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Supporting Information

Competing Pathways in O-Arylations with Diaryliodonium Salts: Mechanistic Insights

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Supporting Information

1. General Experimental Procedure

All reactions were carried out without any precaution to avoid air or moisture unless otherwise stated. Toluene and THF were dried using VAC-purification system and then stored over activated 4Å molecular sieves. MeCN was dried using VAC-purification system. Pentane and anhydrous TBME were dried over activated 4Å molecular sieves. MeOH was used as received. The stabilizer in the CH_2Cl_2 had an impact on the arylation reaction; wet CH_2Cl_2 (*i.e.* CH_2Cl_2 saturated with deionized H_2O) stabilized with amylene should be used. CH_2Cl_2 stabilized with EtOH (<0.2%) gave an undesired ether product, which was difficult to separate from the desired diaryl ether.

All reactants and reagents were purchased from commercial suppliers, except the diaryliodonium salts and the secondary alcohols, which were synthesized according to published procedures. NaOH was powdered and stored in a desiccator. *tert*-Butoxide bases, $NaBH_4$ and $NaBD_4$ were stored under argon atmosphere in a desiccator. *m*CPBA was dried under high vacuum for 3-4 hours and the percentage of active oxidant was determined using iodometric titration.[1] TfOH and $BF_3{\cdot}OEt_2$ were stored and handled under argon atmosphere using Hamilton syringes and oven-dried metal needles. For diaryliodonium salt synthesis CH_2Cl_2 stabilized with EtOH (<0.2%) was used, except in the synthesis of 4-nitrophenyl-(phenyl)iodonium triflate that utilized CH_2Cl_2 stabilized with amylene.

TLC analysis was performed on pre-coated silica gel 60 F_{254} plates using either UV light, $KMnO_4$, or Seebach's "magic" stain (a mixture of phosphormolybdic acid and $Ce(SO_4)_2$) together with heat as developing agent.[2] The crude products were purified by flash column chromatography using 40-60 μm, 60A silica gel as stationary phase or using automated flash system Teledyne ISCO CombiFlash Rf 200 with RediSep Rf columns.

GC-MS analyses were performed using a Shimadzu GC-2010 Plus gas chromatograph (column HP-5MS 30 m x 0.25 mm x 0.25 μm) connected to a GCMS-QP2020 mass spectrometer.

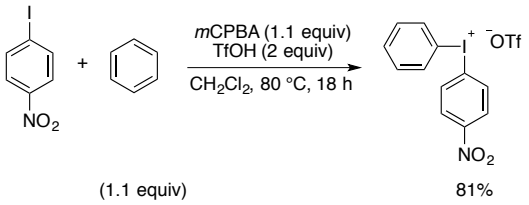
Melting points were measured using a STUART SMP3 and are reported uncorrected. All NMR spectra were recorded using a 400 MHz Bruker AVANCE II with a BBO probe at 298 K using $CDCl_3$, CD_2Cl_2, MeOH-d_4 or DMSO-d_6 as solvents. Chemical shifts are given in ppm relative to the residual solvent peak (^{1}H NMR: $CDCl_3$ δ 7.26; MeOH-d_4 3.31; DMSO-d_6 2.50; ^{13}C NMR: $CDCl_3$ δ 77.16; MeOH-d_4 49.00; DMSO-d_6 39.52) with multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, app = apparent), coupling constants (in Hz) and integration. High-resolution mass analyses were obtained using a Bruker microTOF ESI or APCI.

2. Synthesis of Starting Materials

The diaryliodonium salts used in this investigation were synthesized according to published procedures.

2.1. Synthesis of Diaryliodonium Salts 1

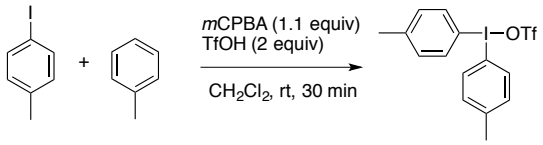
4-Nitrophenyl(phenyl)iodonium Triflate (1a)



(1.1 equiv) 81%

Synthesized according to our published procedure.[3] Spectral data are in agreement with published data. ***Note:*** *For synthesis of this salt CH_2Cl_2 stabilized with EtOH should not be used. The reaction can also be performed at rt.*

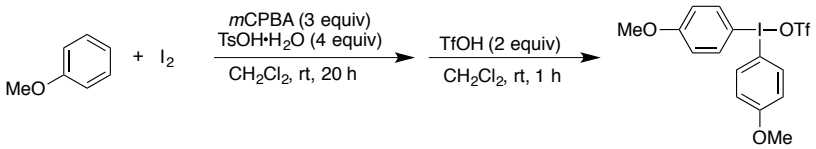
Di(*p*-tolyl)iodonium Triflate (1b)



(1.1 equiv) 84%

Synthesized according to our published procedure.[3] Spectral data are in agreement with published data.

Di(4-methoxyphenyl)iodonium Triflate (1c)



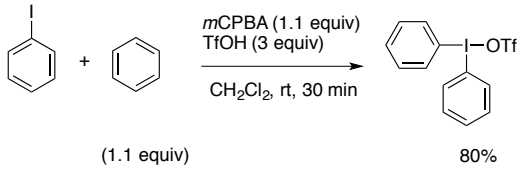
4 equiv 57%

Synthesized according to our published procedure.[4] Remaining tosic acid was removed via filtration over basic alumina after the anion exchange.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 9.0 Hz, 4H), 7.06 (d, *J* = 9.0 Hz, 4H), 3.79 (s, 6H)

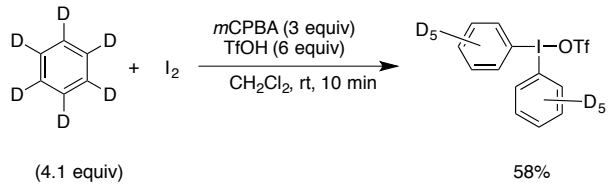
^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8, 136.9, 120.7 (q, *J* = 323 Hz) 117.3, 106.0, 55.7

Diphenyliodonium Triflate (1d)



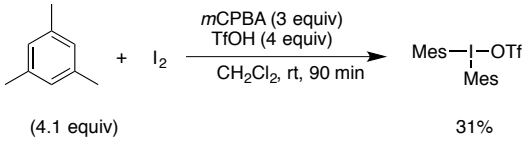
Synthesized according to our published procedure.[6] Spectral data are in agreement with published data.

Diphenyliodonium Triflate-d_{10} (1d-D)



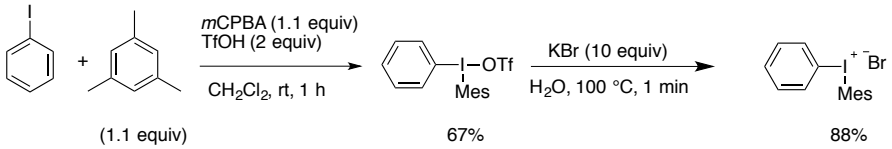
Synthesized according to our published procedure.[6] Spectral data are in agreement with published data.[7]

Dimesityliodonium Triflate (1e)



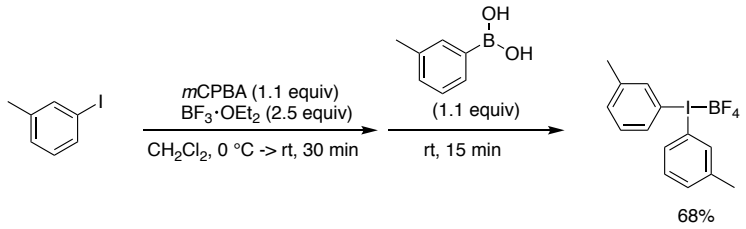
Synthesized according to our published procedure.[6] Spectral data are in agreement with published data.

Mesityl(phenyl)iodonium Bromide (1f)



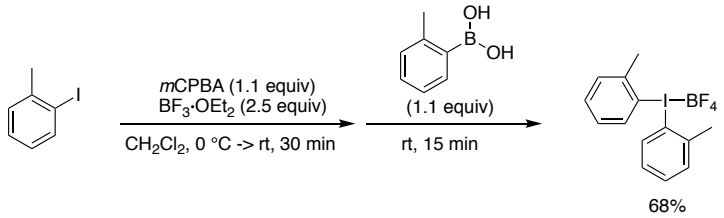
Triflate salt synthesized according to a published procedure.[3] Anion exchange according to a published procedure.[8] Spectral data are in agreement with published data.[9]

Di(*m*-tolyl)iodonium Tetrafluoroborate (1g)



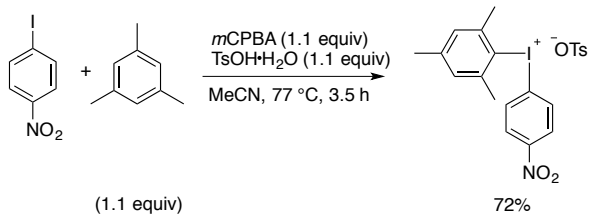
Synthesized according to our published procedure.[10] All spectral data are in agreement with published data.[11]

Di(*o*-tolyl)iodonium Tetrafluoroborate (1h)



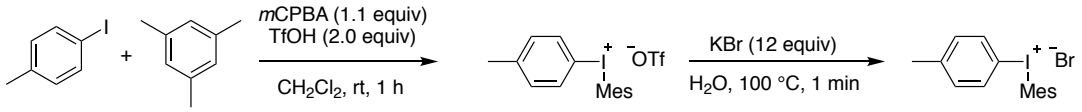
Synthesized according to a published procedure.[10] All spectral data are in agreement with published data.

Mesityl(4-nitrophenyl)iodonium Tosylate (1i)



Synthesized according to a published procedure.[12] The ^{13}C NMR is in full agreement with published data. In the ^{1}H NMR the doublet that was reported at 6.39 ppm was found at 7.20 ppm.[13]

Mesityl(*p*-tolyl)iodonium Bromide (1j)



(1.1 equiv) 74% 85%

Triflate salt synthesized according to our published procedure.[3] Anion exchange according to a published procedure.[8]

mp = 156-158 °C

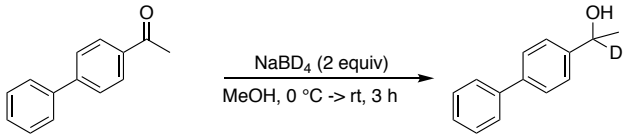
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.63 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.00 (s, 2H), 2.66 (s, 6H), 2.29 (s, 6H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 141.5, 141.0, 132.8, 132.2, 129.9, 126.8, 115.6, 27.2, 21.3, 21.2

HRMS (ESI): calcd for $C_{16}H_{18}I$ $[M-Br]^+$: 337.0453; found: 337.0439.

2.2. Synthesis of Alcohols 3

1-(4-Biphenylyl)ethanol-d_1 (3b-D)



3b-D 94%

Synthesized according to a slightly modified literature procedure.[14] An oven-dried two-necked round-bottomed flask was evacuated and backfilled with argon three times, then charged with 4-phenylacetophenone (785 mg, 4 mmol) and MeOH (50 mL). The mixture was cooled to 0 °C and $NaBD_4$ (335 mg, 8 mmol, 2 equiv) was added in portions during 1 h after which the mixture was stirred at rt for 3 h. The reaction was quenched with HCl (1 M), and then extracted with EtOAc (x3), the combined organic phases were dried over Na_2SO_4, filtered and concentrated down. The crude residue was purified using flash chromatography (SiO_2, pentane -> pentane/EtOAc 75:25 as eluent), which gave the desired alcohol **3b-D** as a white powder (753 mg, 94%).

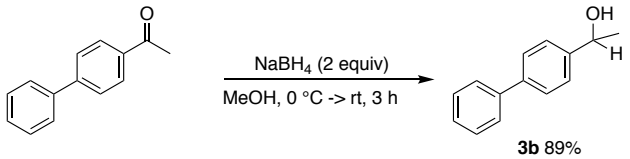
mp = 96-97 °C (ref 95-96 °C)[15]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.57 (m, 4H), 7.49-7.42 (m, 4H), 7.39-7.33 (m, 1H), 1.87 (bs, 1H), 1.54 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 141.0, 140.6, 128.9, 127.4, 127.2, 126,0, *70.3* (H Alcohol), 69.9 (t), 25.2.
Traces of the non-deuterated product could be detected in the NMR spectra.

HRMS (ESI): calcd for $C_{14}H_{13}DNaO$ $[M+Na]^+$: 222.1000; found: 222.1002 .

1-(4-Biphenylyl)ethanol (3b)



Synthesized according to the same procedure as for **3b-D**. The reaction was performed on 10 mmol scale. The desired alcohol **3b** was isolated as a white powder in 89% (1.77 g).

MP: 96-97 °C (ref 95-96 °C)[16]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.55 (m, 4H), 7.52-7.41 (m, 4H), 7.41-7.32 (m, 1H), 4.96 (q, *J* = 6.5 Hz, 1H), 1.94 (bs, 1H), 1.55 (d, *J* = 6.5 Hz, 3H).

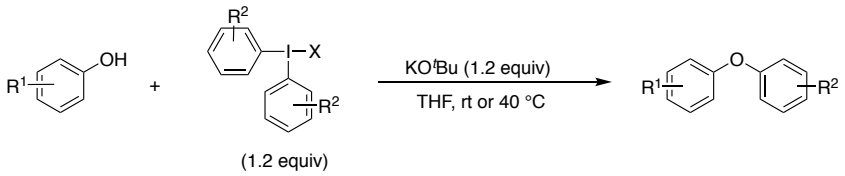
^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 140.9, 140.6, 128.9, 127.4, 127.2, 126.0, 70.3, 25.3.
^{13}C NMR not the same as in reference with HRMS[17] but matches reference including melting point.

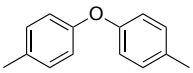
HRMS (ESI): calcd for $C_{14}H_{14}NaO$ $[M+Na]^+$: 221.0937; found: 221.0942 .

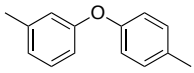
3. Arylation of Hydroxide

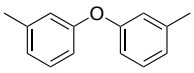
3.1. Synthesis of Reference Diaryl Ethers

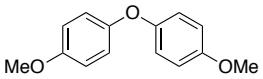
In order to confirm the components in the reaction mixtures during the mechanistic investigations, several diaryl ethers were synthesized. This was done according to a published procedure by the Olofsson group.[18]



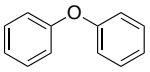

2b[19] 88%

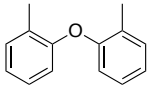

2c[20] 69%

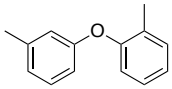

2d[21] 72%

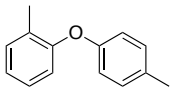


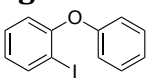
2e[19]

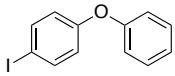

2f[a] 72%


2g[22] 56%

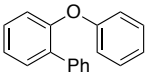

2h[23] 96%


2i[24] 82%


5a[18, 25]86%



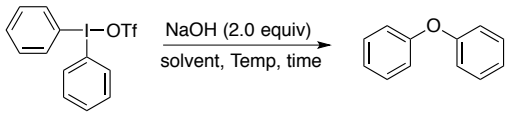
5b[18] 87%



8[26] 65%

[a] Synthesized according to a different procedure.[27]

3.2. Initial Solvent Screening



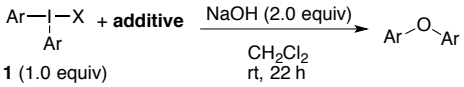
Entry	Time	Temp (°C)	Solvent	Yield (%)[a]	Comment
1	on	60	H_2O	51	
2	on	80	H_2O	66	
3	on	100	H_2O	64	
4	on	40	THF	trace	
5	on	60	THF	21	
6	on	40	1,4-Dioxane	8	
7	on	40	Toluene	26	Impure
8	on	40	CH_2Cl_2	38	Impure
9	4	40	CH_2Cl_2	30	Impure
10	on	rt	CH_2Cl_2	38	Impure

[a] ^1H NMR yield using internal standard.

The reaction was initially performed in water (entries 1-3). When organic solvents were tested, ether solvents such as THF and 1,4-dioxane gave poor results (entries 4-6). When the apolar solvents toluene and CH_2Cl_2 were used the reaction gave conversion into product at lower temperature, which was deemed interesting. Unfortunately efforts to isolate the diphenyl ether were unsuccessful, yielding mixture of ethers as results. This was seen for both the aqueous reaction and in organic solvents.

3.3. General Procedure for the Arylation of Hydroxides

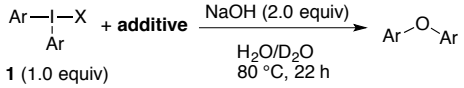
3.3.1. General Procedure A



Sodium hydroxide (1.6 mmol, 2 equiv) was added to a 10-20 mL or 2-5 mL microwave vial and CH_2Cl_2 (3 mL) was added. The indicated additive was added followed by immediate addition of diaryliodonium salt **1** (0.8 mmol, 1 equiv). The reagents were rinsed down from the walls of the vial using CH_2Cl_2 (1 mL). The vial was capped and stirred at rt for 22 h. The reaction mixture was quenched with sat. NH_4Cl and then extracted with CH_2Cl_2 (x3). The combined organic phases were dried over $MgSO_4$, filtrated and the solvent removed *in vacuo*. The crude mixture was then submitted to column chromatography.

Note: The yields of the ethers were calculated based on that 1 equiv Ar_2IX gives maximum 0.5 equiv diaryl ether.

3.3.2. General Procedure B

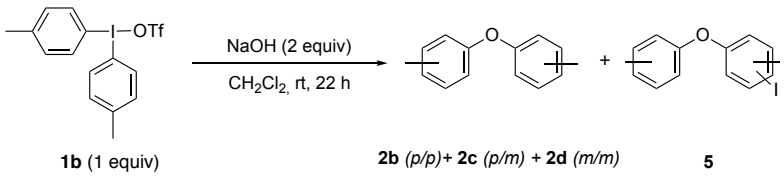


Sodium hydroxide (1.6 mmol, 2 equiv) was added to a 10-20 mL or 2-5 mL microwave vial and deionized H_2O (3 mL) was added. The indicated additive was added followed by immediate addition of diaryliodonium salt **1** (0.8 mmol, 1 equiv). The reagents were rinsed down from the walls of the vial using H_2O (1 mL). The vial was capped and stirred in a pre-heated oil bath at 80 °C for 22 h. The vial was removed from the heat and cooled to rt. It was then extracted with CH_2Cl_2 (x3) and the combined organic phases were dried over $MgSO_4$, filtered and the solvent was removed *in vacuo*. The crude mixture was then submitted to column chromatography or to ^1H NMR yield determination using 1,3,5-trimethoxybenzene (0.4 mmol) as internal standard.

Note: The yields of the ethers were calculated based on that 1 equiv Ar_2IX gives maximum 0.5 equiv diaryl ether.

3.4. Arylations with Salt 1b

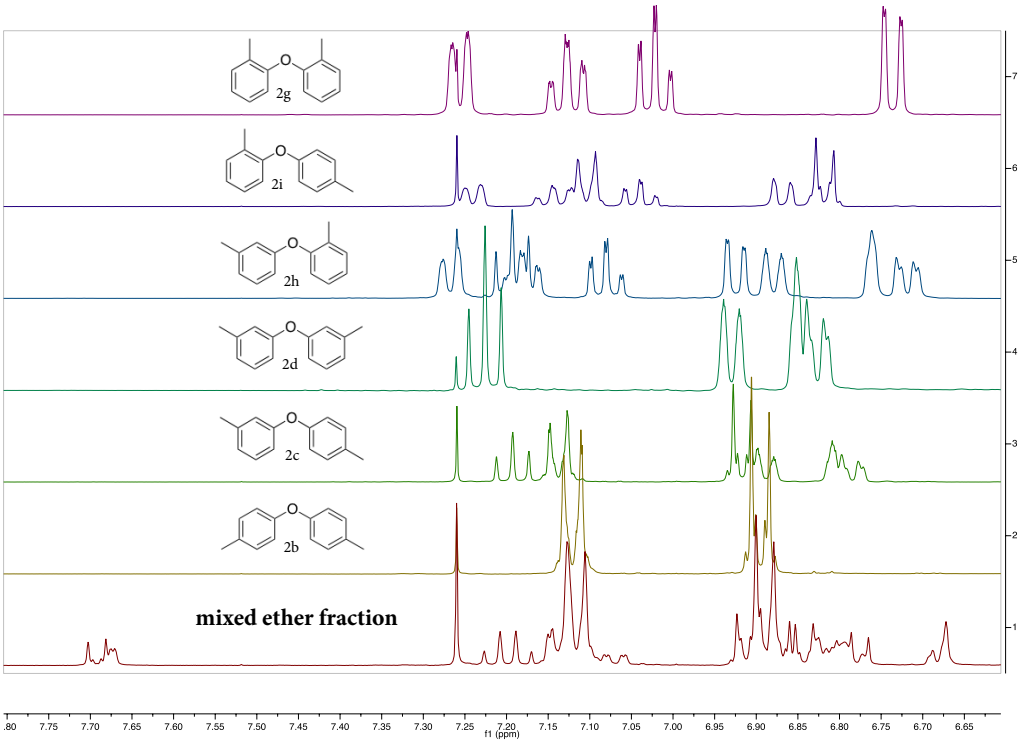
3.4.1. Identification of By-Products



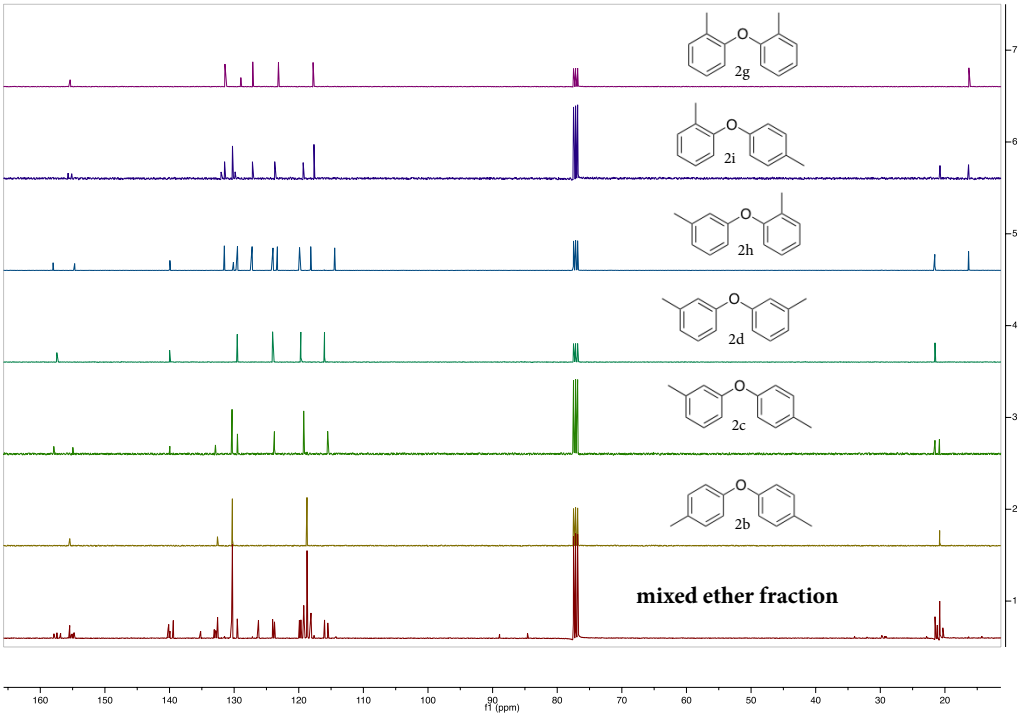
1b (1 equiv) **2b** *(p/p)*+ **2c** *(p/m)* + **2d** *(m/m)* **5**

The reaction was performed according to general procedure A using **1b**. After flash column chromatography (silica gel, pentane → 2% CH_2Cl_2 in pentane) a mixed ether fraction was isolated as a colorless oil (57.1 mg).

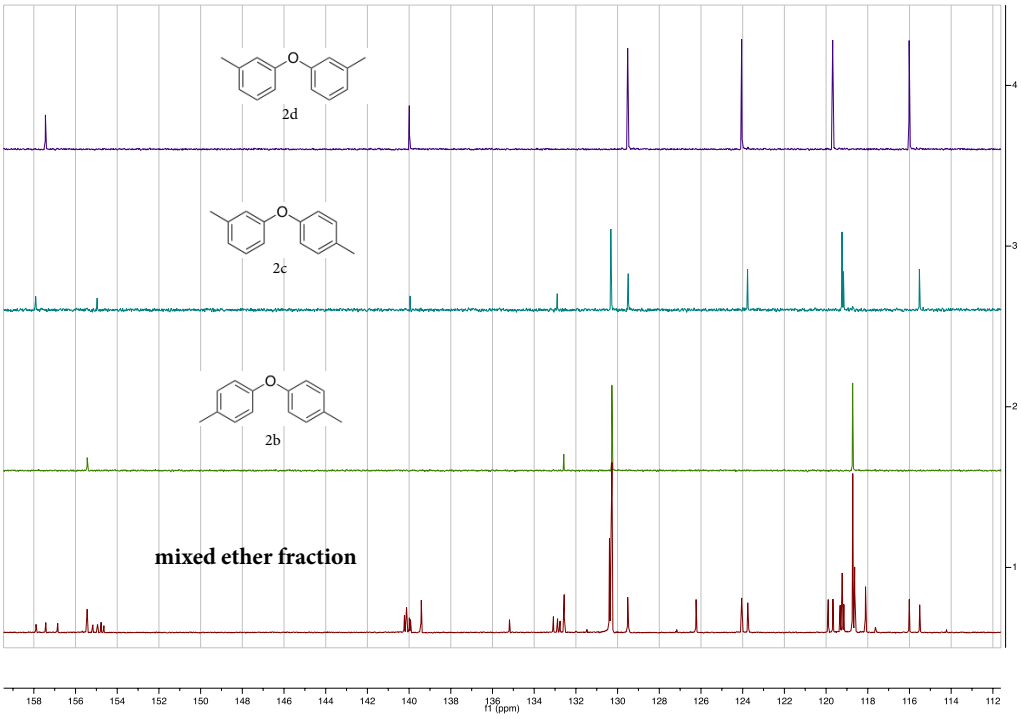
The ^{1}H NMR of the ether fraction was overlapped with the separately synthesized ethers **2b-d** and **2g-i**, which showed that **2b** and **2c** had formed. The formation of **2d** was hard to confirm from ^{1}H NMR. It was difficult to assign the regioisomers with ^{1}H NMR, and the ^{13}C NMR spectrum proved more revealing.



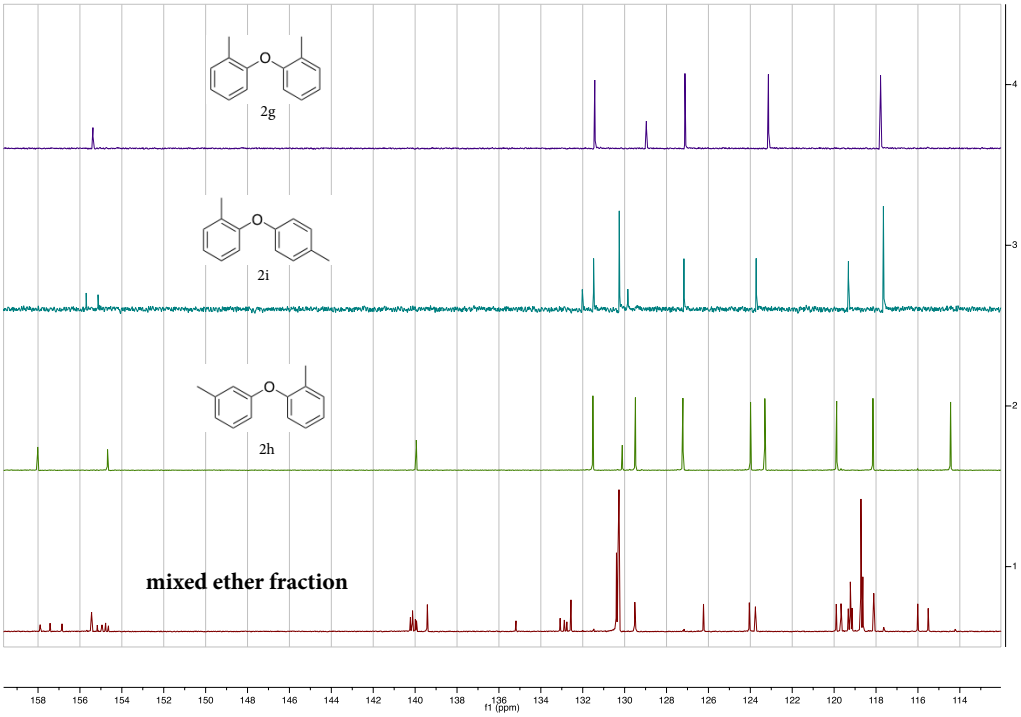
The ^{13}C NMR of the ether fraction was very complex. When the mixed ether fraction was overlapped with the synthesized regioisomers **2b-d** and **2g-i** many of the peaks were matching. It was difficult to assign the peaks to the different regioisomers in the mixture, but the extra peaks at 88.9 and 84.6 ppm support the presence of iodo-substituted products **5**.



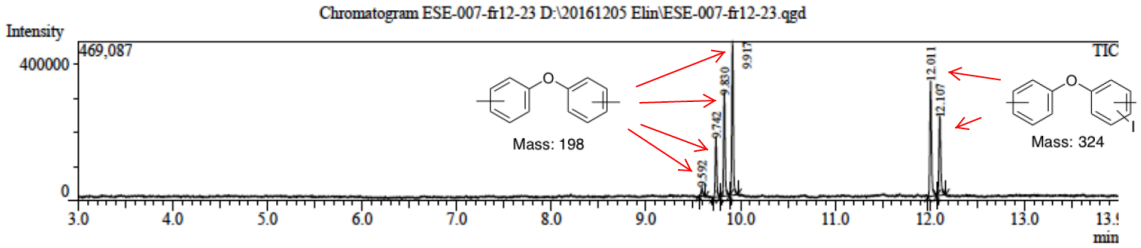
When the ^{13}C NMR spectra of the regioisomers **2b**, **2c** and **2d** were overlapped with the ether fraction the presence of these regioisomers could be confirmed.



When the ^{13}C NMR spectra of the regioisomers **2g**, **2i** and **2h** were overlapped with the ether fraction, only traces of what appears to be **2i** matched. The other regioisomers could not be found in detectable amounts.



When the ether fraction was analyzed using GC-MS, four peaks with the same mass as **2b** and its regioisomers were found. Also, two peaks with the same mass as iodo-substituted products **5** were found.



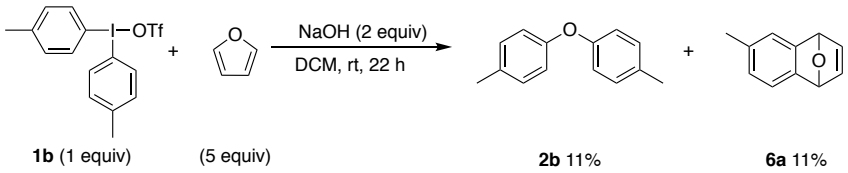
Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	9.592	9.563	9.629	31360	1.78	24665	1.64	1.27		
2	9.742	9.709	9.783	189258	10.74	173460	11.54	1.09		
3	9.830	9.783	9.886	337747	19.17	301920	20.08	1.12	V	
4	9.917	9.886	9.973	492315	27.95	445879	29.65	1.10	V	
5	12.011	11.983	12.076	411184	23.34	331183	22.02	1.24		
6	12.107	12.076	12.169	299810	17.02	226642	15.07	1.32	V	
				1761674	100.00	1503749	100.00			

Conclusion from the experiment:

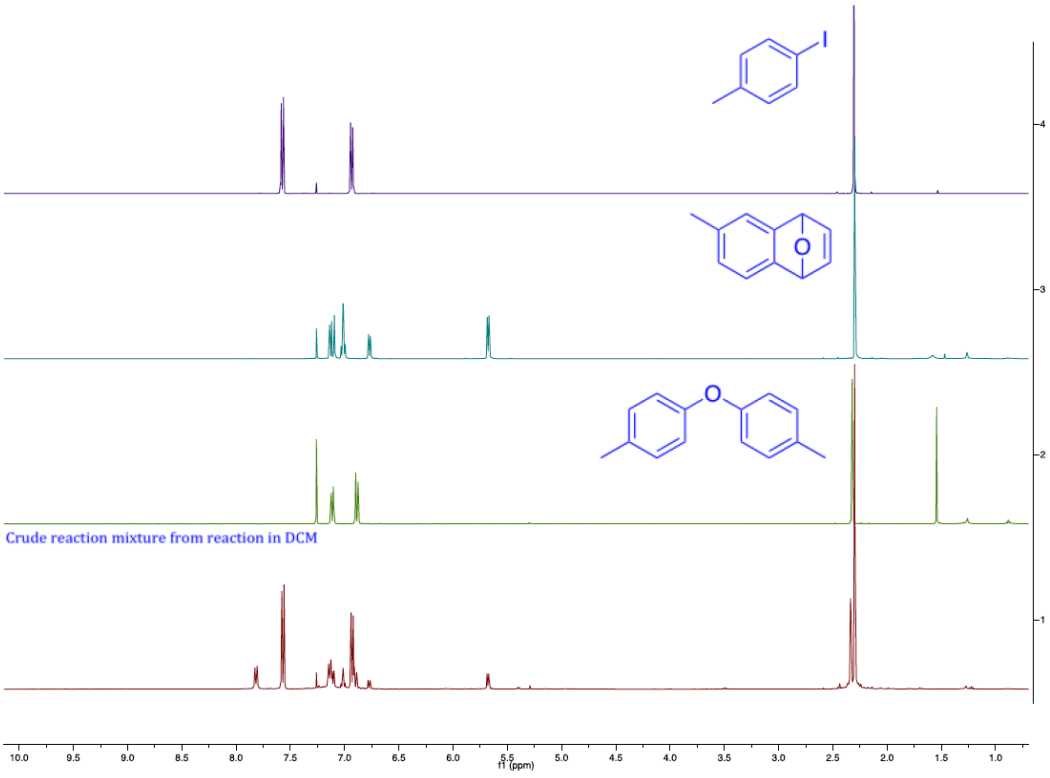
Arylation of hydroxide with **1b** gave a complex mixture of diaryl ethers **2b**, **2c** and **2d**. There probably was a rather large amount of iodo-substituted products **5**.

3.4.2. Trapping of Aryne with Furan

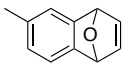


The reaction was performed according to general procedure A using **1b** with furan as additive.

The iodo-arene, the Diels Alder adduct **6a**, and the diaryl ether **2b** were detected in the crude mixture. Only one regioisomer of the diaryl ether was isolated after purification.

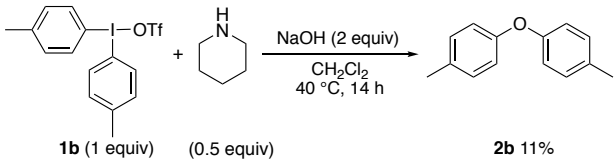


6-Methyl-1,4-epoxy-1,4-dihydronaphthalene (6a)[12, 28]



All spectral data are in agreement with published data.

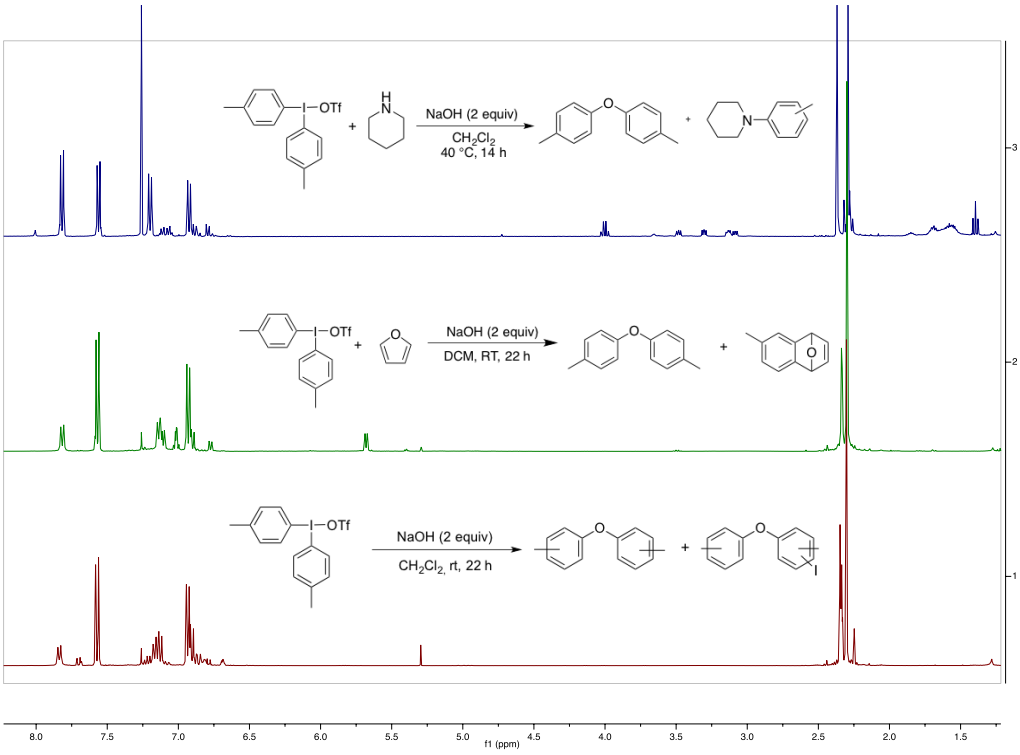
3.4.3. Trapping of Aryne with Piperidine



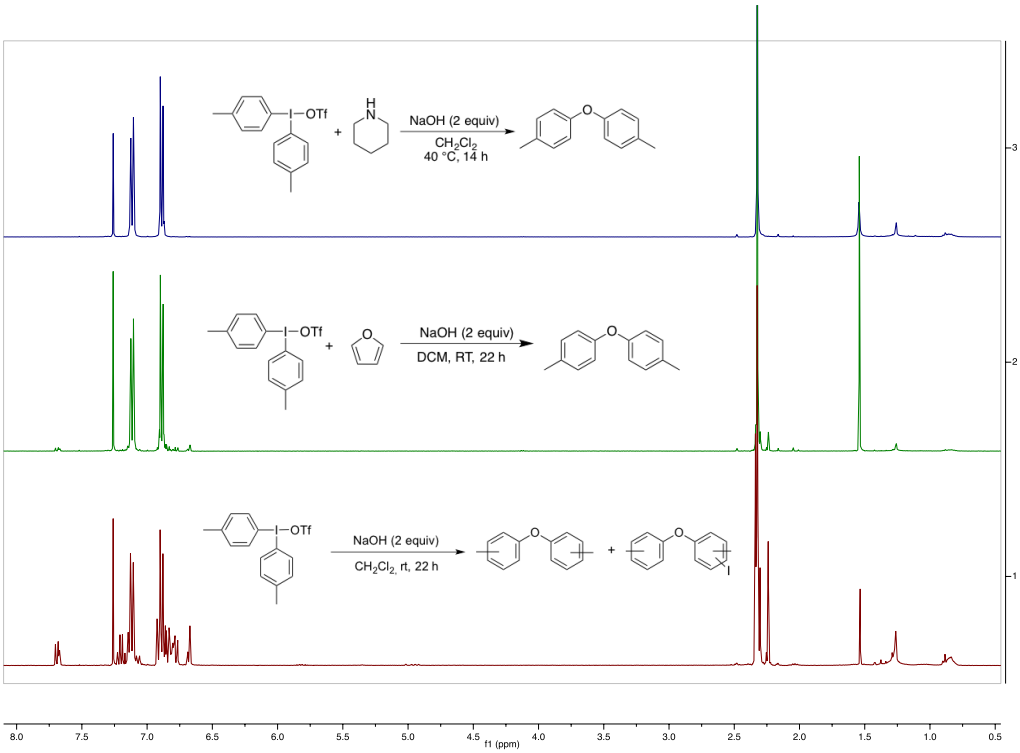
The reaction was performed according to a small modification of general procedure A using **1b** with piperidine as additive, which suppressed the formation of by-products.

3.4.4. Comparison with and without Aryne Traps

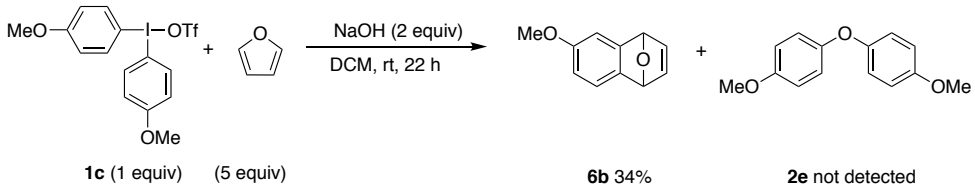
Comparing the crude ^{1}H NMR of the reactions with and without additives showed a cleaner reaction with the additives.



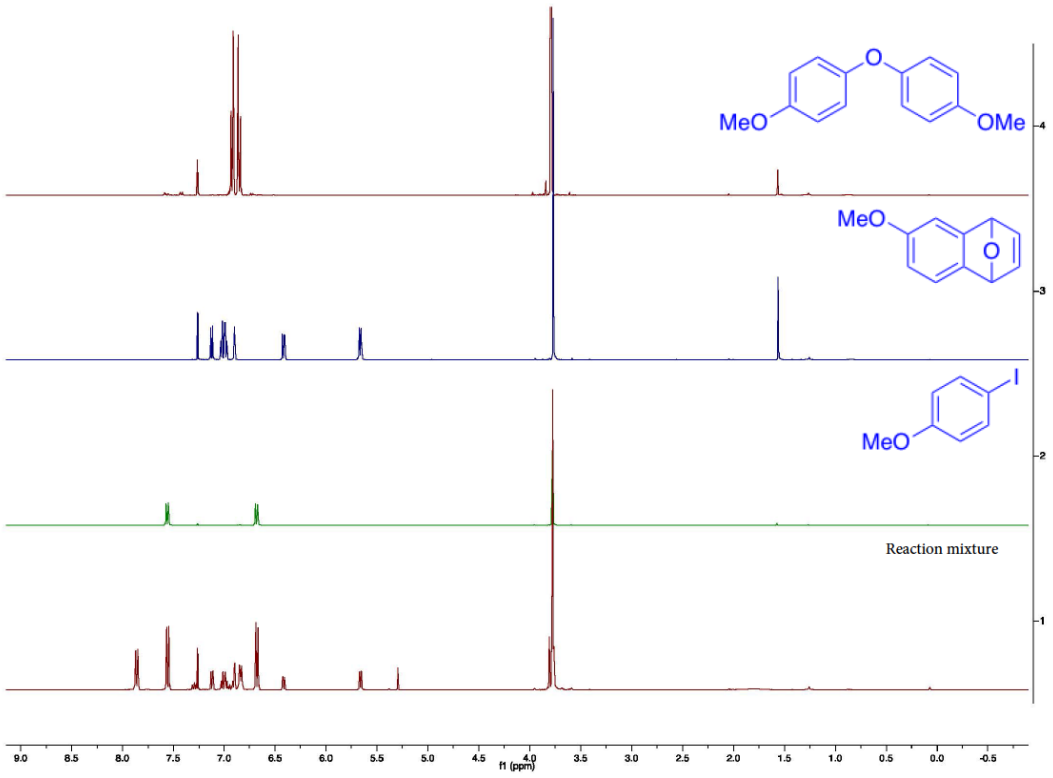
Furthermore, the use of additives allowed for isolation of only the desired diaryl ether **2b**.



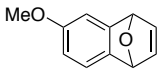
3.5. Arylation with Salt 1c



The reaction was performed according to general procedure A using **1c** with furan as additive. Diaryl ether **2e** could neither be detected nor isolated from the reaction above. The Diels Alder adduct **6b** was isolated in 34% yield and the corresponding aryl iodide was isolated in 59% yield.

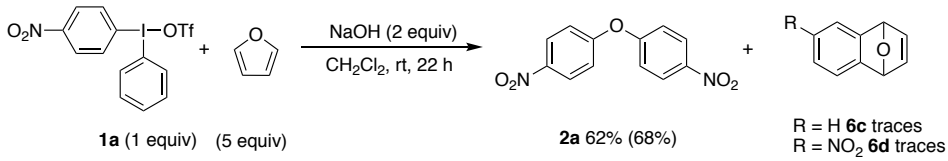


6-Methoxy-1,4-dihydro-1,4-epoxynaphthalene (6b)

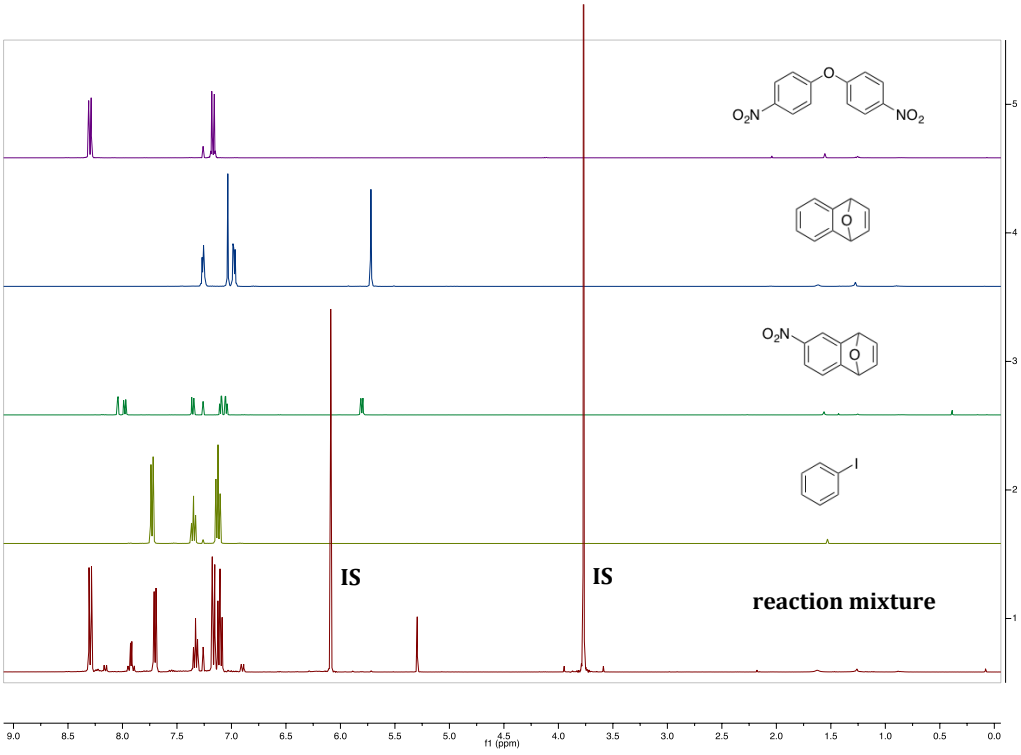


Isolated as a white powder in 34% yield (47 mg). All spectral data are in agreement with published data.[12]

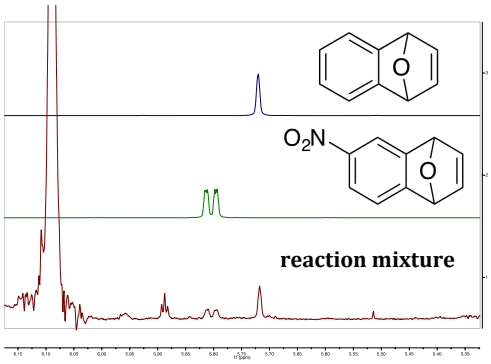
3.6. Arylation with Salt 1a



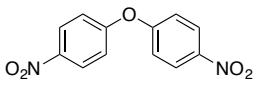
The reaction was performed according to general procedure A using **1a** with furan as additive. After work-up, the NMR-yield was determined to 67% after addition of 1,3,5-trimethoxybenzene as internal standard. Only trace of the Diels-Alder adducts **6c** and **6d** were detected. Then, the crude was purified by flash column chromatography (silica gel, pentane → 15% EtOAc in pentane) to obtain diaryl ether **2a** as a yellow solid in 62%. Some of ether **2a** was obtained in mixed fractions and the total yield was calculated to 68%.
*Note: good stirring was extremely important in this reaction, otherwise the yield of ether **2a** dropped drastically.*



Traces of the Diels-Alder adducts were only seen upon enlargement.

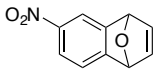


4,4'-Dinitrodiphenyl Ether (2a)



Isolated as yellow solid in 62% (64.3 mg). Spectral data are in agreement with published data.[29]

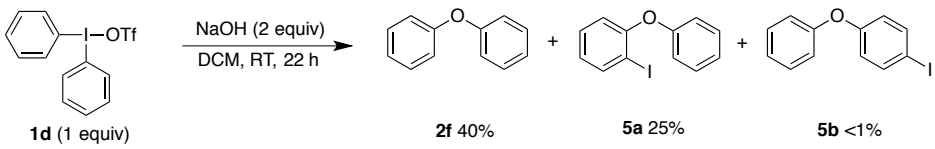
1,4-Dihydro-7-nitro-1,4-epoxynaphthalene (6d)



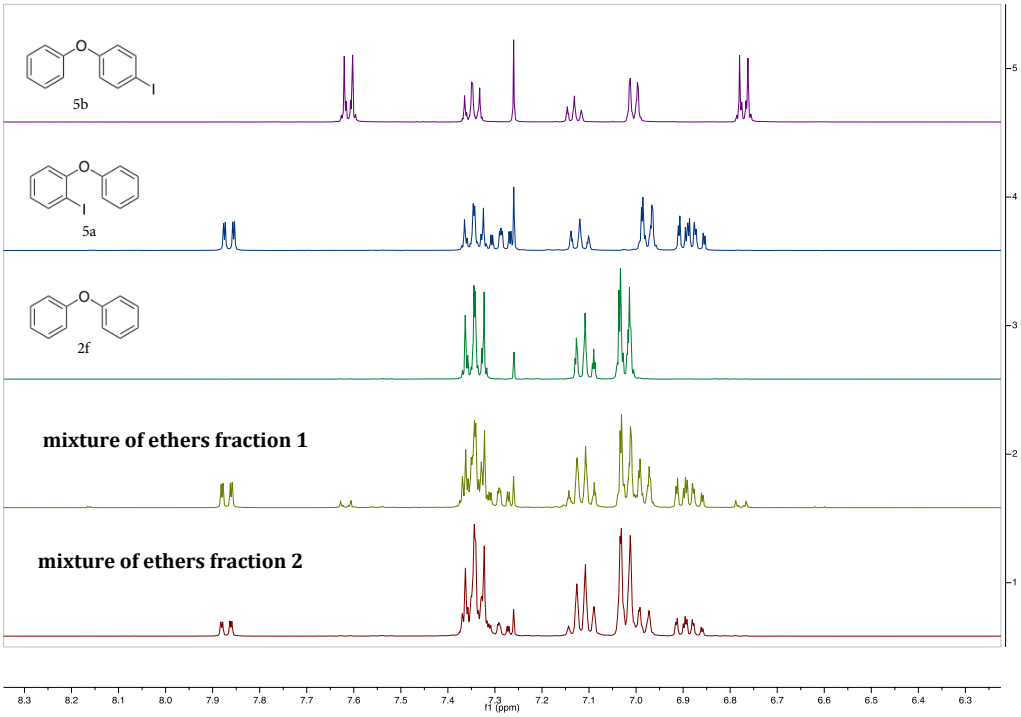
Synthesized according to a modified published procedure to obtain reference material.[12] NaHMDS (0.6 M in toluene) was used as a base instead of LiHMDS (1 M in toluene). The product was obtained as a yellow oil that solidified to an orange solid in 56% yield. The ^{1}H NMR is in full agreement to published data.[30] In ^{13}C NMR one of the two peaks at 143 ppm was not found, but a peak at 82.2 ppm was found instead.

3.7. Arylation with Salt 1d

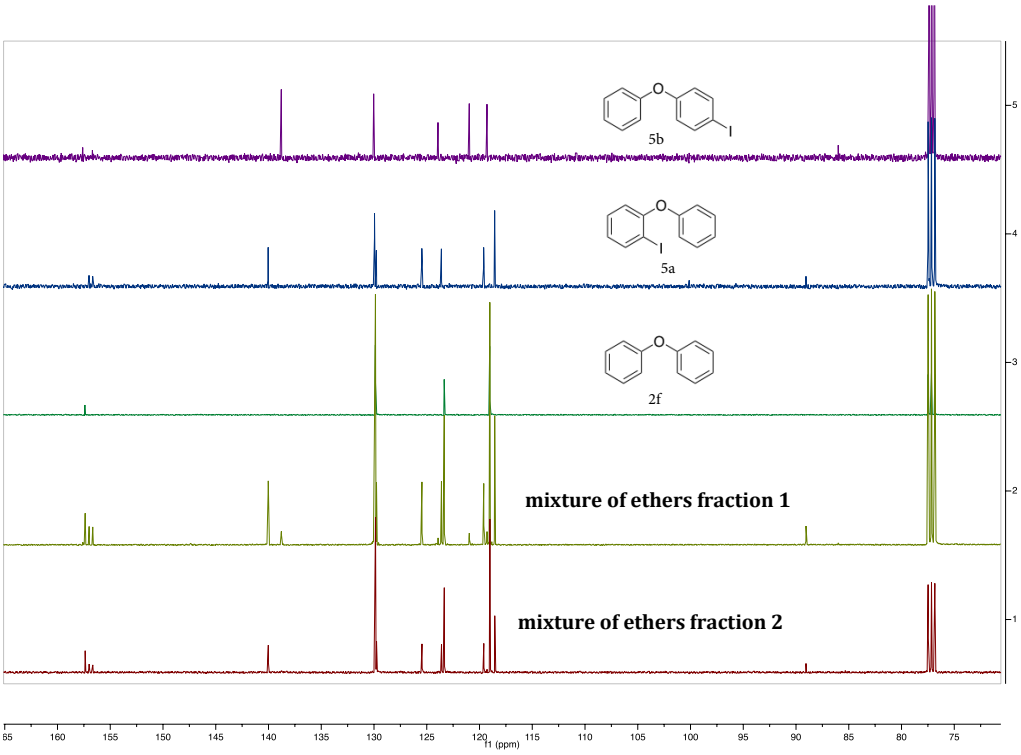
3.7.1. Identification of By-Products



Synthesized according to the general procedure A using **1d**. After purification by flash column chromatography (silica gel, pentane → 2% CH_2Cl_2 in pentane) two mixed fractions of ethers were obtained. The first fraction contained **2f** and **5a** together with traces of **5b**. The second fraction was a mixture of only **2f** and **5a**. From these mixtures, the yields were calculated to 40% of **2f**, 25% of **5a** and approximate 1% of **5b**.

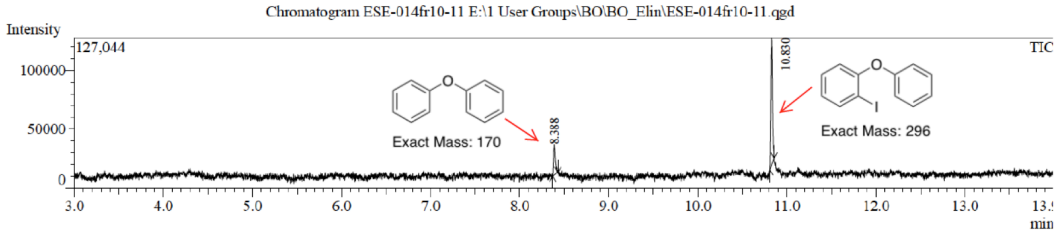


In the ^{13}C NMR the same ethers were seen. **5b** was in such small amounts it was barely detected.



When the two ether fractions were submitted to GC-MS, peaks with the corresponding masses for **2f** and **5a** were found. The amount of **5b** in fraction 1 was below the detection limit.

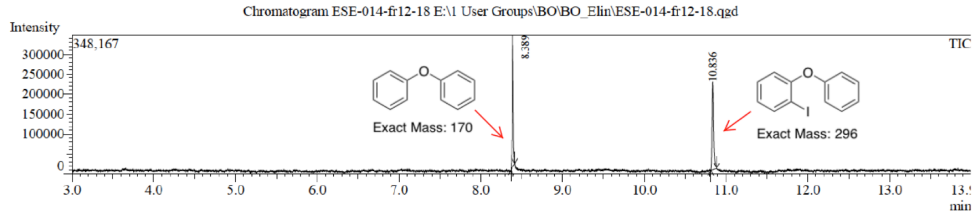
GC-MS Ether fraction 1



Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	8.388	8.372	8.428	34211	21.48	25650	19.30	1.33	MI	
2	10.830	10.812	10.856	125056	78.52	107273	80.70	1.17	MI	
				159267	100.00	132923	100.00			

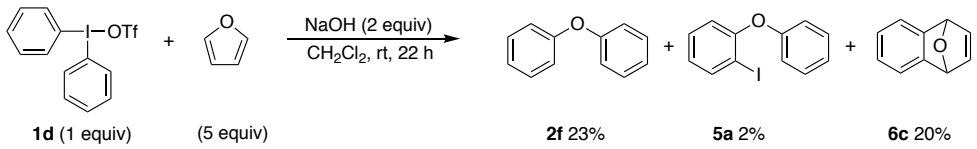
GC-MS Ether fraction 2



Peak Report TIC

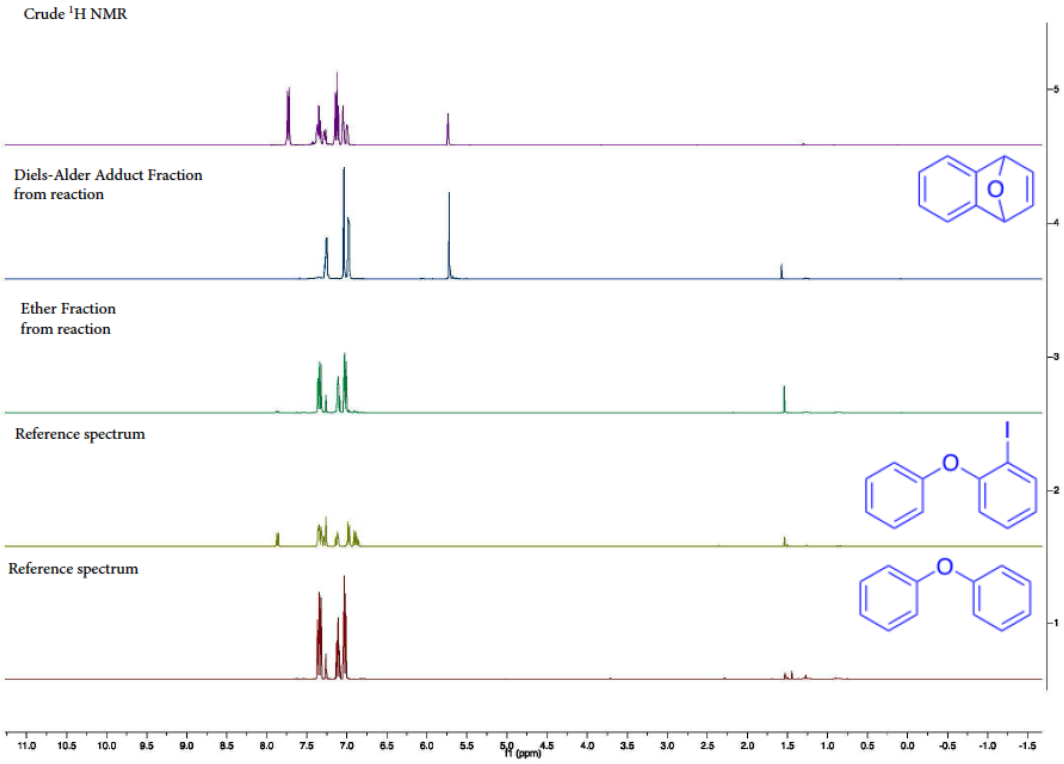
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	8.389	8.369	8.416	338585	55.11	331837	60.09	1.02	MI	
2	10.836	10.814	10.885	275742	44.89	220382	39.91	1.25	MI	
				614327	100.00	552219	100.00			

3.7.2. Trapping of Benzyne with Furan

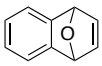


1d (1 equiv) (5 equiv) **2f** 23% **5a** 2% **6c** 20%

The reaction was performed according to general procedure A using **1d** with furan as additive. The desired **2f** was formed in 23%, together with iodo-substituted product **5a** in 2% (calculated yields from ether fraction after flash chromatography). The Diels-Alder adduct **6c** was isolated in 20%. **5a** was detectable in the crude ^{1}H NMR spectrum, but was easier to confirm after purification.

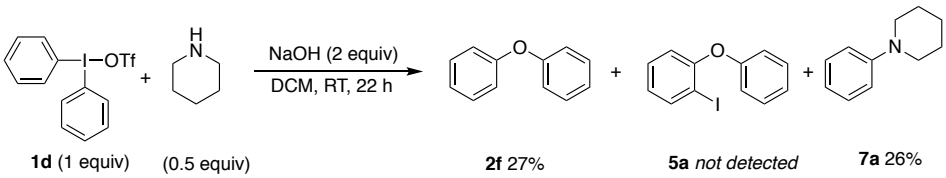


1,4-Dihydro-1,4-epoxynaphthalene (6c)



All spectral data are in agreement with the commercial compound, CAS: [573-57-9].

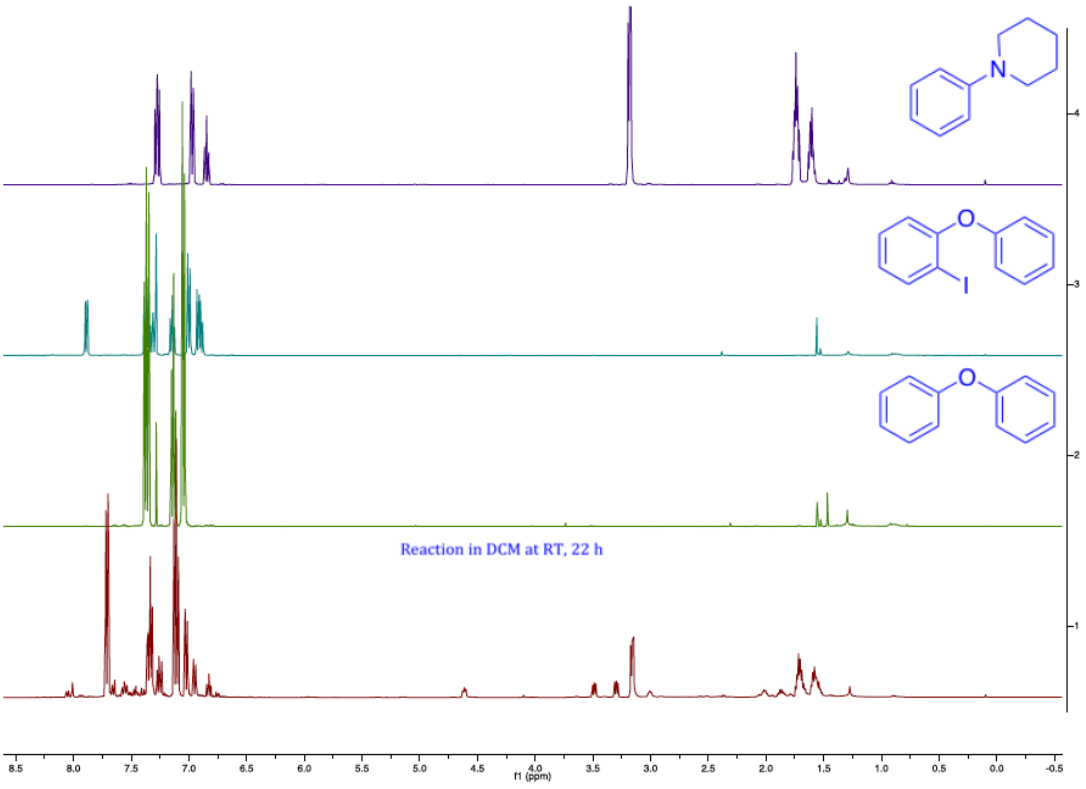
3.7.4. Trapping of Benzyne with Piperidine



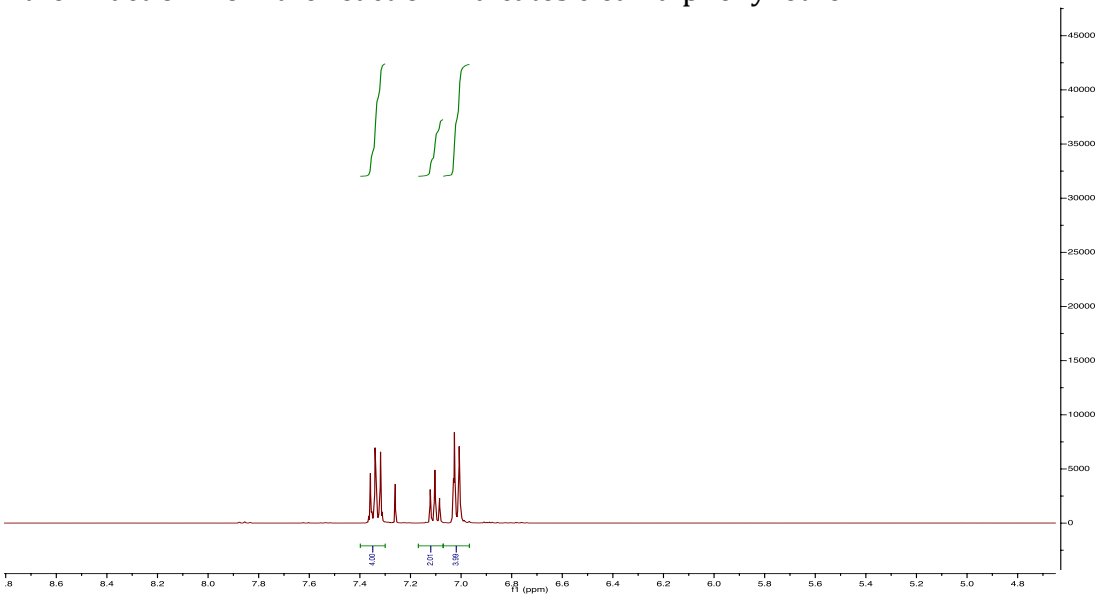
1d (1 equiv) (0.5 equiv) **2f** 27% **5a** *not detected* **7a** 26%

The reaction was performed according to general procedure A using **1d** with piperidine as additive. Piperidine proved to be a more efficient trap than furan as iodo-substituted **5a** was not detected in the mixture. **2f** was isolated as a pure compound.

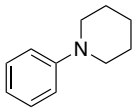
In the crude spectrum **7a** was detected and could be isolated. The iodo-substituted product **5a** was neither detected in the crude ^{1}H NMR nor in the isolated ether fraction, as shown below.



Ether fraction from the reaction indicates clean diphenyl ether **2f**.



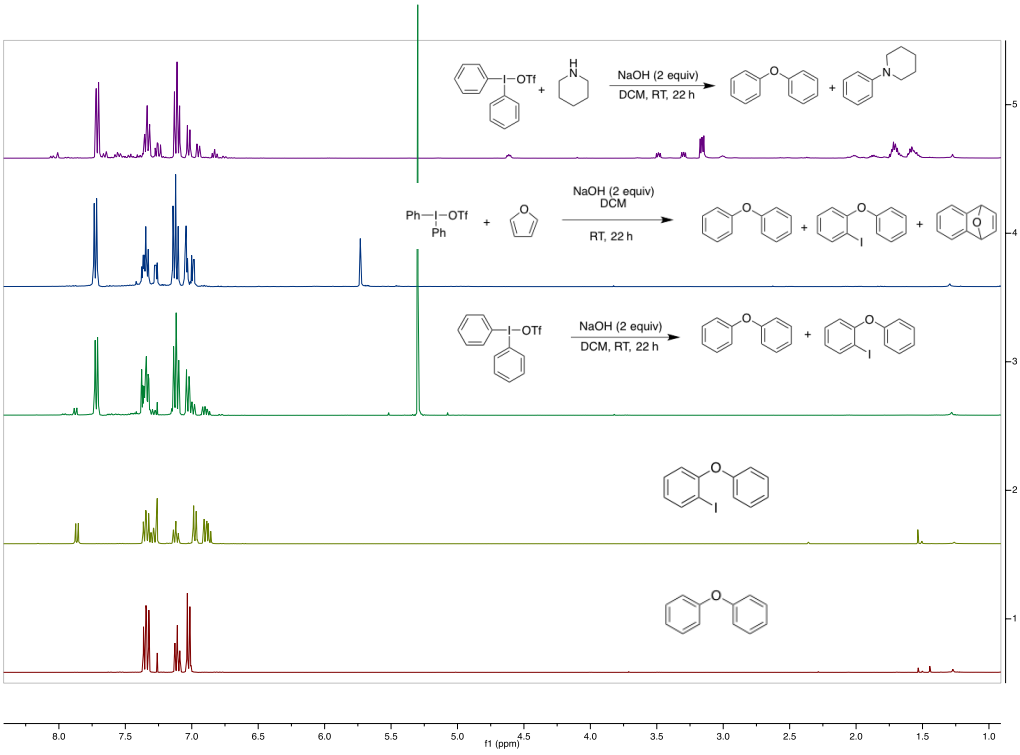
1-Phenylpiperidine (7a)



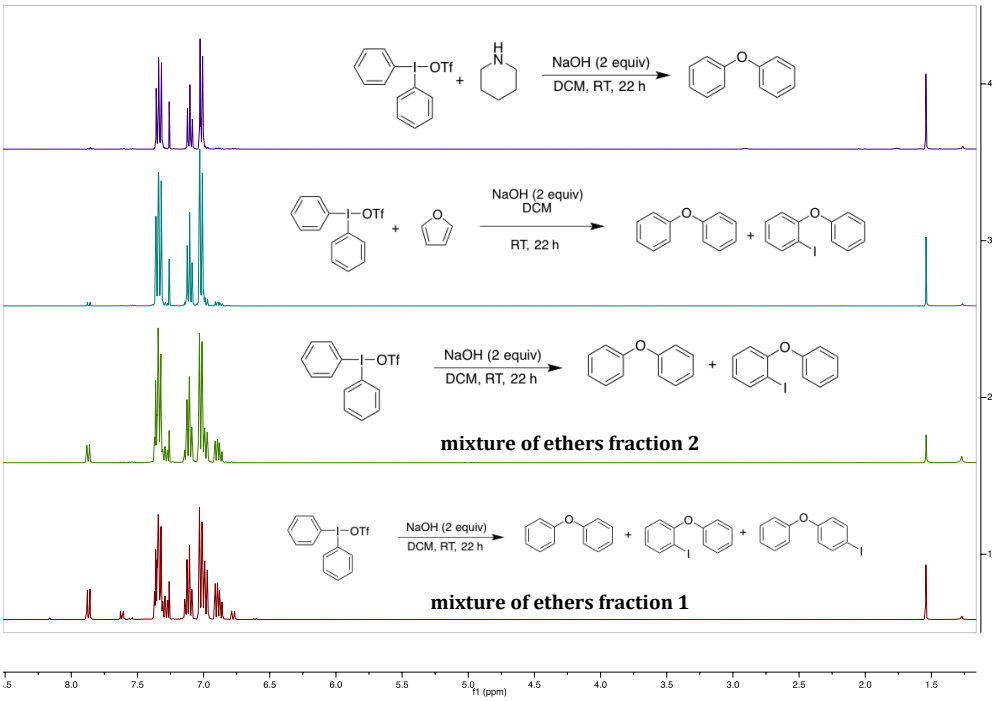
All spectral data are in agreement with published data.[31]

3.7.5. Comparison with and without Aryne Traps

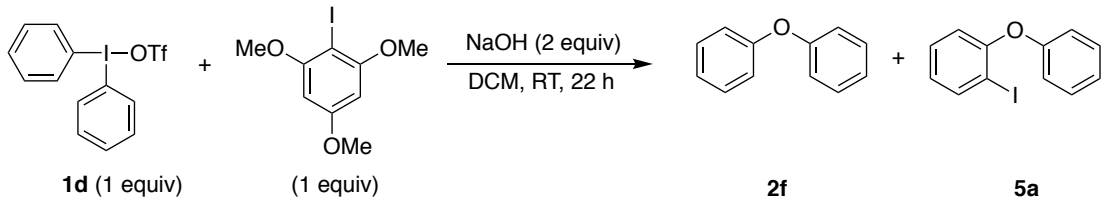
When the crude spectra of reactions with and without additives were compared, it was concluded that iodo-substituted **5a** was not formed with piperidine and in low amounts with furan. Reaction without any additives showed a messier spectrum.



The same trend was more easily seen in the isolated ether fractions from reactions with and without traps. Two ether fractions were isolated in the reaction without traps.



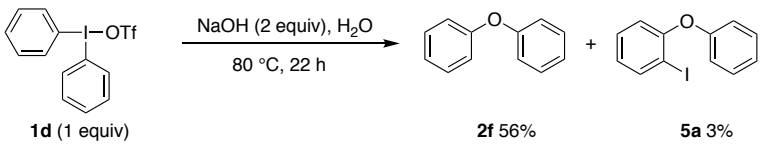
3.7.6. Addition of Another Aryl Iodide



1d (1 equiv) (1 equiv) **2f** **5a**

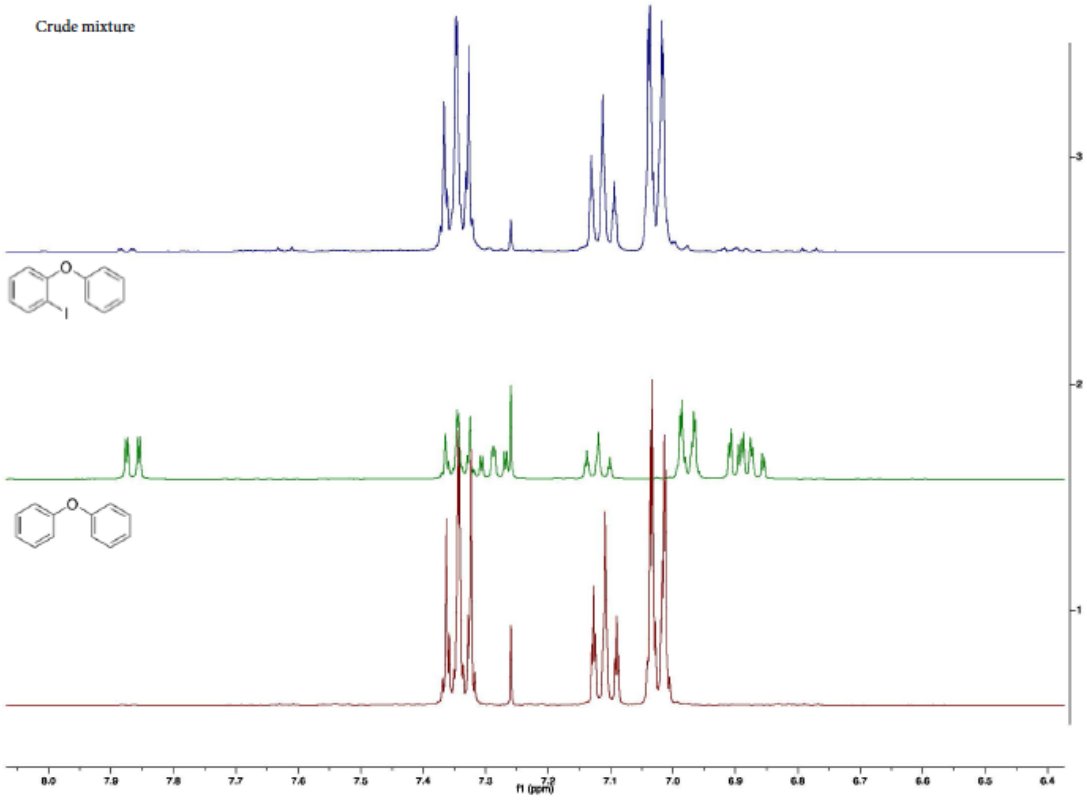
The reaction was performed according to general procedure A using **1d** with 2,4,6-trimethoxyiodobenzene as additive. The ratio between products **2f** and **5a** were determined from the crude ^{1}H NMR and compared to the ratio obtained in the reaction without any additives. It was concluded that the additive did not alter the ratio between these two products.

3.7.7. Salt 1d in H_2O

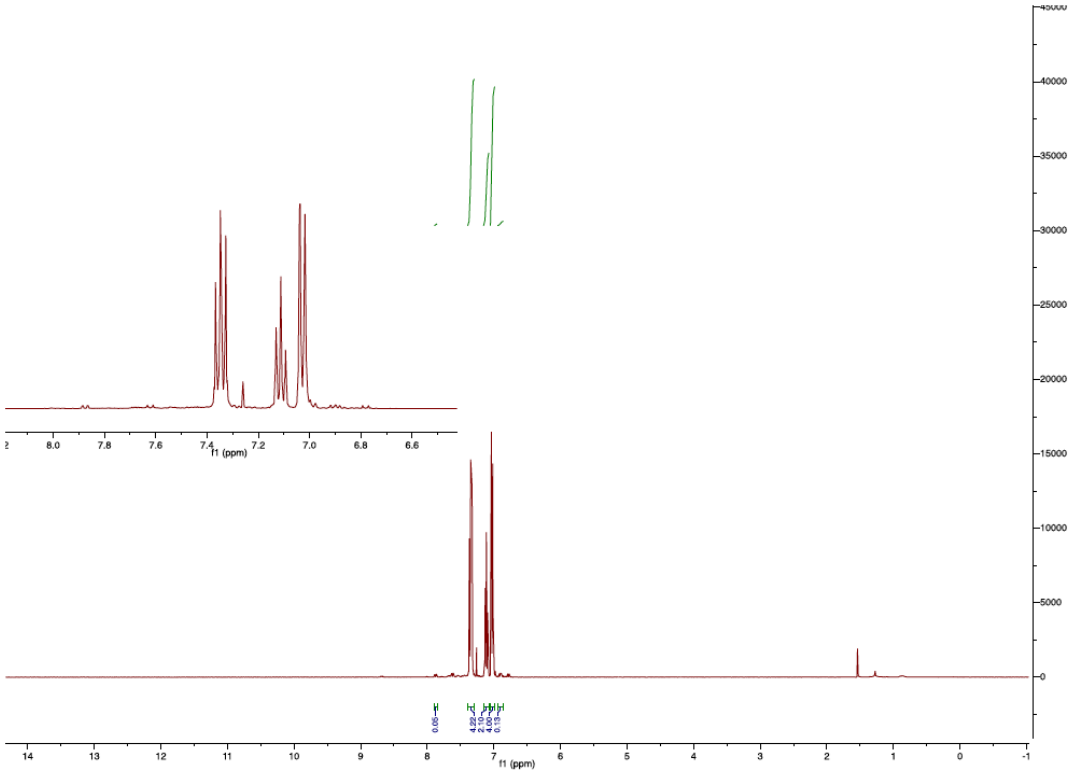


1d (1 equiv) **2f** 56% **5a** 3%

The reaction was performed according to general procedure B using **1d**. The yields were calculated from the ratio obtained in the ^{1}H NMR of the ether fraction. As depicted below, the iodo-substituted product **5a** was formed in minor amounts.

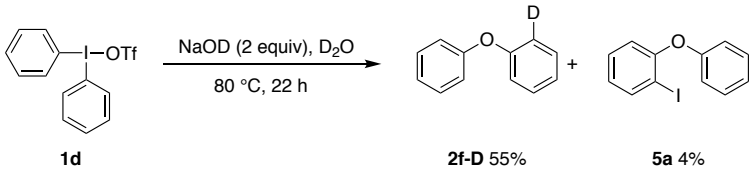


Isolated ether fraction of **2f**, the iodo-substituted product **5a** was barely detected.



3.9. Deuterium-Labeling Experiments

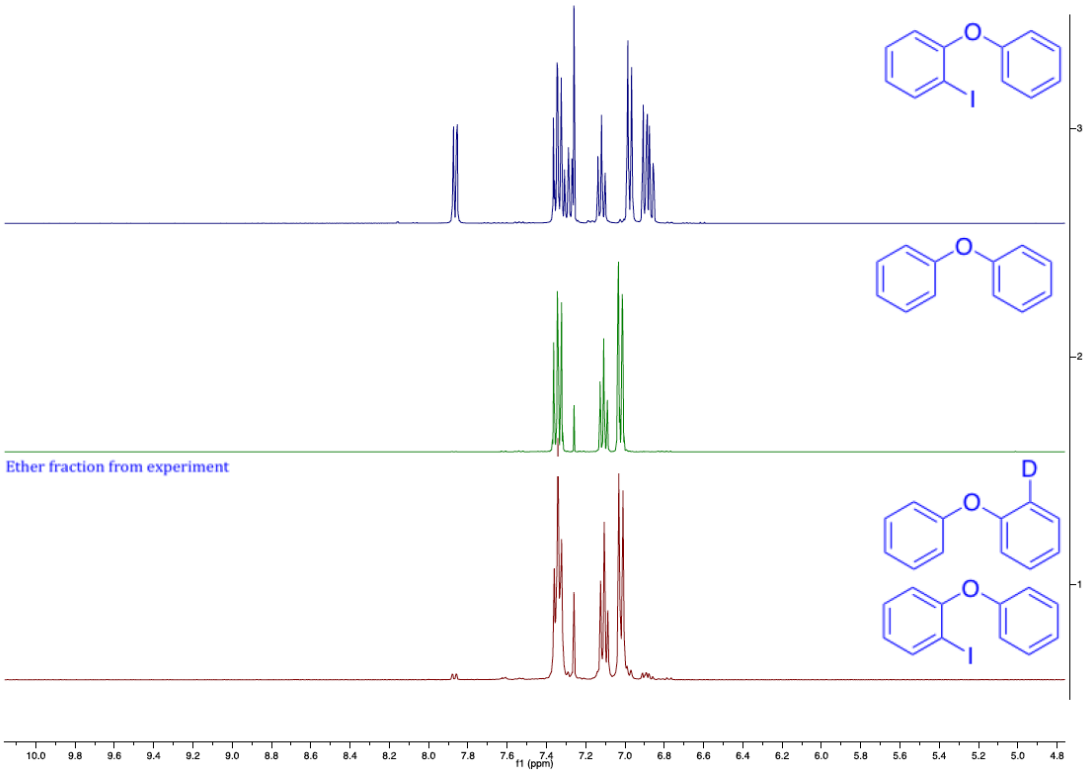
3.9.1. Salt 1d in D_2O without Trap



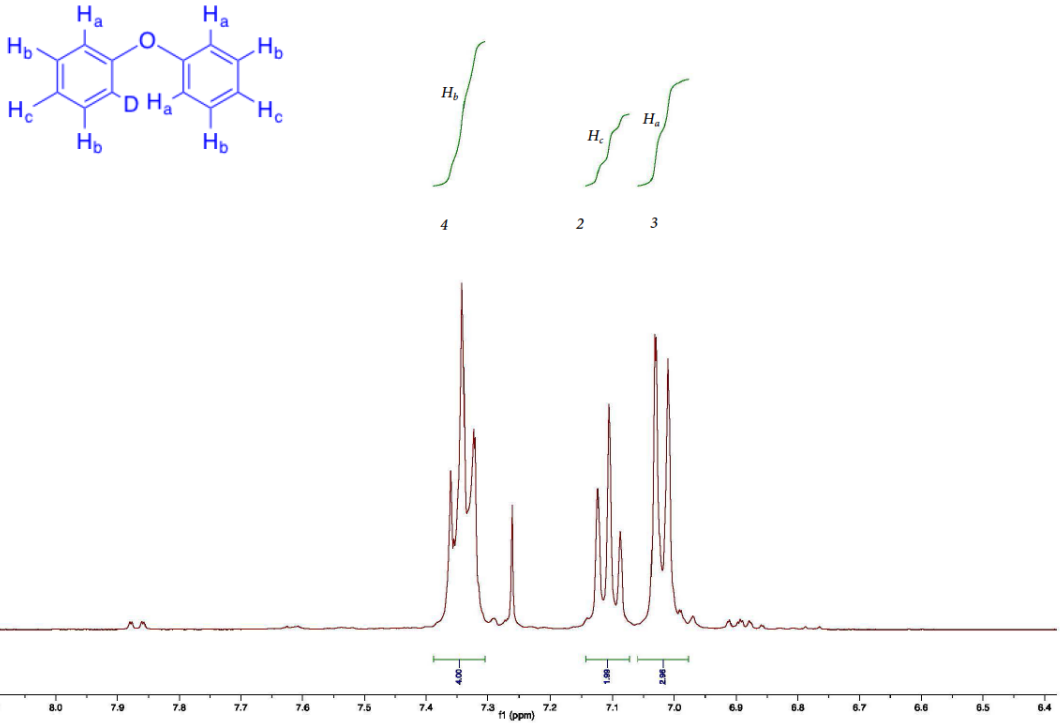
1d **2f-D** 55% **5a** 4%

The reaction was performed according to general procedure B using **1d**. The crude was purified using flash chromatography and the ether fraction was analyzed to investigate how much deuterium that was incorporated into the product. The yields were calculated from the ratio obtained in the ^{1}H NMR of the ether fraction.

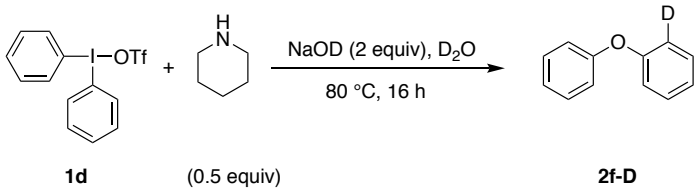
The presence of the product **5a** and the diphenyl ether **2f-D** is shown below.



The incorporation of deuterium was clearly seen when the peaks of the product were integrated. The expected ratio 4:2:4 of **2f** was instead 4:2:3, indicating that a deuterium was incorporated in the *ortho*-position. This correlates well to spectral data for **2f-D** in the literature.[7]



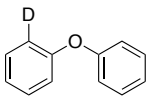
3.9.2. Salt 1d-D D_2O with Trap



1d (0.5 equiv) **2f-D**

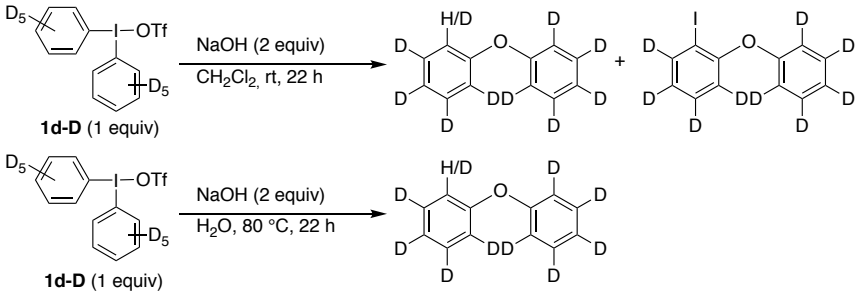
The reaction was performed according to general procedure B using **1d**. The crude was analyzed by GC-MS and a peak corresponding to product **2f-D** was detected. This means that piperidine did not fully suppress the aryne pathway in water.

