Synthesis of Neocannabinoids Using Controlled Friedel-Crafts Reactions

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General Information:

A. Instrumentation and Methods

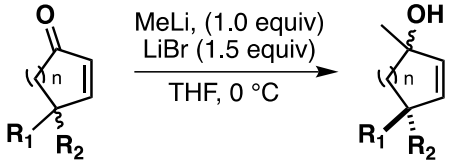
^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a Varian Agilent-500 MHz VNMRS (500 and 126 MHz, respectively), and are internally referenced to the residual protio solvent signal ($CDCl_3$: δ 7.26 and 77.0 ppm). Data for ^{1}H NMR are reported as follows: chemical shift, integration, multiplicity (br s = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, overlap = overlapping peaks) and coupling constants in Hz and data for ^{13}C NMR are reported in terms of chemical shift. High resolution mass spectrometry data was obtained in the Boston University Chemical Instrumentation Center on a Waters Q-TOF (hybrid quadrupolar/time-of-flight) Premier system by electrospray (ESI) in the negative mode. Mass correction was done by an external reference using a Waters Lockspray accessory. Mobile phases were water and acetonitrile with 0.1% formic acid. The MS settings were capillary voltage = 3.2 or 3.0 kV, cone voltage = 10 or 35, source temperature = 120 °C and dissolvation temperature = 350 °C [cone voltage = 10 and dissolvation temperature = 120 °C if experiment was carried out in low T and low V]. Analytical LC–MS experiments were performed using a Waters Acquity UPLC (ultraperformance liquid chromatography) with a binary solvent *manager*, SQ mass spectrometer, Waters 2996 PDA (photodiode array) detector, and evaporative light scattering detector (ELSD). Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator using a water bath. Chromatographic purification of products was accomplished by flash chromatography on Silicycle F60 silica gel. All reactions were carried out in well ventilated fume hoods. Reactions were monitored by thin-layer chromatography (TLC) using Silicycle 250 μm silica gel plates. Visualization of the developed chromatogram was performed by irradiation with a 254 nm Ultra-Violet (UV) light or treatment with iodine-silica chamber. Yields refer to purified compounds unless otherwise noted. Diastereoselectivity and regiochemical selectivity for reactions were determined by crude ^{1}H NMR analysis prior to purification.

B. Reagents and Solvents

Solvents methylene chloride, toluene, chloroform-d, and acetonitrile were purchased from Fischer Scientific. Commercial starting materials α-phellandrene, 4-methylcyclohexanone, 4-t-butylcyclohexanone, 4,4-dimethylcyclohex-2-enone, cyclohept-2-en-1-one, orcinol, and methanesulfonic acid (MsOH) were purchased from Sigma Aldrich. β-pinene was purchased from Acros Organics. The commercial resorcinol reagents olivetol and divarinol were obtained from Shanghai Xishite Biosciences Co., Ltd. 5-(1,1-Dimethyl-heptyl)resorcinol was purchased from Oakwood Chemical.

Experimental Procedures for Cyclic Allylic Alcohol Derivatives:

Procedure A:

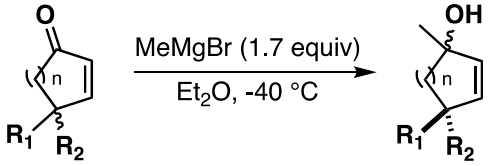


n= 1,
n= 2,
n= 3

R_1 = H, R_2 = *i*-Pr
R_1 = R_2 = H
R_1 = H, R_2 = CH_3
R_1 = R_2 = CH_3
R_1 = H, R_2 = *t*-Bu

To a flame dried round-bottom flask was added lithium bromide (7.80 mmol, 1.5 equiv) under an Ar balloon and the reaction was cooled to 0 °C with an ice bath. After cooling, THF (12 mL) and cyclic allylic ketone (5.20 mmol, 1.0 equiv) is added and the reaction was stirred. Methyl lithium in diethyl ether (1.5 M, 5.20 mL, 7.80 mmol, 1.5 equiv) was added dropwise and the reaction was stirred at 0 °C for 3 h or until full consumption of starting material was observed by TLC analysis. The reaction was then quenched with saturated NH_4Cl solution at 0 °C and was allowed to warm to room temperature. The resulting mixture was extracted with diethyl ether, dried over Na_2SO_4, and evaporated to afford the crude cyclic allylic alcohol without further purification.

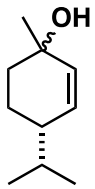
Procedure B:



n= 1,
n= 2,
n= 3

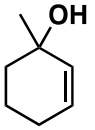
R_1 = H, R_2 = *i*-Pr
R_1 = R_2 = H
R_1 = H, R_2 = CH_3
R_1 = R_2 = CH_3
R_1 = H, R_2 = *t*-Bu

To a flame dried round-bottom flask was added cyclic allylic ketone (3.22 mmol, 1.0 equiv) and dry diethyl ether (6.4 mL) under an Ar balloon. The solution was cooled to -40 °C and was then added dropwise a solution of methyl magnesium bromide in ether (3.0 M, 1.7 equiv, 1.83 mL). The reaction was stirred until full consumption of starting material (3 h to overnight) by TLC analysis. The reaction was quenched with a saturated NH_4Cl solution and extracted with diethyl ether, dried over Na_2SO_4, and evaporated to afford the crude cyclic allylic alcohol which was used without further purification.



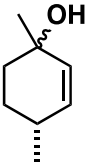
(+/-)-10
***trans*-4-isopropyl-1-methylcyclohex-2-en-1-ol**
Chemical Formula: $C_{10}H_{18}O$
Exact Mass: 154.14

Trans-4-isopropyl-1-methylcyclohex-2-en-1-ol (**±-10**) was prepared as outlined in **Procedure A** and was isolated as a colorless oil and as a 5:1 (*trans/cis*) diastereomeric mixture (706 mg, 5.20 mmol, 88%).[S4, S5, S11] The physical and spectroscopic data of the mixture was consistent with the reported values.[S4]
^{1}H NMR (400 MHz, $CDCl_3$): δ 5.61 (s, 2H), 1.92 – 1.97 (m, 1H), 1.83 – 1.89 (m, 1H), 1.70 – 1.76 (m, 1H), 1.56 – 1.66 (m, 2H), 1.37–1.42 (m, 1H), 1.27 (s, 3H), 0.89 (d, *J* = 6.8 Hz, 3H), 0.87 (d, *J* = 6.8 Hz, 3H) (*trans*). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.7, 131.4, 69.7, 41.8, 38.2, 31.9, 28.6, 23.7, 19.9, 19.5 (*trans*).



(+/-)-10c
1-methylcyclohex-2-en-1-ol
Chemical Formula: $C_7H_{12}O$
Exact Mass: 112.09

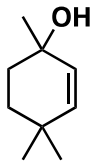
1-Methylcyclohex-2-en-1-ol (**±-10c**) was prepared as outlined in **Procedure B** and was isolated as a colorless oil (220 mg, 3.22 mmol, 61%).[S1] Physical and spectroscopic data were consistent with the reported values.[S1]
^{1}H NMR (200 MHz, $CDCl_3$): δ 5.75 (td, *J* = 4.0, 10.0 Hz, 1H), 5.60 (dm, *J* = 10.0 Hz, 1H), 2.10 (m, 2H), 1.50-1.80 (m, 5H), 1.29 (s, 3H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 133.7, 129.1, 67.9, 37.9, 29.3, 25.1, 19.6.



(+/-)-10d
***trans*-1,4-dimethylcyclohex-2-en-1-ol**
Chemical Formula: $C_8H_{14}O$
Exact Mass: 126.10

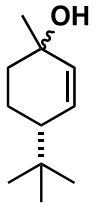
Trans-1,4-dimethylcyclohex-2-en-1-ol (**±-10d**) was prepared as outlined in **Procedure A** and was isolated as a colorless oil and as a 3:1 (*trans/cis*) diastereomeric mixture (526 mg, 5.20 mmol, 80%).[S10] The physical and spectroscopic data of the mixture was consistent with the reported values.[S10]

^{1}H NMR (400 MHz, $CDCl_3$): δ 5.55 (s, 2H), 2.30-1.20 (m, 4H), 1.29 (s, 3H), 0.97 (d, *J* = 7.2 Hz, 3H) (*trans*). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.3, 133.2, 68.9, 36.9, 28.9, 28.8, 27.9, 20.8 (*trans*).



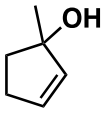
(+/-)-10e
1,4,4-trimethylcyclohex-2-en-1-ol
Chemical Formula: $C_9H_{16}O$
Exact Mass: 140.12

1,4,4-Trimethylcyclohex-2-en-1-ol (**±-10e**) was prepared as outlined in **Procedure B** and was isolated as a colorless oil (360 mg, 3.22 mmol, 80%).[S1] Physical and spectroscopic data were consistent with the reported values.[S2]
^{1}H NMR (300 MHz, $CDCl_3$): δ 5.46 (m, 2H), 1.78-1.68 (m, 2H), 1.64-1.55 (m, 1H), 1.44 (s, 1H), 1.50-1.42 (m, 1H), 1.28 (s, 3H), 1.01 (s, 3H), 0.96 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 139.4, 131.3, 68.2, 35.2, 34.2, 32.0, 29.8, 29.3, 28.3.



(+/-)-10f
***trans*-4-(*tert*-butyl)-1-methylcyclohex-2-en-1-ol**
Chemical Formula: $C_{11}H_{20}O$
Exact Mass: 168.15

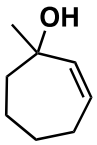
Trans-4-(*tert*-butyl)-1-methylcyclohex-2-en-1-ol (**±-10f**) was prepared as outlined in **Procedure B** and isolated as a colorless solid and as a 98:2 (*trans/cis*) diastereomeric mixture (355 mg, 3.22 mmol, 66%).[S1] The physical and spectroscopic data of the mixture was consistent with the reported values.[S3]
^{1}H NMR (100 MHz, $CDCl_3$): δ 5.59 (br s, 2H), 1.21 (s, 3H), 0.88 (s, 9H) (*trans*).



(+/-)-17
1-methylcyclopent-2-en-1-ol
Chemical Formula: $C_6H_{10}O$
Exact Mass: 98.07

1-Methylcyclopent-2-en-1-ol (**±-17**) was prepared as outlined in **Procedure A** and isolated as a colorless oil (312 mg, 5.20 mmol, 61%).[S8] Physical and spectroscopic data was consistent with literature reported values.[S8, S9]

^{1}H NMR (400 MHz, $CDCl_3$): δ 5.83–5.81 (m, 1H), 5.70–5.69 (m, 1H), 2.51–2.45 (m,1H), 2.35–2.29 (m, 1H), 1.98–1.89 (m, 2H), 1.68 (br s, 1H), 1.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.9, 132.7, 83.4, 39.7, 31.1, 27.4.

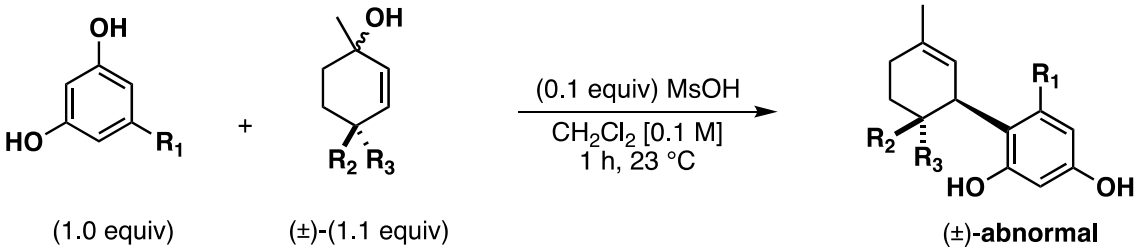


(+/-)-20
1-methylcyclohept-2-en-1-ol
Chemical Formula: $C_8H_{14}O$
Exact Mass: 126.10

1-Methylcyclohept-2-en-1-ol (**±-20**) was prepared as outlined in **Procedure A** and isolated as a colorless oil (302 mg, 5.20 mmol, 46%).[S6, S7] The physical and spectroscopic data of the mixture was consistent with the reported values.[S7]
^{1}H NMR (250.1 MHz, $CDCl_3$): δ 5.64 (dm, *J* = 2.9 Hz, 2H), 2.00-2.40 (m, 3H), 1.50-1.90 (m, 6H), 1.32 (d, *J* = 2.9 Hz, 3H). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 139.7, 129.1, 74.0, 40.8, 28.6, 27.5, 27.3, 24.3.

Experimental Procedures for Neocannabinoid Isomers *via* Friedel-Crafts Reaction:

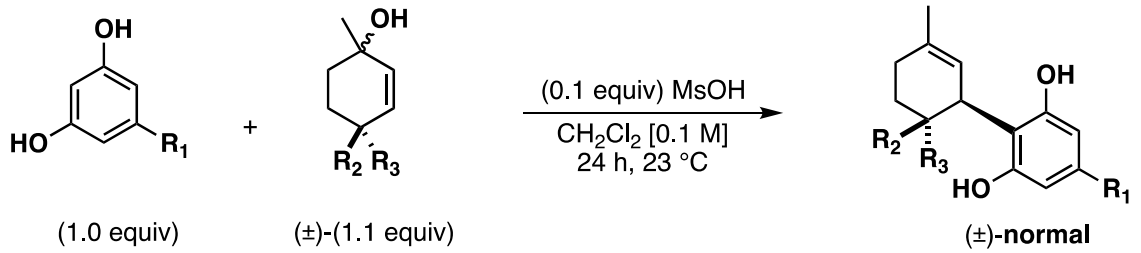
Procedure A:



(1.0 equiv) (±)-(1.1 equiv) (±)-**abnormal**

A scintillation vial was charged with resorcinol derivative (0.13 mmol, 1.0 equiv) and cyclic allylic alcohol (0.14 mmol, 1.1 equiv) along with a magnetic stir bar and the contents of the flask were dissolved in CH_2Cl_2 [0.1 M]. To the stirred solution was added MsOH (0.1 M solution in CH_2Cl_2, 0.1 equiv) dropwise. The reaction was left to stir for 1 h and was then quenched with saturated $NaHCO_3$, extracted 3x with CH_2Cl_2 and dried over Na_2SO_4. The crude material was purified by silica gel column chromatography (10:1 up to 4:1 Hexanes/EtOAc) to provide the abnormal neocannabinoid derivative.

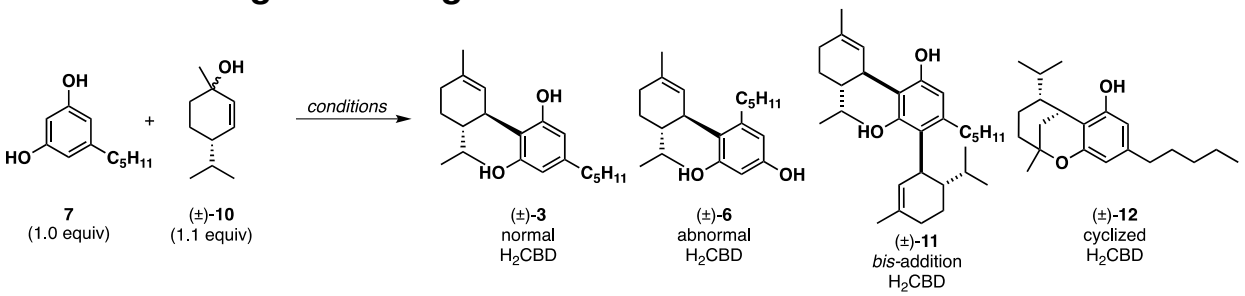
Procedure B:



(1.0 equiv) (±)-(1.1 equiv) (±)-**normal**

A scintillation vial was charged with resorcinol (0.13 mmol, 1.0 equiv) and cyclic allylic alcohol (0.14 mmol, 1.1 equiv) with a magnetic stir bar and the mixture was dissolved in CH_2Cl_2 [0.1 M]. To the stirred solution was added MsOH (0.1 M solution in CH_2Cl_2, 0.1 equiv) dropwise. The reaction was stirred 24 h and then quenched with saturated $NaHCO_3$, extracted 3 x with CH_2Cl_2, and dried over Na_2SO_4. The material was purified by column chromatography (silica gel, 20:1 up to 10:1 Hexanes/EtOAc) to provide the normal neocannabinoid derivative.

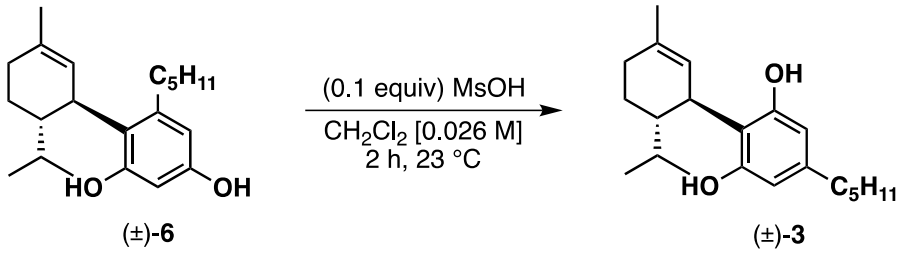
Acid-screening table for general neocannabinoid reactions:



7 (1.0 equiv) + (±)-**10** (1.1 equiv) → conditions → (±)-**3** normal H_2CBD + (±)-**6** abnormal H_2CBD + (±)-**11** *bis*-addition H_2CBD + (±)-**12** cyclized H_2CBD

						Reaction mixture composition				
entry	acid	acid amount	solvent	T (°C)	time (h)	conversion	**3**	**6**	**11**	**12**
1a	$Eu(OTf)_3$	excess	CH_2Cl_2	0	0.5	50%	5	2	1	
1b				rt	1	70%	3	1	1	
1c				40	3	71%	3	1	1	
2a	$La(OTf)_3$	excess	CH_2Cl_2	0	0.5	60%	6	3	1	
2b				rt	1	70%	3	1	1	
2c				40	3	75%	3	1	1	
3a	$La(OTf)_3$	20 mol%	CH_2Cl_2	rt	0.5	25%	2.5	1		
3b					20	80%	12.5	1	5	
4a	$Sc(OTf)_3$	excess	CH_2Cl_2	0	0.5	70%	3	1	1	
4b				rt	1	75%	3	1	1	
5a	$Yb(OTf)_3$	excess	CH_2Cl_2	0	0.5	70%	3	2	1	
5b				rt	1	60%	3	1	1	
5c				40	3	71%	3	1	1	
6a	$Yb(OTf)_3$	20 mol%	CH_2Cl_2	rt	0.25	20%	2.5	1		
6b					0.5	25%	2.5	1		
6c					20	75%	5	1	2	
7	$Yb(OTf)_3$	30 mol%	CH_2Cl_2	rt	0.5	50%	12	5	1	
8	$Ce(OTf)_3$	excess	CH_2Cl_2	rt	1	95%				1
9	$In(OTf)_3$	excess	CH_2Cl_2	rt	1	95%				1
10	MsOH	10 mol%	CH_2Cl_2	rt	16	50%	1	0	0	
11	MsOH + $Yb(OTf)_3$	10 mol% + 20 mol%	CH_2Cl_2	rt	16	95%				1
12	MsOH + $La(OTf)_3$	10 mol% + 20 mol%	CH_2Cl_2	rt	16	95%				1
13a	Schreiner's catalyst	10 mol%	CH_2Cl_2	rt	16	65%	5	7	1	
13b		20 mol%			16	68%	4	6	1	

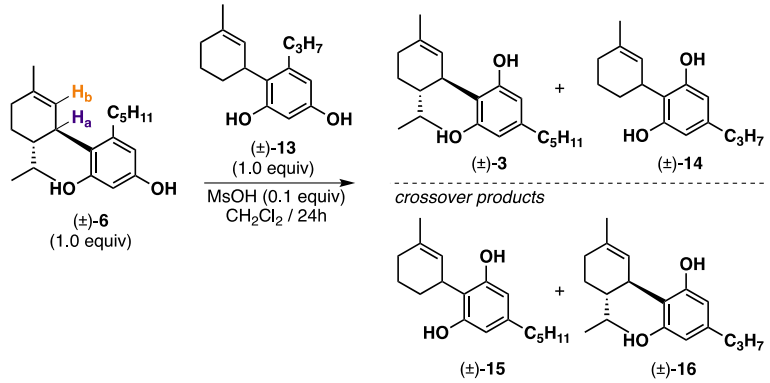
Experimental Procedure for Equilibration of Abnormal 8,9-dihydrocannabidiol:



(±)-**6** (±)-**3**

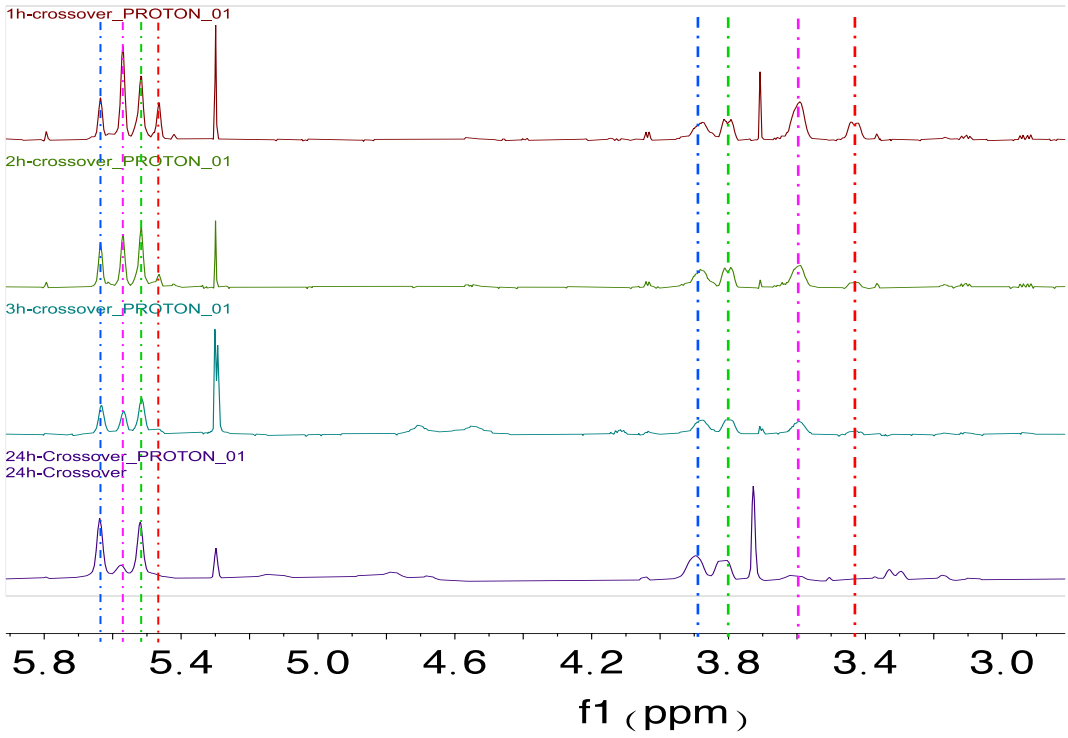
A scintillation vial with magnetic stir bar was charged with **6** (5 mg, 0.016 mmol, 1.0 equiv) and the contents of the flask was dissolved in CH_2Cl_2 [0.026 M]. To the stirred solution was added MsOH (0.1 M solution in CH_2Cl_2, 16 µL, 0.0016 mmol, 0.1 equiv) dropwise. After 2 h, the reaction was quenched with saturated $NaHCO_3$, extracted 3 x with CH_2Cl_2, and dried over Na_2SO_4. Product regioselectivity was determined by crude ^1H NMR analysis.

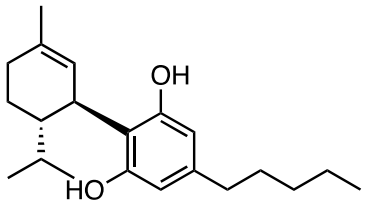
Crossover Experiment and Identification of Product Composition and Ratio:



Product	Allylic-benzylic and vinylic ^{1}H NMR signals	
	H_a	H_b
6	3.44 ppm	5.48 ppm
3	3.83 ppm	5.52 ppm
13	3.60 ppm	5.57 ppm
14	3.90 ppm	5.64 ppm

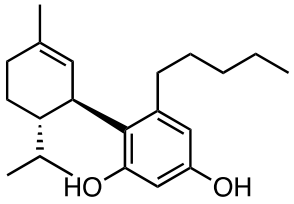
Using a combination of *in situ* ^{1}H NMR and LC/MS analyses, we monitored the ratios of the pure abnormal cannabinoids **6**/**13**, their corresponding normal isomers **3**/**14**, and crossover products **15**/**16**. Normal and abnormal cannabinoids can be distinguished by ^{1}H NMR analysis by examining the chemical shift of the H_2CBD allylic-benzylic methine H_a ^{1}H NMR signal, which appears further downfield in the normal vs. abnormal isomer; this trend of normal vs. abnormal cannabinoid derivatives was found to be consistent for other derivatives (*vide infra*). We therefore used these signature ^{1}H NMR chemical shifts to measure changes from abnormal to normal forms, and HPLC/MS to determine the existence of crossover products, as they differ in molecular weight from the starting structures **3** and **14**. By ^{1}H NMR analysis, we observed products **3** and **14** after 1 h with starting materials **6** and **13** still present; after 24 h we observe only trace amounts of **6** and **13**, and by LC/MS we obtained 26% of crossover products. *It should be noted that the crossover products NMR signals overlap with the other cannabinoids and HPLC/MS confirmed the molecular weight of all products observed.*





(±)-3
Chemical Formula: $C_{21}H_{32}O_2$
Exact Mass: 316.24

Synthesis of **(±)-3** from olivetol and **(±)-10**:
Reaction Time: 24 h
TLC: R_f= 0.53 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellowish oil
% Yield: 88% (36.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.35 – 5.93 (m, 3H), 5.52 (s, 1H), 4.78 (br s, 1H), 3.82 (dtd, *J* = 9.0, 4.6, 2.4 Hz, 1H), 2.52 – 2.34 (m, 2H), 2.23 – 2.01 (m, 2H), 1.84 – 1.74 (m, 4H), 1.66 – 1.51 (m, 4H), 1.44 – 1.36 (m, 1H), 1.35 – 1.26 (m, 4H), 0.88 (dt, *J* = 14.0, 6.7 Hz, 9H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 143.1, 140.2, 124.9, 114.1, 43.8, 35.6, 35.6, 31.7, 30.8, 30.8, 27.9, 23.8, 22.7, 22.2, 21.9, 16.5, 14.2.
HRMS-ESI (m/z): Calc. for $C_{21}H_{32}O_2$: $[M-H]^+$ = 315.2324 ; found: 315.2318

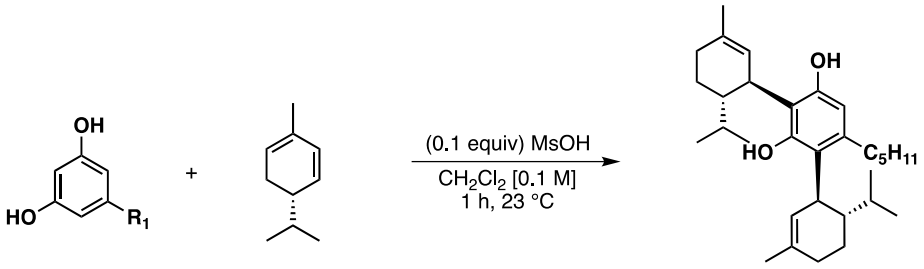


(±)-6
Chemical Formula: $C_{21}H_{32}O_2$
Exact Mass: 316.24

Synthesis of **(±)-6**from olivetol and **(±)-10**:
Reaction Time: 1 h
TLC: R_f= 0.33 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 41% (17.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (d, *J* = 2.7 Hz, 1H), 6.21 (d, *J* = 2.7 Hz, 1H), 6.07 (s, 1H), 5.47 (d, *J* = 2.0 Hz, 1H), 4.81 (br s, 1H), 3.69 – 3.27 (m, 1H), 2.66 (ddd, *J* = 13.8, 9.4, 6.1 Hz, 1H), 2.34 (ddd, *J* = 13.8, 9.5, 6.8 Hz, 1H), 2.22 – 2.05 (m, 2H), 1.82 – 1.78 (m, 1H), 1.80 – 1.74 (m, 3H), 1.73 (ddt, *J* = 12.7, 10.4, 2.3 Hz, 1H), 1.56 – 1.46 (m, 3H), 1.40 – 1.35 (m, 1H), 1.34 – 1.29 (m, 4H), 0.94 – 0.87 (m, 3H), 0.83 (dd, *J* = 7.9, 6.9 Hz, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 154.7, 144.2, 140.1, 125.3, 120.4, 108.7, 102.6, 43.1, 38.4, 34.4, 32.0, 31.4, 30.7, 27.4, 23.8, 22.7, 22.3, 22.1, 16.9, 14.2.
HRMS-ESI (m/z): Calc. for $C_{21}H_{32}O_2$: $[M-H]^+$ = 315.2324 ; found: 315.2328

Experimental Procedure for *Bis*-Addition and Stereochemistry Determination:

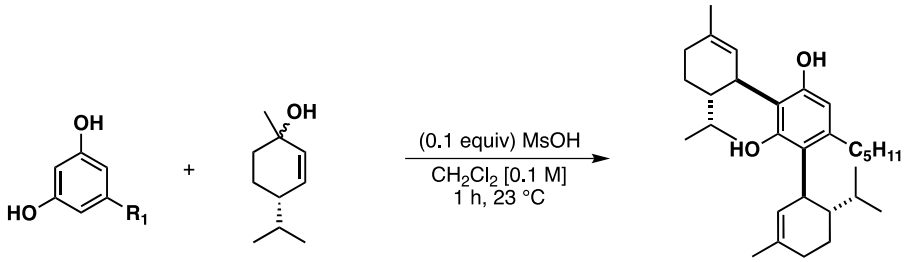
Procedure A:



7 (1.0 equiv) | **(R)-α-phellandrene** (1.1 equiv) | **11a** *bis*-addition H_2CBD

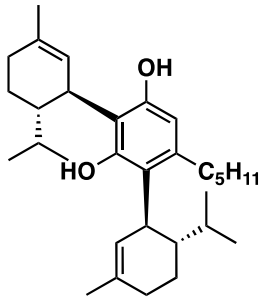
A scintillation vial was charged with olivetol **7** (1.0 equiv) and (1.1 equiv) (*R*)-α-phellandrene (≥95.0% sum of enantiomers, GC) with a magnetic stir bar and the flask contents were dissolved in CH_2Cl_2 [0.1 M]. To the stirred solution was added *p*-MsOH (0.1 M solution in CH_2Cl_2, 0.1 equiv) dropwise. The reaction was stirred for 1 h and was then quenched with saturated $NaHCO_3$, extracted 3 x with CH_2Cl_2, and dried over Na_2SO_4. The material was purified by silica column chromatography (silica gel, 10:1 Hexanes/EtOAc) to provide *bis*-addition product **11a** as a single diastereomer.

Procedure B:



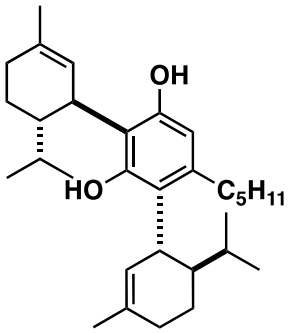
7 (1.0 equiv) | (±)-**10** (1.1 equiv) | **11a and 11b** *bis*-addition H_2CBD

A scintillation vial was charged with olivetol **7** (1.0 equiv) and cyclic allylic alcohol **10** (1.1 equiv) and a magnetic stir bar and the contents of the flask was dissolved in CH_2Cl_2 [0.1 M]. To the stirred solution was added MsOH (0.1 M solution in CH_2Cl_2, 0.1 equiv) dropwise. The reaction was stirred for 1 h then quenched with saturated $NaHCO_3$, extracted 3 x with CH_2Cl_2, and dried over Na_2SO_4. The material was purified by column chromatography (silica gel, 10:1 Hexanes/EtOAc) to provide a mixture of diastereomeric *bis*-addition products **11a** and **11b**. The products were separated by prep-TLC (Silicycle 250 μm silica gel plates, 10:1 Hexanes/Et_2O) to determine each diastereomers stereochemistry. The first diastereomer was determined to be **11a** (*cf.* **Procedure A**) as its spectroscopic properties, ^{1}H, ^{13}C, and 1D NOESY matched the product obtained from the control reaction with (*R*)-α-phellandrene.



(±)-11a
Chemical Formula: $C_{31}H_{48}O_2$
Exact Mass: 452.37

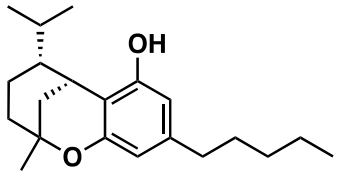
Compound **(±)-11a** from olivetol and **(±)-10**:
Reaction Time: 1 h
TLC: R_f= 0.88 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: orange/yellow oil
% Yield: 6% (3.5 mg) by-product
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (s, 1H), 6.00 (s, 1H), 5.93 (s, 1H), 5.60 – 5.53 (m, 1H), 5.51 (s, 1H), 3.99 – 3.56 (m, 1H), 3.43 (d, *J* = 10.4 Hz, 1H), 2.63 (ddd, *J* = 14.7, 9.4, 6.0 Hz, 1H), 2.32 (ddd, *J* = 13.9, 9.5, 6.9 Hz, 1H), 2.19 – 2.03 (m, 4H), 1.76 (dd, *J* = 10.0, 2.3 Hz, 8H), 1.57 – 1.42 (m, 6H), 1.39 – 1.30 (m, 6H), 0.92 – 0.86 (m, 3H), 0.81 (dd, *J* = 14.5, 6.9 Hz, 9H), 0.75 (d, *J* = 6.9 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 154.4, 154.3, 141.4, 140.1, 139.6, 125.4, 119.2, 115.8, 109.7, 44.0, 42.7, 39.0, 35.6, 34.3, 32.1, 31.5, 31.1, 31.0, 28.1, 27.5, 23.8, 23.8, 22.7, 22.6, 22.5, 22.0, 21.7, 16.9, 16.8, 14.2.
HRMS-ESI (m/z): Calc. for $C_{31}H_{48}O_2$: $[M-H]^+$ = 451.3576 ; found: 451.3697



(±)-11b
Chemical Formula: $C_{31}H_{48}O_2$
Exact Mass: 452.37

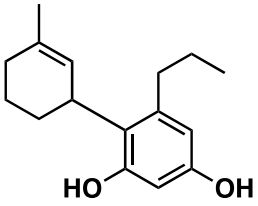
Synthesis of **(±)-11b** from olivetol and **(±)-10**:
Reaction Time: 1 h
TLC: R_f= 0.80 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: orange/yellow oil
% Yield: 6% (3.5 mg) by-product
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (s, 1H), 6.03 (s, 1H), 5.95 (s, 1H), 5.54 (s, 1H), 5.42 (s, 1H), 3.86 (d, *J* = 10.1 Hz, 1H), 3.44 (d, *J* = 10.2 Hz, 1H), 2.68 – 2.53 (m, 1H), 2.46 –

2.26 (m, 1H), 2.21 – 2.01 (m, 4H), 1.79 – 1.72 (m, 8H), 1.62 – 1.54 (m, 3H), 1.54 – 1.46 (m, 3H), 1.39 – 1.29 (m, 6H), 0.91 – 0.87 (m, 3H), 0.85 – 0.77 (m, 12H).
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 154.4, 154.2, 141.3, 140.2, 139.4, 125.7, 125.6, 119.5, 116.1, 109.6, 43.8, 42.6, 38.8, 35.6, 34.2, 32.2, 31.2, 30.9, 30.8, 28.0, 27.5, 23.7, 23.6, 22.7, 22.4, 22.1, 21.8, 16.9, 16.6, 14.2.
HRMS-ESI (m/z): Calc. for $C_{31}H_{48}O_2$: $[M-H]^+$ = 451.3576 ; found: 451.3700



(±)-12
Chemical Formula: $C_{21}H_{32}O_2$
Exact Mass: 316.24

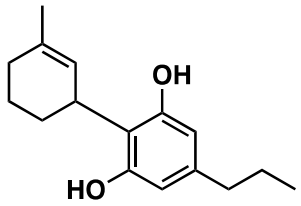
Synthesis of **(±)-12** from olivetol and **(±)-10**:
TLC: R_f= 0.52 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.29 (d, *J* = 1.5 Hz, 1H), 6.12 (d, *J* = 1.5 Hz, 1H), 4.73 (s, 1H), 3.35 (q, *J* = 3.0 Hz, 1H), 2.45 (dd, *J* = 8.9, 6.7 Hz, 2H), 1.90 (dd, *J* = 13.3, 2.6 Hz, 1H), 1.83 (dp, *J* = 10.5, 6.6 Hz, 1H), 1.74 (dq, *J* = 13.3, 3.2 Hz, 1H), 1.62 – 1.54 (m, 4H), 1.53 – 1.49 (m, 2H), 1.35 (s, 3H), 1.34 – 1.26 (m, 5H), 1.10 (d, *J* = 6.6 Hz, 3H), 0.96 (d, *J* = 6.6 Hz, 3H), 0.89 (t, *J* = 6.8 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 152.2, 142.5, 111.9, 107.9, 106.3, 74.7, 44.4, 35.8, 35.1, 31.7, 30.9, 30.7, 29.5, 27.9, 26.4, 22.7, 22.2, 21.2, 20.6, 14.2.
HRMS-ESI (m/z): Calc. for $C_{21}H_{32}O_2$: $[M-H]^+$ = 315.2324 ; found: 315.2309



(±)-13
Chemical Formula: $C_{16}H_{22}O_2$
Exact Mass: 246.16

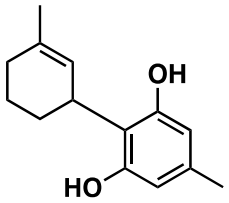
Synthesis of **13** (abnormal isomer) from divarinol and **(±)-10c**:
Reaction Time: 1h
TLC: R_f= R_f= 0.24 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 43% (14.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (d, *J* = 2.7 Hz, 1H), 6.22 (d, *J* = 2.7 Hz, 1H), 6.17 (s, 1H), 5.58 (s, 1H), 4.82 (s, 1H), 3.66 – 3.50 (m, 1H), 2.54 (dt, *J* = 13.8, 7.8 Hz, 1H), 2.44 (dt, *J* = 13.7, 7.9 Hz, 1H), 2.19 – 2.08 (m, 1H), 2.05 – 1.98 (m, 1H), 1.95 – 1.82 (m, 2H), 1.78 (dt, *J* = 2.6, 1.2 Hz, 3H), 1.68 – 1.62 (m, 2H), 1.55 (q, *J* = 7.6 Hz, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 154.7, 142.6, 141.0, 124.4, 121.0, 109.0, 102.2, 36.2, 35.4, 29.9, 28.5, 24.9, 24.2, 23.0, 14.3.
HRMS-ESI (m/z): Calc. for $C_{16}H_{22}O_2$: $[M-H]^+$ = 245.1542 ; found: 245.1540



(±)-14
Chemical Formula: $C_{16}H_{22}O_2$
Exact Mass: 246.16

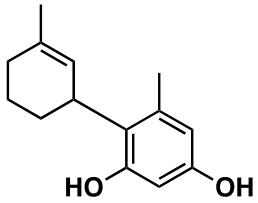
Synthesis of **(±)-14** from divarinol and **(±)-10c**:
Reaction Time: 24 h
TLC: R_f= R_f= 0.36 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 36% (11.5 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.22 (s, 2H), 5.71 – 5.51 (m, 1H), 3.90 (ddt, *J* = 8.9, 6.0, 3.0 Hz, 1H), 2.43 (dd, *J* = 8.6, 6.8 Hz, 2H), 2.18 – 2.09 (m, 1H), 2.06 – 1.99 (m, 1H), 1.98 – 1.92 (m, 1H), 1.88 (dtt, *J* = 13.4, 5.3, 2.9 Hz, 1H), 1.81 – 1.77 (m, 3H), 1.71 – 1.64 (m, 1H), 1.62 – 1.56 (m, 3H), 0.93 (t, *J* = 7.3 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 142.8, 141.2, 123.8, 114.6, 108.7, 37.7, 32.3, 30.1, 28.4, 24.3, 24.2, 22.5, 14.0.
HRMS-ESI (m/z): Calc. for $C_{16}H_{22}O_2$: $[M-H]^+$ = 245.1542 ; found: 245.1537



(±)-3ac
Chemical Formula: $C_{14}H_{18}O_2$
Exact Mass: 218.13

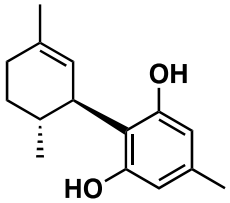
Synthesis of (**±)-3ac** from orcinol and **(±)-10c**:
Reaction Time: 24 h
TLC: R_f= 0.35 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 9% (2.5 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.22 (s, 2H), 5.64 (dq, *J* = 2.9, 1.4 Hz, 1H), 3.91 (ddq, *J* = 8.9, 5.8, 2.8 Hz, 1H), 2.21 (s, 3H), 2.18 – 2.09 (m, 1H), 2.06 – 1.99 (m, 1H), 1.98 – 1.92 (m, 1H), 1.88 (dtt, *J* = 13.6, 5.4, 2.9 Hz, 1H), 1.83 – 1.73 (m, 3H), 1.68 (tddd, *J* = 12.7, 10.1, 5.4, 2.5 Hz, 1H), 1.57 (tdd, *J* = 12.2, 9.6, 2.6 Hz, 1H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 141.2, 137.9, 123.8, 114.4, 109.3, 32.3, 30.1, 28.4, 24.3, 22.5, 21.2.

HRMS-ESI (m/z): Calc. for $C_{14}H_{18}O_2$: $[M-H]^+$ = 217.1229 ; found: 217.1206



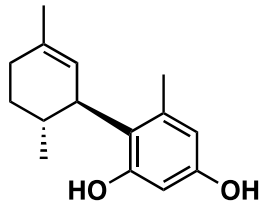
(±)-6ac
Chemical Formula: $C_{14}H_{18}O_2$
Exact Mass: 218.13

Synthesis of **(±)-6ac** from orcinol and **(±)-10c**:
Reaction Time: 1 h
TLC: R_f= 0.33 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
% Yield: 35% (10.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.28 (s, 1H), 6.27 – 6.22 (m, 1H), 6.22 (t, *J* = 1.9 Hz, 1H), 5.62 (s, 1H), 4.97 (s, 1H), 3.60 (s, 1H), 2.24 (s, 3H), 2.18 – 2.08 (m, 1H), 2.02 (dt, *J* = 17.9, 3.5 Hz, 1H), 1.94 – 1.84 (m, 2H), 1.79 (s, 3H), 1.70 – 1.61 (m, 1H), 1.60 – 1.50 (m, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 154.6, 141.1, 138.0, 124.1, 121.2, 109.7, 102.1, 35.6, 30.0, 28.1, 24.2, 22.8, 20.4.
HRMS-ESI (m/z): Calc. for $C_{14}H_{18}O_2$: $[M-H]^+$ = 217.1229 ; found: 217.1239



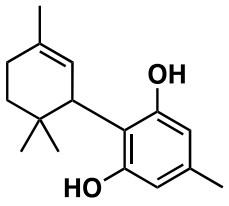
(±)-3ad
Chemical Formula: $C_{15}H_{20}O_2$
Exact Mass: 232.15

Synthesis of **(±)-3ad** from orcinol and **(±)-10d**:
Reaction Time: 24 h
TLC: R_f= 0.40 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 37% (11.3 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.34 – 6.14 (m, 2H), 6.10 – 5.95 (m, 1H), 5.50 (dt, *J* = 2.9, 1.6 Hz, 1H), 4.77 (s, 1H), 3.52 (ddq, *J* = 9.0, 4.6, 2.4 Hz, 1H), 2.25 – 2.16 (m, 4H), 2.08 – 2.00 (m, 1H), 1.84 (ddt, *J* = 13.0, 5.4, 2.6 Hz, 1H), 1.79 – 1.73 (m, 4H), 1.45 (dtd, *J* = 14.1, 11.7, 5.4 Hz, 1H), 0.92 (d, *J* = 6.5 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 140.5, 138.0, 124.1, 113.7, 39.4, 33.6, 31.5, 30.6, 23.9, 21.2, 20.3.
HRMS-ESI (m/z): Calc. for $C_{15}H_{20}O_2$: $[M-H]^+$ = 231.1385 ; found: 231.1412



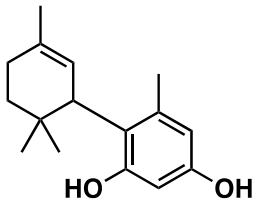
(±)-6ad
Chemical Formula: $C_{15}H_{20}O_2$
Exact Mass: 232.15

Synthesis of **(±)-6ad** from orcinol and **(±)-10d**:
Reaction Time: 1 h
TLC: R_f= 0.36 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
% Yield: 50% (15.2 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.28 – 6.19 (m, 2H), 6.05 (s, 1H), 5.49 (s, 1H), 4.96 (broad s, 1H), 3.29 – 3.18 (m, 1H), 2.23 (s, 3H), 2.21 – 2.16 (m, 1H), 2.09 – 1.99 (m, 1H), 1.88 – 1.81 (m, 2H), 1.77 (s, 3H), 1.48 – 1.40 (m, 1H), 0.87 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 154.7, 140.3, 138.9, 124.4, 120.6, 109.7, 102.4, 42.6, 33.5, 31.6, 30.5, 23.8, 21.3, 20.4.
HRMS-ESI (m/z): Calc. for $C_{15}H_{20}O_2$: $[M-H]^+$ = 231.1385 ; found: 231.1003



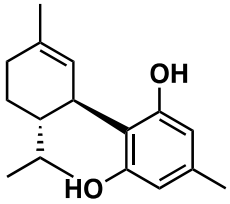
(±)-3ae
Chemical Formula: $C_{16}H_{22}O_2$
Exact Mass: 246.16

Synthesis of **(±)-3ae** from orcinol and **(±)-10e**:
Reaction Time: 24 h
TLC: R_f= 0.42 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 16% (5.2 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.32 (s, 1H), 6.26 (s, 1H), 6.15 (s, 1H), 5.57 (s, 1H), 4.63 (s, 1H), 3.70-3.69 (apparent triplet, 1H), 2.21 (s, 3H), 2.20 – 2.12 (m, 1H), 2.12 – 2.00 (m, 1H), 1.80 (s, 3H), 1.68 – 1.57 (m, 1H), 1.56 – 1.46 (m, 1H), 1.00 (s, 3H), 0.82 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 154.3, 139.4, 138.0, 123.3, 111.1, 110.4, 108.0, 41.7, 35.7, 34.0, 29.1, 27.9, 23.8, 23.7, 21.0.
HRMS-ESI (m/z): Calc. for $C_{16}H_{22}O_2$: $[M-H]^+$ = 245.1542 ; found: 245.1532



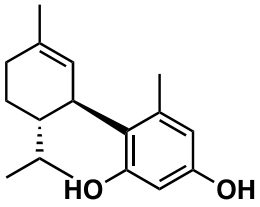
(±)-6ae
Chemical Formula: $C_{16}H_{22}O_2$
Exact Mass: 246.16

Synthesis of **(±)-6ae** from orcinol and **(±)-10e**:
Reaction Time: 1 h
TLC: R_f= 0.47 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 33% (10.7 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.35 (s, 1H), 6.26 (s, 1H), 6.19 (s, 1H), 5.56 (s, 1H), 4.78 (s, 1H), 3.44 (s, 1H), 2.27 (s, 3H), 2.19 – 2.14 (m, 1H), 2.12 – 2.03 (m, 1H), 1.80 (s, 3H), 1.72 – 1.65 (m, 1H), 1.57 – 1.47 (m, 1H), 0.99 (s, 3H), 0.78 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 154.6, 139.8, 139.4, 123.7, 118.2, 110.0, 102.1, 44.7, 36.1, 34.4, 29.8, 27.9, 24.6, 23.8, 22.0.
HRMS-ESI (m/z): Calc. for $C_{16}H_{22}O_2$: $[M-H]^+$ = 245.1542 ; found: 245.1536



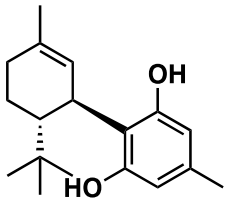
(±)-3a
Chemical Formula: $C_{17}H_{24}O_2$
Exact Mass: 260.18

Synthesis of **(±)-3a** from orcinol and **(±)-10**:
Reaction Time: 24 h
TLC: R_f= 0.44 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 47% (16.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.34 – 5.92 (m, 2H), 5.51 (s, 1H), 4.68 (br s, 1H), 3.81 (apparent dt, *J* = 8.1, 2.1 Hz, 1H), 2.21 (s, 3H), 2.19 – 2.05 (m, 2H), 1.84 – 1.77 (m, 1H), 1.77 (s, 3H), 1.67 – 1.56 (m, 2H), 1.45 – 1.33 (m, 1H), 0.86 (apparent td, *J* = 6.0, 5.6, 1.0 Hz, 6H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 140.2, 137.9, 124.9, 113.9, 110.7, 108.3, 43.8, 35.6, 30.8, 28.0, 23.8, 22.2, 21.9, 21.2, 16.5.
HRMS-ESI (m/z): Calc. for $C_{17}H_{24}O_2$: $[M-H]^+$ = 259.1698 ; found: 259.1687



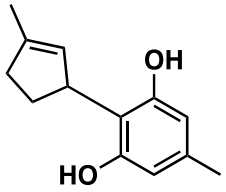
(±)-6a
Chemical Formula: $C_{17}H_{24}O_2$
Exact Mass: 260.18

Synthesis of **(±)-6a** from orcinol and **(±)-10**:
Reaction Time: 1 h
TLC: R_f= 0.31 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 40% (13.5 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.25 – 6.16 (m, 2H), 6.07 (s, 1H), 5.48 (s, 1H), 4.58 (s, 1H), 3.46 (d, *J* = 10.4 Hz, 1H), 2.23 (s, 3H), 2.18 – 2.05 (m, 2H), 1.84 – 1.77 (m, 1H), 1.76 (s, 3H), 1.76 – 1.66 (m, 1H), 1.52 (tt, *J* = 8.0, 4.0 Hz, 1H), 1.35 (qd, *J* = 12.3, 5.5 Hz, 1H), 0.84 (dd, *J* = 6.9, 4.7 Hz, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 154.7, 140.0, 139.0, 125.1, 120.8, 109.8, 102.6, 43.2, 38.8, 30.7, 27.5, 23.7, 22.3, 22.0, 21.2, 16.8.
HRMS-ESI (m/z): Calc. for $C_{17}H_{24}O_2$: $[M-H]^+$ = 259.1698 ; found: 259.1705



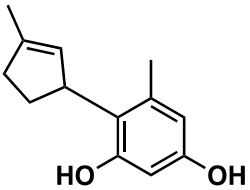
(±)-3af
Chemical Formula: $C_{18}H_{26}O_2$
Exact Mass: 274.19

Synthesis of (**±)-3af** from orcinol and **(±)-10f**:
Reaction Time: 24 h
TLC: R_f= 0.44 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 51% (18.3 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.20 (brd, *J* = 66.0 Hz, 2H), 5.79 (br s, 1H), 5.34 (s, 1H), 4.86 (br s, 1H), 3.95 – 3.88 (m, 1H), 2.20 (s, 3H), 2.16 – 2.10 (m, 1H), 2.08 (d, *J* = 3.2 Hz, 1H), 2.08 – 1.97 (m, 01), 1.77 (ddd, *J* = 11.9, 9.1, 2.8 Hz, 1H), 1.73 (s, 3H), 1.46 (dtd, *J* = 12.5, 10.9, 4.9 Hz, 1H), 0.83 (apparent s, 9H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 156.3, 153.1, 138.2, 137.8, 125.9, 116.8, 111.0, 108.8, 46.5, 34.1, 34.0, 30.8, 28.6, 25.1, 23.4, 21.1.
HRMS-ESI (m/z): Calc. for $C_{18}H_{26}O_2$: $[M-H]^+$ = 273.1855 ; found: 273.1842



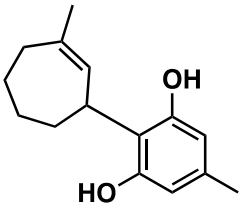
(±)-19a
Chemical Formula: $C_{13}H_{16}O_2$
Exact Mass: 204.12

Synthesis of **(±)-19a** from orcinol and **(±)-17**:
Reaction Time: 24 h
TLC: R_f= 0.24 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 9% (2.4 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.22 (s, 2H), 5.61 (s, 2H), 5.57 (s, 1H), 4.43 (ddq, *J* = 8.6, 6.1, 2.8 Hz, 1H), 2.56 – 2.40 (m, 3H), 2.20 (s, 3H), 1.88 – 1.85 (m, 4H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 155.2, 147.3, 137.9, 126.7, 113.8, 109.3, 40.9, 37.5, 31.5, 21.1, 17.1.
HRMS-ESI (m/z): Calc. for $C_{13}H_{16}O_2$: $[M-H]^+$ = 203.1072 ; found: 203.0864



(±)-18a
Chemical Formula: $C_{13}H_{16}O_2$
Exact Mass: 204.12

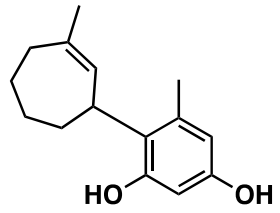
Synthesis of **(±)-18a** from orcinol and **(±)-17**:
Reaction Time: 1 h
TLC: R_f= 0.33 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 9% (2.5 mg)
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.30 (s, 1H), 6.25 – 6.19 (m, 2H), 5.58 (s, 1H), 4.16 (qt, *J* = 6.0, 2.7 Hz, 1H), 2.55 – 2.37 (m, 3H), 2.25 (s, 3H), 1.86 (s, 3H), 1.83 – 1.78 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 154.7, 147.3, 137.9, 127.1, 120.4, 109.5, 102.0, 44.5, 37.5, 31.2, 20.7, 17.1.
HRMS-ESI (m/z): Calc. for $C_{13}H_{16}O_2$: $[M-H]^+$ = 203.1072 ; found: 203.0865



(±)-22a

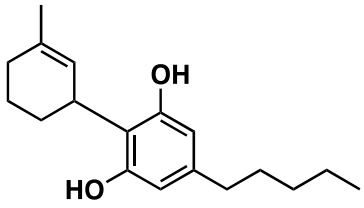
Chemical Formula: $C_{15}H_{20}O_2$
Exact Mass: 232.15

Synthesis of **(±)-22a** from orcinol and **(±)-20**:
Reaction Time: 24 h
TLC: R_f= 0.28 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 17% (5.2 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (s, 2H), 5.55 (s, 1H), 5.41 (s, 1H), 4.03 (d, *J* = 8.5 Hz, 1H), 2.36 – 2.27 (m, 1H), 2.25 – 2.21 (m, 1H), 2.20 (s, 3H), 1.97 – 1.89 (m, 2H), 1.88 – 1.82 (m, 1H), 1.80 (s, 3H), 1.78 – 1.74 (m, 1H), 1.69 – 1.61 (m, 1H), 1.60 – 1.50 (m, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 154.2, 143.6, 137.6, 127.7, 116.9, 109.4, 36.0, 33.9, 32.9, 29.2, 27.6, 26.6, 21.1.
HRMS-ESI (m/z): Calc. for $C_{15}H_{20}O_2$: $[M-H]^+$ = 231.1385 ; found: 231.1381



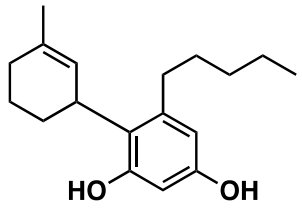
(±)-21a
Chemical Formula: $C_{15}H_{20}O_2$
Exact Mass: 232.15

Synthesis of **(±)-21a** from orcinol and **(±)-20**:
Reaction Time: 1 h
TLC: R_f= 0.21 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
% Yield: 30% (9.1 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.25 (s, 2H), 5.75 (s, 1H), 5.53 (s, 1H), 5.33 (s, 1H), 3.72 (d, *J* = 11.3 Hz, 1H), 2.31 (dd, *J* = 16.1, 8.1 Hz, 1H), 2.24 (s, 3H), 2.21 – 2.15 (m, 1H), 1.98 – 1.90 (m, 2H), 1.89 – 1.82 (m, 1H), 1.80 (s, 3H), 1.73 – 1.65 (m, 1H), 1.63 – 1.49 (m, 2H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 155.6, 154.3, 143.4, 137.0, 128.0, 124.0, 109.9, 102.0, 39.2, 34.1, 33.0, 29.6, 27.6, 26.6, 20.7.
HRMS-ESI (m/z): Calc. for $C_{15}H_{20}O_2$: $[M-H]^+$ = 231.1385 ; found: 231.1376



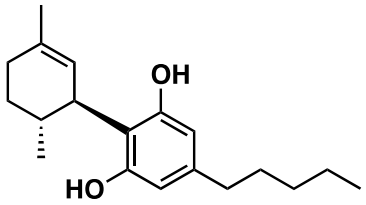
(±)-3c
Chemical Formula: $C_{18}H_{26}O_2$
Exact Mass: 274.19

Synthesis of **(±)-3c** from olivetol and **(±)-10c**:
Reaction Time: 24 h
TLC: R_f= 0.45 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 43% (15.5 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.22 (s, 2H), 5.64 (s, 1H), 3.90 (ddt, *J* = 8.8, 5.9, 2.9 Hz, 1H), 2.44 (dd, *J* = 8.9, 6.8 Hz, 2H), 2.18 – 2.07 (m, 1H), 2.06 – 1.98 (m, 1H), 1.99 – 1.91 (m, 1H), 1.93 – 1.84 (m, 1H), 1.79 (s, 3H), 1.73 – 1.61 (m, 1H), 1.63 – 1.50 (m, 3H), 1.37 – 1.26 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 143.1, 141.2, 123.8, 114.6, 108.6, 35.6, 32.3, 31.7, 30.9, 30.1, 28.4, 24.3, 22.7, 22.5, 14.2.
HRMS-ESI (m/z): Calc. for $C_{18}H_{26}O_2$: $[M-H]^+$ = 273.1855 ; found: 273.1842



(±)-6c
Chemical Formula: $C_{18}H_{26}O_2$
Exact Mass: 274.19

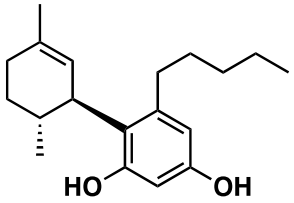
Synthesis of **(±)-6c** from olivetol and **(±)-10c**:
Reaction Time: 1 h
TLC: R_f= 0.39 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
% Yield: 50% (18.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.26 – 6.21 (m, 2H), 6.19 (s, 1H), 5.58 (br s, 1H), 5.11 (s, 1H), 3.60 (s, 1H), 2.55 (dt, *J* = 13.7, 7.8 Hz, 1H), 2.46 (dt, *J* = 14.4, 8.0 Hz, 1H), 2.21 – 2.09 (m, 1H), 2.05 – 1.98 (m, 1H), 1.97 – 1.83 (m, 2H), 1.78 (s, 3H), 1.68 – 1.60 (m, 2H), 1.52 (p, *J* = 7.4 Hz, 2H), 1.37 – 1.27 (m, 4H), 0.96 – 0.83 (m, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 154.7, 142.9, 140.9, 124.3, 120.9, 109.0, 102.2, 35.3, 34.1, 32.0, 31.5, 29.9, 28.6, 24.2, 23.0, 22.7, 14.2.
HRMS-ESI (m/z): Calc. for $C_{18}H_{26}O_2$: $[M-H]^+$ = 273.1855 ; found: 273.1859



(±)-3d
Chemical Formula: $C_{19}H_{28}O_2$
Exact Mass: 288.21

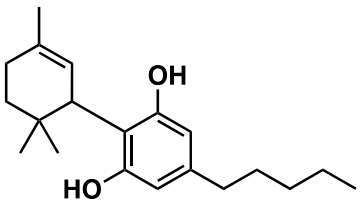
Synthesis of **(±)-3d** from olivetol and **(±)-10d**:
Reaction Time: 24 h

TLC: R_f= 0.52 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 56% (21.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.37 – 5.91 (m, 3H), 5.52 (s, 1H), 4.75 (br s, 1H), 3.52 (ddq, *J* = 9.1, 4.6, 2.4 Hz, 1H), 2.45 (dd, *J* = 8.8, 6.8 Hz, 2H), 2.27 – 2.15 (m, 1H), 2.11 – 1.97 (m, 1H), 1.84 (ddt, *J* = 13.0, 5.4, 2.5 Hz, 1H), 1.80 – 1.74 (m, overlap, 4H), 1.62 – 1.52 (m, 2H), 1.45 (qd, *J* = 11.9, 5.3 Hz, 1H), 1.37 – 1.27 (m, 4H), 0.92 (d, *J* = 6.5 Hz, 3H), 0.89 (t, *J* = 6.9 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 143.1, 140.4, 124.1, 113.9, 39.5, 35.6, 33.6, 31.7, 31.5, 30.8, 30.6, 23.8, 22.7, 20.4, 14.2.
HRMS-ESI (m/z): Calc. for $C_{19}H_{28}O_2$: $[M-H]^+$ = 287.2011 ; found: 287.2002



