47 (d, *J* = 7.4 Hz, 4H), 7.34 (dd, *J* = 13.7, 5.8 Hz, 6H), 7.29 – 7.25 (m, 2H), 7.03 (s, 1H), 3.97 (s, 2H), 2.32 (s, 6H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.5, 144.1, 138.3, 131.8, 130.0, 128.4, 127.6, 126.1, 124.5, 91.8, 48.3, 21.2 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₃H₂₂NO⁺: 328.1696 found: 328.1697.

3'-Phenyl-4'-H-spiro[fluorene-9,5'-isoxazole] (2s)

Yield: 94% (140 mg), Yellow solid; mp 131-132 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.83 – 7.76 (m, 2H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.53 (d, *J* = 7.5 Hz, 2H), 7.50 – 7.45 (m, 3H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 3.87 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.0, 146.2, 139.8, 130.2, 129.7, 129.5, 128.8, 128.5, 126.8 (2C), 123.6, 120.0, 92.2, 45.1 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆NO⁺: 298.1226 found: 298.1228.

3-(Naphthalen-1-yl)-5,5-diphenyl-4,5-dihydroisoxazole (2t)

Yield: 94% (164 mg), White solid; mp 127-128 °C.

¹H NMR (500 MHz, CDCl₃) δ 8.96 (d, *J* = 8.6 Hz, 1H), 7.88 (t, *J* = 7.5 Hz, 2H), 7.63 – 7.51 (m, 7H), 7.48 – 7.43 (m, 1H), 7.42 – 7.36 (m, 4H), 7.34 – 7.28 (m, 2H), 4.20 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.1, 144.0, 133.9, 130.8, 130.6, 128.5, 128.4, 127.6, 127.6, 127.5, 126.9, 126.5, 126.3, 126.1, 124.7, 90.8, 50.9 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₅H₂₀NO⁺: 350.1539 found: 350.1544.

5,5-Diphenyl-3-(pyridin-3-yl)-4,5-dihydroisoxazole (2u)

Yield: 77% (116 mg), White solid; mp 169-170 °C.

¹H NMR (500 MHz, CDCl₃) δ 8.85 (s, 1H), 8.63 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 4H), 7.39 – 7.32 (m, 5H), 7.29 (t, *J* = 7.3 Hz, 2H), 4.00 (s, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 153.9, 151.0, 147.6, 143.6, 133.7, 128.5, 127.8, 126.0 (2C), 123.7, 92.5, 47.6 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₀H₁₇N₂O⁺: 301.1335 found: 301.1340.

5-(4-Chlorophenyl)-3,5-diphenyl-4,5-dihydroisoxazole (2v)

Yield: 88% (147 mg), White solid; mp 161-162 °C.

¹H NMR (500 MHz, CDCl₃) δ 7.69 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.43 – 7.39 (m, 5H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.30 (dd, *J* = 14.6, 7.9 Hz, 3H), 3.96 (q, *J* = 16.5 Hz, 2H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.3, 143.5, 142.7, 133.6, 130.3, 129.4, 128.7, 128.6, 128.5, 127.9, 127.6, 126.7, 126.0, 91.5, 48.2 ppm.

HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇ClNO⁺: 334.0993; found: 334.0992.

5-Methyl-3,5-diphenyl-4,5-dihydroisoxazole (2w)²⁰

Yield: 94% (112 mg), White solid.

¹H NMR (500 MHz, CDCl₃) δ 7.73 – 7.64 (m, 2H), 7.52 (d, *J* = 7.5 Hz, 2H), 7.43 – 7.35 (m, 5H), 7.29 (t, *J* = 7.3 Hz, 1H), 3.51 (q, *J* = 16.4 Hz, 2H), 1.83 (s, 3H) ppm.

¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.1, 145.4, 129.9, 129.8, 128.6, 128.4, 127.3, 126.5, 124.6, 88.0, 48.7, 28.2 ppm.

3,5-Diphenyl-5-(trifluoromethyl)-4,5-dihydroisoxazole (2x)²⁶

Yield: 90% (131 mg), White solid.

¹H NMR (500 MHz, CDCl₃) δ 7.69 – 7.59 (m, 4H), 7.48 – 7.36 (m, 6H), 3.93 (q, *J* = 17.0, 2H) ppm.

^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.0, 135.7, 130.8, 129.3, 128.8, 128.6, 128.1, 126.8, 126.6, 124.3 (q, $J_{\text{C-F}} = 282.5$ Hz), 87.8 (q, $J_{\text{C-F}} = 30.0$ Hz), 44.0 ppm.

3,3-Diphenylacrylonitrile (**4**)²⁷

Yield: 88% (90 mg), Pale yellow oil.

^1H NMR (500 MHz, CDCl_3) δ 7.50 – 7.42 (m, 6H), 7.38 (t, $J = 7.5$ Hz, 2H), 7.31 (d, $J = 7.4$ Hz, 2H), 5.75 (s, 1H) ppm.

^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 163.1, 138.9, 137.0, 130.4, 130.0, 129.5, 128.6, 128.5, 128.4, 117.8, 94.8 ppm.

Ullmann-Type Amination Reaction of Isoxazoline Compound **2f** with pyrazole (**5**):²⁴

A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 5,5-bis(4-bromophenyl)-3-phenyl-4,5-dihydroisoxazole (**2f**, 50 mg, 0.109 mmol), pyrazole (**5**, 30 mg, 0.436 mmol), CuI (10 mg, 0.054 mmol), Cs_2CO_3 (284 mg, 0.87 mmol) in DMF (2.0 mL) was stirred at 140 °C in an oil bath for 24 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na_2SO_4 and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 80:20) to provide 5,5-bis(4-(1H-pyrazol-1-yl)phenyl)-3-phenyl-4,5-dihydroisoxazole (**6**) as white solid (29 mg, 0.067 mmol, 62% yield), mp 173–174 °C.

^1H NMR (500 MHz, CDCl_3) δ 7.91 (d, $J = 2.4$ Hz, 2H), 7.71 (dd, $J = 8.5, 6.0$ Hz, 8H), 7.57 (d, $J = 8.7$ Hz, 4H), 7.43 – 7.39 (m, 3H), 6.48 – 6.44 (m, 2H), 4.02 (s, 2H) ppm.

^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.4, 141.8, 141.3, 139.7, 130.4, 129.3, 128.8, 127.3, 126.7, 125.0, 119.1, 107.8, 91.3, 48.3 ppm.

HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$]⁺ calcd for $\text{C}_{27}\text{H}_{22}\text{N}_5\text{O}$: 432.1819; found: 432.1820.

Conflict of Interest

The authors declare no conflict of interest.

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Supporting Information

YES (this text will be updated with links prior to publication)

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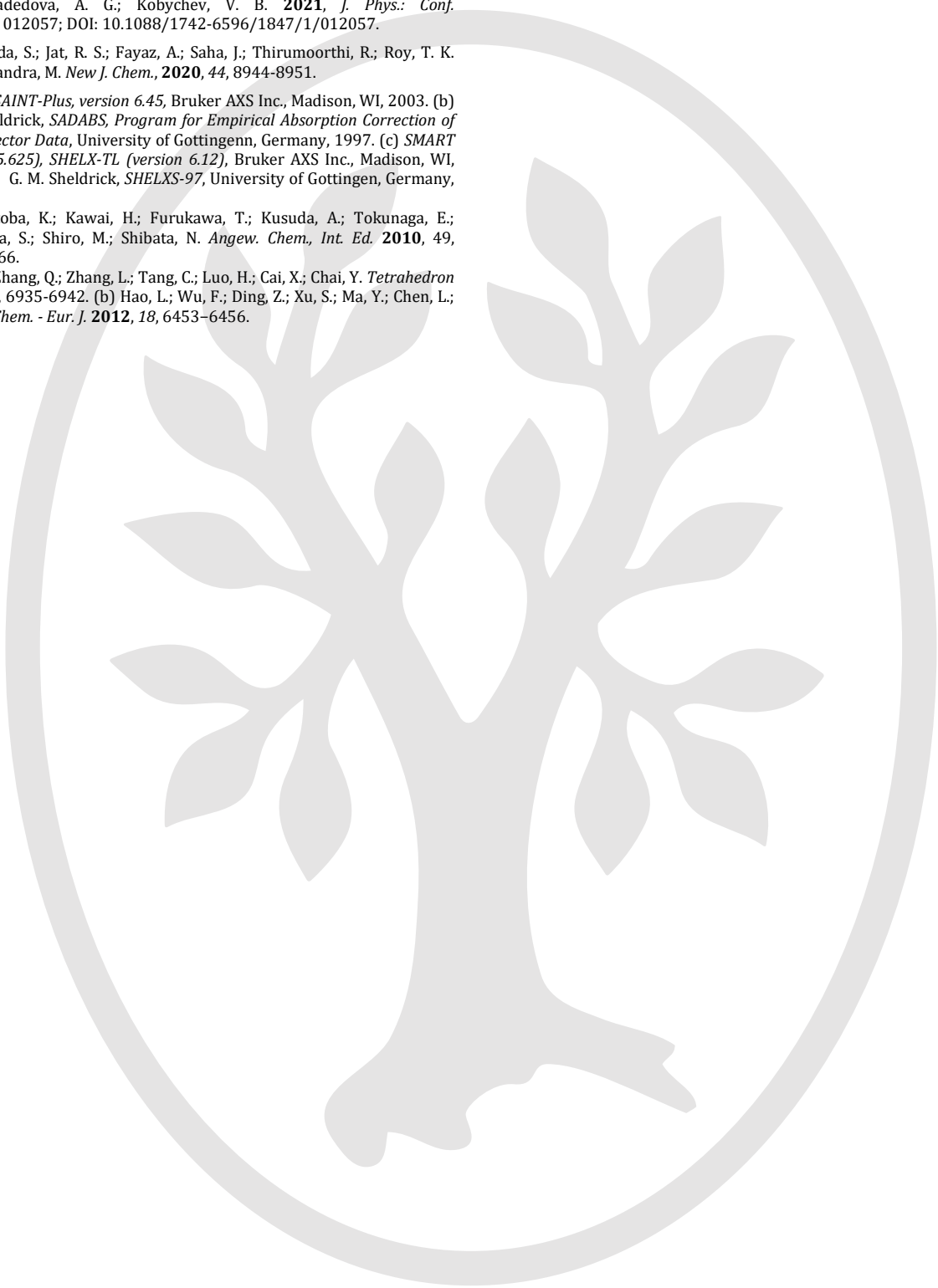
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Supporting Information

for

K₂CO₃-Mediated Intramolecular Oxa-Michael Cyclization of α,β -Unsaturated Ketoximes: Synthesis of Densely Arene-Substituted 2-Isoxazolines Bearing One Quaternary Center

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1. General Information

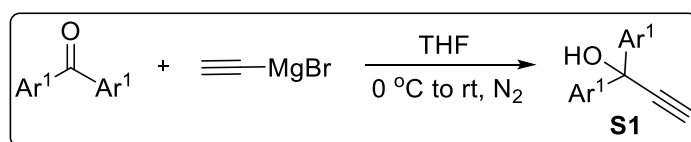
^1H and ^{13}C NMR spectra were recorded at 25 °C on a Bruker Avance III 500 MHz spectrometer operating at 500 MHz for ^1H , 125 MHz for ^{13}C NMR experiments. Chemical shifts were calibrated to the residual proton and carbon resonance of the solvent, CDCl_3 (^1H δ 7.26; ^{13}C δ 77.0)/ DMSO-d_6 (^1H δ 2.50; ^{13}C δ 39.52). The following abbreviations were used to illuminate the diversities: δ = chemical shifts, J = coupling constant, s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, m = multiplet. Chemical shifts are given in ppm relative to the internal standard of tetramethylsilane (TMS). High-resolution mass spectra (HRMS) were obtained by using a TOF analyzer in ESI mode. X-ray data were taken at 273K with a Bruker APEX-II CCD single crystal diffractometer by using graphite monochromated Mo-K α radiation (0.71073 Å). Data integration was done using SAINT.^{1a} Intensities for absorption were corrected using SADABS.^{1b} Structure solution and refinement were carried out using Bruker SHELX-TL.^{1c-d} TLC analysis was performed with pre-coated TLC plates (0.2 mm, Silica gel 60 F-254, Merck). Column chromatography was done using silica gel (100-200 mesh) as an adsorbent. Unless otherwise stated, all reagents and starting materials obtained from commercial suppliers were used without further purification. Benzophenone, Ethynylmagnesium bromide (0.5 M in THF), n-BuLi (1.6 M in hexane), Phenylacetylene, Hydroxylamine hydrochloride, Aryl halides, CuI, $\text{PdCl}_2(\text{PPh}_3)_2$, K_2CO_3 were purchased from standard commercial sources (Sigma-Aldrich, TCI, Avra and CDH India). DMF was vacuum distilled over 4Å molecular sieves and stored under nitrogen. All the reactions were performed in an oven-dried glass pressure tube (capacity 15 mL) procured from the Sigma-Aldrich India (catalogue No. Z181099) under an atmosphere of N_2 . Reactions were monitored by thin-layer chromatography (TLC). The products were purified by column chromatography on silica gel using petroleum ether and ethyl acetate as the eluent. In the case that oximes were obtained as *E/Z*-mixtures, the stereochemistry was assigned by ^{13}C NMR (the chemical shift of α -carbon with *syn* to the OH is farther to the higher field than that with *anti* to the OH).

2. Experimental Section

2.1 General procedure for starting materials

2.1.1 Procedure for the preparation of terminal propargyl alcohols: GP-1

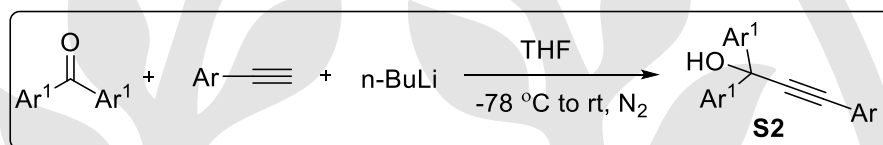
Terminal propargyl alcohols **S1** were synthesized *via* reported procedure.²



In an oven dried round bottom flask added ketone (1.0 equiv.) in THF under N₂ atmosphere with continuous stirrer at room temp. Then the solution of ethynylmagnesium bromide (1.5 equiv.) was added at 0 °C. The reaction mixture was stirred at 0 °C for 30 minutes and at room temperature for 6 h then the reaction was quenched with aqueous ammonium chloride and extracted with EtOAc. The combined organic layers were washed with H₂O and saturated NaHCO₃ solution, dried over Na₂SO₄ and evaporated under reduced pressure. The crude product was purified by column chromatography.

2.1.2 Procedure for the preparation of internal propargyl alcohols: GP-2

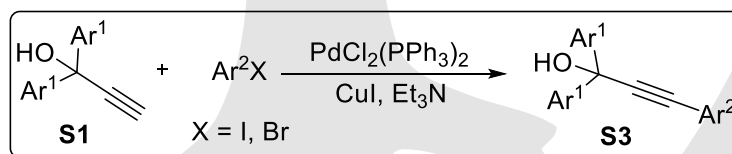
Internal propargyl alcohols **S2** were synthesized *via* reported procedure.³



To a solution of alkyne (3.75 equiv.) in THF at -78 °C was added n-BuLi solution (1.6 M, 1.4 equiv.). The solution was allowed to warm at 0 °C over 1 hour and then the solution was cooled to -78 °C and ketone (1.0 equiv.) was added. The reaction mixture was allowed to warm at room temperature and stirred at room temp for 3 hours. The reaction was quenched with aqueous solution of NH₄Cl and the reaction mixture was extracted with EtOAc. The combined organic layers were washed with H₂O and saturated NaHCO₃ solution, dried over Na₂SO₄, filtered and evaporated under reduced pressure. The crude product was purified by column chromatography.

2.1.3 Procedure for the sonogashira coupling between terminal propargyl alcohol and aryl iodide: GP-3

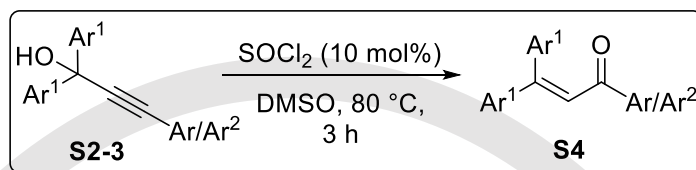
Aryl propargyl alcohols **S3** were synthesized *via* reported procedure.⁴



To a solution of the substituted aryl halide (5 mmol) in Et₃N (5 mL) was added PdCl₂(PPh₃)₂ (4 mol%), CuI (2 mol%) under Ar atmosphere for 5 minutes. A solution of terminal propargyl alcohol **S1** (5 mmol) in Et₃N (5 mL) was dropwise added over a period of 5 minutes at rt. Further, the resulting solution was stirred at rt for overnight and upon completion the reaction (monitored by TLC) mixture was diluted with aqueous solution of NH₄Cl (30 mL) and extracted with ethyl acetate (30 mL), dried over Na₂SO₄, and concentrated under vacuum. The crude product was purified by column chromatography.

2.1.4 General procedure for the synthesis of α,β -unsaturated carbonyl compounds: GP-4

Aryl enones **S4** were synthesized *via* reported procedure.⁵



A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with propargyl alcohols **S2-3** (1 mmol), SOCl₂ (0.1 mmol) in DMSO was stirred at 80 °C in an oil bath and upon completion the reaction (monitored by TLC) mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by silica gel column chromatography to provide the desired α,β -unsaturated carbonyl compounds **S4**.

2.1.5 General procedure for the synthesis of α,β -unsaturated ketoximes: GP-5

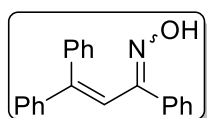
Aryl ketoximes **1** were synthesized *via* reported procedure (**1a** as representative).⁶



A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 1,3,3-triphenylprop-2-en-1-one (142 mg, 0.5 mmol) in EtOH (3 mL) was added hydroxylamine hydrochloride (52 mg, 0.75 mmol) and pyridine (101 μ L, 1.25 mmol) under the argon atmosphere. The reaction mixture was stirred at 60 °C in an oil bath and upon completion the reaction (monitored by TLC) mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by silica gel column chromatography to provide the desired product 1,3,3-triphenylprop-2-en-1-one oxime (**1a**).

The NMR spectrums were described as a mixture. Compounds **1w**,^{7a} **1x**,^{7b} **3^{8a}** are previously reported and showed the identical spectra according to the literature.

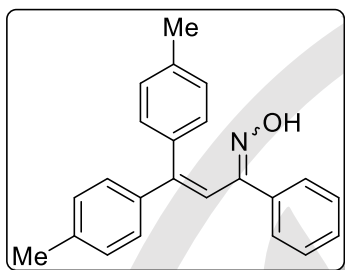
1,3,3-Triphenylprop-2-en-1-one oxime (**1a**):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 10:90); Yield: 92% (138 mg), White solid; (*E/Z* = 1:0.34, inseparable); mp 131-132 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.44 – 7.38 (m, 2H), 7.37 – 7.32 (m, 4.4H), 7.31 – 7.27 (m, 2.7H), 7.16 – 7.12 (m, 1.2H), 7.11 – 7.01 (m, 7.9H), 7.01 – 6.97 (m, 1.8H), 6.80 (s, 0.3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.2, 156.7, 149.8, 148.7, 142.4, 141.6,

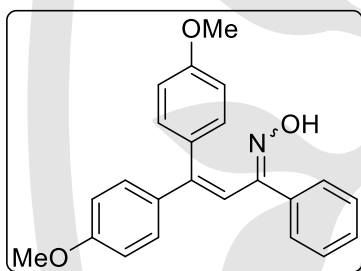
139.2, 139.1, 134.7, 132.2, 130.2, 130.0, 129.0, 128.8, 128.6, 128.5, 128.5, 128.4, 128.2, 128.2, 128.0, 127.9, 127.7, 127.6, 127.6, 127.5, 127.4, 127.2, 123.8, 118.5 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{18}NO^+$: 300.1383; found: 300.1384.

1-Phenyl-3,3-di-*p*-tolylprop-2-en-1-one oxime (1b):



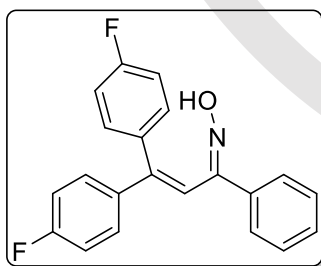
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 90% (147 mg), White solid; (*E/Z* = 1:0.17, inseparable); mp 161-162 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, J = 7.0 Hz, 2.1H), 7.30 (d, J = 8.0 Hz, 2.3H), 7.18-7.03 (m, 6.1H), 6.92 (t, J = 3.8 Hz, 3H), 6.86 (dd, J = 17.8, 6.2 Hz, 2.7H), 2.38 (s, 3H), 2.35 (s, 0.5H), 2.24 (s, 0.5H), 2.18 (s, 3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) Major isomer δ 157.4, 149.8, 139.0, 138.4, 137.7, 136.4, 134.9, 129.9, 128.9, 128.5, 128.4, 128.2, 127.7, 127.5, 117.1, 21.2, 21.1 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{22}NO^+$: 328.1696; found: 328.1697.

3,3-Bis(4-methoxyphenyl)-1-phenylprop-2-en-1-one oxime (1c):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 16:84); Yield: 89% (160 mg), White solid; (*E/Z* = 1:0.76, inseparable); mp 137-138 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.42 (dd, J = 8.8, 2.1 Hz, 4H), 7.37 – 7.31 (m, 3.1H), 7.11 – 7.03 (m, 2.2H), 6.97 (dd, J = 11.8, 8.8 Hz, 3.6H), 6.88 (dd, J = 12.6, 6.1 Hz, 4.4H), 6.56 (d, J = 8.7 Hz, 1.6H), 3.86 (s, 3H), 3.84 (s, 2.3H), 3.82 (s, 3H), 3.68 (s, 2.3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 160.6, 160.0, 159.3, 157.5, 157.1, 149.2, 134.9, 134.5, 131.9, 131.4, 131.1, 129.9, 129.4, 129.4, 129.2, 129.0, 128.4, 127.7, 127.5, 127.4, 124.9, 115.9, 113.7, 113.5, 113.5, 113.1, 113.0, 55.3, 55.3, 55.2, 55.1 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{22}NO_3^+$: 360.1594; found: 360.1596.

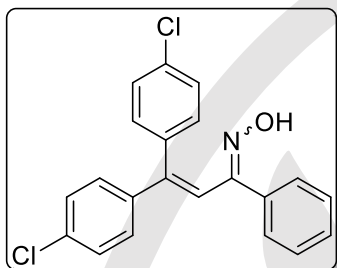
3,3-Bis(4-fluorophenyl)-1-phenylprop-2-en-1-one oxime (1d):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 85% (142 mg), White solid; (single *E*-isomer); mp 151-152 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.33 (m, 2H), 7.31 (d, J = 7.1 Hz, 2H), 7.14 (t, J = 7.3 Hz, 1H), 7.09 (t, J = 7.3 Hz, 2H), 7.04 (t, J = 8.6 Hz, 2H), 6.98 (dd, J = 8.6, 5.5 Hz, 2H), 6.96 (s, 1H), 6.74 (dd, J = 15.1, 6.5 Hz, 2H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 163.1

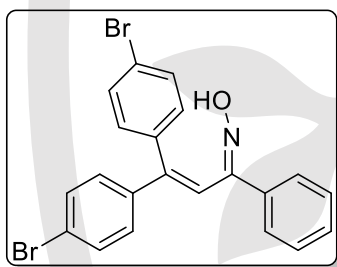
(d, $J_{C-F} = 246.3$ Hz), 162.5 (d, $J_{C-F} = 246.3$ Hz), 156.8, 147.7, 137.5 (d, $J_{C-F} = 2.5$ Hz), 135.0 (d, $J_{C-F} = 2.5$ Hz), 134.4, 131.7 (d, $J_{C-F} = 8.7$ Hz), 130.2 (d, $J_{C-F} = 8.7$ Hz), 128.8, 127.9, 127.4, 118.5, 115.3 (d, $J_{C-F} = 21.2$ Hz), 114.79 (d, $J_{C-F} = 21.2$ Hz) ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{16}F_2NO^+$: 336.1194; found: 336.1195.

3,3-Bis(4-chlorophenyl)-1-phenylprop-2-en-1-one oxime (1e):



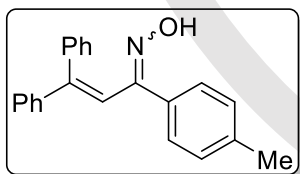
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 83% (152 mg), White solid; ($E/Z = 1:0.19$, inseparable); mp 154-155 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.24 (m, 6.7H), 7.23 – 7.14 (m, 2H), 7.11 (t, $J = 7.4$ Hz, 2H), 7.03 (dd, $J = 8.2, 6.4$ Hz, 2.3H), 6.98 (s, 1H), 6.94 (d, $J = 8.4$ Hz, 1.9H), 6.89 (d, $J = 8.4$ Hz, 0.4H), 6.78 (s, 0.2H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) Major isomer δ 156.5, 147.4, 139.5, 137.2, 134.7, 134.2, 131.4, 131.1, 129.6, 128.9, 128.6, 128.0, 128.0, 127.4, 119.3 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{16}Cl_2NO^+$: 368.0603; found: 368.0602.

3,3-Bis(4-bromophenyl)-1-phenylprop-2-en-1-one oxime (1f):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 81% (185 mg), White solid; (single E -isomer); mp 163-164 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, $J = 8.5$ Hz, 2H), 7.33 – 7.28 (m, 2H), 7.23 (d, $J = 8.5$ Hz, 2H), 7.20 – 7.15 (m, 3H), 7.12 (t, $J = 7.4$ Hz, 2H), 6.96 (s, 1H), 6.87 (d, $J = 8.4$ Hz, 2H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 156.6, 147.4, 139.9, 137.6, 134.3, 131.6, 131.4, 131.0, 129.9, 129.0, 128.0, 127.4, 123.0, 122.5, 119.3 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{16}Br_2NO^+$: 457.9573; found: 457.9571.

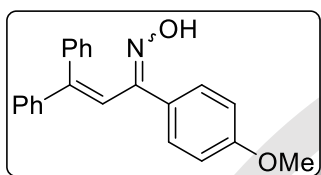
3,3-Diphenyl-1-(*p*-tolyl)prop-2-en-1-one oxime (1g):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 89% (139 mg), Yellow semi-solid; ($E/Z = 1:0.28$, inseparable); 1H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 2.2H), 7.38 – 7.32 (m, 3.1H), 7.30 (s, 1.5H), 7.25 (dd, $J = 11.1, 2.9$ Hz, 2.9H), 7.12 – 7.03 (m, 5.9H), 7.01 (dd, $J = 7.7, 1.7$ Hz, 0.6H), 6.97 (d, $J = 7.9$ Hz, 0.6H), 6.94 (s, 1H), 6.88 (d, $J = 8.0$ Hz, 2H), 6.75 (s, 0.3H), 2.25 (s, 0.8H), 2.20 (s, 3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) Major isomer δ 157.0, 149.4, 141.7, 139.2, 138.6, 131.8, 129.9, 128.5 (2C), 128.4,

128.2, 127.9, 127.6, 127.2, 118.7, 21.1 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{22}H_{20}NO^+$: 314.1539; found: 314.1549.

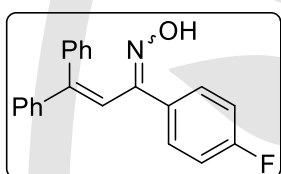
1-(4-Methoxyphenyl)-3,3-diphenylprop-2-en-1-one oxime (1h):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 14:86); Yield: 75% (123 mg), White solid; (E/Z = 1:0.14, inseparable); mp 183-184 °C; 1H NMR (500

MHz, $CDCl_3$) δ 7.40 (dt, J = 6.9, 3.2 Hz, 2.1H), 7.37 – 7.33 (m, 3.1H), 7.30 (d, J = 9.1 Hz, 2.8H), 7.12 – 7.00 (m, 5.8H), 6.94 (s, 1H), 6.61 (d, J = 8.8 Hz, 2H), 3.75 (s, 0.4H), 3.70 (s, 3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) Major isomer δ 159.5, 156.6, 149.5, 141.7, 139.2, 129.9, 128.7, 128.5, 128.4, 128.2, 128.0, 127.6, 127.1, 118.7, 113.3, 55.1 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{22}H_{20}NO_2^+$: 330.1489; found: 330.1491.

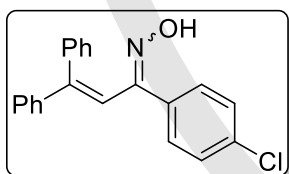
1-(4-Fluorophenyl)-3,3-diphenylprop-2-en-1-one oxime (1i):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 86% (136 mg), White solid; (E/Z = 1:0.14, inseparable); mp 119-120 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.39 (dd,

J = 6.9, 2.8 Hz, 2H), 7.37 – 7.34 (m, 3.1H), 7.32 – 7.27 (m, 3H), 7.11 – 7.03 (m, 3.6H), 7.03 – 6.99 (m, 3H), 6.96 (d, J = 6.7 Hz, 0.4H), 6.74 (t, J = 8.7 Hz, 2.1H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) Major isomer δ 162.8 (d, J_{C-F} = 246.2 Hz), 156.4, 150.1, 141.4, 139.0, 130.8 (d, J_{C-F} = 3.7 Hz), 130.0, 129.3 (d, J_{C-F} = 7.5 Hz), 128.6, 128.5, 128.3, 128.1, 127.7, 118.2, 114.7 (d, J_{C-F} = 21.2 Hz) ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{17}FNO^+$: 318.1289; found: 318.1292.

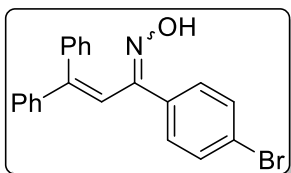
1-(4-Chlorophenyl)-3,3-diphenylprop-2-en-1-one oxime (1j):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 84% (140 mg), White solid; (E/Z = 1:0.29, inseparable); mp 133-134 °C; 1H NMR (500 MHz, $CDCl_3$) δ

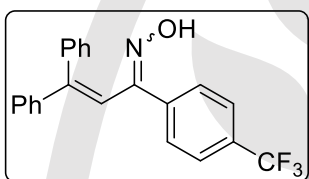
7.39 (dd, J = 7.0, 2.9 Hz, 1.8H), 7.37 – 7.33 (m, 2.7H), 7.33 – 7.28 (m, 1.4H), 7.25 (d, J = 8.8 Hz, 2.1H), 7.18 (d, J = 8.5 Hz, 0.6H), 7.13 – 6.99 (m, 7.6H), 6.97 (s, 1H), 6.81 (s, 0.3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) Major isomer δ 156.5, 150.1, 141.3, 139.0, 134.5, 133.2, 130.5, 130.0, 128.7, 128.5, 128.3, 128.2, 128.0, 127.7, 117.9 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{17}ClNO^+$: 334.0993; found: 334.0993.

1-(4-Bromophenyl)-3,3-diphenylprop-2-en-1-one oxime (1k):



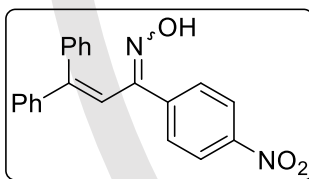
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 82% (161 mg), White solid; (*E/Z* = 1:0.20, inseparable); mp 138-139 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.39 (dd, *J* = 7.1, 2.7 Hz, 1.9H), 7.36 (dd, *J* = 5.3, 1.7 Hz, 2.9H), 7.30 (d, *J* = 1.7 Hz, 1H), 7.18 (s, 3.8H), 7.09 (ddd, *J* = 19.4, 10.4, 5.1 Hz, 3.9H), 7.03 – 6.99 (m, 1.9H), 6.98 (s, 1H), 6.81 (s, 0.2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) Major isomer δ 156.5, 150.2, 141.3, 139.0, 133.7, 130.9, 130.0, 128.9, 128.7, 128.5, 128.3, 128.2, 127.7, 122.8, 117.8 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇BrNO⁺: 378.0488; found: 378.0488.

3,3-Diphenyl-1-(4-(trifluoromethyl)phenyl)prop-2-en-1-one oxime (1l):



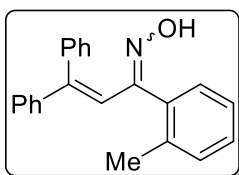
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 13:87); Yield: 78% (143 mg), White solid; (*E/Z* = 1:0.14, inseparable); mp 143-144 °C; ¹H NMR (500 MHz, CDCl₃) δ 9.35 (s, 1H), 7.40 (dd, *J* = 7.3, 2.5 Hz, 4H), 7.39 – 7.35 (m, 2.9H), 7.31 (t, *J* = 7.8 Hz, 2.9H), 7.09 – 7.00 (m, 4.4H), 6.98 (dd, *J* = 7.9, 1.6 Hz, 2.1H), 6.91 (s, 0.1H), 6.90 – 6.87 (m, 0.3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) Major isomer δ 156.5, 150.6, 141.2, 138.9, 138.4, 130.2 (q, *J*_{C-F} = 32.5 Hz), 130.0, 129.3, 128.8, 128.5, 128.3, 127.9, 127.8, 124.6 (q, *J*_{C-F} = 3.7 Hz), 123.9 (q, *J*_{C-F} = 270.0 Hz), 117.5 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₁₇F₃NO⁺: 368.1257; found: 368.1263.

1-(4-Nitrophenyl)-3,3-diphenylprop-2-en-1-one oxime (1m):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 18:82); Yield: 94% (162 mg), Yellow semi-solid; (*E/Z* = 1:0.40, inseparable); ¹H NMR (500 MHz, CDCl₃) δ 7.89 (d, *J* = 8.8 Hz, 2H), 7.44 (d, *J* = 8.9 Hz, 1.4H), 7.39 (dd, *J* = 8.7, 3.8 Hz, 3.4H), 7.34 – 7.26 (m, 2.9H), 7.07 – 6.95 (m, 5.2H), 6.90 (s, 0.4H), 6.89 – 6.86 (m, 0.8H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.0, 156.0, 150.9, 149.9, 147.5, 147.0, 141.6, 141.3, 140.9, 138.9, 138.7, 138.7, 130.3, 130.1, 130.0, 129.0, 128.7, 128.6, 128.5, 128.4, 128.3, 128.3, 127.9, 127.9, 127.8, 127.7, 122.9, 122.8, 122.5, 117.1 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇N₂O₃⁺: 345.1234; found: 345.1233.

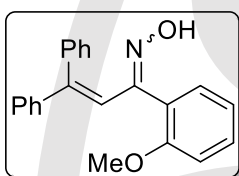
3,3-Diphenyl-1-(*o*-tolyl)prop-2-en-1-one oxime (1n):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 81% (127 mg), Yellow semi-solid; (*E/Z* = 1:0.42, inseparable); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.36 – 7.31 (m, 4.8H), 7.30

(s, 1.1H), 7.27 (d, J = 1.3 Hz, 1.9H), 7.06 – 6.85 (m, 11.2H), 6.82 (t, J = 7.3 Hz, 2.2H), 2.25 (s, 3H), 2.16 (s, 1.2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 158.5, 157.6, 149.1, 147.9, 142.4, 141.6, 138.9, 138.5, 135.8, 135.4, 134.8, 132.6, 130.1, 129.9, 129.6, 129.5, 129.4, 128.5, 128.2, 128.2, 128.2, 128.1, 128.1, 127.9, 127.6, 127.6, 127.3, 127.3, 126.9, 124.9, 123.8, 118.9, 20.8, 20.1 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{20}\text{NO}^+$: 314.1539; found: 314.1550.

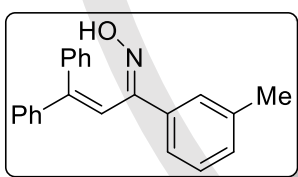
1-(2-Methoxyphenyl)-3,3-diphenylprop-2-en-1-one oxime (1o):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 14:86); Yield: 77% (127 mg), White solid; (*E/Z* = 1:0.41, inseparable); mp 162-163 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.43 – 7.36

(m, 2H), 7.36 – 7.32 (m, 2.9H), 7.29 (d, J = 6.5 Hz, 2.9H), 7.09 – 6.98 (m, 6.9H), 6.98 – 6.90 (m, 3.3H), 6.72 (t, J = 7.4 Hz, 0.4H), 6.63 (t, J = 7.4 Hz, 1H), 6.52 (dd, J = 8.4, 3.4 Hz, 1.4H), 3.72 (s, 4.2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 156.6, 156.0, 155.4, 155.1, 147.7, 147.1, 142.6, 142.1, 139.0, 138.5, 130.7, 129.8, 129.8, 129.6, 129.4, 129.4, 128.3, 128.1, 128.0 (2C), 127.9, 127.7, 127.4, 127.1, 126.9, 126.8, 124.4, 124.0, 121.8, 119.8, 119.7, 119.1, 110.2, 110.1, 55.2, 55.0 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{20}\text{NO}_2^+$: 330.1489; found: 330.1502.

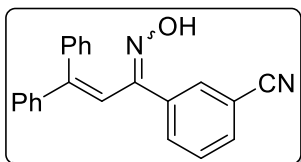
3,3-Diphenyl-1-(*m*-tolyl)prop-2-en-1-one oxime (1p):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 82% (128 mg), White solid; (single *E*-isomer); mp 147-148 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.46 –

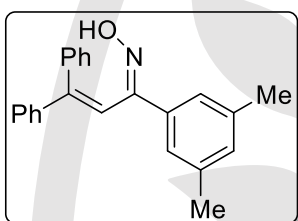
7.39 (m, 2H), 7.39 – 7.34 (m, 3H), 7.18 (d, J = 7.7 Hz, 1H), 7.12 (s, 1H), 7.09 – 7.04 (m, 5H), 7.03 (s, 1H), 6.98 (t, J = 7.6 Hz, 1H), 6.92 (d, J = 7.5 Hz, 1H), 2.18 (s, 3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 157.1, 149.7, 141.6, 139.3, 137.1, 134.5, 129.9, 129.3, 128.5, 128.4, 128.3, 128.2, 127.9, 127.7, 127.5, 124.6, 118.5, 21.1 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{20}\text{NO}^+$: 314.1539; found: 314.1539.

3-(1-(Hydroxyimino)-3,3-diphenylallyl)benzotrile (1q):



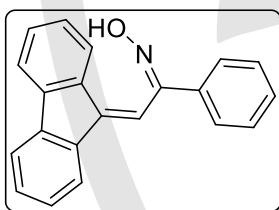
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 16:84); Yield: 72% (117 mg), White solid; (*E/Z* = 1:0.47, inseparable); mp 126-127 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.52 (d, *J* = 9.0 Hz, 1.4H), 7.43 – 7.27 (m, 7H), 7.19 – 7.11 (m, 1.1H), 7.09 – 7.02 (m, 3.8H), 7.01 – 6.95 (m, 1.4H), 6.92 – 6.86 (m, 1.1H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.8, 155.5, 150.8, 149.7, 141.6, 140.9, 138.8, 138.6, 136.0, 133.2, 133.2, 132.8, 131.7, 131.6, 131.4, 131.3, 130.2, 130.0, 128.9, 128.6, 128.5 (2C), 128.4, 128.3, 128.3, 128.1, 127.9, 127.8, 127.8, 127.7, 122.8, 118.3, 118.3, 117.1, 111.7, 111.5 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₁₇N₂O⁺: 325.1335; found: 325.1334.

1-(3,5-Dimethylphenyl)-3,3-diphenylprop-2-en-1-one oxime (1r):



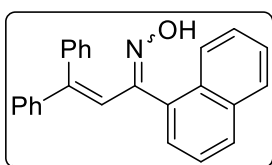
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 11:89); Yield: 85% (139 mg), White solid; (single *E*-isomer); mp 133-134 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.49 – 7.42 (m, 2H), 7.41 – 7.34 (m, 3H), 7.11 – 7.06 (m, 5H), 7.05 (s, 1H), 6.97 (s, 2H), 6.75 (s, 1H), 2.17 (s, 6H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.0, 149.5, 141.7, 139.3, 137.0, 134.3, 130.1, 129.9, 128.5, 128.4, 128.2, 127.8, 127.4, 125.4, 118.6, 21.0 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₃H₂₂NO⁺: 328.1696; found: 328.1698.

2-(9H-Fluoren-9-ylidene)-1-phenylethan-1-one oxime (1s):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 12:88); Yield: 74% (110 mg), Yellow solid; (single *E*-isomer); mp 210-211 °C; ¹H NMR (500 MHz, CDCl₃) δ 9.03 (s, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.76 – 7.72 (m, 2H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.44 – 7.32 (m, 6H), 7.28 (dd, *J* = 14.9, 7.6 Hz, 1H), 7.24 (s, 1H), 7.04 (t, *J* = 7.6 Hz, 1H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.3, 141.4, 140.8, 140.0, 138.2, 135.9, 134.1, 129.9, 129.2, 128.8, 127.2, 127.2, 127.0 (2C), 125.6, 121.0, 119.7, 119.6, 114.9 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆NO⁺: 298.1226; found: 298.1232.

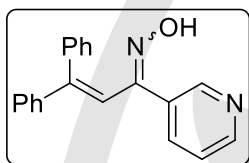
1-(Naphthalen-1-yl)-3,3-diphenylprop-2-en-1-one oxime (1t):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 13:87); Yield: 92% (161 mg), Yellow semi-solid; (*E/Z* = 1:0.37, inseparable); ¹H NMR (500 MHz, CDCl₃) δ 8.08 (d, *J* = 8.4 Hz, 1H),

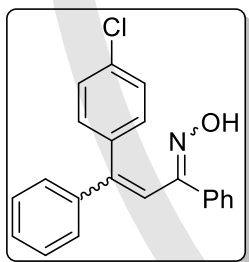
7.72 – 7.60 (m, 2H), 7.53 (d, $J = 4.1$ Hz, 1.3H), 7.50 (d, $J = 8.3$ Hz, 1.3H), 7.46 – 7.40 (m, 2H), 7.40 – 7.29 (m, 6.3H), 7.14 (dd, $J = 8.8, 5.0$ Hz, 2H), 7.07 (dd, $J = 15.3, 7.7$ Hz, 1.5H) 6.77 (t, $J = 7.3$ Hz, 1.1H), 6.73 – 6.64 (m, 2.3H), 6.60 (dd, $J = 15.4, 7.9$ Hz, 3.8H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 158.1, 157.0, 150.0, 148.4, 142.3, 141.7, 138.6, 138.1, 133.3, 133.0, 132.9, 131.4, 130.9, 130.1, 129.4, 129.3, 128.6, 128.6, 128.5, 128.2, 128.2 (2C), 128.2, 128.1, 128.0, 127.9, 127.6, 127.2, 126.8, 126.6, 126.5, 126.1, 126.1, 125.9, 125.8, 125.6, 125.6, 125.3, 124.7, 124.6, 124.3, 118.9 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{20}\text{NO}^+$: 350.1539; found: 350.1539.

3,3-Diphenyl-1-(pyridin-3-yl)prop-2-en-1-one oxime (1u):



Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 30:70); Yield: 73% (110 mg), White solid; ($E/Z = 1:0.44$, inseparable); mp 147-148 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.63 (d, $J = 1.7$ Hz, 1H), 8.50 (d, $J = 1.4$ Hz, 0.4H), 8.29 – 8.22 (m, 1.5H), 7.56 (d, $J = 8.0$ Hz, 1.1H), 7.46 (d, $J = 7.9$ Hz, 0.6H), 7.39 (dd, $J = 7.1, 2.2$ Hz, 2.1H), 7.34 (dd, $J = 5.2, 1.5$ Hz, 3.1H), 7.29 (s, 2.4H), 7.20 (d, $J = 4.3$ Hz, 0.7H), 7.12 (s, 1.3H), 7.01 (d, $J = 16.3$ Hz, 7.2H), 6.96 – 6.87 (m, 2.6H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 154.0, 153.8, 149.6, 149.3, 148.3, 148.1, 148.0, 147.8, 143.4, 142.0, 141.2, 138.9, 138.8, 136.9, 135.1, 131.6, 130.3, 130.0, 129.1, 128.6, 128.5, 128.3, 128.2, 128.2, 127.9, 127.8, 127.4, 126.4, 123.9, 122.5, 122.4, 117.9 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}^+$: 301.1335; found: 301.1334.

3-(4-Chlorophenyl)-1,3-diphenylprop-2-en-1-one oxime (1v):



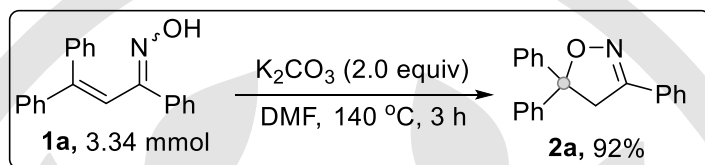
Following the general synthetic procedure GP-5. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 10:90); Yield: 84% (140 mg), White solid; ($E/Z = 0.9:1$, inseparable); mp 131-132 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.36 (s, 2.1H), 7.35 – 7.29 (m, 3.3H), 7.29 – 7.25 (m, 1.1H), 7.21 – 6.94 (m, 9.3H), 6.92 (d, $J = 8.4$ Hz, 0.3H), 6.79 (d, $J = 13.7$ Hz, 0.3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 156.8, 148.6, 148.5, 141.1, 140.1, 138.7, 137.7, 134.5, 134.5, 133.9, 131.5, 131.2, 130.1, 129.9, 129.7, 128.8, 128.7, 128.7, 128.4, 128.4, 128.3, 128.2, 127.9, 127.8, 127.8, 127.7, 127.4, 119.0, 118.8 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{17}\text{ClNO}^+$: 334.0993; found: 334.0992.

2.2 General procedure for the synthesis of isoxazolines (2a as representative): GP-6

A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 1,3,3-triphenylprop-2-en-1-one oxime (**1a**, 150 mg, 0.5 mmol), and K_2CO_3 (138 mg, 1.0 mmol)

in DMF (2.0 mL) was stirred at 140 °C in an oil bath for 3 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 98:2) to provide 3,5,5-triphenyl-4,5-dihydroisoxazole (**2a**) as white solid (144 mg, 0.48 mmol, 96% yield).

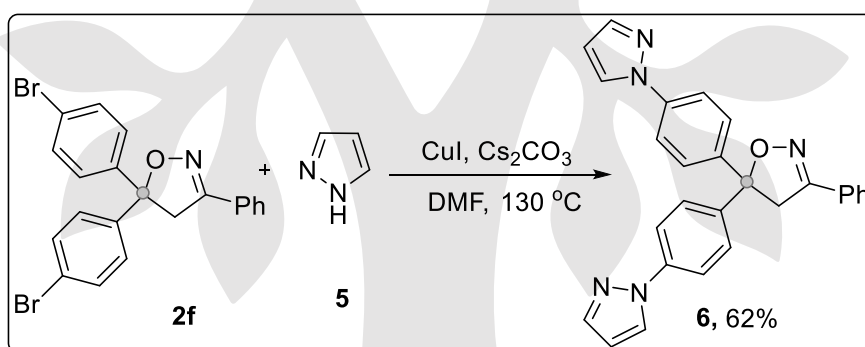
2.3 Large-scale reaction of **2a**



A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 1,3,3-triphenylprop-2-en-1-one oxime (**1a**, 1.0 g, 3.34 mmol), and K₂CO₃ (923 mg, 6.69 mmol) in DMF (5.0 mL) was stirred at 140 °C in an oil bath for 3 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 98:2) to provide 3,5,5-triphenyl-4,5-dihydroisoxazole (**2a**) as white solid (0.92 g, 3.07 mmol, 92% yield).

2.4 Post-functionalization of 2-isoxazolines

2.4.1 Ullmann-type amination reaction of 2-isoxazoline compound **2f** with pyrazole (**5**):⁹

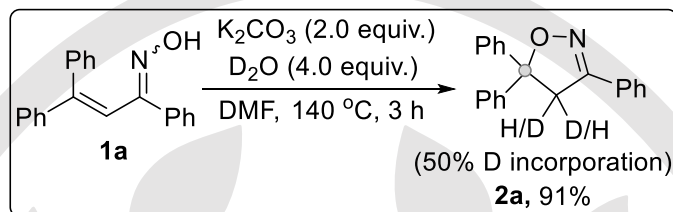


A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 5,5-bis(4-bromophenyl)-3-phenyl-4,5-dihydroisoxazole (**2f**, 50 mg, 0.109 mmol), pyrazole (**5**, 30 mg, 0.436 mmol), CuI (10 mg, 0.054 mmol), Cs₂CO₃ (284 mg, 0.87 mmol) in DMF (2.0 mL) was stirred at 140 °C in an oil bath for 24 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 80:20) to provide 5,5-bis(4-(1*H*-pyrazol-1-yl)phenyl)-3-phenyl-4,5-dihydroisoxazole (**6**) as white solid (29 mg, 0.067 mmol, 62% yield), mp 173-174 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.91 (d, *J* = 2.4 Hz, 2H), 7.71 (dd, *J* = 8.5, 6.0 Hz, 8H), 7.57 (d, *J* = 8.7 Hz, 4H), 7.43 – 7.39 (m, 3H), 6.48 – 6.44 (m, 2H), 4.02 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.4, 141.8, 141.3, 139.7, 130.4,

129.3, 128.8, 127.3, 126.7, 125.0, 119.1, 107.8, 91.3, 48.3 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{22}N_5O^+$: 432.1819; found: 432.1820.

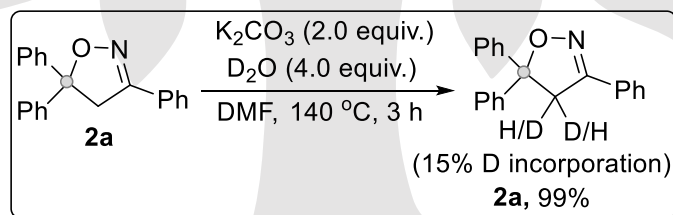
2.5 Deuterium scrambling experiments

2.5.1 Reaction of 1,3,3-triphenylprop-2-en-1-one oxime (1a) with D₂O (4.0 equiv.):



A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 1,3,3-triphenylprop-2-en-1-one oxime (**1a**, 150 mg, 0.5 mmol), K₂CO₃ (138 mg, 1.0 mmol), and D₂O (36 μ L, 2.0 mmol) in DMF (2.0 mL) was stirred at 140 °C in an oil bath for 3 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 98:2) to provide 50 % D incorporated 3,5,5-triphenyl-4,5-dihydroisoxazole (**2a**) as white solid (137 mg, 0.455 mmol, 91% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.70 (dd, J = 6.6, 3.0 Hz, 2H), 7.48 (d, J = 7.7 Hz, 4H), 7.43 – 7.31 (m, 7H), 7.31 – 7.24 (m, 2H), 3.99 (d, J = 7.1 Hz, 1H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.2, 144.1, 130.1, 129.6, 128.7, 128.4, 127.6, 126.7, 126.1, 91.9, 48.2, 47.9 (t, J_{C-D} = 20.0 Hz) ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{17}DNO^+$: 301.1446; found: 301.1441.

2.5.2 Reaction of 3,5,5-triphenyl-4,5-dihydroisoxazole (2a) with D₂O (4.0 equiv.):



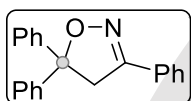
A dry screw cap pressure tube (15 mL) equipped with a magnetic stirring bar was charged with 3,5,5-triphenyl-4,5-dihydroisoxazole (**2a**, 150 mg, 0.5 mmol), K₂CO₃ (138 mg, 1.0 mmol), and D₂O (36 μ L, 2.0 mmol) in DMF (2.0 mL) was stirred at 140 °C in an oil bath for 3 h and mixture was diluted with water and extracted with ethyl acetate, dried over Na₂SO₄ and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane-EtOAc, 98:2) to provide 15 % D incorporated 3,5,5-triphenyl-4,5-dihydroisoxazole (**2a**) as white solid (149 mg, 0.496 mmol, 99% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.71 (dd, J = 6.6, 3.0 Hz, 2H), 7.50 (d, J = 7.7 Hz, 4H), 7.45 – 7.33 (m, 7H), 7.29 (t, J = 7.3 Hz, 2H), 4.00 (d, J = 7.0 Hz,

1.7H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.2, 144.0, 130.1, 129.5, 128.7, 128.4, 127.6, 126.6, 126.1, 91.9, 48.2, 47.9 (t, $J_{\text{C-D}} = 20.0$ Hz) ppm.

3. Characterization data for products

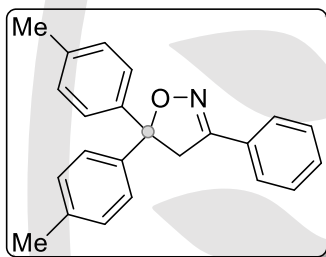
Compounds **2a**,⁶ **2g-h**,⁶ **2k-l**,⁶ **2w**,^{7c} **2x**,^{7b} **4⁸** are previously reported and showed the identical spectra according to the literature.

3,5,5-Triphenyl-4,5-dihydroisoxazole (**2a**):⁶



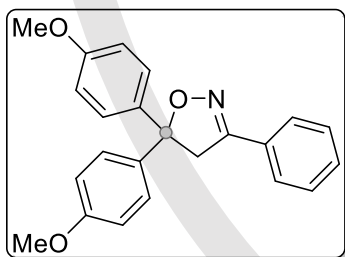
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 96% (144 mg), White solid; mp 143-144 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.73 – 7.67 (m, 2H), 7.51 – 7.45 (m, 4H), 7.42 – 7.32 (m, 7H), 7.31 – 7.26 (m, 2H), 4.00 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.2, 144.0, 130.1, 129.6, 128.7, 128.4, 127.6, 126.7, 126.1, 92.0, 48.2 ppm.

3-Phenyl-5,5-di-p-tolyl-4,5-dihydroisoxazole (**2b**):



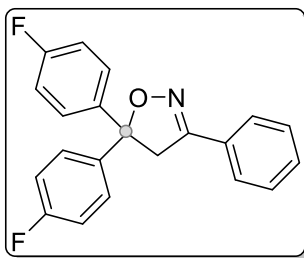
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 3:97); Yield: 91% (149 mg), White solid; mp 107-108 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.70 (dd, $J = 6.4, 2.8$ Hz, 2H), 7.45 – 7.33 (m, 7H), 7.16 (d, $J = 8.0$ Hz, 4H), 3.96 (s, 2H), 2.34 (s, 6H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.2, 141.3, 137.3, 130.0, 129.7, 129.0, 128.6, 126.6, 126.0, 91.9, 48.1, 21.0 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{23}\text{H}_{22}\text{NO}^+$: 328.1696; found: 328.1697.

5,5-Bis(4-methoxyphenyl)-3-phenyl-4,5-dihydroisoxazole (**2c**):



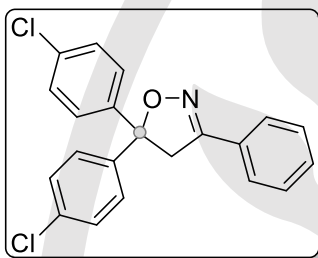
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 5:95); Yield: 92% (165 mg), Yellow solid; mp 90-91 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.74 – 7.63 (m, 2H), 7.38 (dd, $J = 9.9, 6.0$ Hz, 7H), 6.88 (d, $J = 8.7$ Hz, 4H), 3.93 (s, 2H), 3.79 (s, 6H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 159.0, 156.2, 136.3, 132.2, 130.0, 128.6, 127.4, 126.6, 113.6, 91.6, 55.2, 48.3 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{23}\text{H}_{22}\text{NO}_3^+$: 360.1594; found: 360.1596.

5,5-Bis(4-fluorophenyl)-3-phenyl-4,5-dihydroisoxazole (**2d**):



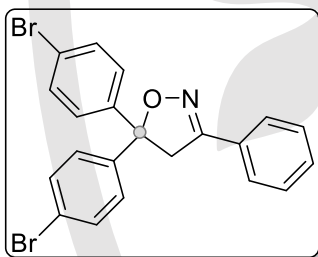
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 88% (147 mg), White solid; mp 105-106 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.75 – 7.64 (m, 2H), 7.42 (dd, $J = 8.6, 5.3$ Hz, 7H), 7.04 (t, $J = 8.6$ Hz, 4H), 3.95 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 162.2 (d, $J_{\text{C-F}} = 250.0$ Hz), 156.3, 139.6 (d, $J_{\text{C-F}} = 3.7$ Hz), 130.3, 129.3, 128.8, 127.9 (d, $J_{\text{C-F}} = 7.5$ Hz), 126.7, 115.3 (d, $J_{\text{C-F}} = 21.2$ Hz), 91.1, 48.4 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{F}_2\text{NO}^+$: 336.1194; found: 336.1190.

5,5-Bis(4-chlorophenyl)-3-phenyl-4,5-dihydroisoxazole (2e):



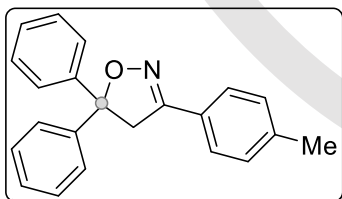
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 84% (155 mg), White solid; mp 100-101 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.74 – 7.63 (m, 2H), 7.46 – 7.36 (m, 7H), 7.32 (d, $J = 8.5$ Hz, 4H), 3.94 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.3, 142.0, 133.9, 130.4, 129.1, 128.8, 128.7, 127.5, 126.7, 91.0, 48.1 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{Cl}_2\text{NO}^+$: 368.0603; found: 368.0606.

5,5-Bis(4-bromophenyl)-3-phenyl-4,5-dihydroisoxazole (2f):



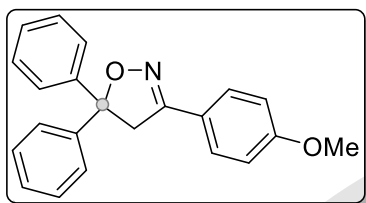
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 81% (185 mg), White solid; mp 118-119 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.67 (d, $J = 5.4$ Hz, 2H), 7.48 (d, $J = 8.4$ Hz, 4H), 7.40 (d, $J = 5.7$ Hz, 3H), 7.32 (d, $J = 8.3$ Hz, 4H), 3.92 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.3, 142.5, 131.7, 130.4, 129.1, 128.8, 127.8, 126.7, 122.1, 91.1, 48.0 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{Br}_2\text{NO}^+$: 457.9573; found: 457.9571.

5,5-Diphenyl-3-(p-tolyl)-4,5-dihydroisoxazole (2g):⁶



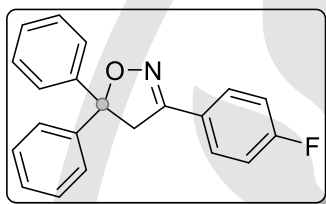
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 86% (135 mg), White solid; mp 129-130 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.60 (d, $J = 8.1$ Hz, 2H), 7.49 (d, $J = 7.7$ Hz, 4H), 7.36 (t, $J = 7.6$ Hz, 4H), 7.28 (dd, $J = 12.8, 5.5$ Hz, 2H), 7.21 (d, $J = 8.0$ Hz, 2H), 3.99 (s, 2H), 2.38 (s, 3H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.2, 144.1, 140.3, 129.3, 128.4, 127.6, 126.7, 126.6, 126.1, 91.7, 48.3, 21.4 ppm.

3-(4-Methoxyphenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2h):⁶



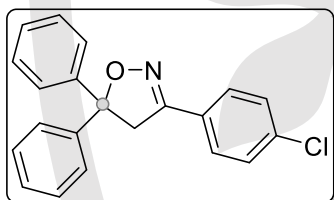
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 4:96); Yield: 84% (138 mg), Yellow solid; mp 143-144 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.65 (d, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 7.7 Hz, 4H), 7.35 (t, *J* = 7.6 Hz, 4H), 7.28 (dd, *J* = 12.5, 5.3 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 3.98 (s, 2H), 3.82 (s, 3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 161.0, 155.8, 144.2, 128.3, 128.2, 127.5, 126.1, 122.1, 114.1, 91.6, 55.3, 48.4 ppm.

3-(4-Fluorophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2i):



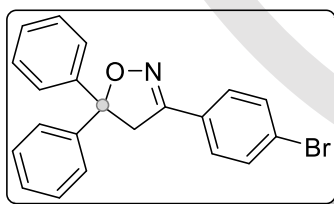
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 74% (117 mg), White solid; mp 121-122 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.72 – 7.64 (m, 2H), 7.49 – 7.42 (m, 4H), 7.38 – 7.32 (m, 4H), 7.27 (t, *J* = 7.3 Hz, 2H), 7.07 (t, *J* = 8.7 Hz, 2H), 3.96 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 163.8 (d, *J*_{C-F} = 248.7 Hz), 155.2, 143.9, 128.6, 128.6, 128.4, 127.7, 126.0, 115.8 (d, *J*_{C-F} = 21.2 Hz), 92.1, 48.3 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇FNO⁺: 318.1289; found: 318.1287.

3-(4-Chlorophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2j):



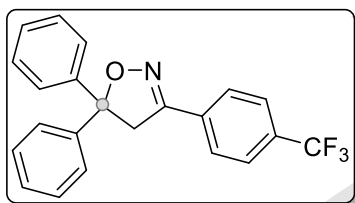
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 71% (119 mg), White solid; mp 139-140 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.63 (d, *J* = 8.5 Hz, 2H), 7.46 (d, *J* = 7.6 Hz, 4H), 7.36 (dd, *J* = 12.1, 4.9 Hz, 6H), 7.28 (t, *J* = 7.3 Hz, 2H), 3.96 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.3, 143.9, 136.1, 129.0, 128.5, 128.1, 127.9, 127.7, 126.0, 92.3, 48.0 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇ClNO⁺: 334.0993 found: 334.0991.