Diphenyl ether*o-d1* (2f-D)

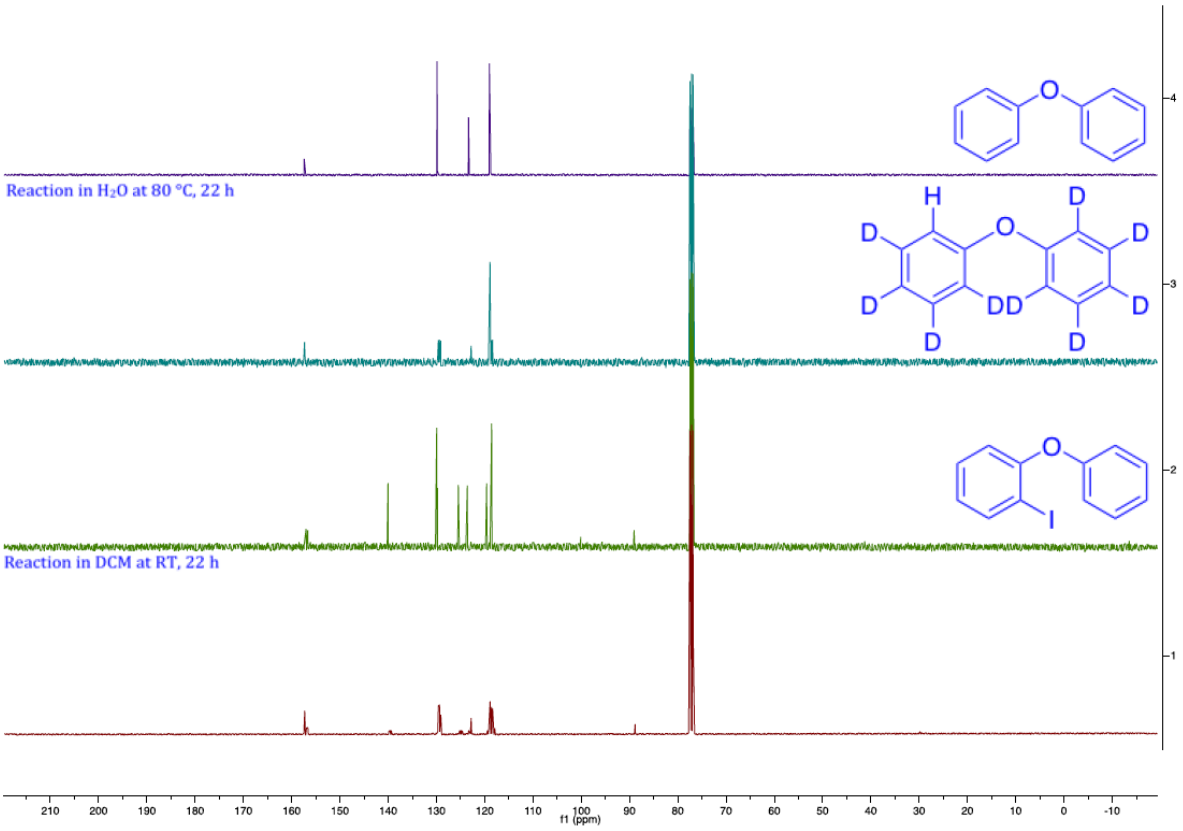


Spectral data corresponds to literature.[32]

3.9.3. Salt 1d-D in CH_2Cl_2 and H_2O

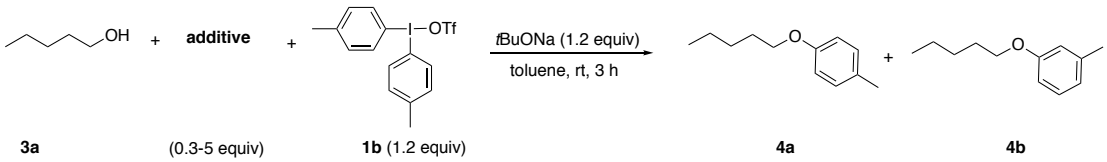


For comparison, the fully labeled salt **1d-D** was submitted to the general procedures A and B. After work-up and purification the ether fractions were compared. As can be seen in the ^{13}C NMR:s below there is more than one compound in the spectrum for the CH_2Cl_2 reaction, and one compound is probably when iodine is incorporated into the *ortho*-position.



4. Arylation of Primary Alcohol 3a

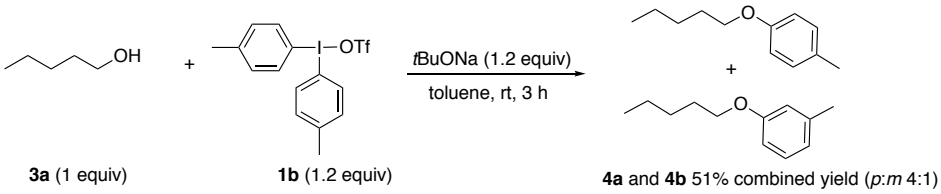
4.1. General Procedure C



A dry 10 mL Schlenk tube was evacuated and backfilled with argon three times. *t*BuONa (58 mg, 0.6 mmol, 1.2 equiv) was added, followed by anhydrous toluene (1.5 mL). The mixture was cooled to 0 °C and 1-pentanol (54 μL, 0.5 mmol, 1 equiv) was added and rinsed down using toluene (0.5 mL). After stirring at rt for 15 min the mixture was cooled to 0 °C and additive (0.3-5.0 equiv) was added followed by **1b** (275 mg, 0.6 mmol, 1.2 equiv). After rinsing down using toluene (0.5 mL) the mixture was left to stir at rt for 3 hours. The reaction was quenched using sat. NH_4Cl, extracted with CH_2Cl_2 (3x10 mL), dried over $MgSO_4$, filtered and concentrated *in vacuo*. The crude was then submitted to flash column chromatography to obtain the product.

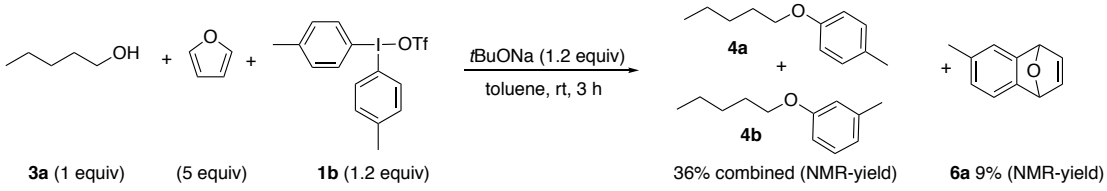
NB! The oxidized product (1-pentanal) has a boiling point of 102-103 °C, and is therefore difficult to study.

4.2. Identification of By-Products



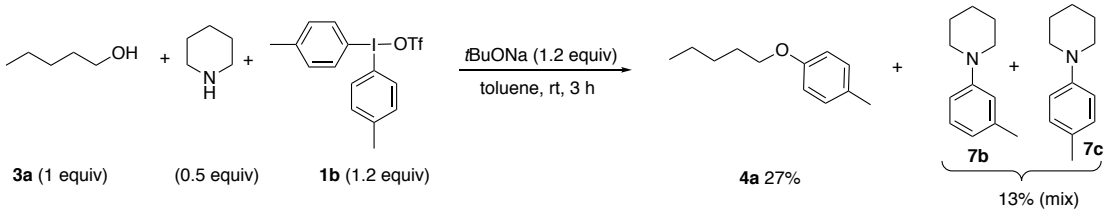
The reaction was performed according to the general procedure C. The ethers were isolated as a mixture, and the ratio was determined via ^{1}H NMR.

4.3. Trapping of Aryne with Furan



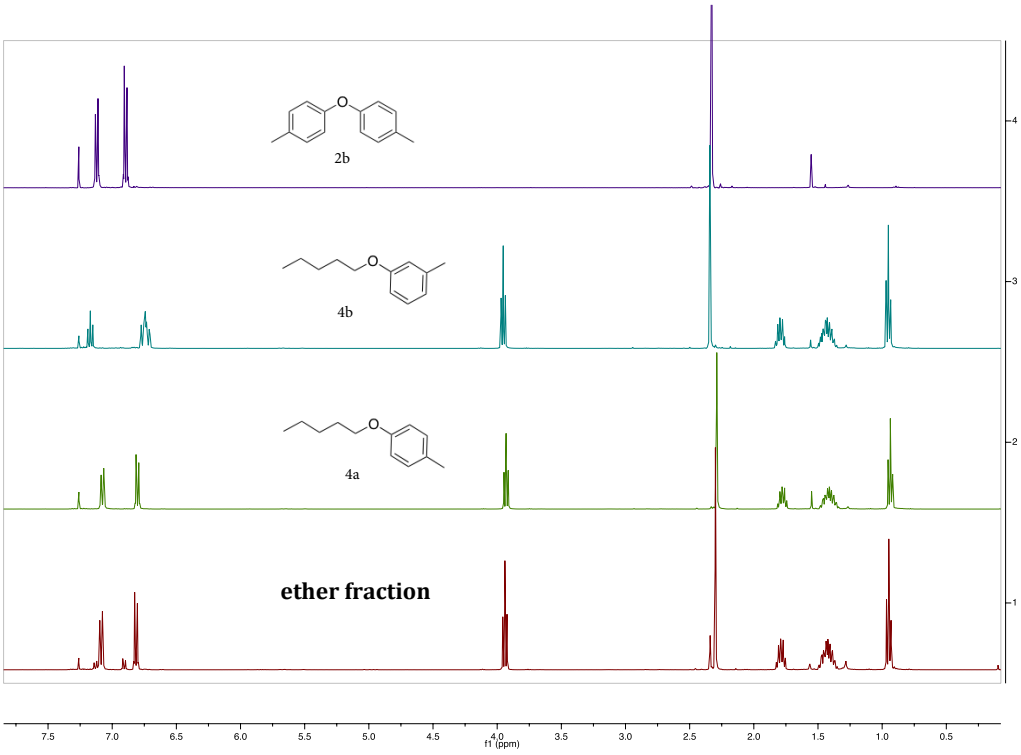
The reaction was performed according to the general procedure C using furan as additive. *Modified work-up for ^{1}H NMR yield determination:* To the reaction mixture D_2O (0.1 mL) was added and the mixture was then diluted with EtOAc. 1,3,5-trimethoxybenzene (0.5 mmol) was added as internal standard. A sample was taken, concentrated and then evaluated by ^{1}H NMR ($CDCl_3$) to determine the yield and products that were formed. *Note: due to overlapping peaks in the crude, the ratio between **4a** and **4b** could not be determined.*

4.4. Trapping of Aryne with Piperidine

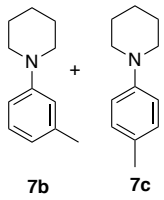


The reaction was performed according to the general procedure C using piperidine as additive. The crude product was purified using flash column chromatography (SiO_2, pentane -> 2% CH_2Cl_2 in pentane) to elute ether **4a** (25.8 mg, 0.14 mmol) in 27% yield. Then the eluent was changed (5% EtOAc in pentane -> 10% EtOAc in pentane) to elute coupling products **7b** and **7c** (13.6 mg, 0.08 mmol, 1.3:1 *m*:*p*) in 13% yield.

The ether product **4a** was isolated as one regioisomer, but contained inseparable diaryl ether **2b** in a ratio of 1:0.08 (**4a**:**2b**).



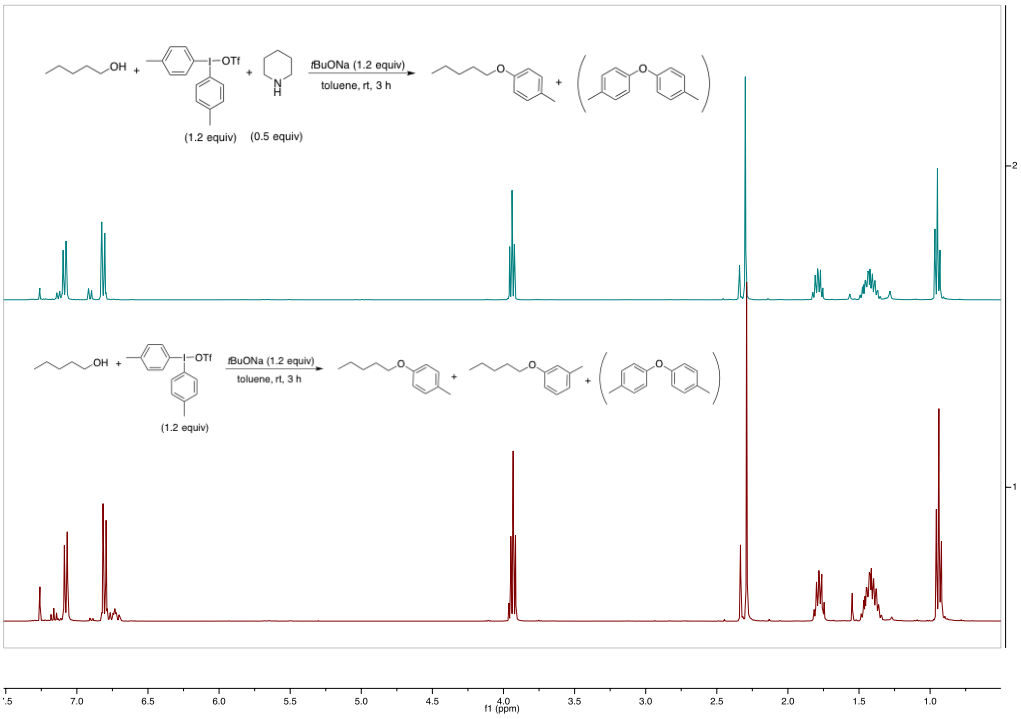
1-Tolylpiperidine (7b and 7c)



Isolated as a mixture (1.3:1 *m*:*p*). Spectral data are in agreement with published data,[33] except that one carbon peak in the *para*-regioisomer **7c** at 129 ppm was difficult to assign due to overlapping and minor impurities.

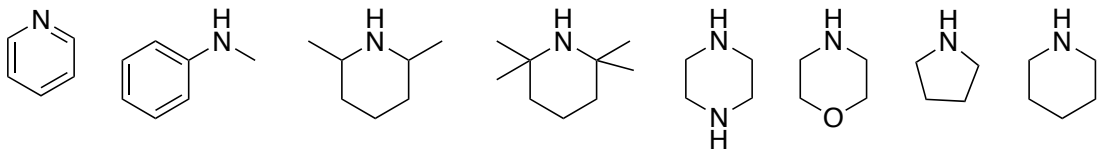
4.5. Comparison with and without Aryne Trap

Comparing the ether fractions spectra with and without traps showed that the *meta*-isomer could not be seen when piperidine was added.

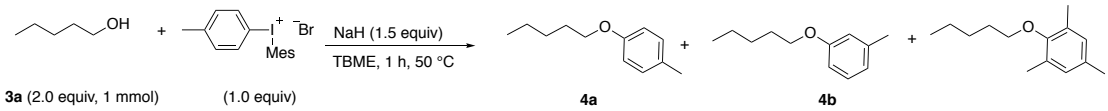


4.6. Screening of Amines as Aryne Trap

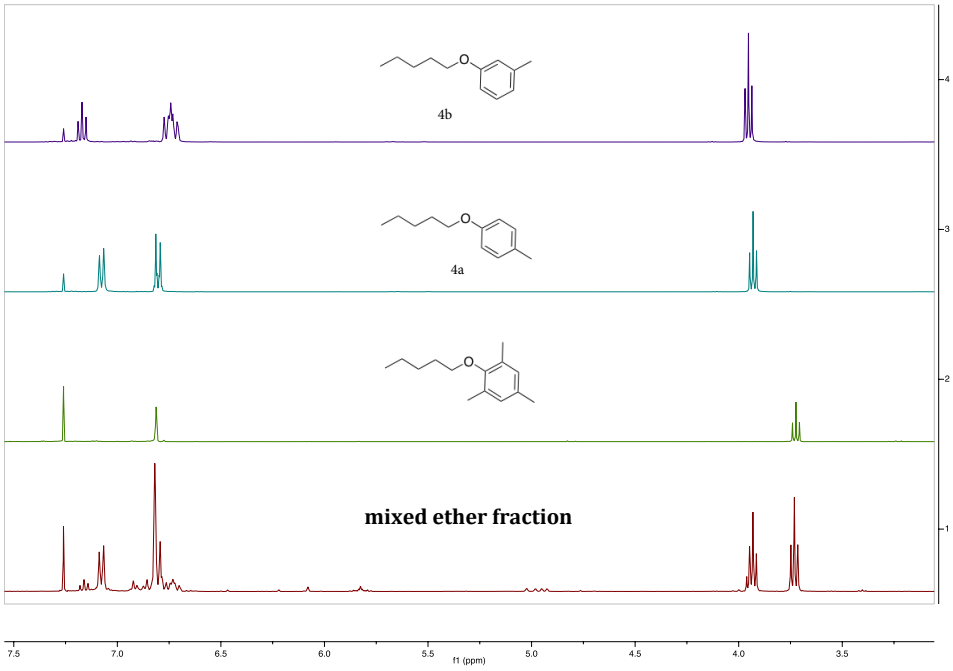
Different amines were screened as aryne trap, and piperidine was found to be superior. Morpholine was second best. *N*-Methylaniline was only tested in phenylation of hydroxides.



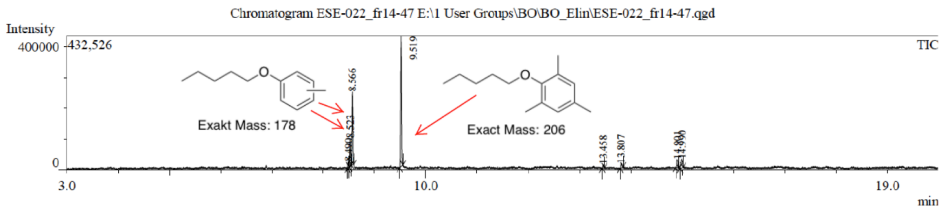
4.7. Comparing with Published Protocol



The reaction was performed according to a published procedure.[12] The crude residue was purified using flash chromatography (SiO_2, using a gradient: pentane (100%) -> DCM (100%) -> pentane:EtOAc, 9:1) to yield an ether fraction containing several products. When overlapping with reference compounds it was seen that regioisomers **4a** and **4b** were present. It also seemed like the ether resulting from transfer of the mesityl was formed. This was further supported by GC-MS analysis.



GC-MS

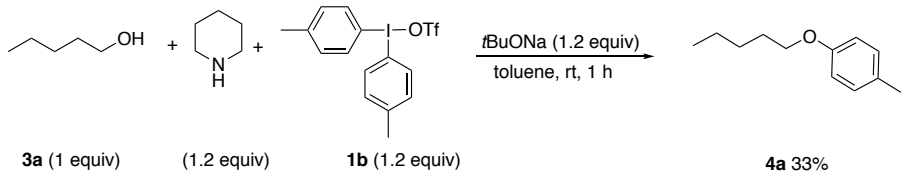


Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	8.490	8.472	8.506	17122	1.85	17775	2.11	0.96	MI	
2	8.523	8.506	8.546	84591	9.13	89375	10.59	0.95	MI	
3	8.566	8.545	8.598	244786	26.41	235411	27.90	1.04	MI	
4	9.519	9.492	9.554	450543	48.62	419954	49.78	1.07	MI	
5	13.458	13.441	13.484	12254	1.32	11416	1.35	1.07	MI	
6	13.807	13.790	13.848	18929	2.04	14464	1.71	1.31	MI	
7	14.901	14.876	14.931	44259	4.78	26841	3.18	1.65	MI	
8	14.990	14.957	15.017	54224	5.85	28401	3.37	1.91	MI	
				926708	100.00	843637	100.00			

4.8. Analytical Data for Arylation of Primary Alcohols

1-Pentyloxy-4-toluene (4a)



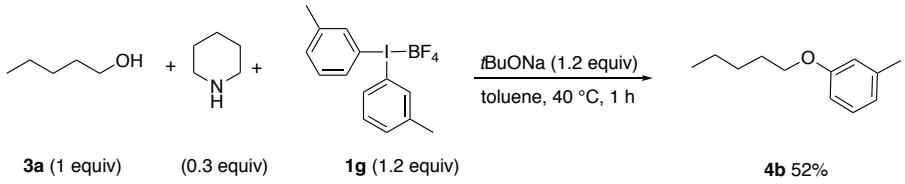
The reaction was performed according to the general procedure C. Isolated as a transparent oil 29 mg (33%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 – 7.04 (m, 2H), 6.83 – 6.78 (m, 2H), 3.93 (t, *J* = 6.6 Hz, 2H), 2.29 (s, 3H), 1.85 – 1.72 (m, 2H), 1.50 – 1.34 (m, 4H), 0.94 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.15, 129.97, 129.76, 114.50, 68.20, 29.19, 28.38, 22.63, 20.60, 14.18.

HRMS (APCI); calcd for $C_{12}H_{19}O$ (M+H): 179.1430 found: 179.1428

1-Pentyloxy-3-toluene (4b)



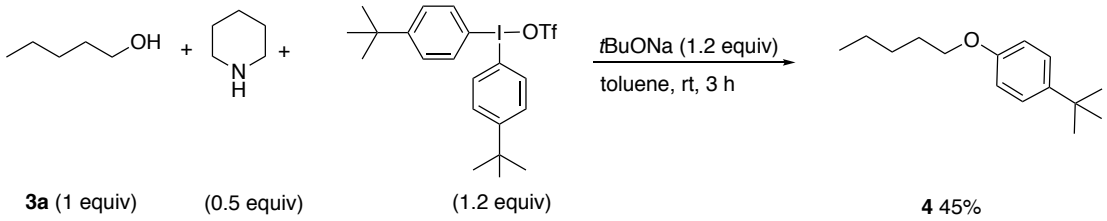
The reaction was performed according to the general procedure C. Isolated as transparent oil in 46 mg (52%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (t, *J* = 7.7 Hz, 1H), 6.79 – 6.69 (m, 3H), 3.95 (t, *J* = 6.6 Hz, 2H), 2.34 (s, 3H), 1.86 – 1.73 (m, 2H), 1.52 – 1.35 (m, 4H), 0.95 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.31, 139.53, 129.27, 121.41, 119.68, 115.52, 111.48, 67.96, 29.19, 28.39, 22.63, 21.67, 14.18.

HRMS (APCI); calcd for $C_{12}H_{19}O$ (M+H): 179.1430 found: 179.1422

4.9. Other Salts with 1-Pentanol

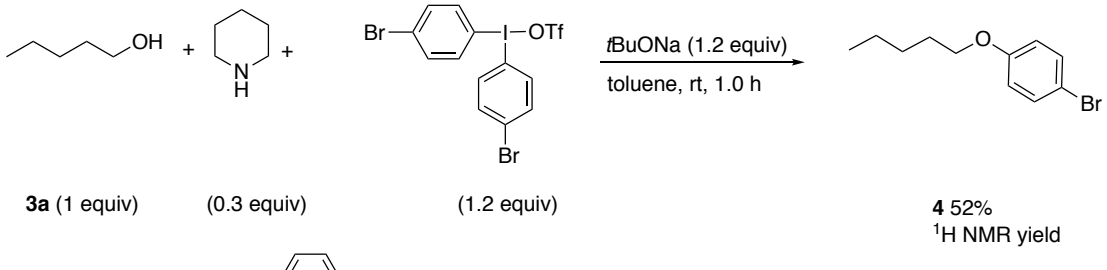


3a (1 equiv) (0.5 equiv) (1.2 equiv) **4** 45%

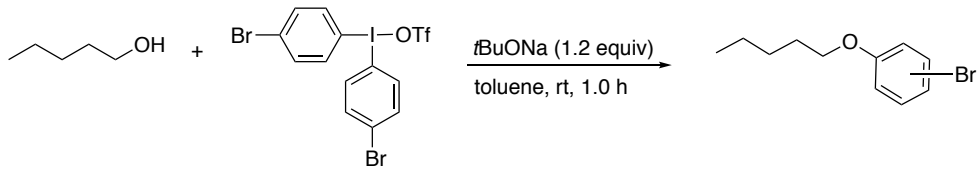
The reaction was performed according to the general procedure C. Isolated as transparent oil in 50 mg (45%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 3.96 (t, *J* = 6.6 Hz, 2H), 1.80 (p, *J* = 6.8 Hz, 2H), 1.52 – 1.38 (m, 4H), 1.33 (s, 9H), 0.96 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.03, 143.21, 126.29, 114.06, 68.06, 34.18, 31.69, 29.22, 28.41, 22.63, 14.19.
HRMS (APCI); calcd for $C_{15}H_{25}O$ (M+H): 221.1900 found: 221.1906

Reaction was performed with a bromo substituted diaryliodonium salt. The outcome showed that with piperidine as additive, the reaction was cleaner.



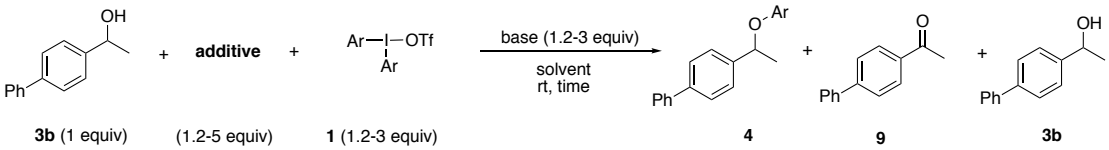
3a (1 equiv) (0.3 equiv) (1.2 equiv) **4** 52% ^{1}H NMR yield



3a (1 equiv) (1.2 equiv) **4** 73% ^{1}H NMR yield

5. Arylation of Secondary Alcohols 3b and 3b-D

5.1. General Procedure for Arylation of Secondary Alcohols



3b (1 equiv) (1.2-5 equiv) **1** (1.2-3 equiv) **4** **9** **3b**

5.1.1. General Procedure D

A dry 10 mL Schlenk tube was evacuated and backfilled with argon three times. *t*BuONa (1.2 equiv) was added followed by anhydrous toluene or THF (1 mL). The mixture was cooled to 0 °C and the alcohol **3b** (40 mg, 0.20 mmol, 1 equiv) was added and rinsed down using toluene or THF (0.5 mL). The mixture was stirred at rt for 15 min and then cooled to 0 °C. Additive (1.2-5 equiv) and diaryliodonium salt **1** (1.2 equiv) were added and rinsed down using toluene (0.5 mL). The reaction mixture was stirred at rt for 90 min.

Work-up ^{1}H NMR yield:
The mixture was quenched with D_2O (0.1 mL) and diluted with EtOAc. 1,3,5-trimethoxybenzene (0.2 mmol) was added as internal standard. The mixture was stirred for 5 min, then allowed to settle, a sample was taken, concentrated and then evaluated by ^{1}H NMR ($CDCl_3$) to determine the yield and products that had formed.

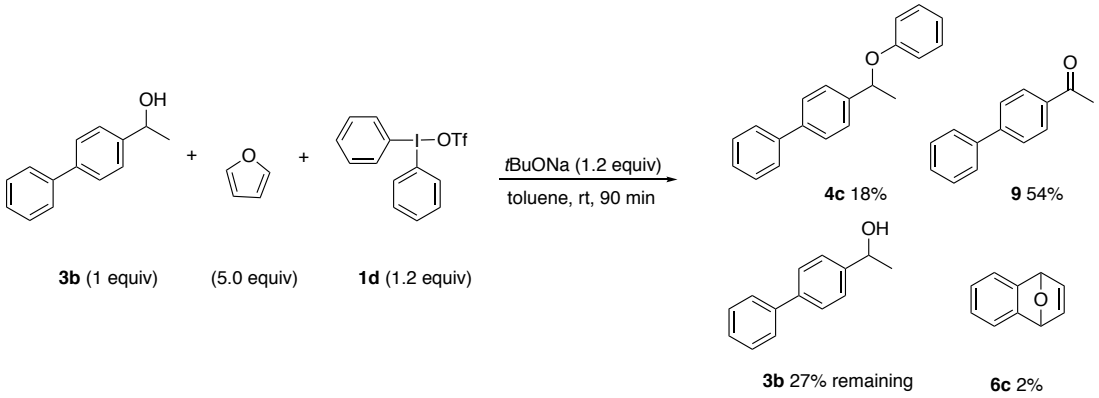
Work-up isolated reactions:
The reaction was quenched with sat. NH_4Cl, extracted with CH_2Cl_2 (x3), dried over $MgSO_4$, filtered and concentrated *in vacuo*. The crude was purified using flash column chromatography, either using ISCO CombiFlash or manual flash chromatography.

5.1.2. General Procedure E

A dry 10 mL Schlenk tube was evacuated and backfilled with argon three times, then charged with alcohol **3b** (40 mg, 0.20 mmol, 1 equiv). Pentane (1 mL) was added and the mixture was cooled to 0 °C. NaHMDS (0.6 M in toluene, 1.0 equiv, 0.34 mL) was added dropwise and then the reaction mixture was stirred at rt for 10 min before the diaryliodonium salt **1** (0.20 mmol, 1 equiv) and pentane (1 mL) were added. The reaction was stirred at rt for 90 min.

The mixture was quenched with D_2O (0.1 mL) and diluted with EtOAc. 1,3,5-trimethoxybenzene (0.2 mmol) was added as internal standard. The mixture was stirred for 5 min, then allowed to settle, a sample was taken, concentrated and then evaluated by ^{1}H NMR ($CDCl_3$) to determine the yield and products that had formed.

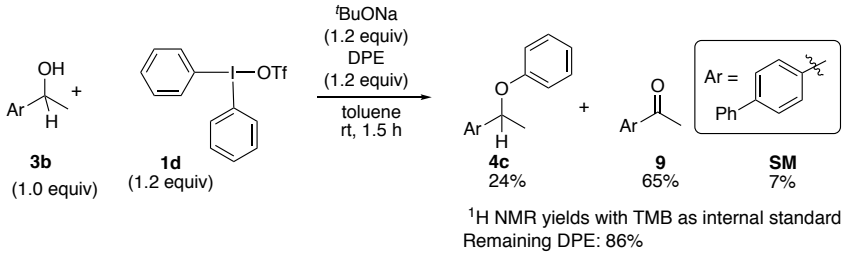
5.2. Trapping of Benzyne with Furan



The reaction was performed according to general procedure D using salt **1d**, with furan (5 equiv) as additive. Yields were determined with ^{1}H NMR analysis.

5.3. Effect of Radical Traps

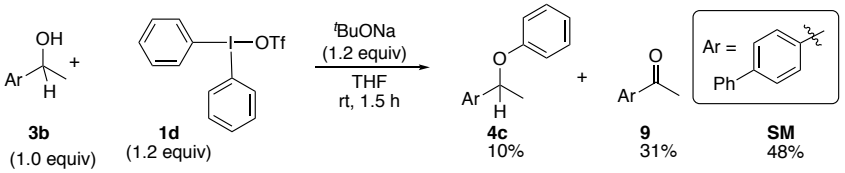
5.3.1. DPE in Toluene



^{1}H NMR yields with TMB as internal standard
Remaining DPE: 86%

The reaction was performed according to general procedure D using salt **1d**, with DPE (1.2 equiv) as additive. Yields were determined with ^{1}H NMR analysis.

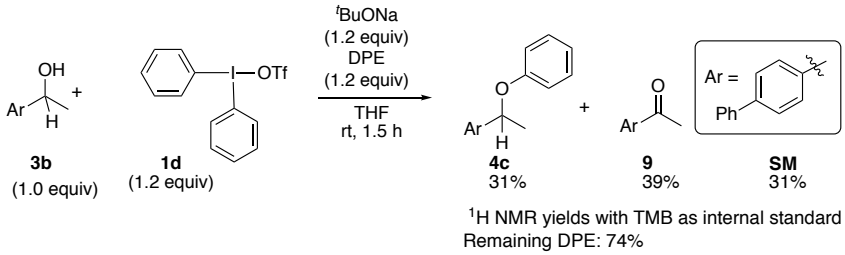
5.3.2. Reaction in THF



^{1}H NMR yields with TMB as internal standard

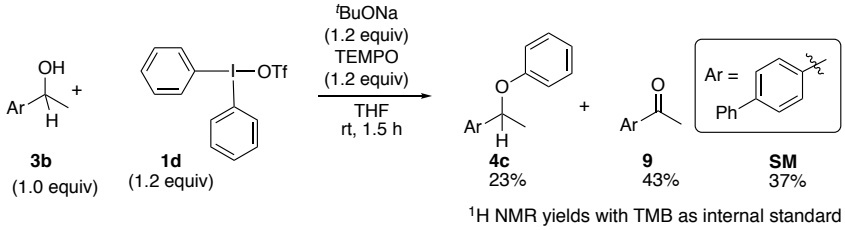
The reaction was performed according to general procedure D using salt **1d**. Yields were determined with ^{1}H NMR analysis.

5.3.3. DPE in THF



The reaction was performed according to general procedure D using salt **1d** with DPE (1.2 equiv) as additive. Yields were determined with ^{1}H NMR analysis.

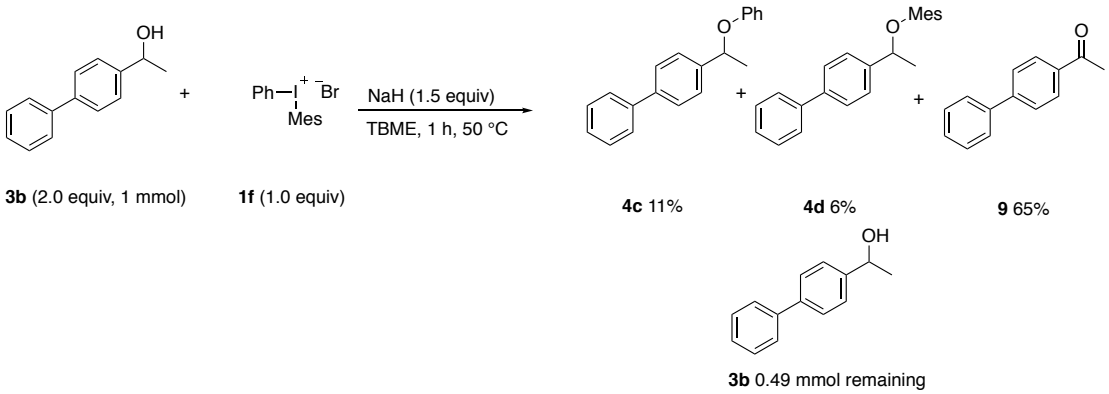
5.3.4. TEMPO in THF



The reaction was performed according to general procedure D using salt **1d** with TEMPO (1.2 equiv) as additive. Yields were determined with ^{1}H NMR analysis.

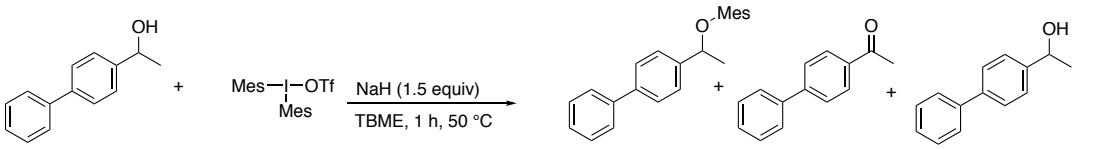
5.4. Comparing Oxidation with Published Protocols

5.4.1. Reaction with Salt 1f



The reaction was performed according to a literature procedure.[34] The products were isolated using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV).

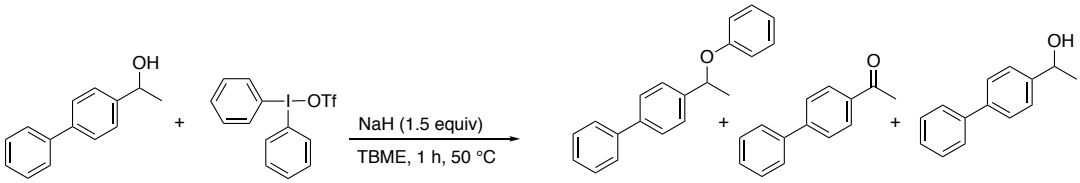
5.4.2. Reaction with Salt 1e



3b (2.0 equiv, 1 mmol) **1e** (1.0 equiv) **4d** 45% **9** 30% **3b** 0.51 mmol remaining

The reaction was performed according to a literature procedure.[34] The products were isolated using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV).

5.4.3. Reaction with Salt 1d

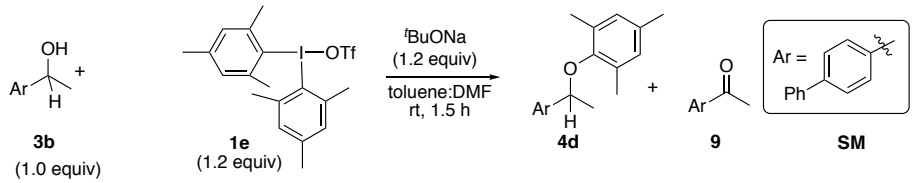


3b (2.0 equiv, 1 mmol) **1d** (1.0 equiv) **4c** 30% **9** 53% **3b** 0.52 mmol remaining

The reaction was performed according to a literature procedure.[34] The products were isolated using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV).

5.5. Oxidation Mechanism with Salt 1e

In order to investigate the oxidation mechanism without aryne interference, salt **1e** was selected. Dilution and excess base did not affect the reaction outcome to any great extent. In toluene, the reactions were not homogenous, and therefore a mixture of toluene and DMF were used. Diluting the reaction did not affect the outcome, however, excess base lowered both the formation of ether and the ketone.

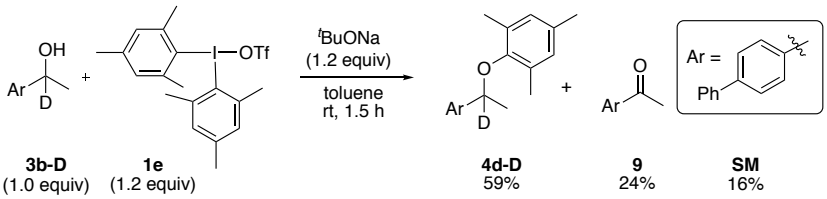


3b (1.0 equiv) **1e** (1.2 equiv) **4d** **9** **SM**

Entry	NaO^{t}Bu (equiv)	M (mmol/mL)	Ratio toluene:DMF	4d	9	3b
1[a]	1.2	0.1	Only toluene	40	32[b]	19
2[a]	1.2	0.02	Only toluene	41	34	24
3[a]	2.0	0.1	Only toluene	44	32	20
4[b]	1.2	0.1	7.3:1	35	28	26
5[b]	1.2	0.02	41:1	39	31	18
6[b]	1.2	0.02	7.3:1	43	29	20
7[b]	2.2	0.1	7.3:1	21	13	33

[a] Isolated yields. [b] H NMR yields using 1,3,5-trimethoxybenzene as internal standard.

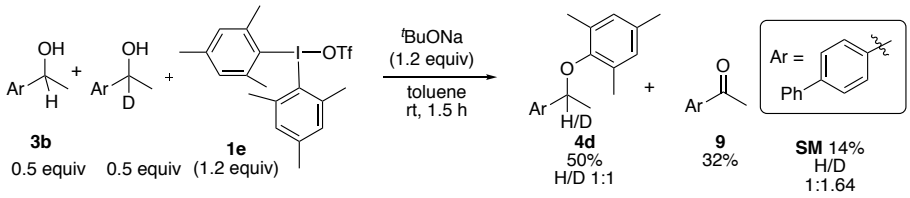
5.6. Oxidation Mechanism with Salt 1e and 3b-D



3b-D (1.0 equiv) **1e** (1.2 equiv) **4d-D** 59% **9** 24% **SM** 16%

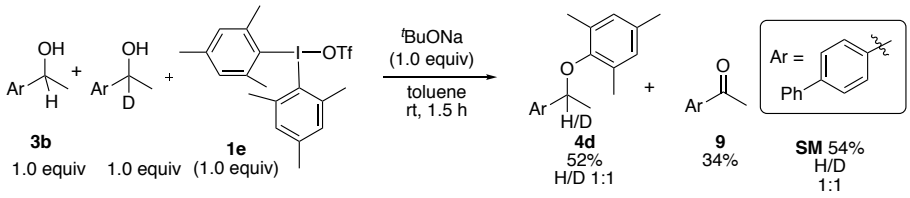
The reaction was performed according to general procedure D using salt **1e** with. The products were isolated using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV).
Submitting this reaction to GC-MS analysis showed a peak with a mass corresponding to deuterated mesitylene.

5.7. Competition Experiments



3b 0.5 equiv 0.5 equiv **1e** (1.2 equiv) **4d** 50% H/D 1:1 **9** 32% **SM** 14% H/D 1:1.64

The reaction was performed according to general procedure D using salt **1e** with. The products were isolated using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV).

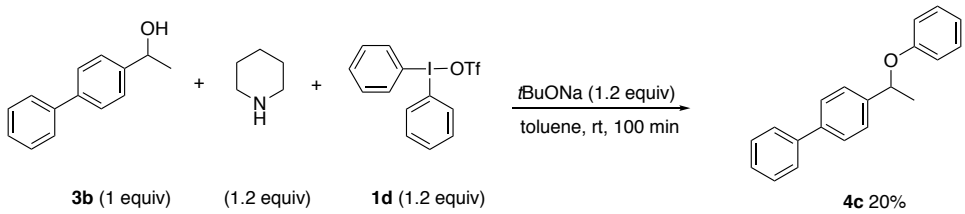


3b 1.0 equiv 1.0 equiv **1e** (1.0 equiv) **4d** 52% H/D 1:1 **9** 34% **SM** 54% H/D 1:1

The reaction was performed according to general procedure D using salt **1e** with. The products were isolated using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV).

5.8. Analytical Data for Arylation of Secondary Alcohols

4(1-Phenoxyethyl)-1,1'-biphenyl (4c)



The reaction was performed according to general procedure **D** on a 0.5 mmol scale, using piperidine (1.2 equiv) as additive. The reaction was stirred at rt for 100 min and quenched using HCl (3M, aq). The organic phase was washed three times with HCl (3M, aq), then with brine and dried over $MgSO_4$. The solution was filtered and concentrated *in vacuo*. The crude was purified using flash column chromatography (silica, gradient pentane → 16% CH_2Cl_2 in pentane). The product was obtained as colorless crystals (27.1 mg, 0.10 mmol) in 20% yield.

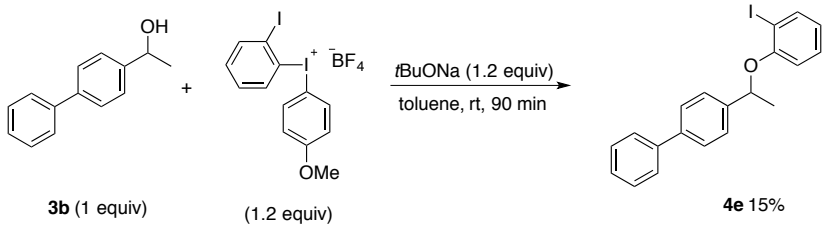
mp = 94-96 °C

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63-7.55 (m, 4H), 7.50-7.41 (m, 4H), 7.39-7.32 (m, 1H), 7.28-2.20 (m, 2H), 6.96-6.88 (m, 3H), 5.39 (q, *J* = 6.4 Hz, 1H), 1.70 (d, J = 6.5 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.1, 142.4, 140.9, 140.5, 129.5, 128.9, 127.5, 127.4, 127.2, 126.1, 120.8, 116.1, 75.8, 24.6.

HRMS (ESI): calcd for $C_{20}H_{18}ONa$ $[M+Na]^+$: 297.1250; found: 297.1249.

4(1-(2-Iodophenoxy)ethyl)-1,1'-biphenyl (4e)



The reaction was performed according to general procedure **D** on 0.5 mmol scale. The crude was purified using flash column chromatography (silica, gradient pentane → 2% EtOAc in pentane). The product contained some impurities and was submitted to a second flash column chromatography (silica, gradient pentane → 10% CH_2Cl_2 in pentane). The product was obtained as a colorless oil that solidified upon standing (30.9 mg, 0.08 mmol) in 15% yield.

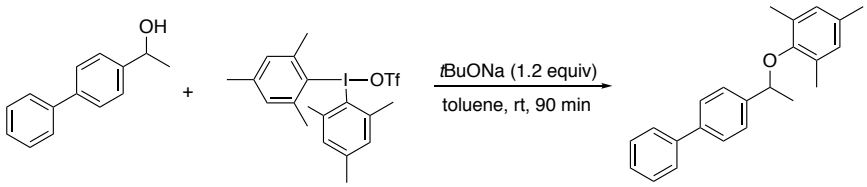
mp = 93-95 °C

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.62-7.55 (m, 4H), 7.52-7.41 (m, 4H), 7.39-7.32 (m, 1H), 7.16 (ddd, *J* = 8.2, 7.3, 1.6 Hz, 1H), 6.71 (dd, *J* = 8.3, 1.4 Hz, 1H), 6.66 (td, *J* = 7.6, 1.4 Hz, 1H), 5.42 (q, *J* = 6.4 Hz, 1H), 1.75 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.5, 141.7, 140.8, 140.6, 139.6, 129.3, 128.9, 127.5, 127.4, 127.2, 126.2, 122.6, 114.2, 87.8, 77.2, 24.6.

HRMS (ESI): calcd for $C_{20}H_{17}IONa$ $[M+Na]^+$: 423.0216; found: 423.0208.

4(1-(Mesityloxy)ethyl)-1,1'-biphenyl (4d)



3b (1 equiv) **1e** (1.2 equiv) **4d** 41%

The reaction was performed according to the general procedure **D**. The crude residue was purified using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV). The desired ether **4d** was isolated in 32 mg (41%) as transparent oil, which solidified upon standing.

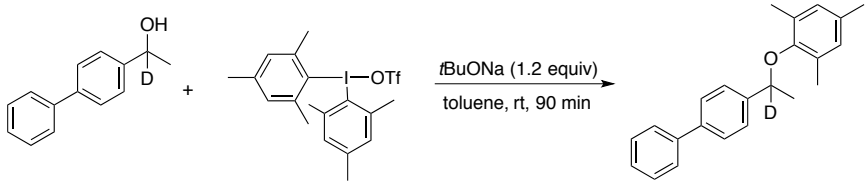
mp = 61-63 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.57 (m, 4H), 7.53-7.42 (m, 4H), 7.39-7.32 (m, 1H), 6.81 (s, 2H), 4.96 (q, *J* = 6.5 Hz, 1H), 2.25 (s, 3H), 2.15 (s, 6H), 1.64 (d, *J* = 6.5 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.2, 141.0, 140.7, 132.7, 131.1, 129.6, 128.9, 127.4, 127.2, 127.2, 127.2, 80.1, 22.4, 20.8, 17.3

HRMS (ESI): calcd for $C_{23}H_{24}NaO$ $[M+Na]^+$: 339.1719; found: 339.1716 .

4-(1-(Mesityloxy)ethyl-1-*d*)-1,1'-biphenyl (4d-D)



3b-D (1 equiv) **1e** (1.2 equiv) **4d-D** 59%

The reaction was performed according to general procedure **D**. The crude residue was purified using flash chromatography (ISCO CombiFlash, 12 g column, gradient of pentane:EtOAc 0->75:25, 25 CV). The desired ether **4d-D** was isolated in 94 mg (59%) as transparent oil, which solidified upon standing.

mp = 58-60 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.57 (m, 4H), 7.53-7.42 (m, 4H), 7.40-7.33 (m, 1H), 6.81 (s, 2H), 2.25 (s, 3H), 2.15 (s, 6H), 1.63 (s, 3H). *Traces of the non-deuterated ether, same amount as in the alcohol, quartet at 4.96.*

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.2, 141.0, 140.8, 132.8, 131.1, 129.6, 128.9, 127.4, 127.2, 127.2, 127.1, *80.1* (from H alcohol), 79.7 (t), 22.3, 20.8, 17.3.

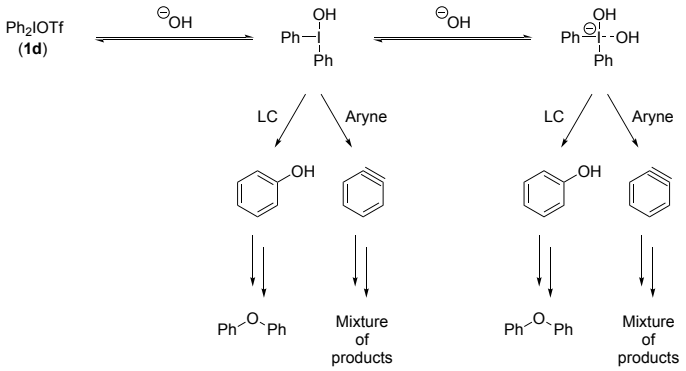
HRMS (ESI): calcd for $C_{23}H_{23}DNaO$ $[M+Na]^+$: 340.1782; found: 340.1775 .

6. Computational Details

Calculations were performed using the Gaussian09 package[35]. Optimization was generally done using the Becke Three-Parameter Lee-Yang-Parr functional[36] with the class III correction to dispersion by Grimme[37] (B3LYP-D3). The Minnesota functional (M06-2X)[38] was also used as comparison in a few cases, which will be stated when necessary. The SDD basis set with an applied effective core potential (MWB46) was used for iodine,[39] Pople's triple-zeta basis set with polarization and diffusion functions (6-311+G(d,p))[40] were used for N, O, F, Cl and Na atoms while the triple-zeta basis set with polarization (6-311G(d,p))[40b, c] were used for H-, C- and S-atoms. All structures were optimized in the respective solvent (CH_2Cl_2, water or toluene) using the polarizable continuum model (PCM, Surface=SES, Radii=UFF).[41] A vibrational analysis was conducted to verify a lowest energy structure or in some cases to verify a transition state as indicated by a single imaginary frequency. All energies are given in kJ/mol.

7. Arylation of Hydroxide

The Minnesota functional (M06-2X) was initially chosen as our method to study the system (Scheme S1) based on previous studies in the group.[42] Toluene was used as the solvent based on early results from the arylation of secondary alcohols (*vide infra*).



Scheme S1 General depiction of the analyzed reaction. The steps studied are the aryne formation and the ligand coupling (LC).

7.1. Diphenyliodonium Triflate (1d) and Hydroxide in Toluene (M06-2X)

Addition of hydroxides to **1d** leads to a large decrease in energy to form the stable intermediate **1d-(OH)$_2$** (-182 kJ/mol). Due to the fast equilibrium between **1d-(OH)OH** and **1d-(OH)$_2$** all transition state energies are calculated from the lowest intermediate according to the Curtin-Hammet principle. The external aryne formation via **TS1-1d** (+33 kJ/mol) is heavily favored over other TSs for aryne formation and ligand coupling (Figure S1).

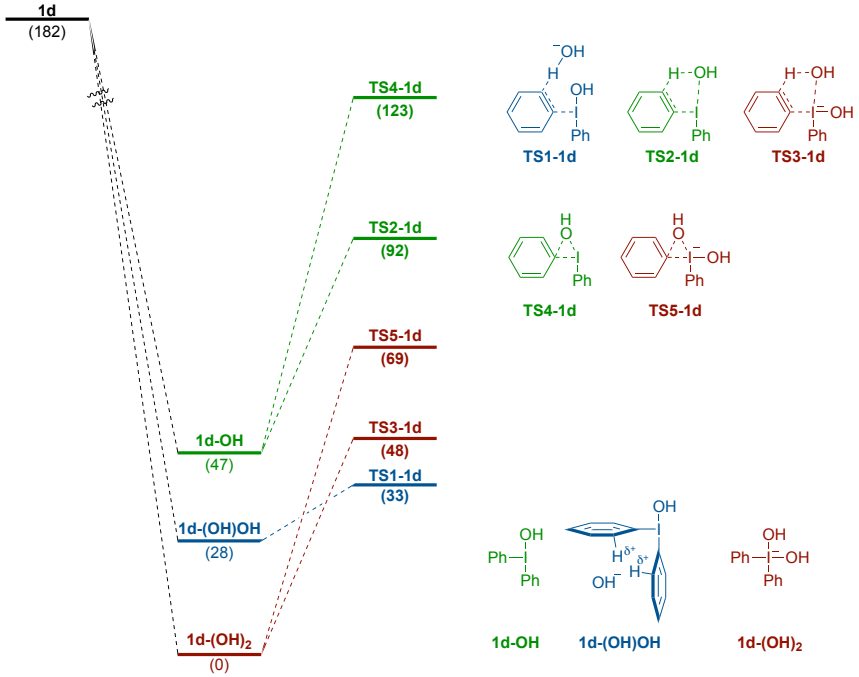
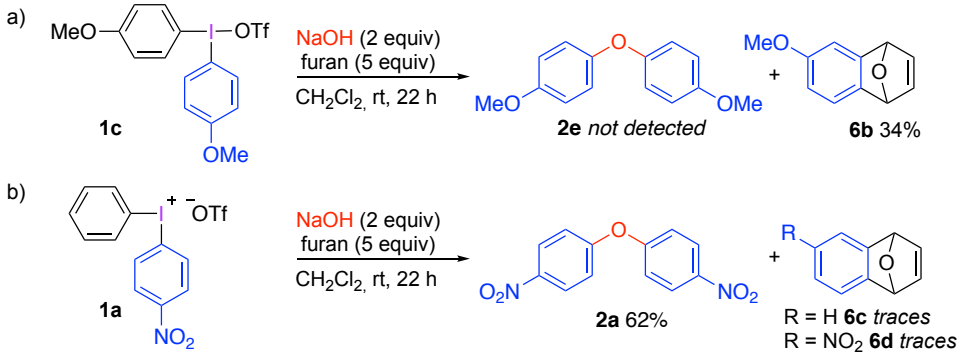


Figure S1. Free energy surface of the reaction between **1d** and hydroxide in toluene using M06-2X. Free triflates and hydroxides are omitted for clarity.

7.2. Electronic Effects of Ar_2IOTf with Hydroxide in Toluene (M06-2X)

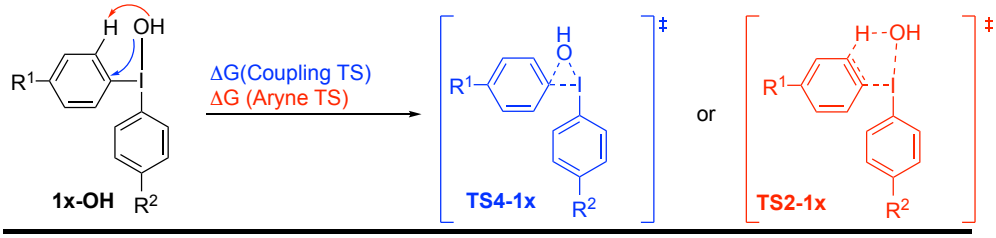
The product distribution (aryne vs. ligand coupling) was experimentally seen to drastically change based on the substituent on the iodonium salt. Employing the electron-rich salt **1c** to the reaction with sodium hydroxide in the presence of furan furnished exclusively the Diels-Alder (DA) product **6b** derived from the formation of arynes (Figure S2a). However, when using the electron-poor salt **1a** under the same conditions, the major product was the diarylether **2a** as a single regioisomer (Figure S2b), which indicates that it forms via a ligand coupling and not via an aryne.



Scheme S2. (a) DA-adduct **6b** as the major product when using **1c** as the iodonium salt. (b) Diarylether **2a** as the major product when using iodonium salt **1a**.

The change in product distribution between **1a** and **1c** indicates large changes in the energies of the inherent transition states, hence, the energy difference between **TS4-1x** (3-coordinated ligand coupling) and **TS2-1x** (3-coordinated aryne formation) were investigated for a range of different substituents (Table S1). To our surprise, none of the investigated substitution patterns showed a preference for ligand coupling via **TS1** ($\Delta\Delta G < 0$).

Table S1. Electronic effects on the energy difference between **TS2-1x** and **TS4-1x**

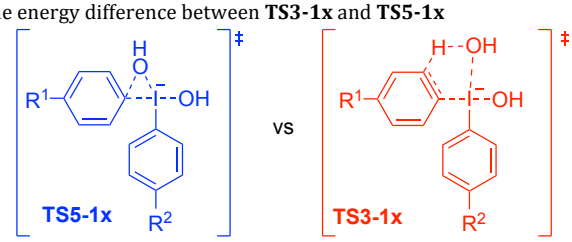


R¹	R²	x	ΔG (**TS4-1x**)	ΔG (**TS2-1x**)	ΔΔG (TS1-TS2)
NO_2	H	a	60.7	39.2	21.6
CN	H	l	61.2	37.8	23.4
H	NO_2	m	81.0	52.5	28.4
H	H	d	76.2	45.1	31.1
Cl	Cl	n	79.1	45.6	33.5
F	F	o	81.4	45.3	36.2
OMe	OMe	c	87.0	46.9	40.1

7.4. Solvation Effects of Ar_2IOTf with Hydroxide (M06-2X)

Since we could not match the experimental selectivity between aryne formation and ligand coupling for **1a** and **1c** as shown in Scheme S2 we investigated the effect of the solvent on the energies (Table S2) on the 4-coordinated **TS3** (aryne) and **TS5** (LC). While the energy difference (ΔΔG) decreases, none of the entries shows a preference for substitution (ΔΔG < 0).

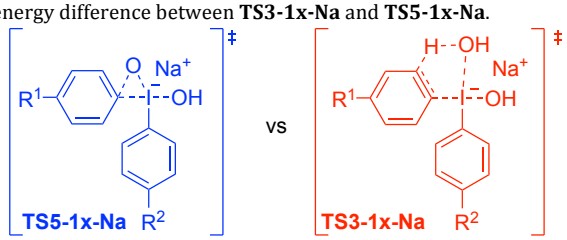
Table S2. Solvent effects on the energy difference between **TS3-1x** and **TS5-1x**



R¹	R²	x	Solvent	ΔΔG (TS5-TS3)
NO_2	H	a	CH_2Cl_2	6.8
NO_2	H	a	H_2O	11.5
OMe	OMe	c	CH_2Cl_2	36.5
OMe	OMe	c	H_2O	43.1

We postulated that the inclusion of Na^+ (NaOH used as Nu) to these anionic systems could alter the selectivity (Table S3). No explicit solvation was included in these calculations. Unfortunately, the addition of Na^+ increased the gap (ΔΔG), *i.e*. aryne formation was even more favored and the energies resemble more those of 3-coordinated TSs, probably due the coordination of Na^+ to the "non-reacting" hydroxide, decreasing its coordinative ability to the iodonium.

Table S3. Effect of Na^+ on the energy difference between **TS3-1x-Na** and **TS5-1x-Na**.



R¹	R²	Solvent	ΔΔG (TS5-TS3)
NO_2	H	CH_2Cl_2	24.9
NO_2	H	H_2O	17.2
OMe	OMe	CH_2Cl_2	55.5
OMe	OMe	H_2O	42.2

7.5. Diphenyliodonium Triflate (1d) and Hydroxide in CH_2Cl_2 and Water (B3LYP-D3)

Due to the difficulties in achieving the proper selectivity for the reaction shown above we tried using the B3LYP-D3 functional and initially we modeled the standard reaction between **1d** and hydroxide in CH_2Cl_2 and water (Figure S2). In both solvents the preferred pathway is via the external elimination (**TS3-1d**, +43 kJ/mol [water], +33 kJ/mol [CH_2Cl_2]) similar to M06-2X in toluene (Figure S1).

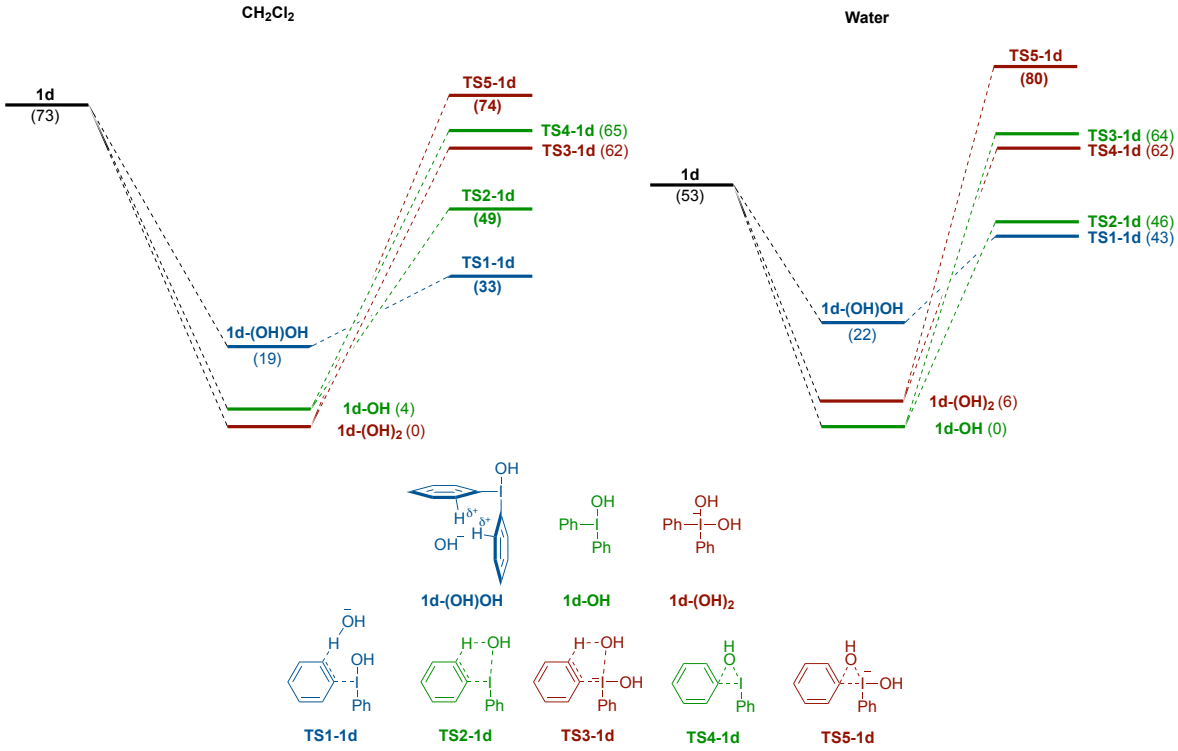
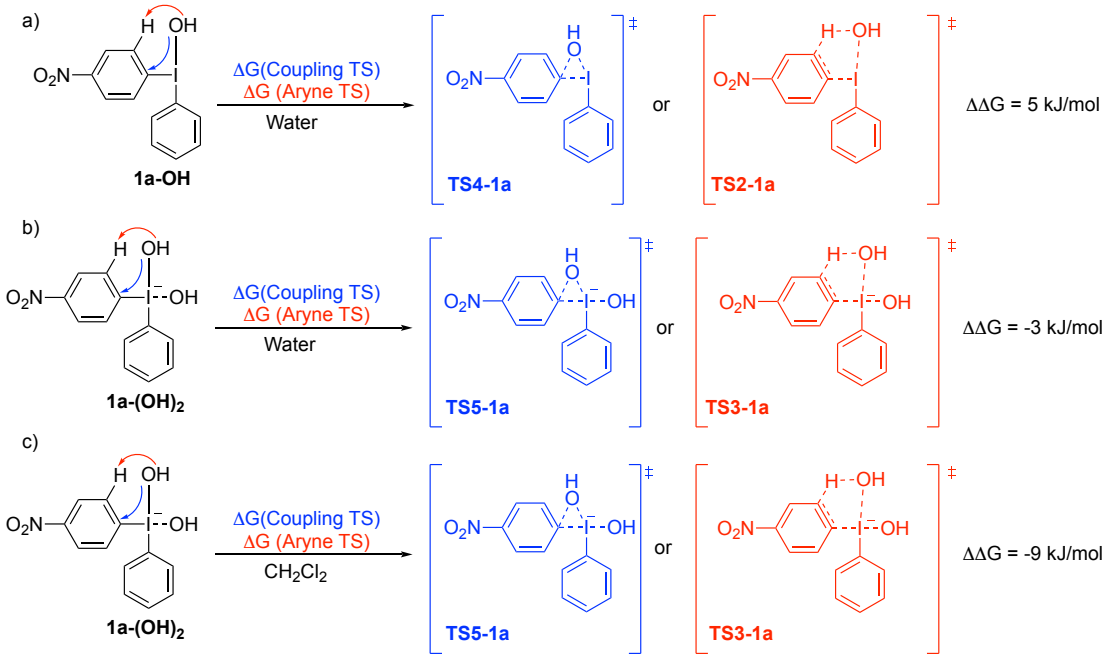


Figure S2. Free energy surface of the reaction between **1d** and hydroxide in CH_2Cl_2 (left) and water (right) using B3LYP-D3. Free triflates and hydroxides are omitted for clarity.

7.6. *p*-Nitrophenyl(phenyl)iodonium Triflate (1a) and Hydroxide in CH_2Cl_2 and Water (B3LYP-D3)

We then investigated the 3- and 4-coordinated TSs for elimination and substitution in various solvents. In water, elimination via **TS2-1a** is still favored by 5 kJ/mol (Scheme 3a). To our delight, the selectivity changed for the 4-coordinated TSs where substitution via **TS5-1a** is favored in both water (Scheme S3b, -3 kJ/mol) and in CH_2Cl_2 (Scheme S3c, -9 kJ/mol).



Scheme S3. Calculations using B3LYP-D3 (a) Energy difference between **TS4-1a** and **TS2-1a** in toluene. (b) Energy difference between **TS5-1a** and **TS3-1a** in water. (c) Energy difference between **TS5-1a** and **TS3-1a** in CH_2Cl_2.

However, the external elimination (**TS1-1a**) still had a lower barrier (+30 kJ/mol in CH_2Cl_2, +40 kJ/mol in water) than the 4-coordinated substitution via **TS5-1a** (+38 kJ/mol in CH_2Cl_2, +46 kJ/mol in water), which is depicted in the free energy surface in Figure S3. Surprisingly, the direct attack of the hydroxide on **1a**, without prior coordination to iodine, resulted in **TS6-1a** (+6 kJ/mol in CH_2Cl_2, +28 kJ/mol in water) that is lower in energy than that of the external elimination (**TS3-1a**) in both water and CH_2Cl_2, which explains the selectivity seen experimentally.

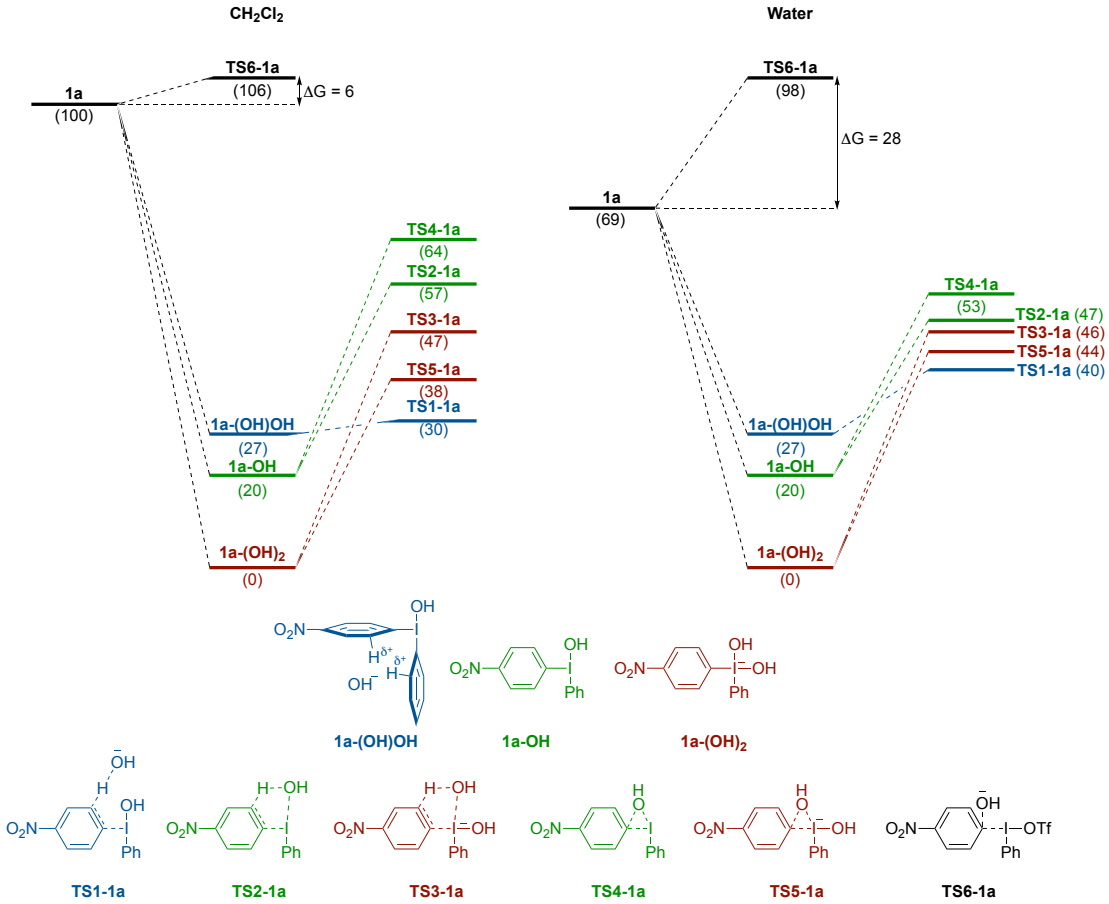


Figure S3 Free energy surface of the reaction between **1a** and hydroxide in CH_2Cl_2 (left) and water (right) using B3LYP-D3

7.7. Dianisyliodonium Triflate (1c) and Hydroxide in CH_2Cl_2 and Water (B3LYP-D3)

In order to verify that we also have the correct selectivity in the system employing **1c** we modeled it with together with hydroxide and the free energy surface is depicted in Figure S4. All possible aryne pathways (via **TS1-1c**, **TS2-1c** or **TS3-1c**) are lower than the corresponding ligand coupling pathways (via **TS4-1c** and **TS5-1c**), with the external elimination via **TS1-1c** being the major pathway in CH_2Cl while competing with the 3-coordinated internal elimination via **TS2-1c** ($\Delta\Delta G$ = 2 kJ/mol) in water. The direct attack by the hydroxide on **1c** was not obtained despite numerous tries using constrained and unconstrained geometries. The imaginary frequency corresponding to the *O-C* coupling could be found, however, other imaginary frequencies corresponding to *O-I* interaction were also detected. The same behavior was seen for salt **1d**.

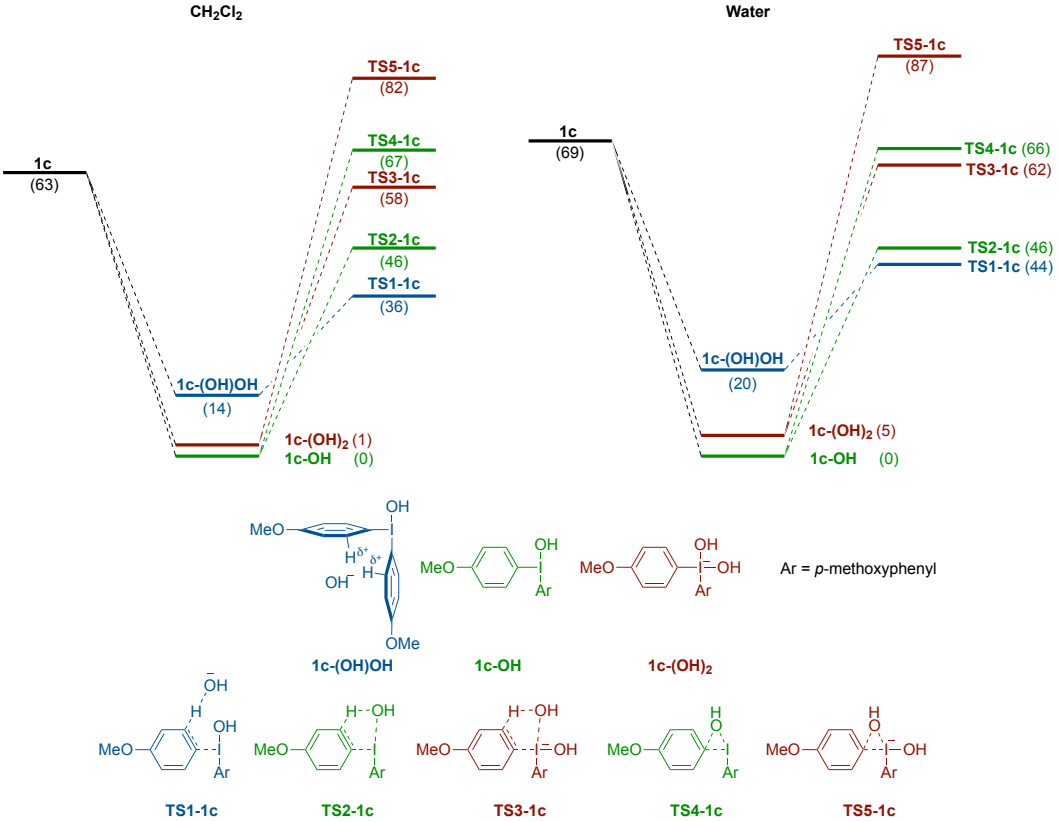
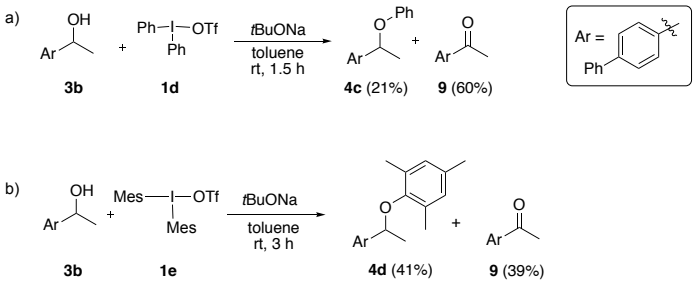


Figure S4. Free energy surface of the reaction between **1c** and hydroxide in CH_2Cl_2 and water using B3LYP-D3.

8. Arylation vs. Oxidation of Secondary Alcohol

In the reaction between activated alcohol **3b** and diphenyliodonium triflate (**1d**), the unexpected oxidation product **9** was obtained as the major product (Scheme S4a). Severe oxidation also occurred when using dimesityliodonium triflate (**1e**) indicating that the oxidation does not form via an aryne type of intermediate (Scheme S4b). We set out to elucidate the mechanism between these competing pathways (ligand coupling vs. oxidation) using DFT calculations (both M06-2X and B3LYP-D3). 1-Phenylethanol was chosen as the alcohol to simplify the calculations.



Scheme S4. Competing ligand coupling and oxidation pathways between **3b** and iodonium salts **1d** (a) and **1e** (b).

8.1. Diphenyliodonium Triflate (1d) and 1-Phenylethoxide in Toluene (B3LYP-D3 and M06-2X)

Both methods were unable to predict the product distribution seen in Scheme S4a. The 4-coordinated ligand coupling going via **TS7-1d** is atleast 14 kJ/mol (B3LYP-D3) lower than any of the other TSs (**TS8-TS11**), suggesting a clear preference for ligand coupling over oxidation as seen in Figure S5.

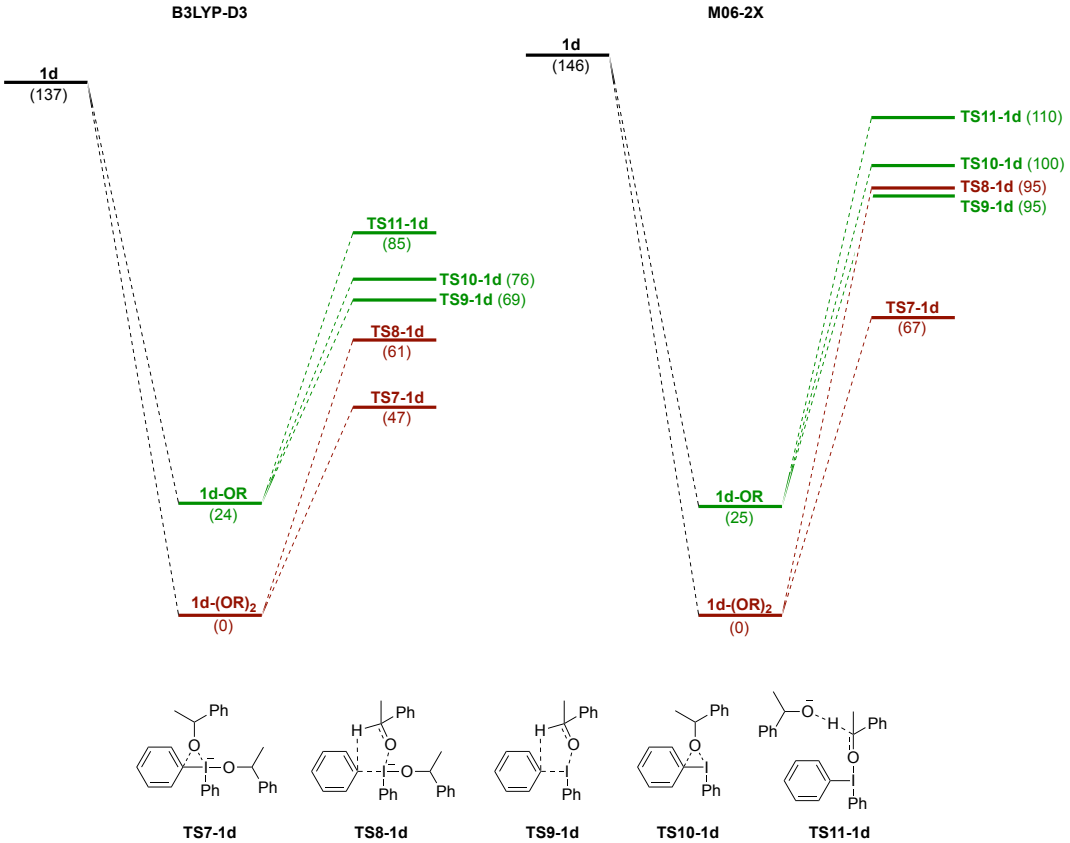


Figure S5. Free energy surface for the reaction between **1d** and 1-phenylethoxide using B3LYP-D3 (left) and M06-2X (right). Free alkoxides and triflates are omitted for clarity.

8.2. Dimesityliodonium Triflate (1e) and 1-Phenylethoxide in Toluene (B3LYP-D3 and M06-2X)

A similar discrepancy was seen for the calculation between **1e** and 1-phenylethoxide where the 4-coordinated ligand coupling going via **TS7-1e** is much lower in energy than any of the other TSs (**TS8**-**TS11**), again showing a clear preference for ligand coupling (Scheme S6).

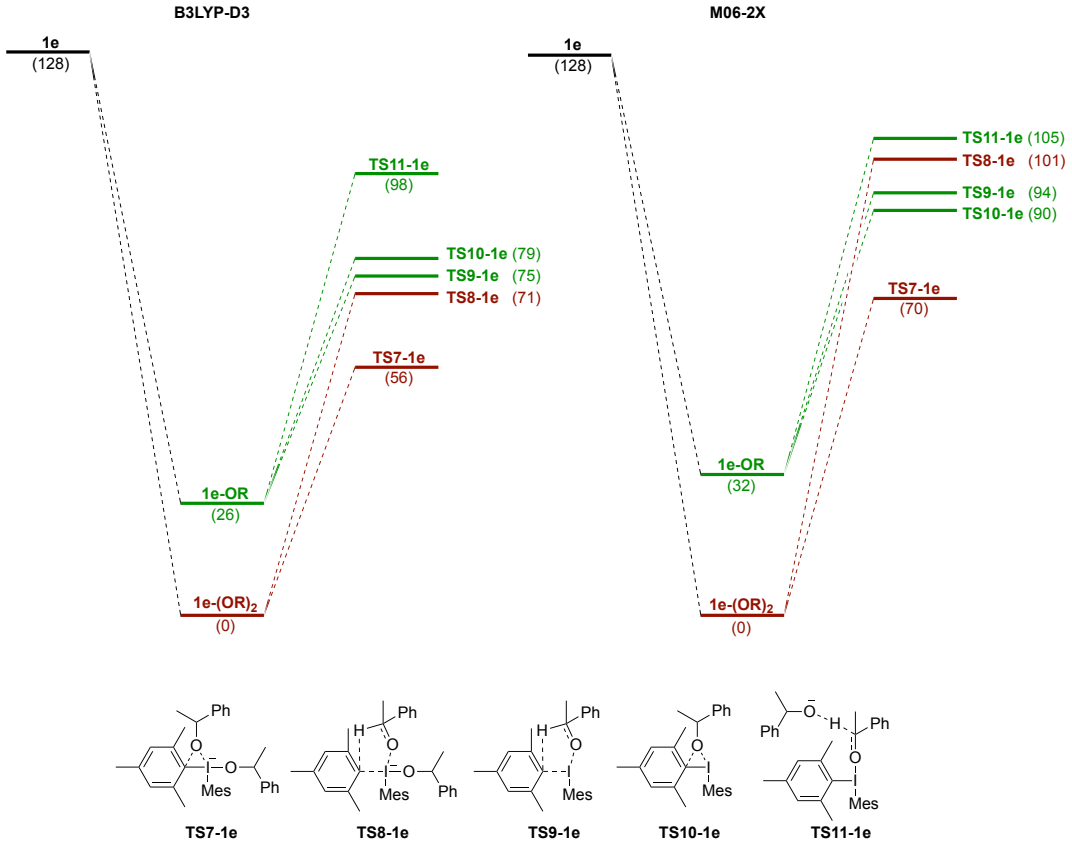
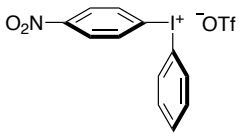


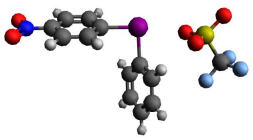
Figure S6. Free energy surface for the reaction between **1e** and 1-phenylethoxide using B3LYP-D3 (left) and M06-2X (right). Free alkoxides and triflates are omitted for clarity.

9. Selected Optimized Intermediates and Transition States

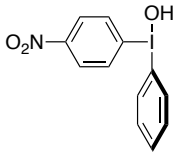
Optimized structures of the intermediates and transition states for iodonium salt **1a** are presented in Figure S7. The calculations are done using the B3LYP-D3 level of theory using dichloromethane as the solvent.

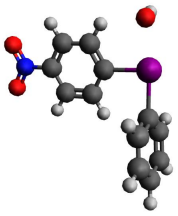
1a



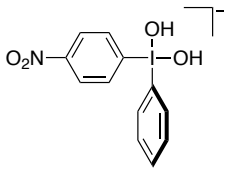


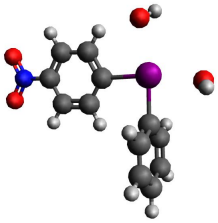
1a-OH



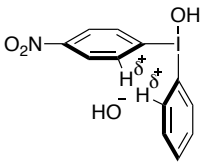


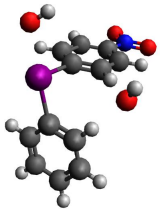
1a-(OH)$_2$



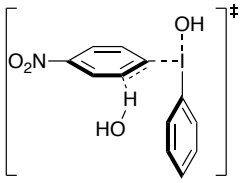


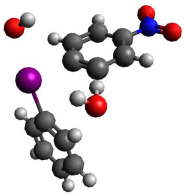
1a-(OH)OH



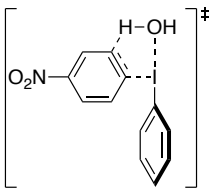


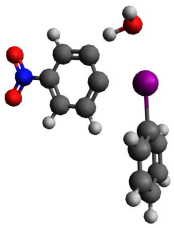
TS1-1a



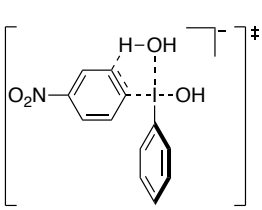


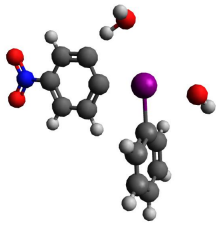
TS2-1a



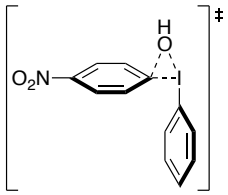


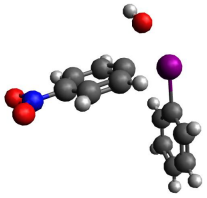
TS3-1a



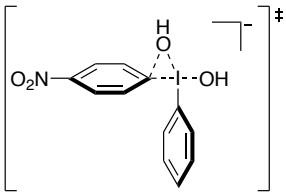


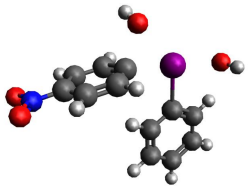
TS4-1a



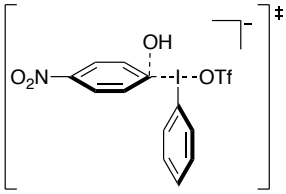


TS5-1a





TS6-1a



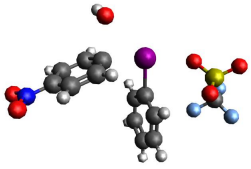


Figure S7. Structures of intermediates and transition state for the reaction between iodonium salt **1a** and hydroxide.