(±)-6d
Chemical Formula: $C_{19}H_{28}O_2$
Exact Mass: 288.21

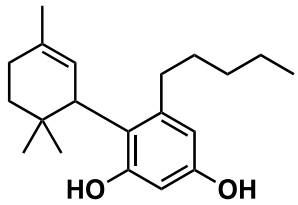
Synthesis of **(±)-6d** from olivetol and **(±)-10d**:
Reaction Time: 1 h
TLC: R_f= 0.36 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
% Yield: 37% (14.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (d, *J* = 2.7 Hz, 1H), 6.21 (d, *J* = 2.7 Hz, 1H), 6.00 (s, 1H), 5.47 (s, 1H), 3.23 (ddq, *J* = 9.2, 4.7, 2.5 Hz, 1H), 2.69 (ddd, *J* = 13.9, 8.9, 6.5 Hz, 1H), 2.43 – 2.27 (m, 1H), 2.27 – 2.16 (m, 1H), 2.09 – 2.01 (m, 1H), 1.89 – 1.81 (m, 2H), 1.77 (s, 3H), 1.52 – 1.46 (m, 2H), 1.43 (dd, *J* = 12.6, 5.4 Hz, 1H), 1.34 – 1.30 (m, 4H), 0.90 (t, *J* = 7.0 Hz, 3H), 0.86 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 154.7, 144.0, 140.3, 124.5, 120.0, 108.7, 102.4, 42.3, 34.4, 33.2, 32.0, 31.7, 31.3, 30.6, 23.8, 22.7, 20.5, 14.2.
HRMS-ESI (m/z): Calc. for $C_{19}H_{28}O_2$: $[M-H]^+$ = 287.2011 ; found: 287.2890



(±)-3e
Chemical Formula: $C_{20}H_{30}O_2$
Exact Mass: 302.22

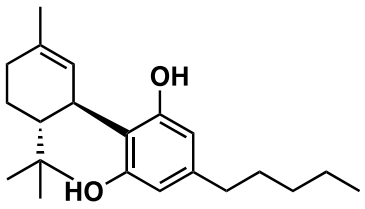
Synthesis of **(±)-3e** from olivetol and **(±)-10e**:
Reaction Time: 24 h

TLC: R_f= 0.50 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 18% (7.2 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.33 (s, 1H), 6.27 (s, 1H), 6.15 (s, 1H), 5.62 – 5.51 (m, 1H), 4.65 (s, 1H), 3.71 – 3.66 (m, 1H), 2.45 (t, *J* = 7.8 Hz, 2H), 2.23 – 2.11 (m, 1H), 2.11 – 1.95 (m, 1H), 1.80 (s, 3H), 1.64 (dt, *J* = 12.2, 6.0 Hz, 2H), 1.52 (dt, *J* = 13.4, 6.7 Hz, 2H), 1.34 – 1.28 (m, 4H), 1.00 (s, 3H), 0.89 (t, *J* = 6.7 Hz, 3H), 0.82 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 154.4, 143.3, 139.5, 123.5, 111.4, 109.8, 107.5, 41.9, 35.8, 35.6, 34.1, 31.7, 30.8, 29.2, 28.1, 24.0, 23.8, 22.7, 14.2.
HRMS-ESI (m/z): Calc. for $C_{20}H_{30}O_2$: $[M-H]^+$ = 301.2168 ; found: 301.2160



(±)-6e
Chemical Formula: $C_{20}H_{30}O_2$
Exact Mass: 302.22

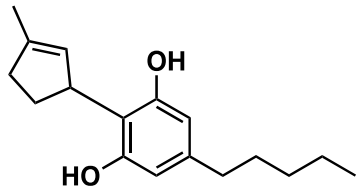
Synthesis of **(±)-6e** from olivetol and **(±)-10e**:
Reaction Time: 1 h
TLC: R_f= 0.48 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: orange/brown oil
% Yield: 24% (9.5 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.41 (s, 1H), 6.26 (d, *J* = 2.7 Hz, 1H), 6.18 (d, *J* = 2.7 Hz, 1H), 5.63 – 5.36 (m, 1H), 4.93 (s, 1H), 3.43 (t, *J* = 2.9 Hz, 1H), 2.75 (dt, *J* = 13.9, 7.7 Hz, 1H), 2.37 (dt, *J* = 13.8, 8.1 Hz, 1H), 2.20 – 2.12 (m, 1H), 2.13 – 2.08 (m, 1H), 1.81 – 1.79 (m, 3H), 1.70 (dt, *J* = 13.1, 6.4 Hz, 1H), 1.53 – 1.44 (m, 3H), 1.32 (qd, *J* = 6.3, 3.6 Hz, 4H), 1.00 (s, 3H), 0.93 – 0.86 (m, 3H), 0.75 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 154.8, 145.0, 139.5, 123.8, 117.3, 109.0, 102.0, 44.1, 35.9, 34.8, 34.0, 32.0, 31.5, 29.7, 27.9, 25.1, 23.8, 22.7, 14.2.
HRMS-ESI (m/z): Calc. for $C_{20}H_{30}O_2$: $[M-H]^+$ = 301.2168 ; found: 301.2152



(±)-3f
Chemical Formula: $C_{22}H_{34}O_2$
Exact Mass: 330.26

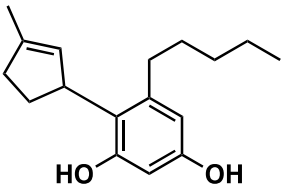
Synthesis of **(±)-3f** from olivetol and **(±)-10f**:
Reaction Time: 24 h
TLC: R_f= 0.52 in 10:1 Hex/EtOAc, Stain= iodine

Physical State: orange/brown oil
% Yield: 75% (32.3 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.32 – 6.06 (m, 2H), 5.82 (br s, 1H), 5.37 (d, *J* = 1.4 Hz, 1H), 4.90 (br s, 1H), 3.92 (dt, *J* = 8.8, 2.8 Hz, 1H), 2.43 (t, *J* = 7.8 Hz, 2H), 2.15 – 2.06 (m, 1H), 2.07 – 1.97 (m, 1H), 1.77 (td, *J* = 9.0, 4.6 Hz, 1H), 1.73 (s, 3H), 1.55 (p, *J* = 7.5 Hz, 2H), 1.51 – 1.41 (m, 1H), 1.34 – 1.24 (m, 5H), 0.92 – 0.85 (m, 3H), 0.83 (d, *J* = 1.1 Hz, 9H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 156.2, 153.1, 142.9, 138.2, 125.9, 116.9, 110.2, 108.1, 46.5, 35.5, 34.1, 34.0, 31.6, 30.8, 30.8, 28.5, 25.1, 23.4, 22.7, 14.2.
HRMS-ESI (m/z): Calc. for $C_{22}H_{34}O_2$: $[M-H]^+$ = 329.2481 ; found: 329.2478



(±)-19
Chemical Formula: $C_{17}H_{24}O_2$
Exact Mass: 260.18

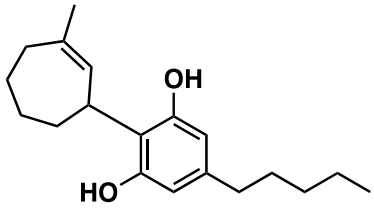
Synthesis of **(±)-19** from olivetol and **(±)-17**:
Reaction Time: 24 h
TLC: R_f= 0.35 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow oil
% Yield: 21% (7.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.22 (s, 2H), 5.61 – 5.54 (m, 1H), 5.50 (s, 2H), 4.42 (dtq, *J* = 8.7, 5.5, 2.7 Hz, 1H), 2.53 – 2.40 (m, 5H), 1.89 – 1.84 (m, 4H), 1.56 (p, *J* = 7.5 Hz, 2H), 1.34 – 1.28 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 155.1, 147.3, 143.1, 126.8, 113.9, 108.5, 40.9, 37.5, 35.6, 31.7, 31.4, 30.9, 22.7, 17.1, 14.2.
HRMS-ESI (m/z): Calc. for $C_{17}H_{24}O_2$: $[M-H]^+$ = 259.1698 ; found: 259.0579



(±)-18
Chemical Formula: $C_{17}H_{24}O_2$
Exact Mass: 260.18

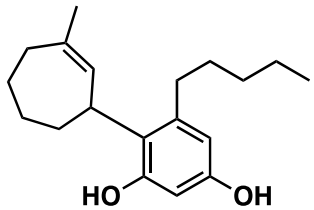
Synthesis of **(±)-18** from olivetol and **(±)-17**:
Reaction Time: 1 h
TLC: R_f= 0.42 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 14% (4.8 mg)

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.25 (s, 1H), 6.21 (s, 2H), 5.54 (s, 1H), 4.63 (s, 1H), 4.24 – 4.08 (m, 1H), 2.53 (s, 3H), 2.47 – 2.33 (m, 2H), 1.92 – 1.88 (m, 4H), 1.86 (s, 3H), 1.52 (t, *J* = 7.7 Hz, 2H), 1.37 – 1.30 (m, 4H), 1.26 (s, 1H), 0.92 – 0.85 (m, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 154.7, 147.1, 142.9, 127.6, 120.0, 108.7, 102.1, 44.1, 37.5, 34.4, 32.0, 31.7, 31.6, 22.7, 17.1, 14.2.
HRMS-ESI (m/z): Calc. for $C_{17}H_{24}O_2$: $[M-H]^+$ = 259.1698 ; found: 259.1139



(±)-22
Chemical Formula: $C_{19}H_{28}O_2$
Exact Mass: 288.21

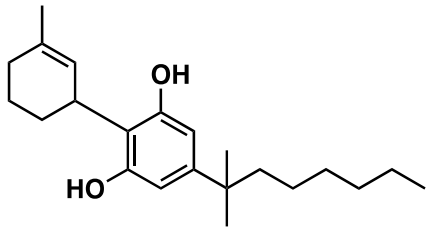
Synthesis of **(±)-22** from olivetol and **(±)-20**:
Reaction Time: 1 h
TLC: R_f= 0.33 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow oil
% Yield: 40% (15.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.23 (s, 2H), 5.59 – 5.51 (m, 1H), 5.17 (s, 2H), 4.06 – 3.87 (m, 1H), 2.55 – 2.36 (m, 2H), 2.36 – 2.28 (m, 1H), 2.21 (dd, *J* = 16.2, 9.5 Hz, 1H), 1.95 – 1.88 (m, 2H), 1.88 – 1.83 (m, 1H), 1.80 (d, *J* = 1.9 Hz, 3H), 1.78 – 1.73 (m, 1H), 1.68 – 1.62 (m, 1H), 1.59 – 1.51 (m, 3H), 1.35 – 1.27 (m, 4H), 0.91 – 0.78 (m, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 143.7, 142.8, 127.7, 117.0, 108.7, 36.1, 35.6, 34.0, 32.9, 31.7, 30.9, 29.2, 27.6, 26.6, 22.7, 14.2.
HRMS-ESI (m/z): Calc. for $C_{19}H_{28}O_2$: $[M-H]^+$ = 287.2011 ; found: 287.2003



(±)-21
Chemical Formula: $C_{19}H_{28}O_2$
Exact Mass: 288.21

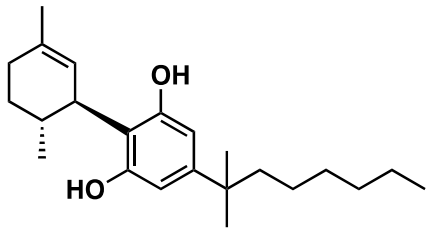
Synthesis of **(±)-21** from olivetol and **(±)-20**:
Reaction Time: 1 h
TLC: R_f= 0.33 in 5:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 32% (12.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.29 – 6.11 (m, 2H), 5.64 (s, 1H), 5.59 – 5.47 (m, 1H), 5.11 (s, 1H), 3.84 – 3.52 (m, 1H), 2.57 – 2.45 (m, 2H), 2.36 – 2.24 (m, 1H), 2.24 – 2.13 (m,

1H), 2.01 – 1.92 (m, 2H), 1.91 – 1.83 (m, 1H), 1.79 (t, *J* = 1.9 Hz, 3H), 1.71 – 1.64 (m, 1H), 1.64 – 1.59 (m, 1H), 1.53 – 1.46 (m, 3H), 1.36 – 1.30 (m, 4H), 0.92 – 0.85 (m, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 155.9, 154.4, 143.6, 141.8, 128.3, 123.9, 109.1, 102.2, 38.8, 34.4, 34.1, 33.5, 31.9, 31.2, 29.7, 27.5, 26.5, 22.6, 14.2.
HRMS-ESI (m/z): Calc. for $C_{19}H_{28}O_2$: $[M-H]^+$ = 287.2011 ; found: 287.2021



(±)-3bc
Chemical Formula: $C_{22}H_{34}O_2$
Exact Mass: 330.26

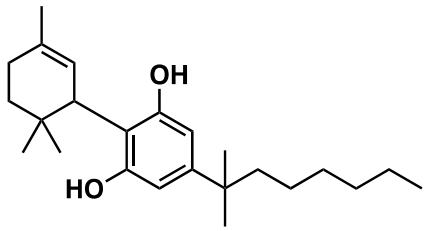
Synthesis of **(±)-3bc** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10c**:
Reaction Time: 24 h
TLC: R_f= 0.53 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 98% (42.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.34 (s, 2H), 5.65 (s, 1H), 3.88 (ddq, *J* = 8.4, 5.4, 2.6 Hz, 1H), 2.18 – 2.09 (m, 1H), 2.05 – 1.99 (m, 1H), 1.98 – 1.92 (m, 1H), 1.91 – 1.86 (m, 1H), 1.79 (s, 3H), 1.70 – 1.64 (m, 1H), 1.62 – 1.56 (m, 1H), 1.53 – 1.47 (m, 2H), 1.27 – 1.21 (m, 3H), 1.21 – 1.18 (m, 9H), 1.10 – 1.02 (m, 2H), 0.85 (t, *J* = 6.9 Hz, 3H).
^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 150.3, 141.1, 123.9, 114.2, 44.6, 37.5, 32.4, 32.0, 30.2, 30.1, 28.9, 28.9, 28.4, 24.8, 24.3, 22.9, 22.5, 14.3.
HRMS-ESI (m/z): Calc. for $C_{22}H_{34}O_2$: $[M-H]^+$ = 329.2481; found: 329.2494



(±)-3bd
Chemical Formula: $C_{23}H_{36}O_2$
Exact Mass: 344.27

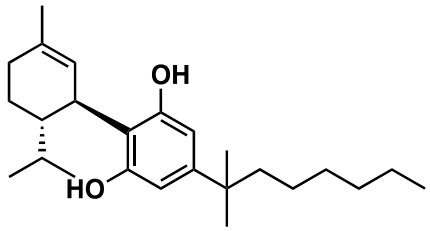
Synthesis of **(±)-3bd** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10d**:
Reaction Time: 24 h
TLC: R_f= 0.56 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow oil
% Yield: 98% (43.8 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.45 – 6.16 (m, 2H), 6.00 (br s, 1H), 5.53 (d, *J* = 2.1 Hz, 1H), 4.97 – 4.78 (m, 1H), 3.51 (ddq, *J* = 9.0, 4.5, 2.4 Hz, 1H), 2.27 – 2.16 (m, 1H), 2.10 –

1.98 (m, 1H), 1.91 – 1.81 (m, 1H), 1.78 – 1.75 (m, 4H), 1.54 – 1.40 (m, 3H), 1.24 – 1.15 (m, 12H), 1.10 – 1.01 (m, 2H), 0.92 (d, *J* = 6.5 Hz, 3H), 0.84 (t, *J* = 7.0 Hz, 3H).
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 150.4, 140.4, 124.1, 113.5, 44.6, 39.5, 37.5, 33.6, 31.9, 31.5, 30.6, 30.2, 28.9, 28.8, 24.8, 23.8, 22.8, 20.4, 14.2.
HRMS-ESI (m/z): Calc. for $C_{23}H_{36}O_2$: $[M-H]^+$ = 343.2637 ; found: 343.2633



(±)-3be
Chemical Formula: $C_{24}H_{38}O_2$
Exact Mass: 358.29

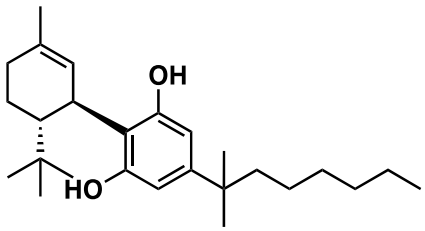
Synthesis of **(±)-3be** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10e**:
Reaction Time: 24 h
TLC: R_f= 0.56 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: orange oil
% Yield: 72% (33.5 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.38 (d, *J* = 3.7 Hz, 1H), 6.34 (d, *J* = 3.1 Hz, 1H), 6.27 (d, *J* = 2.8 Hz, 1H), 5.60 (s, 1H), 4.76 (s, 1H), 3.77 – 3.54 (m, 1H), 2.18 (d, *J* = 19.4 Hz, 1H), 2.07 (d, *J* = 19.1 Hz, 1H), 1.80 (s, 3H), 1.69 – 1.61 (m, 1H), 1.53 – 1.43 (m, 3H), 1.20 (d, *J* = 3.2 Hz, 12H), 1.09 – 1.03 (m, 2H), 1.01 (d, *J* = 3.1 Hz, 3H), 0.89 – 0.78 (m, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 154.2, 150.5, 139.4, 123.6, 111.1, 107.6, 105.3, 44.6, 41.9, 37.5, 35.7, 34.1, 31.9, 30.1, 29.2, 28.8, 28.1, 24.8, 24.1, 23.8, 22.8, 14.2.
HRMS-ESI (m/z): Calc. for $C_{24}H_{38}O_2$: $[M-H]^+$ = 357.2794 ; found: 357.2787



(±)-3b
Chemical Formula: $C_{25}H_{40}O_2$
Exact Mass: 372.30

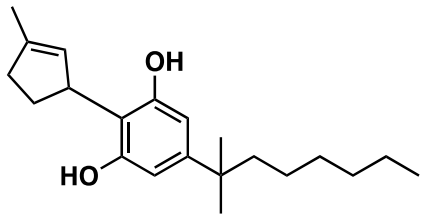
Synthesis of **(±)-3b** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10**:
Reaction Time: 24 h
TLC: R_f= 0.58 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 79% (38.4 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.41 – 6.21 (m, 2H), 6.05 (br s, 1H), 5.53 (s, 1H), 4.62 (br s, 1H), 3.80 (ddq, *J* = 8.9, 4.6, 2.4 Hz, 1H), 2.21 – 2.05 (m, 2H), 1.82 – 1.78 (m, 1H), 1.77

(s, 3H), 1.66 – 1.57 (m, 2H), 1.53 – 1.46 (m, 2H), 1.45 – 1.33 (m, 1H), 1.24 – 1.21 (m, 3H), 1.20 (s, 6H), 1.19 – 1.16 (m, 3H), 1.08 – 1.02 (m, 2H), 0.87 – 0.83 (m, 9H).
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 150.3, 140.2, 124.9, 113.7, 44.6, 43.8, 37.5, 35.6, 31.9, 30.8, 30.1, 28.9, 28.8, 27.9, 24.8, 23.8, 22.8, 22.3, 21.8, 16.6, 14.2.
HRMS-ESI (m/z): Calc. for $C_{25}H_{40}O_2$: $[M-H]^+$ = 371.2950 ; found: 371.2756



(±)-3bf
Chemical Formula: $C_{26}H_{42}O_2$
Exact Mass: 386.32

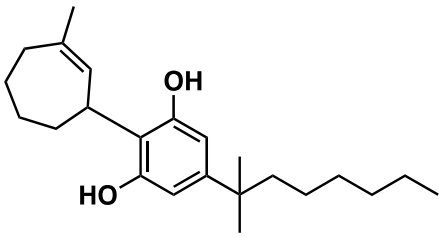
Synthesis of **(±)-3bf** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10f**:
Reaction Time: 24 h
TLC: R_f= 0.58 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/orange oil
% Yield: 56% (28.2 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.55 – 6.08 (m, 2H), 5.90 – 5.79 (m, 1H), 5.42 – 5.31 (m, 1H), 5.00 (br s, 1H), 3.92 (dt, *J* = 9.8, 3.1 Hz, 1H), 2.20 – 2.11 (m, 1H), 2.10 – 1.97 (m, 2H), 1.81 – 1.75 (m, 1H), 1.74 (s, 3H), 1.52 – 1.43 (m, 3H), 1.23 – 1.18 (m, 8H), 1.18 – 1.11 (m, 4H), 1.03 – 0.96 (m, 2H), 0.84 (dd, *J* = 7.0, 1.4 Hz, 3H), 0.82 (d, *J* = 1.4 Hz, 9H).
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 150.1, 138.2, 125.9, 116.5, 46.5, 44.7, 37.4, 34.2, 34.0, 31.9, 30.8, 30.1, 28.9, 28.8, 28.5, 25.1, 24.7, 23.4, 22.7, 14.2.
HRMS-ESI (m/z): Calc. for $C_{26}H_{42}O_2$: $[M-H]^+$ = 385.3107 ; found: 385.3122



(±)-19b
Chemical Formula: $C_{21}H_{32}O_2$
Exact Mass: 316.24

Synthesis of **(±)-19b** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-17**:
Reaction Time: 24 h
TLC: R_f= 0.41 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow oil
% Yield: 55% (22.7 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.34 (s, 2H), 5.58 (t, *J* = 2.0 Hz, 1H), 5.48 (s, 2H), 4.41 (dtq, *J* = 8.5, 5.4, 2.5 Hz, 1H), 2.55 – 2.39 (m, 3H), 1.89 – 1.83 (m, 4H), 1.55 – 1.44 (m, 2H),

1.27 – 1.22 (m, 3H), 1.20 (s, H), 1.07 (qd, *J* = 7.7, 7.2, 4.2 Hz, 2H), 0.85 (t, *J* = 6.9 Hz, 3H).
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 154.8, 150.4, 147.2, 126.8, 113.6, 106.4, 44.6, 41.0, 37.5, 37.5, 31.9, 31.4, 30.2, 28.9, 24.8, 22.8, 17.1, 14.2.
HRMS-ESI (m/z): Calc. for $C_{21}H_{32}O_2$: $[M-H]^+$ = 315.2324 ; found: 315.2324



(±)-22b
Chemical Formula: $C_{23}H_{36}O_2$
Exact Mass: 344.27

Synthesis of **(±)-22b** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-20**:
Reaction Time: 24 h
TLC: R_f= 0.41 in 10:1 Hex/EtOAc, Stain= iodine
Physical State: yellow/brown oil
% Yield: 51% (23.0 mg)
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.36 (d, *J* = 2.0 Hz, 2H), 5.57 (s, 1H), 5.20 (s, 2H), 4.04 – 3.96 (m, 1H), 2.34 – 2.28 (m, 1H), 2.21 (dd, *J* = 16.1, 9.4 Hz, 1H), 1.93 (td, *J* = 11.0, 10.5, 2.2 Hz, 2H), 1.88 – 1.82 (m, 1H), 1.83 – 1.75 (m, 4H), 1.69 – 1.61 (m, 1H), 1.56 (dqd, *J* = 11.4, 5.0, 2.5 Hz, 1H), 1.52 – 1.45 (m, 2H), 1.28 – 1.14 (m, 12H), 1.09 – 1.02 (m, 2H), 0.85 (td, *J* = 7.0, 2.0 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 153.8, 150.0, 143.6, 127.8, 116.6, 106.6, 44.6, 37.5, 36.1, 33.9, 32.9, 31.9, 30.2, 29.2, 28.9, 28.9, 27.6, 26.6, 24.8, 22.8, 14.2.
HRMS-ESI (m/z): Calc. for $C_{23}H_{36}O_2$: $[M-H]^+$ = 343.2637 ; found: 343.2631

Computational Studies:

Constrained conformational analyses of the transition states were performed with Grimme's Conformer-Rotamer Ensemble Sampling Tool[S12] (CREST). The resulting conformers were then optimized with ORCA[S13-S16] at the composite r^{2}SCAN-3C[S17]/CPCM(CH_2Cl_2) level and verified as stationary points by inspection of harmonic vibrational frequencies. For **3ad** and **6ad**, the conformers were all confirmed as transition states connecting the desired reactants and products based on inspection of intrinsic reaction coordinate (IRC) scans. Products were similarly modeled by first performing unconstrained conformational analyses followed by r^{2}SCAN-3C/CPCM(CH_2Cl_2) optimizations.

Benchmarking was performed on the global minimum structures for 3ae‡ and 6ae‡ against results at the DLPNO-CCSD(T)[S18-S19]/CBS(3,CC)[S20]/CPCM(CH_2Cl_2)//r^{2}SCAN-3C/CPCM(CH_2Cl_2) level, with the results shown in **Table S1**. Inspection of **Table S1** indicates that the r^{2}SCAN-3C composite method shows very nice agreement with the benchmark DLPNO-CCSD(T) results thus justifying our choice of computational model.

Listed in **Table S2** are computational summaries for transition state structures. The experimental value listed in **Table S2** assumes that the 1 h ratio of products is completely kinetically controlled. As can be seen from **Table S2**, this assumption does not appear to hold in all cases. In particular, for systems with the **10f** allylic alcohol, we see a large divergence between the computational and experimental ratios. We tentatively attribute this discrepancy to a breakdown of the kinetic assumption listed above. Conformational analysis for each of the systems are listed in **Tables S3-S62**. Representative structures are given in **Tables S63-S122**. **Figure S1** shows the Löwdin partial charges for the *ortho* and *para* carbons (relative to the alkyl group) for **7-7b**. The structures used here were the minima as determined by CREST, with optimizations at the same level of theory as listed above.

Table S1. Summary of benchmarking for **3ae**‡ and **6ae**‡.

Theory[i]	BS	E	E	G	G	ΔE[ii]	ΔG[iii]
		6ae‡	3ae‡	6ae‡	3ae‡	kcal	kcal
		au	au	au	au		
CCSD(T)[iv]	CBS(3,CC)	-733.558628	-733.558314	-733.275080	-733.274932	-0.20	-0.09
r^2SCAN-3C		-734.345630	-734.344590	-734.062082	-734.061209	-0.65	-0.55
PBEH-3C		-732.914515	-732.913404	-732.619010	-732.617607	-0.70	-0.88
M06	DEF2-SV(P)	-733.382846	-733.383136	-733.100011	-733.099214	0.18	-0.50
M06	DEF2-TZVP	-734.245852	-734.244673	-733.960794	-733.959563	-0.74	-0.77
M06-2X	DEF2-SV(P)	-733.568303	-733.568621	-733.280398	-733.280928	0.20	0.33
M06-2X	DEF2-TZVP	-734.453233	-734.452865	-734.165339	-734.164311	-0.23	-0.65
B3LYP[v]	DEF2-SV(P)	-733.527409	-733.526976	-733.243021	-733.242338	-0.27	-0.43
B3LYP[v]	DEF2-TZVP	-734.401946	-734.400525	-734.115812	-734.114699	-0.89	-0.70
PBE0[v]	DEF2-TZVP	-733.953871	-733.952908	-733.667888	-733.666829	-0.60	-0.66
WB97X-D3BJ	DEF2-SV(P)	-734.259902	-734.260550	-733.971218	-733.972000	0.41	0.49
WB97X-D3BJ	DEF2-TZVP	-735.118529	-735.118001	-734.829503	-734.828868	-0.33	-0.40
WB97X-V	DEF2-SV(P)	-733.710349	-733.710851	-733.423273	-733.423223	0.31	-0.03
WB97X-V	DEF2-TZVP	-734.569268	-734.568997	-734.281293	-734.281979	-0.17	0.43

[I] All models used the CPCM(CH_2Cl_2) implicit solvation model with the Gaussian charge scheme.
[ii] DE = E(Abnormal) – E(Normal)
[iii] DG = G(Abnormal) – G(Normal)
[iv] DLPNO-CCSD(T)//r^2SCAN-3C
[v] D3BJ dispersion model was used.

Table S2. Summary of computational results.

System	k^3/k^6		
	E	G	Expt.
3ac	0.33	0.48	0.33
3ad	0.18	0.24	0.40
3ae	0.41	0.48	0.1
3a	1.00	1.20	0.67
3af	0.20	0.34	5.00
3c	1.02	0.67	0.70
3d	1.74	0.85	1.00
3e	0.55	0.51	0.25
3	0.46	0.49	1.10
3f	5.28	2.34	27
3bc	2.32	4.52	> 100
3bd	3.48	8.80	> 100
3be	214.88	206.01	> 100
3b	40.60	49.72	> 100
3bf	43.00	117.65	17

Table S3. Conformational analysis for **3ac**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-695.040902	-694.784449	1.2	1.0
2	-695.042754	-694.785975	0.0	0.0
3	-695.040806	-694.782988	1.2	1.9
4	-695.036347	-694.779231	4.0	4.2
5	-695.042334	-694.784389	0.3	1.0
6	-695.038989	-694.780489	2.4	3.4
7	-695.039122	-694.780409	2.3	3.5
Avg.	-695.042280	-694.785447		

Table S4. Conformational analysis for **3ac**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-694.6426066	-694.3949300	0.0	0.0
2	-694.6413948	-694.3942055	0.8	0.5
3	-694.6405366	-694.3929628	1.3	1.2
Avg.	-694.6421988	-694.3945643		

Table S5. Conformational analysis for **6ac**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-695.043855	-694.786599	0.0	0.0
2	-695.041395	-694.784419	1.5	1.4
3	-695.042175	-694.784158	1.1	1.5
4	-695.042770	-694.784092	0.7	1.6
5	-695.036967	-694.779060	4.3	4.7
6	-695.038860	-694.779692	3.1	4.3
Avg.	-695.043319	-694.786131		

Table S6. Conformational analysis for **6ac**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-694.6416823	-694.3926803	0.0	0.0
2	-694.6397086	-694.3902285	1.2	1.5
Avg.	-694.6414653	-694.3925106		

Table S7. Conformational analysis for **3ad**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-734.342834	-734.059655	1.2	1.0
2	-734.344604	-734.061245	0.1	0.0
3	-734.344690	-734.060382	0.0	0.5
4	-734.344181	-734.059967	0.3	0.8
5	-734.344229	-734.059910	0.3	0.8
6	-734.343398	-734.058867	0.8	1.5
7	-734.342415	-734.058871	1.4	1.5
8	-734.343353	-734.059511	0.8	1.1
9	-734.343231	-734.058432	0.9	1.8
Avg.	-734.344175	-734.060392		

Table S8. Conformational analysis for **3ad**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-733.9464598	-733.6725199	0.0	0.0
2	-733.9447891	-733.6709757	1.1	1.0
3	-733.9465133	-733.6719802	0.0	0.3
Avg.	-733.9463576	-733.6721758		

Table S9. Conformational analysis for **6ad**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-734.346141	-734.061660	0.0	0.3
2	-734.345644	-734.062161	0.3	0.0
3	-734.346134	-734.061201	0.0	0.6
4	-734.345518	-734.061860	0.4	0.2
5	-734.344669	-734.059692	0.9	1.5
6	-734.343801	-734.058625	1.5	2.2
Avg.	-734.345809	-734.061756		

Table S10. Conformational analysis for **6ad**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-733.9451078	-733.6696136	0.0	0.0
2	-733.9451554	-733.6695269	0.0	0.1
3	-733.9424533	-733.6665897	1.7	1.9
4	-733.9424183	-733.6665334	1.7	1.9
Avg.	-733.9449858	-733.6694531		

Table S11. Conformational analysis for **3ae**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-773.644200	-773.333030	0.2	0.1
2	-773.642660	-773.331497	1.2	1.1
3	-773.644436	-773.333124	0.1	0.1
4	-773.642231	-773.331986	1.5	0.8
5	-773.644576	-773.333265	0.0	0.0
Avg.	-773.644278	-773.332969		

Table S12. Conformational analysis for **3ae**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-773.246127	-772.945009	0.1	0.0
2	-773.246222	-772.944557	0.0	0.3
Avg.	-773.246177	-772.944836		

Table S13. Conformational analysis for **6ae**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-773.645613	-773.334124	0.0	0.0
2	-773.643223	-773.331717	1.5	1.5
3	-773.643243	-773.332048	1.5	1.3
4	-773.643595	-773.331505	1.3	1.6
Avg.	-773.645128	-773.333660		

Table S14. Conformational analysis for **6ae**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-773.238073	-772.935667	0.1	0.2
2	-773.237674	-772.935309	0.4	0.4
3	-773.238306	-772.935938	0.0	0.0
4	-773.236347	-772.934262	1.2	1.1
5	-773.237508	-772.935459	0.5	0.3
6	-773.236056	-772.934252	1.4	1.1
7	-773.237958	-772.935609	0.2	0.2
8	-773.237144	-772.935239	0.7	0.4
Avg.	-773.237827	-772.935494		

Table S15. Conformational analysis for **3a**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-812.947249	-812.609165	0.1	0.0
2	-812.947349	-812.609087	0.0	0.0
3	-812.946129	-812.609048	0.8	0.1
4	-812.945090	-812.607915	1.4	0.8
5	-812.945093	-812.607908	1.4	0.8
6	-812.945158	-812.607240	1.4	1.2
Avg.	-812.946920	-812.608850		

Table S16. Conformational analysis for **3a**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-812.5469972	-812.2195526	0.0	0.0
2	-812.5449901	-812.2175753	1.3	1.2
3	-812.5442272	-812.2159939	1.7	2.2
Avg.	-812.5466676	-812.2192689		

Table S17. Conformational analysis for **6a**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-812.947767	-812.609006	0.0	0.2
2	-812.946622	-812.609248	0.7	0.0
3	-812.945723	-812.607357	1.3	1.2
4	-812.945657	-812.607255	1.3	1.3
5	-812.946514	-812.608662	0.8	0.4
6	-812.945793	-812.607017	1.2	1.4
7	-812.946369	-812.608053	0.9	0.7
8	-812.945474	-812.606604	1.4	1.7
Avg.	-812.946914	-812.608680		

Table S18. Conformational analysis for **6a**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-812.540312	-812.211749	0.2	0.0
2	-812.539903	-812.211568	0.4	0.1
3	-812.540602	-812.211680	0.0	0.0
4	-812.538010	-812.209144	1.6	1.6
5	-812.537488	-812.208888	2.0	1.8
Avg.	-812.540245	-812.211569		

Table S19. Conformational analysis for **3af**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-852.246587	-851.880393	0.3	1.6
2	-852.246243	-851.880556	0.5	1.5
3	-852.246994	-851.882921	0.1	0.0
4	-852.247086	-851.882647	0.0	0.2
5	-852.245031	-851.879790	1.3	2.0
Avg.	-852.246770	-851.882567		

Table S20. Conformational analysis for **3af**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-851.842902	-851.488988	0.0	0.0
2	-851.841912	-851.486364	0.6	1.6
3	-851.840876	-851.485889	1.3	1.9
4	-851.841916	-851.486371	0.6	1.6
Avg.	-851.842390	-851.488607		

Table S21. Conformational analysis for **6af**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-852.248105	-851.882371	0.4	1.1
2	-852.248760	-851.884061	0.0	0.0
3	-852.247436	-851.880340	0.8	2.3
4	-852.248226	-851.883357	0.3	0.4
5	-852.246646	-851.881230	1.3	1.8
Avg.	-852.248272	-851.883576		

Table S22. Conformational analysis for **6af**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-851.837324	-851.482272	0.3	0.0
2	-851.837498	-851.481832	0.2	0.3
3	-851.837788	-851.482262	0.0	0.0
Avg.	-851.837576	-851.482163		

Table S23. Conformational analysis for **3c**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-852.246553	-851.881831	0.0	0.3
2	-852.244519	-851.879668	1.3	1.6
3	-852.246623	-851.882080	0.0	0.1
4	-852.246406	-851.882294	0.1	0.0
5	-852.245382	-851.880987	0.8	0.8
6	-852.245263	-851.880988	0.9	0.8
7	-852.245700	-851.880005	0.6	1.4
8	-852.245362	-851.882064	0.8	0.1
9	-852.246031	-851.880773	0.4	1.0
10	-852.245527	-851.879008	0.7	2.1
11	-852.245099	-851.880388	1.0	1.2
12	-852.245554	-851.880477	0.7	1.1
13	-852.245745	-851.880350	0.6	1.2
14	-852.245758	-851.880368	0.5	1.2
15	-852.245349	-851.881209	0.8	0.7
16	-852.245426	-851.880931	0.8	0.9
17	-852.245093	-851.880375	1.0	1.2
18	-852.244893	-851.879873	1.1	1.5
19	-852.244912	-851.880168	1.1	1.3
20	-852.244488	-851.879861	1.3	1.5
21	-852.244462	-851.880376	1.4	1.2
22	-852.245473	-851.881196	0.7	0.7
23	-852.244482	-851.880538	1.3	1.1
24	-852.244292	-851.879786	1.5	1.6
25	-852.245864	-851.879805	0.5	1.6
26	-852.244470	-851.880393	1.4	1.2
27	-852.244397	-851.880194	1.4	1.3
28	-852.246258	-851.880854	0.2	0.9
29	-852.244230	-851.879348	1.5	1.8
30	-852.244817	-851.879354	1.1	1.8
31	-852.245249	-851.880035	0.9	1.4
32	-852.245258	-851.879291	0.9	1.9
33	-852.245259	-851.879354	0.9	1.8
34	-852.246384	-851.879393	0.1	1.8
35	-852.244326	-851.878660	1.4	2.3
36	-852.244211	-851.879630	1.5	1.7
37	-852.246475	-851.881142	0.1	0.7
38	-852.244684	-851.878801	1.2	2.2
39	-852.246489	-851.880963	0.1	0.8
40	-852.244979	-851.879635	1.0	1.7

41	-852.244808	-851.879746	1.1	1.6
42	-852.244958	-851.880147	1.0	1.3
43	-852.245789	-851.879872	0.5	1.5
44	-852.244961	-851.879753	1.0	1.6
45	-852.244536	-851.878351	1.3	2.5
46	-852.244963	-851.879797	1.0	1.6
47	-852.245716	-851.880006	0.6	1.4
48	-852.244882	-851.879733	1.1	1.6
49	-852.244992	-851.879985	1.0	1.4
50	-852.245180	-851.878112	0.9	2.6
51	-852.244791	-851.879475	1.1	1.8
52	-852.244984	-851.879954	1.0	1.5
53	-852.245165	-851.879530	0.9	1.7
54	-852.244996	-851.880058	1.0	1.4
55	-852.244905	-851.878656	1.1	2.3
56	-852.245187	-851.879652	0.9	1.7
57	-852.245800	-851.879664	0.5	1.7
58	-852.244391	-851.878815	1.4	2.2
59	-852.245834	-851.879921	0.5	2.5
60	-852.245122	-851.878811	0.9	2.2
61	-852.244584	-851.878653	1.3	2.3
62	-852.245047	-851.878737	1.0	2.2
63	-852.245747	-851.879920	0.5	1.5
64	-852.245034	-851.879025	1.0	2.1
65	-852.245002	-851.880084	1.0	1.4
66	-852.245087	-851.880282	1.0	1.3
Avg.	-852.245665	-851.880949		

Table S24. Conformational analysis for **3c**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-851.845097	-851.489506	0.1	0.3
2	-851.845154	-851.489440	0.1	0.4
3	-851.845119	-851.489624	0.1	0.3
4	-851.845254	-851.490055	0.0	0.0
5	-851.844777	-851.488497	0.3	1.0
6	-851.844847	-851.488577	0.3	0.9
7	-851.844889	-851.488745	0.2	0.8
8	-851.844249	-851.488427	0.6	1.0
9	-851.844175	-851.488145	0.7	1.2
10	-851.844105	-851.488351	0.7	1.1
11	-851.844069	-851.488189	0.7	1.2
12	-851.844035	-851.488217	0.8	1.2
13	-851.844210	-851.488658	0.7	0.9
14	-851.844190	-851.488687	0.7	0.9
15	-851.844285	-851.488689	0.6	0.9
16	-851.844201	-851.488793	0.7	0.8
17	-851.843119	-851.487043	1.3	1.9
18	-851.843067	-851.486749	1.4	2.1
19	-851.842932	-851.486887	1.5	2.0
20	-851.842359	-851.485686	1.8	2.7
21	-851.843839	-851.488176	0.9	1.2
22	-851.844148	-851.487252	0.7	1.8
23	-851.842351	-851.485539	1.8	2.8
24	-851.844115	-851.487243	0.7	1.8
25	-851.844130	-851.487202	0.7	1.8
26	-851.843818	-851.488057	0.9	1.3
27	-851.843814	-851.487706	0.9	1.5
28	-851.843894	-851.487934	0.9	1.3
29	-851.843982	-851.487831	0.8	1.4
30	-851.842326	-851.486004	1.8	2.5
31	-851.842317	-851.485573	1.8	2.8
32	-851.844061	-851.487850	0.7	1.4
33	-851.843845	-851.488304	0.9	1.1
34	-851.843859	-851.488317	0.9	1.1
35	-851.843646	-851.486887	1.0	2.0
36	-851.843581	-851.486730	1.0	2.1
37	-851.843539	-851.486914	1.1	2.0
38	-851.843564	-851.486996	1.1	1.9
39	-851.842953	-851.486722	1.4	2.1
40	-851.843250	-851.486763	1.3	2.1
41	-851.842950	-851.486663	1.4	2.1
42	-851.842788	-851.486555	1.5	2.2

43	-851.842874	-851.486613	1.5	2.2
44	-851.842872	-851.486699	1.5	2.1
45	-851.842859	-851.486703	1.5	2.1
46	-851.843284	-851.488657	1.2	0.9
47	-851.842930	-851.487201	1.5	1.8
48	-851.842915	-851.486948	1.5	1.9
49	-851.842916	-851.487287	1.5	1.7
50	-851.842954	-851.487126	1.4	1.8
51	-851.842920	-851.487007	1.5	1.9
52	-851.842146	-851.485448	2.0	2.9
53	-851.842886	-851.487000	1.5	1.9
54	-851.842926	-851.485680	1.5	2.7
55	-851.842825	-851.485813	1.5	2.7
56	-851.842956	-851.485912	1.4	2.6
57	-851.842820	-851.485775	1.5	2.7
58	-851.842709	-851.486161	1.6	2.4
59	-851.842696	-851.486290	1.6	2.4
60	-851.842550	-851.486959	1.7	1.9
61	-851.842732	-851.486080	1.6	2.5
62	-851.842709	-851.486277	1.6	2.4
63	-851.843049	-851.488137	1.4	1.2
64	-851.842273	-851.487627	1.9	1.5
65	-851.843179	-851.488246	1.3	1.1
66	-851.844778	-851.488340	0.3	1.1
Avg.	-851.844229	-851.488642		

Table S25. Conformational analysis for **6c**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-852.246482	-851.882016	0.1	0.2
2	-852.246567	-851.882298	0.0	0.0
3	-852.246485	-851.882363	0.1	0.0
4	-852.244265	-851.880548	1.4	1.1
5	-852.245952	-851.881281	0.4	0.7
6	-852.246142	-851.881141	0.3	0.8
7	-852.244783	-851.878442	1.1	2.5
8	-852.245668	-851.880714	0.6	1.0
9	-852.245691	-851.881070	0.5	0.8
10	-852.245618	-851.881498	0.6	0.5
11	-852.245456	-851.880619	0.7	1.1
12	-852.245412	-851.880663	0.7	1.1
13	-852.245726	-851.881366	0.5	0.6
14	-852.245536	-851.881218	0.6	0.7
15	-852.245662	-851.881289	0.6	0.7
16	-852.246259	-851.881766	0.2	0.4

17	-852.244256	-851.880351	1.5	1.3
18	-852.244556	-851.878207	1.3	2.6
19	-852.244499	-851.879161	1.3	2.0
20	-852.244789	-851.879063	1.1	2.1
21	-852.245294	-851.879887	0.8	1.6
22	-852.245602	-851.880036	0.6	1.5
23	-852.244700	-851.879512	1.2	1.8
24	-852.245440	-851.880401	0.7	1.2
25	-852.245546	-851.880500	0.6	1.2
26	-852.244741	-851.880493	1.1	1.2
27	-852.245606	-851.880091	0.6	1.4
28	-852.244806	-851.880288	1.1	1.3
29	-852.244345	-851.878398	1.4	2.5
30	-852.245230	-851.880374	0.8	1.2
31	-852.244641	-851.879286	1.2	1.9
32	-852.244744	-851.878723	1.1	2.3
33	-852.244794	-851.879023	1.1	2.1
34	-852.245300	-851.880501	0.8	1.2
35	-852.244479	-851.880423	1.3	1.2
36	-852.244209	-851.879101	1.5	2.0
37	-852.246429	-851.881781	0.1	0.4
38	-852.245642	-851.879878	0.6	1.6
39	-852.245739	-851.880564	0.5	1.1
40	-852.244868	-851.880254	1.1	1.3
41	-852.245068	-851.879664	0.9	1.7
42	-852.245266	-851.879215	0.8	2.0
43	-852.244926	-851.879514	1.0	1.8
44	-852.244757	-851.878683	1.1	2.3
45	-852.244843	-851.879319	1.1	1.9
46	-852.244770	-851.878794	1.1	2.2
47	-852.244558	-851.878453	1.3	2.5
48	-852.244804	-851.879254	1.1	2.0
49	-852.244875	-851.878624	1.1	2.3
50	-852.244608	-851.877817	1.2	2.9
51	-852.244603	-851.878579	1.2	2.4
52	-852.244747	-851.879581	1.1	1.7
53	-852.244280	-851.878488	1.4	2.4
Avg.	-852.245639	-851.881249		

Table S26. Conformational analysis for **6c**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-851.843567	-851.487439	0.3	0.4
2	-851.844007	-851.488112	0.0	0.0
3	-851.843144	-851.486635	0.6	0.9
4	-851.843233	-851.486952	0.5	0.7
5	-851.843008	-851.486233	0.6	1.2
6	-851.843071	-851.487124	0.6	0.6
7	-851.843529	-851.487470	0.3	0.4
8	-851.842771	-851.486268	0.8	1.2
9	-851.843077	-851.486971	0.6	0.7
10	-851.843602	-851.487399	0.3	0.4
11	-851.842643	-851.485673	0.9	1.5
12	-851.842493	-851.486060	1.0	1.3
13	-851.843225	-851.486921	0.5	0.7
14	-851.842456	-851.485430	1.0	1.7
15	-851.844037	-851.487978	0.0	0.1
16	-851.842798	-851.485848	0.8	1.4
17	-851.841781	-851.484875	1.4	2.0
18	-851.842479	-851.486377	1.0	1.1
19	-851.843380	-851.486685	0.4	0.9
20	-851.843336	-851.487610	0.4	0.3
21	-851.842046	-851.485180	1.2	1.8
22	-851.841313	-851.484123	1.7	2.5
23	-851.842449	-851.486249	1.0	1.2
24	-851.841941	-851.485823	1.3	1.4
25	-851.842038	-851.485553	1.3	1.6
26	-851.842106	-851.485607	1.2	1.6
27	-851.842071	-851.485673	1.2	1.5
28	-851.841365	-851.485424	1.7	1.7
29	-851.842787	-851.486360	0.8	1.1
30	-851.842896	-851.485962	0.7	1.3
31	-851.842209	-851.485000	1.1	2.0
32	-851.841836	-851.484924	1.4	2.0
33	-851.841737	-851.485526	1.4	1.6
34	-851.841314	-851.484056	1.7	2.5
35	-851.840918	-851.484360	2.0	2.4
36	-851.841688	-851.485951	1.5	1.4
37	-851.841232	-851.484617	1.8	2.2
38	-851.840902	-851.483992	2.0	2.6
Avg.	-851.843128	-851.487077		

Table S27. Conformational analysis for 3d‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-891.549995	-891.156939	0.0	0.3
2	-891.548978	-891.156205	0.6	0.8
3	-891.548765	-891.156915	0.8	0.3
4	-891.548477	-891.155338	1.0	1.3
5	-891.548532	-891.156960	0.9	0.3
6	-891.548338	-891.155351	1.0	1.3
7	-891.548641	-891.155451	0.9	1.2
8	-891.548017	-891.155025	1.2	1.5
9	-891.545226	-891.154695	3.0	1.7
10	-891.547932	-891.154692	1.3	1.7
11	-891.547368	-891.155177	1.7	1.4
12	-891.548180	-891.155109	1.1	1.5
13	-891.547369	-891.155352	1.7	1.3
14	-891.547386	-891.155874	1.6	1.0
15	-891.548300	-891.157441	1.1	0.0
16	-891.547209	-891.156246	1.8	0.7
17	-891.547158	-891.155993	1.8	0.9
18	-891.547582	-891.155613	1.5	1.1
19	-891.547631	-891.155664	1.5	1.1
20	-891.547679	-891.155549	1.5	1.2
21	-891.548090	-891.154944	1.2	1.6
22	-891.547228	-891.156496	1.7	0.6
23	-891.548021	-891.156045	1.2	0.9
24	-891.547797	-891.155904	1.4	1.0
25	-891.547929	-891.155908	1.3	1.0
26	-891.547477	-891.156117	1.6	0.8
27	-891.547508	-891.156327	1.6	0.7
28	-891.548094	-891.155224	1.2	1.4
29	-891.547942	-891.154283	1.3	2.0
30	-891.547970	-891.155040	1.3	1.5
31	-891.546862	-891.154498	2.0	1.8
32	-891.547676	-891.156198	1.5	0.8
33	-891.546909	-891.154328	1.9	2.0
34	-891.547713	-891.155077	1.4	1.5
35	-891.547295	-891.156251	1.7	0.7
36	-891.547532	-891.154144	1.6	2.1
37	-891.546876	-891.155060	2.0	1.5
38	-891.547975	-891.155316	1.3	1.3
39	-891.547655	-891.156395	1.5	0.7
40	-891.547493	-891.155574	1.6	1.2
41	-891.547552	-891.156437	1.5	0.6
42	-891.547566	-891.154699	1.5	1.7

43	-891.547400	-891.154911	1.6	1.6
44	-891.547989	-891.153756	1.3	2.3
45	-891.547277	-891.154713	1.7	1.7
46	-891.549639	-891.156578	0.2	0.5
47	-891.547994	-891.155442	1.3	1.3
48	-891.547195	-891.155490	1.8	1.2
49	-891.547204	-891.155429	1.8	1.3
Avg.	-891.548485	-891.156220		

Table S28. Conformational analysis for **3d.**

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-891.148925	-890.766835	0.0	0.3
2	-891.148966	-890.766912	0.0	0.3
3	-891.148947	-890.766912	0.0	0.3
4	-891.148971	-890.766861	0.0	0.3
5	-891.148979	-890.766798	0.0	0.3
6	-891.148955	-890.767181	0.0	0.1
7	-891.148585	-890.765921	0.2	0.9
8	-891.148691	-890.766029	0.2	0.8
9	-891.148552	-890.765933	0.3	0.9
10	-891.148631	-890.766072	0.2	0.8
11	-891.147991	-890.765501	0.6	1.1
12	-891.148113	-890.765794	0.5	1.0
13	-891.147771	-890.765508	0.8	1.1
14	-891.147938	-890.765400	0.7	1.2
15	-891.147497	-890.764428	0.9	1.8
16	-891.148023	-890.766333	0.6	0.6
17	-891.148088	-890.766699	0.6	0.4
18	-891.147300	-890.764568	1.1	1.7
19	-891.147933	-890.765965	0.7	0.9
20	-891.147976	-890.766271	0.6	0.7
21	-891.147994	-890.766166	0.6	0.7
22	-891.146865	-890.764240	1.3	1.9
23	-891.146544	-890.763354	1.5	2.5
24	-891.146591	-890.763292	1.5	2.5
25	-891.147890	-890.764631	0.7	1.7
26	-891.146104	-890.762825	1.8	2.8
27	-891.147844	-890.764518	0.7	1.8
28	-891.147975	-890.764624	0.6	1.7
29	-891.147963	-890.764987	0.6	1.5
30	-891.147764	-890.765536	0.8	1.1
31	-891.146109	-890.762999	1.8	2.7
32	-891.147759	-890.765136	0.8	1.4
33	-891.148938	-890.767334	0.0	0.0

34	-891.146461	-890.763868	1.6	2.2
35	-891.146554	-890.764021	1.5	2.1
36	-891.146547	-890.764274	1.5	1.9
37	-891.146428	-890.763836	1.6	2.2
38	-891.147196	-890.765439	1.1	1.2
39	-891.146527	-890.764481	1.5	1.8
40	-891.147277	-890.765779	1.1	1.0
41	-891.146496	-890.764450	1.6	1.8
Avg.	-891.148393	-890.766425		

Table S29. Conformational analysis for **6d**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-891.548923	-891.156934	0.0	0.5
2	-891.548559	-891.156597	0.2	0.7
3	-891.548883	-891.156954	0.0	0.5
4	-891.548387	-891.157190	0.3	0.3
5	-891.548094	-891.155290	0.5	1.5
6	-891.548055	-891.155607	0.5	1.3
7	-891.548097	-891.156010	0.5	1.1
8	-891.547791	-891.155896	0.7	1.2
9	-891.547987	-891.155884	0.6	1.2
10	-891.548323	-891.157742	0.4	0.0
11	-891.545865	-891.154945	1.9	1.8
12	-891.547333	-891.154818	1.0	1.8
13	-891.547837	-891.155972	0.7	1.1
14	-891.546691	-891.153823	1.4	2.5
15	-891.547142	-891.154740	1.1	1.9
16	-891.547834	-891.156365	0.7	0.9
17	-891.545999	-891.155862	1.8	1.2
18	-891.548028	-891.156256	0.6	0.9
19	-891.548849	-891.156628	0.0	0.7
20	-891.547411	-891.156090	0.9	1.0
21	-891.545865	-891.154812	1.9	1.8
22	-891.545844	-891.154215	1.9	2.2
23	-891.548029	-891.154846	0.6	1.8
24	-891.546532	-891.153626	1.5	2.6
25	-891.547299	-891.155934	1.0	1.1
26	-891.547483	-891.156494	0.9	0.8
27	-891.546156	-891.153031	1.7	3.0
28	-891.547176	-891.154070	1.1	2.3
29	-891.548054	-891.155343	0.5	1.5
30	-891.547852	-891.156715	0.7	0.6
31	-891.547721	-891.155300	0.8	1.5
32	-891.547456	-891.156413	0.9	0.8

33	-891.547451	-891.156387	0.9	0.9
34	-891.547183	-891.155211	1.1	1.6
35	-891.547324	-891.155488	1.0	1.4
36	-891.546012	-891.155493	1.8	1.4
37	-891.546972	-891.155454	1.2	1.4
38	-891.547188	-891.155954	1.1	1.1
39	-891.547749	-891.155601	0.7	1.3
40	-891.547338	-891.155571	1.0	1.4
41	-891.546866	-891.156237	1.3	0.9
42	-891.546870	-891.155792	1.3	1.2
43	-891.546946	-891.155379	1.2	1.5
44	-891.546818	-891.153825	1.3	2.5
45	-891.547473	-891.155334	0.9	1.5
46	-891.547052	-891.154846	1.2	1.8
47	-891.548092	-891.156277	0.5	0.9
48	-891.547252	-891.155221	1.0	1.6
49	-891.547071	-891.155229	1.2	1.6
50	-891.546549	-891.154673	1.5	1.9
51	-891.547060	-891.154652	1.2	1.9
52	-891.547841	-891.156012	0.7	1.1
Avg.	-891.547961	-891.156373		

Table S30. Conformational analysis for **6d**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-891.143484	-890.761076	0.0	0.0
2	-891.142706	-890.760054	0.5	0.6
3	-891.142589	-890.760799	0.6	0.2
4	-891.142823	-890.760066	0.4	0.6
5	-891.141920	-890.759398	1.0	1.1
6	-891.142444	-890.759539	0.7	1.0
7	-891.142543	-890.759831	0.6	0.8
8	-891.142364	-890.759283	0.7	1.1
9	-891.142266	-890.759754	0.8	0.8
10	-891.143093	-890.760900	0.2	0.1
11	-891.142302	-890.759756	0.7	0.8
12	-891.142516	-890.760399	0.6	0.4
13	-891.142035	-890.759761	0.9	0.8
14	-891.140525	-890.757301	1.9	2.4
15	-891.141632	-890.759424	1.2	1.0
16	-891.142908	-890.760813	0.4	0.2
17	-891.140833	-890.758299	1.7	1.7
18	-891.141590	-890.759113	1.2	1.2
19	-891.142085	-890.759222	0.9	1.2
20	-891.142111	-890.759542	0.9	1.0

21	-891.141866	-890.759604	1.0	0.9
22	-891.141048	-890.758849	1.5	1.4
23	-891.142060	-890.758919	0.9	1.4
24	-891.142598	-890.760354	0.6	0.5
25	-891.142050	-890.758816	0.9	1.4
26	-891.142014	-890.759400	0.9	1.1
27	-891.141631	-890.759501	1.2	1.0
28	-891.141470	-890.758764	1.3	1.5
29	-891.141532	-890.759114	1.2	1.2
30	-891.140933	-890.757822	1.6	2.0
31	-891.141901	-890.759696	1.0	0.9
32	-891.142235	-890.760126	0.8	0.6
33	-891.140961	-890.757802	1.6	2.1
34	-891.142737	-890.760059	0.5	0.6
35	-891.140325	-890.757764	2.0	2.1
36	-891.142003	-890.759865	0.9	0.8
37	-891.140447	-890.757901	1.9	2.0
38	-891.140880	-890.758444	1.6	1.7
39	-891.140386	-890.757022	1.9	2.5
40	-891.140724	-890.757950	1.7	2.0
41	-891.140452	-890.756978	1.9	2.6
42	-891.140909	-890.759193	1.6	1.2
43	-891.141259	-890.757931	1.4	2.0
44	-891.141685	-890.759024	1.1	1.3
45	-891.140331	-890.756429	2.0	2.9
Avg.	-891.142375	-890.760065		

Table S31. Conformational analysis for **3e**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-930.846885	-930.427415	0.7	1.3
2	-930.847514	-930.427702	0.3	1.1
3	-930.847957	-930.429431	0.0	0.0
4	-930.845969	-930.427633	1.2	1.1
5	-930.845088	-930.426705	1.8	1.7
6	-930.845633	-930.426275	1.5	2.0
7	-930.845025	-930.426658	1.8	1.7
8	-930.846665	-930.426950	0.8	1.6
9	-930.845467	-930.425819	1.6	2.3
10	-930.847378	-930.427542	0.4	1.2
11	-930.846029	-930.426942	1.2	1.6
12	-930.846878	-930.427977	0.7	0.9
13	-930.847025	-930.428228	0.6	0.8
14	-930.847010	-930.428256	0.6	0.7
15	-930.846660	-930.426954	0.8	1.6

16	-930.845656	-930.427600	1.4	1.1
17	-930.845029	-930.427305	1.8	1.3
18	-930.846961	-930.428387	0.6	0.7
19	-930.845119	-930.426411	1.8	1.9
20	-930.845654	-930.427957	1.4	0.9
21	-930.845660	-930.425833	1.4	2.3
22	-930.845019	-930.426664	1.8	1.7
23	-930.845891	-930.427481	1.3	1.2
24	-930.845788	-930.426121	1.4	2.1
25	-930.845785	-930.426254	1.4	2.0
26	-930.846523	-930.426776	0.9	1.7
27	-930.846157	-930.426495	1.1	1.8
28	-930.846450	-930.426447	0.9	1.9
29	-930.845010	-930.426481	1.8	1.9
30	-930.845206	-930.426637	1.7	1.8
31	-930.846718	-930.427591	0.8	1.2
32	-930.846727	-930.428135	0.8	0.8
33	-930.847151	-930.429151	0.5	0.2
34	-930.844811	-930.425903	2.0	2.2
35	-930.845431	-930.426386	1.6	1.9
36	-930.845705	-930.426546	1.4	1.8
37	-930.846584	-930.426997	0.9	1.5
38	-930.845084	-930.426514	1.8	1.8
39	-930.844847	-930.426739	2.0	1.7
40	-930.846157	-930.427602	1.1	1.1
41	-930.844954	-930.426535	1.9	1.8
42	-930.846096	-930.427598	1.2	1.2
43	-930.845464	-930.425829	1.6	2.3
44	-930.845813	-930.426610	1.3	1.8
45	-930.845190	-930.427971	1.7	0.9
46	-930.846096	-930.427337	1.2	1.3
47	-930.845092	-930.426522	1.8	1.8
48	-930.844973	-930.425446	1.9	2.5
49	-930.844985	-930.426121	1.9	2.1
50	-930.845098	-930.426225	1.8	2.0
51	-930.845711	-930.425838	1.4	2.3
52	-930.846306	-930.426604	1.0	1.8
53	-930.845713	-930.425219	1.4	2.6
54	-930.844920	-930.425766	1.9	2.3
55	-930.846602	-930.427261	0.9	1.4
56	-930.845778	-930.425343	1.4	2.6
57	-930.845614	-930.426137	1.5	2.1
58	-930.846600	-930.427065	0.9	1.5
59	-930.845889	-930.425777	1.3	2.3
60	-930.845890	-930.425786	1.3	2.3