3-(4-Bromophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2k):⁶



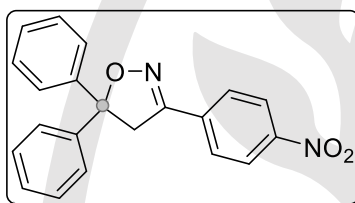
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 68% (129 mg), White solid; mp 170-171 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.51 (dd, *J* = 13.3, 8.2 Hz, 6H), 7.37 (t, *J* = 7.5 Hz, 4H), 7.30 (t, *J* = 7.1 Hz, 2H), 3.98 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.4, 143.8, 131.8, 128.4, 128.0, 127.7, 126.0 (2C), 124.3, 92.3, 47.9 ppm.

5,5-Diphenyl-3-(4-(trifluoromethyl)phenyl)-4,5-dihydroisoxazole (2l):⁶



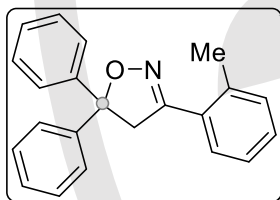
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 3:97); Yield: 65% (119 mg), White solid; mp 134-135 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.52 – 7.44 (m, 4H), 7.40 – 7.33 (m, 4H), 7.33 – 7.27 (m, 2H), 4.00 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.2, 143.7, 133.0, 131.8 (q, *J*_{C-F} = 32.6 Hz), 128.5, 127.8, 126.9, 126.0, 125.7 (q, *J*_{C-F} = 4.0 Hz), 123.8 (q, *J*_{C-F} = 270.6 Hz), 92.7, 47.8 ppm.

3-(4-Nitrophenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2m):



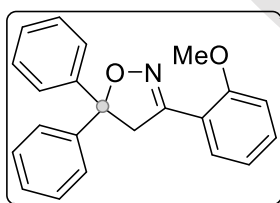
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 5:95); Yield: 63% (108 mg), Yellow solid; mp 139-140 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.25 (d, *J* = 8.8 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 4H), 7.37 (t, *J* = 7.6 Hz, 4H), 7.30 (t, *J* = 7.3 Hz, 2H), 4.02 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 154.7, 148.4, 143.4, 135.6, 128.5, 127.9, 127.3, 125.9, 124.0, 93.3, 47.6 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₇N₂O₃⁺: 345.1234 found: 345.1226.

5,5-Diphenyl-3-(*o*-tolyl)-4,5-dihydroisoxazole (2n):



Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 71% (111 mg), White solid; mp 93-94 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.49 (d, *J* = 7.8 Hz, 4H), 7.35 (dd, *J* = 15.8, 7.9 Hz, 5H), 7.27 (dd, *J* = 12.6, 4.7 Hz, 4H), 7.21 (t, *J* = 7.1 Hz, 1H), 4.03 (s, 2H), 2.53 (s, 3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 157.3, 144.0, 138.0, 131.5, 129.4, 128.7, 128.7, 128.4, 127.6, 126.1, 125.7, 90.9, 50.5, 22.7 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₂H₂₀NO⁺: 314.1539 found: 314.1541.

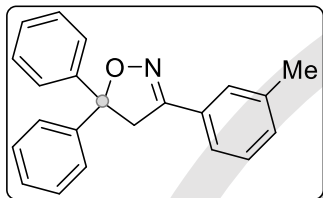
3-(2-Methoxyphenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2o):



Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 3:97); Yield: 75% (123 mg), White solid; mp 151-152 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.76 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.52 – 7.46 (m, 4H), 7.34 (ddd, *J* = 10.0, 6.1, 2.6 Hz, 5H), 7.27 (ddd, *J* = 7.7, 4.1, 1.4 Hz, 2H), 6.95 (td, *J* = 7.6, 1.0 Hz, 1H), 6.91 (d, *J* = 8.3 Hz, 1H), 4.09 (s, 2H), 3.83 (s, 3H) ppm; ¹³C {¹H} NMR

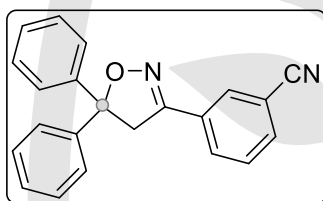
(125 MHz, CDCl₃) δ 157.5, 144.3, 131.3, 129.4, 128.4, 128.3, 127.4, 126.5, 126.2, 120.8, 111.4, 91.6, 55.5, 50.6 ppm; HRMS (ESI-TOF): m/z [M+H]⁺ calcd for C₂₂H₂₀NO₂⁺: 330.1489 found: 330.1490.

5,5-Diphenyl-3-(*m*-tolyl)-4,5-dihydroisoxazole (2p):



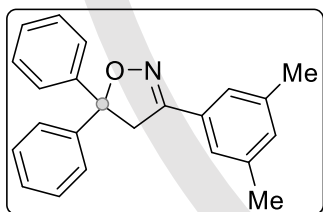
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 78% (122 mg), White solid; mp 118-119 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.54 (s, 1H), 7.48 (dd, J = 8.2, 0.9 Hz, 5H), 7.35 (dd, J = 10.4, 4.8 Hz, 4H), 7.30 – 7.25 (m, 3H), 7.21 (d, J = 7.6 Hz, 1H), 3.99 (s, 2H), 2.37 (s, 3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.4, 144.1, 138.4, 130.9, 129.4, 128.6, 128.4, 127.6, 127.2, 126.1, 123.8, 91.9, 48.3, 21.3 ppm; HRMS (ESI-TOF): m/z [M+H]⁺ calcd for C₂₂H₂₀NO⁺: 314.1539 found: 314.1539.

3-(5,5-Diphenyl-4,5-dihydroisoxazol-3-yl)benzonitrile (2q):



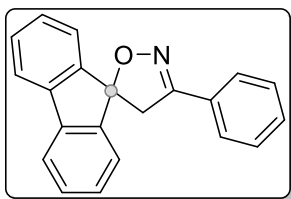
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 4:96); Yield: 66% (107 mg), White solid; mp 141-142 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.96 (d, J = 7.9 Hz, 1H), 7.93 (s, 1H), 7.66 (d, J = 7.6 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.47 (d, J = 7.6 Hz, 4H), 7.37 (t, J = 7.5 Hz, 4H), 7.30 (t, J = 7.2 Hz, 2H), 3.99 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 154.5, 143.4, 133.1, 130.9, 130.5, 130.0, 129.6, 128.5, 127.8, 125.9, 118.0, 113.0, 92.8, 47.5 ppm; HRMS (ESI-TOF): m/z [M+H]⁺ calcd for C₂₂H₁₇N₂O⁺: 325.1335 found: 325.1338.

3-(3,5-Dimethylphenyl)-5,5-diphenyl-4,5-dihydroisoxazole (2r):



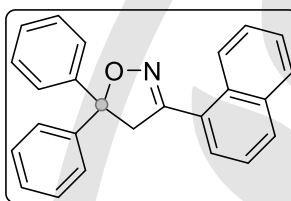
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 86% (141 mg), White solid; mp 133-134 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.47 (d, J = 7.4 Hz, 4H), 7.34 (dd, J = 13.7, 5.8 Hz, 6H), 7.29 – 7.25 (m, 2H), 7.03 (s, 1H), 3.97 (s, 2H), 2.32 (s, 6H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.5, 144.1, 138.3, 131.8, 130.0, 128.4, 127.6, 126.1, 124.5, 91.8, 48.3, 21.2 ppm; HRMS (ESI-TOF): m/z [M+H]⁺ calcd for C₂₃H₂₂NO⁺: 328.1696 found: 328.1697.

3'-Phenyl-4'H-spiro[fluorene-9,5'-isoxazole] (2s):



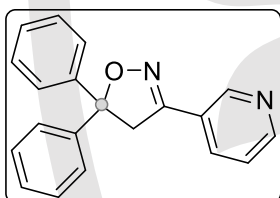
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 94% (140 mg), Yellow solid; mp 131-132 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.83 – 7.76 (m, 2H), 7.65 (d, $J = 7.5$ Hz, 2H), 7.53 (d, $J = 7.5$ Hz, 2H), 7.50 – 7.45 (m, 3H), 7.41 (t, $J = 7.5$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 2H), 3.87 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 157.0, 146.2, 139.8, 130.2, 129.7, 129.5, 128.8, 128.5, 126.8 (2C), 123.6, 120.0, 92.2, 45.1 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{NO}^+$: 298.1226 found: 298.1228.

3-(Naphthalen-1-yl)-5,5-diphenyl-4,5-dihydroisoxazole (2t):



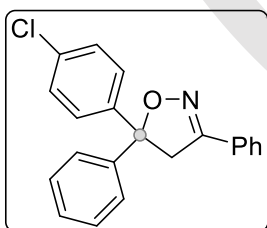
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 94% (164 mg), White solid; mp 127-128 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.96 (d, $J = 8.6$ Hz, 1H), 7.88 (t, $J = 7.5$ Hz, 2H), 7.63 – 7.51 (m, 7H), 7.48 – 7.43 (m, 1H), 7.42 – 7.36 (m, 4H), 7.34 – 7.28 (m, 2H), 4.20 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 157.1, 144.0, 133.9, 130.8, 130.6, 128.5, 128.4, 127.6, 127.6, 127.5, 126.9, 126.5, 126.3, 126.1, 124.7, 90.8, 50.9 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{25}\text{H}_{20}\text{NO}^+$: 350.1539 found: 350.1544.

5,5-Diphenyl-3-(pyridin-3-yl)-4,5-dihydroisoxazole (2u):



Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 5:95); Yield: 77% (116 mg), White solid; mp 169-170 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.85 (s, 1H), 8.63 (s, 1H), 8.09 (d, $J = 8.0$ Hz, 1H), 7.47 (d, $J = 7.5$ Hz, 4H), 7.39 – 7.32 (m, 5H), 7.29 (t, $J = 7.3$ Hz, 2H), 4.00 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 153.9, 151.0, 147.6, 143.6, 133.7, 128.5, 127.8, 126.0 (2C), 123.7, 92.5, 47.6 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}^+$: 301.1335 found: 301.1340.

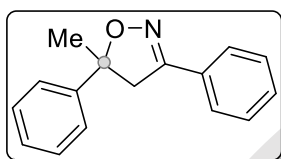
5-(4-Chlorophenyl)-3,5-diphenyl-4,5-dihydroisoxazole (2v):



Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 4:96); Yield: 88% (147 mg), White solid; mp 161-162 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.69 (dd, $J = 6.5, 3.0$ Hz, 2H), 7.46 (d, $J = 7.6$ Hz, 2H), 7.43 – 7.39 (m, 5H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.30 (dd, $J = 14.6, 7.9$ Hz, 3H), 3.96 (q, $J = 16.5$ Hz, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 156.3,

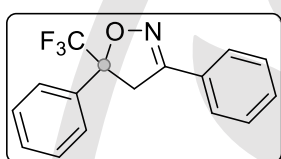
143.5, 142.7, 133.6, 130.3, 129.4, 128.7, 128.6, 128.5, 127.9, 127.6, 126.7, 126.0, 91.5, 48.2 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{17}ClNO^+$: 334.0993; found: 334.0992.

5-Methyl-3,5-diphenyl-4,5-dihydroisoxazole (2w):^{7c}



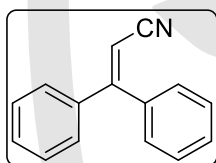
Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 94% (112 mg), White solid; 1H NMR (500 MHz, $CDCl_3$) δ 7.73 – 7.64 (m, 2H), 7.52 (d, J = 7.5 Hz, 2H), 7.43 – 7.35 (m, 5H), 7.29 (t, J = 7.3 Hz, 1H), 3.51 (q, J = 16.4 Hz, 2H), 1.83 (s, 3H) ppm; ^{13}C { 1H } NMR (125 MHz, $CDCl_3$) δ 156.1, 145.4, 129.9, 129.8, 128.6, 128.4, 127.3, 126.5, 124.6, 88.0, 48.7, 28.2 ppm.

3,5-Diphenyl-5-(trifluoromethyl)-4,5-dihydroisoxazole (2x):^{7b}



Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 2:98); Yield: 90% (131 mg), White solid; 1H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.59 (m, 4H), 7.48 – 7.36 (m, 6H), 3.93 (q, J = 17.0, 2H) ppm; ^{13}C { 1H } NMR (125 MHz, $CDCl_3$) δ 156.0, 135.7, 130.8, 129.3, 128.8, 128.6, 128.1, 126.8, 126.6, 124.3 (q, J_{C-F} = 282.5 Hz), 87.8 (q, J_{C-F} = 30.0 Hz), 44.0 ppm.

3,3-Diphenylacrylonitrile (4):⁸



Following the general synthetic procedure GP-6. The reaction mixture was purified by silica gel column chromatography (EtOAc: petroleum ether, 1:99); Yield: 88% (90 mg), Pale yellow oil; 1H NMR (500 MHz, $CDCl_3$) δ 7.50 – 7.42 (m, 6H), 7.38 (t, J = 7.5 Hz, 2H), 7.31 (d, J = 7.4 Hz, 2H), 5.75 (s, 1H) ppm; ^{13}C { 1H } NMR (125 MHz, $CDCl_3$) δ 163.1, 138.9, 137.0, 130.4, 130.0, 129.5, 128.6, 128.5, 128.4, 117.8, 94.8 ppm.

4. Single Crystal X-ray Structure of 2o

Crystallization: Crystal of compound **2o** (15 mg) was grown in 1 mL of $CHCl_3$ by slow evaporation method for 5 days.

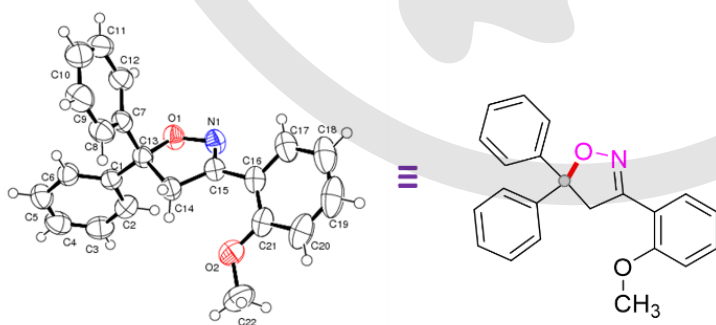


Figure S1: X-ray crystallography of **2o** (the ellipsoid contour probability level is 50%).

Table S1: Crystal data and structure refinement for **2o**.

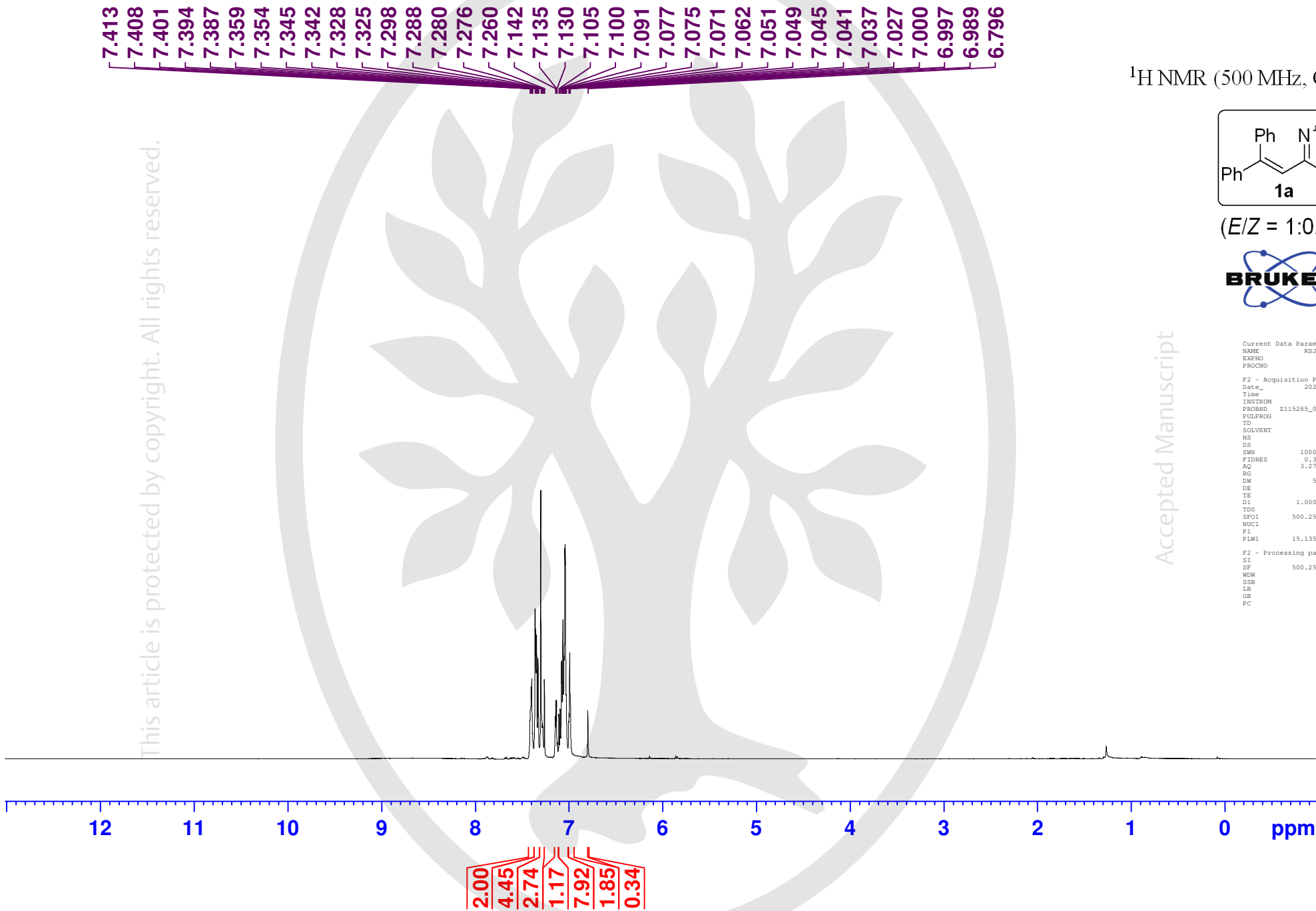
CCDC Number	2313318
Empirical formula	C ₂₂ H ₁₉ NO ₂
Formula weight	329.38
Temperature	298(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 9.4474(2) Å α = 66.3850(10)°. b = 10.4369(2) Å β = 89.6330(10)°. c = 10.8920(2) Å γ = 63.8430(10)°.
Volume	864.14(3) Å ³
Z	2
Density (calculated)	1.266 Mg/m ³
Absorption coefficient	0.641 mm ⁻¹
F(000)	348
Crystal size	0.155 x 0.145 x 0.070 mm ³
Theta range for data collection	4.528 to 70.452°.
Index ranges	-10 ≤ h ≤ 11, -12 ≤ k ≤ 12, -13 ≤ l ≤ 13
Reflections collected	28945
Independent reflections	3304 [R(int) = 0.0473]
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9424 and 0.8388
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3304 / 0 / 228
Goodness-of-fit on F ²	1.032
Final R indices [I > 2σ(I)]	R ₁ = 0.0386, wR ₂ = 0.0938
R indices (all data)	R ₁ = 0.0497, wR ₂ = 0.1031
Extinction coefficient	0.0076(9)
Largest diff. peak and hole	0.158 and -0.152 e.Å ⁻³

5. References

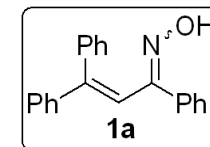
1. (a) *SAINT-Plus, version 6.45*, Bruker AXS Inc., Madison, WI, 2003. (b) G. M. Sheldrick, *SADABS, Program for Empirical Absorption Correction of Area Detector Data*, University of Gottingen, Germany, 1997. (c) *SMART (version 5.625), SHELX-TL (version 6.12)*, Bruker AXS Inc., Madison, WI, 2000. (d) G. M. Sheldrick, *SHELXS-97*, University of Gottingen, Germany, 1997.
2. (a) Liu, T.; Qiao, J. X.; Poss, M. A.; Yu, J.-Q. *Angew. Chem. Int. Ed.* **2017**, *56*, 10924. (b) Zhang, X.; Teo, W. T.; Chan, P. W. H. *Org. Lett.* **2009**, *11*, 4990–4993.
3. (a) Zheng, H.; Lejkowski, M.; Hall, D. G. *Chem. Sci.* **2011**, *2*, 1305–1310.
4. (a) Zhou, N.-N.; Ning, S.-S.; Tong, X.-J.; Luo, T.-T.; Yang, J.; Li, L.-Q.; Fan, M.-J.; Yang, D.-S.; Zhu, H.-T. *J. Org. Chem.*, **2019**, *84*, 8497-8508. (b) Zhu, H.-T.; Dong, X.; Wang, L.-J.; Zhong, M.-J.; Liu, X.-Y.; Liang, Y.-M. *Chem. Commun.*, **2012**, *48*, 10748-10750. (c) Olaizola, I.; Campano, T. E.; Iriarte, I.; Vera, S.; Mielgo, A.; Garcia, J. M.; Odriozola, J. M.; Oiarbide, M.; Palomo, C. *Chem.–Eur. J.* **2018**, *24*, 3893–3901.
5. Jat, R. S.; Bhanuchandra, M. *J. Org. Chem.* **2023**, *88*, 13184-13190.
6. Zhu, X.; Wang, Y. F.; Ren, W.; Zang, F. L.; Chiba, S. *Org. Lett.* **2013**, *15*, 3214-3217.
7. (a) Luo, G.; Huang, Z.; Zhuo, S.; Mou, C.; Wu, J.; Jin, Z.; Chi, Y. R. *Angew. Chem. Int. Ed.* **2019**, *58*, 17189-17193; *Angew. Chem.* **2019**, *131*, 17349-17353. (b) Matoba, K.; Kawai, H.; Furukawa, T.; Kusuda, A.; Tokunaga, E.; Nakamura, S.; Shiro, M.; Shibata, N. *Angew. Chem., Int. Ed.* **2010**, *49*, 5762–5766. (c) Mondal, S.; Biswas, S.; Ghosh, K. G.; Sureshkumar, D. *Chem Asian J.* **2021**, *16*, 2439–2446.
8. (a) Zhang, Q.; Zhang, L.; Tang, C.; Luo, H.; Cai, X.; Chai, Y. *Tetrahedron* **2016**, *72*, 6935-6942. (b) Hao, L.; Wu, F.; Ding, Z.; Xu, S.; Ma, Y.; Chen, L.; Zhan, Z. *Chem. - Eur. J.* **2012**, *18*, 6453–6456.
9. Panda, S.; Jat, R. S.; Fayaz, A.; Saha, J.; Thirumoorthi, R.; Roy, T. K. Bhanuchandra, M. *New J. Chem.* **2020**, *44*, 8944-8951.

6. NMR Spectra

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.34)



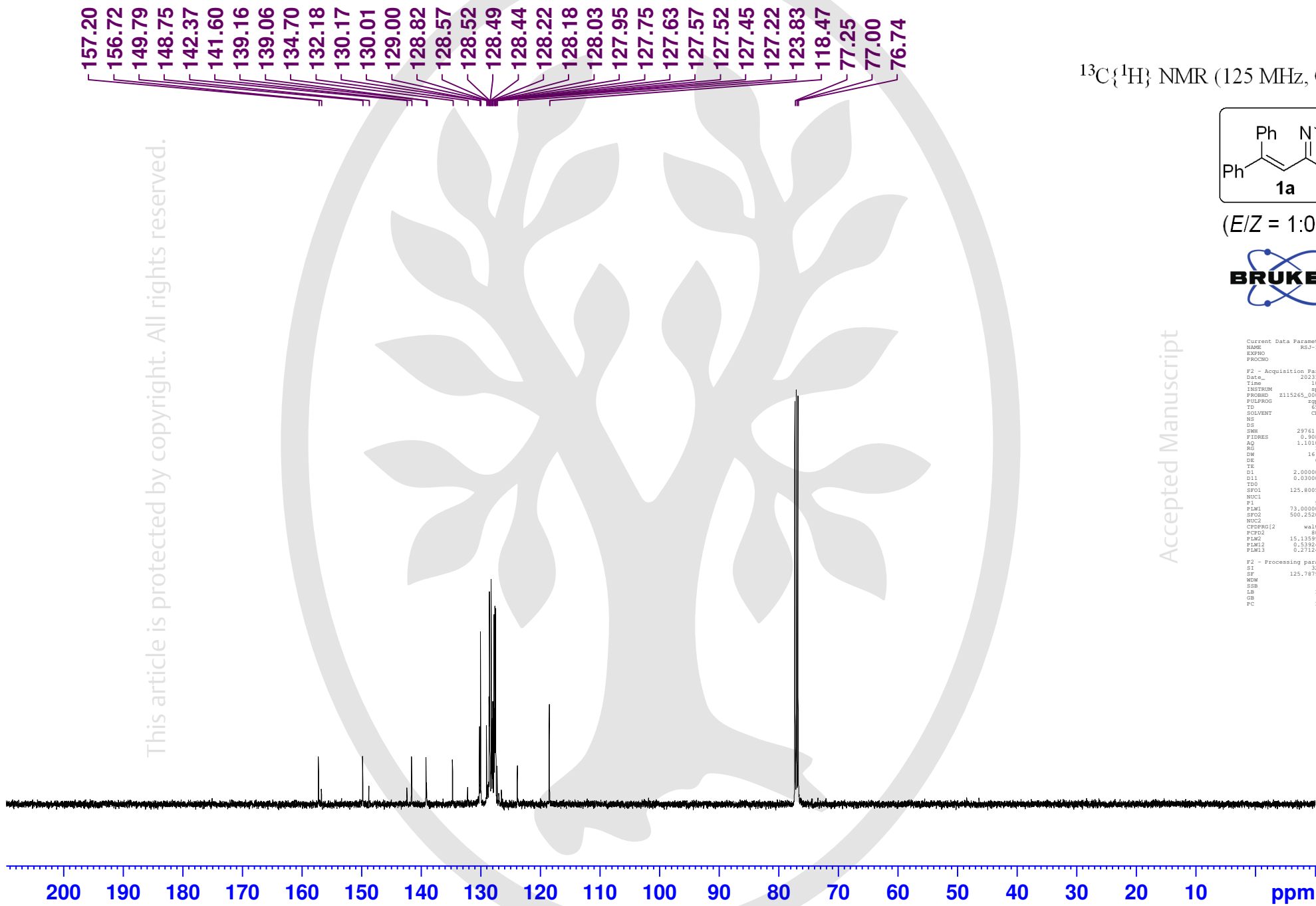
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PROCNO    1

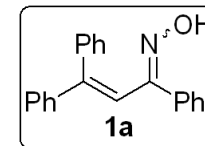
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RG         228
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SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
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SF         500.2500137 MHz
WDW        EM
SSB        0
LB         0.30 Hz
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PC         1.00
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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.34)



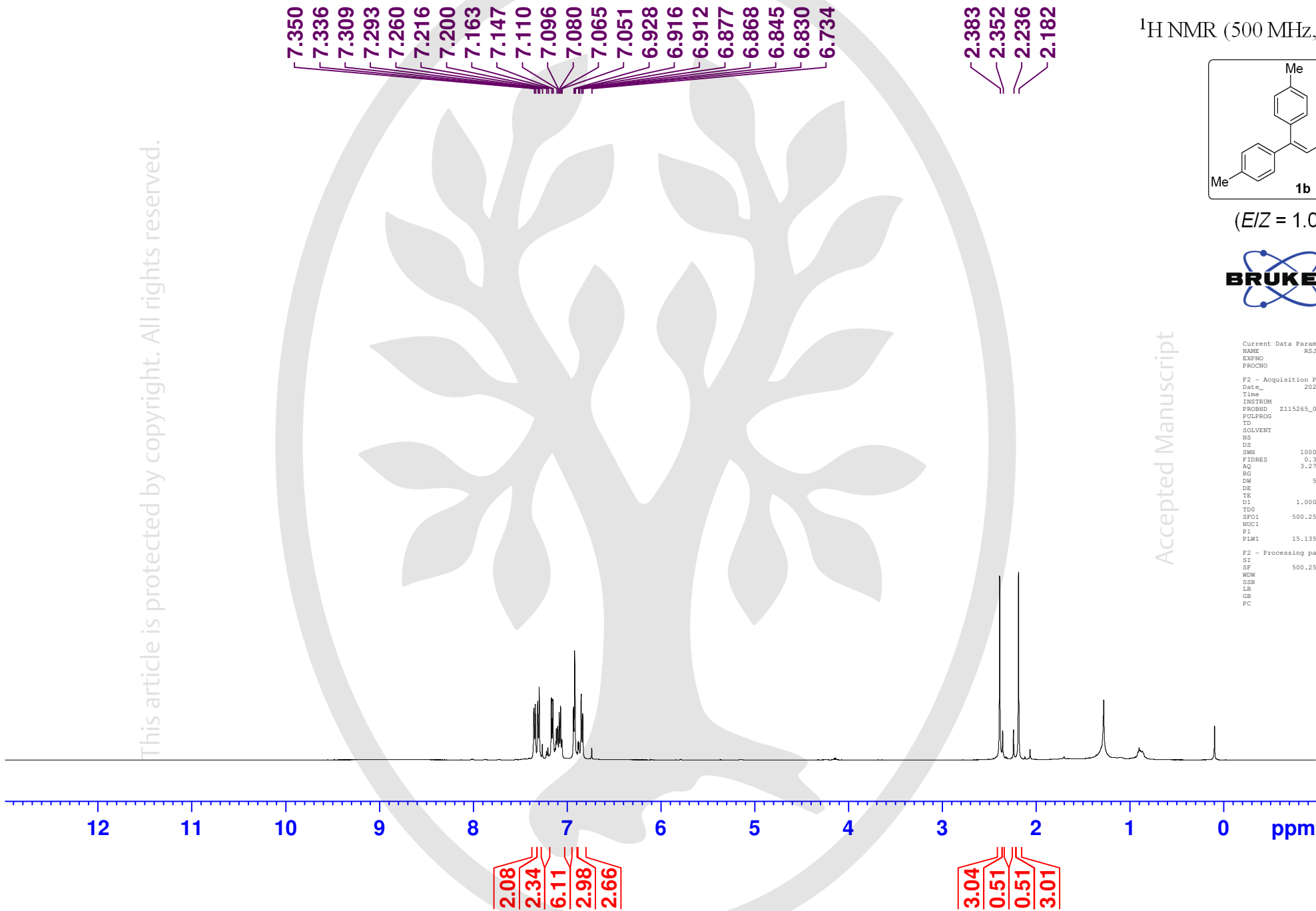
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FIDRES    0.908261 Hz
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D11        0.0300000 sec
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PLM1      73.0000000 W
SFO2      500.2550010 MHz
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PLM13     0.27124000 W

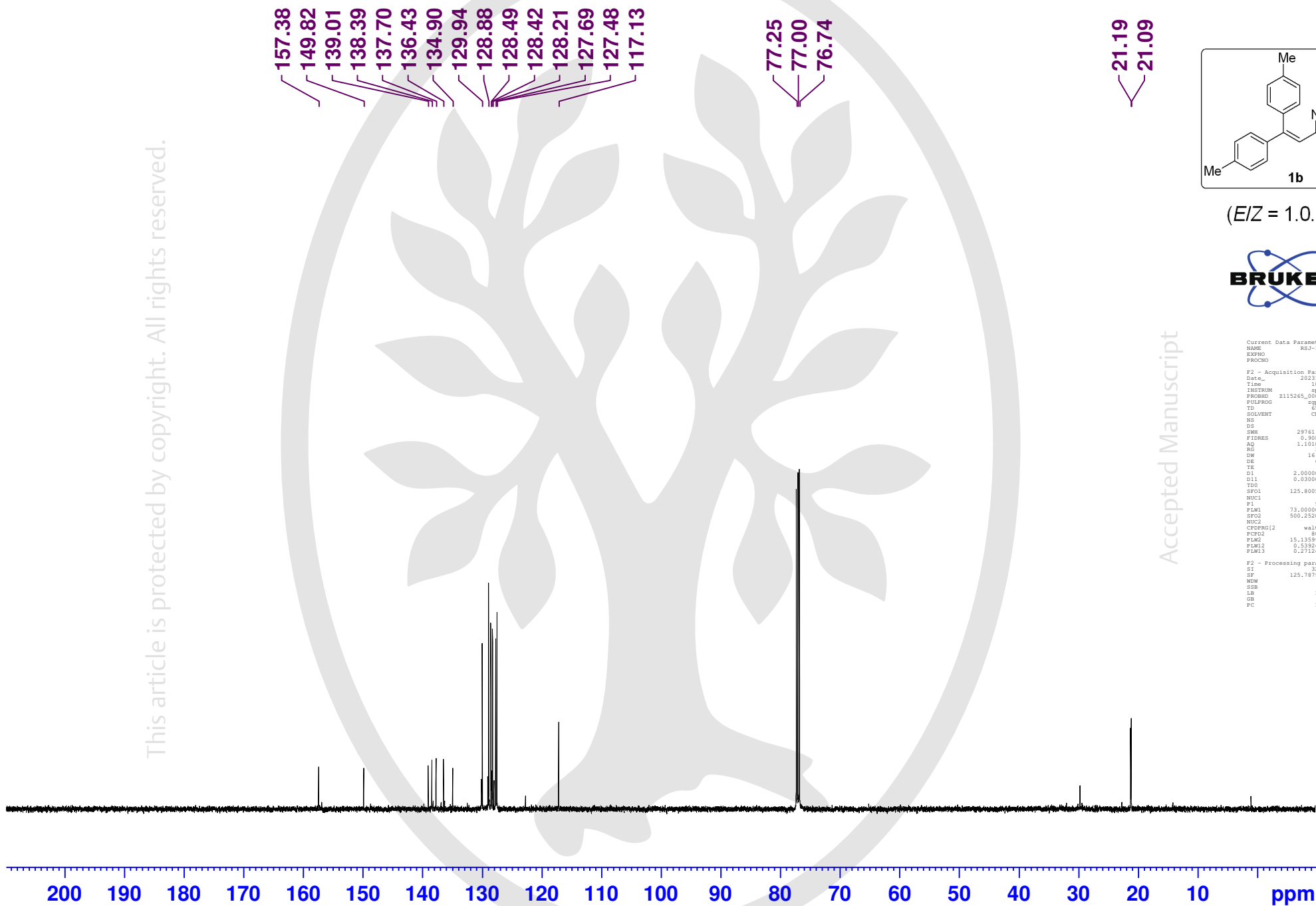
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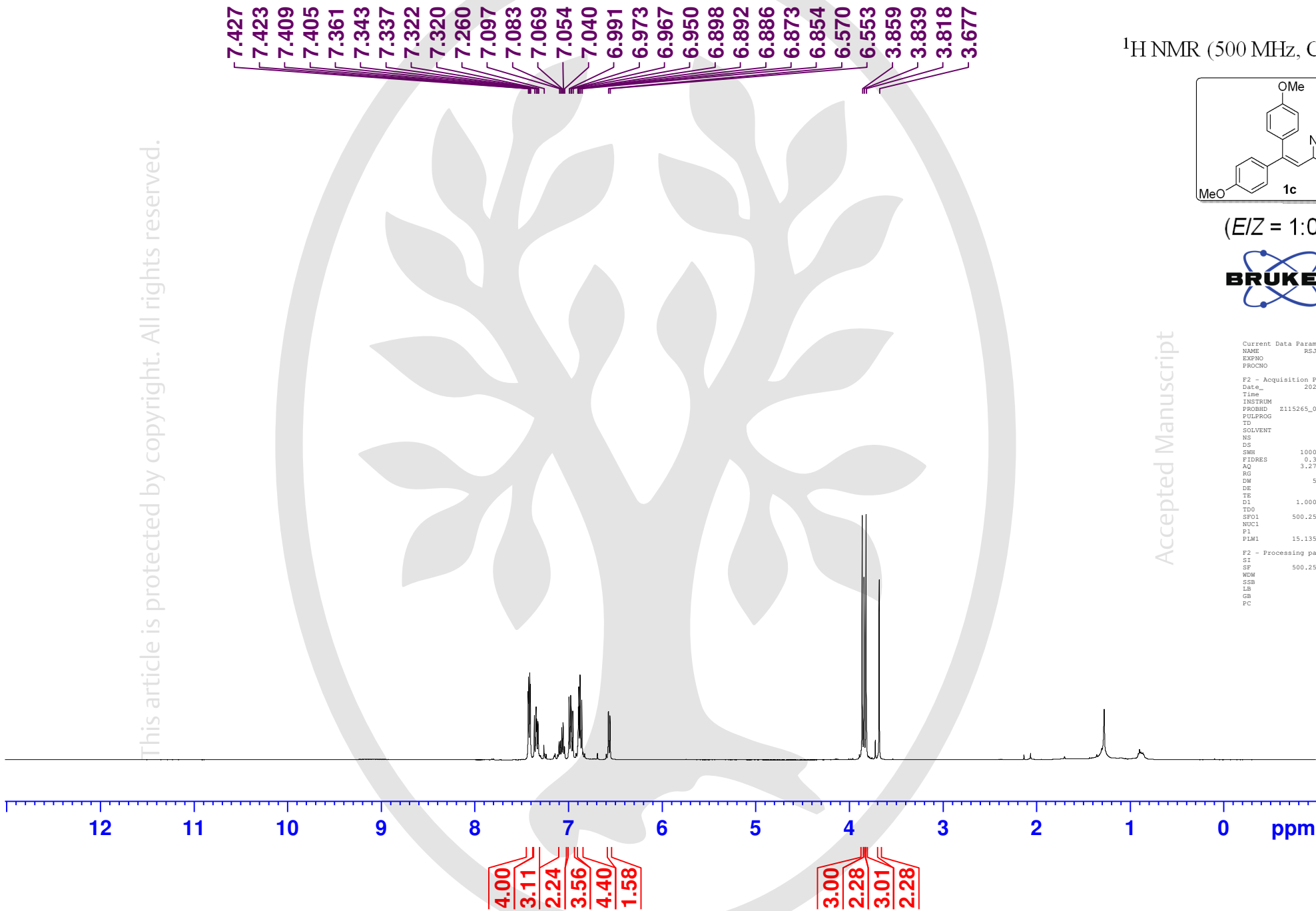
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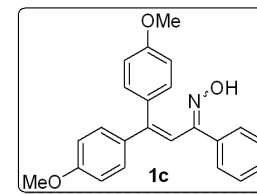
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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.76)



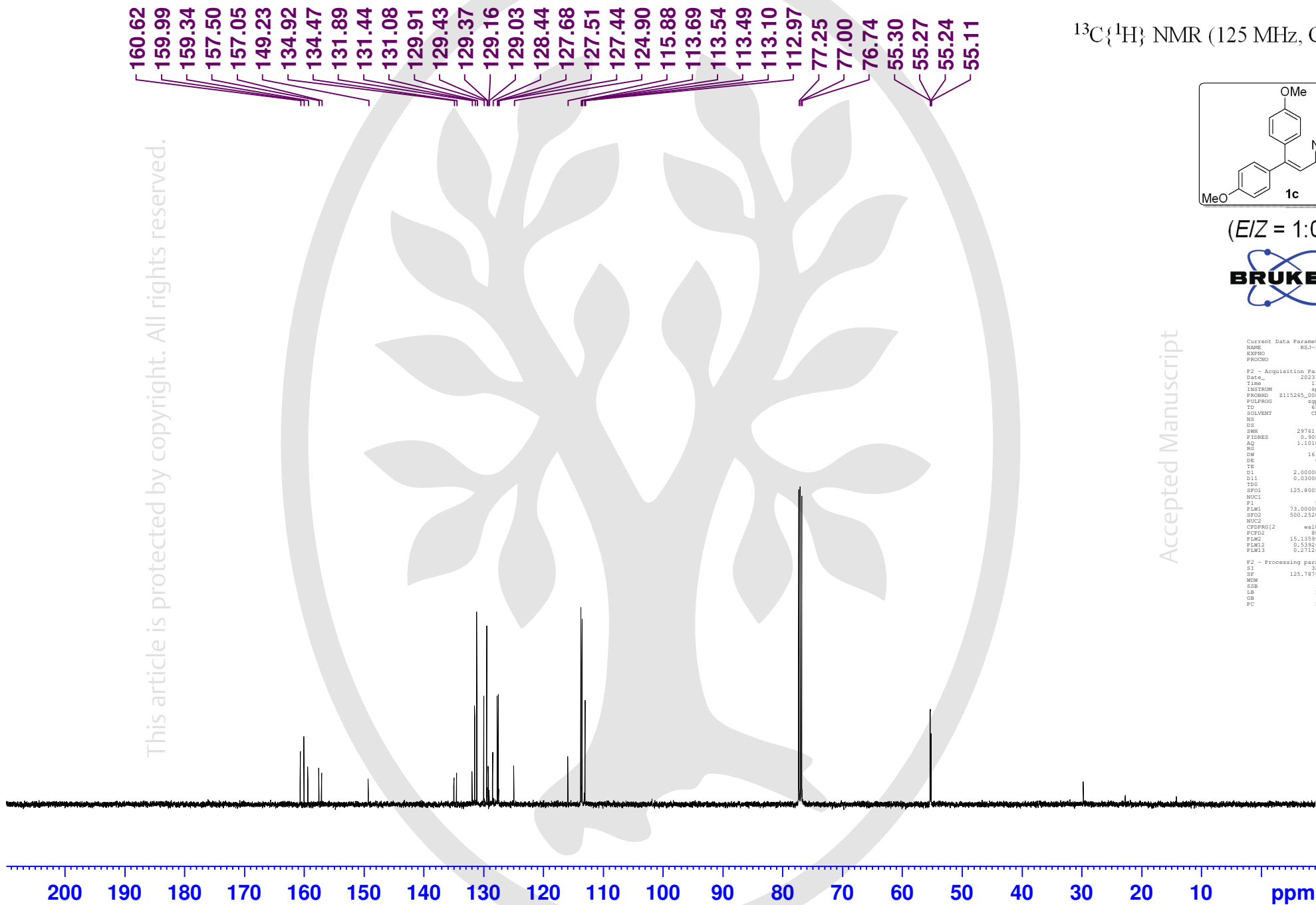
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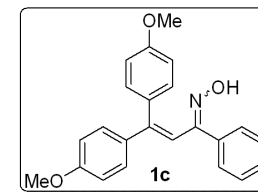
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SSB        0
LB         0.30 Hz
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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.76)



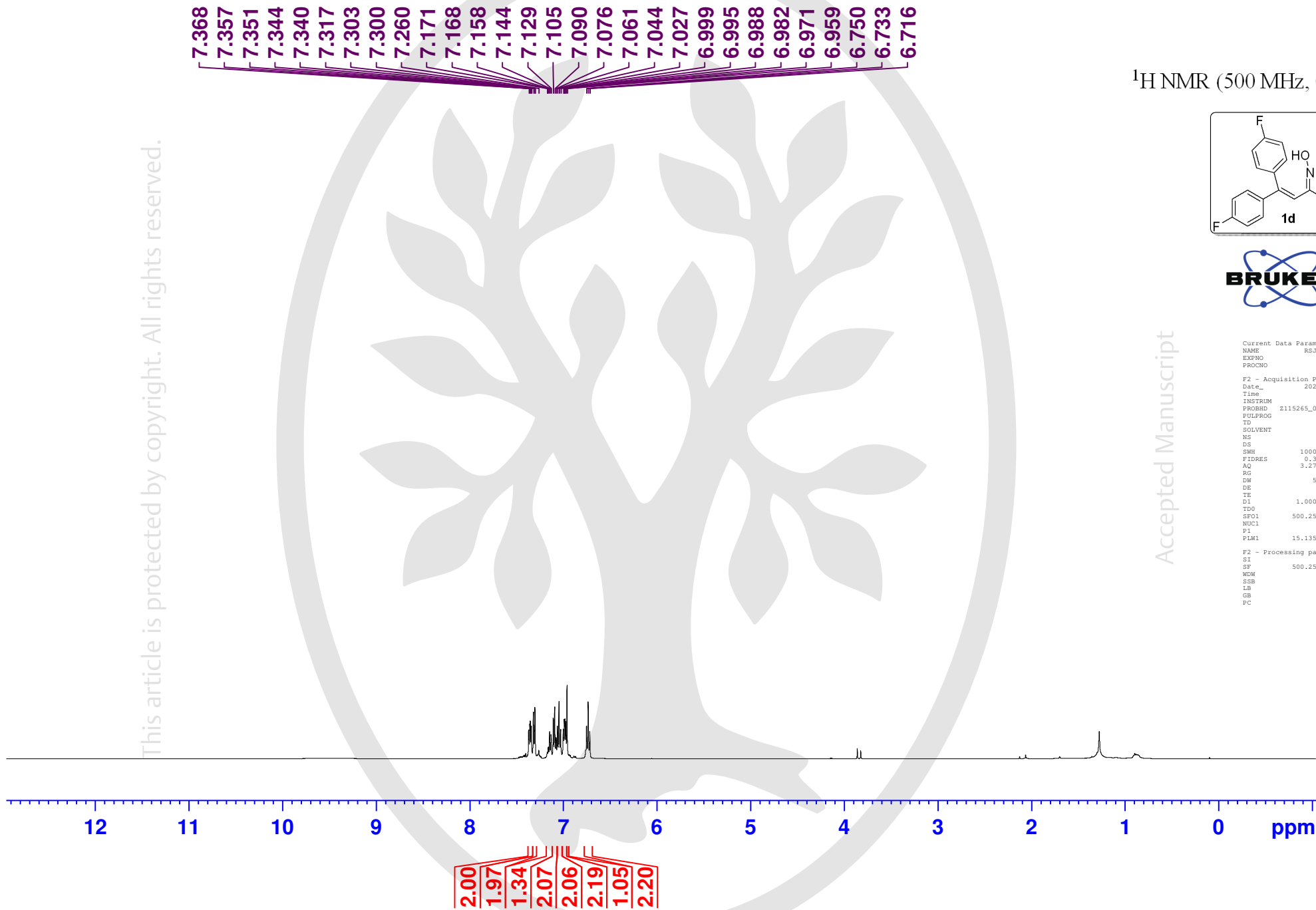
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SFO2       500.2550010 MHz
NUC2       1H
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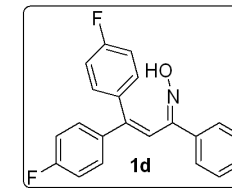
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PC         1.40
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^1H NMR (500 MHz, CDCl_3)



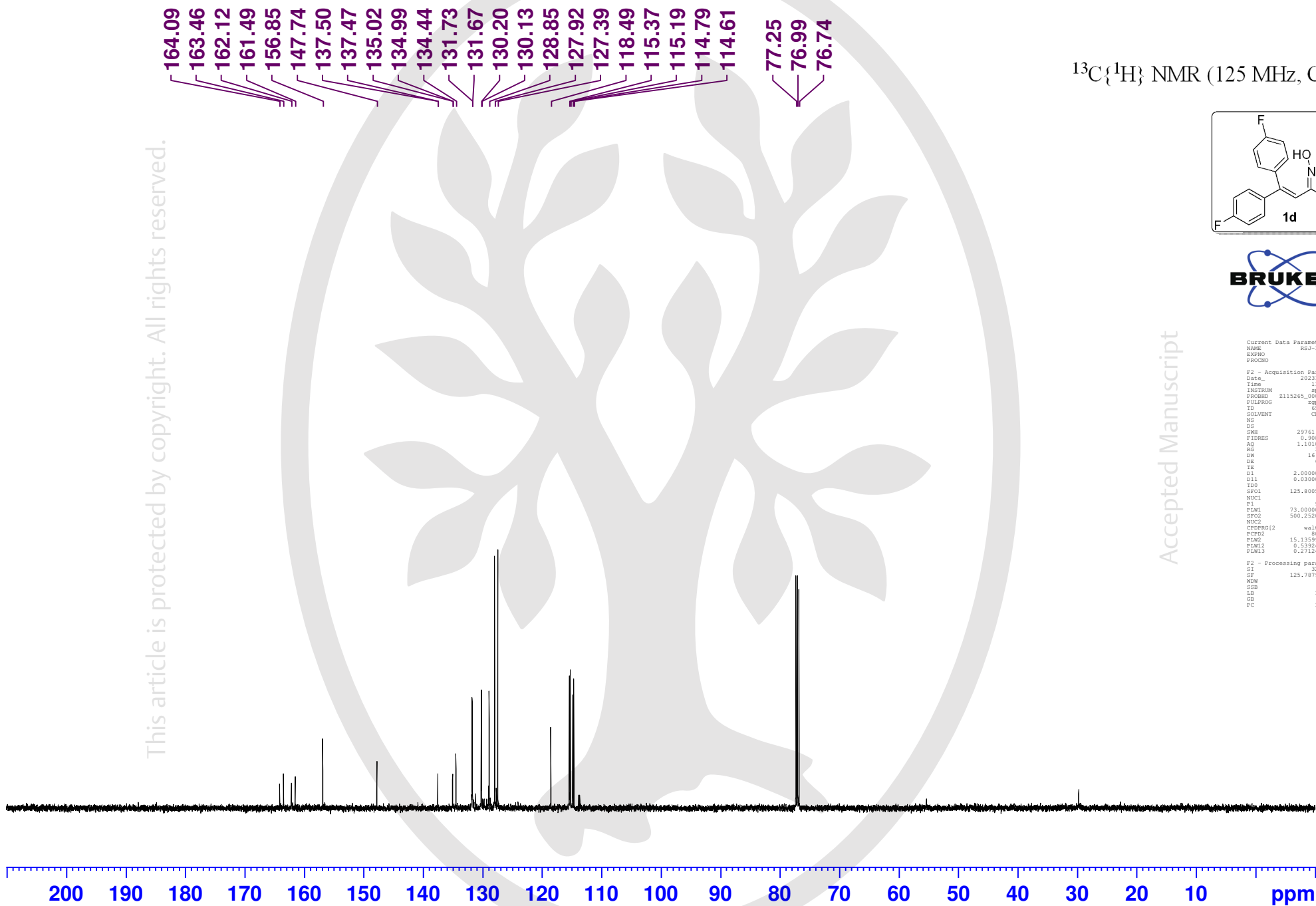
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AQ         3.2767999 sec
RG         114
DW         50.000 usec
DE         6.50 usec
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TDO       1
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NUC1       1H
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PL1        15.13599968 W

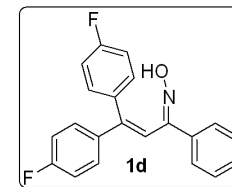
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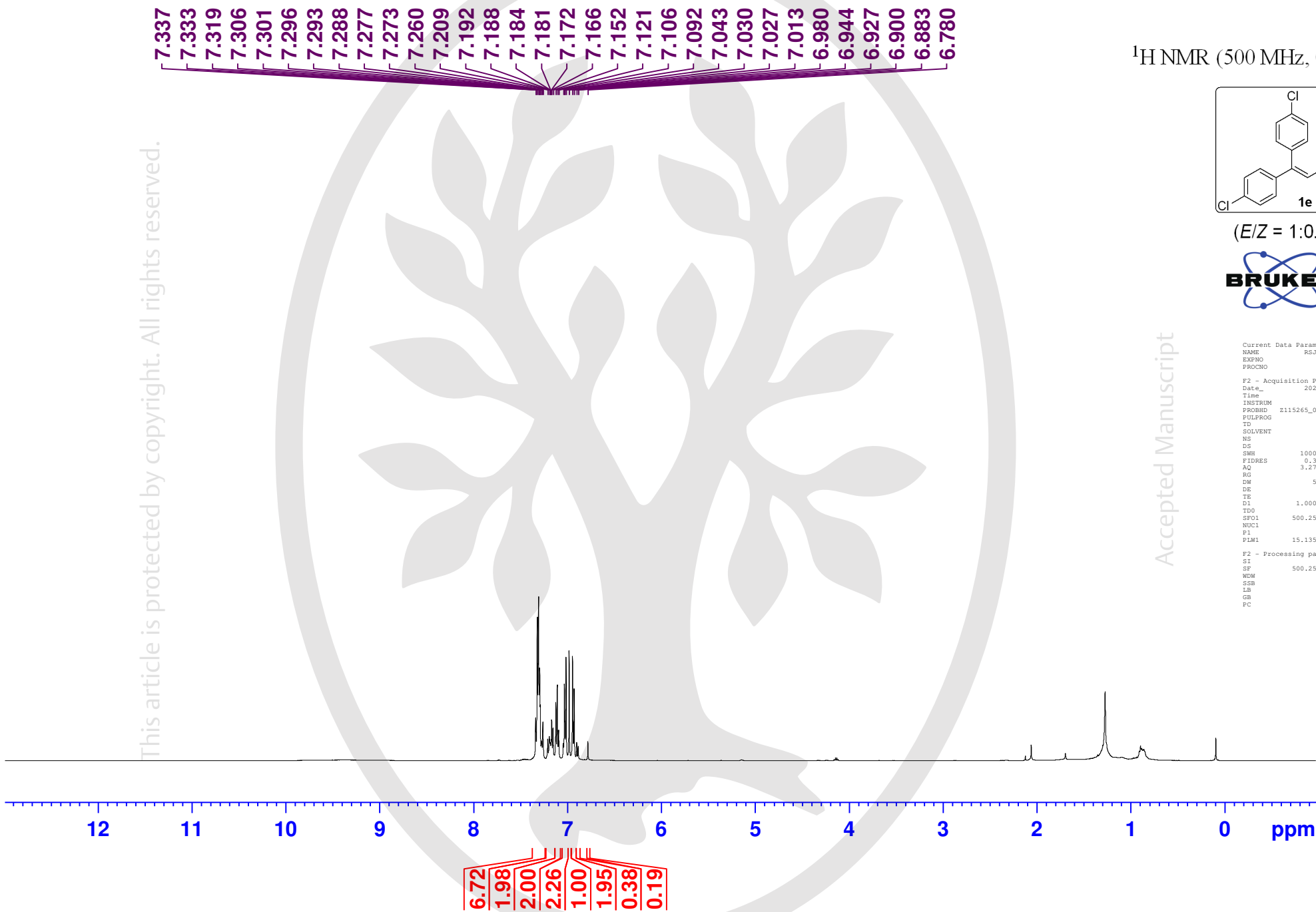
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



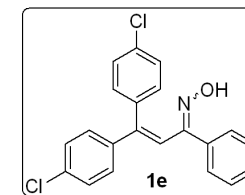
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INSTRUM  spect
PROBHD   z115265_0004 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       111
DS       4
SWE      29761.904 Hz
FIDRES   0.908261 Hz
AQ       1.1010048 sec
RG       1030
DM       16.800 usec
DE       6.50 usec
TE       0 K
D1       2.0000000 sec
D11      0.0300000 sec
TDO      1
SFO1     125.8005413 MHz
NUC1     13C
P1       9.70 usec
PLW1     73.0000000 W
SFO2     500.2550010 MHz
NUC2     1H
PCPD2    waitz16
PLW2     80.00 usec
PLW3     15.13599968 W
PLW4     0.53924000 W
PLW5     0.27124000 W
F2 - Processing parameters
SI       32768
SF       125.7879683 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.19)



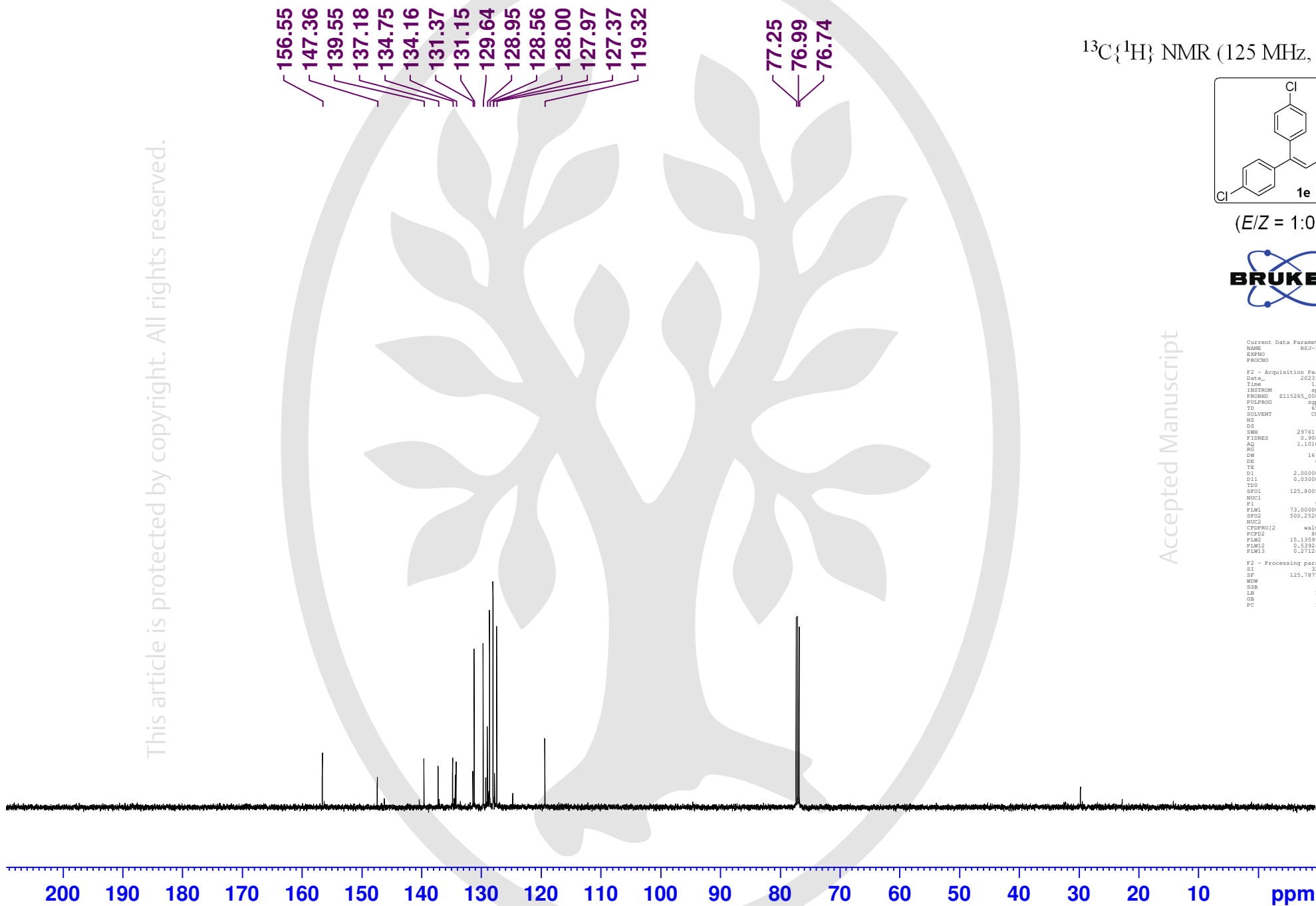
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Current Data Parameters
NAME      RSJ-1104
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
Date_     20231126
Time      11.28 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         114
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

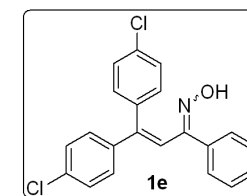
F2 - Processing parameters
SI         65536
SF         500.2500137 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.19)



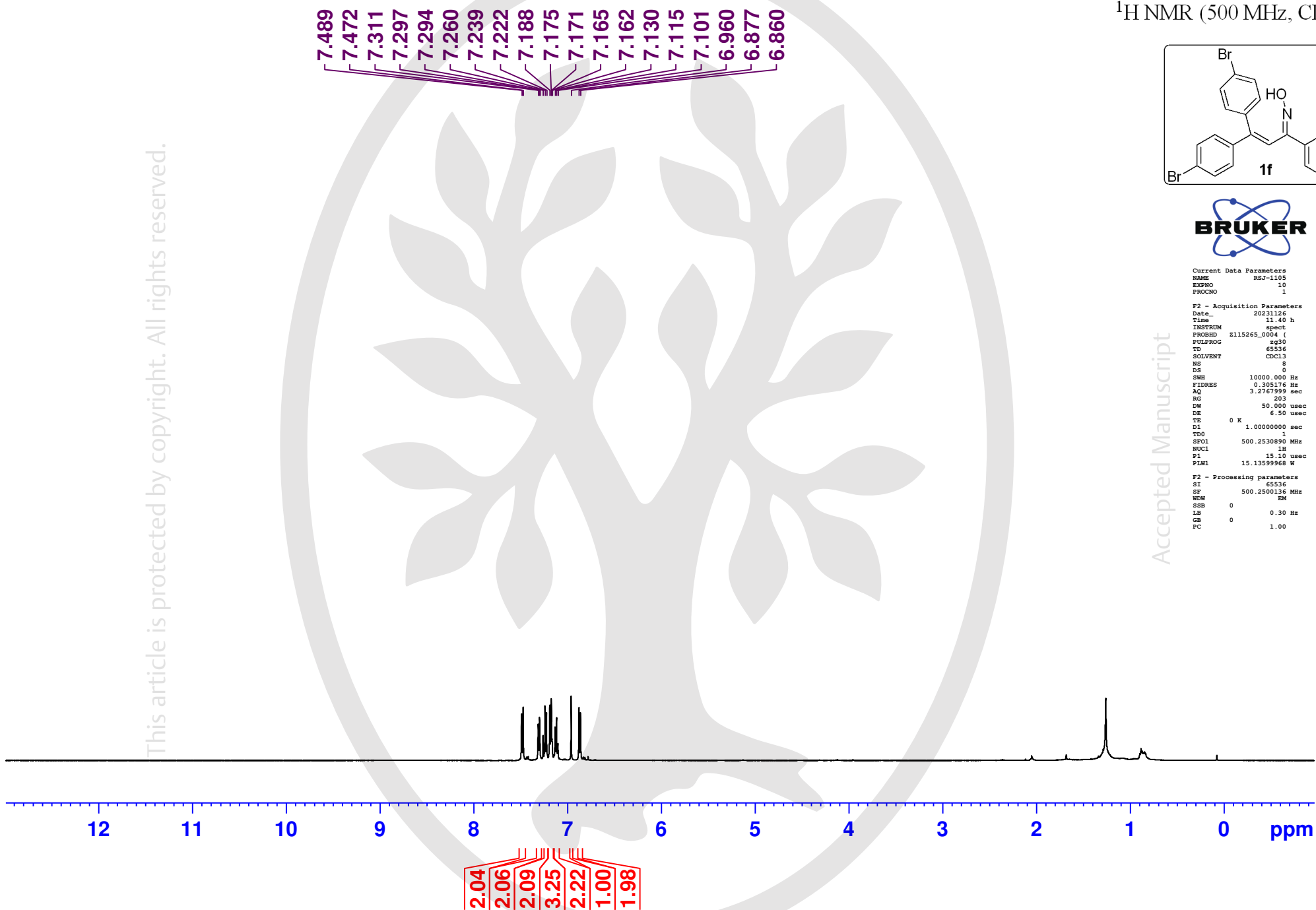
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Current Data Parameters
NAME      hcp-1104
EXPNO     9
PROCNO    1