10. Cartesian Coordinates, Energies and Selected Vibrational Frequencies

Energies are given in Hartree and frequencies in cm^{-1}

Sum of electronic and zero-point energies	=	$\varepsilon_0 + \varepsilon_{ZPE}$
Sum of electronic and thermal energies	=	$\varepsilon_0 + E_{tot}$
Sum of electronic and thermal enthalpies	=	$\varepsilon_0 + H_{corr}$
Sum of electronic and thermal free energies	=	$\varepsilon_0 + G_{corr}$

1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = 1640.781740
$\varepsilon_0 + E_{tot}$ = 1640.758385
$\varepsilon_0 + H_{corr}$ = 1640.757441
$\varepsilon_0 + G_{corr}$ = 1640.841263

Coordinates:

H	2.8147440000	-1.2728790000	-2.1170290000
H	0.9526070000	1.5808210000	-2.0288910000
H	0.4968140000	4.0083150000	-1.8769830000
H	5.2522860000	-0.8936160000	-1.8158630000
C	0.3446870000	1.9735470000	-1.2252890000
F	-5.2656020000	0.0473680000	-1.2238320000
C	3.1954310000	-0.9156010000	-1.1700440000
C	0.0834640000	3.3407840000	-1.1308110000
C	4.5615880000	-0.7026880000	-1.0071340000
O	-2.5050620000	-1.0664210000	-0.7122640000
O	7.2078900000	-0.2389220000	-0.5643850000
I	0.2266000000	-0.9735360000	-0.3510070000
C	-0.2032630000	1.1599340000	-0.2464910000
C	2.3513090000	-0.6504620000	-0.0983290000
C	-0.7064340000	3.8379170000	-0.0947810000
H	-0.9067810000	4.9007100000	-0.0347110000
F	-4.0588980000	1.4029000000	-0.0264550000
C	-4.7027760000	0.2253210000	-0.0192500000
C	5.0220800000	-0.2319750000	0.2167010000
O	-4.3566200000	-2.3871490000	0.3099600000
S	-3.5151190000	-1.1844170000	0.3800010000
N	6.4749340000	-0.0000340000	0.3871860000
C	-0.9957200000	1.6039930000	0.7965360000
C	-1.2442490000	2.9768000000	0.8586910000
F	-5.6812710000	0.2885640000	0.8968740000
C	2.8105260000	-0.1875830000	1.1298420000
C	4.1743730000	0.0311360000	1.2881690000
O	6.8636620000	0.4186800000	1.4703740000
H	-1.4300600000	0.9233340000	1.5154340000
H	-1.8661450000	3.3602260000	1.6582660000
O	-2.9856150000	-0.8359000000	1.7128040000
H	2.1334500000	0.0088250000	1.9498800000
H	4.5724410000	0.3940600000	2.2249000000

1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1640.788699
$\varepsilon_0 + E_{tot}$ = −1640.765253
$\varepsilon_0 + H_{corr}$ = −1640.764308
$\varepsilon_0 + G_{corr}$ = −1640.848479

Coordinates:

H	2.6874160000	-0.4477470000	-2.2804820000
H	-0.1430730000	1.4261310000	-2.2310500000
H	5.1059250000	0.0566230000	-2.0143660000
H	-0.8286720000	3.7863960000	-1.9287400000
C	3.1300240000	-0.4113980000	-1.2949020000
F	-5.0905840000	0.1446390000	-1.2820770000
C	-0.3952060000	1.8015710000	-1.2491990000
C	4.4844230000	-0.1280780000	-1.1501230000
C	-0.7833160000	3.1295120000	-1.0687240000
O	7.1145300000	0.4404450000	-0.7307890000
O	-2.5032360000	-1.3175710000	-0.7044740000
I	0.2664340000	-1.0676880000	-0.3725820000
F	-3.6629090000	1.4168050000	-0.2497340000
C	2.3761950000	-0.6377550000	-0.1493850000
C	-0.3510920000	0.9986350000	-0.1206190000
C	-4.4665050000	0.3544460000	-0.1112430000
C	5.0243590000	-0.0872170000	0.1307480000
C	-1.1090800000	3.6024420000	0.2013680000
N	6.4655060000	0.2130000000	0.2831440000
H	-1.4101190000	4.6351310000	0.3291340000
S	-3.4889770000	-1.1744830000	0.4034690000
O	-4.5094940000	-2.2356260000	0.4510670000
F	-5.3975900000	0.6486580000	0.8116190000
C	2.9130690000	-0.6029630000	1.1323500000
C	-0.6747570000	1.4217180000	1.1576800000
C	4.2675750000	-0.3196490000	1.2742650000
C	-1.0562850000	2.7555360000	1.3064490000
O	6.9339960000	0.2187120000	1.4151640000
O	-2.8880540000	-0.7966130000	1.6952770000
H	-0.6568090000	0.7503860000	2.0030940000
H	2.3041240000	-0.7847160000	2.0070100000
H	4.7246280000	-0.2812270000	2.2524880000
H	-1.3179600000	3.1207480000	2.2920030000

1c (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1665.282537
$\varepsilon_0 + E_{tot}$ = −1665.256424
$\varepsilon_0 + H_{corr}$ = −1665.255480
$\varepsilon_0 + G_{corr}$ = −1665.345042

Coordinates:

H	3.1094880000	-0.4439340000	-2.1299760000
H	0.1391110000	1.2085490000	-2.1232180000
H	-0.7558590000	3.4641840000	-1.7822970000
H	5.4490040000	0.1805180000	-1.7704700000
F	-4.8033380000	-0.5542440000	-1.3335470000
H	-2.4529900000	4.9952430000	-1.2071610000
C	-0.1938590000	1.5074680000	-1.1385050000
C	3.5113440000	-0.4469520000	-1.1252760000
H	7.6665450000	-0.1968310000	-1.0801890000
C	-0.7037390000	2.7896630000	-0.9398230000
C	4.8425860000	-0.0895170000	-0.9178450000
H	7.1803400000	1.5157240000	-0.8810960000
H	-0.8128930000	5.6179210000	-0.8449540000
O	-2.0931740000	-1.8248720000	-0.8196700000
C	-1.7876090000	5.3612650000	-0.4201520000
C	7.5378760000	0.6203470000	-0.3649300000
I	0.6670880000	-1.3315320000	-0.3586300000
F	-3.4540270000	0.7869450000	-0.2842390000
C	-4.1776230000	-0.3357610000	-0.1644300000
C	-0.1341290000	0.6471280000	-0.0560640000
C	2.7265450000	-0.7947760000	-0.0351820000
H	-2.2244610000	6.2408660000	0.0468470000
H	8.4876660000	0.8335970000	0.1197400000
S	-3.0847930000	-1.8047650000	0.2909520000
O	-4.0203270000	-2.9410670000	0.2987420000
C	-1.1399840000	3.1757690000	0.3336300000
C	5.3673580000	-0.0865700000	0.3803790000
O	-1.6530240000	4.3943210000	0.6281940000
O	6.6431810000	0.2438790000	0.6894310000
F	-5.1138830000	-0.1312490000	0.7770870000
C	-0.5667570000	0.9961740000	1.2182320000
C	3.2314370000	-0.8034250000	1.2647840000
C	-1.0665640000	2.2742390000	1.4056150000
C	4.5540160000	-0.4454130000	1.4665180000
O	-2.5103020000	-1.4294990000	1.5964790000
H	-0.5473950000	0.2902450000	2.0352090000
H	2.6112050000	-1.0794620000	2.1071810000
H	-1.4222590000	2.5870220000	2.3791480000
H	4.9785200000	-0.4392200000	2.4625520000

1c (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1665.288846
$\varepsilon_0 + E_{tot}$ = −1665.262647
$\varepsilon_0 + H_{corr}$ = −1665.261703
$\varepsilon_0 + G_{corr}$ = −1665.351898

Coordinates:

H	3.1215390000	-0.4693560000	-2.1291840000
H	0.1613390000	1.2072550000	-2.1152230000
H	-0.7370910000	3.4618120000	-1.7789010000
H	5.4628260000	0.1539390000	-1.7776990000
F	-4.8170680000	-0.5466300000	-1.3526930000
H	-2.4211020000	5.0064110000	-1.2161080000
C	-0.1806320000	1.5044290000	-1.1330690000
C	3.5247580000	-0.4628330000	-1.1252850000
H	7.6790020000	-0.2238420000	-1.0854460000
C	-0.6917220000	2.7865700000	-0.9366530000
C	4.8567180000	-0.1060360000	-0.9218590000
H	7.1982500000	1.4921970000	-0.9068820000
H	-0.7810950000	5.6143400000	-0.8306270000
O	-2.1244320000	-1.8449120000	-0.8096960000
C	-1.7630340000	5.3643280000	-0.4195870000
C	7.5541760000	0.6024740000	-0.3804340000
I	0.6820700000	-1.3329890000	-0.3490720000
F	-3.4652290000	0.7913650000	-0.3020420000
C	-4.1974830000	-0.3238590000	-0.1808950000
C	-0.1264640000	0.6431770000	-0.0506050000
C	2.7417060000	-0.7963760000	-0.0297010000
H	-2.1988760000	6.2451340000	0.0459720000
H	8.5050310000	0.8188160000	0.1007080000
S	-3.1215710000	-1.7998170000	0.2918340000
O	-4.0740600000	-2.9252390000	0.3036290000
C	-1.1340480000	3.1723730000	0.3348490000
C	5.3817890000	-0.0898150000	0.3761900000
O	-1.6487480000	4.3910090000	0.6271190000
O	6.6588950000	0.2412230000	0.6803640000
F	-5.1392360000	-0.1079770000	0.7535090000
C	-0.5623100000	0.9933680000	1.2225270000
C	3.2445490000	-0.7915610000	1.2707390000
C	-1.0641600000	2.2711490000	1.4076030000
C	4.5682080000	-0.4338870000	1.4671000000
O	-2.5580820000	-1.4241890000	1.6020380000
H	-0.5381460000	0.2905420000	2.0421220000
H	2.6232930000	-1.0550470000	2.1162530000
H	-1.4189070000	2.5852880000	2.3811580000
H	4.9922570000	-0.4169220000	2.4632270000

1d (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1436.219593
$\varepsilon_0 + E_{tot}$ = −1436.198747
$\varepsilon_0 + H_{corr}$ = −1436.197803
$\varepsilon_0 + G_{corr}$ = −1436.275356

Coordinates:

H	3.6310440000	-0.7966130000	-2.0404760000
H	1.9187580000	1.7536600000	-1.7249610000
H	6.0460290000	-0.4810560000	-1.6010310000
H	1.4271340000	4.1661480000	-1.4804470000
F	-4.5884590000	0.0644310000	-1.3166540000
C	3.9866580000	-0.6557960000	-1.0283590000
C	1.2108250000	2.0938570000	-0.9814940000
C	0.9291690000	3.4525630000	-0.8352830000
O	-1.7846130000	-0.9679890000	-0.8257550000
C	5.3469030000	-0.4760330000	-0.7736230000
I	1.0024210000	-0.9067940000	-0.3252190000
C	0.5520230000	1.2172450000	-0.1345080000
C	-4.0549000000	0.1695510000	-0.0898000000
F	-3.4655060000	1.3721850000	0.0087100000
O	-3.5979900000	-2.4429330000	0.0446270000
C	3.1143430000	-0.6415920000	0.0531000000
C	0.0118640000	3.8829940000	0.1225610000
H	-0.2037180000	4.9397600000	0.2236230000
S	-2.8111350000	-1.2135520000	0.2244940000
C	5.7990110000	-0.2906090000	0.5310940000
H	6.8565160000	-0.1509290000	0.7200690000
F	-5.0528160000	0.1193570000	0.8068350000
C	-0.3653730000	1.5964190000	0.8289800000
C	-0.6319490000	2.9622990000	0.9459970000
C	3.5357570000	-0.4679740000	1.3660160000
H	-0.8744340000	0.8720550000	1.4499150000
O	-2.3326420000	-0.9457670000	1.5959330000
C	4.8985810000	-0.2860740000	1.5959540000
H	-1.3498130000	3.2941550000	1.6861490000
H	2.8334810000	-0.4671310000	2.1889070000
H	5.2503700000	-0.1444850000	2.6106880000

1d (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1436.224956
$\varepsilon_0 + E_{tot}$ = −1436.204132
$\varepsilon_0 + H_{corr}$ = −1436.203188
$\varepsilon_0 + G_{corr}$ = −1436.280356

Coordinates:

H	3.6424350000	-0.6210140000	-2.0567720000
H	1.5354690000	1.7232400000	-1.9398360000
H	0.9514010000	4.1135300000	-1.6702730000
H	6.0444170000	-0.2229380000	-1.6145570000
F	-4.5486630000	0.1068080000	-1.2960480000
C	0.9438910000	2.0493080000	-1.0954690000
C	3.9992860000	-0.5159320000	-1.0410720000
C	0.6108520000	3.3948040000	-0.9349320000
O	-1.7913930000	-1.0716610000	-0.8471080000
C	5.3522240000	-0.2903470000	-0.7841150000
I	1.0335490000	-0.9294340000	-0.3370700000
C	0.4892730000	1.1650270000	-0.1295550000
C	-3.9787570000	0.2045830000	-0.0840070000
F	-3.3222860000	1.3722920000	-0.0229080000
C	3.1371280000	-0.5940030000	0.0452680000
O	-3.6742700000	-2.4253660000	0.0669890000
C	-0.1552820000	3.8058550000	0.1553100000
S	-2.8090670000	-1.2429300000	0.2230640000
H	-0.4106950000	4.8524740000	0.2684460000
C	5.8057250000	-0.1520330000	0.5261930000
H	6.8576510000	0.0234330000	0.7163060000
F	-4.9562590000	0.2243830000	0.8370480000
C	-0.2767120000	1.5268210000	0.9654350000
C	-0.5981670000	2.8790720000	1.0964900000
C	3.5579870000	-0.4679540000	1.3633900000
O	-2.2978890000	-0.9986440000	1.5861590000
C	4.9140280000	-0.2398560000	1.5946960000
H	-0.6378330000	0.7954090000	1.6743560000
H	-1.2004920000	3.1966030000	1.9389180000
H	2.8623650000	-0.5376090000	2.1887000000
H	5.2667060000	-0.1342970000	2.6134570000

1d (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1436.206741
$\varepsilon_0 + E_{tot}$ = −1436.185969

$\varepsilon_0 + H_{corr}$ = −1436.185025
$\varepsilon_0 + G_{corr}$ = −1436.262517
Coordinates:

H	3.5322400000	-1.0273420000	-2.0364580000
H	5.9680620000	-0.7540230000	-1.6940090000
H	2.1585920000	1.7087390000	-1.5073710000
F	-4.5149700000	-0.0414580000	-1.4285690000
H	1.7452120000	4.1432700000	-1.3268750000
C	3.9217340000	-0.8080980000	-1.0505940000
C	1.3771670000	2.0844830000	-0.8606990000
C	5.2940410000	-0.6517280000	-0.8519800000
C	1.1401520000	3.4547450000	-0.7492830000
O	-1.7249050000	-0.9315280000	-0.7375510000
I	0.9497040000	-0.9068840000	-0.2556340000
C	-4.0695840000	0.1370220000	-0.1772340000
C	0.5789920000	1.2428270000	-0.1039500000
F	-3.5319830000	1.3685850000	-0.0963330000
C	3.0773080000	-0.6703880000	0.0452960000
C	0.1300130000	3.9287550000	0.0864950000
O	-3.5046930000	-2.4453780000	0.1414780000
H	-0.0512400000	4.9943380000	0.1598820000
S	-2.7926900000	-1.1731530000	0.2827480000
C	5.7904350000	-0.3651340000	0.4174580000
H	6.8569490000	-0.2440680000	0.5646780000
F	-5.1194960000	0.0877370000	0.6551550000
C	-0.4309170000	1.6631250000	0.7404830000
C	-0.6493310000	3.0404110000	0.8229890000
H	-1.0392780000	0.9661090000	1.3014790000
C	3.5487230000	-0.3937880000	1.3237960000
H	-1.4383390000	3.4045840000	1.4696360000
C	4.9219010000	-0.2358750000	1.5007850000
O	-2.3765340000	-0.7902860000	1.6472340000
H	2.8714620000	-0.2948660000	2.1620380000
H	5.3083540000	-0.0158030000	2.4887130000

1d (M06-2X, Toluene)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −1435.707736
$\varepsilon_0 + E_{tot}$ = −1435.687463
$\varepsilon_0 + H_{corr}$ = −1435.686519
$\varepsilon_0 + G_{corr}$ = −1435.761618
Coordinates:

H	3.4977130000	-1.1846490000	-1.9836960000
H	5.9308260000	-0.8893140000	-1.6462070000
H	2.1669510000	1.6542150000	-1.5028310000
F	-4.3947110000	0.0518650000	-1.4185860000
H	1.7509930000	4.0892130000	-1.3611410000
C	3.8819070000	-0.8874100000	-1.0156780000
C	1.3772420000	2.0404140000	-0.8706760000
C	5.2504840000	-0.7187710000	-0.8211950000
C	1.1382580000	3.4084720000	-0.7834110000
O	-1.6821630000	-0.8701380000	-0.7138420000
I	0.9316070000	-0.9109640000	-0.2352170000
C	-4.0047440000	0.1456020000	-0.1517180000
C	0.5679180000	1.2072880000	-0.1191770000
C	0.1156020000	3.8920940000	0.0266170000
F	-3.4782660000	1.3584460000	0.0354560000
O	-3.4631740000	-2.4141630000	0.0401490000
C	3.0307850000	-0.6626460000	0.0571280000
H	-0.0674930000	4.9579550000	0.0814680000
S	-2.7622120000	-1.1623230000	0.2599210000
C	5.7369090000	-0.3316890000	0.4217620000
H	6.8021360000	-0.1996570000	0.5661000000
F	-5.0757120000	0.0344860000	0.6282730000
C	-0.4537840000	1.6410730000	0.7021480000
C	-0.6741690000	3.0160050000	0.7612630000
H	-1.0668190000	0.9501000000	1.2692750000
C	3.4945720000	-0.2842500000	1.3097860000
H	-1.4721420000	3.3900460000	1.3905380000
C	4.8633450000	-0.1138260000	1.4831860000
O	-2.3774490000	-0.8500550000	1.6367560000
H	2.8089540000	-0.1183200000	2.1315810000
H	5.2436320000	0.1862270000	2.4516670000

1e (B3LYP-D3, Toluene)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −1672.033524
$\varepsilon_0 + E_{tot}$ = −1672.003296
$\varepsilon_0 + H_{corr}$ = −1672.002352
$\varepsilon_0 + G_{corr}$ = −1672.098179
Coordinates:

H	1.0272950000	2.6518570000	-3.0199860000
H	-0.2088510000	1.3935220000	-2.9578700000
H	-2.4764010000	0.6906480000	-2.7265910000
H	1.4641560000	1.0082980000	-2.5254850000
C	0.6894000000	1.7757680000	-2.4671620000
H	-3.8309280000	1.7409480000	-2.3089270000
C	-2.9938940000	1.1781170000	-1.8963720000
H	-2.2993380000	1.8893760000	-1.4437940000
H	1.1206800000	4.1386950000	-1.2819820000
O	2.2443830000	-0.6618770000	-1.0364690000
C	0.4345650000	2.1337320000	-1.0278000000
F	5.0850470000	-1.6359450000	-0.9929800000
H	-5.4956010000	0.8723010000	-0.9921620000
C	-3.4793410000	0.1689510000	-0.8891110000
I	-0.5138700000	-0.7937530000	-0.7226290000
C	0.7333140000	3.4202290000	-0.5678690000
C	-4.8312570000	0.1485710000	-0.5318560000
C	-2.6502320000	-0.7706220000	-0.2663140000
C	-0.0509580000	1.2507190000	-0.0614560000
O	3.8292730000	0.9267810000	0.0477330000
H	-7.3497550000	-1.4834080000	0.0729040000
C	4.3734220000	-1.6740450000	0.1445170000
S	3.0632660000	-0.3187400000	0.1678850000
F	3.8030850000	-2.8888310000	0.2376010000
C	-5.3464600000	-0.7663780000	0.3850570000
H	0.7913390000	5.9199230000	0.4381670000
H	-1.7954120000	-3.4417810000	0.5658590000
H	-7.2676140000	0.2027500000	0.5862310000
C	-3.1111300000	-1.7237570000	0.6527300000
C	-6.8160010000	-0.7817280000	0.7223900000
C	0.5723490000	3.7954570000	0.7650840000
C	-4.4747190000	-1.6922730000	0.9581170000
F	5.2228870000	-1.5340260000	1.1740050000
C	0.9547310000	5.1796120000	1.2241690000
C	-0.2130920000	1.5388290000	1.2930430000
C	-2.2308710000	-2.7625420000	1.3041760000
O	2.3504250000	-0.5393810000	1.4396720000
H	2.0166380000	5.2075850000	1.4884290000
H	-4.8601270000	-2.4156880000	1.6688310000
C	0.1009600000	2.8480080000	1.6718920000
H	-6.9835960000	-1.0978070000	1.7541280000
H	-1.4050510000	-2.3084370000	1.8566130000
H	-2.8094960000	-3.3657830000	2.0036160000
H	0.3858540000	5.4802870000	2.1062300000
H	-1.6628510000	0.1775430000	2.1398480000

C	-0.6490420000	0.5392020000	2.3279800000
H	0.0406470000	-0.3081740000	2.3297470000
H	-0.0086510000	3.1161640000	2.7170490000
H	-0.6323700000	0.9898810000	3.3198950000

1e (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1671.393691
$\varepsilon_0 + E_{tot}$ = −1671.363975
$\varepsilon_0 + H_{corr}$ = −1671.363031
$\varepsilon_0 + G_{corr}$ = −1671.456308

Coordinates:

H	1.0469600000	2.6117970000	-3.0185170000
H	-0.2061730000	1.3694640000	-2.9510210000
H	-2.4390910000	0.6921580000	-2.7344270000
H	1.4699720000	0.9563130000	-2.5455750000
C	0.7058440000	1.7336930000	-2.4725240000
H	-3.7715010000	1.7707930000	-2.3145760000
C	-2.9370090000	1.2027400000	-1.9063540000
H	-2.2273620000	1.9087570000	-1.4680160000
H	1.2027830000	4.0770050000	-1.2727950000
O	2.2203920000	-0.6810980000	-1.0694180000
C	0.4751740000	2.0869300000	-1.0296550000
H	-5.4367820000	0.9481790000	-0.9789660000
F	5.0817240000	-1.4558920000	-0.9365390000
C	-3.4313700000	0.2139830000	-0.8861080000
I	-0.5153690000	-0.7917950000	-0.7346660000
C	0.8030310000	3.3598490000	-0.5635050000
C	-4.7798550000	0.2156810000	-0.5217390000
C	-2.6146810000	-0.7336360000	-0.2704640000
C	-0.0233400000	1.2056020000	-0.0711550000
F	3.8317000000	-2.8552550000	0.1285500000
C	4.3234350000	-1.6162620000	0.1452530000
S	2.9543560000	-0.3729690000	0.1806700000
O	3.6349080000	0.9121360000	0.1855140000
H	-7.2827960000	0.1467200000	0.2801050000
C	-5.3001580000	-0.6903450000	0.3949530000
H	0.9199810000	5.8403850000	0.4604980000
H	-7.2391790000	-1.6106130000	0.4743210000
H	-1.8020120000	-3.4181660000	0.5386150000
C	-3.0858220000	-1.6821470000	0.6460600000
C	-6.7583190000	-0.6746650000	0.7678390000
C	0.6557390000	3.7249050000	0.7714320000
C	-4.4418250000	-1.6327140000	0.9588100000
F	5.0973760000	-1.4904820000	1.2203930000
C	1.0700740000	5.0933620000	1.2407930000
C	-0.1804920000	1.4899740000	1.2825790000
C	-2.2136580000	-2.7327570000	1.2836300000
O	2.2012380000	-0.7221140000	1.3855660000
H	2.1316860000	5.0904770000	1.5014960000
H	-4.8365910000	-2.3541460000	1.6673610000
C	0.1651760000	2.7845770000	1.6714270000
H	-1.3741310000	-2.2888410000	1.8234710000
H	-6.8785600000	-0.5673740000	1.8479710000
H	-2.7965370000	-3.3227390000	1.9893210000
H	-1.6780780000	0.1799800000	2.1202220000
H	0.5081090000	5.3938050000	2.1256910000
H	0.0099840000	-0.3798890000	2.2836480000
C	-0.6469090000	0.4931520000	2.3044520000
H	0.0628420000	3.0485020000	2.7186740000
H	-0.5983550000	0.9318180000	3.2997920000

TfO^- (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −961.784737
$\varepsilon_0 + E_{tot}$ = −961.777512
$\varepsilon_0 + H_{corr}$ = −961.776568
$\varepsilon_0 + G_{corr}$ = −961.817180

Coordinates:

O	-1.2568480000	0.3701510000	-1.3908820000
F	1.4497760000	-0.8896880000	-0.8856580000
F	1.4496650000	1.2120300000	-0.3278060000
C	0.9648720000	0.0000740000	-0.0001540000
S	-0.9239170000	-0.0000470000	0.0000640000
O	-1.2557470000	-1.3899810000	0.3749800000
O	-1.2560260000	1.0195970000	1.0162570000
F	1.4497170000	-0.3221020000	1.2131370000

TfO^- (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −961.793784
$\varepsilon_0 + E_{tot}$ = −961.786530
$\varepsilon_0 + H_{corr}$ = −961.785586
$\varepsilon_0 + G_{corr}$ = −961.826335

Coordinates:

F	1.4476980000	0.3197380000	-1.2140660000
O	-1.2563540000	-1.0223980000	-1.0129510000
O	-1.2563320000	1.3884450000	-0.3789820000
S	-0.9209500000	0.0000020000	0.0000080000
C	0.9666380000	-0.0000680000	0.0001050000
F	1.4478560000	-1.2114830000	0.3302180000
F	1.4478320000	0.8917580000	0.8838870000
O	-1.2567010000	-0.3660140000	1.3917950000

TfO^- (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −961.757411
$\varepsilon_0 + E_{tot}$ = −961.750213
$\varepsilon_0 + H_{corr}$ = −961.749269
$\varepsilon_0 + G_{corr}$ = −961.789779

Coordinates:

F	1.4548680000	-0.3115290000	-1.2152500000
O	-1.2546450000	1.0315800000	-1.0055410000
O	-1.2559160000	-1.3865110000	-0.3905720000
S	-0.9313300000	-0.0001360000	-0.0001940000
C	0.9608100000	-0.0000820000	0.0002550000
F	1.4543110000	1.2087270000	0.3382460000
F	1.4543810000	-0.8974110000	0.8777710000
O	-1.2563920000	0.3555060000	1.3954470000

TfO^- (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −961.530473
$\varepsilon_0 + E_{tot}$ = −961.523537
$\varepsilon_0 + H_{corr}$ = −961.522593
$\varepsilon_0 + G_{corr}$ = −961.562407

Coordinates:

F	1.4296880000	0.0708100000	-1.2448200000
O	-1.2367350000	-1.0712110000	-0.9586110000
O	-1.2339130000	1.3669490000	-0.4479210000
C	0.9426710000	-0.0002300000	-0.0000510000
S	-0.9145480000	0.0000130000	0.0002390000
F	1.4310770000	-1.1133860000	0.5603290000
F	1.4305590000	1.0418220000	0.6835590000
O	-1.2349990000	-0.2947440000	1.4071400000

HO^- (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −75.936860
$\varepsilon_0 + E_{tot}$ = −75.934499
$\varepsilon_0 + H_{corr}$ = −75.933555
$\varepsilon_0 + G_{corr}$ = −75.953110

Coordinates:

	0.000000000	0.000000000	-
H	0	0	0.8566970000
	0.000000000	0.000000000	
O	0	0	0.1070870000

HO^- (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −75.950621
$\varepsilon_0 + E_{tot}$ = −75.948260
$\varepsilon_0 + H_{corr}$ = −75.947316
$\varepsilon_0 + G_{corr}$ = −75.966871

Coordinates:

	0.000000000	0.000000000	-
H	0	0	0.8566010000
	0.000000000	0.000000000	
O	0	0	0.1070750000

HO^- (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −75.852788
$\varepsilon_0 + E_{tot}$ = −75.850427
$\varepsilon_0 + H_{corr}$ = −75.849483
$\varepsilon_0 + G_{corr}$ = −75.869034

Coordinates:

	0.000000000	0.000000000	-
H	0	0	0.8545720000
	0.000000000	0.000000000	
O	0	0	0.1068210000

1-phenylethoxide (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −385.521650
$\varepsilon_0 + E_{tot}$ = −385.513858
$\varepsilon_0 + H_{corr}$ = −385.512913
$\varepsilon_0 + G_{corr}$ = −385.554042

Coordinates:

H	-1.8928490000	-0.7275710000	-1.2709400000
H	0.1197260000	-2.1206170000	-0.6403190000
O	-2.3114950000	1.1445460000	-0.4840020000
C	-1.7359560000	-0.0673960000	-0.3696900000
C	0.5976640000	-1.1830100000	-0.3658350000
H	2.5738060000	-2.0392870000	-0.3285020000
C	-0.1936050000	-0.0386820000	-0.2038170000
C	1.9801170000	-1.1394610000	-0.1925870000
C	0.4449750000	1.1590350000	0.1240810000
C	2.6037420000	0.0622510000	0.1510440000
H	-0.1837510000	2.0382080000	0.2150780000
H	3.6802090000	0.1018140000	0.2867300000
C	1.8276400000	1.2111130000	0.3072560000
H	2.3047880000	2.1525250000	0.5661730000
H	-3.3944460000	-0.9749550000	0.7033030000
C	-2.3106900000	-0.8924820000	0.8279530000
H	-1.8853260000	-1.9022870000	0.9091240000
H	-2.1135260000	-0.3524030000	1.7609380000

1-phenylethoxide (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −385.331538
$\varepsilon_0 + E_{tot}$ = −385.323845
$\varepsilon_0 + H_{corr}$ = −385.322901
$\varepsilon_0 + G_{corr}$ = −385.363773

Coordinates:

H	-1.8919470000	-0.7289410000	-1.2679870000
H	0.1177600000	-2.1200120000	-0.6411360000
O	-2.3009840000	1.1385410000	-0.4779700000
C	-1.7320450000	-0.0721060000	-0.3710230000
C	0.5947950000	-1.1819830000	-0.3662530000
H	2.5693480000	-2.0328240000	-0.3230350000
C	-0.1961820000	-0.0406620000	-0.2087460000
C	1.9737530000	-1.1351970000	-0.1899010000
C	0.4357790000	1.1567630000	0.1188570000
C	2.5918930000	0.0662210000	0.1524040000
H	-0.1964430000	2.0336260000	0.2051940000
H	3.6668270000	0.1080220000	0.2911030000
C	1.8153960000	1.2114330000	0.3047280000
H	2.2910040000	2.1527970000	0.5620850000
H	-3.3738520000	-0.9704370000	0.7195950000
C	-2.2894400000	-0.8894320000	0.8292930000
H	-1.8618280000	-1.8964970000	0.9070100000
H	-2.0766870000	-0.3442880000	1.7547770000

1a-OH (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.960597
$\varepsilon_0 + E_{tot}$ = −754.944333
$\varepsilon_0 + H_{corr}$ = −754.943389
$\varepsilon_0 + G_{corr}$ = −755.007521

Coordinates:

H	-2.5760730000	0.6591140000	-2.0927890000
H	-3.7036180000	2.8606790000	-2.0116490000
C	-2.7073270000	1.1648290000	-1.1431430000
C	-3.3420580000	2.4069720000	-1.0959980000
H	0.0028440000	-3.7897620000	-0.8913040000
H	2.2553770000	2.4388420000	-0.4797920000
H	-0.0291100000	1.4782630000	-0.4795650000
C	0.8227250000	0.8437370000	-0.2842590000
C	2.1035870000	1.3875000000	-0.2815970000
O	4.6582790000	2.3369990000	-0.2317430000
C	0.6864610000	-0.5135980000	-0.0335250000
I	-1.3183320000	-1.4261180000	-0.0228300000
C	3.1874100000	0.5547650000	-0.0209200000
N	4.5438800000	1.1351140000	-0.0140280000
O	-0.1717690000	-3.5005910000	0.0133340000
C	-2.2421910000	0.5895140000	0.0375390000
C	-3.5073670000	3.0604790000	0.1243060000
H	-3.9997660000	4.0253530000	0.1585550000
O	5.4895240000	0.3869150000	0.2093610000
C	1.7572380000	-1.3538610000	0.2225660000
C	3.0360970000	-0.8054110000	0.2317120000
H	1.5737670000	-2.4103910000	0.3897320000
H	3.8995630000	-1.4235650000	0.4323870000
C	-2.4092840000	1.2327750000	1.2623360000
C	-3.0428990000	2.4745690000	1.3019790000
H	-2.0477730000	0.7786910000	2.1775700000
H	-3.1733710000	2.9810280000	2.2514760000

1a-OH (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.964227
$\varepsilon_0 + E_{tot}$ = −754.947886
$\varepsilon_0 + H_{corr}$ = −754.946942
$\varepsilon_0 + G_{corr}$ = −755.011344

Coordinates:

H	-2.6061940000	0.6482700000	-2.0832090000
H	-3.7326130000	2.8503270000	-1.9941300000
C	-2.7242320000	1.1578000000	-1.1341670000
C	-3.3579800000	2.4002750000	-1.0820390000
H	0.0590300000	-3.7732390000	-0.8954280000
H	-0.0247380000	1.4652190000	-0.5401390000
H	2.2575290000	2.4260030000	-0.5387360000
C	0.8244810000	0.8357050000	-0.3189310000
C	2.1051130000	1.3797940000	-0.3158090000
O	4.6589280000	2.3321640000	-0.2522410000

C	0.6857990000	-0.5148680000	-0.0358220000
I	-1.3192000000	-1.4208440000	-0.0261890000
C	3.1862020000	0.5539050000	-0.0234170000
N	4.5410950000	1.1337710000	-0.0158730000
O	-0.1740680000	-3.5203010000	0.0069670000
C	-2.2422640000	0.5890330000	0.0427130000
C	-3.5046000000	3.0587560000	0.1380490000
H	-3.9960480000	4.0239500000	0.1756140000
O	5.4864930000	0.3902260000	0.2270070000
C	1.7541220000	-1.3488210000	0.2504190000
C	3.0325560000	-0.8003190000	0.2597290000
H	1.5721980000	-2.4013050000	0.4391220000
H	3.8934130000	-1.4139170000	0.4837930000
C	-2.3893310000	1.2358980000	1.2679400000
C	-3.0219990000	2.4781130000	1.3111710000
H	-2.0133240000	0.7858440000	2.1790970000
H	-3.1373620000	2.9888570000	2.2602440000

1a-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.564042
$\varepsilon_0 + E_{tot}$ = −754.548099
$\varepsilon_0 + H_{corr}$ = −754.547154
$\varepsilon_0 + G_{corr}$ = −754.611051

Coordinates:

H	-2.7376040000	0.6111650000	-2.0151180000
H	-3.7869620000	2.8456410000	-1.9054020000
C	-2.7515830000	1.1550330000	-1.0761710000
C	-3.3425420000	2.4150830000	-1.0158860000
H	-0.0417950000	-3.6938300000	-0.9160100000
H	2.2613620000	2.3308250000	-0.7553090000
H	-0.0317920000	1.3831320000	-0.7518190000
C	0.8050750000	0.7707850000	-0.4460310000
C	2.0856510000	1.3099610000	-0.4457810000
O	4.6225480000	2.2462640000	-0.3681470000
C	0.6422980000	-0.5487520000	-0.0538530000
C	3.1417190000	0.5104040000	-0.0397340000
N	4.5016060000	1.0876070000	-0.0325080000
O	-0.2281950000	-3.3747540000	-0.0278740000
I	-1.3398180000	-1.4244100000	-0.0268840000
C	-2.1773280000	0.6023220000	0.0641590000
C	-3.3580880000	3.1168310000	0.1844580000
H	-3.8162300000	4.0973990000	0.2328850000
O	5.4157930000	0.3691000000	0.3081320000
C	1.6983510000	-1.3536690000	0.3425870000
C	2.9761660000	-0.8074220000	0.3550510000
H	1.5090800000	-2.3877500000	0.6047120000
H	3.8301480000	-1.3946980000	0.6637230000
C	-2.1996660000	1.3007330000	1.2677520000
C	-2.7880240000	2.5600980000	1.3260830000
H	-1.7564530000	0.8701280000	2.1596280000
H	-2.8039860000	3.1051620000	2.2624170000

1c-OH (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.455498
$\varepsilon_0 + E_{tot}$ = −779.436549
$\varepsilon_0 + H_{corr}$ = −779.435605
$\varepsilon_0 + G_{corr}$ = −779.504785

Coordinates:

H	3.3519340000	1.1082250000	-2.4051190000
H	1.3688790000	-0.3686920000	-2.2404580000
C	3.0368350000	0.7100970000	-1.4480100000
C	1.9302600000	-0.1189250000	-1.3476460000
H	-3.1716990000	4.5027040000	-0.5659060000
O	4.8391700000	1.8658630000	-0.5064200000
H	-4.8369210000	0.3694680000	-0.4937040000
H	-3.2216360000	-1.5578410000	-0.4168030000
C	3.7719850000	1.0469710000	-0.3018100000
C	-3.7881070000	0.5320440000	-0.2767140000
C	-2.9016680000	-0.5358250000	-0.2485170000
C	1.5407050000	-0.6178460000	-0.1018160000
O	-4.2942560000	2.8079010000	-0.0776350000
C	-3.3421370000	1.8367760000	-0.0260190000
C	-1.5679730000	-0.2749810000	0.0291330000
I	-0.1819860000	-1.9895030000	0.0521880000
H	-4.8160460000	4.7516840000	0.0740940000
O	-2.1389800000	-3.3608430000	0.1029560000
C	-3.9067450000	4.1622250000	0.1696640000
H	6.4176190000	2.8932550000	0.2193690000
C	-1.9920290000	2.0673110000	0.2546550000
C	-1.0929040000	0.9975010000	0.2798620000
H	-1.6189570000	3.0615880000	0.4557360000
H	-0.0494080000	1.1855690000	0.4898360000
C	5.6374480000	2.2480880000	0.6174600000
C	3.3871240000	0.5443410000	0.9451530000
H	-2.4649310000	-3.4400240000	1.0082350000
C	2.2688800000	-0.2878780000	1.0351690000
H	6.0930010000	1.3743510000	1.0930640000
H	-3.5005810000	4.2784960000	1.1790380000
H	5.0448060000	2.8015430000	1.3520350000
H	3.9372150000	0.7886110000	1.8432480000
H	1.9744600000	-0.6680240000	2.0067650000

1c-OH (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.459300
$\varepsilon_0 + E_{tot}$ = −779.440279
$\varepsilon_0 + H_{corr}$ = −779.439335
$\varepsilon_0 + G_{corr}$ = −779.508743

Coordinates:

H	3.3580460000	1.0909040000	-2.4093620000
H	1.3780910000	-0.3884490000	-2.2438530000
C	3.0410510000	0.6978890000	-1.4507700000
C	1.9354970000	-0.1324680000	-1.3505630000
H	-3.1689490000	4.5039650000	-0.5632990000
O	4.8366780000	1.8629650000	-0.5080730000
H	-4.8353660000	0.3688190000	-0.5020010000
H	-3.2211610000	-1.5565830000	-0.4237400000
C	3.7707400000	1.0431760000	-0.3033490000
C	-3.7871250000	0.5321550000	-0.2826670000
C	-2.9002670000	-0.5355040000	-0.2535560000
C	1.5435400000	-0.6231400000	-0.1024150000
O	-4.2936880000	2.8078510000	-0.0820190000
C	-3.3418840000	1.8368260000	-0.0292980000
C	-1.5674300000	-0.2744010000	0.0274440000
I	-0.1778150000	-1.9851000000	0.0543680000
H	-4.8151470000	4.7526240000	0.0724170000
O	-2.1503210000	-3.3805800000	0.1081520000
C	-3.9061320000	4.1631440000	0.1695040000
H	6.4036580000	2.9074740000	0.2209170000
C	-1.9924700000	2.0673120000	0.2553310000
C	-1.0931820000	0.9978080000	0.2818010000
H	-1.6200450000	3.0611630000	0.4592030000
H	-0.0507030000	1.1864980000	0.4962150000
C	5.6251290000	2.2607100000	0.6193910000
C	3.3823470000	0.5469440000	0.9453100000
H	-2.4960860000	-3.4240860000	1.0085380000

C	2.2656520000	-0.2866220000	1.0366000000
H	6.0824050000	1.3939140000	1.1052370000
H	-3.5029490000	4.2761870000	1.1800750000
H	5.0227720000	2.8161650000	1.3439780000
H	3.9278700000	0.7979250000	1.8441850000
H	1.9676220000	-0.6610860000	2.0089670000

1c-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.040117
$\varepsilon_0 + E_{tot}$ = −779.021599
$\varepsilon_0 + H_{corr}$ = −779.020654
$\varepsilon_0 + G_{corr}$ = −779.089059

Coordinates:

H	-2.2394930000	-0.9145210000	-1.8794780000
H	-4.1851550000	0.5634380000	-1.7169320000
H	-5.1934850000	2.6155690000	-1.4225180000
H	1.5328650000	3.0182350000	-0.9901570000
C	-2.4227100000	-0.3888290000	-0.9478490000
H	2.3685020000	-3.2796540000	-0.9458120000
H	-0.0355260000	1.1041780000	-0.9178860000
C	-3.5322000000	0.4548690000	-0.8616480000
H	-6.2036400000	1.2593880000	-0.8414130000
C	1.8570890000	2.0547020000	-0.6172260000
C	0.9847220000	0.9802610000	-0.5793740000
C	-5.7114910000	2.1936910000	-0.5564450000
H	5.8421350000	2.2005920000	-0.3995770000
O	3.9431020000	3.0275330000	-0.2431740000
H	-6.4547400000	2.9009300000	-0.1973700000
C	3.1744300000	1.9142740000	-0.1718430000
C	1.4504420000	-0.2383940000	-0.1039430000
O	2.0255370000	-3.1587480000	-0.0553380000
I	0.1236310000	-1.9410730000	-0.0121770000
H	5.7199440000	3.9182290000	0.0559710000
C	-1.5636400000	-0.5521750000	0.1274610000
C	5.2868990000	2.9310380000	0.1955620000
C	3.6186880000	0.6812510000	0.3033190000
C	-3.7742070000	1.1422030000	0.3258150000
C	2.7485250000	-0.4079140000	0.3317260000
O	-4.8153320000	1.9881090000	0.5207860000
H	4.6324820000	0.5441080000	0.6530090000
H	3.0778920000	-1.3856360000	0.6607320000
H	5.3345830000	2.6567050000	1.2530810000
C	-1.8202810000	0.1360040000	1.3151490000
C	-2.9118090000	0.9784810000	1.4160110000
H	-1.1573680000	0.0214610000	2.1665810000
H	-3.1246460000	1.5219030000	2.3286540000

1d-OH (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.394654
$\varepsilon_0 + E_{tot}$ = −550.380914
$\varepsilon_0 + H_{corr}$ = −550.379969
$\varepsilon_0 + G_{corr}$ = −550.437422

Coordinates:

H	-2.0655070000	-0.4246750000	-2.0597200000
H	-4.2188490000	0.7935680000	-1.9771790000
C	-2.4222260000	-0.0201050000	-1.1193970000
C	-3.6356150000	0.6689250000	-1.0718680000
H	2.6914230000	-2.4951450000	-0.8494590000
H	1.0567950000	3.8164090000	-0.7429340000
H	-0.2910320000	1.7477000000	-0.7154140000
C	1.5196300000	2.8843480000	-0.4403860000
C	0.7513120000	1.7177020000	-0.4319190000
H	3.4484920000	3.7607650000	-0.0751090000
C	2.8617090000	2.8497980000	-0.0677800000
C	1.3734950000	0.5411500000	-0.0497690000
I	0.2131300000	-1.3398830000	-0.0146360000
O	2.3161120000	-2.4495550000	0.0389350000
C	-1.6754700000	-0.1745920000	0.0463340000
C	-4.0917350000	1.1965230000	0.1349890000
H	-5.0331570000	1.7325570000	0.1698590000
C	3.4492350000	1.6442380000	0.3112510000
C	2.7035850000	0.4631100000	0.3205500000
H	3.1326630000	-0.4971900000	0.5818460000
H	4.4925560000	1.6108560000	0.6029480000
C	-2.1279560000	0.3446730000	1.2575200000
C	-3.3393800000	1.0344340000	1.2986260000
H	-1.5438180000	0.2214620000	2.1621560000
H	-3.6938790000	1.4427010000	2.2383280000

1d-OH (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.397657
$\varepsilon_0 + E_{tot}$ = −550.383852
$\varepsilon_0 + H_{corr}$ = −550.382908
$\varepsilon_0 + G_{corr}$ = −550.440604

Coordinates:

H	-2.0672850000	-0.4275200000	-2.0577920000
H	-4.2178250000	0.7954350000	-1.9727770000
C	-2.4225530000	-0.0223810000	-1.1174680000
C	-3.6342640000	0.6694870000	-1.0680100000
H	2.7194050000	-2.4741460000	-0.8478740000
H	1.0663010000	3.8108210000	-0.7677970000
H	-0.2829030000	1.7436080000	-0.7426130000
C	1.5253540000	2.8806070000	-0.4543160000
C	0.7560940000	1.7144570000	-0.4468920000
H	3.4507940000	3.7582450000	-0.0740580000
C	2.8634750000	2.8477130000	-0.0671590000
C	1.3736470000	0.5403100000	-0.0500850000
I	0.2081500000	-1.3362570000	-0.0164750000
O	2.3281760000	-2.4667190000	0.0348100000
C	-1.6763550000	-0.1768550000	0.0484170000
C	-4.0875240000	1.1985710000	0.1393720000
H	-5.0273790000	1.7371580000	0.1750440000
C	3.4465400000	1.6442210000	0.3254640000
C	2.6998380000	0.4636620000	0.3343850000
H	3.1268980000	-0.4942540000	0.6058820000
H	4.4867800000	1.6121840000	0.6279650000
C	-2.1244030000	0.3429900000	1.2608570000
C	-3.3342550000	1.0355170000	1.3024350000
H	-1.5392870000	0.2187880000	2.1644970000
H	-3.6864110000	1.4452620000	2.2422550000

1d-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.077588
$\varepsilon_0 + E_{tot}$ = −550.064193
$\varepsilon_0 + H_{corr}$ = −550.063249
$\varepsilon_0 + G_{corr}$ = −550.119669

Coordinates:

H	-2.2052350000	-0.6839100000	-1.9469120000
H	-4.3428470000	0.5495440000	-1.8417750000
C	-2.4770930000	-0.1542520000	-1.0395170000
H	1.0552460000	3.7139010000	-1.0275280000
C	-3.6833240000	0.5416670000	-0.9818740000
H	-0.2674100000	1.6333100000	-0.9619090000
H	2.6480180000	-2.4124460000	-0.8236480000
C	1.4989300000	2.8138400000	-0.6195490000
C	0.7484520000	1.6404960000	-0.5902220000

H	3.3754340000	3.7473810000	-0.1539750000
C	2.8008620000	2.8293380000	-0.1328490000
C	1.3435710000	0.5007150000	-0.0774820000
I	0.2198950000	-1.3520340000	-0.0020840000
O	2.2465490000	-2.3389890000	0.0475540000
C	-1.6277100000	-0.1656150000	0.0614960000
C	-4.0354340000	1.2253010000	0.1761390000
H	-4.9720080000	1.7681370000	0.2213610000
C	3.3661590000	1.6659280000	0.3769210000
C	2.6400970000	0.4773320000	0.4040340000
H	4.3808090000	1.6723630000	0.7563070000
H	3.0614440000	-0.4552810000	0.7580810000
C	-1.9843680000	0.5126090000	1.2236820000
C	-3.1859640000	1.2110860000	1.2793370000
H	-1.3249360000	0.5047690000	2.0855460000
H	-3.4604350000	1.7412740000	2.1837720000

1l-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −642.318268
$\varepsilon_0 + E_{tot}$ = −642.303091
$\varepsilon_0 + H_{corr}$ = −642.302147
$\varepsilon_0 + G_{corr}$ = −642.363137

Coordinates:

H	2.5391690000	0.4049210000	-2.0140580000
H	3.7886010000	2.5337610000	-1.9177170000
C	2.5863000000	0.9600960000	-1.0828130000
C	3.2906060000	2.1611560000	-1.0303920000
H	-0.6461640000	-3.5724840000	-0.8702980000
H	-2.2989460000	2.6074510000	-0.8692800000
H	-0.1239700000	1.4395220000	-0.8461910000
C	-2.2349500000	1.5890110000	-0.5082100000
C	-1.0126370000	0.9291060000	-0.5006520000
N	-5.6500000000	2.1749000000	-0.0623050000
C	-4.6408600000	1.6232640000	-0.0569830000
C	-3.3794600000	0.9347380000	-0.0515440000
C	-0.9738090000	-0.3800250000	-0.0489450000
I	0.9078760000	-1.4543530000	-0.0162960000
O	-0.4037920000	-3.2745250000	0.0116370000
C	1.9434080000	0.4823800000	0.0543600000
C	3.3500400000	2.8795280000	0.1587010000
H	3.8961400000	3.8143300000	0.1995510000
C	-2.0963190000	-1.0550680000	0.4005760000
C	-3.3112210000	-0.3826560000	0.4042650000
H	-2.0086540000	-2.0902220000	0.7068580000
H	-4.2050460000	-0.8812550000	0.7572610000
C	2.0097300000	1.1970440000	1.2470130000
C	2.7109050000	2.3975230000	1.2976350000
H	1.5117690000	0.8254920000	2.1366330000
H	2.7596090000	2.9545320000	2.2258840000

1m-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.565816
$\varepsilon_0 + E_{tot}$ = −754.549966
$\varepsilon_0 + H_{corr}$ = −754.549021
$\varepsilon_0 + G_{corr}$ = −754.612014

Coordinates:

H	2.9622170000	1.1623190000	-1.8851060000
H	0.5610950000	0.5112790000	-1.8564990000
C	2.5605250000	0.5392190000	-1.0977580000
C	1.2241360000	0.1657880000	-1.0705030000
O	5.1959120000	1.1624700000	-1.0241320000
H	-3.7458900000	0.3411530000	-1.0185950000
H	-4.4521820000	2.7338870000	-0.9125470000
C	-3.1472330000	1.0855170000	-0.5103490000
C	-3.5389790000	2.4190910000	-0.4223620000
O	-3.5376560000	-1.7669000000	-0.1760880000
N	4.8128130000	0.4775490000	-0.0999290000
C	3.3884440000	0.0870160000	-0.0790040000
I	-1.3634730000	-1.3489660000	-0.0559000000
C	0.7372520000	-0.6367480000	-0.0409100000
C	-1.9699140000	0.7165880000	0.1154790000
C	-2.7719890000	3.3359860000	0.2879730000
H	-3.0884710000	4.3696740000	0.3545160000
H	-3.9699880000	-1.7386920000	0.6827680000
O	5.5172290000	0.0914260000	0.8083270000
C	-1.1834770000	1.6014930000	0.8325860000
C	-1.6029330000	2.9267910000	0.9191320000
C	2.9361170000	-0.7155610000	0.9552520000
C	1.5920370000	-1.0746830000	0.9654810000
H	-0.2708780000	1.2841290000	1.3200920000
H	-1.0087930000	3.6330890000	1.4858730000
H	3.6191450000	-1.0429340000	1.7271860000
H	1.2203220000	-1.7004870000	1.7695650000

1n-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1469.297103
$\varepsilon_0 + E_{tot}$ = −1469.281272
$\varepsilon_0 + H_{corr}$ = −1469.280328
$\varepsilon_0 + G_{corr}$ = −1469.343890

Coordinates:

H	2.0802850000	-0.9544270000	-2.0323650000
H	4.0629180000	0.5282190000	-1.9768760000
C	2.3270540000	-0.4272170000	-1.1167770000
C	3.4437120000	0.4049100000	-1.0973660000
H	-1.5903850000	2.9817140000	-0.9606390000
H	-0.0351520000	1.0645260000	-0.9445960000
H	-2.4198140000	-3.3480110000	-0.7895930000
C	-1.9095780000	2.0273560000	-0.5624940000
C	-1.0369900000	0.9437500000	-0.5551110000
Cl	-4.2794040000	3.2343060000	-0.0590470000
C	-3.1919750000	1.8719890000	-0.0552810000
C	-1.4850250000	-0.2647390000	-0.0498670000
I	-0.1619390000	-1.9755350000	-0.0076600000
C	1.5373780000	-0.5765970000	0.0175740000
C	3.7528490000	1.0818430000	0.0737730000
O	-2.0515150000	-3.1690620000	0.0808920000
Cl	5.1460970000	2.1307500000	0.1114410000
C	-2.7649550000	-0.4363140000	0.4480220000
C	-3.6279620000	0.6545890000	0.4494430000
H	-3.0784760000	-1.4123350000	0.7969510000
H	-4.6325730000	0.5536960000	0.8394460000
C	1.8705180000	0.1049160000	1.1846290000
C	2.9792200000	0.9425610000	1.2195310000
H	1.2643910000	-0.0049810000	2.0778180000
H	3.2444390000	1.4791980000	2.1215650000

1o-OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −748.577084
$\varepsilon_0 + E_{tot}$ = −748.562073
$\varepsilon_0 + H_{corr}$ = −748.561129
$\varepsilon_0 + G_{corr}$ = −748.621577

Coordinates:

H	2.1123300000	-0.7440270000	-2.0132340000
H	4.1828700000	0.6423910000	-1.9320620000
C	2.3788160000	-0.2279390000	-1.0969700000
C	3.5379260000	0.5437890000	-1.0680550000

H	-1.4272070000	3.3618000000	-0.9490460000
H	0.0714770000	1.3771860000	-0.9238490000
H	-2.4874170000	-2.9487000000	-0.8097090000
C	-1.7713150000	2.4103560000	-0.5645600000
C	-0.9402980000	1.2944780000	-0.5507040000
F	-3.8571510000	3.3667240000	-0.0838350000
C	-3.0585410000	2.2862160000	-0.0752760000
C	-1.4409510000	0.1006710000	-0.0579860000
I	-0.1830860000	-1.6568720000	-0.0060680000
C	1.5725520000	-0.3348820000	0.0316200000
O	-2.1187810000	-2.7873320000	0.0641150000
C	3.8585970000	1.1965680000	0.1074660000
F	4.9743120000	1.9465500000	0.1463340000
C	-3.5570570000	1.0940950000	0.4174840000
C	-2.7336920000	-0.0269170000	0.4221220000
H	-3.0843210000	-0.9936760000	0.7615490000
H	-4.5728370000	1.0452320000	0.7880710000
C	1.9283340000	0.3309660000	1.2020110000
C	3.0790110000	1.1095120000	1.2481790000
H	1.3072950000	0.2527950000	2.0880860000
H	3.3769060000	1.6389500000	2.1444110000

1a-(OH)$_2$ (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.917695
$\varepsilon_0 + E_{tot}$ = −830.898289
$\varepsilon_0 + H_{corr}$ = −830.897345
$\varepsilon_0 + G_{corr}$ = −830.968297

Coordinates:

H	-2.1299940000	1.0177790000	-2.1387560000
H	-2.9118670000	3.3658390000	-2.1216030000
C	-2.2549590000	1.5397580000	-1.1976320000
C	-2.6967340000	2.8630660000	-1.1852600000
H	-0.5670950000	-3.9859890000	-0.6945570000
H	2.7342780000	2.3522710000	-0.1033460000
H	0.3651200000	1.6580930000	-0.1028830000
O	-3.7312730000	-1.6628640000	-0.1025960000
C	1.1374590000	0.9029550000	-0.0620930000
C	2.4688660000	1.3051480000	-0.0619330000
O	5.1202540000	1.9548520000	-0.0482980000
C	0.8170210000	-0.4538200000	-0.0116050000
C	3.4636440000	0.3310230000	-0.0087220000
N	4.8697190000	0.7509920000	-0.0074010000
I	-1.3247780000	-1.2032660000	-0.0001110000
C	-1.9804840000	0.8976530000	0.0065370000
C	-2.8620400000	3.5351600000	0.0256670000
H	-3.2062090000	4.5630710000	0.0327300000
O	5.7391310000	-0.1175500000	0.0345160000
C	1.8234230000	-1.4176630000	0.0412530000
C	3.1584800000	-1.0286200000	0.0424630000
H	1.5318930000	-2.4656550000	0.0718660000
O	-0.2472340000	-3.5112360000	0.0818900000
H	3.9524190000	-1.7616630000	0.0824580000
H	-4.1143250000	-1.4992900000	0.7677790000
C	-2.1435670000	1.5599570000	1.2199350000
C	-2.5867900000	2.8834250000	1.2270590000
H	-1.9267260000	1.0564270000	2.1548740000
H	-2.7152500000	3.4014250000	2.1709870000

1a-(OH)$_2$ (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.930568
$\varepsilon_0 + E_{tot}$ = −830.910957
$\varepsilon_0 + H_{corr}$ = −830.910013
$\varepsilon_0 + G_{corr}$ = −830.982197

Coordinates:

H	-2.2417610000	0.9909230000	-2.1040200000
H	-3.0627260000	3.3249380000	-2.0501550000
C	-2.3315510000	1.5112540000	-1.1579050000
C	-2.7931620000	2.8281880000	-1.1250600000
H	-0.2157340000	-3.8667080000	-0.8796720000
H	-4.2020780000	-0.9791990000	-0.4606270000
H	2.7235790000	2.3394400000	-0.3559050000
H	0.3581000000	1.6302630000	-0.3534040000
C	2.4626270000	1.3010970000	-0.2073850000
C	1.1333580000	0.8915880000	-0.2059860000
O	5.1104260000	1.9668920000	-0.1785600000
C	0.8225450000	-0.4542280000	-0.0180650000
N	4.8629020000	0.7734050000	-0.0159460000
C	3.4585130000	0.3460800000	-0.0153390000
I	-1.3012020000	-1.2045900000	-0.0139180000
O	-0.2616600000	-3.5383090000	0.0266220000
C	-1.9857200000	0.8800810000	0.0336760000
O	-3.7616490000	-1.6742640000	0.0430140000
C	-2.9028740000	3.5010550000	0.0911530000
H	-3.2595250000	4.5242670000	0.1136830000
O	5.7329160000	-0.0802150000	0.1457300000
C	1.8277420000	-1.4003920000	0.1699310000
C	3.1597880000	-1.0023160000	0.1738500000
H	1.5432510000	-2.4422090000	0.2941660000
H	3.9551050000	-1.7198860000	0.3201520000
C	-2.0937520000	1.5412760000	1.2537290000
C	-2.5537100000	2.8583180000	1.2787630000
H	-1.8203330000	1.0438630000	2.1764900000
H	-2.6375610000	3.3789000000	2.2259780000

1c-(OH)$_2$ (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.404802
$\varepsilon_0 + E_{tot}$ = −855.382778
$\varepsilon_0 + H_{corr}$ = −855.381834
$\varepsilon_0 + G_{corr}$ = −855.457599

Coordinates:

H	-1.4682730000	0.0407700000	-2.0285460000
H	-3.2149600000	1.7572020000	-1.9497350000
H	-5.3887340000	2.5512890000	-1.5320200000
H	-4.1397800000	3.8065440000	-1.2791720000
C	-1.9222950000	0.2875310000	-1.0761210000
C	-2.9157600000	1.2687010000	-1.0326520000
C	-4.9472000000	3.2397360000	-0.8048100000
H	4.8822000000	0.1706700000	-0.6708260000
H	3.1024550000	-1.6037970000	-0.6075150000
H	-5.7108740000	3.9274570000	-0.4469090000
H	3.5982040000	4.4319270000	-0.4146520000
C	3.8636910000	0.4121640000	-0.3881940000
C	2.8790310000	-0.5678900000	-0.3682430000
O	2.0354700000	-3.4714200000	-0.2349690000
O	4.5951940000	2.6230980000	-0.0926120000
H	-1.6941350000	-4.2544090000	-0.0799670000
C	3.5557830000	1.7327750000	-0.0402870000
I	0.0451610000	-1.8827410000	-0.0054010000
C	1.5751160000	-0.2350770000	-0.0053110000
O	-2.0328500000	-3.3596400000	0.0472060000
C	-1.5168290000	-0.3563930000	0.0843080000
H	5.2898820000	4.5033760000	0.1404870000
C	-3.5051330000	1.5979000000	0.1914250000
C	4.3403180000	3.9836390000	0.2539980000
C	2.2506660000	2.0624130000	0.3306040000

C	1.2630940000	1.0704810000	0.3437910000
O	-4.4796430000	2.5416140000	0.3504450000
H	1.9826590000	3.0723610000	0.6100760000
H	0.2565020000	1.3463960000	0.6296070000
H	2.2798240000	-3.7877620000	0.6431160000
H	3.9987130000	4.0729970000	1.2903840000
C	-2.1103600000	-0.0333390000	1.3039260000
C	-3.0993000000	0.9400130000	1.3592360000
H	-1.8063440000	-0.5382130000	2.2128380000
H	-3.5711530000	1.2033340000	2.2984870000

1c-(OH)$_2$ (B3LYP-D3, H$_2$O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.419794
$\varepsilon_0 + E_{tot}$ = −855.397491
$\varepsilon_0 + H_{corr}$ = −855.396547
$\varepsilon_0 + G_{corr}$ = −855.473706

Coordinates:

H	-1.4069270000	0.0909110000	-2.0215560000
H	-3.1557620000	1.8037850000	-1.9572050000
H	-5.3333420000	2.6066610000	-1.5905230000
H	-4.0877060000	3.8475880000	-1.2601210000
C	-1.8881370000	0.3170970000	-1.0774200000
C	-2.8832630000	1.2964970000	-1.0421710000
H	4.8262040000	0.2100050000	-0.8723790000
C	-4.9135370000	3.2725580000	-0.8307250000
H	3.0590870000	-1.5668330000	-0.7986950000
C	3.8302390000	0.4307500000	-0.5056010000
C	2.8483370000	-0.5516340000	-0.4795110000
H	-5.6854550000	3.9532510000	-0.4779970000
H	3.5682980000	4.4446550000	-0.2615980000
O	2.0098390000	-3.4996840000	-0.2346430000
O	4.5801290000	2.6198010000	-0.1234630000
C	3.5479390000	1.7265420000	-0.0552450000
H	-1.6936740000	-4.2992390000	-0.0087340000
C	1.5743210000	-0.2436870000	-0.0074850000
I	0.0459500000	-1.8727070000	0.0065850000
O	-2.0500690000	-3.4047700000	0.0558290000
C	-1.5160740000	-0.3486670000	0.0823570000
C	-3.5076470000	1.6015000000	0.1715110000
H	5.2947440000	4.4841390000	0.1779620000
O	-4.4869210000	2.5382650000	0.3208970000
C	4.3535870000	3.9582260000	0.3251790000
C	2.2713560000	2.0281340000	0.4254310000
C	1.2863180000	1.0350140000	0.4454200000
H	2.4466660000	-3.6141500000	0.6180570000
H	2.0246520000	3.0174630000	0.7855680000
H	0.3018040000	1.2873200000	0.8171360000
C	-2.1408350000	-0.0486710000	1.2926180000
C	-3.1324570000	0.9221460000	1.3381160000
H	4.0856340000	3.9803010000	1.3859990000
H	-1.8576940000	-0.5660020000	2.2012430000
H	-3.6266000000	1.1698940000	2.2700380000

1d-(OH)$_2$ (B3LYP-D3, CH$_2$Cl$_2$)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.344999
$\varepsilon_0 + E_{tot}$ = −626.327986
$\varepsilon_0 + H_{corr}$ = −626.327042
$\varepsilon_0 + G_{corr}$ = −626.392039

Frequency:

H	2.0403880000	3.4387300000	-1.5308120000
H	-2.6875950000	-0.5364540000	-1.4907720000
H	0.3462560000	1.6450500000	-1.4175530000
H	-4.4556720000	1.2102710000	-1.3889250000
C	2.2329250000	2.5556740000	-0.9311520000
C	1.2770060000	1.5403620000	-0.8732670000
C	-2.6167940000	0.2772520000	-0.7809310000
C	-3.6143280000	1.2510350000	-0.7056560000
H	4.1698250000	3.2228450000	-0.2688210000
C	3.4288560000	2.4323860000	-0.2246590000
C	1.5251790000	0.4073110000	-0.1040020000
O	-1.9619530000	-2.7847190000	-0.0941240000
I	0.0245080000	-1.2295980000	-0.0085620000
O	2.1793360000	-2.6257830000	0.0456530000
H	1.8493600000	-3.5326930000	0.0517450000
C	-1.5374900000	0.3374190000	0.0921120000
C	-3.5316320000	2.2684430000	0.2448550000
H	-4.3090360000	3.0219970000	0.3030770000
C	3.6718770000	1.2861610000	0.5310750000
C	2.7212000000	0.2648180000	0.5901030000
H	-2.4817930000	-2.6864660000	0.7126480000
C	-1.4475400000	1.3435130000	1.0485910000
H	4.6046780000	1.1799280000	1.0744230000
C	-2.4499180000	2.3118770000	1.1239840000
H	2.9139160000	-0.6497130000	1.1361910000
H	-0.6009800000	1.3855110000	1.7240030000
H	-2.3833600000	3.0962200000	1.8700550000

1d-(OH)$_2$ (B3LYP-D3, H$_2$O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.358748
$\varepsilon_0 + E_{tot}$ = −626.341728
$\varepsilon_0 + H_{corr}$ = −626.340784
$\varepsilon_0 + G_{corr}$ = −626.405315

Frequency:

H	-2.2298110000	-0.1121900000	-1.9291520000
H	-4.0604280000	1.5492090000	-1.8000080000
H	1.9063060000	3.5899920000	-1.3075740000
H	0.2619050000	1.7490020000	-1.2680970000
C	-2.3781120000	0.4604800000	-1.0215820000
C	-3.4102040000	1.3978170000	-0.9458070000
C	2.1413430000	2.6733810000	-0.7781110000
C	1.2115730000	1.6318550000	-0.7611270000
H	1.9426020000	-3.5025200000	-0.1429870000
H	4.0819240000	3.3455480000	-0.1337820000
H	-2.7197070000	-2.3713100000	-0.1328970000
C	3.3631350000	2.5341750000	-0.1209820000
O	2.2558080000	-2.5914280000	-0.0838280000
C	1.5191920000	0.4570830000	-0.0827390000
I	0.0684840000	-1.2141140000	-0.0289110000
C	-1.5442140000	0.2744070000	0.0765200000
O	-1.9201580000	-2.8677070000	0.0772440000
C	-3.5993910000	2.1377240000	0.2206010000
H	-4.4001710000	2.8660050000	0.2766160000
C	3.6595280000	1.3473250000	0.5483330000
C	2.7376420000	0.2987180000	0.5673630000
H	2.9682270000	-0.6404570000	1.0528270000
H	4.6101470000	1.2314370000	1.0572780000
C	-1.7261290000	1.0041800000	1.2471110000
C	-2.7580650000	1.9408400000	1.3155670000
H	-1.0706450000	0.8553590000	2.0969370000
H	-2.9030040000	2.5131750000	2.2248970000

1d-(OH)$_2$ (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −625.962078
$\varepsilon_0 + E_{tot}$ = −625.946024
$\varepsilon_0 + H_{corr}$ = −625.945080
$\varepsilon_0 + G_{corr}$ = −626.006676

Coordinates:

H	2.1816650000	3.2288520000	-1.7242930000
H	0.4336000000	1.4917120000	-1.5544810000
H	-2.8943600000	-0.6936830000	-1.1164020000
H	-4.5819410000	1.1432800000	-1.0491150000
C	2.3155430000	2.3956080000	-1.0435710000
C	1.3345270000	1.4113990000	-0.9549090000
H	2.4242540000	-2.7732140000	-0.6641900000
C	-2.6987960000	0.2271820000	-0.5789220000
C	-3.6457020000	1.2473440000	-0.5118250000
H	4.2272040000	3.0724410000	-0.3290350000
C	3.4638410000	2.3053390000	-0.2631120000
O	-2.1124210000	-2.4981430000	-0.1260360000
C	1.5030900000	0.3356890000	-0.0908660000
H	-1.8773740000	-3.4245450000	-0.0219960000
I	-0.0133180000	-1.2484810000	0.0050970000
C	-1.4963380000	0.3624350000	0.1039090000
O	1.9590210000	-2.6497270000	0.1680930000
C	-3.4033120000	2.3866610000	0.2486780000
H	-4.1447330000	3.1760240000	0.3015720000
C	3.6331020000	1.2213270000	0.5927950000
C	2.6585630000	0.2286140000	0.6722850000
C	-1.2576190000	1.4891770000	0.8827930000
C	-2.2102590000	2.5019300000	0.9548410000
H	4.5308410000	1.1414640000	1.1959840000
H	2.7980980000	-0.6523560000	1.2877620000
H	-0.3265470000	1.5888660000	1.4300110000
H	-2.0175170000	3.3773900000	1.5649760000

1d-OR (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −860.016004
$\varepsilon_0 + E_{tot}$ = −859.995157
$\varepsilon_0 + H_{corr}$ = −859.994213
$\varepsilon_0 + G_{corr}$ = −860.069981

Coordinates:

H	-4.3696800000	0.3068430000	-2.0393040000
H	-3.9437610000	2.0249960000	-1.9858980000
O	-1.7544810000	0.6240040000	-1.6502610000
H	3.3505700000	0.6950290000	-1.5060210000
H	-3.2451780000	-1.7861320000	-1.4126100000
C	-4.0742600000	1.1258860000	-1.3787710000
H	-0.6032260000	2.6736720000	-1.2615570000
I	0.3082980000	-0.2750250000	-1.0380090000
C	3.4717080000	-0.1498850000	-0.8373020000
H	5.6156870000	-0.0005030000	-0.7965090000
C	-2.7512170000	0.7883380000	-0.6767270000
H	-4.8757550000	1.2988790000	-0.6532280000
C	4.7477860000	-0.5400760000	-0.4337870000
C	2.3579420000	-0.8423120000	-0.3674520000
C	-3.1248000000	-1.7013100000	-0.3382690000
C	-0.0722390000	2.6933050000	-0.3186060000
H	-2.5092180000	1.6369850000	-0.0097140000
H	-3.3741350000	-3.8064830000	0.0148740000
H	-0.3946730000	4.7762130000	0.0774590000
C	0.4895780000	1.5314090000	0.1824220000
C	-2.8833170000	-0.4405270000	0.2205050000
C	4.9071690000	-1.6227020000	0.4317440000
C	0.0328900000	3.8530210000	0.4509750000
C	-3.1848780000	-2.8368930000	0.4634920000
C	2.5108600000	-1.9250150000	0.4947750000
H	5.9004480000	-1.9249240000	0.7435620000
H	1.6422970000	-2.4612700000	0.8615240000
C	3.7907320000	-2.3158150000	0.8943720000
C	1.1310660000	1.4632230000	1.4080870000
H	3.9111270000	-3.1571520000	1.5678280000
C	-2.6987200000	-0.3482950000	1.6009250000
C	0.6745060000	3.8233960000	1.6879190000
H	1.5596710000	0.5386370000	1.7704320000
C	-2.9993580000	-2.7324530000	1.8444520000
H	-2.4932350000	0.6215060000	2.0440020000
C	1.2170120000	2.6321500000	2.1661750000
H	0.7477190000	4.7270560000	2.2816380000
C	-2.7561210000	-1.4839090000	2.4112920000
H	-3.0435090000	-3.6176560000	2.4694600000
H	1.7092280000	2.6020490000	3.1313200000
H	-2.6063410000	-1.3927040000	3.4819490000

1d-OR (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.230809
$\varepsilon_0 + E_{tot}$ = −1095.200421
$\varepsilon_0 + H_{corr}$ = −1095.199477
$\varepsilon_0 + G_{corr}$ = −1095.294157

Coordinates:

H	-4.0204450000	1.5687810000	-1.7402230000
H	-3.0296480000	-1.1756850000	-1.6899640000
H	3.4354450000	0.1254490000	-1.4934500000
O	-1.5195230000	0.8355940000	-1.4006390000
H	-0.1885440000	2.6786880000	-1.3028400000
H	-3.0384480000	2.9702590000	-1.2690670000
C	-3.5026400000	2.0502190000	-0.9070890000
I	0.3295340000	-0.3339050000	-0.8585540000
H	5.5876790000	-0.8928330000	-0.8328980000
H	-4.1349230000	-3.2249180000	-0.8110490000
C	3.4506690000	-0.6932290000	-0.7812030000
C	-3.3239640000	-1.2427780000	-0.6481510000
C	0.4458680000	2.6947430000	-0.4257310000
C	4.6626140000	-1.2632530000	-0.4066300000
C	-2.4203130000	1.1054720000	-0.3767110000
C	2.2627580000	-1.1655530000	-0.2311470000
H	0.4889090000	4.8255920000	-0.2241360000
C	-3.9378290000	-2.3873790000	-0.1511580000
H	-4.2329960000	2.2966910000	-0.1317580000
C	0.8803320000	1.5056740000	0.1339340000
C	-3.0634550000	-0.1565270000	0.1876080000
C	0.8135030000	3.8829730000	0.1999310000
H	-1.9205480000	1.6135960000	0.4712180000
C	4.6865590000	-2.3089540000	0.5126990000
C	2.2846110000	-2.2111110000	0.6847480000
H	5.6313070000	-2.7525590000	0.8036030000
C	3.4992530000	-2.7845970000	1.0567190000
H	1.3596410000	-2.5814940000	1.1150850000
C	-4.3003080000	-2.4617930000	1.1913720000
C	1.6480170000	1.4498580000	1.2837480000
C	1.5839670000	3.8624930000	1.3578080000
C	-3.4299940000	-0.2397020000	1.5295740000
H	-4.7750930000	-3.3550620000	1.5799550000
H	1.9758560000	0.5049270000	1.6979930000
H	3.5148440000	-3.5985740000	1.7719920000
H	1.8613060000	4.7916790000	1.8403790000
C	1.9948660000	2.6502070000	1.8996560000
C	-4.0456100000	-1.3826800000	2.0315830000
H	-3.2242460000	0.5987140000	2.1890900000
H	2.5876800000	2.6281050000	2.8060130000
H	-4.3203130000	-1.4336500000	3.0791780000

1e-OR (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.838917
$\varepsilon_0 + E_{tot}$ = −1095.808531
$\varepsilon_0 + H_{corr}$ = −1095.807586
$\varepsilon_0 + G_{corr}$ = −1095.900957

Coordinates:

H	2.0841440000	0.9007790000	-3.0277020000
H	0.3908150000	0.3951700000	-3.0041790000
H	-1.8925860000	0.5302170000	-2.7912520000
H	-2.7961700000	2.0451250000	-2.7364090000
C	1.3258490000	0.3860330000	-2.4375120000
H	1.6294810000	-0.6528660000	-2.2937090000
C	-2.2477540000	1.3238080000	-2.1291280000
H	5.5557180000	0.2302730000	-1.8647990000
H	-1.3688430000	1.8266310000	-1.7194640000
H	3.8480010000	-1.5572340000	-1.6299150000
H	2.5361930000	2.6157350000	-1.5837630000
H	-4.6899740000	2.1703740000	-1.4519680000
C	1.1591910000	1.0584270000	-1.1015600000
C	-3.1242470000	0.7673130000	-1.0347290000
C	4.9933060000	0.1334190000	-0.9417970000
C	-4.3850370000	1.3368660000	-0.8260190000
C	1.8712700000	2.2262220000	-0.8207080000
C	4.0435180000	-0.8748970000	-0.8108550000
O	1.4390360000	-2.2134470000	-0.6326970000
I	-0.7297540000	-1.3019330000	-0.4603630000
H	-7.3555300000	1.0050690000	-0.3265380000
C	-2.7361520000	-0.3000510000	-0.2132460000
H	2.6550900000	4.7680410000	-0.1786810000
H	3.5722360000	-3.7340660000	-0.1609940000
C	0.3348640000	0.5757010000	-0.0788470000
H	5.9602820000	1.8114570000	0.0093460000
H	-6.6154260000	2.5494130000	0.0943500000
C	5.2230800000	1.0222540000	0.1107510000
C	-5.2587710000	0.8675330000	0.1531900000
C	-6.6245690000	1.4836700000	0.3340150000
C	3.3023570000	-1.0149930000	0.3673680000
C	1.7816720000	2.8805960000	0.4064740000
C	2.2666490000	-2.1334860000	0.4894040000
C	2.6255540000	4.0979840000	0.6840500000
C	2.9679350000	-3.4848750000	0.7155830000
C	-3.5981050000	-0.8166220000	0.7672680000
H	2.2173260000	-4.2682660000	0.8498930000
H	3.6554750000	3.7945150000	0.8988070000
C	-4.8493270000	-0.2132910000	0.9326370000
H	-3.0578140000	-2.8988240000	1.0588200000
C	0.2052280000	1.1755520000	1.1741030000
C	4.4933470000	0.8899860000	1.2894810000
H	-6.9829060000	1.3666190000	1.3591470000
C	0.9451630000	2.3460580000	1.3819250000
H	1.6821770000	-1.9157650000	1.4068230000
C	3.5412890000	-0.1218520000	1.4123380000
H	2.2537670000	4.6596740000	1.5431850000
H	3.6219990000	-3.4590980000	1.5936550000
C	-3.2413870000	-1.9948850000	1.6465940000
H	-5.5188960000	-0.6019810000	1.6941470000
H	-1.7013090000	0.6491450000	2.0420590000
H	4.6554400000	1.5815860000	2.1096350000
H	-2.3413710000	-1.8056370000	2.2367830000
C	-0.6395020000	0.6298820000	2.2953860000
H	2.9606360000	-0.2056620000	2.3257760000
H	-4.0542830000	-2.2149070000	2.3399470000
H	0.8733410000	2.8333490000	2.3488290000
H	-0.3696980000	-0.4052520000	2.5203110000
H	-0.4951820000	1.2183180000	3.2016950000

1e-OR (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.200421
$\varepsilon_0 + E_{tot}$ = −1095.200421
$\varepsilon_0 + H_{corr}$ = −1095.199477
$\varepsilon_0 + G_{corr}$ = −1095.294157

Coordinates:

H	-3.3685910000	1.0921120000	-2.9323580000
H	0.2206970000	0.7676780000	-2.8724340000
H	1.5251720000	1.9586750000	-2.8585190000
H	-1.9196060000	0.0973340000	-2.7773970000
C	1.0193820000	1.1996290000	-2.2633250000
C	-2.6297080000	0.7165660000	-2.2247650000
H	1.7168330000	0.3963990000	-2.0133710000
H	-2.0840220000	1.5721920000	-1.8195800000
H	-5.2474090000	0.5965690000	-1.7329790000
H	1.1046420000	3.7758560000	-1.5636440000
H	6.1155310000	-3.0671800000	-1.2371580000
C	-3.3036690000	-0.0775510000	-1.1358640000
C	-4.6959100000	-0.0276420000	-1.0360040000
C	0.4641850000	1.8157800000	-1.0086680000
H	3.7273970000	-2.4463000000	-0.8475490000
C	0.5995730000	3.1914120000	-0.8015080000
C	5.8685270000	-2.1430680000	-0.7262530000
H	-7.3334960000	-1.5292360000	-0.5914390000
C	4.5342220000	-1.8080540000	-0.5087340000
H	7.9228010000	-1.5546100000	-0.4712990000
H	-7.2823370000	0.2261300000	-0.4182000000
O	1.8978350000	-1.0290130000	-0.3721280000
H	0.7752270000	5.7694790000	-0.3158500000
C	6.8846380000	-1.2958070000	-0.2980330000
I	-0.4004440000	-1.0287220000	-0.2865220000
C	-2.6001780000	-0.8745610000	-0.2271490000
C	-5.3939550000	-0.7572620000	-0.0807610000
C	-6.8979350000	-0.7103780000	-0.0122190000
C	-0.1908590000	1.0968390000	-0.0075740000
C	4.1999640000	-0.6248010000	0.1443610000
H	2.6392330000	0.8100730000	0.1968210000
C	0.1174280000	3.8237100000	0.3381540000
C	6.5581510000	-0.1064430000	0.3493770000
C	2.7411200000	-0.2721750000	0.4191690000
C	0.2771660000	5.3078420000	0.5366100000
C	5.2256450000	0.2231940000	0.5667550000
H	-0.6961210000	5.7865990000	0.6659950000
H	7.3429560000	0.5646450000	0.6801380000
C	-3.2752310000	-1.6444100000	0.7307560000
C	-4.6661930000	-1.5670740000	0.7869170000
H	-7.2477340000	-0.8107880000	1.0163660000
H	4.9744300000	1.1547490000	1.0666830000
C	-0.6823430000	1.6717900000	1.1675770000
H	-2.0093350000	-3.3441340000	1.1813820000
C	-0.5132590000	3.0489550000	1.3078470000
H	0.8678990000	5.5160900000	1.4315970000
H	-5.1943150000	-2.1550490000	1.5318460000
C	-2.5613990000	-2.5562790000	1.7001670000
C	2.4500860000	-0.4527850000	1.9186500000
H	-2.3493030000	0.5539890000	1.9538100000
H	1.4435340000	-0.0956880000	2.1546090000

H	2.5168710000	-1.5146510000	2.1715340000
H	-0.8843540000	3.5241530000	2.2106970000
C	-1.3633350000	0.9033950000	2.2682420000
H	-1.8458970000	-2.0104220000	2.3196140000
H	-3.2798890000	-3.0382730000	2.3627030000
H	3.1577030000	0.1026800000	2.5389860000
H	-0.7774270000	0.0306720000	2.5657230000
H	-1.4869310000	1.5397000000	3.1435930000

1d-$(OR)_2$ (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1245.567999
$\varepsilon_0 + E_{tot}$ = −1245.537736
$\varepsilon_0 + H_{corr}$ = −1245.536791
$\varepsilon_0 + G_{corr}$ = −1245.633072

Coordinates:

H	1.6661620000	-1.2595960000	-2.3727250000
H	1.9949200000	-3.0101900000	-2.3684560000
H	-5.1886600000	2.4539730000	-2.0242350000
H	-2.7952380000	1.7455500000	-1.9215830000
H	0.3881660000	-2.4034220000	-1.9172970000
C	1.4614360000	-2.2021380000	-1.8555020000
C	-4.8558360000	1.7747910000	-1.2460700000
C	-3.5229810000	1.3616310000	-1.2163770000
O	-0.5750950000	2.1708630000	-1.1265030000
H	-3.1888250000	-2.2462240000	-1.0828410000
H	-0.6044620000	4.2100090000	-1.0813330000
H	3.3658820000	0.1640320000	-0.5900570000
H	5.8386550000	0.4310280000	-0.5794190000
H	-3.8082870000	-4.5729760000	-0.5138540000
C	4.0129700000	-0.6955740000	-0.4719210000
C	5.3979400000	-0.5536580000	-0.4574890000
C	-0.3860750000	3.3417900000	-0.4217290000
C	1.8927840000	-2.0802310000	-0.3732050000
C	3.4179680000	-1.9521830000	-0.3179450000
C	-2.6471530000	-2.7745890000	-0.3067880000
H	-6.7878850000	1.6540010000	-0.2995010000
C	6.2184540000	-1.6704440000	-0.2814390000
C	-5.7536980000	1.3272430000	-0.2769300000
H	7.2978570000	-1.5603180000	-0.2627840000
C	-3.0982670000	0.4898100000	-0.2198690000
I	-0.9489770000	-0.0940390000	-0.1764080000
C	4.2473070000	-3.0624540000	-0.1415450000
C	5.6368590000	-2.9270900000	-0.1221400000
H	3.7989610000	-4.0438170000	-0.0109930000
C	-2.9994950000	-4.0849190000	0.0202020000
H	6.2641270000	-3.8012300000	0.0240350000
H	0.8984850000	5.7043910000	0.0485300000
C	1.0519810000	3.5601670000	0.0781970000
H	1.6430880000	-3.0555500000	0.1021960000
H	1.5568650000	1.4693010000	0.2072620000
O	1.2840850000	-1.0285450000	0.2832050000
C	1.5371820000	4.8571080000	0.2861280000
C	-1.6080750000	-2.1479580000	0.3749430000
C	1.8939970000	2.4844910000	0.3771150000
H	-2.3793400000	3.3743540000	0.4511810000
C	-5.3148180000	0.4654880000	0.7270310000
C	-3.9842400000	0.0440130000	0.7556990000
C	2.8196990000	5.0814840000	0.7840080000
C	-1.3457210000	3.4795430000	0.7895870000
C	3.1755720000	2.7033840000	0.8847850000
H	3.1751230000	6.0973980000	0.9287160000
C	-2.3129280000	-4.7631240000	1.0265580000
C	3.6463140000	4.0001220000	1.0901280000
H	3.8052770000	1.8512860000	1.1185390000
H	-2.5863990000	-5.7817590000	1.2801600000
H	-1.2302990000	4.4453240000	1.2939180000
C	-0.9080910000	-2.8222080000	1.3700270000
H	4.6459510000	4.1664270000	1.4786960000
H	-6.0034460000	0.1213730000	1.4918380000
H	-1.1411210000	2.6891280000	1.5184500000
H	-3.6482520000	-0.6311280000	1.5337360000
C	-1.2672450000	-4.1305740000	1.6981680000
H	-0.0664000000	-2.3334580000	1.8466190000
H	-0.7220930000	-4.6559240000	2.4754530000

1d-$(OR)_2$ (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1244.917269
$\varepsilon_0 + E_{tot}$ = −1244.887307
$\varepsilon_0 + H_{corr}$ = −1244.886363
$\varepsilon_0 + G_{corr}$ = −1244.982335

Coordinates:

H	0.5716830000	-4.5104340000	-2.6730490000
H	-0.0545400000	-2.2118460000	-1.9338080000
C	1.1144420000	-4.0342500000	-1.8640510000
H	-4.1945830000	4.3728120000	-1.7939920000
H	3.4521060000	-0.5192870000	-1.6115130000
H	2.4015680000	-5.7230530000	-1.5202830000
H	5.8379420000	0.1164180000	-1.5135550000
C	0.7718080000	-2.7414730000	-1.4723060000
H	1.4944690000	2.6401400000	-1.3180430000
C	-3.2459590000	4.1525070000	-1.3172690000
H	-3.5772730000	2.0262750000	-1.2505660000
H	-2.6224550000	6.2106860000	-1.2236360000
C	2.1409410000	-4.7154040000	-1.2173610000
H	1.6136060000	4.3879570000	-1.0457780000
C	-2.9000440000	2.8400880000	-1.0112970000
C	-2.3621950000	5.1812900000	-0.9998210000
C	3.8350590000	0.0135680000	-0.7474940000
C	5.1805740000	0.3670280000	-0.6887100000
C	1.6529350000	3.4103100000	-0.5556230000
H	-1.8963080000	-2.9526610000	-0.5140780000
C	1.4710000000	-2.1292330000	-0.4397360000
C	-1.6835790000	2.5535380000	-0.3939930000
C	-1.1472800000	4.8887200000	-0.3903620000
O	-1.3447280000	-0.9751400000	-0.3345860000
C	2.8272400000	-4.1019290000	-0.1738190000
H	-1.4400800000	1.5249270000	-0.1506840000
H	-0.4632150000	5.6961320000	-0.1405940000
H	2.6468850000	3.2659070000	-0.1241710000
C	-0.7862520000	3.5742410000	-0.0818860000
H	-4.0841210000	-3.8760220000	0.1168820000
C	-2.0063580000	-2.0703160000	0.1561060000
I	0.8683260000	-0.1335900000	0.2039740000
C	2.4936560000	-2.8076220000	0.2146770000
C	-4.4362240000	-2.8567840000	0.2540400000
C	-3.5093950000	-1.8144880000	0.2736120000
C	2.9879800000	0.3423750000	0.3036500000
H	3.6219770000	-4.6294430000	0.3417820000
H	-6.5052310000	-3.4292320000	0.3743430000
C	-5.7978580000	-2.6071280000	0.3992140000
C	5.6759250000	1.0403170000	0.4233030000
C	-3.9745220000	-0.5114190000	0.4417330000
H	-3.2421190000	0.2871990000	0.4491210000
H	6.7240200000	1.3132960000	0.4701390000

C	0.5795020000	3.2755230000	0.5486300000
C	-6.2524320000	-1.3019380000	0.5681930000
C	-5.3342070000	-0.2552180000	0.5902270000
H	-7.3126150000	-1.1029610000	0.6782180000
H	-5.6781590000	0.7655770000	0.7208200000
H	3.0349070000	-2.3306640000	1.0251840000
O	0.6417320000	2.0734790000	1.2047290000
H	0.7615460000	4.1085590000	1.2594470000
C	3.4716680000	1.0287250000	1.4092050000
H	-0.4318130000	-2.7912590000	1.4705330000
C	4.8207430000	1.3695420000	1.4707860000
C	-1.4874600000	-2.5127820000	1.5407410000
H	-2.0473310000	-3.3681060000	1.9312000000
H	2.7781590000	1.3319030000	2.1845090000
H	-1.5846330000	-1.6782860000	2.2419060000
H	5.2000040000	1.9022800000	2.3355790000