61	-930.845890	-930.426248	1.3	2.0
62	-930.846024	-930.426705	1.2	1.7
63	-930.844920	-930.424618	1.9	3.0
64	-930.845273	-930.425324	1.7	2.6
65	-930.845917	-930.426569	1.3	1.8
66	-930.844850	-930.425323	1.9	2.6
67	-930.845917	-930.427776	1.3	1.0
68	-930.846658	-930.427081	0.8	1.5
69	-930.845812	-930.427578	1.3	1.2
Avg.	-930.846556	-930.427858		

Table S32. Conformational analysis for **3e**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-930.448677	-930.039514	0.1	0.3
2	-930.448456	-930.039420	0.2	0.3
3	-930.448409	-930.039326	0.3	0.4
4	-930.448635	-930.039287	0.1	0.4
5	-930.448712	-930.039876	0.1	0.0
6	-930.448650	-930.039320	0.1	0.4
7	-930.448568	-930.039827	0.2	0.1
8	-930.448693	-930.039342	0.1	0.4
9	-930.448750	-930.039397	0.0	0.3
10	-930.448817	-930.039314	0.0	0.4
11	-930.448156	-930.038369	0.4	1.0
12	-930.448433	-930.038473	0.2	0.9
13	-930.448095	-930.038380	0.5	1.0
14	-930.448729	-930.039594	0.1	0.2
15	-930.448396	-930.038569	0.3	0.8
16	-930.447767	-930.038388	0.7	1.0
17	-930.447468	-930.037948	0.8	1.2
18	-930.447254	-930.037208	1.0	1.7
19	-930.447568	-930.038181	0.8	1.1
20	-930.447447	-930.038049	0.9	1.2
21	-930.448541	-930.038497	0.2	0.9
22	-930.448307	-930.038373	0.3	1.0
23	-930.447556	-930.038648	0.8	0.8
24	-930.447652	-930.038444	0.7	0.9
25	-930.447634	-930.037199	0.7	1.7
26	-930.447651	-930.038605	0.7	0.8
27	-930.447583	-930.038555	0.8	0.9
28	-930.448428	-930.038467	0.2	0.9
29	-930.446474	-930.036058	1.5	2.4
30	-930.447652	-930.038610	0.7	0.8
31	-930.447819	-930.038323	0.6	1.0

32	-930.447614	-930.038634	0.8	0.8
33	-930.447897	-930.038015	0.6	1.2
34	-930.447532	-930.037912	0.8	1.3
35	-930.447540	-930.037239	0.8	1.7
36	-930.447748	-930.037931	0.7	1.2
37	-930.446506	-930.036517	1.5	2.1
38	-930.446357	-930.036742	1.5	2.0
39	-930.447822	-930.038776	0.6	0.7
40	-930.447698	-930.038589	0.7	0.8
41	-930.447857	-930.038686	0.6	0.8
42	-930.447717	-930.038351	0.7	1.0
43	-930.446327	-930.036742	1.6	2.0
44	-930.447711	-930.038361	0.7	1.0
45	-930.447705	-930.038521	0.7	0.9
46	-930.447721	-930.038520	0.7	0.9
47	-930.447463	-930.037153	0.8	1.7
48	-930.447476	-930.037087	0.8	1.8
49	-930.446622	-930.036757	1.4	2.0
50	-930.447690	-930.037232	0.7	1.7
51	-930.446434	-930.036444	1.5	2.2
52	-930.447382	-930.037699	0.9	1.4
53	-930.447457	-930.037722	0.9	1.4
54	-930.445744	-930.035914	1.9	2.5
55	-930.447445	-930.037599	0.9	1.5
56	-930.447401	-930.037626	0.9	1.4
57	-930.447714	-930.037074	0.7	1.8
58	-930.445890	-930.035303	1.8	2.9
59	-930.447748	-930.037130	0.7	1.7
60	-930.447426	-930.037724	0.9	1.4
61	-930.447603	-930.037723	0.8	1.4
62	-930.447607	-930.037564	0.8	1.5
63	-930.447565	-930.037384	0.8	1.6
64	-930.446690	-930.038090	1.3	1.1
65	-930.448666	-930.039913	0.1	0.0
66	-930.446736	-930.038804	1.3	0.7
Avg.	-930.448123	-930.038934		

Table S33. Conformational analysis for **6e**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-930.848149	-930.428928	0.0	0.6
2	-930.848189	-930.429914	0.0	0.0
3	-930.848075	-930.429871	0.1	0.0
4	-930.847801	-930.428521	0.3	0.9
5	-930.847333	-930.427981	0.5	1.2
6	-930.846440	-930.427005	1.1	1.8
7	-930.847810	-930.428248	0.2	1.0
8	-930.847157	-930.428045	0.7	1.2
9	-930.847317	-930.428272	0.6	1.0
10	-930.847379	-930.428666	0.5	0.8
11	-930.847303	-930.428565	0.6	0.8
12	-930.847116	-930.428155	0.7	1.1
13	-930.847155	-930.428710	0.7	0.8
14	-930.847209	-930.428743	0.6	0.7
15	-930.846545	-930.427583	1.0	1.5
16	-930.846222	-930.426390	1.2	2.2
17	-930.845344	-930.426772	1.8	2.0
18	-930.845632	-930.427003	1.6	1.8
19	-930.845350	-930.427365	1.8	1.6
20	-930.847157	-930.429178	0.7	0.5
21	-930.846268	-930.427519	1.2	1.5
22	-930.847097	-930.427281	0.7	1.7
23	-930.847154	-930.427252	0.7	1.7
24	-930.847178	-930.427455	0.6	1.5
25	-930.846223	-930.425947	1.2	2.5
26	-930.846052	-930.427667	1.4	1.4
27	-930.847402	-930.427716	0.5	1.4
28	-930.846927	-930.427463	0.8	1.5
29	-930.845048	-930.425477	2.0	2.8
30	-930.846067	-930.427486	1.3	1.5
31	-930.846021	-930.426906	1.4	1.9
32	-930.847328	-930.428397	0.6	1.0
33	-930.845519	-930.426113	1.7	2.4
34	-930.846697	-930.426372	0.9	2.2
35	-930.844570	-930.425327	2.3	2.9
36	-930.846387	-930.427475	1.1	1.5
37	-930.847408	-930.428608	0.5	0.8
38	-930.845529	-930.426337	1.7	2.2
39	-930.846016	-930.426673	1.4	2.0
40	-930.846277	-930.427521	1.2	1.5
41	-930.846028	-930.426782	1.4	2.0
42	-930.845533	-930.426376	1.7	2.2

43	-930.845425	-930.426231	1.7	2.3
44	-930.845133	-930.426678	1.9	2.0
45	-930.845217	-930.426402	1.9	2.2
46	-930.846399	-930.427369	1.1	1.6
47	-930.846326	-930.427528	1.2	1.5
48	-930.846523	-930.426657	1.1	2.0
49	-930.845257	-930.426930	1.9	1.9
50	-930.846452	-930.427642	1.1	1.4
51	-930.845164	-930.426723	1.9	2.0
52	-930.846778	-930.427444	0.9	1.6
53	-930.846306	-930.427049	1.2	1.8
54	-930.846111	-930.426466	1.3	2.2
55	-930.845036	-930.425388	2.0	2.8
56	-930.845425	-930.427370	1.7	1.6
57	-930.845447	-930.426800	1.7	2.0
58	-930.846524	-930.426555	1.1	2.1
59	-930.846832	-930.427706	0.9	1.4
60	-930.846233	-930.426931	1.2	1.9
61	-930.845364	-930.426000	1.8	2.5
62	-930.846289	-930.427727	1.2	1.4
63	-930.845545	-930.425431	1.7	2.8
64	-930.847060	-930.427052	0.7	1.8
65	-930.846769	-930.428268	0.9	1.0
66	-930.845357	-930.426751	1.8	2.0
67	-930.845188	-930.426611	1.9	2.1
68	-930.846064	-930.425828	1.3	2.6
69	-930.845233	-930.425146	1.9	3.0
Avg.	-930.847121	-930.428490		

Table S34. Conformational analysis for **6e**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-930.445612	-930.035836	0.3	0.5
2	-930.446149	-930.036623	0.0	0.0
3	-930.445783	-930.035914	0.2	0.4
4	-930.445757	-930.035460	0.2	0.7
5	-930.445419	-930.035132	0.5	0.9
6	-930.445868	-930.036117	0.2	0.3
7	-930.445979	-930.036240	0.1	0.2
8	-930.445052	-930.034707	0.7	1.2
9	-930.445721	-930.034587	0.3	1.3
10	-930.444747	-930.034621	0.9	1.3
11	-930.445272	-930.035569	0.6	0.7
12	-930.445914	-930.035739	0.1	0.6
13	-930.445411	-930.035639	0.5	0.6

14	-930.445422	-930.034705	0.5	1.2
15	-930.446099	-930.035555	0.0	0.7
16	-930.444380	-930.034302	1.1	1.5
17	-930.444578	-930.034505	1.0	1.3
18	-930.444962	-930.034415	0.7	1.4
19	-930.444430	-930.034186	1.1	1.5
20	-930.444735	-930.034365	0.9	1.4
21	-930.445187	-930.035036	0.6	1.0
22	-930.444654	-930.033920	0.9	1.7
23	-930.445307	-930.034915	0.5	1.1
24	-930.443769	-930.033466	1.5	2.0
25	-930.444564	-930.033966	1.0	1.7
26	-930.445857	-930.035067	0.2	1.0
27	-930.443236	-930.033279	1.8	2.1
28	-930.445118	-930.034770	0.6	1.2
29	-930.443970	-930.033158	1.4	2.2
30	-930.444294	-930.033506	1.2	2.0
31	-930.444958	-930.033984	0.7	1.7
32	-930.444189	-930.032896	1.2	2.3
33	-930.443740	-930.033289	1.5	2.1
34	-930.443265	-930.033445	1.8	2.0
35	-930.443360	-930.034220	1.8	1.5
Avg.	-930.445484	-930.035539		

Table S35. Conformational analysis for **3**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-970.149986	-969.702432	0.8	2.0
2	-970.149657	-969.702714	1.0	1.9
3	-970.150959	-969.705430	0.2	0.2
4	-970.150051	-969.701891	0.7	2.4
5	-970.149943	-969.704785	0.8	0.6
6	-970.150353	-969.704788	0.5	0.6
7	-970.149361	-969.701516	1.2	2.6
8	-970.151216	-969.704513	0.0	0.7
9	-970.148727	-969.702113	1.6	2.2
10	-970.148406	-969.703503	1.8	1.4
11	-970.148991	-969.703339	1.4	1.5
12	-970.149076	-969.703186	1.3	1.6
13	-970.150015	-969.704918	0.8	0.5
14	-970.149571	-969.702810	1.0	1.8
15	-970.150382	-969.704315	0.5	0.9
16	-970.148851	-969.703496	1.5	1.4
17	-970.149107	-969.702954	1.3	1.7
18	-970.148443	-969.700737	1.7	3.1

19	-970.149036	-969.703456	1.4	1.4
20	-970.149047	-969.703657	1.4	1.3
21	-970.149399	-969.703876	1.1	1.1
22	-970.148882	-969.702192	1.5	2.2
23	-970.149917	-969.704068	0.8	1.0
24	-970.148787	-969.701814	1.5	2.4
25	-970.148922	-969.701161	1.4	2.8
26	-970.148911	-969.703762	1.4	1.2
27	-970.150618	-969.705681	0.4	0.0
28	-970.150526	-969.703895	0.4	1.1
29	-970.149103	-969.701101	1.3	2.9
30	-970.150124	-969.704138	0.7	1.0
31	-970.148497	-969.700165	1.7	3.5
32	-970.148240	-969.701313	1.9	2.7
33	-970.148149	-969.700881	1.9	3.0
34	-970.148646	-969.704034	1.6	1.0
35	-970.148819	-969.703753	1.5	1.2
36	-970.149181	-969.702369	1.3	2.1
37	-970.148288	-969.700542	1.8	3.2
38	-970.148704	-969.704373	1.6	0.8
39	-970.148888	-969.702478	1.5	2.0
40	-970.148835	-969.702389	1.5	2.1
41	-970.148874	-969.702885	1.5	1.8
42	-970.150191	-969.703347	0.6	1.5
43	-970.148428	-969.700671	1.7	3.1
44	-970.148420	-969.702972	1.8	1.7
45	-970.148156	-969.701030	1.9	2.9
46	-970.149392	-969.704329	1.1	0.8
47	-970.149337	-969.703999	1.2	1.1
48	-970.149096	-969.703276	1.3	1.5
49	-970.149147	-969.704446	1.3	0.8
50	-970.149358	-969.703964	1.2	1.1
51	-970.148617	-969.702477	1.6	2.0
52	-970.149442	-969.702475	1.1	2.0
53	-970.148090	-969.702073	2.0	2.3
54	-970.149050	-969.702803	1.4	1.8
55	-970.148354	-969.702959	1.8	1.7
65	-970.148577	-969.703023	1.7	1.7
57	-970.148739	-969.702198	1.6	2.2
58	-970.148351	-969.699770	1.8	3.7
59	-970.148697	-969.702457	1.6	2.0
60	-970.148952	-969.703212	1.4	1.5
61	-970.147645	-969.702877	2.2	1.8
62	-970.147399	-969.703433	2.4	1.4
63	-970.148788	-969.702985	1.5	1.7

64	-970.149224	-969.702948	1.3	1.7
65	-970.148103	-969.702568	2.0	2.0
66	-970.148998	-969.702645	1.4	1.9
67	-970.148171	-969.703075	1.9	1.6
68	-970.148179	-969.703298	1.9	1.5
69	-970.149223	-969.703443	1.3	1.4
70	-970.148733	-969.703206	1.6	1.6
71	-970.149213	-969.703368	1.3	1.5
Avg.	-970.149801	-969.704235		

Table S36. Conformational analysis for **3**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-969.749488	-969.313668	0.1	0.4
2	-969.749585	-969.313988	0.0	0.2
3	-969.749589	-969.313840	0.0	0.3
4	-969.749541	-969.314285	0.0	0.0
5	-969.749511	-969.314204	0.0	0.1
6	-969.748738	-969.311936	0.5	1.5
7	-969.749217	-969.312672	0.2	1.0
8	-969.748395	-969.311813	0.7	1.6
9	-969.749348	-969.313063	0.2	0.8
10	-969.749157	-969.312829	0.3	0.9
11	-969.749267	-969.312779	0.2	0.9
12	-969.748655	-969.312527	0.6	1.1
13	-969.748490	-969.312409	0.7	1.2
14	-969.747530	-969.310756	1.3	2.2
15	-969.746865	-969.311067	1.7	2.0
16	-969.746830	-969.311241	1.7	1.9
17	-969.748590	-969.312958	0.6	0.8
18	-969.748586	-969.312943	0.6	0.8
19	-969.748568	-969.313014	0.6	0.8
20	-969.748673	-969.313174	0.6	0.7
21	-969.748551	-969.313168	0.7	0.7
22	-969.747437	-969.311048	1.4	2.0
23	-969.747502	-969.310991	1.3	2.1
24	-969.748579	-969.311508	0.6	1.7
25	-969.748452	-969.311566	0.7	1.7
26	-969.748662	-969.311923	0.6	1.5
27	-969.748563	-969.311756	0.6	1.6
28	-969.746588	-969.310127	1.9	2.6
29	-969.748393	-969.312080	0.8	1.4
30	-969.748325	-969.312155	0.8	1.3
31	-969.746739	-969.310175	1.8	2.6
32	-969.748403	-969.312225	0.7	1.3

33	-969.748402	-969.312325	0.7	1.2
34	-969.749001	-969.313797	0.4	0.3
35	-969.747519	-969.313772	1.3	0.3
Avg.	-969.748976	-969.313407		

Table S37. Conformational analysis for **6**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-970.151611	-969.705475	0.0	0.5
2	-970.150983	-969.705090	0.4	0.7
3	-970.151103	-969.704330	0.3	1.2
4	-970.150612	-969.703863	0.6	1.5
5	-970.150697	-969.704512	0.6	1.1
6	-970.150465	-969.703822	0.7	1.5
7	-970.150627	-969.704667	0.6	1.0
8	-970.150532	-969.704657	0.7	1.0
9	-970.149938	-969.703583	1.0	1.6
10	-970.149180	-969.702673	1.5	2.2
11	-970.149921	-969.703549	1.1	1.7
12	-970.150546	-969.703315	0.7	1.8
13	-970.149928	-969.704924	1.1	0.8
14	-970.149688	-969.702591	1.2	2.3
15	-970.148670	-969.701924	1.8	2.7
16	-970.150108	-969.705078	0.9	0.7
17	-970.150401	-969.703800	0.8	1.5
18	-970.150059	-969.705883	1.0	0.2
19	-970.149140	-969.701860	1.6	2.7
20	-970.148589	-969.701570	1.9	2.9
21	-970.149057	-969.704102	1.6	1.3
22	-970.149018	-969.703816	1.6	1.5
23	-970.148754	-969.702214	1.8	2.5
24	-970.149622	-969.704205	1.2	1.3
25	-970.149082	-969.704337	1.6	1.2
26	-970.149115	-969.704440	1.6	1.1
27	-970.151501	-969.706202	0.1	0.0
28	-970.149097	-969.704296	1.6	1.2
29	-970.148982	-969.703721	1.6	1.6
30	-970.148886	-969.704310	1.7	1.2
31	-970.149064	-969.704529	1.6	1.0
32	-970.149924	-969.703080	1.1	2.0
33	-970.150970	-969.705255	0.4	0.6
34	-970.150073	-969.703983	1.0	1.4
35	-970.148594	-969.702862	1.9	2.1
36	-970.148480	-969.702567	2.0	2.3
37	-970.150286	-969.704567	0.8	1.0

38	-970.148870	-969.703212	1.7	1.9
39	-970.148730	-969.702794	1.8	2.1
40	-970.150580	-969.703816	0.6	1.5
41	-970.149991	-969.703299	1.0	1.8
42	-970.148718	-969.702819	1.8	2.1
43	-970.148452	-969.703017	2.0	2.0
44	-970.149688	-969.702925	1.2	2.1
Avg.	-970.150525	-969.704908		

Table S38. Conformational analysis for **6**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-969.747643	-969.311119	0.4	0.4
2	-969.748115	-969.311749	0.1	0.0
3	-969.748074	-969.311139	0.2	0.4
4	-969.747219	-969.310609	0.7	0.7
5	-969.747002	-969.310271	0.8	0.9
6	-969.747237	-969.309971	0.7	1.1
7	-969.746590	-969.309780	1.1	1.2
8	-969.747172	-969.310703	0.7	0.7
9	-969.748334	-969.310634	0.0	0.7
10	-969.747523	-969.310702	0.5	0.7
11	-969.746188	-969.309053	1.3	1.7
12	-969.747264	-969.309676	0.7	1.3
13	-969.746077	-969.309264	1.4	1.6
14	-969.745974	-969.308991	1.5	1.7
15	-969.746464	-969.308857	1.2	1.8
16	-969.747075	-969.309921	0.8	1.1
17	-969.746159	-969.309822	1.4	1.2
18	-969.745545	-969.308591	1.7	2.0
19	-969.745439	-969.308130	1.8	2.3
20	-969.745283	-969.308708	1.9	1.9
21	-969.745568	-969.309427	1.7	1.5
Avg.	-969.747510	-969.310722		

Table S39. Conformational analysis for **3f**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.452222	-1008.977090	0.2	1.4
2	-1009.452238	-1008.976750	0.1	1.6
3	-1009.451004	-1008.976976	0.9	1.4
4	-1009.451343	-1008.976320	0.7	1.9
5	-1009.450590	-1008.975591	1.2	2.3
6	-1009.450179	-1008.975325	1.4	2.5
7	-1009.451774	-1008.978942	0.4	0.2

8	-1009.449292	-1008.975307	2.0	2.5
9	-1009.450700	-1008.976364	1.1	1.8
10	-1009.450406	-1008.976435	1.3	1.8
11	-1009.449979	-1008.975732	1.6	2.2
12	-1009.452462	-1008.979188	0.0	0.1
13	-1009.449815	-1008.975852	1.7	2.1
14	-1009.449779	-1008.975285	1.7	2.5
15	-1009.450463	-1008.975681	1.3	2.3
16	-1009.449873	-1008.975060	1.6	2.6
17	-1009.450102	-1008.974734	1.5	2.8
18	-1009.452247	-1008.978635	0.1	0.4
19	-1009.451697	-1008.979275	0.5	0.0
20	-1009.449769	-1008.974882	1.7	2.8
21	-1009.450444	-1008.977599	1.3	1.1
22	-1009.450887	-1008.978303	1.0	0.6
23	-1009.449755	-1008.974950	1.7	2.7
24	-1009.451138	-1008.978406	0.8	0.5
25	-1009.449740	-1008.975078	1.7	2.6
26	-1009.451249	-1008.978078	0.8	0.8
27	-1009.450647	-1008.978056	1.1	0.8
28	-1009.449602	-1008.974001	1.8	3.3
29	-1009.449949	-1008.974312	1.6	3.1
30	-1009.449605	-1008.977691	1.8	1.0
31	-1009.451307	-1008.978414	0.7	0.5
32	-1009.449613	-1008.974887	1.8	2.8
33	-1009.450233	-1008.977756	1.4	1.0
34	-1009.450534	-1008.978043	1.2	0.8
35	-1009.449631	-1008.977872	1.8	0.9
36	-1009.450451	-1008.978004	1.3	0.8
37	-1009.450481	-1008.976953	1.2	1.5
38	-1009.450120	-1008.976601	1.5	1.7
39	-1009.450180	-1008.977312	1.4	1.2
Avg.	-1009.451434	-1008.978332		

Table S40. Conformational analysis for **3f**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.045872	-1008.583862	0.0	0.0
2	-1009.045881	-1008.583905	0.0	0.0
3	-1009.045830	-1008.583706	0.0	0.1
4	-1009.045381	-1008.582880	0.3	0.6
5	-1009.045723	-1008.583727	0.1	0.1
6	-1009.045720	-1008.583725	0.1	0.1
7	-1009.045350	-1008.583764	0.3	0.1
8	-1009.044896	-1008.582752	0.6	0.7

9	-1009.045327	-1008.583627	0.3	0.2
10	-1009.045551	-1008.582520	0.2	0.9
11	-1009.045550	-1008.582526	0.2	0.9
12	-1009.045353	-1008.583788	0.3	0.1
13	-1009.044961	-1008.582031	0.6	1.2
14	-1009.044222	-1008.581441	1.0	1.5
15	-1009.045534	-1008.582554	0.2	0.8
16	-1009.045536	-1008.582553	0.2	0.8
17	-1009.045542	-1008.582562	0.2	0.8
18	-1009.044609	-1008.583184	0.8	0.5
19	-1009.044876	-1008.582336	0.6	1.0
20	-1009.044891	-1008.582363	0.6	1.0
21	-1009.045344	-1008.582857	0.3	0.7
22	-1009.044464	-1008.581962	0.9	1.2
23	-1009.044229	-1008.581430	1.0	1.6
24	-1009.044276	-1008.581833	1.0	1.3
25	-1009.044474	-1008.582442	0.9	0.9
26	-1009.044374	-1008.582951	0.9	0.6
27	-1009.044381	-1008.582316	0.9	1.0
28	-1009.043528	-1008.579824	1.5	2.6
29	-1009.044451	-1008.582538	0.9	0.9
30	-1009.044373	-1008.582242	0.9	1.0
31	-1009.043650	-1008.580409	1.4	2.2
32	-1009.043375	-1008.580489	1.6	2.1
33	-1009.043375	-1008.580492	1.6	2.1
34	-1009.044386	-1008.582213	0.9	1.1
35	-1009.043228	-1008.580297	1.7	2.3
36	-1009.044547	-1008.581217	0.8	1.7
37	-1009.044546	-1008.581351	0.8	1.6
38	-1009.043322	-1008.580557	1.6	2.1
39	-1009.043222	-1008.580230	1.7	2.3
40	-1009.044762	-1008.581570	0.7	1.5
41	-1009.044263	-1008.580662	1.0	2.0
42	-1009.044252	-1008.580976	1.0	1.8
43	-1009.044613	-1008.582419	0.8	0.9
44	-1009.044625	-1008.581168	0.8	1.7
45	-1009.044089	-1008.581647	1.1	1.4
46	-1009.044239	-1008.580590	1.0	2.1
47	-1009.044090	-1008.581223	1.1	1.7
48	-1009.044276	-1008.580659	1.0	2.0
49	-1009.044223	-1008.581601	1.0	1.4
50	-1009.044197	-1008.581718	1.1	1.4
51	-1009.044212	-1008.581377	1.0	1.6
52	-1009.044192	-1008.581113	1.1	1.8
53	-1009.045470	-1008.583582	0.3	0.2

54	-1009.045346	-1008.583621	0.3	0.2
Avg.	-1009.045155	-1008.583145		

Table S41. Conformational analysis for **6f**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.450306	-1008.976013	0.4	1.8
2	-1009.450386	-1008.976595	0.3	1.4
3	-1009.449968	-1008.975535	0.6	2.1
4	-1009.450923	-1008.978470	0.0	0.2
5	-1009.450838	-1008.978807	0.1	0.0
6	-1009.447769	-1008.975444	2.0	2.1
7	-1009.450740	-1008.977980	0.1	0.5
8	-1009.449741	-1008.974852	0.7	2.5
9	-1009.447901	-1008.975990	1.9	1.8
10	-1009.449584	-1008.974724	0.8	2.6
11	-1009.449606	-1008.977332	0.8	0.9
12	-1009.449406	-1008.974720	1.0	2.6
13	-1009.450480	-1008.977701	0.3	0.7
14	-1009.450533	-1008.977242	0.2	1.0
15	-1009.449590	-1008.975574	0.8	2.0
16	-1009.449167	-1008.974506	1.1	2.7
17	-1009.449939	-1008.977388	0.6	0.9
18	-1009.447828	-1008.975992	1.9	1.8
19	-1009.449415	-1008.975112	0.9	2.3
20	-1009.449775	-1008.977374	0.7	0.9
21	-1009.450284	-1008.978139	0.4	0.4
22	-1009.450127	-1008.978222	0.5	0.4
23	-1009.448781	-1008.974082	1.3	3.0
24	-1009.448939	-1008.976259	1.2	1.6
25	-1009.448367	-1008.973459	1.6	3.4
26	-1009.448710	-1008.974180	1.4	2.9
27	-1009.449189	-1008.977266	1.1	1.0
28	-1009.448459	-1008.974353	1.5	2.8
29	-1009.447928	-1008.976297	1.9	1.6
30	-1009.448584	-1008.975265	1.5	2.2
31	-1009.449484	-1008.974313	0.9	2.8
32	-1009.449595	-1008.974449	0.8	2.7
33	-1009.448471	-1008.973126	1.5	3.6
34	-1009.450047	-1008.976560	0.5	1.4
35	-1009.449894	-1008.977217	0.6	1.0
36	-1009.450031	-1008.977092	0.6	1.1
37	-1009.449479	-1008.977020	0.9	1.1
38	-1009.449442	-1008.976219	0.9	1.6
39	-1009.448536	-1008.974845	1.5	2.5

40	-1009.448511	-1008.974794	1.5	2.5
41	-1009.447780	-1008.972305	2.0	4.1
42	-1009.450317	-1008.977981	0.4	0.5
43	-1009.448574	-1008.975286	1.5	2.2
44	-1009.449287	-1008.978004	1.0	0.5
45	-1009.448560	-1008.975199	1.5	2.3
46	-1009.449533	-1008.975642	0.9	2.0
47	-1009.449290	-1008.975567	1.0	2.0
48	-1009.448834	-1008.975247	1.3	2.2
49	-1009.449546	-1008.975690	0.9	2.0
50	-1009.449000	-1008.975786	1.2	1.9
51	-1009.448426	-1008.975230	1.6	2.2
52	-1009.448852	-1008.976584	1.3	1.4
53	-1009.449498	-1008.976963	0.9	1.2
54	-1009.448672	-1008.974995	1.4	2.4
55	-1009.448646	-1008.975479	1.4	2.1
56	-1009.449477	-1008.977079	0.9	1.1
57	-1009.447931	-1008.974369	1.9	2.8
58	-1009.448241	-1008.974761	1.7	2.5
59	-1009.448958	-1008.974797	1.2	2.5
60	-1009.449294	-1008.976751	1.0	1.3
61	-1009.449481	-1008.976952	0.9	1.2
62	-1009.449401	-1008.976681	1.0	1.3
63	-1009.449498	-1008.975419	0.9	2.1
64	-1009.448879	-1008.974406	1.3	2.8
65	-1009.448464	-1008.976074	1.5	1.7
66	-1009.448580	-1008.974295	1.5	2.8
67	-1009.448599	-1008.976691	1.5	1.3
Avg.	-1009.449865	-1008.977530		

Table S42. Conformational analysis for **6f**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.043661	-1008.580852	0.0	0.0
2	-1009.040614	-1008.577587	1.9	2.0
3	-1009.043468	-1008.580364	0.1	0.3
4	-1009.042842	-1008.579528	0.5	0.8
5	-1009.040522	-1008.576776	2.0	2.6
Avg.	-1009.043343	-1008.580442		

Table S43. Conformational analysis for **3bc**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.448213	-1008.974824	1.0	1.9
2	-1009.447915	-1008.975930	1.2	1.2
3	-1009.448222	-1008.975080	1.0	1.7
4	-1009.449846	-1008.977784	0.0	0.0
5	-1009.447780	-1008.975279	1.3	1.6
6	-1009.449454	-1008.977840	0.2	0.0
7	-1009.448121	-1008.974372	1.1	2.2
8	-1009.449247	-1008.977039	0.4	0.5
9	-1009.448969	-1008.976453	0.6	0.9
10	-1009.448883	-1008.975824	0.6	1.3
11	-1009.448983	-1008.977720	0.5	0.1
12	-1009.448973	-1008.977592	0.5	0.2
13	-1009.448849	-1008.976695	0.6	0.7
14	-1009.448789	-1008.977206	0.7	0.4
15	-1009.448983	-1008.976214	0.5	1.0
16	-1009.448546	-1008.976568	0.8	0.8
17	-1009.448562	-1008.976322	0.8	1.0
18	-1009.448541	-1008.976498	0.8	0.8
19	-1009.448885	-1008.976075	0.6	1.1
20	-1009.448321	-1008.976465	1.0	0.9
21	-1009.448108	-1008.976642	1.1	0.8
22	-1009.449000	-1008.976384	0.5	0.9
23	-1009.448138	-1008.976404	1.1	0.9
24	-1009.448096	-1008.976950	1.1	0.6
25	-1009.448023	-1008.976288	1.1	1.0
26	-1009.448129	-1008.976577	1.1	0.8
27	-1009.448008	-1008.976629	1.2	0.8
28	-1009.448012	-1008.976655	1.2	0.7
29	-1009.447958	-1008.976396	1.2	0.9
30	-1009.447889	-1008.976829	1.2	0.6
31	-1009.448130	-1008.975886	1.1	1.2
32	-1009.447545	-1008.975534	1.4	1.4
33	-1009.447999	-1008.975580	1.2	1.4
34	-1009.447596	-1008.974823	1.4	1.9
35	-1009.447503	-1008.975301	1.5	1.6
36	-1009.448219	-1008.975121	1.0	1.7
37	-1009.447491	-1008.975160	1.5	1.7
38	-1009.448144	-1008.973834	1.1	2.5
39	-1009.448125	-1008.976041	1.1	1.1
40	-1009.448204	-1008.975800	1.0	1.3
41	-1009.447750	-1008.975831	1.3	1.3
42	-1009.447733	-1008.975632	1.3	1.4

43	-1009.448156	-1008.975243	1.1	1.6
44	-1009.447668	-1008.974810	1.4	1.9
45	-1009.448303	-1008.975629	1.0	1.4
46	-1009.448015	-1008.976004	1.1	1.2
47	-1009.447492	-1008.974834	1.5	1.9
48	-1009.447513	-1008.974764	1.5	1.9
49	-1009.447461	-1008.974154	1.5	2.3
50	-1009.448214	-1008.976249	1.0	1.0
51	-1009.447911	-1008.974818	1.2	1.9
52	-1009.448233	-1008.975988	1.0	1.2
53	-1009.448290	-1008.976306	1.0	1.0
54	-1009.447956	-1008.974908	1.2	1.8
55	-1009.448481	-1008.974653	0.9	2.0
56	-1009.448071	-1008.973272	1.1	2.9
57	-1009.447470	-1008.975222	1.5	1.6
58	-1009.448235	-1008.976636	1.0	0.8
59	-1009.447502	-1008.975383	1.5	1.5
60	-1009.448706	-1008.976266	0.7	1.0
61	-1009.449504	-1008.975367	0.2	1.6
62	-1009.448290	-1008.974546	1.0	2.1
63	-1009.448255	-1008.975178	1.0	1.7
64	-1009.448369	-1008.975074	0.9	1.7
Avg.	-1009.448616	-1008.976711		

Table S44. Conformational analysis for **3bc**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.049017	-1008.585263	0.0	0.4
2	-1009.048066	-1008.583191	0.6	1.7
3	-1009.048932	-1008.584622	0.1	0.8
4	-1009.047878	-1008.583132	0.7	1.7
5	-1009.047300	-1008.582937	1.1	1.8
6	-1009.048728	-1008.584834	0.2	0.6
7	-1009.046764	-1008.582075	1.4	2.4
8	-1009.048683	-1008.584993	0.2	0.5
9	-1009.048033	-1008.585800	0.6	0.0
10	-1009.048059	-1008.585862	0.6	0.0
11	-1009.046991	-1008.583607	1.3	1.4
12	-1009.047469	-1008.583425	1.0	1.5
13	-1009.046381	-1008.581592	1.7	2.7
14	-1009.047207	-1008.584251	1.1	1.0
15	-1009.046357	-1008.583055	1.7	1.8
16	-1009.047314	-1008.584606	1.1	0.8
17	-1009.047619	-1008.583804	0.9	1.3
18	-1009.047121	-1008.584548	1.2	0.8

19	-1009.047283	-1008.584759	1.1	0.7
20	-1009.047237	-1008.584466	1.1	0.9
21	-1009.047144	-1008.584721	1.2	0.7
22	-1009.047289	-1008.584881	1.1	0.6
23	-1009.047065	-1008.584711	1.2	0.7
24	-1009.047253	-1008.585090	1.1	0.5
25	-1009.047212	-1008.584512	1.1	0.8
26	-1009.047310	-1008.584748	1.1	0.7
27	-1009.047130	-1008.584659	1.2	0.8
28	-1009.047136	-1008.584720	1.2	0.7
29	-1009.047171	-1008.584979	1.2	0.6
30	-1009.047114	-1008.584550	1.2	0.8
31	-1009.047298	-1008.584692	1.1	0.7
32	-1009.045947	-1008.582615	1.9	2.0
33	-1009.047664	-1008.583614	0.8	1.4
34	-1009.047324	-1008.583021	1.1	1.8
35	-1009.047081	-1008.584646	1.2	0.8
36	-1009.047165	-1008.584474	1.2	0.9
37	-1009.047602	-1008.583553	0.9	1.4
38	-1009.047123	-1008.584603	1.2	0.8
39	-1009.047081	-1008.584631	1.2	0.8
40	-1009.047515	-1008.584097	0.9	1.1
41	-1009.047595	-1008.584514	0.9	0.8
42	-1009.047660	-1008.584404	0.9	0.9
43	-1009.045982	-1008.582984	1.9	1.8
44	-1009.046409	-1008.583191	1.6	1.7
45	-1009.047576	-1008.583652	0.9	1.4
46	-1009.045872	-1008.582935	2.0	1.8
47	-1009.046014	-1008.581853	1.9	2.5
48	-1009.047503	-1008.584308	0.9	1.0
49	-1009.046068	-1008.582863	1.9	1.9
50	-1009.047097	-1008.583499	1.2	1.5
51	-1009.046359	-1008.583106	1.7	1.7
52	-1009.047028	-1008.583746	1.2	1.3
53	-1009.046332	-1008.583605	1.7	1.4
54	-1009.046374	-1008.583387	1.7	1.6
55	-1009.046314	-1008.583342	1.7	1.6
56	-1009.046702	-1008.584081	1.5	1.1
57	-1009.046796	-1008.584108	1.4	1.1
58	-1009.046854	-1008.584361	1.4	0.9
59	-1009.045973	-1008.583182	1.9	1.7
60	-1009.047589	-1008.583039	0.9	1.8
61	-1009.046131	-1008.583337	1.8	1.6
62	-1009.045950	-1008.583310	1.9	1.6
63	-1009.046008	-1008.583201	1.9	1.7

64	-1009.046844	-1008.583486	1.4	1.5
65	-1009.046101	-1008.583872	1.8	1.2
66	-1009.046103	-1008.583494	1.8	1.5
Avg.	-1009.047740	-1008.584639		

Table S45. Conformational analysis for **6bc**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.448830	-1008.975497	0.0	0.7
2	-1009.447955	-1008.974668	0.6	1.2
3	-1009.448392	-1008.976603	0.3	0.0
4	-1009.448576	-1008.975116	0.2	0.9
5	-1009.447665	-1008.975897	0.8	0.4
6	-1009.447703	-1008.975859	0.7	0.5
7	-1009.446680	-1008.972730	1.4	2.4
8	-1009.448231	-1008.975484	0.4	0.7
9	-1009.447615	-1008.975559	0.8	0.7
10	-1009.447114	-1008.974035	1.1	1.6
11	-1009.447033	-1008.974269	1.1	1.5
12	-1009.447595	-1008.975495	0.8	0.7
13	-1009.447666	-1008.975158	0.8	0.9
14	-1009.447521	-1008.974990	0.8	1.0
15	-1009.447510	-1008.973320	0.8	2.1
16	-1009.447540	-1008.975162	0.8	0.9
17	-1009.446696	-1008.973796	1.4	1.8
18	-1009.446480	-1008.972799	1.5	2.4
19	-1009.447992	-1008.974092	0.5	1.6
20	-1009.447748	-1008.974805	0.7	1.1
21	-1009.446775	-1008.975007	1.3	1.0
22	-1009.447350	-1008.974451	0.9	1.4
23	-1009.447676	-1008.975144	0.7	0.9
24	-1009.447202	-1008.974360	1.0	1.4
25	-1009.447235	-1008.974942	1.0	1.0
26	-1009.446687	-1008.974212	1.4	1.5
27	-1009.446469	-1008.972024	1.5	2.9
28	-1009.446639	-1008.973958	1.4	1.7
29	-1009.447019	-1008.973255	1.2	2.1
30	-1009.447451	-1008.974293	0.9	1.4
31	-1009.447202	-1008.974223	1.0	1.5
32	-1009.446528	-1008.974460	1.5	1.3
33	-1009.447331	-1008.973492	1.0	2.0
34	-1009.446592	-1008.973797	1.4	1.8
35	-1009.446935	-1008.973381	1.2	2.0
36	-1009.446472	-1008.973702	1.5	1.8
37	-1009.446553	-1008.973022	1.4	2.2

38	-1009.447083	-1008.974167	1.1	1.5
39	-1009.446684	-1008.973451	1.4	2.0
40	-1009.446705	-1008.973315	1.4	2.1
41	-1009.447618	-1008.974918	0.8	1.1
42	-1009.447543	-1008.975417	0.8	0.7
43	-1009.448863	-1008.975348	0.0	0.8
Avg.	-1009.447822	-1008.975288		

Table S46. Conformational analysis for **6bc**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1009.037584	-1008.573797	0.0	0.0
2	-1009.036967	-1008.573869	0.4	0.0
3	-1009.037330	-1008.573063	0.2	0.5
4	-1009.036702	-1008.573081	0.6	0.5
5	-1009.036929	-1008.573118	0.4	0.5
6	-1009.036751	-1008.572933	0.5	0.6
7	-1009.036758	-1008.572594	0.5	0.8
8	-1009.036650	-1008.573631	0.6	0.1
9	-1009.036971	-1008.572810	0.4	0.7
10	-1009.036896	-1008.572746	0.4	0.7
11	-1009.036761	-1008.572599	0.5	0.8
12	-1009.036186	-1008.572464	0.9	0.9
13	-1009.036229	-1008.572917	0.8	0.6
14	-1009.036520	-1008.571868	0.7	1.3
15	-1009.037578	-1008.573800	0.0	0.0
16	-1009.035519	-1008.569835	1.3	2.5
17	-1009.037196	-1008.572953	0.2	0.6
18	-1009.036846	-1008.572458	0.5	0.9
19	-1009.036933	-1008.571417	0.4	1.5
20	-1009.036578	-1008.571717	0.6	1.4
21	-1009.035875	-1008.571583	1.1	1.4
22	-1009.036740	-1008.573065	0.5	0.5
23	-1009.037022	-1008.573035	0.4	0.5
24	-1009.036836	-1008.572705	0.5	0.7
25	-1009.035595	-1008.571736	1.2	1.3
26	-1009.035899	-1008.571370	1.1	1.6
27	-1009.035705	-1008.571329	1.2	1.6
28	-1009.035361	-1008.571705	1.4	1.4
29	-1009.035604	-1008.571301	1.2	1.6
30	-1009.035989	-1008.571372	1.0	1.6
31	-1009.035877	-1008.570932	1.1	1.8
32	-1009.035901	-1008.571365	1.1	1.6
33	-1009.034619	-1008.570641	1.9	2.0
34	-1009.035346	-1008.571530	1.4	1.5

35	-1009.034800	-1008.571283	1.7	1.6
36	-1009.036001	-1008.570386	1.0	2.2
37	-1009.036606	-1008.571892	0.6	1.2
38	-1009.035216	-1008.570671	1.5	2.0
39	-1009.034633	-1008.570963	1.9	1.8
40	-1009.035550	-1008.571373	1.3	1.6
41	-1009.035083	-1008.571094	1.6	1.7
42	-1009.035627	-1008.571371	1.2	1.6
43	-1009.036769	-1008.572611	0.5	0.8
44	-1009.034918	-1008.569300	1.7	2.9
45	-1009.034490	-1008.569376	1.9	2.8
46	-1009.036329	-1008.571005	0.8	1.8
Avg.	-1009.036739	-1008.572953		

Table S47. Conformational analysis for **3bd**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1048.748907	-1048.249156	2.1	2.7
2	-1048.750138	-1048.250446	1.3	1.9
3	-1048.750178	-1048.250245	1.3	2.0
4	-1048.752115	-1048.253509	0.1	0.0
5	-1048.751834	-1048.252657	0.2	0.5
6	-1048.750313	-1048.251744	1.2	1.1
7	-1048.752217	-1048.253216	0.0	0.2
8	-1048.752083	-1048.252062	0.1	0.9
9	-1048.751613	-1048.252386	0.4	0.7
10	-1048.751096	-1048.250818	0.7	1.7
11	-1048.751382	-1048.251124	0.5	1.5
12	-1048.750911	-1048.251778	0.8	1.1
13	-1048.751004	-1048.251904	0.8	1.0
14	-1048.749313	-1048.251645	1.8	1.2
15	-1048.749704	-1048.250760	1.6	1.7
16	-1048.749234	-1048.251600	1.9	1.2
17	-1048.749103	-1048.249532	2.0	2.5
18	-1048.749293	-1048.251322	1.8	1.4
19	-1048.750560	-1048.251463	1.0	1.3
20	-1048.749661	-1048.250065	1.6	2.2
21	-1048.749098	-1048.249647	2.0	2.4
22	-1048.751210	-1048.251837	0.6	1.0
23	-1048.750451	-1048.249334	1.1	2.6
24	-1048.750944	-1048.251399	0.8	1.3
25	-1048.751323	-1048.251741	0.6	1.1
26	-1048.750919	-1048.252300	0.8	0.8
27	-1048.750778	-1048.253133	0.9	0.2
28	-1048.750849	-1048.253078	0.9	0.3

29	-1048.749214	-1048.249924	1.9	2.2
30	-1048.750600	-1048.251281	1.0	1.4
31	-1048.750564	-1048.251470	1.0	1.3
32	-1048.750551	-1048.250963	1.0	1.6
33	-1048.750020	-1048.250463	1.4	1.9
34	-1048.750533	-1048.250002	1.1	2.2
35	-1048.750237	-1048.250294	1.2	2.0
36	-1048.751110	-1048.250284	0.7	2.0
37	-1048.750321	-1048.250987	1.2	1.6
38	-1048.750260	-1048.251125	1.2	1.5
39	-1048.750265	-1048.251327	1.2	1.4
40	-1048.749716	-1048.248905	1.6	2.9
41	-1048.751290	-1048.250594	0.6	1.8
42	-1048.750770	-1048.250814	0.9	1.7
43	-1048.750445	-1048.251845	1.1	1.0
44	-1048.749244	-1048.249960	1.9	2.2
45	-1048.749908	-1048.252440	1.4	0.7
46	-1048.749302	-1048.251339	1.8	1.4
47	-1048.750011	-1048.252928	1.4	0.4
48	-1048.749307	-1048.249095	1.8	2.8
49	-1048.749918	-1048.250925	1.4	1.6
50	-1048.750111	-1048.251588	1.3	1.2
51	-1048.750618	-1048.250081	1.0	2.2
52	-1048.749969	-1048.251972	1.4	1.0
53	-1048.749966	-1048.251600	1.4	1.2
54	-1048.749553	-1048.251424	1.7	1.3
55	-1048.749937	-1048.251710	1.4	1.1
56	-1048.750226	-1048.249769	1.2	2.3
57	-1048.750244	-1048.250842	1.2	1.7
58	-1048.750595	-1048.250919	1.0	1.6
59	-1048.750535	-1048.250154	1.1	2.1
60	-1048.750398	-1048.249947	1.1	2.2
61	-1048.749908	-1048.251700	1.4	1.1
62	-1048.750041	-1048.250046	1.4	2.2
63	-1048.750006	-1048.250122	1.4	2.1
64	-1048.751281	-1048.251619	0.6	1.2
65	-1048.749297	-1048.249762	1.8	2.4
66	-1048.750944	-1048.252171	0.8	0.8
67	-1048.749475	-1048.249723	1.7	2.4
68	-1048.749807	-1048.249865	1.5	2.3
69	-1048.749432	-1048.250383	1.7	2.0
70	-1048.750074	-1048.250563	1.3	1.8
71	-1048.749077	-1048.250757	2.0	1.7
72	-1048.749803	-1048.250891	1.5	1.6
73	-1048.749858	-1048.251194	1.5	1.5

74	-1048.749892	-1048.250809	1.5	1.7
75	-1048.750172	-1048.250507	1.3	1.9
76	-1048.749051	-1048.250467	2.0	1.9
77	-1048.749581	-1048.248743	1.7	3.0
78	-1048.750305	-1048.252131	1.2	0.9
79	-1048.749639	-1048.250655	1.6	1.8
80	-1048.749467	-1048.250420	1.7	1.9
Avg.	-1048.750953	-1048.252142		

Table S48. Conformational analysis for **3bd**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1048.353459	-1047.862457	0.0	0.5
2	-1048.352822	-1047.862416	0.4	0.6
3	-1048.352058	-1047.860819	0.9	1.6
4	-1048.352264	-1047.860678	0.8	1.6
5	-1048.353027	-1047.862389	0.3	0.6
6	-1048.351306	-1047.860434	1.4	1.8
7	-1048.350654	-1047.859474	1.8	2.4
8	-1048.351862	-1047.863179	1.0	0.1
9	-1048.351907	-1047.863169	1.0	0.1
10	-1048.351922	-1047.863297	1.0	0.0
11	-1048.352724	-1047.861877	0.5	0.9
12	-1048.350875	-1047.860889	1.6	1.5
13	-1048.352175	-1047.861539	0.8	1.1
14	-1048.350436	-1047.859436	1.9	2.4
15	-1048.351999	-1047.861437	0.9	1.2
16	-1048.351474	-1047.862324	1.2	0.6
17	-1048.352078	-1047.861776	0.9	1.0
18	-1048.351439	-1047.861918	1.3	0.9
19	-1048.350860	-1047.860785	1.6	1.6
20	-1048.350417	-1047.860649	1.9	1.7
21	-1048.351361	-1047.862752	1.3	0.3
22	-1048.350963	-1047.861760	1.6	1.0
23	-1048.351045	-1047.862039	1.5	0.8
24	-1048.351294	-1047.863028	1.4	0.2
25	-1048.351120	-1047.861879	1.5	0.9
26	-1048.351029	-1047.861986	1.5	0.8
27	-1048.351082	-1047.862584	1.5	0.4
28	-1048.351066	-1047.861940	1.5	0.9
29	-1048.351085	-1047.862359	1.5	0.6
30	-1048.351275	-1047.861091	1.4	1.4
31	-1048.351161	-1047.862023	1.4	0.8
32	-1048.351050	-1047.862118	1.5	0.7
33	-1048.351834	-1047.861783	1.0	0.9

34	-1048.351036	-1047.862249	1.5	0.7
35	-1048.351035	-1047.862153	1.5	0.7
36	-1048.351345	-1047.860924	1.3	1.5
37	-1048.351108	-1047.862010	1.5	0.8
38	-1048.351412	-1047.861629	1.3	1.0
39	-1048.350394	-1047.860178	1.9	2.0
40	-1048.350992	-1047.861874	1.5	0.9
41	-1048.350299	-1047.859282	2.0	2.5
42	-1048.350972	-1047.861998	1.6	0.8
43	-1048.351340	-1047.862336	1.3	0.6
44	-1048.351520	-1047.860972	1.2	1.5
45	-1048.350367	-1047.860091	1.9	2.0
46	-1048.350923	-1047.859405	1.6	2.4
47	-1048.350989	-1047.862000	1.5	0.8
48	-1048.350997	-1047.861875	1.5	0.9
49	-1048.350976	-1047.862096	1.6	0.8
50	-1048.350600	-1047.858466	1.8	3.0
51	-1048.351276	-1047.861228	1.4	1.3
52	-1048.351261	-1047.860792	1.4	1.6
53	-1048.351815	-1047.861069	1.0	1.4
54	-1048.351125	-1047.861097	1.5	1.4
55	-1048.350481	-1047.859112	1.9	2.6
56	-1048.350911	-1047.860903	1.6	1.5
57	-1048.351236	-1047.861908	1.4	0.9
58	-1048.350394	-1047.859775	1.9	2.2
59	-1048.350929	-1047.861042	1.6	1.4
60	-1048.350912	-1047.860906	1.6	1.5
Avg.	-1048.351958	-1047.862265		

Table S49. Conformational analysis for **6bd**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1048.750882	-1048.250645	0.0	0.7
2	-1048.750126	-1048.249575	0.5	1.4
3	-1048.750802	-1048.250732	0.1	0.6
4	-1048.750443	-1048.250745	0.3	0.6
5	-1048.750733	-1048.250185	0.1	1.0
6	-1048.748458	-1048.247345	1.5	2.8
7	-1048.750340	-1048.249729	0.4	1.3
8	-1048.749882	-1048.250749	0.6	0.6
9	-1048.748584	-1048.248054	1.5	2.3
10	-1048.750303	-1048.250055	0.4	1.1
11	-1048.749141	-1048.249122	1.1	1.6
12	-1048.750502	-1048.249322	0.3	1.5
13	-1048.749153	-1048.249805	1.1	1.2

14	-1048.748151	-1048.248298	1.7	2.2
15	-1048.749603	-1048.250234	0.8	0.9
16	-1048.749482	-1048.250529	0.9	0.8
17	-1048.749432	-1048.248527	0.9	2.0
18	-1048.749694	-1048.250310	0.8	0.9
19	-1048.748278	-1048.246727	1.7	3.1
20	-1048.748729	-1048.248531	1.4	2.0
21	-1048.749472	-1048.249572	0.9	1.4
22	-1048.749297	-1048.249802	1.0	1.2
23	-1048.750080	-1048.249482	0.5	1.4
24	-1048.749261	-1048.249671	1.0	1.3
25	-1048.748801	-1048.249466	1.3	1.4
26	-1048.748794	-1048.249467	1.3	1.4
27	-1048.748787	-1048.249390	1.3	1.5
28	-1048.748072	-1048.247884	1.8	2.4
29	-1048.749026	-1048.249593	1.2	1.3
30	-1048.749567	-1048.249356	0.8	1.5
31	-1048.749288	-1048.248118	1.0	2.3
32	-1048.749211	-1048.250383	1.1	0.8
33	-1048.748113	-1048.247972	1.8	2.4
34	-1048.748792	-1048.249201	1.3	1.6
35	-1048.748023	-1048.247870	1.8	2.4
36	-1048.748581	-1048.249334	1.5	1.5
37	-1048.748118	-1048.247991	1.8	2.3
38	-1048.748768	-1048.249333	1.3	1.5
39	-1048.747958	-1048.246174	1.9	3.5
40	-1048.748773	-1048.247103	1.3	2.9
41	-1048.749415	-1048.248775	0.9	1.9
42	-1048.748570	-1048.249661	1.5	1.3
43	-1048.749332	-1048.249706	1.0	1.3
44	-1048.748410	-1048.248993	1.6	1.7
45	-1048.748600	-1048.249381	1.4	1.5
46	-1048.748891	-1048.248913	1.3	1.8
47	-1048.748420	-1048.248181	1.6	2.2
48	-1048.748553	-1048.247990	1.5	2.3
49	-1048.749686	-1048.250557	0.8	0.7
50	-1048.748898	-1048.248637	1.3	1.9
51	-1048.748100	-1048.248069	1.8	2.3
52	-1048.748533	-1048.249002	1.5	1.7
53	-1048.748031	-1048.248637	1.8	1.9
54	-1048.747853	-1048.247562	1.9	2.6
55	-1048.747896	-1048.248659	1.9	1.9
56	-1048.747959	-1048.247306	1.9	2.8
57	-1048.748339	-1048.249166	1.6	1.6
58	-1048.748986	-1048.248808	1.2	1.8

59	-1048.748234	-1048.249401	1.7	1.5
60	-1048.749004	-1048.248242	1.2	2.2
61	-1048.748332	-1048.248583	1.6	2.0
62	-1048.748412	-1048.248764	1.6	1.9
63	-1048.748481	-1048.248776	1.5	1.9
64	-1048.748218	-1048.248894	1.7	1.8
65	-1048.750497	-1048.251730	0.3	0.0
66	-1048.748380	-1048.248972	1.6	1.7
67	-1048.747845	-1048.247810	1.9	2.5
68	-1048.749892	-1048.250489	0.6	0.8
69	-1048.747946	-1048.248281	1.9	2.2
70	-1048.747896	-1048.248233	1.9	2.2
71	-1048.748459	-1048.248013	1.5	2.3
72	-1048.748093	-1048.248437	1.8	2.1
73	-1048.747819	-1048.248654	1.9	1.9
74	-1048.748550	-1048.247907	1.5	2.4
75	-1048.748848	-1048.248300	1.3	2.2
76	-1048.747781	-1048.248390	2.0	2.1
77	-1048.750910	-1048.250803	0.0	0.6
78	-1048.748845	-1048.248302	1.3	2.2
79	-1048.748727	-1048.248800	1.4	1.8
80	-1048.749364	-1048.249071	1.0	1.7
81	-1048.748223	-1048.247857	1.7	2.4
82	-1048.748114	-1048.247233	1.8	2.8
83	-1048.748586	-1048.247806	1.5	2.5
Avg.	-1048.749777	-1048.250090		

Table S50. Conformational analysis for **6bd**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1048.338555	-1047.848307	0.0	0.0
2	-1048.338251	-1047.847702	0.2	0.4
3	-1048.337961	-1047.847258	0.4	0.7
4	-1048.338103	-1047.847316	0.3	0.7
5	-1048.337461	-1047.846817	0.7	1.0
6	-1048.337654	-1047.847263	0.6	0.7
7	-1048.338598	-1047.848371	0.0	0.0
8	-1048.338159	-1047.847553	0.3	0.5
9	-1048.338314	-1047.847647	0.2	0.5
10	-1048.337399	-1047.846002	0.8	1.5
11	-1048.337536	-1047.846990	0.7	0.9
12	-1048.337927	-1047.847345	0.4	0.6
13	-1048.337434	-1047.846205	0.7	1.4
14	-1048.338126	-1047.847284	0.3	0.7
15	-1048.336364	-1047.845657	1.4	1.7

16	-1048.336628	-1047.845911	1.2	1.5
17	-1048.337436	-1047.846984	0.7	0.9
18	-1048.335749	-1047.843189	1.8	3.3
19	-1048.337650	-1047.847497	0.6	0.5
20	-1048.335739	-1047.844354	1.8	2.5
21	-1048.336837	-1047.846672	1.1	1.1
22	-1048.337805	-1047.847768	0.5	0.4
23	-1048.336733	-1047.845079	1.2	2.1
24	-1048.335730	-1047.844626	1.8	2.3
25	-1048.335510	-1047.844156	1.9	2.6
26	-1048.337742	-1047.845565	0.5	1.8
27	-1048.336762	-1047.844230	1.2	2.6
28	-1048.336910	-1047.844551	1.1	2.4
29	-1048.336233	-1047.845060	1.5	2.1
30	-1048.335989	-1047.843790	1.6	2.9
31	-1048.336095	-1047.844566	1.6	2.4
32	-1048.336756	-1047.845939	1.2	1.5
33	-1048.337339	-1047.846139	0.8	1.4
34	-1048.335678	-1047.844275	1.8	2.6
35	-1048.337440	-1047.846217	0.7	1.4
36	-1048.337142	-1047.846944	0.9	0.9
37	-1048.336486	-1047.843987	1.3	2.8
38	-1048.336370	-1047.845649	1.4	1.7
39	-1048.336876	-1047.846688	1.1	1.1
40	-1048.336651	-1047.845876	1.2	1.6
41	-1048.336713	-1047.846548	1.2	1.1
42	-1048.335757	-1047.843145	1.8	3.3
Avg.	-1048.337739	-1047.847376		

Table S51. Conformational analysis for **3be**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1088.051930	-1087.522997	0.0	0.9
2	-1088.049523	-1087.523764	1.5	0.4
3	-1088.049513	-1087.523213	1.5	0.8
4	-1088.048879	-1087.523236	1.9	0.8
5	-1088.049892	-1087.523643	1.3	0.5
6	-1088.049782	-1087.522608	1.3	1.2
7	-1088.050251	-1087.523122	1.1	0.8
8	-1088.048786	-1087.522605	2.0	1.2
9	-1088.050207	-1087.522461	1.1	1.3
10	-1088.050285	-1087.523304	1.0	0.7
11	-1088.050023	-1087.521986	1.2	1.5
12	-1088.048867	-1087.522018	1.9	1.5
13	-1088.049338	-1087.522810	1.6	1.0

14	-1088.049801	-1087.523254	1.3	0.8
15	-1088.050324	-1087.522556	1.0	1.2
16	-1088.050190	-1087.524131	1.1	0.2
17	-1088.050085	-1087.522001	1.2	1.5
18	-1088.050107	-1087.524454	1.1	0.0
19	-1088.049374	-1087.523456	1.6	0.6
20	-1088.049817	-1087.522134	1.3	1.5
21	-1088.048967	-1087.522647	1.9	1.1
22	-1088.049009	-1087.522394	1.8	1.3
23	-1088.048842	-1087.522532	1.9	1.2
24	-1088.050211	-1087.522546	1.1	1.2
25	-1088.049689	-1087.522397	1.4	1.3
26	-1088.049194	-1087.523252	1.7	0.8
27	-1088.049850	-1087.522850	1.3	1.0
28	-1088.049259	-1087.523923	1.7	0.3
29	-1088.049015	-1087.522704	1.8	1.1
30	-1088.049327	-1087.523225	1.6	0.8
31	-1088.049197	-1087.523279	1.7	0.7
32	-1088.049331	-1087.523289	1.6	0.7
33	-1088.049093	-1087.522696	1.8	1.1
34	-1088.049156	-1087.523031	1.7	0.9
35	-1088.049182	-1087.523250	1.7	0.8
36	-1088.048860	-1087.521753	1.9	1.7
37	-1088.049180	-1087.523419	1.7	0.6
38	-1088.050006	-1087.522997	1.2	0.9
39	-1088.049000	-1087.522849	1.8	1.0
40	-1088.049505	-1087.521896	1.5	1.6
41	-1088.049391	-1087.521965	1.6	1.6
42	-1088.049256	-1087.523374	1.7	0.7
Avg.	-1088.050222	-1087.523324		

Table S52. Conformational analysis for **3be**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1087.652493	-1087.134702	0.3	0.7
2	-1087.651591	-1087.133294	0.9	1.6
3	-1087.652863	-1087.135092	0.1	0.5
4	-1087.652570	-1087.134696	0.2	0.7
5	-1087.651850	-1087.133111	0.7	1.7
6	-1087.652401	-1087.134575	0.4	0.8
7	-1087.652830	-1087.135405	0.1	0.3
8	-1087.650875	-1087.132752	1.3	1.9
9	-1087.652853	-1087.134891	0.1	0.6
10	-1087.652961	-1087.134674	0.0	0.7
11	-1087.651550	-1087.135603	0.9	0.2