F2 - Acquisition Parameters
Date_     20231126
Time      11.36 h
INSTRUM   spect
PROBHD    z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         107
DS         4
SWE        29761.904 Hz
FIDRES     0.908261 Hz
AQ          1.1010048 sec
RG          1030
DM          16.800 usec
DE          6.50 usec
TE          0 K
D1          2.0000000 sec
D11         0.0300000 sec
TD0         1
SF01        125.8005413 MHz
NUC1        13C
P1          9.70 usec
PL1         73.0000000 W
SFO2        500.2550010 MHz
NUC2         1H
CPDPRG2    waltz16
PCPD2       80.00 usec
PLM2        15.13599968 W
PLM12       0.53924000 W
PLM13       0.27124000 W

F2 - Processing parameters
SI          32768
SF          125.7879692 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
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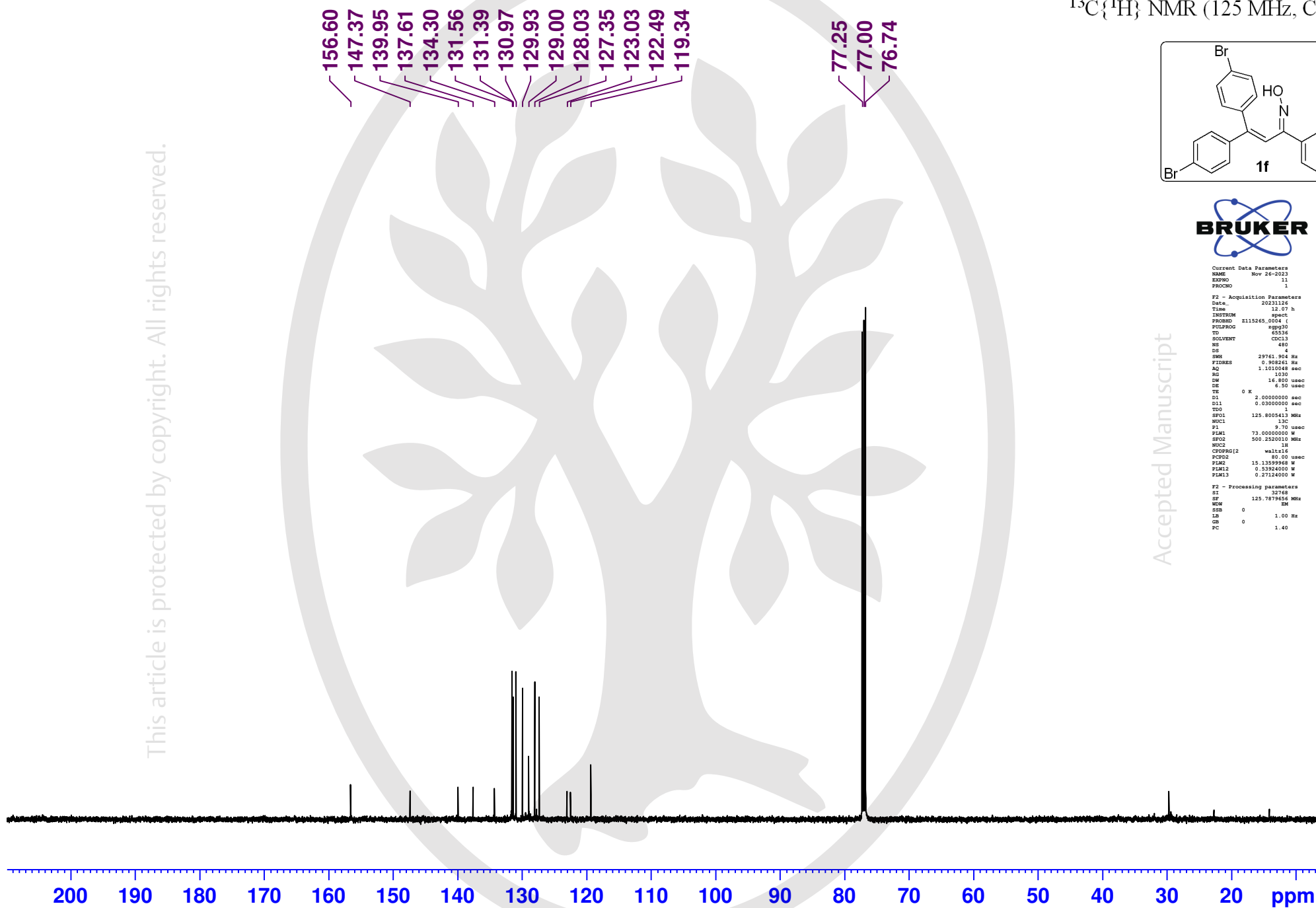
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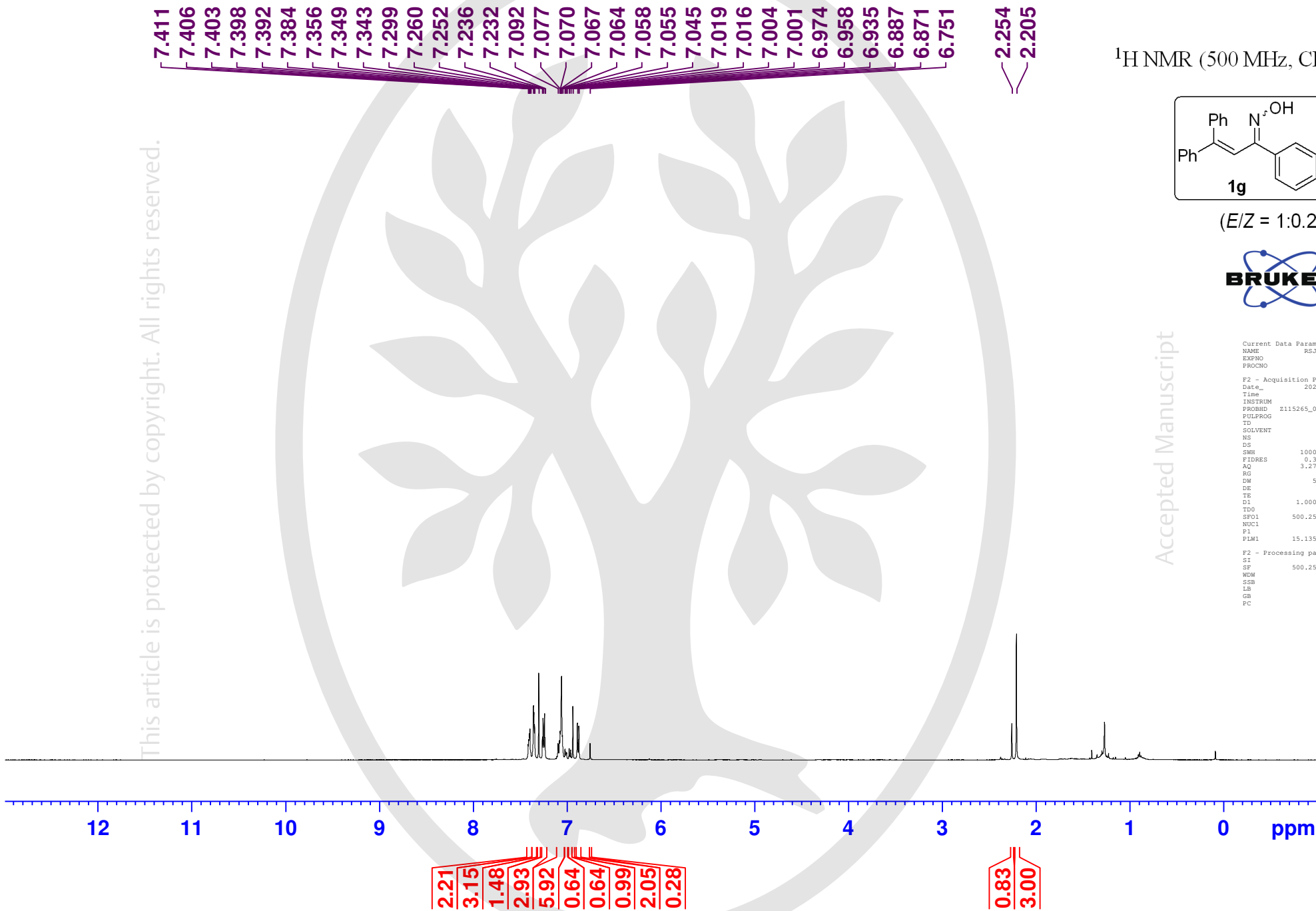
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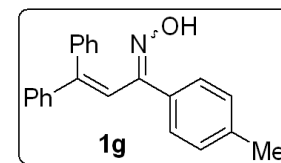


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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.28)



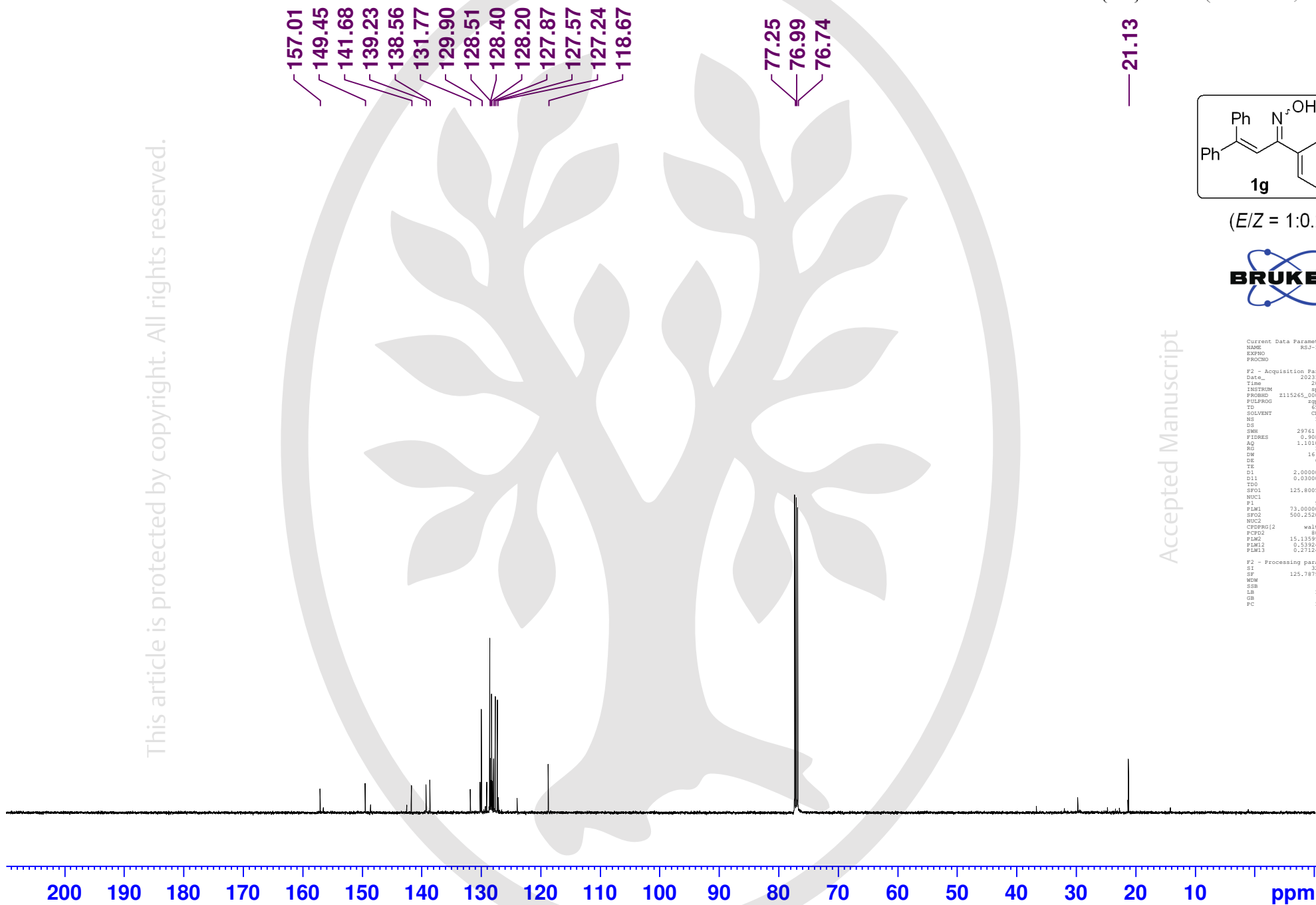
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```
Current Data Parameters
NAME      RSJ-1106
EXPNO     16
PROCNO    1

F2 - Acquisition Parameters
Date_     20231125
Time      19.04 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         10
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         161
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

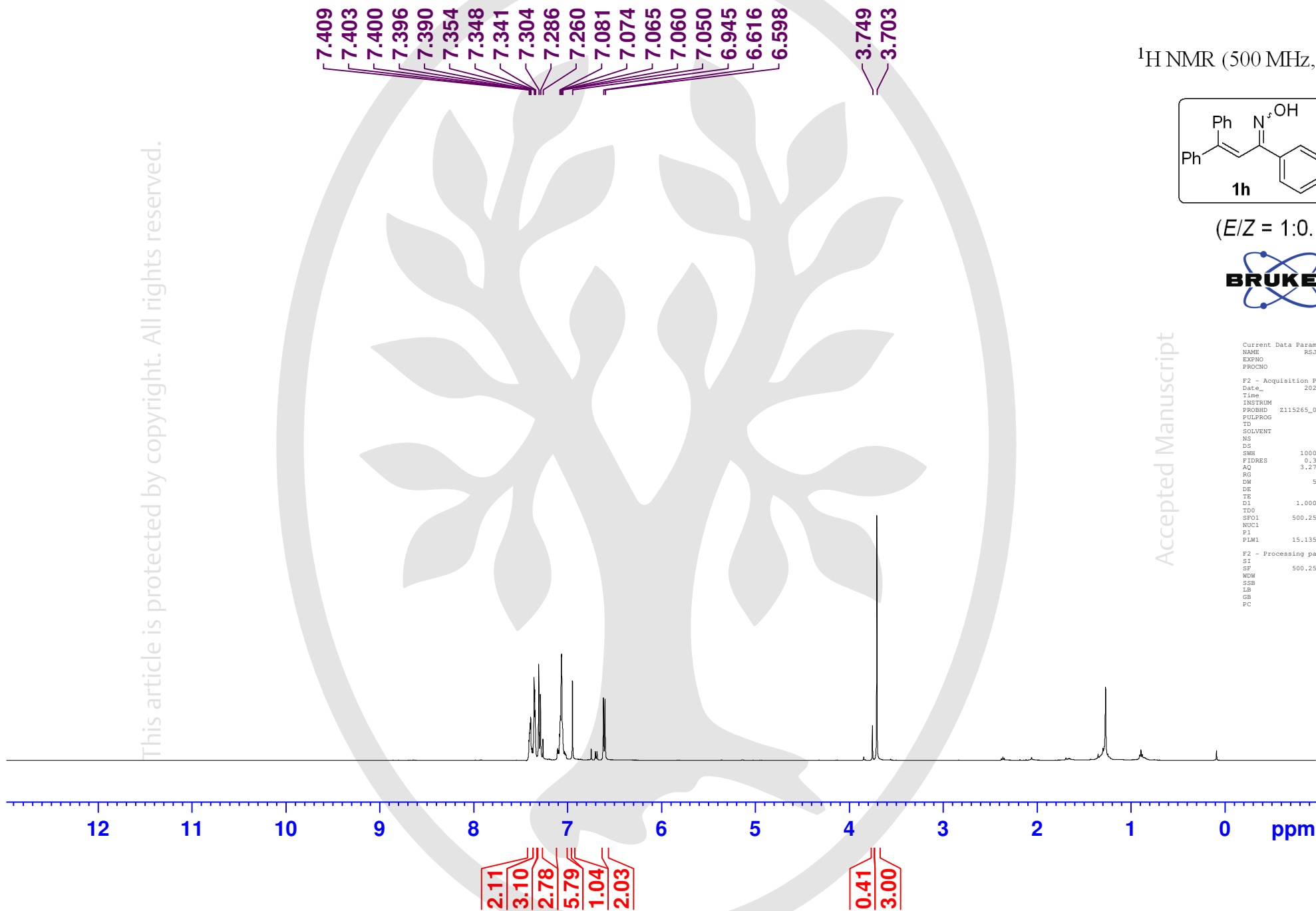
F2 - Processing parameters
SI         65536
SF         500.2500140 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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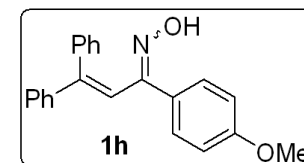


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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.14)



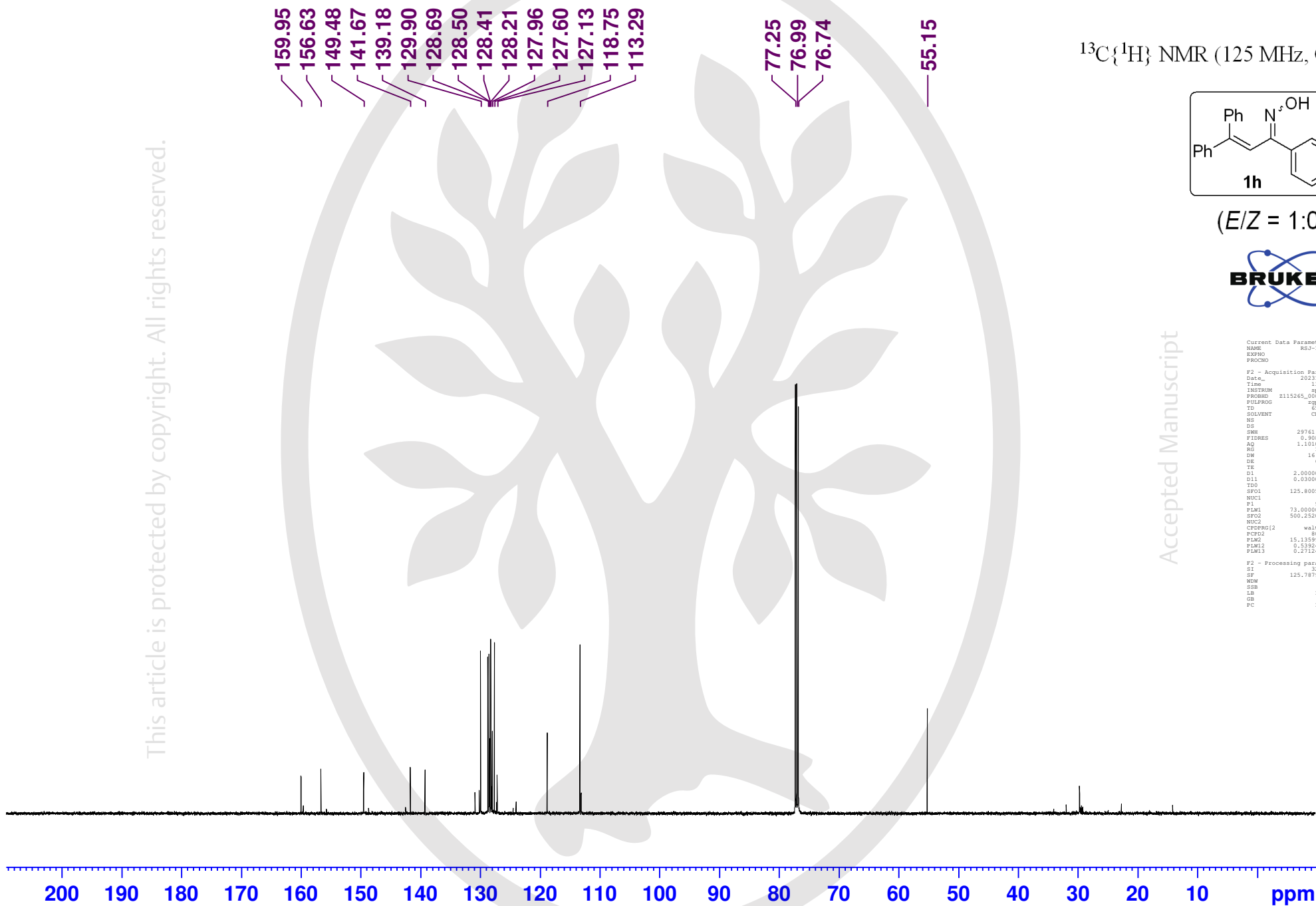
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Current Data Parameters
NAME      RSJ-1107
EXPNO     20
PROCNO    1

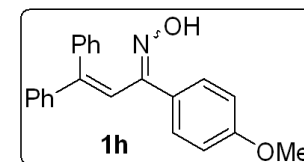
F2 - Acquisition Parameters
Date_     20231126
Time      13.12 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767959 sec
RG         161
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.0000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
SI         65536
SF         500.2500131 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(E/Z = 1:0.14)



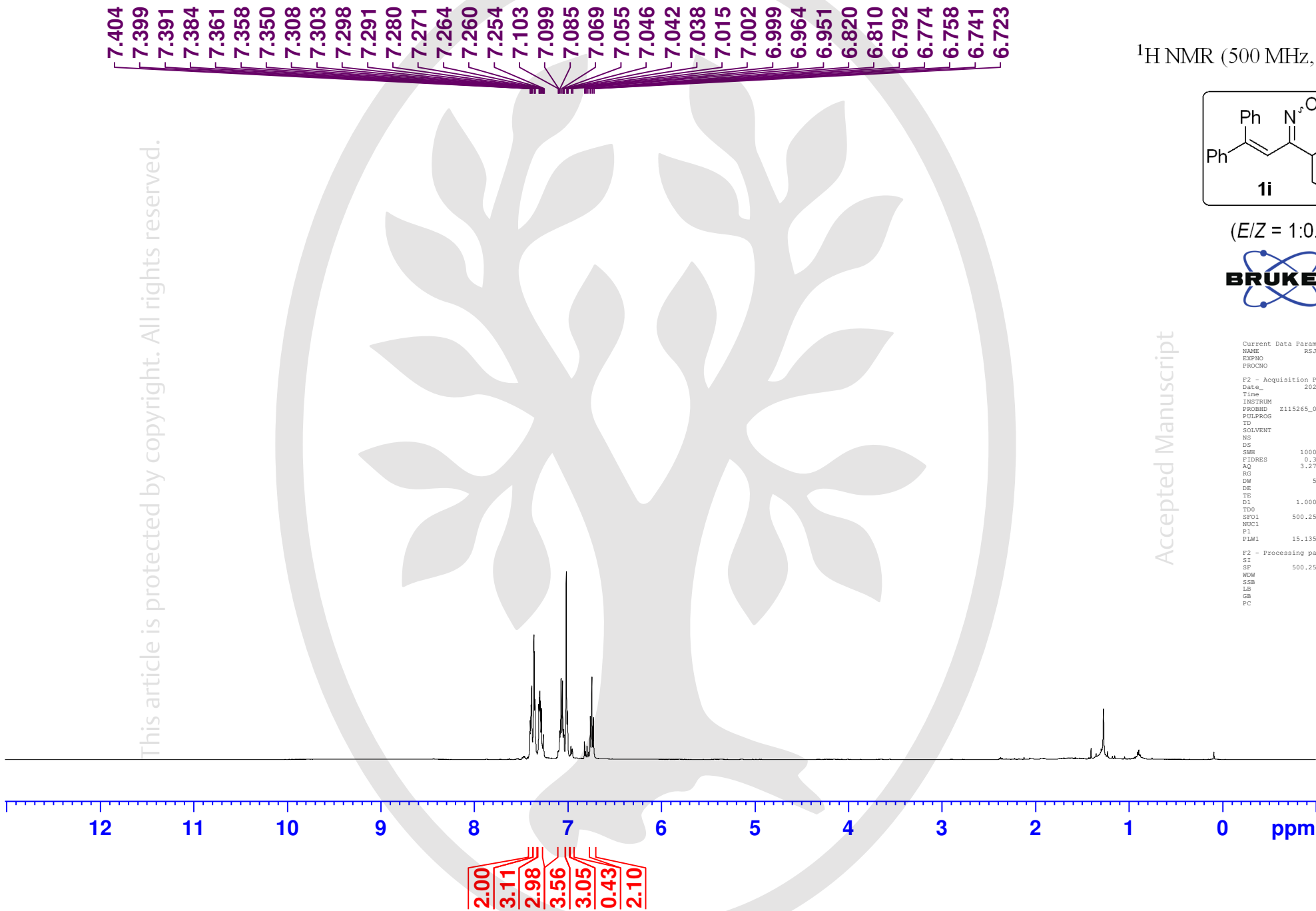
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Current Data Parameters
NAME      hcp-1107
EXPNO     21
PROCNO    1

F2 - Acquisition Parameters
Date_     20231126
Time      13.59 h
INSTRUM   spect
PROBHD    z115265_0004 (
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        862
DS        4
SWE       29761.904 Hz
FIDRES    0.908261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TDO        1
SFO1       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PLM1       73.0000000 W
SFO2       500.2550010 MHz
NUC2       1H
PCPD2      waitrl6
PLM2       80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

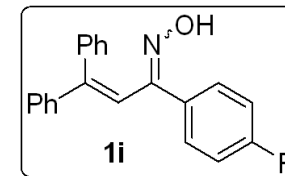
F2 - Processing parameters
SI         32768
SF         125.7879674 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.14)



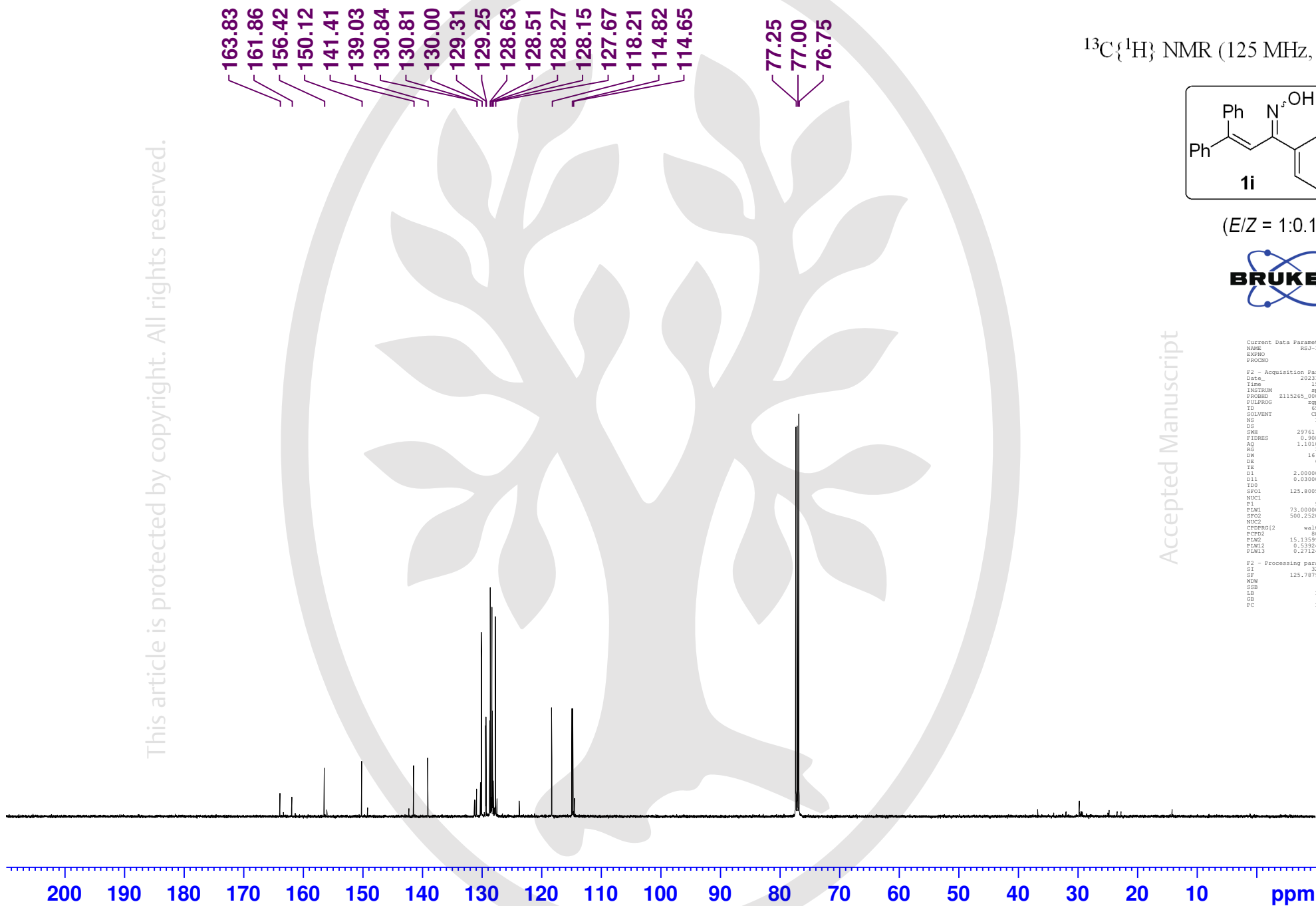
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Current Data Parameters
NAME      RSJ-1108
EXPNO     22
PROCNO    1

F2 - Acquisition Parameters
Date_     20231126
Time      14.04 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         161
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1        1H
P1         15.10 usec
PL1        15.13559968 W

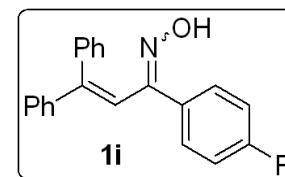
F2 - Processing parameters
SI         65536
SF         500.2500139 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.14)



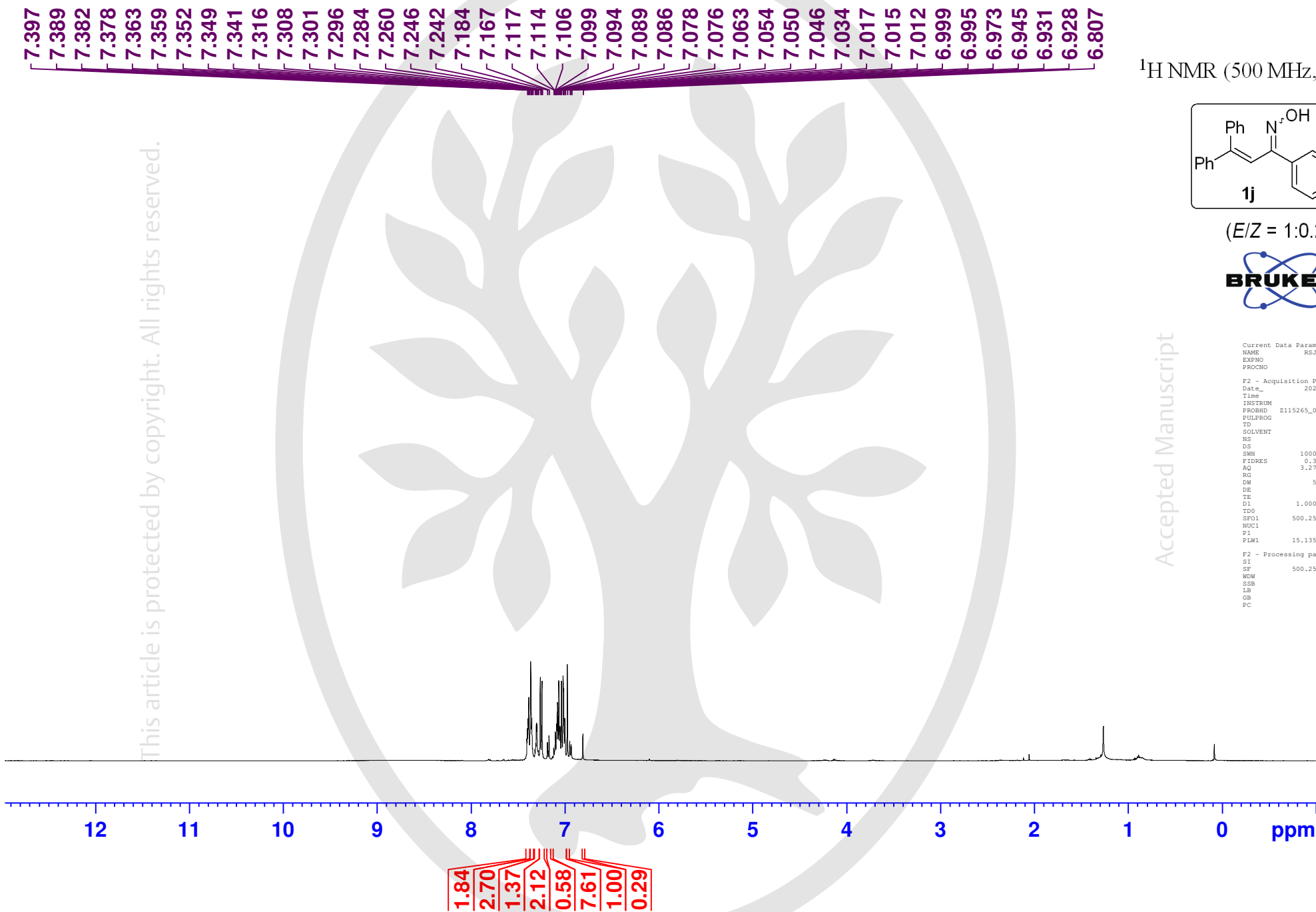
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Current Data Parameters
NAME      hcp-1108
EXPNO    23
PROCNO   1

F2 - Acquisition Parameters
Date_    20231126
Time     15.00 h
INSTRUM  spect
PROBHD   z115265_0004 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWE      29761.904 Hz
FIDRES   0.908261 Hz
AQ        1.1010048 sec
RG        1030
DM        16.800 usec
DE        6.50 usec
TE        0 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
SFO1     125.8005413 MHz
NUC1      13C
P1        9.70 usec
PLM1     73.00000000 W
SFO2     500.2550010 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLM2     15.13599968 W
PLM12    0.53924000 W
PLM13    0.27124000 W

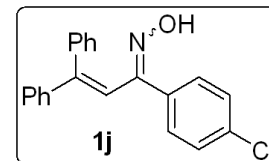
F2 - Processing parameters
SI        32768
SF        125.7879674 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.29)



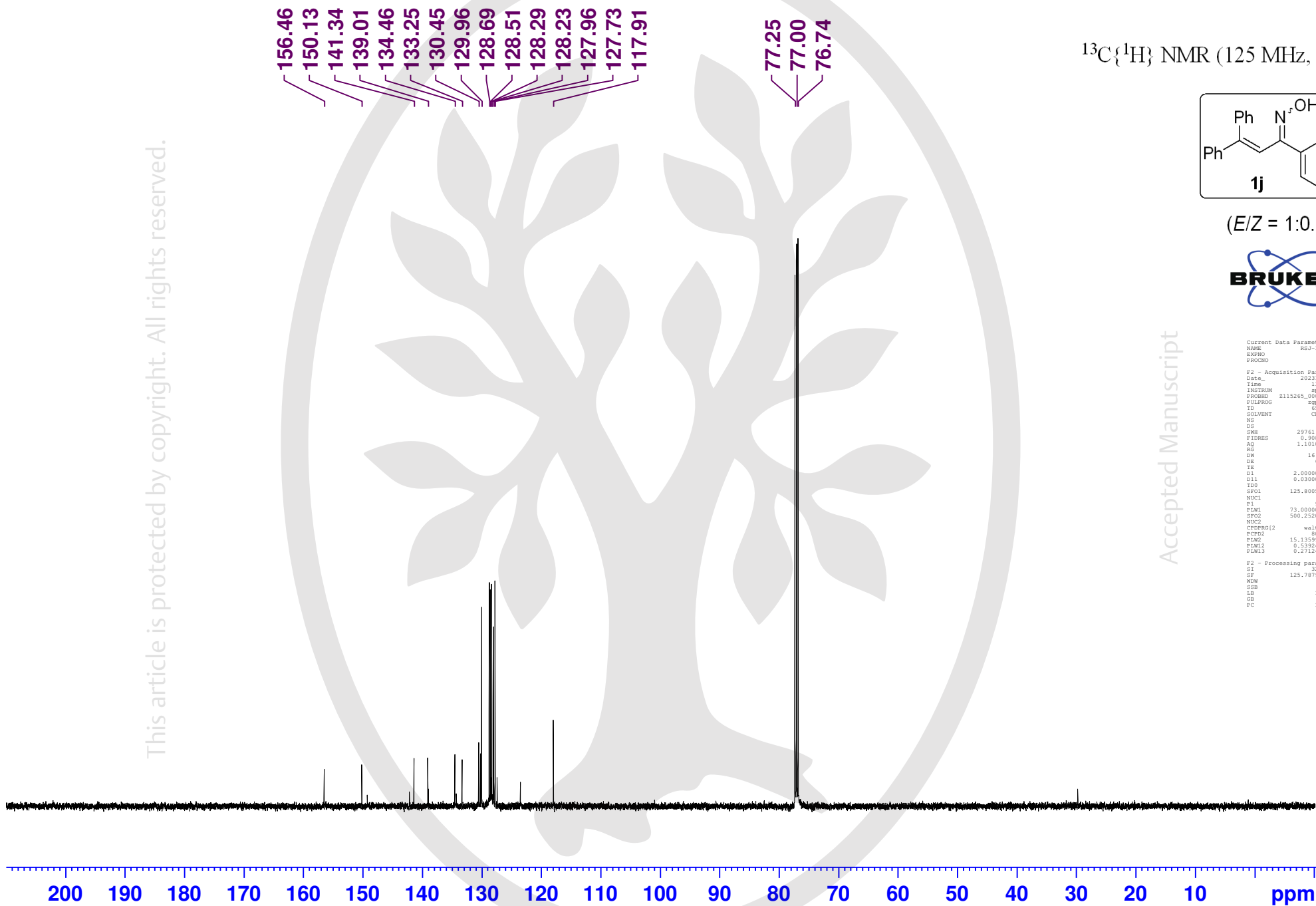
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Current Data Parameters
NAME      RSJ-1109
EXPNO    18
PROCNO   1

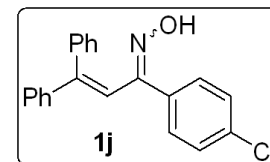
F2 - Acquisition Parameters
Date_    20231126
Time     12.30 h
INSTRUM  spect
PROBHD   Z115265_0004 (
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.2767999 sec
RG       161
DW       50.000 usec
DE       6.50 usec
TE       0 K
D1       1.00000000 sec
TDO      1
SFO1     500.2530890 MHz
NUC1     1H
P1       15.10 usec
PL1      15.13599968 W

F2 - Processing parameters
SI       65536
SF       500.2500139 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



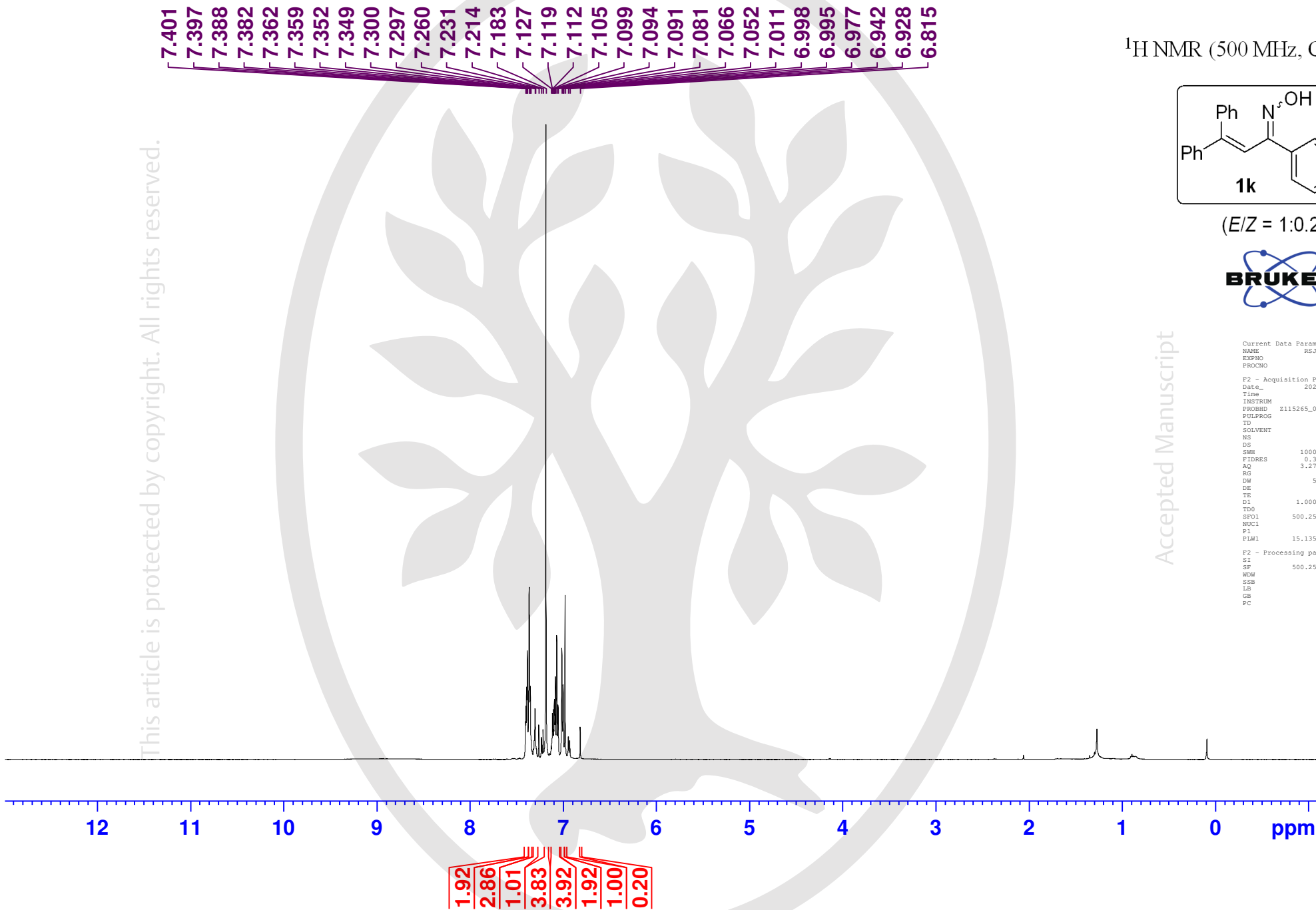
(*E/Z* = 1:0.29)



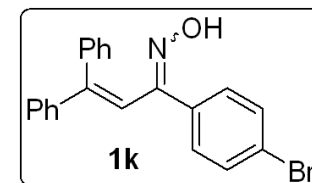
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Current Data Parameters
NAME      hcp-1109
EXPNO    19
PROCNO   1
F2 - Acquisition Parameters
Date_    20231126
Time     13.07 h
INSTRUM  spect
PROBHD   z115265_0004 (
PULPROG  zgpg30
TD       65536
SOLVENT  cdcl3
NS       659
DS       4
SFO1     29761.904 Hz
FIDRES   0.908261 Hz
AQ       1.1010048 sec
RG       322
DM       16.800 usec
DE       6.50 usec
TE       0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
SF01     125.8005413 MHz
NUC1     13C
P1       9.70 usec
PLW1     73.0000000 W
SFO2     500.2550010 MHz
NUC2     1H
PCPD2    waitz16
PLW2     80.00 usec
PLM2     15.13599968 W
PLW12    0.53924000 W
PLW13    0.27124000 W
F2 - Processing parameters
SI       32768
SF       125.7879656 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.20)



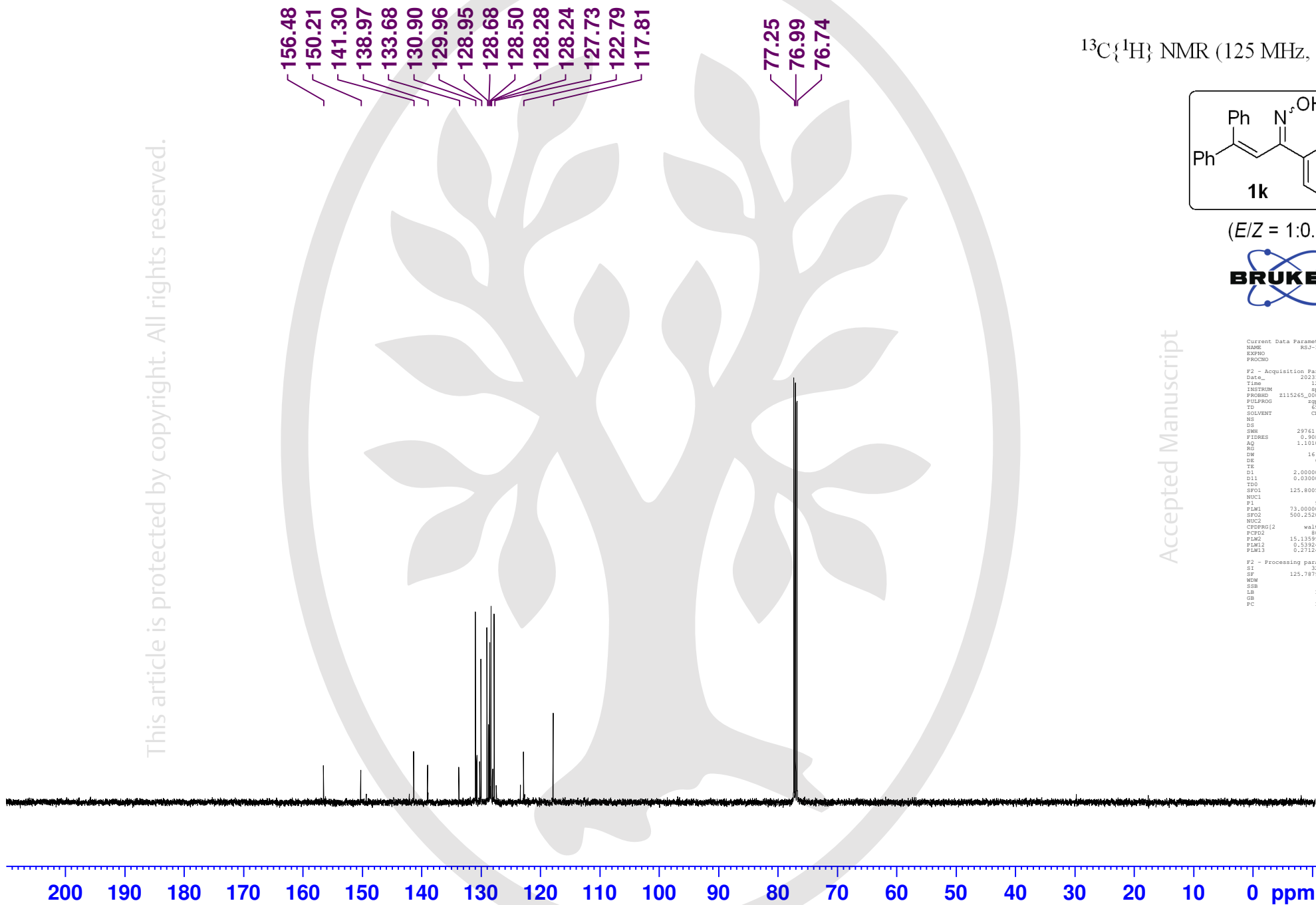
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Current Data Parameters
NAME      RSJ-1110
EXPNO     12
PROCNO    1

F2 - Acquisition Parameters
Date_     20231126
Time      12.12 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767939 sec
RG         161
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
SI         65536
SF         500.2500135 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

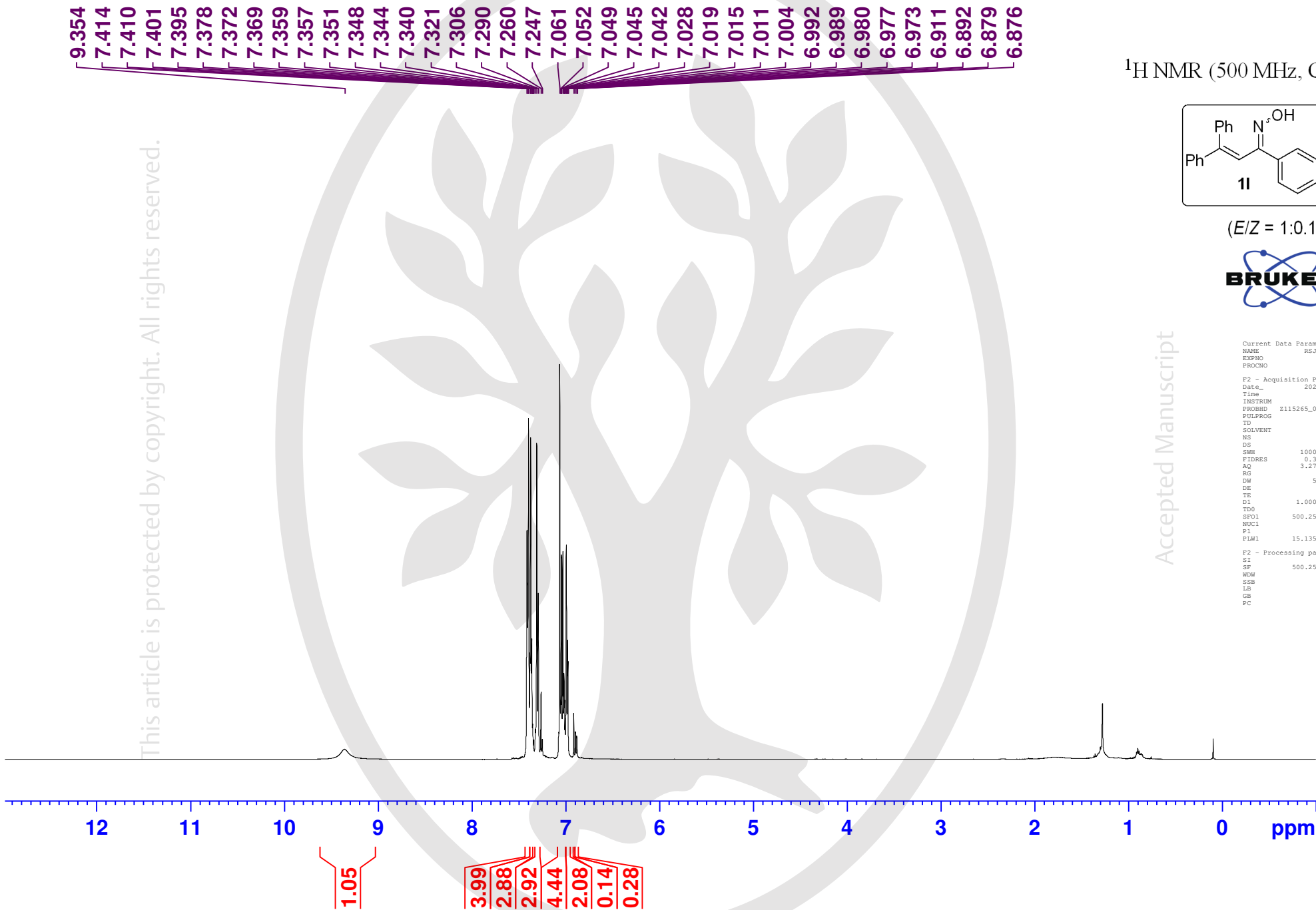
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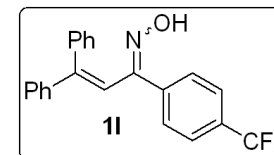


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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.14)



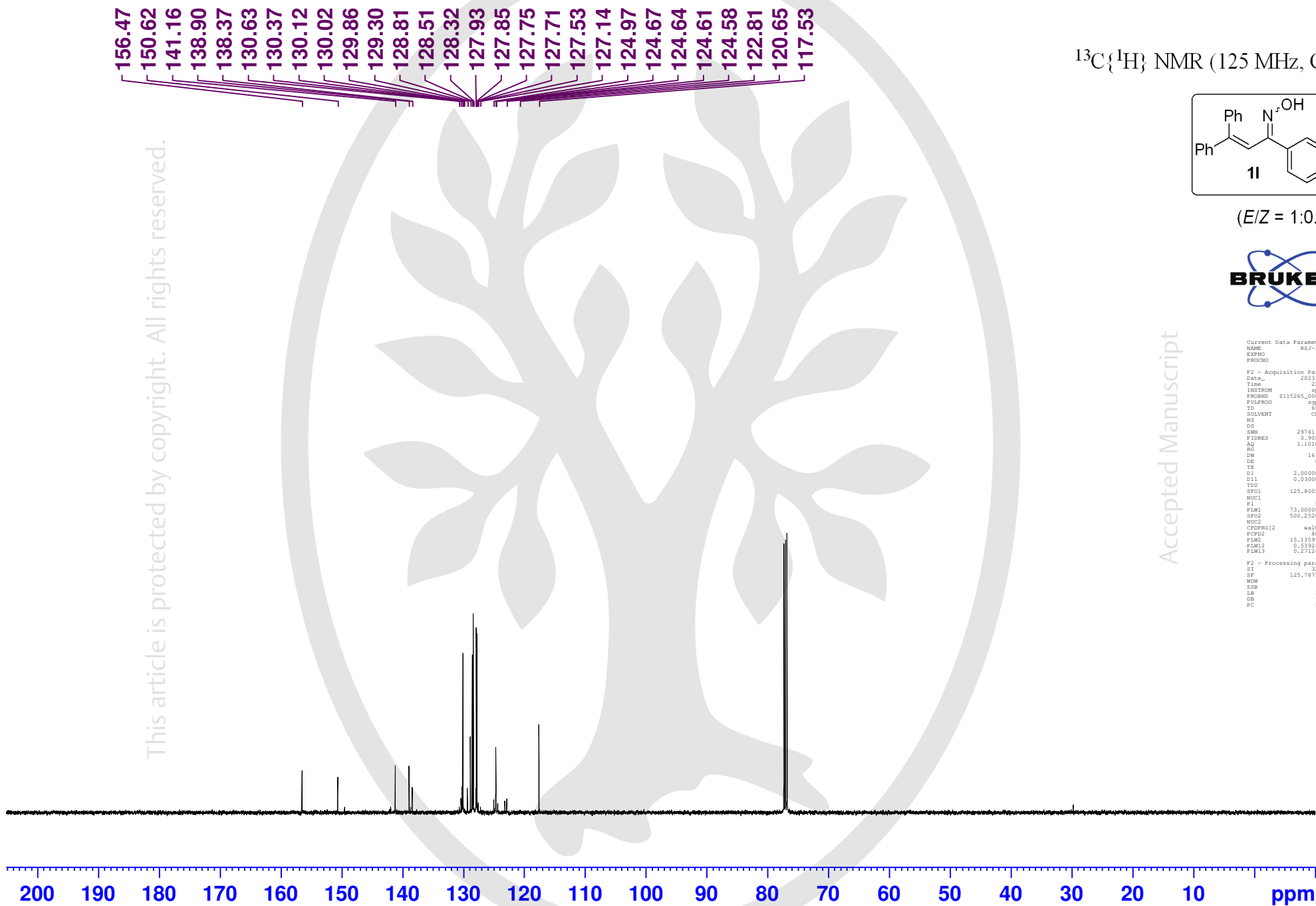
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Current Data Parameters
NAME      RSJ-1111
EXPNO     6
PROCNO    1

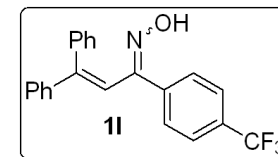
F2 - Acquisition Parameters
Date_     20231201
Time      22.16 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         144
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TD0        1
SF01       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
SI         65536
SF         500.2500134 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.14)



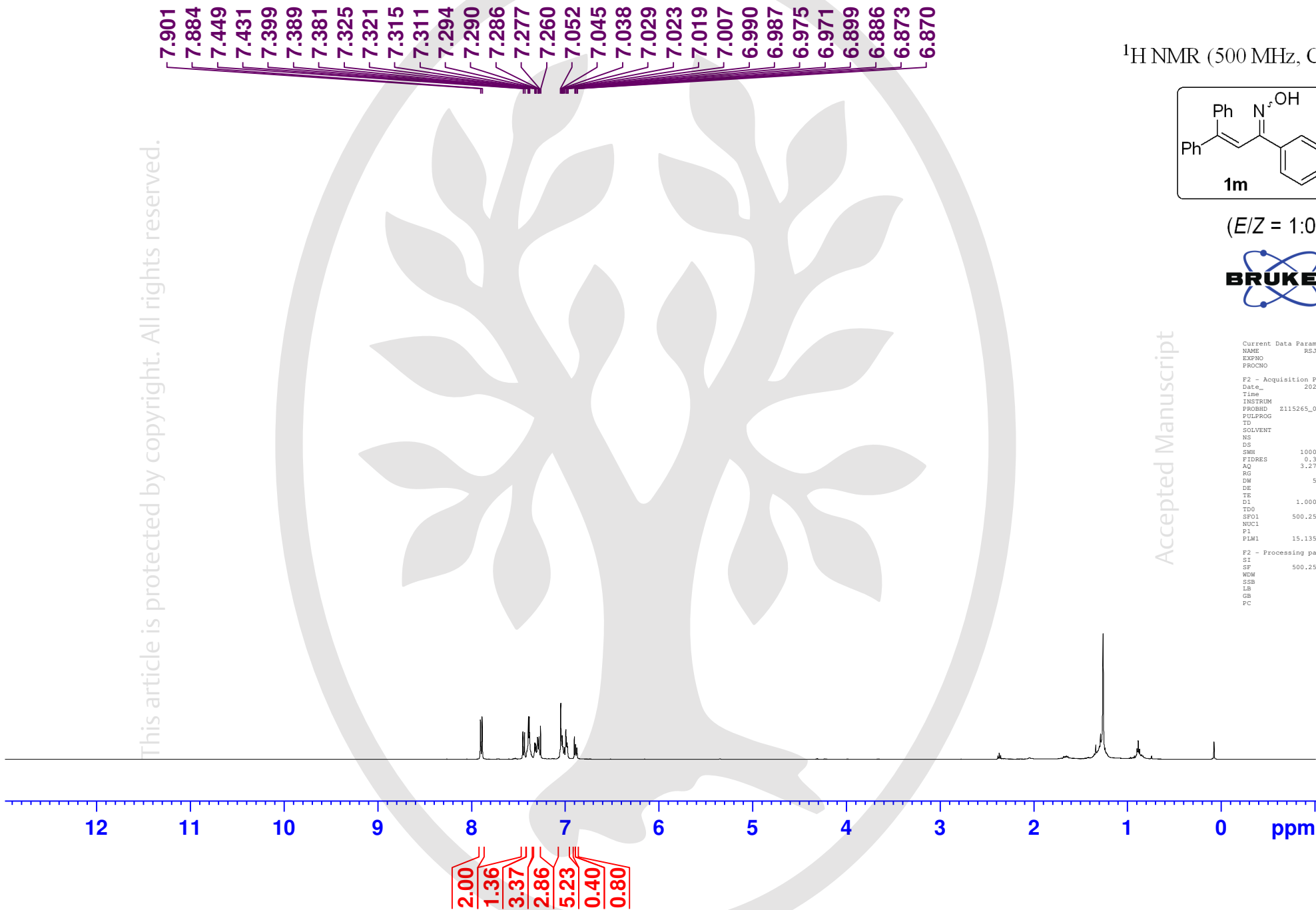
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Current Data Parameters
NAME      hnp-1111
EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
Date_    20231201
Time     22.28 h
INSTRUM  spect
PROBHD   z115265_0004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        200
DS        4
SFE      29761.904 Hz
FIDRES   0.908261 Hz
AQ        1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SFO1      125.8005413 MHz
NUC1       13C
P1         9.70 usec
PLM1       73.0000000 W
SFO2       500.2550010 MHz
NUC2        1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

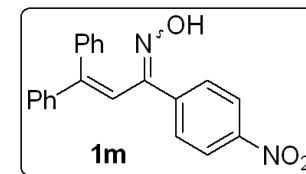
F2 - Processing parameters
SI          32768
SF          125.7879674 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.40)