1e-$(OR)_2$ (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1481.389611
$\varepsilon_0 + E_{tot}$ = −1481.349771
$\varepsilon_0 + H_{corr}$ = −1481.348826
$\varepsilon_0 + G_{corr}$ = −1481.465065

Coordinates:

H	-3.4408720000	0.9208120000	-3.5723600000
H	-2.1209230000	-0.1512170000	-3.0847140000
C	-2.7186590000	0.7122950000	-2.7799820000
H	2.3845440000	-1.0351510000	-2.7651500000
H	-2.0321840000	1.5591470000	-2.6668680000
H	-1.1603290000	-2.2192850000	-2.3925380000
H	2.8408580000	-2.7067760000	-2.3476510000
H	-5.3603480000	0.7495370000	-2.3365820000
H	-2.1355210000	-3.6781010000	-2.1845880000
C	2.2550550000	-1.8362680000	-2.0316540000
H	1.2004360000	-2.1215580000	-2.0102590000
C	-1.8301090000	-2.7451580000	-1.7072640000
H	-2.7156710000	-2.1195400000	-1.5779970000
C	-3.4218200000	0.4656150000	-1.4693170000
C	-4.8174530000	0.5451600000	-1.4177200000
O	-0.6227010000	2.4520620000	-1.2919710000
H	-0.9629220000	4.4583500000	-1.1397570000
H	-7.4840730000	0.0927440000	-1.1086290000
H	6.3850360000	1.5503660000	-0.6975580000
C	6.0341030000	0.5230800000	-0.6743750000
H	8.0186350000	-0.3238490000	-0.6652460000
C	6.9525390000	-0.5266340000	-0.6572820000
C	4.6643340000	0.2611490000	-0.6568290000
H	3.9335080000	1.0600510000	-0.6554340000
C	2.6751870000	-1.3213360000	-0.6323440000
C	4.1868920000	-1.0514670000	-0.6287310000
C	6.4868150000	-1.8419670000	-0.6226270000
C	5.1163200000	-2.0971950000	-0.6088700000
H	7.1921250000	-2.6672930000	-0.6014190000
H	4.7591950000	-3.1231690000	-0.5747460000
C	-0.7263070000	3.5749270000	-0.5039630000
H	-1.5719400000	-5.1161870000	-0.5010010000
C	-1.1538270000	-3.0154070000	-0.3858020000
I	-0.5028020000	0.1026010000	-0.3517140000
C	-2.7312880000	0.1950410000	-0.2765970000
H	1.6396180000	2.1596480000	-0.2602990000
O	1.9672240000	-0.2096260000	-0.2460440000
C	-5.5286800000	0.3807470000	-0.2293900000
C	-7.0332290000	0.5095280000	-0.2039890000
H	-7.3338650000	1.5614740000	-0.1451260000
H	-2.8107340000	3.2105040000	-0.0153730000
H	2.5191230000	-2.1742630000	0.0690780000
C	-1.1090500000	-4.3308130000	0.0902720000
C	0.5662520000	3.9563660000	0.2439580000
C	1.6690220000	3.0986170000	0.2761820000
C	-0.5508020000	-2.0094170000	0.3816750000
C	-1.8912110000	3.4675630000	0.5165410000
H	-7.4639910000	-0.0045730000	0.6586660000
H	-0.1744890000	5.8725160000	0.8908480000
C	0.6630730000	5.1805630000	0.9213760000
C	-4.8069490000	0.1372860000	0.9363110000
C	-3.4094880000	0.0457200000	0.9395280000
H	-0.4981550000	-6.8012290000	0.9737500000
C	2.8169590000	3.4390890000	0.9956740000
H	3.6492390000	2.7432580000	1.0221020000
H	-2.0493670000	4.3956430000	1.0764490000
H	-1.6834410000	2.6685570000	1.2340950000
C	-0.4808990000	-4.6611330000	1.2897180000
C	0.1134680000	-2.3056170000	1.5826870000
C	1.8110780000	5.5305390000	1.6283850000
C	2.8959780000	4.6528930000	1.6754440000
H	1.5598230000	-0.7371030000	1.7692160000
C	-0.4742840000	-6.0833680000	1.7975550000
H	-5.3399820000	0.0199090000	1.8758750000
C	0.1284040000	-3.6379640000	2.0132870000
H	1.8602730000	6.4856980000	2.1430310000
H	3.7903770000	4.9158110000	2.2313590000
C	-2.7045690000	-0.1872880000	2.2526400000
H	-2.2417470000	-1.1762130000	2.2871270000
C	0.8319540000	-1.2612710000	2.3991700000
H	0.4144070000	-6.2869230000	2.4001730000
H	-1.9106860000	0.5471960000	2.4077230000
H	-1.3494800000	-6.2784050000	2.4275800000
H	0.1375500000	-0.5068660000	2.7799560000
H	0.6439210000	-3.8777260000	2.9391090000
H	-3.4043270000	-0.1084200000	3.0866940000
H	1.3358340000	-1.7179770000	3.2534330000

1e-$(OR)_2$ (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1480.596517
$\varepsilon_0 + E_{tot}$ = −1480.557083
$\varepsilon_0 + H_{corr}$ = −1480.556139
$\varepsilon_0 + G_{corr}$ = −1480.670346

Coordinates:

H	-3.3521070000	0.7623030000	-3.6249630000
H	-2.0366310000	-0.2957430000	-3.0959540000
C	-2.6321530000	0.5803060000	-2.8258810000
H	-1.9495150000	1.4312710000	-2.7316340000
H	2.3214960000	-1.1793140000	-2.6929760000
H	-5.2743750000	0.6283280000	-2.4077780000
H	-1.0641920000	-2.2381870000	-2.3637840000
H	2.9016850000	-2.7886000000	-2.1887700000
H	-1.9982620000	-3.7224950000	-2.1455180000
C	2.2696940000	-1.9403450000	-1.9081390000
H	1.2375230000	-2.2928890000	-1.8280920000
C	-1.7380900000	-2.7685500000	-1.6857370000
H	-2.6482970000	-2.1714620000	-1.5917090000
C	-3.3458180000	0.3754860000	-1.5159190000
C	-4.7383340000	0.4489200000	-1.4797140000
O	-0.7021350000	2.3905470000	-1.2929850000
H	-1.0519860000	4.3970600000	-1.1518940000

H	-7.3992260000	-0.0839390000	-1.1463100000
H	6.2450710000	1.7308220000	-0.8677830000
H	7.9673530000	-0.0547020000	-0.8266580000
C	5.9465380000	0.6900180000	-0.7967670000
C	6.9145610000	-0.3094200000	-0.7751580000
H	3.8208770000	1.1204830000	-0.7275310000
C	4.5952770000	0.3617300000	-0.7234660000
C	6.5193600000	-1.6418390000	-0.6809480000
H	7.2659460000	-2.4286320000	-0.6554680000
C	4.1894390000	-0.9679560000	-0.6325490000
C	5.1678540000	-1.9638410000	-0.6115350000
C	2.6961500000	-1.3033910000	-0.5686310000
H	4.8644510000	-3.0044050000	-0.5284330000
C	-0.8309740000	3.5110040000	-0.5183340000
H	-1.4904860000	-5.0946590000	-0.4051190000
I	-0.4789780000	0.0941950000	-0.3673250000
C	-1.0858410000	-2.9923520000	-0.3457620000
H	-7.2637630000	1.4771350000	-0.3385810000
C	-2.6627170000	0.1414530000	-0.3135690000
C	-5.4568900000	0.3090020000	-0.2950490000
H	1.5564580000	2.1322830000	-0.2899950000
C	-6.9596540000	0.4277990000	-0.2877490000
O	1.9505750000	-0.2021770000	-0.2586430000
H	-2.9136750000	3.1186860000	-0.0800680000
C	-1.0382050000	-4.2886920000	0.1666740000
H	2.6005730000	-2.1028970000	0.2034540000
C	0.4360380000	3.8861910000	0.2657750000
C	1.5519230000	3.0493620000	0.2881380000
C	-0.5000070000	-1.9578340000	0.3955790000
C	-2.0111030000	3.3923580000	0.4735330000
H	-7.3842440000	0.0003820000	0.6218570000
C	-4.7466710000	0.0954430000	0.8792540000
C	-3.3512310000	0.0119120000	0.8951390000
H	-0.3581640000	5.7572260000	0.9671840000
C	0.4924510000	5.0812390000	0.9918660000
H	-2.1943560000	4.3183860000	1.0266000000
C	2.6734800000	3.3809180000	1.0490250000
H	3.5189690000	2.7008660000	1.0686470000
H	-0.0073430000	-6.6826600000	1.1631640000
H	-1.8040360000	2.5976750000	1.1976810000
C	-0.4210950000	-4.5783970000	1.3804540000
C	0.1525560000	-2.2168420000	1.6069100000
C	1.6141920000	5.4227980000	1.7380790000
H	1.5640180000	-0.6148680000	1.7745740000
C	2.7113400000	4.5647070000	1.7771270000
H	-5.2864510000	-0.0026590000	1.8169750000
C	-0.3983690000	-5.9891350000	1.9112480000
C	0.1727270000	-3.5337670000	2.0774960000
H	-1.4060300000	-6.3221400000	2.1737430000
C	-2.6574270000	-0.1809550000	2.2183920000
H	-2.1960740000	-1.1694030000	2.2884270000
H	1.6330550000	6.3554600000	2.2922300000
H	-1.8674770000	0.5614940000	2.3551950000
H	3.5854990000	4.8209270000	2.3657120000
C	0.8450950000	-1.1455310000	2.4084310000
H	0.1296680000	-0.4068490000	2.7805990000
H	0.2249380000	-6.0629370000	2.8033730000
H	0.6782980000	-3.7407190000	3.0162970000
H	-3.3685850000	-0.0746530000	3.0380760000
H	1.3531440000	-1.5860310000	3.2672060000

1a-(OH)OH (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.907560
$\varepsilon_0 + E_{tot}$ = −830.888177
$\varepsilon_0 + H_{corr}$ = −830.887232
$\varepsilon_0 + G_{corr}$ = −830.958021

Coordinates:

H	3.4324570000	2.6097400000	-2.7468260000
H	2.5284130000	0.3306340000	-2.4034640000
H	-3.3659170000	-0.5912870000	-2.0772830000
H	-1.0656110000	-1.5442360000	-1.9840510000
C	3.0833040000	2.3106470000	-1.7645940000
C	2.5747150000	1.0249890000	-1.5718540000
C	-2.7191550000	-0.3957160000	-1.2341630000
O	-5.2226340000	0.6776020000	-1.2003380000
C	-1.4337510000	-0.9193710000	-1.1831260000
H	3.5286890000	4.2044230000	-0.8464290000
C	3.1356490000	3.2049730000	-0.6957900000
C	2.1266700000	0.6538870000	-0.3065020000
N	-4.5244090000	0.9485700000	-0.2264820000
C	-3.1610180000	0.3915460000	-0.1712720000
C	-0.6496860000	-0.6240820000	-0.0738340000
I	1.3678670000	-1.4187360000	-0.0207040000
O	0.2178490000	-3.5224200000	0.0815860000
C	2.6819820000	2.8156020000	0.5644240000
O	-4.8997340000	1.6578840000	0.7021420000
C	2.1739120000	1.5305070000	0.7741470000
H	-0.2310240000	-3.5996190000	0.9325160000
C	-2.3648530000	0.6654780000	0.9368720000
C	-1.0705880000	0.1473310000	0.9970030000
H	2.7207220000	3.5129100000	1.3944780000
H	-2.7476420000	1.2709000000	1.7468840000
H	1.8017030000	1.2288850000	1.7561160000
H	-0.4316690000	0.3354690000	1.8836000000
O	0.6639200000	0.6703820000	3.3289900000
H	0.6654740000	0.0928720000	4.1002400000

1a-(OH)OH (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.920679
$\varepsilon_0 + E_{tot}$ = −830.900839
$\varepsilon_0 + H_{corr}$ = −830.899895
$\varepsilon_0 + G_{corr}$ = −830.972110

Coordinates:

H	3.4045580000	2.6582070000	-2.7248750000
H	2.5172030000	0.3681600000	-2.4148030000
H	-3.3311830000	-0.5112400000	-2.1264090000
H	-1.0287570000	-1.4527620000	-2.0498260000
C	3.0622060000	2.3413680000	-1.7461030000
C	2.5633210000	1.0489690000	-1.5726410000
C	-2.6975060000	-0.3512820000	-1.2660250000
C	-1.4101170000	-0.8720820000	-1.2221390000
O	-5.2088210000	0.7044000000	-1.2120780000
H	3.5005990000	4.2230550000	-0.8004740000
C	3.1144930000	3.2192100000	-0.6637440000
C	2.1245320000	0.6559340000	-0.3112200000
N	-4.5211360000	0.9400970000	-0.2225730000
C	-3.1558260000	0.3867130000	-0.1759670000
C	-0.6413940000	-0.6251410000	-0.0907910000
I	1.3737270000	-1.4167740000	-0.0407030000
O	0.2117720000	-3.5280160000	0.1000500000
C	2.6698920000	2.8076530000	0.5927580000
O	-4.9077500000	1.6113620000	0.7295920000
C	2.1719170000	1.5159100000	0.7830130000
C	-2.3737300000	0.6190260000	0.9514640000

H	-0.2204650000	-3.5913370000	0.9607330000
C	-1.0792010000	0.1026950000	1.0049530000
H	2.7090750000	3.4923030000	1.4331870000
H	1.8096000000	1.1985390000	1.7604740000
H	-2.7680590000	1.1915020000	1.7795890000
H	-0.4512530000	0.2703400000	1.8973190000
O	0.6648780000	0.6325210000	3.3895040000
H	0.5269380000	0.2056050000	4.2424740000

1c-(OH)OH (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.399393
$\varepsilon_0 + E_{tot}$ = −855.377118
$\varepsilon_0 + H_{corr}$ = −855.376174
$\varepsilon_0 + G_{corr}$ = −855.452677

Coordinates:

H	-3.6003230000	0.9791500000	-2.5463070000
H	-2.0286550000	-0.9282210000	-2.2716990000
H	4.0760850000	0.5115560000	-2.0258590000
H	2.1679590000	-1.0272260000	-2.0202220000
H	5.0777920000	2.6348510000	-1.8843410000
C	-3.0581690000	0.8390810000	-1.6190840000
C	-2.1760550000	-0.2205570000	-1.4672410000
H	6.1442930000	1.3334600000	-1.2776830000
C	3.4652710000	0.4333780000	-1.1369580000
C	2.3770360000	-0.4442720000	-1.1299920000
C	5.6315920000	2.2645460000	-1.0156850000
O	-4.1487870000	2.7493070000	-0.8213720000
H	6.3655800000	3.0080090000	-0.7108370000
C	-3.2601830000	1.7457060000	-0.5681870000
C	-1.5033490000	-0.3486000000	-0.2562630000
O	-2.0860750000	-3.3908930000	-0.2493220000
H	-5.1358090000	4.3992350000	-0.2072500000
I	-0.1118640000	-1.9914840000	-0.0184580000
C	1.5769770000	-0.5584170000	-0.0008150000
C	3.7369530000	1.1947640000	0.0034780000
O	4.7703950000	2.0832140000	0.1083120000
C	-4.4075470000	3.7060170000	0.2089330000
H	-2.7567900000	-3.1143290000	0.3867910000
H	-3.4979280000	4.2503350000	0.4803640000
C	-2.5725040000	1.5832280000	0.6373860000
C	-1.6777770000	0.5198840000	0.8043590000
H	-4.8267380000	3.2254850000	1.0981190000
C	2.9217090000	1.0723100000	1.1362650000
C	1.8427120000	0.1967530000	1.1434830000
H	-2.7159460000	2.2655860000	1.4638810000
H	-1.1529190000	0.4002430000	1.7647790000
H	3.1478990000	1.6759260000	2.0080130000
H	1.2029400000	0.1260280000	2.0281120000
O	-0.2107220000	0.3268160000	3.4709440000
H	-0.5171300000	-0.2419410000	4.1858590000

1c-(OH)OH (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.414195
$\varepsilon_0 + E_{tot}$ = −855.391710
$\varepsilon_0 + H_{corr}$ = −855.390766
$\varepsilon_0 + G_{corr}$ = −855.467906

Coordinates:

H	-3.5242480000	1.0408790000	-2.5836580000
H	-1.9513990000	-0.8635730000	-2.3199180000
H	2.1610590000	-0.9947240000	-2.0419190000
H	4.0632200000	0.5495230000	-2.0281870000
H	5.0671550000	2.6691090000	-1.8518340000
C	-3.0119310000	0.8753240000	-1.6438100000
C	-2.1302410000	-0.1852790000	-1.4967700000
H	6.1376690000	1.3593730000	-1.2697030000
C	2.3730040000	-0.4283140000	-1.1423050000
C	3.4578070000	0.4529080000	-1.1376390000
C	5.6244820000	2.2850130000	-0.9921660000
O	-4.1340450000	2.7561770000	-0.8233080000
H	6.3565760000	3.0245180000	-0.6744490000
C	-3.2503590000	1.7506640000	-0.5736720000
C	-1.4948040000	-0.3486180000	-0.2697040000
O	-2.1112500000	-3.3904560000	-0.2203740000
H	-5.1456500000	4.3871000000	-0.1953750000
I	-0.1066230000	-1.9907690000	-0.0351430000
C	1.5801620000	-0.5662440000	-0.0107200000
C	3.7346630000	1.1935200000	0.0156360000
O	4.7638750000	2.0815350000	0.1321210000
C	-4.4263060000	3.6871430000	0.2241820000
H	-2.8016530000	-3.0438550000	0.3577590000
H	-3.5267980000	4.2277380000	0.5329580000
C	-2.5966960000	1.5562840000	0.6468920000
C	-1.7042800000	0.4908370000	0.8089770000
H	-4.8680760000	3.1820640000	1.0880760000
C	1.8504550000	0.1675100000	1.1465450000
C	2.9261500000	1.0466110000	1.1512390000
H	-2.7669140000	2.2167590000	1.4861190000
H	-1.2009180000	0.3516180000	1.7743800000
H	1.2185860000	0.0778030000	2.0309580000
H	3.1569590000	1.6332700000	2.0332760000
O	-0.2332010000	0.2902320000	3.5157460000
H	-0.6001840000	-0.0708660000	4.3305120000

1d-(OH)OH (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.338416
$\varepsilon_0 + E_{tot}$ = −626.321460
$\varepsilon_0 + H_{corr}$ = −626.320515
$\varepsilon_0 + G_{corr}$ = −626.384645

Coordinates

H	-3.4277780000	1.5256080000	-2.6830680000
H	4.0490060000	0.0373050000	-2.5826080000
H	1.9586700000	-1.2016350000	-2.1104190000
H	-2.1122270000	-0.4987690000	-2.1063730000
C	-2.8477170000	1.5036940000	-1.7676240000
C	3.5125950000	0.2179390000	-1.6573830000
C	-2.1059930000	0.3644630000	-1.4553840000
C	2.3343950000	-0.4821350000	-1.3912330000
H	-3.4232720000	3.4830310000	-1.1534910000
H	4.9044510000	1.6954900000	-0.9445920000
C	-2.8424130000	2.6016220000	-0.9062200000
C	3.9907560000	1.1495280000	-0.7363000000
C	-1.3736230000	0.3766160000	-0.2770440000
C	1.6516350000	-0.2388870000	-0.2020220000
I	-0.2060140000	-1.3916400000	0.2072790000
C	-2.0967490000	2.5653300000	0.2700930000
O	-2.3692830000	-2.4638220000	0.3886230000
C	3.2938980000	1.3796840000	0.4499210000
C	-1.3398080000	1.4379670000	0.6105070000
C	2.1150910000	0.6835960000	0.7320790000
H	-2.0969260000	3.4146780000	0.9445080000
H	-2.8933230000	-2.0209700000	1.0671800000
H	3.6642690000	2.1058790000	1.1656920000
H	-0.7616820000	1.4135380000	1.5478920000
H	1.5629070000	0.8756440000	1.6561940000
O	0.3326940000	1.5095040000	3.1359750000

H	0.0349690000	1.2051750000	4.0001750000

1d-(OH)OH (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.352324
$\varepsilon_0 + E_{tot}$ = −626.335084
$\varepsilon_0 + H_{corr}$ = −626.334140
$\varepsilon_0 + G_{corr}$ = −626.398950

Coordinates

H	-3.3173680000	1.5964950000	-2.7489870000
H	4.0571730000	0.0804380000	-2.5668160000
H	-2.0089910000	-0.4342220000	-2.1907220000
H	1.9709990000	-1.1756270000	-2.1256970000
C	-2.7814950000	1.5450640000	-1.8084180000
C	3.5142330000	0.2461070000	-1.6429590000
C	-2.0448950000	0.4000450000	-1.5035290000
C	2.3380490000	-0.4643120000	-1.3946310000
H	-3.4008410000	3.4973560000	-1.1528430000
C	-2.8250160000	2.6117740000	-0.9101580000
H	4.8949600000	1.7198540000	-0.9017050000
C	3.9826310000	1.1673600000	-0.7067220000
C	-1.3681980000	0.3726150000	-0.2923070000
C	1.6479570000	-0.2401190000	-0.2064880000
I	-0.2054000000	-1.3968960000	0.1874680000
C	-2.1306200000	2.5406610000	0.2958790000
O	-2.3829680000	-2.4701140000	0.4088690000
C	3.2779660000	1.3786280000	0.4785400000
C	-1.3815240000	1.4066960000	0.6294230000
C	2.1015620000	0.6719990000	0.7429170000
H	-2.1655920000	3.3687930000	0.9951500000
H	-2.8926180000	-2.0202560000	1.0938630000
H	3.6422570000	2.0964320000	1.2057880000
H	-0.8339060000	1.3605850000	1.5784330000
H	1.5466430000	0.8482070000	1.6651210000
O	0.3050700000	1.4607110000	3.2148990000
H	0.0327890000	1.3535520000	4.1331600000

1d-(OH)OH (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = 625.950965
$\varepsilon_0 + E_{tot}$ = −625.934650
$\varepsilon_0 + H_{corr}$ = −625.933706
$\varepsilon_0 + G_{corr}$ = −625.996162

Coordinates

H	3.8474090000	0.3033230000	-2.7175380000
H	-3.6633280000	1.5866300000	-2.3609720000
H	1.7444580000	-0.9102260000	-2.2483680000
H	-2.3678500000	-0.4907000000	-1.8923660000
C	3.3869680000	0.3787690000	-1.7385420000
C	-2.9762980000	1.5534620000	-1.5234980000
C	2.2032250000	-0.3045810000	-1.4728710000
C	-2.2450560000	0.3948460000	-1.2829070000
H	4.8921140000	1.6927680000	-0.9482760000
H	-3.4033950000	3.5576480000	-0.8795940000
C	3.9705050000	1.1586530000	-0.7445570000
C	-2.8284820000	2.6585930000	-0.6880680000
C	1.6131930000	-0.2039600000	-0.2163350000
C	-1.3705780000	0.3993880000	-0.2079650000
I	-0.2116060000	-1.3701090000	0.1441460000
O	-2.2882600000	-2.3838520000	0.1586990000
C	-1.9595200000	2.6072550000	0.3957040000
C	3.3695030000	1.2545090000	0.5067420000
C	-1.2044840000	1.4616460000	0.6604820000
C	2.1837420000	0.5739150000	0.7863250000
H	-2.8445890000	-2.0550010000	0.8706780000
H	-1.8665360000	3.4569860000	1.0621450000
H	3.8197070000	1.8675540000	1.2797320000
H	-0.5580620000	1.3842460000	1.5546870000
H	1.6910000000	0.6630500000	1.7635940000
O	0.4181590000	1.0454430000	3.1073410000
H	0.0287080000	0.6718320000	3.9011660000

TS1-1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.905137
$\varepsilon_0 + E_{tot}$ = −830.885673
$\varepsilon_0 + H_{corr}$ = −830.884729
$\varepsilon_0 + G_{corr}$ = −830.956727

Frequency: -1254.990

Coordinates:

H	3.6227100000	2.8142950000	-2.4440340000
H	2.7474420000	0.5053330000	-2.2836910000
H	-3.2559190000	-0.2900040000	-2.2358440000
H	-0.9367090000	-1.2158740000	-2.1552200000
C	3.1955180000	2.4639070000	-1.5107490000
C	2.7032890000	1.1604930000	-1.4206900000
C	-2.6597350000	-0.2199790000	-1.3375510000
O	-5.1660530000	0.8444570000	-1.2928530000
C	-1.3688050000	-0.7293380000	-1.2916530000
H	3.5123170000	4.3238920000	-0.4764150000
C	3.1317650000	3.3110470000	-0.4051220000
N	-4.5382480000	0.9344330000	-0.2384470000
C	2.1547110000	0.7164670000	-0.2198890000
C	-3.1709840000	0.3888850000	-0.1876320000
O	0.3457490000	-3.5520690000	-0.1360180000
I	1.4121690000	-1.3764630000	-0.0931410000
C	-0.6829590000	-0.5787770000	-0.0906120000
H	-0.2309880000	-3.6403830000	0.6326300000
O	-4.9963690000	1.4591030000	0.7740520000
C	2.5775590000	2.8555770000	0.7912150000
C	2.0869560000	1.5520540000	0.8924820000
C	-2.4377110000	0.4958510000	0.9940730000
C	-1.1271560000	-0.0058870000	1.0650000000
H	2.5248550000	3.5140060000	1.6516220000
H	1.6427560000	1.1951240000	1.8169230000
H	-2.8939750000	0.9685100000	1.8556630000
H	-0.3958670000	0.0306430000	2.2322160000
O	0.2606840000	0.0686310000	3.2724990000
H	0.6193530000	-0.8168410000	3.3970920000

TS1-1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.916212
$\varepsilon_0 + E_{tot}$ = −830.896575
$\varepsilon_0 + H_{corr}$ = −830.895631
$\varepsilon_0 + G_{corr}$ = −830.968876

Frequency: -1270.12

Coordinates:

H	3.5870410000	2.9438870000	-2.3361050000
H	-3.1968030000	-0.1068920000	-2.2877570000
H	2.7610480000	0.6123060000	-2.2662850000
H	-0.8716220000	-1.0160190000	-2.2405480000
C	3.1595070000	2.5518250000	-1.4199760000
C	2.6956400000	1.2352560000	-1.3815650000
C	-2.6220740000	-0.1149730000	-1.3729800000
C	-1.3278360000	-0.6182460000	-1.3443110000
O	-5.1588990000	0.8718940000	-1.2736770000

H	3.4265640000	4.3807020000	-0.3188100000
C	3.0676160000	3.3582780000	-0.2862050000
N	-4.5335320000	0.9217200000	-0.2156860000
C	2.1464920000	0.7399440000	-0.2018180000
O	0.3585140000	-3.5595670000	-0.1991740000
C	-3.1620340000	0.3858340000	-0.1850510000
I	1.4291970000	-1.3589200000	-0.1408340000
C	-0.6724750000	-0.5750050000	-0.1177490000
H	-0.1502170000	-3.6755610000	0.6126100000
O	-4.9984560000	1.3972980000	0.8180930000
C	2.5136500000	2.8499870000	0.8889410000
C	2.0514560000	1.5333940000	0.9388780000
C	-2.4545060000	0.3942280000	1.0172660000
C	-1.1428640000	-0.1068610000	1.0742010000
H	2.4402710000	3.4767040000	1.7710450000
H	1.6075300000	1.1352840000	1.8457650000
H	-2.9335850000	0.7893040000	1.9052000000
H	-0.4115090000	-0.1466520000	2.2600760000
H	0.7858150000	-0.9525690000	3.2522930000
O	0.2272540000	-0.1685950000	3.2946010000

TS1-1c (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.391237
$\varepsilon_0 + E_{tot}$ = −855.369371
$\varepsilon_0 + H_{corr}$ = −855.368427
$\varepsilon_0 + G_{corr}$ = −855.444359
Frequency: -1176.000
Coordinates:

H	-1.9769720000	-0.3632570000	-2.1801420000
H	2.1993710000	-0.7104010000	-2.1509850000
H	-3.5610350000	1.5291360000	-2.0622780000
H	4.0942360000	0.8338630000	-1.9867980000
H	-4.1756910000	3.7536480000	-1.6574740000
H	5.0861040000	2.9227720000	-1.5914540000
H	-5.4966540000	2.6046770000	-1.2955110000
C	-2.1515810000	0.1417620000	-1.2388770000
C	2.4191290000	-0.2475890000	-1.1951790000
H	6.1720320000	1.5664490000	-1.1682900000
C	-3.0491480000	1.2102730000	-1.1649280000
C	3.5002170000	0.6346960000	-1.1053420000
C	-4.8474130000	3.3808820000	-0.8769930000
C	5.6566450000	2.4526300000	-0.7841220000
O	-2.0337730000	-3.3720250000	-0.6189030000
H	-5.4591680000	4.2015520000	-0.5061020000
H	6.3897100000	3.1592380000	-0.3997640000
I	-0.0529110000	-1.9366910000	-0.2625150000
C	1.6370160000	-0.5221080000	-0.0806800000
C	-1.5220920000	-0.2207480000	-0.0610690000
H	-2.7478440000	-3.0690950000	-0.0453470000
C	-3.2604550000	1.8399350000	0.0696200000
C	3.7868540000	1.2451380000	0.1184600000
O	-4.1179030000	2.8959190000	0.2482880000
O	4.8147590000	2.1238180000	0.3209440000
C	1.9240720000	0.0857690000	1.1437510000
C	-1.6757580000	0.3295060000	1.1748860000
C	-2.5828160000	1.3985190000	1.2144450000
C	2.9932550000	0.9672330000	1.2389110000
H	1.3041730000	-0.1166620000	2.0121010000
H	-2.7901970000	1.9141900000	2.1493480000
H	3.2303860000	1.4531850000	2.1784230000
H	-1.0414600000	-0.1649530000	2.3488920000
H	-0.6210180000	-1.5418510000	3.2952090000
O	-0.5092360000	-0.5856180000	3.3316910000

TS1-1c (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.404715
$\varepsilon_0 + E_{tot}$ = −855.382542
$\varepsilon_0 + H_{corr}$ = −855.381597
$\varepsilon_0 + G_{corr}$ = −855.458775
Frequency: -1143.760
Coordinates:

H	-1.7775890000	-0.1379010000	-2.2413420000
H	2.2451190000	-0.6925250000	-2.1523940000
H	-3.3397400000	1.7668570000	-2.0751530000
H	4.1239510000	0.8615770000	-1.9204110000
H	-3.9446920000	3.9616360000	-1.5053830000
H	5.0900350000	2.9532370000	-1.4749600000
H	-5.3155330000	2.8205630000	-1.3798750000
C	-2.0294180000	0.2744780000	-1.2727080000
C	2.4385860000	-0.2417130000	-1.1857140000
C	-2.9137410000	1.3517880000	-1.1724080000
C	3.5102400000	0.6467490000	-1.0565460000
H	6.1763200000	1.5999300000	-1.0417730000
C	-4.6924540000	3.5333430000	-0.8304560000
C	5.6450240000	2.4773730000	-0.6608360000
O	-2.0902980000	-3.3542010000	-0.6513740000
H	-5.3188990000	4.3297250000	-0.4330180000
I	-0.0557380000	-1.9344910000	-0.3190280000
H	6.3613920000	3.1844940000	-0.2477910000
C	1.6325020000	-0.5349890000	-0.0935460000
C	-1.5127180000	-0.2133050000	-0.0847050000
H	-2.7852940000	-3.0146110000	-0.0749020000
C	-3.2229160000	1.8659060000	0.0950070000
C	3.7630310000	1.2437340000	0.1817830000
O	-4.0762600000	2.9175550000	0.3018670000
O	4.7765240000	2.1264910000	0.4200120000
C	1.8854410000	0.0575310000	1.1456170000
C	-1.7598610000	0.2222810000	1.1816710000
C	-2.6512320000	1.3037420000	1.2458500000
C	2.9448150000	0.9449620000	1.2799090000
H	1.2482300000	-0.1604770000	1.9962290000
H	-2.9278660000	1.7390270000	2.2036710000
H	3.1558110000	1.4185420000	2.2318030000
H	-1.1753660000	-0.3834450000	2.3491080000
H	-0.4815880000	-1.7867750000	3.0484410000
O	-0.6854650000	-0.8802340000	3.3030870000

TS1-1d (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.331982
$\varepsilon_0 + E_{tot}$ = −626.314966
$\varepsilon_0 + H_{corr}$ = −626.314021
$\varepsilon_0 + G_{corr}$ = −626.379538
Frequency: -1228.320
Coordinates:

H	-3.1317760000	1.8382730000	-2.7873070000
H	-1.7402250000	-0.1820420000	-2.3374410000
H	4.3222800000	0.4200610000	-2.2247970000
H	2.2878420000	-0.9747330000	-2.0252120000
C	-2.6947360000	1.6895200000	-1.8060140000
C	-1.9148700000	0.5565700000	-1.5663600000
C	3.6830210000	0.5215370000	-1.3544070000
C	2.5362590000	-0.2672600000	-1.2417460000

H	-3.5135750000	3.4969880000	-0.9738960000
C	-2.9049760000	2.6185060000	-0.7819380000
H	4.8890510000	2.0530150000	-0.4422850000
C	3.9995530000	1.4391760000	-0.3535250000
C	-1.3946430000	0.4528170000	-0.2845670000
C	1.7159250000	-0.1334260000	-0.1238760000
I	-0.0964020000	-1.4069730000	0.0469370000
O	-2.2055630000	-2.6784030000	0.0614310000
C	-2.3403880000	2.4197900000	0.4783410000
H	-2.8358260000	-2.2169410000	0.6275360000
C	3.1698810000	1.5671090000	0.7605350000
C	-1.5436650000	1.2900290000	0.7685380000
C	2.0237460000	0.7791140000	0.8833090000
H	-2.5237140000	3.1542750000	1.2596150000
H	3.4125500000	2.2817010000	1.5398250000
H	1.3708720000	0.8832630000	1.7443390000
H	-0.9986820000	1.0472470000	2.0460450000
O	-0.5229690000	0.8381380000	3.1311810000
H	-0.6118700000	-0.1103040000	3.2752850000

TS1-1d (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.343837
$\varepsilon_0 + E_{tot}$ = −626.326845
$\varepsilon_0 + H_{corr}$ = −626.325901
$\varepsilon_0 + G_{corr}$ = −626.391100

Frequency: -1217.270
Coordinates:

H	-2.9048040000	2.0846750000	-2.8015240000
H	-1.5444560000	0.0298930000	-2.4208130000
H	4.3843260000	0.5132940000	-2.0952370000
H	2.3595560000	-0.9059150000	-2.0086400000
C	-2.5506900000	1.8476170000	-1.8044950000
C	-1.7891950000	0.6945520000	-1.6027910000
C	3.7148730000	0.5828080000	-1.2449950000
C	2.5733370000	-0.2203380000	-1.1965660000
H	-3.4404260000	3.5779150000	-0.8862660000
C	-2.8475500000	2.6833510000	-0.7230550000
C	-1.3785080000	0.4769170000	-0.2957050000
H	4.8733230000	2.0971100000	-0.2474450000
C	3.9878460000	1.4729430000	-0.2072280000
C	1.7154970000	-0.1260440000	-0.1036520000
O	-2.2209960000	-2.6962730000	-0.0605240000
I	-0.0899180000	-1.4056160000	-0.0254610000
C	-2.3873150000	2.3726450000	0.5572750000
H	-2.7963590000	-2.3382150000	0.6262920000
C	-1.6134460000	1.2177350000	0.8118250000
C	3.1207280000	1.5596870000	0.8822490000
C	1.9802170000	0.7568220000	0.9413790000
H	-2.6351500000	3.0394440000	1.3803500000
H	3.3306450000	2.2515740000	1.6906830000
H	1.3005150000	0.8279090000	1.7840600000
H	-1.1385190000	0.8626280000	2.1047070000
H	-0.5503480000	-0.3827740000	3.1403510000
O	-0.7324320000	0.5622670000	3.1852060000

TS1-1d (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −625.947943
$\varepsilon_0 + E_{tot}$ = −625.931756
$\varepsilon_0 + H_{corr}$ = −625.930812
$\varepsilon_0 + G_{corr}$ = −625.994000

Frequency: -1175.400
Coordinates:

H	3.9999310000	-0.0215210000	-2.6317680000
H	-4.0720210000	0.9387340000	-2.2496710000
H	1.8733650000	-1.1358440000	-2.0710030000
C	3.5198770000	0.1823210000	-1.6806720000
H	-2.5960380000	-0.9579230000	-1.5571190000
C	-3.2706160000	1.1017530000	-1.5383080000
C	2.3184880000	-0.4441060000	-1.3624540000
H	-3.7009220000	3.1935810000	-1.2841990000
C	-2.4386810000	0.0448030000	-1.1793730000
H	5.0367630000	1.5510190000	-1.0151870000
C	-3.0527480000	2.3709090000	-0.9991490000
C	4.0998680000	1.0614570000	-0.7751580000
C	-1.4382620000	0.3438120000	-0.2648440000
C	1.6848070000	-0.1854640000	-0.1462310000
C	-2.0375580000	2.5693670000	-0.0734620000
I	-0.1320840000	-1.3473970000	0.2909770000
C	-1.1887100000	1.5286050000	0.3478290000
H	-1.9146240000	3.5483910000	0.3836720000
C	3.4652020000	1.3297450000	0.4322320000
O	-2.1409320000	-2.5008280000	0.5022020000
C	2.2573570000	0.7159370000	0.7619600000
H	-2.7739950000	-2.0243880000	1.0470860000
H	3.9084420000	2.0296100000	1.1309700000
H	-0.3895340000	1.7709900000	1.5406320000
H	1.7846260000	1.0030700000	1.7063730000
O	0.0239660000	2.0183820000	2.6625390000
H	-0.7339400000	1.6610560000	3.1262640000

TS2-1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.945733
$\varepsilon_0 + E_{tot}$ = −754.929531
$\varepsilon_0 + H_{corr}$ = −754.928587
$\varepsilon_0 + G_{corr}$ = −754.993321

Frequency: -1216.100
Coordinates:

H	2.4701730000	-0.5885600000	-2.1531450000
H	3.6832830000	-2.7455000000	-2.1350080000
C	2.7350700000	-1.0555860000	-1.2133680000
C	3.4169190000	-2.2720580000	-1.1975270000
O	-0.4535770000	3.4821380000	-0.0568600000
H	-1.2814780000	2.6100870000	-0.0253010000
H	-3.9732770000	1.3707710000	-0.0190740000
C	-1.7992090000	1.3131140000	-0.0153580000
C	-3.0853330000	0.7515550000	-0.0116390000
I	1.3085660000	1.4059640000	-0.0101610000
O	-4.6772570000	-2.4504410000	-0.0084000000
C	-0.8017380000	0.4100610000	-0.0075920000
C	-0.8402560000	-0.9722490000	-0.0023500000
C	-3.2189200000	-0.6386840000	-0.0016300000
H	0.0340380000	-1.6083580000	-0.0000500000
C	2.3997640000	-0.4627790000	0.0009600000
C	-2.1249030000	-1.5096090000	0.0021250000
N	-4.5729590000	-1.2263310000	0.0031410000
H	-2.2755470000	-2.5794920000	0.0091620000
C	3.7510440000	-2.8737470000	0.0149000000
O	-5.5352430000	-0.4645320000	0.0184980000
H	4.2796840000	-3.8195170000	0.0203570000
H	-0.4782990000	3.9089670000	0.8080400000
C	3.4082880000	-2.2629730000	1.2203730000
C	2.7265560000	-1.0463710000	1.2221060000
H	2.4551170000	-0.5721290000	2.1564280000
H	3.6679380000	-2.7294240000	2.1632380000

TS2-1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.949131

$\varepsilon_0 + E_{tot}$ = −754.932849
$\varepsilon_0 + H_{corr}$ = −754.931904
$\varepsilon_0 + G_{corr}$ = −754.997314
Frequency: -1214.980
Coordinates:

H	-2.4735220000	0.5837020000	-2.1537130000
H	-3.6985460000	2.7340800000	-2.1339770000
C	-2.7411910000	1.0488880000	-1.2140300000
C	-3.4298140000	2.2615490000	-1.1967930000
O	0.4905600000	-3.5055780000	-0.0557080000
H	1.2939700000	-2.6174850000	-0.0231030000
H	3.9770500000	-1.3614360000	-0.0186910000
C	1.8033950000	-1.3113460000	-0.0169220000
C	3.0872150000	-0.7448430000	-0.0120970000
I	-1.3052830000	-1.4023070000	-0.0109810000
O	4.6723130000	2.4605760000	-0.0108290000
C	0.8024440000	-0.4102300000	-0.0092720000
C	0.8382620000	0.9723180000	-0.0025540000
C	3.2173870000	0.6460450000	-0.0015400000
H	-0.0373880000	1.6064810000	0.0005700000
C	-2.4034730000	0.4592640000	0.0009140000
C	2.1209330000	1.5139160000	0.0024560000
N	4.5686670000	1.2360990000	0.0035710000
H	2.2667810000	2.5843870000	0.0104650000
C	-3.7673160000	2.8602890000	0.0162640000
O	5.5341390000	0.4771230000	0.0217180000
H	-4.3010910000	3.8031130000	0.0223020000
H	0.4983290000	-3.9072170000	0.8216190000
C	-3.4214900000	2.2507950000	1.2216030000
C	-2.7329630000	1.0379620000	1.2233710000
H	-2.4589310000	0.5642660000	2.1569740000
H	-3.6837400000	2.7150740000	2.1647310000

TS2-1a (M06-2X, Toluene)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.550115
$\varepsilon_0 + E_{tot}$ = −754.534352
$\varepsilon_0 + H_{corr}$ = −754.533408
$\varepsilon_0 + G_{corr}$ = −754.596122
Frequency: -1178.02
Coordinates:

H	-2.3920980000	0.5944970000	-2.1502960000
H	-3.5542050000	2.7778050000	-2.1452750000
C	-2.6530600000	1.0700880000	-1.2125140000
C	-3.3049910000	2.2994360000	-1.2060720000
O	0.2873800000	-3.3995530000	-0.0675170000
H	1.2127560000	-2.5961890000	-0.0411810000
H	3.9250350000	-1.3899300000	-0.0375490000
C	1.7525170000	-1.3410570000	-0.0216720000
C	3.0343370000	-0.7742350000	-0.0207990000
I	-1.2903390000	-1.4016240000	-0.0032920000
C	3.1664960000	0.6077630000	-0.0005470000
C	0.7454020000	-0.4336970000	-0.0003180000
C	-2.3358640000	0.4686180000	0.0000600000
C	-3.6314560000	2.9103880000	0.0002360000
H	-4.1370730000	3.8682770000	0.0003080000
N	4.5243480000	1.1934300000	0.0021670000
O	5.4686440000	0.4335110000	0.0032330000
O	4.6199870000	2.4036530000	0.0037680000
C	0.8013900000	0.9494890000	0.0149600000
C	2.0840140000	1.4825470000	0.0160970000
H	-0.0670920000	1.5947330000	0.0266840000
H	2.2455630000	2.5511200000	0.0299250000
H	0.3370300000	-3.9303240000	0.7330280000
C	-3.3125880000	2.2953000000	1.2064980000
C	-2.6606710000	1.0659280000	1.2126700000
H	-3.5678880000	2.7705070000	2.1456830000
H	-2.4057160000	0.5872660000	2.1505450000

TS2-1c (B3LYP-D3, CH_2Cl_2)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.437494
$\varepsilon_0 + E_{tot}$ = −779.418572
$\varepsilon_0 + H_{corr}$ = −779.417628
$\varepsilon_0 + G_{corr}$ = −779.487374
Frequency: -1195.640
Coordinates:

H	-1.9955800000	-0.5183890000	-2.0389760000
H	-3.9530430000	0.9475510000	-1.9219830000
H	-5.0706800000	2.9448420000	-1.3693860000
H	-6.1528940000	1.5200020000	-1.3054160000
C	-2.3647250000	-0.2042100000	-1.0710490000
H	2.6785530000	-3.3736030000	-1.0062520000
C	-3.4780750000	0.6331850000	-1.0034170000
H	5.9238030000	2.1760150000	-0.9370630000
C	-5.7276690000	2.3476300000	-0.7304110000
H	-6.5296550000	2.9738400000	-0.3462230000
O	2.5192620000	-3.0517330000	-0.1111110000
H	2.8899890000	-1.9195680000	-0.1004470000
H	4.8509490000	0.2867060000	-0.0799780000
C	2.8383950000	-0.5054470000	-0.0524240000
C	3.7959410000	0.5296340000	-0.0480610000
C	5.6320450000	2.7014950000	-0.0222570000
I	0.0080460000	-1.8692760000	-0.0124120000
C	1.5703700000	-0.0865090000	-0.0085430000
H	6.1018640000	3.6830340000	-0.0024600000
C	3.3785480000	1.8670140000	0.0007710000
O	4.2247810000	2.9426790000	0.0100180000
C	1.0455080000	1.1908040000	0.0434080000
C	2.0104360000	2.1937670000	0.0455190000
H	-0.0113100000	1.4200220000	0.0788230000
H	1.7193380000	3.2365930000	0.0822270000
C	-1.7406370000	-0.6201690000	0.0987380000
C	-3.9564020000	1.0514900000	0.2435410000
O	-5.0266200000	1.8668940000	0.4217330000
H	5.9555410000	2.1245080000	0.8497850000
C	-2.2118800000	-0.2094320000	1.3476890000
C	-3.3168220000	0.6239440000	1.4163700000
H	-1.7220450000	-0.5293140000	2.2583320000
H	-3.7008680000	0.9575140000	2.3724780000

TS2-1c (B3LYP-D3, H_2O)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.440859
$\varepsilon_0 + E_{tot}$ = −779.421842
$\varepsilon_0 + H_{corr}$ = −779.420898
$\varepsilon_0 + G_{corr}$ = −779.491078
Frequency: -1192.360
Coordinates:

H	-1.9832820000	-0.5035000000	-2.0405100000
H	-3.9433310000	0.9581700000	-1.9246160000
H	-5.0694300000	2.9473710000	-1.3654520000
H	-6.1488690000	1.5198980000	-1.3183860000
C	-2.3591320000	-0.1972490000	-1.0728580000
H	2.6922770000	-3.3683990000	-1.0261810000
C	-3.4741020000	0.6375490000	-1.0054030000

H	5.9167010000	2.1860190000	-0.9442570000
C	-5.7295620000	2.3446460000	-0.7354430000
H	-6.5351500000	2.9663240000	-0.3516220000
O	2.5655030000	-3.0615210000	-0.1205020000
H	2.9043640000	-1.9242340000	-0.1114000000
H	4.8518310000	0.2924100000	-0.0868690000
C	2.8410900000	-0.5055210000	-0.0548630000
C	3.7962540000	0.5324430000	-0.0495200000
C	5.6303380000	2.7073900000	-0.0256990000
I	0.0051260000	-1.8647100000	-0.0118630000
H	6.0982670000	3.6896960000	-0.0050730000
C	1.5714820000	-0.0887430000	-0.0049660000
C	3.3769690000	1.8691280000	0.0056230000
O	4.2216480000	2.9459550000	0.0163000000
C	1.0455150000	1.1881360000	0.0526350000
C	2.0083810000	2.1930650000	0.0557090000
H	-0.0114320000	1.4162130000	0.0911090000
H	1.7140290000	3.2348520000	0.0966280000
C	-1.7431980000	-0.6196770000	0.0989030000
C	-3.9612300000	1.0451440000	0.2418960000
O	-5.0340900000	1.8568360000	0.4188460000
H	5.9597500000	2.1278440000	0.8421660000
C	-2.2216340000	-0.2210230000	1.3487450000
C	-3.3287190000	0.6096790000	1.4158620000
H	-1.7375000000	-0.5474200000	2.2599070000
H	-3.7190860000	0.9344260000	2.3724450000

TS2-1c (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.022794
$\varepsilon_0 + E_{tot}$ = −779.004493
$\varepsilon_0 + H_{corr}$ = −779.003549
$\varepsilon_0 + G_{corr}$ = −779.071182

Frequency: -1107.61
Coordinates:

H	1.9608530000	0.5273550000	-2.0349950000
H	3.9312620000	-0.9234890000	-1.9078520000
H	5.0224300000	-2.8855570000	-1.3589890000
H	6.0868250000	-1.4492840000	-1.2814660000
C	2.3232900000	0.2090870000	-1.0648430000
C	3.4422530000	-0.6183220000	-0.9931380000
H	-2.6157830000	3.4249490000	-0.9194110000
H	-5.8370070000	-2.1640930000	-0.9067970000
C	5.6769320000	-2.2907220000	-0.7161630000
H	6.4891190000	-2.9123660000	-0.3489910000
O	-2.3657360000	3.0145740000	-0.0867430000
H	-2.8356430000	1.8995590000	-0.0782790000
H	-4.7963100000	-0.3093580000	-0.0544820000
C	-2.8034910000	0.5122520000	-0.0470530000
C	-3.7377770000	-0.5390360000	-0.0402060000
C	-1.5164400000	0.1132050000	-0.0239530000
I	-0.0509030000	1.8503850000	-0.0163050000
C	-3.3084070000	-1.8666500000	-0.0102700000
C	-5.5335800000	-2.7000210000	-0.0027740000
O	-4.1398290000	-2.9445020000	0.0013640000
C	-0.9917850000	-1.1679400000	0.0070080000
C	-1.9402950000	-2.1781960000	0.0113190000
H	-6.0104240000	-3.6771790000	0.0179910000
H	0.0669100000	-1.3943510000	0.0258100000
H	-1.6428500000	-3.2194250000	0.0332020000
C	1.6813250000	0.6137270000	0.0950640000
C	3.9091830000	-1.0368260000	0.2532780000
O	4.9820030000	-1.8378540000	0.4339410000
H	-5.8350730000	-2.1271740000	0.8788970000
C	2.1470950000	0.1972420000	1.3426080000
C	3.2554680000	-0.6246620000	1.4201270000
H	1.6428010000	0.5076140000	2.2498290000
H	3.6366260000	-0.9641810000	2.3751960000

TS2-1d (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.377094
$\varepsilon_0 + E_{tot}$ = −550.363404
$\varepsilon_0 + H_{corr}$ = −550.362460
$\varepsilon_0 + G_{corr}$ = −550.420120

Frequency: -1249.870
Coordinates:

H	-1.8966520000	-0.1050080000	-2.1537320000
H	-3.9889190000	1.2150950000	-2.1372360000
C	-2.3553830000	0.1738010000	-1.2138380000
C	-3.5339490000	0.9195120000	-1.1991920000
O	2.6528370000	-2.2933360000	-0.0560060000
H	2.9432510000	-1.1235040000	-0.0286470000
H	4.7392560000	1.2208130000	-0.0154160000
C	2.7907710000	0.2648880000	-0.0145340000
I	0.0664490000	-1.3193980000	-0.0114680000
C	3.6639370000	1.3740200000	-0.0073660000
C	1.5010660000	0.6072590000	-0.0050430000
C	-1.7821920000	-0.1985300000	-0.0006100000
C	0.8731910000	1.8329610000	0.0048590000
C	3.1535310000	2.6744410000	0.0071330000
H	-0.1983890000	1.9797170000	0.0079860000
C	-4.1201540000	1.2828380000	0.0123700000
C	1.7737330000	2.9063760000	0.0127080000
H	3.8326170000	3.5206180000	0.0127370000
H	-5.0352620000	1.8631120000	0.0174630000
H	1.3847130000	3.9182840000	0.0234560000
H	2.8717930000	-2.6390540000	0.8175340000
C	-3.5315620000	0.9021320000	1.2174210000
C	-2.3529380000	0.1563810000	1.2189800000
H	-1.8924300000	-0.1359540000	2.1539120000
H	-3.9847790000	1.1841790000	2.1604760000

TS2-1d (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.379793
$\varepsilon_0 + E_{tot}$ = −550.366032
$\varepsilon_0 + H_{corr}$ = −550.365088
$\varepsilon_0 + G_{corr}$ = −550.422998

Frequency: -1252.090
Coordinates:

H	-1.9103110000	-0.1211380000	-2.1534520000
H	-4.0058110000	1.1937120000	-2.1318480000
C	-2.3644280000	0.1617680000	-1.2127610000
C	-3.5449130000	0.9045180000	-1.1948100000
O	2.7044460000	-2.2964180000	-0.0499830000
H	2.9589710000	-1.1230830000	-0.0156880000
I	0.0636040000	-1.3160780000	-0.0134540000
C	2.7922580000	0.2683800000	-0.0089310000
C	1.5006500000	0.6068900000	-0.0078020000
H	-0.2026570000	1.9749010000	-0.0077220000
C	0.8692690000	1.8310670000	-0.0055810000
H	4.7369370000	1.2330060000	-0.0030340000
C	3.6608520000	1.3817590000	-0.0020670000
C	-1.7853980000	-0.2009550000	0.0003000000
C	1.7657990000	2.9078440000	0.0021110000
C	3.1464230000	2.6807670000	0.0042420000
H	1.3727360000	3.9181420000	0.0068680000
H	3.8226610000	3.5291570000	0.0099070000

C	-4.1248850000	1.2729970000	0.0182830000
H	-5.0412450000	1.8511380000	0.0253590000
H	2.8884320000	-2.6321620000	0.8355470000
C	-2.3482060000	0.1577940000	1.2221640000
C	-3.5286910000	0.9007060000	1.2223350000
H	-1.8815930000	-0.1283710000	2.1557450000
H	-3.9770690000	1.1869620000	2.1663280000

TS2-1d (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.060434
$\varepsilon_0 + E_{tot}$ = −550.047179
$\varepsilon_0 + H_{corr}$ = −550.046235
$\varepsilon_0 + G_{corr}$ = −550.102493
Frequency: -1140.71
Coordinates:

H	-1.8207850000	-0.0984150000	-2.1513540000
H	-3.9394100000	1.1779820000	-2.1409350000
C	-2.2938620000	0.1632280000	-1.2126120000
C	-3.4850280000	0.8827940000	-1.2029730000
O	2.5200570000	-2.2473420000	-0.0619640000
H	2.8976760000	-1.0918090000	-0.0380690000
H	4.6529420000	1.3002990000	-0.0338010000
C	2.7472540000	0.2808470000	-0.0175140000
C	3.5740800000	1.4196790000	-0.0148220000
I	0.1216970000	-1.3005710000	-0.0094760000
C	-1.7189360000	-0.2094240000	-0.0029530000
C	-4.0868680000	1.2215720000	0.0044350000
C	1.4335040000	0.5785480000	0.0045970000
H	-5.0133650000	1.7827150000	0.0073390000
C	3.0327470000	2.7018160000	0.0083660000
H	3.6875700000	3.5661600000	0.0097350000
C	0.7869370000	1.7985030000	0.0241400000
C	1.6505740000	2.8933950000	0.0277560000
H	-0.2878460000	1.9249010000	0.0369970000
H	1.2340390000	3.8935120000	0.0457750000
H	2.8305450000	-2.6676610000	0.7451770000
C	-3.5017670000	0.8429730000	1.2081750000
C	-2.3105070000	0.1234840000	1.2103110000
H	-1.8510400000	-0.1695520000	2.1466460000
H	-3.9694870000	1.1063950000	2.1489990000

TS2-1l (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −642.303847
$\varepsilon_0 + E_{tot}$ = −642.288834
$\varepsilon_0 + H_{corr}$ = −642.287890
$\varepsilon_0 + G_{corr}$ = −642.348740
Frequency: -1182.98
Coordinates:

H	2.2324520000	0.4092110000	-2.1433690000
H	3.6240350000	2.4542260000	-2.1403090000
C	2.5065480000	0.8796670000	-1.2067920000
C	3.2870890000	2.0318740000	-1.2014540000
H	-1.0233160000	-3.7693610000	-0.7269100000
H	-2.2653240000	2.8691230000	-0.0679910000
H	-0.0709100000	1.6940620000	-0.0621060000
C	-2.2244030000	1.7876810000	-0.0413550000
C	-0.9975370000	1.1356170000	-0.0389240000
N	-5.6790010000	2.2783240000	-0.0130340000
C	-4.6685020000	1.7279650000	-0.0109280000
C	-3.4070550000	1.0379930000	-0.0092750000
C	-1.0766800000	-0.2449100000	-0.0071320000
H	4.2390520000	3.5329740000	0.0024210000
C	3.6319370000	2.6358800000	0.0030730000
C	2.0815720000	0.3468060000	0.0049090000
I	0.8601830000	-1.4100330000	0.0081190000
C	-3.3833220000	-0.3600010000	0.0250070000
C	-2.1651020000	-1.0500540000	0.0266180000
H	-1.7520100000	-2.3496320000	0.0504900000
H	-4.3244230000	-0.8987990000	0.0529910000
O	-0.9134130000	-3.2473040000	0.0731600000
C	3.2021370000	2.0909750000	1.2087410000
C	2.4227480000	0.9381960000	1.2159360000
H	3.4717870000	2.5603100000	2.1468670000
H	2.0827060000	0.5136960000	2.1530230000

TS2-1m (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.545377
$\varepsilon_0 + E_{tot}$ = −754.529591
$\varepsilon_0 + H_{corr}$ = −754.528647
$\varepsilon_0 + G_{corr}$ = −754.592000
Frequency: -1141.78
Coordinates:

H	-0.9679670000	-0.7046240000	-2.1466510000
H	-3.3443350000	0.0418500000	-2.1415070000
C	-2.8055330000	-0.1122670000	-1.2167320000
C	-1.4806760000	-0.5296220000	-1.2090520000
O	-5.3812390000	0.7029990000	-1.0768900000
H	4.1336270000	-2.0420780000	-0.7365530000
H	1.1120280000	3.9923790000	-0.0436250000
H	0.0760640000	1.7303360000	-0.0369380000
C	1.7450860000	3.1130880000	-0.0277800000
C	1.1512390000	1.8509500000	-0.0246670000
H	3.5750960000	4.2311700000	-0.0108470000
C	3.1347950000	3.2404440000	-0.0097330000
C	2.0638160000	0.8162060000	-0.0064110000
N	-4.8434470000	0.5504950000	-0.0022330000
C	-3.4318400000	0.1068430000	0.0002370000
C	-0.8253020000	-0.7152570000	0.0045140000
I	1.2271590000	-1.3418730000	0.0085970000
C	3.9551540000	2.1160890000	0.0119890000
C	3.4062020000	0.8198380000	0.0146240000
H	5.0325970000	2.2452490000	0.0299640000
H	3.8568670000	-0.4885810000	0.0388120000
O	3.7331360000	-1.6946750000	0.0659160000
O	-5.3753080000	0.7338580000	1.0704350000
C	-1.4723580000	-0.4913740000	1.2161290000
C	-2.7970840000	-0.0734010000	1.2192380000
H	-3.3296940000	0.1103280000	2.1422290000
H	-0.9533020000	-0.6369110000	2.1552680000

TS2-1n (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1469.280224
$\varepsilon_0 + E_{tot}$ = −1469.264565
$\varepsilon_0 + H_{corr}$ = −1469.263621
$\varepsilon_0 + G_{corr}$ = −1469.326520
Frequency: -1139.37
Coordinates:

H	1.8188890000	-0.5879490000	-2.1425350000
H	3.7994280000	0.9015800000	-2.1412030000
C	3.3370120000	0.6027930000	-1.2093260000
C	2.2267240000	-0.2336980000	-1.2035240000
H	-2.5833940000	-3.5242040000	-0.7376820000
H	-1.7249520000	3.1690900000	-0.0591390000

H	0.0066850000	1.3737240000	-0.0524780000
C	-2.0150880000	2.1265660000	-0.0359770000
C	-1.0468950000	1.1262560000	-0.0329280000
Cl	-4.5620280000	3.0446540000	-0.0110130000
C	-3.3614670000	1.7689800000	-0.0086380000
C	-1.5496400000	-0.1601930000	-0.0059840000
Cl	5.2393430000	2.1003350000	-0.0028700000
C	3.8489460000	1.0538400000	0.0007180000
C	1.6503500000	-0.6034180000	0.0061580000
I	-0.0669740000	-1.8795460000	0.0105660000
C	-3.7807300000	0.4446940000	0.0213380000
C	-2.8314740000	-0.5875770000	0.0232320000
H	-2.8357710000	-1.9643510000	0.0451080000
H	-4.8429910000	0.2277280000	0.0457900000
O	-2.3197290000	-3.0668600000	0.0662040000
C	3.2779430000	0.6890590000	1.2133230000
C	2.1686650000	-0.1486100000	1.2135170000
H	3.6946750000	1.0544500000	2.1431060000
H	1.7144690000	-0.4361840000	2.1539770000

TS2-1o (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −748.559989
$\varepsilon_0 + E_{tot}$ = −748.545165
$\varepsilon_0 + H_{corr}$ = −748.544221
$\varepsilon_0 + G_{corr}$ = −748.604341

Frequency: -1121.60
Coordinates:

H	1.8641880000	-0.3998120000	-2.1397910000
H	3.9254300000	1.0054190000	-2.1318310000
C	3.4262100000	0.7360310000	-1.2101070000
C	2.2780680000	-0.0475760000	-1.2028270000
H	-2.6715010000	-3.1455360000	-0.7283310000
H	-1.5844230000	3.5245000000	-0.0790320000
H	0.0982900000	1.6592890000	-0.0691350000
C	-1.8946070000	2.4878470000	-0.0505140000
C	-0.9639350000	1.4530740000	-0.0454140000
F	-4.1313820000	3.1861220000	-0.0213580000
C	-3.2459460000	2.1676630000	-0.0177980000
C	-1.5135620000	0.1851790000	-0.0108710000
F	5.0404640000	1.9296760000	-0.0020250000
C	3.9323100000	1.1742450000	0.0010170000
C	1.6726030000	-0.3706230000	0.0071010000
I	-0.0895780000	-1.5799090000	0.0140220000
C	-3.7220230000	0.8687450000	0.0184690000
C	-2.8106940000	-0.1971870000	0.0230700000
H	-4.7942530000	0.7065430000	0.0456010000
H	-2.8608010000	-1.5788570000	0.0498800000
O	-2.3883380000	-2.6955530000	0.0729870000
C	2.1972330000	0.0805250000	1.2142300000
C	3.3439590000	0.8658150000	1.2151060000
H	3.7795390000	1.2348040000	2.1347610000
H	1.7184130000	-0.1713470000	2.1525070000

TS3-1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.899261
$\varepsilon_0 + E_{tot}$ = −830.880150
$\varepsilon_0 + H_{corr}$ = −830.879205
$\varepsilon_0 + G_{corr}$ = −830.950415

Frequency: -501.620
Coordinates:

H	-2.1584380000	0.9206070000	-2.1473020000
H	-3.0985220000	3.2099580000	-2.1244780000
C	-2.3613540000	1.4153520000	-1.2062820000
C	-2.8899820000	2.7065290000	-1.1876240000
H	-4.1799020000	-1.3222970000	-0.5809040000
O	0.5513260000	-3.6516450000	-0.0565850000
H	0.2853680000	1.7150590000	-0.0301870000
C	1.0900930000	0.9914850000	-0.0224680000
I	-1.2706630000	-1.2016090000	-0.0197660000
C	0.8645260000	-0.3845600000	-0.0191260000
H	1.2439230000	-2.7606270000	-0.0169130000
C	1.8342490000	-1.3676770000	-0.0135050000
C	2.4077520000	1.4333260000	-0.0130530000
H	2.6461380000	2.4874500000	-0.0125560000
C	3.1561270000	-0.8981370000	-0.0045090000
C	3.4247090000	0.4753080000	-0.0027490000
O	5.0338630000	2.1556950000	-0.0025690000
H	3.9937280000	-1.5869010000	-0.0002330000
C	-2.1012120000	0.7819950000	0.0039690000
N	4.8165260000	0.9420630000	0.0087010000
C	-3.1453260000	3.3433880000	0.0254550000
O	5.7187910000	0.1046010000	0.0290380000
H	-3.5546510000	4.3467340000	0.0343670000
O	-3.6996510000	-1.7991190000	0.1069680000
H	0.4992550000	-3.9936880000	0.8430910000
C	-2.3486030000	1.3998030000	1.2248960000
C	-2.8754720000	2.6908300000	1.2278970000
H	-2.1410120000	0.8901020000	2.1564270000
H	-3.0741170000	3.1823400000	2.1731870000

TS3-1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.911375
$\varepsilon_0 + E_{tot}$ = −830.891935
$\varepsilon_0 + H_{corr}$ = −830.890991
$\varepsilon_0 + G_{corr}$ = −830.964546

Frequency: -475.440
Coordinates:

H	-2.2010210000	0.9235590000	-2.1428350000
H	-3.1812850000	3.1956980000	-2.0901320000
C	-2.4036390000	1.4072040000	-1.1965020000
C	-2.9563910000	2.6871400000	-1.1600900000
O	-3.6957200000	-1.8657110000	-0.1357060000
H	0.2785270000	1.7241640000	-0.0535870000
H	2.6361490000	2.5081780000	-0.0460920000
O	5.0279500000	2.1838270000	-0.0368480000
C	1.0876670000	1.0057910000	-0.0349440000
C	2.4036430000	1.4529350000	-0.0312270000
I	-1.2505030000	-1.1932610000	-0.0279710000
C	0.8729150000	-0.3710700000	-0.0148400000
C	3.4241010000	0.4989590000	-0.0075650000
N	4.8143780000	0.9704700000	-0.0050120000
C	-2.1223540000	0.7712550000	0.0074400000
C	1.8428990000	-1.3523600000	0.0076760000
C	3.1625620000	-0.8755560000	0.0113310000
H	4.0035820000	-1.5598280000	0.0272450000
O	5.7193270000	0.1360750000	0.0285020000
O	0.6376220000	-3.6887240000	0.0286400000
H	1.2789960000	-2.7628490000	0.0386560000
C	-3.2165440000	3.3066870000	0.0618220000
H	-3.6455180000	4.3014190000	0.0828550000
H	-4.1946430000	-1.3210260000	0.4851350000
H	0.5626650000	-3.9698990000	0.9477630000
C	-2.3707710000	1.3693440000	1.2376830000
C	-2.9255700000	2.6495770000	1.2560820000
H	-2.1398960000	0.8586400000	2.1633580000
H	-3.1260770000	3.1283170000	2.2072940000

TS3-1a (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.475392
$\varepsilon_0 + E_{tot}$ = −830.456782
$\varepsilon_0 + H_{corr}$ = −830.455837
$\varepsilon_0 + G_{corr}$ = −830.524713
Frequency: -907.850
Coordinates:

H	-2.0409650000	0.9388640000	-2.1449950000
H	-2.9554320000	3.2380870000	-2.1141210000
C	-2.2745930000	1.4206150000	-1.2037540000
C	-2.7896660000	2.7135700000	-1.1809410000
H	-3.8335400000	-2.5086230000	-0.1092160000
O	-3.6571900000	-1.5650390000	-0.0424230000
O	0.4275650000	-3.5592520000	-0.0253950000
I	-1.2501910000	-1.1948370000	-0.0203120000
O	4.9954410000	2.1161930000	-0.0047380000
C	1.7958100000	-1.3724770000	-0.0002480000
H	3.9533460000	-1.5989670000	-0.0000880000
C	-2.0711480000	0.7603820000	-0.0000520000
C	0.8193340000	-0.3862670000	0.0015750000
C	3.1167380000	-0.9091800000	0.0024090000
N	4.7811510000	0.9175070000	0.0033150000
H	1.2074780000	-2.6840200000	0.0046890000
C	3.3837840000	0.4571150000	0.0053120000
C	1.0630370000	0.9856670000	0.0072770000
C	2.3817150000	1.4201810000	0.0086710000
O	5.6647820000	0.0818930000	0.0095600000
H	0.2667090000	1.7199880000	0.0097720000
H	2.6293930000	2.4725510000	0.0117490000
C	-3.0916060000	3.3252110000	0.0316340000
H	-3.4913300000	4.3318760000	0.0444210000
H	0.4638100000	-4.0099560000	0.8233820000
C	-2.3694990000	1.3521580000	1.2189590000
C	-2.8841450000	2.6456460000	1.2277740000
H	-2.2084150000	0.8189940000	2.1473780000
H	-3.1223510000	3.1189220000	2.1726250000

TS3-1a (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.487453
$\varepsilon_0 + E_{tot}$ = −830.468685
$\varepsilon_0 + H_{corr}$ = −830.467741
$\varepsilon_0 + G_{corr}$ = −830.537592
Frequency: -873.000
Coordinates:

H	-2.0766030000	0.9201620000	-2.1519180000
H	-3.0245310000	3.2050460000	-2.1326810000
C	-2.3019020000	1.4094080000	-1.2124670000
C	-2.8357110000	2.6945410000	-1.1962060000
O	-3.6190950000	-1.7840600000	-0.1048110000
O	0.4398710000	-3.5668130000	-0.0449060000
H	3.9560870000	-1.5920910000	-0.0196680000
C	1.7978390000	-1.3687610000	-0.0153960000
H	1.2065350000	-2.6898260000	-0.0130530000
C	3.1185490000	-0.9035140000	-0.0115670000
I	-1.2435740000	-1.1876420000	-0.0108480000
C	0.8233800000	-0.3812630000	-0.0043010000
C	-2.0668730000	0.7689830000	-0.0028440000
O	5.6651230000	0.0864990000	0.0010180000
C	3.3842620000	0.4627890000	0.0017110000
N	4.7819700000	0.9227770000	0.0043410000
O	4.9968680000	2.1208790000	0.0096160000
C	1.0637250000	0.9909260000	0.0097500000
C	2.3823200000	1.4257680000	0.0126710000
C	-3.1251840000	3.3178880000	0.0140730000
H	0.2672660000	1.7247120000	0.0190180000
H	-3.5399220000	4.3183570000	0.0206680000
H	2.6278970000	2.4785390000	0.0235490000
H	-4.1076040000	-1.4270470000	0.6432040000
H	0.4695010000	-4.0073110000	0.8097400000
C	-2.3479180000	1.3738310000	1.2145350000
C	-2.8828860000	2.6594800000	1.2153620000
H	-2.1554940000	0.8596360000	2.1481110000
H	-3.1072710000	3.1429250000	2.1583160000

TS3-1a-Na (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −992.709334
$\varepsilon_0 + E_{tot}$ = −992.688618
$\varepsilon_0 + H_{corr}$ = −992.687674
$\varepsilon_0 + G_{corr}$ = −992.763017
Frequency: -893.640
Coordinates:

H	-2.5706890000	3.6430300000	-2.3538840000
H	-1.8510120000	1.2849600000	-2.1342080000
C	-2.4456380000	3.2092360000	-1.3694300000
C	-2.0418640000	1.8829870000	-1.2521270000
Na	-2.0237750000	-3.7762670000	-0.6952310000
H	-3.0033700000	5.0018460000	-0.3287450000
C	-2.6881010000	3.9704420000	-0.2302400000
O	5.3897180000	1.6858990000	-0.1471770000
O	5.7618670000	-0.4236940000	-0.1164780000
N	5.0117190000	0.5314010000	-0.1021790000
O	-3.4171170000	-2.1874390000	-0.0968570000
H	3.1028310000	2.3777490000	-0.0269060000
C	3.5612540000	0.2748670000	-0.0248490000
H	3.8447410000	-1.8402900000	-0.0124390000
C	2.7086960000	1.3718440000	0.0053900000
C	3.1129920000	-1.0415650000	0.0163250000
C	-1.8850040000	1.3491720000	0.0208010000
C	1.3418340000	1.1344050000	0.0799610000
C	1.7431990000	-1.3202210000	0.0904860000
H	0.6489880000	1.9667030000	0.1070720000
C	0.9353620000	-0.1920570000	0.1181360000
H	0.9568160000	-2.5220520000	0.1497160000
O	0.0483890000	-3.2632440000	0.1741020000
I	-1.2341120000	-0.6633870000	0.2099390000
H	-4.3024760000	-2.2005030000	0.2716000000
H	0.1206690000	-3.7239260000	1.0167230000
C	-2.5319150000	3.4131160000	1.0348170000
C	-2.1266260000	2.0886160000	1.1714550000
H	-2.7257970000	4.0046610000	1.9209610000
H	-2.0012810000	1.6492100000	2.1530960000

TS3-1a-Na (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −992.716216
$\varepsilon_0 + E_{tot}$ = −992.695186
$\varepsilon_0 + H_{corr}$ = −992.694242
$\varepsilon_0 + G_{corr}$ = −992.771164
Frequency: -859.450
Coordinates:

H	-2.0594170000	3.6880290000	-2.2734330000
H	-1.4967640000	1.2849140000	-2.1074390000
C	-2.0057460000	3.2154280000	-1.3003140000
C	-1.6912410000	1.8624050000	-1.2121660000
Na	-4.6056060000	-2.6182750000	-0.7569420000
H	-2.4943560000	5.0064930000	-0.2207670000

O	5.8862430000	-0.7367520000	-0.1525110000
O	5.5818880000	1.3829750000	-0.1483710000
C	-2.2504300000	3.9538660000	-0.1464600000
N	5.1635770000	0.2406630000	-0.1243880000
H	3.9177360000	-2.0924050000	-0.0919620000
C	3.7079850000	0.0300290000	-0.0570880000
C	3.2123310000	-1.2703450000	-0.0475850000
H	3.3140590000	2.1464330000	-0.0085850000
C	2.8897850000	1.1522610000	-0.0025810000
C	1.8331100000	-1.5027560000	0.0159650000
C	-1.6271560000	1.2744250000	0.0437320000
C	1.5166970000	0.9539710000	0.0615960000
H	1.0174320000	-2.6973670000	0.0653030000
C	1.0516860000	-0.3574580000	0.0661170000
O	0.1065290000	-3.4238570000	0.0842960000
H	0.8578490000	1.8121780000	0.1072270000
I	-1.1229930000	-0.7828030000	0.1776410000
O	-3.6305930000	-0.9399570000	0.2258620000
H	-4.0293080000	-0.2393180000	0.7476620000
H	0.1294860000	-3.8870170000	0.9271090000
C	-2.1838080000	3.3445700000	1.1022550000
C	-1.8678470000	1.9921390000	1.2071950000
H	-2.3754490000	3.9176890000	2.0011160000
H	-1.8107120000	1.5148420000	2.1776750000

TS3-1c (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.382716
$\varepsilon_0 + E_{tot}$ = −855.361065
$\varepsilon_0 + H_{corr}$ = −855.360121
$\varepsilon_0 + G_{corr}$ = −855.435496

Frequency: -1149.000
Coordinates:

H	-1.8859760000	-0.2488580000	-2.0272940000
H	-3.6958980000	1.3996850000	-1.9180570000
H	-4.6356430000	3.4845030000	-1.3870870000
H	-5.8340320000	2.1589020000	-1.2973820000
C	-2.2173560000	0.1102460000	-1.0615220000
C	-3.2482450000	1.0497620000	-0.9984370000
H	2.5967350000	-3.3656120000	-0.9933700000
H	6.0421660000	2.0715890000	-0.9626160000
C	-5.3369330000	2.9549470000	-0.7347450000
H	-6.0816710000	3.6538760000	-0.3595430000
O	2.4650070000	-3.0210250000	-0.1023750000
H	2.8738930000	-1.9020940000	-0.0897070000
H	4.9001020000	0.2412540000	-0.0809650000
O	-2.0871540000	-3.3608910000	-0.0793420000
C	5.7809990000	2.6164930000	-0.0492360000
C	3.8522360000	0.5195330000	-0.0443170000
H	6.2969820000	3.5754860000	-0.0411450000
C	2.8702400000	-0.4871180000	-0.0393690000
O	4.3893220000	2.9195930000	-0.0038220000
I	-0.0047550000	-1.7542590000	-0.0036330000
C	3.4941260000	1.8727040000	-0.0014740000
C	1.5632310000	-0.0623680000	0.0099730000
H	-1.7159900000	-4.2471730000	0.0118680000
C	2.1442950000	2.2450040000	0.0484780000
C	1.1540020000	1.2660170000	0.0558180000
H	1.8877220000	3.2979160000	0.0815840000
H	0.1112380000	1.5567700000	0.0958820000
C	-1.6296450000	-0.3552440000	0.1055840000
C	-3.6822460000	1.5174330000	0.2454830000
O	-4.6753780000	2.4347830000	0.4205840000
H	6.0911860000	2.0300110000	0.8220320000
C	-2.0604260000	0.1040890000	1.3495490000
C	-3.0835070000	1.0385500000	1.4180840000
H	-1.6033520000	-0.2592310000	2.2610180000
H	-3.4344550000	1.4087160000	2.3737580000

TS3-1c (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.396610
$\varepsilon_0 + E_{tot}$ = −855.374713
$\varepsilon_0 + H_{corr}$ = −855.373768
$\varepsilon_0 + G_{corr}$ = −855.450279

Frequency: -1156.410
Coordinates:

H	-1.8638850000	-0.2131750000	-2.0349110000
H	-3.6804500000	1.4257290000	-1.9202580000
H	-4.6237410000	3.5048000000	-1.3636950000
H	-5.8260670000	2.1801350000	-1.3163100000
C	-2.2091560000	0.1269940000	-1.0670670000
H	2.6279050000	-3.3664120000	-1.0084990000
C	-3.2437870000	1.0617390000	-1.0009670000
H	6.0512980000	2.0768110000	-0.9449130000
C	-5.3356280000	2.9646540000	-0.7327620000
H	-6.0836310000	3.6572020000	-0.3530830000
O	2.5089500000	-3.0338040000	-0.1110110000
H	2.8888670000	-1.9095890000	-0.0993000000
H	4.9067860000	0.2413620000	-0.0724870000
C	2.8769550000	-0.4895710000	-0.0414110000
C	3.8586050000	0.5183080000	-0.0394340000
O	-2.1128550000	-3.3840310000	-0.0368860000
C	5.7861860000	2.6181740000	-0.0310370000
H	-1.7306790000	-4.2702170000	-0.0300600000
H	6.2985270000	3.5787230000	-0.0183590000
I	-0.0066660000	-1.7448600000	-0.0110550000
C	1.5724730000	-0.0623490000	0.0026410000
C	3.4988630000	1.8713840000	0.0049210000
O	4.3913600000	2.9176430000	0.0095030000
C	2.1476400000	2.2424580000	0.0489790000
C	1.1573550000	1.2639310000	0.0491630000
H	1.8892810000	3.2947720000	0.0824760000
H	0.1142030000	1.5531440000	0.0840830000
C	-1.6347090000	-0.3537700000	0.1009280000
C	-3.6929570000	1.5102070000	0.2454160000
O	-4.6895570000	2.4195880000	0.4228370000
H	6.0930900000	2.0308500000	0.8403730000
C	-2.0773000000	0.0867090000	1.3479220000
C	-3.1045560000	1.0162080000	1.4178630000
H	-1.6268850000	-0.2852190000	2.2591560000
H	-3.4644180000	1.3730330000	2.3752200000

TS3-1c (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −854.939212
$\varepsilon_0 + E_{tot}$ = −854.918102
$\varepsilon_0 + H_{corr}$ = −854.917158
$\varepsilon_0 + G_{corr}$ = −854.991512

Frequency: -274.100
Coordinates:

H	-1.3826970000	0.2336940000	-1.9790230000
H	-3.2463640000	1.8208830000	-1.8896350000
H	-5.4368960000	2.4481490000	-1.6119930000
H	-4.2903340000	3.7107380000	-1.0764160000
C	-1.9398450000	0.3455650000	-1.0566750000

H	5.7859120000	2.2808450000	-1.0564120000
C	-2.9976900000	1.2529690000	-1.0039120000
C	-5.1188170000	3.0671650000	-0.7690180000
O	2.6004510000	-3.0367110000	-0.4420690000
H	-5.9513960000	3.6797360000	-0.4332170000
H	2.8804190000	-1.9465700000	-0.3792680000
H	4.8014990000	0.3500270000	-0.3416620000
H	-2.6978410000	-3.0133870000	-0.2940090000
C	2.8054310000	-0.4533210000	-0.2116920000
C	3.7575480000	0.5825990000	-0.1569510000
C	5.6358760000	2.6798420000	-0.0490670000
I	0.0297330000	-1.7324410000	-0.0313360000
C	1.5036980000	-0.0698660000	0.0342940000
H	6.1551390000	3.6310360000	0.0455910000
C	-1.6052810000	-0.3922480000	0.0651250000
O	-1.8889610000	-3.3720590000	0.0832890000
C	3.3935220000	1.8986930000	0.1309390000
C	-3.7107840000	1.4077900000	0.1837120000
O	4.2688460000	2.9510330000	0.1956720000
C	1.0913610000	1.2249830000	0.3395030000
O	-4.7500080000	2.2636410000	0.3412480000
H	2.9545160000	-3.4591520000	0.3458560000
C	2.0570900000	2.2199710000	0.3850930000
H	0.0572530000	1.4793910000	0.5434010000
H	1.7959790000	3.2459120000	0.6177310000
H	6.0358710000	1.9715310000	0.6821820000
C	-2.3180200000	-0.2488690000	1.2522090000
C	-3.3677570000	0.6505490000	1.3097540000
H	-2.0598930000	-0.8400040000	2.1216950000
H	-3.9376010000	0.7844010000	2.2209890000

TS3-1c (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −854.953370
$\varepsilon_0 + E_{tot}$ = −854.931989
$\varepsilon_0 + H_{corr}$ = −854.931044
$\varepsilon_0 + G_{corr}$ = −855.006243

Frequency: -183.420
Coordinates:

H	-1.5254540000	0.1030390000	-2.0191610000
H	-3.3966560000	1.6784070000	-1.9204720000
H	-5.5903520000	2.2850020000	-1.5404400000
H	-4.4316590000	3.6016040000	-1.1897650000
C	-2.0225190000	0.2763790000	-1.0724480000
H	5.8429190000	2.2236470000	-1.0557060000
C	-3.0862090000	1.1756470000	-1.0151890000
C	-5.2239070000	2.9734580000	-0.7749680000
H	-6.0409330000	3.5994180000	-0.4265460000
O	2.5986200000	-3.0606910000	-0.3938390000
H	2.8830190000	-1.9822150000	-0.3312030000
H	4.8291990000	0.3175100000	-0.3039890000
C	2.8241750000	-0.4683140000	-0.1870270000
C	3.7839950000	0.5619200000	-0.1443830000
H	-2.7702090000	-2.9745200000	-0.1321160000
C	5.6785230000	2.6470880000	-0.0609450000
I	0.0331260000	-1.7032970000	-0.0244520000
H	6.2019010000	3.5969440000	0.0205550000
C	1.5263290000	-0.0612260000	0.0256430000
O	-1.9269590000	-3.4055140000	0.0364970000
C	-1.6094960000	-0.3765030000	0.0761540000
C	3.4253560000	1.8888940000	0.0992120000
O	4.3073320000	2.9335440000	0.1521230000
C	-3.7255580000	1.4081800000	0.2026130000
C	1.1117620000	1.2430130000	0.2809410000
C	2.0861220000	2.2295770000	0.3154950000
O	-4.7613710000	2.2631690000	0.3659930000
H	2.9443670000	-3.4827070000	0.3983300000
H	0.0750410000	1.5092000000	0.4531600000
H	1.8289300000	3.2642210000	0.5103840000
H	6.0593280000	1.9544120000	0.6946520000
C	-2.2451970000	-0.1546990000	1.2951330000
C	-3.3017670000	0.7364160000	1.3551590000
H	-1.9222040000	-0.6720290000	2.1898490000
H	-3.8135310000	0.9297760000	2.2898830000

TS3-1c-Na (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1017.178413
$\varepsilon_0 + E_{tot}$ = −1017.155196
$\varepsilon_0 + H_{corr}$ = −1017.154252
$\varepsilon_0 + G_{corr}$ = −1017.234210

Frequency: -283.790
Coordinates:

H	3.8836880000	-1.1865510000	-2.0097430000
H	1.8168180000	0.1255360000	-1.9584760000
H	5.1729210000	-3.0410910000	-1.5772260000
H	6.1256050000	-1.5270170000	-1.5742710000
H	-5.5648190000	-2.8862730000	-1.2091440000
C	3.4598600000	-0.9122490000	-1.0540280000
C	2.2847680000	-0.1663170000	-1.0266530000
C	5.8332130000	-2.4009080000	-0.9869920000
Na	-1.4662480000	4.2173480000	-0.8580550000
H	6.7189650000	-2.9593900000	-0.6969860000
H	-5.7858990000	-4.4119440000	-0.3172110000
C	-5.3477410000	-3.4174000000	-0.2782050000
H	-4.7028060000	-1.0106800000	-0.2369830000
O	0.5739150000	4.0398010000	-0.1207660000
O	-3.9538470000	-3.6087400000	-0.1128130000
C	-3.6399360000	-1.1857640000	-0.1114390000
C	-3.1652060000	-2.4976150000	-0.0360830000
C	-2.7716780000	-0.0816660000	-0.0311770000
H	-2.9298750000	1.4144050000	-0.0156250000
O	-2.7091970000	2.5181960000	0.0450510000
C	-1.4438900000	-0.4184580000	0.1288420000
C	-1.7987890000	-2.7514590000	0.1289970000
H	1.2206590000	4.7017870000	0.1303970000
C	4.0668400000	-1.2870910000	0.1459560000
H	-1.4566020000	-3.7776080000	0.1878790000
C	1.7285780000	0.1929130000	0.1906320000
C	-0.9047390000	-1.6947810000	0.2143130000
I	-0.0613460000	1.3196890000	0.2207790000
O	5.2056990000	-2.0071630000	0.2259040000
H	0.1547030000	-1.8865980000	0.3407060000
H	-5.7721340000	-2.8636690000	0.5639250000
H	-3.0489900000	2.7949310000	0.9024410000
C	3.4947510000	-0.9143700000	1.3679150000
C	2.3274100000	-0.1739630000	1.3946190000
H	3.9844830000	-1.2148840000	2.2857080000
H	1.8901290000	0.1127220000	2.3427270000

TS3-1c-Na (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1017.183032
$\varepsilon_0 + E_{tot}$ = −1017.159593
$\varepsilon_0 + H_{corr}$ = −1017.158648
$\varepsilon_0 + G_{corr}$ = −1017.240483

Frequency: -169.840
Coordinates:

H	1.6466830000	-0.4424440000	-2.0622670000

H	3.2995790000	-2.2420960000	-1.8963830000
H	5.3296360000	-3.1465310000	-1.3259410000
H	4.0061200000	-4.3458190000	-1.2290990000
C	1.9885780000	-0.7606920000	-1.0851790000
C	2.9288090000	-1.7850280000	-0.9896230000
H	-6.3371610000	-1.5341830000	-0.9388690000
C	4.8028800000	-3.8463220000	-0.6725080000
H	5.5018250000	-4.5858380000	-0.2913250000
H	3.0680390000	2.1375050000	-0.2179700000
O	-2.2763330000	3.1311150000	-0.1875250000
H	-2.7220370000	2.1070740000	-0.1629350000
O	2.3226410000	2.7379990000	-0.1484310000
H	-4.9967170000	0.1260010000	-0.1390040000
C	-2.8926250000	0.5958150000	-0.1068950000
I	0.0624730000	1.3759290000	-0.0873700000
C	-3.9935710000	-0.2820530000	-0.0719780000
C	-1.6637910000	-0.0181160000	-0.0151940000
C	-6.1743340000	-2.0649440000	0.0031890000
C	-3.8266040000	-1.6633020000	0.0457530000
H	-6.8300320000	-2.9313290000	0.0494220000
C	1.5030410000	-0.1629290000	0.0653550000
O	-4.8516230000	-2.5673260000	0.0838010000
C	-1.4330550000	-1.3851210000	0.1017190000
C	-2.5440140000	-2.2152260000	0.1334930000
H	-0.4401890000	-1.8146840000	0.1682750000
Na	2.2362710000	4.8694090000	0.1877090000
H	-2.4356020000	-3.2896540000	0.2246180000
C	3.3715330000	-2.1977500000	0.2676400000
O	4.2802250000	-3.1786890000	0.4686050000
H	-2.4575500000	3.5273000000	0.6700190000
H	-6.3933350000	-1.3954600000	0.8395840000
C	1.9387090000	-0.5675560000	1.3247480000
C	2.8720950000	-1.5840880000	1.4221560000
H	1.5559740000	-0.0981410000	2.2223780000
H	3.2295080000	-1.9203820000	2.3876450000

TS3-1d (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.322537
$\varepsilon_0 + E_{tot}$ = −626.306149
$\varepsilon_0 + H_{corr}$ = −626.305205
$\varepsilon_0 + G_{corr}$ = −626.368318

Frequency: -1192. 740

Coordinates:

H	-1.8337980000	0.1824000000	-2.1390470000
H	-3.6718710000	1.8399810000	-2.1219780000
C	-2.1852800000	0.5934900000	-1.2014870000
C	-3.2208820000	1.5281150000	-1.1868250000
H	0.0888440000	2.1217890000	-0.0576790000
O	2.5111920000	-2.4088140000	-0.0429420000
C	1.1380140000	1.8544250000	-0.0400700000
H	1.8201080000	3.8956360000	-0.0376200000
C	2.1185180000	2.8522530000	-0.0291460000
C	1.5783570000	0.5375230000	-0.0256800000
H	2.9115240000	-1.2718230000	-0.0188270000
I	0.0290910000	-1.1929540000	-0.0146410000
C	2.8918410000	0.1248280000	-0.0109440000
C	3.4698020000	2.5020930000	-0.0081060000
C	3.8468620000	1.1557930000	-0.0017710000
H	4.2261400000	3.2817050000	0.0006630000
C	-1.6144880000	0.1991880000	0.0033620000
H	4.9073360000	0.9105530000	0.0084150000
H	-1.7498500000	-3.6356460000	0.0089850000
C	-3.6724540000	2.0564160000	0.0217690000
H	-4.4767720000	2.7829940000	0.0288180000
O	-2.0879200000	-2.7334960000	0.0684380000
H	2.6731430000	-2.7908670000	0.8276350000
C	-2.0552590000	0.7139860000	1.2175380000
C	-3.0916370000	1.6479550000	1.2214190000
H	-1.6016190000	0.3985110000	2.1483400000
H	-3.4415620000	2.0534200000	2.1639270000

TS3-1d (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.335779
$\varepsilon_0 + E_{tot}$ = −626.318987
$\varepsilon_0 + H_{corr}$ = −626.318043
$\varepsilon_0 + G_{corr}$ = −626.383078

Frequency: -1205.870

Coordinates:

H	-1.7977200000	0.2376270000	-2.1457380000
H	-3.6498690000	1.8791700000	-2.1247700000
C	-2.1715530000	0.6223520000	-1.2056790000
C	-3.2147760000	1.5487630000	-1.1887010000
O	2.5517670000	-2.4236000000	-0.0414050000
H	0.0996950000	2.1231260000	-0.0388250000
C	1.1484980000	1.8545950000	-0.0276540000
H	1.8358420000	3.8932040000	-0.0235160000
C	2.1321240000	2.8495140000	-0.0193100000
C	1.5914560000	0.5391610000	-0.0191240000
I	0.0246370000	-1.1788900000	-0.0139350000
H	2.9245940000	-1.2822150000	-0.0111770000
C	2.9006560000	0.1190110000	-0.0100330000
C	3.4828520000	2.4959390000	-0.0055540000
C	3.8579580000	1.1491030000	-0.0027040000
H	4.2405600000	3.2737770000	0.0012570000
C	-1.6225020000	0.2065360000	0.0024260000
H	4.9178710000	0.9021900000	0.0041300000
C	-3.6919030000	2.0468130000	0.0229950000
H	-1.7322240000	-3.6763600000	0.0291780000
O	-2.0998220000	-2.7839430000	0.0300230000
H	-4.5010610000	2.7676490000	0.0309380000
H	2.6943480000	-2.7961870000	0.8368050000
C	-2.0856590000	0.6921440000	1.2206260000
C	-3.1290720000	1.6184090000	1.2244550000
H	-1.6446230000	0.3622700000	2.1524400000
H	-3.4972230000	2.0032290000	2.1684290000

TS3-1d (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −625.943884
$\varepsilon_0 + E_{tot}$ = −625.927915
$\varepsilon_0 + H_{corr}$ = −625.926971
$\varepsilon_0 + G_{corr}$ = −625.988516

Frequency: -807.170

Coordinates:

H	-2.7815430000	-0.8239940000	-1.3407810000
H	-4.6463950000	0.8360310000	-1.2356210000
H	1.9562020000	3.6859160000	-1.0874430000
H	0.1878160000	1.9626540000	-0.9708190000
C	-2.7218400000	0.0538360000	-0.7112850000
C	2.1855100000	2.7034950000	-0.6886680000
C	1.1883430000	1.7336220000	-0.6200690000
C	-3.7651050000	0.9709640000	-0.6194030000
H	4.2516020000	3.1529750000	-0.3050360000
C	3.4729730000	2.3974160000	-0.2525390000
O	-1.9934950000	-2.5868100000	-0.2025220000
H	3.0761270000	-2.8509770000	-0.2021060000
C	1.5258340000	0.4880170000	-0.1003190000

I	0.0158670000	-1.1516570000	-0.0311290000
H	-1.6992930000	-3.4832450000	-0.0185910000
C	-1.6021170000	0.2408170000	0.0843020000
C	3.7613290000	1.1212860000	0.2269200000
C	-3.6877420000	2.0431910000	0.2639850000
C	2.7898930000	0.1087330000	0.3155420000
H	-4.5058980000	2.7508330000	0.3321760000
O	2.5450060000	-2.4557150000	0.4943420000
H	2.8361350000	-1.3255850000	0.5224960000
H	4.7831150000	0.9088600000	0.5369220000
C	-1.5118150000	1.2930740000	0.9842310000
C	-2.5649070000	2.1998030000	1.0693950000
H	-0.6298650000	1.4143620000	1.6020480000
H	-2.5032110000	3.0246930000	1.7694680000

TS4-1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.944523
$\varepsilon_0 + E_{tot}$ = −754.928699
$\varepsilon_0 + H_{corr}$ = −754.927755
$\varepsilon_0 + G_{corr}$ = −754.990968

Frequency: -304.380
Coordinates:

H	-0.7458320000	-0.7701690000	-2.1701870000
H	-2.9312620000	0.3945710000	-2.1486820000
H	2.2369680000	0.7927830000	-2.1450470000
H	2.9896390000	3.1500240000	-2.1408820000
C	-1.2364510000	-0.5458410000	-1.2340870000
C	-2.4587160000	0.1007160000	-1.2219290000
C	2.4017400000	1.3086460000	-1.2076310000
C	2.8258920000	2.6372170000	-1.2004330000
O	-4.8575470000	1.3934290000	-1.0742160000
O	-0.3941150000	-3.0679530000	-0.1592850000
C	-0.6728470000	-0.9367100000	-0.0144730000
C	-3.0809550000	0.3795390000	-0.0007200000
I	1.4923930000	-1.3951870000	0.0060700000
N	-4.3583830000	1.0686550000	0.0061210000
H	3.3657290000	4.3318720000	0.0074420000
C	3.0363950000	3.2995920000	0.0081690000
C	2.1982030000	0.6659190000	0.0101480000
H	-0.7292620000	-3.4305050000	0.6719670000
O	-4.8955180000	1.3011950000	1.0922280000
C	-1.2604690000	-0.6143380000	1.2142010000
C	-2.4857070000	0.0288180000	1.2145220000
C	2.8243370000	2.6393800000	1.2177180000
C	2.3994920000	1.3110130000	1.2268940000
H	-2.9757710000	0.2713440000	2.1469850000
H	-0.7860800000	-0.8837670000	2.1474210000
H	2.9869500000	3.1540340000	2.1573570000
H	2.2327440000	0.7970820000	2.1649860000

TS4-1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.948781
$\varepsilon_0 + E_{tot}$ = −754.932943
$\varepsilon_0 + H_{corr}$ = −754.931999
$\varepsilon_0 + G_{corr}$ = −754.995271

Frequency: -306.470
Coordinates:

H	-2.2313490000	0.7894390000	-2.1657550000
H	-2.9893480000	3.1454950000	-2.1610340000
H	2.9708440000	0.2705650000	-2.1480320000
H	0.7861730000	-0.8887940000	-2.1475020000
C	-2.3987160000	1.3048580000	-1.2287700000
C	-2.8253030000	2.6327930000	-1.2206620000
C	2.4826330000	0.0279520000	-1.2146810000
C	1.2600600000	-0.6189640000	-1.2142420000
O	4.8885460000	1.3091960000	-1.0922960000
H	0.7509700000	-3.4047670000	-0.6958510000
H	-3.3691500000	4.3260350000	-0.0125630000
C	-3.0378230000	3.2944150000	-0.0117860000
C	-2.1965220000	0.6641110000	-0.0099600000
N	4.3504560000	1.0728810000	-0.0061810000
I	-1.4932600000	-1.3942530000	-0.0036570000
C	3.0769400000	0.3827250000	0.0008690000
C	0.6724710000	-0.9427450000	0.0151210000
O	0.4304110000	-3.0735000000	0.1541330000
O	4.8528310000	1.3975450000	1.0741670000
C	-2.8257460000	2.6345490000	1.1980790000
C	-2.3998770000	1.3064320000	1.2079620000
C	2.4526390000	0.1065560000	1.2225330000
C	1.2328090000	-0.5435380000	1.2347930000
H	-2.9900040000	3.1484400000	2.1377740000
H	-2.2337950000	0.7921070000	2.1457940000
H	2.9203810000	0.4068500000	2.1496060000
H	0.7391300000	-0.7608920000	2.1710660000

TS4-1a (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.541526
$\varepsilon_0 + E_{tot}$ = −754.525854
$\varepsilon_0 + H_{corr}$ = −754.524909
$\varepsilon_0 + G_{corr}$ = −754.587913

Frequency: -391.86
Coordinates:

H	2.9811380000	3.1189410000	-2.1602930000
H	-0.7574180000	-0.8458660000	-2.1558210000
H	2.2155910000	0.7695920000	-2.1505300000
H	-2.9624000000	0.3031940000	-2.1424640000
C	-1.2347580000	-0.5802260000	-1.2231020000
C	2.8094520000	2.6141320000	-1.2174790000
C	-2.4648230000	0.0491790000	-1.2163580000
C	2.3768840000	1.2918300000	-1.2150160000
O	-4.8584570000	1.3138230000	-1.0726910000
O	-0.3048070000	-2.9926000000	-0.1253100000
H	3.3569230000	4.3116610000	-0.0225340000
C	3.0191660000	3.2825510000	-0.0158080000
C	-0.6508310000	-0.9205000000	-0.0013010000
C	-3.0632120000	0.3625400000	0.0000270000
N	-4.3542640000	1.0451620000	0.0006340000
C	2.1630020000	0.6540880000	0.0013300000
I	1.4795540000	-1.3835310000	0.0139120000
H	-0.6848360000	-3.5055810000	0.5962380000
O	-4.8593250000	1.3106100000	1.0747640000
C	2.7958240000	2.6345560000	1.1945250000
C	2.3625880000	1.3126210000	1.2090420000
C	-2.4552640000	0.0700980000	1.2147570000
C	-1.2215750000	-0.5566640000	1.2196580000
H	2.9571950000	3.1549320000	2.1306540000
H	-2.9405290000	0.3464300000	2.1410170000
H	2.1901770000	0.8061080000	2.1512210000
H	-0.7303440000	-0.7882960000	2.1549940000

TS4-1c (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.429641
$\varepsilon_0 + E_{tot}$ = −779.410978
$\varepsilon_0 + H_{corr}$ = −779.410033

$\varepsilon_0 + G_{corr}$ = −779.479248
Frequency: -358.380
Coordinates:

H	3.4264960000	1.0393750000	-2.3892710000
H	1.5837310000	-0.6138780000	-2.2885060000
H	-1.9534940000	-0.3611060000	-2.0292970000
H	-3.0846490000	1.8126440000	-1.8903070000
C	3.0651380000	0.6739230000	-1.4357970000
C	2.0350870000	-0.2515400000	-1.3734260000
H	-3.2766150000	4.0843600000	-1.3250390000
H	-4.8538760000	3.2431830000	-1.2599840000
C	-2.1511700000	0.0790660000	-1.0619520000
C	-2.8001390000	1.3153060000	-0.9732230000
C	-4.1210220000	3.8154360000	-0.6817600000
O	4.6580040000	2.0574980000	-0.4300920000
H	-4.5884340000	4.7219160000	-0.3019480000
C	3.6569470000	1.1547320000	-0.2589940000
C	1.5938750000	-0.7074520000	-0.1288530000
I	-0.0572680000	-2.1005330000	-0.0265630000
O	-2.5912030000	-2.5853130000	-0.0012750000
C	-1.7997120000	-0.5684650000	0.1072300000
C	-3.0650840000	1.8831130000	0.2752030000
H	6.0657730000	3.2755150000	0.3499770000
O	-3.6868240000	3.0888780000	0.4670010000
C	5.3126450000	2.5872080000	0.7270720000
H	-3.0085660000	-2.7291010000	0.8587120000
C	3.2050800000	0.6997920000	0.9847050000
C	2.1679180000	-0.2312960000	1.0439580000
H	5.7978370000	1.7932880000	1.3025120000
C	-2.0245570000	-0.0190930000	1.3636080000
H	4.6080140000	3.1292800000	1.3645250000
C	-2.6729390000	1.2084840000	1.4368560000
H	3.6426570000	1.0571240000	1.9062280000
H	1.8208540000	-0.5756700000	2.0101960000
H	-1.7224290000	-0.5326390000	2.2661970000
H	-2.8743350000	1.6601930000	2.4009920000

TS4-1c (B3LYP-D3, H_2O)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.433699
$\varepsilon_0 + E_{tot}$ = −779.415011
$\varepsilon_0 + H_{corr}$ = −779.414067
$\varepsilon_0 + G_{corr}$ = −779.483444
Frequency: -364.90
Coordinates:

H	3.3950080000	1.0589350000	-2.3868720000
H	1.5542990000	-0.5955720000	-2.2915030000
H	-1.9513210000	-0.3540850000	-2.0291470000
H	-3.0514430000	1.8342080000	-1.8880570000
C	3.0424780000	0.6820170000	-1.4345580000
C	2.0131400000	-0.2445940000	-1.3759380000
H	-3.1956000000	4.1097240000	-1.3116270000
H	-4.7902710000	3.3009620000	-1.2680500000
C	-2.1499030000	0.0832650000	-1.0605830000
C	-2.7802180000	1.3294450000	-0.9710360000
C	-4.0522400000	3.8551390000	-0.6793220000
O	4.6435670000	2.0527070000	-0.4241660000
H	-4.5049940000	4.7686280000	-0.2988410000
C	3.6442820000	1.1478490000	-0.2565100000
C	1.5837920000	-0.7149290000	-0.1326430000
I	-0.0622160000	-2.1077580000	-0.0335280000
O	-2.6366010000	-2.5713220000	0.0114960000
C	-1.8126230000	-0.5725770000	0.1084270000
C	-3.0404640000	1.8980540000	0.2781340000
H	6.0594690000	3.2599500000	0.3602280000
O	-3.6444870000	3.1126190000	0.4706930000
C	5.3093750000	2.5673320000	0.7352340000
H	-3.0123150000	-2.6937280000	0.8938010000
C	3.2032260000	0.6770500000	0.9854250000
C	2.1668960000	-0.2549130000	1.0423300000
H	5.7985550000	1.7653590000	1.2953710000
C	-2.0320400000	-0.0229200000	1.3657460000
H	4.6103490000	3.1010600000	1.3853240000
C	-2.6618600000	1.2145520000	1.4394770000
H	3.6488220000	1.0221560000	1.9076540000
H	1.8288650000	-0.6123510000	2.0068070000
H	-1.7375990000	-0.5414570000	2.2679140000
H	-2.8572630000	1.6667540000	2.4046760000

TS4-1c (M06-2X, Toluene)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −779.007349
$\varepsilon_0 + E_{tot}$ = −778.989118
$\varepsilon_0 + H_{corr}$ = −778.988174
$\varepsilon_0 + G_{corr}$ = −779.055916
Frequency: -430.89
Coordinates:

H	3.3470310000	1.0579060000	-2.3889320000
H	1.5053220000	-0.6000190000	-2.2818430000
H	-1.8880170000	-0.3454850000	-2.0248020000
H	-3.0157430000	1.8282680000	-1.8767310000
C	2.9956230000	0.6782570000	-1.4374550000
C	1.9694560000	-0.2455570000	-1.3692360000
H	-3.2152500000	4.0518980000	-1.3162350000
H	-4.7785960000	3.1890770000	-1.2402400000
C	-2.0775970000	0.0960950000	-1.0558280000
C	-2.7293550000	1.3271460000	-0.9619220000
C	-4.0571770000	3.7830370000	-0.6705770000
O	4.5950610000	2.0466140000	-0.4381390000
H	-4.5383370000	4.6890430000	-0.3096140000
C	3.6024010000	1.1442990000	-0.2663640000
C	1.5433410000	-0.7161840000	-0.1269770000
O	-2.5011700000	-2.5158430000	-0.0261740000
I	-0.0853330000	-2.0941580000	-0.0206550000
C	-1.7334500000	-0.5682650000	0.1058770000
C	-2.9952600000	1.8873960000	0.2841040000
H	5.9979870000	3.2447950000	0.3575820000
O	-3.6175250000	3.0866840000	0.4776020000
H	-3.1193170000	-2.7459340000	0.6762300000
C	5.2496140000	2.5433370000	0.7168870000
C	3.1723660000	0.6767450000	0.9753690000
C	2.1365080000	-0.2528630000	1.0370340000
H	5.7393480000	1.7348290000	1.2667300000
C	-1.9505160000	-0.0097880000	1.3614270000
H	4.5458210000	3.0633950000	1.3725170000
C	-2.5998930000	1.2116640000	1.4393740000
H	3.6235310000	1.0242910000	1.8943640000
H	1.8030290000	-0.6092020000	2.0045400000
H	-1.6505250000	-0.5293740000	2.2620350000
H	-2.8009100000	1.6653110000	2.4025300000

TS4-1d (B3LYP-D3, CH_2Cl_2)
$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.371368
$\varepsilon_0 + E_{tot}$ = −550.357931
$\varepsilon_0 + H_{corr}$ = −550.356987
$\varepsilon_0 + G_{corr}$ = −550.414342
Frequency: -353.030
Coordinates:

H	-2.6662720000	2.5697420000	-2.1785220000

H	-1.6389900000	0.3190250000	-2.1722830000
H	3.8406430000	1.3594930000	-2.1479080000
H	1.9027210000	-0.1781590000	-2.1355740000
C	-1.8832650000	0.8129050000	-1.2423800000
C	-2.4667260000	2.0801840000	-1.2317050000
C	3.3842640000	1.0786560000	-1.2058420000
C	2.2924380000	0.2106580000	-1.2032190000
O	-2.5644360000	-1.7709830000	-0.1326290000
H	-3.2352440000	3.6984770000	-0.0353170000
C	-2.7876290000	2.7121620000	-0.0302540000
C	-1.6562240000	0.1987630000	-0.0192730000
H	4.7297270000	2.2585750000	-0.0130400000
C	3.8823250000	1.5831390000	-0.0053690000
C	1.7180050000	-0.1449710000	0.0145630000
I	-0.0280470000	-1.4417670000	0.0227280000
H	-3.0425970000	-1.8682890000	0.7018130000
C	-2.5176640000	2.0698880000	1.1769840000
C	-1.9308740000	0.8028070000	1.1995960000
C	3.2920470000	1.2217320000	1.2049210000
C	2.2006930000	0.3533880000	1.2220900000
H	-2.7529600000	2.5516280000	2.1195740000
H	-1.7168570000	0.3068420000	2.1363650000
H	3.6768480000	1.6142190000	2.1390390000
H	1.7405990000	0.0741160000	2.1615980000

TS4-1d (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.374835
$\varepsilon_0 + E_{tot}$ = −550.361335
$\varepsilon_0 + H_{corr}$ = −550.360391
$\varepsilon_0 + G_{corr}$ = −550.418094
Frequency: -360.050
Coordinates:

H	-1.6322990000	0.3383920000	-2.1689340000
H	-2.6227610000	2.6052680000	-2.1580710000
H	1.8532370000	-0.1173930000	-2.1450960000
H	3.7865410000	1.4266820000	-2.1434680000
C	-1.8734770000	0.8265620000	-1.2350910000
C	-2.4349590000	2.1041120000	-1.2149400000
C	2.2600300000	0.2420450000	-1.2084720000
C	3.3491650000	1.1136050000	-1.2026480000
O	-2.6086690000	-1.7446060000	-0.1263220000
C	-1.6587540000	0.1990270000	-0.0160620000
C	-2.7459270000	2.7322070000	-0.0086860000
H	-3.1753340000	3.7265710000	-0.0062610000
H	4.7146720000	2.2571840000	0.0026250000
C	3.8690730000	1.5795440000	0.0043240000
C	1.7115520000	-0.1536940000	0.0088510000
I	-0.0294610000	-1.4498380000	0.0095940000
H	-3.0513640000	-1.8212940000	0.7296530000
C	-2.4871370000	2.0761750000	1.1940110000
C	-1.9226040000	0.7987230000	1.2075910000
C	3.3035070000	1.1766530000	1.2134810000
C	2.2143430000	0.3052460000	1.2237220000
H	-2.7132020000	2.5550450000	2.1402680000
H	-1.7151290000	0.2931500000	2.1406930000
H	3.7054210000	1.5389040000	2.1524790000
H	1.7721510000	-0.0055040000	2.1617140000

TS4-1d (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −550.048331
$\varepsilon_0 + E_{tot}$ = −550.035107
$\varepsilon_0 + H_{corr}$ = −550.034163
$\varepsilon_0 + G_{corr}$ = −550.090652
Frequency: -424.580
Coordinates:

H	2.5872670000	2.3724310000	-2.3907430000
H	1.4614400000	0.1826660000	-2.2150540000
H	-4.3621640000	0.6347830000	-1.8528030000
H	-2.4204630000	-0.8918740000	-1.7951320000
C	2.4256150000	1.9378090000	-1.4108360000
C	1.7851100000	0.7041170000	-1.3240700000
C	-3.6605230000	0.6893440000	-1.0292660000
C	-2.5691030000	-0.1734860000	-0.9976630000
H	3.0013820000	-2.0165290000	-0.6054170000
H	3.3256550000	3.5758490000	-0.3488430000
C	2.8369300000	2.6134070000	-0.2680770000
C	1.6087690000	0.1500480000	-0.0633680000
H	-4.6907360000	2.2949690000	-0.0439220000
C	-3.8428240000	1.6216140000	-0.0137710000
C	-1.6789560000	-0.1017210000	0.0670750000
I	0.0190910000	-1.4166480000	0.1031340000
O	2.4305620000	-1.7750680000	0.1323540000
C	2.6027700000	2.0456430000	0.9815430000
C	-2.9375700000	1.6924510000	1.0399900000
C	-1.8502220000	0.8255730000	1.0882850000
C	1.9703670000	0.8138750000	1.1021590000
H	-3.0767230000	2.4203840000	1.8301230000
H	2.9142690000	2.5620500000	1.8822140000
H	-1.1486690000	0.8774960000	1.9125510000
H	1.8102290000	0.3586020000	2.0701060000

TS4-1l (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −642.294248
$\varepsilon_0 + E_{tot}$ = −642.279179
$\varepsilon_0 + H_{corr}$ = −642.278235
$\varepsilon_0 + G_{corr}$ = −642.339843
Frequency: -392.26
Coordinates:

H	-1.8675640000	0.7312530000	-2.1571010000
H	1.1156330000	-0.6565670000	-2.1479100000
H	3.1743380000	0.7089370000	-2.1331140000
H	-2.8250720000	3.0092760000	-2.1258280000
C	-2.1341400000	1.1953790000	-1.2149700000
C	1.5621180000	-0.3533040000	-1.2103730000
C	2.7201740000	0.4055670000	-1.1977940000
C	-2.6737760000	2.4775190000	-1.1944250000
H	1.3401200000	-3.3296270000	-0.5480130000
I	-1.0643710000	-1.4383800000	-0.0265590000
C	-1.9462910000	0.5222410000	-0.0133340000
C	1.0180470000	-0.7578530000	0.0078160000
C	3.2958300000	0.7963110000	0.0142960000
C	-3.0141550000	3.0722810000	0.0158620000
C	4.4838630000	1.5958570000	0.0174890000
N	5.4383380000	2.2403690000	0.0185770000
H	-3.4318890000	4.0715350000	0.0275090000
O	0.8860170000	-2.8453170000	0.1504470000
C	-2.2778000000	1.1071700000	1.2030820000
C	-2.8171080000	2.3896960000	1.2115560000
C	2.6965420000	0.4253480000	1.2232300000
C	1.5417880000	-0.3352870000	1.2288790000
H	-2.1221080000	0.5760780000	2.1345780000
H	-3.0794080000	2.8540150000	2.1543360000
H	1.0831910000	-0.6363070000	2.1604620000
H	3.1373900000	0.7399460000	2.1612100000

TS4-1m (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −754.534401

$\varepsilon_0 + E_{tot}$ = −754.518674
$\varepsilon_0 + H_{corr}$ = −754.517730
$\varepsilon_0 + G_{corr}$ = −754.581171
Frequency: -439.75
Coordinates:

H	-0.8470890000	-0.7079810000	-2.1601430000
H	2.1521490000	0.7618330000	-2.1443960000
H	-3.1969670000	0.1148820000	-2.1385950000
H	2.3289560000	3.2261400000	-2.1223630000
C	-1.3635730000	-0.5660790000	-1.2189480000
C	-2.6741050000	-0.1068340000	-1.2184590000
C	2.2008150000	1.2995780000	-1.2067840000
C	2.3063780000	2.6884830000	-1.1816180000
O	-5.2212090000	0.7915260000	-1.0620060000
H	4.3074550000	-0.8500690000	-0.5952390000
I	1.3359200000	-1.4509920000	-0.0198850000
C	-0.7291130000	-0.8390580000	-0.0109240000
C	-3.3078480000	0.0683420000	0.0017840000
C	2.1993160000	0.6305240000	0.0080060000
N	-4.7024480000	0.5596060000	0.0082580000
C	2.3690430000	3.3793650000	0.0226980000
H	2.4432610000	4.4590810000	0.0292610000
O	3.6608210000	-0.8699320000	0.1191910000
O	-5.2433660000	0.7007840000	1.0831980000
C	-1.3818030000	-0.6528330000	1.2037690000
C	-2.6928250000	-0.1944380000	1.2158460000
C	2.3269200000	2.6714080000	1.2203370000
C	2.2264070000	1.2843630000	1.2305640000
H	-0.8789550000	-0.8616380000	2.1398470000
H	-3.2293900000	-0.0393410000	2.1417280000
H	2.2136940000	0.7292710000	2.1583610000
H	2.3726400000	3.1971740000	2.1669780000

TS4-1n (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1469.267200
$\varepsilon_0 + E_{tot}$ = −1469.251571
$\varepsilon_0 + H_{corr}$ = −1469.250627
$\varepsilon_0 + G_{corr}$ = −1469.313757
Frequency: -423.21
Coordinates:

H	1.7013560000	-0.3886240000	-2.1524010000
H	-1.6492530000	-0.5756940000	-2.1509550000
H	2.8825060000	1.7879750000	-2.1420170000
H	-3.5002340000	1.0709010000	-2.1383940000
C	1.9795000000	0.0743510000	-1.2150270000
C	-3.0947640000	0.6936800000	-1.2083250000
C	-2.0555310000	-0.2291300000	-1.2082590000
C	2.6487960000	1.2939620000	-1.2073700000
H	3.0900710000	-2.7255650000	-0.5942630000
I	0.0946580000	-2.0765260000	-0.0105170000
C	2.9997480000	1.8803130000	-0.0009060000
C	-1.5520810000	-0.6999050000	-0.0008270000
C	1.7174020000	-0.5468010000	-0.0007190000
Cl	3.8265670000	3.4216020000	0.0010340000
C	-3.6073030000	1.1319030000	0.0056000000
Cl	-4.9093480000	2.2901320000	0.0097020000
O	2.4756700000	-2.4921830000	0.1104670000
C	2.6911050000	1.2683530000	1.2071780000
C	-2.0671690000	-0.2516230000	1.2100190000
C	2.0276720000	0.0488930000	1.2154700000
C	-3.1063150000	0.6714670000	1.2162800000
H	2.9656640000	1.7407090000	2.1419320000
H	-3.5207760000	1.0320240000	2.1489630000
H	1.7993200000	-0.4454260000	2.1494890000
H	-1.6700100000	-0.6152210000	2.1501010000

TS4-1o (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −748.546024
$\varepsilon_0 + E_{tot}$ = −748.531159
$\varepsilon_0 + H_{corr}$ = −748.530215
$\varepsilon_0 + G_{corr}$ = −748.590562
Frequency: -430.39
Coordinates:

H	1.7175140000	-0.0114010000	-2.1307810000
H	-1.3802010000	0.1291760000	-2.1106510000
H	-3.2813030000	1.7403940000	-2.0577910000
H	2.8400520000	2.2149900000	-2.0560950000
C	-1.9348890000	0.2830460000	-1.1929540000
C	1.9519530000	0.4524000000	-1.1819280000
C	-2.9942230000	1.1823220000	-1.1758590000
C	2.5862900000	1.6911240000	-1.1431890000
H	3.1157290000	-2.3301070000	-0.5683670000
I	0.0706850000	-1.7526730000	-0.0573840000
C	-1.6013140000	-0.4115780000	-0.0345520000
C	-3.6900960000	1.3578690000	0.0069810000
C	1.6727830000	-0.1881740000	0.0183050000
F	-4.7153270000	2.2241720000	0.0265340000
C	2.8800240000	2.2593300000	0.0808800000
O	2.4651530000	-2.1201260000	0.1109640000
F	3.4826690000	3.4674000000	0.1130890000
C	-2.3083450000	-0.2134780000	1.1464480000
C	-3.3733050000	0.6795300000	1.1703380000
C	1.9333480000	0.3989570000	1.2499250000
C	2.5626710000	1.6374450000	1.2751360000
H	-2.0400170000	-0.7499400000	2.0482860000
H	-3.9473580000	0.8567650000	2.0706170000
H	1.6895190000	-0.1133010000	2.1700900000
H	2.8030500000	2.1192220000	2.2145540000

TS5-1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.905548
$\varepsilon_0 + E_{tot}$ = −830.887314
$\varepsilon_0 + H_{corr}$ = −830.886370
$\varepsilon_0 + G_{corr}$ = −830.953681
Frequency: -246.290
Coordinates:

H	-0.9322940000	-0.8946510000	-2.1567690000
H	-3.2331450000	-0.0031670000	-2.1197340000
C	-1.4148070000	-0.6742170000	-1.2131840000
C	-2.6970990000	-0.1787590000	-1.1970940000
O	-5.2313520000	0.8380600000	-1.0311580000
H	4.2711540000	-1.4905310000	-0.8210300000
H	-0.1881230000	1.5316090000	-0.4973160000
H	0.2716040000	3.9488510000	-0.4728320000
C	0.8135280000	1.8810710000	-0.2917070000
C	1.0787190000	3.2523920000	-0.2753700000
C	1.8584550000	0.9995970000	-0.0425950000
O	-0.4886830000	-2.9968270000	-0.0235790000
I	1.4791090000	-1.1858250000	-0.0223060000
C	2.3641100000	3.7199130000	-0.0096490000
C	-0.7232700000	-0.9179840000	0.0000570000
H	2.5620840000	4.7856550000	0.0031740000
C	-3.3152150000	0.1246780000	0.0316800000
N	-4.6374870000	0.6620870000	0.0478730000
O	3.9333520000	-1.3999600000	0.0785800000
C	3.1465660000	1.4388850000	0.2232140000
C	3.3934120000	2.8131100000	0.2383770000

H	3.9241650000	0.7012410000	0.3943710000
H	4.3965590000	3.1689820000	0.4460190000
H	-0.7933610000	-3.2238260000	0.8646930000
O	-5.1646970000	0.9390450000	1.1404090000
C	-1.3352700000	-0.5512060000	1.2234010000
C	-2.6210900000	-0.0581800000	1.2405610000
H	-0.7908850000	-0.6632470000	2.1530470000
H	-3.0953310000	0.2148200000	2.1732980000

TS5-1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.915875
$\varepsilon_0 + E_{tot}$ = −830.897591
$\varepsilon_0 + H_{corr}$ = −830.896646
$\varepsilon_0 + G_{corr}$ = −830.965545
Frequency: -271.450
Coordinates:

H	-0.8955850000	-0.8059700000	-2.1639980000
H	-3.1912930000	0.0962140000	-2.1386940000
C	-1.3972170000	-0.6235830000	-1.2222570000
C	-2.6774800000	-0.1206620000	-1.2122250000
O	-5.2115920000	0.9215930000	-1.0707250000
H	4.2472040000	-1.5970070000	-0.8306610000
H	-0.2012000000	1.5606850000	-0.2629320000
H	0.2931810000	3.9705100000	-0.2447940000
C	0.8203710000	1.8935980000	-0.1496520000
C	1.1058820000	3.2610660000	-0.1381840000
O	-0.5362390000	-2.9854050000	-0.0676390000
C	1.8736880000	0.9974690000	-0.0161560000
I	1.4695970000	-1.1821530000	-0.0130580000
C	-0.7347830000	-0.9227880000	-0.0050990000
C	2.4176240000	3.7081480000	0.0071340000
C	-3.3205220000	0.1354570000	0.0145240000
H	2.6307070000	4.7708320000	0.0151320000
N	-4.6453170000	0.6735770000	0.0249550000
O	3.9377710000	-1.4537420000	0.0723730000
C	3.1874500000	1.4141340000	0.1324300000
C	3.4534970000	2.7851980000	0.1422140000
H	3.9673940000	0.6655230000	0.2291200000
H	4.4766110000	3.1254240000	0.2572090000
H	-0.8363910000	-3.2182210000	0.8208250000
O	-5.2108160000	0.8807380000	1.1294950000
C	-1.3649920000	-0.5911070000	1.2197540000
C	-2.6498060000	-0.0942300000	1.2293440000
H	-0.8378450000	-0.7375110000	2.1543350000
H	-3.1394460000	0.1468980000	2.1628860000

TS5-1a (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.474331
$\varepsilon_0 + E_{tot}$ = −830.456302
$\varepsilon_0 + H_{corr}$ = −830.455358
$\varepsilon_0 + G_{corr}$ = −830.522110
Frequency: -332.800
Coordinates:

H	-0.9461640000	-0.9794450000	-2.1312910000
H	-3.2637700000	-0.1246950000	-2.0830180000
C	-1.4070520000	-0.7076780000	-1.1893170000
C	-2.6967690000	-0.2353150000	-1.1682560000
O	-5.2239380000	0.7507810000	-0.9827170000
H	-0.0666240000	1.4550750000	-0.9379650000
H	0.3766270000	3.8719930000	-0.9130840000
H	4.2337550000	-1.2065420000	-0.8531090000
C	0.8756680000	1.8196260000	-0.5500940000
C	1.1271120000	3.1902840000	-0.5307750000
C	1.8471910000	0.9512710000	-0.0694400000
I	1.4687350000	-1.1889610000	-0.0377880000
C	2.3275910000	3.6780870000	-0.0275710000
H	2.5164350000	4.7447830000	-0.0124030000
O	3.8391270000	-1.3488130000	0.0129150000
C	-0.6816450000	-0.8713160000	0.0152660000
C	-3.2771180000	0.1269880000	0.0552920000
N	-4.6159060000	0.6480230000	0.0757540000
O	-0.4736740000	-2.9432750000	0.0840440000
C	3.0527180000	1.4187080000	0.4335440000
C	3.2855850000	2.7916060000	0.4540330000
H	3.7931330000	0.7048380000	0.7728010000
H	4.2238080000	3.1647000000	0.8481980000
H	-0.7992900000	-3.1447270000	0.9677810000
O	-5.1071490000	0.9707240000	1.1505760000
C	-1.2605340000	-0.4283990000	1.2247930000
C	-2.5556470000	0.0414780000	1.2489500000
H	-0.6866170000	-0.4647770000	2.1434330000
H	-3.0104170000	0.3701950000	2.1740590000

TS5-1a (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −830.485259
$\varepsilon_0 + E_{tot}$ = −830.467250
$\varepsilon_0 + H_{corr}$ = −830.466306
$\varepsilon_0 + G_{corr}$ = −830.533199
Frequency: -357.390
Coordinates:

H	-0.9508290000	-0.9925340000	-2.1289900000
H	-3.2640650000	-0.1321580000	-2.0718240000
H	0.0533600000	1.4058300000	-1.1965260000
C	-1.4062500000	-0.7180280000	-1.1850530000
H	0.4757190000	3.8299570000	-1.1653580000
C	-2.6941140000	-0.2414900000	-1.1587500000
O	-5.2241570000	0.7339290000	-0.9614700000
H	4.2710220000	-0.9484990000	-0.7894900000
C	0.9345830000	1.7890220000	-0.6982020000
C	1.1732680000	3.1619820000	-0.6744810000
C	1.8414330000	0.9420330000	-0.0763790000
I	1.4728890000	-1.1905710000	-0.0506260000
C	2.2952530000	3.6690170000	-0.0290500000
H	2.4742080000	4.7372260000	-0.0118500000
O	3.8568080000	-1.3265850000	-0.0074380000
C	-0.6777310000	-0.8838820000	0.0182420000
C	-3.2664700000	0.1286220000	0.0664610000
N	-4.6040120000	0.6488260000	0.0920350000
O	-0.5041240000	-2.9383410000	0.1143000000
C	2.9687360000	1.4270670000	0.5700080000
C	3.1887980000	2.8018810000	0.5923860000
H	-0.7949910000	-3.1148680000	1.0157490000
H	3.6663420000	0.7304420000	1.0165760000
H	4.0650460000	3.1917560000	1.0966180000
O	-5.0856960000	0.9883320000	1.1664110000
C	-1.2430860000	-0.4210870000	1.2279070000
C	-2.5358600000	0.0536030000	1.2560470000
H	-0.6633210000	-0.4525080000	2.1429150000
H	-2.9815220000	0.3927370000	2.1818670000

TS5-1a-Na (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −992.701779
$\varepsilon_0 + E_{tot}$ = −992.681481
$\varepsilon_0 + H_{corr}$ = −992.680537
$\varepsilon_0 + G_{corr}$ = −992.753520
Frequency: -336.030
Coordinates:

H	-1.1326650000	-0.7615600000	-2.1868960000

H	-3.5550530000	-0.2908730000	-2.0454260000
H	-0.0526720000	1.5790330000	-1.6707250000
H	-0.0145190000	4.0443520000	-1.5736340000
C	-1.6104440000	-0.6503750000	-1.2215300000
C	-2.9606380000	-0.3959710000	-1.1477120000
C	0.5819150000	2.0810280000	-0.9507740000
C	0.6033690000	3.4727680000	-0.8918020000
O	-5.6134490000	0.1178550000	-0.8587240000
H	4.0940850000	0.3131440000	-0.4723430000
O	-0.3144310000	-2.8357100000	-0.1484440000
I	1.3126340000	-0.7821520000	-0.1172740000
C	1.3832790000	1.3632990000	-0.0744330000
O	3.7818470000	-0.5002470000	-0.0686730000
C	-0.8598670000	-0.8278030000	-0.0397860000
C	1.4146490000	4.1220170000	0.0316200000
H	1.4273390000	5.2042730000	0.0734090000
C	-3.5664310000	-0.2610550000	0.1057090000
N	-4.9800100000	0.0182910000	0.1820780000
Na	4.9258440000	-2.3192390000	0.2358030000
H	-0.6610780000	-3.1730260000	0.6843710000
C	2.1989550000	1.9922610000	0.8553720000
C	2.2107690000	3.3832290000	0.9022000000
C	-1.4673600000	-0.5925450000	1.2099390000
C	-2.8220250000	-0.3433810000	1.2826700000
O	-5.4932460000	0.1424830000	1.2847780000
H	2.8235230000	1.4057550000	1.5166760000
H	2.8417280000	3.8867540000	1.6246530000
H	-0.8803660000	-0.6363320000	2.1192140000
H	-3.3069200000	-0.1897530000	2.2375060000

TS5-1a-Na (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −992.712806
$\varepsilon_0 + E_{tot}$ = −992.692612
$\varepsilon_0 + H_{corr}$ = −992.691668
$\varepsilon_0 + G_{corr}$ = −992.764629

Frequency: -360.150
Coordinates:

H	-1.1663670000	-0.7563000000	-2.1978000000
H	-3.5778680000	-0.2580970000	-2.0248830000
H	0.0030280000	1.5512440000	-1.7564400000
H	0.0196290000	4.0161360000	-1.6201870000
C	-1.6316050000	-0.6537580000	-1.2250740000
C	-2.9765990000	-0.3826360000	-1.1341580000
C	0.5951720000	2.0465460000	-0.9968390000
C	0.6054710000	3.4376810000	-0.9162730000
O	-5.6216310000	0.1518390000	-0.8103910000
H	3.9932530000	0.3314240000	-0.5822180000
O	3.7331250000	-0.4981770000	-0.1731680000
I	1.3035160000	-0.8225310000	-0.1676080000
O	-0.3834050000	-2.8584700000	-0.1599540000
C	1.3566920000	1.3204390000	-0.0924250000
C	-0.8666700000	-0.8546940000	-0.0533630000
C	1.3664630000	4.0768290000	0.0560780000
H	1.3711330000	5.1583900000	0.1143480000
C	-3.5680780000	-0.2505240000	0.1278760000
N	-4.9729580000	0.0432710000	0.2221030000
Na	5.2030720000	-1.9929590000	0.4429160000
H	-0.6249430000	-3.1695100000	0.7194190000
C	2.1220410000	1.9391820000	0.8861080000
C	2.1230630000	3.3292880000	0.9543170000
C	-1.4590090000	-0.6126360000	1.2055920000
C	-2.8078970000	-0.3467990000	1.2961250000
O	-5.4745900000	0.1709740000	1.3315500000
H	2.7154750000	1.3482070000	1.5716030000
H	2.7140370000	3.8252800000	1.7147610000
H	-0.8612510000	-0.6654430000	2.1076120000
H	-3.2777830000	-0.1903780000	2.2581250000

TS5-1c (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.374957
$\varepsilon_0 + E_{tot}$ = −855.353609
$\varepsilon_0 + H_{corr}$ = −855.352664
$\varepsilon_0 + G_{corr}$ = −855.426573

Frequency: -362.260
Coordinates:

H	-1.7840290000	-0.5823430000	-2.0777930000
H	-3.2211390000	1.3898450000	-1.9364570000
H	-5.1901560000	2.5525980000	-1.3953760000
H	-3.7410550000	3.5927380000	-1.2997040000
C	-2.1150250000	-0.2378720000	-1.1065510000
C	-2.9337620000	0.8909120000	-1.0202070000
C	-4.5883260000	3.1870240000	-0.7349970000
H	2.6875900000	4.7084600000	-0.6911100000
H	2.6410310000	-3.9948610000	-0.6297430000
H	-5.2018550000	4.0084540000	-0.3680040000
H	3.3568780000	-1.3038970000	-0.2557060000
H	4.7678630000	0.7941160000	-0.2550240000
C	2.9235710000	-0.3119040000	-0.1460620000
C	3.6908000000	0.8463570000	-0.1448980000
O	-2.2540140000	-2.8495740000	-0.1435940000
O	2.8546950000	-3.2243790000	-0.0903430000
O	3.9361290000	3.1749310000	-0.0136830000
I	0.3285970000	-2.0218080000	-0.0133520000
C	1.5434920000	-0.2012740000	-0.0022100000
C	3.0885350000	2.1021750000	-0.0002480000
C	-1.7277910000	-0.9189990000	0.0494620000
H	4.2231170000	5.1698950000	0.0864280000
C	3.3802380000	4.4825510000	0.1259760000
C	0.9247530000	1.0310360000	0.1465670000
C	1.7022760000	2.1934440000	0.1467380000
C	-3.3551430000	1.3637260000	0.2244970000
H	-0.1471000000	1.1167030000	0.2596820000
H	1.2088280000	3.1485590000	0.2624470000
O	-4.1528220000	2.4742180000	0.4170870000
H	-2.7351510000	-2.9917160000	0.6823280000
H	2.8639760000	4.5943460000	1.0847960000
C	-2.1220000000	-0.4251330000	1.3027460000
C	-2.9404910000	0.6958690000	1.3803930000
H	-1.7894910000	-0.9120020000	2.2112880000
H	-3.2536110000	1.0758810000	2.3466290000

TS5-1c (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −855.388211
$\varepsilon_0 + E_{tot}$ = −855.366547
$\varepsilon_0 + H_{corr}$ = −855.365602
$\varepsilon_0 + G_{corr}$ = −855.440713

Frequency: -375.850
Coordinates:

H	-1.7876870000	-0.5890840000	-2.0808700000
H	-3.2342660000	1.3784750000	-1.9422570000
H	-5.1942720000	2.5563270000	-1.4150540000

H	-3.7403000000	3.5874370000	-1.2889790000
C	-2.1245310000	-0.2467590000	-1.1110380000
C	-2.9490440000	0.8790550000	-1.0258980000
C	-4.5973770000	3.1805320000	-0.7414890000
H	2.6782640000	4.7252960000	-0.6690880000
H	2.6761540000	-4.0365770000	-0.5973020000
H	-5.2108220000	4.0000460000	-0.3711600000
H	4.7638510000	0.8071000000	-0.2903540000
H	3.3562000000	-1.2888120000	-0.2858790000
C	3.6885330000	0.8586030000	-0.1640890000
C	2.9214180000	-0.2996940000	-0.1637390000
O	-2.2389920000	-2.8820340000	-0.1414330000
O	2.9414260000	-3.2550750000	-0.0982160000
O	3.9336120000	3.1848380000	-0.0182460000
I	0.3310550000	-2.0091340000	-0.0106350000
C	3.0876970000	2.1135500000	-0.0011140000
C	1.5436420000	-0.1898380000	0.0014710000
C	-1.7421810000	-0.9194530000	0.0477300000
H	4.2239740000	5.1799760000	0.0921190000
C	3.3803500000	4.4943850000	0.1378200000
C	1.7030080000	2.2030150000	0.1660660000
C	0.9258780000	1.0406400000	0.1681530000
C	-3.3768490000	1.3473780000	0.2183850000
H	1.2112850000	3.1570900000	0.2956010000
H	-0.1444920000	1.1249260000	0.2969660000
O	-4.1788480000	2.4506260000	0.4096090000
H	-2.6934480000	-3.0354370000	0.6977290000
H	2.8772470000	4.5986510000	1.1039180000
C	-2.1424780000	-0.4390000000	1.3008030000
C	-2.9657170000	0.6786760000	1.3759660000
H	-1.8140570000	-0.9288560000	2.2087540000
H	-3.2852100000	1.0541870000	2.3416300000

TS5-1c (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −854.926368
$\varepsilon_0 + E_{tot}$ = −854.905418
$\varepsilon_0 + H_{corr}$ = −854.904474
$\varepsilon_0 + G_{corr}$ = −854.977603

Frequency: -404.800
Coordinates:

H	-1.5863160000	-0.4399830000	-2.0829200000
H	-3.0445370000	1.5092320000	-1.9328260000
H	-5.0378490000	2.5637520000	-1.4476130000
H	-3.6211350000	3.6332180000	-1.2637940000
C	-1.9704380000	-0.1425830000	-1.1148800000
C	-2.8016540000	0.9734220000	-1.0238970000
C	-4.4884150000	3.2048320000	-0.7506710000
H	2.6462580000	4.6429250000	-0.5166350000
H	4.7127130000	0.7189810000	-0.5071040000
H	3.2843730000	-1.3499030000	-0.4637020000
H	-5.1381350000	4.0082160000	-0.4100520000
C	3.6523220000	0.7784510000	-0.2921620000
C	2.8691630000	-0.3645000000	-0.2789500000
O	-2.2638040000	-2.7150700000	-0.2000090000
H	2.4434470000	-4.1069880000	-0.1384000000
O	3.9465790000	3.0867800000	-0.0642930000
O	2.6691710000	-3.1752620000	-0.0593290000
C	3.0922410000	2.0301440000	-0.0251550000
I	0.2798370000	-2.0127260000	0.0002360000
C	1.5111980000	-0.2463330000	0.0029570000
C	-1.6472630000	-0.8919790000	0.0246650000
H	4.2495720000	5.0656840000	0.1336450000
C	3.4160050000	4.3722230000	0.2114040000
C	-3.2856760000	1.3956550000	0.2114070000
C	1.7332210000	2.1331370000	0.2609850000
C	0.9382950000	0.9851070000	0.2758420000
O	-4.0996150000	2.4898010000	0.4032290000
H	-2.9649640000	-2.7640420000	0.4590430000
H	1.2713930000	3.0870670000	0.4754980000
H	-0.1159570000	1.0844180000	0.5006330000
H	2.9971670000	4.4155470000	1.2205410000
C	-2.0871920000	-0.4178350000	1.2777780000
C	-2.9139190000	0.6912630000	1.3571110000
H	-1.7866810000	-0.9302840000	2.1843480000
H	-3.2667070000	1.0406290000	2.3214210000

TS5-1c (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −854.938804
$\varepsilon_0 + E_{tot}$ = −854.917899
$\varepsilon_0 + H_{corr}$ = −854.916955
$\varepsilon_0 + G_{corr}$ = −854.989813

Frequency: -425.910
Coordinates:

H	-1.4854560000	-0.4004590000	-2.0866050000
H	-2.9407330000	1.5516320000	-1.9436540000
H	-4.8874210000	2.6870780000	-1.5403660000
H	-3.4479650000	3.6792620000	-1.1825250000
C	-1.9137640000	-0.1322500000	-1.1284670000
C	-2.7434450000	0.9867640000	-1.0414020000
H	4.5997880000	0.8238740000	-0.8014400000
C	-4.3697140000	3.2612940000	-0.7658500000
H	3.2279460000	-1.2771330000	-0.7103330000
C	3.5730520000	0.8433920000	-0.4556160000
H	-5.0127240000	4.0699530000	-0.4258290000
C	2.8160840000	-0.3164120000	-0.4231200000
H	2.4724560000	4.6782720000	-0.3250840000
O	-2.2417120000	-2.7441210000	-0.2813470000
O	3.8520790000	3.1382080000	-0.1131160000
C	3.0281140000	2.0620700000	-0.0401960000
O	2.7567740000	-3.1374810000	-0.0312580000
C	-1.6500010000	-0.9143650000	0.0011950000
I	0.2956960000	-2.0236540000	0.0211830000
C	1.5014650000	-0.2482630000	0.0283050000
H	2.5483790000	-4.0733180000	0.0517170000
H	4.1338570000	5.1146920000	0.1453120000
C	-3.2824000000	1.3725950000	0.1820550000
C	3.3312630000	4.3962600000	0.2894830000
H	-2.9766940000	-2.8091260000	0.3388840000
O	-4.0995300000	2.4623620000	0.3693900000
C	1.7128830000	2.1134870000	0.4167600000
C	0.9448160000	0.9480650000	0.4490150000
H	1.2671820000	3.0401140000	0.7512060000
H	-0.0778910000	1.0042980000	0.8012390000
C	-2.1471240000	-0.4829430000	1.2466560000
C	-2.9700530000	0.6289540000	1.3218900000
H	3.0398720000	4.3796650000	1.3429530000
H	-1.8948500000	-1.0281530000	2.1486770000
H	-3.3655510000	0.9493580000	2.2795460000

TS5-1c-Na (M06-2X, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1017.158232
$\varepsilon_0 + E_{tot}$ = −1017.135151
$\varepsilon_0 + H_{corr}$ = −1017.134206
$\varepsilon_0 + G_{corr}$ = −1017.213074

Frequency: -437.700
Coordinates:

H	-3.2839020000	-0.7384410000	-2.0922830000
H	-0.9276530000	-1.3598420000	-2.0056130000
H	-5.5481800000	-1.1050650000	-1.8313530000
H	-5.0850810000	0.6017080000	-1.5879480000
Na	4.5647530000	-2.0550900000	-1.3061620000
C	-2.8533970000	-0.9957100000	-1.1331020000
C	-5.5661180000	-0.2671370000	-1.1274240000
C	-1.5053690000	-1.3527620000	-1.0897680000
H	-6.5975050000	-0.0223960000	-0.8836180000
H	-1.4940810000	5.2577560000	-0.5928320000
H	2.6762930000	3.7436840000	-0.5623750000
H	3.0123180000	1.2537490000	-0.3498540000
C	1.8568660000	3.0902730000	-0.2877360000
C	2.0453850000	1.7221930000	-0.1850200000
O	0.5232460000	5.0042780000	-0.1636980000
H	-0.5765150000	6.6850640000	-0.0517620000
C	0.6033210000	3.6558170000	-0.0354560000
O	-0.0790600000	-3.4597770000	0.0002110000
C	-3.6137460000	-0.9616050000	0.0319290000
O	-4.9398720000	-0.6116240000	0.0919310000
C	-0.7283180000	5.6193490000	0.0985190000
C	-0.9027760000	-1.7100720000	0.1197350000
O	4.0319010000	-0.5513580000	0.1238490000
C	0.9657530000	0.9225040000	0.1740150000
I	1.2583870000	-1.1976690000	0.3126160000
C	-0.4675790000	2.8393930000	0.3246700000
C	-0.2842360000	1.4599190000	0.4307490000
H	-0.7077200000	-4.0078880000	0.4832540000
H	-1.4466250000	3.2511780000	0.5274300000
H	-1.1259600000	0.8374700000	0.7100130000
H	4.4845650000	-0.1944930000	0.8908440000
H	-1.0455730000	5.4357820000	1.1284860000
C	-3.0045500000	-1.2911320000	1.2437370000
C	-1.6665900000	-1.6444840000	1.3003580000
H	-3.5946230000	-1.2528570000	2.1526120000
H	-1.2081580000	-1.8743770000	2.2545310000

TS5-1c-Na (M06-2X, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1017.167987
$\varepsilon_0 + E_{tot}$ = −1017.144574
$\varepsilon_0 + H_{corr}$ = −1017.143630
$\varepsilon_0 + G_{corr}$ = −1017.224402

Frequency: -445.600
Coordinates:

H	-0.8633670000	-1.2876300000	-2.0679700000
H	-3.2842350000	-1.0035860000	-2.0110500000
H	-5.4600690000	-1.6655520000	-1.6986310000
H	-5.2144600000	0.0598490000	-1.3129360000
C	-1.3881930000	-1.4316370000	-1.1316860000
C	-2.7742150000	-1.2657030000	-1.0930570000
C	-5.5546560000	-0.9030280000	-0.9195150000
H	2.0111300000	4.0555590000	-0.8832320000
H	2.7193290000	1.6535270000	-0.7074140000
H	-6.5960210000	-0.8232960000	-0.6162880000
Na	5.1358150000	-1.6590190000	-0.6155390000
C	1.3389420000	3.3033860000	-0.4878970000
C	1.7298670000	1.9777510000	-0.4060080000
H	-2.2931700000	4.9663170000	-0.3453880000
O	0.3465340000	-3.4134430000	-0.2397340000
O	-0.2209500000	5.0148730000	-0.1873900000
C	0.0656050000	3.6954050000	-0.0622300000
C	-0.6840440000	-1.7863500000	0.0218660000
H	-1.5284910000	6.5272890000	0.0428400000
C	-3.4717470000	-1.4190020000	0.1006470000
C	0.8378700000	1.0433300000	0.1094280000
O	4.0114730000	0.0266850000	0.1469480000
I	1.4143750000	-1.0180020000	0.1733210000
C	-1.5043670000	5.4571220000	0.2303870000
O	-4.8289750000	-1.2647220000	0.2398910000
H	-0.1573650000	-4.0504270000	0.2797180000
C	-0.8173620000	2.7476320000	0.4534360000
C	-0.4260870000	1.4108100000	0.5394770000
H	4.2789060000	0.7231700000	0.7511960000
H	-1.8058180000	3.0240320000	0.7932180000
H	-1.1229860000	0.6828530000	0.9378110000
C	-1.3876640000	-1.9027970000	1.2351890000
C	-2.7624990000	-1.7381350000	1.2604870000
H	-1.6544480000	5.2680420000	1.2964090000
H	-0.8543790000	-2.1269820000	2.1512390000
H	-3.3037310000	-1.8397070000	2.1945300000

TS5-1d (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.319026
$\varepsilon_0 + E_{tot}$ = −626.302922
$\varepsilon_0 + H_{corr}$ = −626.301977
$\varepsilon_0 + G_{corr}$ = −626.364053

Frequency: -344.750
Coordinates:

H	3.4600280000	1.7787880000	-2.1331240000
H	1.8975610000	-0.1238130000	-2.1298050000
C	2.2351510000	0.2994590000	-1.1913480000
C	3.1144510000	1.3805450000	-1.1840930000
H	2.7454140000	-2.2966680000	-0.6886850000
H	0.2792940000	1.8532030000	-0.1256210000
H	-1.0651860000	3.9215880000	-0.1227710000
O	-2.7688260000	-2.4389400000	-0.0825700000
C	-0.7989120000	1.7933460000	-0.0739510000
C	-1.5654290000	2.9608450000	-0.0712480000
I	-0.2752420000	-1.2817720000	-0.0168890000
C	-1.4580040000	0.5704750000	-0.0070710000
C	-2.9560920000	2.8934850000	-0.0043650000
H	-3.5439100000	3.8046110000	-0.0042160000
H	4.2009620000	2.8159110000	0.0091970000
C	3.5301530000	1.9650230000	0.0133670000
C	1.7902200000	-0.2414270000	0.0269000000
C	-2.8408280000	0.4718680000	0.0581260000
C	-3.5879110000	1.6521970000	0.0599810000
H	-3.2875050000	-0.5199140000	0.1035860000
H	-4.6698940000	1.5936540000	0.1098770000
O	2.2690320000	-2.1797470000	0.1437630000
H	-2.6519000000	-3.1410560000	0.5685730000
C	3.0455980000	1.4454010000	1.2176310000
C	2.1726030000	0.3625970000	1.2364360000
H	3.3410740000	1.8950260000	2.1606420000
H	1.7942520000	-0.0208190000	2.1757360000

TS5-1d (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −626.331140
$\varepsilon_0 + E_{tot}$ = −626.314705
$\varepsilon_0 + H_{corr}$ = −626.313760
$\varepsilon_0 + G_{corr}$ = −626.376973

Frequency: -358.810
Coordinates:

H	1.9325240000	-0.1539830000	-2.1252130000
H	3.5006460000	1.7464000000	-2.1247820000

C	2.2614920000	0.2759660000	-1.1872580000
C	3.1441600000	1.3552950000	-1.1772870000
H	2.7050220000	-2.3476670000	-0.6865340000
H	0.2856590000	1.8537390000	-0.1828880000
H	-1.0484620000	3.9285660000	-0.1713210000
C	-0.7915980000	1.7996580000	-0.1081100000
C	-1.5520800000	2.9710990000	-0.1002760000
O	-2.8639760000	-2.4471700000	-0.0670230000
I	-0.2784330000	-1.2702600000	-0.0192280000
C	-1.4555720000	0.5812090000	-0.0157080000
C	-2.9413620000	2.9114640000	-0.0032240000
H	-3.5242210000	3.8254170000	0.0016010000
H	4.2240440000	2.7915660000	0.0187170000
C	3.5501840000	1.9433340000	0.0215240000
C	1.8056490000	-0.2471570000	0.0308020000
C	-2.8376910000	0.4899500000	0.0800110000
C	-3.5784960000	1.6744870000	0.0858480000
H	-3.2951880000	-0.4932760000	0.1459220000
O	2.2537760000	-2.2129880000	0.1574640000
H	-4.6592330000	1.6226140000	0.1599850000
H	-2.6299770000	-3.2806010000	0.3584760000
C	3.0547510000	1.4333170000	1.2245750000
C	2.1765170000	0.3530960000	1.2416490000
H	3.3441710000	1.8862020000	2.1674640000
H	1.7878350000	-0.0242340000	2.1788550000

TS5-1d (M06-2X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −625.936449
$\varepsilon_0 + E_{tot}$ = −625.920947
$\varepsilon_0 + H_{corr}$ = −625.920003
$\varepsilon_0 + G_{corr}$ = −625.980412

Frequency: -342.650
Coordinates:

H	-1.6972010000	0.0553400000	-2.1663920000
H	-3.3220450000	1.8950620000	-2.1511400000
C	-2.0861940000	0.4264890000	-1.2253680000
C	-3.0029020000	1.4636070000	-1.2072860000
H	2.3366180000	-3.2770710000	-0.2751530000
O	-2.2604410000	-2.0491370000	-0.1032300000
H	3.2716200000	-0.6324150000	-0.0551030000
H	4.7059350000	1.4252000000	-0.0394790000
C	2.8451160000	0.3668270000	-0.0278650000
C	3.6260840000	1.5209370000	-0.0213150000
C	-1.6775470000	-0.1840110000	-0.0183110000
C	-3.5030780000	1.9741800000	-0.0062520000
C	1.4630650000	0.5025160000	-0.0046300000
H	-4.2082240000	2.7958230000	-0.0033090000
C	3.0378320000	2.7804230000	0.0097220000
I	0.2297000000	-1.2795280000	0.0116190000
H	3.6549430000	3.6717890000	0.0155620000
O	2.4958030000	-2.3788500000	0.0275850000
C	0.8512860000	1.7510420000	0.0287790000
C	1.6527810000	2.8909580000	0.0343930000
H	-0.2255930000	1.8546220000	0.0499050000
H	1.1808520000	3.8664680000	0.0597890000
H	-2.9088160000	-2.0609490000	0.6079390000
C	-3.0418100000	1.4235780000	1.1875600000
C	-2.1177410000	0.3868670000	1.1961250000
H	-3.3852650000	1.8243500000	2.1365440000
H	-1.7411690000	0.0001950000	2.1368930000

TS6-1a (B3LYP-D3, CH_2Cl_2)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1716.729072
$\varepsilon_0 + E_{tot}$ = −1716.703024
$\varepsilon_0 + H_{corr}$ = −1716.702080
$\varepsilon_0 + G_{corr}$ = −1716.792232

Frequency: -247.450
Coordinates:

H	-4.5291010000	0.0295690000	-2.2930660000
H	-2.3706230000	-1.1716780000	-2.0600100000
H	1.0461820000	3.2003370000	-2.0528870000
H	0.7199910000	0.7475380000	-1.9417790000
O	3.0856880000	-0.4092730000	-1.7428940000
O	-6.4778950000	1.1892290000	-1.4453520000
C	-4.1018070000	-0.1468090000	-1.3159760000
C	-2.8972280000	-0.8136410000	-1.1872040000
C	0.7873620000	2.7366890000	-1.1085580000
C	0.5933750000	1.3567330000	-1.0592040000
F	5.2817410000	1.3703940000	-0.6973220000
O	4.9569490000	-1.6662500000	-0.6693700000
S	3.7590310000	-0.8246320000	-0.4977470000
N	-6.0228830000	1.0149320000	-0.3108190000
C	-4.7667220000	0.3048930000	-0.1694630000
H	0.8137020000	4.5800310000	-0.0042080000
C	0.6594250000	3.5086260000	0.0443970000
C	-2.4071330000	-1.0461100000	0.0979970000
C	0.2726780000	0.7918460000	0.1669640000
C	4.4567380000	0.7879220000	0.1914070000
O	-2.5977390000	-3.3852720000	0.2552660000
I	-0.1035180000	-1.3290610000	0.2559190000
F	3.4774900000	1.6577950000	0.4801730000
O	2.8384390000	-1.2647060000	0.5810780000
O	-6.5908110000	1.4178400000	0.7092210000
C	-4.2333570000	0.1078440000	1.1083370000
H	-2.8349940000	-3.3940830000	1.1909370000
C	-3.0258170000	-0.5549700000	1.2477350000
C	0.3398980000	2.9092830000	1.2617810000
F	5.1560700000	0.5619190000	1.3180130000
C	0.1416340000	1.5310470000	1.3354760000
H	-4.7586730000	0.4785200000	1.9772140000
H	0.2455810000	3.5075790000	2.1601270000
H	-2.5983450000	-0.7104080000	2.2283910000
H	-0.1006340000	1.0587930000	2.2777800000

TS6-1a (B3LYP-D3, H_2O)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1716.740999
$\varepsilon_0 + E_{tot}$ = −1716.714890
$\varepsilon_0 + H_{corr}$ = −1716.713946
$\varepsilon_0 + G_{corr}$ = −1716.804527

Frequency: -252.540
Coordinates:

H	-4.5498860000	0.0168240000	-2.2991060000
H	1.0501980000	3.2309740000	-2.0574810000
H	-2.3609840000	-1.1249340000	-2.0554450000
H	0.6769480000	0.7842360000	-1.9456360000
O	3.0836120000	-0.4627610000	-1.7404760000
O	-6.5372740000	1.1153240000	-1.4602750000
C	-4.1245480000	-0.1496710000	-1.3194770000
C	-2.9026310000	-0.7845560000	-1.1847710000
C	0.8101340000	2.7683910000	-1.1077030000
C	0.5912100000	1.3921560000	-1.0569920000
F	5.3068500000	1.3079030000	-0.7347550000
O	4.9558300000	-1.7187630000	-0.6701850000
S	3.7644050000	-0.8656450000	-0.4953190000
N	-6.0814240000	0.9578080000	-0.3239040000
C	-4.8048730000	0.2844450000	-0.1758170000

H	0.8991730000	4.6073020000	0.0008230000
C	0.7268910000	3.5387990000	0.0507370000
C	-2.4175630000	-1.0035570000	0.1034870000
C	4.4813800000	0.7486750000	0.1677110000
C	0.2914630000	0.8308390000	0.1764220000
I	-0.1142860000	-1.2853680000	0.2688380000
O	-2.6082300000	-3.3418480000	0.2736310000
F	3.5127640000	1.6302410000	0.4496030000
O	2.8526990000	-1.2917240000	0.5956240000
O	-6.6651670000	1.3458930000	0.6922870000
C	-4.2706640000	0.1082270000	1.1046460000
H	-2.7105340000	-3.3733620000	1.2332240000
C	-3.0466990000	-0.5233110000	1.2506200000
C	0.4266430000	2.9421440000	1.2744070000
F	5.1848670000	0.5277060000	1.2923070000
C	0.2032510000	1.5675870000	1.3503950000
H	-4.8060270000	0.4699600000	1.9711050000
H	0.3649780000	3.5396550000	2.1759890000
H	-2.6162630000	-0.6611440000	2.2323390000
H	-0.0269790000	1.0980290000	2.2969890000

TS7-1d (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1245.551281
$\varepsilon_0 + E_{tot}$ = −1245.521527
$\varepsilon_0 + H_{corr}$ = −1245.520583
$\varepsilon_0 + G_{corr}$ = −1245.615336

Frequency: -275.21
Coordinates:

H	-4.1078890000	0.3451970000	-2.7854580000
H	2.9080810000	0.9631060000	-2.4895990000
H	5.1086830000	1.9848010000	-2.0570820000
H	0.4308460000	4.6567190000	-1.9814560000
H	-1.2193260000	4.0043830000	-1.9336910000
H	-2.2218740000	-1.0573660000	-1.9323690000
C	-4.2485570000	-0.2878540000	-1.9148590000
H	-6.3103370000	0.2818450000	-1.6358160000
C	3.1450310000	1.3496490000	-1.5064160000
C	-3.1872350000	-1.0598970000	-1.4414660000
C	-0.3811240000	4.3455360000	-1.3191070000
C	-5.4851650000	-0.3216190000	-1.2723670000
C	4.3830210000	1.9252420000	-1.2511940000
O	0.5443920000	2.1326210000	-1.1998380000
H	-1.9688350000	1.5050040000	-0.8355920000
H	-0.7112050000	5.2062650000	-0.7265990000
O	-1.0408280000	-2.6516850000	-0.6049620000
I	0.6828720000	-0.4868660000	-0.5489710000
C	2.1840000000	1.2812910000	-0.4819370000
C	0.1081980000	3.1948090000	-0.4190320000
C	-3.3325210000	-1.8688590000	-0.3137700000
C	-5.6510980000	-1.1435890000	-0.1555350000
H	0.6204060000	-3.5327090000	-0.0238190000
C	4.7076910000	2.4153470000	0.0196990000
C	2.1125120000	-2.0161860000	0.0999960000
C	-1.9957840000	1.9081460000	0.1693000000
H	0.9503200000	3.5880980000	0.1839260000
H	5.6818580000	2.8499840000	0.2116530000
C	1.6662880000	-3.3259540000	0.2118850000
C	-2.1338710000	-2.6790060000	0.2188860000
H	3.7576100000	-0.6246990000	0.2949900000
C	-4.5847600000	-1.9079470000	0.3135040000
H	-2.5225200000	-3.7199310000	0.3337980000
H	-6.6113010000	-1.1847440000	0.3498030000
C	3.4236130000	-1.6488760000	0.3864640000
C	-0.9868080000	2.7896010000	0.5689310000
C	2.5737160000	-4.3001820000	0.6324100000
H	-3.7617400000	0.8218920000	0.7188520000
H	2.2399630000	-5.3284820000	0.7258750000
C	2.5063360000	1.7487860000	0.8026820000
C	4.3143270000	-2.6396050000	0.8050510000
C	3.8937070000	-3.9625360000	0.9289570000
H	5.3387150000	-2.3659700000	1.0341640000
C	3.7577920000	2.3197830000	1.0353330000
C	-3.0026680000	1.5206380000	1.0490230000
H	-4.7251280000	-2.5439670000	1.1830480000
H	4.5919880000	-4.7259640000	1.2552540000
H	1.7904120000	1.6513860000	1.6093950000
H	-1.5279020000	-1.1350690000	1.6374670000
C	-1.8011400000	-2.1926470000	1.6573750000
C	-1.0102440000	3.2782940000	1.8777820000
H	-0.9470100000	-2.7644070000	2.0315860000
H	3.9910840000	2.6748150000	2.0349300000
H	-0.2246420000	3.9525990000	2.2075760000
H	-2.6389370000	-2.3159390000	2.3528090000
C	-3.0147870000	2.0145650000	2.3544370000
C	-2.0155670000	2.8949700000	2.7671540000
H	-3.7903030000	1.7039250000	3.0466700000
H	-2.0111960000	3.2742440000	3.7844030000

TS7-1d (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1244.894236
$\varepsilon_0 + E_{tot}$ = −1244.864896
$\varepsilon_0 + H_{corr}$ = −1244.863952
$\varepsilon_0 + G_{corr}$ = −1244.956734

Frequency: -324.31
Coordinates:

H	-4.1543180000	0.3272480000	-2.7881590000
H	2.9105290000	0.8156710000	-2.4631590000
H	5.1267710000	1.8203010000	-2.0896180000
H	0.5015380000	4.6445920000	-1.9713590000
H	-1.1535490000	4.0045910000	-1.9359140000
H	-2.2309350000	-1.0207280000	-1.9268410000
C	-4.2756830000	-0.2991000000	-1.9105590000
H	-6.3471240000	0.2215300000	-1.6335460000
C	3.1605070000	1.2457340000	-1.5014210000
C	-3.1961550000	-1.0400340000	-1.4332570000
C	-0.3158740000	4.3363180000	-1.3162310000
C	4.4052290000	1.8116940000	-1.2790940000
C	-5.5071080000	-0.3568250000	-1.2658420000
O	0.5893600000	2.1221280000	-1.2040650000
H	-1.9107840000	1.5062390000	-0.8998560000
H	-0.6404100000	5.1925730000	-0.7165240000
O	-1.0177350000	-2.5306110000	-0.5779480000
I	0.6576250000	-0.4804430000	-0.4784740000
C	2.2083870000	1.2456290000	-0.4699250000
C	0.1597640000	3.1763810000	-0.4285770000
C	-3.3220090000	-1.8392380000	-0.2996720000
H	0.6335080000	-3.5539890000	-0.1908220000
C	-5.6517820000	-1.1705040000	-0.1432810000
C	4.7460730000	2.3528880000	-0.0361540000
C	1.6593750000	-3.3341410000	0.1014010000
C	-1.9583840000	1.9028380000	0.1096010000
C	2.0638400000	-2.0069610000	0.1219760000
H	5.7275860000	2.7795350000	0.1290200000
H	0.9921890000	3.5629280000	0.1936560000

C	-2.1076070000	-2.6094900000	0.2383290000
C	-4.5689610000	-1.9028820000	0.3301680000
H	-2.4595990000	-3.6605430000	0.3489560000
H	-6.6099890000	-1.2320070000	0.3618430000
H	2.2730560000	-5.3535230000	0.4666180000
C	2.5770770000	-4.3127200000	0.4771340000
C	3.3494770000	-1.6342160000	0.4987920000
H	3.6603170000	-0.5971800000	0.5091880000
C	-0.9553550000	2.7762260000	0.5356500000
H	-3.7535260000	0.8385980000	0.6117730000
C	2.5438670000	1.7592400000	0.7898730000
C	3.8681480000	-3.9667510000	0.8616460000
C	4.2498800000	-2.6300260000	0.8711230000
C	-2.9924410000	1.5290280000	0.9606280000
C	3.8041080000	2.3199400000	0.9861610000
H	4.5746840000	-4.7354470000	1.1530470000
H	5.2531850000	-2.3485810000	1.1694390000
H	-4.6919640000	-2.5375930000	1.2035160000
H	1.8336280000	1.7032910000	1.6070660000
H	-1.5938830000	-1.0347060000	1.6512650000
C	-1.8086060000	-2.1070330000	1.6715550000
C	-1.0108610000	3.2682620000	1.8387960000
H	4.0514470000	2.7143980000	1.9665850000
H	-0.9270490000	-2.6326860000	2.0500080000
H	-0.2295180000	3.9390100000	2.1863070000
C	-3.0356490000	2.0270730000	2.2616290000
H	-2.6415220000	-2.2742690000	2.3616550000
C	-2.0429000000	2.8976000000	2.6989270000
H	-3.8339510000	1.7277800000	2.9312810000
H	-2.0656090000	3.2807170000	3.7135090000

TS7-1e (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$	=	−1481.365809
$\varepsilon_0 + E_{tot}$	=	−1481.326081
$\varepsilon_0 + H_{corr}$	=	−1481.325137
$\varepsilon_0 + G_{corr}$	=	−1481.443793

Frequency: -250.16
Coordinates:

H	-0.5740790000	2.7837100000	-3.0553910000
H	3.4205470000	-0.0891850000	-2.8186630000
H	-3.9590730000	-0.6057890000	-2.6258050000
H	-0.4557120000	1.0765120000	-2.6119950000
H	1.6681720000	-0.1051830000	-2.5804270000
H	4.0794450000	2.1217270000	-2.3582600000
H	-2.9195080000	-2.0253250000	-2.3459170000
C	-0.3368670000	2.0973720000	-2.2407180000
H	-2.2426730000	-0.3899300000	-2.2220760000
C	2.6332530000	-0.1302540000	-2.0624470000
C	-3.1288430000	-0.9991390000	-2.0272210000
H	0.7145260000	2.2309200000	-1.9773790000
H	4.8243730000	4.3988080000	-1.9657880000
H	-2.0641280000	4.1123130000	-1.9501530000
H	2.6978150000	-1.0912870000	-1.5511070000
H	4.5455870000	-5.8484310000	-1.4328610000
C	3.5557440000	2.1236110000	-1.4049790000
H	6.4414490000	-4.2452810000	-1.3133990000
H	-6.0092340000	-0.2787010000	-1.1442290000
C	2.7609180000	1.0133960000	-1.0893680000
C	-2.0799990000	3.4669020000	-1.0768970000
H	-4.1812950000	5.1908690000	-1.0764380000
C	-1.2322230000	2.3547050000	-1.0557050000
C	4.4170050000	-4.8864120000	-0.9478650000
C	4.5738330000	4.3932790000	-0.9016710000
C	5.4810820000	-3.9857710000	-0.8787790000
H	-8.1001050000	-1.5446260000	-0.7594680000
H	4.0829240000	5.3440980000	-0.6700760000
C	-5.9706190000	-1.2489130000	-0.6557010000
C	3.6931300000	3.2163670000	-0.5520960000
C	-3.4249870000	-0.9864190000	-0.5030900000
H	2.3490310000	-5.2236260000	-0.4523760000
C	-7.1493180000	-1.9593650000	-0.4379870000
C	3.1854860000	-4.5343630000	-0.3966610000
H	5.5176290000	4.3745990000	-0.3431980000
C	5.3089220000	-2.7489910000	-0.2604790000
H	-3.6696240000	0.0729180000	-0.2534310000
C	-4.7313430000	-1.7580850000	-0.2480570000
H	6.1366010000	-2.0460110000	-0.2210870000
C	-3.8136500000	4.9975070000	-0.0651710000
C	-2.9427540000	3.7647720000	-0.0234160000
C	-1.2741520000	1.5302460000	0.0768900000
C	2.0828960000	1.0204750000	0.1395880000
C	-7.1088930000	-3.2011340000	0.1993280000
I	0.0213180000	-0.2036720000	0.2054930000
C	3.0193680000	-3.2946830000	0.2207870000
O	-2.3716730000	-1.4570510000	0.2301750000
H	-3.2513660000	5.8832420000	0.2513370000
C	4.0784420000	-2.3874880000	0.2991480000
H	4.3990440000	-0.2843070000	0.3358480000
H	-8.0246090000	-3.7570510000	0.3735250000
C	-4.7047920000	-2.9955210000	0.3978580000
H	-4.6760350000	4.8996830000	0.5977520000
C	-5.8809490000	-3.7140090000	0.6164810000
H	2.0639190000	-2.9985330000	0.6371330000
C	3.0100320000	3.1692160000	0.6682290000
H	-3.7403820000	-3.3648590000	0.7261370000
C	3.8881340000	-1.0287230000	0.9834030000
C	2.2016770000	2.0946660000	1.0371360000
C	-2.9614930000	2.9057310000	1.0724050000
H	-5.8402060000	-4.6757910000	1.1193740000
O	2.5616920000	-0.6926260000	1.1363050000
C	-2.1419580000	1.7738440000	1.1520550000
H	3.1124940000	3.9971550000	1.3665300000
H	-3.6446620000	3.1036290000	1.8926160000
H	-2.5180320000	-0.1525830000	1.9943530000
H	5.6863620000	-1.2476980000	2.2446610000
H	0.4289110000	2.2823060000	2.2512540000
C	-2.2609580000	0.8562480000	2.3395610000
C	4.6207970000	-1.0122210000	2.3442480000
C	1.4983420000	2.0798690000	2.3687440000
H	4.5176300000	-0.0206110000	2.7924150000
H	1.6055040000	1.0982370000	2.8331850000
H	-1.3128950000	0.7822790000	2.8809750000
H	4.1628240000	-1.7460660000	3.0139820000
H	-3.0223590000	1.2206250000	3.0315840000
H	1.9096130000	2.8389760000	3.0385530000

TS7-1e (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$	=	−1480.569330
$\varepsilon_0 + E_{tot}$	=	−1480.530088
$\varepsilon_0 + H_{corr}$	=	−1480.529144
$\varepsilon_0 + G_{corr}$	=	−1480.643617

Frequency: -334.06
Coordinates:

H	-0.4144780000	2.7421020000	-3.0626880000

H	3.3280920000	-0.6548630000	-2.6421560000
H	-0.4397900000	1.0239620000	-2.6334480000
H	1.5747260000	-0.3987630000	-2.5853340000
H	-3.2697900000	-1.3849790000	-2.4313850000
H	-4.4329570000	-0.0385550000	-2.3403520000
C	-0.2471630000	2.0310830000	-2.2534090000
H	4.2132520000	1.4848810000	-2.2304770000
H	-2.7077290000	0.2537260000	-2.0347800000
H	5.7348250000	-4.6129910000	-2.0238450000
H	-1.8467430000	4.1601080000	-1.9832450000
C	2.4723090000	-0.5433950000	-1.9733640000
H	0.8051100000	2.0808990000	-1.9606830000
C	-3.5235130000	-0.4620060000	-1.9012170000
H	5.0958850000	3.7584660000	-1.9009320000
H	6.9304960000	-2.4888040000	-1.5726660000
H	2.3515120000	-1.4763550000	-1.4199270000
C	5.3221930000	-3.8926630000	-1.3263620000
C	3.6286700000	1.5937090000	-1.3192410000
H	-3.7433120000	5.4549180000	-1.1518120000
C	-1.9236460000	3.5071950000	-1.1190720000
C	-1.1495910000	2.3453510000	-1.0902670000
C	5.9924470000	-2.7010140000	-1.0710600000
C	2.6829900000	0.6103330000	-1.0304180000
H	3.5763180000	-5.0710050000	-0.8910290000
C	4.8875630000	3.7362170000	-0.8290460000
H	-6.3458500000	-0.1800530000	-0.6935060000
C	4.1094060000	-4.1484580000	-0.6883850000
H	4.5633020000	4.7355140000	-0.5290620000
C	3.8407420000	2.7009060000	-0.5013000000
H	-8.2973600000	-1.6796020000	-0.4509210000
C	-6.1969700000	-1.2240280000	-0.4290630000
C	-3.6774240000	-0.7789510000	-0.3953030000
H	5.8323650000	3.5312680000	-0.3148850000
C	-7.2956390000	-2.0650010000	-0.2919020000
C	-4.8975320000	-1.6940480000	-0.2222680000
C	5.4520520000	-1.7728510000	-0.1830220000
C	-3.5869830000	5.1212780000	-0.1248870000
C	-2.7878000000	3.8442990000	-0.0832070000
H	5.9635640000	-0.8318210000	-0.0005890000
C	-1.2745130000	1.5147950000	0.0254230000
C	-7.1103570000	-3.4014710000	0.0564250000
H	-3.9730920000	0.1839980000	0.0895120000
C	-4.7245290000	-3.0289720000	0.1358480000
O	-2.5430980000	-1.3044630000	0.1381220000
C	1.9363500000	0.7318620000	0.1556370000
H	-7.9637630000	-4.0614240000	0.1656670000
I	-0.1231440000	-0.2830890000	0.1688080000
C	3.5752010000	-3.2176290000	0.1945070000
C	-5.8205650000	-3.8779930000	0.2701320000
H	-3.7097460000	-3.3663000000	0.3128990000
H	-4.5622370000	4.9895750000	0.3469900000
H	-3.0644240000	5.9199180000	0.4093710000
C	4.2406500000	-2.0191450000	0.4587540000
H	-5.6687840000	-4.9156600000	0.5489450000
C	3.0748420000	2.7868250000	0.6606070000
H	2.6123510000	-3.3832030000	0.6677060000
C	-2.8820750000	2.9819610000	1.0043750000
C	2.1234460000	1.8319900000	1.0109440000
C	-2.1376860000	1.8047540000	1.0888090000
H	4.1168840000	-0.0395140000	1.2254610000
O	2.2612100000	-0.8914310000	1.2567170000
H	3.2227020000	3.6293740000	1.3330520000
C	3.6204380000	-1.0123280000	1.4223660000
H	-3.5632080000	3.2202340000	1.8158690000
H	-2.5943600000	-0.0984990000	1.9395980000
H	0.3378080000	2.3418510000	2.1161260000
C	-2.3048150000	0.9021810000	2.2796890000
C	1.3479060000	1.9584620000	2.2954970000
H	1.2653390000	0.9801420000	2.7743370000
H	-1.3639990000	0.8066510000	2.8300460000
C	3.9578630000	-1.4090600000	2.8678790000
H	-3.0597910000	1.3055210000	2.9549850000
H	1.8478600000	2.6470940000	2.9792920000
H	5.0383030000	-1.4846650000	3.0267730000
H	3.5008640000	-2.3757520000	3.0967900000
H	3.5459990000	-0.6616800000	3.5501870000

TS8-1d (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1245.544591
$\varepsilon_0 + E_{tot}$ = −1245.514515
$\varepsilon_0 + H_{corr}$ = −1245.513571
$\varepsilon_0 + G_{corr}$ = −1245.609694

Frequency: -473.94
Coordinates:

H	-4.0888480000	-2.9796690000	-2.4070720000
H	-4.6583480000	-0.1318400000	-2.3499080000
H	6.2483080000	-2.3446200000	-2.3454690000
H	3.1775410000	2.8808870000	-2.2214080000
H	7.7299520000	-0.4204440000	-1.8250030000
H	-2.5367730000	-3.6320220000	-1.8133800000
H	-6.7516360000	1.0463020000	-1.7519850000
H	-1.8070330000	3.7703400000	-1.6950680000
H	2.5580010000	0.5475310000	-1.6891210000
H	-2.6340900000	-1.1606250000	-1.5558940000
C	5.9879510000	-1.6604090000	-1.5439140000
H	-0.2084890000	1.8957930000	-1.5196760000
C	-3.4660720000	-3.1370710000	-1.5173890000
C	-5.0918500000	-0.2683350000	-1.3628950000
C	2.7287590000	2.6524270000	-1.2597880000
C	6.8221500000	-0.5810390000	-1.2528800000
H	4.1455110000	-2.6820780000	-1.0348920000
C	-6.2679100000	0.4001140000	-1.0257470000
C	2.3735080000	1.3367260000	-0.9696710000
C	-1.9733720000	2.9916570000	-0.9583620000
C	-1.0727910000	1.9295340000	-0.8693760000
H	-4.0014360000	-3.7977100000	-0.8276050000
C	4.8175030000	-1.8616180000	-0.8134870000
C	-3.1225810000	-1.8106440000	-0.7923250000
H	2.7794950000	4.6931960000	-0.5626330000
C	-4.4347160000	-1.0867870000	-0.4401390000
C	2.5094750000	3.6694510000	-0.3292370000
C	6.4738590000	0.2979340000	-0.2261850000
H	-3.7832890000	3.8693680000	-0.1909370000
C	-3.0786350000	3.0487370000	-0.1109880000
H	7.1060260000	1.1514800000	-0.0034210000
C	-1.2924500000	0.9313820000	0.0738160000
C	4.4691220000	-0.9981940000	0.2287400000
I	0.0487740000	-0.7735290000	0.2368040000
C	-6.8139410000	0.2522590000	0.2495450000
C	1.7979430000	1.0277580000	0.2686830000
O	-2.3154640000	-2.0238900000	0.2955220000
O	2.3046690000	-2.0551830000	0.4550500000
C	5.3079470000	0.0894030000	0.5056410000