12	-1087.651408	-1087.135633	1.0	0.1
13	-1087.651026	-1087.133048	1.2	1.8
14	-1087.651328	-1087.134476	1.0	0.9
15	-1087.651148	-1087.133277	1.1	1.6
16	-1087.651250	-1087.135084	1.1	0.5
17	-1087.651431	-1087.135357	1.0	0.3
18	-1087.650568	-1087.134354	1.5	0.9
19	-1087.652266	-1087.134144	0.4	1.1
20	-1087.650590	-1087.133417	1.5	1.5
21	-1087.651608	-1087.135842	0.8	0.0
22	-1087.651687	-1087.135593	0.8	0.2
23	-1087.652510	-1087.134469	0.3	0.9
24	-1087.652554	-1087.134025	0.3	1.1
25	-1087.651386	-1087.134653	1.0	0.7
26	-1087.651997	-1087.134823	0.6	0.6
27	-1087.650525	-1087.133495	1.5	1.5
28	-1087.650839	-1087.134458	1.3	0.9
29	-1087.650681	-1087.134181	1.4	1.0
30	-1087.650947	-1087.135674	1.3	0.1
31	-1087.652021	-1087.134729	0.6	0.7
32	-1087.650313	-1087.133080	1.7	1.7
33	-1087.650780	-1087.134635	1.4	0.8
34	-1087.650740	-1087.134459	1.4	0.9
35	-1087.651274	-1087.135246	1.1	0.4
36	-1087.651439	-1087.135535	1.0	0.2
37	-1087.650741	-1087.134749	1.4	0.7
38	-1087.651282	-1087.134215	1.1	1.0
39	-1087.650297	-1087.132928	1.7	1.8
40	-1087.650134	-1087.132251	1.8	2.3
41	-1087.650710	-1087.134359	1.4	0.9
42	-1087.651416	-1087.135635	1.0	0.1
43	-1087.650751	-1087.134515	1.4	0.8
44	-1087.650559	-1087.135105	1.5	0.5
45	-1087.650716	-1087.134379	1.4	0.9
46	-1087.650849	-1087.132495	1.3	2.1
47	-1087.650676	-1087.134575	1.4	0.8
48	-1087.650824	-1087.135006	1.3	0.5
49	-1087.650088	-1087.132441	1.8	2.1
50	-1087.650590	-1087.134501	1.5	0.8
51	-1087.650833	-1087.133749	1.3	1.3
52	-1087.652166	-1087.134509	0.5	0.8
53	-1087.651410	-1087.134152	1.0	1.1
54	-1087.650942	-1087.134586	1.3	0.8
55	-1087.650891	-1087.134628	1.3	0.8
56	-1087.651479	-1087.133907	0.9	1.2

57	-1087.650928	-1087.134660	1.3	0.7
58	-1087.650824	-1087.134412	1.3	0.9
59	-1087.650923	-1087.134537	1.3	0.8
60	-1087.650955	-1087.134185	1.3	1.0
61	-1087.650442	-1087.132950	1.6	1.8
62	-1087.651117	-1087.133651	1.2	1.4
63	-1087.650796	-1087.134357	1.4	0.9
64	-1087.650652	-1087.132781	1.4	1.9
65	-1087.650717	-1087.134181	1.4	1.0
66	-1087.650849	-1087.134414	1.3	0.9
67	-1087.650720	-1087.133799	1.4	1.3
68	-1087.650173	-1087.132232	1.7	2.3
69	-1087.650112	-1087.133807	1.8	1.3
70	-1087.650910	-1087.134219	1.3	1.0
71	-1087.650236	-1087.132492	1.7	2.1
72	-1087.650657	-1087.133352	1.4	1.6
73	-1087.650179	-1087.134345	1.7	0.9
74	-1087.650681	-1087.133617	1.4	1.4
75	-1087.650626	-1087.133667	1.5	1.4
76	-1087.649968	-1087.133224	1.9	1.6
77	-1087.650925	-1087.134455	1.3	0.9
78	-1087.649788	-1087.133040	2.0	1.8
79	-1087.650560	-1087.133655	1.5	1.4
80	-1087.650000	-1087.133478	1.9	1.5
81	-1087.649942	-1087.133394	1.9	1.5
82	-1087.649839	-1087.133682	2.0	1.4
83	-1087.649822	-1087.133359	2.0	1.6
84	-1087.649828	-1087.133607	2.0	1.4
85	-1087.649885	-1087.134413	1.9	0.9
86	-1087.649838	-1087.133186	2.0	1.7
87	-1087.649875	-1087.133830	1.9	1.3
88	-1087.649867	-1087.133904	1.9	1.2
89	-1087.650896	-1087.133114	1.3	1.7
90	-1087.650443	-1087.133762	1.6	1.3
91	-1087.649836	-1087.133175	2.0	1.7
92	-1087.650440	-1087.133617	1.6	1.4
Avg.	-1087.651789	-1087.134791		

Table S53. Conformational analysis for **6be**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1088.046467	-1087.518322	0.0	0.9
2	-1088.045880	-1087.519481	0.4	0.2
3	-1088.046402	-1087.518251	0.0	1.0
4	-1088.045660	-1087.517501	0.5	1.4
5	-1088.045346	-1087.518837	0.7	0.6
6	-1088.045414	-1087.517826	0.7	1.2
7	-1088.045296	-1087.519129	0.7	0.4
8	-1088.045300	-1087.517515	0.7	1.4
9	-1088.044964	-1087.516630	0.9	2.0
10	-1088.045115	-1087.518445	0.8	0.9
11	-1088.044959	-1087.517297	0.9	1.6
12	-1088.044980	-1087.518461	0.9	0.8
13	-1088.044847	-1087.517410	1.0	1.5
14	-1088.043988	-1087.515520	1.6	2.7
15	-1088.045453	-1087.517329	0.6	1.6
16	-1088.044542	-1087.516769	1.2	1.9
17	-1088.044311	-1087.517604	1.4	1.4
18	-1088.045832	-1087.519803	0.4	0.0
19	-1088.044692	-1087.518181	1.1	1.0
20	-1088.045478	-1087.518033	0.6	1.1
21	-1088.045025	-1087.517708	0.9	1.3
22	-1088.045341	-1087.516525	0.7	2.1
23	-1088.044099	-1087.516944	1.5	1.8
24	-1088.044097	-1087.515994	1.5	2.4
25	-1088.044258	-1087.517492	1.4	1.5
26	-1088.044844	-1087.517944	1.0	1.2
27	-1088.044964	-1087.517272	0.9	1.6
28	-1088.044711	-1087.517674	1.1	1.3
29	-1088.043877	-1087.516706	1.6	1.9
30	-1088.044110	-1087.517075	1.5	1.7
31	-1088.043799	-1087.516049	1.7	2.4
32	-1088.043907	-1087.516585	1.6	2.0
33	-1088.043706	-1087.516455	1.7	2.1
34	-1088.045189	-1087.518288	0.8	1.0
35	-1088.043805	-1087.516710	1.7	1.9
36	-1088.043695	-1087.516018	1.7	2.4
37	-1088.045196	-1087.518682	0.8	0.7
38	-1088.045026	-1087.518251	0.9	1.0
39	-1088.043838	-1087.516867	1.6	1.8
40	-1088.043815	-1087.516693	1.7	2.0
41	-1088.044152	-1087.517630	1.5	1.4
42	-1088.043456	-1087.516754	1.9	1.9

43	-1088.043901	-1087.516868	1.6	1.8
44	-1088.044210	-1087.515986	1.4	2.4
45	-1088.044616	-1087.516649	1.2	2.0
46	-1088.044711	-1087.517245	1.1	1.6
47	-1088.044168	-1087.516800	1.4	1.9
48	-1088.044623	-1087.516593	1.2	2.0
49	-1088.044316	-1087.516934	1.3	1.8
50	-1088.043328	-1087.515512	2.0	2.7
51	-1088.043983	-1087.517123	1.6	1.7
52	-1088.043384	-1087.516338	1.9	2.2
53	-1088.043518	-1087.517391	1.9	1.5
54	-1088.044778	-1087.516865	1.1	1.8
55	-1088.043328	-1087.516549	2.0	2.0
56	-1088.043412	-1087.516751	1.9	1.9
57	-1088.043442	-1087.517065	1.9	1.7
58	-1088.043776	-1087.516684	1.7	2.0
59	-1088.044219	-1087.516258	1.4	2.2
60	-1088.043501	-1087.516841	1.9	1.9
61	-1088.044168	-1087.516611	1.4	2.0
62	-1088.043520	-1087.514885	1.8	3.1
63	-1088.043825	-1087.515111	1.7	2.9
64	-1088.044417	-1087.518480	1.3	0.8
65	-1088.044174	-1087.516809	1.4	1.9
66	-1088.043896	-1087.516197	1.6	2.3
67	-1088.044402	-1087.516563	1.3	2.0
68	-1088.043544	-1087.515796	1.8	2.5
69	-1088.043456	-1087.515639	1.9	2.6
Avg.	-1088.045156	-1087.518297		

Table S54. Conformational analysis for **6be**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1087.634767	-1087.117858	0.1	0.0
2	-1087.634766	-1087.117498	0.1	0.2
3	-1087.634253	-1087.117176	0.5	0.4
4	-1087.634588	-1087.116753	0.2	0.7
5	-1087.634088	-1087.116455	0.6	0.9
6	-1087.634566	-1087.117275	0.3	0.4
7	-1087.633895	-1087.116855	0.7	0.6
8	-1087.634818	-1087.117704	0.1	0.1
9	-1087.634981	-1087.116507	0.0	0.8
10	-1087.634896	-1087.116806	0.1	0.7
11	-1087.634173	-1087.116680	0.5	0.7
12	-1087.632682	-1087.113607	1.4	2.7
13	-1087.633972	-1087.116430	0.6	0.9

14	-1087.633681	-1087.116159	0.8	1.1
15	-1087.633911	-1087.115516	0.7	1.5
16	-1087.633236	-1087.115617	1.1	1.4
17	-1087.633823	-1087.115700	0.7	1.4
18	-1087.633815	-1087.116410	0.7	0.9
19	-1087.633652	-1087.115710	0.8	1.3
20	-1087.633155	-1087.115339	1.1	1.6
21	-1087.633378	-1087.114981	1.0	1.8
22	-1087.632389	-1087.113931	1.6	2.5
23	-1087.634012	-1087.114672	0.6	2.0
24	-1087.632817	-1087.115386	1.4	1.6
25	-1087.632554	-1087.115449	1.5	1.5
26	-1087.634546	-1087.115043	0.3	1.8
27	-1087.632265	-1087.113887	1.7	2.5
28	-1087.633219	-1087.115228	1.1	1.7
29	-1087.633945	-1087.115350	0.7	1.6
30	-1087.633414	-1087.115084	1.0	1.7
31	-1087.633981	-1087.114524	0.6	2.1
32	-1087.632363	-1087.115026	1.6	1.8
33	-1087.632508	-1087.115190	1.6	1.7
34	-1087.632447	-1087.115003	1.6	1.8
35	-1087.632699	-1087.115255	1.4	1.6
36	-1087.632816	-1087.114651	1.4	2.0
37	-1087.633974	-1087.116359	0.6	0.9
38	-1087.633446	-1087.114990	1.0	1.8
39	-1087.632087	-1087.113875	1.8	2.5
40	-1087.632199	-1087.114682	1.7	2.0
41	-1087.632332	-1087.113776	1.7	2.6
42	-1087.632681	-1087.113451	1.4	2.8
43	-1087.632265	-1087.113883	1.7	2.5
44	-1087.633436	-1087.114199	1.0	2.3
45	-1087.633809	-1087.116378	0.7	0.9
46	-1087.631887	-1087.114504	1.9	2.1
47	-1087.632462	-1087.115209	1.6	1.7
48	-1087.633152	-1087.115334	1.1	1.6
49	-1087.631944	-1087.113460	1.9	2.8
50	-1087.632018	-1087.114292	1.9	2.2
51	-1087.631869	-1087.113031	2.0	3.0
52	-1087.631831	-1087.113898	2.0	2.5
53	-1087.632378	-1087.115701	1.6	1.4
54	-1087.632323	-1087.113255	1.7	2.9
55	-1087.632422	-1087.114507	1.6	2.1
Avg.	-1087.634089	-1087.116701		

Table S55. Conformational analysis for **3b**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1127.355495	-1126.800826	0.0	0.7
2	-1127.353364	-1126.798268	1.3	2.3
3	-1127.354822	-1126.801658	0.4	0.1
4	-1127.353421	-1126.798519	1.3	2.1
5	-1127.353116	-1126.800086	1.5	1.1
6	-1127.354345	-1126.800836	0.7	0.7
7	-1127.352471	-1126.799647	1.9	1.4
8	-1127.352459	-1126.799743	1.9	1.3
9	-1127.352449	-1126.799691	1.9	1.4
10	-1127.354156	-1126.800528	0.8	0.8
11	-1127.352802	-1126.799444	1.7	1.5
12	-1127.352797	-1126.799457	1.7	1.5
13	-1127.354002	-1126.799711	0.9	1.4
14	-1127.354235	-1126.800147	0.8	1.1
15	-1127.353266	-1126.798865	1.4	1.9
16	-1127.353997	-1126.801161	0.9	0.4
17	-1127.353509	-1126.799788	1.2	1.3
18	-1127.354599	-1126.799495	0.6	1.5
19	-1127.353043	-1126.800366	1.5	0.9
20	-1127.352810	-1126.798192	1.7	2.3
21	-1127.354629	-1126.800082	0.5	1.1
22	-1127.352936	-1126.799569	1.6	1.4
23	-1127.354257	-1126.799717	0.8	1.4
24	-1127.352868	-1126.799927	1.6	1.2
25	-1127.352704	-1126.799392	1.8	1.6
26	-1127.352646	-1126.799500	1.8	1.5
27	-1127.353238	-1126.799580	1.4	1.4
28	-1127.353223	-1126.799406	1.4	1.6
29	-1127.353472	-1126.800314	1.3	1.0
30	-1127.352314	-1126.797262	2.0	2.9
31	-1127.353213	-1126.798683	1.4	2.0
32	-1127.353046	-1126.798146	1.5	2.3
33	-1127.353338	-1126.799348	1.4	1.6
34	-1127.353013	-1126.799303	1.6	1.6
35	-1127.352980	-1126.799574	1.6	1.4
36	-1127.354258	-1126.799002	0.8	1.8
37	-1127.352886	-1126.798328	1.6	2.2
38	-1127.353072	-1126.799862	1.5	1.3
39	-1127.352799	-1126.800077	1.7	1.1
40	-1127.352856	-1126.800030	1.7	1.2
41	-1127.352741	-1126.798531	1.7	2.1
42	-1127.354285	-1126.798612	0.8	2.0

43	-1127.352884	-1126.798987	1.6	1.8
44	-1127.354213	-1126.799063	0.8	1.8
45	-1127.352639	-1126.799576	1.8	1.4
46	-1127.352838	-1126.799915	1.7	1.2
47	-1127.352957	-1126.799067	1.6	1.8
48	-1127.352660	-1126.800693	1.8	0.7
49	-1127.352502	-1126.798512	1.9	2.1
50	-1127.352911	-1126.798902	1.6	1.9
51	-1127.352731	-1126.801029	1.7	0.5
52	-1127.353392	-1126.799050	1.3	1.8
53	-1127.352962	-1126.799235	1.6	1.7
54	-1127.353764	-1126.800577	1.1	0.8
55	-1127.352888	-1126.799693	1.6	1.4
56	-1127.352677	-1126.799043	1.8	1.8
57	-1127.353113	-1126.798498	1.5	2.1
58	-1127.352419	-1126.798334	1.9	2.2
59	-1127.354075	-1126.799293	0.9	1.6
60	-1127.354988	-1126.801877	0.3	0.0
61	-1127.352809	-1126.799189	1.7	1.7
62	-1127.352378	-1126.798909	2.0	1.9
Avg.	-1127.354036	-1126.800442		

Table S56. Conformational analysis for **3b**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1126.953548	-1126.409296	0.6	1.1
2	-1126.954115	-1126.409266	0.3	1.1
3	-1126.954559	-1126.409719	0.0	0.8
4	-1126.953217	-1126.407818	0.8	2.0
5	-1126.951916	-1126.407213	1.7	2.4
6	-1126.952932	-1126.409521	1.0	0.9
7	-1126.952550	-1126.410724	1.3	0.2
8	-1126.952294	-1126.410082	1.4	0.6
9	-1126.952682	-1126.410479	1.2	0.3
10	-1126.953251	-1126.408743	0.8	1.4
11	-1126.952569	-1126.411013	1.2	0.0
12	-1126.951401	-1126.408627	2.0	1.5
13	-1126.953507	-1126.408317	0.7	1.7
14	-1126.953608	-1126.409090	0.6	1.2
15	-1126.952074	-1126.407430	1.6	2.2
16	-1126.952451	-1126.407834	1.3	2.0
17	-1126.951501	-1126.408259	1.9	1.7
18	-1126.952548	-1126.408512	1.3	1.6
19	-1126.952336	-1126.409315	1.4	1.1
20	-1126.951339	-1126.406960	2.0	2.5

21	-1126.951798	-1126.408722	1.7	1.4
22	-1126.951663	-1126.408749	1.8	1.4
23	-1126.951724	-1126.409174	1.8	1.2
24	-1126.951682	-1126.407642	1.8	2.1
25	-1126.951703	-1126.409148	1.8	1.2
26	-1126.951708	-1126.409045	1.8	1.2
27	-1126.953110	-1126.409358	0.9	1.0
28	-1126.951527	-1126.408668	1.9	1.5
29	-1126.951516	-1126.408918	1.9	1.3
30	-1126.952057	-1126.407851	1.6	2.0
31	-1126.951390	-1126.406409	2.0	2.9
32	-1126.952310	-1126.407705	1.4	2.1
33	-1126.951666	-1126.409235	1.8	1.1
34	-1126.949780	-1126.406549	3.0	2.8
35	-1126.951427	-1126.406767	2.0	2.7
36	-1126.951650	-1126.408843	1.8	1.4
37	-1126.951731	-1126.407322	1.8	2.3
38	-1126.952020	-1126.407644	1.6	2.1
39	-1126.951501	-1126.409054	1.9	1.2
40	-1126.951664	-1126.409192	1.8	1.1
41	-1126.951554	-1126.407855	1.9	2.0
42	-1126.951383	-1126.407961	2.0	1.9
43	-1126.951823	-1126.408713	1.7	1.4
44	-1126.951567	-1126.407211	1.9	2.4
Avg.	-1126.953158	-1126.409714		

Table S57. Conformational analysis for **6b**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1127.351993	-1126.798273	0.0	0.0
2	-1127.350850	-1126.796072	0.7	1.4
3	-1127.350470	-1126.797383	1.0	0.6
4	-1127.351076	-1126.796578	0.6	1.1
5	-1127.349955	-1126.795258	1.3	1.9
6	-1127.351209	-1126.797303	0.5	0.6
7	-1127.351010	-1126.796764	0.6	0.9
8	-1127.350998	-1126.797155	0.6	0.7
9	-1127.351179	-1126.796943	0.5	0.8
10	-1127.351197	-1126.796830	0.5	0.9
11	-1127.349842	-1126.796339	1.3	1.2
12	-1127.350493	-1126.796954	0.9	0.8
13	-1127.350796	-1126.796643	0.8	1.0
14	-1127.349591	-1126.795628	1.5	1.7
15	-1127.351109	-1126.796439	0.6	1.2
16	-1127.351632	-1126.796320	0.2	1.2

17	-1127.351481	-1126.796726	0.3	1.0
18	-1127.350787	-1126.798101	0.8	0.1
19	-1127.349662	-1126.796129	1.5	1.3
20	-1127.349144	-1126.794792	1.8	2.2
21	-1127.349633	-1126.795860	1.5	1.5
22	-1127.351362	-1126.796785	0.4	0.9
23	-1127.350268	-1126.794922	1.1	2.1
24	-1127.350001	-1126.796535	1.2	1.1
25	-1127.350147	-1126.795382	1.2	1.8
26	-1127.350729	-1126.796430	0.8	1.2
27	-1127.349822	-1126.795222	1.4	1.9
28	-1127.350838	-1126.796275	0.7	1.3
29	-1127.350195	-1126.796182	1.1	1.3
30	-1127.350097	-1126.796546	1.2	1.1
31	-1127.350107	-1126.797326	1.2	0.6
32	-1127.349579	-1126.794551	1.5	2.3
33	-1127.349702	-1126.795391	1.4	1.8
34	-1127.350711	-1126.796057	0.8	1.4
35	-1127.349645	-1126.796045	1.5	1.4
36	-1127.349558	-1126.795429	1.5	1.8
37	-1127.350076	-1126.796282	1.2	1.2
38	-1127.349990	-1126.796568	1.3	1.1
39	-1127.349289	-1126.795474	1.7	1.8
40	-1127.349749	-1126.795971	1.4	1.4
41	-1127.350070	-1126.795624	1.2	1.7
42	-1127.350055	-1126.795988	1.2	1.4
43	-1127.350688	-1126.797070	0.8	0.8
44	-1127.350673	-1126.795616	0.8	1.7
45	-1127.349485	-1126.796076	1.6	1.4
46	-1127.349992	-1126.796530	1.3	1.1
47	-1127.350466	-1126.795782	1.0	1.6
48	-1127.350342	-1126.797253	1.0	0.6
49	-1127.350569	-1126.796390	0.9	1.2
50	-1127.349776	-1126.794950	1.4	2.1
51	-1127.350352	-1126.795807	1.0	1.5
52	-1127.350140	-1126.796328	1.2	1.2
53	-1127.349177	-1126.795514	1.8	1.7
54	-1127.349667	-1126.795548	1.5	1.7
55	-1127.349376	-1126.794556	1.6	2.3
56	-1127.350493	-1126.795587	0.9	1.7
57	-1127.349085	-1126.795224	1.8	1.9
58	-1127.349198	-1126.795934	1.8	1.5
59	-1127.349780	-1126.795602	1.4	1.7
60	-1127.349778	-1126.795180	1.4	1.9
61	-1127.350819	-1126.796481	0.7	1.1

62	-1127.349760	-1126.796837	1.4	0.9
63	-1127.349176	-1126.794463	1.8	2.4
64	-1127.349323	-1126.794562	1.7	2.3
65	-1127.349125	-1126.794359	1.8	2.5
66	-1127.348975	-1126.793871	1.9	2.8
67	-1127.350364	-1126.797822	1.0	0.3
68	-1127.349152	-1126.795310	1.8	1.9
69	-1127.350612	-1126.795979	0.9	1.4
70	-1127.349305	-1126.794810	1.7	2.2
71	-1127.349474	-1126.796186	1.6	1.3
72	-1127.349559	-1126.797157	1.5	0.7
73	-1127.349534	-1126.795781	1.5	1.6
74	-1127.349078	-1126.795704	1.8	1.6
75	-1127.349432	-1126.796736	1.6	1.0
76	-1127.349356	-1126.795254	1.7	1.9
77	-1127.349235	-1126.795855	1.7	1.5
78	-1127.349901	-1126.795522	1.3	1.7
79	-1127.349641	-1126.796288	1.5	1.2
80	-1127.349102	-1126.795530	1.8	1.7
81	-1127.350397	-1126.797461	1.0	0.5
82	-1127.348966	-1126.795944	1.9	1.5
83	-1127.348847	-1126.795427	2.0	1.8
84	-1127.349194	-1126.794586	1.8	2.3
85	-1127.348922	-1126.795929	1.9	1.5
86	-1127.349403	-1126.795040	1.6	2.0
87	-1127.350273	-1126.794556	1.1	2.3
88	-1127.349351	-1126.796395	1.7	1.2
89	-1127.349136	-1126.795209	1.8	1.9
90	-1127.348957	-1126.795286	1.9	1.9
91	-1127.349120	-1126.794339	1.8	2.5
92	-1127.350034	-1126.795324	1.2	1.9
93	-1127.350102	-1126.795099	1.2	2.0
94	-1127.349547	-1126.796168	1.5	1.3
95	-1127.349095	-1126.794511	1.8	2.4
96	-1127.349262	-1126.796058	1.7	1.4
97	-1127.348952	-1126.794217	1.9	2.5
98	-1127.349252	-1126.795459	1.7	1.8
99	-1127.349477	-1126.795385	1.6	1.8
100	-1127.348820	-1126.793899	2.0	2.7
101	-1127.349036	-1126.794338	1.9	2.5
102	-1127.349104	-1126.795835	1.8	1.5
103	-1127.349353	-1126.796224	1.7	1.3
104	-1127.349723	-1126.794653	1.4	2.3
105	-1127.349685	-1126.795785	1.4	1.6
106	-1127.348987	-1126.793659	1.9	2.9

Avg.	-1127.350541	-1126.796757		

Table S58. Conformational analysis for **6b**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1126.937573	-1126.393509	0.0	0.0
2	-1126.937289	-1126.392590	0.2	0.6
3	-1126.937030	-1126.392480	0.4	0.6
4	-1126.936672	-1126.392109	0.6	0.9
5	-1126.936568	-1126.392219	0.7	0.8
6	-1126.936848	-1126.392200	0.5	0.8
7	-1126.937645	-1126.393450	0.0	0.0
8	-1126.936528	-1126.392631	0.7	0.6
9	-1126.937347	-1126.391800	0.2	1.1
10	-1126.936424	-1126.391467	0.8	1.3
11	-1126.934813	-1126.390862	1.8	1.7
12	-1126.936428	-1126.391174	0.8	1.5
13	-1126.934933	-1126.390866	1.7	1.7
14	-1126.935630	-1126.391322	1.3	1.4
15	-1126.935319	-1126.390803	1.5	1.7
16	-1126.935657	-1126.391434	1.2	1.3
17	-1126.934501	-1126.389084	2.0	2.8
18	-1126.935463	-1126.390660	1.4	1.8
19	-1126.935976	-1126.390695	1.0	1.8
20	-1126.935300	-1126.390326	1.5	2.0
21	-1126.934571	-1126.389580	1.9	2.5
22	-1126.934893	-1126.390122	1.7	2.1
23	-1126.935633	-1126.389758	1.3	2.4
24	-1126.936446	-1126.391448	0.8	1.3
25	-1126.936647	-1126.390367	0.6	2.0
26	-1126.935178	-1126.389203	1.5	2.7
27	-1126.935420	-1126.390513	1.4	1.9
28	-1126.934611	-1126.389401	1.9	2.6
29	-1126.934645	-1126.389212	1.9	2.7
30	-1126.935443	-1126.390008	1.4	2.2
31	-1126.935300	-1126.389983	1.5	2.2
32	-1126.934835	-1126.390195	1.8	2.1
33	-1126.934656	-1126.389822	1.9	2.3
34	-1126.934506	-1126.390237	2.0	2.1
35	-1126.934543	-1126.388612	1.9	3.1
Avg.	-1126.936728	-1126.392441		

Table S59. Conformational analysis for **3bf**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1166.652315	-1166.070981	1.6	3.1
2	-1166.651978	-1166.069466	1.8	4.1
3	-1166.654674	-1166.072561	0.2	2.1
4	-1166.654152	-1166.073140	0.5	1.8
5	-1166.654312	-1166.072017	0.4	2.5
6	-1166.653317	-1166.070337	1.0	3.5
7	-1166.653575	-1166.072302	0.8	2.3
8	-1166.653260	-1166.072870	1.0	1.9
9	-1166.653250	-1166.071469	1.0	2.8
10	-1166.653355	-1166.072156	1.0	2.4
11	-1166.653253	-1166.072027	1.0	2.5
12	-1166.652528	-1166.072135	1.5	2.4
13	-1166.652488	-1166.072307	1.5	2.3
14	-1166.654597	-1166.071962	0.2	2.5
15	-1166.652687	-1166.071713	1.4	2.7
16	-1166.654149	-1166.071309	0.5	2.9
17	-1166.652284	-1166.071192	1.7	3.0
18	-1166.652953	-1166.070564	1.2	3.4
19	-1166.652606	-1166.071598	1.5	2.7
20	-1166.654923	-1166.075940	0.0	0.0
21	-1166.652661	-1166.071188	1.4	3.0
22	-1166.652568	-1166.071288	1.5	2.9
23	-1166.652585	-1166.071566	1.5	2.7
24	-1166.652370	-1166.071589	1.6	2.7
25	-1166.652424	-1166.071108	1.6	3.0
26	-1166.652081	-1166.072599	1.8	2.1
27	-1166.652919	-1166.070720	1.3	3.3
28	-1166.653473	-1166.070947	0.9	3.1
29	-1166.652116	-1166.073110	1.8	1.8
30	-1166.651808	-1166.071173	2.0	3.0
31	-1166.654029	-1166.073359	0.6	1.6
32	-1166.652618	-1166.072052	1.4	2.4
33	-1166.652452	-1166.071383	1.6	2.9
34	-1166.652090	-1166.071457	1.8	2.8
35	-1166.652071	-1166.070807	1.8	3.2
36	-1166.652433	-1166.071906	1.6	2.5
37	-1166.652139	-1166.072157	1.7	2.4
38	-1166.652351	-1166.071617	1.6	2.7
39	-1166.652406	-1166.070277	1.6	3.6
40	-1166.653249	-1166.072835	1.1	1.9
41	-1166.654004	-1166.074030	0.6	1.2
42	-1166.652545	-1166.071600	1.5	2.7

43	-1166.654893	-1166.074431	0.0	0.9
44	-1166.653010	-1166.070422	1.2	3.5
45	-1166.653929	-1166.074792	0.6	0.7
46	-1166.652621	-1166.069731	1.4	3.9
47	-1166.653818	-1166.073393	0.7	1.6
48	-1166.652029	-1166.071561	1.8	2.7
49	-1166.654328	-1166.073919	0.4	1.3
50	-1166.653865	-1166.073580	0.7	1.5
51	-1166.652418	-1166.070594	1.6	3.4
52	-1166.652898	-1166.070878	1.3	3.2
53	-1166.652507	-1166.072270	1.5	2.3
54	-1166.653197	-1166.073763	1.1	1.4
55	-1166.651815	-1166.070005	2.0	3.7
Avg.	-1166.653854	-1166.074378		

Table S60. Conformational analysis for **3bf**.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1166.248655	-1165.677740	1.0	1.8
2	-1166.248731	-1165.677768	0.9	1.8
3	-1166.250051	-1165.679529	0.1	0.7
4	-1166.250218	-1165.679129	0.0	0.9
5	-1166.248099	-1165.677103	1.3	2.2
6	-1166.249938	-1165.679838	0.2	0.5
7	-1166.248970	-1165.680482	0.8	0.1
8	-1166.248956	-1165.680260	0.8	0.2
9	-1166.249119	-1165.679356	0.7	0.8
10	-1166.248973	-1165.680430	0.8	0.1
11	-1166.248789	-1165.679167	0.9	0.9
12	-1166.249116	-1165.678999	0.7	1.0
13	-1166.248969	-1165.680570	0.8	0.0
14	-1166.250005	-1165.679165	0.1	0.9
15	-1166.249597	-1165.678148	0.4	1.5
16	-1166.248356	-1165.678747	1.2	1.1
17	-1166.248325	-1165.680049	1.2	0.3
18	-1166.249190	-1165.678418	0.6	1.4
19	-1166.249465	-1165.677726	0.5	1.8
20	-1166.248272	-1165.678607	1.2	1.2
21	-1166.248259	-1165.678741	1.2	1.1
22	-1166.248397	-1165.679365	1.1	0.8
23	-1166.249177	-1165.678658	0.7	1.2
24	-1166.247174	-1165.675813	1.9	3.0
25	-1166.248015	-1165.678697	1.4	1.2
26	-1166.247839	-1165.678339	1.5	1.4

27	-1166.248062	-1165.677280	1.4	2.1
28	-1166.248009	-1165.678889	1.4	1.1
29	-1166.247522	-1165.676720	1.7	2.4
30	-1166.248008	-1165.678920	1.4	1.0
31	-1166.247972	-1165.678961	1.4	1.0
32	-1166.249455	-1165.677675	0.5	1.8
33	-1166.247771	-1165.678215	1.5	1.5
34	-1166.247839	-1165.678488	1.5	1.3
35	-1166.247398	-1165.676860	1.8	2.3
36	-1166.248237	-1165.677470	1.2	1.9
37	-1166.248231	-1165.677801	1.2	1.7
38	-1166.247743	-1165.675519	1.6	3.2
39	-1166.249002	-1165.680261	0.8	0.2
40	-1166.247572	-1165.678205	1.7	1.5
41	-1166.247625	-1165.678425	1.6	1.3
42	-1166.247816	-1165.678397	1.5	1.4
43	-1166.247770	-1165.678620	1.5	1.2
44	-1166.247127	-1165.676325	1.9	2.7
45	-1166.248302	-1165.679748	1.2	0.5
46	-1166.247960	-1165.678473	1.4	1.3
47	-1166.248036	-1165.679195	1.4	0.9
48	-1166.247528	-1165.678637	1.7	1.2
49	-1166.247591	-1165.676408	1.6	2.6
50	-1166.247096	-1165.677103	2.0	2.2
51	-1166.248009	-1165.678890	1.4	1.1
52	-1166.247360	-1165.678822	1.8	1.1
53	-1166.248052	-1165.676803	1.4	2.4
54	-1166.248009	-1165.678967	1.4	1.0
55	-1166.247627	-1165.679060	1.6	0.9
56	-1166.247441	-1165.675909	1.7	2.9
57	-1166.248026	-1165.676521	1.4	2.5
58	-1166.247404	-1165.677732	1.8	1.8
59	-1166.247147	-1165.677786	1.9	1.7
60	-1166.247127	-1165.677468	1.9	1.9
61	-1166.247403	-1165.679039	1.8	1.0
62	-1166.247128	-1165.677653	1.9	1.8
63	-1166.247982	-1165.679330	1.4	0.8
64	-1166.248269	-1165.678622	1.2	1.2
65	-1166.247101	-1165.677492	2.0	1.9
66	-1166.247881	-1165.677301	1.5	2.1
67	-1166.247795	-1165.678164	1.5	1.5
68	-1166.247669	-1165.678014	1.6	1.6
69	-1166.247032	-1165.678973	2.0	1.0
70	-1166.247051	-1165.677983	2.0	1.6
71	-1166.247755	-1165.678542	1.5	1.3

72	-1166.247386	-1165.677572	1.8	1.9
73	-1166.247626	-1165.678084	1.6	1.6
74	-1166.247664	-1165.677274	1.6	2.1
75	-1166.247101	-1165.676746	2.0	2.4
76	-1166.247132	-1165.674821	1.9	3.6
77	-1166.247643	-1165.678595	1.6	1.2
78	-1166.247884	-1165.678094	1.5	1.6
79	-1166.247685	-1165.678246	1.6	1.5
80	-1166.248315	-1165.675624	1.2	3.1
81	-1166.247163	-1165.677111	1.9	2.2
82	-1166.247872	-1165.675808	1.5	3.0
83	-1166.247285	-1165.674947	1.8	3.5
84	-1166.247192	-1165.676809	1.9	2.4
85	-1166.248728	-1165.675764	0.9	3.0
Avg.	-1166.248897	-1165.679380		

Table S61. Conformational analysis for **6bf**‡.

Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1166.651170	-1166.068813	0.3	1.6
2	-1166.651603	-1166.069689	0.0	1.1
3	-1166.648900	-1166.065119	1.7	4.0
4	-1166.650413	-1166.069149	0.7	1.4
5	-1166.651124	-1166.070573	0.3	0.5
6	-1166.650518	-1166.070061	0.7	0.9
7	-1166.650479	-1166.069643	0.7	1.1
8	-1166.650391	-1166.068176	0.8	2.0
9	-1166.651396	-1166.071438	0.1	0.0
10	-1166.650354	-1166.068887	0.8	1.6
11	-1166.648846	-1166.067215	1.7	2.6
12	-1166.649521	-1166.067793	1.3	2.3
13	-1166.650535	-1166.069466	0.7	1.2
14	-1166.650562	-1166.069691	0.7	1.1
15	-1166.650200	-1166.069016	0.9	1.5
16	-1166.649968	-1166.068776	1.0	1.7
17	-1166.650392	-1166.070269	0.8	0.7
18	-1166.650349	-1166.069966	0.8	0.9
19	-1166.650262	-1166.069340	0.8	1.3
20	-1166.650262	-1166.069398	0.8	1.3
21	-1166.650275	-1166.068890	0.8	1.6
22	-1166.649956	-1166.069014	1.0	1.5
23	-1166.649180	-1166.070060	1.5	0.9
24	-1166.649254	-1166.068735	1.5	1.7
25	-1166.650292	-1166.069604	0.8	1.2
26	-1166.650430	-1166.068614	0.7	1.8

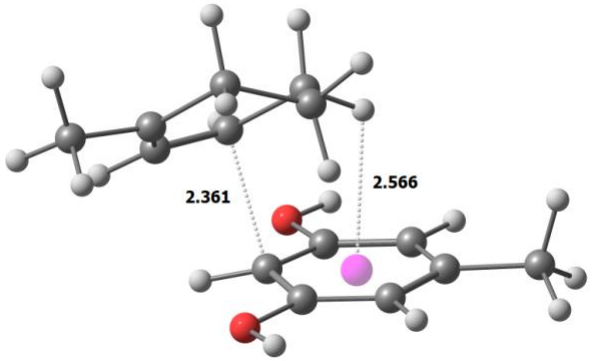
27	-1166.650274	-1166.071168	0.8	0.2
28	-1166.649354	-1166.069890	1.4	1.0
29	-1166.650642	-1166.070230	0.6	0.8
30	-1166.649173	-1166.069231	1.5	1.4
31	-1166.650223	-1166.069875	0.9	1.0
32	-1166.649213	-1166.069036	1.5	1.5
33	-1166.650517	-1166.068885	0.7	1.6
34	-1166.648844	-1166.066052	1.7	3.4
35	-1166.649846	-1166.067844	1.1	2.3
36	-1166.649705	-1166.069493	1.2	1.2
37	-1166.649257	-1166.068555	1.5	1.8
38	-1166.649356	-1166.067586	1.4	2.4
39	-1166.648876	-1166.065263	1.7	3.9
40	-1166.649435	-1166.068751	1.4	1.7
41	-1166.649474	-1166.067496	1.3	2.5
42	-1166.649488	-1166.068640	1.3	1.8
43	-1166.649383	-1166.068402	1.4	1.9
44	-1166.650954	-1166.069712	0.4	1.1
45	-1166.649424	-1166.069700	1.4	1.1
46	-1166.648698	-1166.067225	1.8	2.6
47	-1166.649425	-1166.069203	1.4	1.4
48	-1166.650130	-1166.068457	0.9	1.9
49	-1166.649270	-1166.069666	1.5	1.1
50	-1166.649659	-1166.069082	1.2	1.5
51	-1166.649308	-1166.069167	1.4	1.4
52	-1166.649044	-1166.069148	1.6	1.4
53	-1166.649304	-1166.069931	1.4	0.9
54	-1166.649950	-1166.066875	1.0	2.9
55	-1166.649922	-1166.067328	1.1	2.6
56	-1166.650015	-1166.068911	1.0	1.6
57	-1166.650079	-1166.069171	1.0	1.4
58	-1166.648723	-1166.067370	1.8	2.6
59	-1166.648803	-1166.067363	1.8	2.6
60	-1166.648694	-1166.066713	1.8	3.0
61	-1166.648826	-1166.067334	1.7	2.6
62	-1166.649207	-1166.069758	1.5	1.1
63	-1166.649239	-1166.068912	1.5	1.6
64	-1166.649120	-1166.068200	1.6	2.0
65	-1166.649797	-1166.069535	1.1	1.2
66	-1166.650170	-1166.067833	0.9	2.3
67	-1166.649229	-1166.069321	1.5	1.3
68	-1166.649223	-1166.068194	1.5	2.0
69	-1166.650165	-1166.067930	0.9	2.2
70	-1166.649517	-1166.067319	1.3	2.6
71	-1166.648437	-1166.066083	2.0	3.4

72	-1166.649712	-1166.068209	1.2	2.0
73	-1166.648564	-1166.068188	1.9	2.0
74	-1166.649339	-1166.068443	1.4	1.9
75	-1166.649325	-1166.068208	1.4	2.0
76	-1166.648741	-1166.065868	1.8	3.5
77	-1166.649836	-1166.068017	1.1	2.1
Avg.	-1166.650305	-1166.069880		

Table S62. Conformational analysis for **6bf**.

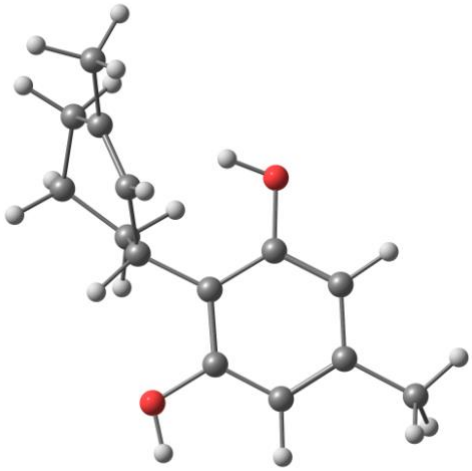
Conformer #	E	G	DE	DG
	au	au	kcal/mol	kcal/mol
1	-1166.232884	-1165.661685	0.0	0.0
2	-1166.232359	-1165.660518	0.3	0.7
3	-1166.232322	-1165.660381	0.4	0.8
4	-1166.230007	-1165.658169	1.8	2.2
5	-1166.230066	-1165.657569	1.8	2.6
6	-1166.232005	-1165.660407	0.6	0.8
7	-1166.231738	-1165.659924	0.7	1.1
8	-1166.231816	-1165.659861	0.7	1.1
9	-1166.232347	-1165.660413	0.3	0.8
10	-1166.232506	-1165.659854	0.2	1.1
11	-1166.231733	-1165.659409	0.7	1.4
12	-1166.230967	-1165.658837	1.2	1.8
13	-1166.230805	-1165.658761	1.3	1.8
14	-1166.231850	-1165.659960	0.6	1.1
15	-1166.231125	-1165.659116	1.1	1.6
16	-1166.231053	-1165.659027	1.1	1.7
17	-1166.229962	-1165.658855	1.8	1.8
18	-1166.230374	-1165.658353	1.6	2.1
19	-1166.231043	-1165.658200	1.2	2.2
20	-1166.231681	-1165.659420	0.8	1.4
21	-1166.230003	-1165.657632	1.8	2.5
22	-1166.231131	-1165.659095	1.1	1.6
Avg.	-1166.232023	-1165.660437		

Table S63. Coordinates for global minimum of **3ac**‡.



C	-0.863091	-1.100226	-0.642569
C	-2.039228	-1.042961	0.125538
C	-2.981620	-0.069673	-0.084443
C	-4.284300	-0.095353	0.622242
H	-4.363377	0.800561	1.254214
H	-5.108730	-0.025381	-0.098935
H	-4.408665	-0.984457	1.243106
C	-2.771506	0.999967	-1.103155
C	-1.299324	1.245386	-1.415796
H	-0.834203	1.760279	-0.568476
H	-1.200746	1.901816	-2.285390
C	-0.569446	-0.070767	-1.668163
H	0.513783	0.071659	-1.771695
H	-3.313816	0.675146	-2.008391
H	-3.271885	1.920182	-0.778645
H	-2.243785	-1.840973	0.834911
H	-0.381098	-2.068123	-0.755195
C	0.634556	0.457092	1.326800
C	0.775812	-0.918174	1.046706
C	1.888096	-1.332887	0.281185
C	2.746771	-0.406629	-0.286886
C	2.547194	0.962407	-0.050156
C	1.494585	1.392048	0.761965
H	1.354696	2.451476	0.962676
C	3.457113	1.966102	-0.691981
H	3.105708	2.190363	-1.707218
H	4.475658	1.577696	-0.778166
H	3.580299	-0.738010	-0.901443
O	2.015209	-2.668894	0.112124
H	2.774926	-2.860377	-0.456979
H	0.222420	-1.648090	1.627941
O	-0.392511	0.788880	2.136248
H	-0.435093	1.750766	2.244333
H	3.474127	2.904260	-0.131882
H	-0.890379	-0.516206	-2.627794

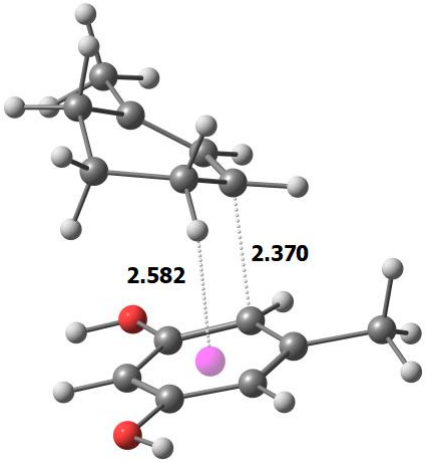
Table S64. Coordinates for global minimum of **3ac**.



C	-0.858487	-0.792503	0.206676
C	-1.759396	0.184457	0.932315
C	-2.990943	0.531635	0.529473
C	-3.822641	1.527781	1.281158
H	-4.135741	2.344313	0.617159
H	-3.279271	1.954806	2.128675
H	-4.742433	1.058097	1.652773
C	-3.617103	-0.062584	-0.706643
C	-2.902183	-1.330556	-1.173482
C	-1.392715	-1.106303	-1.204744
H	-0.867481	-1.983692	-1.599403
H	-1.163804	-0.265717	-1.875089
H	-3.267970	-1.628572	-2.162848
H	-3.131658	-2.152685	-0.481470
H	-4.676580	-0.268366	-0.501438
H	-3.611539	0.695167	-1.506167
H	-1.362571	0.614398	1.854092
H	-0.861481	-1.727488	0.782766
C	0.578925	-0.314265	0.147029
C	1.646239	-1.188657	0.402172
C	2.976231	-0.785432	0.300740
C	3.284330	0.524017	-0.074829
C	2.246573	1.413003	-0.335171
C	0.917574	0.994678	-0.229080
O	-0.035219	1.929060	-0.529783
H	-0.909812	1.597758	-0.244220
H	2.450213	2.440216	-0.624354
C	4.720969	0.954828	-0.204548
H	5.299824	0.667277	0.679896
H	5.193925	0.475698	-1.070368
H	4.799697	2.037582	-0.333192
H	3.771899	-1.497571	0.512175
O	1.325048	-2.475215	0.752048

H	2.139748	-2.971714	0.905455

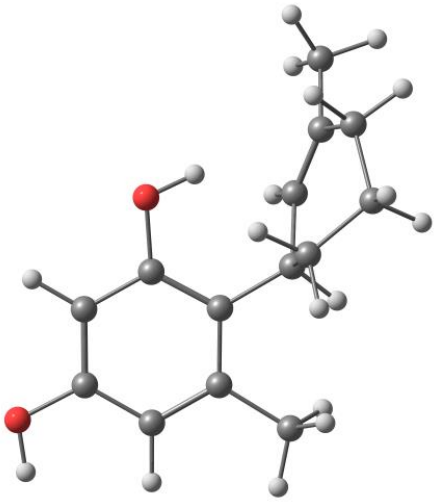
Table S65. Coordinates for global minimum of **6ac**‡.



C	0.882471	1.131521	-0.718120
C	2.036798	1.064192	0.081847
C	2.960495	0.065167	-0.080898
C	4.241843	0.070920	0.665115
H	4.368190	0.966553	1.276271
H	4.280585	-0.816124	1.313143
H	5.086571	-0.028902	-0.028605
C	2.753962	-1.016504	-1.088440
C	1.284579	-1.239754	-1.430598
H	0.791464	-1.730864	-0.585014
H	1.193325	-1.910259	-2.290276
C	0.582808	0.083960	-1.722676
H	-0.503086	-0.042335	-1.831431
H	3.322725	-0.716976	-1.986014
H	3.227769	-1.941407	-0.738433
H	2.240454	1.871911	0.780436
H	0.437168	2.109941	-0.872332
C	-2.468961	-1.009925	-0.007457
C	-1.410347	-1.336191	0.838711
C	-0.609113	-0.310233	1.317426
C	-0.825173	1.030670	0.921669
C	-1.950691	1.346552	0.122563
C	-2.744305	0.325298	-0.362465
H	-3.598160	0.544057	-0.999763
C	-2.229663	2.775285	-0.234888
H	-1.955108	3.448520	0.582029
H	-3.284311	2.921062	-0.480180
H	-0.302527	1.818553	1.455055
O	0.424342	-0.523042	2.156370
H	0.523568	-1.470059	2.336886
H	-1.236903	-2.370909	1.120599

O	-3.225079	-2.033039	-0.454617
H	-3.939545	-1.701018	-1.017845
H	-1.645163	3.072632	-1.116275
H	0.916101	0.498320	-2.691543

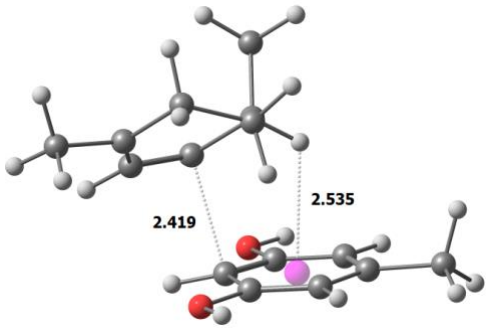
Table S66. Coordinates for global minimum of **6ac**.



C	0.868581	0.804710	0.198510
C	1.767023	-0.161278	0.942669
C	2.996785	-0.522039	0.545791
C	3.825369	-1.505934	1.316649
H	4.136902	-2.335893	0.668799
H	3.280647	-1.914943	2.172106
H	4.746244	-1.031403	1.679333
C	3.623419	0.043367	-0.703654
C	2.913552	1.304494	-1.195701
C	1.402969	1.086492	-1.219456
H	0.881217	1.957866	-1.632289
H	1.168281	0.234118	-1.872432
H	3.279705	1.580808	-2.191226
H	3.148009	2.139760	-0.521120
H	4.684486	0.247650	-0.505566
H	3.612191	-0.731011	-1.487111
H	1.368980	-0.571341	1.872987
H	0.895322	1.750296	0.756503
C	-0.577577	0.343332	0.154612
C	-0.898212	-0.975521	-0.221149
C	-2.216265	-1.412801	-0.333934
C	-3.245825	-0.517648	-0.077923
C	-2.964640	0.796220	0.293107
C	-1.640869	1.228123	0.407949
C	-1.386601	2.661816	0.801605
H	-0.849404	2.726700	1.755045
H	-0.781048	3.185463	0.053299

H	-2.330304	3.201739	0.910172
H	-3.780227	1.488426	0.490931
O	-4.527744	-0.983231	-0.203126
H	-5.146442	-0.270072	0.003077
H	-2.427274	-2.438341	-0.620232
O	0.061276	-1.904332	-0.518776
H	0.931257	-1.571228	-0.220988

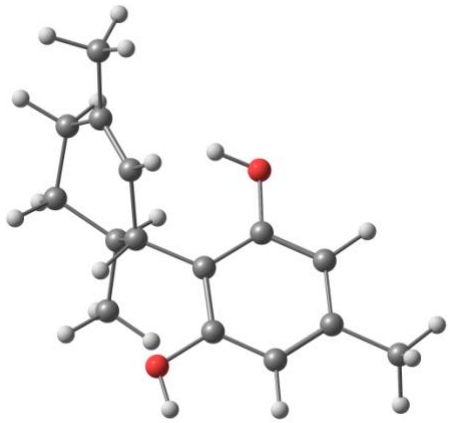
Table S67. Coordinates for global minimum of **3ad**‡



C	-0.889779	-1.016673	0.459623
C	-1.992377	-0.346526	1.005361
C	-2.915647	0.282495	0.206128
C	-4.151071	0.867779	0.776461
H	-4.262479	0.660146	1.842162
H	-4.128946	1.956161	0.622080
H	-5.031692	0.507427	0.229703
C	-2.752552	0.322557	-1.273318
C	-1.311780	0.111306	-1.727206
H	-0.742422	1.023622	-1.521363
H	-1.276713	-0.051111	-2.809328
C	-0.644715	-1.063597	-1.006101
H	0.439867	-1.031533	-1.181819
C	-1.140567	-2.441884	-1.507507
H	-0.935860	-2.523570	-2.579174
H	-3.422649	-0.454817	-1.678026
H	-3.153862	1.267930	-1.659087
H	-2.165121	-0.401988	2.077259
H	-0.423495	-1.794456	1.060204
C	1.952455	-0.703441	1.189487
C	0.923780	0.216683	1.480041
C	0.825639	1.380107	0.693196
C	1.656415	1.570114	-0.406544
C	2.629576	0.616020	-0.712309
C	2.779089	-0.524125	0.091992
H	3.549347	-1.256675	-0.137112
C	3.504818	0.793066	-1.917080
H	4.519620	0.434216	-1.722742
H	3.546415	1.839066	-2.229995

H	1.552710	2.462595	-1.018755
O	-0.132527	2.260216	1.056340
H	-0.145353	3.010041	0.443002
H	0.385568	0.147130	2.419183
O	2.039181	-1.769713	2.019833
H	2.742822	-2.364752	1.722219
H	3.107744	0.207556	-2.755959
H	-0.624002	-3.255947	-0.990628
H	-2.216768	-2.560339	-1.346917

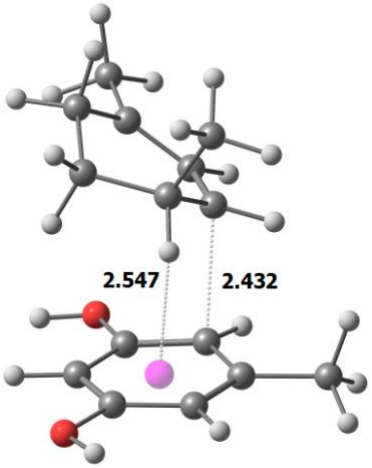
Table S68. Coordinates for global minimum of **3ad**.



C	0.830204	0.575788	0.425779
C	1.677462	-0.552593	0.978700
C	2.907165	-0.870455	0.549362
C	3.677416	-2.026581	1.114426
H	3.092883	-2.586963	1.849479
H	3.982208	-2.711896	0.312514
H	4.600968	-1.675979	1.592847
C	3.591323	-0.076541	-0.532262
C	2.923558	1.275137	-0.771264
C	1.406189	1.133705	-0.897992
C	0.749760	2.457926	-1.279295
H	-0.338461	2.359317	-1.352229
H	0.970075	3.225571	-0.527136
H	1.125932	2.811701	-2.245545
H	1.200530	0.399822	-1.693364
H	3.146144	1.949504	0.068929
H	3.331411	1.744502	-1.675197
H	3.597466	-0.670959	-1.459809
H	4.647700	0.056244	-0.260613
H	1.230809	-1.136416	1.785645
H	0.848211	1.393494	1.160018
C	-0.617670	0.150299	0.267433
C	-1.675143	0.937625	0.747825
C	-3.009562	0.588552	0.548162

C	-3.333565	-0.579904	-0.144580
C	-2.305671	-1.388696	-0.618668
C	-0.972580	-1.027045	-0.410107
O	-0.029941	-1.876208	-0.922825
H	0.841974	-1.653104	-0.542054
H	-2.520440	-2.309673	-1.153503
C	-4.774972	-0.965128	-0.345282
H	-5.227341	-1.283036	0.601676
H	-5.360864	-0.116764	-0.714291
H	-4.868270	-1.788869	-1.057602
H	-3.796746	1.233931	0.933999
O	-1.345580	2.085000	1.422144
H	-2.158539	2.533579	1.689881

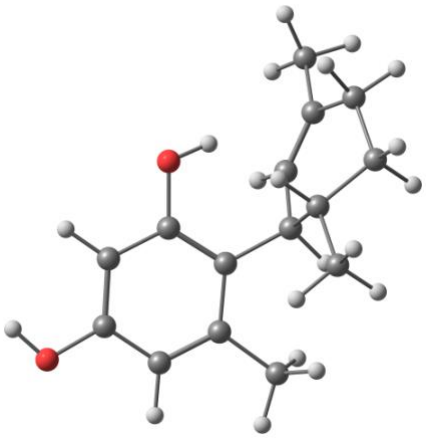
Table S69. Coordinates for global minimum of **6ad**‡.



C	-0.910463	-1.076363	0.484849
C	-1.992070	-0.352457	1.002763
C	-2.891178	0.278859	0.178967
C	-4.109092	0.924595	0.722239
H	-5.000074	0.567041	0.190391
H	-4.227044	0.764752	1.795525
H	-4.055854	2.004433	0.522614
C	-2.721996	0.258449	-1.300839
C	-1.284127	-0.002854	-1.738351
H	-0.694807	0.902080	-1.558380
H	-1.246830	-0.201572	-2.814327
C	-0.647900	-1.168932	-0.974813
H	0.440781	-1.157053	-1.133441
C	-1.153618	-2.551778	-1.451456
H	-0.929605	-2.664790	-2.516371
H	-3.408464	-0.517488	-1.679858
H	-3.097457	1.197973	-1.724961
H	-2.170553	-0.366758	2.075016
H	-0.483991	-1.857004	1.109118

C	2.539222	0.681016	-0.739970
C	1.554252	1.592867	-0.364023
C	0.787088	1.309113	0.756836
C	0.966101	0.108579	1.478252
C	2.012082	-0.770742	1.118845
C	2.773803	-0.494331	-0.001741
H	3.568909	-1.169968	-0.308642
C	2.244520	-2.017833	1.918586
H	1.584106	-2.824526	1.572448
H	2.032230	-1.853949	2.978779
H	0.459355	-0.006510	2.431195
O	-0.178310	2.138335	1.206331
H	-0.238736	2.920828	0.638358
H	1.410314	2.505514	-0.935489
O	3.264720	0.986544	-1.836770
H	3.923486	0.296563	-2.003492
H	3.273147	-2.369841	1.809820
H	-2.234496	-2.650294	-1.309223
H	-0.659834	-3.359900	-0.903628

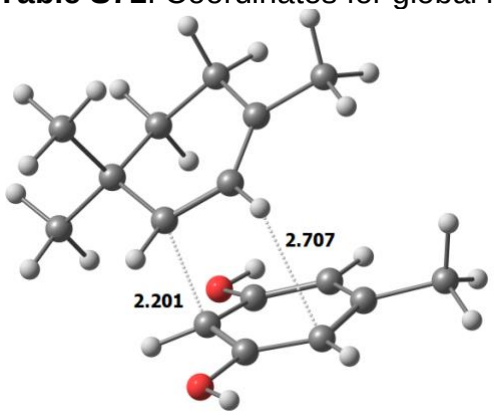
Table S70. Coordinates for global minimum of **6ad**.



C	0.840397	0.597651	0.412458
C	1.677239	-0.521307	1.001285
C	2.903684	-0.866973	0.583866
C	3.659911	-2.013215	1.186847
H	4.586572	-1.657685	1.655587
H	3.067585	-2.542542	1.938478
H	3.958060	-2.727453	0.408053
C	3.596639	-0.116702	-0.522872
C	2.944764	1.234599	-0.804637
C	1.425523	1.108763	-0.927283
C	0.788772	2.429887	-1.350642
H	1.028127	3.220638	-0.628520
H	1.164933	2.743054	-2.330746
H	-0.301466	2.345699	-1.415806

H	1.210313	0.356616	-1.702035
H	3.176099	1.932471	0.013843
H	3.358347	1.670283	-1.722816
H	3.594499	-0.740883	-1.430759
H	4.654860	0.011948	-0.256515
H	1.222831	-1.075504	1.824742
H	0.882097	1.436667	1.121130
C	-0.616344	0.185232	0.273972
C	-0.950900	-0.996598	-0.412637
C	-2.274677	-1.376988	-0.631690
C	-3.295507	-0.570281	-0.146309
C	-2.999539	0.590088	0.565705
C	-1.672899	0.967210	0.780548
C	-1.411555	2.224127	1.573142
H	-2.354519	2.673811	1.893495
H	-0.815208	2.015504	2.468973
H	-0.863627	2.969939	0.987647
H	-3.813587	1.196009	0.952849
O	-4.617199	-0.878876	-0.326982
H	-4.688491	-1.700599	-0.830683
H	-2.485393	-2.298565	-1.168567
O	-0.001810	-1.841320	-0.922020
H	0.862089	-1.627712	-0.518054

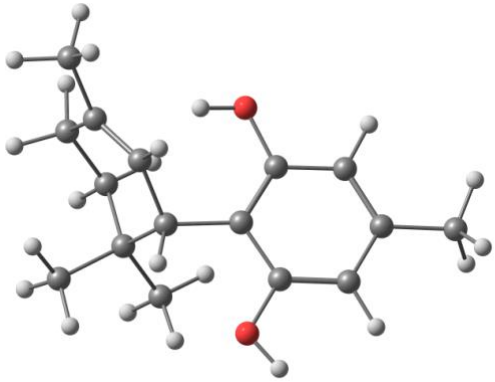
Table S71. Coordinates for global minimum of **3ae**‡.