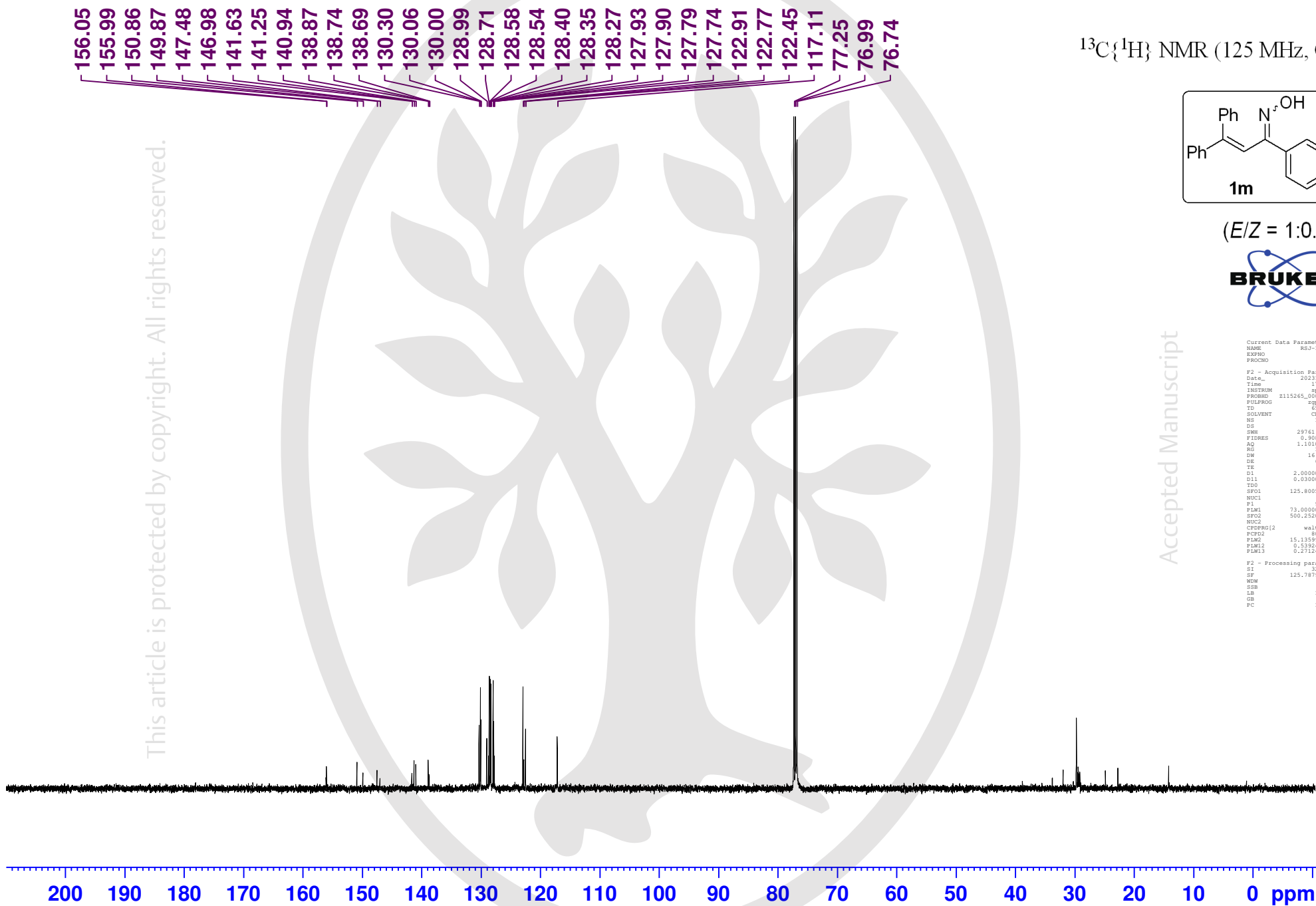
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```
Current Data Parameters
NAME      RSJ-1112
EXPNO     3
PROCNO    1

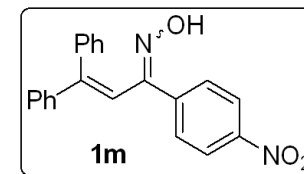
F2 - Acquisition Parameters
Date_     20231127
Time      16.19 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         203
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
SI         65536
SF         500.2500131 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

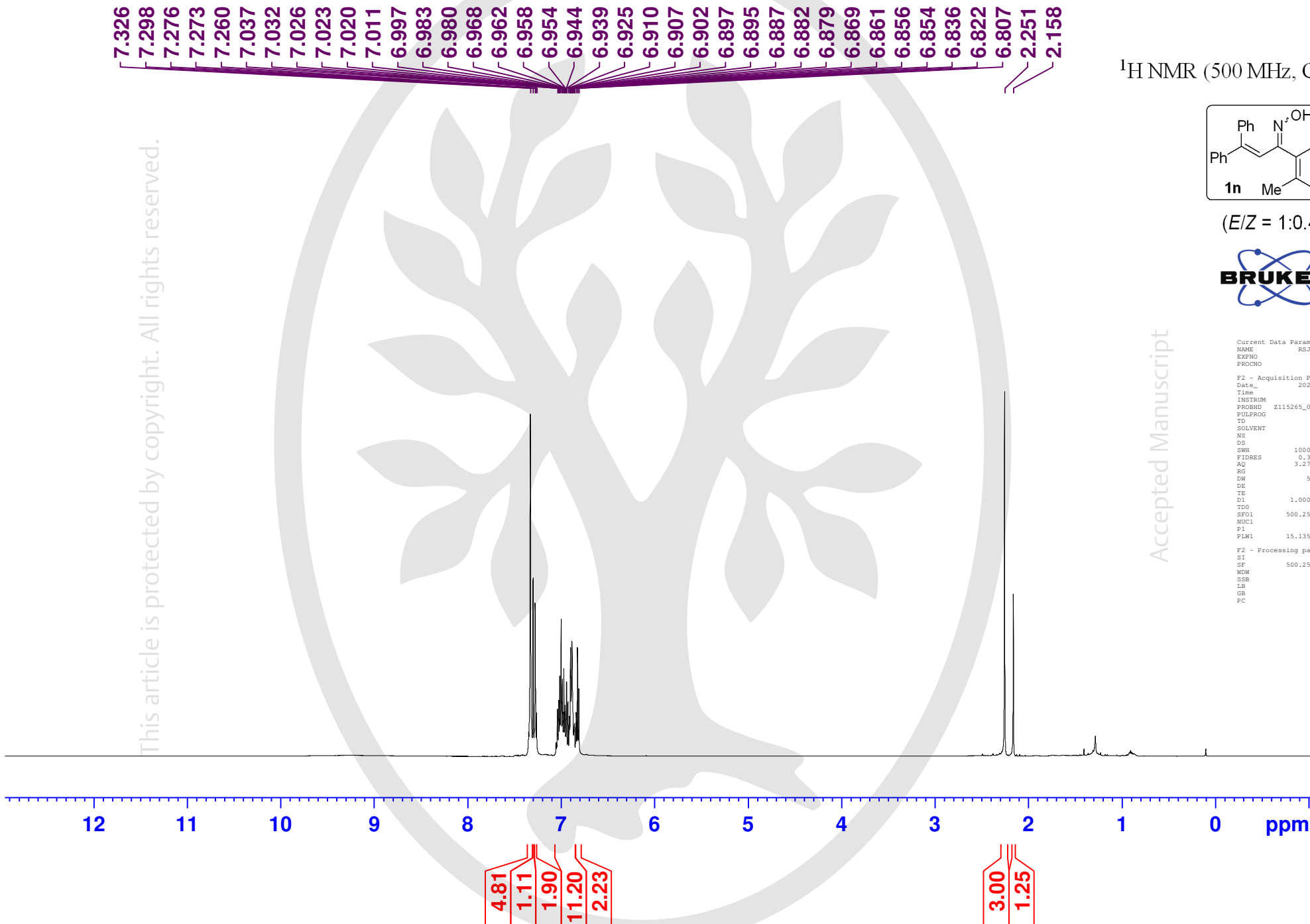


(E/Z = 1:0.40)

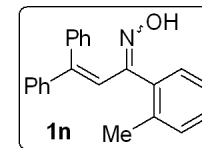


```
Current Data Parameters
NAME      hcp-1112
EXPNO     4
PROCNO    1
F2 - Acquisition Parameters
Date_     20231127
Time      17.15 h
INSTRUM   spect
PROBHD    z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWE        29761.904 Hz
FIDRES    0.908261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SF01       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PLM1       73.0000000 W
SFO2       500.2550010 MHz
NUC2       1H
CPCPRG12   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W
F2 - Processing parameters
SI         32768
SF         125.7879646 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.42)



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```
Current Data Parameters
NAME      RSJ-1113
EXPNO     8
PROCNO    1

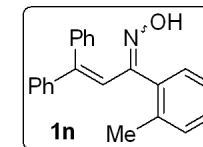
F2 - Acquisition Parameters
Date_     20231201
Time      22.33 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         101
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
SI         65536
SF         500.2500135 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

158.52
157.60
149.12
147.88
142.38
141.61
138.85
138.46
135.80
135.40
134.78
132.57
130.07
129.92
129.60
129.50
129.38
128.46
128.22
128.19
128.18
128.13
128.05
127.90
127.65
127.63
127.33
127.29
126.95
124.95
123.82
118.87
77.25
76.99
76.74

20.81
20.06



(*E/Z* = 1:0.42)



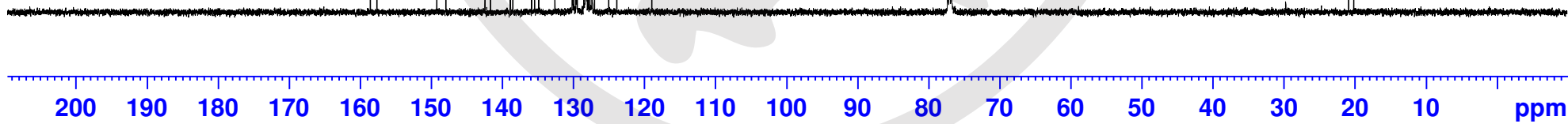
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Current Data Parameters
NAME      hcp-1113
EXPNO     9
PROCNO    1

F2 - Acquisition Parameters
Date_     20231201
Time      22.57 h
INSTRUM   spect
PROBHD    z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         417
DS         4
SWE        29761.904 Hz
FIDRES     0.908261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SF01       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PLM1       73.00000000 W
SFO2       500.2550010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

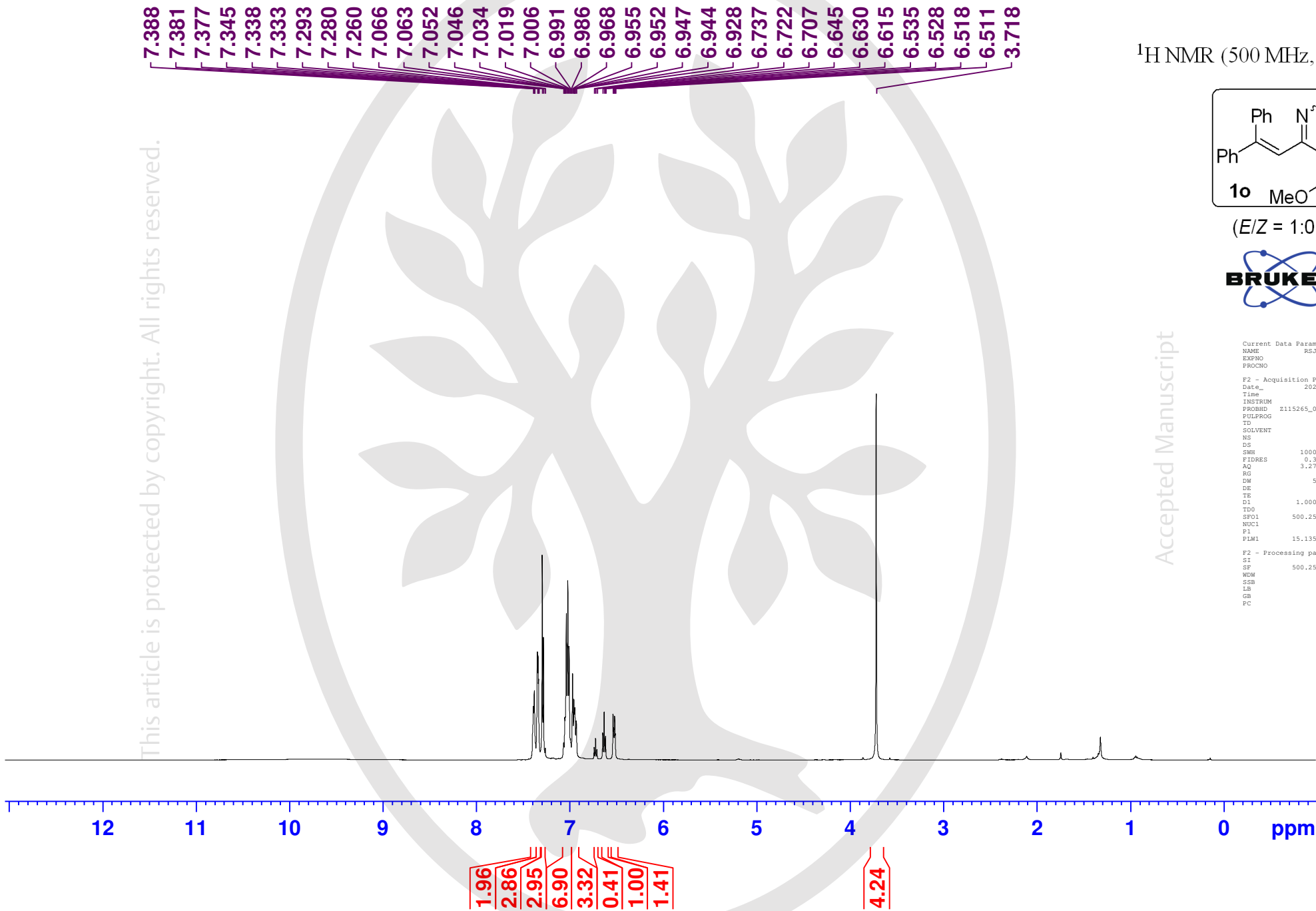
F2 - Processing parameters
SI         32768
SF         125.7879701 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

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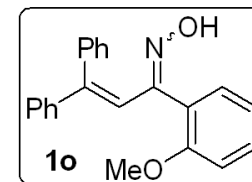
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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.41)

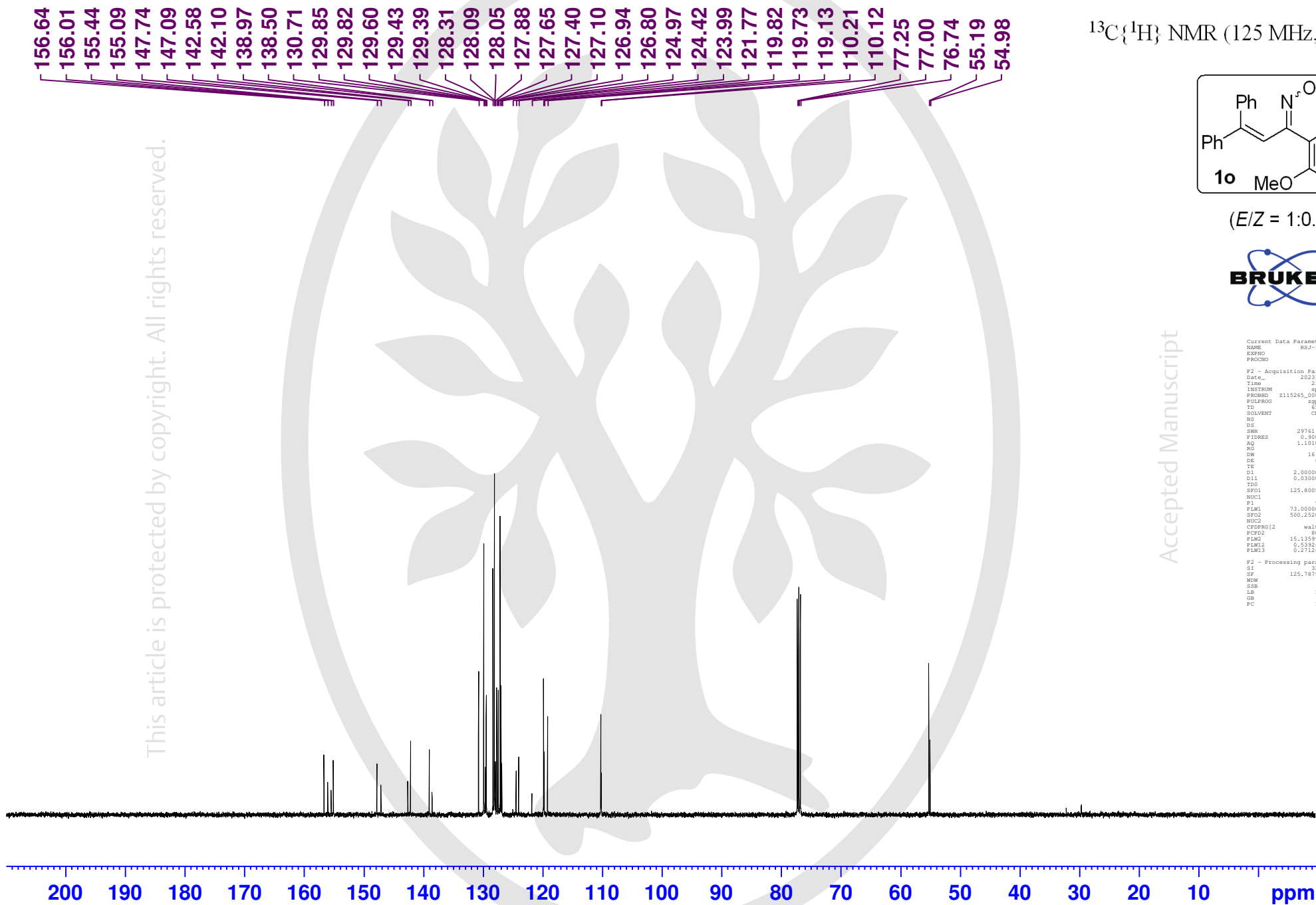


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Current Data Parameters
NAME      RSJ-1114
EXPNO    10
PROCNO   1

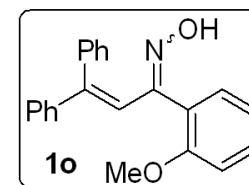
F2 - Acquisition Parameters
Date_    20231201
Time     23.02 h
INSTRUM  spect
PROBHD   Z115265_0004 (
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.2767959 sec
RG       32
DW       50.000 usec
DE       6.50 usec
TE       0 K
D1       1.00000000 sec
TD0      1
SF01     500.2530890 MHz
NUC1     1H
P1       15.10 usec
PL1     15.13559968 W

F2 - Processing parameters
SI       65536
SF       500.2500138 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.41)



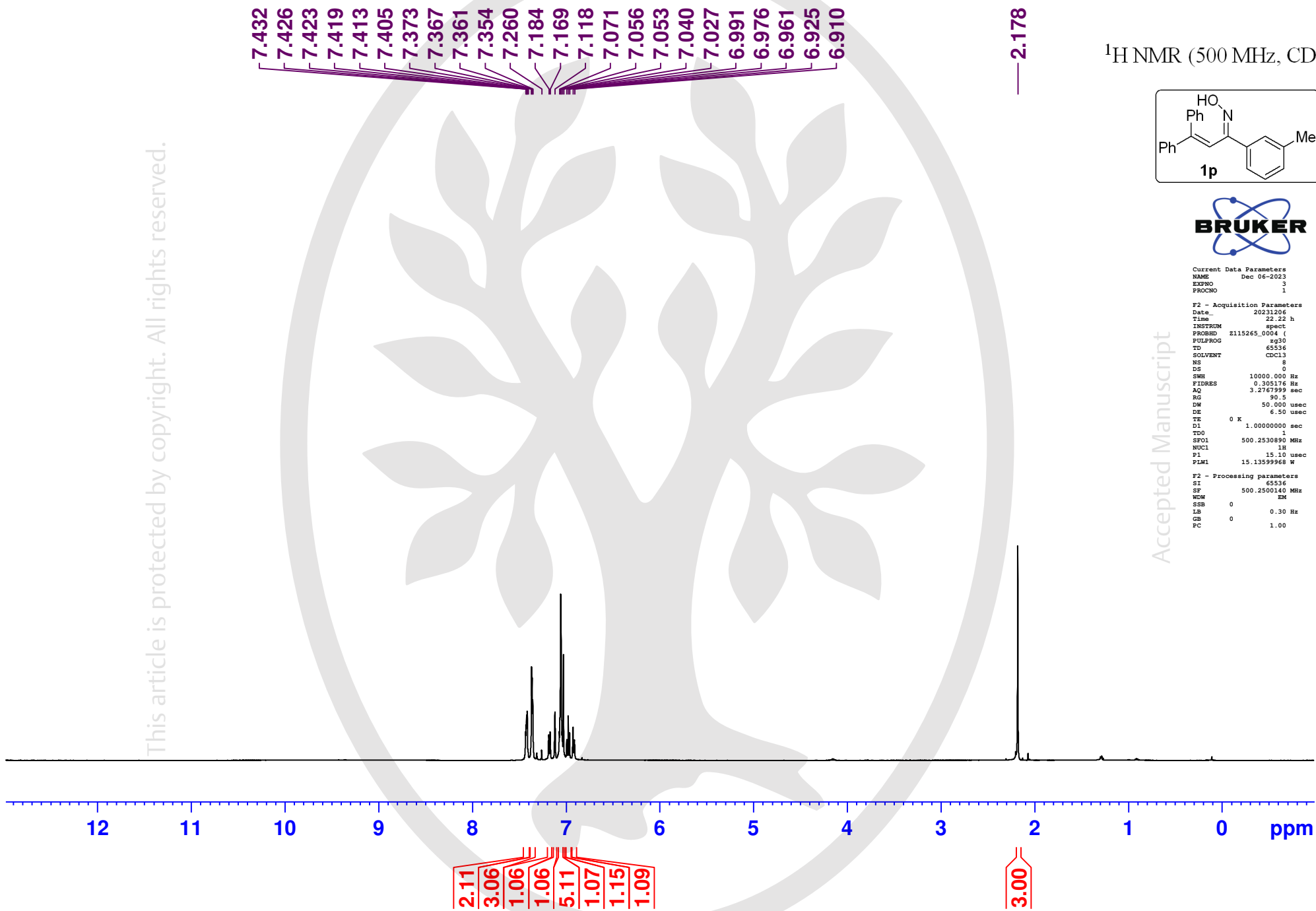
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Current Data Parameters
NAME      hmr-1114
EXPNO     11
PROCNO    1

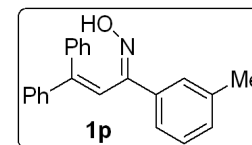
F2 - Acquisition Parameters
Date_     20231201
Time     23.09 h
INSTRUM   spect
PROBHD    z115265_0004 (
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        104
DS        4
SFR       29761.904 Hz
FIDRES    0.908261 Hz
AQ        1.1010048 sec
RG        1030
DM        16.800 usec
DE        6.50 usec
TE        0 K
D1        2.00000000 sec
D11       0.03000000 sec
TDO       1
SFO1      125.8005413 MHz
NUC1      13C
P1        9.70 usec
PLM1      73.00000000 W
SFO2      500.2550010 MHz
NUC2      1H
PCPD2     waitx16
PLM2      15.13599968 W
PLM12     0.53924000 W
PLM13     0.27124000 W

F2 - Processing parameters
SI        32768
SF        125.7879910 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

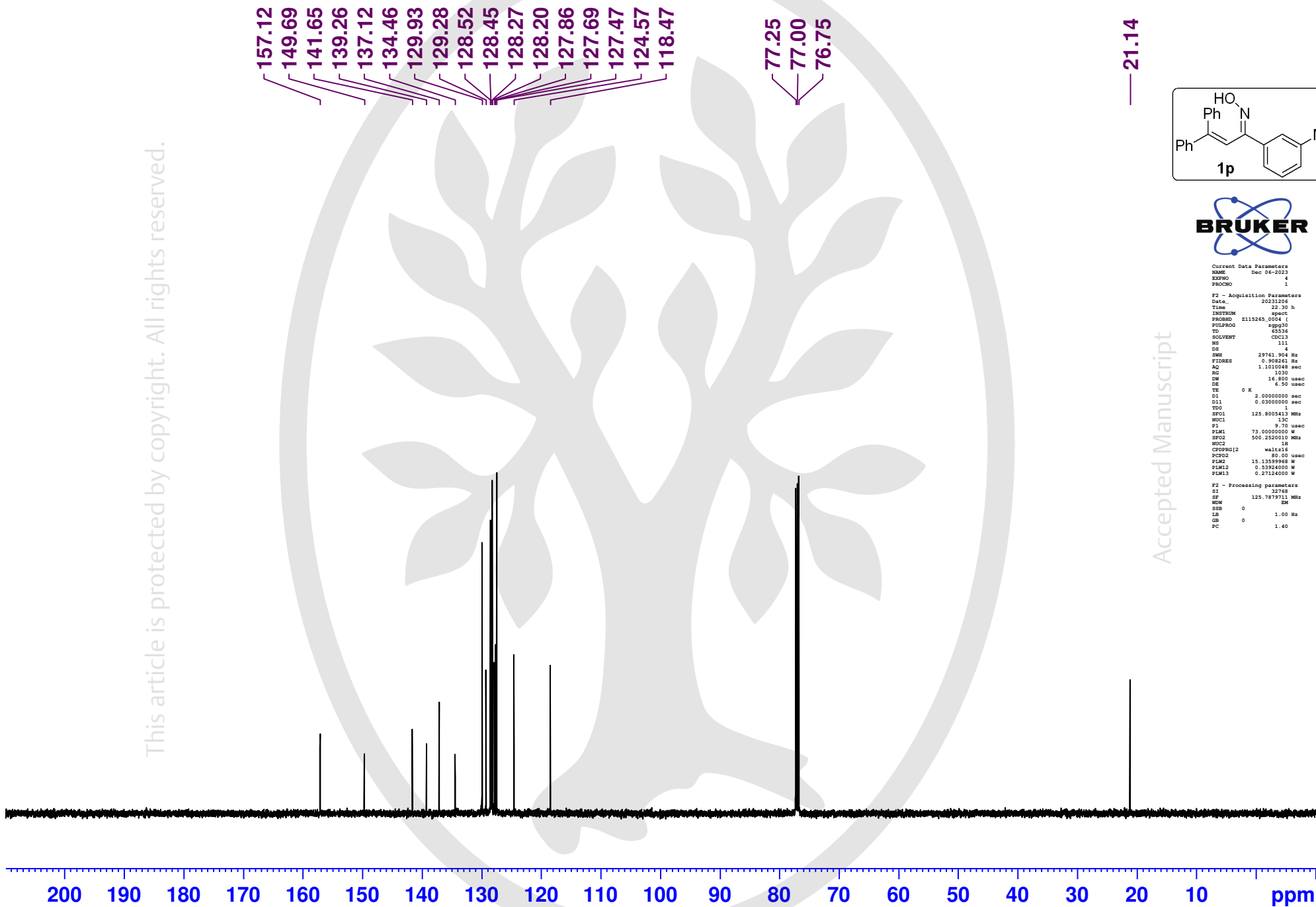
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¹H NMR (500 MHz, CDCl₃)



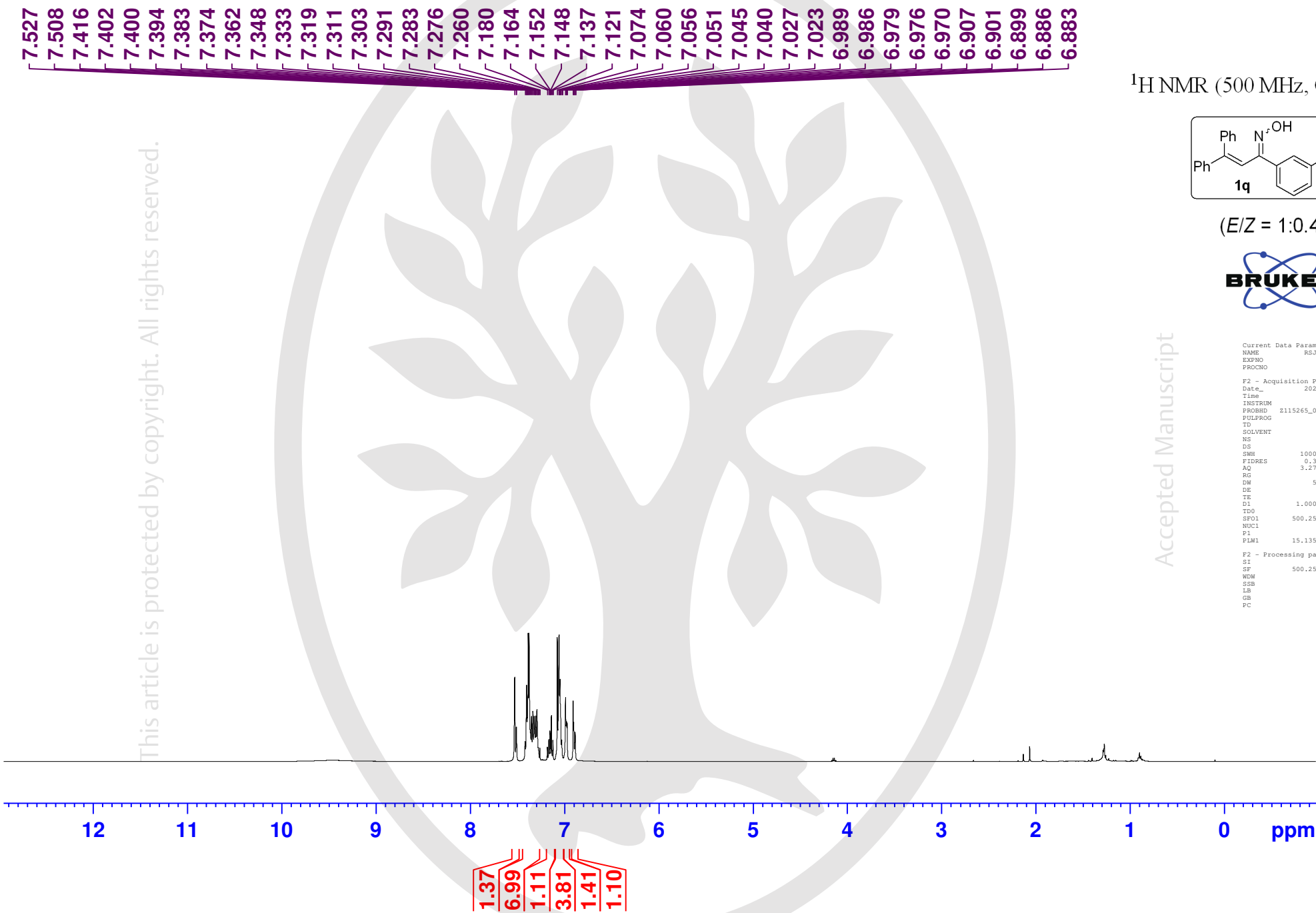
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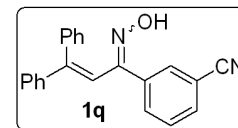
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¹H NMR (500 MHz, CDCl₃)



(E/Z = 1:0.47)



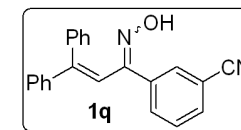
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```
Current Data Parameters
NAME      RSJ-1116
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20231206
Time      22.34 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         90.5
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1        1H
P1         15.10 usec
PL1        15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.2500136 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(E/Z = 1:0.47)

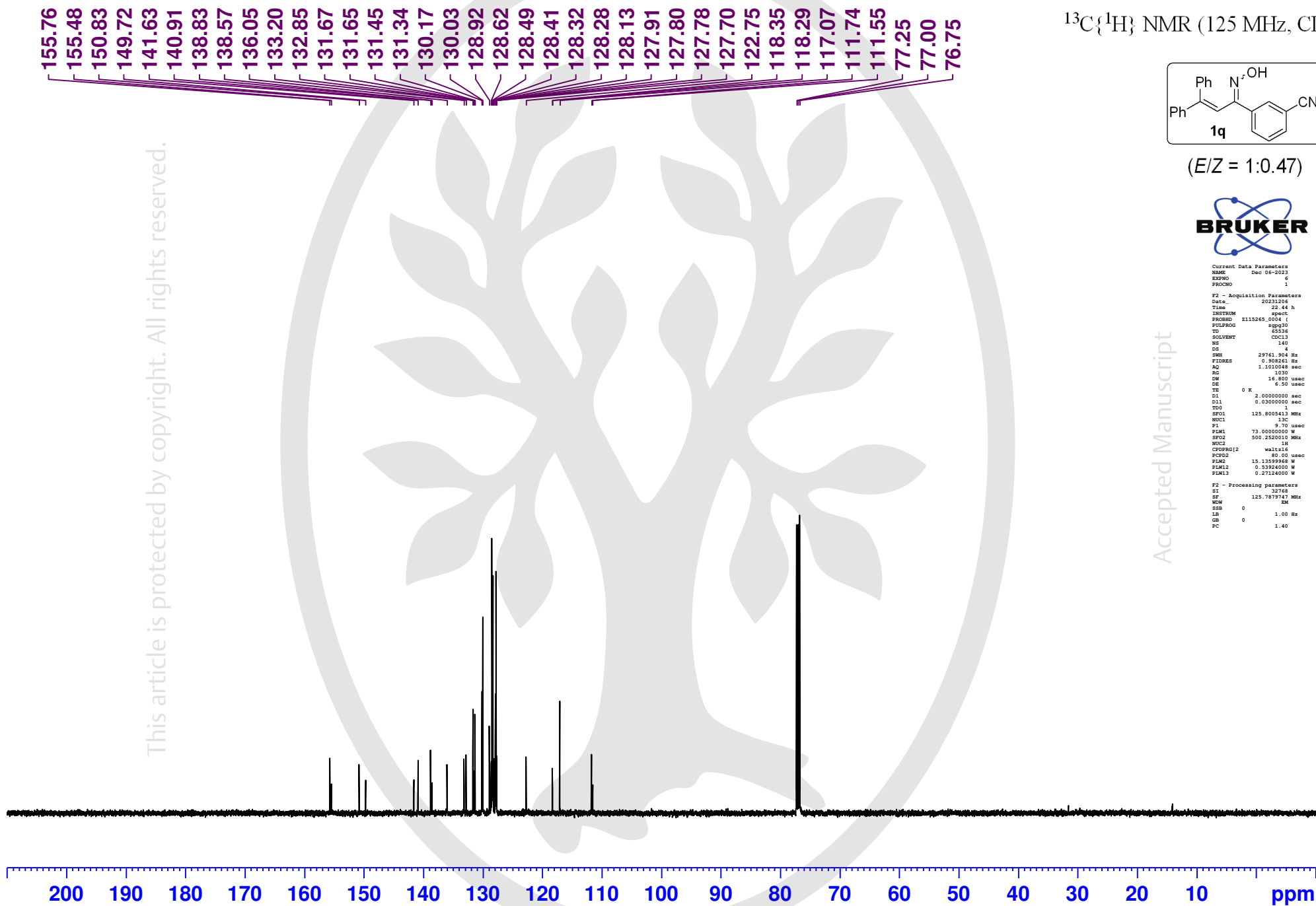


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Current Data Parameters
NAME          Dec 06-2023
EXPNO         6
PROCNO        1

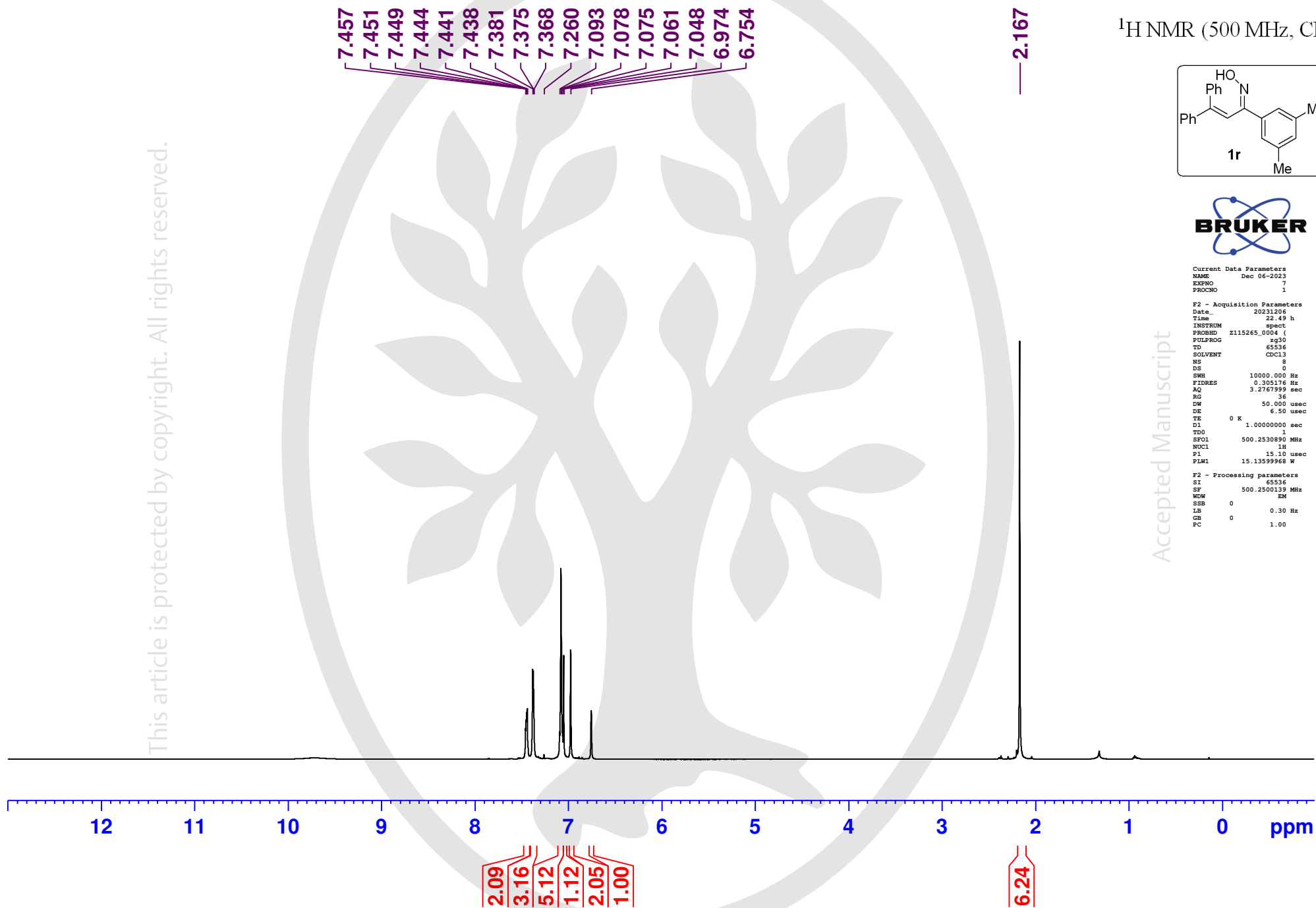
F2 - Acquisition Parameters
Date_         20231206
Time          22:44 h
INSTRUM       spect
PROBHD        5mmBBO
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            140
DS            4
SWH           29761.904 Hz
FIDRES        0.998261 Hz
AQ            1.1010048 sec
RG            1030
DE            16.800 usec
TE            0 K
D1            2.0000000 sec
d11           0.0300000 sec
SFO1          125.805413 MHz
NUC1          13C
P1            9.70 usec
PL1           73.0000000 W
SFO2          500.2520010 MHz
NUC2          1H
PCPDPRG2     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7679747 MHz
SBS           0
LS            1.00 Hz
GB            0
PC            1.40
```

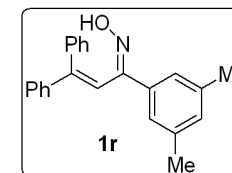
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^1H NMR (500 MHz, CDCl_3)

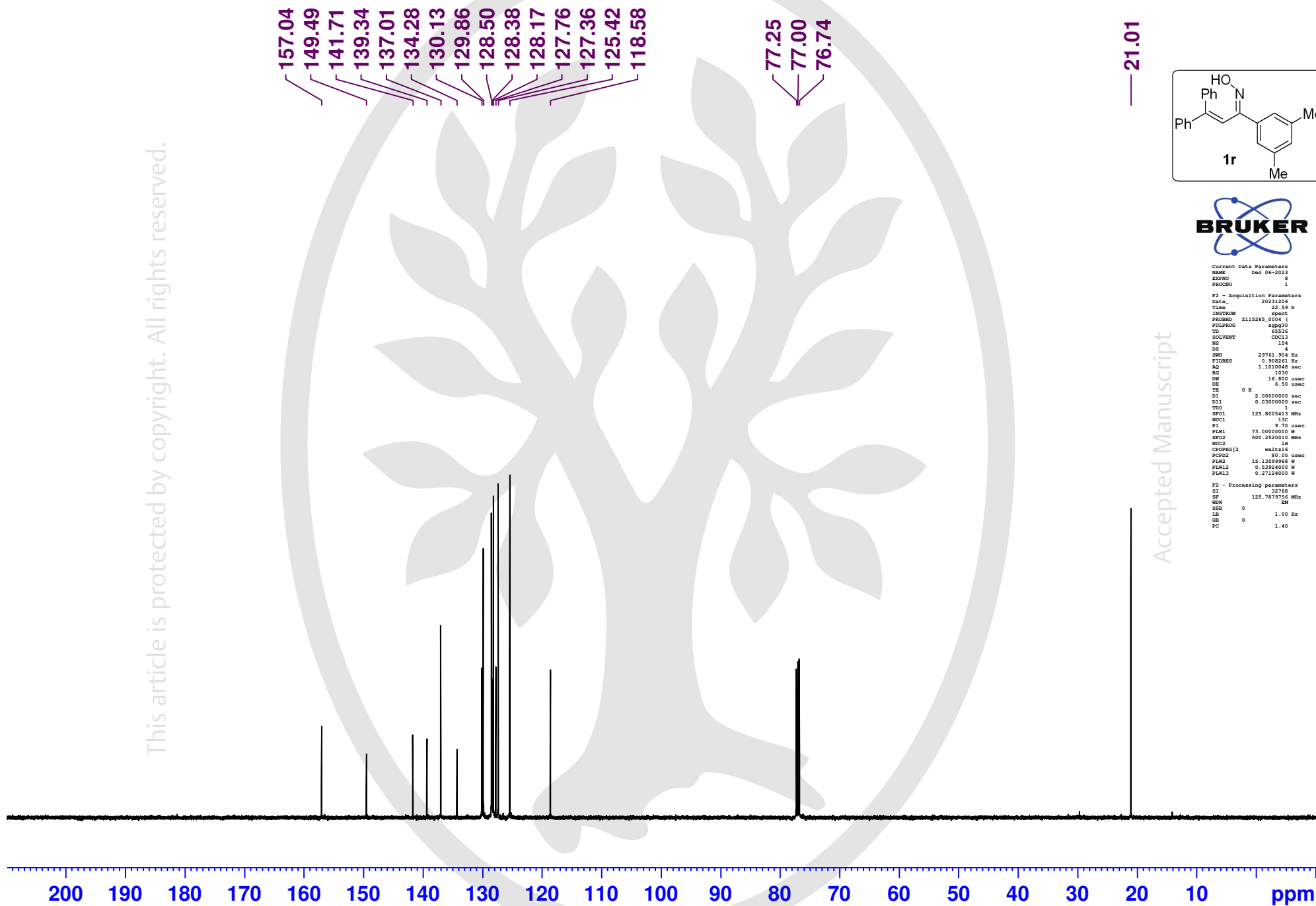


Current Data Parameters
NAME Dec 06-2023
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231206
Time 22.49 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 36
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.0000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

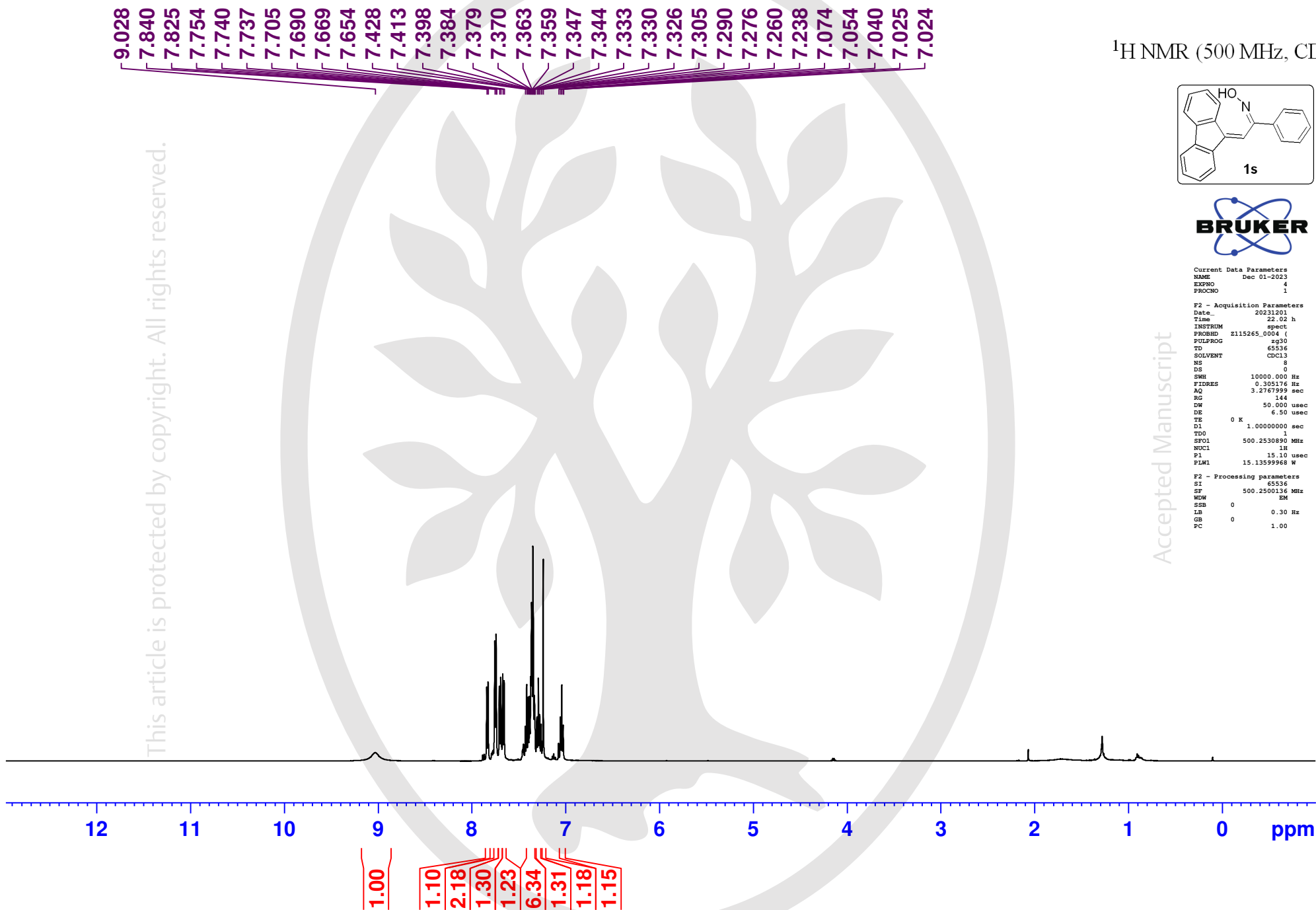
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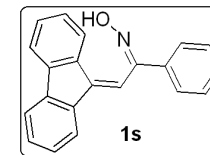
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^1H NMR (500 MHz, CDCl_3)



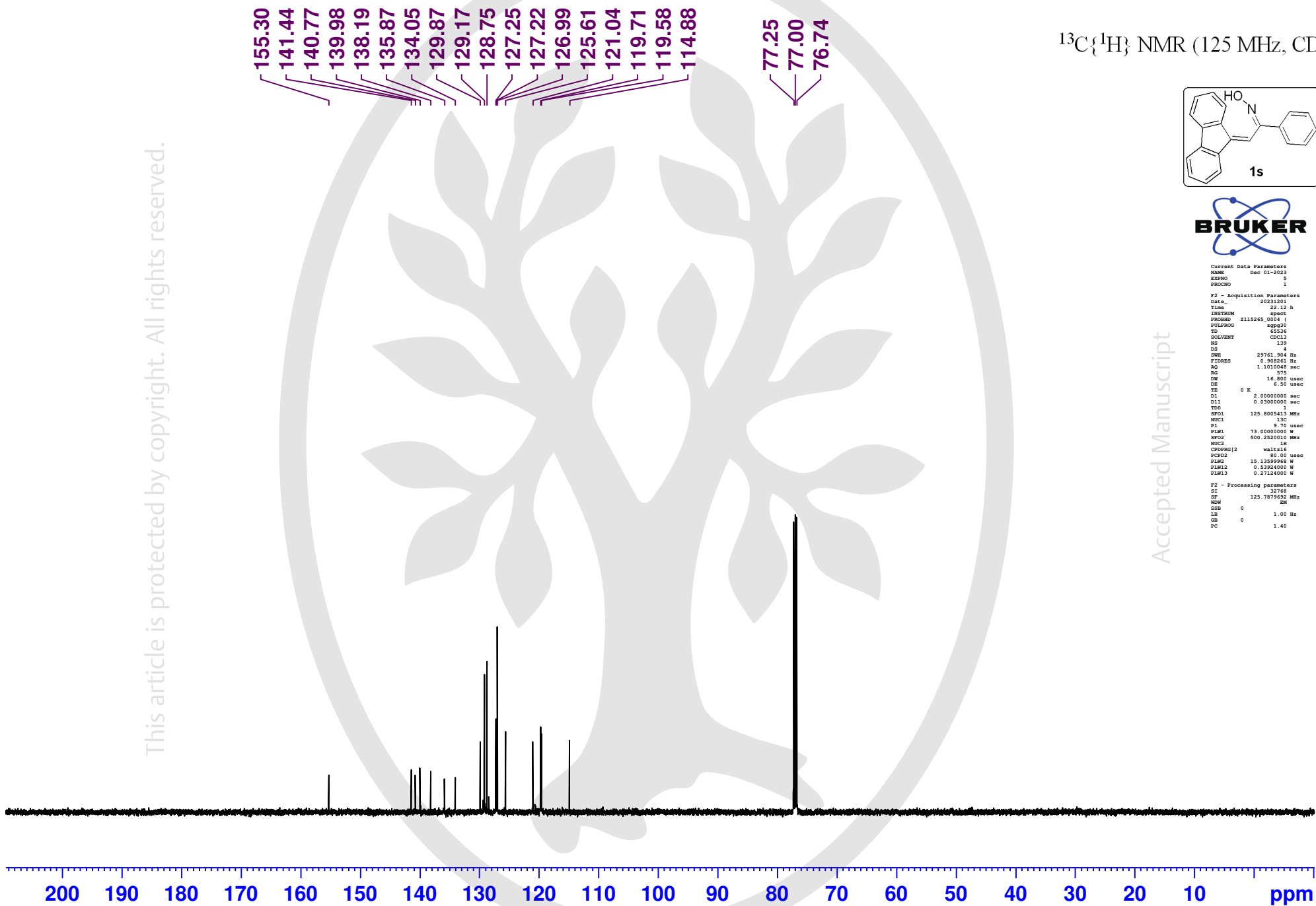
Current Data Parameters
NAME Dec 01-2023
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231201
Time 22.02 h
INSTRUM spect
PROBHD Z115265_0004 ((
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.276799 sec
RG 144
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

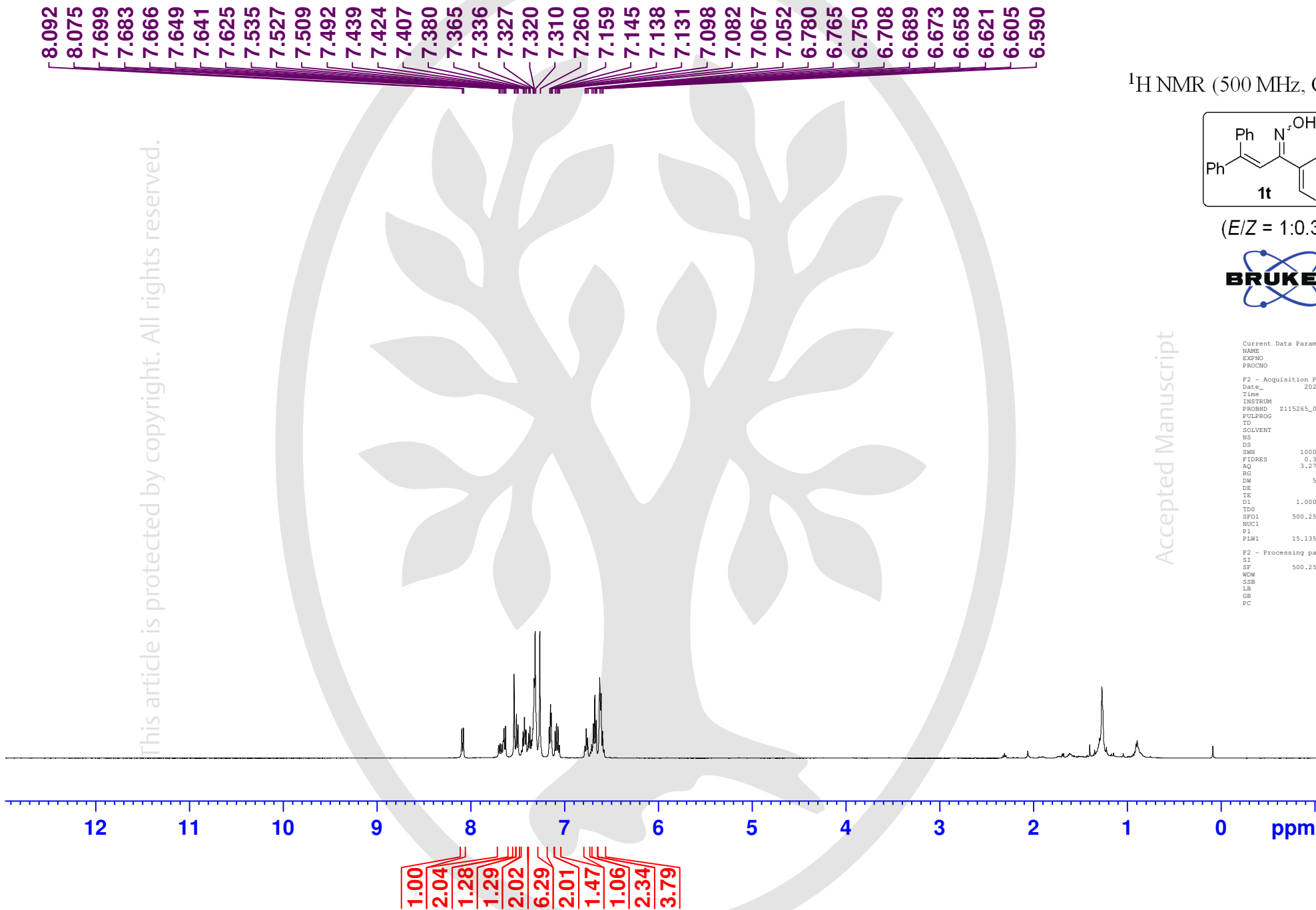
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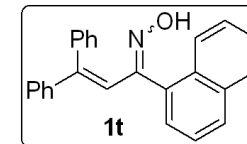


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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.37)