H	-7.7254410000	0.7759130000	0.5193830000
C	-3.2860540000	2.0391770000	0.8263950000
C	-4.9917690000	-1.2286830000	0.8333460000
H	2.6526950000	-0.1127310000	0.8631200000
C	1.9325930000	3.3554960000	0.9027000000
C	-2.3909310000	0.9749930000	0.9237060000
C	3.1667580000	-1.2026750000	0.9865620000
C	-6.1704460000	-0.5692410000	1.1770920000
C	1.5691880000	2.0443860000	1.2024220000
H	5.0303860000	0.7924140000	1.2842040000
H	-4.1617000000	2.0542650000	1.4649590000
H	-4.4557220000	-1.8393020000	1.5513580000
H	-2.5770410000	0.1515490000	1.5987600000
H	1.7537010000	4.1369080000	1.6347430000
H	1.0980060000	1.8155140000	2.1516940000
H	-6.5853700000	-0.6867200000	2.1739080000
C	3.3419750000	-1.3168690000	2.5143650000
H	3.8101730000	-2.2775450000	2.7530120000
H	3.9584740000	-0.5160490000	2.9326030000
H	2.3569670000	-1.2897260000	2.9867500000

TS8-1d (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1244.883789
$\varepsilon_0 + E_{tot}$ = −1244.854203
$\varepsilon_0 + H_{corr}$ = −1244.853259
$\varepsilon_0 + G_{corr}$ = −1244.946129

Frequency: -637.54

Coordinates:

H	-4.0871460000	-2.9520760000	-2.4088910000
H	6.3108310000	-2.0839730000	-2.3561200000
H	-4.2492900000	0.1039680000	-2.3280560000
H	3.0310450000	2.8836780000	-2.1788980000
H	7.6297870000	-0.0475960000	-1.8518170000
H	-2.0378590000	3.4202660000	-1.8285270000
H	-2.6025070000	-3.7383540000	-1.8062600000
H	-6.2315840000	1.4613260000	-1.7327370000
H	-0.4484680000	1.5340400000	-1.6811810000
H	2.4753320000	0.5291640000	-1.6634490000
H	-2.4610030000	-1.2697540000	-1.6115130000
C	5.9962470000	-1.4190120000	-1.5589540000
C	-3.4778710000	-3.1505850000	-1.5200140000
C	-4.7496430000	-0.0566170000	-1.3765610000
C	6.7390810000	-0.2763640000	-1.2774980000
C	2.5701000000	2.6391380000	-1.2279130000
C	-5.8618040000	0.7117190000	-1.0406880000
H	4.2439160000	-2.5837840000	-1.0399040000
C	-2.1178410000	2.7143970000	-1.0098140000
C	2.2525640000	1.3137700000	-0.9478640000
C	-1.2266010000	1.6474040000	-0.9352510000
C	-3.0077480000	-1.8524990000	-0.8324540000
C	4.8480360000	-1.7094990000	-0.8260250000
H	-4.0696190000	-3.7362230000	-0.8102270000
H	2.5418780000	4.6756550000	-0.5276550000
C	-4.2406550000	-1.0074870000	-0.4946410000
C	2.2996640000	3.6439860000	-0.3020920000
C	6.3229320000	0.5799520000	-0.2603480000
H	-3.8024090000	3.6973990000	-0.1063430000
H	6.8830270000	1.4837170000	-0.0470120000
C	-3.1040280000	2.8710490000	-0.0413160000
C	-1.3364650000	0.7431220000	0.1124210000
C	-6.4884870000	0.5311800000	0.1879200000
C	4.4365660000	-0.8697250000	0.2070940000
I	0.0195660000	-0.9070010000	0.2599940000
O	-2.2325300000	-2.1167160000	0.2604680000
C	1.6649930000	0.9897180000	0.2763910000
O	2.3460420000	-2.0600160000	0.4533730000
H	-7.3517290000	1.1308130000	0.4556400000
C	5.1804760000	0.2840040000	0.4724200000
C	-4.8785560000	-1.1826630000	0.7348400000
H	2.5885600000	-0.1013930000	0.8604910000
C	1.7069280000	3.3106420000	0.9139780000
C	3.1642990000	-1.1608200000	0.9771800000
C	-3.2054910000	1.9554290000	0.9999730000
C	-5.9932960000	-0.4249380000	1.0741640000
C	-2.3216270000	0.8834190000	1.0794450000
C	1.3779810000	1.9910190000	1.2050930000
H	4.8395850000	0.9705130000	1.2428200000
H	-4.4554180000	-1.9039920000	1.4262460000
H	1.4872310000	4.0849200000	1.6412880000
H	-3.9900440000	2.0556500000	1.7409890000
H	-2.4264500000	0.1345800000	1.8545270000
H	-6.4753650000	-0.5708230000	2.0356100000
H	0.8874250000	1.7463250000	2.1410740000
C	3.3775290000	-1.2778680000	2.4925050000
H	3.8897130000	-2.2198370000	2.7107520000
H	3.9688530000	-0.4543410000	2.9004720000
H	2.4029470000	-1.2961850000	2.9863340000

TS8-1e (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1481.363727
$\varepsilon_0 + E_{tot}$ = −1481.324235
$\varepsilon_0 + H_{corr}$ = −1481.323291
$\varepsilon_0 + G_{corr}$ = −1481.437878

Frequency: -462.81

Coordinates:

H	-0.5396300000	2.5265240000	-3.0205680000
H	1.9735250000	-0.1079990000	-2.8619040000
H	3.7057890000	-0.3945840000	-2.6419950000
H	-0.3824330000	0.8200830000	-2.5869120000
H	-4.2417030000	0.0474070000	-2.5854260000
H	-3.5116580000	-1.5787770000	-2.5805340000
H	-2.5070140000	-0.1536680000	-2.2576460000
C	-0.2259690000	1.8398820000	-2.2318810000
H	4.0559890000	2.0161600000	-2.2147920000
C	2.7480330000	-0.3341900000	-2.1196600000
C	-3.4944230000	-0.5943330000	-2.1035480000
H	0.8456090000	1.9708040000	-2.0730970000
H	2.5201870000	-1.3090200000	-1.6931160000
H	6.0561720000	-4.0447550000	-1.6662940000
H	-1.5674060000	4.0587510000	-1.6467640000
C	3.5084510000	1.9152760000	-1.2806880000
H	5.1794910000	4.0380410000	-1.2663040000
H	3.6779900000	4.9548230000	-1.1449510000
C	2.7829900000	0.7408010000	-1.0608790000
H	7.7890990000	-2.3767780000	-1.0454460000
C	5.8085280000	-3.2292040000	-0.9940290000
C	-0.9908410000	2.1123380000	-0.9615520000
H	-6.1441730000	0.5234880000	-0.9496150000
C	-1.6425010000	3.3453120000	-0.8312590000
H	3.7355430000	-3.8130720000	-0.7705750000
C	6.7839760000	-2.2941830000	-0.6453120000
C	4.3114070000	4.2243990000	-0.6282990000
H	-8.4331160000	-0.3524090000	-0.6044910000
C	-6.2855630000	-0.4972170000	-0.6038750000

C	-3.7348260000	-0.7591580000	-0.5797130000
H	-3.1915090000	5.4984510000	-0.5452230000
C	4.5152790000	-3.1156130000	-0.4884550000
C	-7.5747970000	-0.9881040000	-0.4078820000
C	-5.1612610000	-1.2937970000	-0.3538280000
C	3.5536820000	2.9491930000	-0.3436120000
H	-3.7565990000	0.2769600000	-0.1648180000
I	-0.1178030000	-0.7423660000	-0.0082800000
O	-2.7785930000	-1.5345680000	0.0121580000
C	-7.7635500000	-2.2947710000	0.0471430000
C	-1.0970350000	1.1994150000	0.0956920000
C	-5.3621400000	-2.5953350000	0.1103010000
C	2.0914030000	0.6156010000	0.1516850000
O	1.8098510000	-2.5491560000	0.1945330000
H	-8.7659450000	-2.6802250000	0.2038850000
C	6.4541340000	-1.2455340000	0.2142570000
H	4.6641410000	4.6943850000	0.2936060000
C	-2.3830820000	3.6782910000	0.2989460000
C	-6.6505760000	-3.0943000000	0.3058600000
H	-4.4810420000	-3.1896510000	0.3225470000
C	4.1787500000	-2.0766770000	0.3830380000
C	-3.0439110000	5.0295320000	0.4305000000
H	7.2007380000	-0.5030270000	0.4770920000
H	-6.7868030000	-4.1093350000	0.6673950000
C	5.1621320000	-1.1410050000	0.7247010000
H	2.5533530000	-0.7659650000	0.7791290000
C	2.8634940000	2.7732220000	0.8563320000
C	2.7535540000	-1.9478450000	0.9052030000
H	-4.0180190000	4.9496900000	0.9202030000
H	-2.4303890000	5.7082860000	1.0334580000
C	2.1292880000	1.6140330000	1.1299770000
C	-1.8771760000	1.4751280000	1.2329220000
C	-2.4964090000	2.7261940000	1.3108410000
H	4.9022230000	-0.3094100000	1.3719680000
H	2.9053490000	3.5508590000	1.6152870000
H	-2.5568760000	-0.4395770000	1.8753270000
H	-3.1031120000	2.9481760000	2.1839440000
C	-2.1233600000	0.4640900000	2.3220060000
C	2.6584440000	-2.1701370000	2.4301350000
H	0.4411440000	1.9101410000	2.4320840000
C	1.4377130000	1.4621210000	2.4607460000
H	2.8857270000	-3.2176450000	2.6546880000
H	1.3213000000	0.4112000000	2.7258450000
H	1.6356600000	-1.9663060000	2.7539940000
H	-1.1948900000	0.1699630000	2.8189170000
H	3.3496450000	-1.5343580000	2.9917220000
H	-2.8003550000	0.8699820000	3.0762660000
H	2.0044900000	1.9570300000	3.2535620000

TS8-1e (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1480.559973
$\varepsilon_0 + E_{tot}$ = −1480.521064
$\varepsilon_0 + H_{corr}$ = −1480.520120
$\varepsilon_0 + G_{corr}$ = −1480.631707

Frequency: -915.66

Coordinates:

H	-0.5977550000	2.2696500000	-3.0406240000
H	2.1015780000	-0.1942850000	-2.9036860000
H	-3.4250070000	-1.4204820000	-2.5432400000
H	-4.1633480000	0.2020750000	-2.5263060000
H	-0.1549190000	0.6749180000	-2.4214430000
H	3.7272010000	-0.6841950000	-2.3982940000
H	3.9470560000	1.8715720000	-2.2612210000
C	-0.1479090000	1.7421620000	-2.1977470000
H	-2.4365950000	-0.0000990000	-2.1500530000
H	0.8933260000	2.0597960000	-2.1096070000
C	2.7131790000	-0.4839550000	-2.0418850000
C	-3.4276560000	-0.4486010000	-2.0409150000
H	5.7776460000	-4.0524980000	-1.8068130000
H	-1.4565880000	3.9840470000	-1.6899550000
H	2.3124530000	-1.4082450000	-1.6286120000
H	4.9544350000	3.9821050000	-1.5335070000
H	7.5213720000	-2.3286840000	-1.4427690000
C	3.4243120000	1.8050130000	-1.3094490000
H	3.4898180000	4.9014490000	-1.1825830000
C	5.5848990000	-3.2198070000	-1.1392050000
H	-6.1380850000	0.5355900000	-1.0657890000
C	2.7301920000	0.6280850000	-1.0226890000
C	-0.9090050000	2.0577380000	-0.9360110000
C	6.5666010000	-2.2523870000	-0.9348930000
H	-8.4071560000	-0.4259120000	-0.8572360000
C	-1.5451730000	3.2981780000	-0.8516990000
C	4.1844370000	4.1579800000	-0.7802200000
C	-6.2627100000	-0.4869590000	-0.7182120000
H	3.5655610000	-3.8369990000	-0.6681840000
H	-3.4503980000	5.2719630000	-0.6034580000
C	-7.5395070000	-1.0245580000	-0.5990000000
C	-3.7097620000	-0.6649480000	-0.5345140000
C	4.3559130000	-3.1146130000	-0.4981430000
C	3.4649600000	2.8805180000	-0.4287860000
C	-5.1294510000	-1.2364640000	-0.3896430000
C	-7.7061070000	-2.3312870000	-0.1434040000
H	-3.7749300000	0.3598080000	-0.0891590000
C	6.3127280000	-1.1834630000	-0.0798500000
H	-8.7001600000	-2.7541240000	-0.0471040000
O	-2.7620030000	-1.4348440000	0.0532170000
H	7.0664980000	-0.4188700000	0.0721300000
C	-5.3085320000	-2.5373410000	0.0752940000
H	4.6610700000	4.5969840000	0.0988650000
I	-0.0843920000	-0.7517740000	0.1351350000
C	-1.0365460000	1.1791060000	0.1446080000
C	-6.5848300000	-3.0831420000	0.1940420000
C	2.0607950000	0.5368360000	0.2047350000
C	-2.2886460000	3.6756260000	0.2604290000
C	-2.9311770000	5.0373990000	0.3282410000
H	-4.4152920000	-3.0892850000	0.3459960000
C	4.0965830000	-2.0510980000	0.3657890000
O	1.7351730000	-2.5228270000	0.4255550000
H	-2.1779600000	5.8135950000	0.4898570000
H	-6.7064480000	-4.0983770000	0.5578090000
C	5.0858040000	-1.0868380000	0.5687020000
C	2.8028710000	2.7433500000	0.7915850000
H	2.5227440000	-0.7137530000	0.8664080000
C	2.7350290000	-1.9271920000	1.0219780000
C	2.1070430000	1.5870180000	1.1344420000
H	-3.6520320000	5.0929280000	1.1449300000
H	4.8761160000	-0.2361100000	1.2121340000
C	-1.8291570000	1.4977860000	1.2565780000
C	-2.4283840000	2.7579270000	1.2955030000

H	2.8445730000	3.5547860000	1.5143550000
H	-2.5530400000	-0.3836530000	1.9151400000
H	-3.0417440000	3.0132280000	2.1546390000
C	-2.1112510000	0.5167050000	2.3610910000
H	0.4284050000	1.8379990000	2.4553400000
C	1.4584090000	1.4728390000	2.4877880000
C	2.7851690000	-2.0704270000	2.5495450000
H	3.0726090000	-3.0967160000	2.7997360000
H	1.4376890000	0.4341490000	2.8233680000
H	-1.1969620000	0.2177500000	2.8815360000
H	1.7880010000	-1.8878450000	2.9564780000
H	3.5019940000	-1.3843960000	3.0086150000
H	-2.7953750000	0.9535150000	3.0895500000
H	2.0023090000	2.0649290000	3.2259460000

TS9-1d (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −859.999203
$\varepsilon_0 + E_{tot}$ = −859.978818
$\varepsilon_0 + H_{corr}$ = −859.977873
$\varepsilon_0 + G_{corr}$ = −860.052669

Frequency: -315.15
Coordinates:

H	-4.8140180000	-0.3759730000	-3.4190890000
H	3.9264590000	-1.0987000000	-3.2599030000
C	-4.3058510000	-0.2971680000	-2.4643320000
H	-4.4417710000	1.8511400000	-2.3840390000
H	-4.0068290000	-2.4187170000	-2.2619890000
H	0.3257920000	3.1245950000	-2.2352310000
C	3.7998290000	-0.8500230000	-2.2122210000
H	1.7901770000	-1.6164320000	-2.1264240000
H	5.7658210000	-0.0015340000	-2.0064730000
C	-4.0991570000	0.9534080000	-1.8806990000
C	-3.8512790000	-1.4432490000	-1.8132400000
H	-0.4337520000	0.8553020000	-1.5830110000
C	2.5946330000	-1.1451800000	-1.5741900000
C	4.8317590000	-0.2332830000	-1.5077250000
C	0.4644140000	2.7864370000	-1.2143420000
C	0.0383130000	1.5063110000	-0.8590250000
C	-3.4482570000	1.0516420000	-0.6534720000
C	-3.1962510000	-1.3409570000	-0.5867470000
H	1.3956430000	4.6116010000	-0.5569280000
C	1.0600440000	3.6221500000	-0.2700420000
C	2.4359280000	-0.8226670000	-0.2291930000
H	-3.2767050000	2.0293960000	-0.2152620000
C	4.6625830000	0.0865270000	-0.1614150000
H	-2.8288310000	-2.2200970000	-0.0717810000
C	-2.9979610000	-0.0954700000	0.0127890000
H	5.4632070000	0.5666340000	0.3899720000
C	0.2119580000	1.1038480000	0.4573850000
C	3.4620890000	-0.2085520000	0.4834080000
I	0.5382090000	-1.2870820000	0.7581110000
C	1.2281700000	3.1824090000	1.0420970000
H	-1.3722040000	0.7327250000	1.0486820000
C	-2.2359390000	0.0096670000	1.3299020000
C	0.8092350000	1.9052040000	1.4202710000
H	3.3306400000	0.0468980000	1.5277530000
O	-1.6491500000	-1.1273240000	1.7447210000
H	1.6884640000	3.8284060000	1.7815080000
H	-3.3800620000	1.7091610000	2.1247400000
H	0.9333540000	1.5576890000	2.4378620000
C	-3.0002530000	0.7372320000	2.4481070000
H	-3.8458920000	0.1213160000	2.7657290000
H	-2.3354090000	0.8807780000	3.3023720000

TS9-1d (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −859.530377
$\varepsilon_0 + E_{tot}$ = −859.510218
$\varepsilon_0 + H_{corr}$ = −859.509274
$\varepsilon_0 + G_{corr}$ = −859.582461

Frequency: -456.93
Coordinates:

H	-4.6676800000	-0.4499670000	-2.8344200000
H	4.0724710000	2.0606670000	-2.2154380000
H	1.9347720000	0.8339770000	-2.0330410000
H	-5.5628090000	1.7151690000	-2.0299360000
C	-4.3626860000	-0.0630080000	-1.8686720000
C	3.9649730000	1.2737860000	-1.4783250000
H	-3.0520020000	-1.7265800000	-1.4228400000
C	-4.8678750000	1.1524430000	-1.4177400000
C	2.7626920000	0.5808290000	-1.3806730000
H	-1.0227150000	1.1072920000	-1.2139420000
C	-3.4655250000	-0.7836770000	-1.0848000000
H	-0.5964310000	3.5358990000	-1.0111520000
H	5.9595920000	1.4996280000	-0.7116950000
C	5.0250790000	0.9570750000	-0.6343220000
C	2.6306300000	-0.4273530000	-0.4329210000
C	-0.4430210000	1.4950860000	-0.3840150000
C	-0.2042210000	2.8617220000	-0.2585760000
I	0.7644070000	-1.4929390000	-0.2307540000
C	-4.4721230000	1.6452010000	-0.1766880000
C	-3.0756080000	-0.3032150000	0.1633710000
H	-4.8525580000	2.5968600000	0.1763680000
C	4.8862320000	-0.0557080000	0.3078760000
O	-1.4428330000	-2.0591130000	0.3504350000
C	3.6842680000	-0.7512140000	0.4131290000
C	0.0630020000	0.6444540000	0.5902540000
C	-3.5813650000	0.9217260000	0.6064960000
C	0.5294660000	3.3562670000	0.8139670000
H	0.7173220000	4.4191780000	0.8999030000
H	5.7096050000	-0.3042080000	0.9669310000
C	-2.0450460000	-1.0570630000	0.9823250000
H	-1.2192320000	-0.2205150000	1.1236100000
H	3.5730080000	-1.5341020000	1.1548490000
H	-3.2549510000	1.3237550000	1.5610510000
C	0.8037270000	1.1107640000	1.6686850000
C	1.0257070000	2.4802970000	1.7757620000
H	-3.2749740000	-2.1377170000	2.3772470000
H	1.2014980000	0.4272750000	2.4091760000
C	-2.4818900000	-1.3869390000	2.4128880000
H	1.5940430000	2.8580030000	2.6177040000
H	-2.8545450000	-0.5101930000	2.9453960000
H	-1.6338380000	-1.8045970000	2.9586110000

TS9-1e (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.820908
$\varepsilon_0 + E_{tot}$ = −1095.790889
$\varepsilon_0 + H_{corr}$ = −1095.789945
$\varepsilon_0 + G_{corr}$ = −1095.882647

Frequency: -317.18
Coordinates:

H	-2.6373600000	1.6114630000	-2.9747380000
H	-1.5866440000	0.1939910000	-2.8795810000

H	0.8985670000	0.6316480000	-2.8043470000
H	2.4610900000	1.3533340000	-2.3955080000
C	-2.0583360000	0.9858990000	-2.2939440000
C	1.6492790000	0.7328950000	-2.0132540000
H	-1.2622350000	1.5992110000	-1.8682900000
H	2.0404580000	-0.2592100000	-1.7984660000
H	6.3739450000	-1.0992420000	-1.6861120000
H	-4.5272820000	1.7822810000	-1.6822390000
H	1.5528260000	3.3530280000	-1.3995850000
C	-2.9421880000	0.4215060000	-1.2104940000
H	4.2047780000	-2.1836650000	-1.1077760000
C	-4.2195450000	0.9661790000	-1.0356640000
C	5.7172890000	-0.6463300000	-0.9507050000
C	1.0303560000	1.3704720000	-0.7958860000
H	-6.8092480000	1.6110980000	-0.7896800000
C	1.0549990000	2.7620140000	-0.6364350000
C	4.5112330000	-1.2635120000	-0.6249690000
H	7.0165500000	1.0365240000	-0.5964230000
I	-0.5640920000	-1.5549300000	-0.5394350000
C	-2.5565820000	-0.6306440000	-0.3687140000
C	6.0806260000	0.5533370000	-0.3381150000
O	1.8155860000	-2.1424030000	-0.2972610000
C	-5.1044030000	0.4925390000	-0.0701260000
H	1.3668870000	5.3334750000	0.0903170000
H	-0.3967450000	5.3391450000	0.1037160000
C	-6.4594490000	1.1268710000	0.1245420000
C	0.3929080000	0.6563990000	0.2137420000
C	3.6578960000	-0.6953160000	0.3232570000
H	-7.2052750000	0.3884570000	0.4279020000
C	0.4750310000	3.3992080000	0.4610820000
C	0.4892060000	4.9041310000	0.5785740000
C	-3.4328900000	-1.1636960000	0.5933630000
C	5.2301620000	1.1307340000	0.6048590000
C	2.3350000000	-1.3660620000	0.6703220000
C	-4.6964740000	-0.5801520000	0.7225090000
H	1.6136060000	-0.4612460000	0.7837540000
H	-2.9106510000	-3.2454980000	0.8793820000
H	-6.4187130000	1.8916340000	0.9076660000
C	4.0278910000	0.5077780000	0.9327200000
H	5.4997490000	2.0691330000	1.0776270000
C	-0.1817760000	1.2138310000	1.3484750000
C	-0.1270170000	2.6107650000	1.4423060000
H	-5.3810070000	-0.9832340000	1.4626040000
C	-3.0889160000	-2.3445530000	1.4725630000
H	0.4901800000	5.2224690000	1.6235150000
H	3.3585440000	0.9693810000	1.6522040000
H	3.0601050000	-2.8689740000	2.0473430000
C	2.3584530000	-2.0299480000	2.0619800000
H	-2.1869540000	-2.1673930000	2.0624010000
H	-3.9066450000	-2.5563170000	2.1627470000
H	-1.8523520000	0.2031680000	2.2434890000
H	1.3642040000	-2.4183860000	2.2964400000
H	-0.5512090000	3.0820830000	2.3241050000
C	-0.7982700000	0.3992450000	2.4533790000
H	-0.2911420000	-0.5602990000	2.5648120000
H	2.6663890000	-1.3311260000	2.8447350000
H	-0.7391630000	0.9320240000	3.4039000000

TS9-1e (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.210218
$\varepsilon_0 + E_{tot}$ = −1095.180476
$\varepsilon_0 + H_{corr}$ = −1095.179532
$\varepsilon_0 + G_{corr}$ = −1095.270924

Frequency: -522.21
Coordinates:

H	-2.4756280000	1.7013820000	-2.8915090000
H	1.2289870000	0.8718680000	-2.8431550000
H	-1.1840030000	0.5485950000	-2.5394530000
C	-1.8972960000	1.2397810000	-2.0900830000
H	2.7981660000	1.1206820000	-2.0630390000
C	1.8086990000	0.6756930000	-1.9351610000
H	1.9355830000	-0.3990480000	-1.8207580000
H	6.2932770000	-0.9594260000	-1.6561610000
H	-1.3321700000	2.0276660000	-1.5856750000
H	-4.3591650000	1.9968400000	-1.4996680000
H	1.6384110000	3.2773240000	-1.3454860000
C	-2.8229000000	0.5548550000	-1.1192970000
H	4.1690550000	-2.1464110000	-1.1086290000
C	-4.0955440000	1.1078680000	-0.9342810000
C	5.6151100000	-0.5507410000	-0.9154670000
C	1.1184360000	1.2966960000	-0.7478040000
C	4.4379980000	-1.2240540000	-0.6065340000
C	1.1148580000	2.6851660000	-0.5992820000
H	-6.5561530000	1.9799360000	-0.5828580000
I	-0.5541020000	-1.5469190000	-0.5737310000
H	6.8369960000	1.1773160000	-0.5267910000
H	0.3786420000	5.3039360000	-0.3908040000
C	-2.4933870000	-0.5888330000	-0.3903930000
O	1.7620720000	-2.1722020000	-0.3133890000
C	5.9231300000	0.6496090000	-0.2801130000
C	-5.0238130000	0.5562270000	-0.0642470000
H	-7.1711310000	0.4309060000	0.0117220000
C	-6.3822170000	1.1761830000	0.1328630000
C	0.4396890000	0.5727110000	0.2273520000
C	3.5625030000	-0.7084450000	0.3473890000
C	0.4631490000	3.3229350000	0.4531370000
C	-3.4158860000	-1.1914920000	0.4836330000
C	0.4988240000	4.8241890000	0.5821910000
H	-2.8816480000	-3.2849690000	0.6113090000
C	-4.6671750000	-0.6001920000	0.6289960000
C	2.2649610000	-1.4287930000	0.6647190000
C	5.0515950000	1.1705450000	0.6721590000
H	1.5169390000	-0.5131520000	0.7971860000
C	3.8787290000	0.4915140000	0.9845810000
H	1.4553280000	5.1541700000	0.9965310000
H	-6.4742180000	1.5919330000	1.1394770000
H	5.2815370000	2.1083740000	1.1645830000
H	-0.2929480000	5.1819340000	1.2411550000
C	-3.1107260000	-2.4437090000	1.2689610000
H	-5.3859730000	-1.0574880000	1.3027040000
C	-0.2046110000	1.1394660000	1.3211760000
C	-0.1852870000	2.5341280000	1.4005960000
H	3.1856510000	0.9090390000	1.7108280000
H	-3.9676050000	-2.7186180000	1.8835090000
H	-2.2488060000	-2.3039000000	1.9266430000
H	3.0000190000	-2.9241790000	2.0278730000
C	2.2757290000	-2.1051230000	2.0420380000
H	-1.9059250000	0.1292130000	2.1659710000
H	-0.6749510000	3.0066670000	2.2473800000
H	1.2879770000	-2.5251280000	2.2479490000
C	-0.8559730000	0.3223130000	2.4027700000
H	-0.3491020000	-0.6375970000	2.5225490000
H	2.5494570000	-1.4089370000	2.8383360000
H	-0.8173720000	0.8544050000	3.3537380000

TS10-1d (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −859.995867
$\varepsilon_0 + E_{tot}$ = −859.975215
$\varepsilon_0 + H_{corr}$ = −859.974270
$\varepsilon_0 + G_{corr}$ = −860.050240

Frequency: -287.65
Coordinates:

H	-3.9437820000	1.0396720000	-2.2198970000
H	3.4152590000	-0.3043520000	-1.9583020000
H	-2.9080250000	-1.2515730000	-1.7731070000
H	-3.4440850000	2.6744130000	-1.7486230000
H	1.2198610000	2.4665300000	-1.7084840000
C	-3.7596400000	1.7001320000	-1.3681220000
O	-1.4507220000	1.0333550000	-1.1927110000
H	5.7039810000	-0.7608470000	-1.1357220000
C	3.5629870000	-0.7254800000	-0.9714440000
H	-3.5314620000	-3.4666590000	-0.8518160000
I	0.4597600000	-0.5636420000	-0.8445400000
H	-4.6949970000	1.8193160000	-0.8111180000
C	-3.1331810000	-1.3587360000	-0.7173110000
C	0.9531980000	2.5724290000	-0.6664490000
C	4.8514520000	-0.9831080000	-0.5041750000
H	1.7199670000	4.5612190000	-0.4862910000
C	-2.6456040000	1.1180370000	-0.4809340000
C	-3.4763310000	-2.6031850000	-0.1972110000
C	2.4746820000	-1.0176170000	-0.1531100000
C	0.2868840000	1.5599440000	0.0094400000
C	1.2237400000	3.7480100000	0.0320370000
C	-3.0572480000	-0.2299920000	0.1078510000
H	-2.5116910000	1.8105150000	0.3731590000
C	5.0412840000	-1.5201760000	0.7679830000
C	2.6505820000	-1.5487810000	1.1222780000
H	6.0444560000	-1.7174150000	1.1276770000
C	-3.7489140000	-2.7433090000	1.1655020000
C	-0.0698870000	1.6452190000	1.3477620000
C	0.8620690000	3.8850280000	1.3730800000
C	-3.3342140000	-0.3820610000	1.4678640000
H	-4.0131990000	-3.7129330000	1.5728090000
C	3.9433890000	-1.8020390000	1.5792720000
H	1.7969290000	-1.7636140000	1.7532650000
H	-0.5710630000	0.8277830000	1.8478660000
H	1.0841350000	4.8014330000	1.9063230000
C	-3.6775180000	-1.6279480000	1.9967350000
C	0.2195190000	2.8338130000	2.0222510000
H	-3.2751100000	0.4832770000	2.1212420000
H	4.0888500000	-2.2173820000	2.5699090000
H	-3.8861290000	-1.7263910000	3.0568660000
H	-0.0588910000	2.9221320000	3.0667790000

TS10-1d (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −859.527174
$\varepsilon_0 + E_{tot}$ = −859.506853
$\varepsilon_0 + H_{corr}$ = −859.505909
$\varepsilon_0 + G_{corr}$ = −859.580641

Frequency: -346.17
Coordinates:

H	0.8134660000	1.8217520000	-2.2661450000
H	-4.8855400000	-2.2994870000	-1.8694560000
H	1.5656670000	4.1380510000	-1.8363540000
H	-2.9903210000	-0.6828440000	-1.7673860000
C	0.9070920000	2.1952840000	-1.2556510000
C	1.3167380000	3.4954580000	-0.9996810000
C	-4.7009880000	-1.7336940000	-0.9630190000
C	-3.6417500000	-0.8304490000	-0.9139690000
H	-3.2810510000	2.4781260000	-0.7763380000
O	-1.3214550000	0.6905270000	-0.7029970000
H	3.2585990000	0.8074510000	-0.5226020000
I	0.5632490000	-0.8372290000	-0.4508950000
C	0.5544600000	1.3959700000	-0.1715320000
C	3.5651610000	-0.1657130000	-0.1557480000
C	2.6407090000	-1.1874670000	0.0160190000
H	5.6286370000	0.3845810000	0.0299120000
H	-6.3463860000	-2.6154800000	0.1059140000
C	-5.5229640000	-1.9119640000	0.1440980000
C	4.8998320000	-0.4065470000	0.1591460000
C	-2.7883040000	2.3477570000	0.1900650000
C	-3.3934040000	-0.0944990000	0.2425340000
H	-1.9489500000	3.0455720000	0.2534850000
C	-2.2537860000	0.9140240000	0.2916530000
C	1.4029930000	3.9785340000	0.3071450000
H	1.7276940000	4.9941900000	0.4929500000
C	3.0183430000	-2.4336020000	0.4986940000
C	5.2964200000	-1.6525710000	0.6323820000
H	2.2858040000	-3.2199130000	0.6412270000
C	4.3574020000	-2.6644260000	0.8006160000
H	6.3368570000	-1.8349600000	0.8722890000
H	-3.5032190000	2.5726440000	0.9862460000
C	0.6750460000	1.8229470000	1.1427670000
H	4.6615470000	-3.6352490000	1.1729400000
H	-1.7909770000	0.8043480000	1.2951580000
C	-5.2795280000	-1.1815270000	1.3048930000
C	-4.2215740000	-0.2816110000	1.3505370000
C	1.0850230000	3.1391700000	1.3649270000
H	0.4575780000	1.1654960000	1.9734810000
H	-5.9122330000	-1.3181720000	2.1745750000
H	-4.0285080000	0.2810020000	2.2596970000
H	1.1692220000	3.4913820000	2.3865360000

TS10-1e (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.817006
$\varepsilon_0 + E_{tot}$ = −1095.786613
$\varepsilon_0 + H_{corr}$ = −1095.785668
$\varepsilon_0 + G_{corr}$ = −1095.880884

Frequency: -236.80
Coordinates:

H	-2.7140480000	0.5803090000	-3.2517220000
H	-1.3919720000	-0.4980270000	-2.7939170000
H	2.1034470000	1.5463080000	-2.6236750000
H	0.7519570000	0.4121810000	-2.6179950000
C	-2.1109950000	0.2316290000	-2.4127270000
H	-4.7861730000	0.1239570000	-2.3829860000
H	6.4494220000	-0.8821180000	-2.0255610000
H	-1.5469590000	1.0830680000	-2.0252480000
C	1.4781540000	0.9248850000	-1.9810620000
H	1.1858310000	3.6005880000	-1.9697080000
H	5.8242710000	-3.2828350000	-1.9069440000
H	-7.0095700000	-0.7209600000	-1.7684570000
H	2.1101520000	0.1630280000	-1.5260550000
C	-4.3727580000	-0.3394250000	-1.4927380000
C	5.6275260000	-1.1990560000	-1.3920090000
C	-2.9826810000	-0.3739820000	-1.3430140000

C	5.2765780000	-2.5476580000	-1.3275160000
C	0.7234320000	3.1635610000	-1.0896260000
H	0.8149360000	5.8372870000	-1.0261330000
C	0.7901350000	1.7698850000	-0.9409380000
H	-0.9365340000	5.7659400000	-0.8243920000
C	-6.7326590000	-0.7993750000	-0.7150760000
H	5.1885320000	0.7938310000	-0.7122900000
C	4.9182420000	-0.2565020000	-0.6499550000
C	-5.2361930000	-0.8814380000	-0.5423420000
C	4.2136220000	-2.9413090000	-0.5151130000
H	3.9349520000	-3.9885370000	-0.4577440000
C	0.0184360000	5.4834290000	-0.3678550000
H	-7.2309220000	-1.6755840000	-0.2940280000
H	-7.1315080000	0.0824410000	-0.2024460000
C	-2.4698150000	-0.9783160000	-0.1881780000
C	0.0987930000	3.9902230000	-0.1580890000
C	3.8491600000	-0.6396320000	0.1663270000
I	-0.3003510000	-1.0217770000	0.1782720000
C	0.1890670000	1.2612660000	0.2053220000
C	3.5070280000	-1.9931450000	0.2237860000
H	3.0799980000	1.3325870000	0.4018090000
H	0.0982140000	6.0225270000	0.5794670000
C	-4.6795970000	-1.4811130000	0.5869030000
C	-3.2984230000	-1.5423230000	0.7951750000
H	2.6751700000	-2.2864640000	0.8535240000
C	-0.4655300000	3.3963150000	0.9729580000
C	3.0704030000	0.3891450000	0.9892040000
C	-0.4401460000	2.0146260000	1.1888920000
O	1.7687040000	0.0071010000	1.2418410000
H	-5.3357770000	-1.9186100000	1.3327660000
H	-0.9284560000	4.0211870000	1.7309930000
H	-2.1626230000	-3.0907660000	1.7972460000
C	-2.7754380000	-2.2184160000	2.0408090000
H	4.8385550000	1.0290180000	2.1337250000
H	-1.9124790000	0.8288470000	2.2245910000
C	3.8149390000	0.6813920000	2.3093060000
C	-1.0122050000	1.4121340000	2.4424560000
H	-2.1539670000	-1.5454260000	2.6367600000
H	-3.6016680000	-2.5571850000	2.6668370000
H	3.2686520000	1.4477450000	2.8651360000
H	-0.2757840000	0.7497750000	2.9013060000
H	3.8529640000	-0.2280440000	2.9157260000
H	-1.2841070000	2.1904670000	3.1568350000

TS10-1e (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1095.208872
$\varepsilon_0 + E_{tot}$ = −1095.178728
$\varepsilon_0 + H_{corr}$ = −1095.177784
$\varepsilon_0 + G_{corr}$ = −1095.272367

Frequency: -320.77
Coordinates:

H	2.7754130000	-0.7136820000	-3.2208890000
H	1.5010270000	0.4434960000	-2.8207050000
H	-0.7063880000	-0.2997340000	-2.6333620000
H	-2.0794890000	-1.4114110000	-2.6283220000
C	2.1678180000	-0.3176420000	-2.4080600000
H	4.8434030000	-0.3483310000	-2.3167600000
H	1.5516630000	-1.1307210000	-2.0156950000
C	-1.4456830000	-0.7911810000	-1.9939560000
H	-1.2266720000	-3.4800680000	-1.9134680000
H	-6.3823260000	2.9176740000	-1.7151790000
H	7.0847860000	0.5225190000	-1.6866360000
H	-6.8423210000	0.4836760000	-1.5866660000
H	-2.0637490000	-0.0142970000	-1.5387740000
C	4.4321190000	0.1594410000	-1.4499680000
C	3.0464710000	0.2649880000	-1.3342780000
C	-5.7016450000	2.2622320000	-1.1845110000
C	-5.9592320000	0.8955130000	-1.1111170000
H	-0.7294840000	-5.6601830000	-1.0934010000
C	-0.7607330000	-3.0290540000	-1.0421180000
C	-0.7829350000	-1.6333070000	-0.9392880000
C	6.7874650000	0.5301300000	-0.6370410000
H	-4.3562320000	3.8413260000	-0.6284520000
C	-4.5623400000	2.7779230000	-0.5755080000
C	5.2968140000	0.6890400000	-0.4968330000
C	-5.0806450000	0.0572900000	-0.4343080000
H	-5.2787500000	-1.0100720000	-0.3869290000
H	0.8510850000	-5.7218400000	-0.3069310000
C	-0.1697880000	-5.3430700000	-0.2127480000
C	2.5408320000	0.9256860000	-0.2110680000
H	7.1131310000	-0.4142780000	-0.1924520000
H	7.3190730000	1.3372810000	-0.1317540000
C	-0.1807540000	-3.8418730000	-0.0756070000
I	0.4121100000	1.0936480000	0.0860110000
C	-3.6854890000	1.9336670000	0.1011260000
C	-3.9347350000	0.5649160000	0.1804970000
C	-0.1862060000	-1.0992010000	0.1959180000
H	-2.9366810000	-1.3004730000	0.3549950000
H	-2.7904750000	2.3198740000	0.5763590000
C	4.7483270000	1.3508790000	0.5971820000
H	-0.6176210000	-5.8190510000	0.6626240000
C	3.3703910000	1.4836080000	0.7694570000
C	-2.9774580000	-0.3531920000	0.9375770000
C	0.3860620000	-3.2283270000	1.0414670000
O	-1.7206530000	0.1763380000	1.0703390000
C	0.4104630000	-1.8445870000	1.2067690000
H	5.4088330000	1.7821510000	1.3428480000
H	2.2997020000	3.1274690000	1.6751830000
H	0.8200270000	-3.8425980000	1.8256340000
C	2.8494440000	2.2307650000	1.9713460000
H	1.9396690000	-0.7094170000	2.2105360000
H	-4.5614870000	-1.1576700000	2.2297590000
C	-3.5698960000	-0.7032490000	2.3122880000
C	0.9943380000	-1.2131400000	2.4383050000
H	2.1716040000	1.6156160000	2.5677090000
H	3.6778680000	2.5401110000	2.6075160000
H	-2.8977610000	-1.3997790000	2.8193570000
H	0.2929450000	-0.4786940000	2.8406260000
H	-3.6476690000	0.2076300000	2.9117270000
H	1.1922550000	-1.9701220000	3.1970440000

TS11-1d (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1245.535112
$\varepsilon_0 + E_{tot}$ = −1245.504819
$\varepsilon_0 + H_{corr}$ = −1245.503875
$\varepsilon_0 + G_{corr}$ = −1245.600596

Frequency: -1344.44
Coordinates:

H	-2.1753570000	-1.7297410000	-3.3612830000
H	-3.7715390000	-1.5239350000	-2.6432500000

C	-2.7845310000	-1.9710210000	-2.4852390000
H	-2.9102190000	-3.0664250000	-2.4552920000
H	-4.2070970000	1.6486570000	-2.3305980000
H	-2.1289180000	2.9910210000	-2.2306490000
O	-1.6260900000	1.0394110000	-2.0002670000
H	-1.9923010000	-0.0003970000	-1.5893430000
C	-2.2808980000	2.1795630000	-1.5011620000
H	1.1383090000	-3.3661770000	-1.4032680000
C	-3.7986080000	1.9676800000	-1.3672050000
H	4.1315630000	-0.3912490000	-1.2472990000
C	-2.0992450000	-1.4405430000	-1.2309160000
O	-0.7883020000	-1.8949320000	-1.1378260000
H	-4.2978220000	2.8929060000	-1.0599520000
H	-0.9847540000	4.5349120000	-0.9683670000
I	0.8060690000	-0.2848510000	-0.8881910000
H	6.0592650000	1.0901600000	-0.7760340000
H	-4.8189730000	-1.1572830000	-0.7693030000
C	3.9731350000	0.5547770000	-0.7381250000
H	-4.0215200000	1.1943950000	-0.6289270000
C	1.7084430000	-3.2355490000	-0.4948640000
C	5.0612070000	1.3851000000	-0.4660010000
C	2.6894420000	0.9268950000	-0.3429420000
H	2.2267630000	-5.3093440000	-0.2958710000
C	-1.6720270000	2.6577290000	-0.1833200000
C	-1.0381320000	3.8990720000	-0.0893200000
C	-2.8320730000	-1.4955510000	0.0310240000
C	1.8213810000	-1.9751950000	0.0801860000
C	-4.2317610000	-1.2776270000	0.1341860000
C	2.3092370000	-4.3213710000	0.1441160000
C	4.8670020000	2.5938620000	0.2052740000
C	2.4952290000	2.1356080000	0.3215770000
H	5.7127180000	3.2392190000	0.4185590000
C	3.5827480000	2.9680890000	0.5982360000
H	1.4985550000	2.4361990000	0.6269750000
H	-2.1848670000	0.8721010000	0.9043740000
C	-1.7165300000	1.8464630000	0.9570180000
C	-0.4649580000	4.3279510000	1.1097280000
H	3.4232840000	3.9044210000	1.1243310000
H	0.0274900000	5.2939530000	1.1587070000
H	-1.0811170000	-1.9040560000	1.2123540000
C	-2.1397110000	-1.6827630000	1.2579810000
C	2.4943740000	-1.7793310000	1.2786130000
C	3.0006430000	-4.1426500000	1.3412160000
C	-4.8714700000	-1.1922210000	1.3645520000
H	-5.9430280000	-1.0120330000	1.3936680000
H	2.5643410000	-0.7900290000	1.7129970000
H	3.4627110000	-4.9912780000	1.8337610000
C	3.0897910000	-2.8726640000	1.9089510000
C	-1.1411220000	2.2644230000	2.1525070000
C	-0.5131270000	3.5095100000	2.2366110000
C	-2.7876310000	-1.5965740000	2.4842290000
C	-4.1597410000	-1.3380640000	2.5606180000
H	3.6197890000	-2.7266530000	2.8441080000
H	-1.1813360000	1.6119150000	3.0184510000
H	-0.0612880000	3.8336160000	3.1682240000
H	-2.2154450000	-1.7418100000	3.3973100000
H	-4.6621360000	-1.2654020000	3.5192970000

TS11-1d (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1244.879549
$\varepsilon_0 + E_{tot}$ = −1244.850787
$\varepsilon_0 + H_{corr}$ = −1244.849842
$\varepsilon_0 + G_{corr}$ = −1244.940316

Frequency: -1255.21
Coordinates:

H	4.6163820000	-1.3202900000	-3.5284580000
H	2.1768190000	-1.8047220000	-3.3933970000
H	0.1894300000	3.8731640000	-3.1681500000
H	1.2109890000	1.6102800000	-2.9855960000
H	-3.8832070000	-2.6973640000	-2.6681090000
C	4.1176390000	-1.3841460000	-2.5684480000
C	2.7499180000	-1.6455750000	-2.4840990000
C	0.6005530000	3.5334510000	-2.2239730000
C	1.1741200000	2.2653450000	-2.1217310000
C	-3.2578300000	-2.8509670000	-1.7963540000
H	-3.5421160000	-4.9801380000	-1.7605420000
H	-2.7940400000	-0.7579960000	-1.5877650000
H	5.9015510000	-1.0444800000	-1.4127590000
C	4.8312040000	-1.2256730000	-1.3784630000
C	-3.0638070000	-4.1304330000	-1.2874340000
C	2.1070220000	-1.7199440000	-1.2563570000
H	1.0479570000	-1.9454570000	-1.2039730000
C	-2.6453790000	-1.7554690000	-1.1926710000
H	-3.1681680000	3.9253000000	-1.1807740000
H	0.1097740000	5.3429870000	-1.1723070000
C	0.5576140000	4.3572910000	-1.1047850000
C	1.7023220000	1.8316090000	-0.9126490000
H	2.1382350000	0.8395150000	-0.8393110000
H	-1.3400540000	2.3454430000	-0.6623150000
C	-3.3861260000	3.0110190000	-0.6390250000
H	-5.4905070000	3.4167250000	-0.4628700000
C	-2.3558420000	2.1175810000	-0.3486620000
C	-4.6865130000	2.7250400000	-0.2383290000
C	-2.2461470000	-4.3187850000	-0.1781620000
C	4.1978270000	-1.3012460000	-0.1469620000
C	-1.8453520000	-1.9629620000	-0.0793130000
C	2.8011680000	-1.5174290000	-0.0360350000
C	1.0860780000	3.9138970000	0.1078110000
H	-2.0809880000	-5.3153650000	0.2143740000
C	1.6662950000	2.6521760000	0.2191190000
C	-2.6221360000	0.9390890000	0.3399550000
C	-1.6237100000	-3.2339650000	0.4340300000
C	-4.9549080000	1.5471340000	0.4564860000
H	3.9486840000	1.1398220000	0.6555660000
C	-3.9235220000	0.6583310000	0.7462020000
H	4.7879310000	-1.1693810000	0.7537610000
H	-5.9677820000	1.3235430000	0.7738100000
I	-0.8401110000	-0.3068930000	0.8631510000
H	1.0439290000	4.5559280000	0.9827370000
H	4.2736400000	2.8255460000	1.1093970000
O	0.7621420000	-1.9089420000	1.1139960000
C	2.0692600000	-1.4471060000	1.2228900000
H	-0.9462150000	-3.3610470000	1.2668750000
H	-4.1398960000	-0.2615610000	1.2819980000
C	3.7519780000	1.9106950000	1.4054480000
C	2.2435310000	2.1527480000	1.5407760000
H	1.9498770000	-0.0107150000	1.5922940000
O	1.5733140000	1.0232870000	2.0084800000
H	2.1018040000	2.9639930000	2.2719900000
H	4.1503130000	1.5673360000	2.3640930000
H	2.8513270000	-3.0987020000	2.4231460000
C	2.7526480000	-2.0023180000	2.4626100000
H	3.7498400000	-1.5769990000	2.6114030000
H	2.1592970000	-1.7511100000	3.3468150000

TS11-1e (B3LYP-D3, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1481.353837
$\varepsilon_0 + E_{tot}$ = −1481.314088
$\varepsilon_0 + H_{corr}$ = −1481.313144
$\varepsilon_0 + G_{corr}$ = −1481.427908

Frequency: -1303.60

Coordinates:

H	-2.2714420000	-1.7886310000	-3.5466630000
H	-4.6476530000	0.6669450000	-2.8184420000
H	-2.7112080000	-3.3253310000	-2.7752230000
H	-3.8316340000	-1.9470890000	-2.7442150000
C	-2.7751270000	-2.2279060000	-2.6811050000
H	2.4848130000	-2.1047870000	-2.6765640000
H	3.4792000000	-0.0585280000	-2.4373230000
H	2.4893100000	-3.8498600000	-2.3883000000
H	0.9644830000	-2.9215130000	-2.2996340000
H	-3.1818330000	2.5949640000	-2.2310170000
C	2.0357130000	-2.9053120000	-2.0818000000
O	-2.1548490000	0.8730650000	-1.9033850000
H	5.1086100000	0.3075730000	-1.8592200000
C	-4.5903220000	1.0401670000	-1.7922100000
H	-5.4123580000	1.7431480000	-1.6208370000
H	-2.2951220000	-0.2547600000	-1.5992410000
C	-3.2265010000	1.7180140000	-1.5651620000
C	4.0759240000	0.1418090000	-1.5442210000
O	-0.7366780000	-1.9239950000	-1.4329430000
C	-2.1117820000	-1.7187690000	-1.4069080000
H	-4.7116870000	0.1969330000	-1.1088710000
I	0.5506100000	-0.0767370000	-1.0762510000
H	4.0487080000	-0.7604350000	-0.9299970000
H	-4.7970960000	-2.1338720000	-0.8103970000
C	3.5415730000	1.3395240000	-0.7951120000
H	-3.2321680000	4.3178020000	-0.6859380000
H	5.4944720000	2.2274300000	-0.6637290000
C	2.2383690000	-2.6723370000	-0.6074370000
C	2.1836800000	1.4895740000	-0.4775130000
H	-0.3359770000	2.8735710000	-0.4675380000
C	4.4410520000	2.3466820000	-0.4213030000
H	3.3736000000	-4.4699140000	-0.3610710000
C	-3.1292830000	2.2446530000	-0.1328720000
C	-2.7385810000	-2.0266860000	-0.1290200000
H	5.8869250000	4.5789430000	0.0116390000
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C	1.7136330000	-1.5644520000	0.0711150000
C	-3.1514800000	3.6143890000	0.1382250000
C	2.9562510000	-3.6048530000	0.1464000000
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C	4.0247780000	3.4994700000	0.2421300000
C	0.2689570000	2.9102210000	0.4405550000
C	2.6634480000	3.6440660000	0.5056230000
C	5.0184450000	4.5517210000	0.6750880000
H	4.5674160000	5.5474460000	0.6846730000
H	-2.9856250000	0.2916990000	0.7583960000
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C	-3.0124010000	1.3566350000	0.9434970000
H	2.3117840000	4.5477850000	0.9972700000
C	-1.9496020000	-2.1242080000	1.0504270000
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C	-3.0534720000	4.0931880000	1.4461810000
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C	3.1381720000	-3.4680700000	1.5233080000
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H	0.1396050000	-0.1840570000	2.0069820000
H	5.0117350000	-4.3640070000	2.1147950000
C	2.5637000000	-2.3698180000	2.1555970000
C	1.2076100000	-0.2629240000	2.2228230000
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C	-2.5247240000	-2.2390700000	2.3094200000
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C	-2.9332160000	3.1998790000	2.5080950000
H	-2.8217570000	1.1160720000	3.0628330000
H	-1.8785650000	-2.2993840000	3.1819540000
H	2.6665310000	-2.2605200000	3.2311690000
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H	-4.3614910000	-2.3701440000	3.4533140000
H	-2.8508630000	3.5669600000	3.5258760000

TS711-1e (M062-X, Toluene)

$\varepsilon_0 + \varepsilon_{ZPE}$ = −1480.558598
$\varepsilon_0 + E_{tot}$ = −1480.519480
$\varepsilon_0 + H_{corr}$ = −1480.518536
$\varepsilon_0 + G_{corr}$ = −1480.630285

Frequency: -1204.05

Coordinates:

H	-2.3748180000	-1.6710800000	-3.6078130000
H	-2.8844410000	-3.1828390000	-2.8345370000
H	-3.9162070000	-1.7388580000	-2.7565860000
C	-2.8781870000	-2.0858540000	-2.7305920000
H	-4.6219010000	0.8414590000	-2.7181160000
H	2.3914840000	-2.2465120000	-2.6505450000
H	2.3625740000	-3.9740210000	-2.2719490000
H	0.8511220000	-3.0134350000	-2.2489170000
H	-3.1344710000	2.7281550000	-2.0821790000
H	3.5065220000	-0.4847400000	-2.0775050000
C	1.9212520000	-3.0085960000	-2.0228280000
O	-2.1150910000	0.9876430000	-1.8336570000
C	-4.5324510000	1.1558820000	-1.6749860000
H	5.1279820000	0.0663760000	-1.6435210000
H	-2.2853540000	-0.1498100000	-1.5859060000
O	-0.7824850000	-1.8771190000	-1.5627980000
C	-2.1478970000	-1.6275010000	-1.4788410000
C	-3.1681950000	1.8225580000	-1.4555390000
H	-5.3499670000	1.8418170000	-1.4347470000
C	4.1215690000	-0.1077310000	-1.2592500000
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H	-0.3091400000	2.7534380000	-0.8285530000
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C	2.1120870000	-2.7104810000	-0.5612170000
C	2.1791170000	1.3918520000	-0.5386910000
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H	3.1881600000	-4.5232450000	-0.2075970000	H	-5.7353760000	-2.2163310000	1.4380960000
C	-2.7347670000	-1.9651410000	-0.1963010000	C	2.9596760000	-3.4159380000	1.6150750000
C	1.7179270000	2.6263600000	-0.0525120000	C	-2.8338180000	4.0438600000	1.6515950000
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C	-4.1327220000	-2.0682690000	0.0309420000	H	0.0457960000	-0.0187030000	1.8174110000
C	1.6146920000	-1.5576680000	0.0525030000	H	-2.7950990000	5.1014970000	1.8902310000
C	0.2474900000	2.9328140000	0.0952380000	H	1.6200130000	0.7782710000	1.9070830000
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H	2.2856930000	4.5566520000	0.6846270000	C	-2.7059750000	3.0970080000	2.6612930000
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C	-1.9113600000	-2.1009360000	0.9523890000	H	2.4920180000	-2.1186850000	3.2549980000
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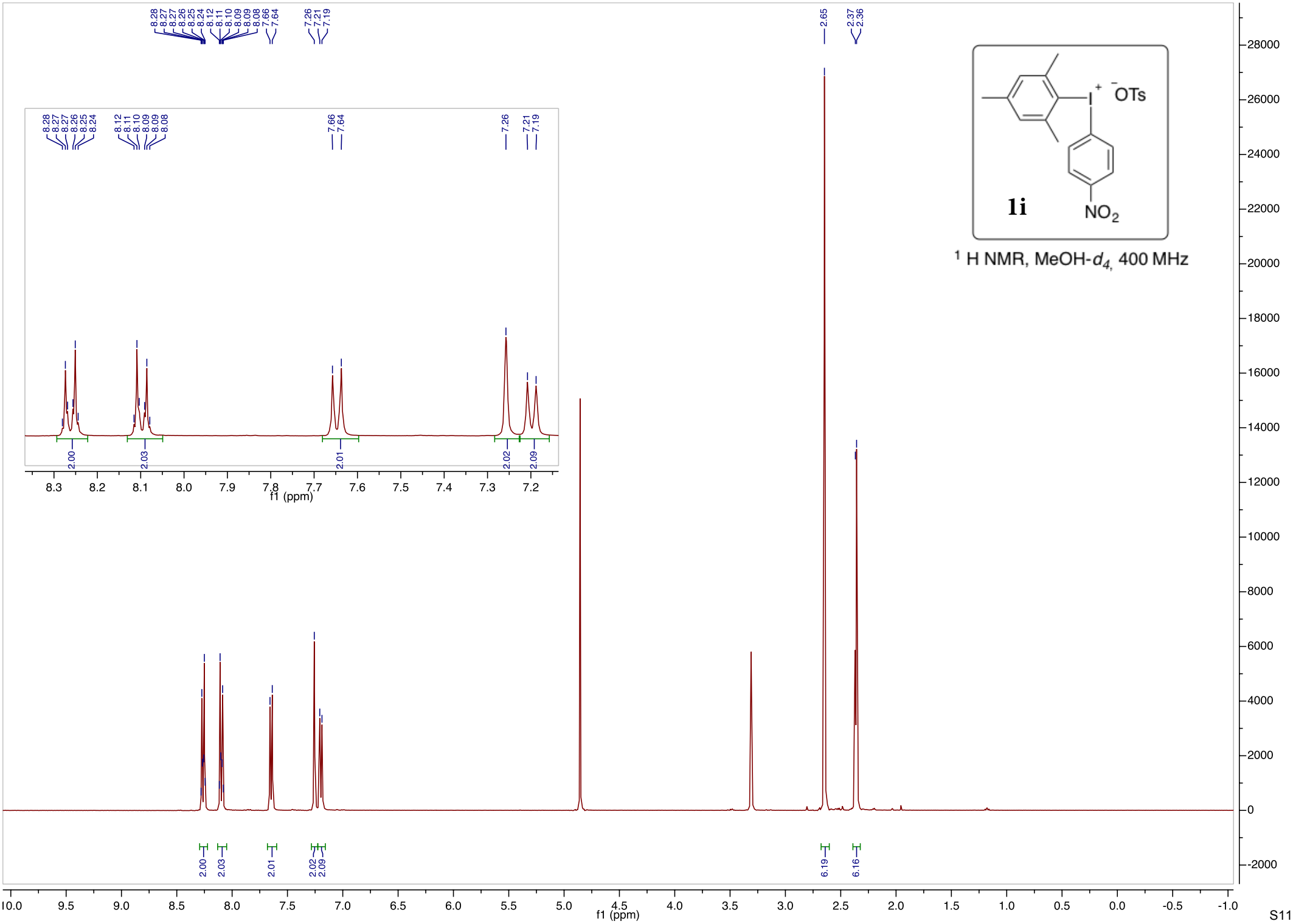
12. Copies of ^{1}H and ^{13}C NMR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7.64
7.26
7.21
7.19
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2.37
2.36
OTs
1i
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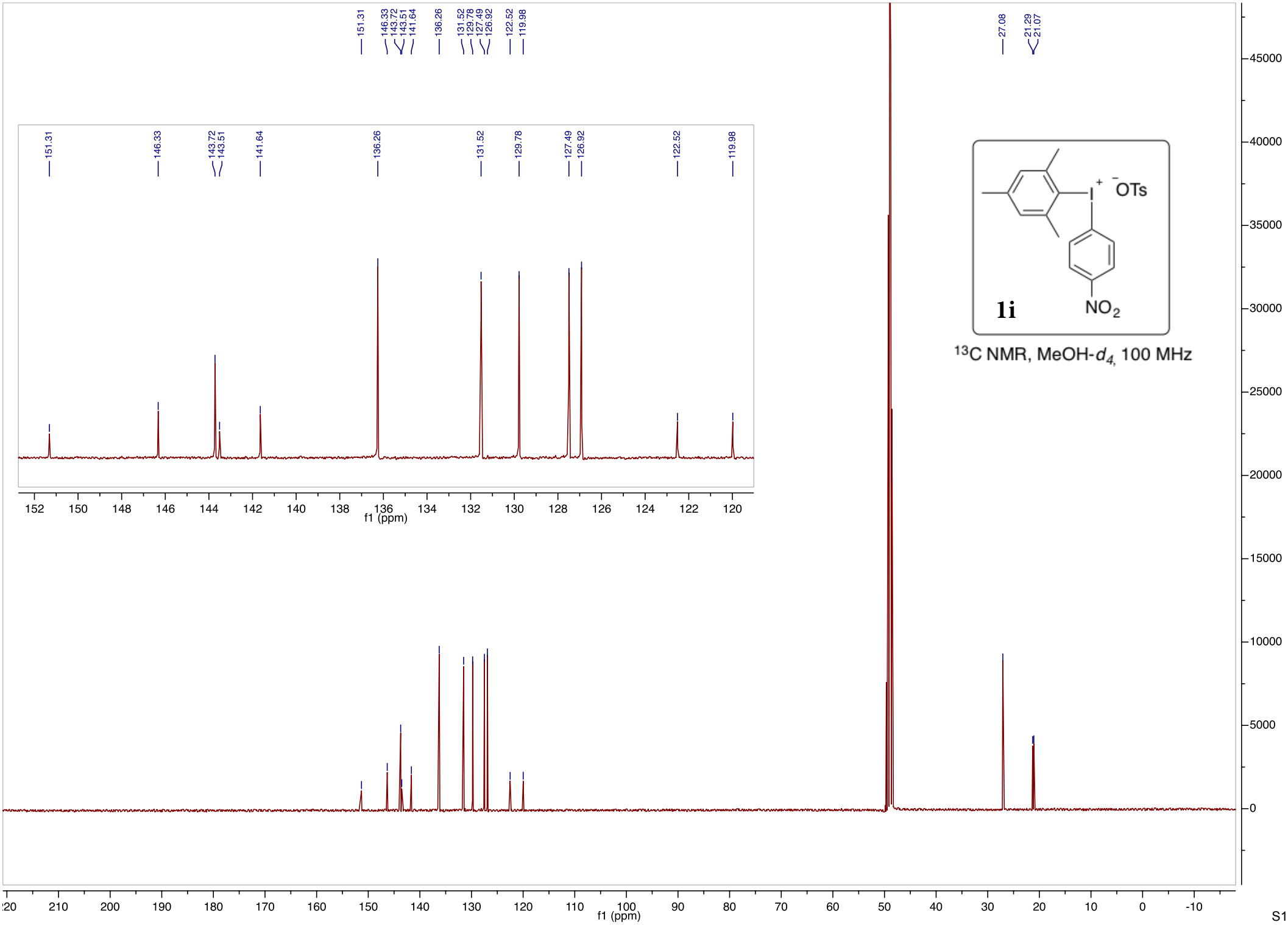
6.16
f1 (ppm)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1i
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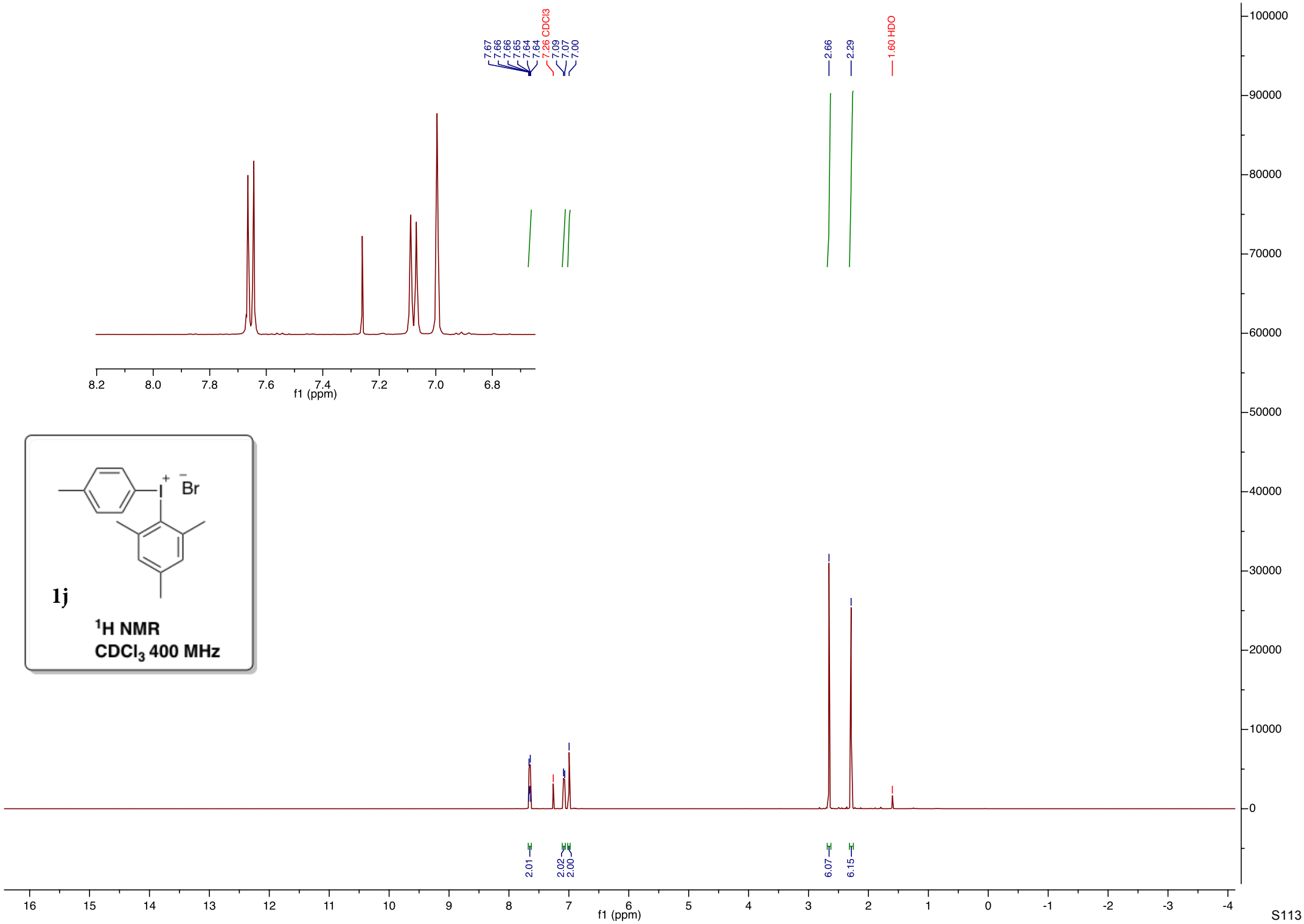
f1 (ppm)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7.00
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2.29
1.60 HDO
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
f1 (ppm)
Br
1j
1H NMR
CDCl3 400 MHz
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2.02
2.00
6.07
6.15
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
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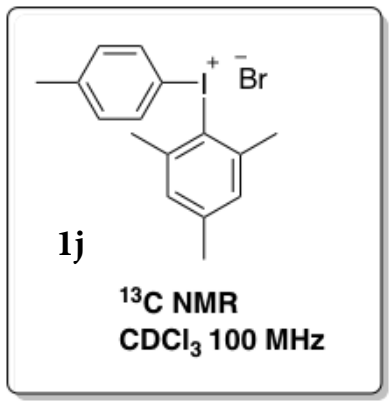

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27.20
21.28
21.20

130000
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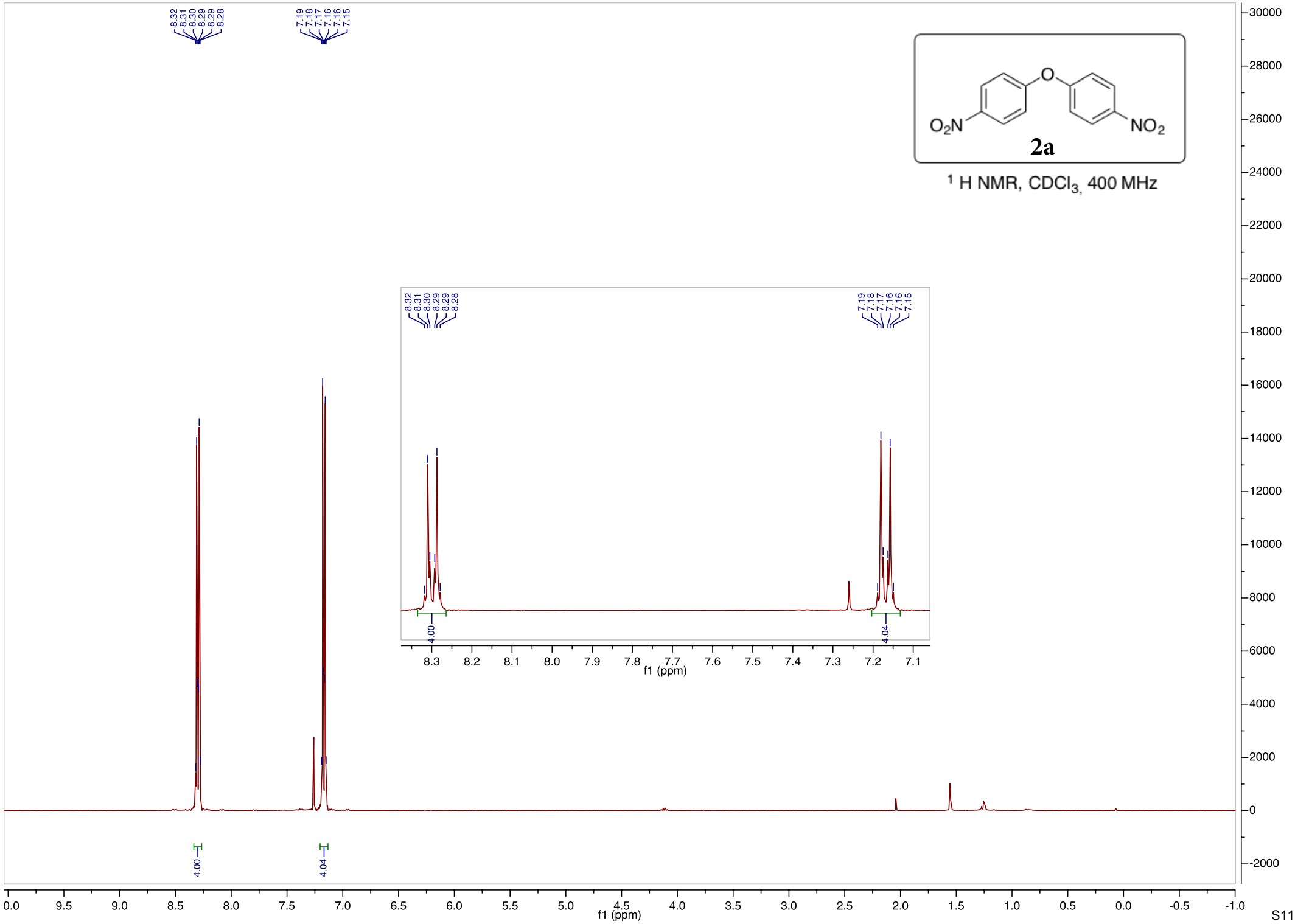
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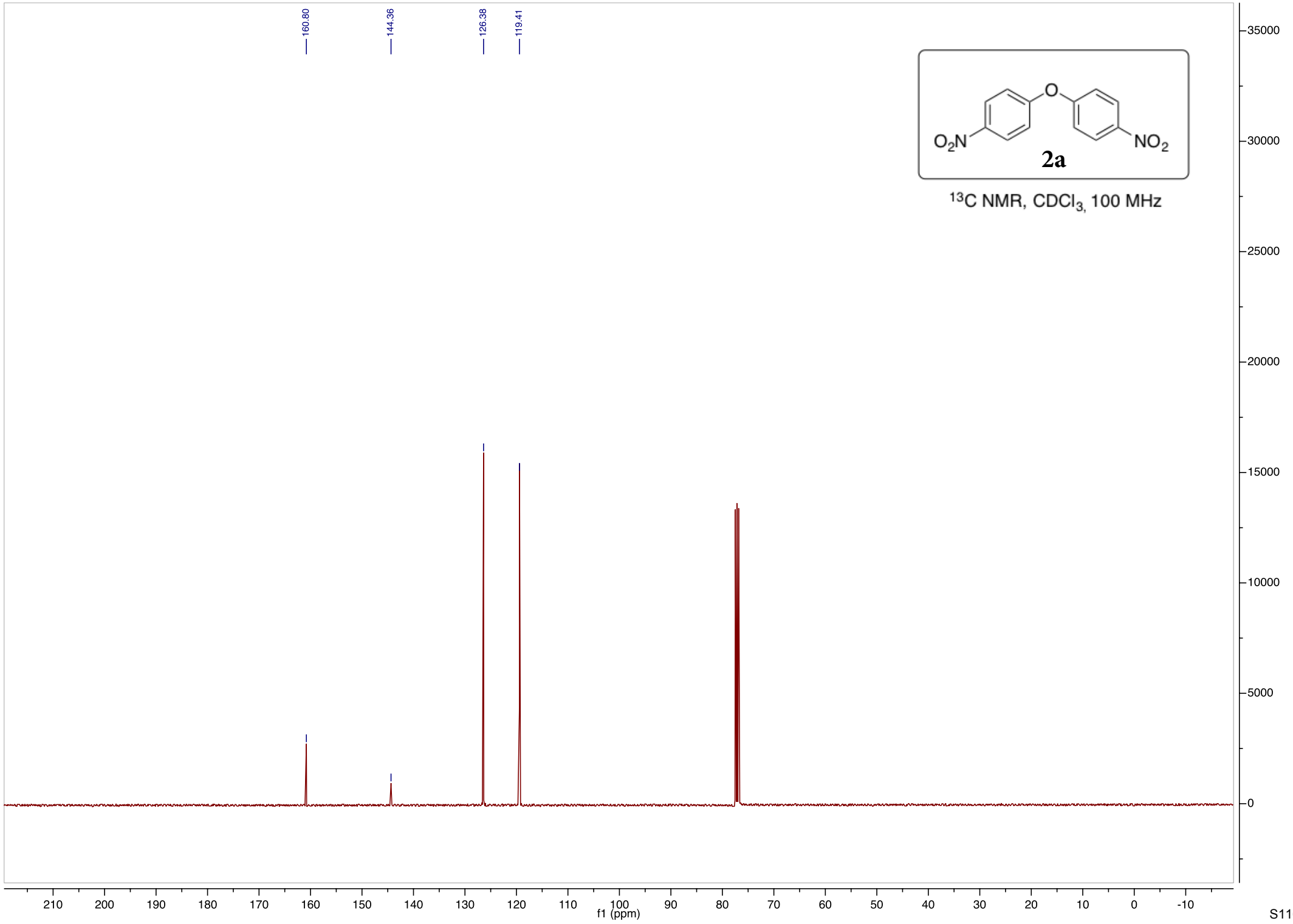
f1 (ppm)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20000
15000
10000
5000
0
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200
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180
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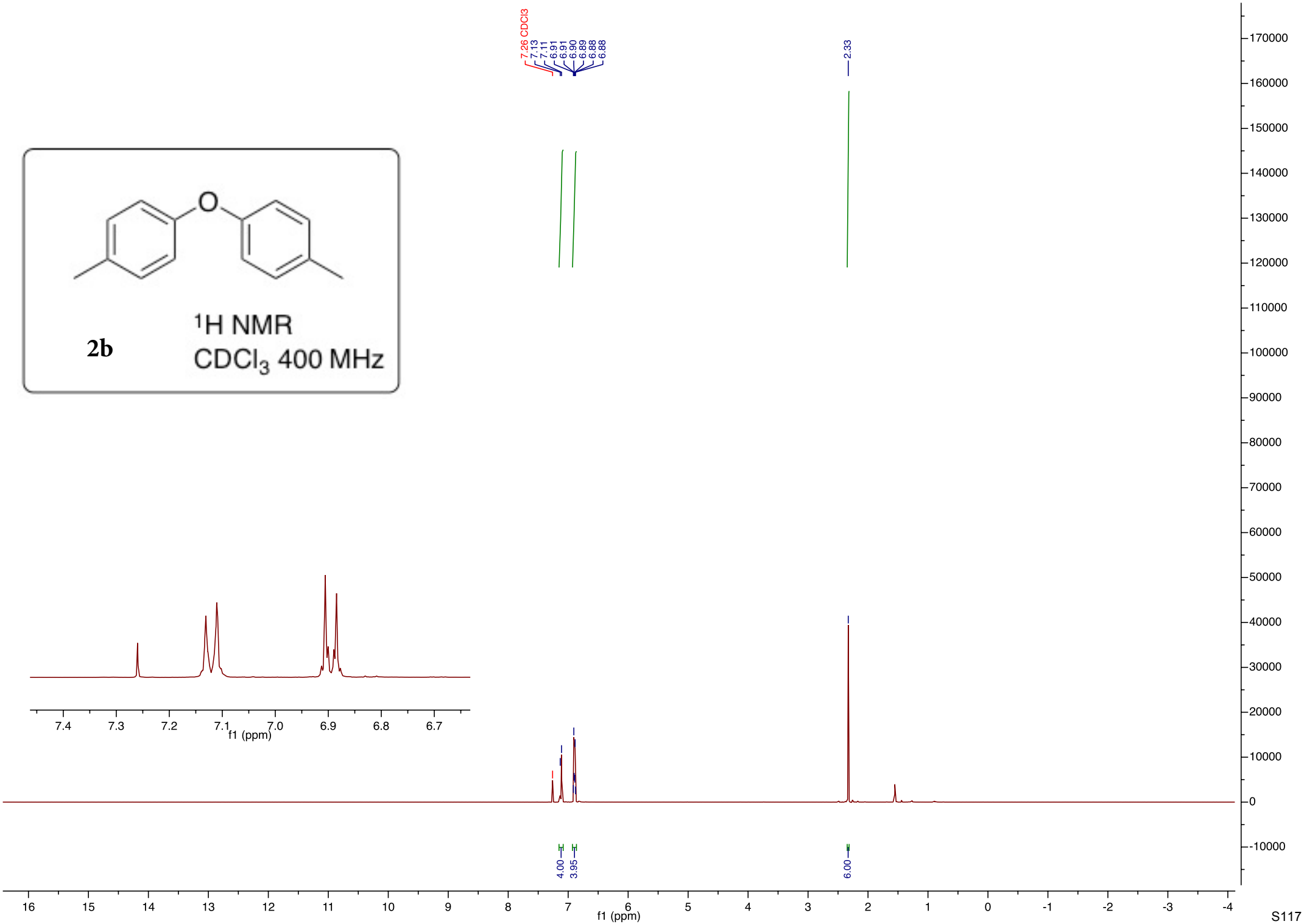
f1 (ppm)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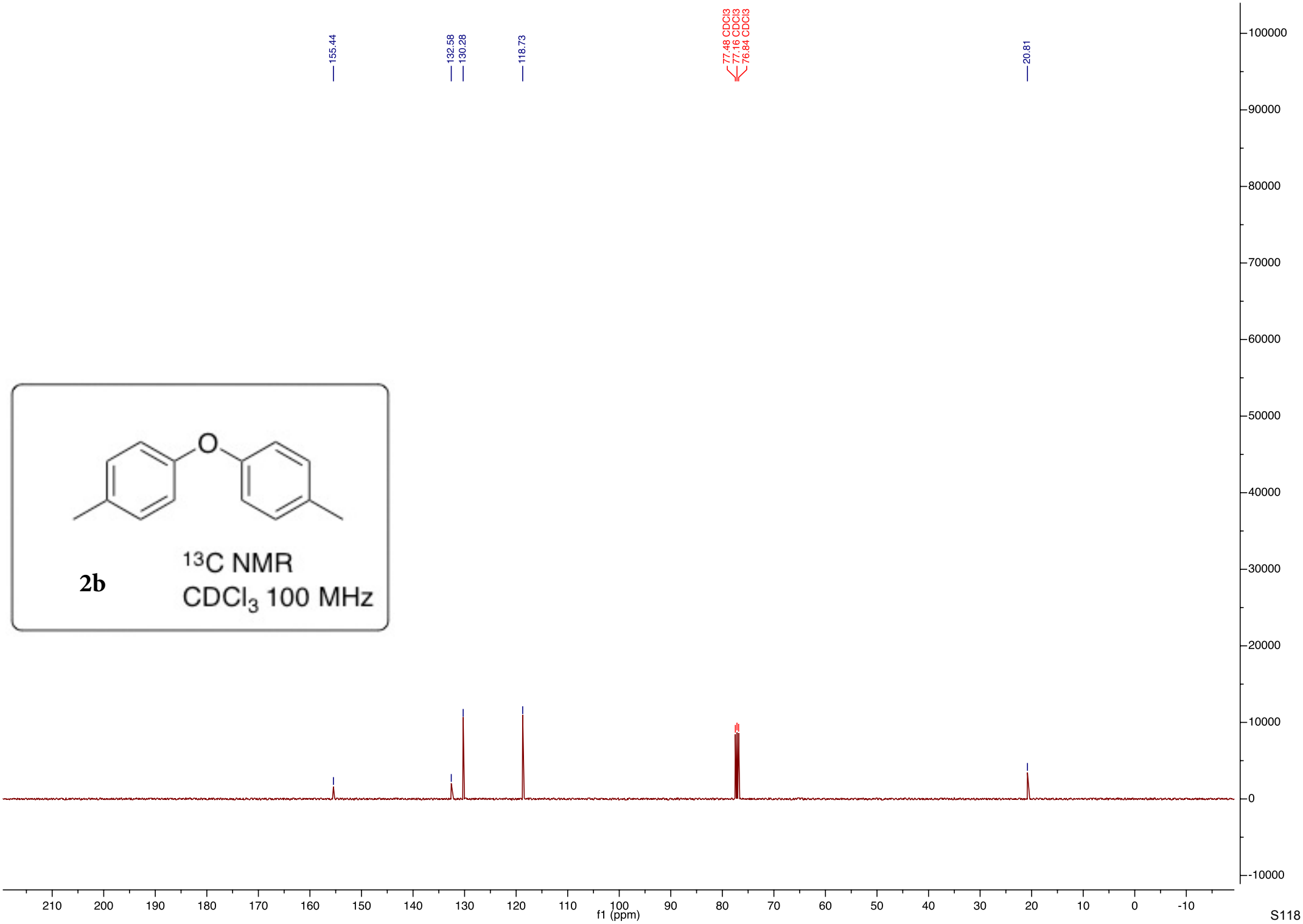
f1 (ppm)
f1 (ppm)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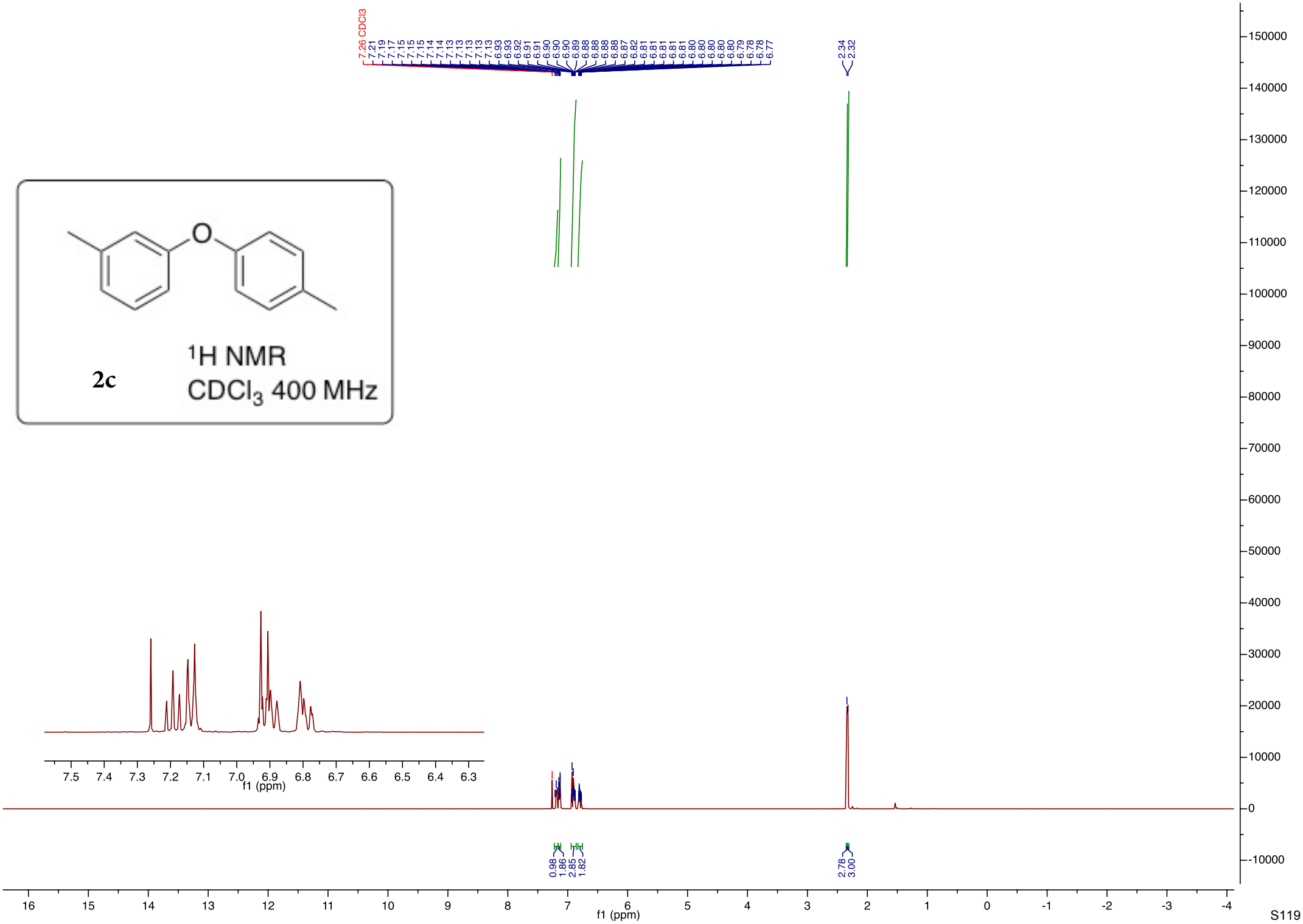
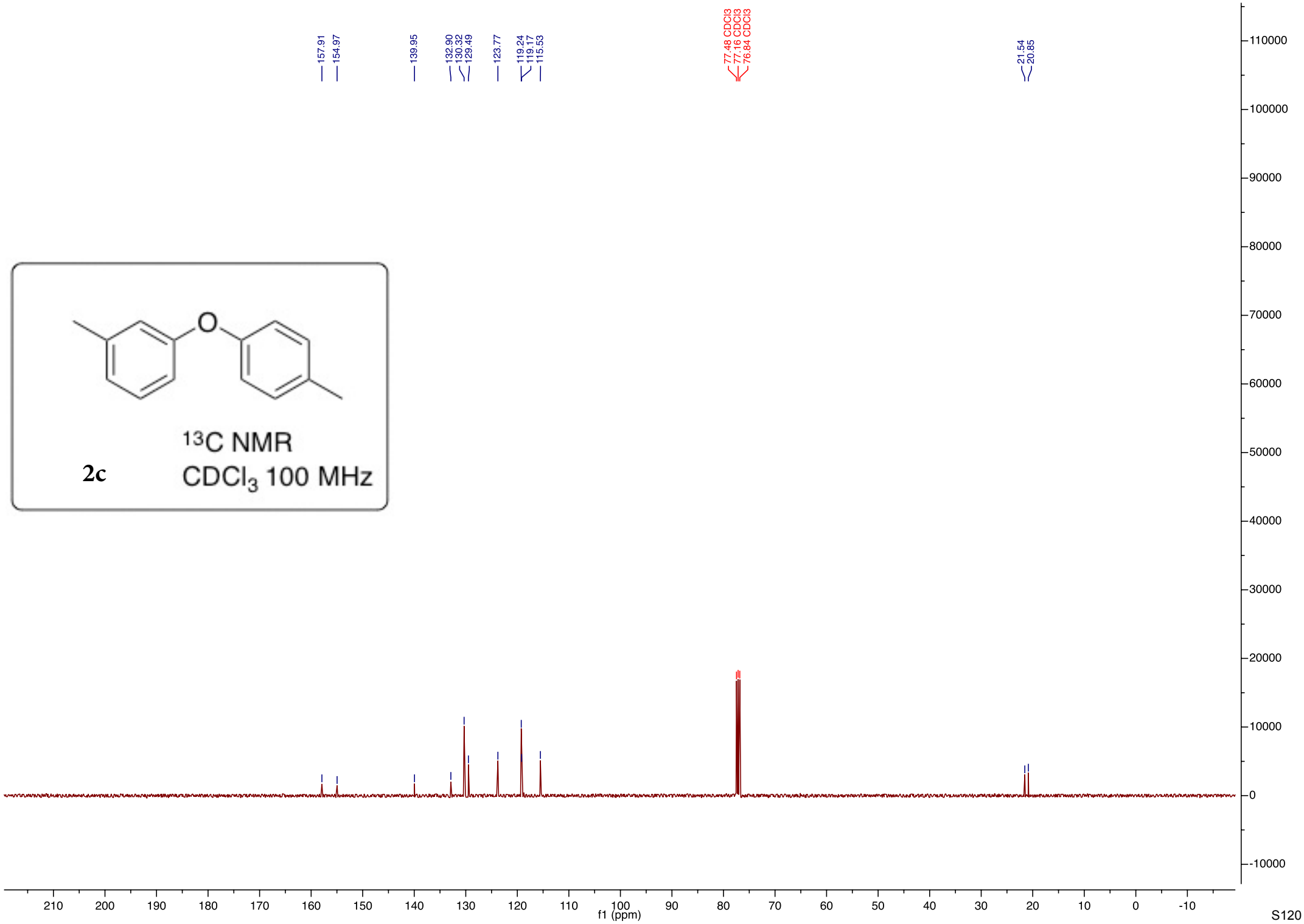
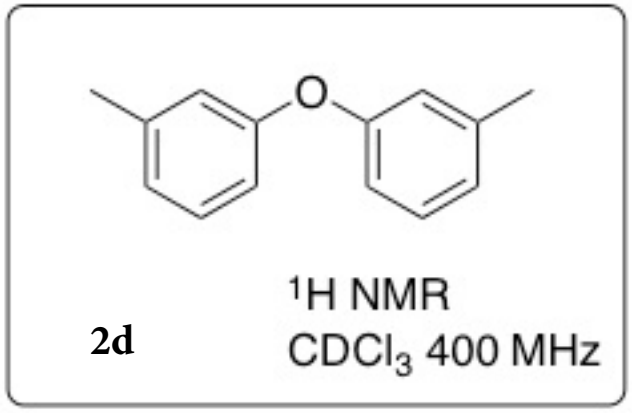
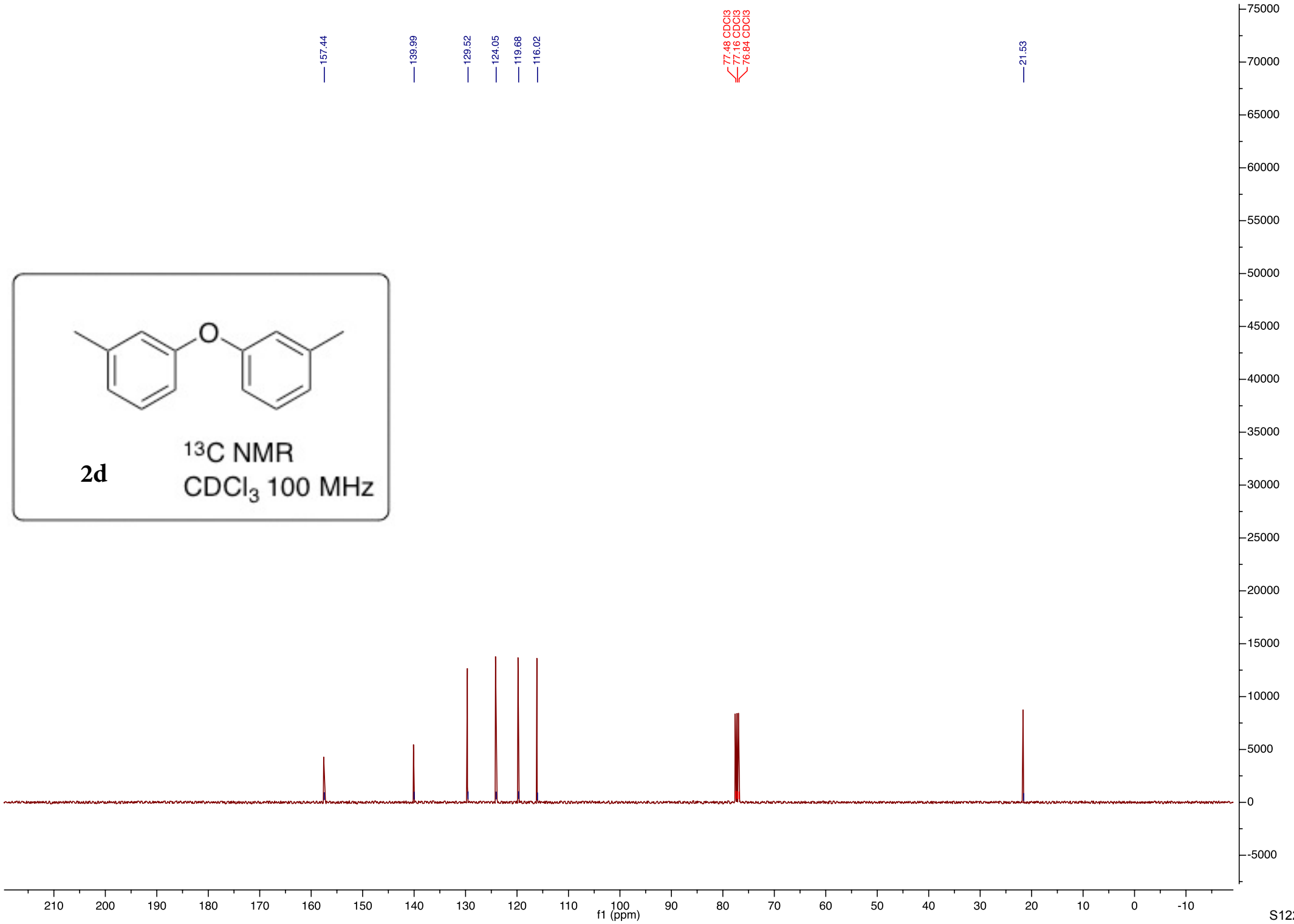
13C NMR
CDCl3 100 MHz
f1 (ppm)