C	-0.986473	-0.525385	0.748822
C	-0.288266	0.611531	1.246296
C	-0.583117	1.880410	0.853258
C	0.135026	3.051403	1.425551
H	0.852650	2.760509	2.195892
H	0.667705	3.580237	0.623404
H	-0.578447	3.772475	1.844283
C	-1.692738	2.166059	-0.102976
C	-2.189765	0.944934	-0.873825
H	-1.514078	0.749461	-1.711750
H	-3.176442	1.151030	-1.304599

C	-2.276813	-0.317683	-0.005404
H	-2.504614	2.610831	0.496135
H	-1.384786	2.963595	-0.791429
H	0.492310	0.458484	1.985343
H	-0.967823	-1.418953	1.372552
C	1.437634	-1.728189	0.541378
C	0.471537	-1.600931	-0.500207
C	0.778304	-0.702422	-1.558477
C	1.780112	0.239026	-1.413984
C	2.616418	0.194984	-0.288538
C	2.476229	-0.823139	0.662978
H	3.165202	-0.889673	1.501371
C	3.673756	1.238253	-0.109053
H	3.255508	2.084082	0.453059
H	4.021562	1.624226	-1.070631
H	1.955219	0.977518	-2.192421
O	0.032721	-0.818751	-2.675001
H	0.293274	-0.143308	-3.319614
H	-0.181116	-2.445157	-0.698525
O	1.210276	-2.723028	1.417068
H	1.863382	-2.699508	2.133127
H	4.522694	0.852749	0.461171
C	-2.703573	-1.527756	-0.841346
H	-2.675535	-2.445596	-0.243162
H	-3.731278	-1.380437	-1.189074
H	-2.067023	-1.656165	-1.719217
C	-3.333135	-0.132104	1.121570
H	-3.411592	-1.037843	1.731505
H	-3.092595	0.707150	1.779542
H	-4.305554	0.053384	0.652620

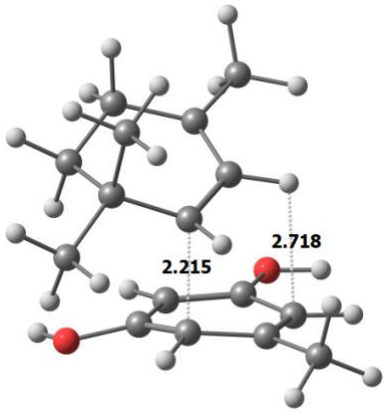
Table S72. Coordinates for global minimum of **3ae**.



C	0.747779	0.550845	0.600025
C	1.611779	-0.563020	1.148589
C	2.709641	-1.061254	0.560476
C	3.548095	-2.124634	1.206600

H	4.582479	-1.774856	1.321616
H	3.589930	-3.021852	0.575890
H	3.163840	-2.403969	2.191521
C	3.171143	-0.576481	-0.786230
C	2.120381	0.259999	-1.514310
C	1.438366	1.288574	-0.597702
C	0.437316	2.097781	-1.426387
H	0.969429	2.647127	-2.212223
H	-0.301827	1.446731	-1.905589
H	-0.098141	2.823087	-0.805664
C	2.488082	2.249015	-0.017330
H	3.172223	1.736315	0.666920
H	3.081535	2.699719	-0.821773
H	1.998025	3.056375	0.539078
H	1.352251	-0.398038	-1.941509
H	2.585695	0.786022	-2.358060
H	3.460210	-1.442045	-1.398973
H	4.097618	0.001666	-0.646410
H	1.309170	-0.960388	2.118911
H	0.676387	1.291605	1.407267
C	-0.685841	0.099142	0.351373
C	-1.040454	-1.127785	-0.234513
C	-2.372811	-1.470401	-0.487702
C	-3.402903	-0.601334	-0.149515
C	-3.084126	0.611108	0.465836
C	-1.754076	0.941896	0.709895
O	-1.435843	2.127967	1.320148
H	-2.251988	2.606033	1.518373
H	-3.872113	1.302201	0.759866
C	-4.838411	-0.952314	-0.434099
H	-5.250463	-0.300898	-1.213838
H	-4.933262	-1.987263	-0.772316
H	-5.459506	-0.819700	0.458217
H	-2.582209	-2.432944	-0.946100
O	-0.112498	-2.062287	-0.600920
H	0.743802	-1.827225	-0.188826

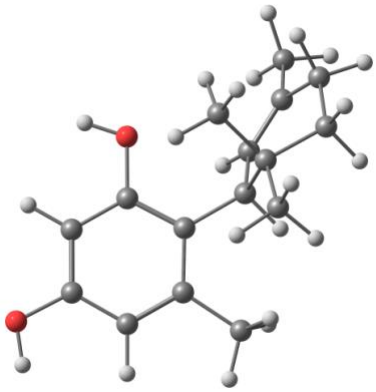
Table S73. Coordinates for global minimum of **6ae**‡.



C	-0.978220	-0.565591	0.847205
C	-0.400422	0.675124	1.234234
C	-0.771137	1.858472	0.673067
C	-0.162788	3.144605	1.108992
H	0.382931	3.591091	0.266349
H	-0.942279	3.866095	1.384224
H	0.526109	3.014200	1.946721
C	-1.860749	1.935235	-0.344148
C	-2.245807	0.593475	-0.967109
H	-1.538626	0.353680	-1.765707
H	-3.234592	0.669848	-1.433893
C	-2.257300	-0.558370	0.047309
H	-2.722895	2.391275	0.170259
H	-1.584218	2.660297	-1.120531
H	0.355577	0.676702	2.013457
H	-0.908879	-1.383750	1.562641
C	2.439706	0.525500	-0.399822
C	1.608908	0.267332	-1.494463
C	0.789803	-0.842825	-1.443015
C	0.652685	-1.594965	-0.241390
C	1.641024	-1.418320	0.779199
C	2.503826	-0.350475	0.703308
H	3.227161	-0.162802	1.493734
C	1.650014	-2.332590	1.962842
H	2.631736	-2.340636	2.442155
H	1.373833	-3.352339	1.681026
H	0.132209	-2.546491	-0.300596
O	0.081269	-1.271051	-2.505532
H	0.225106	-0.686783	-3.265495
H	1.665448	0.895659	-2.379066
O	3.216370	1.617252	-0.482008
H	3.781480	1.694823	0.301681
H	0.923722	-1.991500	2.713942
C	-2.558186	-1.897489	-0.632219
H	-3.577471	-1.879600	-1.031934

H	-1.874011	-2.096385	-1.458368
H	-2.491632	-2.720172	0.088926
C	-3.360407	-0.324580	1.118963
H	-3.376707	-1.146997	1.841390
H	-3.215051	0.611310	1.665021
H	-4.330846	-0.291894	0.611759

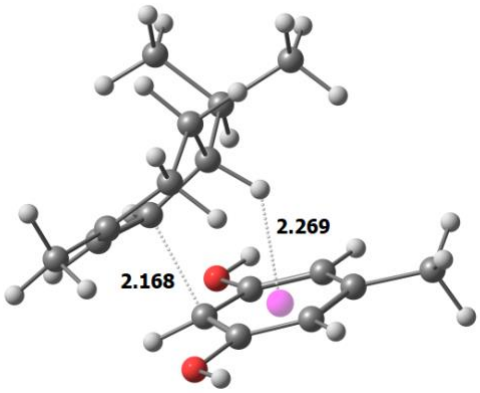
Table S74. Coordinates for global minimum of **6ae**.



C	0.751527	0.435844	0.457885
C	1.551390	-0.741642	0.974130
C	2.847336	-0.953664	0.729984
C	3.581057	-2.148553	1.267639
H	4.018877	-2.734023	0.447392
H	4.416372	-1.841364	1.911035
H	2.921550	-2.804098	1.844272
C	3.650557	-0.011713	-0.126130
C	2.927352	1.309748	-0.376225
H	3.437899	1.876955	-1.166305
C	1.447979	1.125194	-0.762060
C	1.347590	0.314901	-2.058309
H	1.735901	-0.698788	-1.942646
H	1.920054	0.821987	-2.845160
H	0.307394	0.238645	-2.392075
C	0.835115	2.506920	-1.010891
H	1.304121	2.974889	-1.884663
H	-0.241597	2.434079	-1.203683
H	0.990905	3.169238	-0.151535
H	2.971763	1.922528	0.535785
H	3.895179	-0.509946	-1.077734
H	4.619943	0.179316	0.356765
H	1.010349	-1.449187	1.602844
H	0.788765	1.195042	1.252105
C	-0.727327	0.113819	0.279655
C	-1.167565	-1.043381	-0.393614
C	-2.519123	-1.330174	-0.585389
C	-3.475446	-0.463822	-0.075789

C	-3.082758	0.662739	0.639946
C	-1.726379	0.946238	0.829050
C	-1.391509	2.147151	1.680946
H	-0.787252	1.862384	2.550138
H	-2.308202	2.612969	2.050906
H	-0.828384	2.905700	1.130860
H	-3.837568	1.319153	1.066987
O	-4.789489	-0.778902	-0.292406
H	-5.349681	-0.105014	0.115251
H	-2.824045	-2.226314	-1.120661
O	-0.229927	-1.921363	-0.860120
H	-0.678586	-2.660726	-1.291759

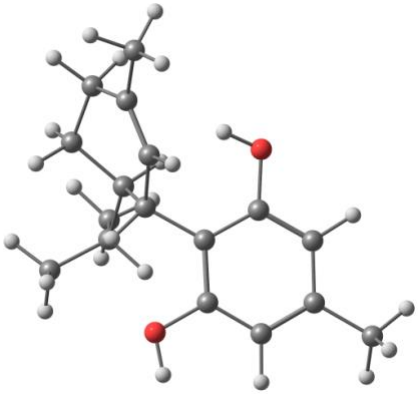
Table S75. Coordinates for global minimum of **3a**‡.



C	0.811504	0.441945	0.953730
C	2.044704	-0.257777	1.043403
C	2.795045	-0.530165	-0.060559
C	4.046190	-1.324389	0.009928
H	3.999843	-2.150084	-0.712688
H	4.898429	-0.703880	-0.298635
H	4.231987	-1.725257	1.008633
C	2.368138	-0.001535	-1.393178
C	1.616871	1.321355	-1.247106
H	1.278812	1.670057	-2.227561
H	2.311038	2.071469	-0.848981
C	0.413015	1.166501	-0.305635
H	3.241678	0.108209	-2.045869
H	1.720659	-0.755892	-1.871970
H	2.353681	-0.640316	2.013576
H	0.419338	0.848396	1.884836
C	-0.371569	-1.984205	0.143110
C	-0.605313	-1.165572	1.281864
C	-1.808353	-0.406431	1.311674
C	-2.612359	-0.306426	0.191243
C	-2.291997	-1.039771	-0.961756
C	-1.171911	-1.880756	-0.983051

H	-0.944233	-2.465308	-1.870873
C	-3.180169	-0.953160	-2.163905
H	-3.648475	0.031523	-2.240981
H	-3.985422	-1.694420	-2.078491
H	-3.495922	0.326926	0.206308
O	-2.052621	0.237165	2.469154
H	-2.848496	0.784492	2.388075
H	-0.138179	-1.434920	2.223935
O	0.696729	-2.794139	0.226267
H	0.824083	-3.274530	-0.606603
H	-2.629366	-1.167658	-3.082911
H	-0.314907	0.537622	-0.843930
C	-0.320795	2.488340	0.026124
H	-1.108061	2.224736	0.747885
C	-1.004436	3.067644	-1.212458
C	0.588981	3.526327	0.688773
H	1.133529	3.108238	1.543756
H	1.324674	3.923469	-0.018939
H	-0.006357	4.370286	1.052430
H	-1.611672	3.937748	-0.941536
H	-1.660976	2.327120	-1.684966
H	-0.269205	3.396337	-1.955205

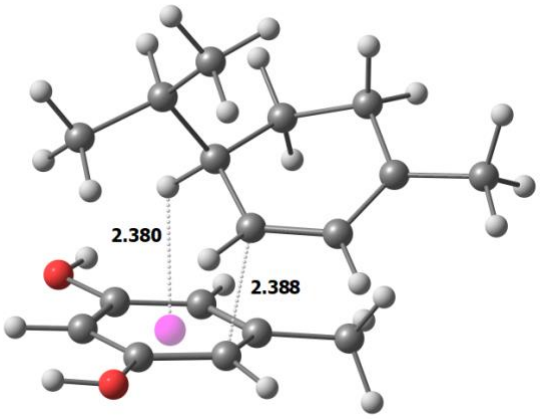
Table S76. Coordinates for global minimum of **3a**.



C	-0.706071	-0.017253	-0.675694
C	-1.399827	-1.342732	-0.920568
C	-2.600595	-1.685632	-0.432520
C	-3.206681	-3.035759	-0.675248
H	-4.144486	-2.940727	-1.237579
H	-3.461512	-3.517848	0.277803
H	-2.530781	-3.693222	-1.229214
C	-3.416864	-0.721055	0.386382
C	-2.924984	0.716726	0.239186
H	-3.177720	1.078896	-0.766719
C	-1.409430	0.798988	0.439070
H	-1.176128	0.306340	1.397066

C	-0.872966	2.243405	0.539837
C	-1.371672	3.154183	-0.585997
H	-0.841669	4.112822	-0.559288
H	-2.442023	3.364985	-0.477248
H	-1.210320	2.713418	-1.575056
C	-1.195415	2.860756	1.904159
H	-2.277578	2.956584	2.052980
H	-0.793499	2.249092	2.719911
H	-0.762398	3.864030	1.986470
H	0.221866	2.177397	0.462757
H	-3.445107	1.364860	0.954293
H	-3.388459	-1.032607	1.442762
H	-4.469839	-0.801295	0.082355
H	-0.855053	-2.059553	-1.537802
H	-0.764318	0.559590	-1.608253
C	0.767014	-0.224266	-0.372119
C	1.764356	0.514306	-1.026353
C	3.115323	0.383209	-0.708500
C	3.517874	-0.511108	0.285215
C	2.552405	-1.269392	0.940275
C	1.202629	-1.128201	0.610259
O	0.325017	-1.907598	1.313330
H	-0.541963	-1.896929	0.862122
H	2.830170	-1.981970	1.712008
C	4.978331	-0.673952	0.612057
H	5.485747	0.295679	0.644873
H	5.115174	-1.173121	1.575138
H	5.481261	-1.278139	-0.153197
H	3.852368	0.984505	-1.237974
O	1.354951	1.394264	-1.994956
H	2.130202	1.841259	-2.359354

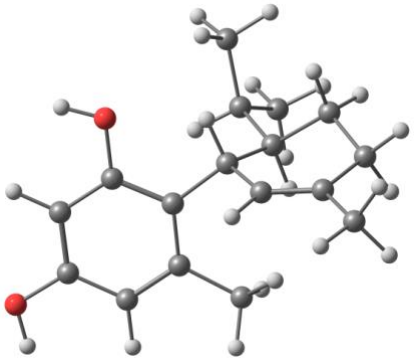
Table S77. Coordinates for global minimum of **6a**‡.



C	-0.839187	-0.336387	0.742380
C	-1.876722	0.544812	1.098319

C	-2.803686	0.981640	0.188536
C	-3.980569	1.779130	0.614077
H	-4.905568	1.314756	0.249022
H	-4.033171	1.902452	1.697494
H	-3.934367	2.769669	0.140405
C	-2.708267	0.615499	-1.250694
C	-1.331055	0.102872	-1.667617
H	-0.677614	0.971640	-1.806894
H	-1.394356	-0.402348	-2.636919
C	-0.651775	-0.822951	-0.645378
H	-3.505825	-0.117587	-1.445856
H	-2.987883	1.488926	-1.855284
H	-1.999142	0.805268	2.147284
H	-0.427747	-0.944450	1.543679
C	2.790364	0.309393	-0.826645
C	2.798164	-0.501280	0.313599
C	1.972654	-0.158817	1.369503
C	1.099087	0.950051	1.282258
C	1.161409	1.798644	0.151456
C	1.982009	1.456399	-0.908862
H	2.023480	2.078988	-1.799483
C	0.315176	3.030079	0.116502
H	0.476105	3.602262	-0.799554
H	0.528720	3.668987	0.980305
H	0.589231	1.278269	2.182744
O	1.907632	-0.875448	2.514137
H	2.498145	-1.641892	2.467106
H	3.446305	-1.372087	0.356906
O	3.606541	-0.062496	-1.832410
H	3.533076	0.557342	-2.573145
H	-0.748474	2.761454	0.181154
H	0.427229	-0.804701	-0.864024
C	-1.024910	-2.342519	-0.744746
H	-0.995221	-2.558388	-1.821947
C	-2.421900	-2.683623	-0.222501
C	0.032458	-3.214194	-0.063500
H	1.032830	-3.010577	-0.460696
H	0.055415	-3.052830	1.020997
H	-0.191170	-4.273185	-0.229523
H	-2.625532	-3.747814	-0.381233
H	-3.207520	-2.118969	-0.731290
H	-2.503575	-2.489203	0.853593

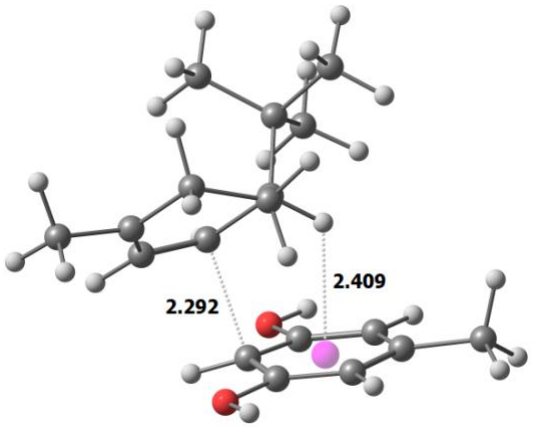
Table S78. Coordinates for global minimum of **6a**.



C	-0.712462	-0.072605	-0.589969
C	-1.402705	-1.395897	-0.846502
C	-2.652923	-1.691045	-0.476807
C	-3.269285	-3.036707	-0.725828
H	-2.568881	-3.720417	-1.214699
H	-4.166359	-2.947695	-1.352662
H	-3.593971	-3.491561	0.220261
C	-3.513307	-0.686083	0.243885
C	-2.967211	0.736079	0.128219
C	-1.471339	0.779281	0.453686
H	-1.337915	0.302160	1.434841
C	-0.901095	2.210150	0.573075
C	-1.308175	2.860443	1.898960
H	-1.003003	2.243412	2.751977
H	-2.394117	3.003194	1.955080
H	-0.841222	3.845927	2.008224
C	-1.279340	3.118895	-0.600594
H	-2.349732	3.355800	-0.586463
H	-1.043844	2.662180	-1.567465
H	-0.730673	4.065501	-0.538140
H	0.194816	2.109034	0.580937
H	-3.526808	1.406289	0.792071
H	-3.124349	1.096006	-0.897912
H	-4.536829	-0.734912	-0.154640
H	-3.593819	-0.980372	1.303400
H	-0.810457	-2.149385	-1.368265
H	-0.750197	0.483768	-1.535435
C	0.765484	-0.254447	-0.268368
C	1.727306	0.341970	-1.106584
C	3.096796	0.226596	-0.881685
C	3.537232	-0.510626	0.210684
C	2.618885	-1.119860	1.058606
C	1.243496	-0.994066	0.829855
C	0.325415	-1.657298	1.827055
H	-0.623801	-1.956974	1.378971
H	0.101620	-0.975302	2.656816

H	0.807653	-2.541341	2.254947
H	2.971185	-1.698918	1.910092
O	4.889787	-0.605900	0.398142
H	5.064044	-1.144368	1.181519
H	3.814414	0.698059	-1.548728
O	1.276999	1.063096	-2.182835
H	2.035764	1.417818	-2.664598

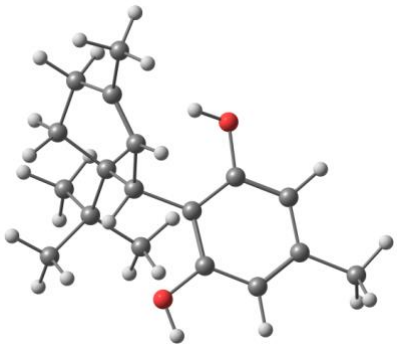
Table S79. Coordinates for global minimum of **3af**‡.



C	0.717829	0.094342	-0.877699
C	1.485660	1.255904	-1.117037
C	2.321788	1.784318	-0.174061
C	3.247336	2.897923	-0.502265
H	4.275518	2.630166	-0.227120
H	3.210151	3.175847	-1.557341
H	2.989556	3.773311	0.109762
C	2.391237	1.215943	1.200883
C	1.182867	0.356026	1.550565
H	0.339617	1.029638	1.739817
H	1.354497	-0.183899	2.483949
C	0.744088	-0.607601	0.435610
H	3.338424	0.660138	1.279008
H	2.493983	2.039707	1.919980
H	1.483893	1.676285	-2.120249
H	0.480972	-0.504111	-1.753411
C	-1.598449	1.607405	-0.079349
C	-1.406069	0.862707	-1.264681
C	-2.052161	-0.392140	-1.376598
C	-2.727596	-0.942302	-0.302419
C	-2.833760	-0.217641	0.896279
C	-2.277151	1.060026	1.002675
H	-2.383860	1.628884	1.923057
C	-3.530447	-0.834441	2.070793
H	-2.854101	-1.537067	2.574113
H	-4.408848	-1.403291	1.752339

H	-3.181832	-1.926563	-0.386395
O	-1.907397	-1.015069	-2.566860
H	-2.324762	-1.888908	-2.538419
H	-1.056863	1.362515	-2.162117
O	-1.050871	2.837948	-0.067455
H	-1.193089	3.262718	0.792049
H	-3.832428	-0.078860	2.799581
H	-0.282002	-0.923223	0.677073
C	1.520202	-1.982226	0.289149
C	0.632542	-2.956998	-0.501730
C	1.754188	-2.575449	1.683390
H	2.130757	-3.599156	1.579236
H	2.496243	-2.006363	2.252103
H	0.823958	-2.613320	2.262694
H	-0.320708	-3.123823	0.013515
H	1.140675	-3.922598	-0.598563
H	0.416322	-2.600576	-1.514547
C	2.868662	-1.838882	-0.430578
H	3.540864	-1.150623	0.090006
H	3.362738	-2.816195	-0.469387
H	2.748895	-1.487981	-1.461438

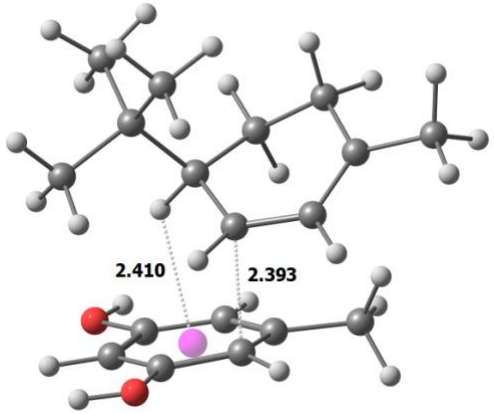
Table S80. Coordinates for global minimum of **3af**.



C	-0.659029	-0.149302	-0.682888
C	-1.186302	-1.559302	-0.899735
C	-2.333223	-2.054563	-0.418527
C	-2.734481	-3.487273	-0.605895
H	-1.961948	-4.063002	-1.123423
H	-2.931061	-3.959838	0.365601
H	-3.667720	-3.554346	-1.179862
C	-3.289496	-1.167953	0.326848
C	-2.998224	0.308411	0.076981
H	-3.249299	0.544302	-0.966518
H	-3.655943	0.908936	0.709822
C	-1.522661	0.653947	0.339037
H	-1.278252	0.288647	1.349070
C	-1.267217	2.197143	0.380814

C	0.174084	2.515087	0.813233
H	0.902903	2.253928	0.045242
H	0.440280	1.977004	1.731376
H	0.269559	3.589649	1.009591
C	-2.192385	2.834639	1.437360
H	-3.242253	2.838181	1.131370
H	-1.898589	3.877653	1.599230
H	-2.114467	2.309578	2.397677
C	-1.538896	2.869322	-0.972488
H	-2.569631	2.705858	-1.305209
H	-1.386683	3.951618	-0.883039
H	-0.860546	2.504375	-1.750669
H	-3.241525	-1.394561	1.404306
H	-4.315938	-1.410429	0.018031
H	-0.522256	-2.215286	-1.464979
H	-0.715680	0.370147	-1.646989
C	0.815504	-0.273455	-0.329378
C	1.819681	0.296969	-1.125022
C	3.169049	0.214044	-0.790076
C	3.565608	-0.468908	0.362117
C	2.595571	-1.091268	1.141342
C	1.247863	-1.007430	0.785076
O	0.364561	-1.671961	1.594042
H	-0.466087	-1.808486	1.100985
H	2.869581	-1.662350	2.024027
C	5.020399	-0.530063	0.743147
H	5.640517	-0.817213	-0.112675
H	5.373600	0.450605	1.083817
H	5.188485	-1.247842	1.550254
H	3.911481	0.689343	-1.428885
O	1.417320	0.978980	-2.245485
H	2.196113	1.343937	-2.686041

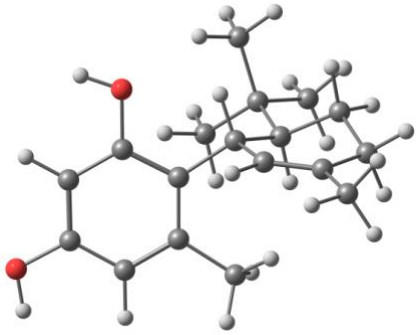
Table S81. Coordinates for global minimum of **6af**‡.



C	-0.767135	-0.069538	-0.884920

C	-1.679542	-1.123628	-1.082703
C	-2.601498	-1.474034	-0.131458
C	-3.674088	-2.456873	-0.422614
H	-3.547557	-3.331339	0.230973
H	-4.654412	-2.033038	-0.169953
H	-3.671369	-2.784721	-1.463880
C	-2.600332	-0.831592	1.211492
C	-1.286148	-0.132338	1.538980
H	-0.544101	-0.903939	1.774664
H	-1.392016	0.473615	2.440983
C	-0.706844	0.699345	0.382643
H	-3.459904	-0.143929	1.244055
H	-2.827777	-1.593675	1.969083
H	-1.722032	-1.594461	-2.062310
H	-0.390440	0.410522	-1.783411
C	2.843543	0.037794	0.860256
C	2.805591	0.621253	-0.410747
C	2.076241	-0.011247	-1.401734
C	1.336057	-1.184666	-1.127668
C	1.446793	-1.796282	0.142949
C	2.172607	-1.165446	1.137925
H	2.246057	-1.604549	2.129893
C	0.756946	-3.099914	0.387241
H	1.110410	-3.859021	-0.319306
H	-0.324307	-2.997042	0.220758
H	0.910000	-1.733351	-1.962144
O	1.984369	0.466095	-2.663421
H	2.489475	1.288079	-2.748482
H	3.349542	1.541601	-0.603420
O	3.567895	0.682108	1.796881
H	3.544049	0.194359	2.633510
H	0.922453	-3.457665	1.405706
H	0.353050	0.879089	0.621668
C	-1.277244	2.161581	0.150380
C	-2.623020	2.166784	-0.588248
C	-0.251933	2.958250	-0.671938
H	-0.069365	2.515137	-1.657101
H	-0.622523	3.975939	-0.836376
H	0.705842	3.025044	-0.143276
H	-2.537131	1.752709	-1.598978
H	-2.979490	3.198640	-0.683302
H	-3.389689	1.602221	-0.049575
C	-1.444355	2.851919	1.509175
H	-2.267768	2.420568	2.086738
H	-0.526809	2.786604	2.105649
H	-1.670885	3.911780	1.348241

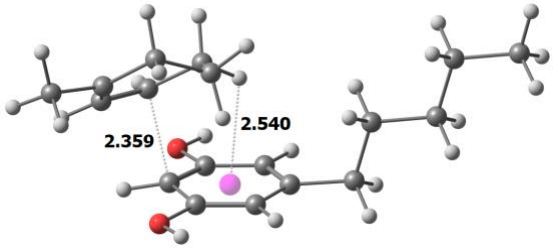
Table S82. Coordinates for global minimum of **6af**.



C	-0.670397	-0.201046	-0.588999
C	-1.180551	-1.614234	-0.810458
C	-2.366291	-2.087736	-0.421181
C	-2.772687	-3.518642	-0.617494
H	-1.980989	-4.104560	-1.093840
H	-3.015738	-3.985075	0.347260
H	-3.678879	-3.588444	-1.233575
C	-3.358557	-1.184411	0.253706
C	-3.043002	0.290227	0.014631
H	-3.236437	0.526460	-1.041090
H	-3.729621	0.896592	0.610944
C	-1.581962	0.628928	0.359121
H	-1.416840	0.292903	1.391091
C	-1.303509	2.169613	0.369908
C	-2.320715	2.866284	1.295489
H	-2.375382	2.365078	2.270199
H	-3.326458	2.892809	0.866280
H	-2.011897	3.903621	1.466904
C	-1.409126	2.795415	-1.027423
H	-2.384813	2.601902	-1.486979
H	-0.629497	2.420927	-1.698574
H	-1.287944	3.882954	-0.953610
C	0.092130	2.473328	0.942058
H	0.892599	2.127879	0.285010
H	0.209120	3.555675	1.074539
H	0.228943	1.994878	1.919891
H	-3.377605	-1.401445	1.334614
H	-4.368636	-1.416515	-0.113280
H	-0.479499	-2.282918	-1.312492
H	-0.717008	0.294349	-1.566170
C	0.810306	-0.285650	-0.229905
C	1.764862	0.157329	-1.164664
C	3.135411	0.095306	-0.927511
C	3.584365	-0.441317	0.272942
C	2.672881	-0.918547	1.208155
C	1.296498	-0.851816	0.962477
C	0.387194	-1.389836	2.038809

H	0.087565	-0.593465	2.731195
H	-0.522705	-1.830031	1.624777
H	0.909105	-2.151617	2.625345
H	3.032525	-1.356144	2.137389
O	4.938038	-0.486305	0.472396
H	5.118820	-0.887901	1.332696
H	3.847990	0.453145	-1.666517
O	1.304170	0.682998	-2.346056
H	2.056312	0.972195	-2.879487

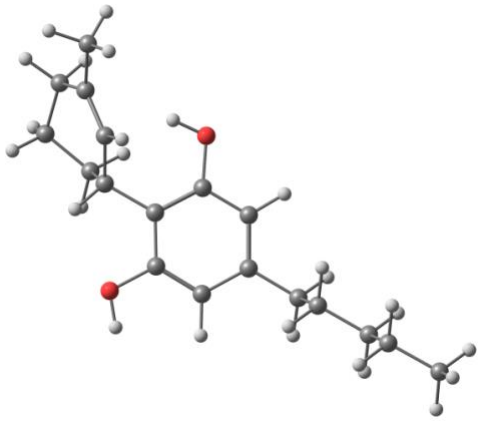
Table S83. Coordinates for global minimum of **3c**‡.



C	-2.089750	0.035472	-1.185686
C	-3.244207	0.584454	-0.599353
C	-3.276995	1.886247	-0.172036
C	-4.533964	2.505231	0.311977
H	-5.394565	1.840792	0.215202
H	-4.409508	2.782108	1.368512
H	-4.726045	3.444732	-0.222087
C	-2.071025	2.759870	-0.265749
C	-0.765236	1.973145	-0.296763
H	-0.565960	1.568169	0.701073
H	0.070145	2.634099	-0.546803
C	-0.840492	0.825531	-1.299620
H	0.036390	0.168296	-1.235145
H	-2.191081	3.354794	-1.187995
H	-2.080784	3.488342	0.553790
H	-4.153598	-0.010476	-0.571034
H	-2.221313	-0.791376	-1.879081
C	-0.746650	-2.454459	-0.543820
C	-1.673042	-1.770076	0.273483
C	-1.180287	-1.034042	1.372334
C	0.186132	-0.879248	1.568850
C	1.085390	-1.501729	0.698401
C	0.617059	-2.297528	-0.357583
H	1.321102	-2.795310	-1.020402
H	0.554189	-0.280050	2.398597
O	-2.113914	-0.476352	2.171214
H	-1.688471	0.039487	2.872611
H	-2.725316	-2.029498	0.224605
O	-1.282305	-3.210438	-1.529443

H	-0.577596	-3.598311	-2.068674
H	-0.830957	1.209538	-2.336120
C	2.557876	-1.257878	0.851949
H	3.120180	-2.118730	0.471102
H	2.805835	-1.136761	1.913372
C	2.989850	0.007347	0.087059
H	2.726082	-0.108717	-0.973613
H	2.414971	0.865835	0.462587
C	4.484418	0.288436	0.220615
H	5.052525	-0.575921	-0.152787
H	4.741664	0.393564	1.284645
C	4.919269	1.545301	-0.532644
H	4.656943	1.438545	-1.594279
H	4.348285	2.406052	-0.157522
C	6.415655	1.821718	-0.397501
H	7.004686	0.986239	-0.792944
H	6.706729	2.725805	-0.942403
H	6.694741	1.958012	0.653757

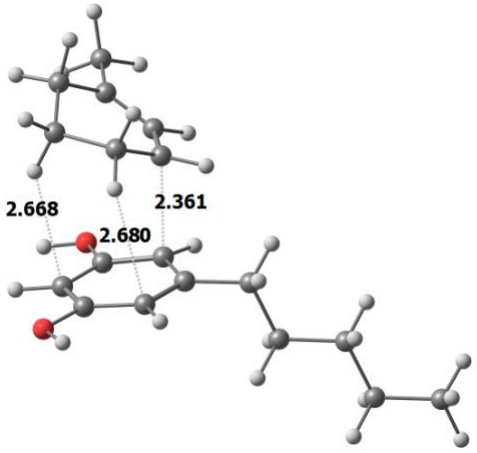
Table S84. Coordinates for global minimum of **3c**.



C	2.509176	0.594388	0.442564
C	3.041741	-0.738209	0.926063
C	4.220970	-1.264775	0.563217
C	4.681207	-2.603562	1.058300
H	3.923734	-3.091614	1.678097
H	4.920736	-3.262258	0.213109
H	5.602977	-2.500195	1.645180
C	5.161434	-0.539935	-0.365769
C	4.822522	0.944131	-0.505025
C	3.327266	1.126474	-0.750279
H	3.039085	0.581258	-1.660430
H	3.077218	2.181012	-0.914392
H	5.105832	1.470083	0.417257
H	5.402987	1.388655	-1.321796
H	5.136646	-1.032262	-1.350920

H	6.188454	-0.668875	0.002801
H	2.411767	-1.283593	1.631545
H	2.618804	1.307443	1.270540
C	1.033032	0.538694	0.100387
C	0.482987	-0.491783	-0.680270
C	-0.863759	-0.501114	-1.046287
C	-1.705777	0.534170	-0.648761
C	-1.185023	1.573808	0.122915
C	0.162111	1.568822	0.483670
O	0.697324	2.593405	1.221905
H	-0.000174	3.229931	1.426787
H	-1.824687	2.395191	0.441423
C	-3.172156	0.501671	-0.993086
H	-3.315534	-0.033079	-1.940651
H	-3.541792	1.525289	-1.136840
C	-4.009937	-0.182158	0.098863
C	-5.495194	-0.244524	-0.250509
C	-6.339933	-0.903751	0.839695
C	-7.821942	-0.973498	0.474727
H	-8.409948	-1.443535	1.270203
H	-7.971362	-1.555160	-0.442388
H	-8.229826	0.029506	0.302825
H	-5.957825	-1.916473	1.029221
H	-6.215980	-0.345579	1.778041
H	-5.623694	-0.796613	-1.193284
H	-5.870063	0.773399	-0.434051
H	-3.624638	-1.198707	0.261009
H	-3.874208	0.359187	1.045811
H	-1.238534	-1.324705	-1.648507
O	1.244393	-1.529110	-1.144619
H	2.110274	-1.520367	-0.690272

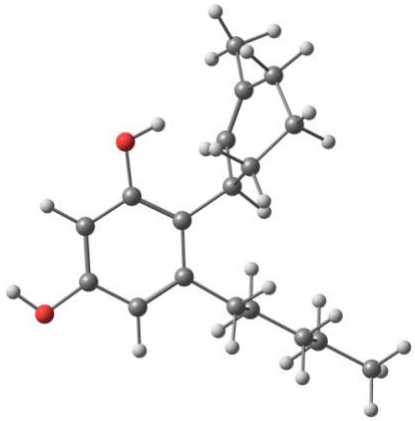
Table S85. Coordinates for global minimum of **6c**‡.



C	1.356270	1.032773	-0.937339

C	2.089592	1.912808	-0.119212
C	3.454632	1.840041	-0.037814
C	4.238697	2.857915	0.703166
H	3.614627	3.658321	1.105379
H	4.772953	2.367354	1.528880
H	5.015986	3.283423	0.055362
C	4.215705	0.789259	-0.776389
C	3.377772	-0.446305	-1.086986
H	3.216813	-1.010562	-0.162368
H	3.915056	-1.105483	-1.775346
C	2.027302	-0.057956	-1.682554
H	1.356377	-0.922648	-1.778745
H	4.575894	1.261102	-1.707060
H	5.119867	0.526276	-0.214407
H	1.566117	2.723673	0.381075
H	0.405999	1.385583	-1.326667
C	0.219620	-2.677098	0.049716
C	1.071832	-2.099674	0.990440
C	0.902574	-0.758141	1.299595
C	-0.077433	0.022209	0.642455
C	-0.984573	-0.605107	-0.245227
C	-0.808195	-1.936511	-0.566401
H	-1.471841	-2.427138	-1.275508
H	-0.298777	1.012709	1.029029
O	1.666317	-0.114125	2.204642
H	2.330728	-0.713758	2.576526
H	1.842539	-2.699299	1.466693
O	0.422519	-3.980084	-0.231671
H	-0.226959	-4.288320	-0.880550
H	2.147203	0.318443	-2.714663
C	-2.140309	0.176574	-0.798389
H	-2.427782	-0.227204	-1.776519
H	-1.850395	1.225508	-0.943567
C	-3.353147	0.126932	0.148344
H	-3.648105	-0.921259	0.293567
H	-3.057153	0.511374	1.134244
C	-4.537757	0.929827	-0.384405
H	-4.818657	0.548935	-1.377164
H	-4.233476	1.976957	-0.527715
C	-5.753277	0.877564	0.540616
H	-6.054867	-0.169548	0.680911
H	-5.468183	1.253464	1.532977
C	-6.933761	1.685489	0.004304
H	-7.252293	1.309897	-0.974948
H	-7.793812	1.633810	0.680020
H	-6.663223	2.740989	-0.115508

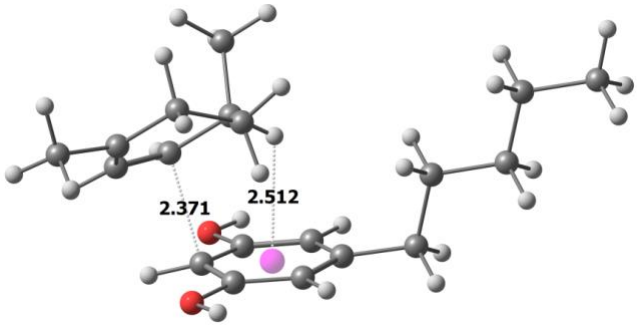
Table S86. Coordinates for global minimum of **6c**.



C	-0.786761	-0.739488	-0.387635
C	-1.465585	-1.387792	0.800723
C	-2.467300	-2.276438	0.716879
C	-3.114500	-2.864955	1.934974
H	-2.715315	-2.433932	2.857391
H	-4.199538	-2.698688	1.910292
H	-2.966099	-3.952214	1.961454
C	-3.004950	-2.740279	-0.613275
C	-2.057994	-2.425138	-1.771154
C	-1.578256	-0.978610	-1.687104
H	-2.445736	-0.304201	-1.718469
H	-0.943519	-0.720394	-2.543137
H	-1.190469	-3.098227	-1.723989
H	-2.557713	-2.610324	-2.729090
H	-3.986110	-2.268858	-0.783162
H	-3.202069	-3.819641	-0.557013
H	-1.085385	-1.108120	1.785348
H	0.184783	-1.238052	-0.497162
C	-0.518876	0.741171	-0.172361
C	-1.541405	1.588083	0.296011
C	-1.352959	2.961880	0.446626
C	-0.122216	3.514273	0.113374
C	0.908843	2.705921	-0.357766
C	0.716420	1.331089	-0.502993
C	1.885793	0.502111	-0.979689
C	2.644503	-0.161293	0.180621
C	3.793569	-1.045063	-0.298755
C	4.563970	-1.700939	0.846720
C	5.707000	-2.587689	0.355427
H	5.329003	-3.392581	-0.285746
H	6.245951	-3.047989	1.190254
H	6.428294	-2.006299	-0.230701
H	4.960568	-0.918911	1.508945
H	3.867889	-2.296330	1.453759

H	3.396216	-1.826570	-0.963531
H	4.486801	-0.444994	-0.906698
H	3.029689	0.625043	0.844764
H	1.946489	-0.759277	0.783453
H	1.556282	-0.267867	-1.688488
H	2.580115	1.150365	-1.527712
H	1.863613	3.156862	-0.614054
O	0.131590	4.854655	0.231937
H	-0.658159	5.302257	0.563135
H	-2.168811	3.577024	0.818267
O	-2.789534	1.125144	0.612902
H	-2.760712	0.149813	0.679206

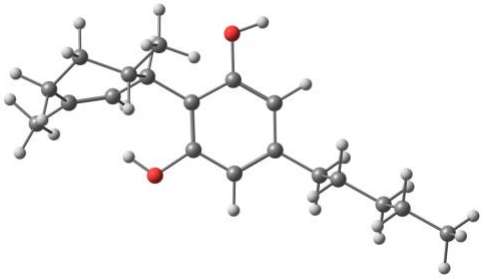
Table S87. Coordinates for global minimum of **3d**‡.



C	2.080794	0.052729	1.015761
C	3.225746	0.498324	0.334974
C	3.262545	1.722022	-0.283027
C	4.516699	2.245637	-0.875401
H	4.722550	3.255881	-0.499560
H	5.373970	1.596970	-0.685939
H	4.379269	2.352336	-1.960790
C	2.067449	2.611283	-0.306216
C	0.755771	1.866699	-0.078904
H	0.501767	1.316292	-0.990722
H	-0.057028	2.577780	0.101824
C	0.844833	0.878897	1.088133
H	-0.027124	0.210424	1.063726
H	2.237538	3.379340	0.467171
H	2.045769	3.166336	-1.252340
H	4.128622	-0.106141	0.374925
H	2.221440	-0.684660	1.803190
C	1.095703	-1.323333	-1.364155
C	1.592559	-1.928650	-0.190711
C	0.667925	-2.483275	0.720995
C	-0.695678	-2.319688	0.537794
C	-1.166313	-1.650383	-0.601554
C	-0.270560	-1.164164	-1.557804
H	-0.641269	-0.662513	-2.448853

H	-1.397965	-2.712374	1.269464
O	1.206141	-3.122512	1.785090
H	0.503374	-3.436120	2.373013
H	2.640954	-2.199382	-0.123378
O	2.025447	-0.886688	-2.239703
H	1.596616	-0.453533	-2.992908
C	-2.634959	-1.386674	-0.759566
H	-3.212351	-2.172741	-0.258748
H	-2.902065	-1.398728	-1.823327
C	-3.015389	-0.018585	-0.162292
H	-2.739251	-0.003721	0.901540
H	-2.418615	0.763215	-0.653317
C	-4.501753	0.293665	-0.315712
H	-5.092485	-0.492307	0.176826
H	-4.772144	0.264402	-1.381294
C	-4.883002	1.654611	0.266451
H	-4.609404	1.681386	1.330344
H	-4.288467	2.436599	-0.226067
C	-6.370735	1.964270	0.109370
H	-6.659543	1.969530	-0.948022
H	-6.983080	1.210858	0.618179
H	-6.622639	2.942809	0.531286
C	0.837521	1.575387	2.469772
H	1.696074	2.244926	2.583129
H	-0.080057	2.163815	2.565419
H	0.865796	0.840240	3.279441

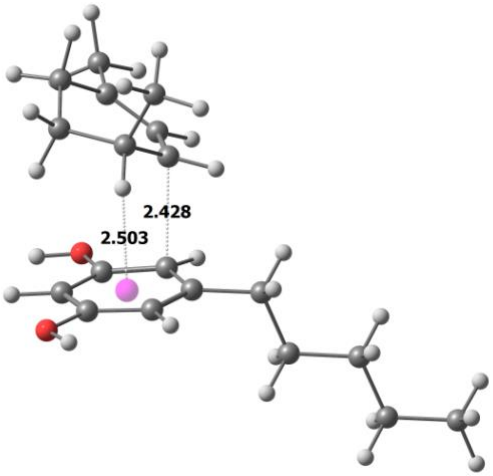
Table S88. Coordinates for global minimum of **3d**.



C	2.378911	0.507923	0.582750
C	3.306190	-0.680668	0.738847
C	4.391134	-0.911907	-0.014061
C	5.245859	-2.130660	0.167852
H	5.336853	-2.679552	-0.778759
H	4.838364	-2.805995	0.925346
H	6.264291	-1.845691	0.461736
C	4.818045	0.049068	-1.092552
C	4.145307	1.412413	-0.955238
C	2.637926	1.271358	-0.738518
C	1.940166	2.628656	-0.745143

H	0.862860	2.525030	-0.577727
H	2.089019	3.135301	-1.705095
H	2.345590	3.272320	0.045293
H	2.232490	0.666484	-1.565073
H	4.338710	2.021531	-1.847015
H	4.576296	1.951252	-0.098458
H	5.911599	0.152196	-1.063084
H	4.589578	-0.393840	-2.074997
H	3.049056	-1.388307	1.529169
H	2.590298	1.202586	1.407830
C	0.925010	0.092776	0.710520
C	0.392718	-0.974835	-0.032172
C	-0.955845	-1.325866	0.039879
C	-1.820728	-0.615760	0.868163
C	-1.316295	0.438807	1.629791
C	0.033766	0.779426	1.547534
O	0.542165	1.814249	2.290113
H	-0.170107	2.202112	2.815336
H	-1.974687	0.999089	2.291384
C	-3.290280	-0.946034	0.905621
H	-3.689260	-0.740125	1.907337
H	-3.432786	-2.016653	0.711258
C	-4.091764	-0.138651	-0.127088
C	-5.584664	-0.459002	-0.096064
C	-6.389710	0.340196	-1.120369
C	-7.882336	0.016936	-1.078309
H	-8.302299	0.237840	-0.090055
H	-8.058192	-1.045189	-1.284767
H	-8.440527	0.600003	-1.818464
H	-6.238675	1.413478	-0.939585
H	-5.995605	0.137876	-2.125962
H	-5.730461	-1.534097	-0.277641
H	-5.978696	-0.259200	0.911479
H	-3.939797	0.933684	0.060381
H	-3.689512	-0.341149	-1.129716
H	-1.313714	-2.162022	-0.555153
O	1.167857	-1.720213	-0.878908
H	2.109958	-1.545240	-0.687798

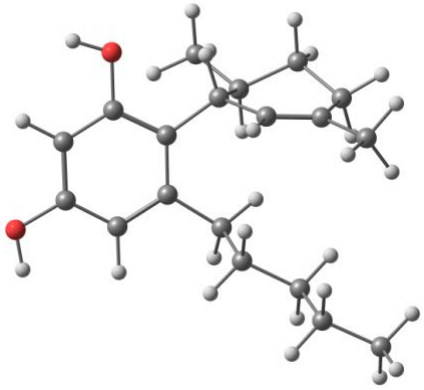
Table S89. Coordinates for global minimum of **6d**‡.



C	-1.304846	-1.090166	-0.653188
C	-1.995771	-1.875552	0.280332
C	-3.356265	-1.775342	0.432224
C	-4.101887	-2.701731	1.316495
H	-4.936177	-3.161501	0.771444
H	-3.465357	-3.478066	1.745008
H	-4.560314	-2.121830	2.130147
C	-4.145861	-0.788354	-0.357132
C	-3.308617	0.384877	-0.855091
H	-3.084180	1.038073	-0.005385
H	-3.879404	0.979690	-1.575489
C	-1.991321	-0.072382	-1.489655
H	-1.321967	0.793847	-1.600556
H	-4.596086	-1.348676	-1.193762
H	-4.997074	-0.439262	0.240086
H	-1.453508	-2.642655	0.827564
H	-0.355941	-1.467316	-1.024334
C	-0.101559	2.710429	-0.071869
C	-0.913819	2.232653	0.956197
C	-0.724253	0.930099	1.396946
C	0.241293	0.093215	0.797315
C	1.101716	0.619254	-0.192268
C	0.905032	1.910272	-0.645606
H	1.536071	2.321762	-1.430479
H	0.465135	-0.863546	1.259627
O	-1.458096	0.380462	2.387733
H	-2.111317	1.016200	2.715739
H	-1.671519	2.875779	1.395124
O	-0.324316	3.977425	-0.481539
H	0.294384	4.215579	-1.187475
C	2.234292	-0.218255	-0.711982
H	2.498919	0.103312	-1.726232
H	1.927690	-1.271266	-0.767241

C	3.473370	-0.113329	0.194810
H	3.784763	0.938696	0.251781
H	3.199793	-0.417202	1.214710
C	4.633321	-0.971132	-0.305526
H	4.895977	-0.667613	-1.329449
H	4.310819	-2.020955	-0.365494
C	5.871444	-0.872201	0.585067
H	6.191270	0.177352	0.642955
H	5.604602	-1.171608	1.607976
C	7.027130	-1.735137	0.081500
H	7.328768	-1.434918	-0.928685
H	7.903302	-1.649997	0.732686
H	6.738453	-2.791913	0.042828
C	-2.175024	-0.676984	-2.902025
H	-2.644615	0.068756	-3.550373
H	-1.210535	-0.957712	-3.335654
H	-2.811696	-1.567163	-2.874554

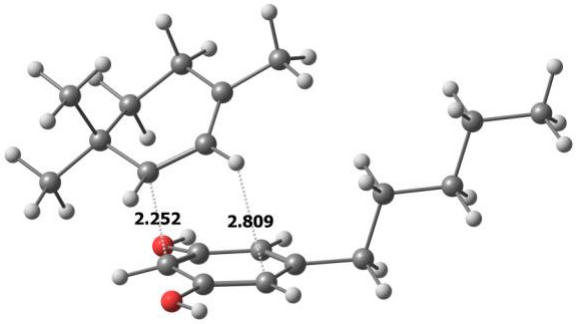
Table S90. Coordinates for global minimum of **6d**.



C	-0.713990	-1.461184	-0.358923
C	0.633877	-1.371705	-1.036736
C	1.723625	-2.054639	-0.675120
C	3.041403	-1.896237	-1.375937
H	3.352918	-2.838107	-1.847070
H	3.829995	-1.631813	-0.658048
H	3.000548	-1.118124	-2.144412
C	1.691228	-3.016514	0.484368
C	0.268431	-3.438426	0.845985
C	-0.661794	-2.231569	0.982322
C	-2.058756	-2.652465	1.433758
H	-2.729343	-1.789740	1.511614
H	-2.019289	-3.142999	2.412865
H	-2.498287	-3.357692	0.717428
H	-0.240430	-1.567010	1.750349
H	0.268481	-4.014616	1.780281
H	-0.124931	-4.101288	0.060699

H	2.300758	-3.898199	0.240715
H	2.182893	-2.547848	1.353165
H	0.691212	-0.692972	-1.888361
H	-1.355867	-2.055225	-1.024554
C	-1.390438	-0.102487	-0.220561
C	-2.695883	0.070472	-0.721109
C	-3.391725	1.271120	-0.604600
C	-2.781341	2.342667	0.037398
C	-1.494237	2.210453	0.544524
C	-0.797254	1.002837	0.417819
C	0.612444	0.980988	0.963327
H	0.971030	-0.042110	1.083558
H	0.614717	1.445611	1.958829
C	1.606372	1.733096	0.064552
C	3.046452	1.576257	0.545945
C	4.062244	2.272244	-0.358451
C	5.501905	2.076793	0.113556
H	5.762930	1.012059	0.135752
H	6.214149	2.583387	-0.546355
H	5.639843	2.474177	1.125961
H	3.829507	3.345115	-0.406948
H	3.954129	1.885662	-1.381755
H	3.287577	0.503991	0.601141
H	3.138083	1.967717	1.570154
H	1.337116	2.797641	0.024904
H	1.522651	1.348611	-0.960612
H	-1.022712	3.051860	1.049297
O	-3.502579	3.501888	0.142788
H	-2.974428	4.164380	0.608030
H	-4.399770	1.372672	-0.999623
O	-3.288476	-0.999878	-1.341298
H	-4.174252	-0.745698	-1.631706

Table S91. Coordinates for global minimum of **3e**‡.

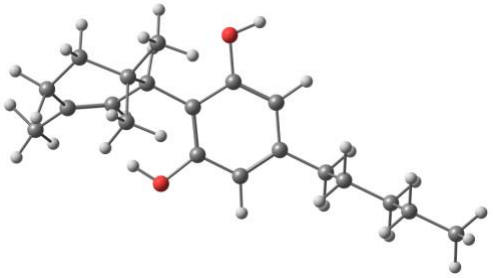


C	-2.050001	-0.174606	-0.867092
C	-0.783866	-0.802453	-1.015449
C	-0.473829	-1.971040	-0.384543
C	0.788826	-2.700166	-0.679187

H	1.381288	-2.805098	0.239153
H	0.560354	-3.721117	-1.011817
H	1.392407	-2.198410	-1.438090
C	-1.427224	-2.627423	0.555873
C	-2.572594	-1.727830	1.008617
H	-2.211472	-1.046542	1.786156
H	-3.370467	-2.331200	1.456451
C	-3.154973	-0.892319	-0.138550
H	-1.807122	-3.524972	0.040794
H	-0.870176	-3.016625	1.418226
H	-0.072531	-0.374316	-1.716222
H	-2.381411	0.454435	-1.692411
C	-1.025707	1.500155	1.352003
C	-1.635080	1.812341	0.108958
C	-0.789161	2.270256	-0.939190
C	0.588569	2.206308	-0.825988
C	1.159283	1.748911	0.367274
C	0.350185	1.401953	1.458255
H	0.807332	1.108076	2.400286
H	1.222802	2.510872	-1.655098
O	-1.423237	2.702014	-2.046469
H	-0.779059	2.933975	-2.732336
H	-2.681995	2.095374	0.087455
O	-1.860936	1.304937	2.393613
H	-1.356924	1.066116	3.186403
C	2.647648	1.603169	0.474077
H	2.966225	1.796728	1.505363
H	3.141178	2.335159	-0.176000
C	3.088686	0.184728	0.069229
H	2.573194	-0.543604	0.709912
H	2.757757	-0.011757	-0.959901
C	4.598032	-0.013756	0.174596
H	4.921063	0.185858	1.206551
H	5.109580	0.723677	-0.460729
C	5.033311	-1.422327	-0.230129
H	4.511350	-2.155859	0.400350
H	4.710597	-1.616232	-1.262514
C	6.542822	-1.626311	-0.114615
H	6.880912	-1.464451	0.915435
H	6.833517	-2.640108	-0.408753
H	7.082720	-0.921490	-0.757318
C	-4.269399	0.027624	0.368724
H	-4.612997	0.702245	-0.423524
H	-5.120536	-0.583383	0.686384
H	-3.943000	0.620355	1.226190
C	-3.775525	-1.809626	-1.233010
H	-3.040962	-2.488016	-1.674993

H	-4.571050	-2.402978	-0.769341
H	-4.215711	-1.207676	-2.034206

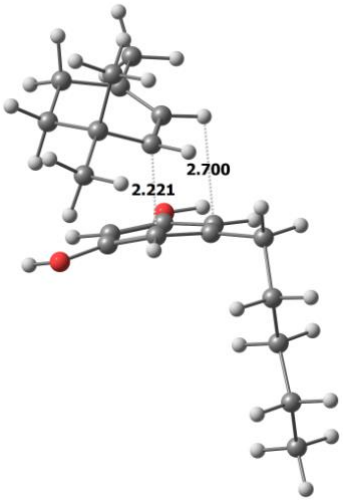
Table S92. Coordinates for global minimum of **3e**.



C	-2.300866	-0.480219	0.272522
C	-3.133153	0.475849	1.103107
C	-4.275049	1.051951	0.702288
C	-5.045666	1.993964	1.578396
H	-4.534435	2.179250	2.527276
H	-6.045565	1.593586	1.789902
H	-5.195818	2.954820	1.068617
C	-4.857944	0.770405	-0.655174
C	-4.219480	-0.447632	-1.320148
C	-2.682122	-0.436405	-1.243186
C	-2.135878	0.801347	-1.966138
H	-2.491783	1.739431	-1.530925
H	-1.040976	0.813381	-1.950968
H	-2.459873	0.778986	-3.013469
C	-2.140858	-1.681720	-1.952507
H	-2.528920	-2.597942	-1.494356
H	-1.047005	-1.717069	-1.907624
H	-2.438395	-1.669378	-3.007770
H	-4.584152	-1.358670	-0.824792
H	-4.527883	-0.508426	-2.372013
H	-4.754894	1.666638	-1.285827
H	-5.940825	0.616365	-0.548216
H	-2.779115	0.662050	2.119324
H	-2.562797	-1.493334	0.609785
C	-0.814156	-0.324887	0.550040
C	-0.180141	0.924057	0.685181
C	1.192029	1.037518	0.919075
C	1.982133	-0.100731	1.041755
C	1.377577	-1.353798	0.946105
C	0.006274	-1.454352	0.713628
O	-0.596414	-2.683935	0.648745
H	0.071041	-3.367325	0.794330
H	1.971375	-2.259198	1.059874
C	3.471835	0.015168	1.232308
H	3.701476	0.934085	1.786751

H	3.833759	-0.827759	1.835381
C	4.228934	0.033951	-0.104360
C	5.741172	0.145009	0.077171
C	6.503832	0.171440	-1.246903
C	8.015461	0.280241	-1.054115
H	8.397942	-0.568718	-0.475483
H	8.276060	1.196852	-0.512153
H	8.542571	0.296788	-2.013962
H	6.268956	-0.738103	-1.817154
H	6.146644	1.016110	-1.852248
H	5.973127	1.056170	0.648386
H	6.097984	-0.699799	0.684903
H	3.989451	-0.880676	-0.665128
H	3.865674	0.876166	-0.710108
H	1.625329	2.029992	1.011051
O	-0.861436	2.105797	0.597224
H	-1.820784	1.925745	0.583405

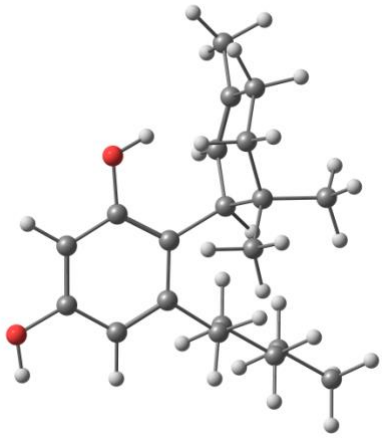
Table S93. Coordinates for global minimum of 6e‡.



C	-1.452366	-0.835076	0.797725
C	-1.763930	0.470528	1.267089
C	-2.836935	1.173052	0.810542
C	-3.152147	2.529332	1.335006
H	-3.085781	3.259621	0.516839
H	-4.187153	2.571084	1.697155
H	-2.473212	2.832150	2.135253
C	-3.793686	0.589024	-0.174874
C	-3.283980	-0.660180	-0.893299
H	-2.639104	-0.357825	-1.722683
H	-4.126266	-1.207382	-1.332033
C	-2.496890	-1.603946	0.025957
H	-4.715389	0.370984	0.389757
H	-4.086403	1.361001	-0.898327

H	-1.130349	0.915516	2.027756
H	-0.837452	-1.453867	1.448655
C	0.460689	2.217512	-0.336875
C	-0.098874	1.587700	-1.452595
C	-0.046353	0.208929	-1.516805
C	0.395622	-0.556900	-0.401622
C	1.135997	0.113461	0.624123
C	1.130386	1.486815	0.667030
H	1.636548	2.019896	1.468466
H	0.563338	-1.618893	-0.555712
O	-0.414244	-0.480185	-2.614459
H	-0.727893	0.126111	-3.302634
H	-0.508489	2.182744	-2.264044
O	0.383912	3.557381	-0.301306
H	0.827234	3.901577	0.489066
C	1.883732	-0.697427	1.640020
H	1.218691	-1.457666	2.071535
H	2.208959	-0.044587	2.457753
C	3.110253	-1.409591	1.035046
H	3.577821	-2.004896	1.829982
H	2.781657	-2.119257	0.264050
C	4.137498	-0.447598	0.443391
H	4.423346	0.293719	1.204619
H	3.681540	0.118270	-0.381920
C	5.388635	-1.160951	-0.067513
H	5.847696	-1.721329	0.758612
H	5.095917	-1.905250	-0.821005
C	6.410956	-0.196533	-0.665908
H	7.298913	-0.726706	-1.025641
H	5.981969	0.353440	-1.511634
H	6.737138	0.538475	0.078860
C	-3.424758	-2.178143	1.133822
H	-2.869551	-2.853065	1.793417
H	-3.873200	-1.390524	1.745294
H	-4.224684	-2.750060	0.650812
C	-1.925905	-2.790611	-0.755489
H	-1.306463	-3.419519	-0.105865
H	-2.749798	-3.404021	-1.135075
H	-1.326701	-2.464479	-1.607394

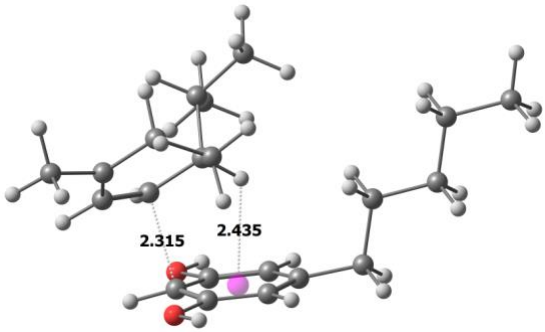
Table S94. Coordinates for global minimum of **6e**.