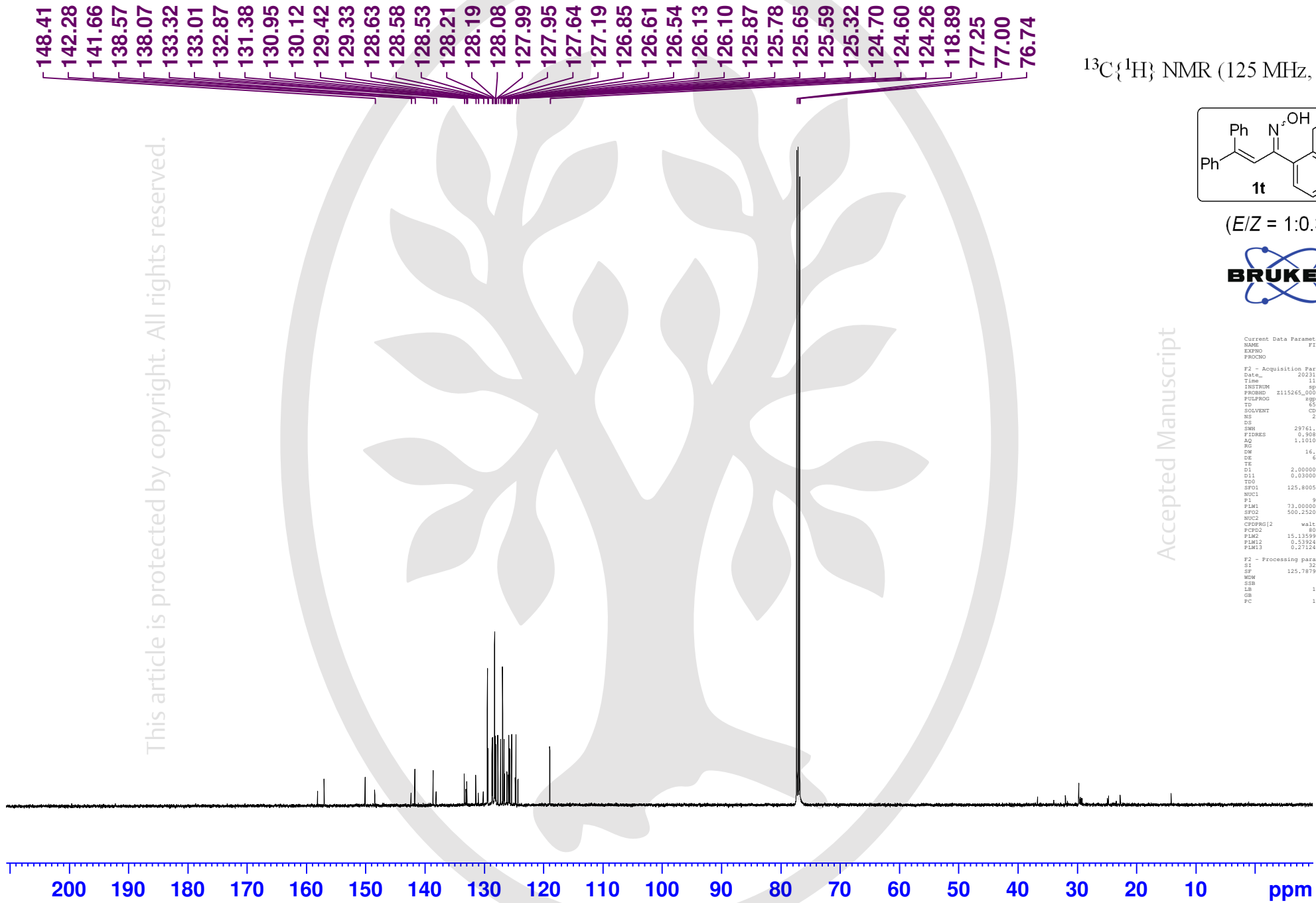


```
Current Data Parameters
NAME          FINAL
EXPNO         5
PROCNO        1

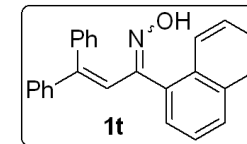
F2 - Acquisition Parameters
Date_         20231130
Time          9.21 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            161
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SFO1          500.2530890 MHz
NUC1           1H
P1            15.10 usec
PL1           15.13559968 W

F2 - Processing parameters
SI            65536
SF            500.2500136 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



(*E/Z* = 1:0.37)



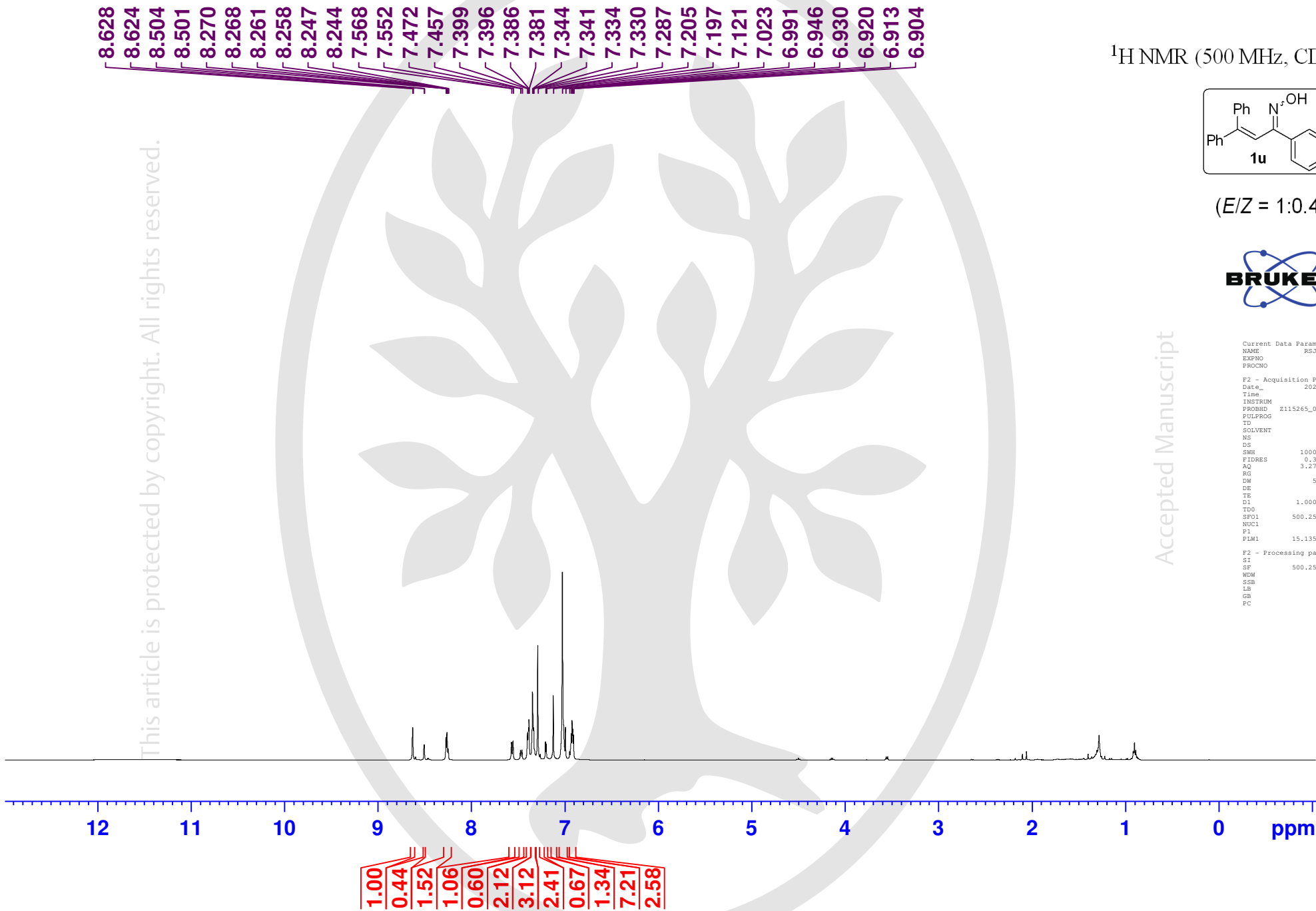
Current Data Parameters
NAME Final
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231110
Time_ 11.11 h
INSTRUM spect
PROBHD z115265_0004 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SFE 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 256
DM 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PL1 73.0000000 W
SFO2 500.2550010 MHz
NUC2 1H
CPCPRG2 waltz16
PCPD2 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27124000 W

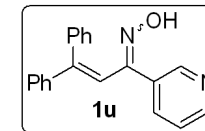
F2 - Processing parameters
SI 32768
SF 125.7879674 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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^1H NMR (500 MHz, CDCl_3)



(*E/Z* = 1:0.44)

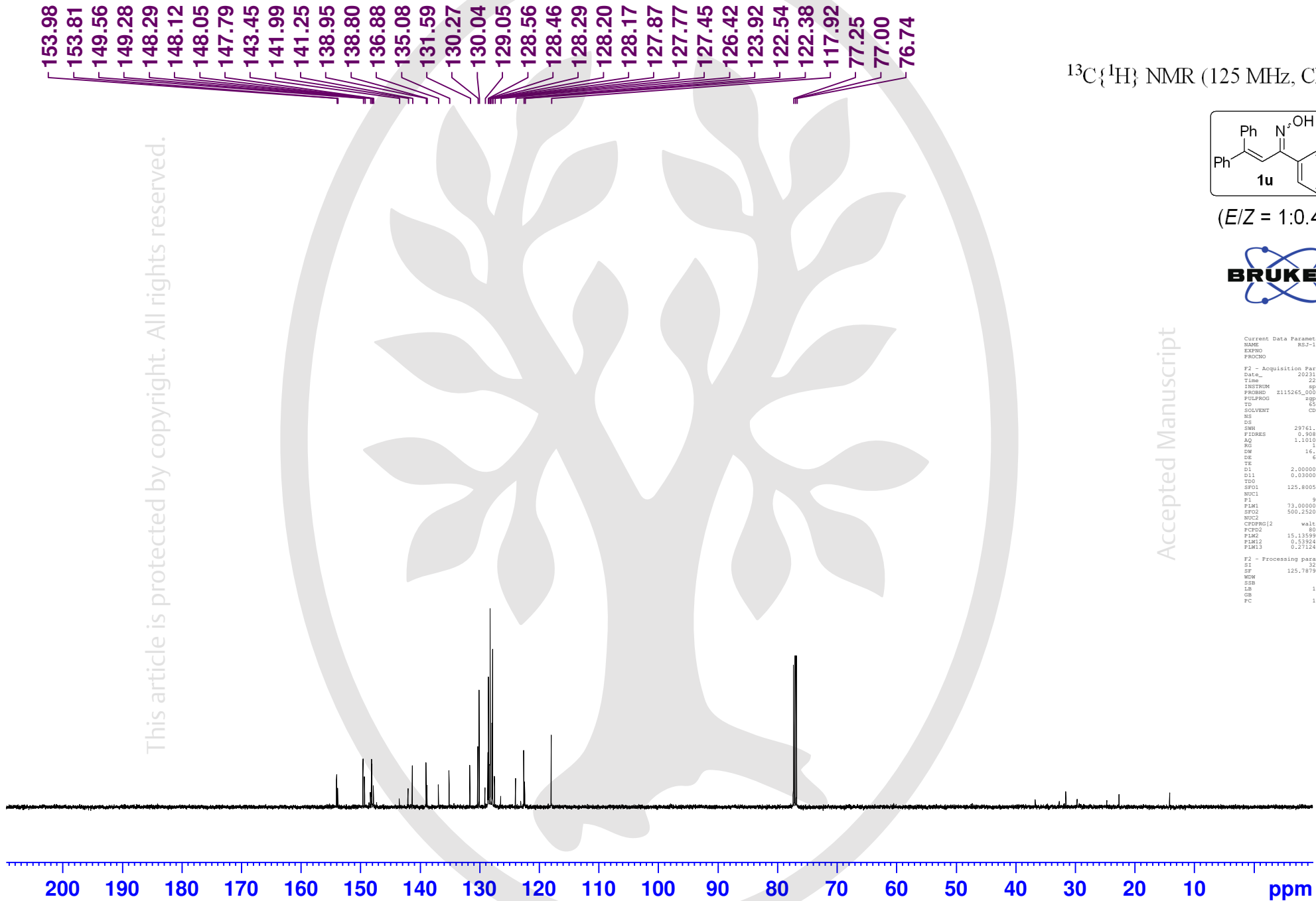


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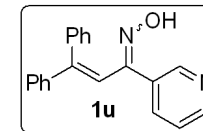
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Current Data Parameters
NAME      RSJ-1120
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20231206
Time      22.10 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         36
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.2500140 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

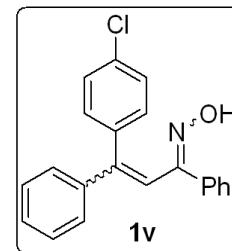


(*E/Z* = 1:0.44)



Current Data Parameters
 NAME hsu-1150
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20231206
 Time 22.16 h
 INSTRUM spect
 PROBHD z115265_0004 (4
 PULPROG zgpg30
 TD 65536
 SOLVENT cdcl3
 NS 88
 DS 4
 SFO1 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 1030
 DW 16.800 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TSD 1
 SFO1 125.8005413 MHz
 NUCL1 13C
 P1 9.70 usec
 PL1 0.00000000 W
 SFO2 500.2550010 MHz
 NUCL2 1H
 CPGPRG2 waltz16
 PCPD2 80.00 usec
 PLM2 15.13599968 W
 PLM12 0.53924000 W
 PLM13 0.27124000 W
 F2 - Processing parameters
 SI 32768
 SF 125.7879765 MHz
 NWDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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(*E/Z* = 0.9:1)

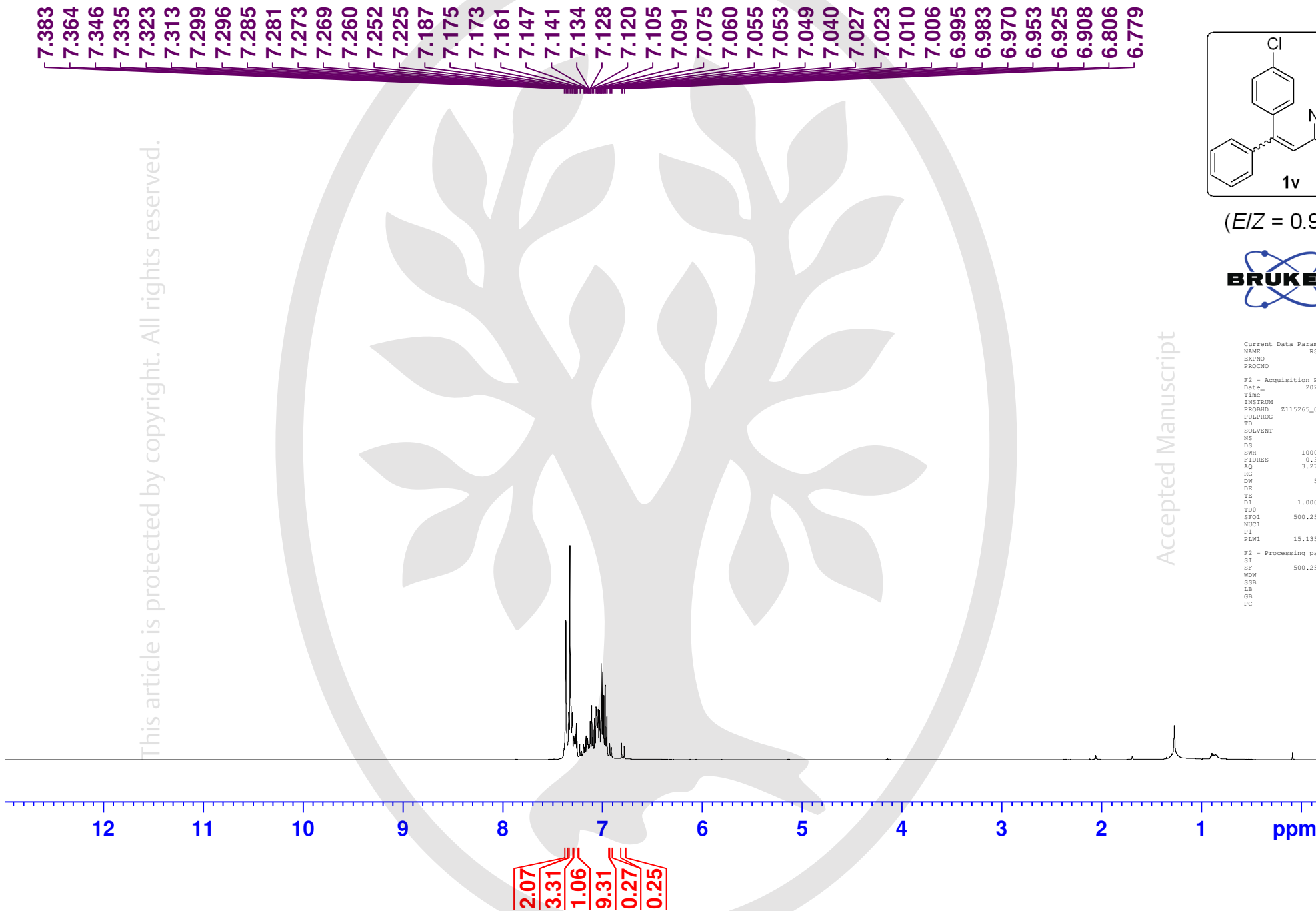


Current Data Parameters
NAME RSJ-957
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230908
Time 15.58 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 144
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PL1 15.13559968 W

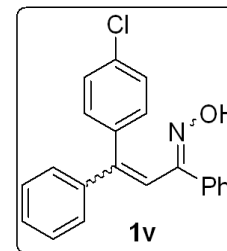
F2 - Processing parameters
SI 65536
SF 500.2500137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



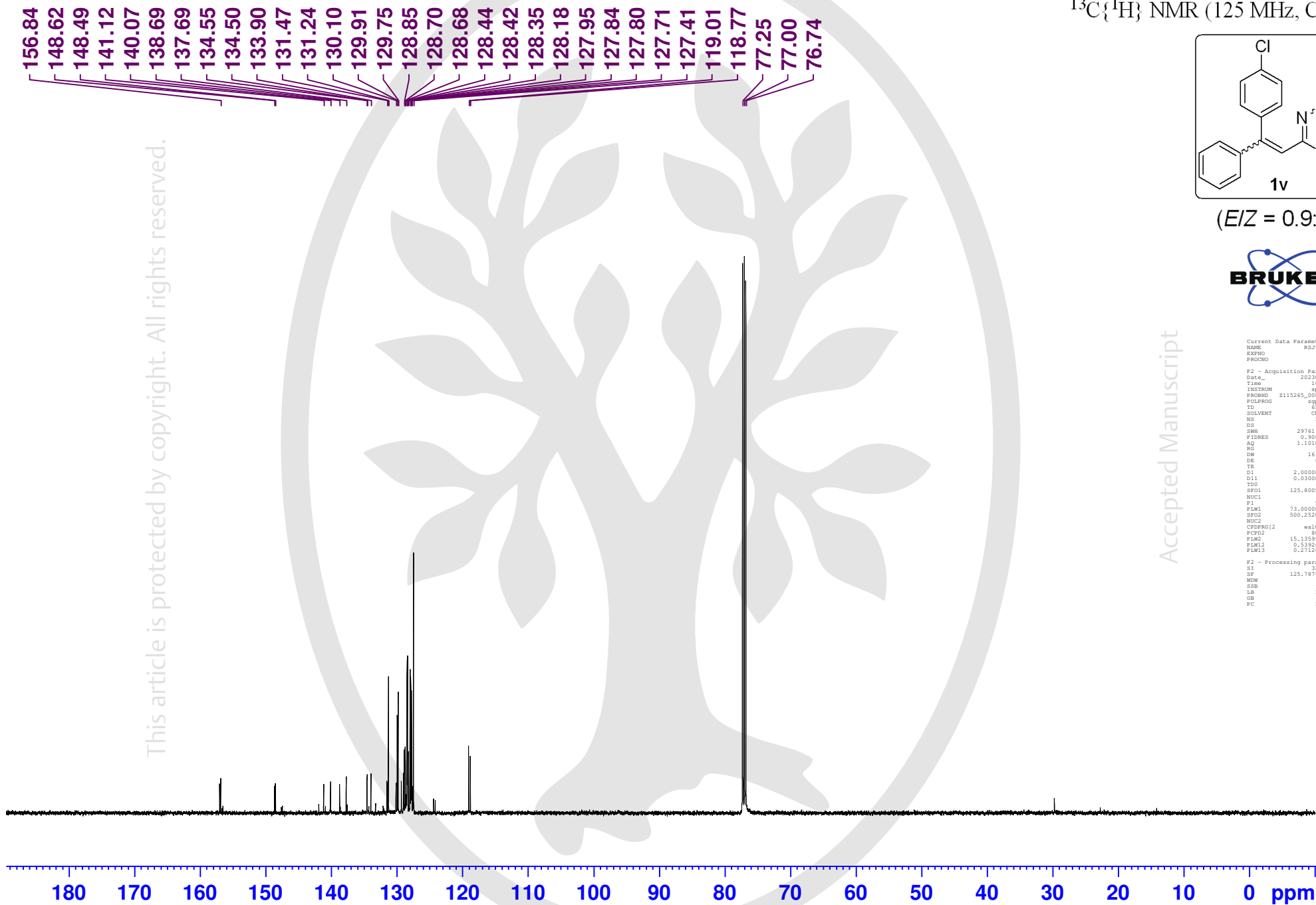
(E/Z = 0.9:1)



```
Current Data Parameters
NAME      R32-957
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
Date_     20230908
Time      16.54 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWE        29761.904 Hz
FIDRES     0.908261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
SFO1       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PL1        73.00000000 W
SFO2        500.2550010 MHz
NUC2       1H
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

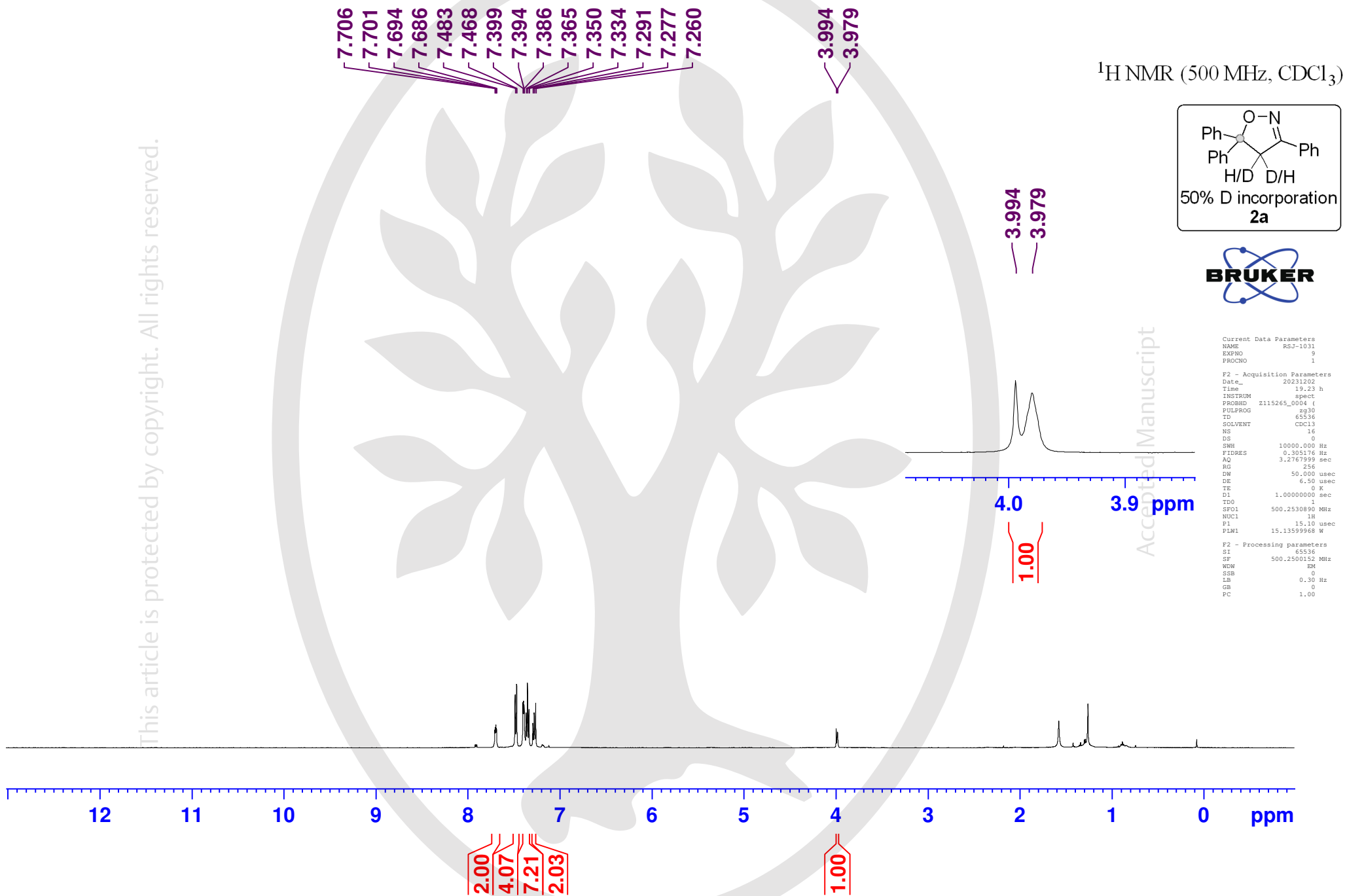
F2 - Processing parameters
SI         32768
SF         125.7879674 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC         1.40
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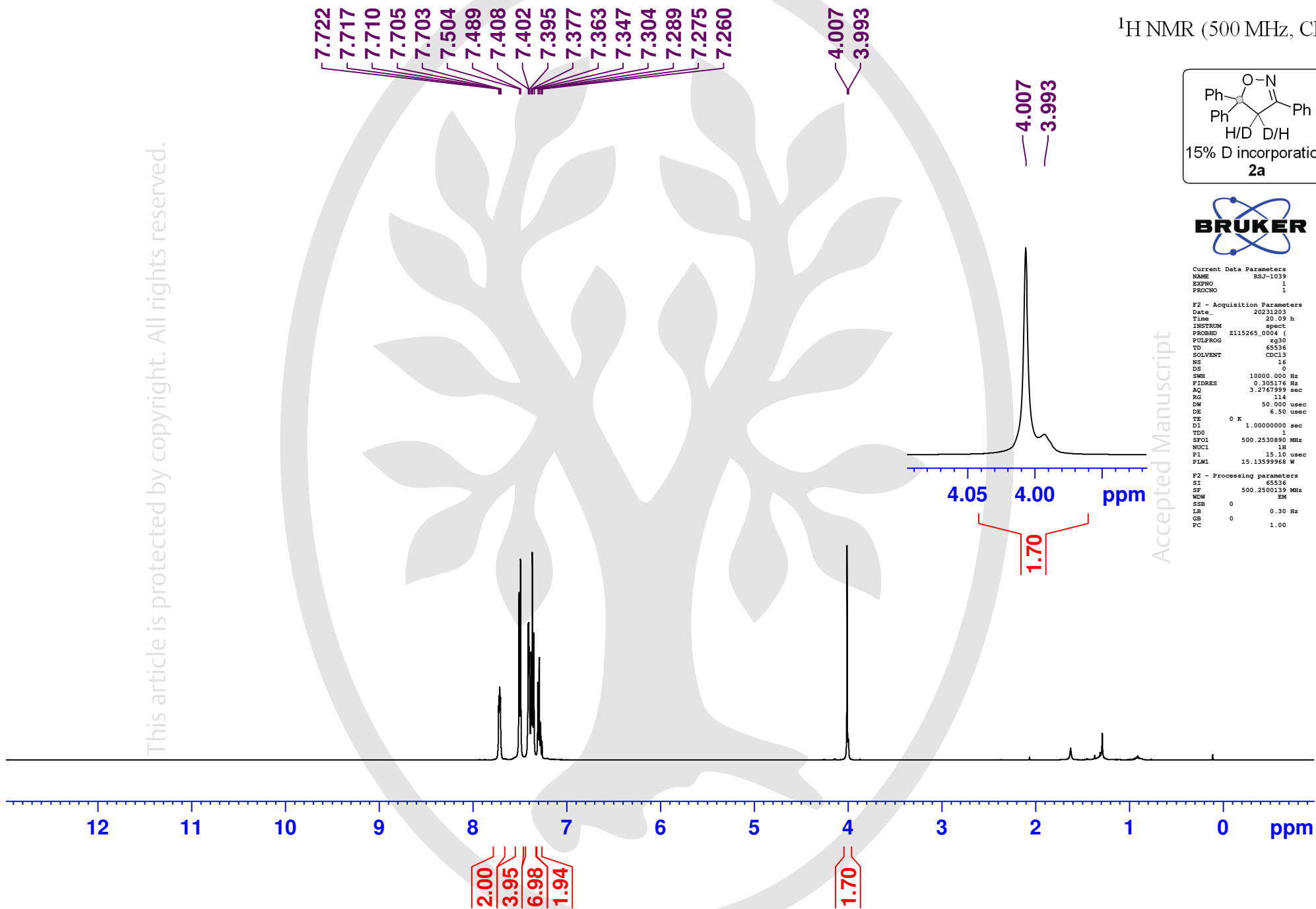
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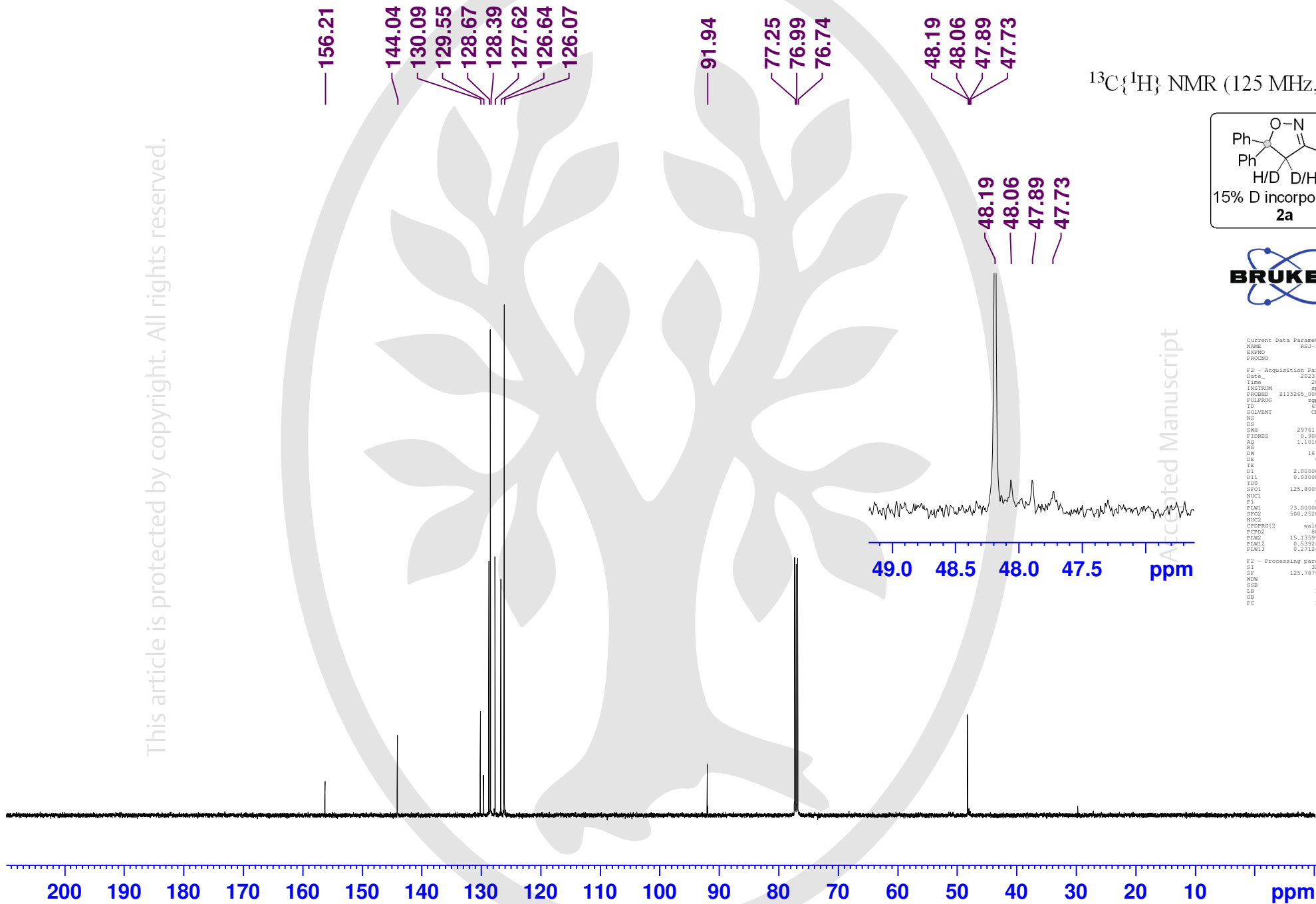


Current Data Parameters
NAME RSJ-1039
EXPNO 1
PROCNO 1

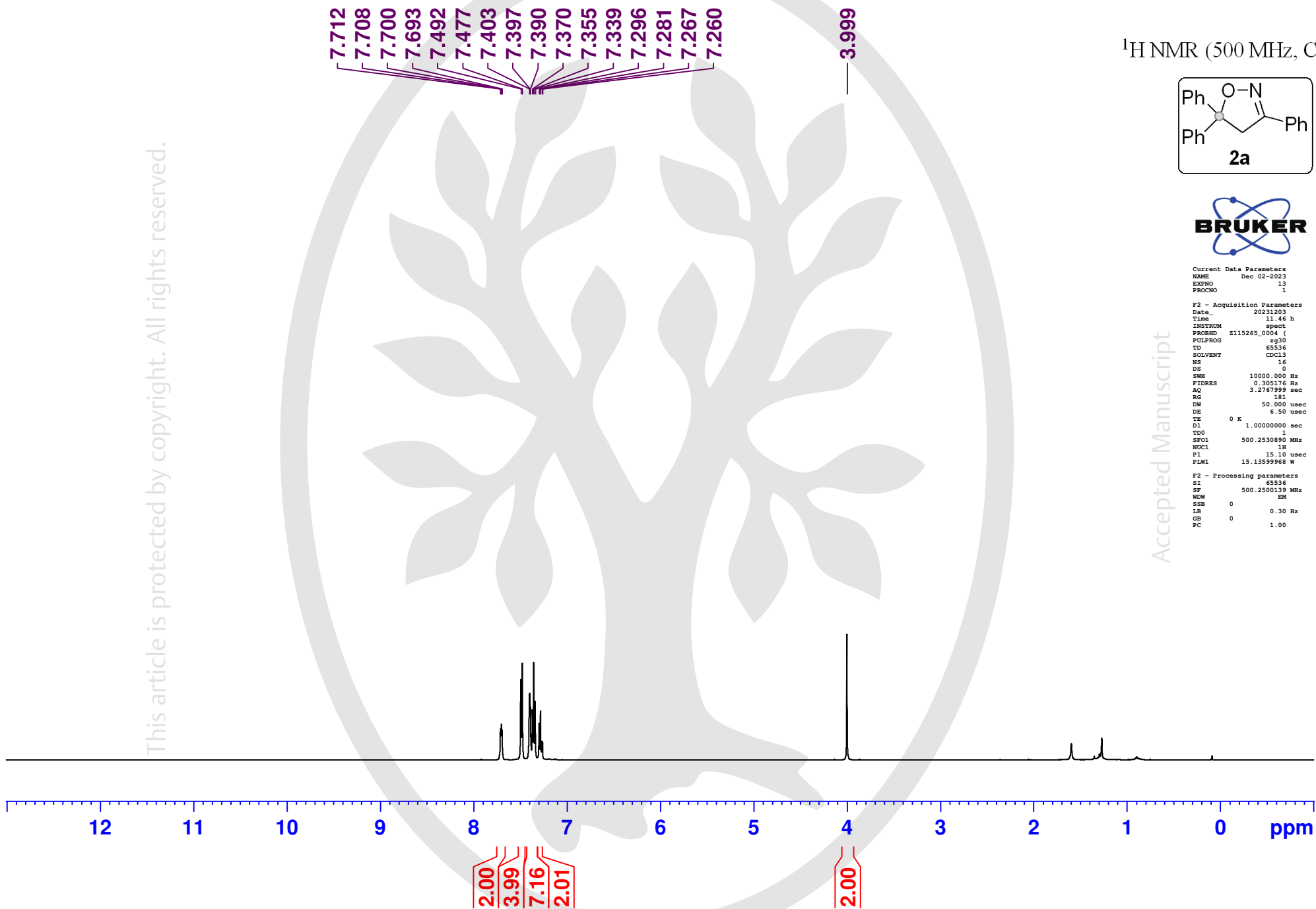
F2 - Acquisition Parameters
Date_ 20231203
Time 20.09 h
INSTRUM spect
PROBHD Z115265_0004 (
FULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 114
DW 50.000 usec
DE 6.50 usec
TE 0 K
DI 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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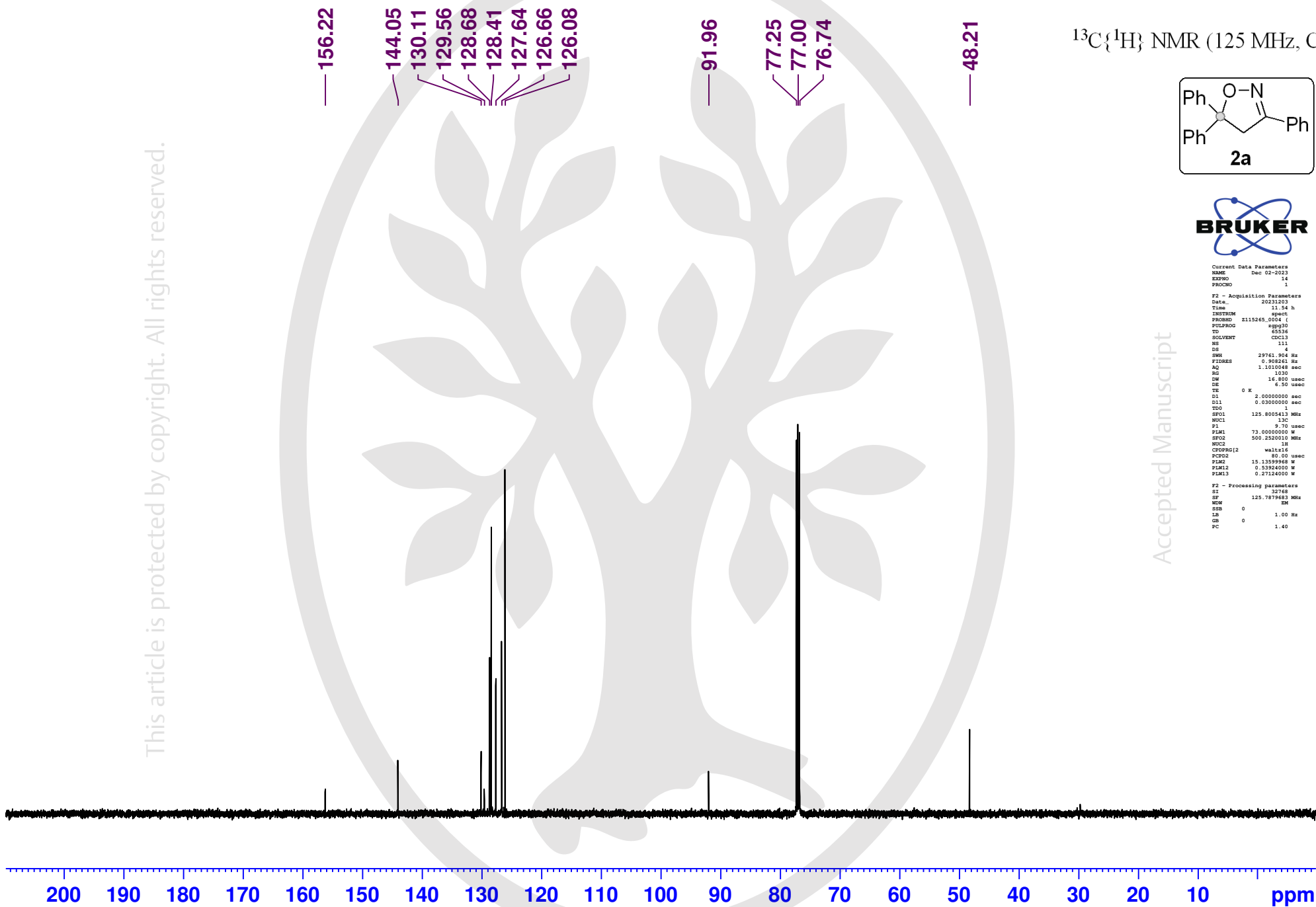


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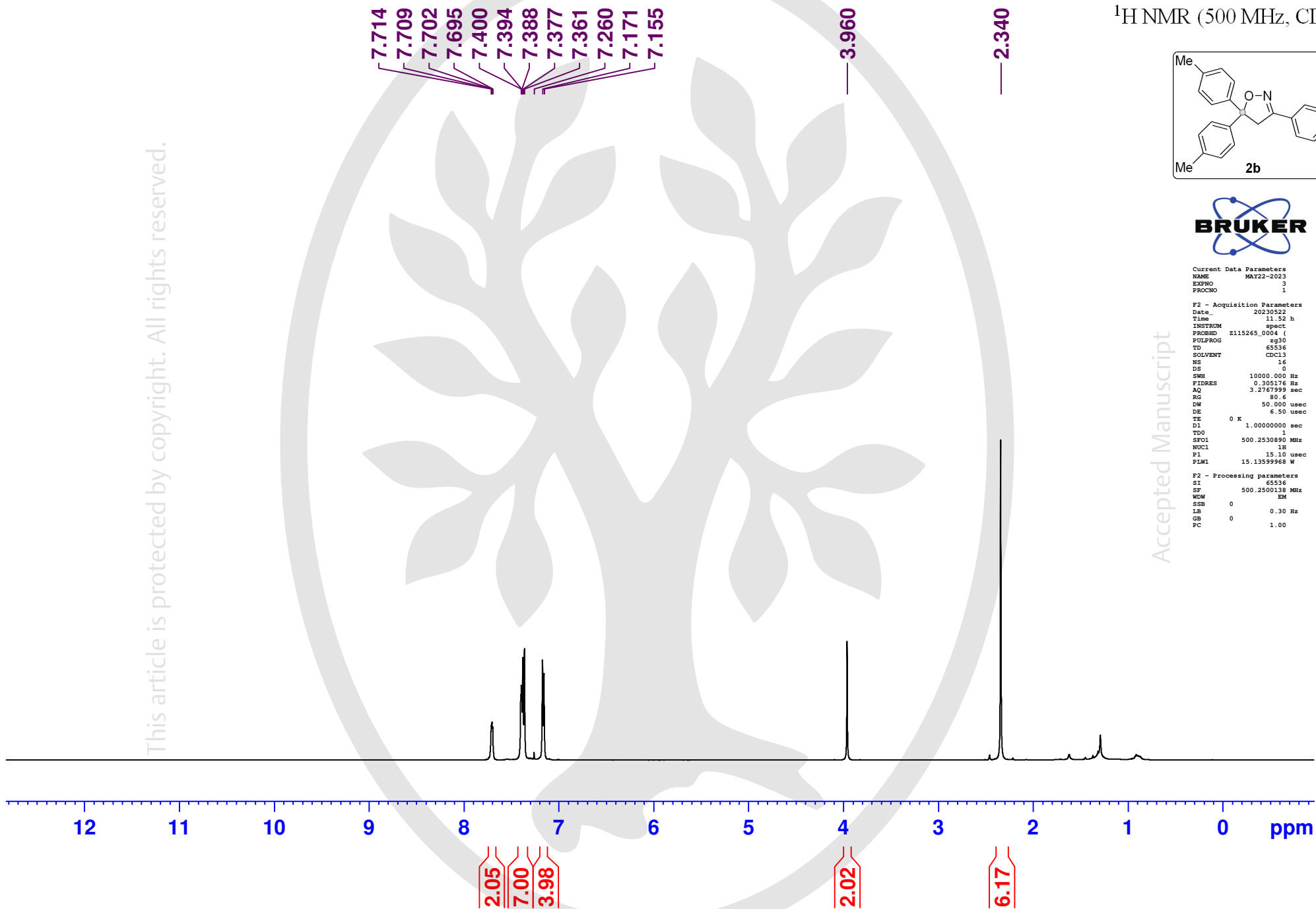
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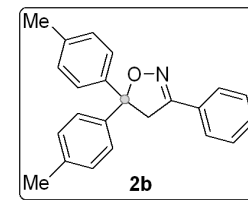
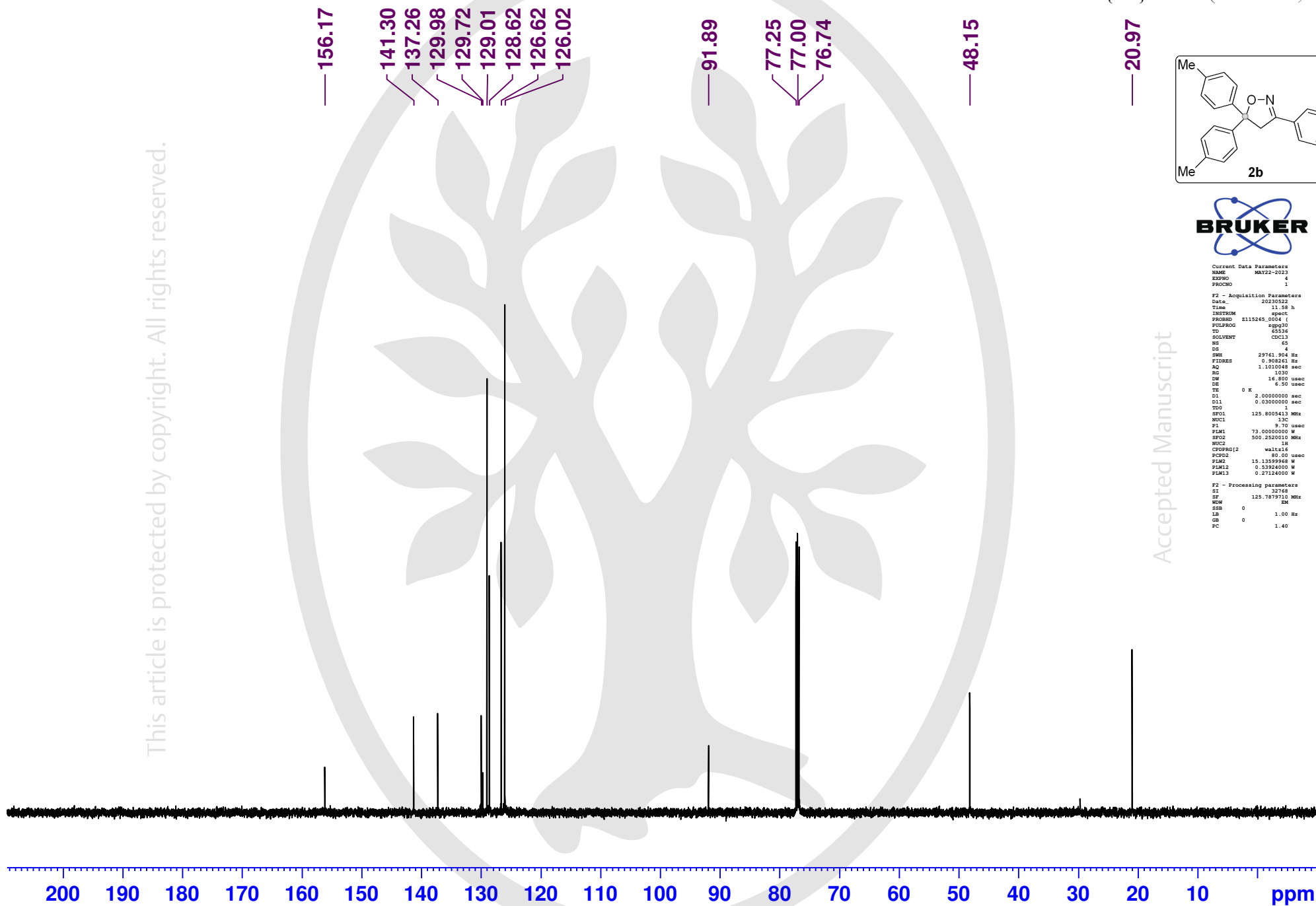


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Current Data Parameters
NAME      MAY22-2023
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20230522
Time     21:58 h
INSTRUM  spect
PROBHD   1H5265.004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        65
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         1030
DSW        16.800 usec
DE         6.50 usec
TE         0 K

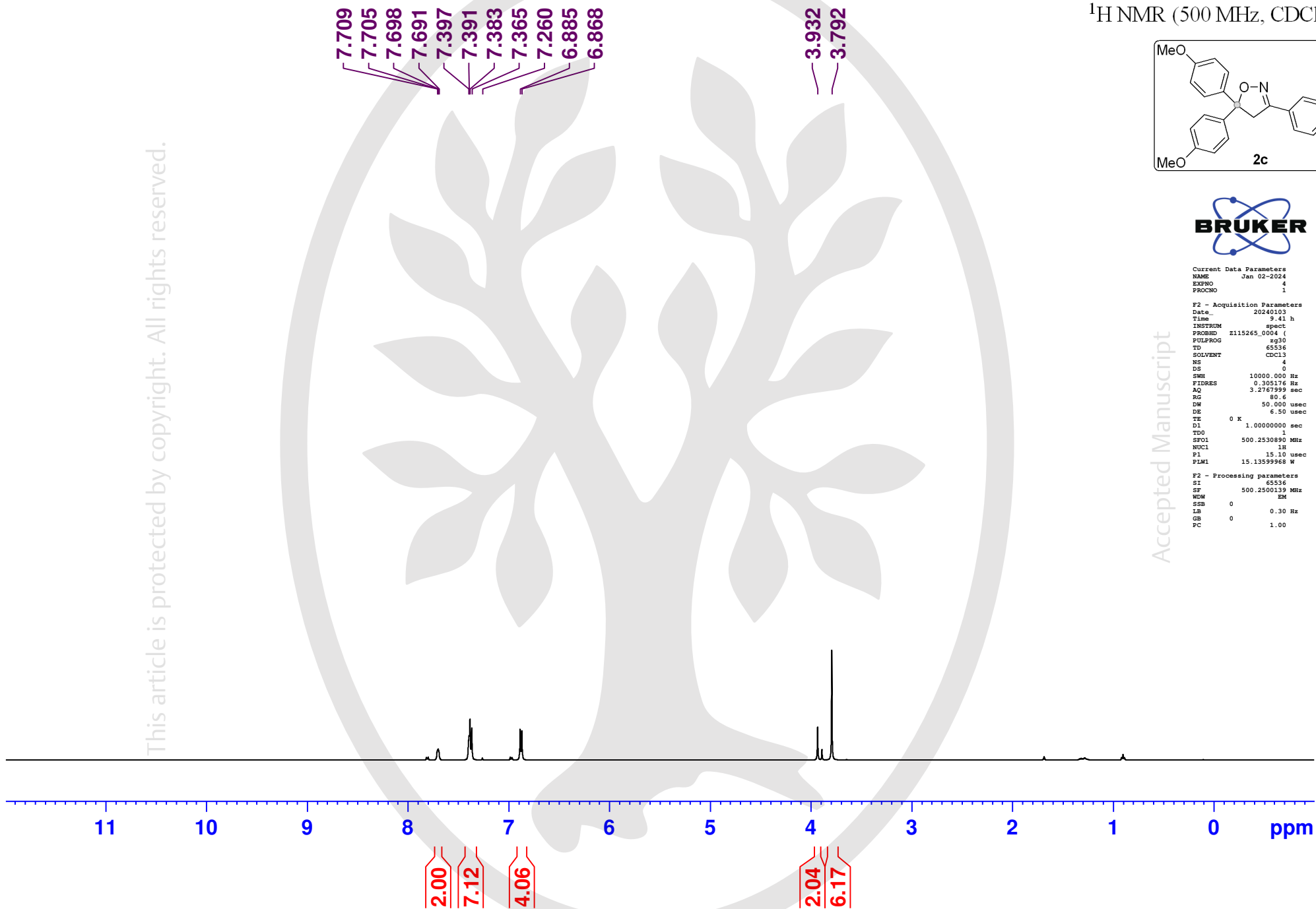
D1         2.0000000 sec
D11        0.0300000 sec
TDO        1
SFO1       125.8005413 MHz
NUC1       13C
D1         9.70 usec
PL1        73.0000000 W
SFO2       500.2520010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7679710 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
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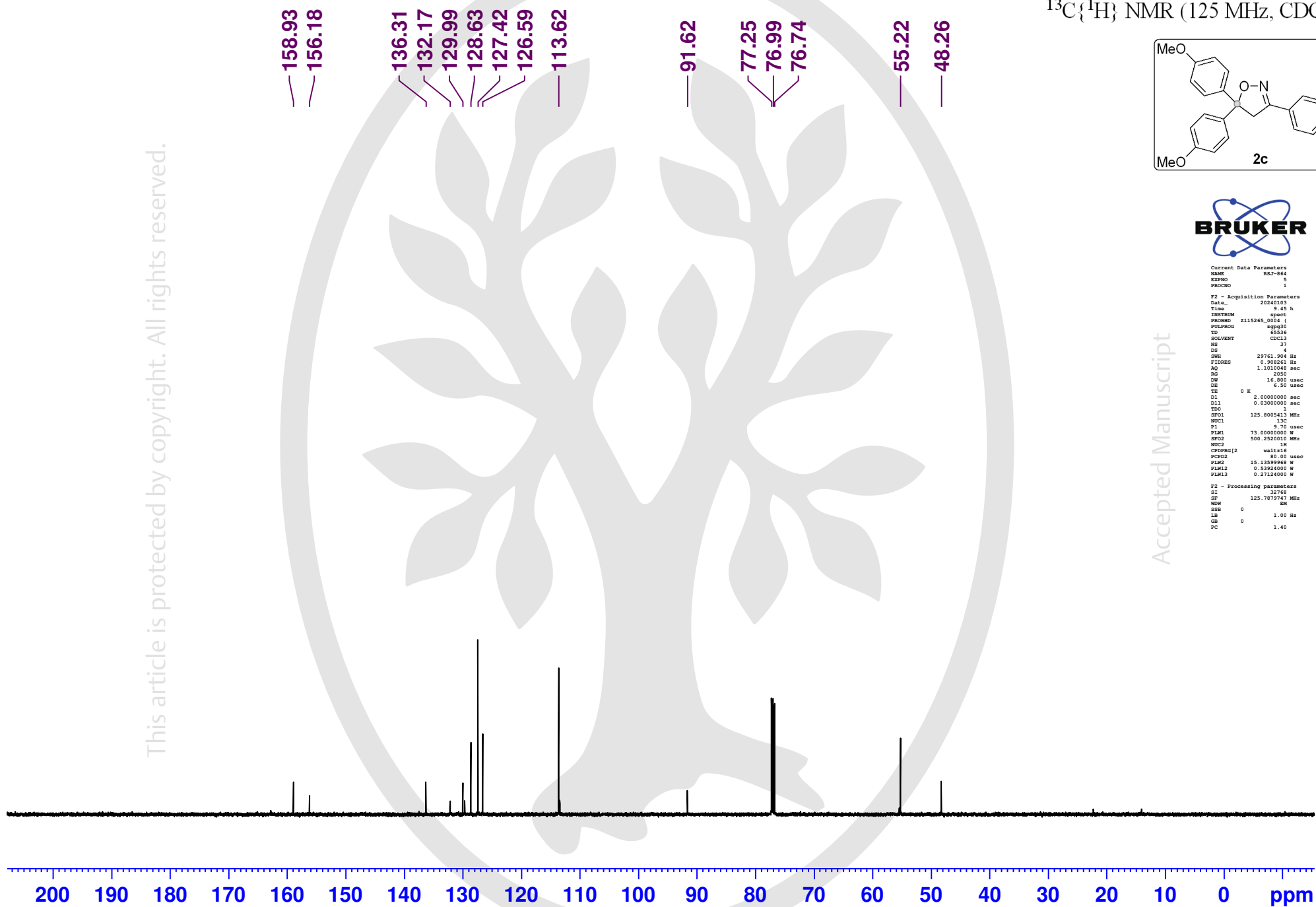


Current Data Parameters
NAME Jan 02-2024
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240103
Time 9:41 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 80.6
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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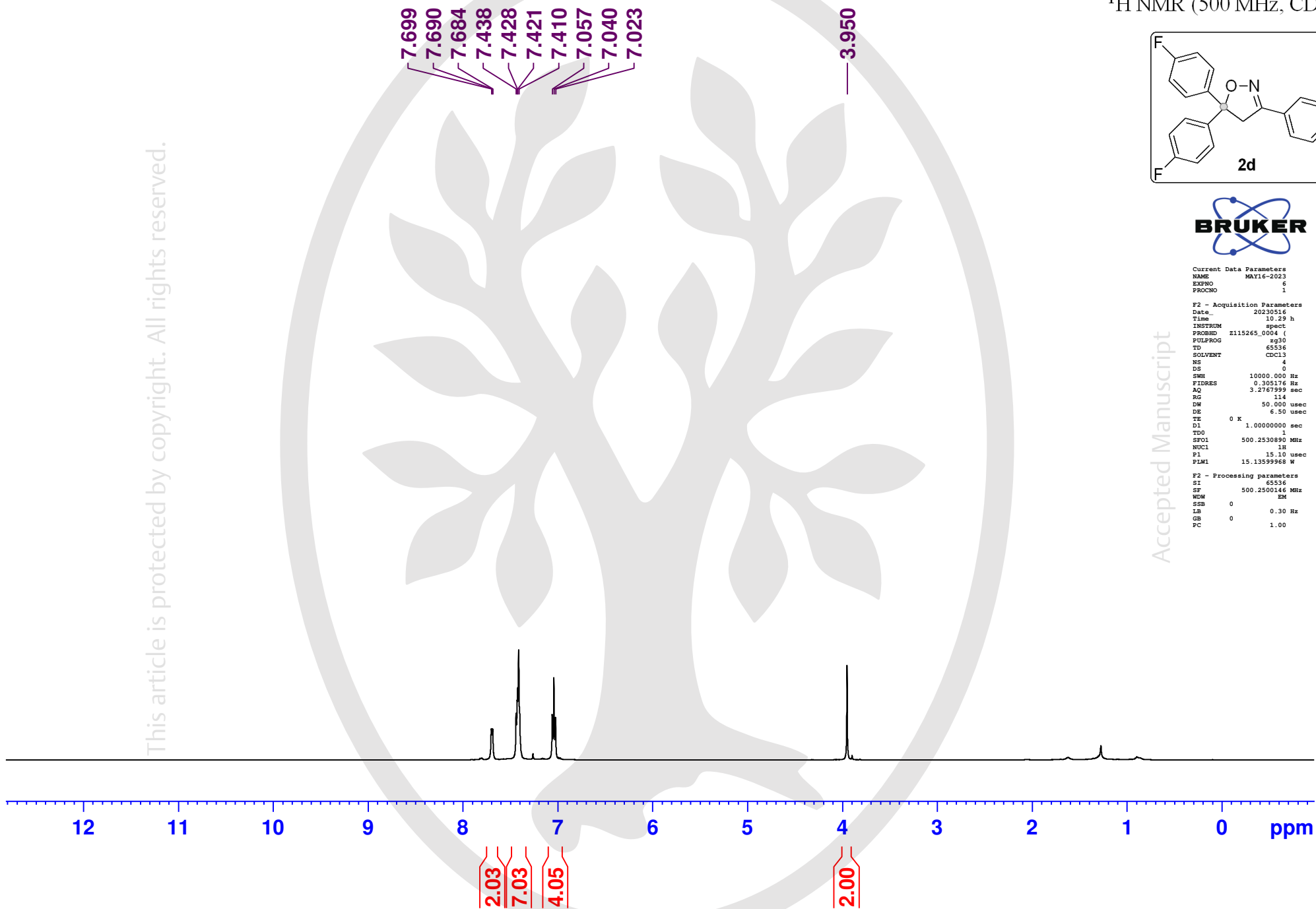


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Current Data Parameters
NAME          RSI-864
EXPNO         5
PROCNO        1

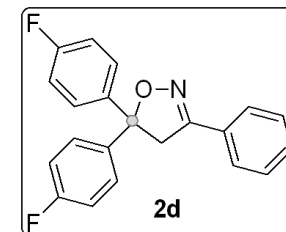
F2 - Acquisition Parameters
Date_         20240103
Time          9.45 h
INSTRUM       spect
PROBHD        1H1256.004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            37
DS            4
SWH           29761.904 Hz
FIDRES        0.998261 Hz
AQ            1.1010048 sec
RG            2050
AQ            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.0000000 sec
d11           0.0300000 sec
TDO           1
SFO1          125.8005413 MHz
NUC1          13C
P1            9.70 usec
SFO2          73.0000000 MHz
SFO2          500.2520010 MHz
NUC2          1H
CPCPRG2       waltz16
PCPD2         80.00 usec
PLM2          15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879747 MHz
SBS           0
LS            1.00 Hz
GB            0
PC            1.40
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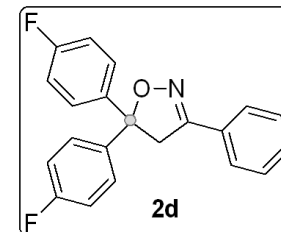


^1H NMR (500 MHz, CDCl_3)



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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



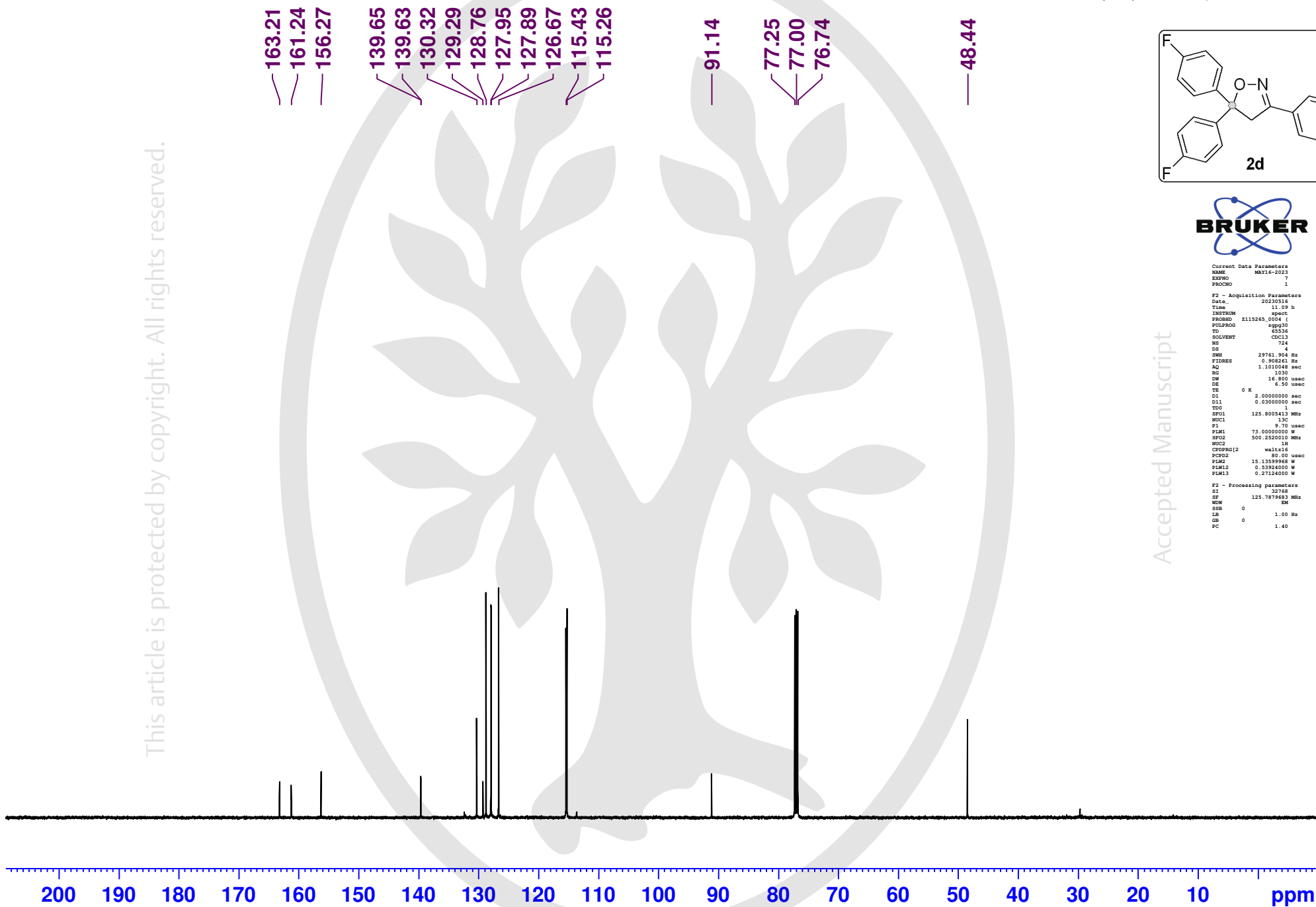
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Current Data Parameters
NAME          MAY16-2023
EXPNO        7
PROCNO       1

F2 - Acquisition Parameters
Date_        20230516
Time         11:09 h
INSTRUM      spect
PROBHD       1H125AS.004 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           724
DS           4
SWH          29761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           1030
SW           16.800 usec
DE           6.50 usec
TE           0 K

D1           2.0000000 sec
d11          0.0300000 sec
TDO          1
SFO1         125.8005413 MHz
NUC1         13C
P1           9.70 usec
PL1         73.0000000 W
SFO2         500.2520010 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27154000 W