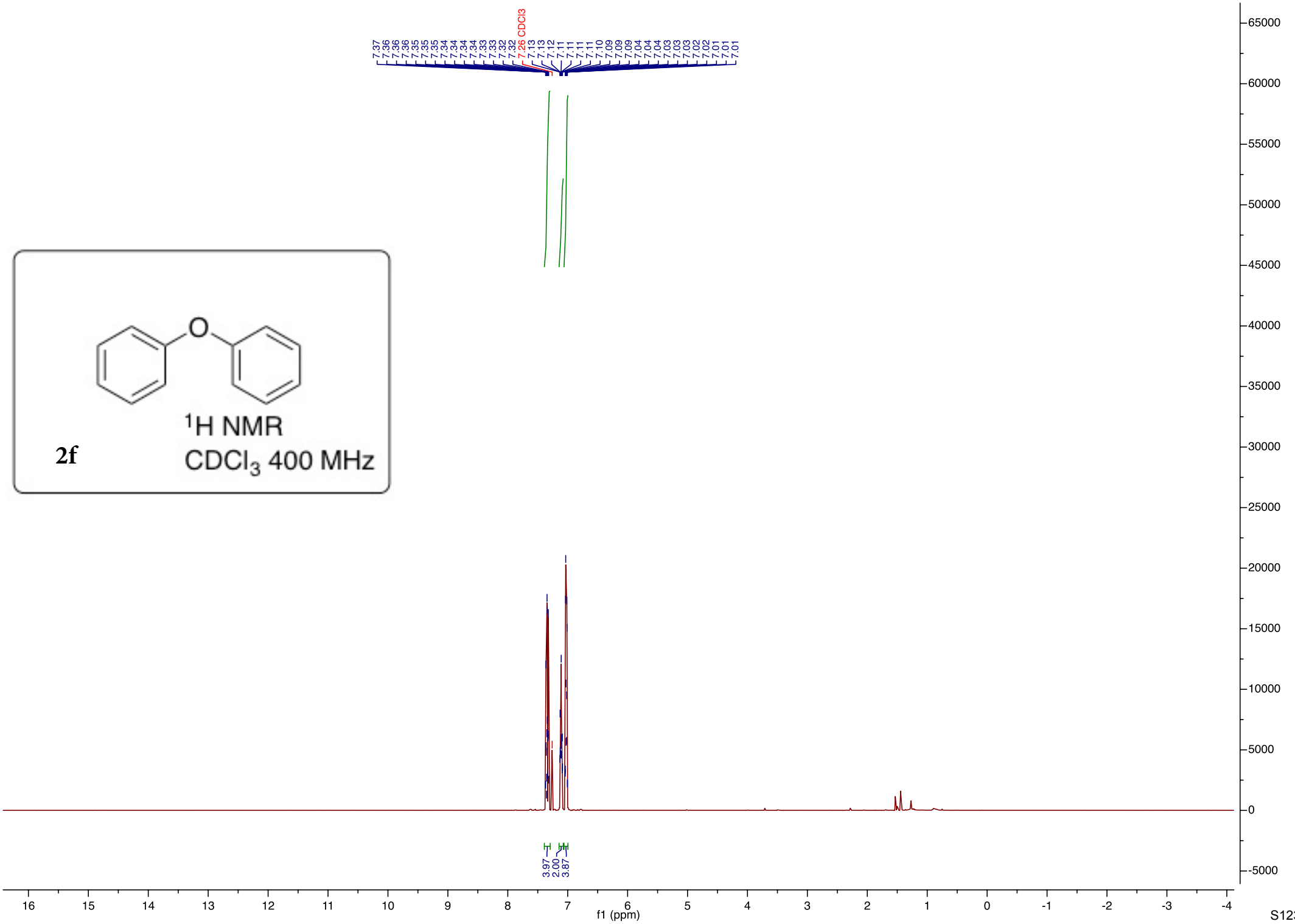

7.26 CDCl3
7.21
7.19
7.17
7.15
7.15
7.15
7.14
7.14
7.13
7.13
7.13
7.13
6.93
6.93
6.92
6.91
6.91
6.90
6.90
6.90
6.89
6.88
6.88
6.88
6.88
6.87
6.82
6.81
6.81
6.81
6.81
6.81
6.80
6.80
6.80
6.80
6.80
6.79
6.78
6.78
6.77
2.34
2.32
O
2c
1H NMR
CDCl3 400 MHz
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3
f1 (ppm)
0.98
1.86
2.85
1.82
2.78
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

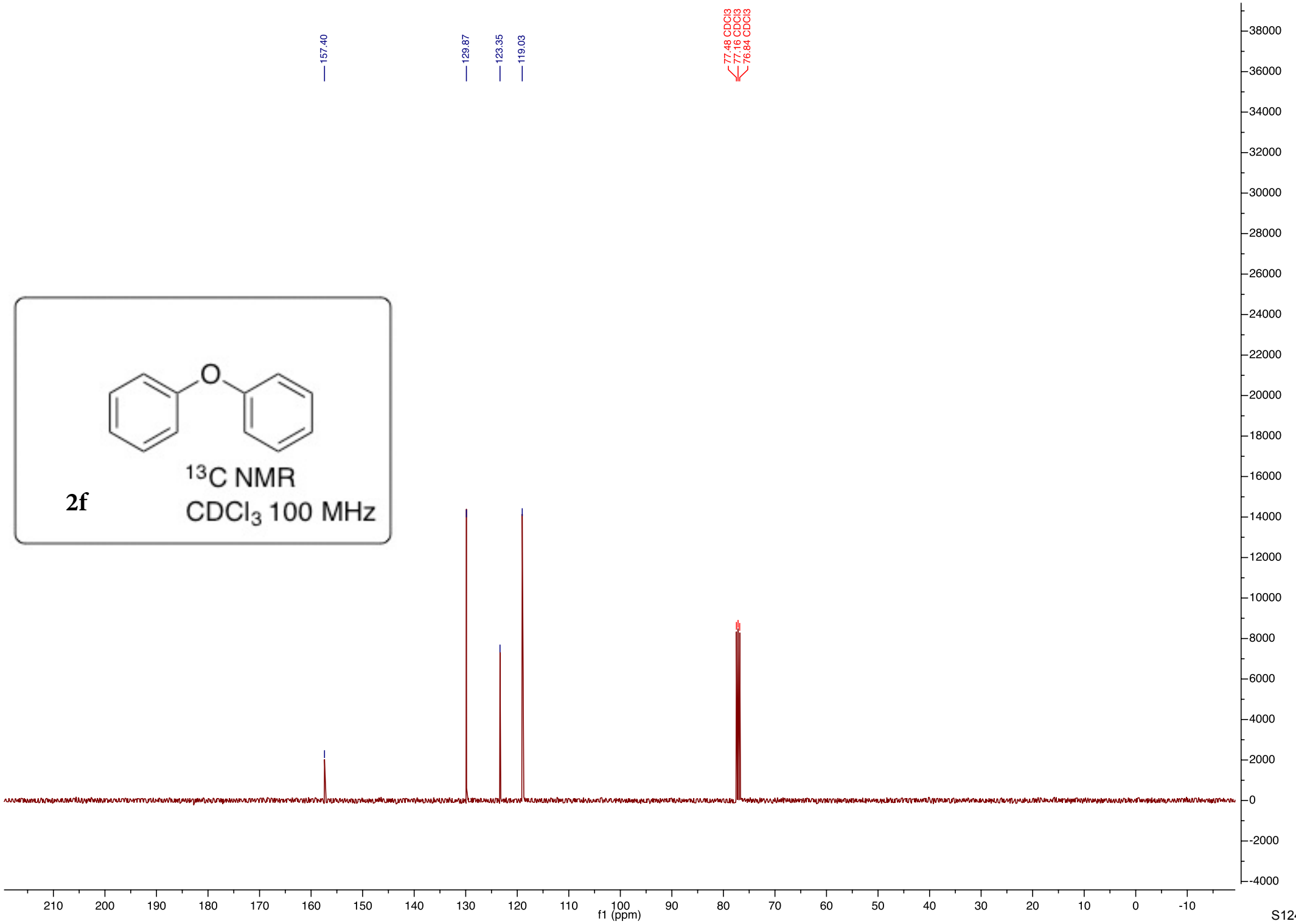

157.91
154.97
139.95
132.90
130.32
129.49
123.77
119.24
119.17
115.53
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
21.54
20.85
O
2c
13C NMR
CDCl3 100 MHz
f1 (ppm)

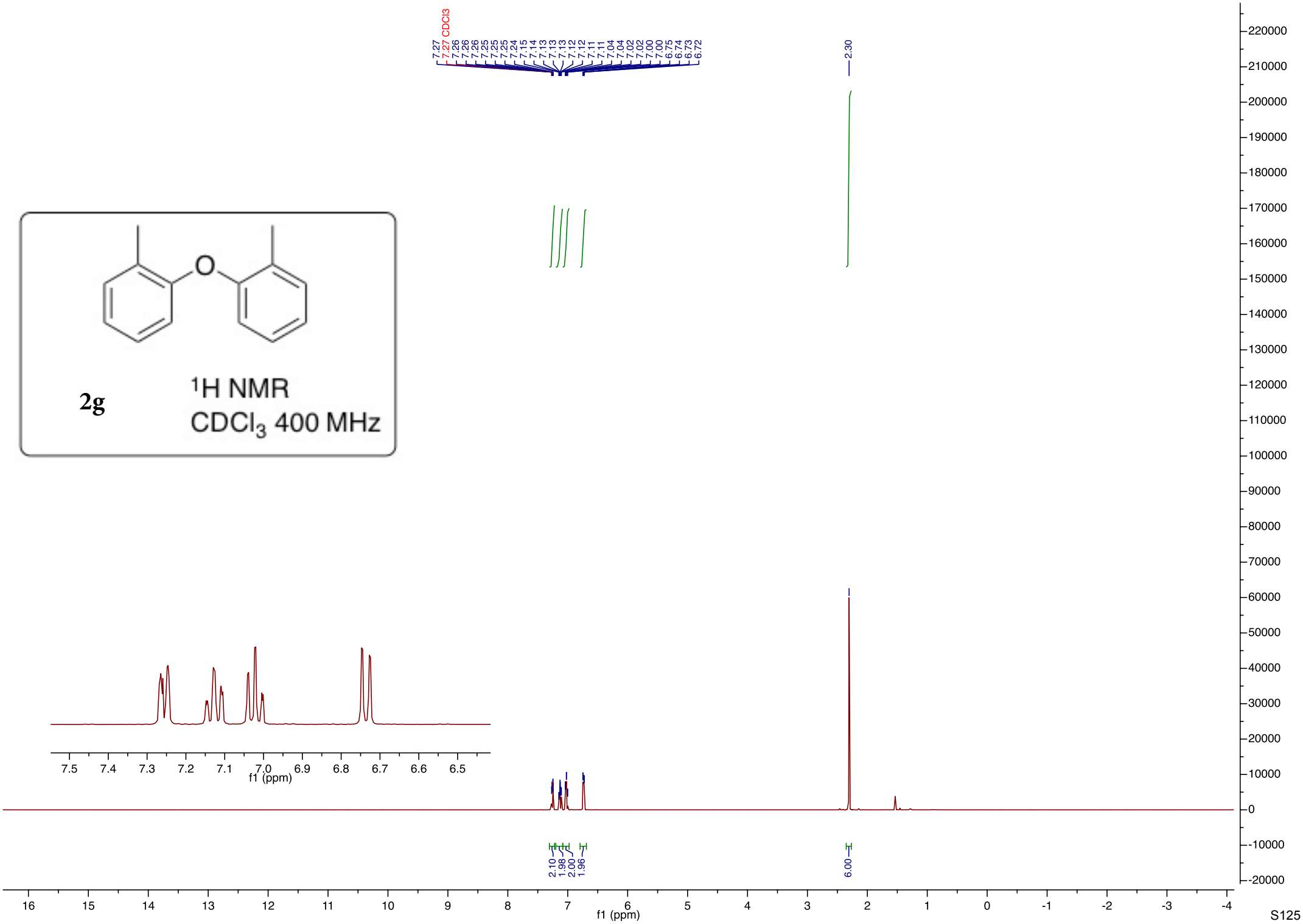

O
2d
^{1}H NMR
$CDCl_3$ 400 MHz

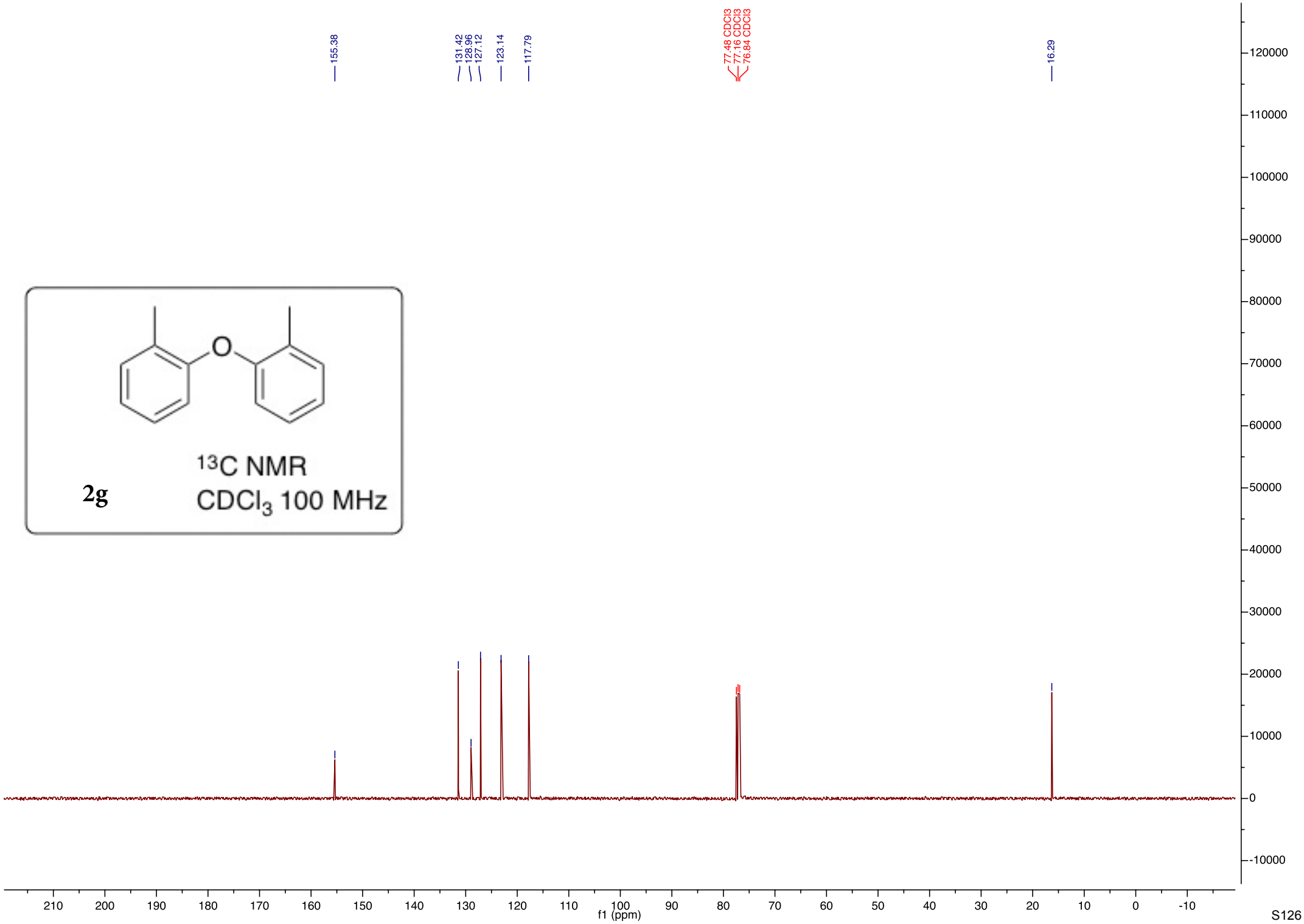
7.28 CDCl3
7.27
7.26
7.25
7.23
6.97
6.96
6.96
6.96
6.96
6.95
6.95
6.94
6.94
6.94
6.88
6.88
6.87
6.87
6.87
6.86
6.86
6.84
6.84
2.37
2.02
1.87
3.88
6.00
f1 (ppm)
7.5
7.0
6.5
6.0

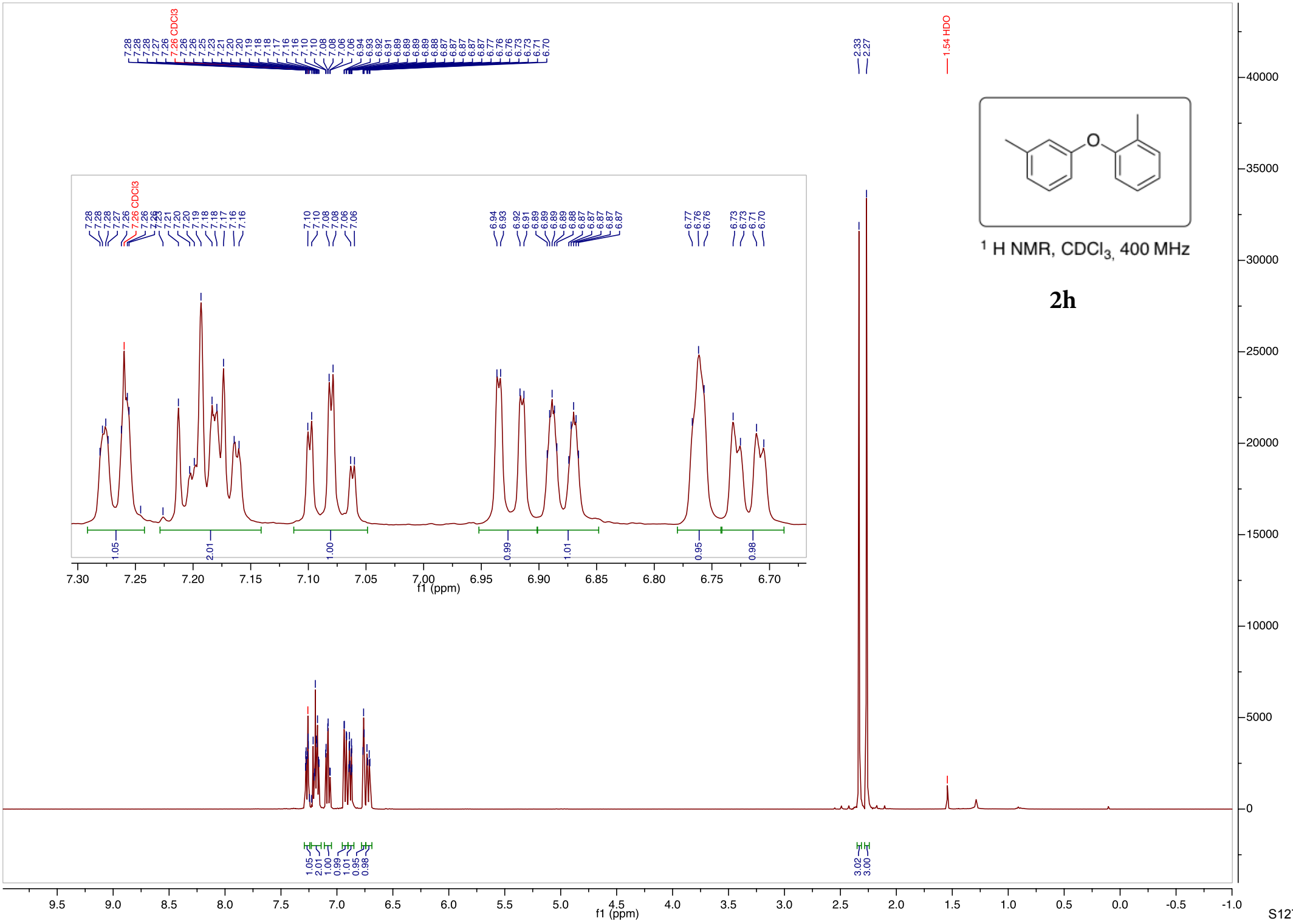

157.44
139.99
129.52
124.05
119.68
116.02
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
21.53
O
2d
13C NMR
CDCl3 100 MHz
f1 (ppm)

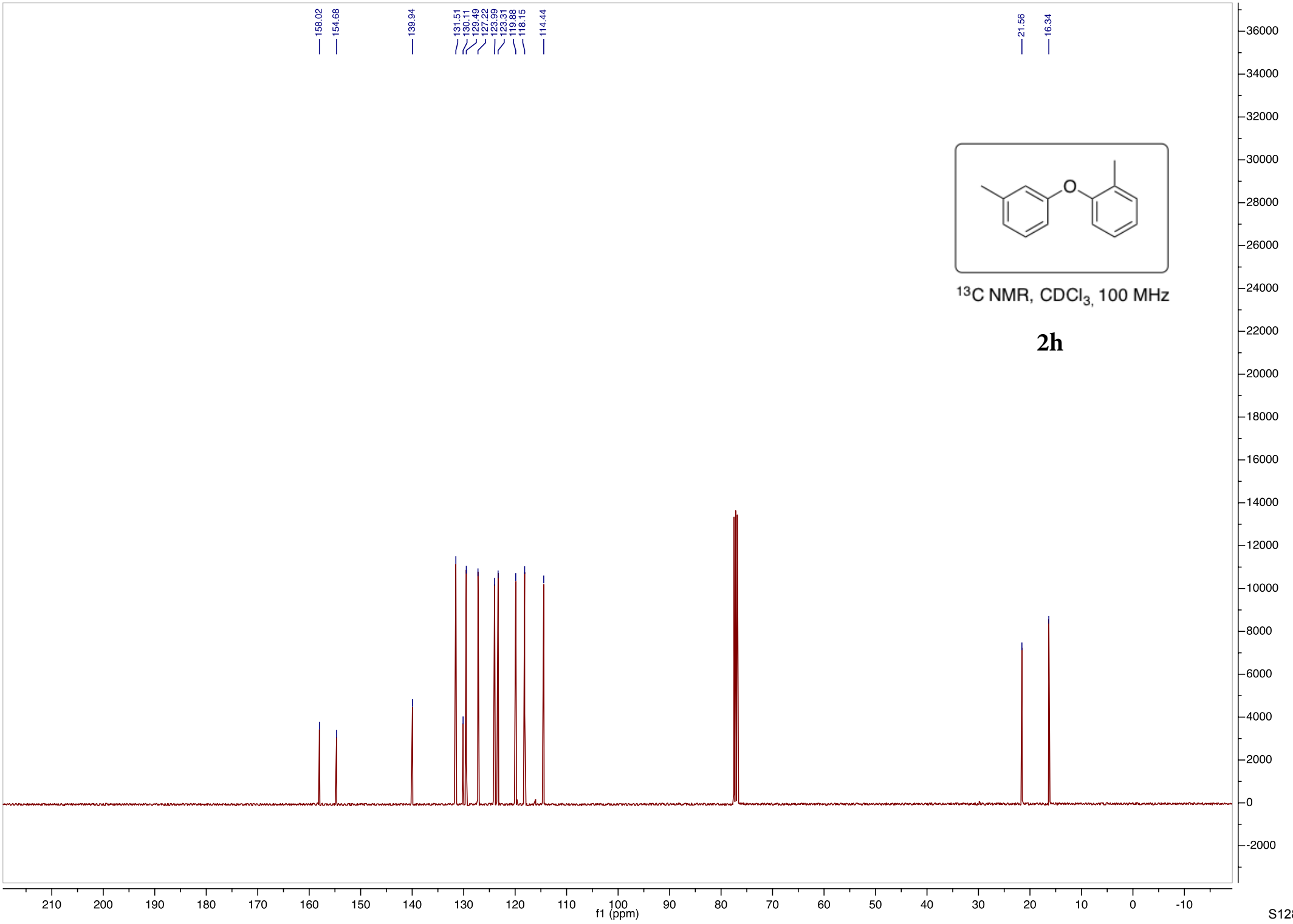

7.37
7.36
7.36
7.36
7.35
7.35
7.35
7.34
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.26 CDCl3
7.13
7.12
7.11
7.11
7.11
7.11
7.10
7.09
7.09
7.09
7.04
7.04
7.04
7.03
7.03
7.03
7.02
7.02
7.01
7.01
7.01
O
1H NMR
2f
CDCl3 400 MHz
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
3.97
2.00
3.87
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

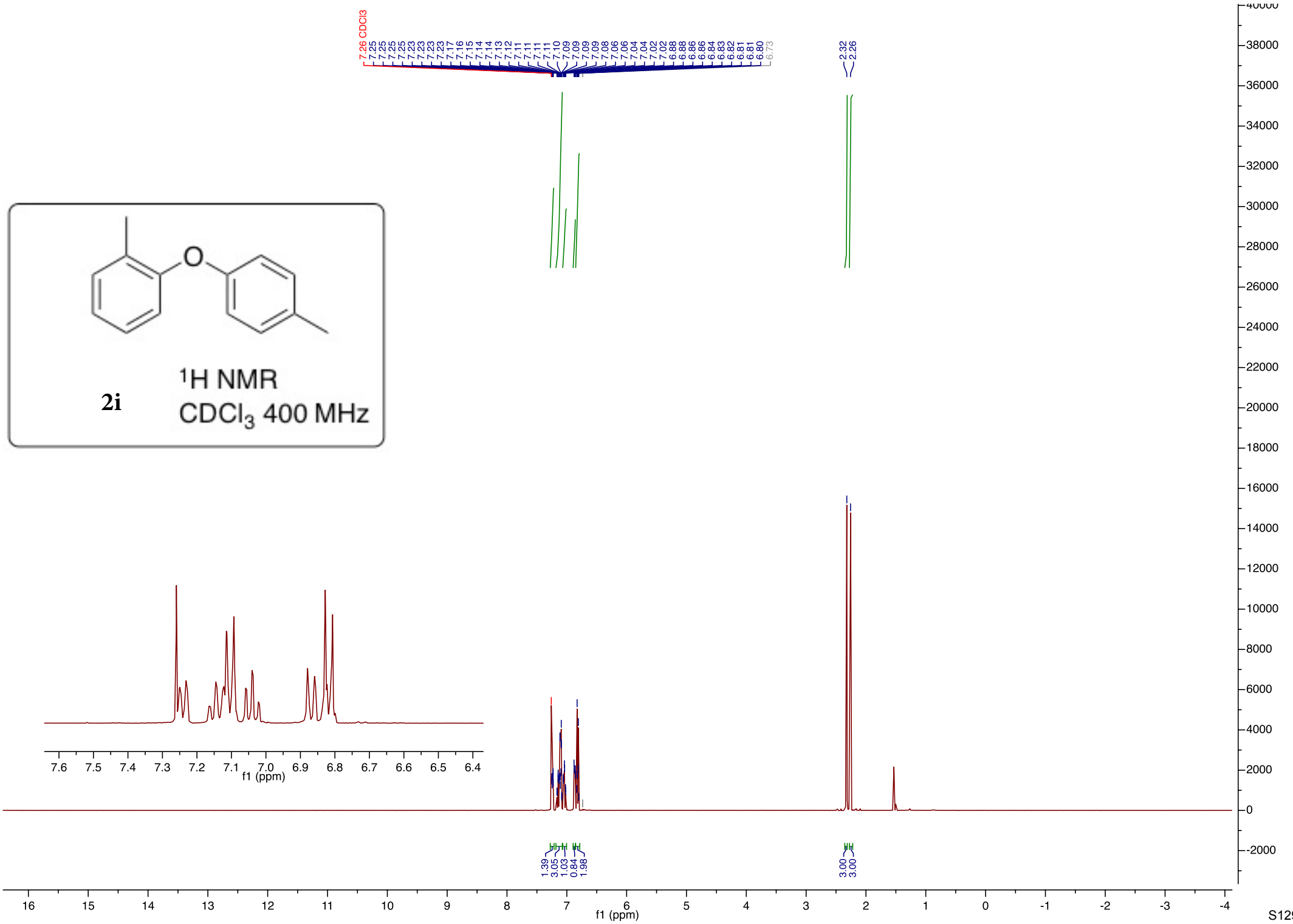

157.40
129.87
123.35
119.03
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
O
2f
13C NMR
CDCl3 100 MHz
f1 (ppm)

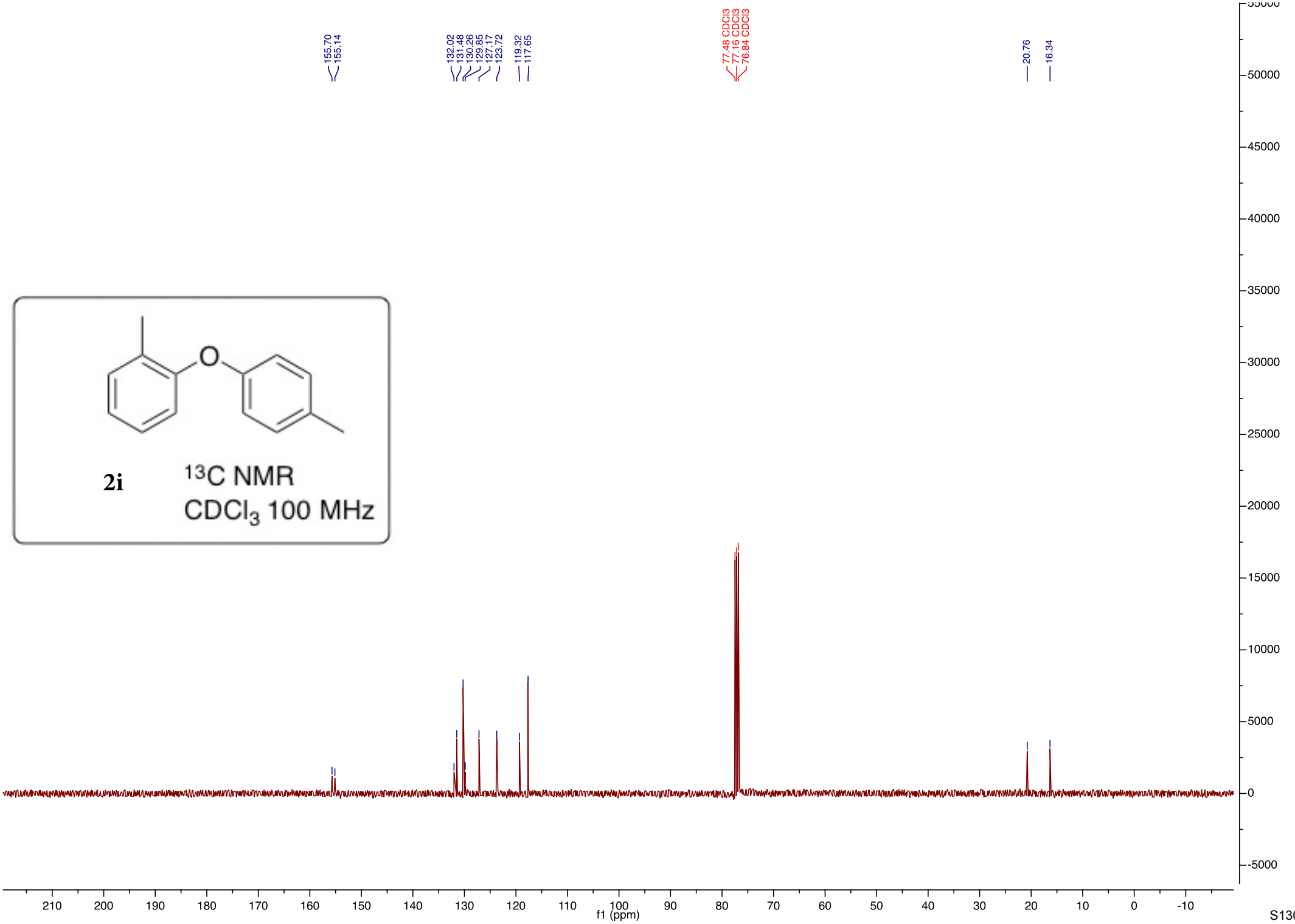

7.27 CDCl3
7.27
7.26
7.26
7.26
7.25
7.25
7.25
7.24
7.15
7.14
7.13
7.13
7.13
7.12
7.12
7.11
7.11
7.04
7.04
7.02
7.02
7.00
7.00
6.75
6.74
6.73
6.72
2.30
O
2g
1H NMR
CDCl3 400 MHz
2.10
1.98
2.00
1.96
6.00
f1 (ppm)
f1 (ppm)

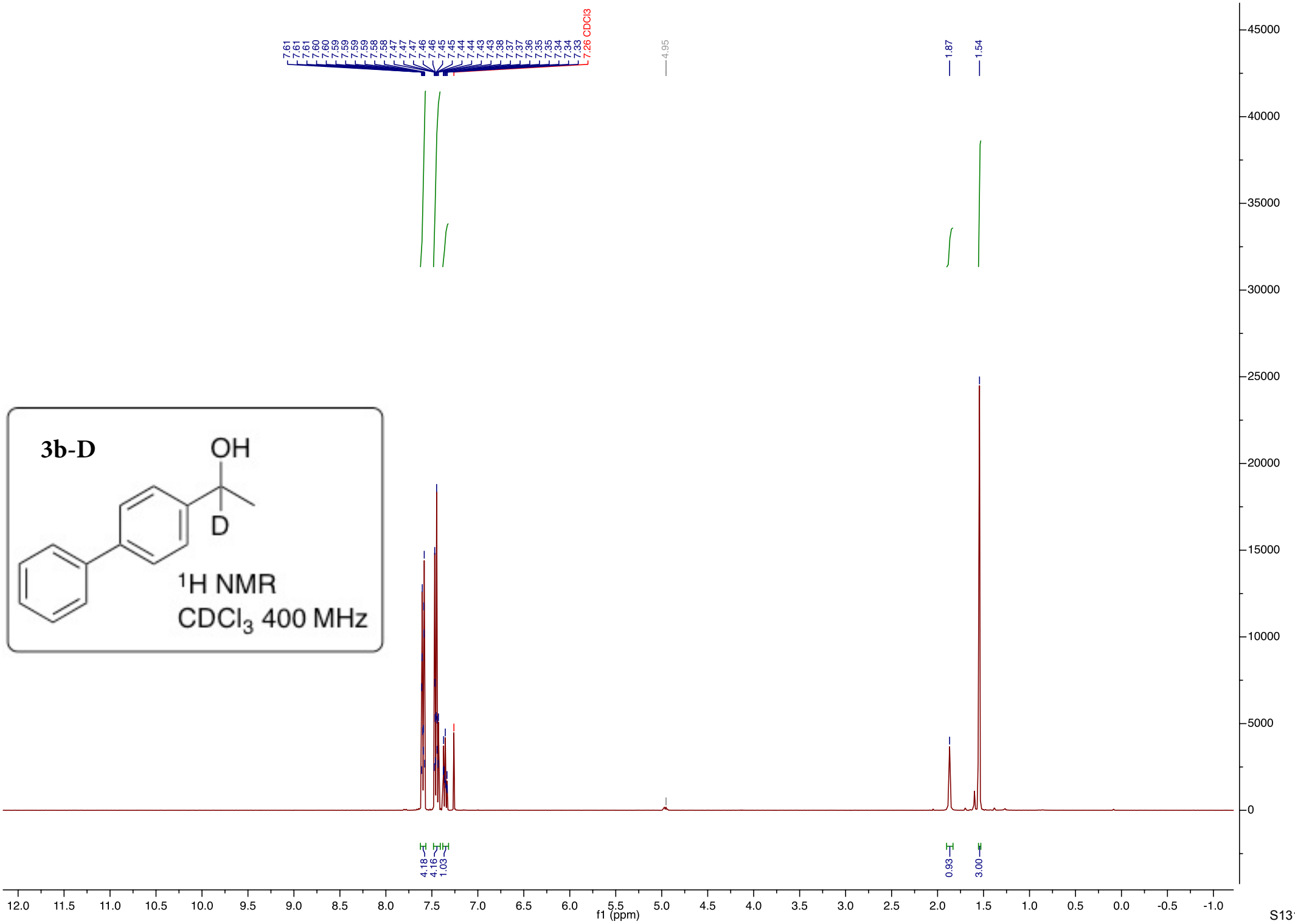

155.38
131.42
128.96
127.12
123.14
117.79
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
16.29
O
2g
13C NMR
CDCl3 100 MHz
f1 (ppm)

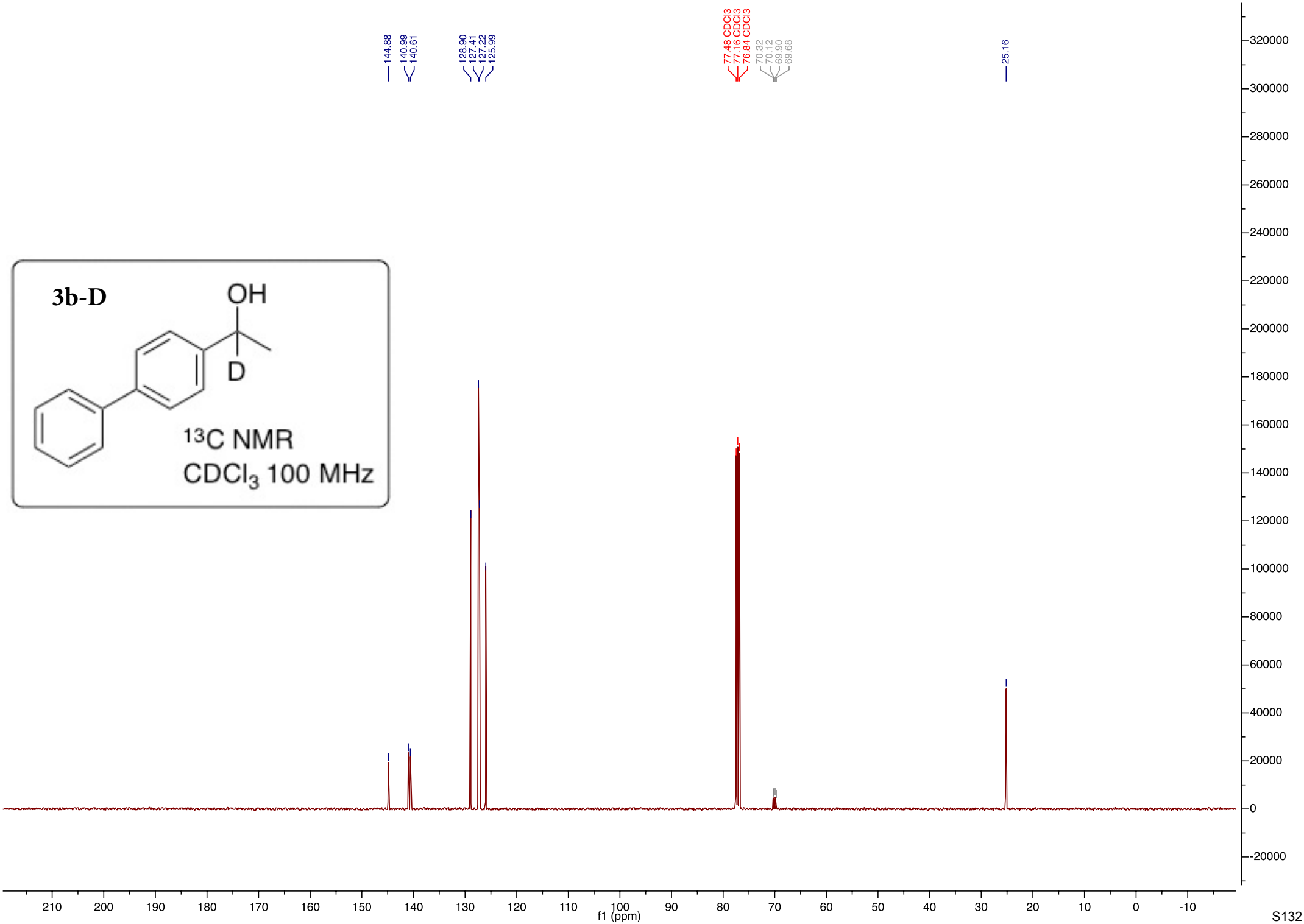

7.26 CDCl3
2.33
2.27
1.54 HDO
1 H NMR, CDCl3, 400 MHz
2h
f1 (ppm)
f1 (ppm)

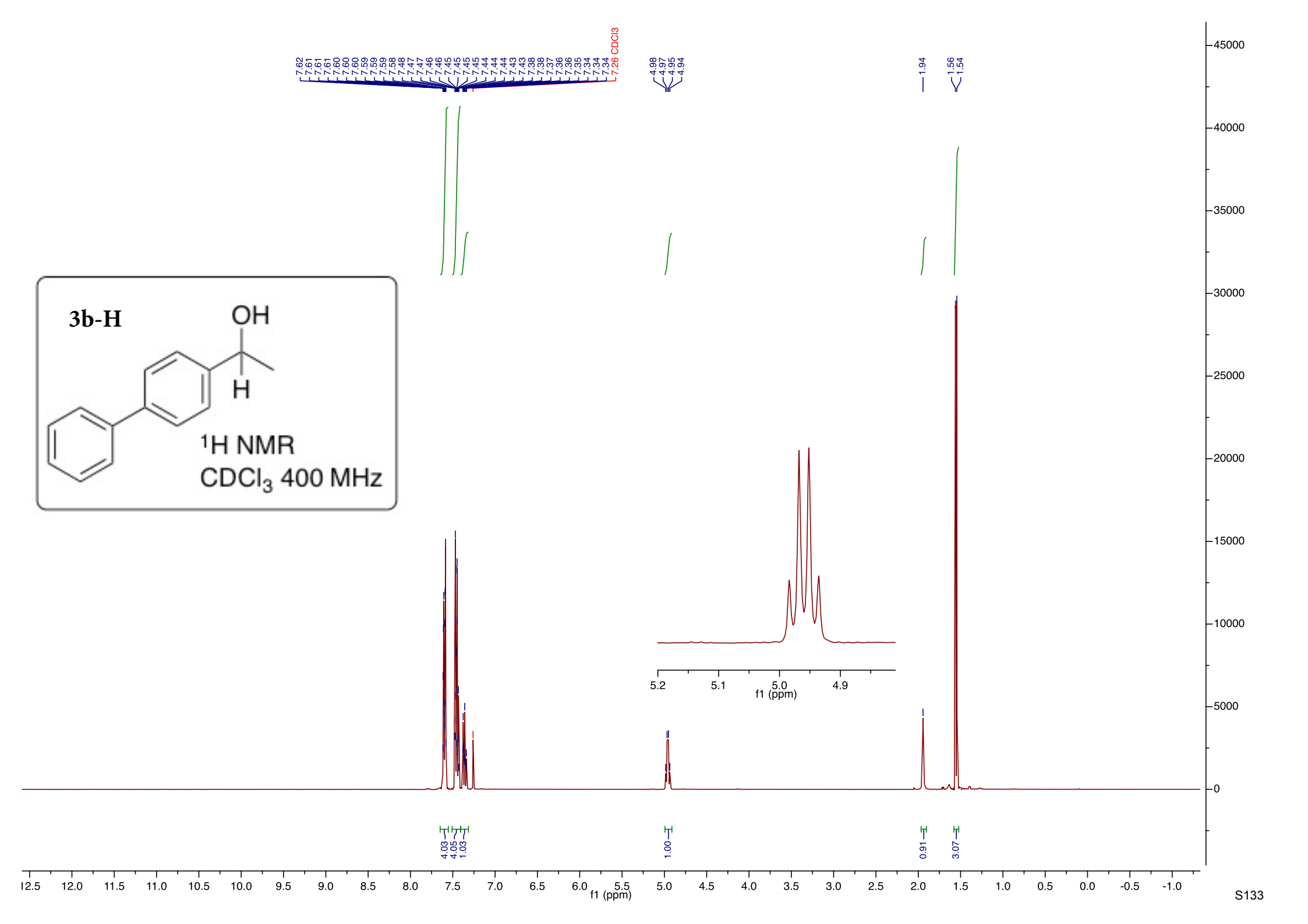

158.02
154.68
139.94
131.51
130.11
129.49
127.22
123.99
123.31
119.88
118.15
114.44
21.56
16.34
O
^{13}C NMR, $CDCl_3$, 100 MHz
2h
f1 (ppm)

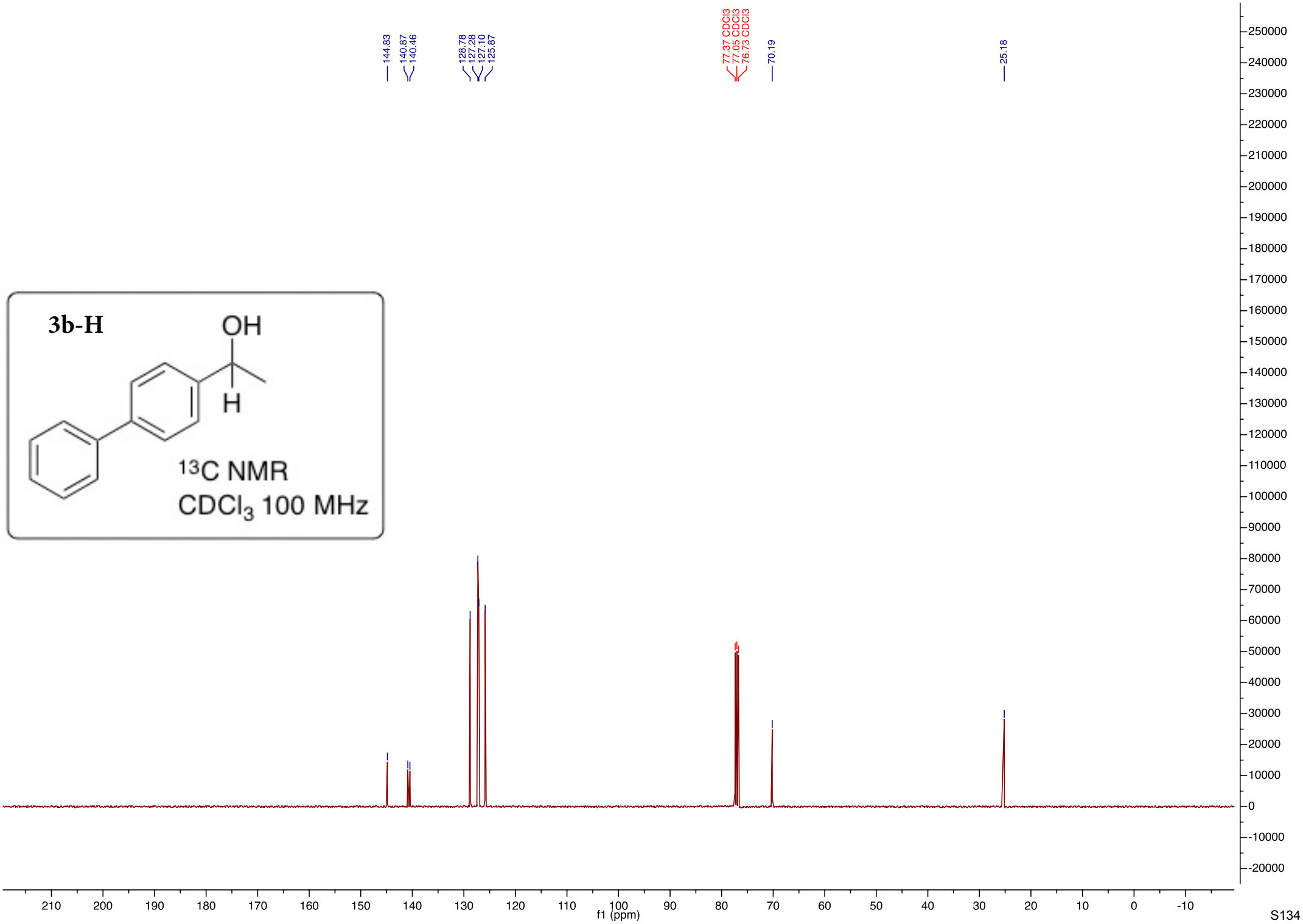

7.26 CDCl3
2.32
2.26
O
2i
1H NMR
CDCl3 400 MHz
1.39
3.05
1.03
0.84
1.98
3.00
3.00
f1 (ppm)

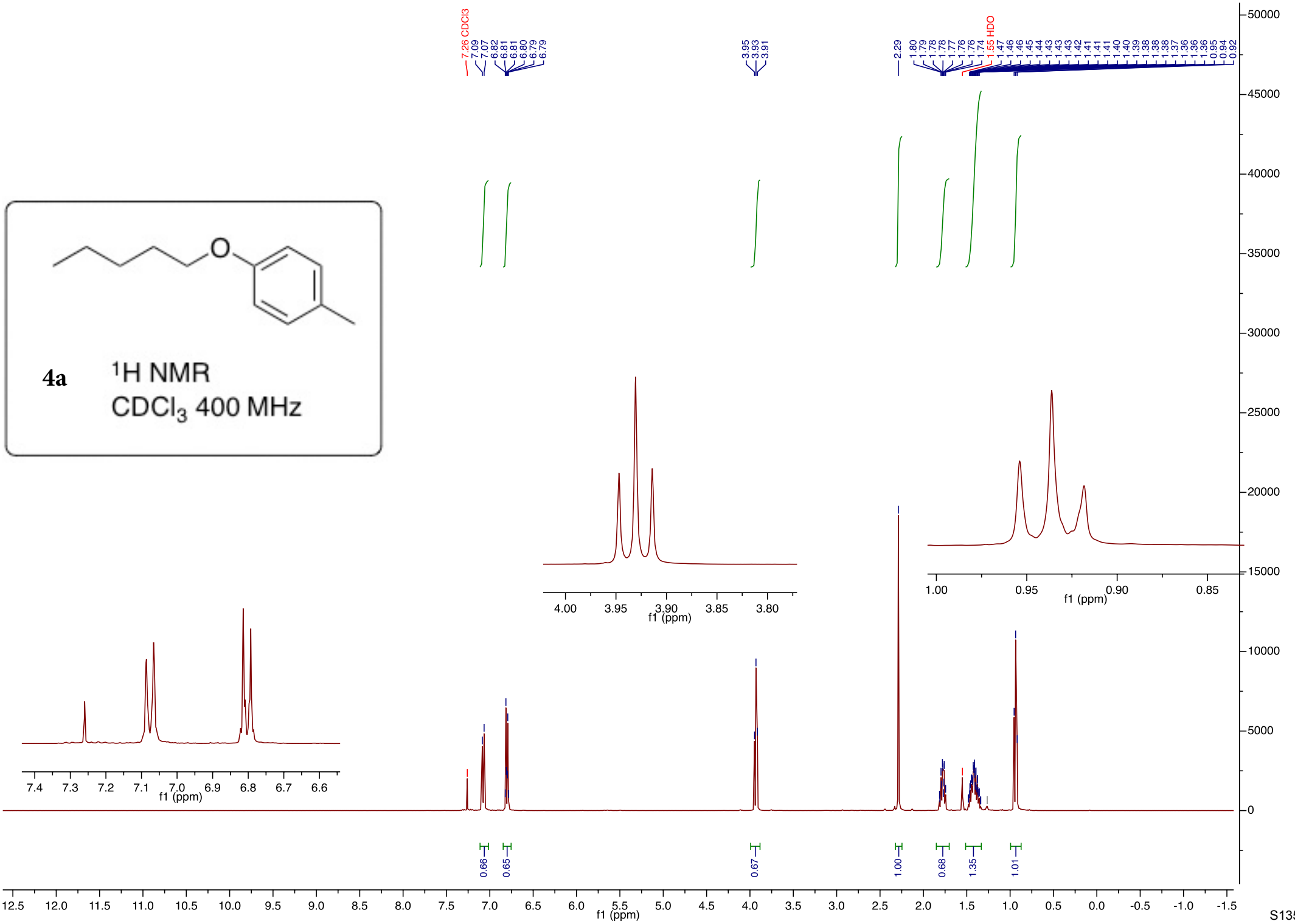

155.70
155.14
132.02
131.48
130.26
129.85
127.17
123.72
119.32
117.65
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
20.76
16.34
O
2i
13C NMR
CDCl3 100 MHz
f1 (ppm)

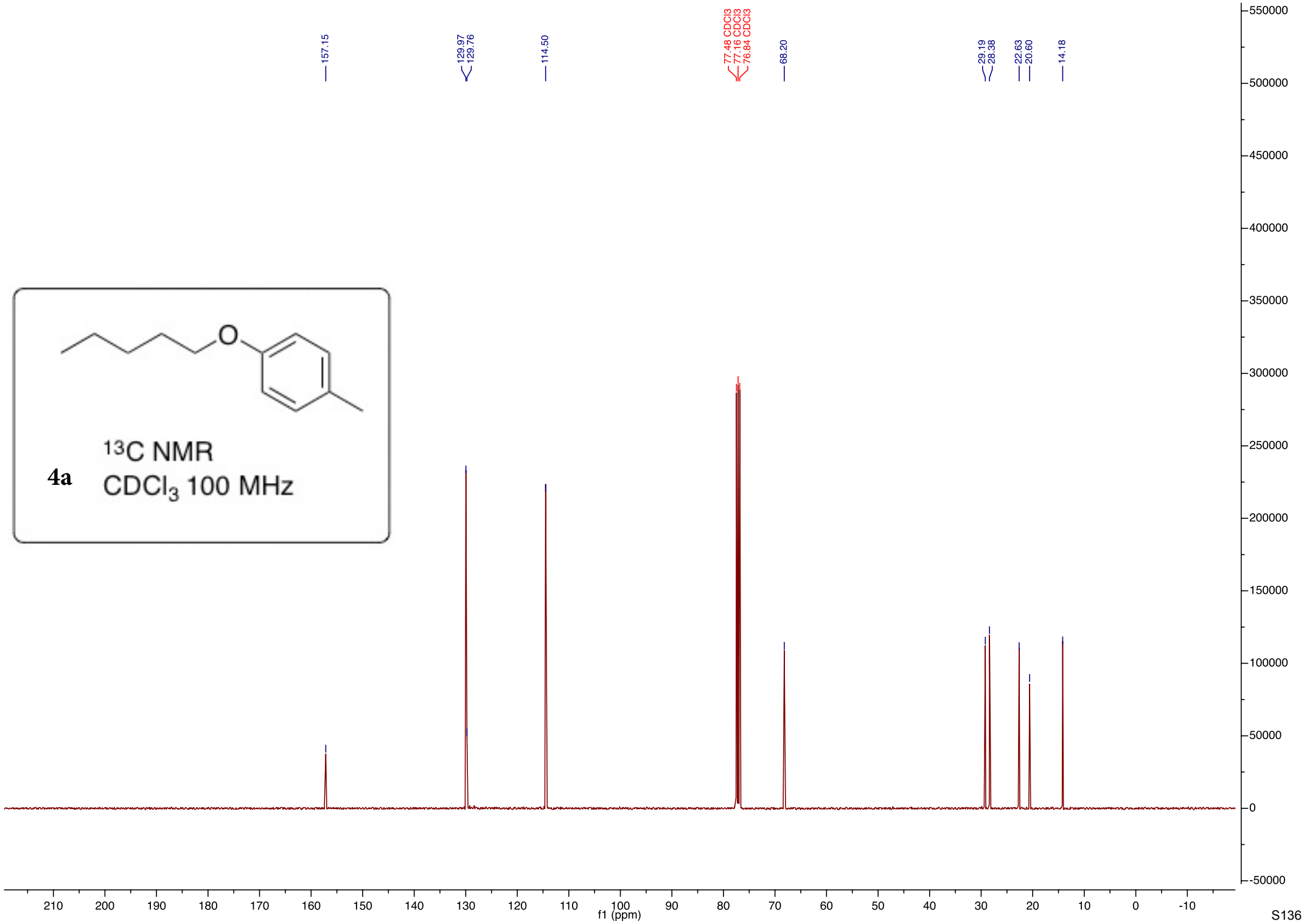

7.61
7.61
7.61
7.60
7.60
7.59
7.59
7.59
7.59
7.58
7.58
7.47
7.47
7.47
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.34
7.33
7.26 CDCl3
4.95
1.87
1.54
3b-D
OH
D
1H NMR
CDCl3 400 MHz
4.18
4.16
1.03
0.93
3.00
f1 (ppm)

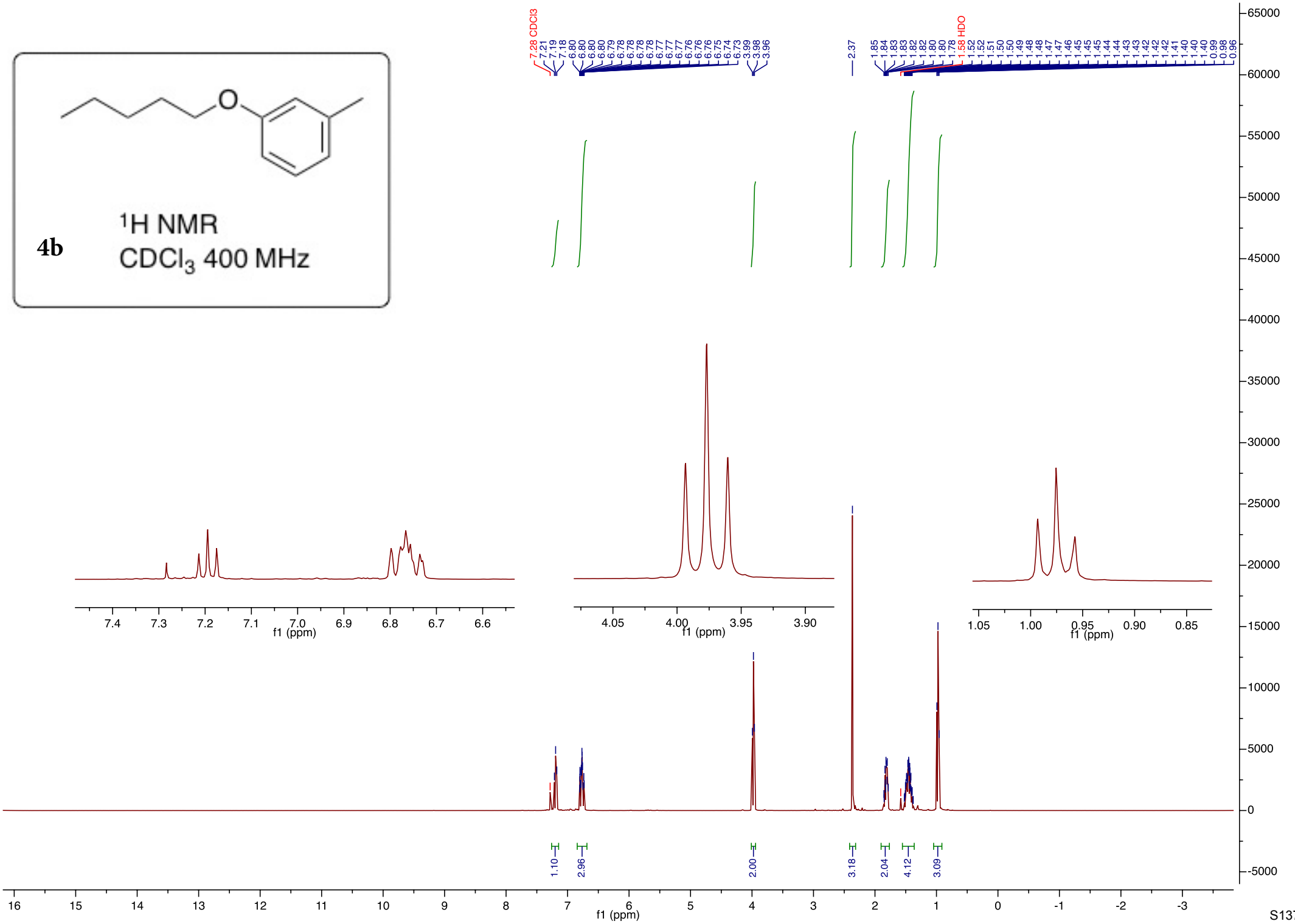

144.88
140.99
140.61
128.90
127.41
127.22
125.99
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
70.32
70.12
69.90
69.68
25.16
3b-D
OH
D
13C NMR
CDCl3 100 MHz
f1 (ppm)

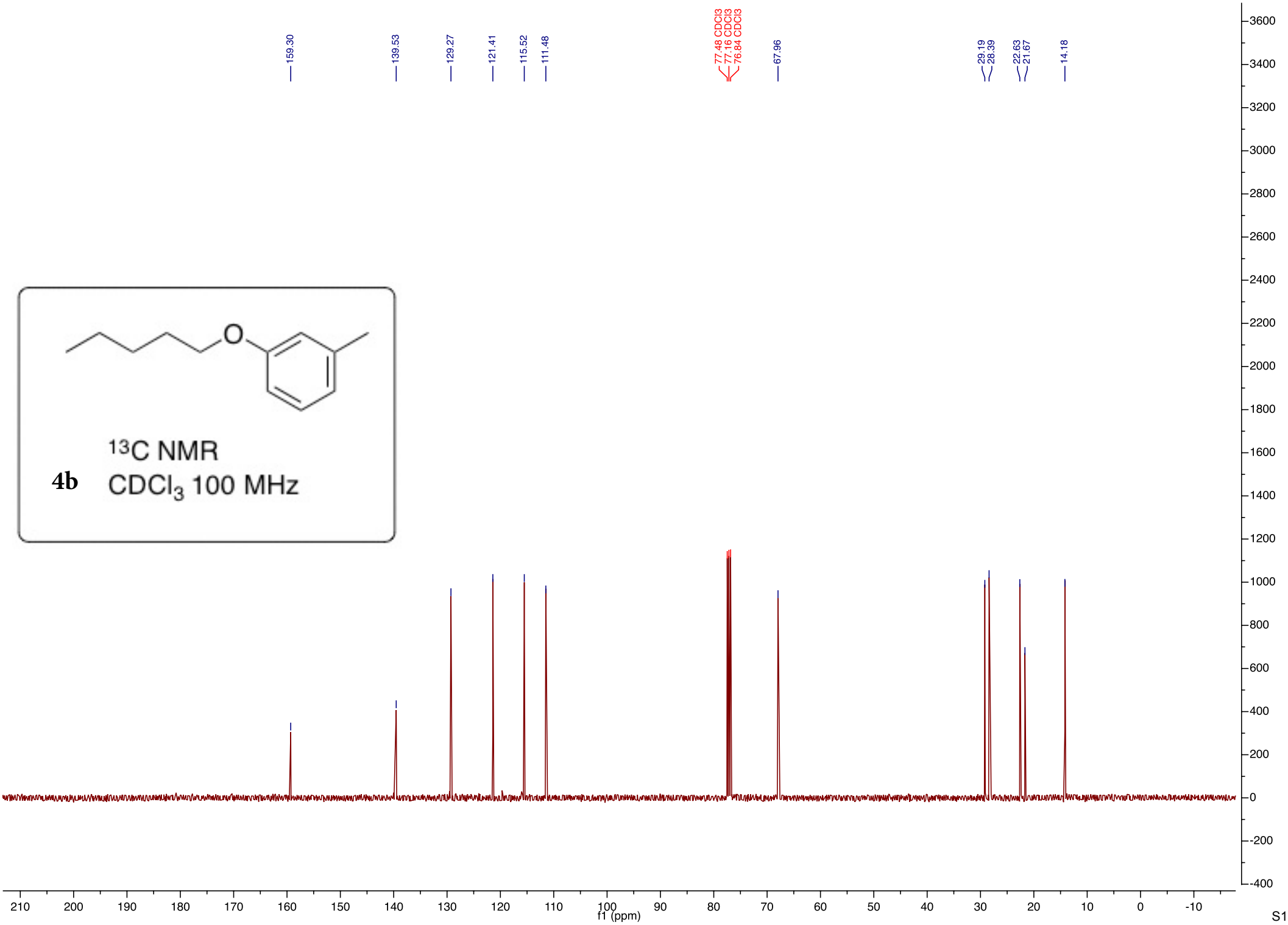

3b-H
OH
H
^{1}H NMR
$CDCl_3$ 400 MHz
7.62 7.61 7.61 7.61 7.60 7.60 7.60 7.59 7.59 7.59 7.58 7.48 7.47 7.47 7.46 7.46 7.45 7.45 7.45 7.44 7.44 7.44 7.43 7.38 7.38 7.37 7.36 7.36 7.35 7.34 7.34 7.26 CDCl3
4.98 4.97 4.95 4.94
1.94
1.56 1.54
4.03 4.05 1.03
1.00
0.91
3.07
f1 (ppm)

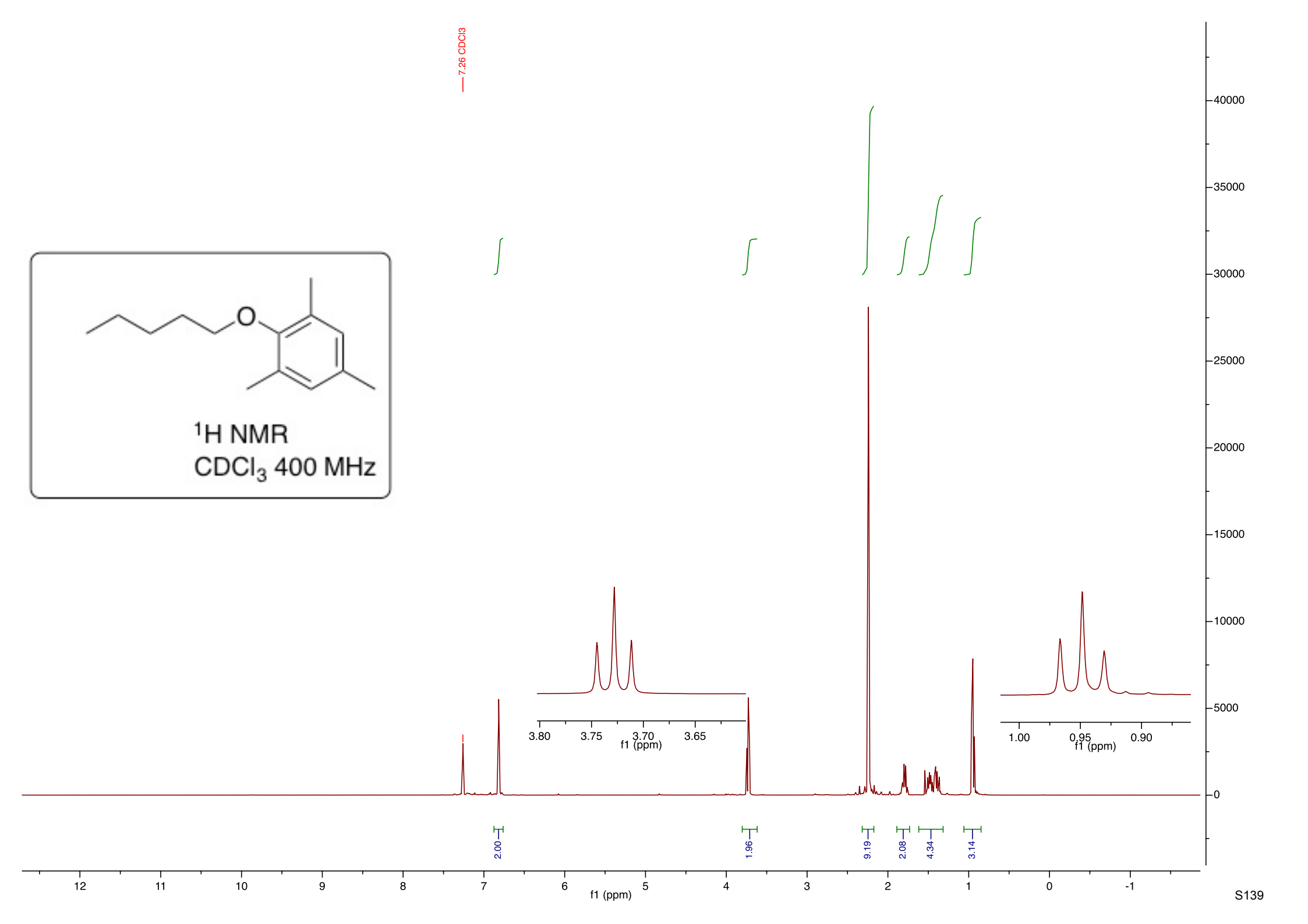

144.83
140.87
140.46
128.78
127.28
127.10
125.87
77.37 CDCl3
77.05 CDCl3
76.73 CDCl3
70.19
25.18
3b-H
OH
H
13C NMR
CDCl3 100 MHz
f1 (ppm)

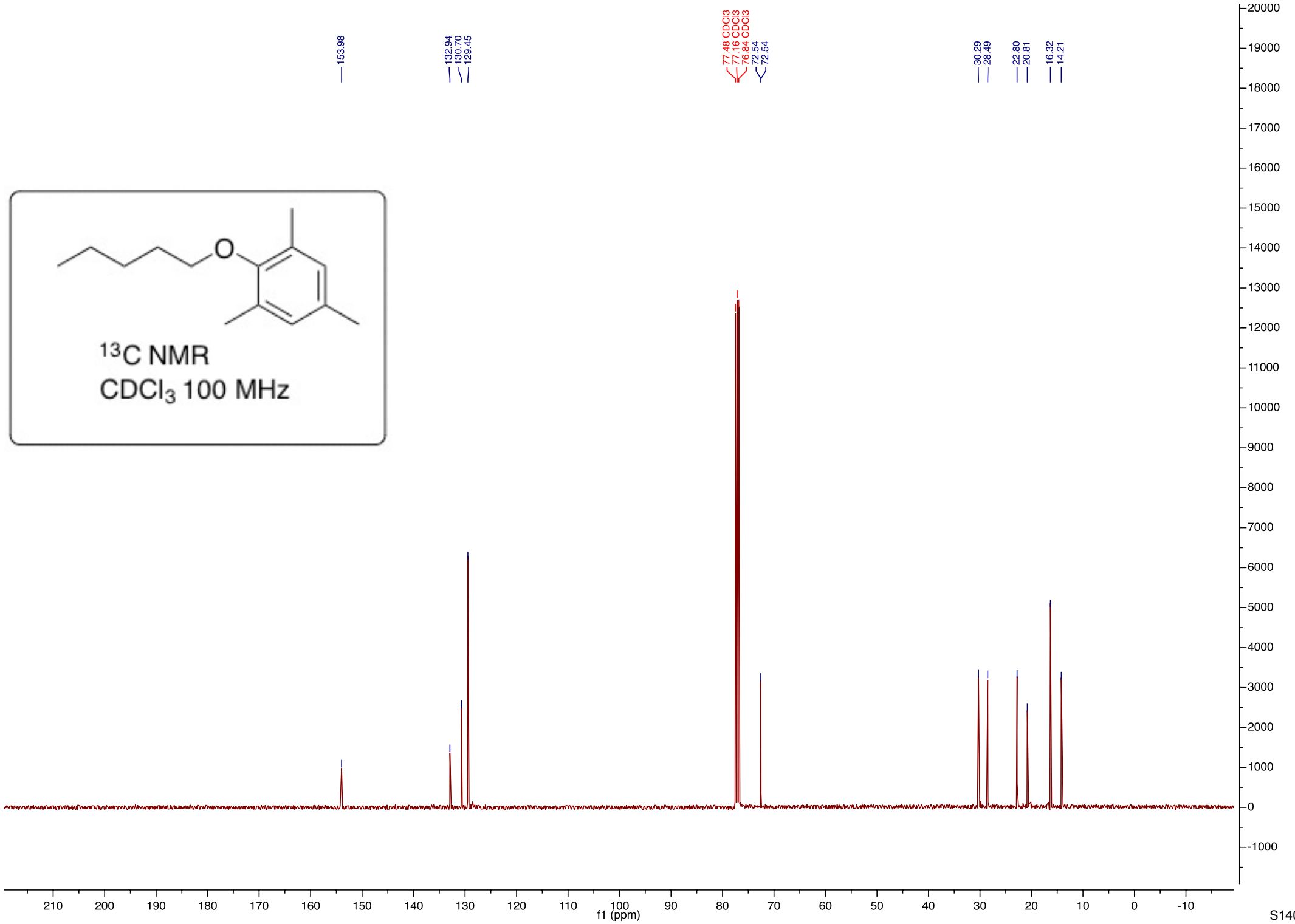

4a
^{1}H NMR
$CDCl_3$ 400 MHz
7.26 CDCl3
7.09
7.07
6.82
6.81
6.81
6.80
6.79
6.79
3.95
3.93
3.91
2.29
1.80
1.79
1.78
1.78
1.77
1.76
1.76
1.74
1.55 HDO
1.47
1.46
1.46
1.45
1.44
1.43
1.43
1.43
1.42
1.41
1.41
1.41
1.40
1.40
1.39
1.38
1.38
1.38
1.37
1.36
1.36
1.36
0.95
0.94
0.92
0.66
0.65
0.67
1.00
0.68
1.35
1.01
f1 (ppm)

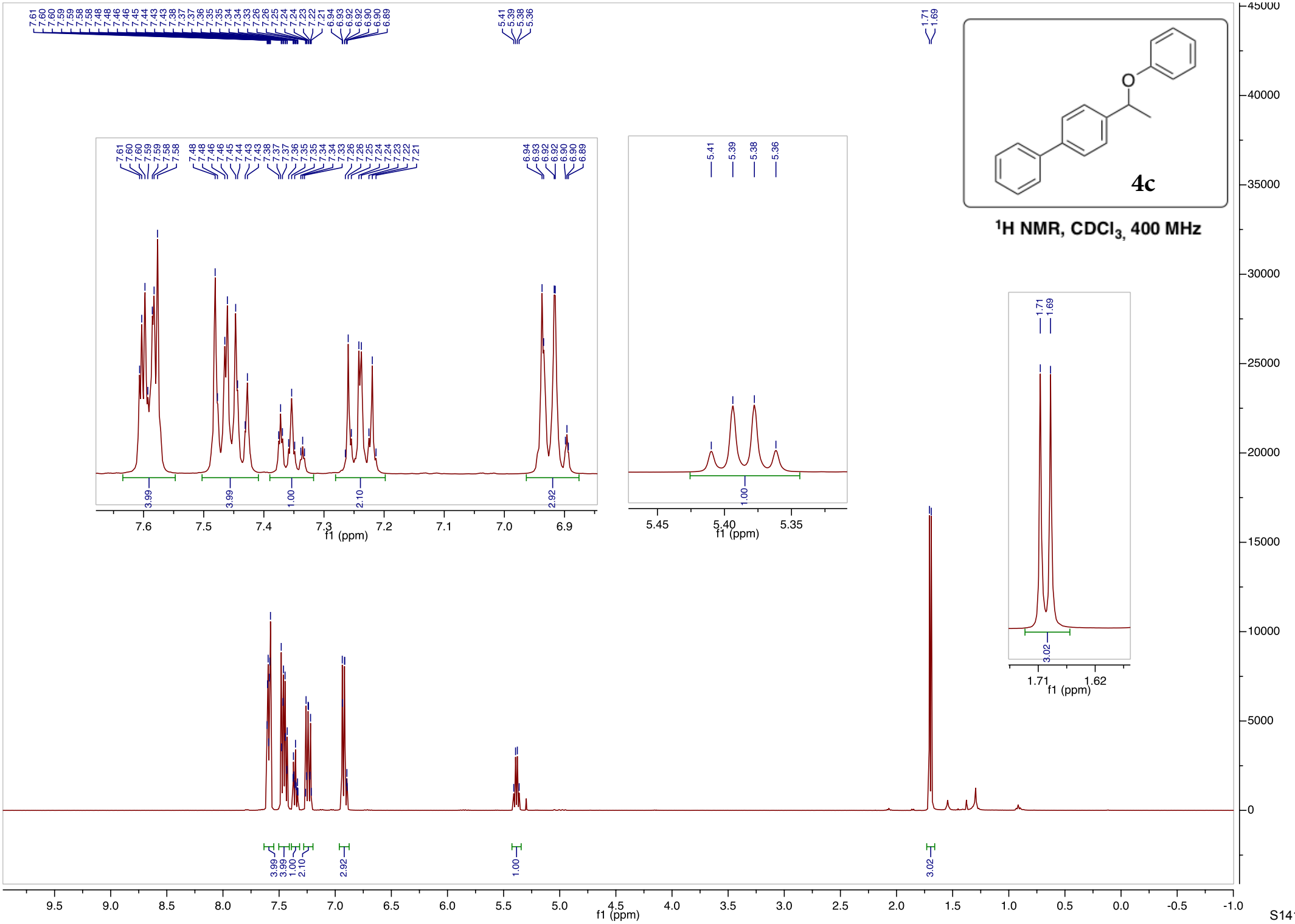

157.15
129.97
129.76
114.50
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
68.20
29.19
28.38
22.63
20.60
14.18
O
^{13}C NMR
4a
$CDCl_3$ 100 MHz
f1 (ppm)

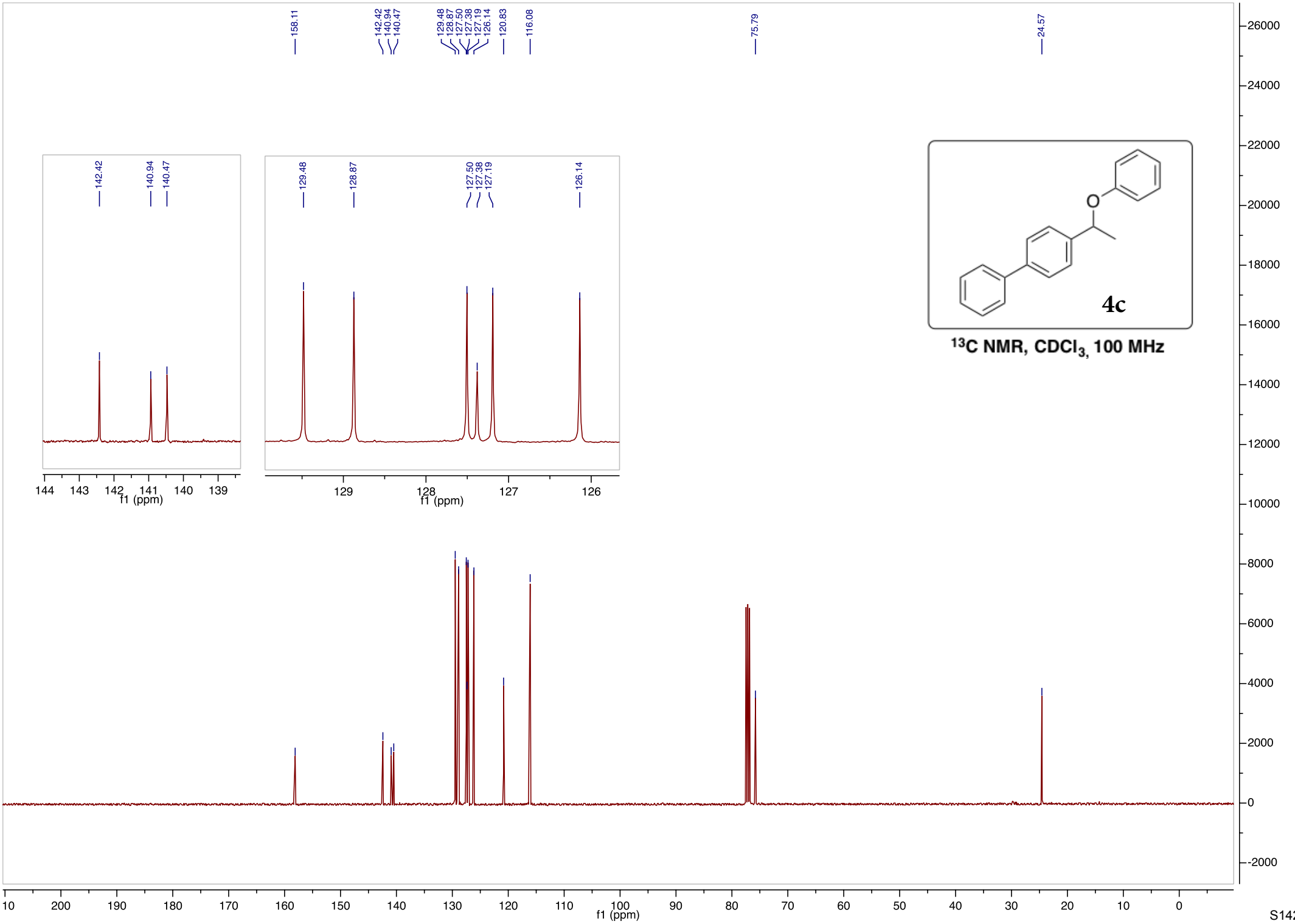

4b
1H NMR
CDCl3 400 MHz
f1 (ppm)