C	-0.668586	-0.700314	-0.135263
C	-1.281999	-1.299798	1.110525
C	-2.463195	-1.931720	1.179828
C	-2.962674	-2.552306	2.451185
H	-3.164557	-3.620870	2.299942
H	-3.912490	-2.095155	2.756793
H	-2.242652	-2.446501	3.267348
C	-3.359589	-2.058020	-0.020831
C	-2.970102	-1.113578	-1.155517
H	-3.300174	-0.094541	-0.917668
C	-1.457338	-1.097369	-1.433168
C	-1.193662	-0.128862	-2.589834
H	-0.127263	-0.055618	-2.826731
H	-1.558465	0.877162	-2.357145
H	-1.713646	-0.483058	-3.488032
C	-0.993038	-2.503340	-1.846713
H	-1.062323	-3.212748	-1.014874
H	0.051899	-2.475790	-2.177904
H	-1.603475	-2.883943	-2.674290
H	-3.494454	-1.404132	-2.075207
H	-4.398904	-1.874156	0.285690
H	-3.338373	-3.104878	-0.361182
H	-0.673193	-1.221402	2.013276
H	0.306039	-1.195434	-0.221633
C	-0.354329	0.784412	0.026455
C	-1.281775	1.692820	0.577157
C	-1.026223	3.060858	0.653484
C	0.184531	3.550535	0.186539
C	1.141870	2.679406	-0.327852
C	0.881873	1.309180	-0.404431
C	2.003139	0.423024	-0.898323
H	2.675215	1.017704	-1.528803
H	1.627321	-0.388462	-1.531228
C	2.817727	-0.177846	0.258948

C	3.912209	-1.125005	-0.226795
C	4.735744	-1.725164	0.912277
C	5.822284	-2.676771	0.414872
H	6.400288	-3.096103	1.245155
H	5.384811	-3.511331	-0.145405
H	6.520417	-2.158196	-0.252529
H	4.064016	-2.256966	1.600442
H	5.193042	-0.912847	1.494004
H	3.454464	-1.937403	-0.811006
H	4.580731	-0.588157	-0.916115
H	2.145446	-0.713009	0.944700
H	3.261768	0.640948	0.842080
H	2.099113	3.067905	-0.670256
O	0.391640	4.901389	0.268738
H	1.269521	5.109021	-0.077854
H	-1.769159	3.726637	1.081398
O	-2.498034	1.302976	1.066644
H	-2.485368	0.332502	1.189378

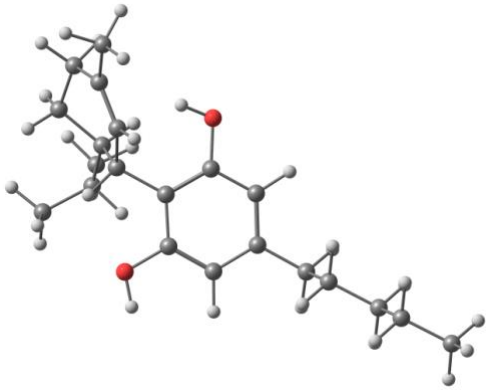
Table S95. Coordinates for global minimum of **3**‡.



C	2.014603	0.171281	0.680813
C	3.201051	0.413855	-0.045410
C	3.275969	1.396548	-0.994252
C	4.568557	1.771395	-1.618983
H	4.735956	2.851961	-1.525089
H	5.414115	1.228655	-1.192124
H	4.516879	1.567925	-2.697707
C	2.068527	2.183969	-1.375597
C	0.775338	1.453120	-1.040580
H	0.679526	0.593024	-1.711595
H	-0.091083	2.091186	-1.228369
C	0.766615	0.936350	0.401741
H	-0.102013	0.274015	0.532753
H	2.134715	3.150811	-0.848458
H	2.117759	2.433870	-2.442747
H	4.104161	-0.118297	0.243840
H	2.142288	-0.226468	1.683154
C	1.128601	-1.957443	-1.060173

C	1.626820	-2.070795	0.256723
C	0.702848	-2.293464	1.304905
C	-0.660191	-2.234597	1.073154
C	-1.131957	-2.018957	-0.231081
C	-0.238218	-1.902264	-1.299647
H	-0.610521	-1.759490	-2.311629
H	-1.362601	-2.346762	1.895931
O	1.245741	-2.492325	2.526550
H	0.546294	-2.577017	3.191180
H	2.677965	-2.286448	0.417499
O	2.058562	-1.858527	-2.031215
H	1.630446	-1.739952	-2.892353
C	-2.599455	-1.813318	-0.463094
H	-3.181241	-2.409718	0.249731
H	-2.867969	-2.137172	-1.475594
C	-2.959848	-0.324679	-0.293931
H	-2.681582	-0.004510	0.720398
H	-2.347909	0.269283	-0.987977
C	-4.439256	-0.040322	-0.537220
H	-5.045636	-0.633624	0.162324
H	-4.713867	-0.373843	-1.548453
C	-4.783823	1.440545	-0.380189
H	-4.504049	1.770975	0.629913
H	-4.171563	2.028210	-1.078485
C	-6.263921	1.729117	-0.624137
H	-6.488378	2.794447	-0.507416
H	-6.558972	1.432471	-1.637287
H	-6.891876	1.173747	0.081965
C	0.614570	2.037279	1.510509
H	1.569402	2.575923	1.600711
C	0.277572	1.399842	2.862216
C	-0.474318	3.045833	1.135782
H	-0.648103	3.724183	1.977726
H	-0.201685	3.654884	0.269573
H	-1.419196	2.533215	0.914480
H	-0.680131	0.867526	2.799800
H	0.182463	2.174657	3.629708
H	1.037045	0.691366	3.206056

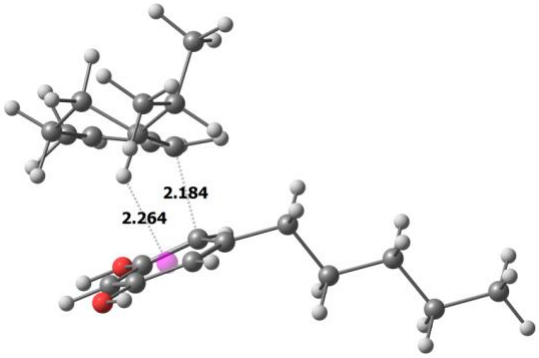
Table S96. Coordinates for global minimum of **3**.



C	-2.058155	-0.125181	-0.678657
C	-2.358479	-1.595818	-0.890811
C	-3.436874	-2.238347	-0.419945
C	-3.646014	-3.708648	-0.628590
H	-2.799233	-4.172346	-1.142255
H	-4.555391	-3.888268	-1.216448
H	-3.792288	-4.215169	0.334541
C	-4.509048	-1.509040	0.345282
C	-4.423753	0.002516	0.152570
H	-5.123707	0.506342	0.829368
H	-4.733862	0.248548	-0.872291
C	-2.996061	0.504515	0.383383
H	-2.670313	0.128680	1.366943
C	-2.878859	2.043203	0.434872
C	-3.574631	2.744677	-0.735567
H	-3.328425	3.812352	-0.735496
H	-4.664594	2.657202	-0.656863
H	-3.269564	2.333632	-1.703547
C	-3.396533	2.594107	1.767092
H	-2.869784	2.140019	2.614101
H	-3.251805	3.679100	1.819580
H	-4.468563	2.399448	1.890448
H	-1.806004	2.279165	0.379773
H	-5.490865	-1.883944	0.024166
H	-4.428383	-1.768405	1.413112
H	-1.619236	-2.155322	-1.467045
H	-2.236296	0.385795	-1.634058
C	-0.595432	0.083401	-0.328616
C	0.027942	-0.634202	0.706547
C	1.352213	-0.398416	1.076192
C	2.105241	0.564464	0.409490
C	1.519513	1.277545	-0.636528
C	0.193298	1.033287	-0.993794
O	-0.398476	1.733649	-2.013812
H	0.242318	2.356820	-2.380891

H	2.092988	2.029941	-1.175584
C	3.553497	0.779376	0.764767
H	3.700155	0.591388	1.836081
H	3.831073	1.824525	0.576325
C	4.488924	-0.139631	-0.036177
C	5.958089	0.043803	0.337694
C	6.896524	-0.862668	-0.458347
C	8.362344	-0.681114	-0.068069
H	9.017476	-1.338452	-0.649485
H	8.514845	-0.908173	0.993501
H	8.687183	0.352227	-0.237013
H	6.600526	-1.910025	-0.306558
H	6.771187	-0.659072	-1.530869
H	6.246838	1.093722	0.180635
H	6.086539	-0.154175	1.412154
H	4.192372	-1.184721	0.131128
H	4.351611	0.055999	-1.109082
H	1.783386	-0.980458	1.886557
O	-0.639307	-1.591067	1.422297
H	-1.457229	-1.832566	0.945334

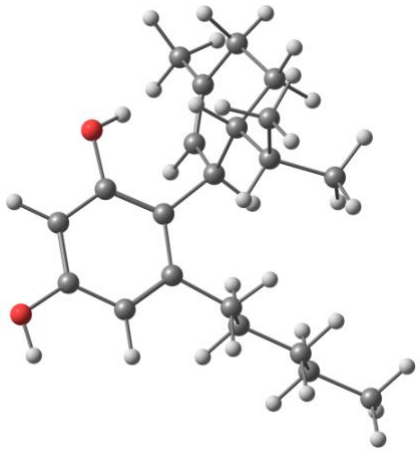
Table S97. Coordinates for global minimum of **6**‡.



C	0.910711	1.216407	-0.653567
C	1.565192	2.317770	-0.039442
C	2.881834	2.267416	0.304679
C	3.560261	3.385447	1.006274
H	2.871074	4.187860	1.278111
H	4.054840	3.007048	1.911029
H	4.361659	3.791188	0.374187
C	3.691854	1.059795	-0.047822
C	3.177080	0.404581	-1.330006
H	3.755519	-0.498182	-1.548492
H	3.325654	1.104425	-2.161332
C	1.687738	0.051276	-1.203124
H	1.631840	-0.769944	-0.469456
H	4.748675	1.335134	-0.140014
H	3.632273	0.346250	0.791658

H	0.975004	3.195872	0.212789
H	-0.033330	1.439364	-1.145245
C	0.516816	-2.181813	1.302164
C	1.148330	-1.186745	2.052750
C	0.698075	0.115111	1.927382
C	-0.315463	0.456285	0.986380
C	-1.016365	-0.594434	0.323997
C	-0.565706	-1.889528	0.445956
H	-1.055413	-2.698954	-0.091442
H	-0.802550	1.421217	1.098326
O	1.209727	1.137081	2.631658
H	1.931261	0.831350	3.203007
H	1.955912	-1.447216	2.731144
O	0.981520	-3.433306	1.451122
H	0.469139	-4.051833	0.908942
C	-2.246447	-0.270030	-0.468392
H	-2.405566	-1.033282	-1.239092
H	-2.123857	0.695156	-0.977561
C	-3.488811	-0.194717	0.438724
H	-3.628659	-1.166570	0.930968
H	-3.313244	0.541125	1.235518
C	-4.747610	0.179767	-0.340329
H	-4.904509	-0.547160	-1.150542
H	-4.598840	1.156431	-0.823475
C	-5.995105	0.233967	0.540739
H	-6.142397	-0.744642	1.017930
H	-5.831538	0.953792	1.354655
C	-7.248809	0.618730	-0.242769
H	-7.445850	-0.103095	-1.043775
H	-8.130973	0.651548	0.404985
H	-7.133332	1.606053	-0.704646
C	1.035574	-0.486382	-2.498635
H	-0.031027	-0.619967	-2.264778
C	1.597565	-1.856920	-2.877497
C	1.138692	0.492784	-3.671217
H	0.794757	1.497537	-3.398339
H	2.169827	0.575035	-4.031626
H	0.524092	0.143824	-4.507455
H	2.652530	-1.789845	-3.166208
H	1.048221	-2.271457	-3.729314
H	1.515392	-2.562870	-2.042274

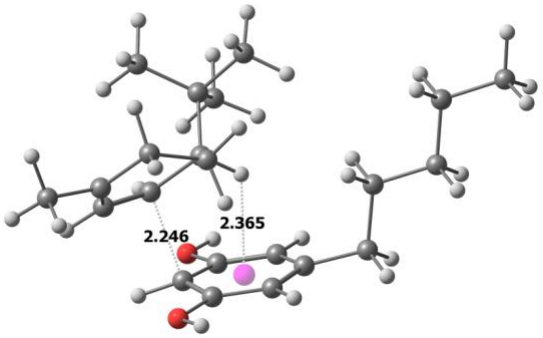
Table S98. Coordinates for global minimum of **6**.



C	-0.636150	-0.595617	0.147177
C	-0.992265	-1.124009	1.523386
C	-2.023761	-1.935352	1.798459
C	-2.351366	-2.366367	3.196968
H	-2.266852	-3.456481	3.293403
H	-3.390638	-2.111407	3.443167
H	-1.692995	-1.896911	3.933280
C	-2.913525	-2.463477	0.704027
C	-2.262388	-2.334448	-0.670067
H	-2.978848	-2.610015	-1.453067
H	-1.427563	-3.045854	-0.732347
C	-1.736367	-0.914406	-0.899298
H	-2.571881	-0.220713	-0.717012
C	-1.254119	-0.663419	-2.344665
C	-2.435446	-0.427801	-3.290917
H	-3.042075	0.423154	-2.961014
H	-2.083171	-0.220159	-4.307698
H	-3.086650	-1.308762	-3.341351
C	-0.359328	-1.783162	-2.887958
H	0.112468	-1.470037	-3.825840
H	0.438319	-2.058355	-2.188831
H	-0.944277	-2.686525	-3.096393
H	-0.666050	0.266191	-2.324084
H	-3.155531	-3.513456	0.919302
H	-3.874962	-1.925778	0.729122
H	-0.356751	-0.780053	2.341612
H	0.278167	-1.117169	-0.164329
C	-0.324149	0.894161	0.211436
C	-1.260405	1.782143	0.781171
C	-1.056924	3.159407	0.808987
C	0.112876	3.678295	0.271253
C	1.074539	2.829661	-0.271585
C	0.863942	1.447981	-0.301923

C	1.970181	0.582887	-0.857405
H	2.625133	1.200247	-1.483915
H	1.564257	-0.195314	-1.513557
C	2.817750	-0.075834	0.242281
C	3.866886	-1.029435	-0.324474
C	4.719305	-1.694939	0.755134
C	5.753292	-2.659584	0.177320
H	5.266147	-3.460088	-0.391675
H	6.437679	-2.138227	-0.502134
H	6.353435	-3.125452	0.966102
H	4.061041	-2.231337	1.452780
H	5.226171	-0.918505	1.344835
H	4.520907	-0.483784	-1.020797
H	3.362782	-1.805977	-0.919577
H	2.164030	-0.621736	0.936858
H	3.305517	0.710999	0.834630
H	1.994975	3.244422	-0.677920
O	0.273860	5.037588	0.311625
H	1.123693	5.267865	-0.086628
H	-1.802874	3.810101	1.254572
O	-2.437296	1.349742	1.330860
H	-2.368460	0.390905	1.507841

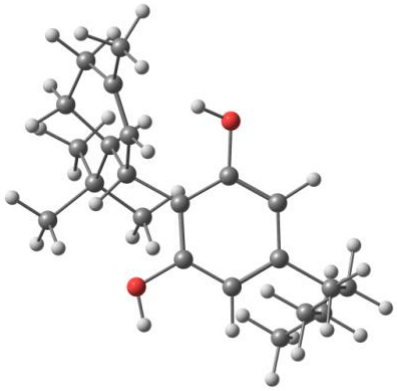
Table S99. Coordinates for global minimum of **3f**‡.



C	-1.947724	-0.119075	0.587775
C	-3.153024	-0.219966	-0.151460
C	-3.275768	-1.025340	-1.245530
C	-4.591203	-1.240296	-1.902642
H	-4.807735	-2.313575	-1.977493
H	-5.407168	-0.737934	-1.379185
H	-4.544405	-0.868362	-2.935358
C	-2.109808	-1.782220	-1.782368
C	-0.772508	-1.226736	-1.307547
H	-0.579293	-0.302041	-1.863224
H	0.038671	-1.909705	-1.568103
C	-0.723352	-0.871602	0.188036
H	0.145038	-0.209470	0.320964
H	-2.246283	-2.838325	-1.502622

H	-2.155971	-1.776286	-2.879638
H	-4.033391	0.290467	0.232846
H	-2.067598	0.096607	1.646361
C	-1.081275	2.169945	-0.852103
C	-1.536229	2.086960	0.486222
C	-0.572005	2.168277	1.523782
C	0.779426	2.134815	1.237865
C	1.204813	2.097053	-0.100519
C	0.275575	2.138030	-1.144130
H	0.612115	2.139168	-2.178250
H	1.511652	2.130418	2.041874
O	-1.072405	2.206507	2.776689
H	-0.351460	2.190806	3.423889
H	-2.573067	2.314309	0.711772
O	-2.042447	2.221473	-1.792182
H	-1.645612	2.212468	-2.676440
C	2.662577	1.915961	-0.400040
H	3.266800	2.469863	0.328719
H	2.894732	2.301965	-1.399154
C	3.032452	0.420796	-0.329515
H	2.771953	0.037920	0.667211
H	2.411385	-0.131962	-1.049066
C	4.508704	0.155562	-0.609280
H	5.123041	0.719322	0.107587
H	4.767777	0.533673	-1.608642
C	4.857769	-1.330275	-0.519759
H	4.585406	-1.703688	0.477371
H	4.240972	-1.888837	-1.237665
C	6.336522	-1.605358	-0.786007
H	6.562935	-2.674513	-0.718294
H	6.624483	-1.263242	-1.786677
H	6.968236	-1.081146	-0.059637
C	-0.443288	-2.040906	1.218994
C	0.054777	-1.418772	2.533617
C	0.671630	-2.939550	0.668790
H	0.334077	-3.536709	-0.184138
H	1.543188	-2.350367	0.358510
H	0.993359	-3.633989	1.452807
H	-0.684018	-0.751524	2.990939
H	0.976073	-0.847407	2.369307
H	0.270198	-2.211066	3.258918
C	-1.686197	-2.893866	1.507229
H	-2.082023	-3.358813	0.599556
H	-1.422615	-3.697982	2.203484
H	-2.486169	-2.305148	1.969139

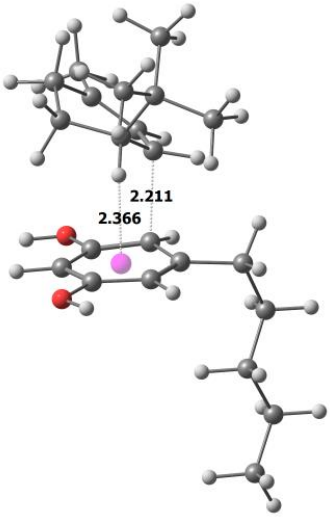
Table S100. Coordinates for global minimum of **3f**.



C	-1.839475	-0.146270	-0.666933
C	-2.857000	-1.257825	-0.464421
C	-3.954148	-1.190352	0.299540
C	-4.861296	-2.365143	0.513962
H	-4.970888	-2.573345	1.586497
H	-4.485379	-3.266049	0.020879
H	-5.867765	-2.148935	0.133159
C	-4.335204	0.098578	0.970042
C	-3.611829	1.292006	0.353529
H	-3.844561	2.184438	0.938985
H	-4.002898	1.458287	-0.659857
C	-2.092060	1.065047	0.284451
H	-1.762518	0.775549	1.295122
C	-1.300886	2.373291	-0.051150
C	-1.600314	2.887538	-1.466146
H	-2.670126	3.075155	-1.609729
H	-1.072004	3.833461	-1.636092
H	-1.266061	2.180169	-2.231775
C	-1.687838	3.472205	0.960201
H	-1.607450	3.106450	1.991584
H	-1.008700	4.324826	0.850976
H	-2.704036	3.845425	0.805712
C	0.217635	2.165183	0.092023
H	0.465305	1.703882	1.056101
H	0.726070	3.135343	0.039889
H	0.628073	1.535298	-0.698268
H	-5.423331	0.232382	0.893370
H	-4.119129	0.031442	2.048538
H	-2.618324	-2.196631	-0.966915
H	-1.949985	0.211832	-1.697618
C	-0.457284	-0.768720	-0.556098
C	0.457984	-0.732996	-1.614867
C	1.753476	-1.235267	-1.491467
C	2.170669	-1.810770	-0.292454
C	1.258253	-1.923672	0.754699

C	-0.036701	-1.428853	0.610858
O	-0.877111	-1.599014	1.679132
H	-1.797478	-1.492822	1.372826
H	1.536579	-2.402533	1.689982
C	3.597306	-2.262651	-0.109610
H	4.085811	-2.333388	-1.089324
H	3.612297	-3.265263	0.336210
C	4.401123	-1.305121	0.789161
C	4.474149	0.119840	0.245185
C	5.309344	1.053814	1.119748
C	5.348545	2.482350	0.579221
H	5.946490	3.139392	1.219574
H	4.337561	2.902339	0.516112
H	5.782167	2.507513	-0.427318
H	4.897844	1.055788	2.138717
H	6.332106	0.659844	1.199923
H	4.891552	0.100371	-0.773063
H	3.457501	0.528158	0.151466
H	3.950460	-1.289622	1.791308
H	5.417678	-1.705233	0.906558
H	2.444552	-1.151812	-2.328318
O	0.048647	-0.135680	-2.780198
H	0.782977	-0.140164	-3.408370

Table S101. Coordinates for global minimum of **6f**‡.

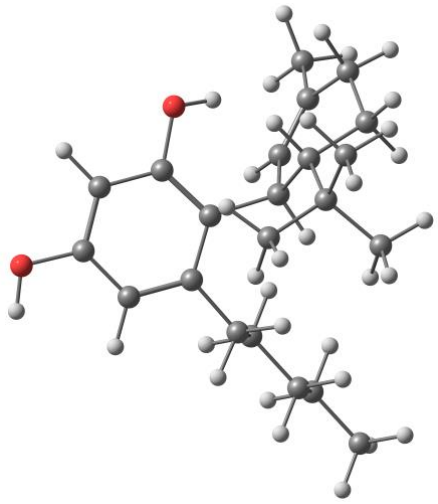


C	-1.270116	-0.079656	-0.888452
C	-1.861875	-1.275227	-1.374134
C	-3.016206	-1.783805	-0.862456
C	-3.683352	-2.962322	-1.476940
H	-3.170402	-3.306679	-2.377330
H	-3.717136	-3.783026	-0.747547
H	-4.727929	-2.726827	-1.717644

C	-3.703571	-1.131191	0.285682
C	-2.812986	-0.172631	1.074250
H	-2.175089	-0.774710	1.730161
H	-3.427943	0.441445	1.736425
C	-1.884870	0.712536	0.220183
H	-1.064761	1.047869	0.875123
H	-4.597675	-0.633785	-0.118498
H	-4.096852	-1.909344	0.953660
H	-1.405835	-1.756856	-2.236571
H	-0.699632	0.477953	-1.622812
C	1.028772	0.328610	2.286096
C	0.449359	-0.936044	2.184284
C	0.332612	-1.505556	0.927020
C	0.719262	-0.793254	-0.240143
C	1.421208	0.438355	-0.094253
C	1.521694	1.012555	1.151999
H	2.014194	1.973899	1.280166
H	0.829424	-1.356042	-1.162347
O	-0.186193	-2.728075	0.724947
H	-0.476029	-3.115938	1.564825
H	0.115351	-1.455822	3.077810
O	1.119117	0.853878	3.519784
H	1.545337	1.723357	3.486140
C	2.035336	1.081059	-1.302756
H	2.306492	2.115969	-1.065718
H	1.301050	1.113573	-2.119129
C	3.283448	0.323717	-1.798937
H	2.998401	-0.691562	-2.106236
H	3.648288	0.833233	-2.700176
C	4.402110	0.250269	-0.762811
H	4.052183	-0.302599	0.120692
H	4.644927	1.265667	-0.415074
C	5.665817	-0.417280	-1.304519
H	5.414745	-1.424986	-1.663675
H	6.023471	0.142826	-2.179400
C	6.776335	-0.505341	-0.259265
H	6.447490	-1.083311	0.612217
H	7.671223	-0.988582	-0.664863
H	7.063016	0.492802	0.091715
C	-2.490936	2.074682	-0.300016
C	-2.880447	2.926851	0.916981
C	-3.721523	1.863516	-1.189153
H	-3.510591	1.176934	-2.017371
H	-4.567039	1.470774	-0.616439
H	-4.033151	2.822138	-1.619558
H	-3.680511	2.469873	1.505865
H	-3.240548	3.903967	0.576800

H	-2.016274	3.091676	1.571736
C	-1.423718	2.853614	-1.087925
H	-1.771688	3.878220	-1.256109
H	-0.479255	2.904797	-0.531769
H	-1.224380	2.417375	-2.071863

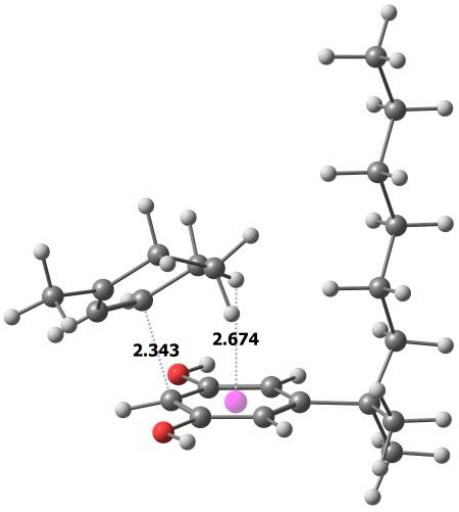
Table S102. Coordinates for global minimum of **6f**.



C	-0.570355	-0.587497	0.151301
C	-0.568066	-1.127077	1.574873
C	-1.509570	-1.901580	2.129392
C	-1.478485	-2.298595	3.575091
H	-0.639595	-1.840264	4.106332
H	-1.404478	-3.389295	3.673521
H	-2.411320	-2.002979	4.073216
C	-2.645336	-2.428804	1.298876
C	-2.328143	-2.337968	-0.188950
H	-3.199014	-2.662205	-0.764749
H	-1.514173	-3.040400	-0.415177
C	-1.899705	-0.919079	-0.599113
H	-2.672169	-0.224102	-0.236875
C	-1.881092	-0.744035	-2.153147
C	-0.987159	-1.786032	-2.841330
H	-0.953220	-1.591121	-3.919688
H	0.042780	-1.752832	-2.468142
H	-1.367706	-2.802804	-2.699383
C	-3.319082	-0.903013	-2.687162
H	-3.337475	-0.700019	-3.763933
H	-3.715816	-1.911295	-2.539698
H	-3.995775	-0.191248	-2.198580
C	-1.416408	0.660955	-2.567179
H	-1.968067	1.438692	-2.025700
H	-1.593327	0.800028	-3.640346
H	-0.352444	0.815705	-2.382465

H	-2.842742	-3.471385	1.584866
H	-3.568833	-1.875766	1.535748
H	0.261003	-0.781182	2.194201
H	0.241766	-1.092599	-0.385749
C	-0.216924	0.894811	0.238464
C	-1.058932	1.776433	0.944222
C	-0.822848	3.147350	1.000567
C	0.307375	3.660421	0.379408
C	1.206337	2.807339	-0.257122
C	0.957464	1.433808	-0.320436
C	2.007122	0.564326	-0.972408
H	2.645902	1.191959	-1.605523
H	1.549191	-0.176963	-1.638820
C	2.887747	-0.161440	0.055551
C	3.931963	-1.065015	-0.596203
C	4.804356	-1.797176	0.422794
C	5.844852	-2.703096	-0.233169
H	6.456237	-3.219299	0.514565
H	5.362664	-3.464738	-0.857037
H	6.518081	-2.124133	-0.876019
H	4.160366	-2.392328	1.085152
H	5.307374	-1.059346	1.063242
H	4.571602	-0.466175	-1.261296
H	3.424221	-1.802024	-1.236430
H	2.255100	-0.760591	0.724377
H	3.384164	0.586685	0.689466
H	2.108956	3.213495	-0.709563
O	0.502796	5.014096	0.446410
H	1.323683	5.238982	-0.011260
H	-1.505213	3.794855	1.542245
O	-2.173039	1.341428	1.614814
H	-2.064727	0.391582	1.807815

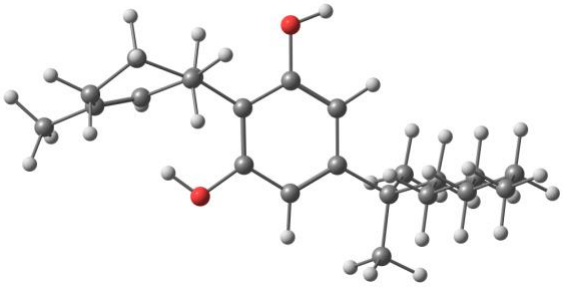
Table S103. Coordinates for global minimum of **3bc**‡.



C	2.027156	1.114709	1.224518
C	3.169945	1.630040	0.587801
C	3.069246	2.477265	-0.484814
C	4.268490	3.120832	-1.072315
H	5.181608	2.893627	-0.518924
H	4.382047	2.780568	-2.111410
H	4.127441	4.207884	-1.128412
C	1.740047	2.855237	-1.048049
C	0.644448	1.840997	-0.735317
H	0.796894	0.944051	-1.345506
H	-0.334698	2.248989	-1.003235
C	0.667339	1.454706	0.740473
H	-0.032645	0.642282	0.970110
H	1.491509	3.841535	-0.618693
H	1.833870	3.023773	-2.127597
H	4.149288	1.408392	1.004415
H	2.121143	0.805627	2.262721
C	2.161691	-1.269753	-0.483442
C	2.348903	-1.184949	0.910836
C	1.313164	-1.669451	1.740826
C	0.115826	-2.110640	1.208122
C	-0.070708	-2.148969	-0.187448
C	0.960248	-1.718100	-1.025244
H	0.853778	-1.743725	-2.104331
H	-0.664569	-2.452628	1.881833
O	1.565301	-1.627911	3.070679
H	0.794744	-1.944272	3.564395
H	3.344635	-1.043420	1.317093
O	3.200097	-0.866356	-1.243460
H	2.968430	-0.928922	-2.182340
H	0.336841	2.302708	1.368414
C	-1.383831	-2.699102	-0.743450

C	-2.577040	-1.888504	-0.177341
H	-3.499899	-2.387395	-0.504693
H	-2.565397	-1.955678	0.918475
C	-2.618074	-0.417637	-0.588082
H	-2.840776	-0.330584	-1.659486
H	-1.625726	0.031672	-0.443635
C	-3.648742	0.385801	0.204225
H	-4.648938	-0.042753	0.042826
H	-3.438149	0.284355	1.279196
C	-3.662329	1.867338	-0.167771
H	-2.665021	2.294442	0.018918
H	-3.845357	1.972405	-1.247438
C	-1.428304	-2.680698	-2.276007
H	-0.668071	-3.343110	-2.704156
H	-2.408685	-3.038184	-2.607835
H	-1.282108	-1.677226	-2.686596
C	-1.524634	-4.165064	-0.280130
H	-1.585011	-4.243218	0.809584
H	-2.439738	-4.594211	-0.702935
H	-0.672782	-4.762901	-0.622047
C	-4.705542	2.676517	0.601911
H	-4.527996	2.561151	1.680221
H	-5.702468	2.257728	0.406484
C	-4.689198	4.159123	0.233981
H	-5.444859	4.720699	0.793248
H	-3.711074	4.604658	0.450351
H	-4.889492	4.298829	-0.834733

Table S104. Coordinates for global minimum of **3bc**.

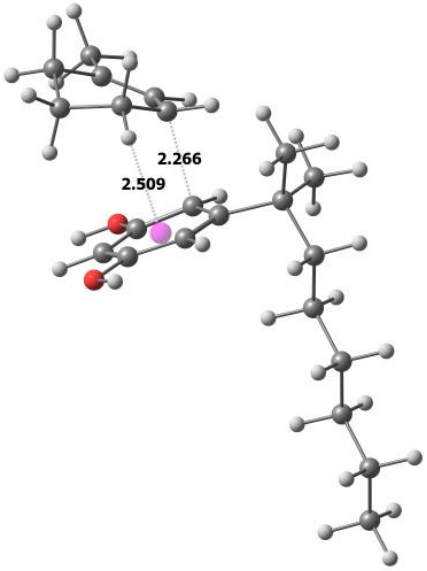


C	2.884768	0.474954	0.842381
C	4.098639	-0.111736	0.153585
C	5.024137	0.603015	-0.503658
C	6.189539	-0.043599	-1.191228
H	6.224113	0.254644	-2.247388
H	6.140617	-1.134824	-1.137467
H	7.134204	0.288746	-0.741857
C	4.949833	2.106425	-0.589677
C	3.998585	2.706310	0.445374
C	2.672900	1.950203	0.449967

H	2.222199	1.997613	-0.551675
H	1.957700	2.405960	1.144490
H	4.457152	2.639747	1.441817
H	3.834113	3.769676	0.236068
H	4.635080	2.388436	-1.606970
H	5.961777	2.516741	-0.468523
H	4.214464	-1.195292	0.220230
H	3.073669	0.436041	1.923552
C	1.630401	-0.335857	0.583078
C	1.273067	-0.778427	-0.697733
C	0.086764	-1.477226	-0.939810
C	-0.799008	-1.751630	0.097935
C	-0.463849	-1.315861	1.385103
C	0.720800	-0.621275	1.612065
O	1.044325	-0.171879	2.867703
H	0.343163	-0.425779	3.482177
H	-1.127395	-1.503317	2.225704
C	-2.116978	-2.497799	-0.123152
C	-2.128565	-3.771105	0.746281
H	-3.061094	-4.325040	0.585949
H	-1.289592	-4.425061	0.482941
H	-2.055122	-3.532945	1.811961
C	-2.307481	-2.929984	-1.582776
H	-2.300043	-2.084306	-2.276480
H	-1.524502	-3.631095	-1.892162
H	-3.272676	-3.438519	-1.682942
C	-3.302880	-1.600093	0.312225
C	-3.407064	-0.254116	-0.402819
C	-4.551673	0.606046	0.133024
C	-4.666433	1.956256	-0.573138
C	-5.811007	2.820163	-0.044200
C	-5.911251	4.168327	-0.756233
H	-4.986120	4.743756	-0.634443
H	-6.078458	4.031337	-1.831012
H	-6.736254	4.771234	-0.362057
H	-5.672684	2.981492	1.034038
H	-6.757233	2.272385	-0.155399
H	-3.718570	2.504139	-0.464791
H	-4.805659	1.792090	-1.652044
H	-4.408378	0.770845	1.211289
H	-5.500317	0.058864	0.027484
H	-2.459374	0.291510	-0.290714
H	-3.552169	-0.408471	-1.480435
H	-4.230440	-2.170302	0.155744
H	-3.231228	-1.420993	1.393935
H	-0.114045	-1.785932	-1.959163
O	2.056218	-0.530309	-1.792692

H	2.930293	-0.208516	-1.494590

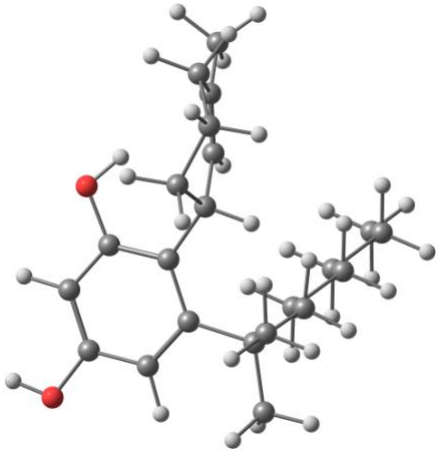
Table S105. Coordinates for global minimum of **6bc**‡.



C	-2.625094	-0.990955	0.149923
C	-3.340478	-0.666719	1.327237
C	-4.541331	-0.019590	1.279036
C	-5.359481	0.183587	2.502164
H	-5.478764	1.261103	2.680963
H	-6.372845	-0.210951	2.352828
H	-4.913199	-0.278109	3.385259
C	-5.130101	0.423375	-0.021155
C	-4.084077	0.617253	-1.113831
H	-3.512653	1.527459	-0.904129
H	-4.570510	0.762319	-2.083265
C	-3.133602	-0.575697	-1.182276
H	-2.298736	-0.397139	-1.873620
H	-5.862988	-0.347493	-0.314769
H	-5.715081	1.338047	0.133687
H	-2.964879	-1.029611	2.281115
H	-2.030570	-1.897460	0.178044
C	-0.226827	1.388221	-1.882063
C	-0.916149	2.041318	-0.860859
C	-1.089787	1.370046	0.336323
C	-0.635756	0.034213	0.505939
C	0.169814	-0.562882	-0.501023
C	0.315154	0.100697	-1.704122
H	0.886159	-0.335909	-2.519010
H	-0.615866	-0.352242	1.517978
O	-1.716553	1.912141	1.396438
H	-2.040931	2.800211	1.182390
H	-1.287673	3.051339	-1.009503

O	-0.083340	2.062754	-3.038854
H	0.425404	1.540112	-3.676560
H	-3.651725	-1.461658	-1.590134
C	0.864170	-1.909026	-0.286509
C	2.386803	-1.728827	-0.526334
H	2.856676	-2.714128	-0.397342
H	2.547586	-1.447556	-1.575394
C	3.084255	-0.709561	0.373276
H	3.020940	-1.023839	1.423247
H	2.568968	0.259679	0.304585
C	4.554885	-0.522005	-0.000534
H	5.069792	-1.492769	0.050168
H	4.623620	-0.189809	-1.046901
C	5.277380	0.481197	0.897215
H	5.211372	0.147522	1.943335
H	4.759752	1.450859	0.849324
C	0.335028	-2.928012	-1.317554
H	-0.744856	-3.081149	-1.215191
H	0.536669	-2.603468	-2.342894
H	0.829207	-3.893297	-1.162557
C	0.640170	-2.479275	1.120634
H	0.987706	-1.803105	1.906686
H	-0.412903	-2.712100	1.311900
H	1.202086	-3.414206	1.213466
C	6.746480	0.675565	0.522793
H	7.261874	-0.293775	0.570934
H	6.811361	1.008062	-0.522629
C	7.457911	1.681038	1.426680
H	6.978285	2.665248	1.370432
H	8.508588	1.803059	1.143015
H	7.428060	1.355665	2.473050

Table S106. Coordinates for global minimum of **6bc**.

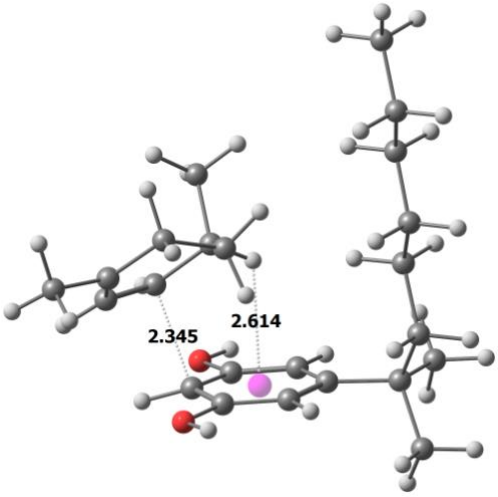


C	1.314543	0.979715	-0.608200

C	0.591039	2.077071	0.147571
C	1.009888	3.349012	0.230468
C	0.261670	4.385489	1.014378
H	0.921281	4.854901	1.756100
H	-0.087988	5.189737	0.354237
H	-0.601159	3.959295	1.533964
C	2.267908	3.813831	-0.458954
C	2.754523	2.831208	-1.524165
C	2.748928	1.404169	-0.981146
H	3.404467	1.345073	-0.102669
H	3.148842	0.700588	-1.720563
H	2.091408	2.887309	-2.398983
H	3.758959	3.109776	-1.863490
H	3.049006	3.972952	0.301783
H	2.082790	4.802409	-0.901195
H	-0.340739	1.789972	0.639234
H	0.775261	0.852359	-1.546446
C	1.288838	-0.348071	0.137387
C	1.805743	-0.358240	1.449772
C	1.932518	-1.522752	2.202809
C	1.515053	-2.715853	1.638768
C	0.948947	-2.737481	0.367099
C	0.814804	-1.574189	-0.398047
C	0.114935	-1.688603	-1.773451
C	1.080381	-1.324572	-2.922846
H	0.573897	-1.471785	-3.884204
H	1.433284	-0.292461	-2.892225
H	1.958475	-1.979742	-2.898327
C	-0.342381	-3.130847	-2.072071
H	-0.838383	-3.140052	-3.048120
H	-1.052718	-3.513502	-1.333927
H	0.505618	-3.821495	-2.126580
C	-1.154588	-0.791177	-1.834349
C	-2.116680	-0.932052	-0.655397
C	-3.313701	0.011832	-0.768330
C	-4.284010	-0.109565	0.405128
C	-5.474002	0.844515	0.306787
C	-6.439488	0.708371	1.482909
H	-7.283582	1.400360	1.392580
H	-5.932132	0.918990	2.431630
H	-6.843550	-0.309075	1.540712
H	-5.103938	1.877790	0.250125
H	-6.010036	0.657165	-0.634218
H	-3.743168	0.080632	1.344255
H	-4.653009	-1.144157	0.466514
H	-2.950351	1.048770	-0.833484
H	-3.851336	-0.186152	-1.707606

H	-1.579612	-0.721620	0.279885
H	-2.479193	-1.966256	-0.579838
H	-1.683645	-1.040057	-2.765774
H	-0.882255	0.265588	-1.926756
H	0.607851	-3.696041	0.000739
O	1.610746	-3.912419	2.299442
H	2.011441	-3.767203	3.166792
H	2.342643	-1.472503	3.208265
O	2.234683	0.782025	2.076058
H	1.876206	1.560690	1.606147

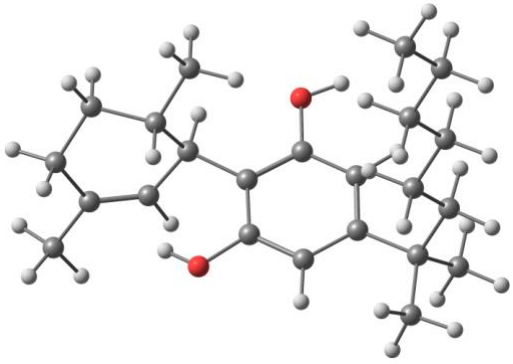
Table S107. Coordinates for global minimum of **3bd**‡.



C	-2.154796	-1.034326	1.014382
C	-3.025082	-1.754381	0.178532
C	-2.558551	-2.674697	-0.723992
C	-3.489406	-3.514527	-1.515342
H	-3.223938	-4.574824	-1.417150
H	-4.533201	-3.365683	-1.232631
H	-3.367213	-3.272745	-2.580675
C	-1.098901	-2.926091	-0.888064
C	-0.224946	-1.780464	-0.385803
H	-0.264638	-0.961506	-1.111617
H	0.819607	-2.103326	-0.325930
C	-0.683265	-1.260572	0.979268
H	-0.179093	-0.310305	1.198626
H	-0.883306	-3.863960	-0.349025
H	-0.885409	-3.151657	-1.940241
H	-4.097619	-1.624377	0.300916
H	-2.562326	-0.634012	1.940303
C	-1.989960	1.125417	-0.963188
C	-2.592264	1.160589	0.313553
C	-1.919074	1.861566	1.335898
C	-0.658131	2.403352	1.127868

C	-0.056182	2.321414	-0.135957
C	-0.733272	1.670819	-1.177134
H	-0.294742	1.608080	-2.168687
H	-0.162942	2.908310	1.950168
O	-2.565770	1.930232	2.522202
H	-2.022835	2.400145	3.172341
H	-3.646093	0.928304	0.424066
O	-2.701739	0.507781	-1.930612
H	-2.199286	0.498340	-2.759119
C	1.300420	2.964177	-0.425657
C	2.282700	1.901862	-0.978955
H	1.849748	1.449352	-1.880979
H	3.189349	2.429368	-1.306753
C	2.665929	0.793695	0.000890
H	1.763456	0.412122	0.499580
H	3.307475	1.197659	0.794815
C	3.381942	-0.370400	-0.681726
H	2.721087	-0.795029	-1.452363
H	4.271152	0.003362	-1.210332
C	3.794613	-1.471034	0.293611
H	4.507211	-1.063152	1.025465
H	2.914547	-1.792897	0.871581
C	1.092648	4.047427	-1.506258
H	0.358038	4.789202	-1.174595
H	2.041836	4.561218	-1.694240
H	0.746347	3.616265	-2.450398
C	1.910468	3.637744	0.809316
H	1.294489	4.476841	1.150630
H	2.040698	2.942631	1.644113
H	2.897400	4.033308	0.546984
C	4.411985	-2.687718	-0.394056
H	5.293013	-2.369872	-0.968750
H	3.695046	-3.088373	-1.124793
C	4.807255	-3.785597	0.591712
H	5.242621	-4.649279	0.078236
H	5.545042	-3.417004	1.313839
H	3.934876	-4.134951	1.156743
C	-0.339523	-2.229509	2.135225
H	-0.652132	-1.817404	3.099219
H	-0.827591	-3.200028	2.000765
H	0.743882	-2.383650	2.156882

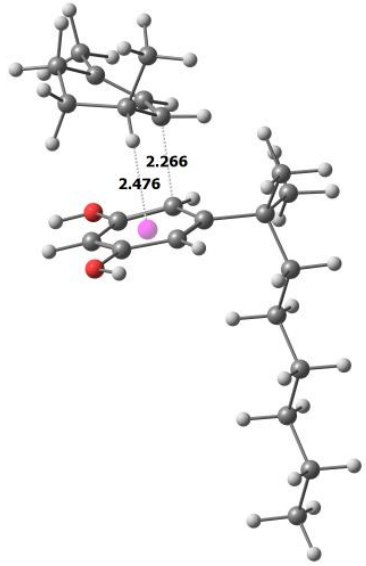
Table S108. Coordinates for global minimum of **3bd**.



C	-2.787435	-0.431827	0.736856
C	-4.011351	0.273520	0.189425
C	-4.988057	-0.317709	-0.513223
C	-6.156943	0.448189	-1.057403
H	-6.069480	1.520423	-0.860908
H	-6.243691	0.296094	-2.141338
H	-7.093836	0.084948	-0.615735
C	-4.967335	-1.797193	-0.795356
C	-3.985813	-2.545876	0.102765
C	-2.623757	-1.851150	0.141064
H	-2.270469	-1.744010	-0.896816
C	-1.597222	-2.668996	0.919760
H	-1.454140	-3.651221	0.455928
H	-0.625794	-2.164476	0.954743
H	-1.934341	-2.826123	1.951809
H	-4.387118	-2.594025	1.125852
H	-3.868450	-3.579963	-0.244677
H	-4.713095	-1.953414	-1.855771
H	-5.984152	-2.195463	-0.673824
H	-4.081178	1.342888	0.397205
H	-2.928599	-0.546249	1.820851
C	-1.534869	0.399433	0.534453
C	-0.621299	0.629290	1.573811
C	0.565095	1.330255	1.377241
C	0.894608	1.836908	0.115151
C	-0.006422	1.639483	-0.926757
C	-1.196403	0.938075	-0.714259
O	-2.007511	0.788307	-1.807495
H	-2.888274	0.485832	-1.510875
H	0.182710	2.015877	-1.925399
C	2.219308	2.579654	-0.073584
C	2.237583	3.818652	0.843764
H	1.408664	4.491739	0.597599
H	2.150876	3.540341	1.898717
H	3.177821	4.367287	0.712670
C	2.418255	3.064060	-1.515429

H	1.646507	3.787827	-1.799584
H	2.398871	2.244634	-2.239878
H	3.390851	3.561808	-1.595752
C	3.396360	1.656034	0.330502
C	3.480185	0.328376	-0.420695
C	4.613999	-0.560916	0.089929
C	4.700154	-1.900211	-0.640357
C	5.831298	-2.793848	-0.132238
C	5.900946	-4.132772	-0.864622
H	4.965997	-4.692494	-0.744647
H	6.063135	-3.983297	-1.938485
H	6.717021	-4.757068	-0.485447
H	5.696714	-2.968461	0.944411
H	6.787257	-2.262758	-0.241127
H	3.742927	-2.432422	-0.535861
H	4.836151	-1.720376	-1.717143
H	5.571351	-0.028420	-0.011925
H	4.475156	-0.742744	1.166061
H	3.622991	0.508805	-1.494605
H	2.525781	-0.207450	-0.318729
H	4.329893	2.219110	0.184700
H	3.329158	1.448393	1.407309
H	1.236465	1.465211	2.221659
O	-0.938876	0.120617	2.808009
H	-0.233222	0.342926	3.429621

Table S109. Coordinates for global minimum of **6bd**‡.

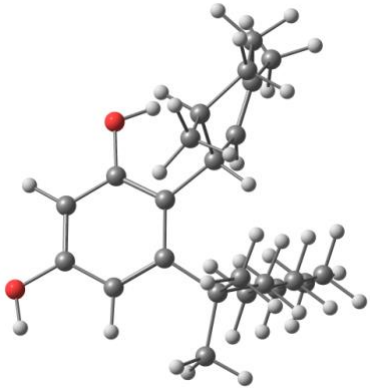


C	-2.605556	-0.707239	0.344528
C	-3.288800	-0.133983	1.442732
C	-4.444676	0.574537	1.281636
C	-5.232538	1.042916	2.451015

H	-4.804601	0.716302	3.400954
H	-5.281643	2.140440	2.437238
H	-6.270237	0.693307	2.375821
C	-5.016035	0.826623	-0.074205
C	-3.985004	0.703429	-1.191649
H	-3.337152	1.585196	-1.168293
H	-4.481707	0.698203	-2.167560
C	-3.122451	-0.555069	-1.046560
H	-2.268414	-0.491688	-1.736675
H	-5.844065	0.111146	-0.207747
H	-5.490732	1.815641	-0.091111
H	-2.926096	-0.343535	2.446534
H	-2.054213	-1.620742	0.543618
C	-0.096563	1.075304	-2.126389
C	-0.746719	1.961882	-1.268356
C	-0.952062	1.562497	0.040089
C	-0.566571	0.270186	0.487577
C	0.208708	-0.561593	-0.365919
C	0.382698	-0.171041	-1.679601
H	0.930484	-0.793385	-2.381829
H	-0.563647	0.103643	1.558202
O	-1.550838	2.343223	0.958064
H	-1.818835	3.186350	0.561900
H	-1.068102	2.935690	-1.626677
O	0.073894	1.480842	-3.398915
H	0.542922	0.803124	-3.908113
C	0.849574	-1.858119	0.131757
C	2.381137	-1.777978	-0.108986
H	2.815639	-2.724563	0.242190
H	2.566786	-1.737680	-1.190451
C	3.099522	-0.607913	0.561250
H	3.009662	-0.681279	1.653004
H	2.619827	0.337943	0.270076
C	4.580882	-0.553249	0.186872
H	5.061068	-1.503657	0.462841
H	4.674856	-0.465475	-0.905619
C	5.326100	0.602111	0.853020
H	5.235678	0.512774	1.945726
H	4.843265	1.552340	0.580334
C	0.299619	-3.049270	-0.680105
H	0.509459	-2.939248	-1.748375
H	0.772053	-3.975226	-0.334237
H	-0.783326	-3.154842	-0.553368
C	0.587607	-2.123554	1.620851
H	0.955194	-1.318006	2.262509
H	-0.476069	-2.272478	1.835684
H	1.108918	-3.041799	1.910091

C	6.805454	0.662281	0.473414
H	7.286136	-0.287743	0.745294
H	6.894019	0.751368	-0.618372
C	7.540848	1.820719	1.144931
H	7.094341	2.782189	0.865516
H	8.597601	1.845698	0.858656
H	7.490520	1.735531	2.236695
C	-3.892263	-1.847822	-1.399253
H	-4.748533	-1.992817	-0.732662
H	-4.258851	-1.780080	-2.428042
H	-3.243375	-2.725174	-1.318592

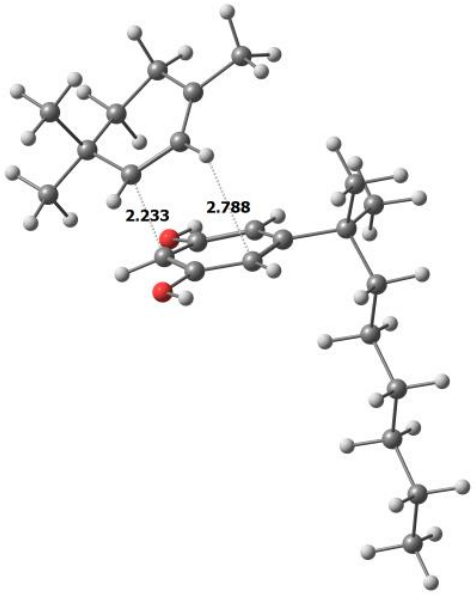
Table S110. Coordinates for global minimum of **6bd**.



C	1.196101	1.000270	-0.484036
C	0.162590	1.945206	0.099021
C	0.344218	3.259312	0.293831
C	-0.708786	4.126798	0.916542
H	-1.034081	4.902856	0.211734
H	-0.306600	4.650422	1.793804
H	-1.582757	3.546546	1.226004
C	1.627148	3.941088	-0.103690
C	2.478487	3.083007	-1.036584
H	3.475148	3.526922	-1.153105
H	2.019025	3.060048	-2.036054
C	2.606885	1.647502	-0.521741
C	3.589918	0.841001	-1.366561
H	3.323070	0.885034	-2.429005
H	3.606834	-0.211756	-1.064430
H	4.602886	1.244524	-1.260179
H	3.002964	1.695213	0.501556
H	2.190926	4.193862	0.808561
H	1.386259	4.903625	-0.576056
H	-0.789802	1.494873	0.384242
H	0.924901	0.826229	-1.527106
C	1.182689	-0.339431	0.244523
C	1.512483	-0.323482	1.617679

C	1.699214	-1.480539	2.365978
C	1.510250	-2.699579	1.739361
C	1.071249	-2.753154	0.418878
C	0.872155	-1.593425	-0.341695
C	0.236757	-1.754771	-1.745347
C	1.218749	-1.381181	-2.875306
H	1.488622	-0.324975	-2.884403
H	0.761204	-1.613665	-3.844274
H	2.142740	-1.963330	-2.786141
C	-0.171206	-3.215212	-2.029265
H	-0.678720	-3.247823	-2.998957
H	-0.857051	-3.619990	-1.280039
H	0.700525	-3.875190	-2.093711
C	-1.051930	-0.892520	-1.865808
C	-2.085239	-1.090261	-0.757251
C	-3.283568	-0.153165	-0.907357
C	-4.306227	-0.307545	0.216538
C	-5.497059	0.641407	0.086267
C	-6.511423	0.474441	1.216253
H	-6.047048	0.668488	2.190194
H	-7.356148	1.162435	1.103988
H	-6.909925	-0.546651	1.235653
H	-5.131525	1.677735	0.067679
H	-5.990632	0.471430	-0.880925
H	-4.670063	-1.345579	0.238438
H	-3.809544	-0.135279	1.183259
H	-2.926836	0.887911	-0.932265
H	-3.774136	-0.333682	-1.875470
H	-1.610831	-0.912517	0.218196
H	-2.440702	-2.129277	-0.745175
H	-1.510765	-1.129396	-2.836784
H	-0.799043	0.171762	-1.911039
H	0.867600	-3.731296	0.000606
O	1.724120	-3.832097	2.479608
H	1.528181	-4.607490	1.936960
H	1.968892	-1.417518	3.415406
O	1.675620	0.845704	2.315175
H	1.259557	1.575088	1.817405

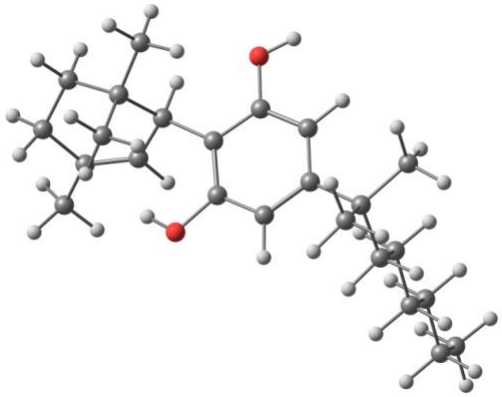
Table S111. Coordinates for global minimum of **3be**‡.



C	2.964789	0.773461	0.813546
C	2.744406	-0.625178	0.944522
C	3.372039	-1.537532	0.150448
C	3.223518	-2.999717	0.382108
H	2.716860	-3.456323	-0.479141
H	4.209667	-3.476467	0.443745
H	2.653821	-3.221359	1.286956
C	4.306249	-1.119663	-0.934309
C	4.213312	0.357572	-1.304631
H	3.345528	0.514777	-1.952680
H	5.098477	0.656532	-1.877759
C	4.075854	1.267021	-0.076466
H	5.320349	-1.377062	-0.586179
H	4.144880	-1.756286	-1.814266
H	2.100492	-0.976699	1.745917
H	2.793263	1.379703	1.702312
C	0.295146	1.169369	1.307362
C	1.007895	1.632991	0.165628
C	0.719084	1.000757	-1.068534
C	-0.004263	-0.180777	-1.112580
C	-0.595571	-0.688303	0.051777
C	-0.459863	0.015137	1.260586
H	-0.945816	-0.335531	2.166120
H	-0.149541	-0.668844	-2.070238
O	1.193604	1.605822	-2.176277
H	0.972650	1.083285	-2.962139
H	1.386266	2.649506	0.168890
O	0.470227	1.895891	2.429002
H	0.006600	1.480694	3.171729

C	-1.424985	-1.968478	0.037743
C	-2.862718	-1.656322	0.530433
H	-3.417010	-2.605281	0.532588
H	-2.818583	-1.325854	1.576546
C	-3.630214	-0.617534	-0.285916
H	-3.787526	-0.981409	-1.309829
H	-3.033979	0.302802	-0.369452
C	-4.985161	-0.280243	0.336763
H	-5.575547	-1.201790	0.447831
H	-4.828498	0.110660	1.353000
C	-5.782662	0.736239	-0.478614
H	-5.184355	1.650865	-0.605220
H	-5.954898	0.338022	-1.489486
C	-1.480976	-2.622993	-1.347594
H	-2.095272	-3.527209	-1.287578
H	-1.923274	-1.969435	-2.104845
H	-0.481924	-2.918439	-1.687024
C	-0.782621	-2.977949	1.011905
H	-0.752968	-2.595721	2.036602
H	-1.365465	-3.905622	1.011131
H	0.240204	-3.214099	0.701123
C	-7.125545	1.097246	0.155969
H	-6.951404	1.498138	1.164245
H	-7.720648	0.182637	0.286261
C	-7.915421	2.110715	-0.670419
H	-8.126780	1.718632	-1.672090
H	-8.872111	2.356538	-0.197535
H	-7.350579	3.042604	-0.790343
C	5.337681	1.166282	0.829345
H	5.505808	0.150586	1.197055
H	6.207193	1.477609	0.240335
H	5.246723	1.835171	1.691039
C	3.932338	2.732755	-0.496777
H	3.133452	2.866988	-1.229530
H	3.733485	3.371595	0.371085
H	4.868733	3.066613	-0.955451

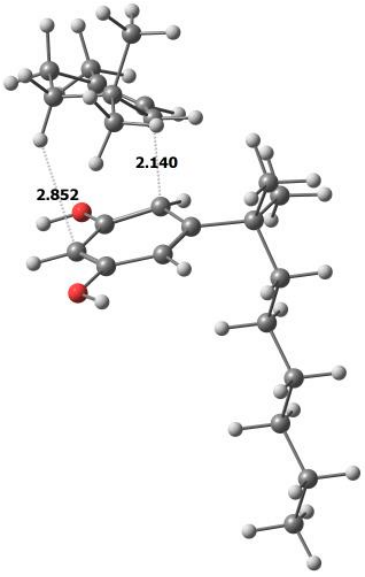
Table S112. Coordinates for global minimum of **3be**.