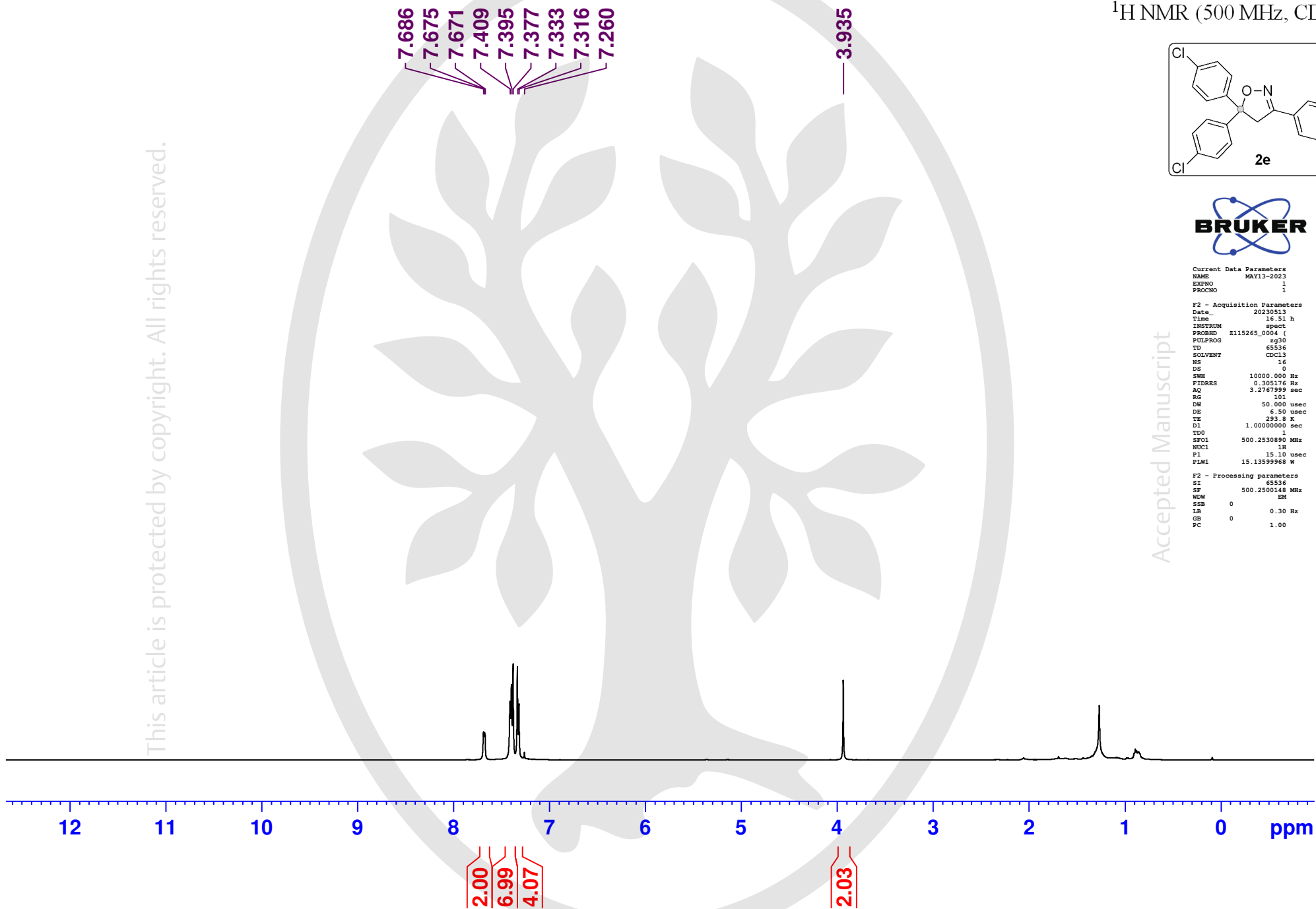
F2 - Processing parameters
SI           32768
SF           125.7879683 MHz
SBS          0
WSW          5M
LB           1.00 Hz
GB           0
PC           1.40
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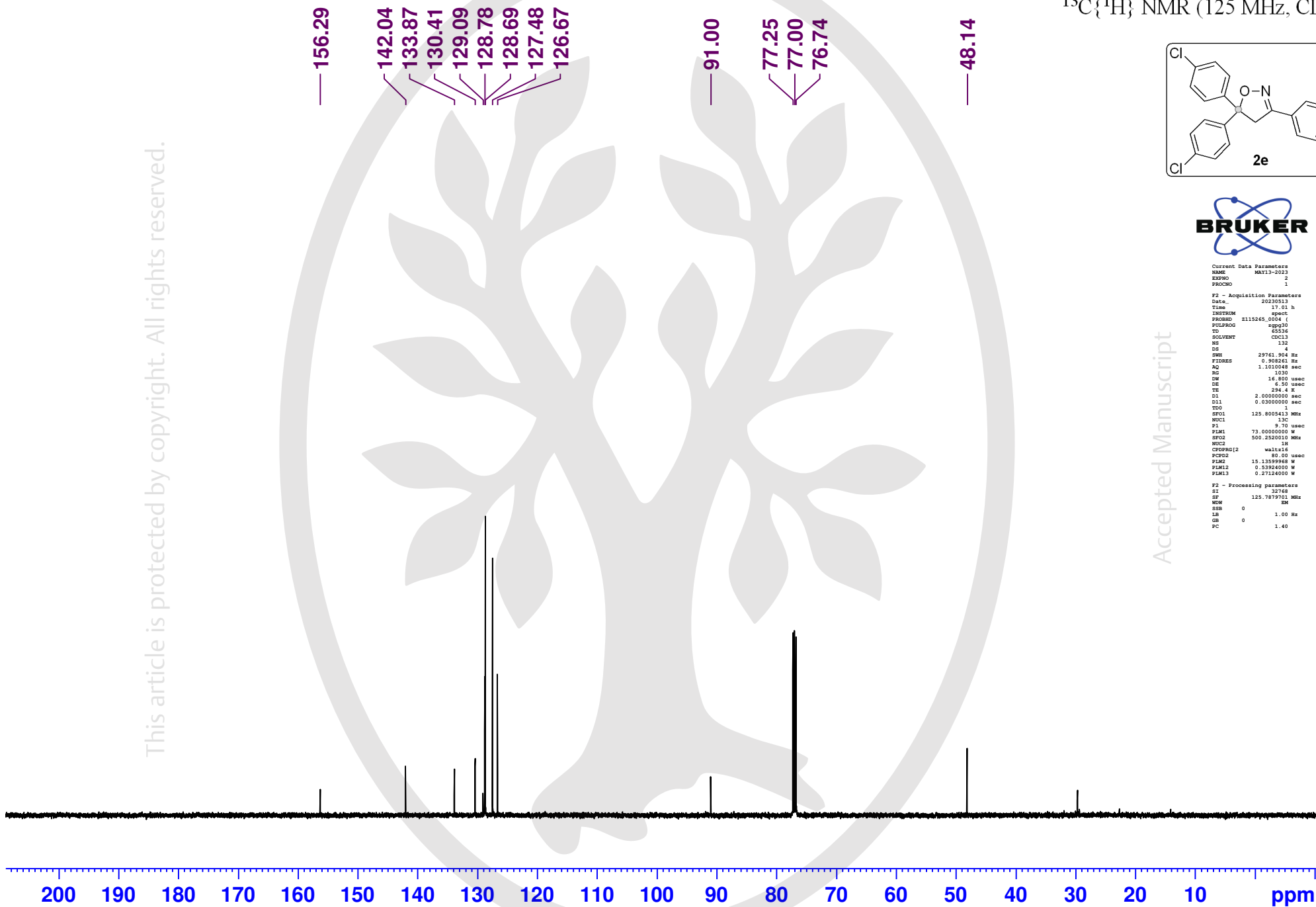
Current Data Parameters
NAME MAY13-2023
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230513
Time 16:51 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2167999 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500148 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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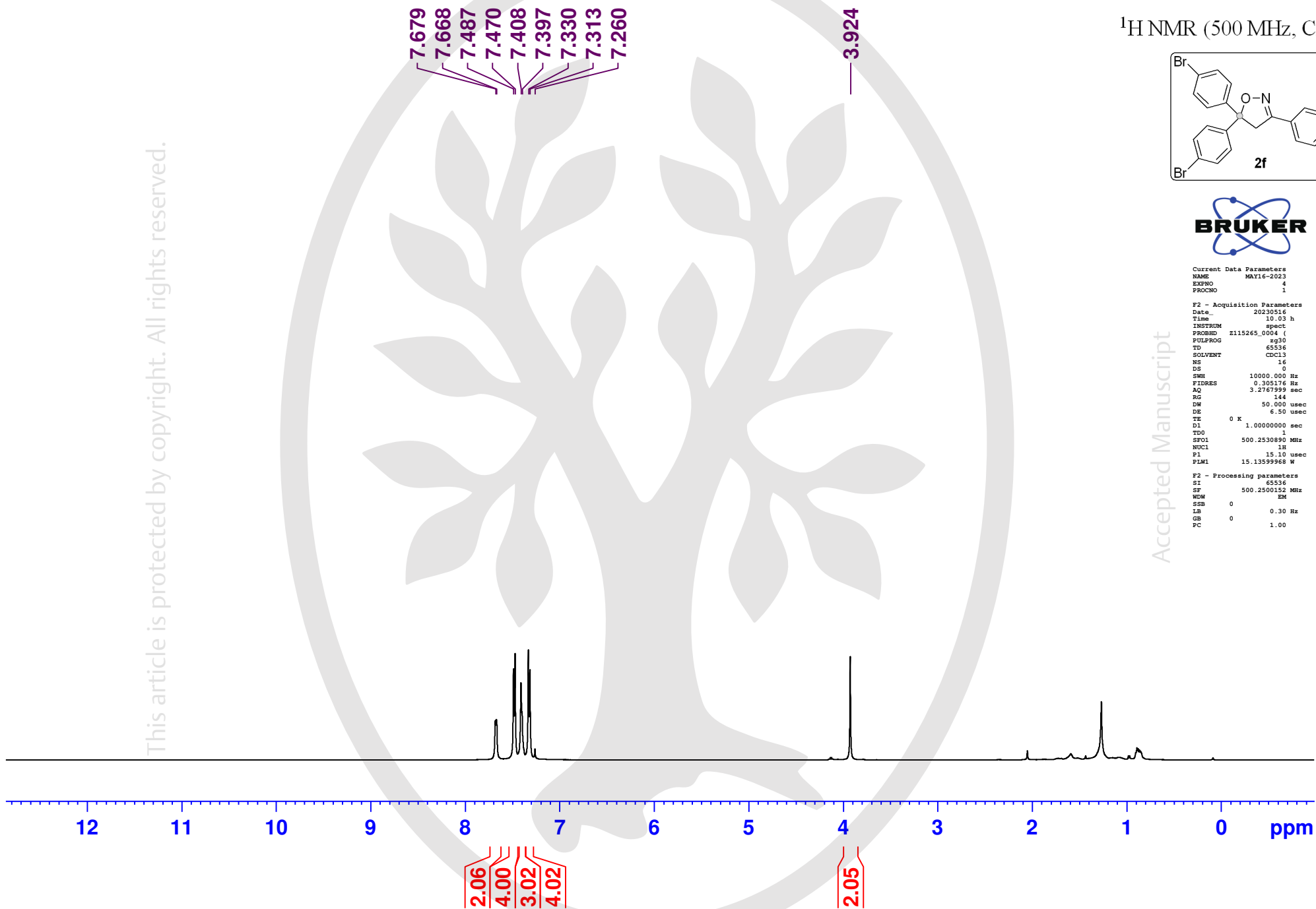
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Current Data Parameters
NAME          MAY13-2023
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        20230513
Time         17.01 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           132
DS           4
SWH          29761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           1030
DW           16.800 usec
DE           6.50 usec
TE           294.4 K
D1           2.0000000 sec
d11          0.0300000 sec
TDO          1
SFO1         125.805413 MHz
NUC1         13C
P1           9.70 usec
PL1          73.0000000 W
SFO2         500.252010 MHz
NUC2         1H
CPCPRG12     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27144000 W

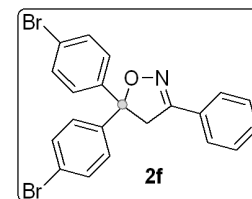
F2 - Processing parameters
SI           32768
SF           125.7679701 MHz
SBS          0
LS           1.00 Hz
GB           0
PC           1.40
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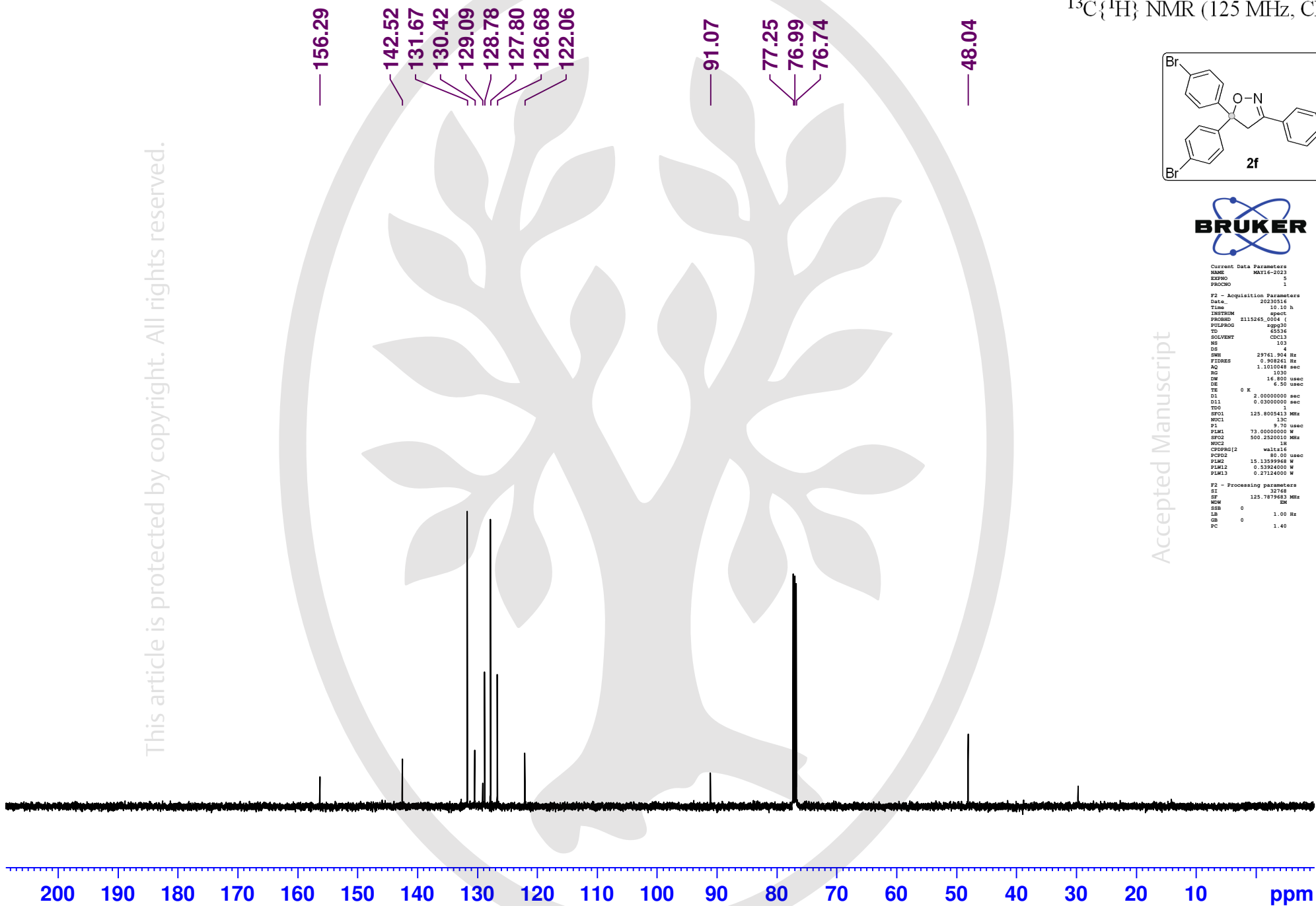


^1H NMR (500 MHz, CDCl_3)



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Current Data Parameters
NAME      MAY16-2023
EXPNO    5
PROCNO   1

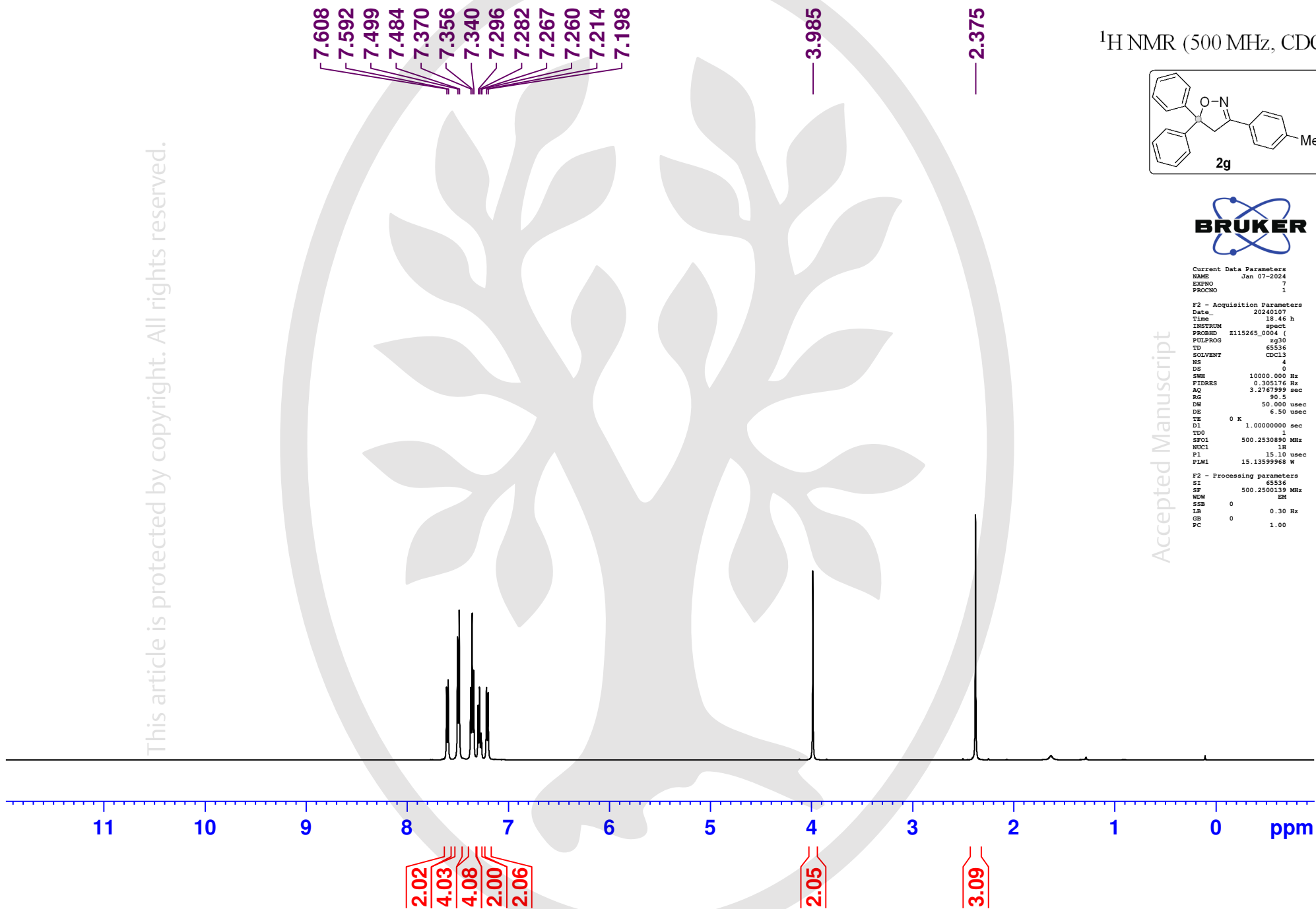
F2 - Acquisition Parameters
Date_    20230516
Time     10:10 h
INSTRUM  spect
PROBHD   1H5265_004 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       103
DS       4
SWH      29761.904 Hz
FIDRES   0.998261 Hz
AQ       1.1010048 sec
RG       1030
DSW      16.800 usec
DE       6.50 usec
TE       0 K

D1       2.0000000 sec
d11      0.0300000 sec
TDO      1
SFO1     125.8005413 MHz
NUC1     13C
P1       73.0000000 usec
SFO2     500.2520010 MHz
NUC2     1H
CPCPRG12 waltz16
PCPD2    80.00 usec
PLM2     15.13599968 u
PLM12    0.53924000 u
PLM13    0.27144000 u

F2 - Processing parameters
SI       32768
SF       125.7879683 MHz
SBS      0
LS       1.00 Hz
GB       0
PC       1.40
```

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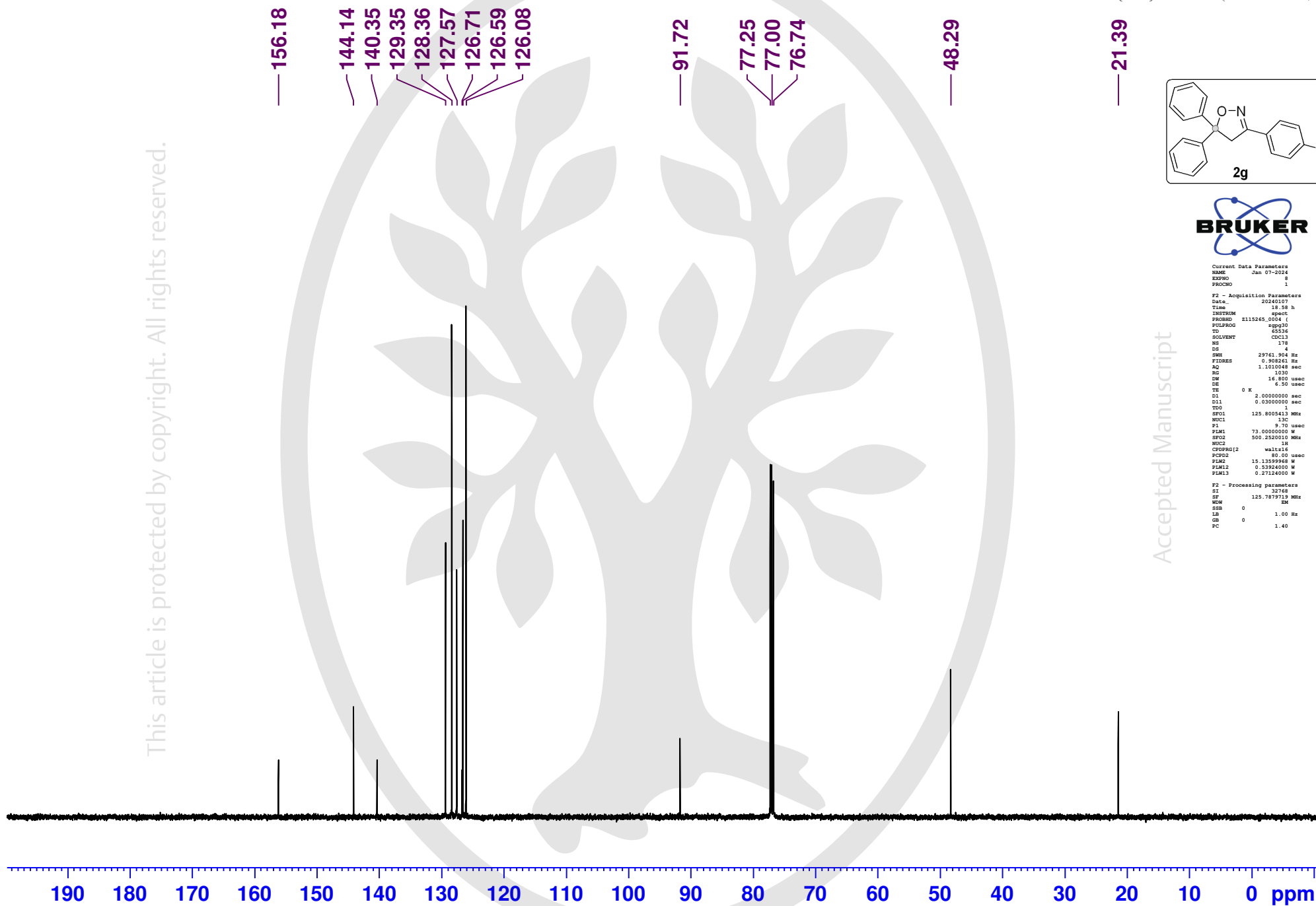
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Current Data Parameters
NAME Jan 07-2024
EXPNO 7
PROCNO 1

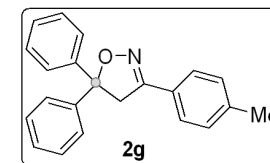
F2 - Acquisition Parameters
Date_ 20240107
Time 18.46 h
INSTRUM spect
PROBHD Z115265_0004 (2g30
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 90.5
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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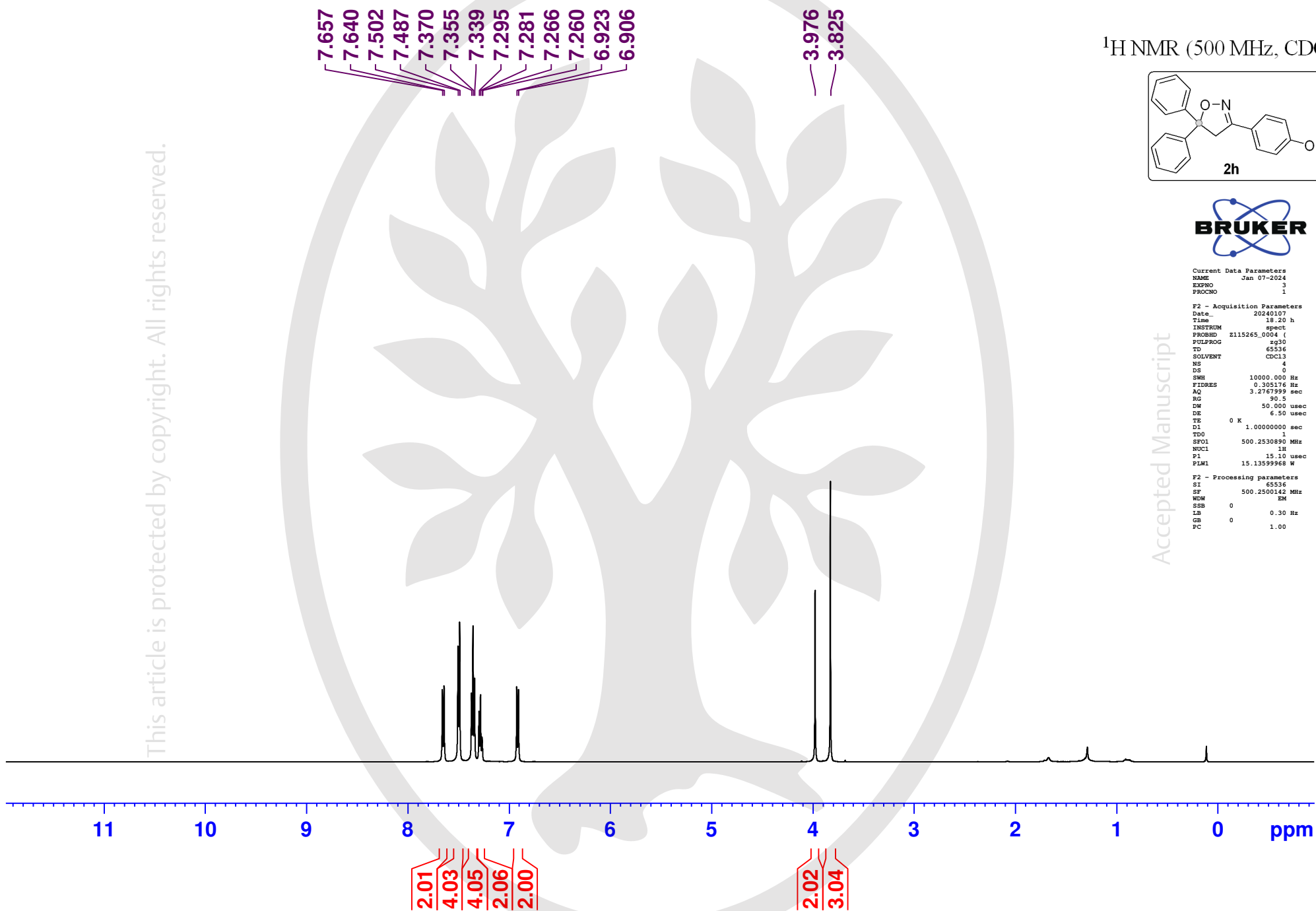


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Current Data Parameters
NAME          Jan 07-2024
EXPNO        8
PROCNO       1

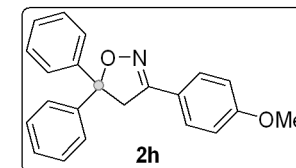
F2 - Acquisition Parameters
Date_        20240107
Time         18:58 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           178
DS           4
SWH          28761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           1030
DSW          16.800 usec
DE           6.50 usec
TE           0 K
D1           2.0000000 sec
d11          0.0300000 sec
SFO1         125.805413 MHz
NUC1         13C
P1           73.0000000 usec
PLA1         0.0000000 usec
SFO2         500.2520010 MHz
NUC2         1H
PCPDPRG2     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27124000 W

F2 - Processing parameters
SI           32768
SF           125.7679719 MHz
SBS          0
LS           1.00 Hz
GB           0
PC           1.40
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^1H NMR (500 MHz, CDCl_3)



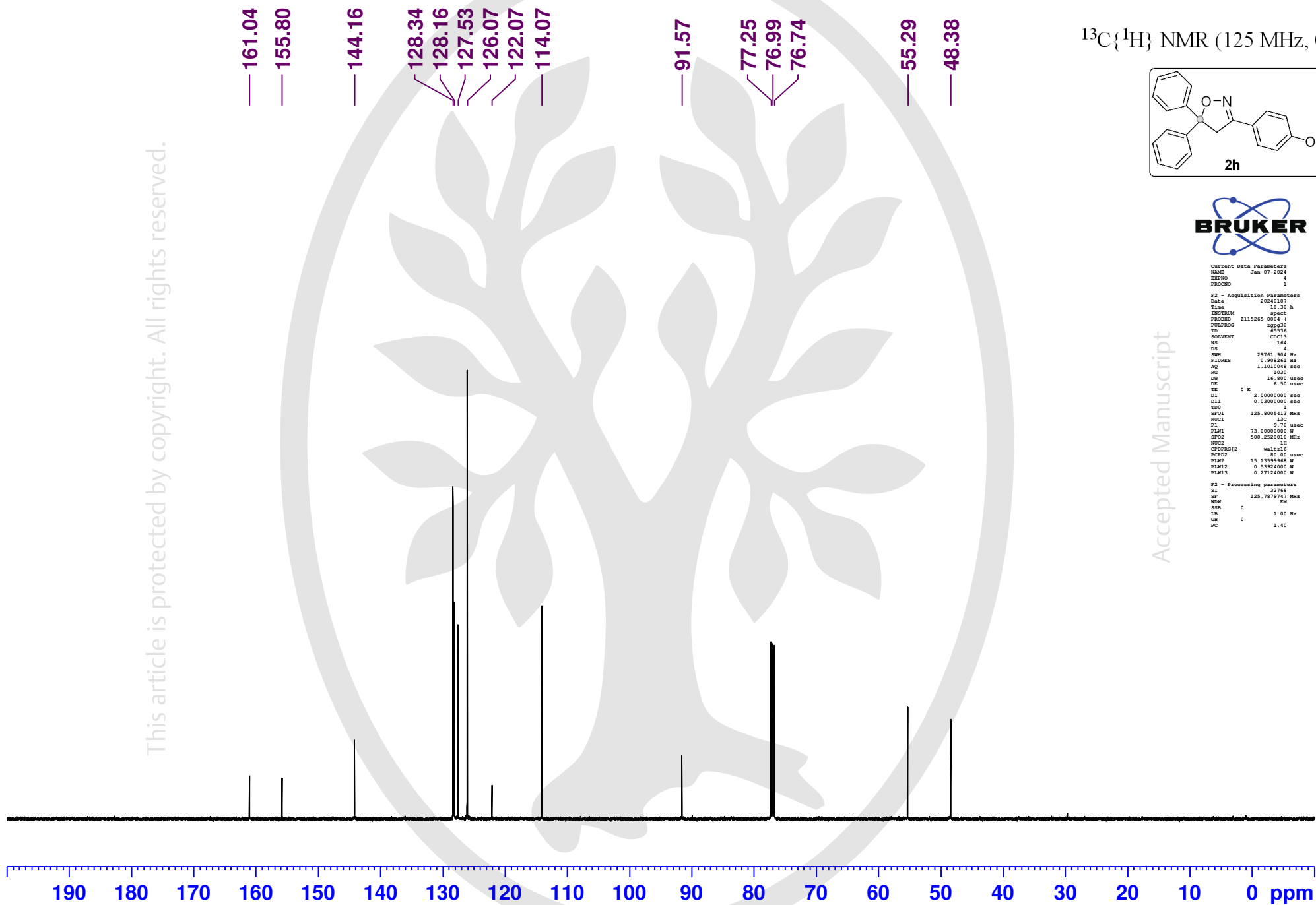
Current Data Parameters
NAME Jan 07-2024
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240107
Time 18.20 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 90.5
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

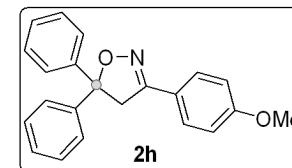
F2 - Processing parameters
SI 65536
SF 500.2500142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME          Jan 07-2024
EXPNO        4
PROCNO       1

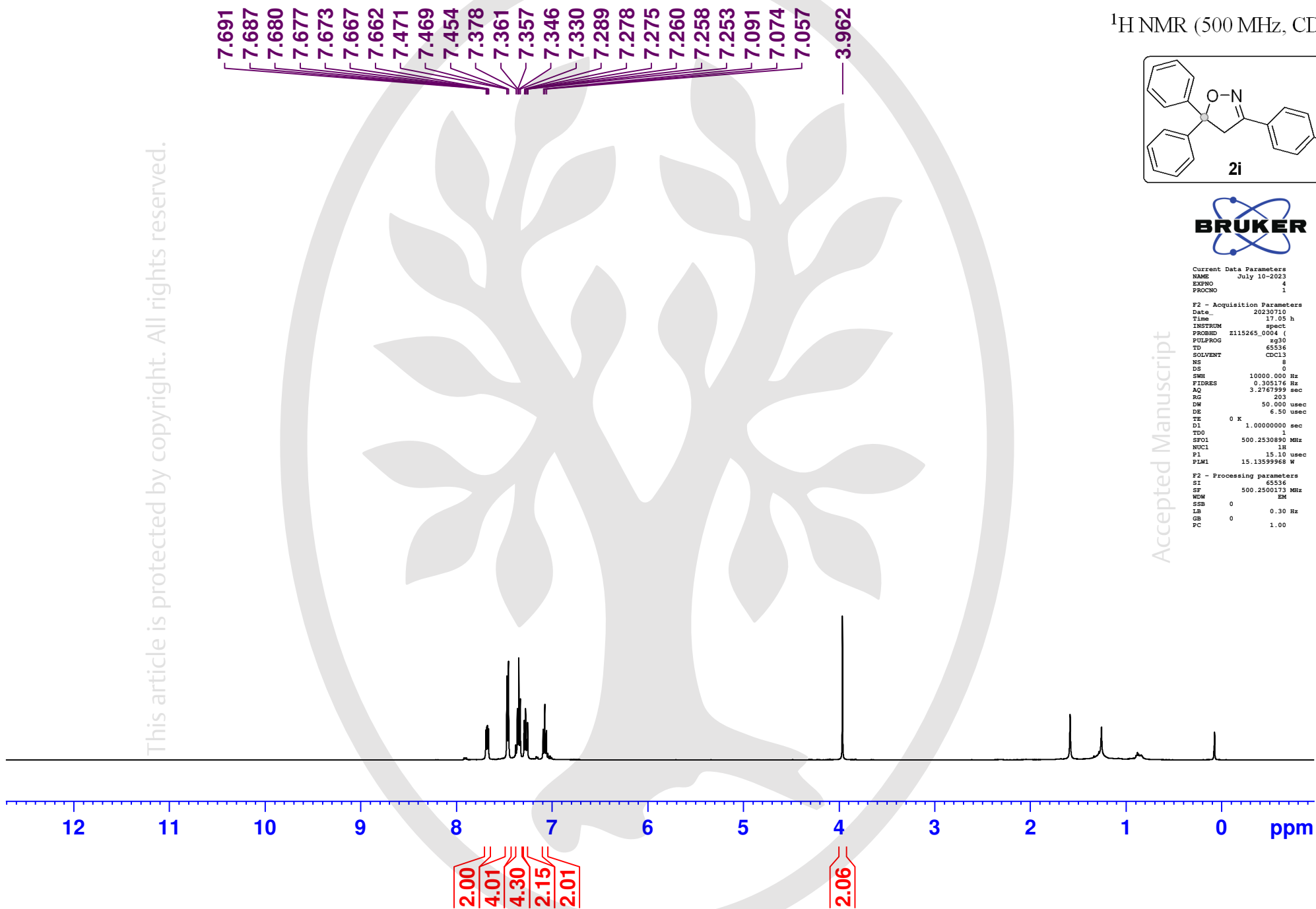
F2 - Acquisition Parameters
Date_        20240107
Time         18:30 h
INSTRUM      spect
PROBHD       1H5265_004 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           164
DS           4
SWH          29761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           1030
AQ           16.800 usec
DE           6.50 usec
TE           0 K

D1           2.0000000 sec
D11          0.0300000 sec
SFO1         125.805413 MHz
NUC1         13C
P1           9.70 usec
PL1          73.0000000 W
SFO2         500.2520010 MHz
NUC2         1H
PCPDPRG2     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27145000 W

F2 - Processing parameters
SI           32768
SF           125.7679747 MHz
SOLVENT      CDCl3
NS           164
DS           4
LB           1.00 Hz
GB           0
PC           1.40
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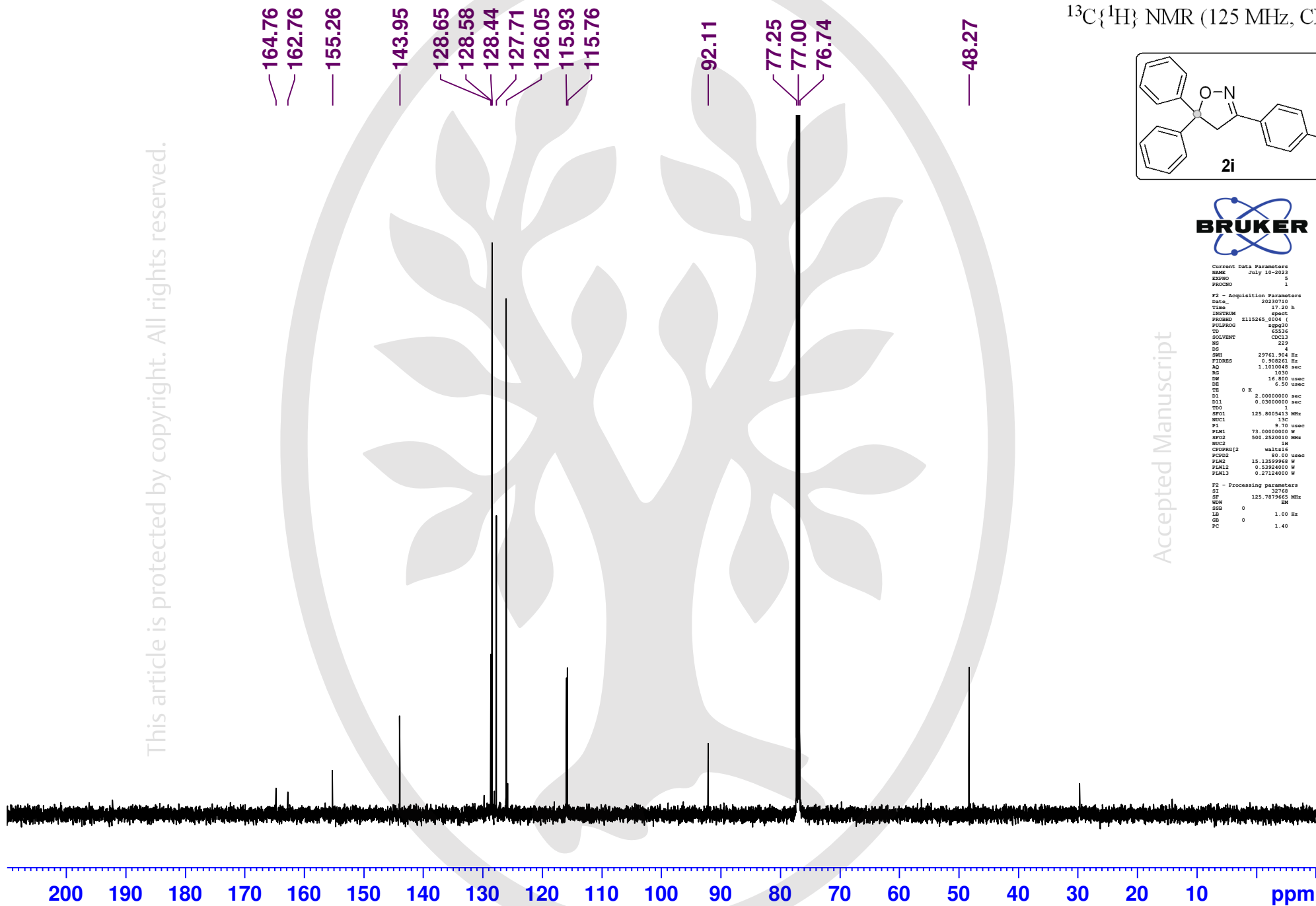
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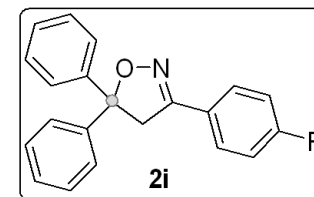


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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      July 10-2023
EXPNO    5
PROCNO   1

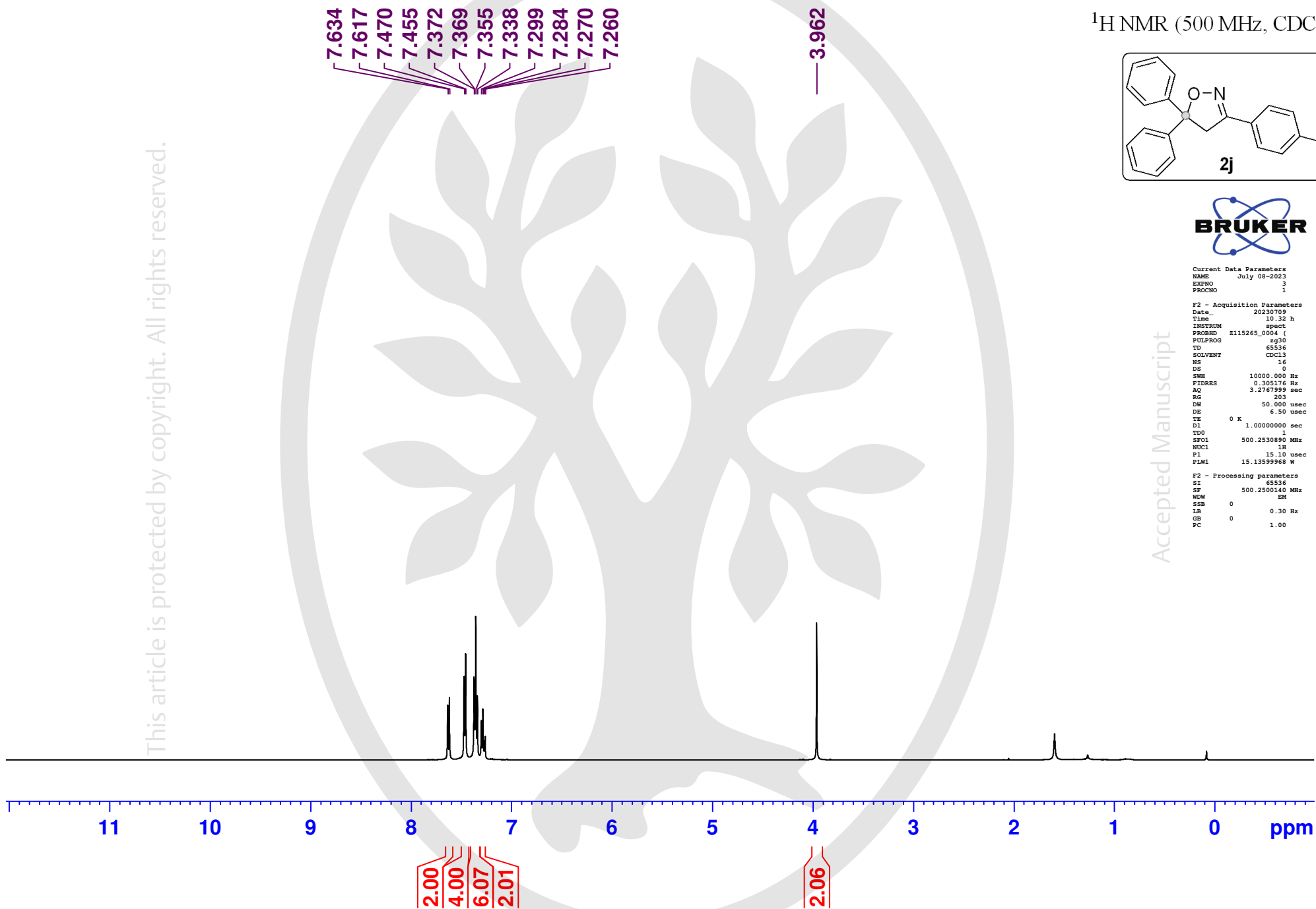
F2 - Acquisition Parameters
Date_    20230710
Time     17:20 h
INSTRUM  spect
PROBHD   1H5265_004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        229
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ        1.1010048 sec
RG         1030
SWH        16.800 usec
DE         6.50 usec
TE        0 K

D1        2.0000000 sec
D11       0.0300000 sec
SFO1      125.8005413 MHz
NUC1       13C
P1         9.70 usec
PL1        73.0000000 W
SFO2      500.2520010 MHz
NUC2       1H
CPCPRG12  waltz16
PCPG2     80.00 usec
PLM2      15.13599968 W
PLM12     0.53924000 W
PLM13     0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7679605 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

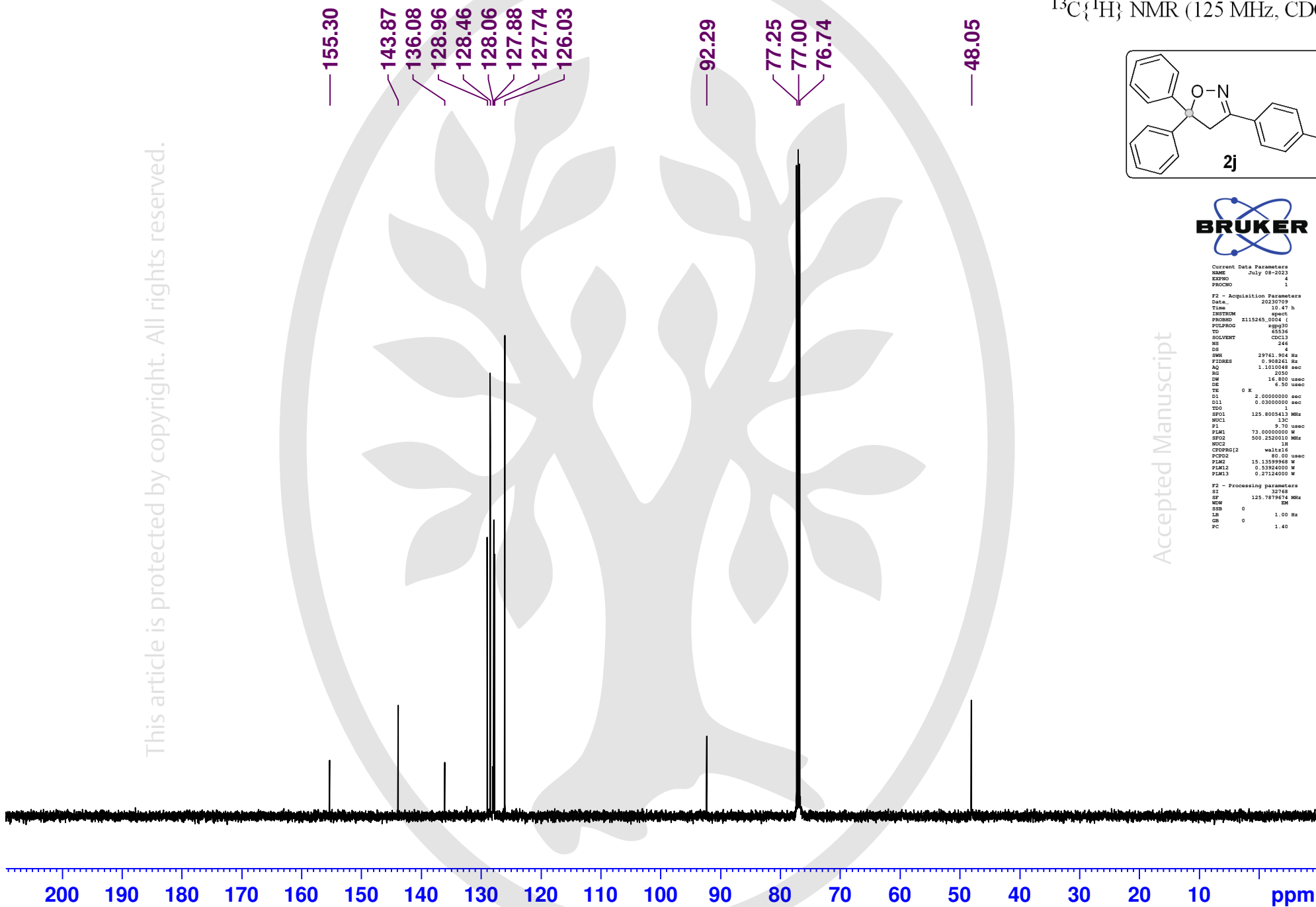
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Current Data Parameters
NAME July 08-2023
EXPRO 4
PROCNO 1

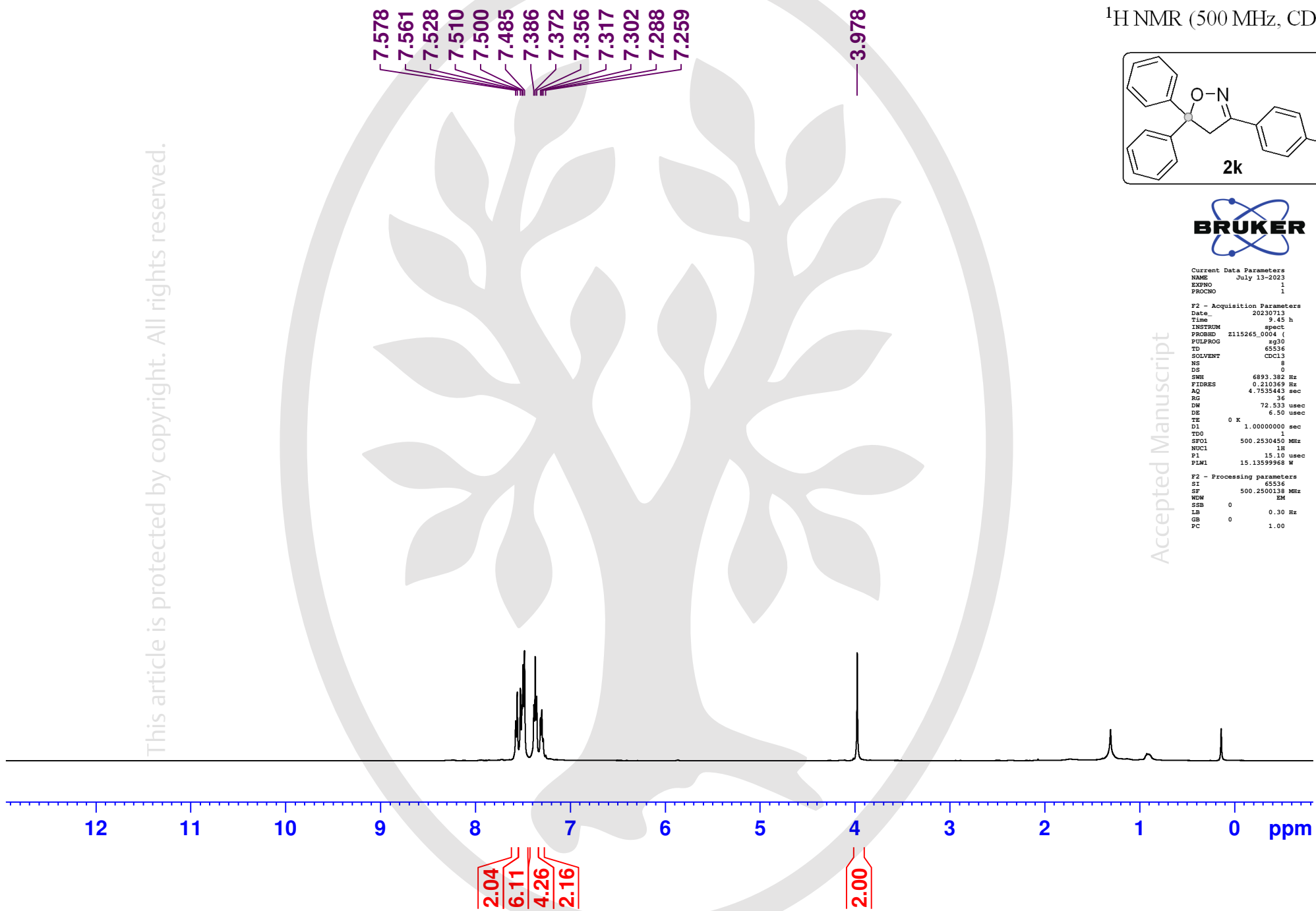
F2 - Acquisition Parameters
Date_ 20230709
Time 10:47 h
INSTRUM spect
PROBHD 1H5265.004 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 246
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 2050
DM 16.800 usec
DE 6.50 usec
TE 0 K

D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLA1 73.0000000 W
SFO2 500.2520010 MHz
NUC2 1H
PCPD12 wait16
PCPD2 80.00 usec
PLM2 15.1359998 W
PLM12 0.53924000 W
PLM13 0.27124000 W

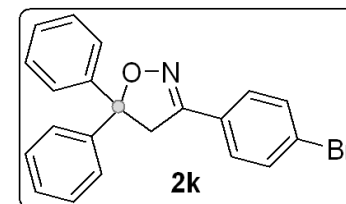
F2 - Processing parameters
SI 32768
SF 125.7879674 MHz
WDW EM
SSB EM
LB 1.00 Hz
GB 0
PC 1.40

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¹H NMR (500 MHz, CDCl₃)



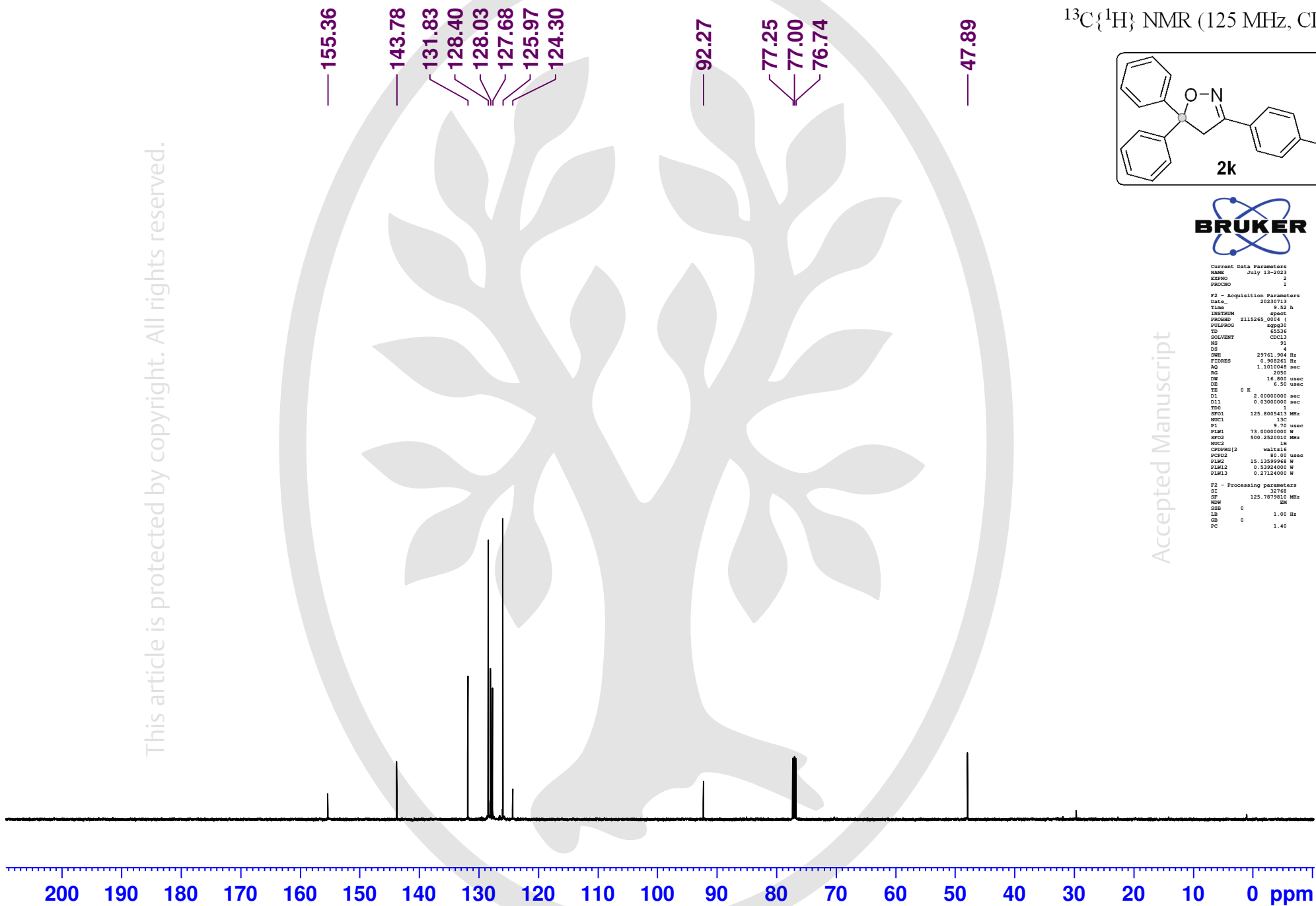
Current Data Parameters
NAME July 13-2023
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 9.45 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6893.382 Hz
FIDRES 0.210369 Hz
AQ 4.7339443 sec
RG 36
DW 72.533 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530450 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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BRUKER

```
Current Data Parameters
NAME      July 13-2023
EXPRO    1
PROCNO   1

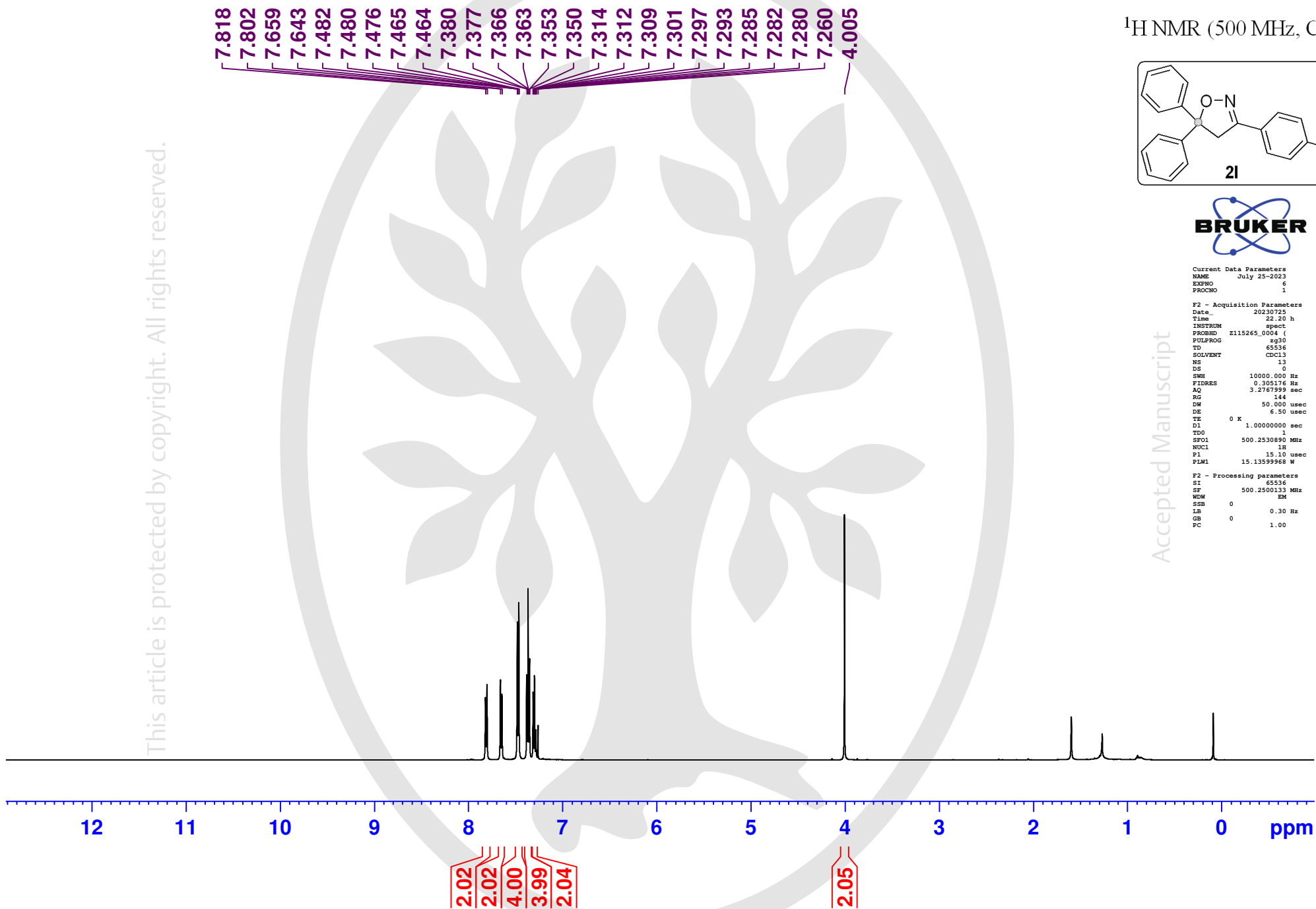
F2 - Acquisition Parameters
Date_    20230713
Time     9.52 h
INSTRUM  spect
PROBHD   1H125AS_004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        91
DS        4
SWH       29761.904 Hz
FIDRES    0.398261 Hz
AQ         1.1010048 sec
RG         2050
SWH        16.800 usec
DE         6.50 usec
TE        0 K

D1         2.0000000 sec
D11        0.0300000 sec
SFO1       125.8005413 MHz
NUC1       13C
P1         73.0000000 usec
PL1        0.0000000 W
SFO2       500.2520010 MHz
NUC2       1H
PCPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27145000 W