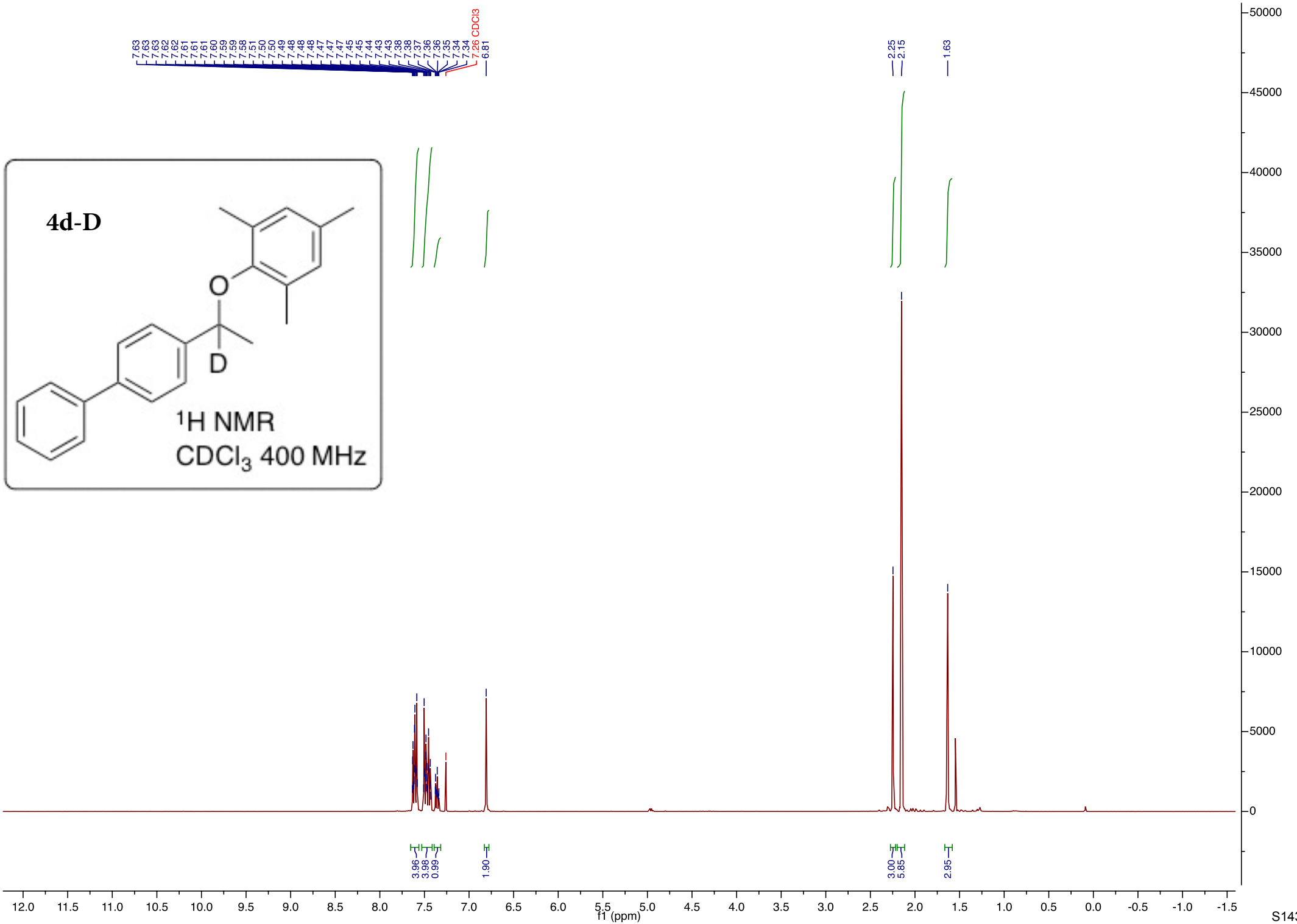

159.30
139.53
129.27
121.41
115.52
111.48
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
67.96
29.19
28.39
22.63
21.67
14.18
O
13C NMR
4b
CDCl3 100 MHz
f1 (ppm)

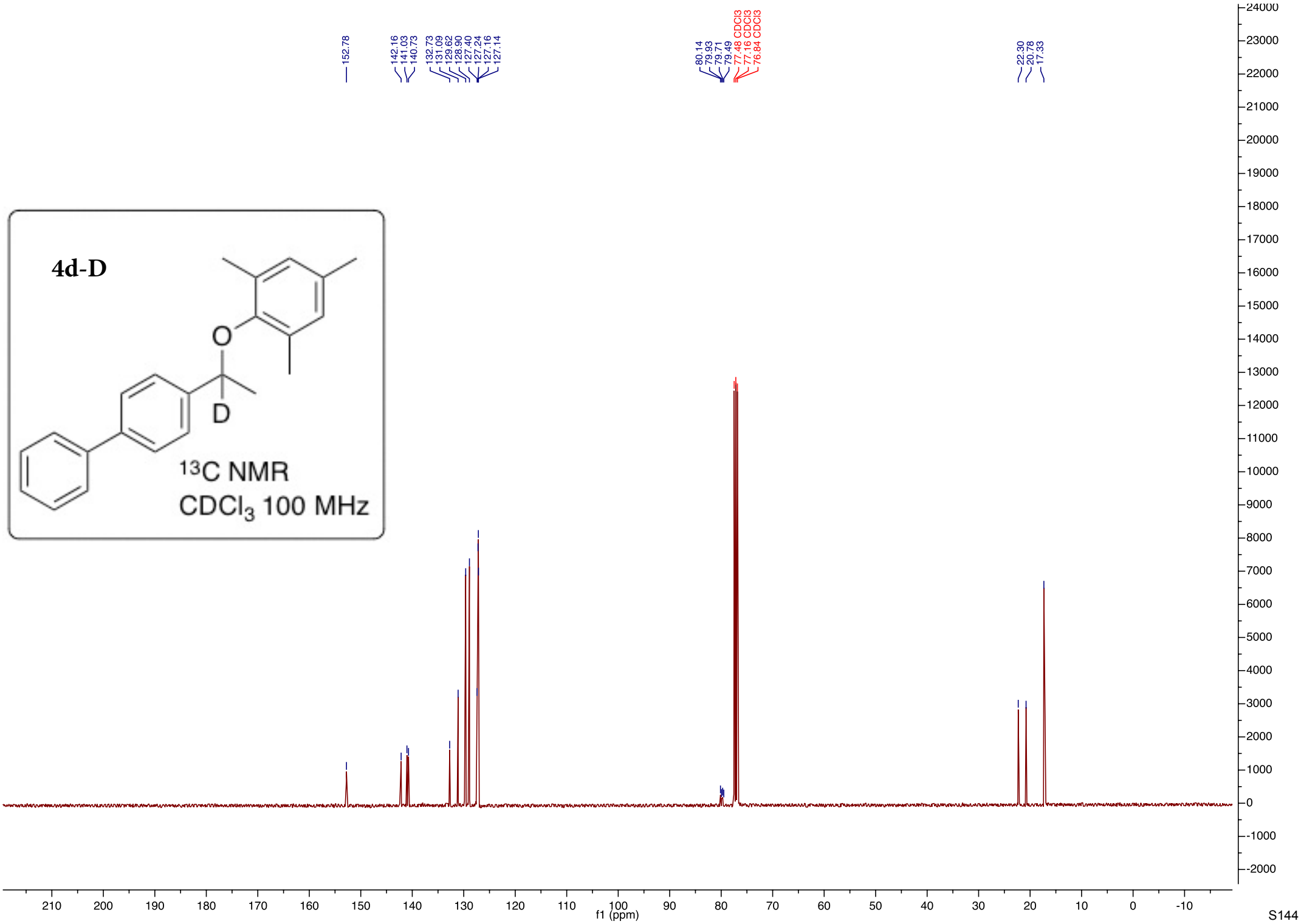

7.26 CDCl3
O
^{1}H NMR
$CDCl_3$ 400 MHz
40000
35000
30000
25000
20000
15000
10000
5000
0
3.80
3.75
3.70
3.65
f1 (ppm)
1.00
0.95
0.90
f1 (ppm)
2.00
1.96
9.19
2.08
4.34
3.14
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

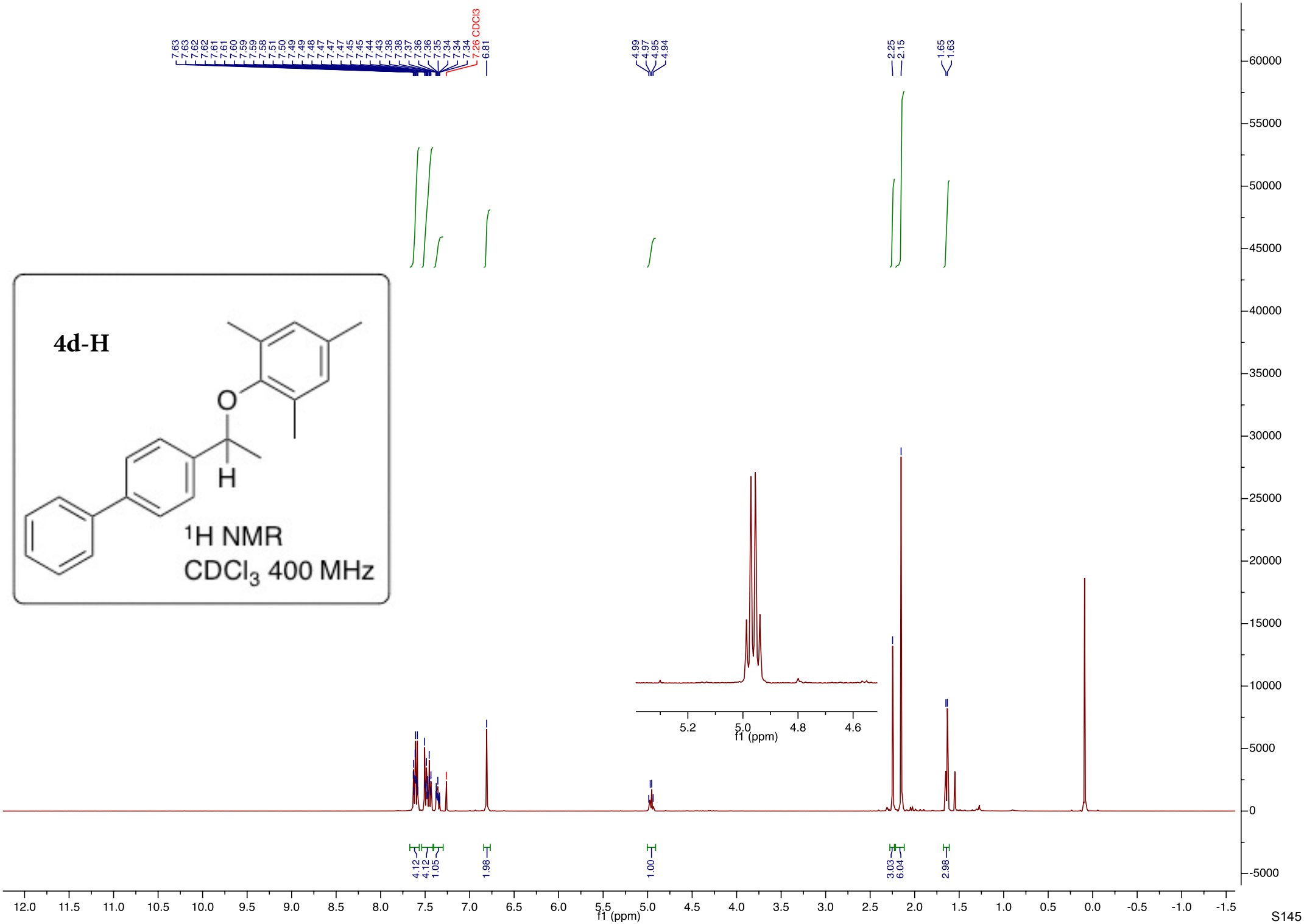

153.98
132.94
130.70
129.45
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
72.54
72.54
30.29
28.49
22.80
20.81
16.32
14.21
O
13C NMR
CDCl3 100 MHz
f1 (ppm)

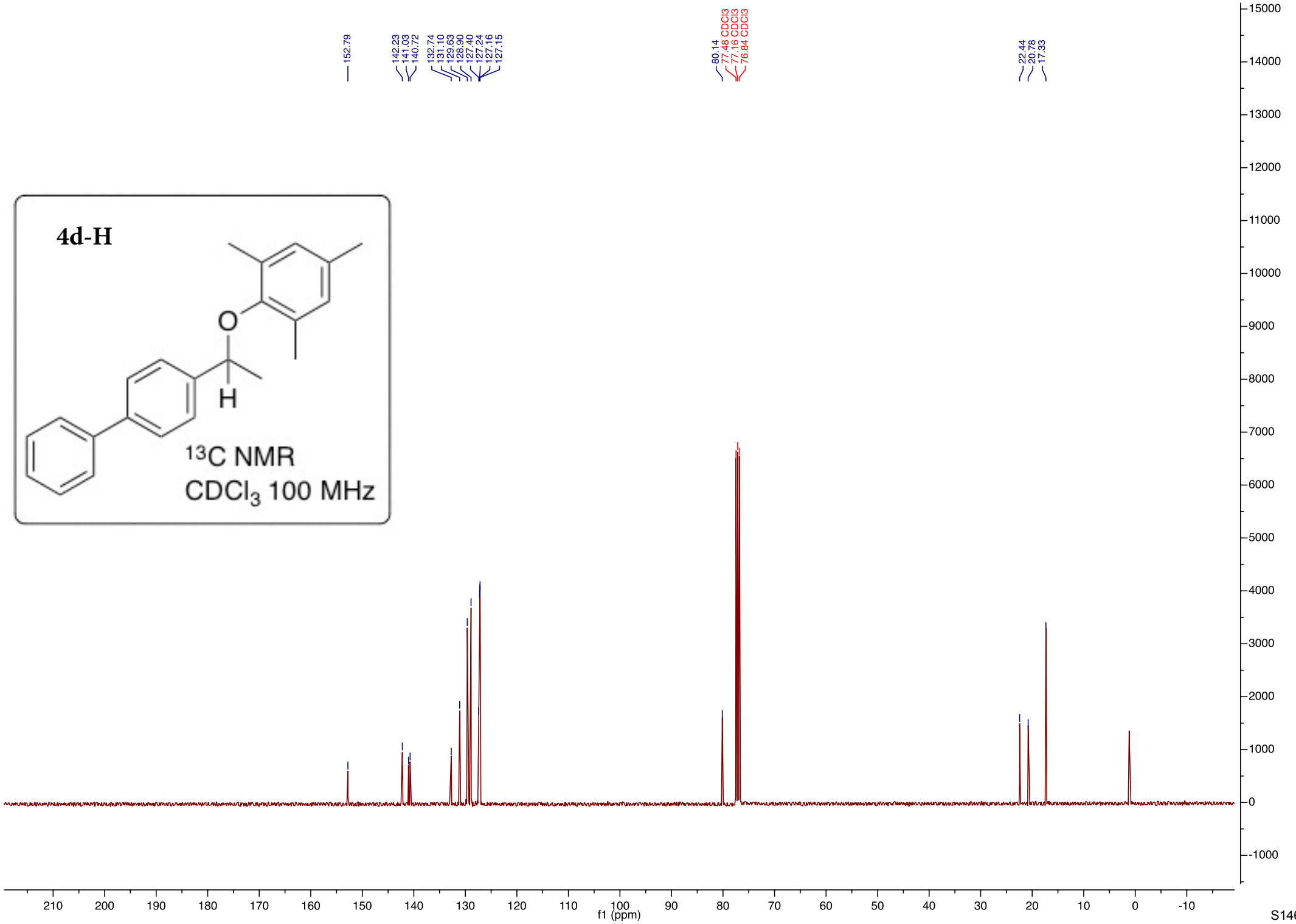

4c
^{1}H NMR, CDCl$_3$, 400 MHz
f1 (ppm)

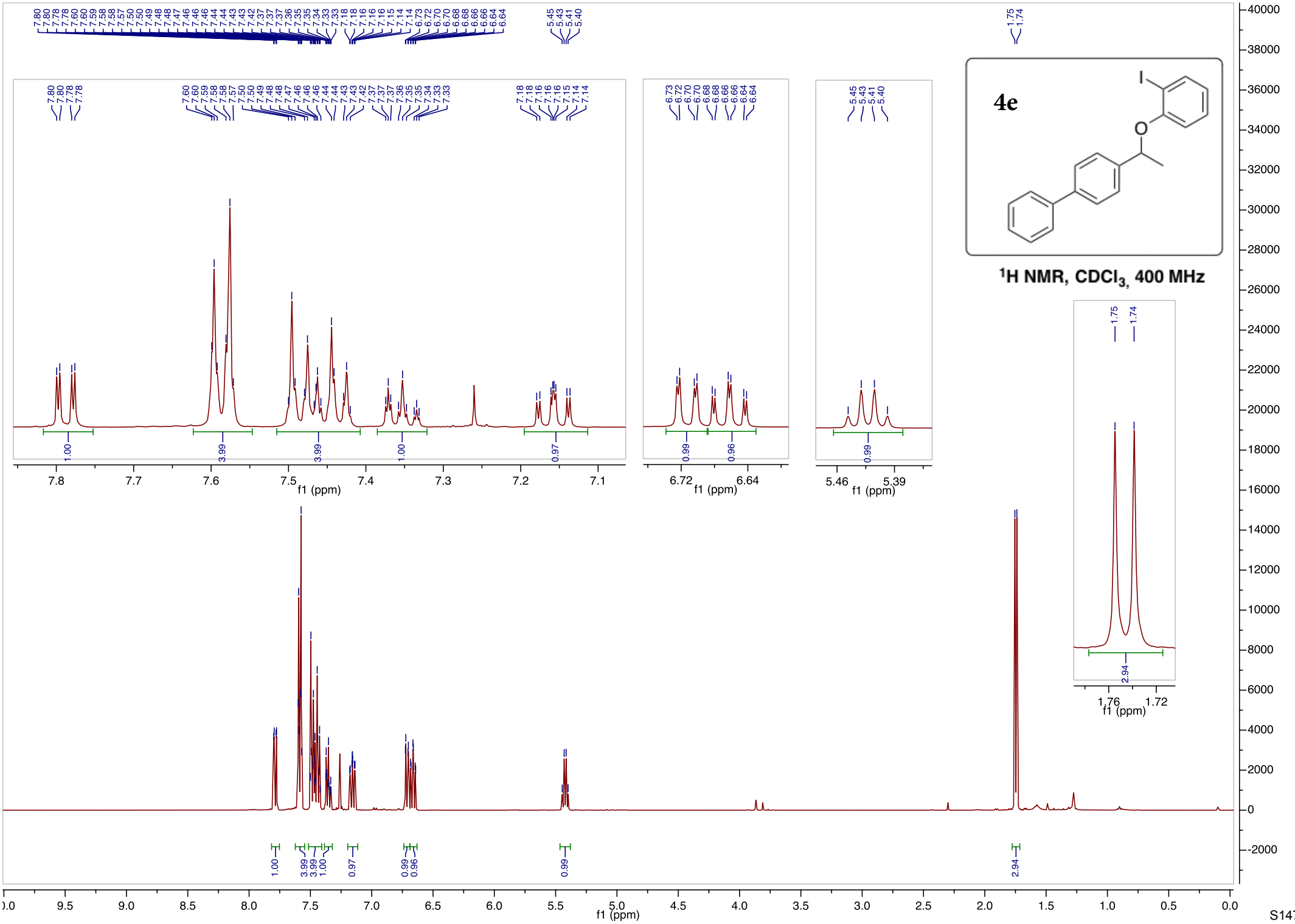

158.11
142.42
140.94
140.47
129.48
128.87
127.50
127.38
127.19
126.14
120.83
116.08
75.79
24.57
O
4c
^{13}C NMR, $CDCl_3$, 100 MHz
f1 (ppm)

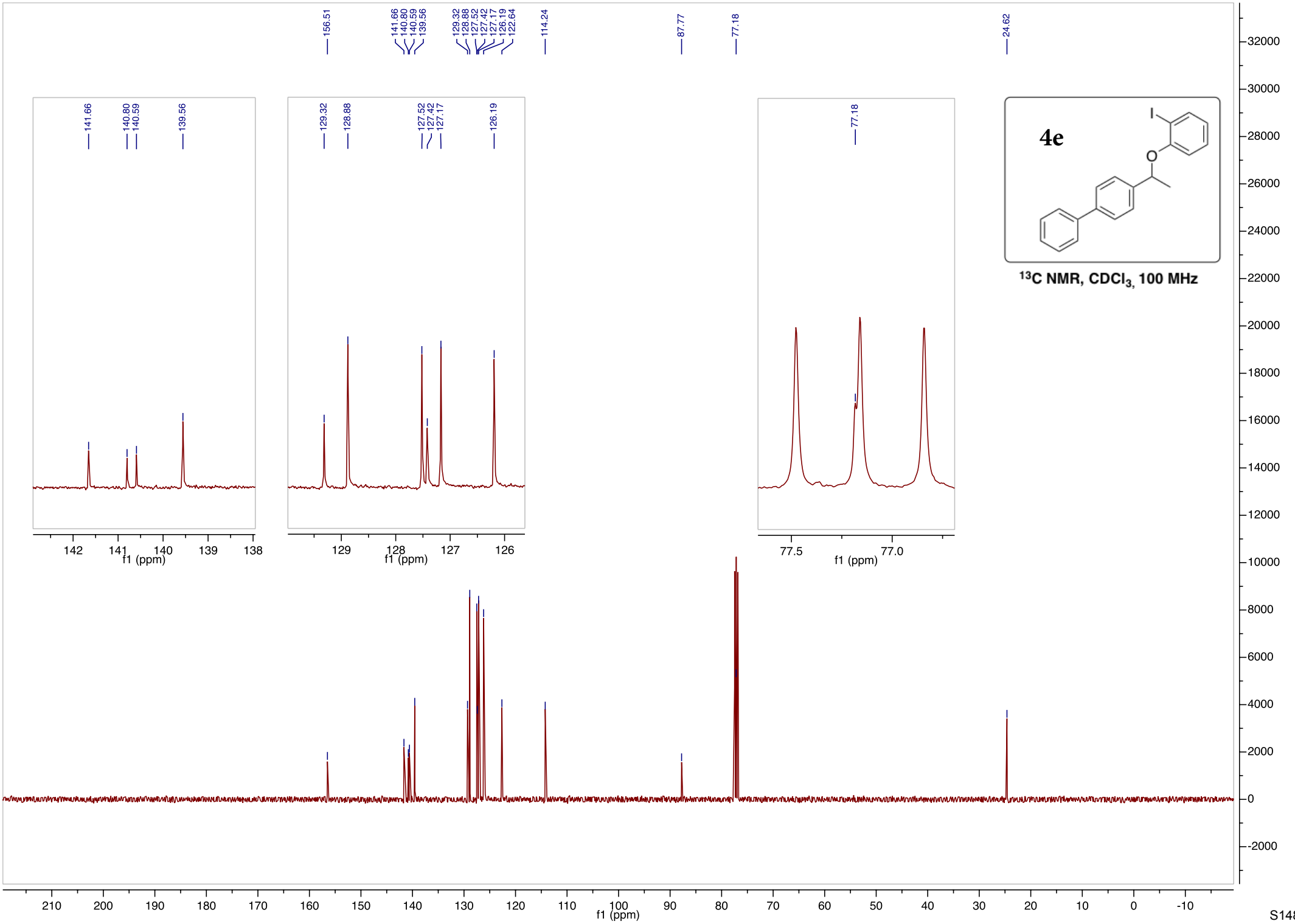

4d-D
O
D
^{1}H NMR
$CDCl_3$ 400 MHz
7.63 7.63 7.63 7.62 7.62 7.61 7.61 7.61 7.60 7.59 7.59 7.58 7.51 7.50 7.50 7.49 7.48 7.48 7.48 7.47 7.47 7.47 7.45 7.45 7.44 7.43 7.43 7.38 7.38 7.37 7.36 7.36 7.35 7.34 7.34 7.26 CDCl3 6.81
2.25 2.15 1.63
3.96 3.98 0.99 1.90 3.00 5.85 2.95
f1 (ppm)

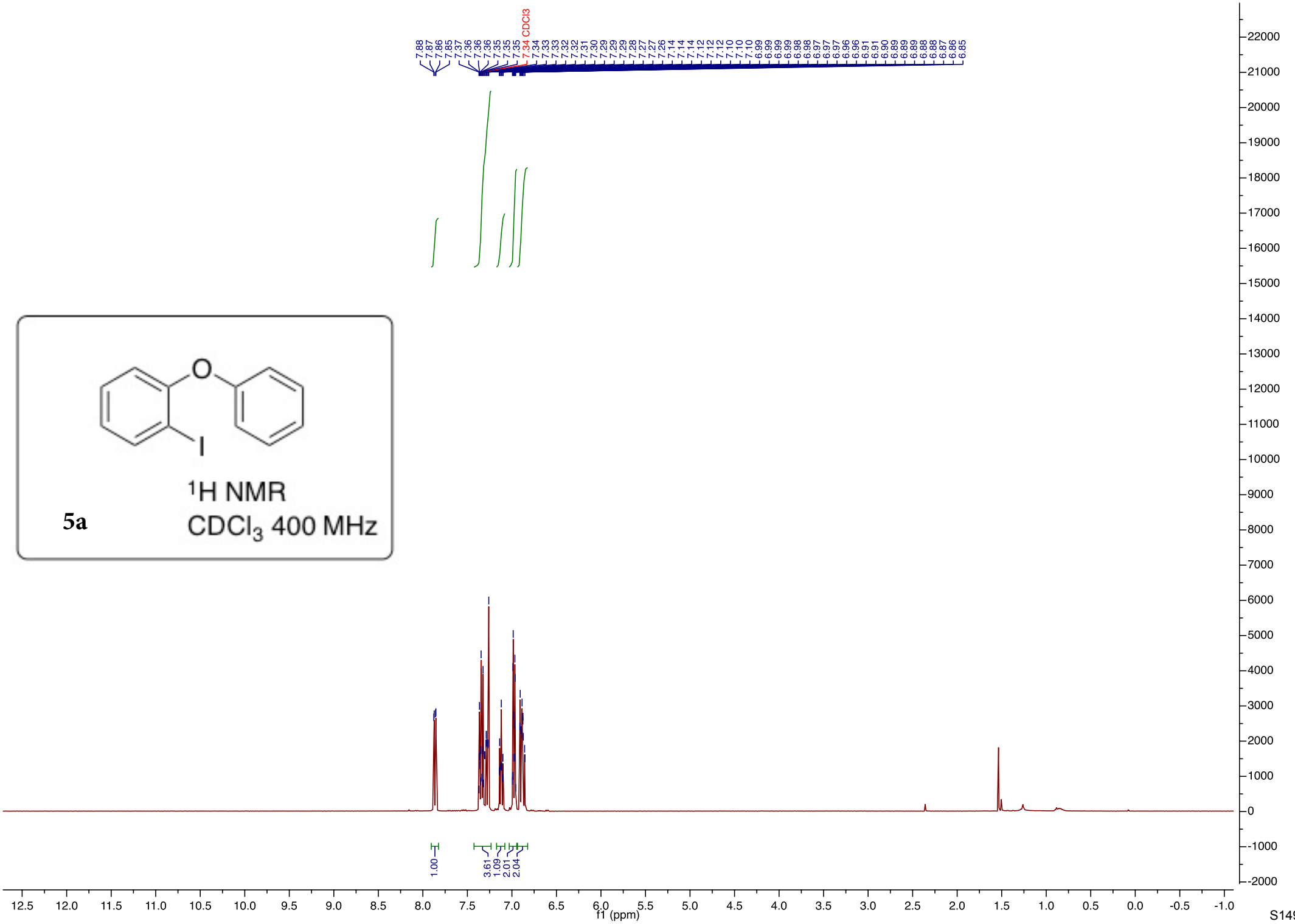

152.78
142.16
141.03
140.73
132.73
131.09
129.62
128.90
127.40
127.24
127.16
127.14
80.14
79.93
79.71
79.49
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
22.30
20.78
17.33
4d-D
O
D
13C NMR
CDCl3 100 MHz
f1 (ppm)

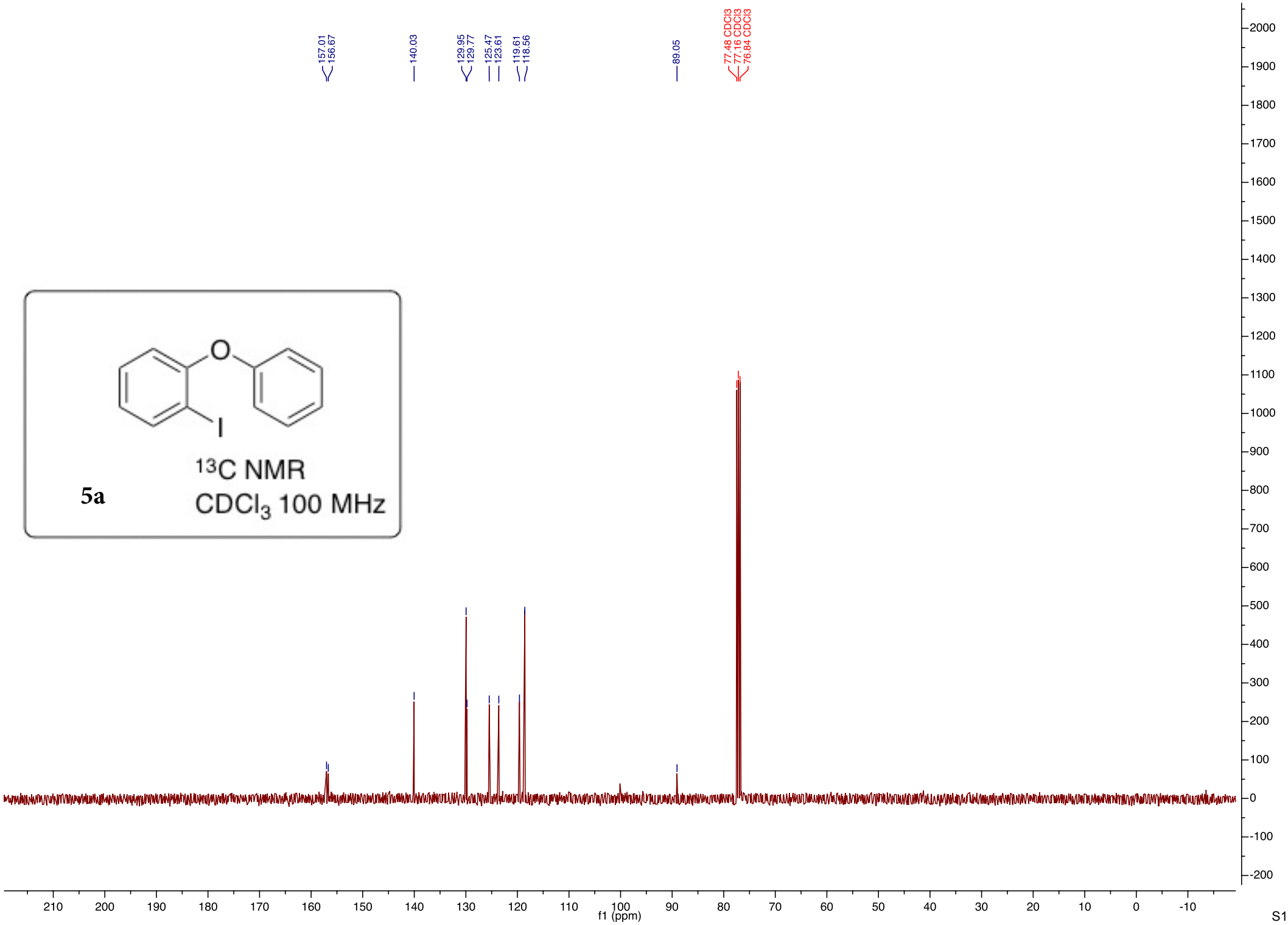

4d-H
O
H
^{1}H NMR
$CDCl_3$ 400 MHz
7.63 7.63 7.62 7.62 7.61 7.61 7.60 7.59 7.59 7.58 7.51 7.50 7.49 7.49 7.48 7.47 7.47 7.47 7.45 7.45 7.44 7.43 7.38 7.38 7.37 7.36 7.36 7.35 7.34 7.34 7.34 7.26 CDCl3 6.81
4.99 4.97 4.95 4.94
2.25 2.15
1.65 1.63
4.12 4.12 1.05 1.98 1.00 3.03 6.04 2.98
f1 (ppm)
S145

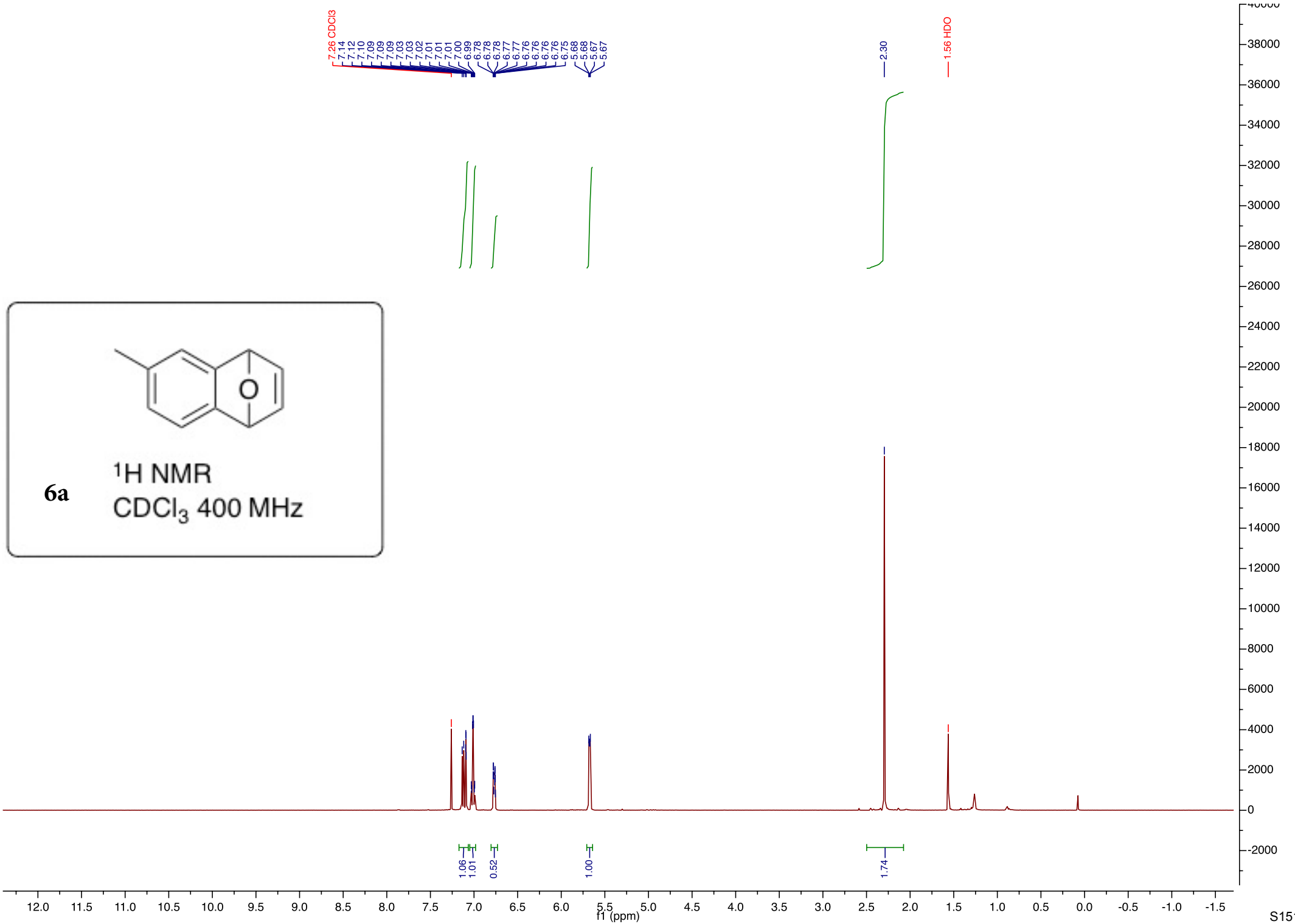

152.79
142.23
141.03
140.72
132.74
131.10
129.63
128.90
127.40
127.24
127.16
127.15
80.14
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
22.44
20.78
17.33
4d-H
O
H
13C NMR
CDCl3 100 MHz
f1 (ppm)

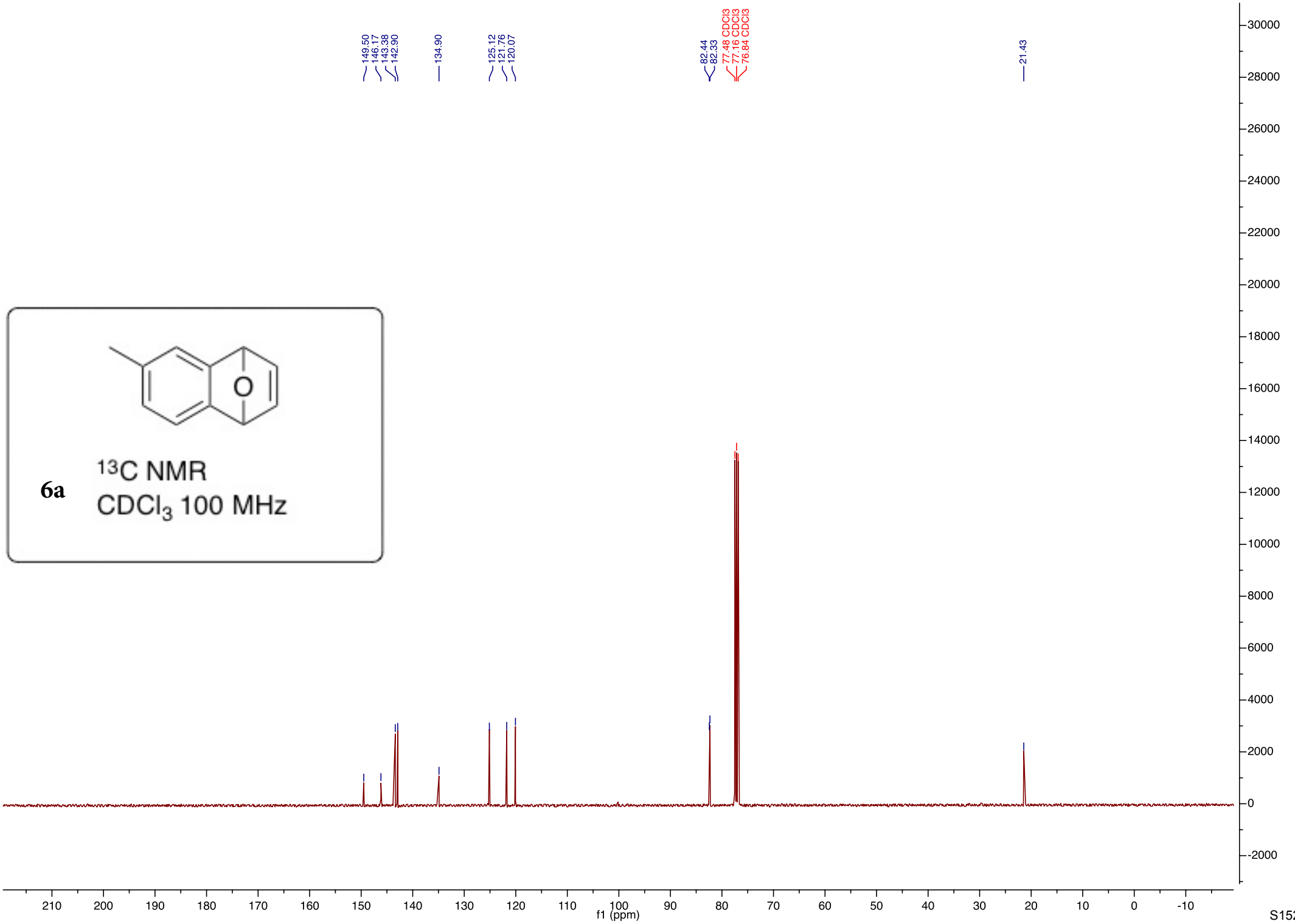

4e
^{1}H NMR, $CDCl_3$, 400 MHz
f1 (ppm)

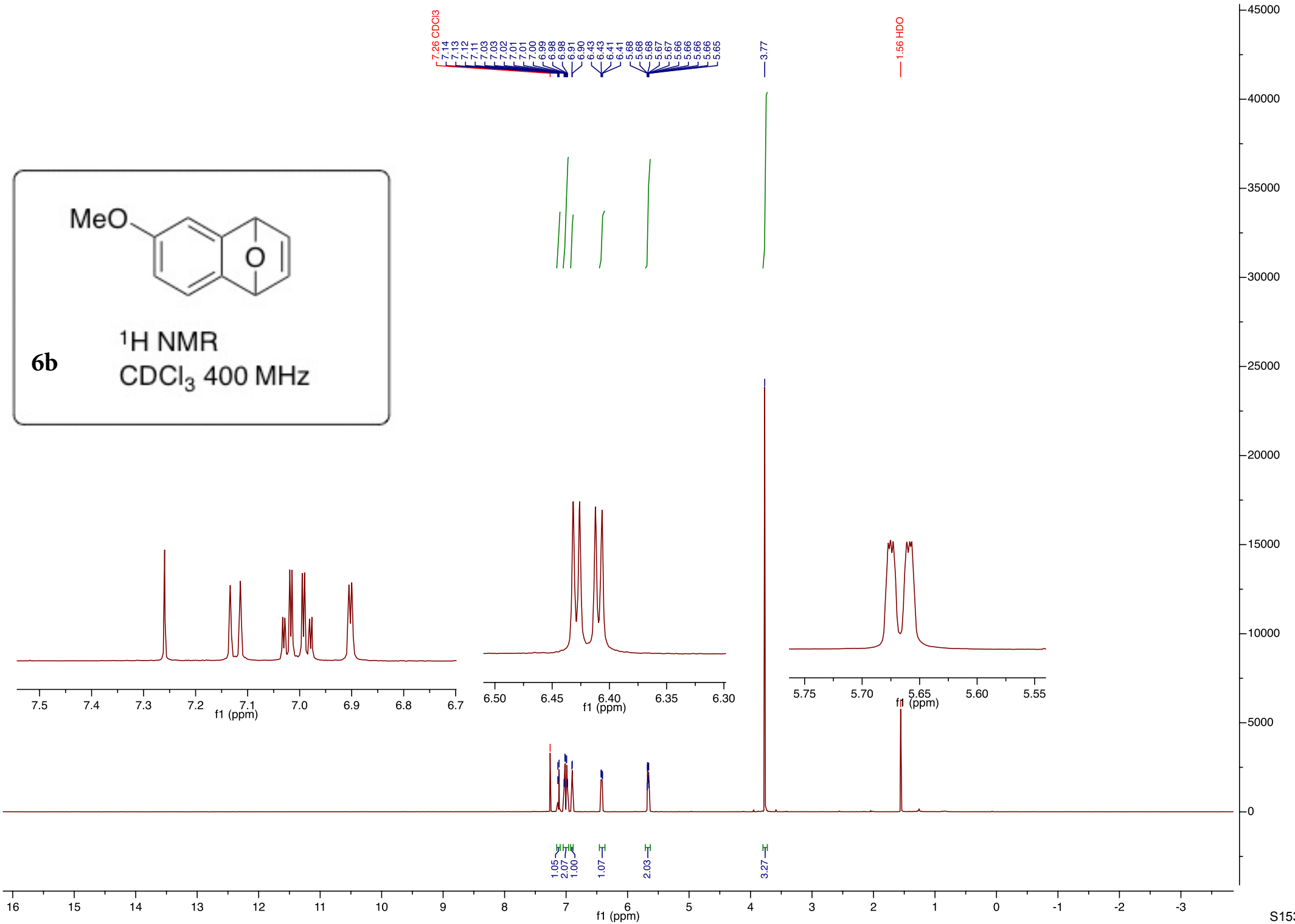

156.51
141.66
140.80
140.59
139.56
129.32
128.88
127.52
127.42
127.17
126.19
122.64
114.24
87.77
77.18
24.62
4e
O
I
13C NMR, CDCl3, 100 MHz
f1 (ppm)
S148

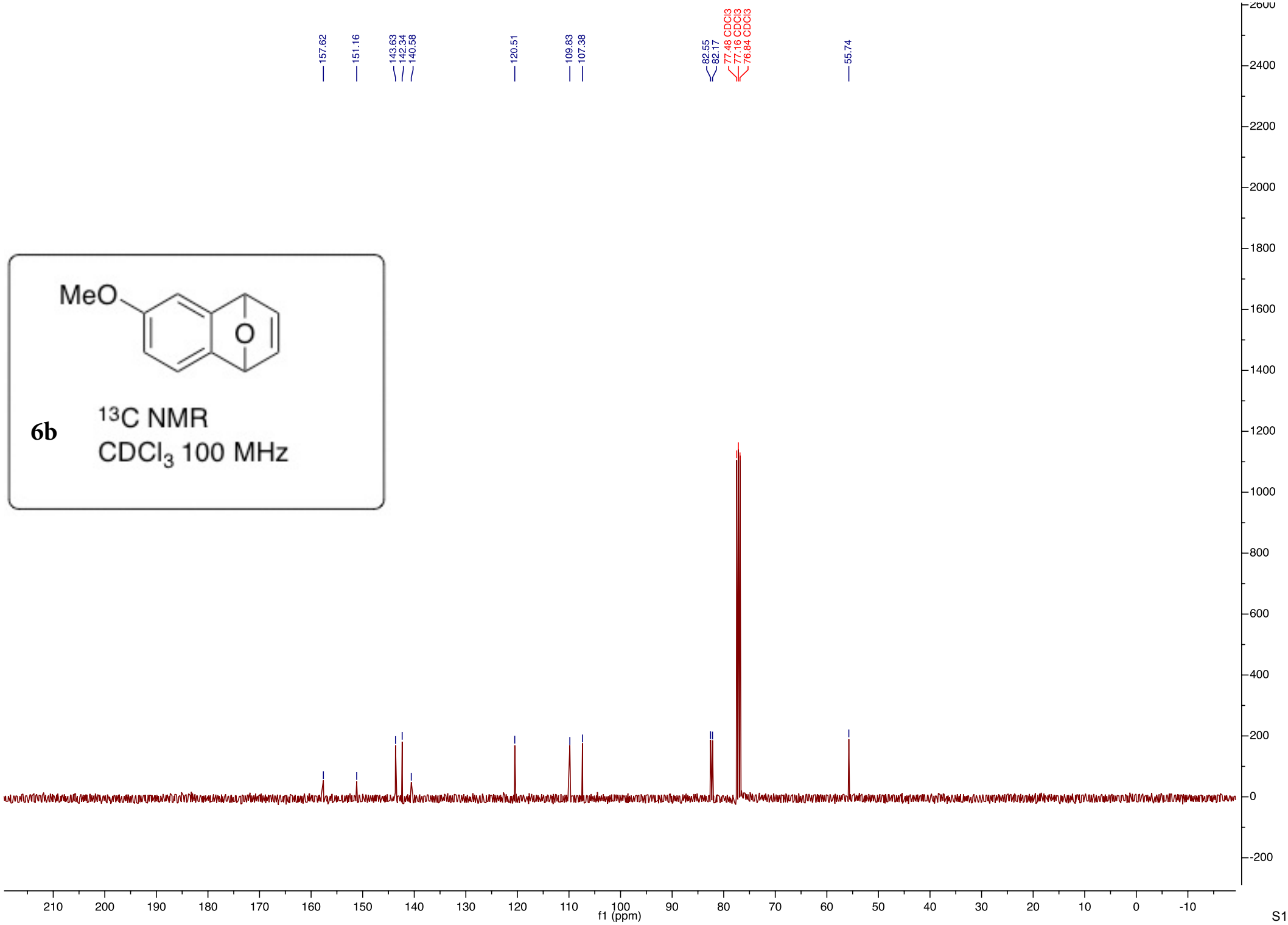

7.88 7.87 7.86 7.85 7.37 7.36 7.36 7.36 7.35 7.35 7.35 7.34 CDCl3 7.34 7.33 7.33 7.32 7.32 7.31 7.30 7.29 7.29 7.29 7.28 7.27 7.27 7.26 7.14 7.14 7.12 7.12 7.12 7.10 7.10 7.10 6.99 6.99 6.99 6.99 6.98 6.98 6.97 6.97 6.97 6.96 6.96 6.96 6.91 6.91 6.90 6.89 6.89 6.89 6.88 6.88 6.87 6.86 6.85
O
I
5a
1H NMR
CDCl3 400 MHz
1.00
3.61
1.09
2.01
2.04
f1 (ppm)

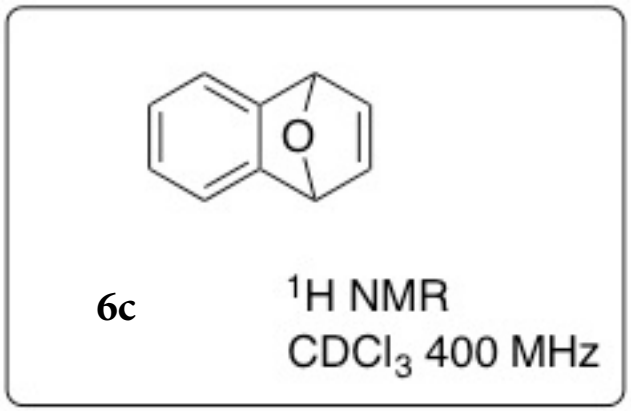

157.01
156.67
140.03
129.95
129.77
125.47
123.61
119.61
118.56
89.05
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
O
I
5a
13C NMR
CDCl3 100 MHz
f1 (ppm)

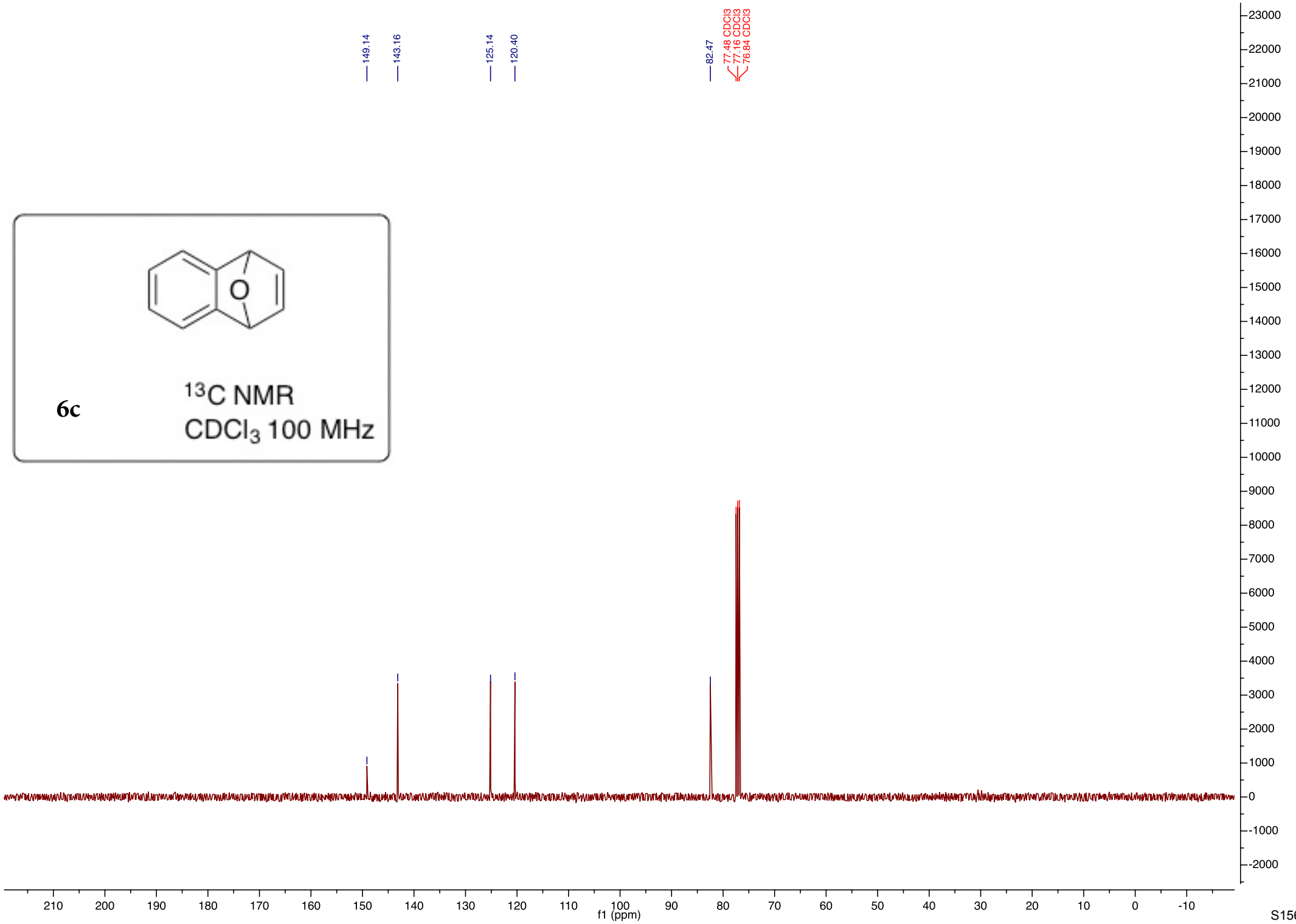

7.26 CDCl3
7.14
7.12
7.10
7.09
7.09
7.09
7.09
7.03
7.03
7.02
7.01
7.01
7.01
7.00
7.00
6.99
6.78
6.78
6.78
6.77
6.77
6.76
6.76
6.76
6.76
6.76
6.75
5.68
5.68
5.67
5.67
2.30
1.56 HDO
O
6a
1H NMR
CDCl3 400 MHz
1.06
1.01
0.52
1.00
1.74
f1 (ppm)

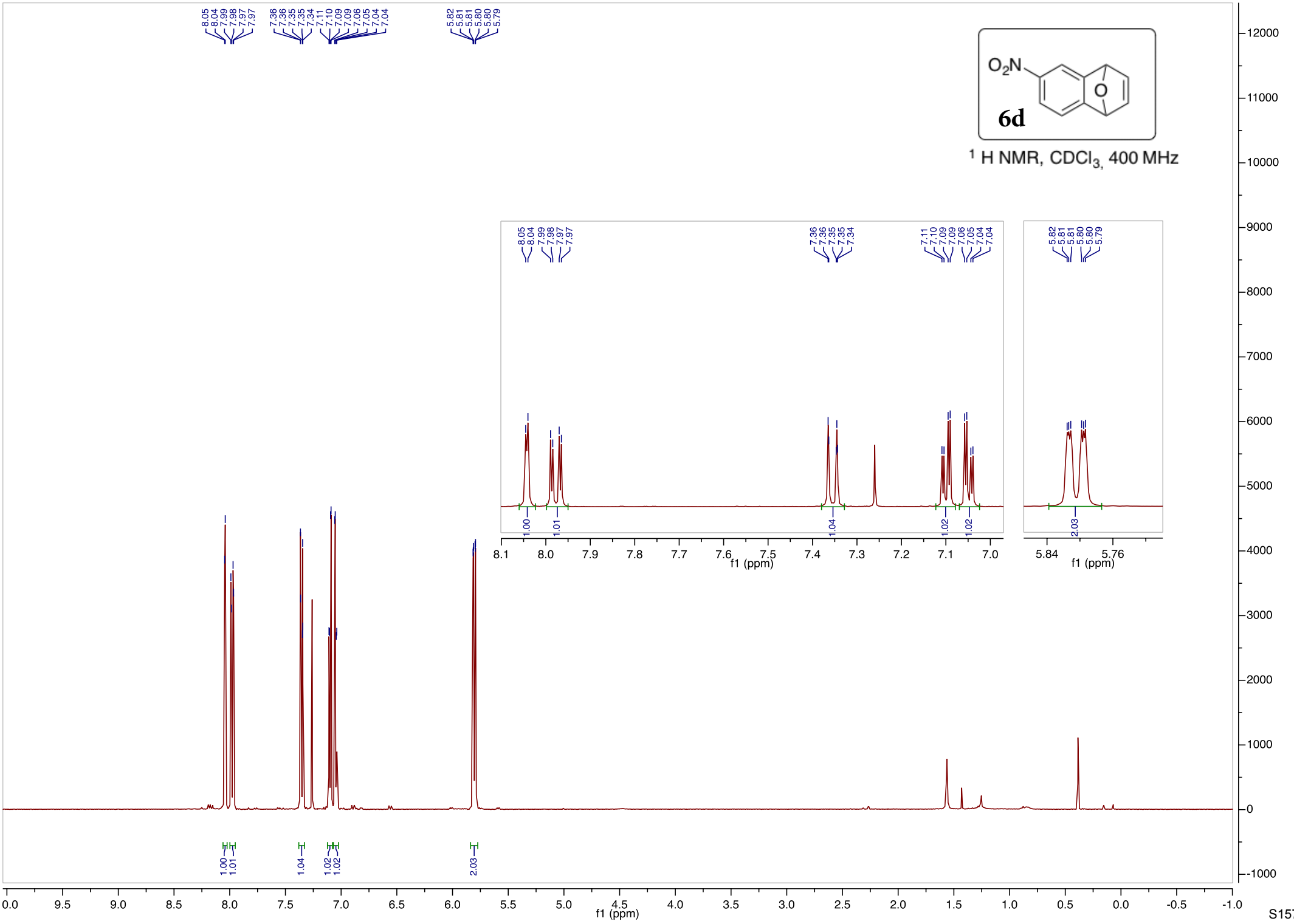

149.50
146.17
143.38
142.90
134.90
125.12
121.76
120.07
82.44
82.33
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
21.43
O
6a
13C NMR
CDCl3 100 MHz
f1 (ppm)

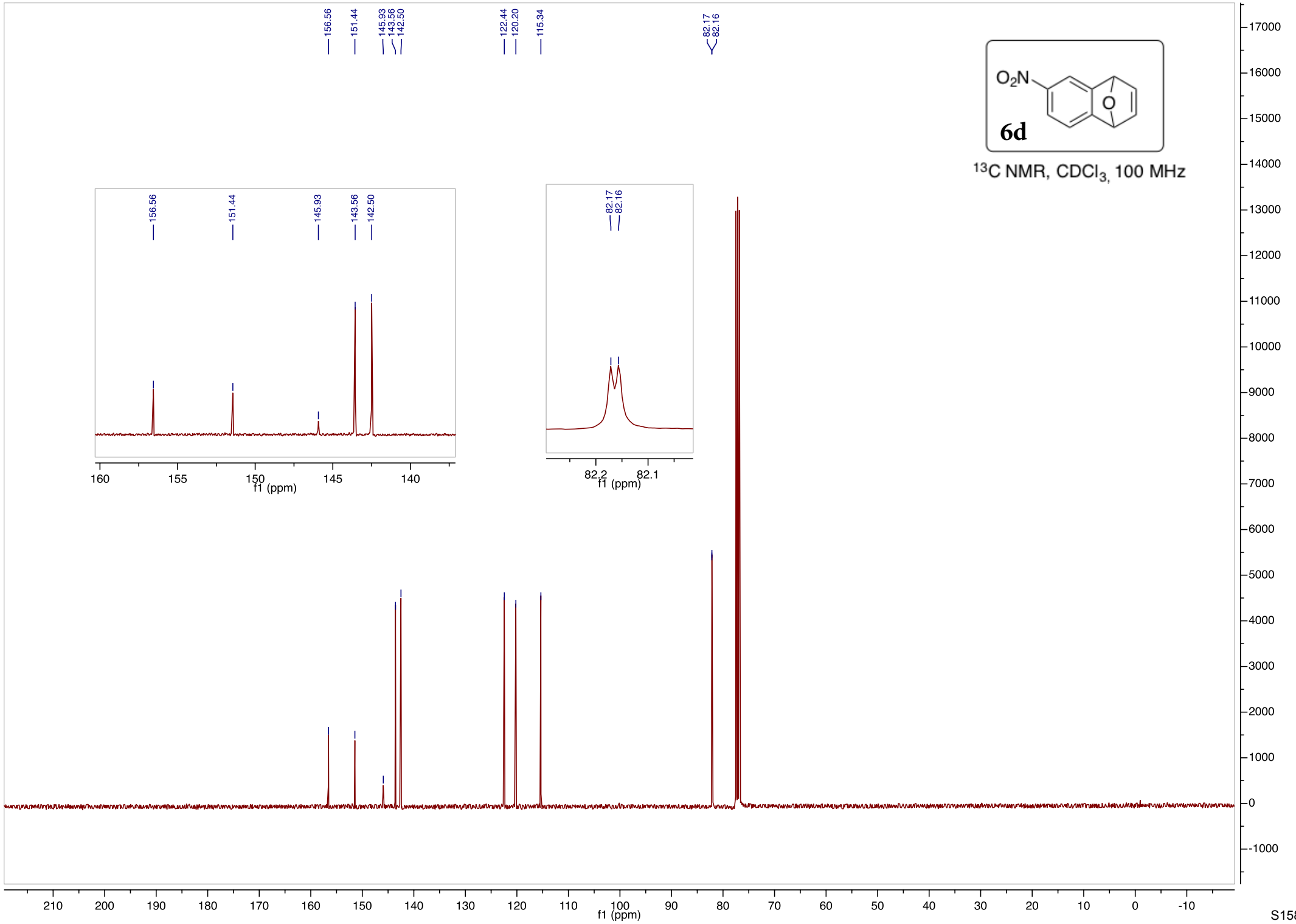

MeO
O
6b
^{1}H NMR
$CDCl_3$ 400 MHz
7.26 CDCl3
7.14
7.13
7.12
7.11
7.03
7.03
7.02
7.01
7.01
7.00
6.99
6.98
6.98
6.91
6.90
6.43
6.43
6.41
6.41
5.68
5.68
5.68
5.67
5.67
5.66
5.66
5.66
5.66
5.65
3.77
1.56 HDO
f1 (ppm)
1.05
2.07
1.00
1.07
2.03
3.27

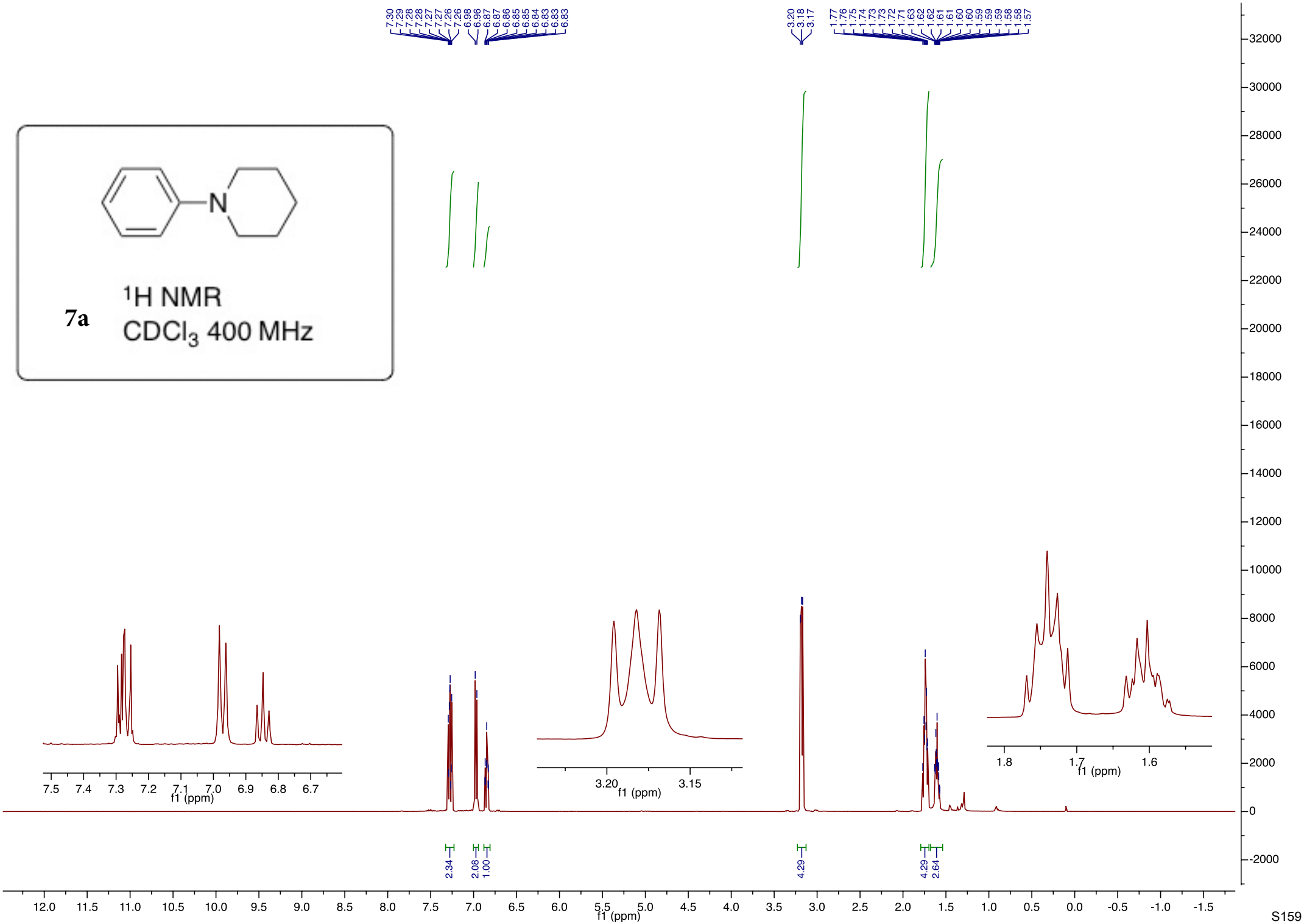

157.62
151.16
143.63
142.34
140.58
120.51
109.83
107.38
82.55
82.17
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
55.74
MeO
O
6b
13C NMR
CDCl3 100 MHz
f1 (ppm)

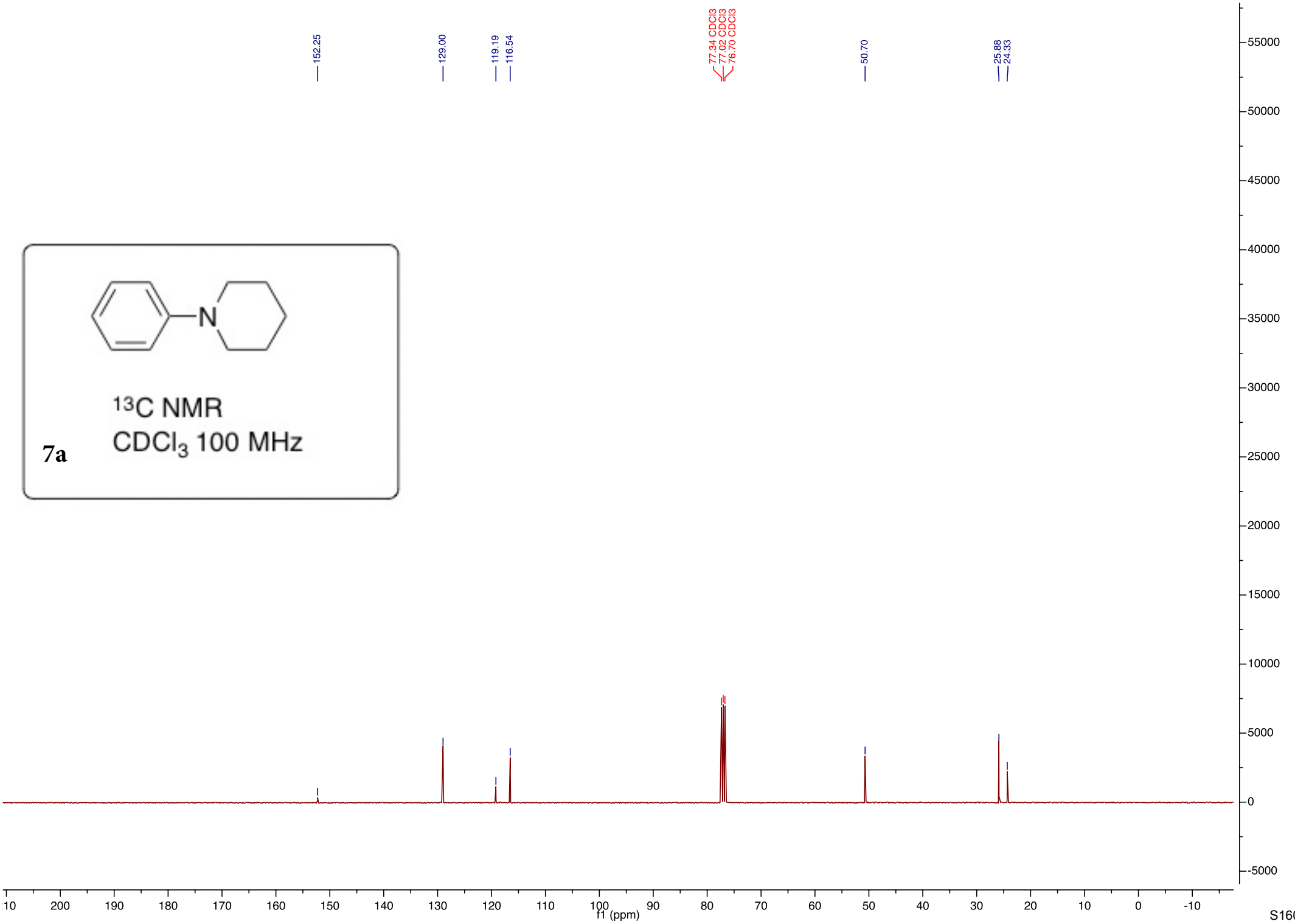

6c
^{1}H NMR
$CDCl_3$ 400 MHz

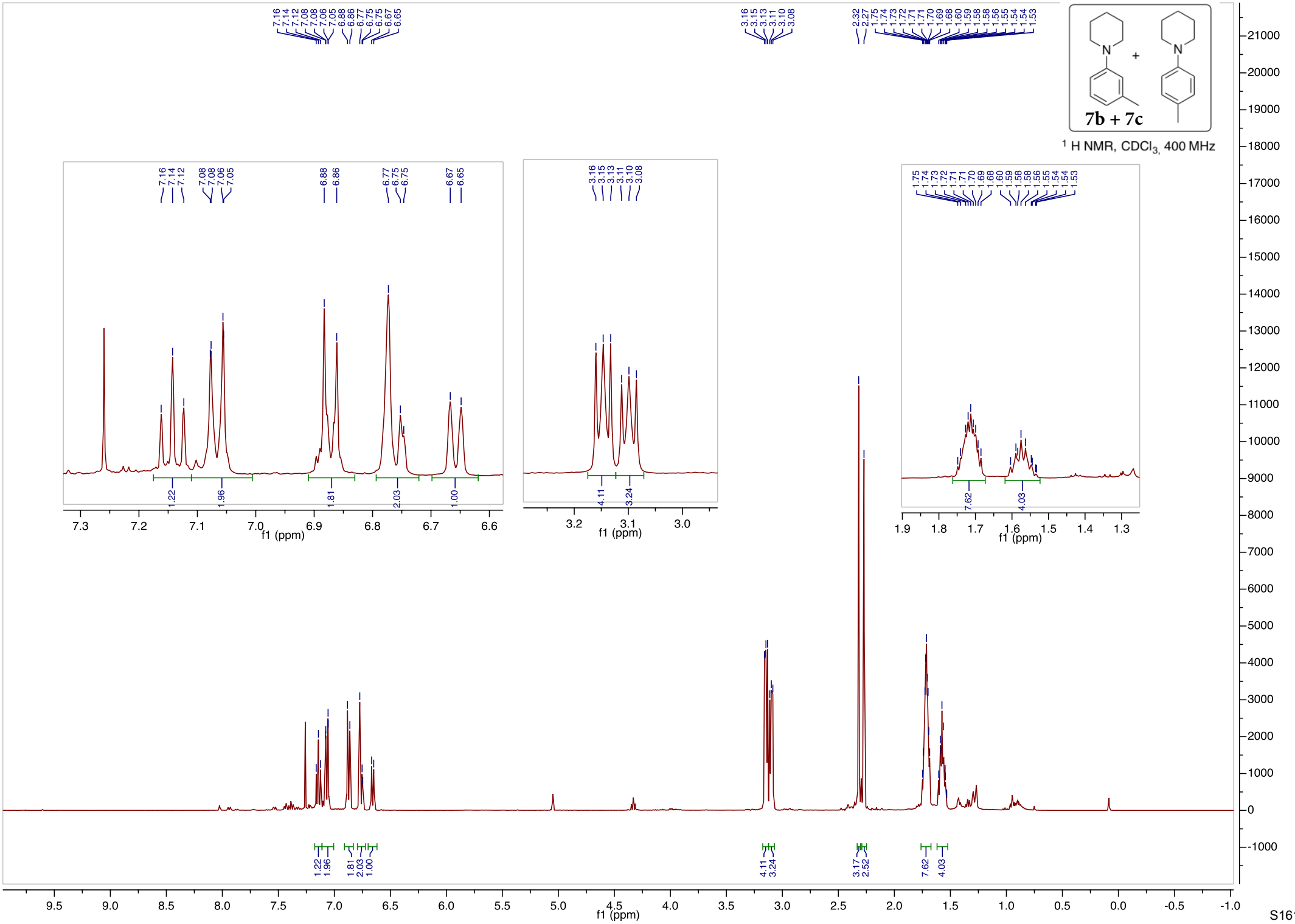

149.14
143.16
125.14
120.40
82.47
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
O
6c
13C NMR
CDCl3 100 MHz
f1 (ppm)

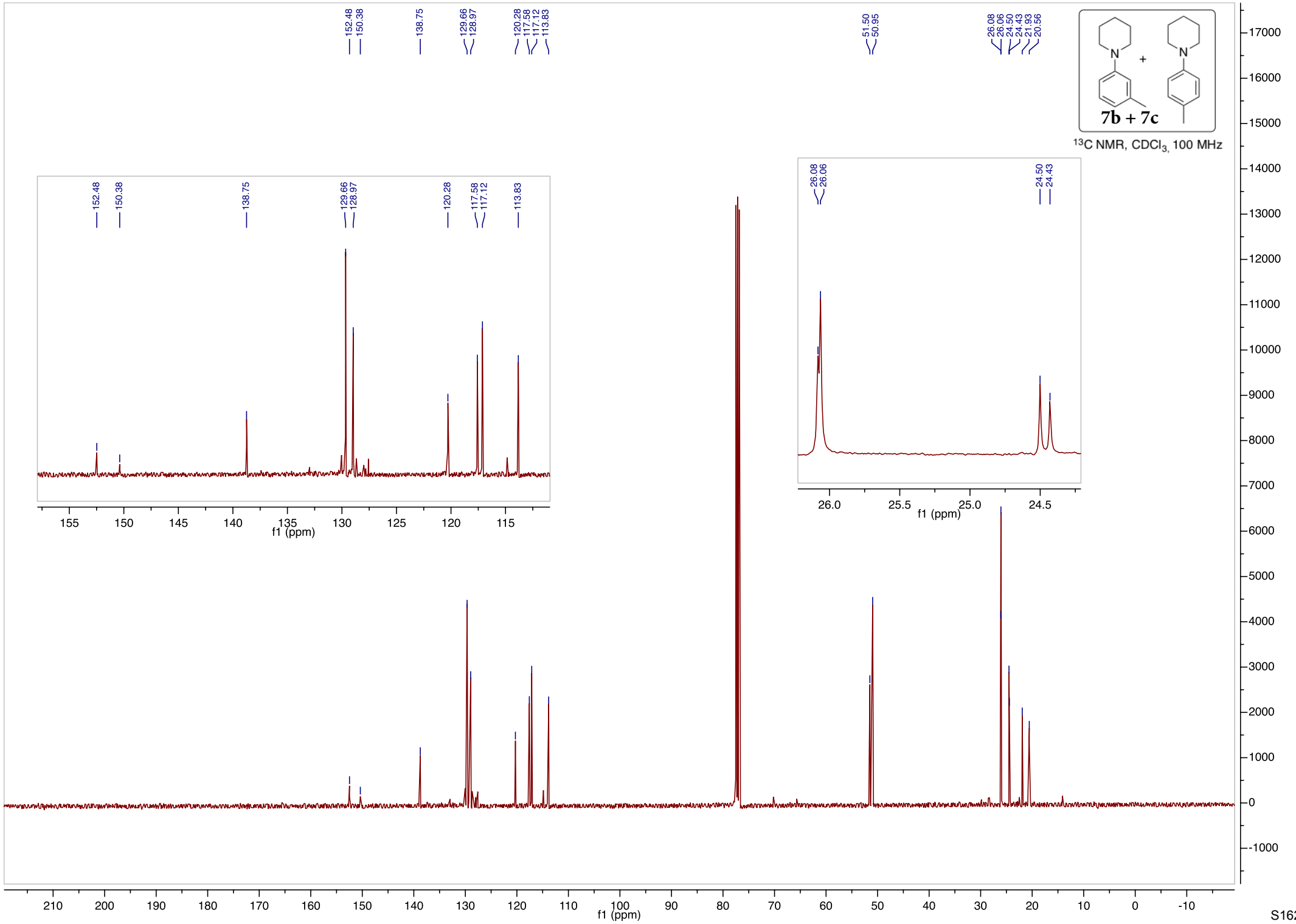

8.05
8.04
7.99
7.98
7.97
7.97
7.36
7.36
7.35
7.35
7.34
7.11
7.10
7.09
7.09
7.06
7.05
7.04
7.04
5.82
5.81
5.81
5.80
5.80
5.79
O2N
O
6d
1 H NMR, CDCl3, 400 MHz
1.00
1.01
1.04
1.02
1.02
2.03
f1 (ppm)

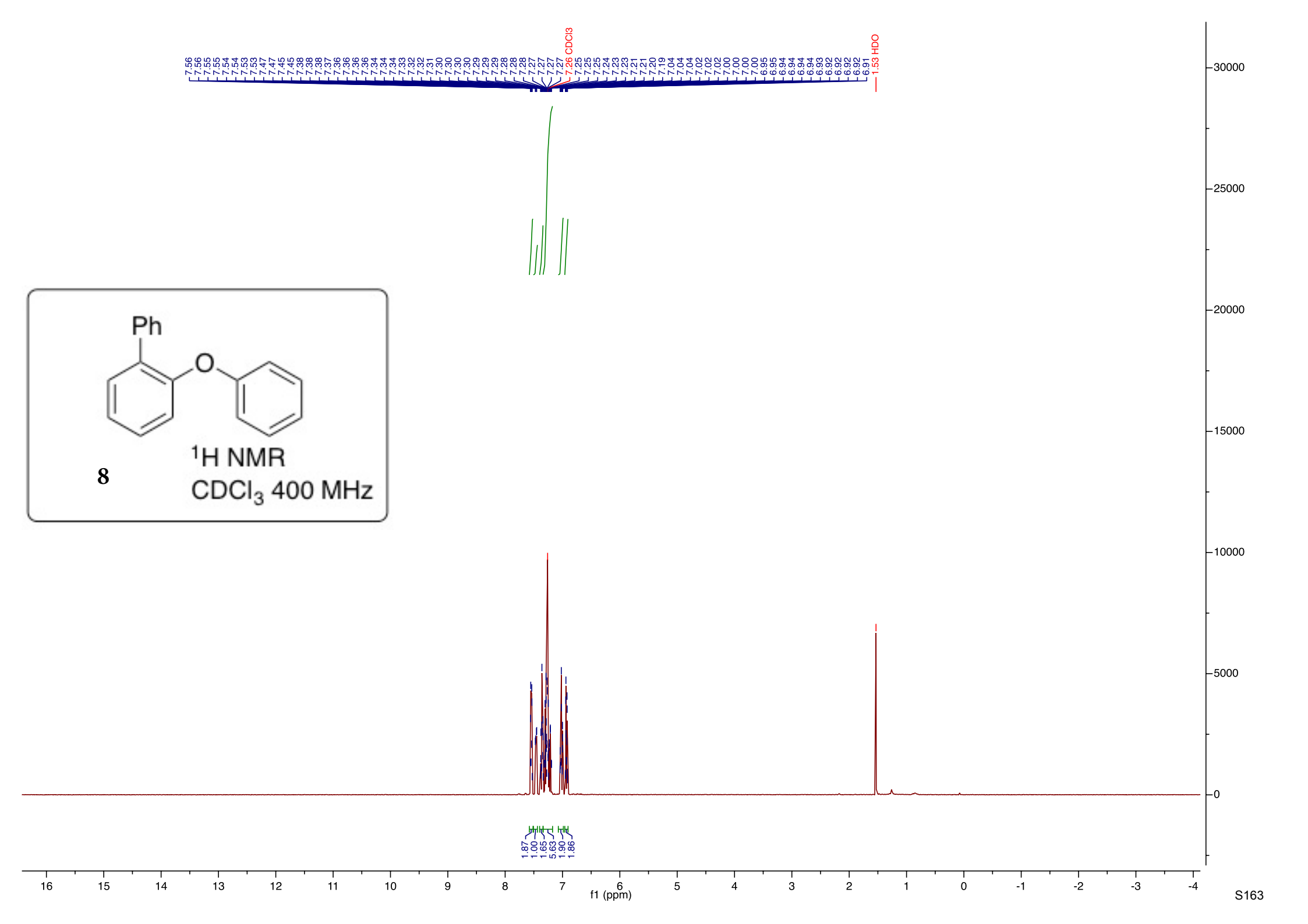

156.56
151.44
145.93
143.56
142.50
122.44
120.20
115.34
82.17
82.16
O2N
O
6d
13C NMR, CDCl3, 100 MHz
f1 (ppm)

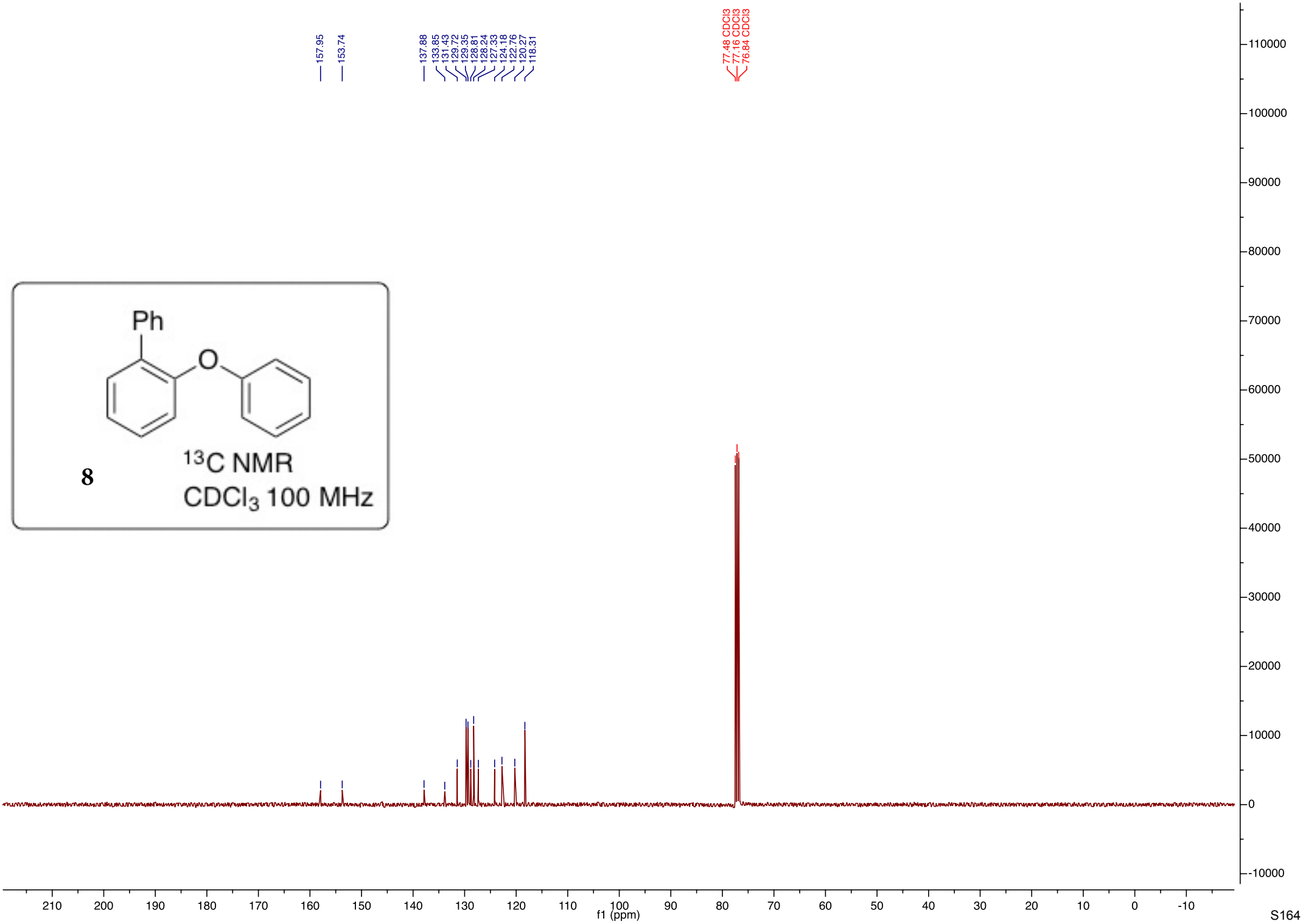

7a
^{1}H NMR
$CDCl_3$ 400 MHz
N
7.30 7.29 7.28 7.28 7.27 7.27 7.26 7.26 6.98 6.96 6.87 6.87 6.86 6.85 6.84 6.83 6.83 6.83
3.20 3.18 3.17
1.77 1.76 1.75 1.74 1.73 1.73 1.72 1.71 1.63 1.62 1.62 1.61 1.61 1.60 1.59 1.59 1.59 1.58 1.57
2.34 2.08 1.00 4.29 4.29 2.64
f1 (ppm)


152.25
129.00
119.19
116.54
77.34 CDCl3
77.02 CDCl3
76.70 CDCl3
50.70
25.88
24.33
N
^{13}C NMR
$CDCl_3$ 100 MHz
7a
f1 (ppm)


7b + 7c
^{1}H NMR, $CDCl_3$, 400 MHz
f1 (ppm)


152.48
150.38
138.75
129.66
128.97
120.28
117.58
117.12
113.83
51.50
50.95
26.08
26.06
24.50
24.43
21.93
20.56
7b + 7c
13C NMR, CDCl3, 100 MHz
f1 (ppm)


Ph
O
8
^{1}H NMR
$CDCl_3$ 400 MHz
7.26 CDCl3
1.53 HDO
1.87
1.00
1.65
5.63
1.90
1.86
f1 (ppm)


157.95
153.74
137.88
133.85
131.43
129.72
129.35
128.81
128.24
127.33
124.18
122.76
120.27
118.31
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
Ph
O
8
13C NMR
CDCl3 100 MHz
f1 (ppm)