F2 - Processing parameters
SI         32768
SF         125.7679610 MHz
SBS        0
LS         1.00 Hz
GB         0
PC         1.40
```

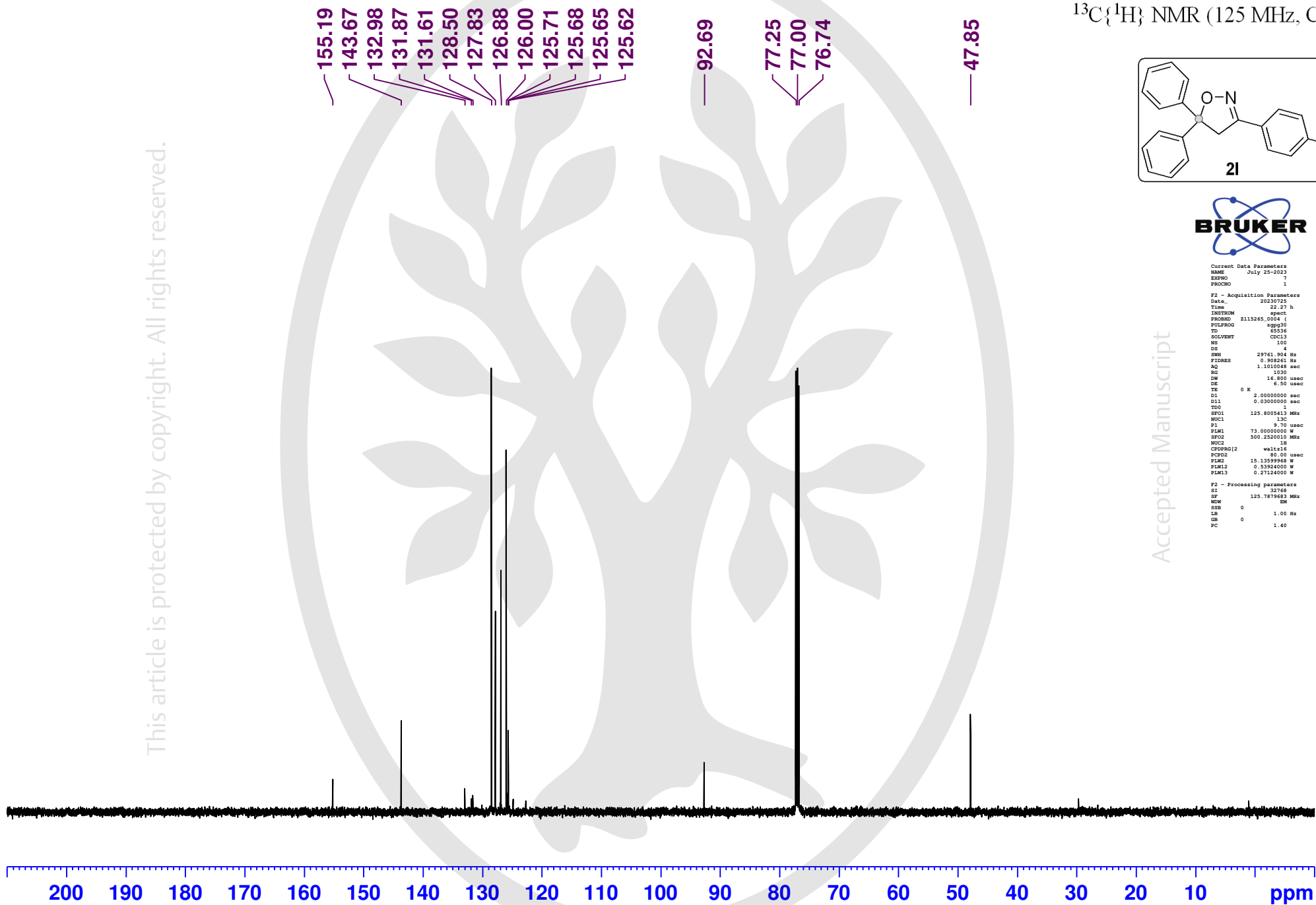
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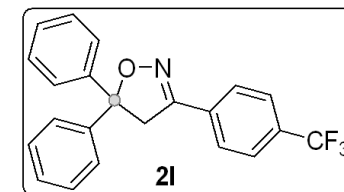


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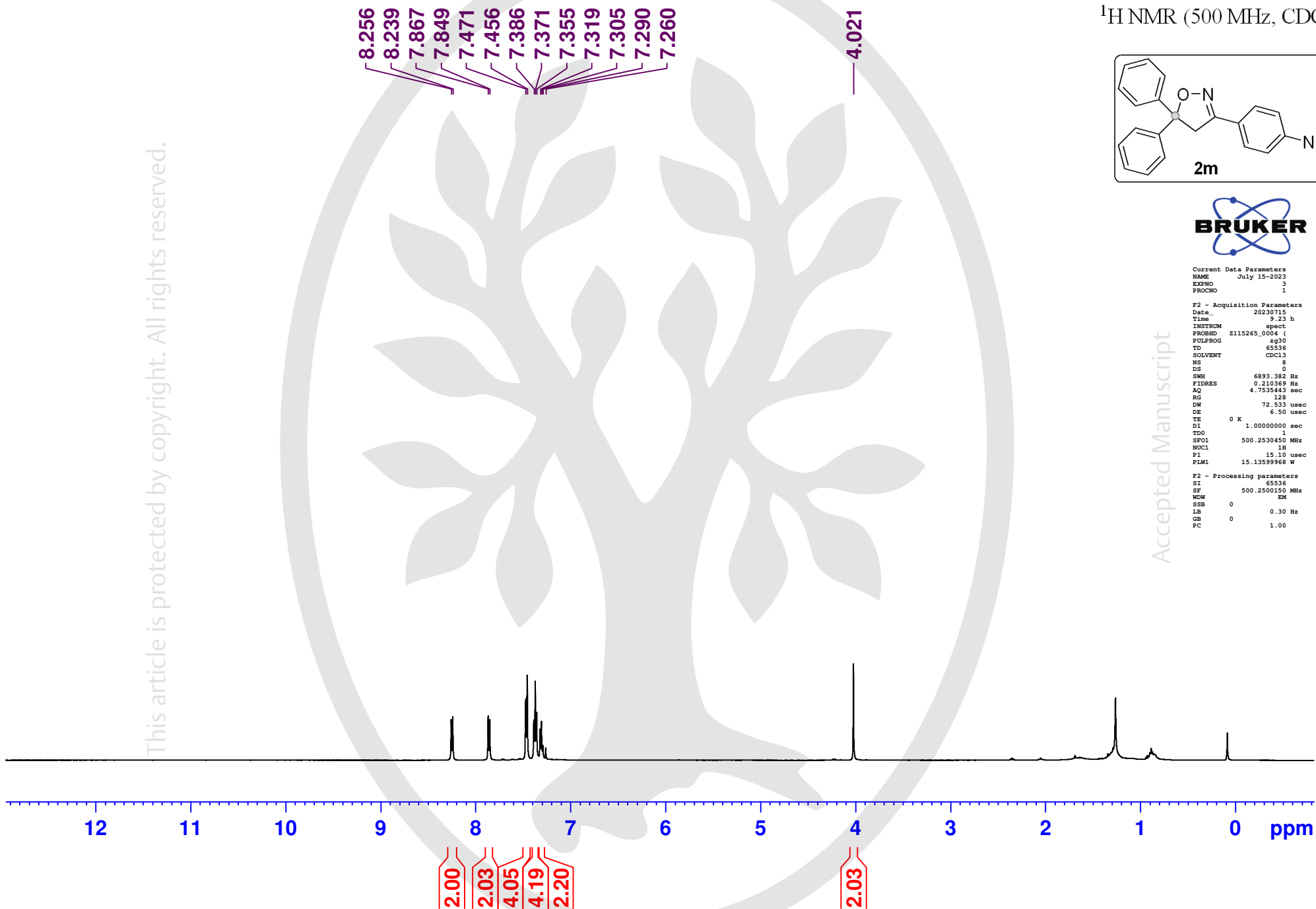


$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



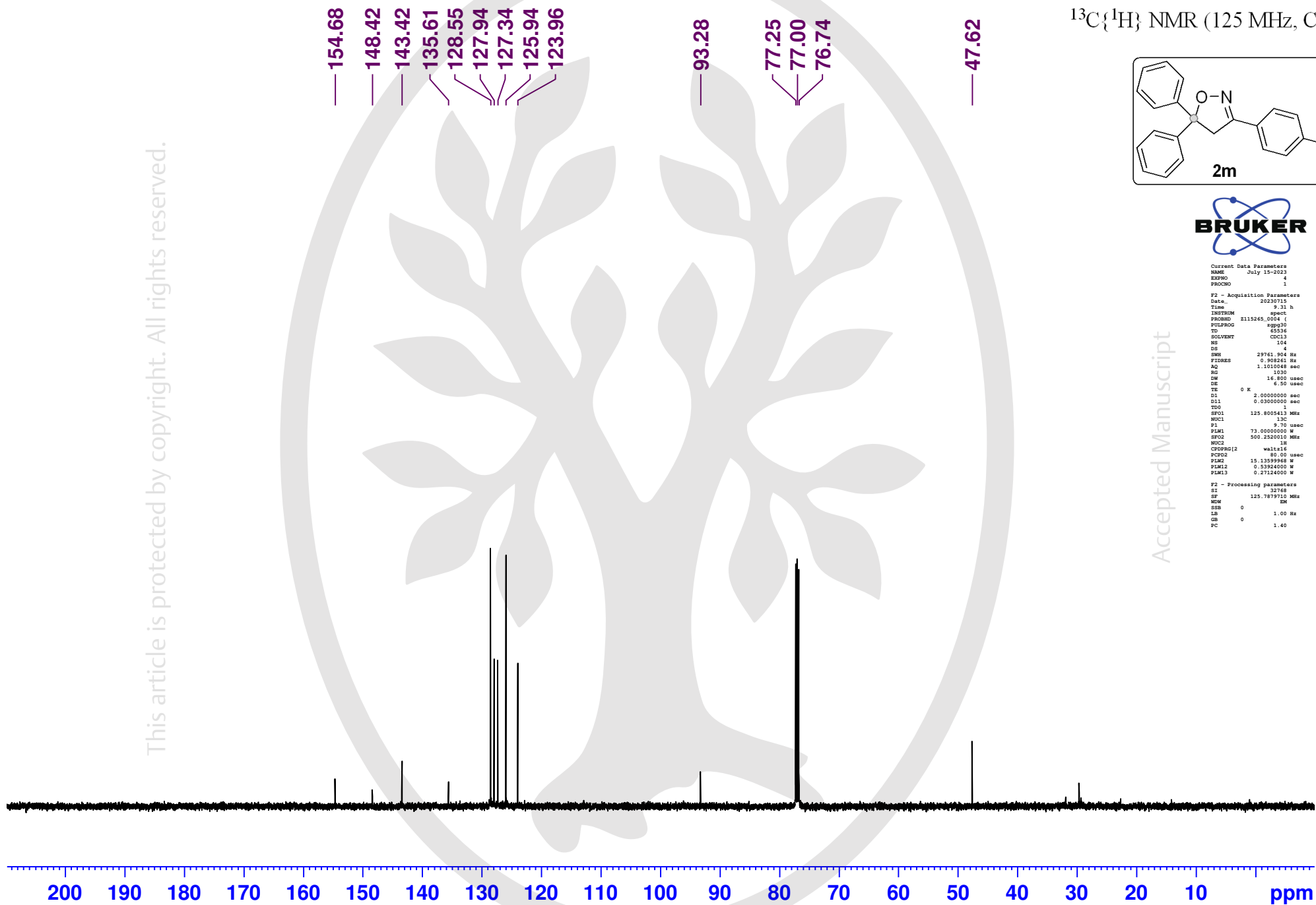
Accepted Manuscript

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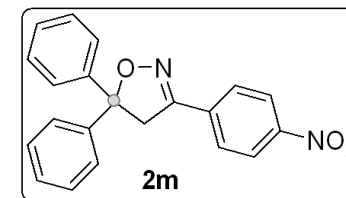


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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



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Current Data Parameters
NAME      July 15-2023
EXPRO    4
PROCNO   1

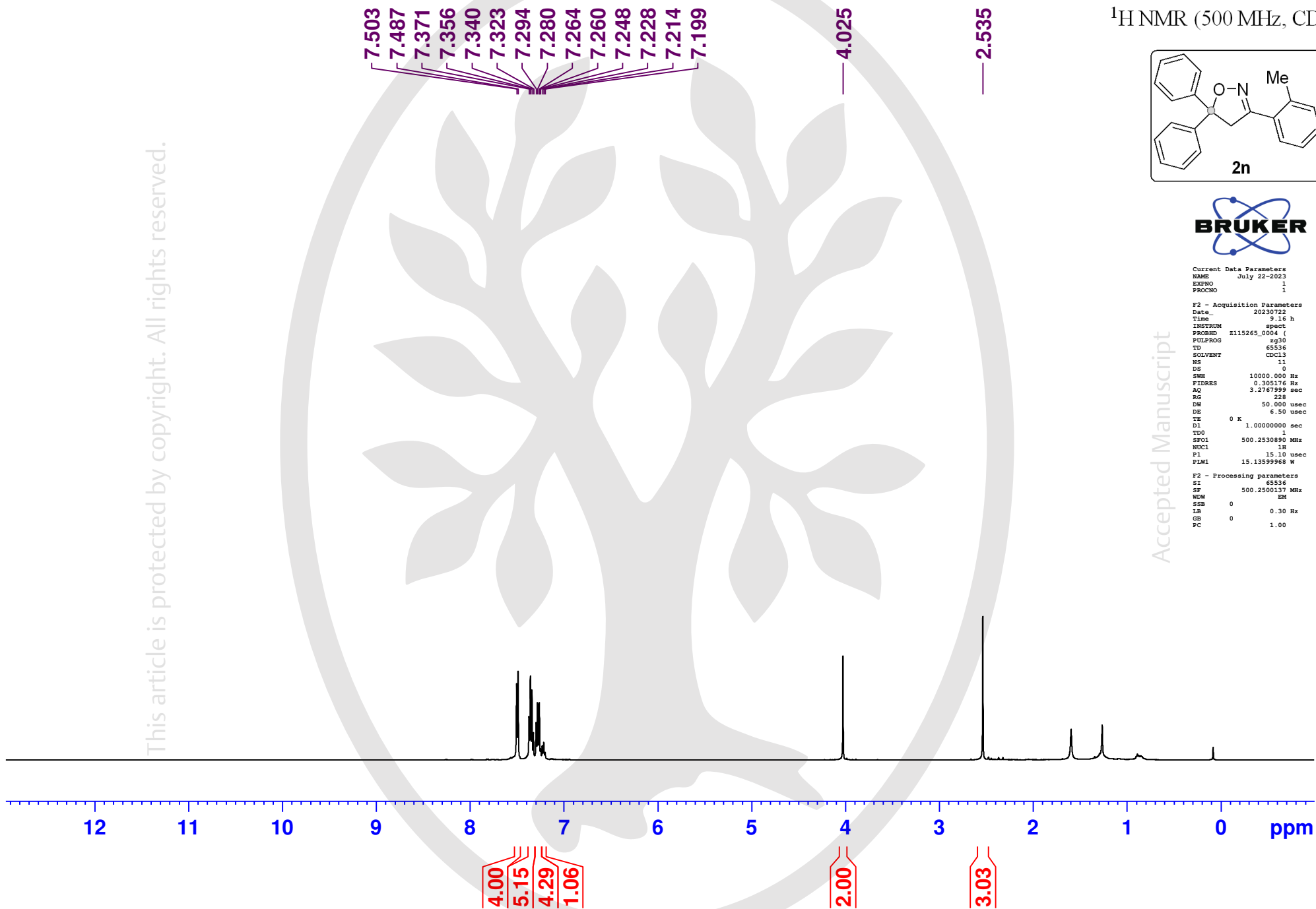
F2 - Acquisition Parameters
Date_    20230715
Time     9:31 h
INSTRUM  spect
PROBHD   115265_004 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       104
DS       4
SWH      29761.904 Hz
FIDRES   0.398261 Hz
AQ       1.1010048 sec
RG       1030
DSW      16.800 usec
DE       6.50 usec
TE       0 K

D1       2.0000000 sec
D11      0.0300000 sec
TDO      1
SFO1     125.8005413 MHz
NUC1     13C
D1       73.0000000 M
PLM1     9.70 usec
SFO2     500.2520010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLM2     15.13599968 M
PEM12    0.53924000 M
PLM13    0.27154000 M

F2 - Processing parameters
SI       32768
SF       125.7879710 MHz
SBS      0
LS       1.00 Hz
GB       0
PC       1.40
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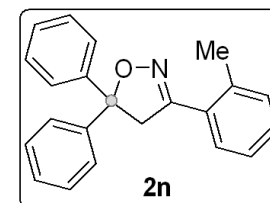
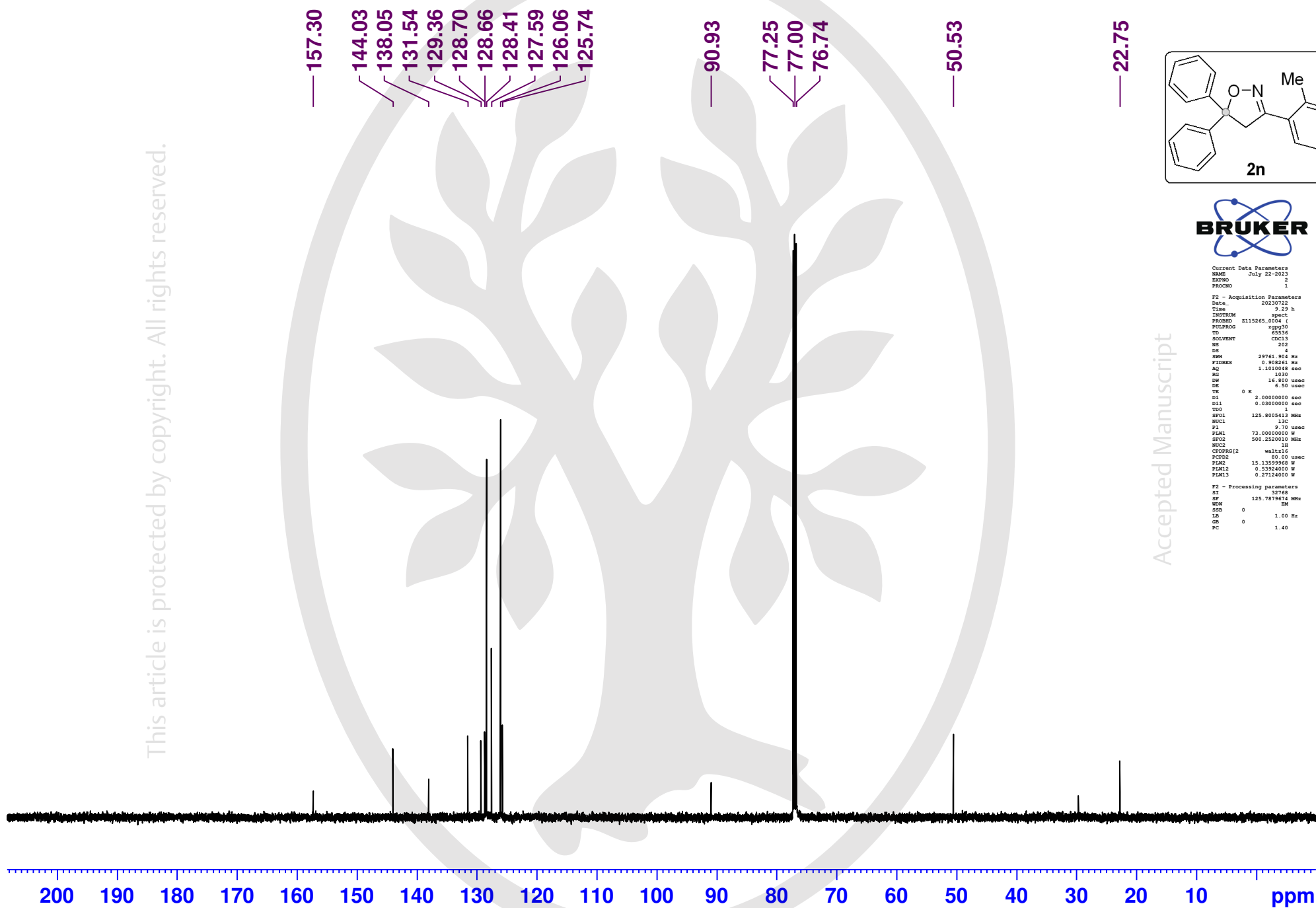
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^1H NMR (500 MHz, CDCl_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



Current Data Parameters
NAME July 22-2023
EXPRO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230722
Time 9:29 h
INSTRUM spect
PROBHD 1H5265.004 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 202
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 1030
DM 16.800 usec
DE 6.50 usec
TE 0 K

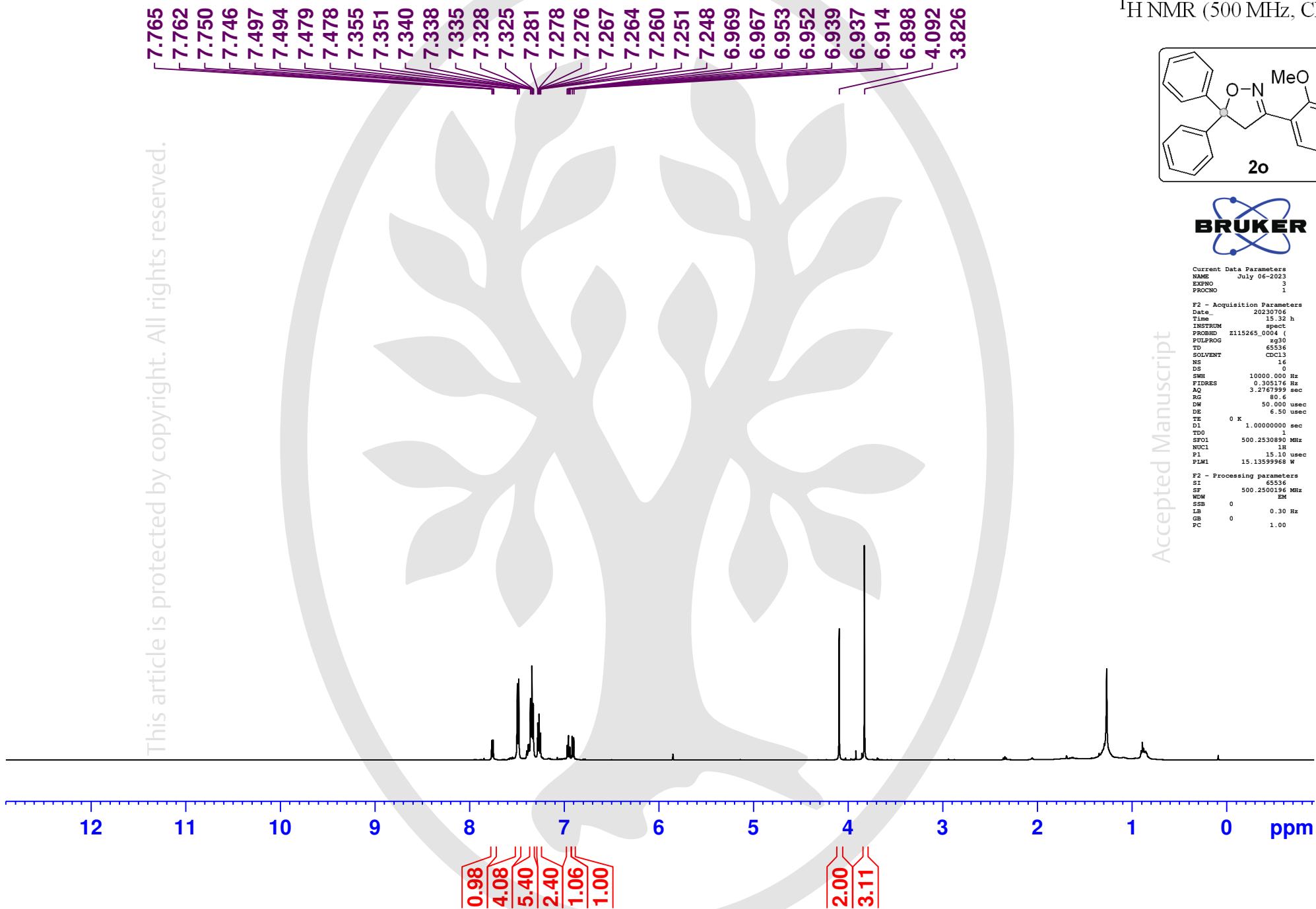
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
P1 73.0000000 W
PLM1 9.70 usec
SFO2 500.2520010 MHz
NUC2 1H
CPCPRG12 waltz16
PCPD2 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27124000 W

F2 - Processing parameters
SI 32768
SF 125.7879674 MHz
SBS 0
SM EM
LS 1.00 Hz
GB 0
PC 1.40

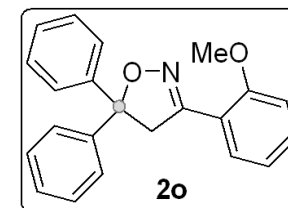
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^1H NMR (500 MHz, CDCl_3)



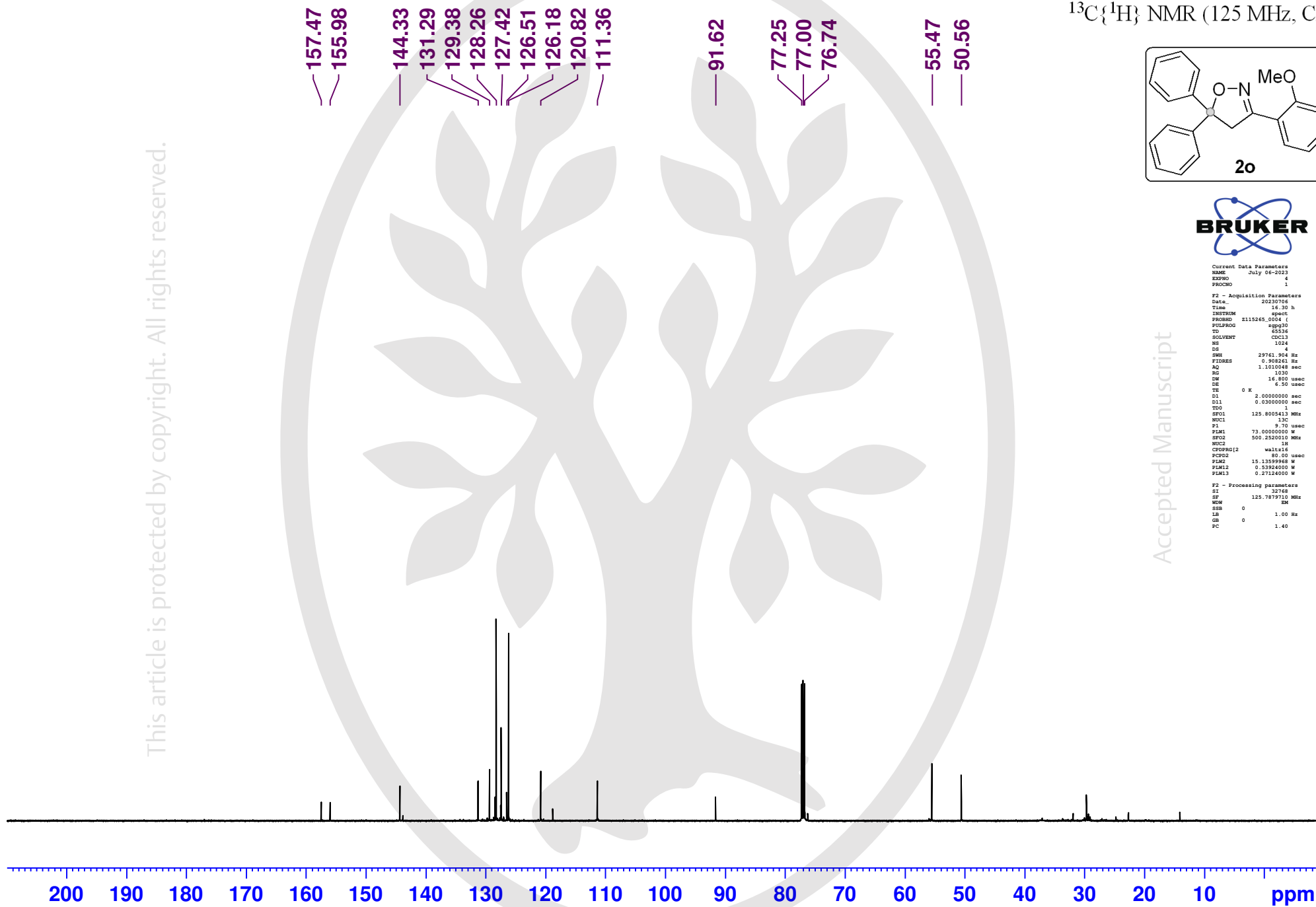
Current Data Parameters
NAME July 06-2023
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230706
Time 15.32 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2167399 sec
RG 80.6
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

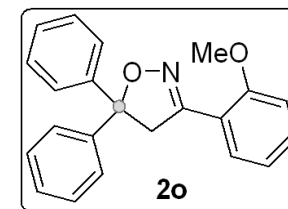
F2 - Processing parameters
SI 65536
SF 500.2500196 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      July 06-2023
EXPRO    4
PROCNO   1

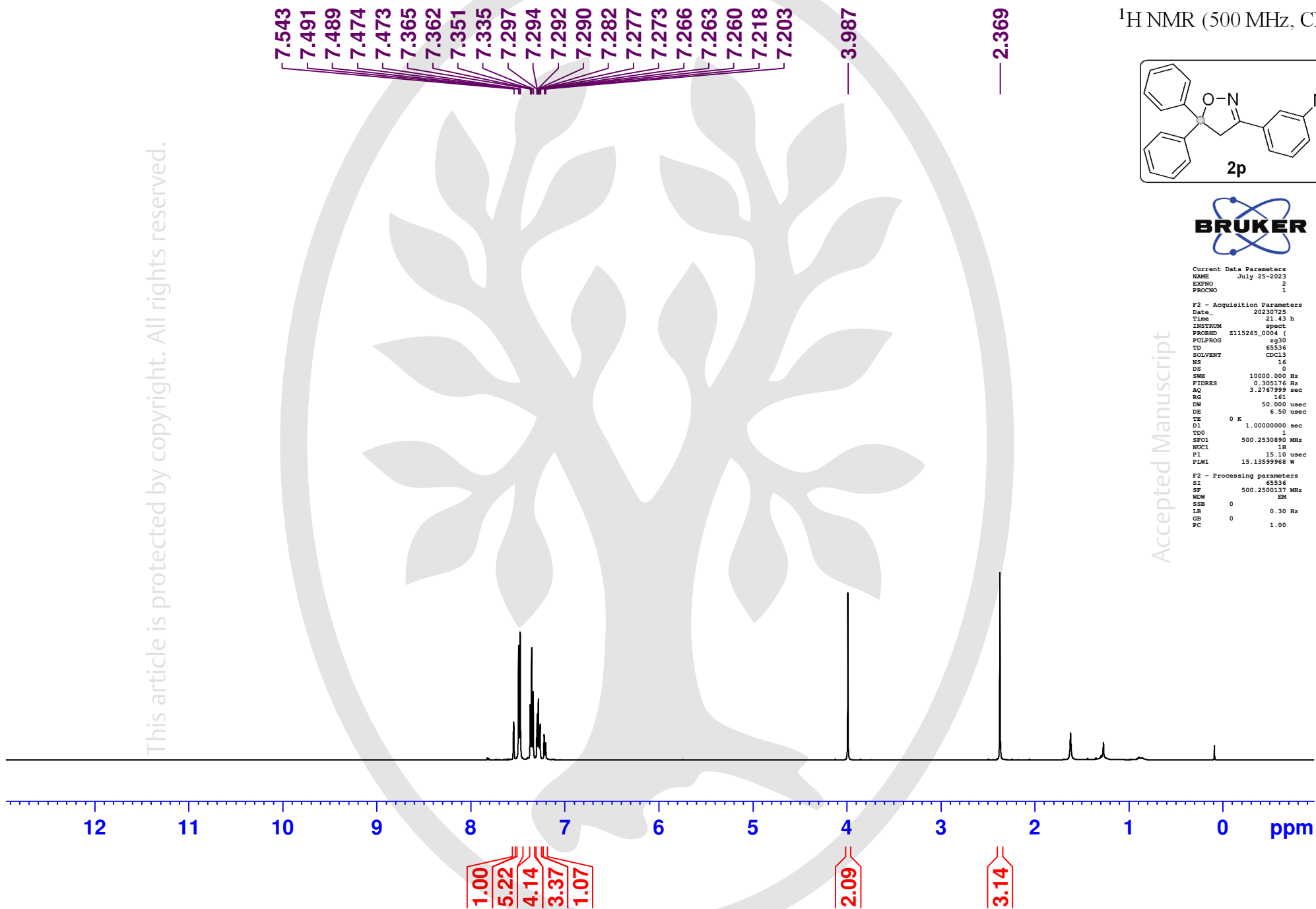
F2 - Acquisition Parameters
Date_    20230706
Time     16:30 h
INSTRUM  spect
PROBHD   1H125AS.004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         1030
RW         16.800 usec
DE         6.50 usec
TE         0 K

D1         2.0000000 sec
D11        0.0300000 sec
TDO        1
SFO1       125.8005413 MHz
NUC1       13C
P1         73.0000000 usec
PLA1       0.70 usec
SFO2       500.2520010 MHz
NUC2       1H
CPCPRG12  waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

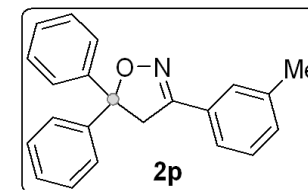
F2 - Processing parameters
SI         32768
SF         125.7679710 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
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^1H NMR (500 MHz, CDCl_3)

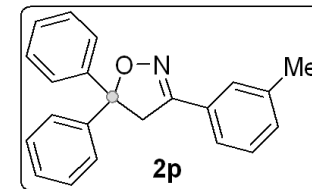
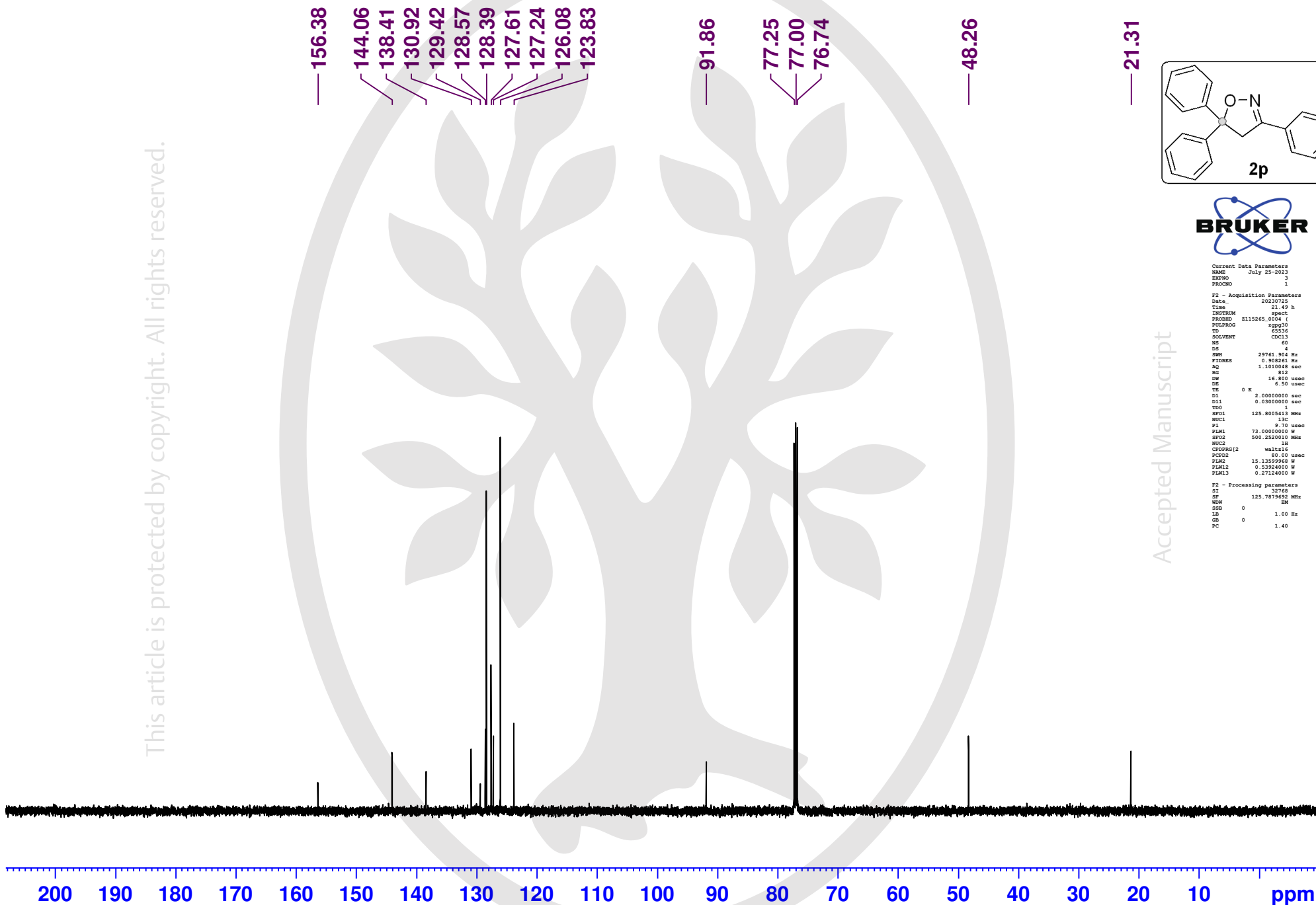


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Current Data Parameters
NAME July 25-2023
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 21.43 h
INSTRUM spect
PROBHD Z115265_0004 (
FULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.276799 sec
RG 161
DW 50.000 usec
DE 6.50 usec
TE 0 K
DI 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUCL1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME July 25-2023
EXPRO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 21:49 h
INSTRUM spect
PROBHD 1H125AS.004 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 60
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 812
SW 16.800 usec
DE 6.50 usec
TE 0 K

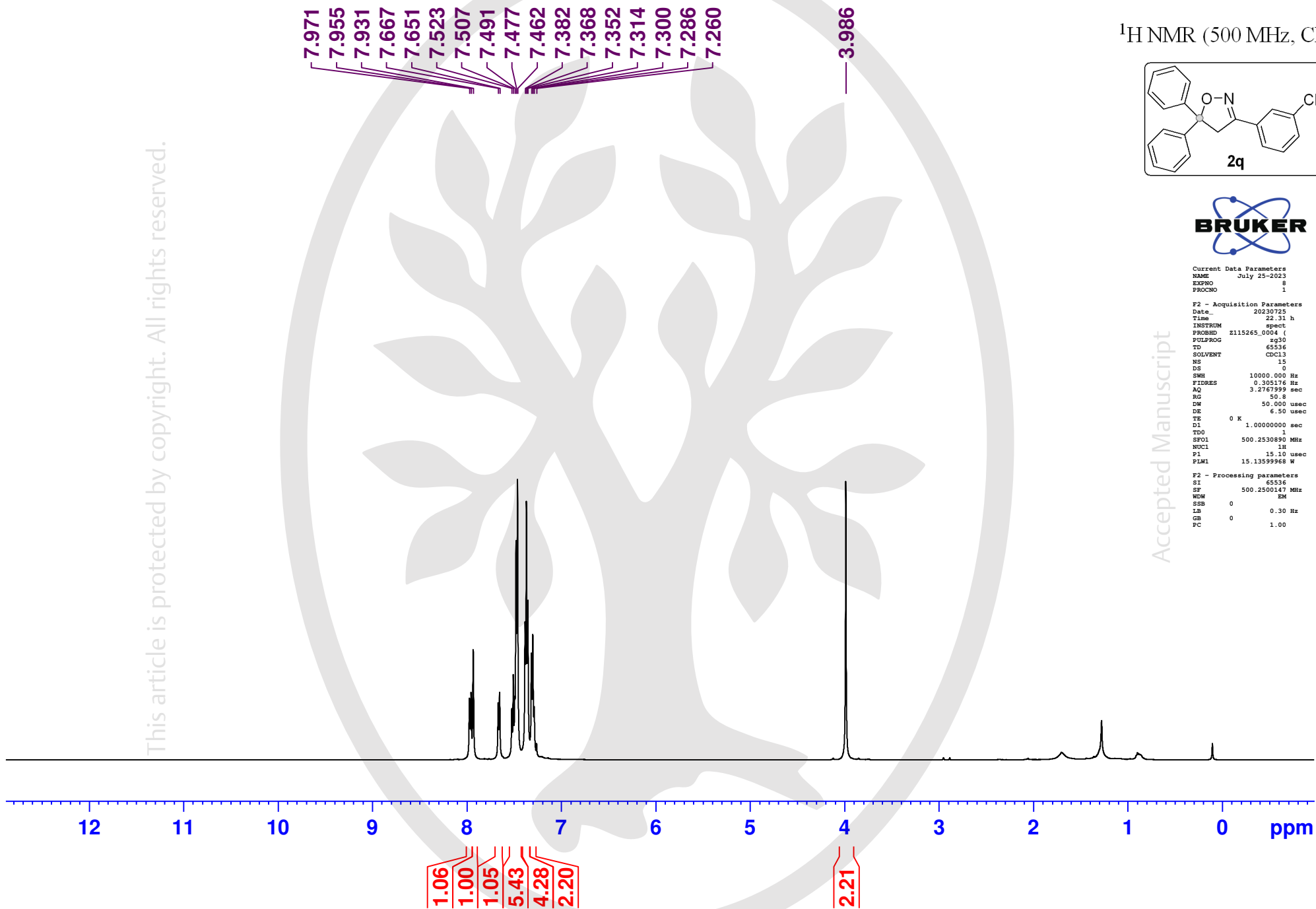
D1 2.0000000 sec
D11 0.0300000 sec
SFO1 125.8005413 MHz
NUC1 13C
P1 73.0000000 usec
PLA1 0.0000000 W
SFO2 500.2520010 MHz
NUC2 1H
PCPPROG2 wait16
PCPD2 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27124000 W

F2 - Processing parameters
SI 32768
SF 125.7879692 MHz
SBS 5M
LS 1.00 Hz
GB 0
PC 1.40

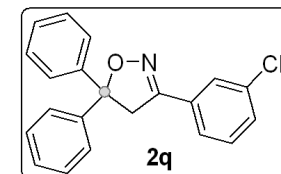
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^1H NMR (500 MHz, CDCl_3)



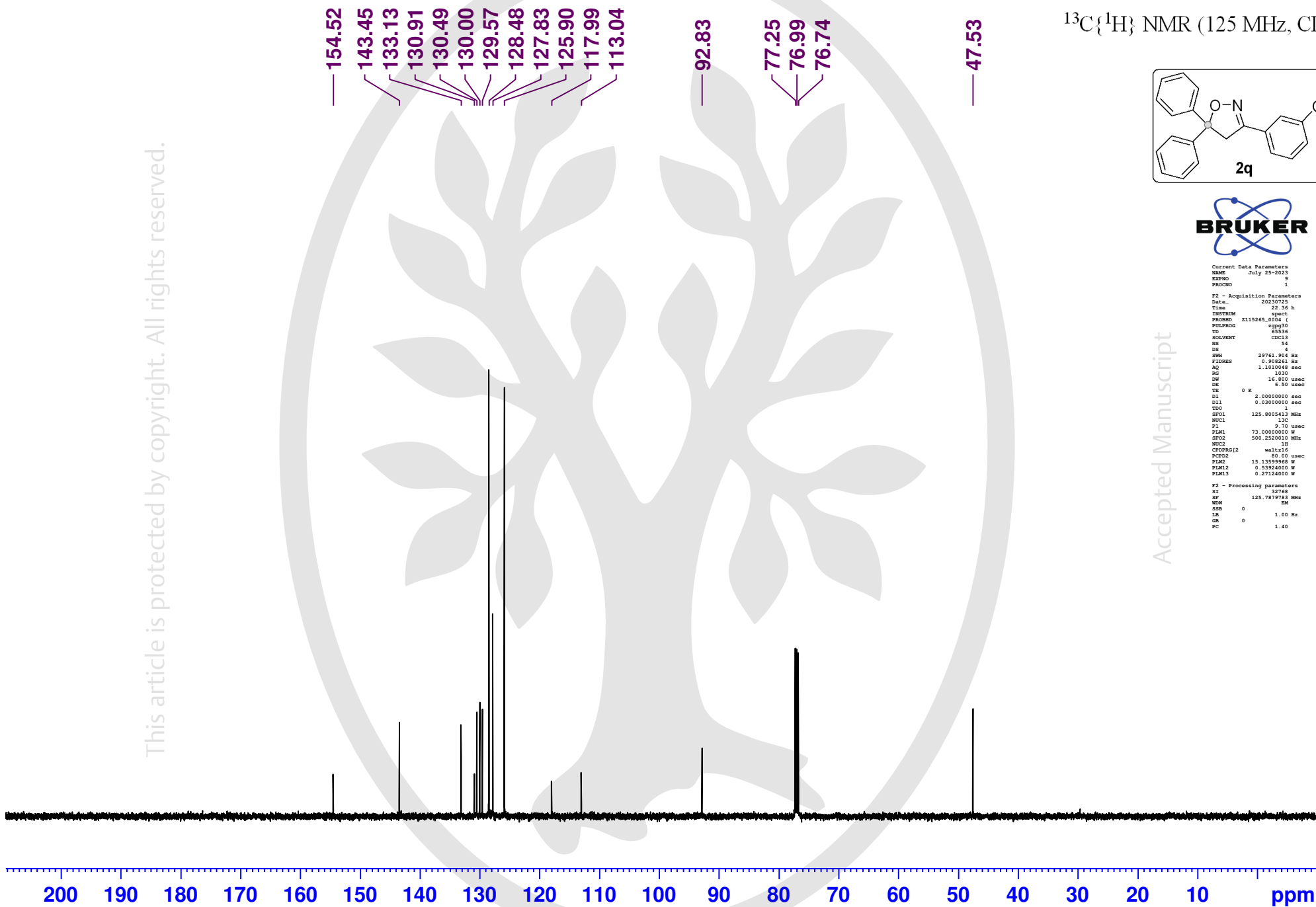
Current Data Parameters
NAME July 25-2023
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 22.31 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 15
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 50.8
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.0000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

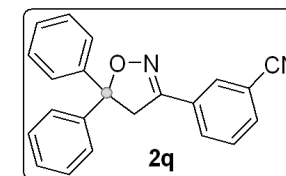
F2 - Processing parameters
SI 65536
SF 500.2500147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



Current Data Parameters
NAME July 25-2023
EXPRO 9
PROCNO 1

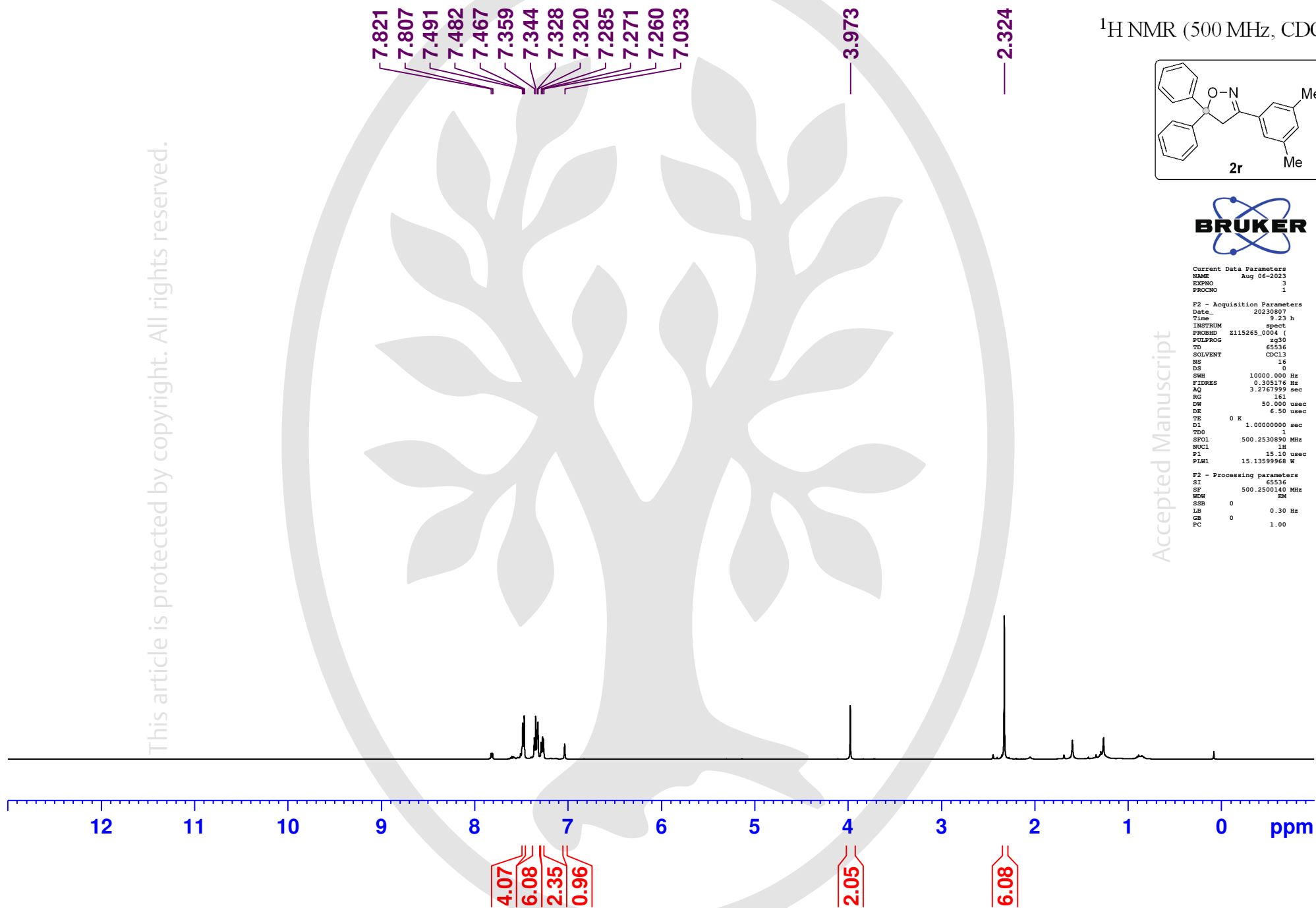
F2 - Acquisition Parameters
Date_ 20230725
Time 22:36 h
INSTRUM spect
PROBHD 1H12565.004 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 54
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 1030
RW 16.800 usec
DE 6.50 usec
TE 0 K

D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLA1 73.0000000 W
SFO2 500.2520010 MHz
NUC2 1H
PCPRG2 wait16
PCPD2 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27124000 W

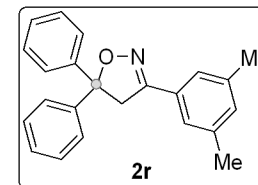
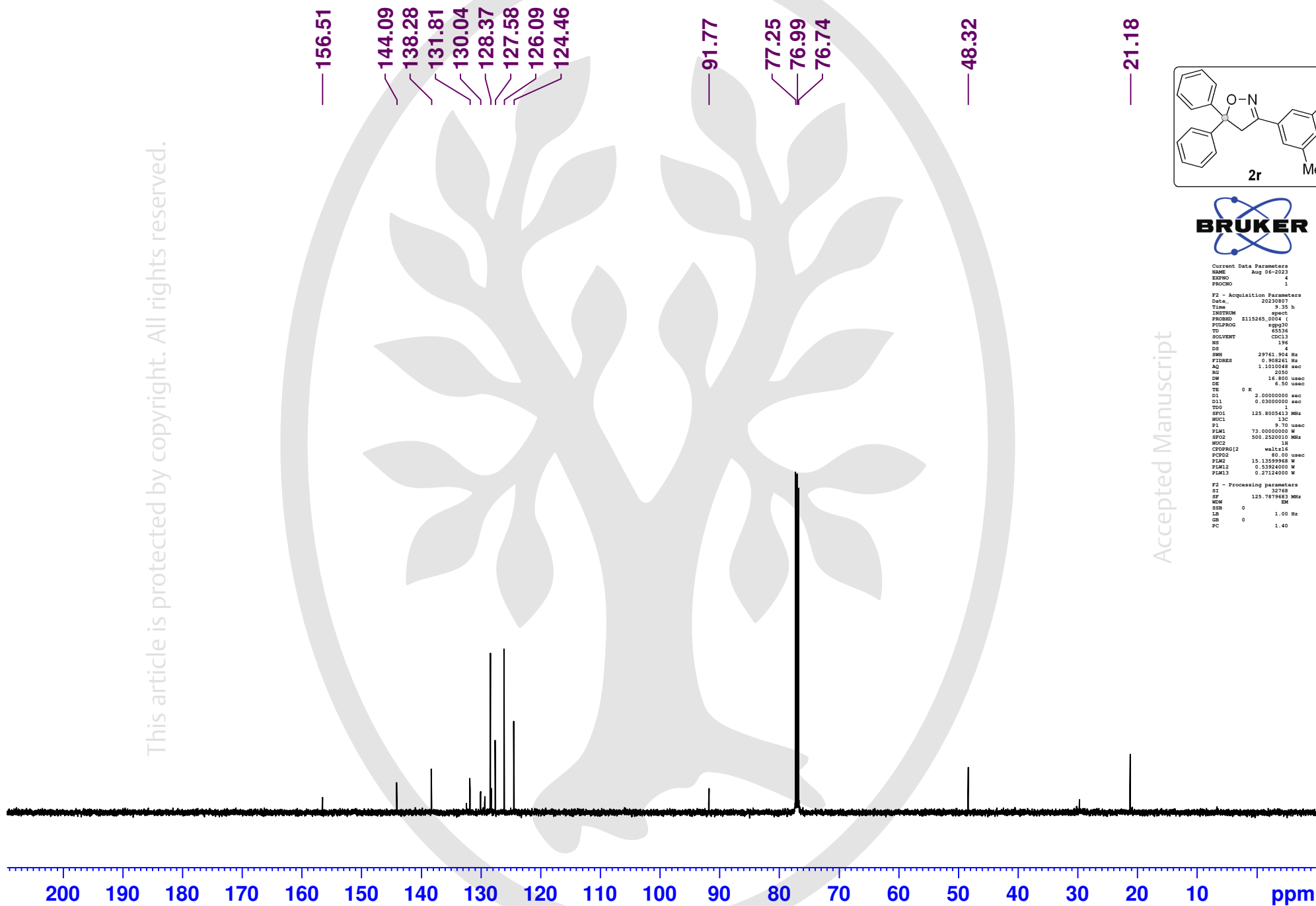
F2 - Processing parameters
SI 32768
SF 125.7679763 MHz
WDW EM
SSB EM
LB 1.00 Hz
GB 0
PC 1.40

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Current Data Parameters
NAME Aug 06-2023
EXPRO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230807
Time 9:25 h
INSTRUM spect
PROBHD 1H125AS.004 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 196
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 2050
SW 16.800 usec
DE 6.50 usec
TE 0 K

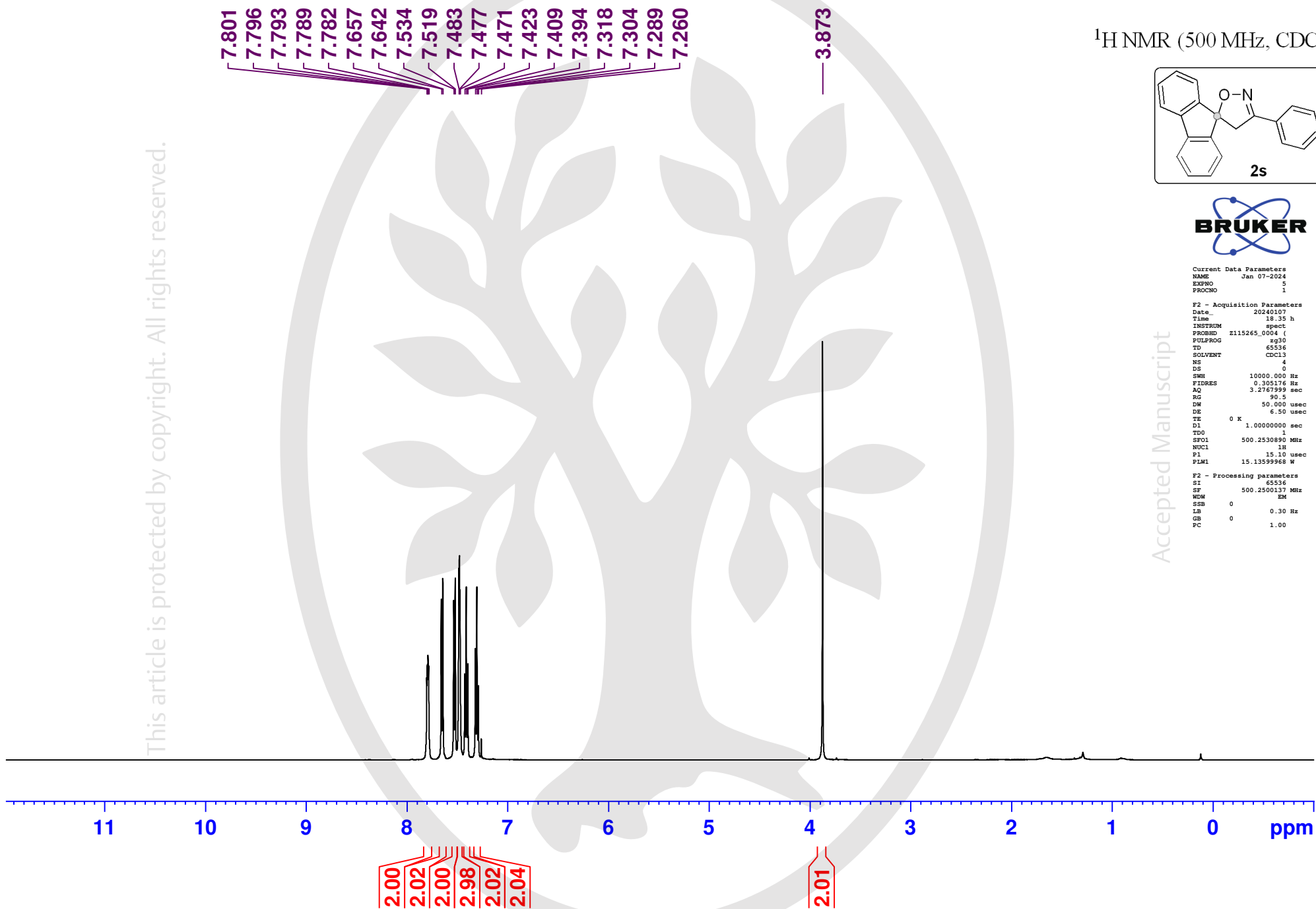
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
P1 73.0000000 usec
PLA1 0.27144000 W
SFO2 500.2520010 MHz
NUC2 1H
PCPPROG2 wait16
PCPD2 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27144000 W

F2 - Processing parameters
SI 32768
SF 125.7879683 MHz
SBS 5M
LS 1.00 Hz
GB 0
PC 1.40

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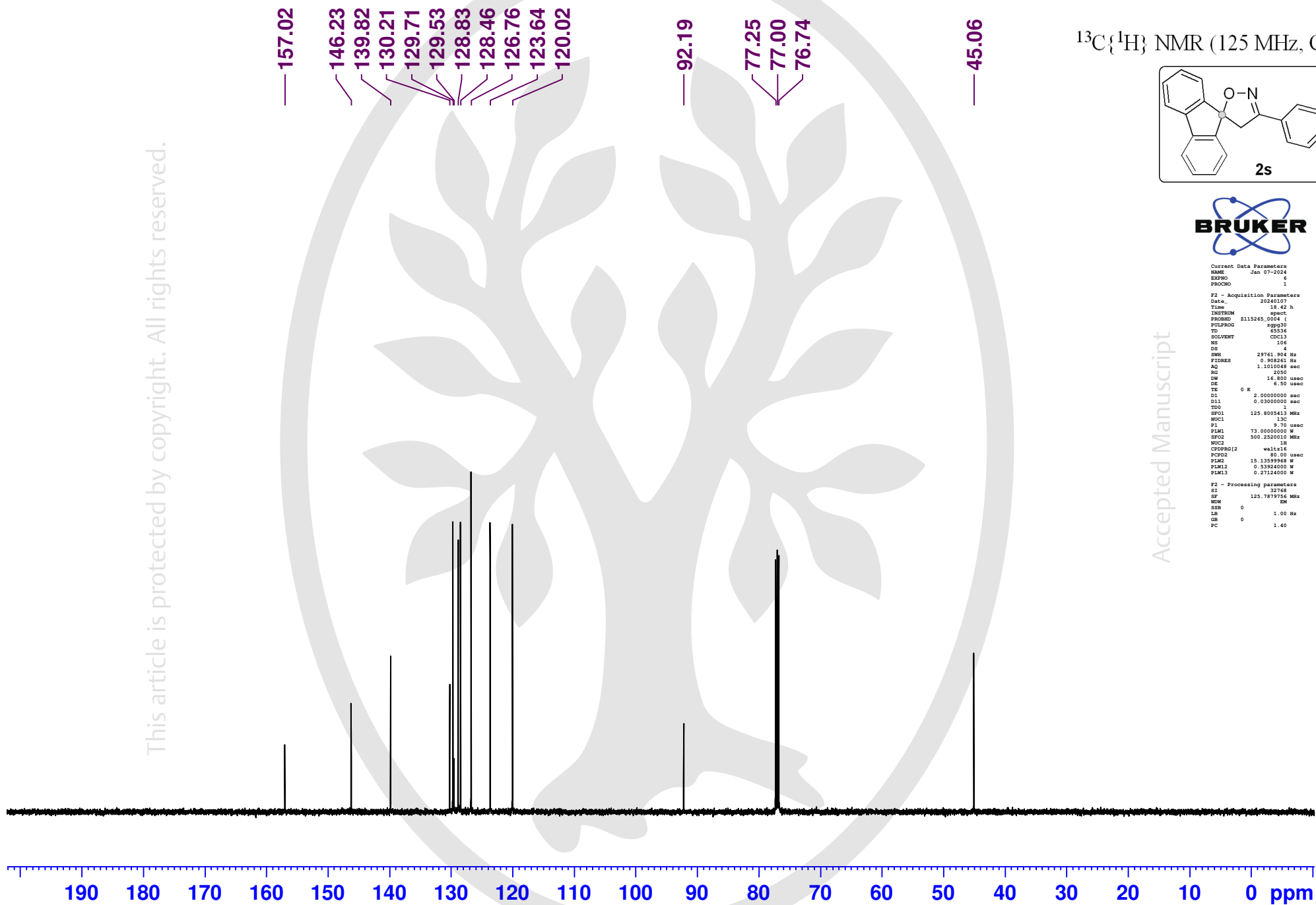
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Current Data Parameters
NAME Jan 07-2024
EXPRO 6
PROCNO 1

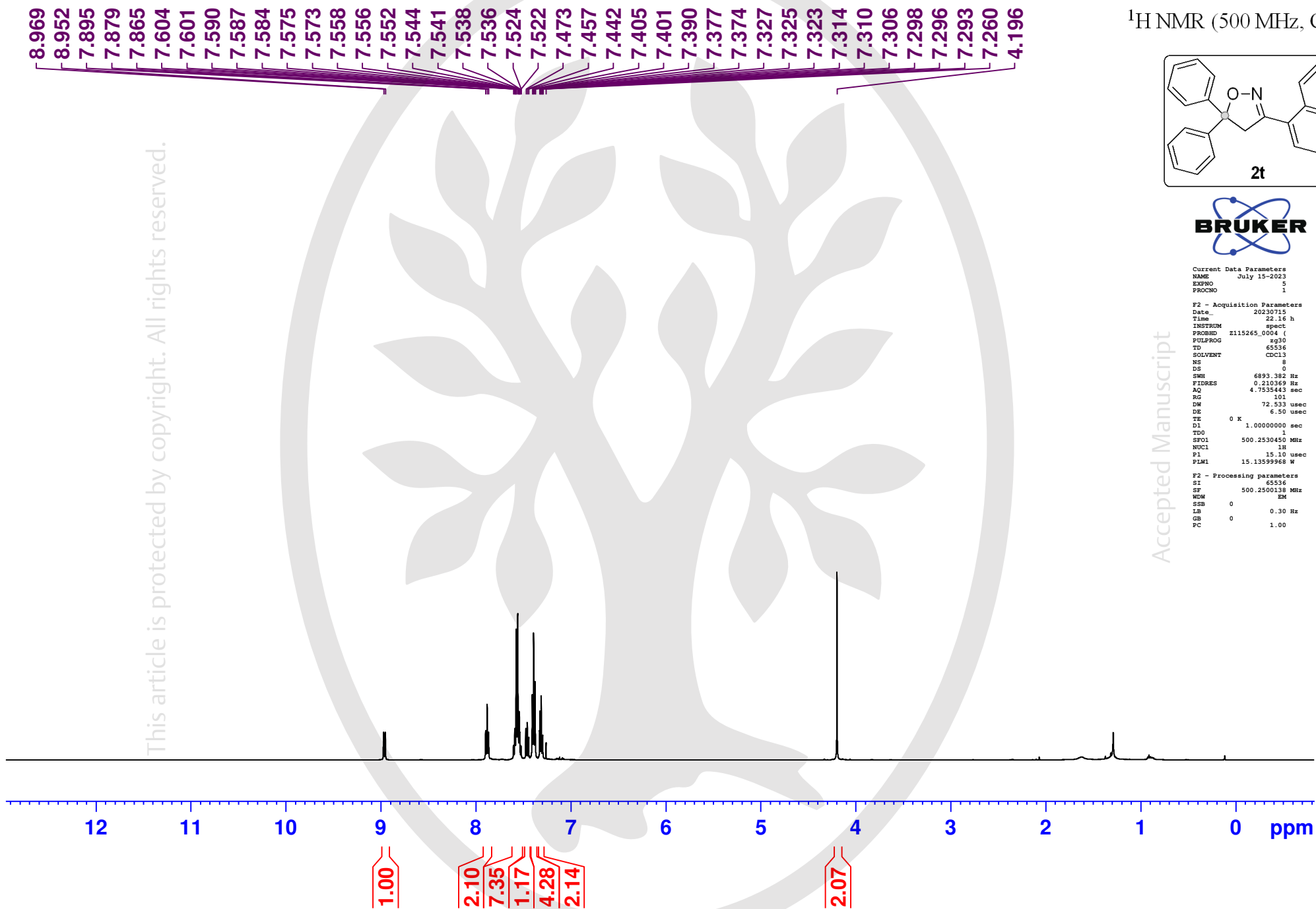
F2 - Acquisition Parameters
Date_ 20240107
Time 18:42 h
INSTRUM spect
PROBHD 1H5265.0014 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 106
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 2050
DM 16.800 usec
DE 6.50 usec
TE 0 K

D1 2.0000000 sec
D11 0.3300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
P1 73.0000000 usec
SFO2 500.2520010 MHz
NUC2 1H
PCPDPRG2 wait16
PCPD2 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27124000 W

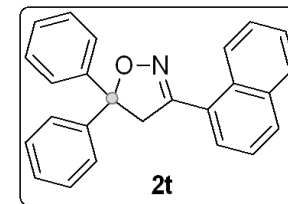
F2 - Processing parameters
SI 32768
SF 125.7879756 MHz
SBS 0 EM
LS 1.00 Hz
GB 0 1.40

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^1H NMR (500 MHz, CDCl_3)



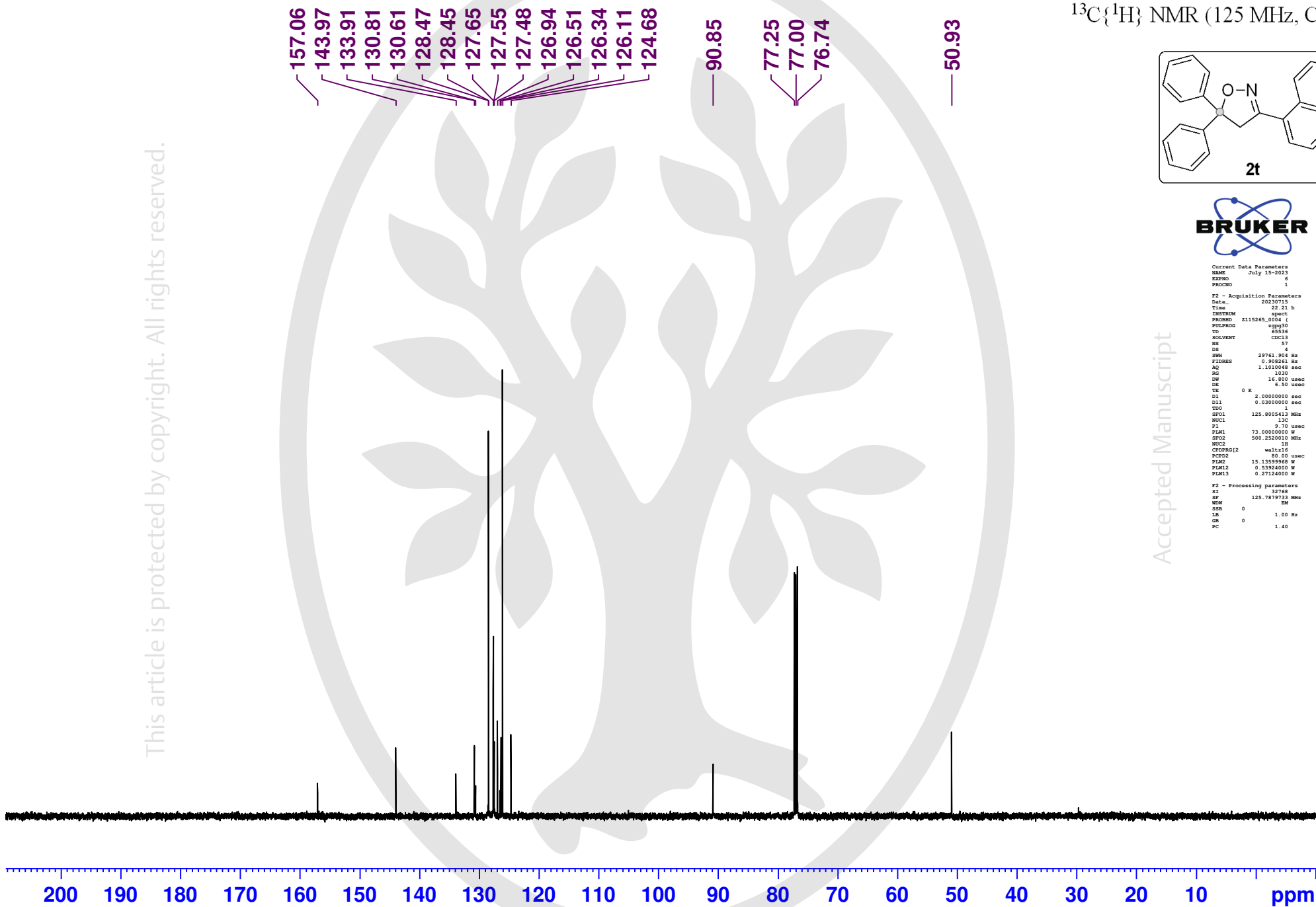
Current Data Parameters
NAME July 15-2023
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230715
Time 22.16 h
INSTRUM spect
PROBHD Z115265_0004 ((
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 8
DS 0
SWH 6893.382 Hz
FIDRES 0.210369 Hz
AQ 4.7535443 sec
RG 101
DW 72.533 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530450 MHz
NUC1 ^1H
F1 15.10 usec
PLM1 15.13599968 W

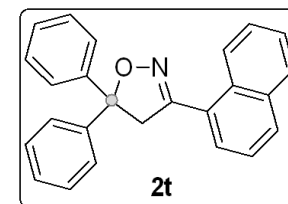
F2 - Processing parameters
SI 65536
SF 500.2500138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      July 15-2023
EXPRO    6
PROCNO   1

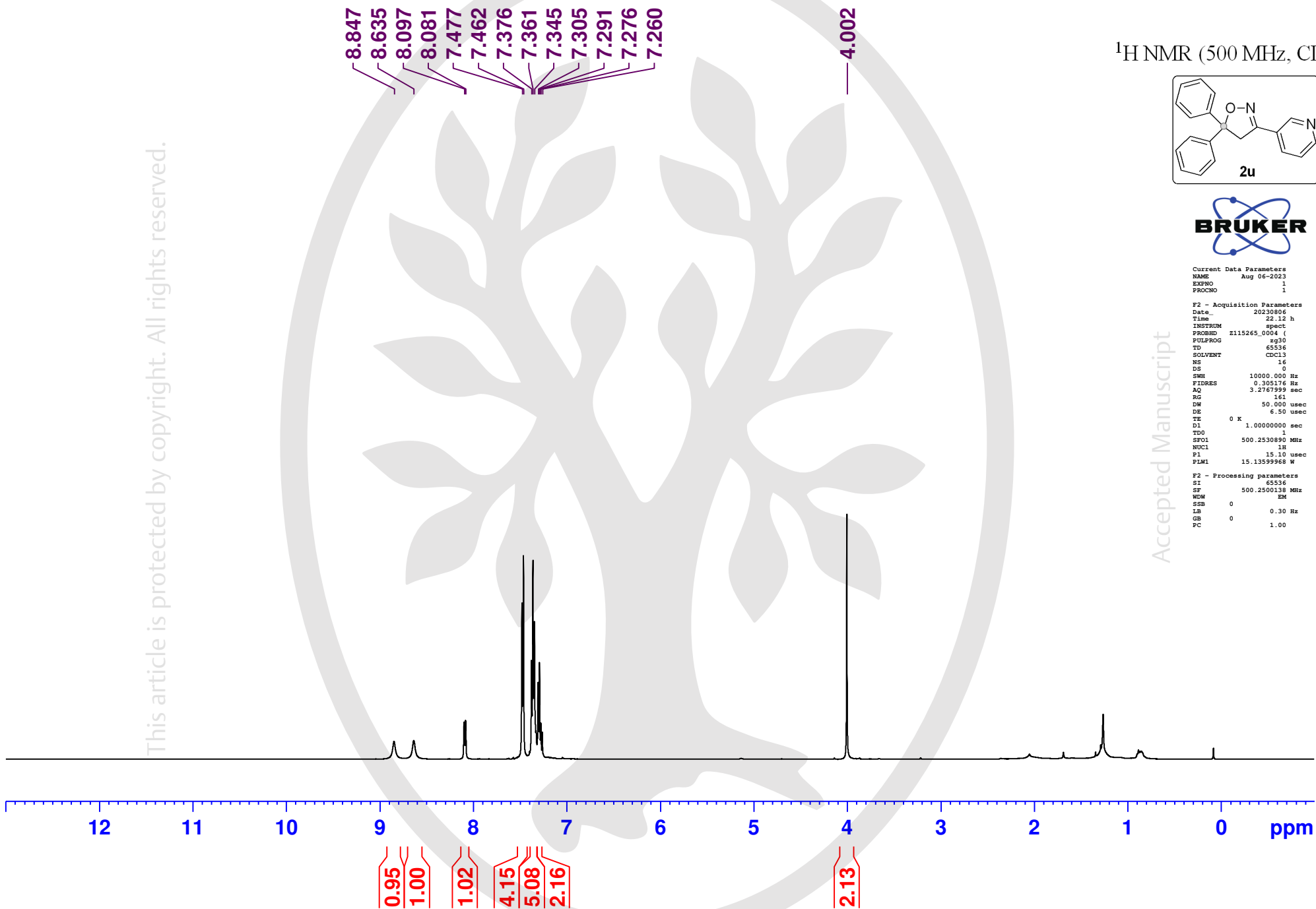
F2 - Acquisition Parameters
Date_    20230715
Time     22:21 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       57
DS       4
SWH      29761.904 Hz
FIDRES   0.998261 Hz
AQ       1.1010048 sec
RG       1030
DSW      16.800 usec
DE       6.50 usec
TE       0 K

D1       2.0000000 sec
D11      0.0300000 sec
TDO      1
SFO1     125.8005413 MHz
NUC1     13C
P1       73.0000000 W
PLM1     9.70 usec
SFO2     500.2520010 MHz
NUC2     1H
PCPDPRG2 waltz16
PCPD2    80.00 usec
PLM2     15.13599968 W
PLM12    0.53924000 W
PLM13    0.27124000 W

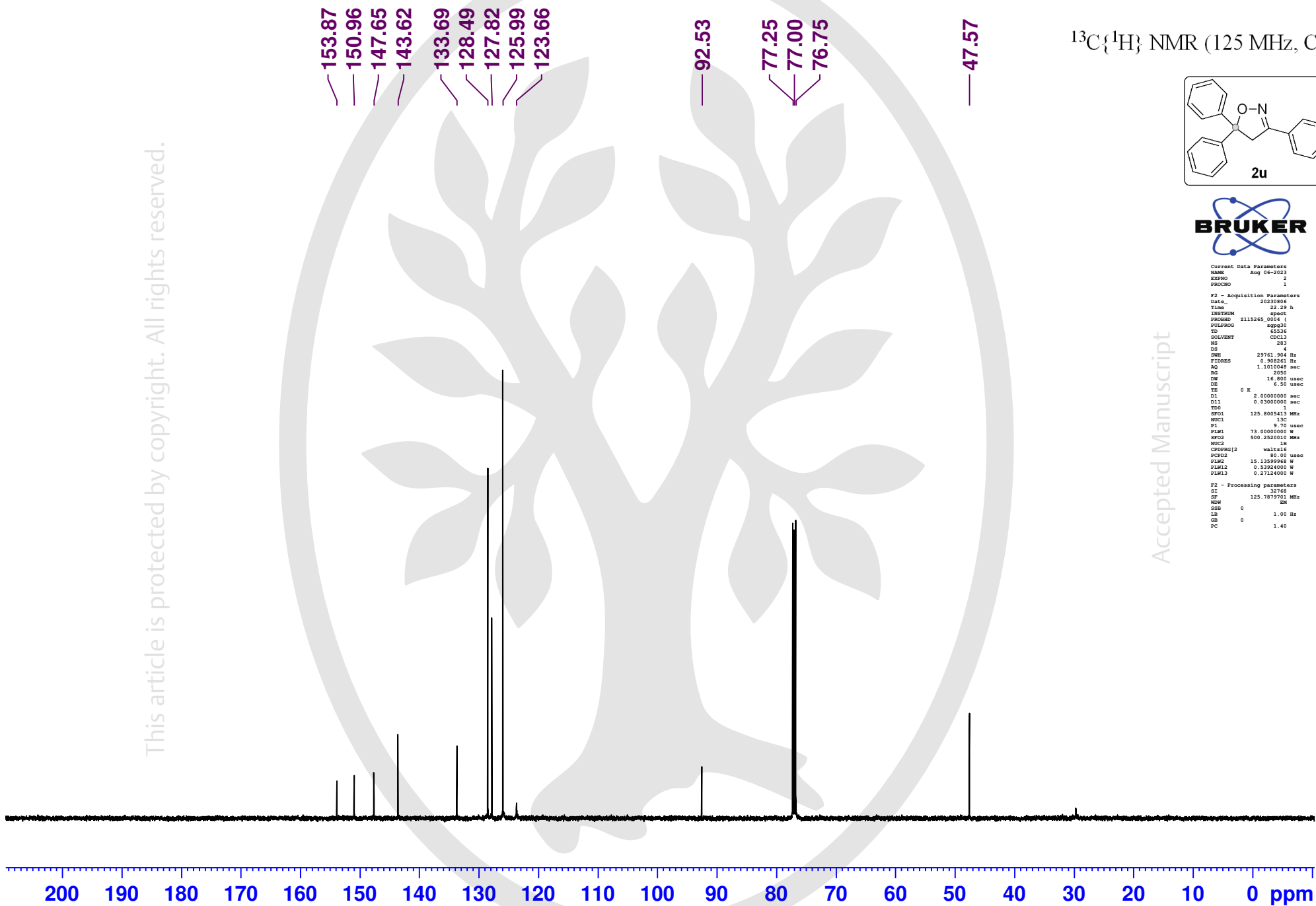
F2 - Processing parameters
SI       32768
SF       125.7679723 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

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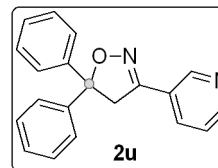
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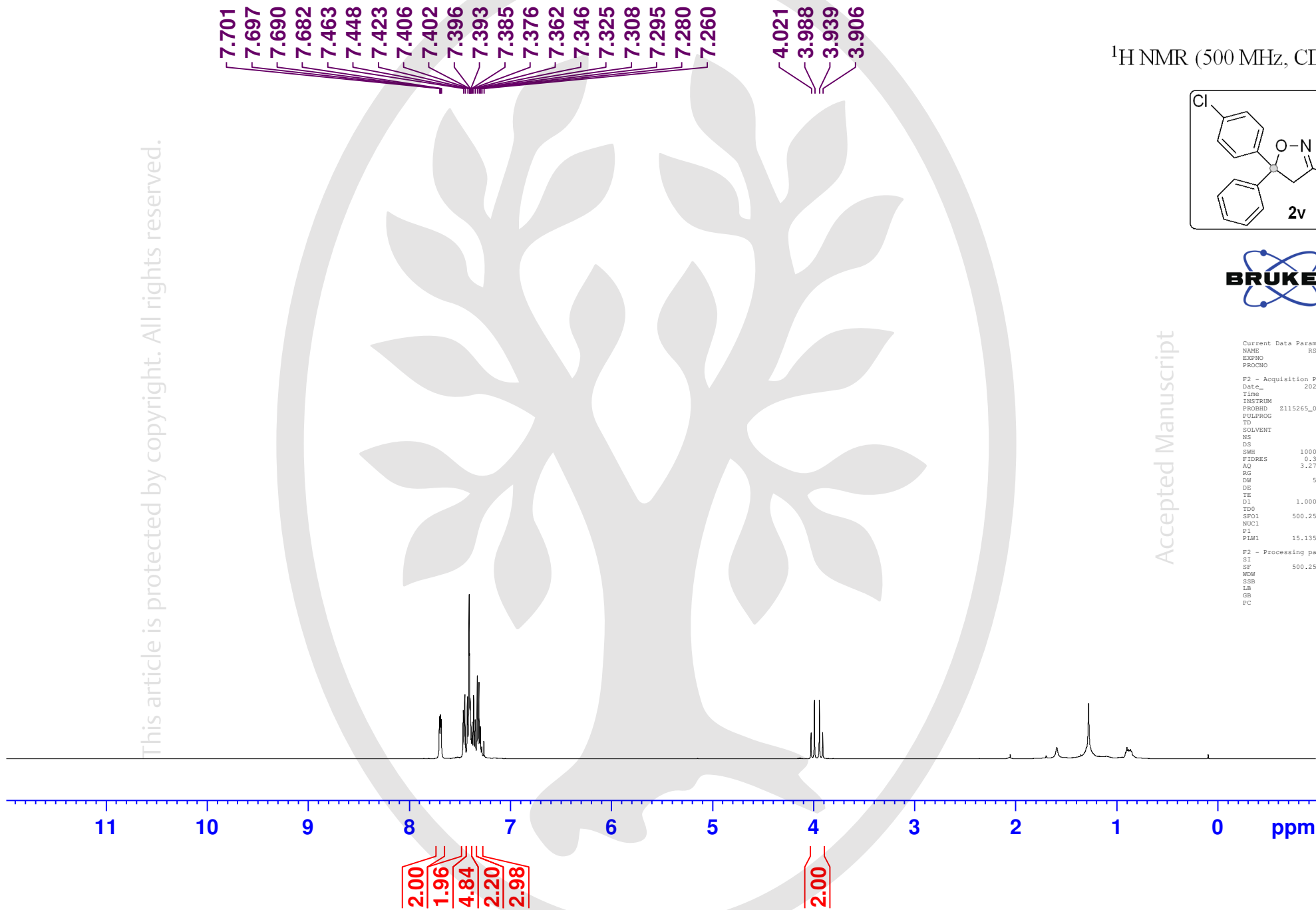
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Current Data Parameters
NAME          Aug 06-2023
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        20230806
Time         22:29 h
INSTRUM      spect
PROBHD       1H5265_004 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           283
DS           4
SWH          29761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           2050
SW           16.800 usec
DE           6.50 usec
TE           0 K

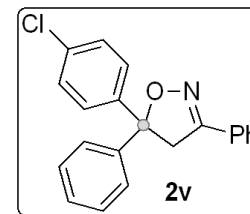
D1           2.0000000 sec
d11          0.0300000 sec
TDO          1
SFO1         125.8005413 MHz
NUC1         13C
P1           73.0000000 usec
PL1         0.970 usec
SFO2         500.2520010 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27144000 W

F2 - Processing parameters
SI           32768
SF           125.7679701 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
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^1H NMR (500 MHz, CDCl_3)



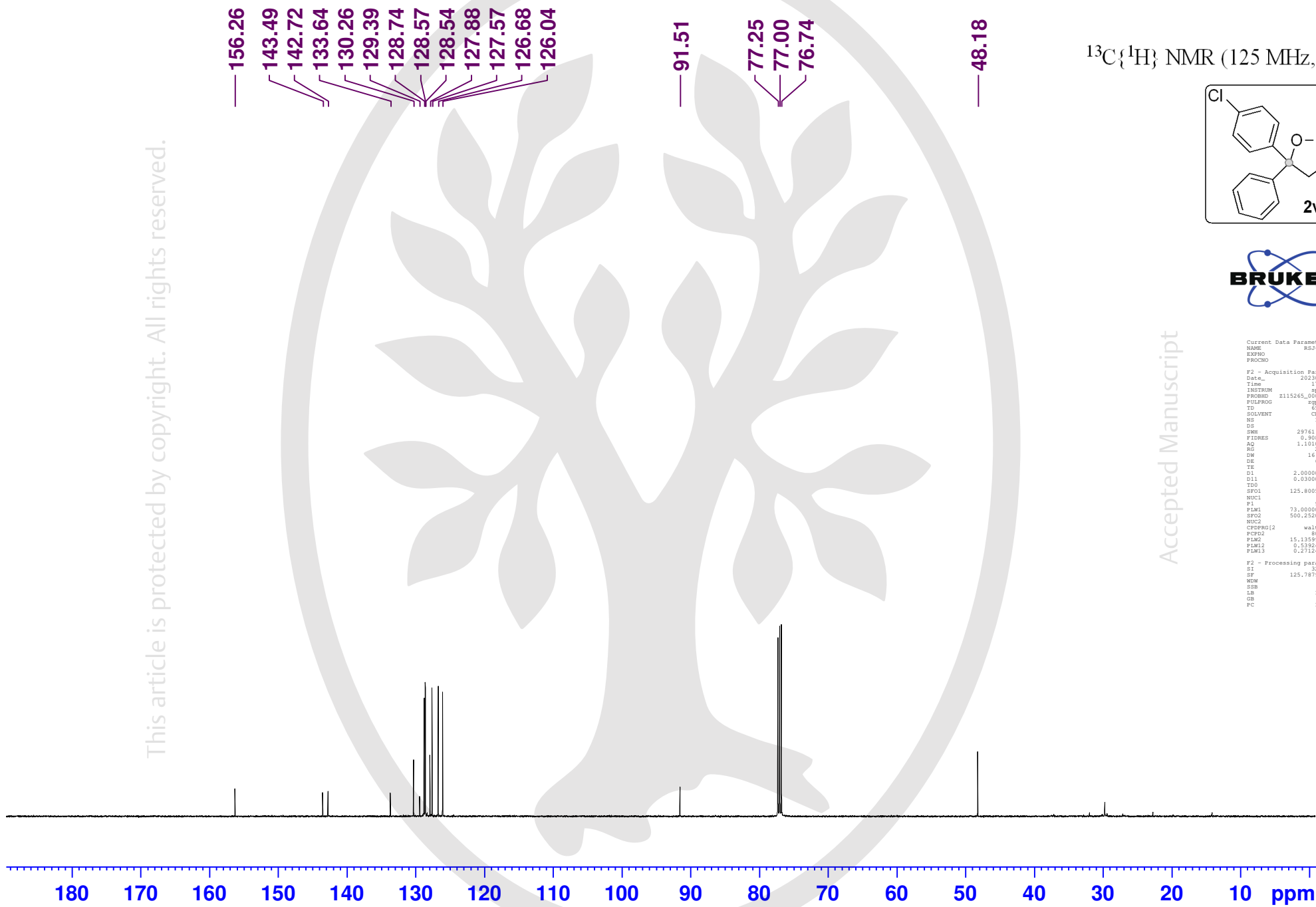
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Current Data Parameters
NAME      RSD-959
EXPNO     3
PROCNO    1

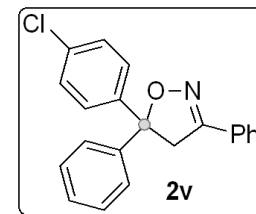
F2 - Acquisition Parameters
Date_     20230909
Time      16.50 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         144
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.2500139 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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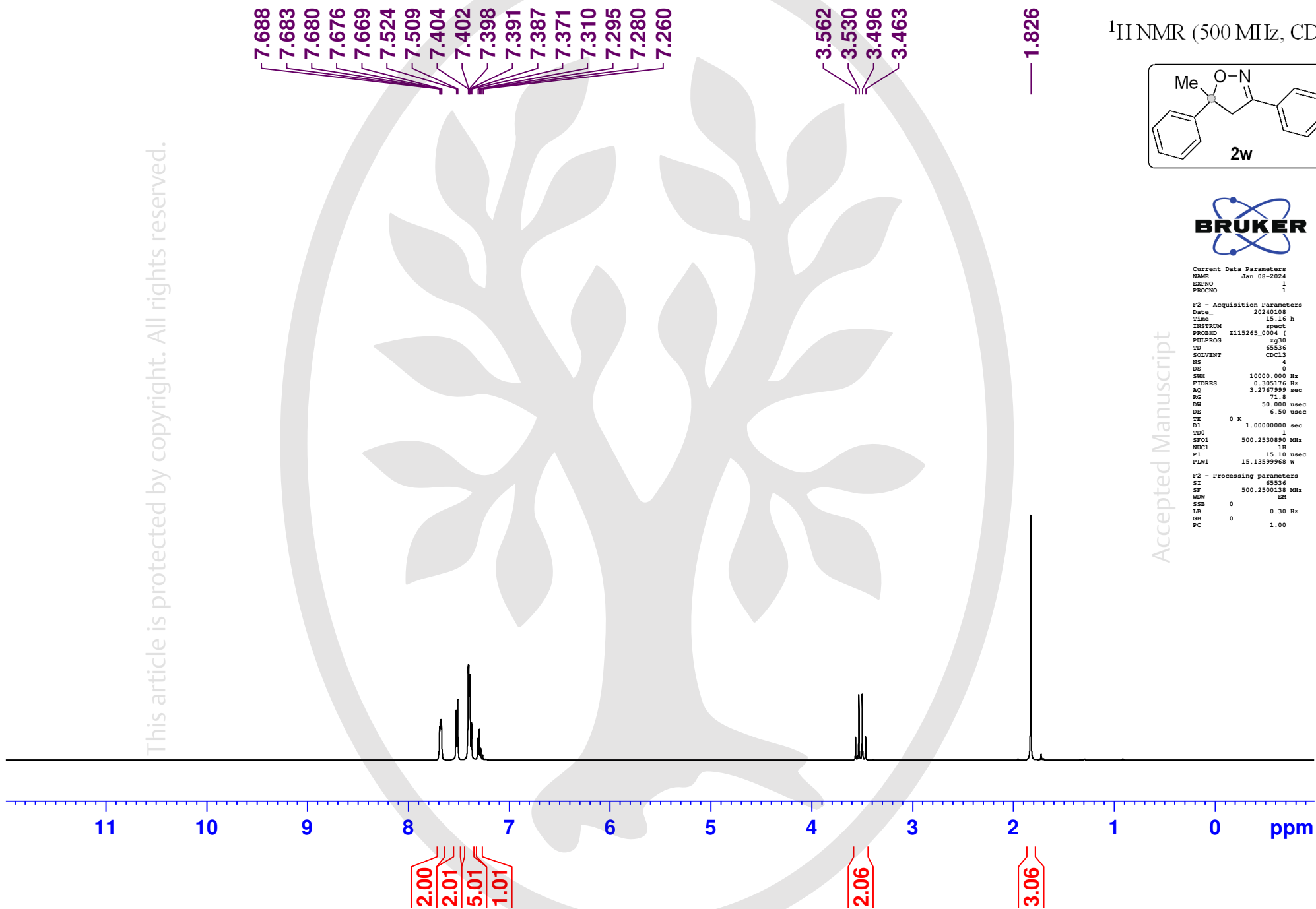


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```
Current Data Parameters
NAME          R02-959
EXPNO        4
PROCNO       1
F2 - Acquisition Parameters
Date_         20230909
Time_        17.46 h
INSTRUM      spect
PROBHD       Z115265_0004 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           1024
DS           4
SWE          29761.904 Hz
FIDRES       0.908261 Hz
AQ           1.1010048 sec
RG           2050
DM           16.800 usec
DE           6.50 usec
TE           0 K
D1           2.0000000 sec
D11          0.0300000 sec
TD0          1
SFO1         125.8005413 MHz
NUC1         13C
P1           9.70 usec
PL1          73.00000000 W
SFO2         500.2550010 MHz
NUC2         1H
CPCPRG12     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27124000 W
F2 - Processing parameters
SI           32768
SF           125.7879656 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```

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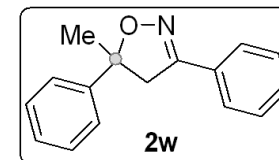
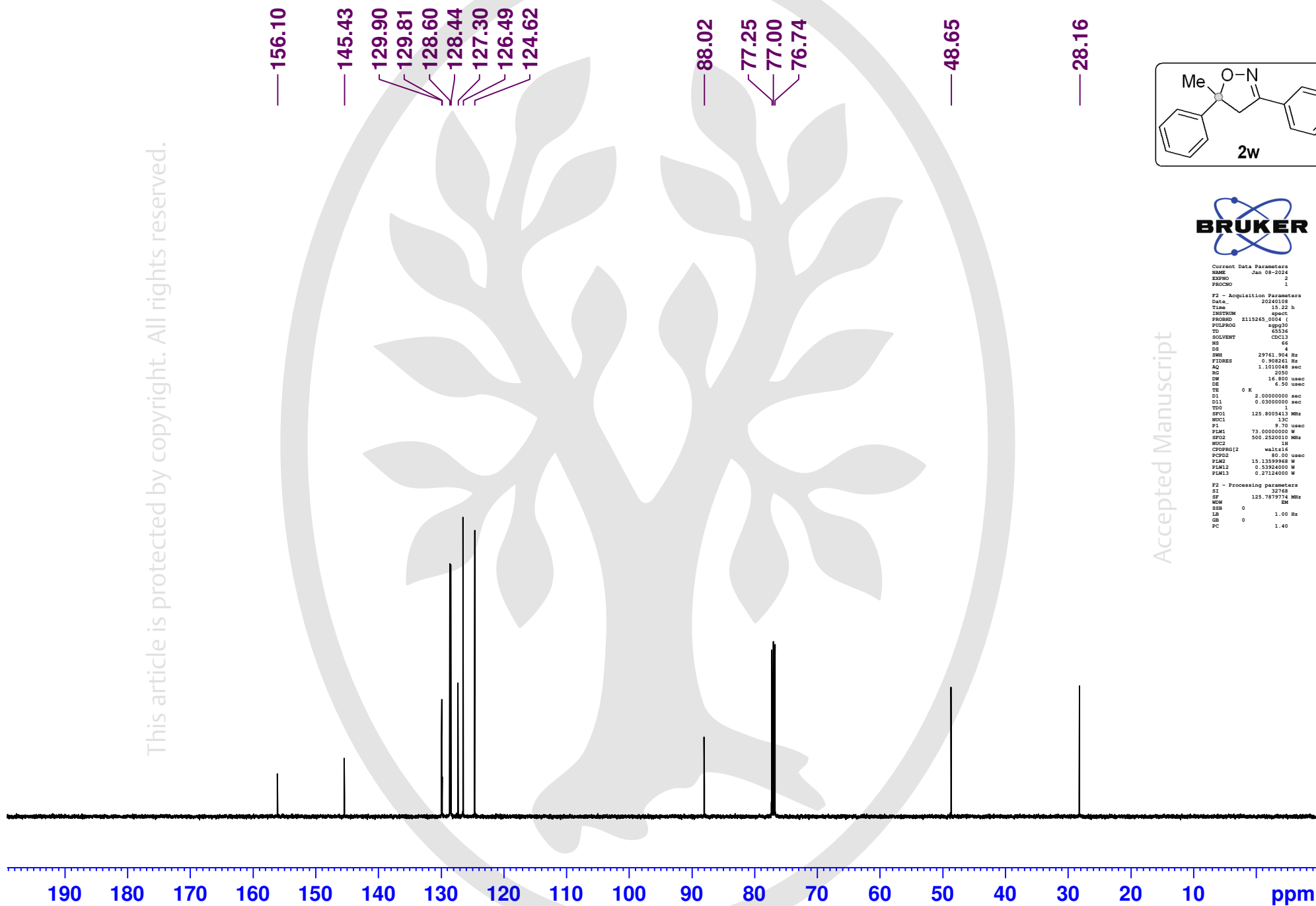
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Current Data Parameters
NAME Jan 08-2024
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240108
Time 15:16 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 71.8
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

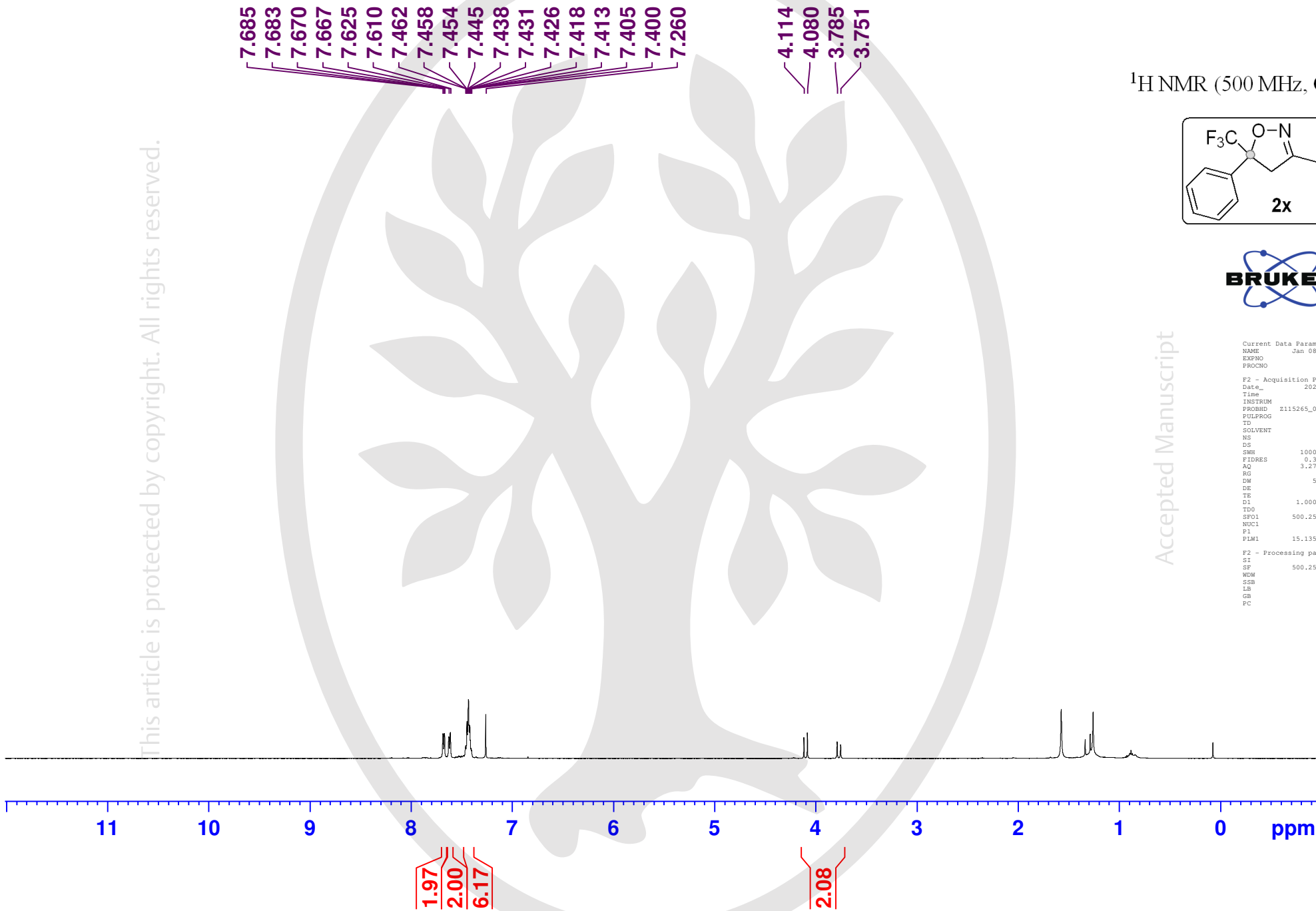


Current Data Parameters
NAME Jan 08-2024
EXPRO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240108
Time 15:22 h
INSTRUM spect
PROBHD 1H5265.004 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 66
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 2050
DM 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.0000000 sec
D11 0.3300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
D1 73.0000000 M
PLM1 500.2520010 MHz
NUC2 1H
CPCPRG12 waltz16
PCPD2 80.00 usec
PLM2 15.13599968 M
PLM12 0.53924000 M
PLM13 0.27144000 M
F2 - Processing parameters
SI 32768
SF 125.7679774 MHz
SBS EM
LS 1.00 Hz
GB 0 1.40

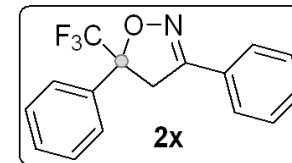
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^1H NMR (500 MHz, CDCl_3)



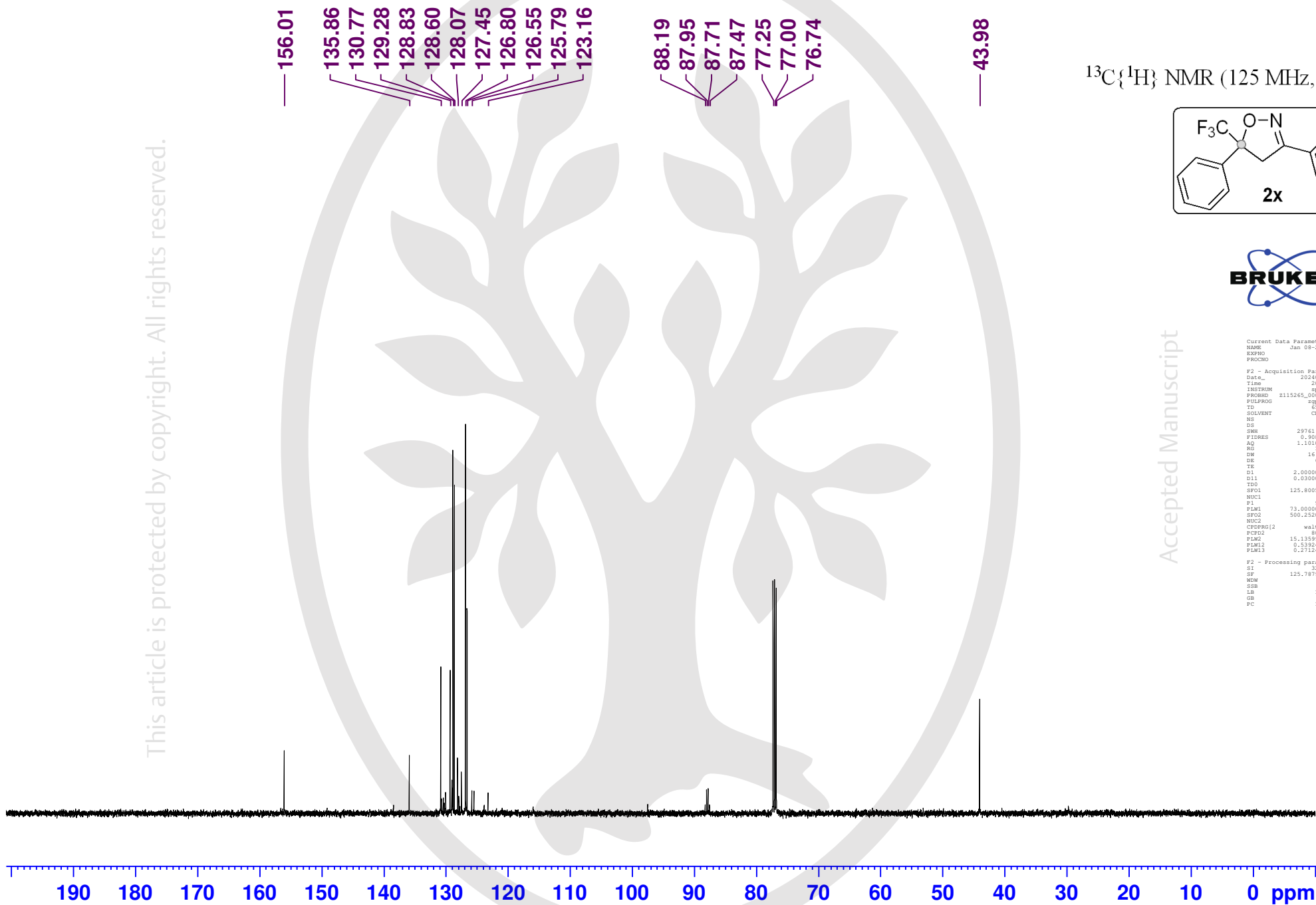
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Current Data Parameters
NAME      Jan 08-2024
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20240108
Time      16.44 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767959 sec
RG         287
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.0000000 sec
TDO        1
SFO1      500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13559968 W

F2 - Processing parameters
SI         65536
SF         500.2500138 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

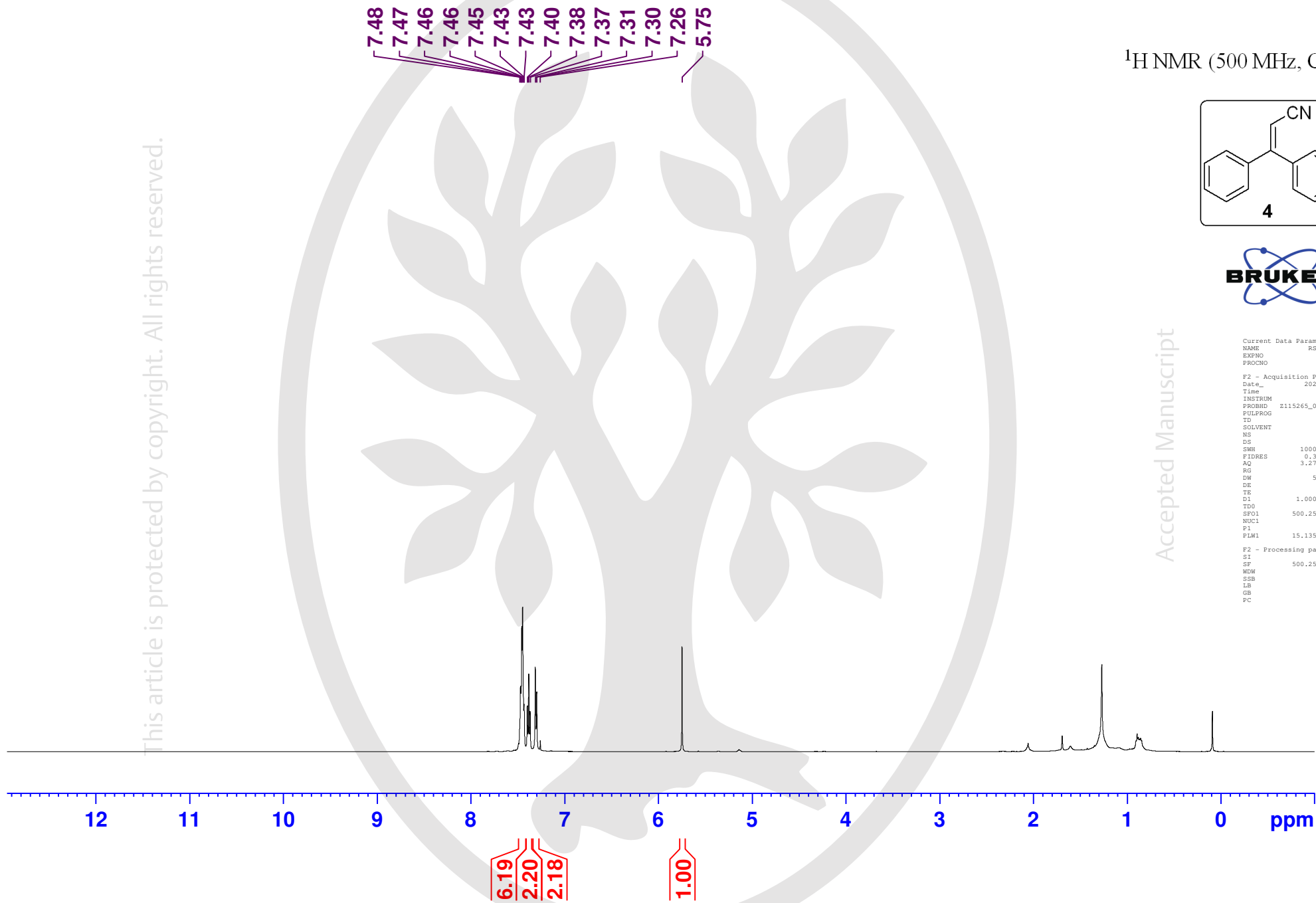
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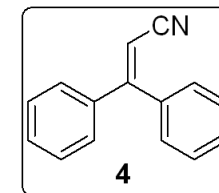
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Current Data Parameters
NAME          Jan 08-2024
EXPNO         6
PROCNO        1
F2 - Acquisition Parameters
Date_         20240108
Time_        20:31 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            48
DS            4
SFE          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG            1030
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SFO1          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.00000000 W
SFO2          500.2550010 MHz
NUC2          1H
PCPD2         waitx16
PLM2          15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W
F2 - Processing parameters
SI            32768
SF            125.7879729 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

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^1H NMR (500 MHz, CDCl_3)



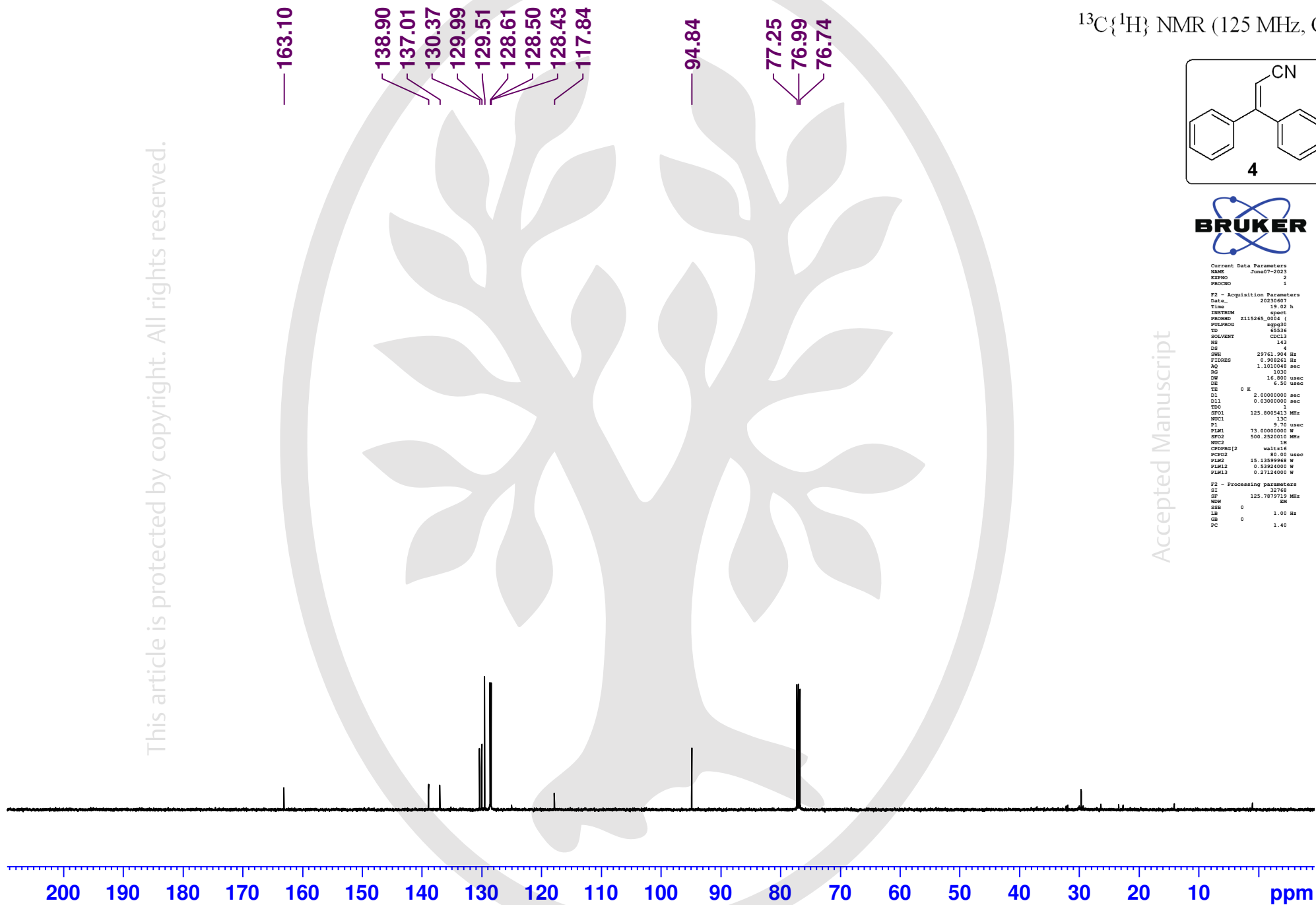
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Current Data Parameters
NAME      R5J-875
EXPNO     1
PROCNO    1

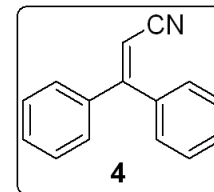
F2 - Acquisition Parameters
Date_     20230607
Time      18.50 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         101
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.2500142 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

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$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      June07-2023
EXPNO    2
PROCNO   1

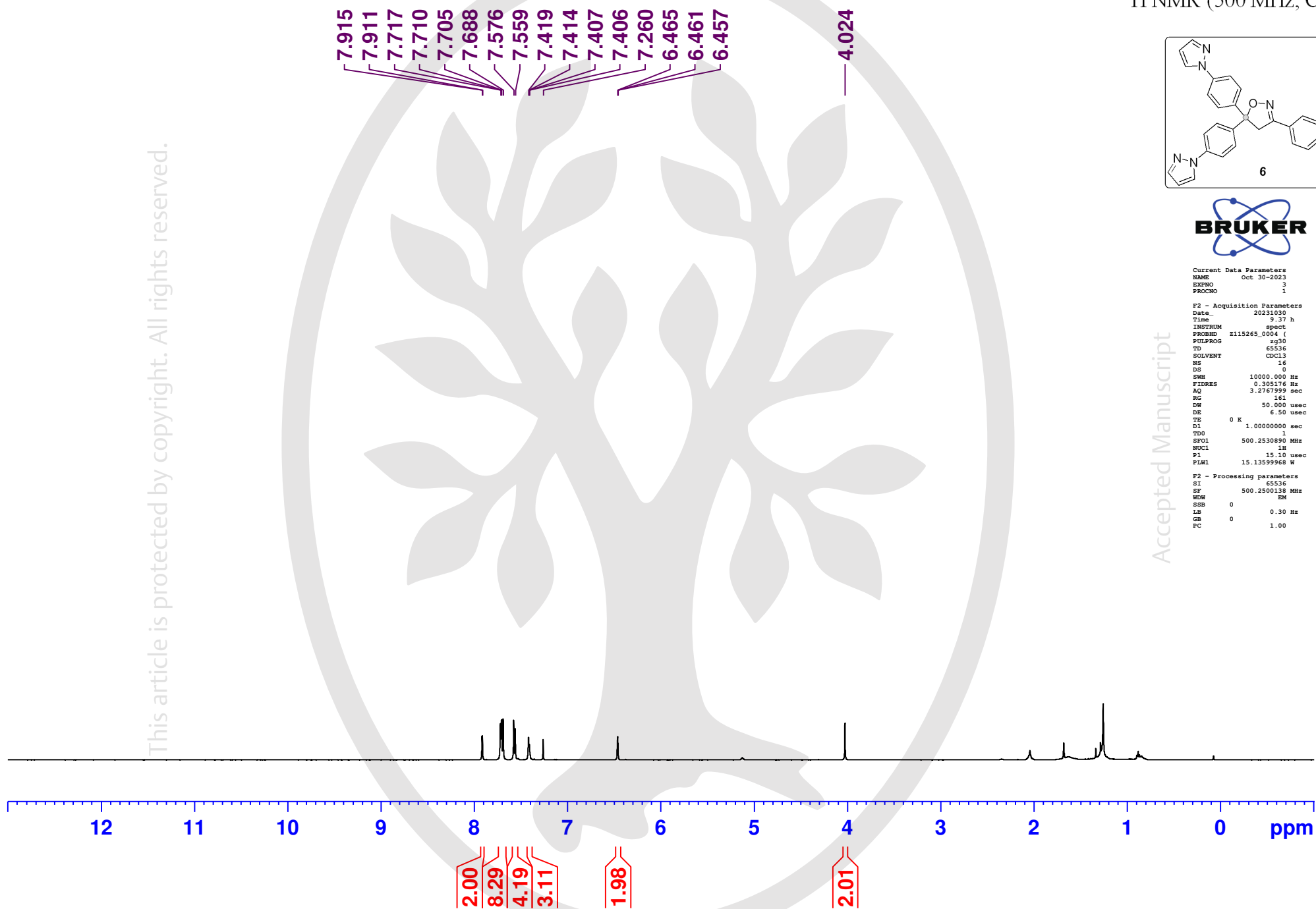
F2 - Acquisition Parameters
Date_    20230607
Time     19:02 h
INSTRUM  spect
PROBHD   1H125AS.004 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       143
DS       4
SWH      29761.904 Hz
FIDRES   0.998261 Hz
AQ       1.1010048 sec
RG       1030
DSW      16.800 usec
DE       6.50 usec
TE       0 K

D1       2.0000000 sec
D11      0.0300000 sec
TDO      1
SFO1     125.8005413 MHz
NUC1     13C
P1       73.0000000 usec
SFO2     500.2520010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLM2     15.13599968 W
PEM12    0.53924000 W
PLM13    0.27144000 W

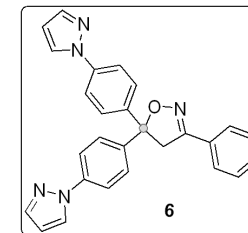
F2 - Processing parameters
SI       32768
SF       125.7879719 MHz
WDW      EM
SSB      EM
LB       1.00 Hz
GB       0
PC       1.40
```

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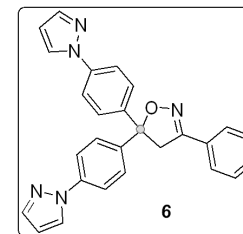
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Current Data Parameters
NAME Oct 30-2023
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231030
Time 9:37 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2167399 sec
RG 161
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



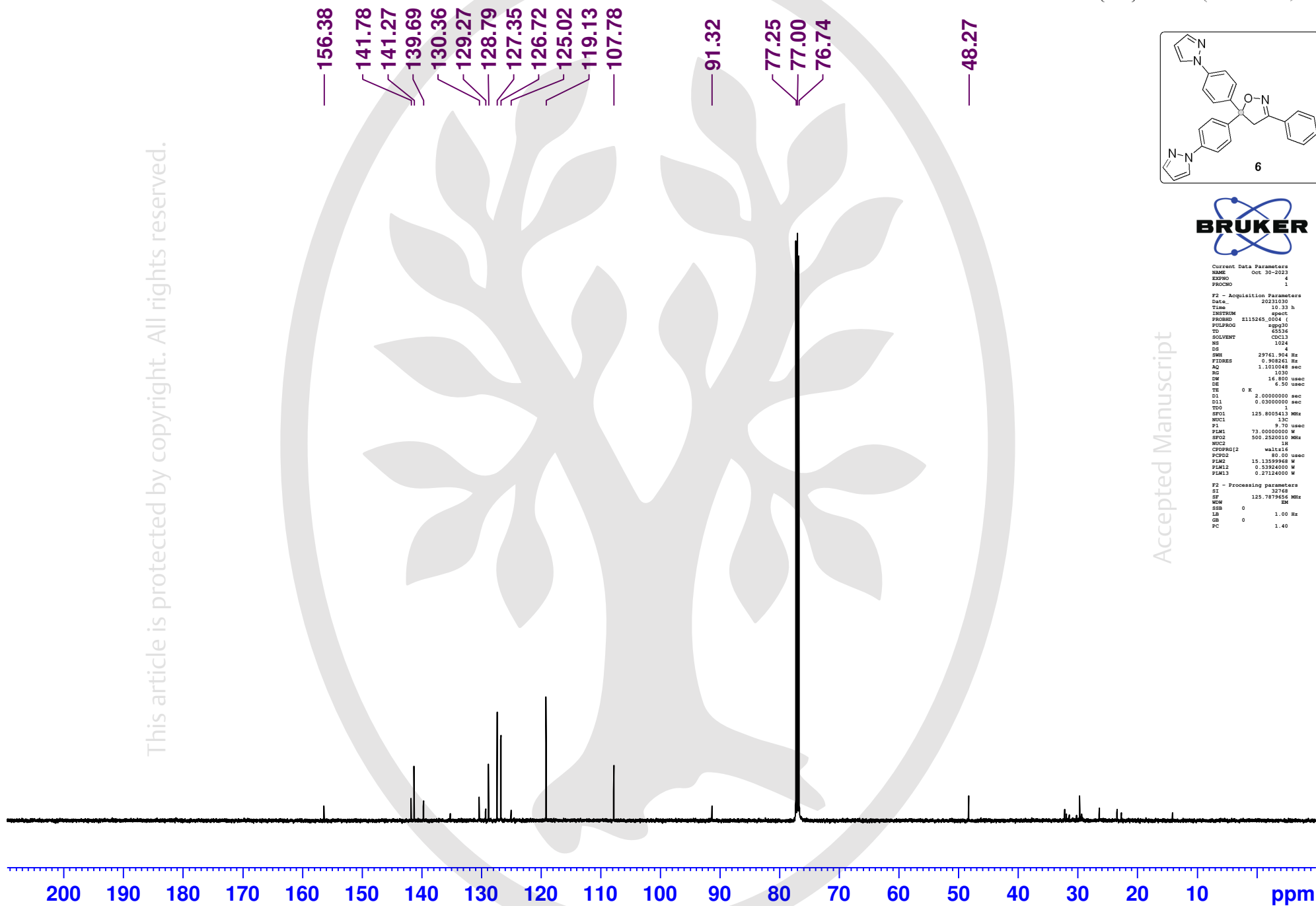
Current Data Parameters
NAME Oct 30-2023
EXPRO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231030
Time 10:23 h
INSTRUM spect
PROBHD 1H125AS.004 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 1030
SW 16.800 usec
DE 6.50 usec
TE 0 K

D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 125.8005413 MHz
NUC1 13C
P1 73.0000000 usec
PLA1 0.53924000 W
SFO2 500.2520010 MHz
NUC2 1H
PCPDPRG2 wait16
PCPDG 80.00 usec
PLM2 15.13599968 W
PLM12 0.53924000 W
PLM13 0.27154000 W

F2 - Processing parameters
SI 32768
SF 125.7879656 MHz
WDW EM
SSB EM
LB 1.00 Hz
GB 0
PC 1.40

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