C	-2.698237	-0.311327	-0.680135
C	-2.713590	-1.753474	-0.214073
C	-3.788621	-2.400693	0.256585
C	-3.727329	-3.830418	0.704719
H	-2.710628	-4.230100	0.654660
H	-4.382413	-4.456758	0.085610
H	-4.089913	-3.925010	1.736831
C	-5.129754	-1.726769	0.343623
C	-5.179592	-0.426239	-0.455759
C	-3.960858	0.480521	-0.205865
C	-3.901806	0.872985	1.275532
H	-3.815291	0.008813	1.940086
H	-4.821613	1.405619	1.545164
H	-3.054805	1.538575	1.472035
C	-4.113988	1.758565	-1.035761
H	-3.255150	2.424110	-0.897673
H	-5.016954	2.299021	-0.727716
H	-4.196736	1.527960	-2.103400
H	-6.097091	0.127886	-0.218002
H	-5.218534	-0.666196	-1.527867
H	-5.380425	-1.553439	1.401373
H	-5.897105	-2.422924	-0.023087
H	-1.774038	-2.300394	-0.316968
H	-2.765269	-0.338329	-1.777343
C	-1.374258	0.366068	-0.365508
C	-0.698573	0.215063	0.860801
C	0.503471	0.865148	1.132110
C	1.107517	1.683757	0.177324
C	0.476988	1.823310	-1.057684
C	-0.731690	1.171499	-1.315841
O	-1.331718	1.298014	-2.542878
H	-0.785289	1.864818	-3.103253
H	0.911841	2.432339	-1.843963
C	2.427887	2.384179	0.507971
C	2.971758	3.198302	-0.673079

H	3.933666	3.640899	-0.392109
H	2.292143	4.015342	-0.939201
H	3.132078	2.584675	-1.564467
C	3.484210	1.339341	0.946480
C	3.802098	0.250019	-0.076153
C	4.784801	-0.787772	0.465719
C	5.123025	-1.880611	-0.547242
C	6.104925	-2.920542	-0.009202
C	6.434624	-4.006632	-1.031882
H	6.884150	-3.572300	-1.932486
H	7.138507	-4.741164	-0.626349
H	5.528818	-4.542878	-1.338154
H	7.029435	-2.415751	0.304234
H	5.683374	-3.380936	0.895249
H	4.196707	-2.384716	-0.860662
H	5.543894	-1.419606	-1.453198
H	5.711349	-0.284330	0.779726
H	4.362740	-1.249159	1.370820
H	4.222266	0.696963	-0.987151
H	2.871387	-0.253102	-0.374890
H	3.145188	0.864098	1.876571
H	4.406604	1.882852	1.198707
C	2.193495	3.355535	1.682146
H	3.125693	3.877994	1.928002
H	1.437959	4.103919	1.417863
H	1.852534	2.826567	2.577727
H	0.955918	0.700864	2.104901
O	-1.178553	-0.576976	1.867550
H	-1.933657	-1.098483	1.535143

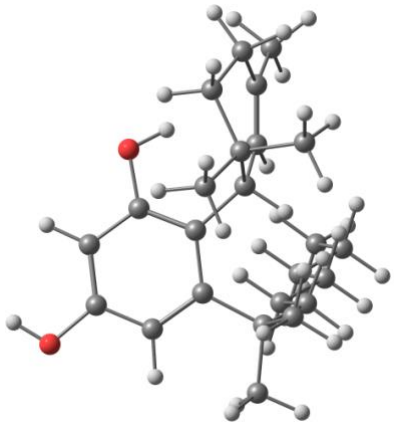
Table S113. Coordinates for global minimum of **6be**‡.



C	-2.362542	-0.102600	-1.006978
C	-2.734888	-1.441251	-1.346901
C	-3.797548	-2.073671	-0.786683
C	-4.192339	-3.445877	-1.210020
H	-3.572871	-3.821667	-2.027342
H	-4.109280	-4.131394	-0.355820
H	-5.246271	-3.464289	-1.515448
C	-4.667374	-1.406912	0.228882
C	-4.072390	-0.129746	0.817061
H	-3.351029	-0.387754	1.600556
H	-4.859198	0.464539	1.295945
C	-3.362511	0.733375	-0.234640
H	-5.631122	-1.200453	-0.264491
H	-4.907774	-2.126189	1.022839
H	-2.140451	-1.964113	-2.094153
H	-1.836518	0.455203	-1.777080
C	0.085238	0.947643	2.205084
C	-0.595675	-0.264161	2.325652
C	-0.809381	-1.001453	1.176686
C	-0.456242	-0.494538	-0.115978
C	0.352002	0.691167	-0.186115
C	0.564402	1.414383	0.965238
H	1.140239	2.335991	0.951556
H	-0.289494	-1.247490	-0.877280
O	-1.352045	-2.228533	1.186416
H	-1.603743	-2.484128	2.087833
H	-0.902323	-0.624985	3.303212
O	0.281616	1.641190	3.338407
H	0.773060	2.456769	3.157203
C	1.019895	1.126771	-1.492235
C	2.541195	1.317621	-1.240115
H	2.988423	1.616284	-2.198457
H	2.688523	2.164570	-0.557585
C	3.283839	0.100235	-0.690876
H	3.186782	-0.748057	-1.380914
H	2.827533	-0.214061	0.258684
C	4.768655	0.384783	-0.462496
H	5.231101	0.689077	-1.412961
H	4.874716	1.240007	0.221157
C	5.525223	-0.814303	0.107140
H	5.407026	-1.674364	-0.568524
H	5.070324	-1.108995	1.064517
C	0.438064	2.484006	-1.939846
H	0.967546	2.826679	-2.835621
H	-0.625894	2.402766	-2.186363
H	0.553064	3.243830	-1.160527
C	0.834889	0.116771	-2.634574

H	1.224605	-0.874342	-2.386206
H	-0.211929	0.007799	-2.935257
H	1.384015	0.478302	-3.509943
C	7.014282	-0.542522	0.319138
H	7.468307	-0.255831	-0.639606
H	7.131963	0.322062	0.987209
C	7.756525	-1.745206	0.899532
H	8.821274	-1.530970	1.039614
H	7.673046	-2.613548	0.235641
H	7.339834	-2.029022	1.872973
C	-4.366098	1.210440	-1.318984
H	-4.835778	0.377605	-1.848450
H	-5.146761	1.803817	-0.830081
H	-3.861594	1.846277	-2.054149
C	-2.763810	1.979479	0.416897
H	-2.158400	2.549285	-0.294955
H	-3.575558	2.624659	0.769321
H	-2.144011	1.722806	1.276290

Table S114. Coordinates for global minimum of **6be**.

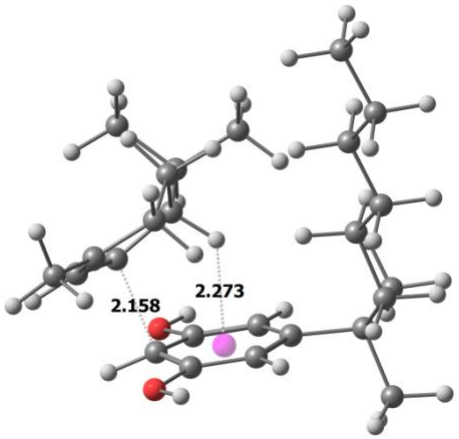


C	1.147386	0.765237	-0.525604
C	0.322496	1.899606	0.037886
C	0.781904	3.109271	0.391810
C	-0.132340	4.190983	0.888101
H	-1.178164	3.870827	0.890326
H	-0.042024	5.084730	0.256726
H	0.145128	4.497498	1.904756
C	2.241184	3.464081	0.298200
C	3.152885	2.245230	0.158063
H	3.293210	1.769498	1.133723
C	2.626133	1.207656	-0.850242
C	3.586081	0.015228	-0.864624
H	3.672198	-0.435261	0.129945
H	3.253753	-0.763070	-1.558484
H	4.583409	0.347072	-1.177790

C	2.612497	1.862788	-2.243899
H	2.400595	1.126739	-3.026937
H	3.588390	2.312164	-2.463220
H	1.852137	2.648929	-2.309661
H	4.148046	2.570114	-0.172625
H	2.526157	4.049463	1.183641
H	2.372795	4.147873	-0.554628
H	-0.745851	1.695918	0.133532
H	0.711097	0.560332	-1.501996
C	0.964945	-0.524860	0.280339
C	1.275962	-0.511844	1.655559
C	1.309857	-1.661994	2.440119
C	0.979665	-2.867381	1.848169
C	0.546638	-2.903633	0.525917
C	0.501374	-1.754294	-0.269876
C	-0.143984	-1.893184	-1.674753
C	0.881513	-1.686769	-2.807362
H	0.394926	-1.855922	-3.775433
H	1.704014	-2.404010	-2.709529
H	1.309498	-0.684594	-2.825478
C	-0.722258	-3.305204	-1.906199
H	-1.205599	-3.320922	-2.888440
H	-1.471086	-3.583450	-1.159440
H	0.060588	-4.070561	-1.914553
C	-1.327523	-0.897341	-1.848432
C	-2.353736	-0.878685	-0.715250
C	-3.439300	0.173367	-0.939011
C	-4.436047	0.262428	0.215373
C	-5.508197	1.330692	0.005343
C	-6.491767	1.418409	1.171111
H	-7.009232	0.463270	1.318874
H	-5.970860	1.661706	2.104581
H	-7.251382	2.188595	0.999946
H	-5.021122	2.304981	-0.141254
H	-6.054936	1.116561	-0.923679
H	-4.919808	-0.715300	0.358064
H	-3.890543	0.474892	1.147158
H	-2.963518	1.155933	-1.080695
H	-3.978693	-0.044792	-1.872728
H	-1.841839	-0.670272	0.234393
H	-2.822771	-1.865820	-0.605435
H	-1.832205	-1.157958	-2.790046
H	-0.960332	0.124869	-1.991068
H	0.225539	-3.863945	0.147337
O	1.009070	-4.055340	2.529158
H	1.312432	-3.898607	3.433347
H	1.577413	-1.588203	3.491139

O	1.577431	0.642472	2.326161
H	1.247761	1.398852	1.801901

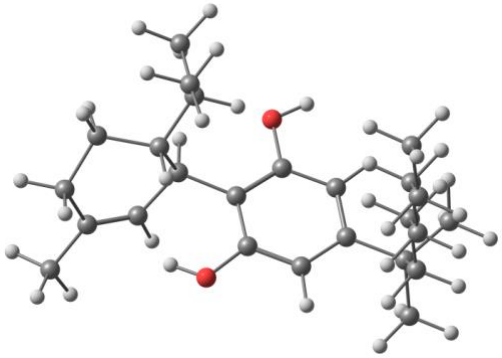
Table S115. Coordinates for global minimum of **3b**‡.



C	-2.233144	-1.232796	0.457264
C	-2.635368	-1.947490	-0.703288
C	-1.726934	-2.416477	-1.604063
C	-2.134361	-3.104247	-2.853826
H	-1.766193	-4.139122	-2.844523
H	-3.217033	-3.105646	-2.997143
H	-1.651934	-2.622749	-3.714903
C	-0.265248	-2.255887	-1.328398
C	0.015754	-2.305733	0.172690
H	1.083013	-2.151797	0.358531
H	-0.245676	-3.304898	0.541570
C	-0.797619	-1.238596	0.917523
H	-0.353271	-0.267790	0.646643
H	0.303935	-3.022972	-1.865549
H	0.059111	-1.285208	-1.742183
H	-3.698998	-2.053694	-0.904428
H	-2.984151	-1.120177	1.237578
C	-1.936232	1.016913	-1.220356
C	-2.757881	0.790016	-0.081053
C	-2.394042	1.457515	1.118804
C	-1.184802	2.122717	1.229946
C	-0.338168	2.241377	0.115372
C	-0.730352	1.685060	-1.112322
H	-0.109283	1.799311	-1.995724
H	-0.917934	2.567056	2.182887
O	-3.273630	1.340370	2.132851
H	-2.923070	1.762404	2.931770
H	-3.797447	0.516905	-0.233003
O	-2.393988	0.494734	-2.370847
H	-1.755843	0.642083	-3.086113
C	0.955467	3.046429	0.192260

C	2.094002	2.386927	-0.623552
H	1.848377	2.418085	-1.693004
H	2.978244	3.028082	-0.504832
C	2.453797	0.954481	-0.235917
H	1.580346	0.303190	-0.380814
H	2.708473	0.900434	0.830901
C	3.618634	0.403149	-1.058330
H	3.393969	0.518281	-2.129103
H	4.518802	1.004430	-0.864404
C	3.911780	-1.066315	-0.761598
H	4.087548	-1.194696	0.317130
H	3.020969	-1.666422	-1.001951
C	0.655196	4.427091	-0.436126
H	0.356244	4.327198	-1.484693
H	-0.147611	4.936496	0.107509
H	1.555192	5.050897	-0.390166
C	1.422823	3.265036	1.638653
H	2.399786	3.758701	1.626044
H	0.736544	3.914075	2.191423
H	1.524240	2.323761	2.187981
C	5.107864	-1.616079	-1.537704
H	6.001769	-1.028365	-1.287192
H	4.935722	-1.473147	-2.613659
C	5.366131	-3.094002	-1.250013
H	5.568577	-3.255381	-0.184793
H	4.494434	-3.702297	-1.518876
H	6.225254	-3.469878	-1.815510
C	-0.716668	-1.335001	2.460767
H	-1.355274	-0.527669	2.849166
C	0.706313	-1.081237	2.958156
C	-1.257884	-2.660458	3.004698
H	-2.258509	-2.885464	2.617536
H	-0.599475	-3.496650	2.746102
H	-1.323510	-2.619017	4.096856
H	1.386893	-1.881102	2.645095
H	0.725320	-1.041860	4.052486
H	1.097713	-0.131454	2.575901

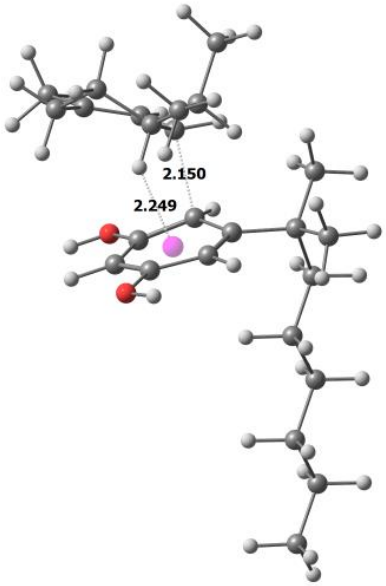
Table S116. Coordinates for global minimum of **3b**.



C	2.740348	0.293211	-0.534346
C	3.725059	0.946016	0.414569
C	4.622752	0.291057	1.164837
C	5.535395	1.000357	2.120266
H	6.583979	0.856483	1.829462
H	5.431463	0.582779	3.130429
H	5.327198	2.073141	2.162465
C	4.769017	-1.205195	1.080144
C	4.117905	-1.775000	-0.177585
H	4.119900	-2.870594	-0.136807
C	2.691408	-1.244684	-0.342429
H	2.158195	-1.435134	0.603395
C	1.888653	-1.953374	-1.454929
C	1.429578	-3.344801	-1.007617
H	0.811022	-3.814585	-1.780679
H	2.283809	-4.007067	-0.822795
H	0.837659	-3.288411	-0.087018
C	2.645161	-2.044522	-2.783584
H	3.483216	-2.747770	-2.712825
H	1.977481	-2.404461	-3.574228
H	3.040227	-1.073411	-3.098989
H	0.984362	-1.350824	-1.622528
H	4.716886	-1.484510	-1.051612
H	5.837764	-1.459099	1.110013
H	4.330532	-1.660984	1.982285
H	3.673385	2.034453	0.480520
H	3.086902	0.498873	-1.555794
C	1.361435	0.913387	-0.400768
C	0.622213	1.314924	-1.518092
C	-0.679244	1.813530	-1.415143
C	-1.293580	1.936688	-0.169609
C	-0.564333	1.569123	0.963192
C	0.729964	1.069695	0.846035
O	1.349375	0.716103	2.014936
H	2.303550	0.590986	1.844153
H	-0.985670	1.655124	1.959919

C	-2.721641	2.464498	-0.009766
C	-3.390053	2.765378	-1.357190
H	-3.430042	1.887729	-2.009497
H	-2.866005	3.565104	-1.892256
H	-4.418141	3.100464	-1.181247
C	-2.679773	3.775530	0.800209
H	-2.253052	3.617082	1.795642
H	-2.073931	4.528531	0.283599
H	-3.694181	4.173892	0.922416
C	-3.576987	1.436742	0.772992
C	-3.659402	0.039794	0.159948
C	-4.435638	-0.937143	1.043484
C	-4.520513	-2.343907	0.453690
C	-5.287744	-3.324674	1.340264
C	-5.363022	-4.728224	0.741609
H	-5.913878	-5.414775	1.393239
H	-5.866860	-4.711592	-0.231786
H	-4.359441	-5.142103	0.589225
H	-6.303079	-2.939722	1.509079
H	-4.807046	-3.369441	2.327380
H	-3.503753	-2.728527	0.284122
H	-5.000906	-2.297044	-0.534854
H	-5.451869	-0.550266	1.210795
H	-3.957789	-0.986803	2.033132
H	-4.136862	0.085611	-0.828092
H	-2.643422	-0.347905	-0.001189
H	-3.180205	1.350902	1.793537
H	-4.590195	1.852904	0.872587
H	-1.199085	2.091280	-2.326965
O	1.220938	1.183776	-2.745708
H	0.604572	1.479431	-3.428516

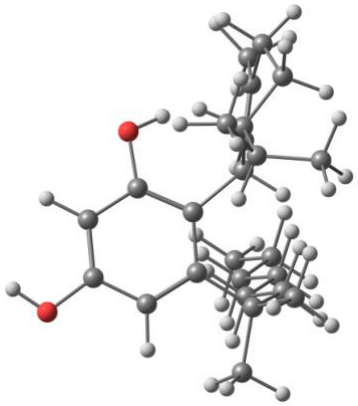
Table S117. Coordinates for global minimum of **6b**‡.



C	-2.212369	-0.065903	-0.972376
C	-2.670124	-1.287863	-1.547969
C	-3.498617	-2.132142	-0.878658
C	-3.939342	-3.430808	-1.448673
H	-3.714677	-4.240090	-0.740731
H	-5.030336	-3.435233	-1.574038
H	-3.463702	-3.648540	-2.407617
C	-4.013819	-1.743697	0.473061
C	-4.162339	-0.226369	0.589435
H	-4.503602	0.042147	1.593924
H	-4.930994	0.101402	-0.121260
C	-2.832775	0.481810	0.285134
H	-2.165241	0.242125	1.128080
H	-4.967504	-2.248158	0.666459
H	-3.309267	-2.116255	1.235567
H	-2.298397	-1.563384	-2.532562
H	-1.855630	0.672927	-1.681233
C	0.005408	-0.098653	2.181782
C	-0.298426	-1.376812	1.712972
C	-0.319906	-1.570822	0.344646
C	-0.143616	-0.483414	-0.563627
C	0.367819	0.757838	-0.055468
C	0.357308	0.954147	1.306930
H	0.681950	1.892539	1.744852
H	0.068568	-0.754129	-1.593916
O	-0.560260	-2.763130	-0.219100
H	-0.746116	-3.430798	0.459367
H	-0.494088	-2.186051	2.410609
O	-0.000954	0.072064	3.513170
H	0.239408	0.983268	3.739267

C	1.033456	1.746007	-1.007235
C	2.372925	1.089459	-1.464878
H	2.137877	0.251899	-2.136249
H	2.896621	1.839624	-2.074349
C	3.302424	0.591550	-0.360280
H	2.814095	-0.215651	0.203404
H	3.503256	1.394873	0.361686
C	4.630136	0.076237	-0.916478
H	4.432376	-0.726207	-1.642568
H	5.129786	0.881862	-1.474028
C	5.568570	-0.444850	0.170574
H	5.065787	-1.246395	0.731963
H	5.769116	0.359239	0.894190
C	1.316605	3.098044	-0.339778
H	2.014385	3.019961	0.498129
H	1.763203	3.770552	-1.078819
H	0.391241	3.560397	0.022652
C	0.202143	2.015444	-2.273974
H	-0.033883	1.099985	-2.826207
H	-0.727778	2.545716	-2.041513
H	0.786188	2.654547	-2.944468
C	6.894769	-0.970059	-0.378358
H	6.693340	-1.775202	-1.098662
H	7.393996	-0.169607	-0.941934
C	7.825433	-1.483347	0.718994
H	8.768419	-1.855286	0.304717
H	7.357274	-2.302406	1.277396
H	8.063627	-0.687075	1.433838
C	-2.920690	2.023825	0.236031
H	-1.910314	2.371984	-0.025198
C	-3.261142	2.607225	1.607758
C	-3.886507	2.538521	-0.834206
H	-4.927254	2.322905	-0.568842
H	-3.790923	3.624623	-0.935953
H	-3.688657	2.092534	-1.816154
H	-4.279556	2.341961	1.913309
H	-3.198631	3.700266	1.582844
H	-2.568603	2.243186	2.376335

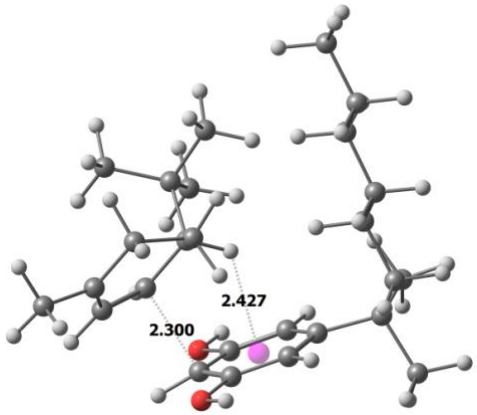
Table S118. Coordinates for global minimum of **6b**.



C	0.960751	0.835558	-0.272891
C	-0.063713	1.829883	0.239438
C	0.194891	3.095272	0.600782
C	-0.862864	3.997782	1.162905
H	-1.011475	4.867231	0.509700
H	-0.553435	4.391060	2.140248
H	-1.819119	3.480094	1.281066
C	1.576263	3.678072	0.460358
C	2.442510	2.864591	-0.497085
H	3.473912	3.237334	-0.478700
H	2.067080	3.007764	-1.519338
C	2.414295	1.374582	-0.143881
C	3.427807	0.533935	-0.955664
C	4.808275	0.557944	-0.292226
H	5.192542	1.583481	-0.223560
H	4.764948	0.144441	0.721676
H	5.531604	-0.028958	-0.869831
C	3.549319	0.965665	-2.422168
H	4.092543	0.206957	-2.996581
H	2.576759	1.115384	-2.902763
H	4.104830	1.906865	-2.506572
H	3.070358	-0.505713	-0.930524
H	2.711903	1.289824	0.909280
H	1.491569	4.717693	0.115096
H	2.046137	3.733123	1.455817
H	-1.080314	1.449494	0.349216
H	0.776822	0.695767	-1.340955
C	0.780845	-0.512686	0.431151
C	1.002773	-0.535931	1.826066
C	1.056198	-1.713020	2.567911
C	0.829229	-2.909755	1.911715
C	0.473735	-2.915616	0.566524
C	0.412134	-1.739099	-0.187928
C	-0.129990	-1.852002	-1.634612
C	-0.665365	-3.265465	-1.943722

H	-1.109429	-3.252578	-2.944723
H	0.136134	-4.011424	-1.951187
H	-1.435326	-3.592680	-1.239658
C	0.976474	-1.596186	-2.676046
H	1.359656	-0.577253	-2.649314
H	0.581355	-1.775889	-3.683116
H	1.819172	-2.277361	-2.512481
C	-1.306493	-0.864422	-1.867227
C	-2.462234	-0.964256	-0.871321
C	-3.525365	0.107592	-1.111312
C	-4.666824	0.058395	-0.097019
C	-5.712724	1.151442	-0.312312
C	-6.850363	1.089305	0.705654
H	-7.586407	1.882364	0.536067
H	-6.467294	1.199151	1.726998
H	-7.373511	0.127602	0.648524
H	-6.121219	1.065417	-1.328922
H	-5.222356	2.133609	-0.259114
H	-5.155156	-0.926305	-0.143573
H	-4.252497	0.149184	0.918360
H	-3.933190	-0.000640	-2.127310
H	-3.052609	1.100919	-1.074602
H	-2.933302	-1.954559	-0.927670
H	-2.072650	-0.862617	0.151602
H	-0.946239	0.169159	-1.870189
H	-1.686000	-1.047698	-2.882969
H	0.228986	-3.874959	0.131614
O	0.887473	-4.121121	2.548515
H	1.137057	-3.984822	3.472114
H	1.252799	-1.668288	3.636045
O	1.187742	0.607823	2.559495
H	0.839583	1.366619	2.053022

Table S119. Coordinates for global minimum of **3bf**‡.

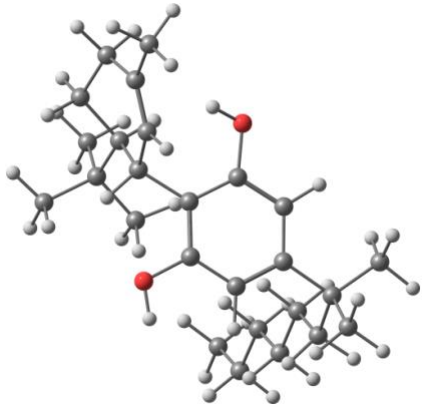


C	-2.406573	-0.542584	0.276276

C	-3.193423	-1.113970	-0.747079
C	-2.722813	-2.107220	-1.560046
C	-3.617383	-2.812973	-2.511400
H	-3.261747	-2.640010	-3.536606
H	-3.560143	-3.897424	-2.352129
H	-4.655429	-2.484368	-2.432463
C	-1.310881	-2.571661	-1.470376
C	-0.399891	-1.576956	-0.760895
H	-0.203528	-0.750347	-1.453830
H	0.569685	-2.033092	-0.552218
C	-0.998743	-0.961890	0.514220
H	-0.409453	-0.059908	0.738592
H	-1.320922	-3.555724	-0.976296
H	-0.938262	-2.774443	-2.483376
H	-4.238210	-0.819891	-0.817893
H	-2.953423	-0.137576	1.123610
C	-1.501584	1.641629	-1.412247
C	-2.414076	1.674545	-0.333634
C	-1.960235	2.210246	0.891459
C	-0.631718	2.559952	1.074719
C	0.275598	2.468174	0.006968
C	-0.174463	2.004089	-1.237956
H	0.500723	1.947931	-2.086477
H	-0.316887	2.925251	2.046214
O	-2.889479	2.300330	1.868982
H	-2.480290	2.613963	2.689062
H	-3.479137	1.597239	-0.523902
O	-2.003571	1.209608	-2.587898
H	-1.306001	1.182016	-3.260106
C	1.714798	2.960872	0.151731
C	2.720963	2.007573	-0.535101
H	2.495957	1.944476	-1.607462
H	3.708967	2.483766	-0.466499
C	2.803101	0.596573	0.042728
H	1.800359	0.147622	0.068929
H	3.154973	0.634020	1.082118
C	3.732768	-0.305536	-0.769404
H	3.358258	-0.372899	-1.801797
H	4.727658	0.159783	-0.831414
C	3.868115	-1.711406	-0.188034
H	4.242169	-1.645724	0.844518
H	2.873044	-2.175443	-0.123490
C	1.786941	4.330173	-0.562366
H	2.794571	4.747130	-0.453206
H	1.566918	4.231395	-1.630383
H	1.071305	5.034472	-0.124698
C	2.119828	3.158513	1.619171

H	1.955959	2.256563	2.217246
H	3.185090	3.407366	1.665754
H	1.568777	3.983612	2.081689
C	4.789612	-2.617786	-1.002968
H	5.789029	-2.164090	-1.055349
H	4.420173	-2.671013	-2.036629
C	4.892920	-4.026313	-0.420726
H	3.908691	-4.508540	-0.388884
H	5.558428	-4.660338	-1.015901
H	5.282629	-3.998399	0.603489
C	-0.911508	-1.796521	1.859439
C	-1.986087	-2.888189	1.958427
C	-1.073230	-0.823639	3.039052
H	-0.282644	-0.063996	3.025793
H	-2.041722	-0.311982	3.031385
H	-1.002276	-1.373276	3.983945
H	-1.849804	-3.446233	2.891565
H	-1.922117	-3.604277	1.133691
H	-2.997222	-2.466962	1.969869
C	0.475659	-2.441012	1.962689
H	0.598110	-2.869939	2.963570
H	0.608845	-3.250107	1.237282
H	1.270876	-1.702176	1.809523

Table S120. Coordinates for global minimum of **3bf.**

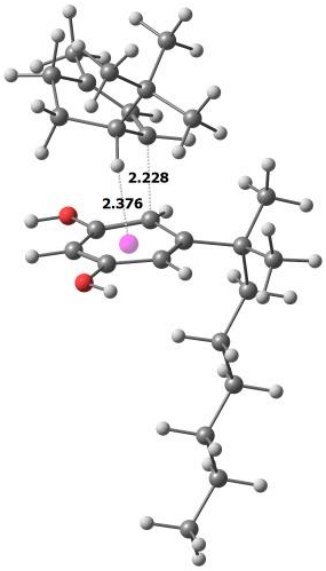


C	-2.560757	-0.070754	0.642854
C	-3.721697	0.875077	0.375888
C	-4.775616	0.626425	-0.411867
C	-5.825955	1.656780	-0.701882
H	-5.930248	1.802435	-1.785225
H	-5.589044	2.620552	-0.242383
H	-6.805482	1.323181	-0.335877
C	-4.960883	-0.732281	-1.027110
C	-4.109370	-1.780823	-0.319874
H	-4.212163	-2.738337	-0.837010
H	-4.501433	-1.920170	0.697015

C	-2.633750	-1.355607	-0.239677
H	-2.316279	-1.080548	-1.257578
C	-1.700909	-2.537355	0.183558
C	-1.761932	-3.631762	-0.900481
H	-1.496945	-3.220784	-1.882472
H	-1.045169	-4.426054	-0.663437
H	-2.748505	-4.096870	-0.978410
C	-2.121127	-3.149293	1.527861
H	-3.124080	-3.586234	1.480921
H	-1.423079	-3.947859	1.805587
H	-2.107475	-2.405458	2.332497
C	-0.229250	-2.102488	0.283592
H	0.090447	-1.552861	-0.609953
H	0.405537	-2.991369	0.382304
H	-0.048410	-1.471066	1.154784
H	-6.024194	-1.005095	-0.974522
H	-4.715771	-0.691774	-2.100746
H	-3.627603	1.858691	0.838823
H	-2.621034	-0.379192	1.693819
C	-1.282865	0.739325	0.485840
C	-0.388711	0.933052	1.547956
C	0.818195	1.605207	1.388518
C	1.180619	2.136027	0.145124
C	0.273668	2.023832	-0.904002
C	-0.942348	1.360061	-0.722500
O	-1.776984	1.325573	-1.809530
H	-2.679424	1.121459	-1.501239
H	0.475251	2.444066	-1.882612
C	2.546491	2.805536	-0.015452
C	2.632807	4.018100	0.931894
H	1.851372	4.748440	0.693516
H	2.515557	3.721189	1.978839
H	3.607225	4.509630	0.825015
C	2.786774	3.308391	-1.444543
H	3.787881	3.748964	-1.506532
H	2.725483	2.505753	-2.185471
H	2.061963	4.082364	-1.719599
C	3.659663	1.799203	0.373696
C	3.657157	0.481808	-0.400031
C	4.697981	-0.506630	0.125581
C	4.689895	-1.838441	-0.622833
C	5.715490	-2.837991	-0.089078
C	5.693084	-4.167151	-0.841910
H	6.434238	-4.867978	-0.443111
H	4.707680	-4.641947	-0.767501
H	5.910388	-4.017707	-1.905996
H	5.523907	-3.015043	0.978478

H	6.718702	-2.393862	-0.152949
H	3.684835	-2.282833	-0.560461
H	4.880843	-1.658254	-1.691153
H	4.512769	-0.690636	1.194364
H	5.699474	-0.056014	0.058671
H	2.660883	0.021223	-0.332330
H	3.843614	0.667009	-1.466473
H	4.628520	2.302560	0.239932
H	3.575002	1.577619	1.446315
H	1.485554	1.688729	2.242802
O	-0.732797	0.387795	2.760194
H	-0.022244	0.556905	3.393043

Table S121. Coordinates for global minimum of **6bf**‡.

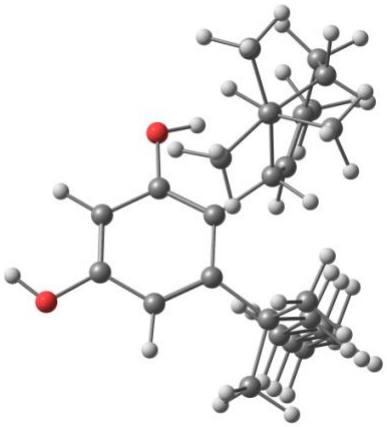


C	2.046697	0.119682	-0.766920
C	2.449484	1.249141	-1.531096
C	3.469368	2.065452	-1.147513
C	3.989625	3.129889	-2.047013
H	3.860416	4.110146	-1.568734
H	5.069776	3.005083	-2.197203
H	3.487581	3.137087	-3.016862
C	4.162207	1.874418	0.159966
C	3.352813	1.034894	1.140862
H	2.534787	1.658592	1.516429
H	3.957362	0.774860	2.012181
C	2.720277	-0.221347	0.520106
H	1.952477	-0.575195	1.225421
H	5.149353	1.432763	-0.047291
H	4.381272	2.858975	0.594512
H	1.988276	1.396396	-2.505637
H	1.669939	-0.714830	-1.345062

C	-0.333555	-0.191952	2.242115
C	-0.009280	1.132260	1.954899
C	0.072532	1.502664	0.623035
C	-0.110484	0.552941	-0.416870
C	-0.627014	-0.740822	-0.098096
C	-0.653704	-1.120263	1.225564
H	-0.984516	-2.109962	1.523433
H	-0.246147	0.947994	-1.418241
O	0.368592	2.753039	0.226822
H	0.541342	3.320891	0.993412
H	0.173062	1.839433	2.758901
O	-0.373162	-0.536667	3.541393
H	-0.623197	-1.467918	3.637075
C	-1.246851	-1.595981	-1.198502
C	-2.590165	-0.909308	-1.597011
H	-2.362224	0.009439	-2.155295
H	-3.089902	-1.587572	-2.303219
C	-3.545531	-0.568844	-0.454753
H	-3.088622	0.187627	0.198289
H	-3.720508	-1.453755	0.172315
C	-4.886870	-0.041943	-0.964887
H	-4.711866	0.827780	-1.615441
H	-5.365296	-0.807299	-1.593173
C	-5.837596	0.355018	0.163595
H	-5.356965	1.121394	0.789589
H	-6.009930	-0.513470	0.816607
C	-1.514863	-3.034225	-0.736469
H	-0.589174	-3.519142	-0.406151
H	-2.242718	-3.089006	0.077661
H	-1.916659	-3.608624	-1.577160
C	-0.377546	-1.668530	-2.467126
H	0.528450	-2.261173	-2.301910
H	-0.951608	-2.166646	-3.255564
H	-0.094461	-0.681643	-2.846878
C	-7.181406	0.883380	-0.336989
H	-7.007458	1.747623	-0.993147
H	-7.662235	0.115488	-0.958795
C	-8.118355	1.284021	0.801403
H	-7.668084	2.069675	1.419235
H	-8.330468	0.428407	1.453114
H	-9.073628	1.661374	0.421587
C	3.650118	-1.490435	0.326307
C	4.502763	-1.424270	-0.949247
C	2.755173	-2.737830	0.263323
H	2.183930	-2.855438	1.191570
H	2.041980	-2.698855	-0.566612
H	3.371779	-3.632642	0.123923

H	5.148890	-0.541546	-0.968283
H	3.885577	-1.417156	-1.854315
H	5.148849	-2.308137	-0.997608
C	4.577245	-1.632706	1.539970
H	4.013323	-1.603827	2.479754
H	5.094870	-2.596800	1.484564
H	5.339290	-0.847432	1.566018

Table S122. Coordinates for global minimum of **6bf**.



C	0.897045	0.784489	-0.261174
C	-0.233146	1.689299	0.214008
C	-0.126722	2.976701	0.568708
C	1.173914	3.709409	0.407236
C	2.136151	2.938350	-0.489045
H	1.753351	2.961294	-1.518862
H	3.106362	3.443495	-0.499687
C	2.287980	1.473212	-0.041186
H	2.494493	1.483933	1.036754
C	3.546085	0.806444	-0.686373
C	3.627558	1.060909	-2.199473
H	2.710974	0.764633	-2.718342
H	3.810208	2.117143	-2.421826
H	4.453510	0.482580	-2.629695
C	3.605279	-0.704847	-0.423990
H	4.568789	-1.095958	-0.772978
H	3.515414	-0.924656	0.646242
H	2.812575	-1.247860	-0.940326
C	4.802108	1.411923	-0.027719
H	5.702749	0.964465	-0.463967
H	4.811550	1.206564	1.049505
H	4.872151	2.494698	-0.169712
H	0.973493	4.705983	-0.011294
H	1.621986	3.887870	1.398159
C	-1.286251	3.751334	1.120766
H	-2.175441	3.124233	1.235325

H	-1.533576	4.595145	0.463768
H	-1.032558	4.180602	2.099042
H	-1.199437	1.199093	0.328701
H	0.791157	0.647620	-1.340283
C	0.697503	-0.576308	0.416541
C	0.892622	-0.634076	1.811601
C	0.938389	-1.829145	2.524638
C	0.714315	-3.007363	1.834781
C	0.349217	-2.973428	0.491894
C	0.293656	-1.777840	-0.231492
C	-0.277473	-1.849786	-1.673234
C	-0.861387	-3.242039	-1.990959
H	-1.616291	-3.561553	-1.267637
H	-1.336707	-3.198681	-2.976787
H	-0.081161	-4.008737	-2.037756
C	0.802154	-1.608832	-2.745953
H	1.622686	-2.326357	-2.637277
H	0.361629	-1.745426	-3.740695
H	1.222133	-0.603721	-2.710045
C	-1.425359	-0.822964	-1.868969
C	-2.590485	-0.928737	-0.884878
C	-3.625617	0.175996	-1.097928
C	-4.766405	0.135000	-0.082718
C	-5.786906	1.255480	-0.277983
C	-6.926928	1.200213	0.737696
H	-7.644180	2.013169	0.582574
H	-6.542799	1.281535	1.761275
H	-7.471869	0.252065	0.661376
H	-6.196065	1.197850	-1.296304
H	-5.273992	2.224981	-0.205874
H	-4.348751	0.199101	0.933364
H	-5.277174	-0.837340	-0.145585
H	-4.037300	0.099266	-2.115160
H	-3.128609	1.156586	-1.042152
H	-3.085460	-1.903976	-0.981235
H	-2.208834	-0.876628	0.144957
H	-1.033139	0.198416	-1.833934
H	-1.806599	-0.958336	-2.891647
H	0.089463	-3.918668	0.035179
O	0.771725	-4.236920	2.436089
H	1.028334	-4.127992	3.361325
H	1.126156	-1.812614	3.595147
O	1.063146	0.493763	2.575163
H	0.697192	1.256683	2.090889

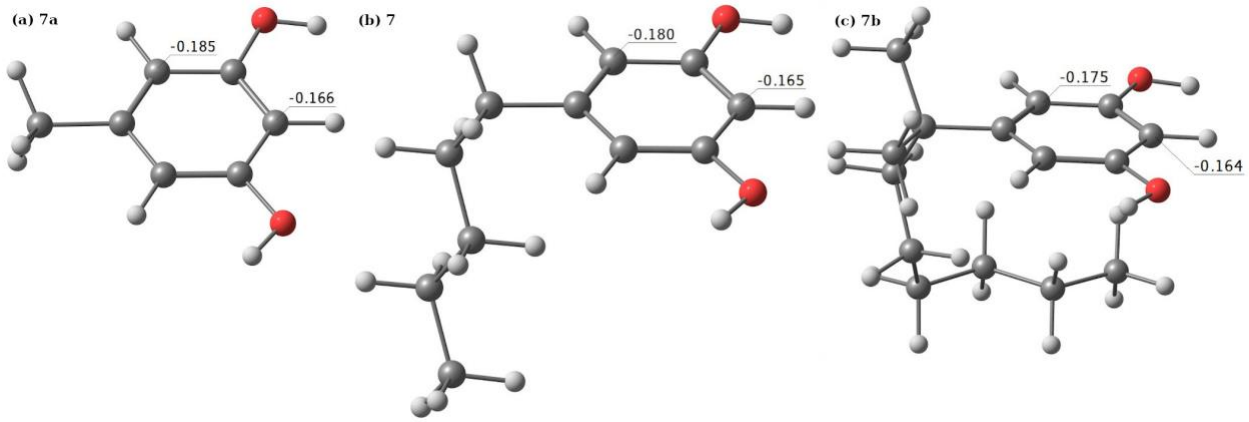


Figure S1. Relevant Löwdin partial charges for **7-7b**.

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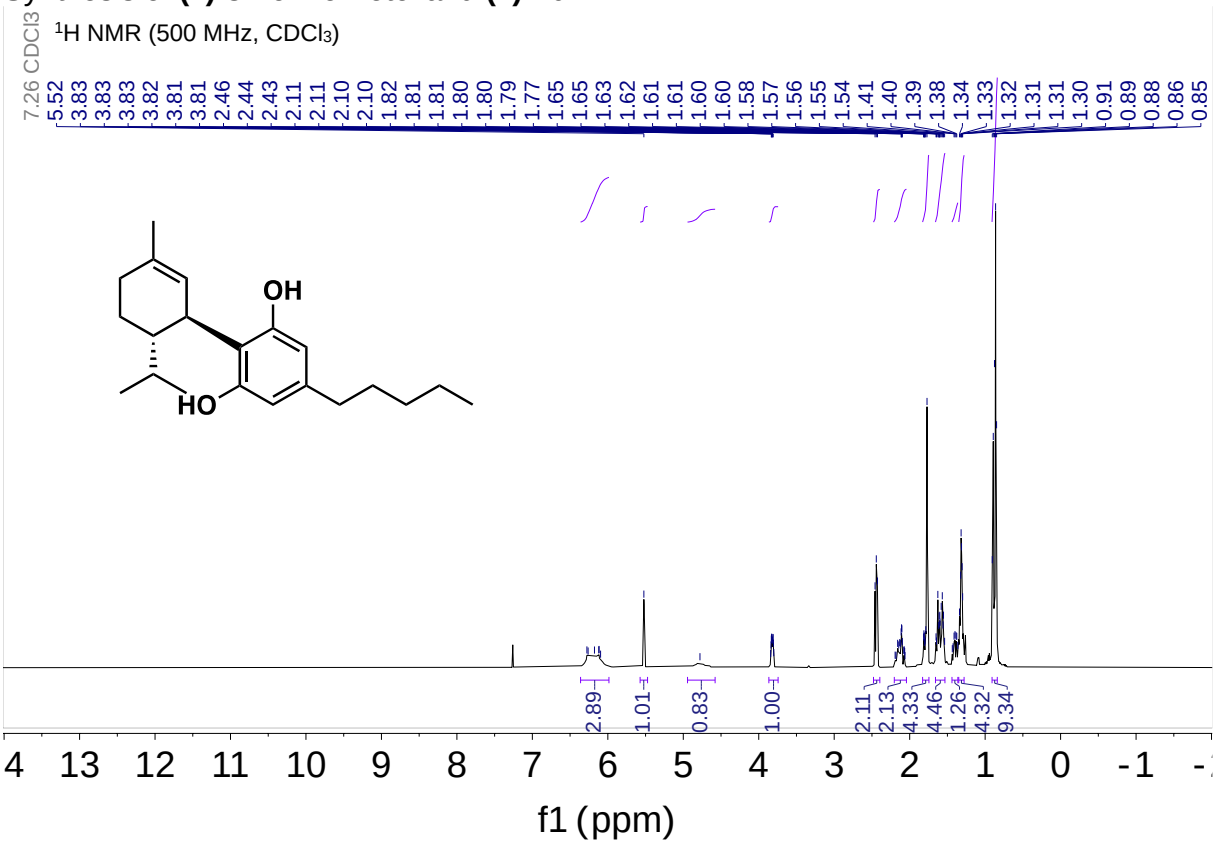
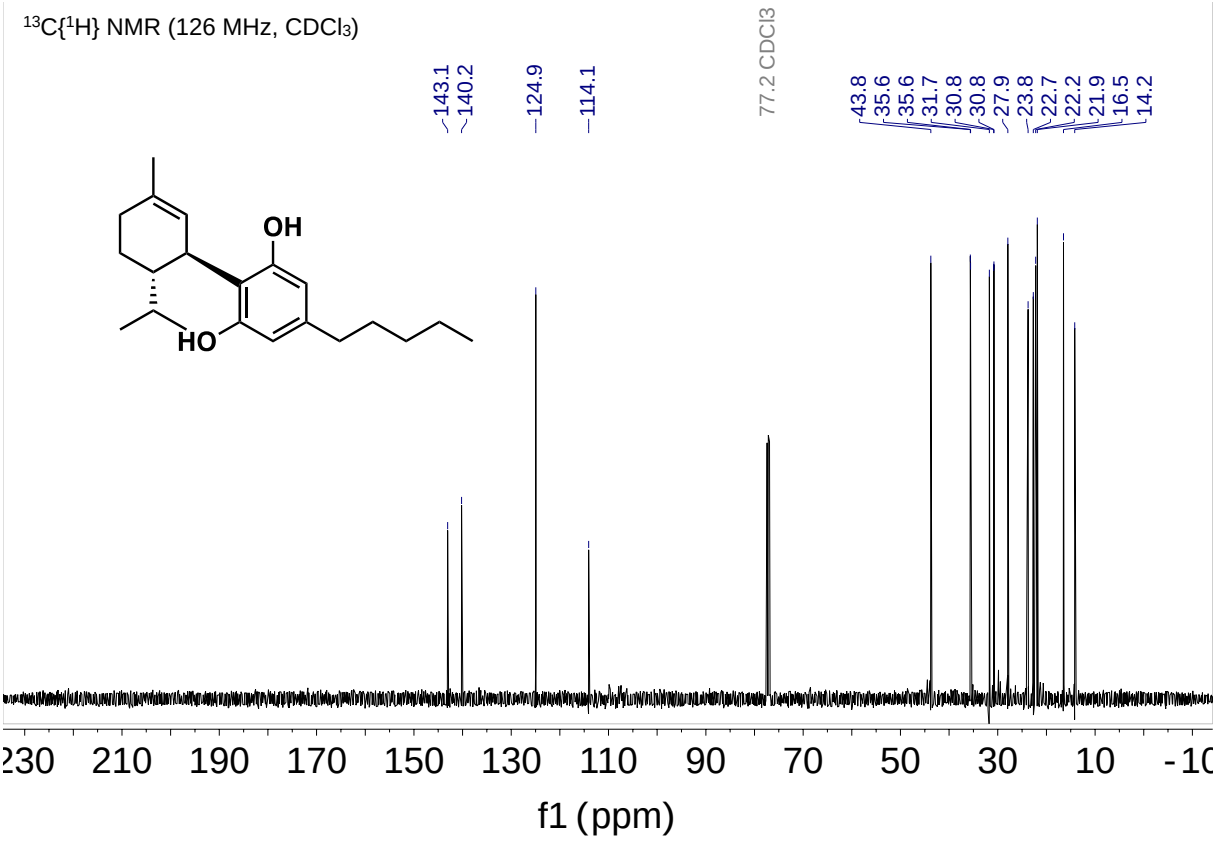
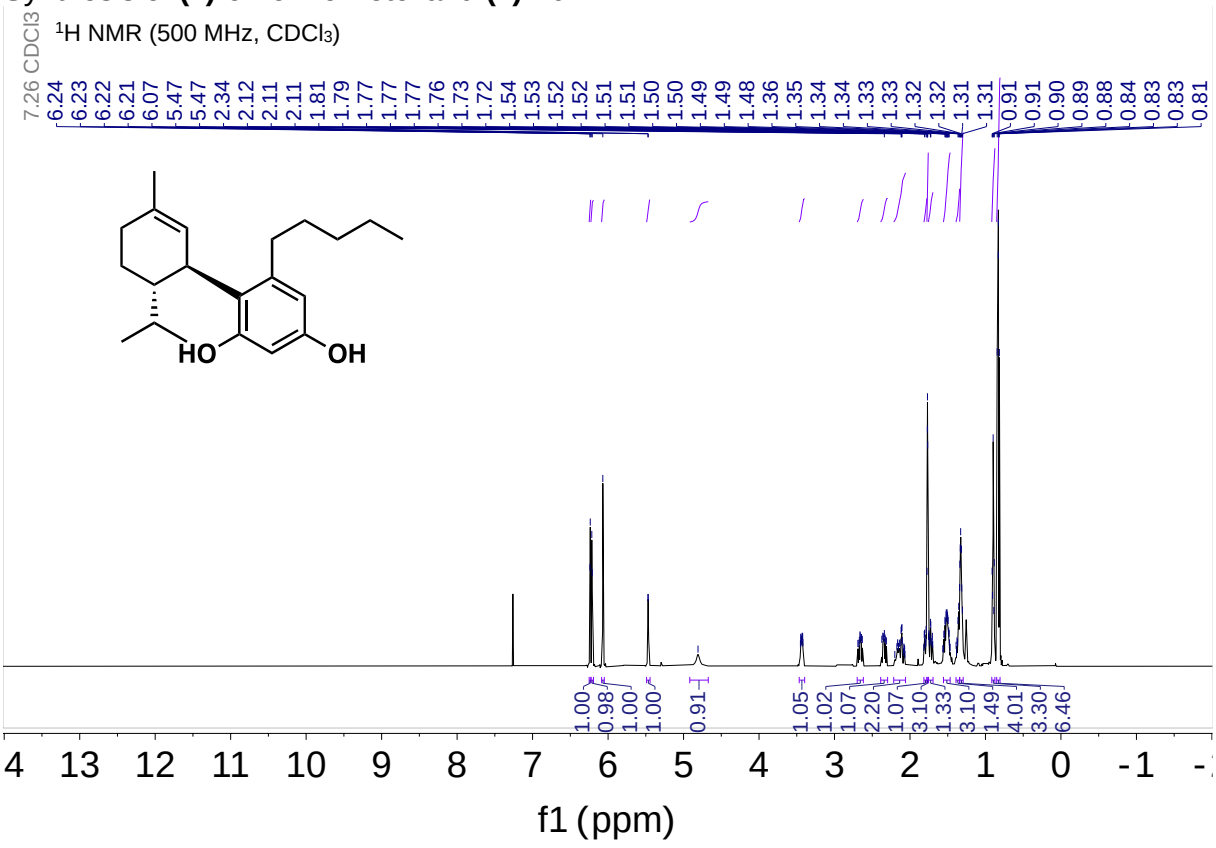
^{1}H and ^{13}C NMR Spectra of Reported Compounds:

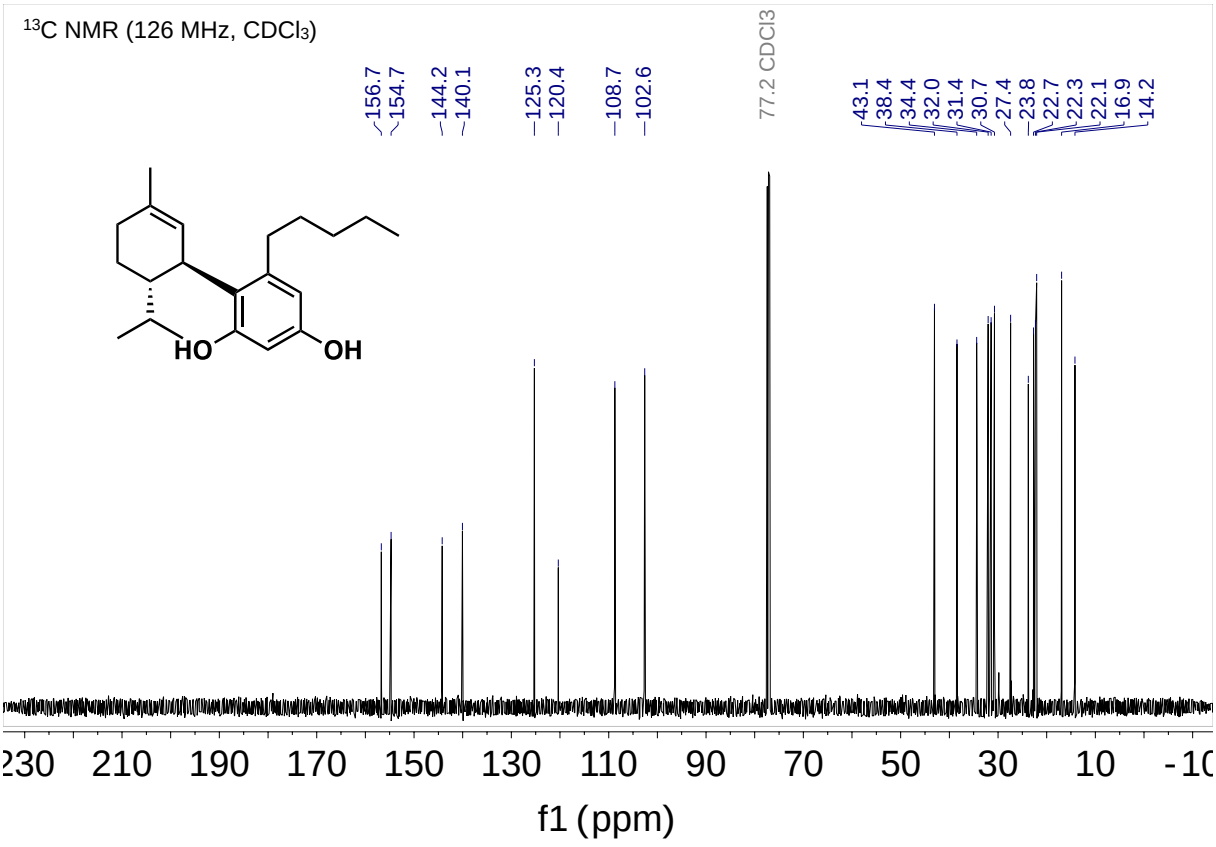
Synthesis of **(±)-3** from olivetol and **(±)-10**:



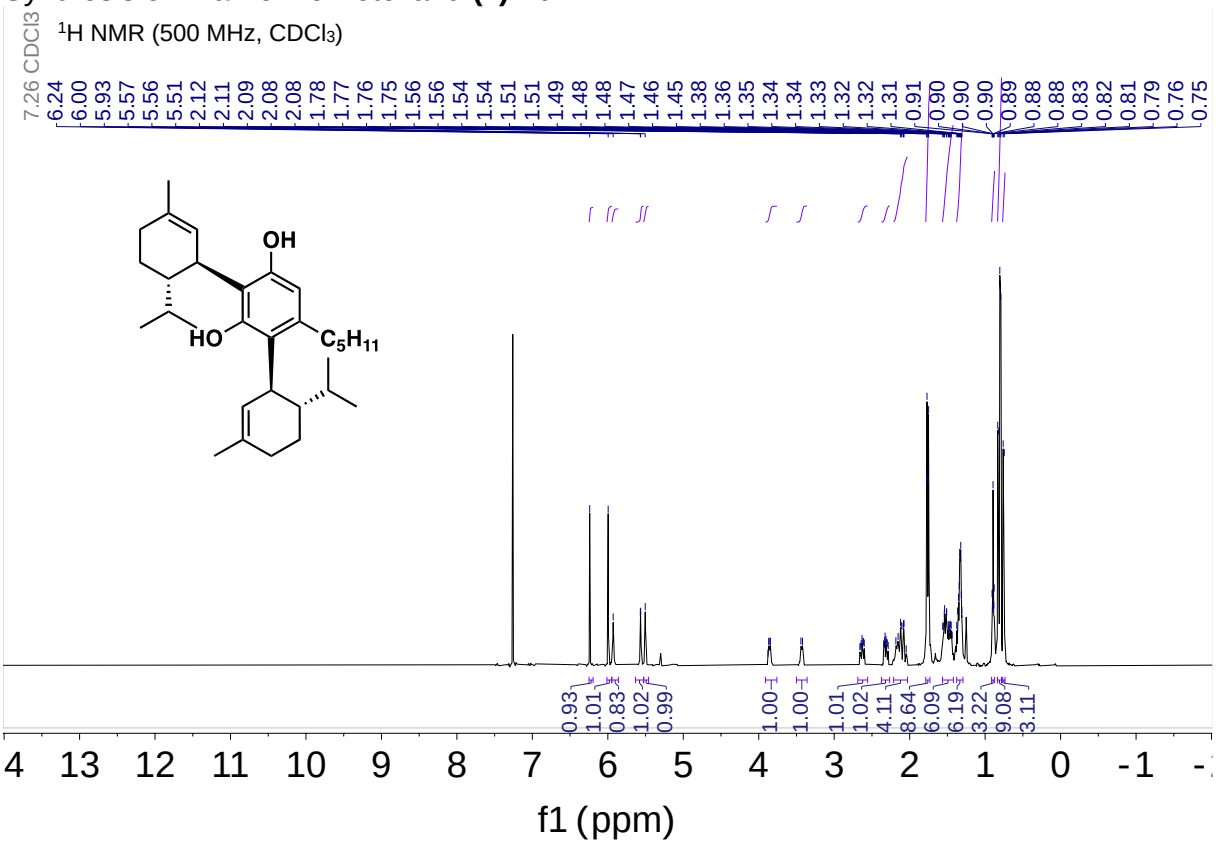


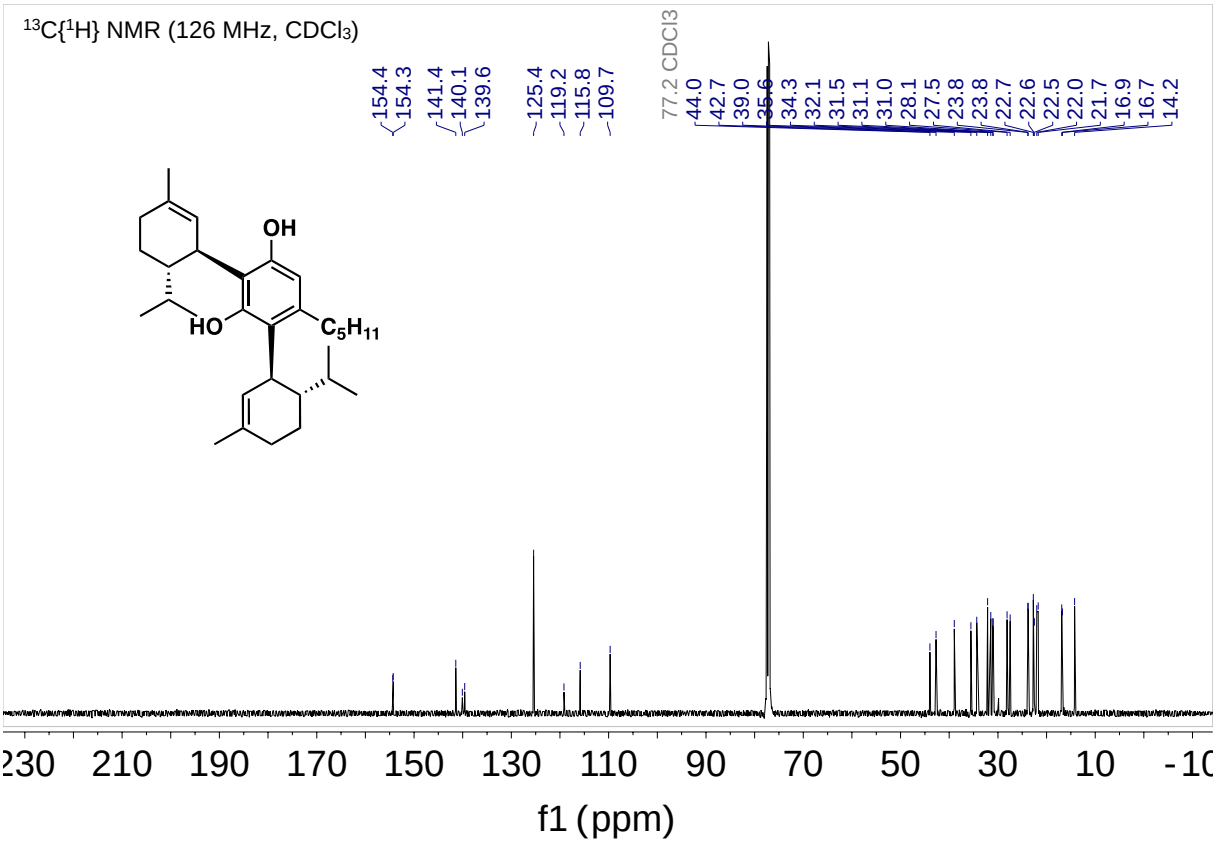
Synthesis of **(±)-6** from olivetol and **(±)-10**:



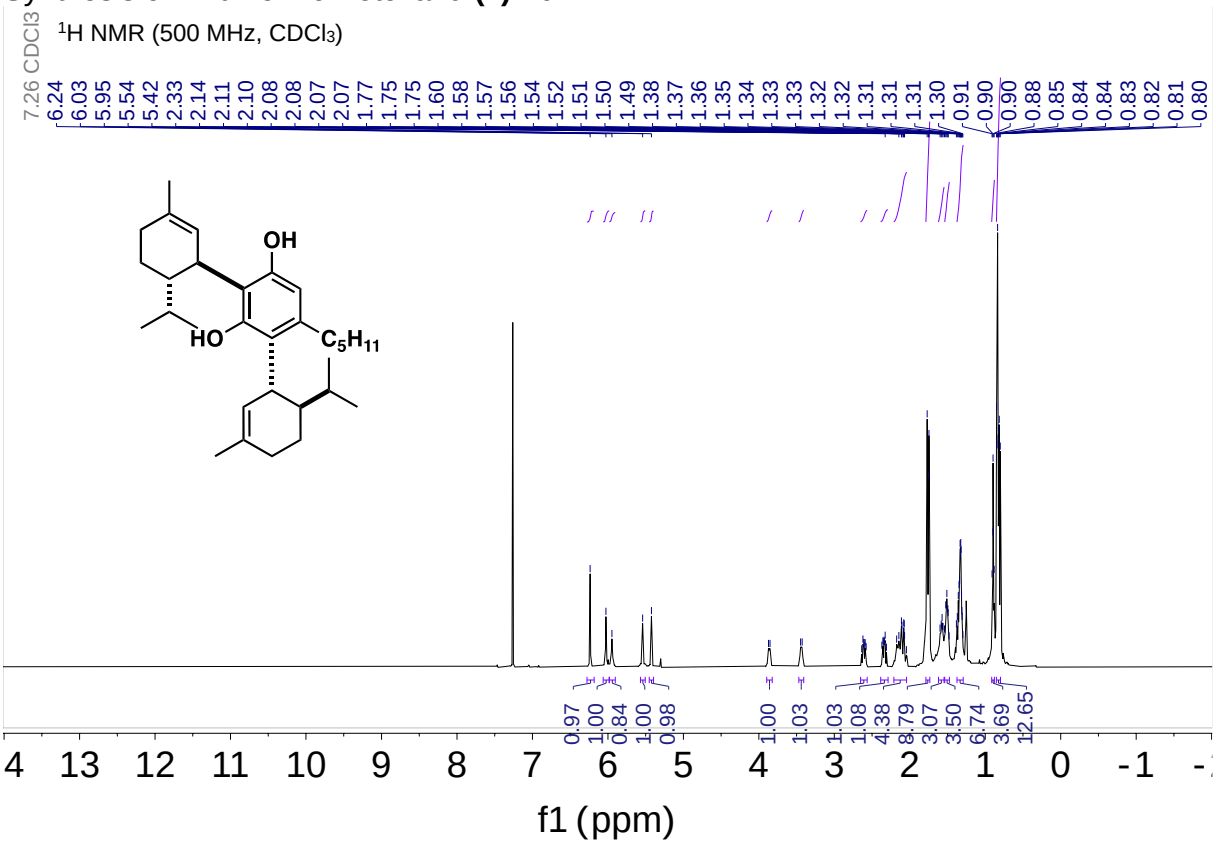


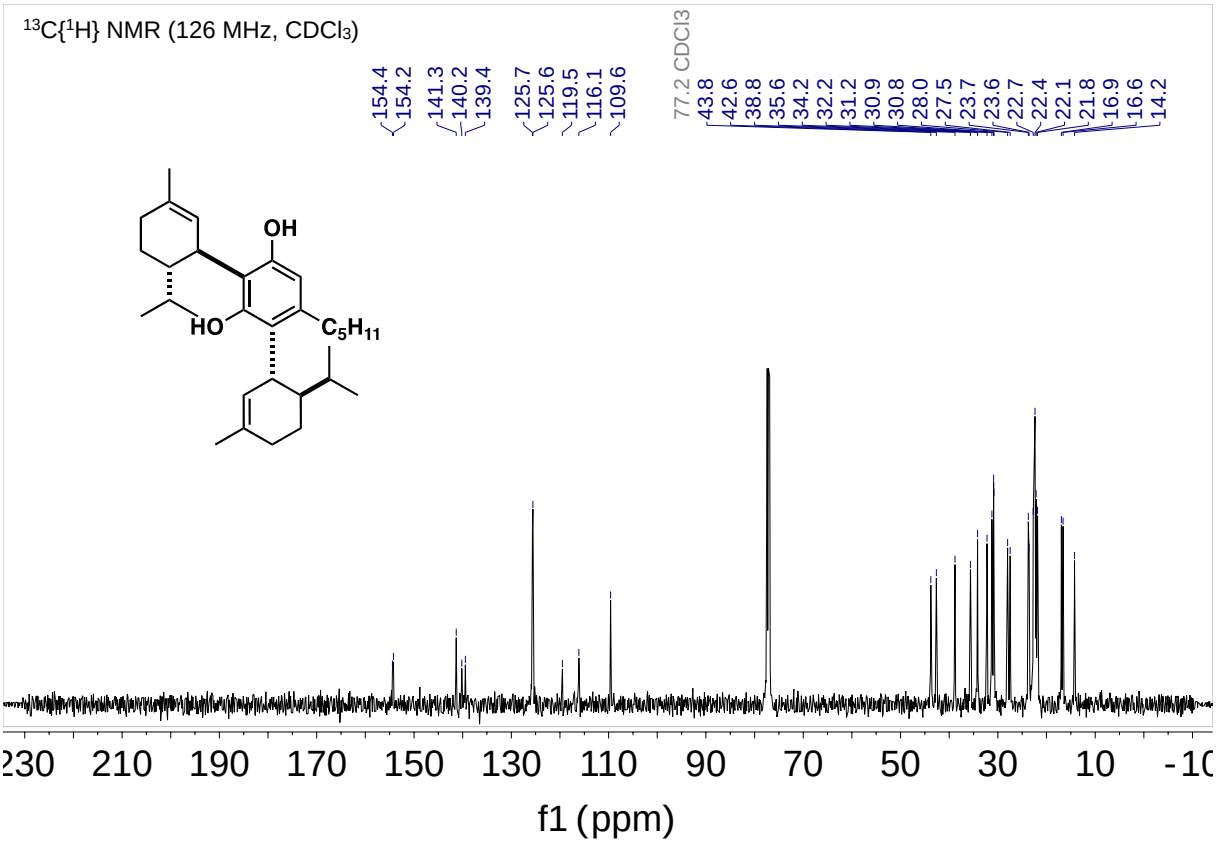
Synthesis of **11a** from olivetol and **(±)-10**:



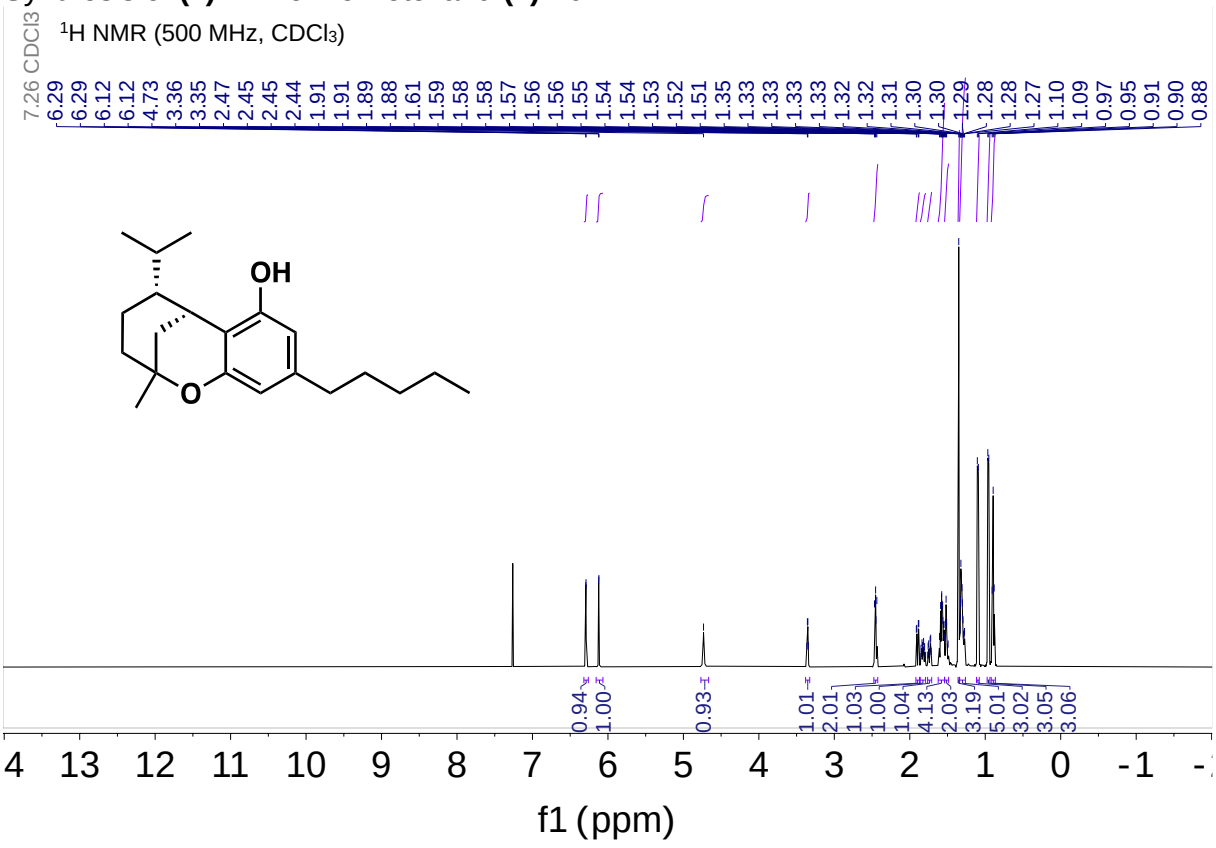


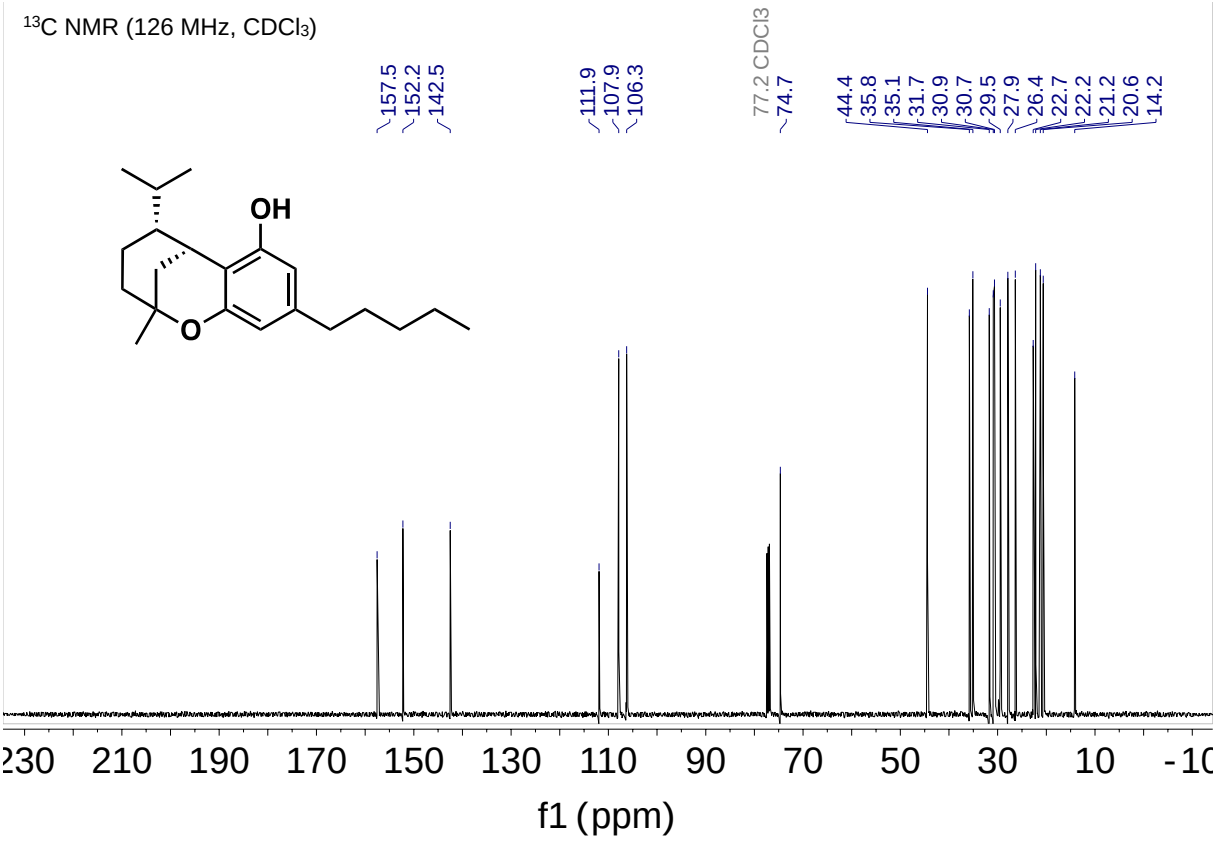
Synthesis of **11b** from olivetol and **(±)-10**:



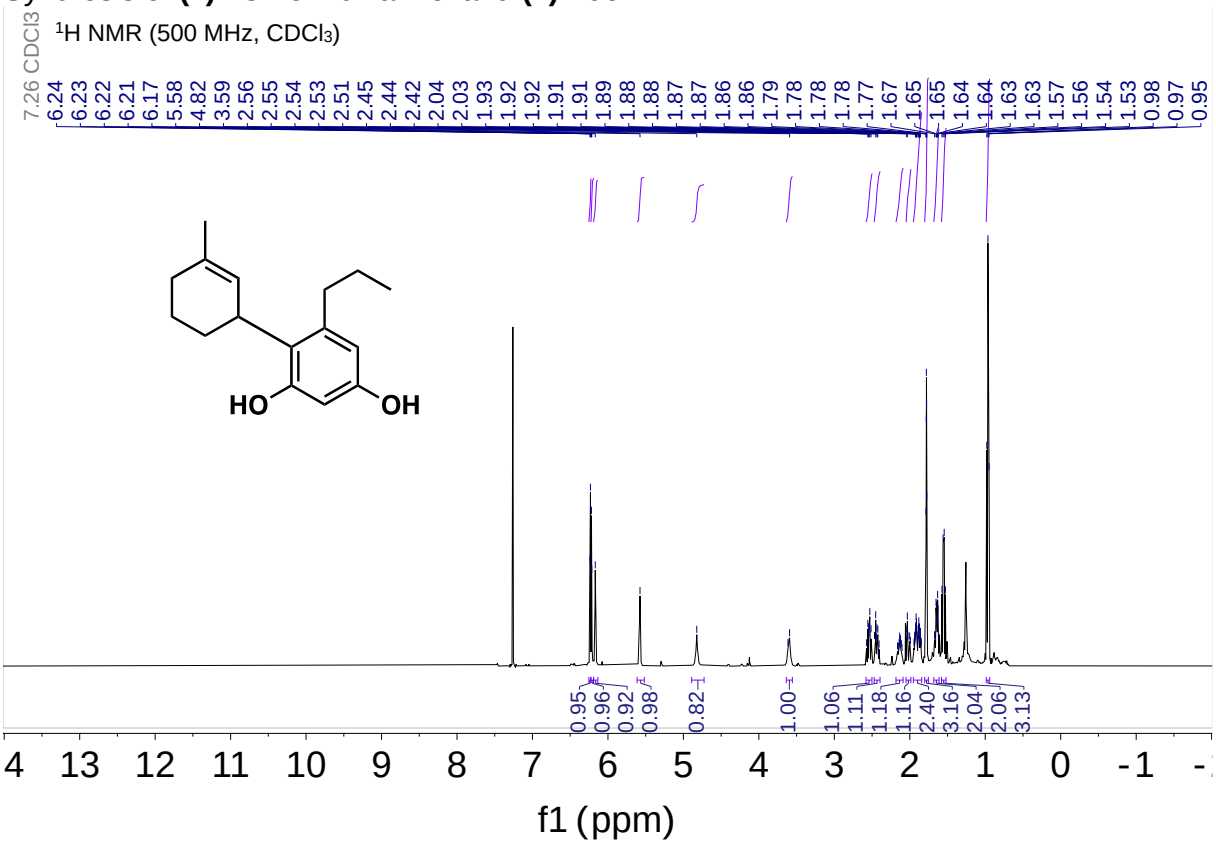


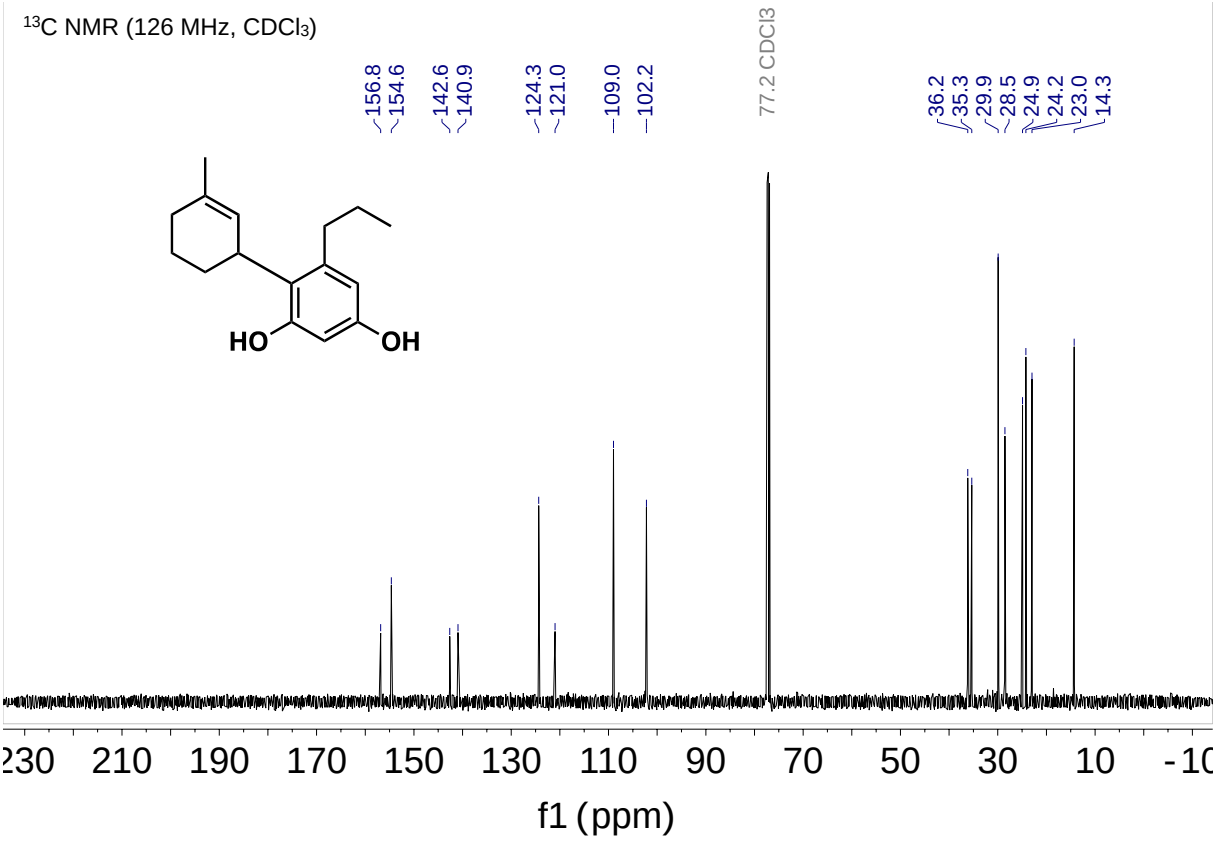
Synthesis of **(±)-12** from olivetol and **(±)-10**:



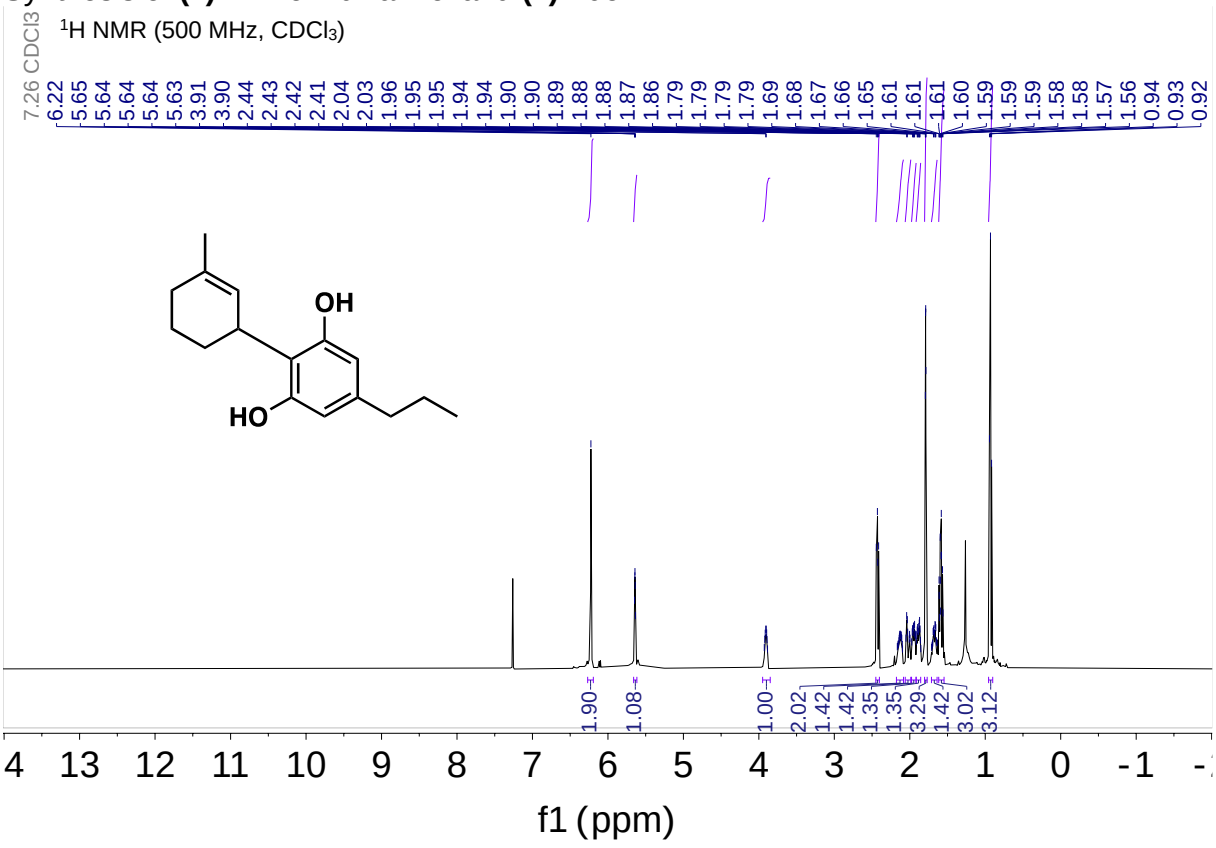


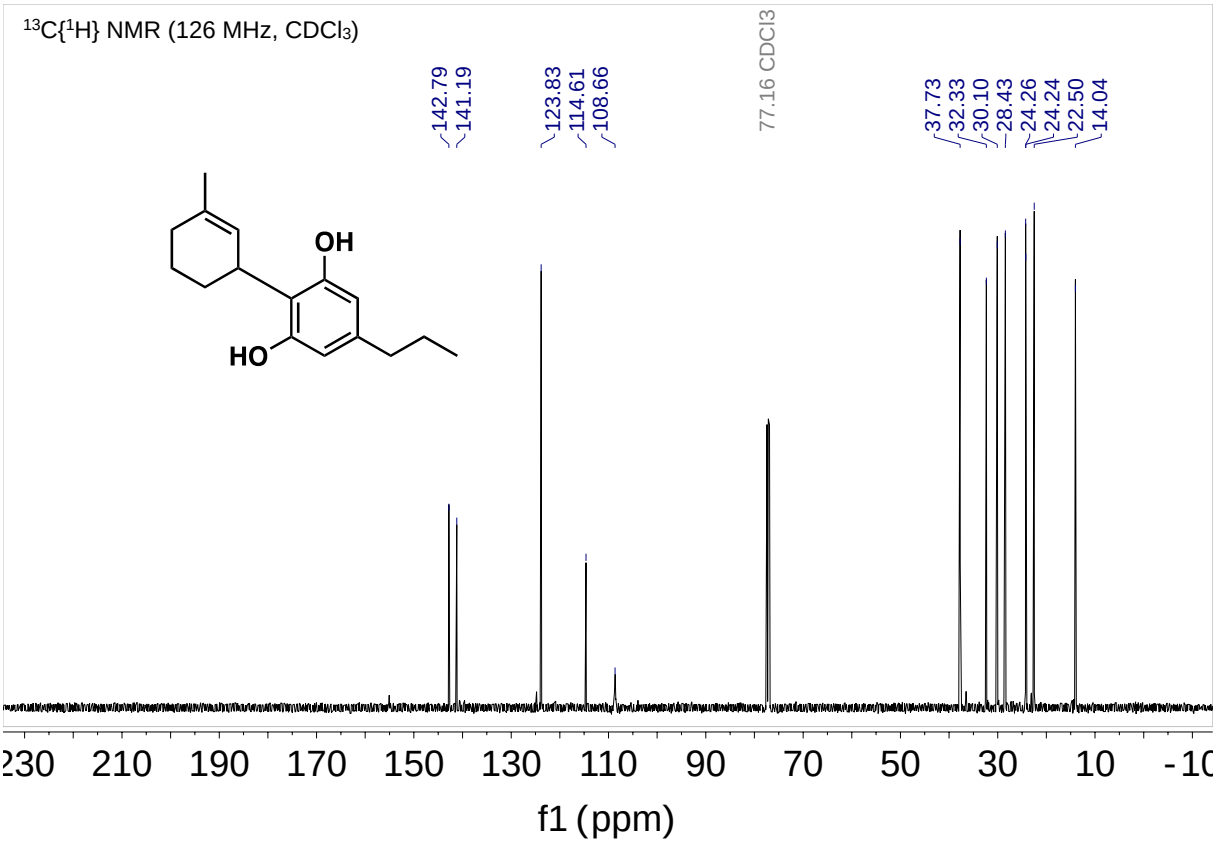
Synthesis of **(±)-13** from divarinol and **(±)-10c**:



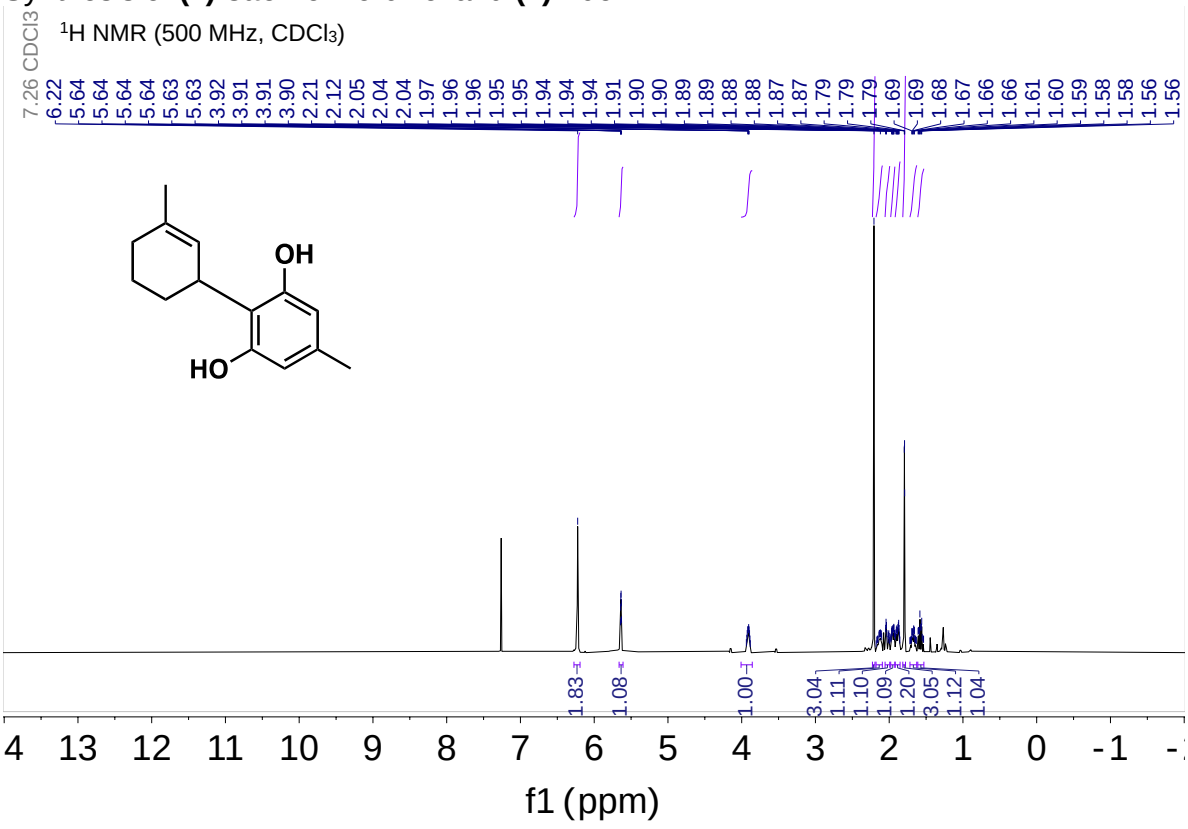


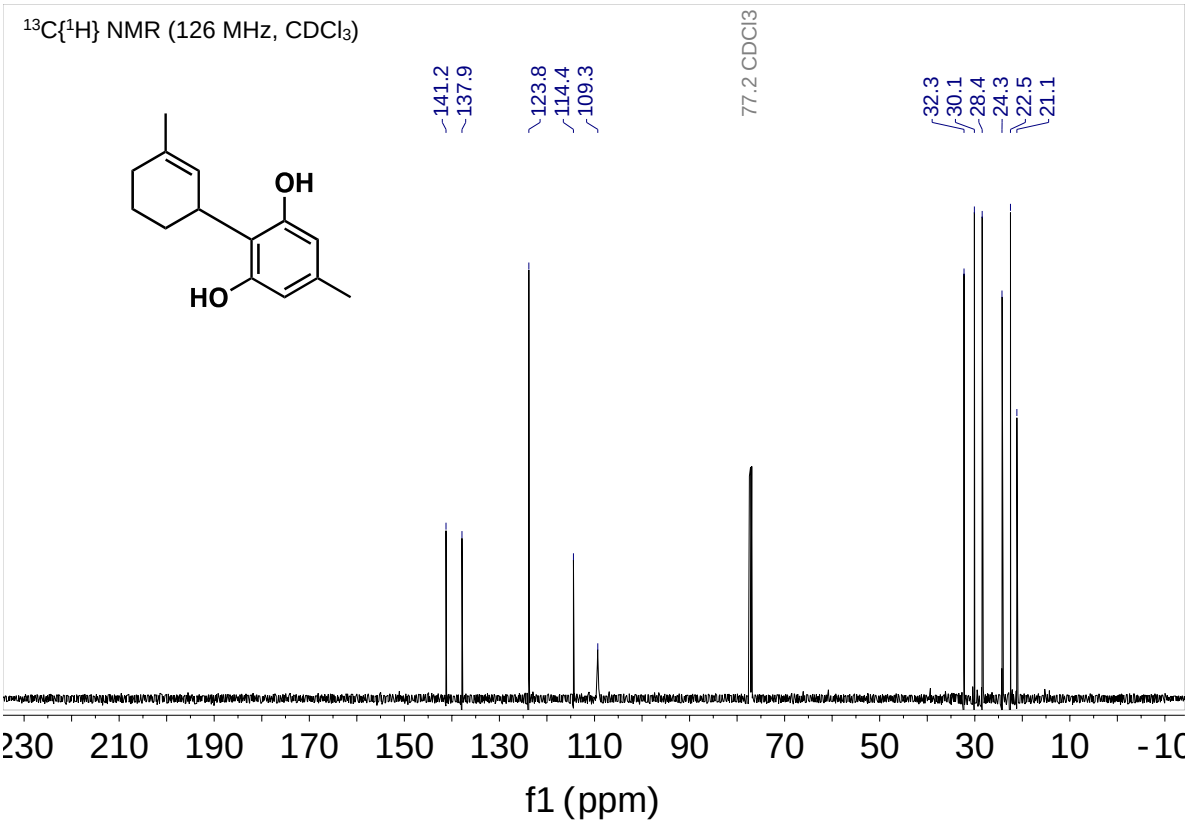
Synthesis of **(±)-14** from divarinol and **(±)-10c**:



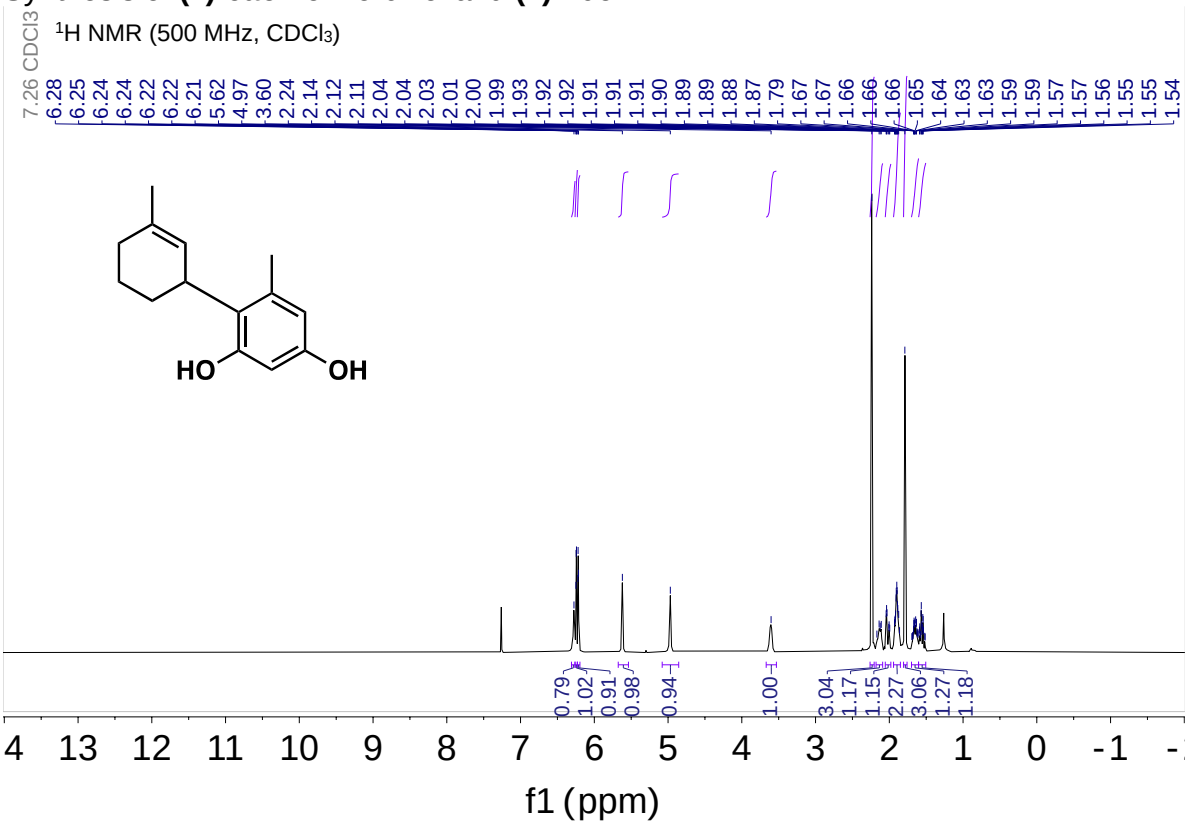


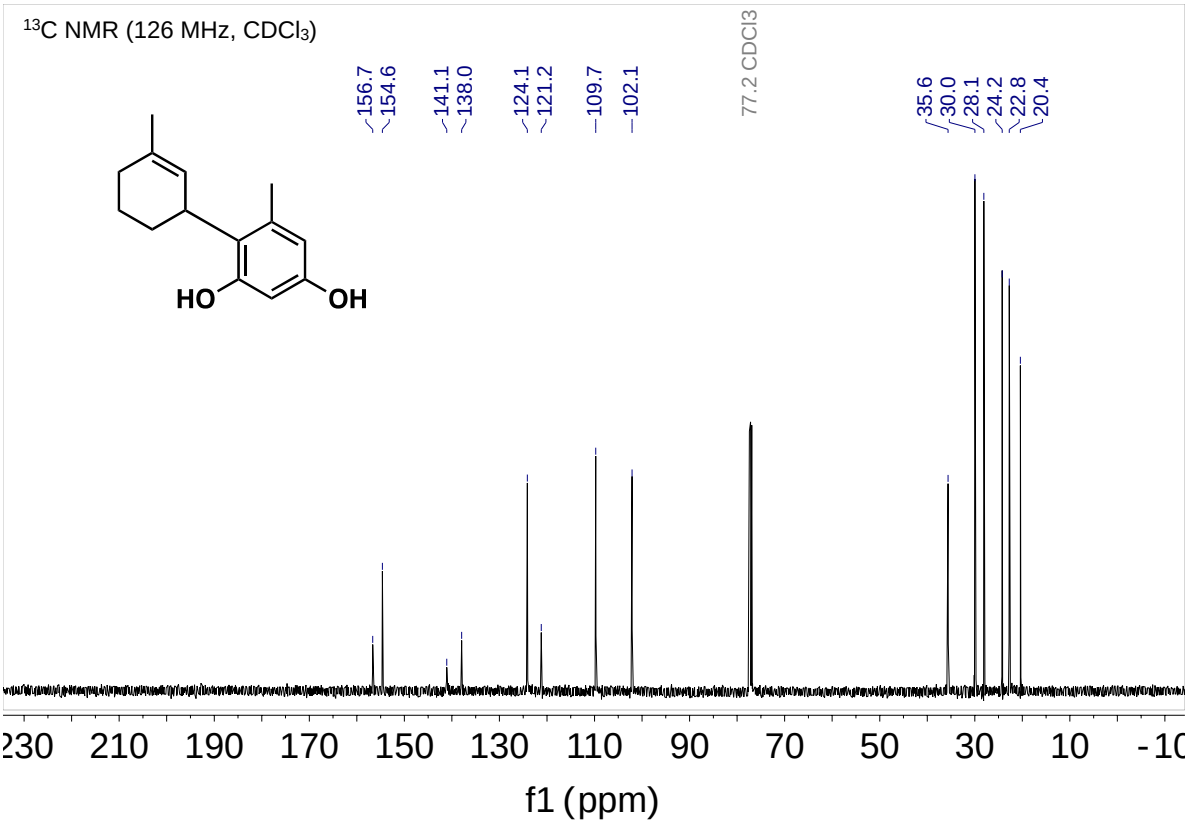
Synthesis of **(±)-3ac** from orcinol and **(±)-10c**:



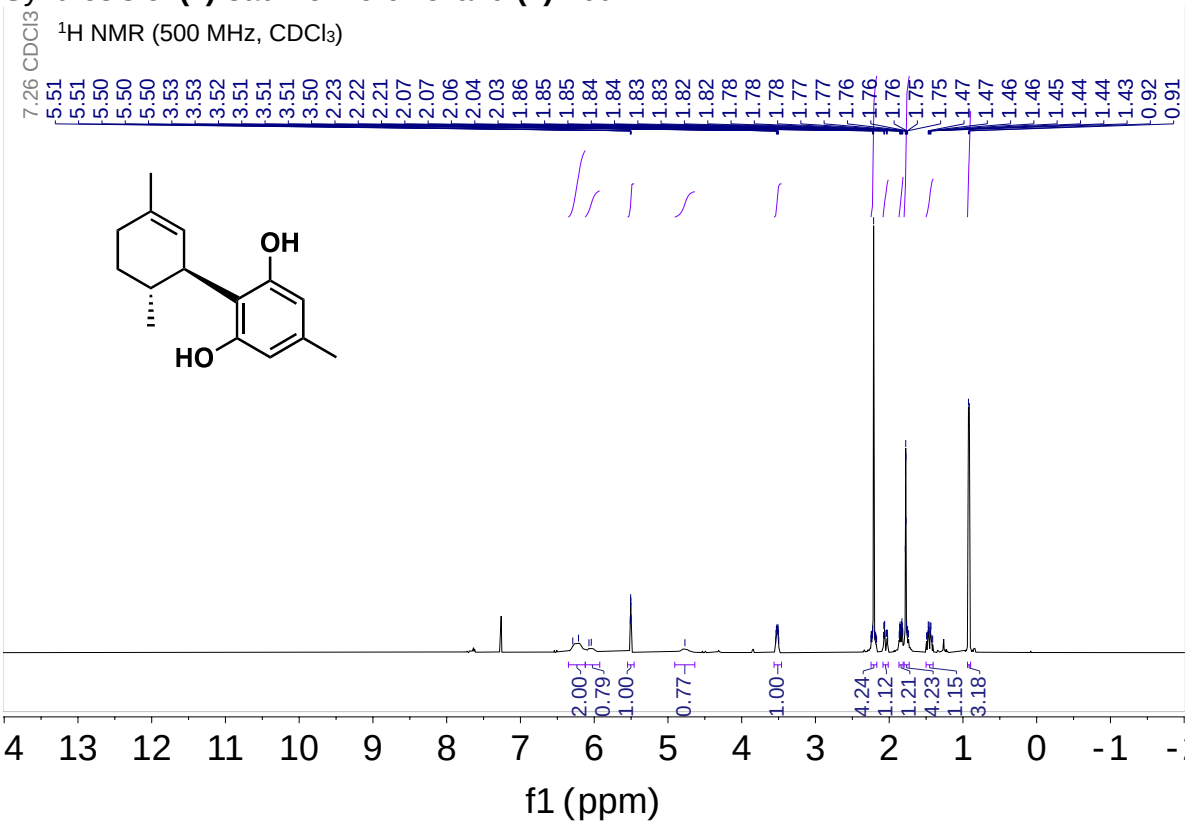


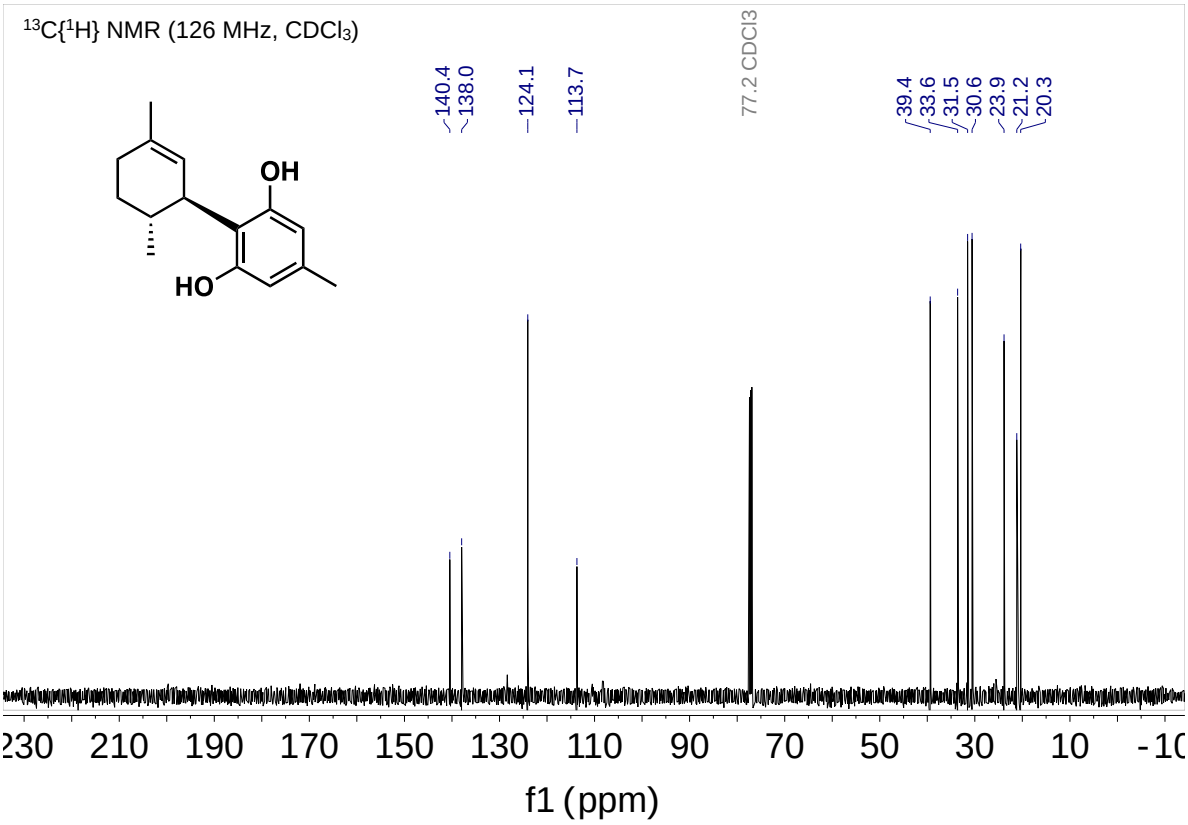
Synthesis of **(±)-6ac** from orcinol and **(±)-10c**:



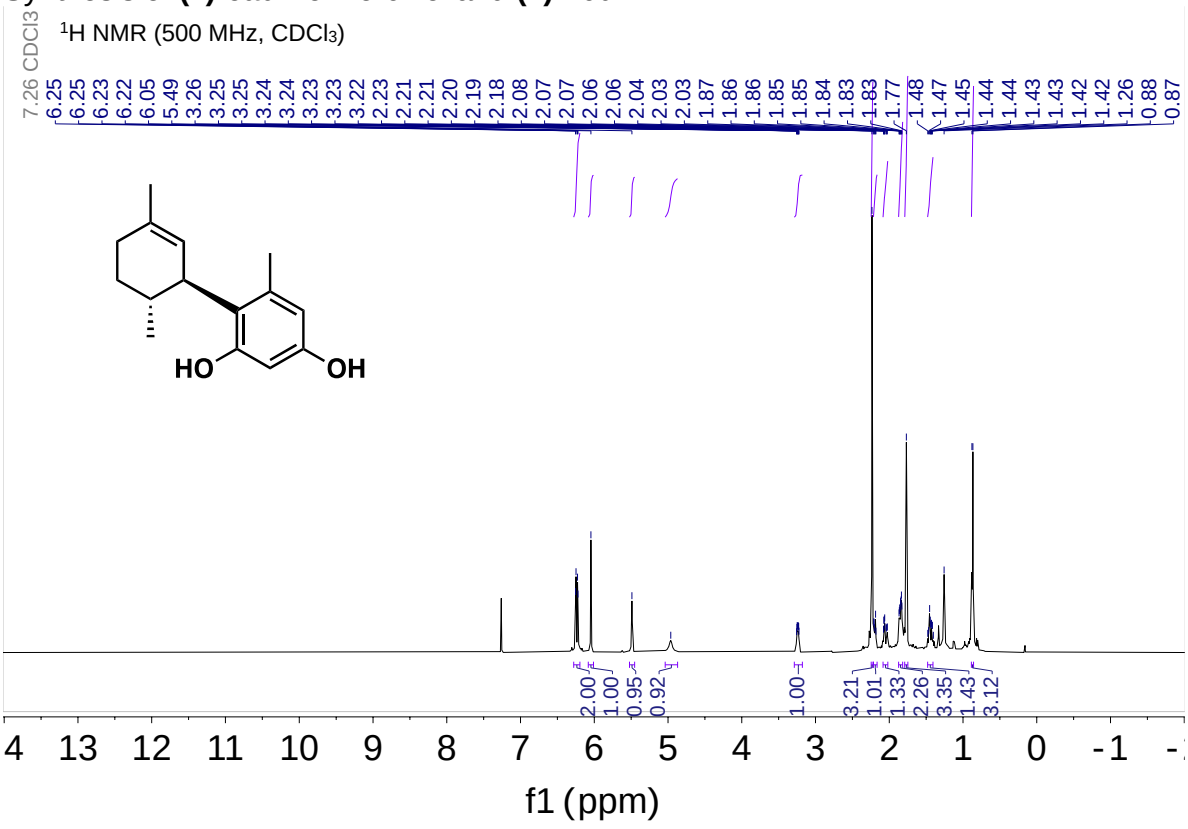


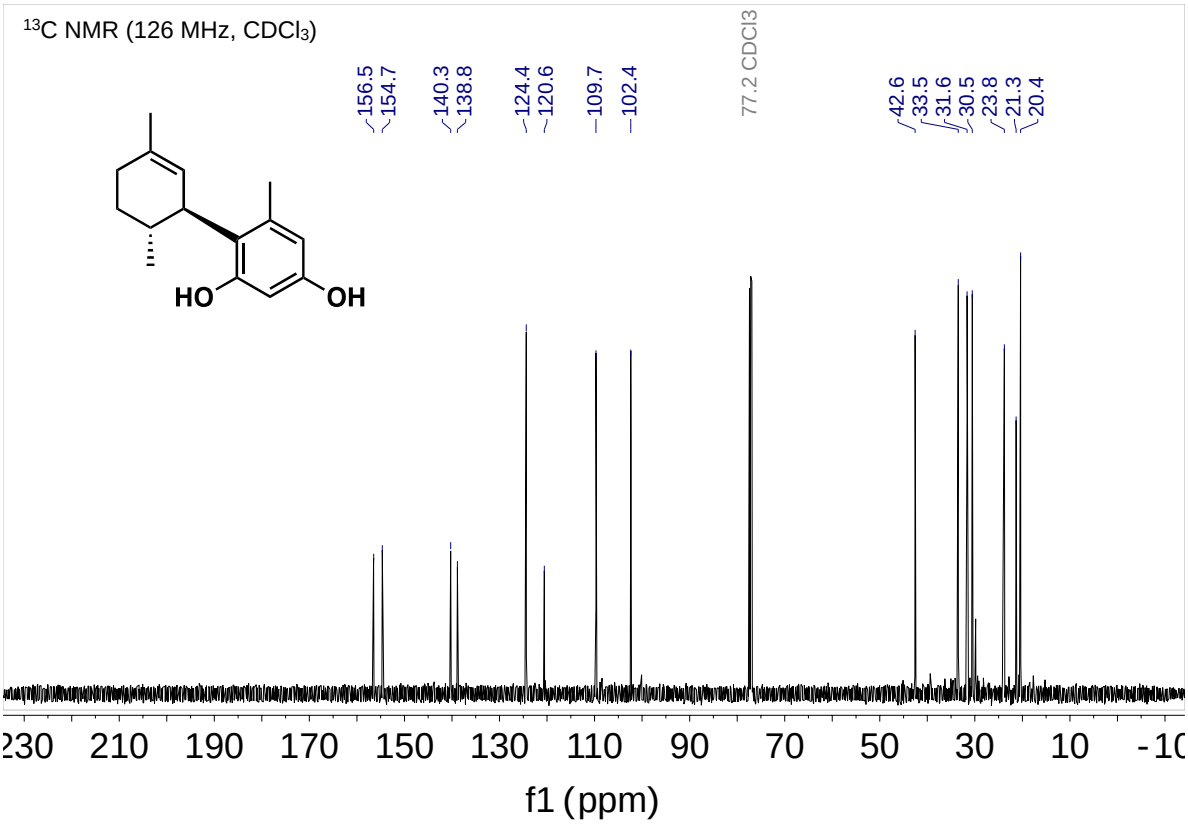
Synthesis of **(±)-3ad** from orcinol and **(±)-10d**:





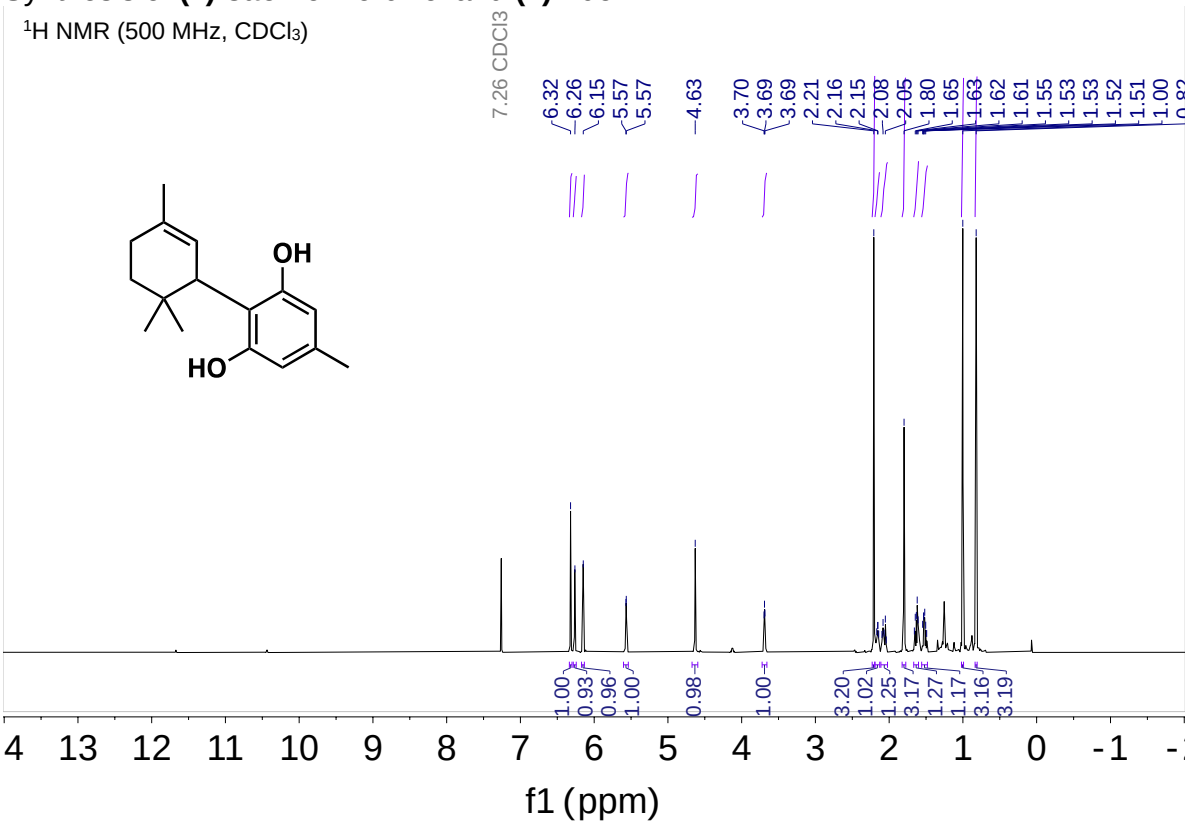
Synthesis of **(±)-6ad** from orcinol and **(±)-10d**:



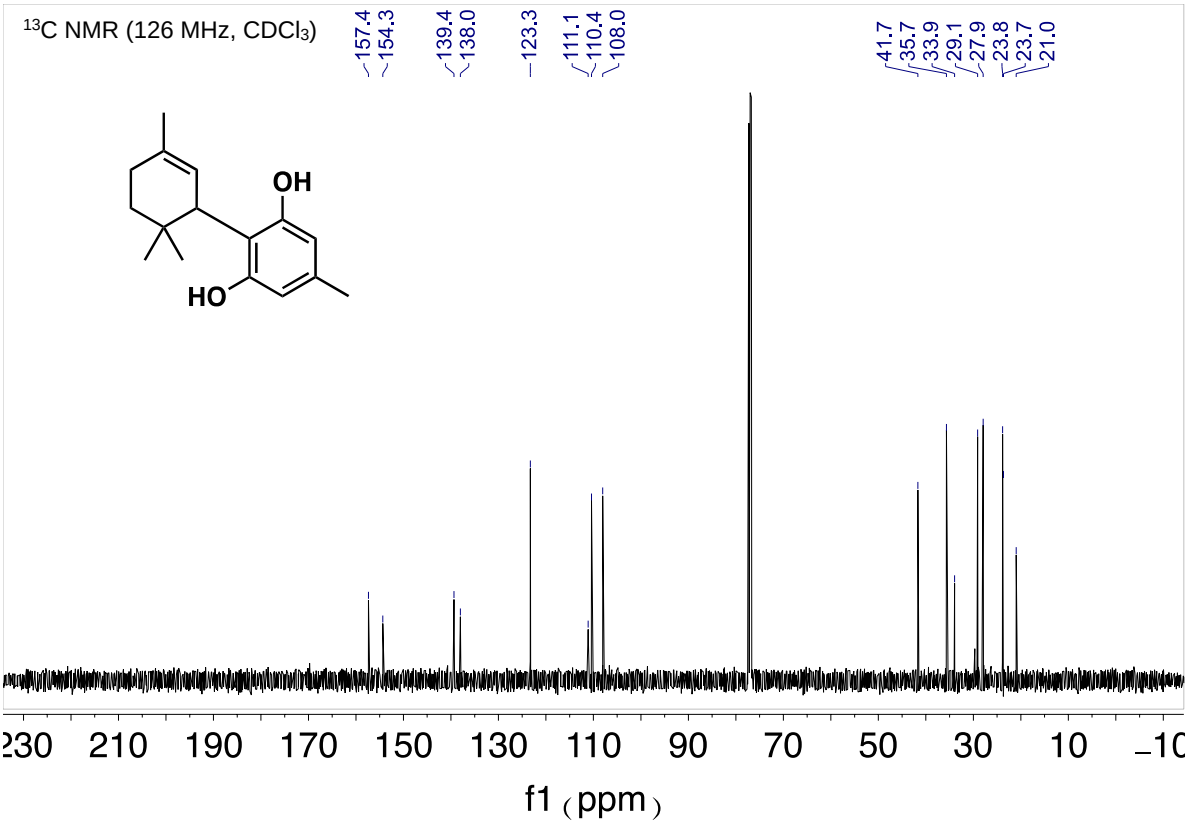


Synthesis of **(±)-3ae** from orcinol and **(±)-10e**:

^{1}H NMR (500 MHz, $CDCl_3$)

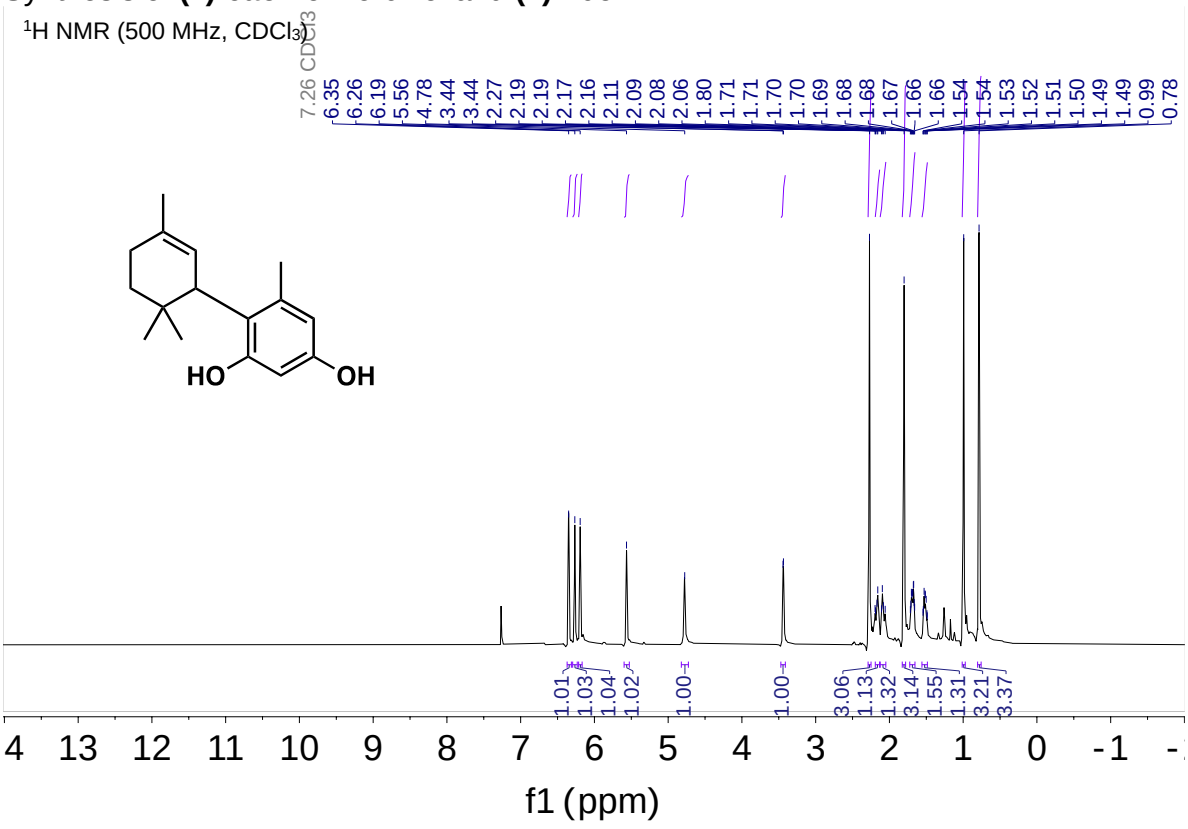


^{13}C NMR (126 MHz, $CDCl_3$)

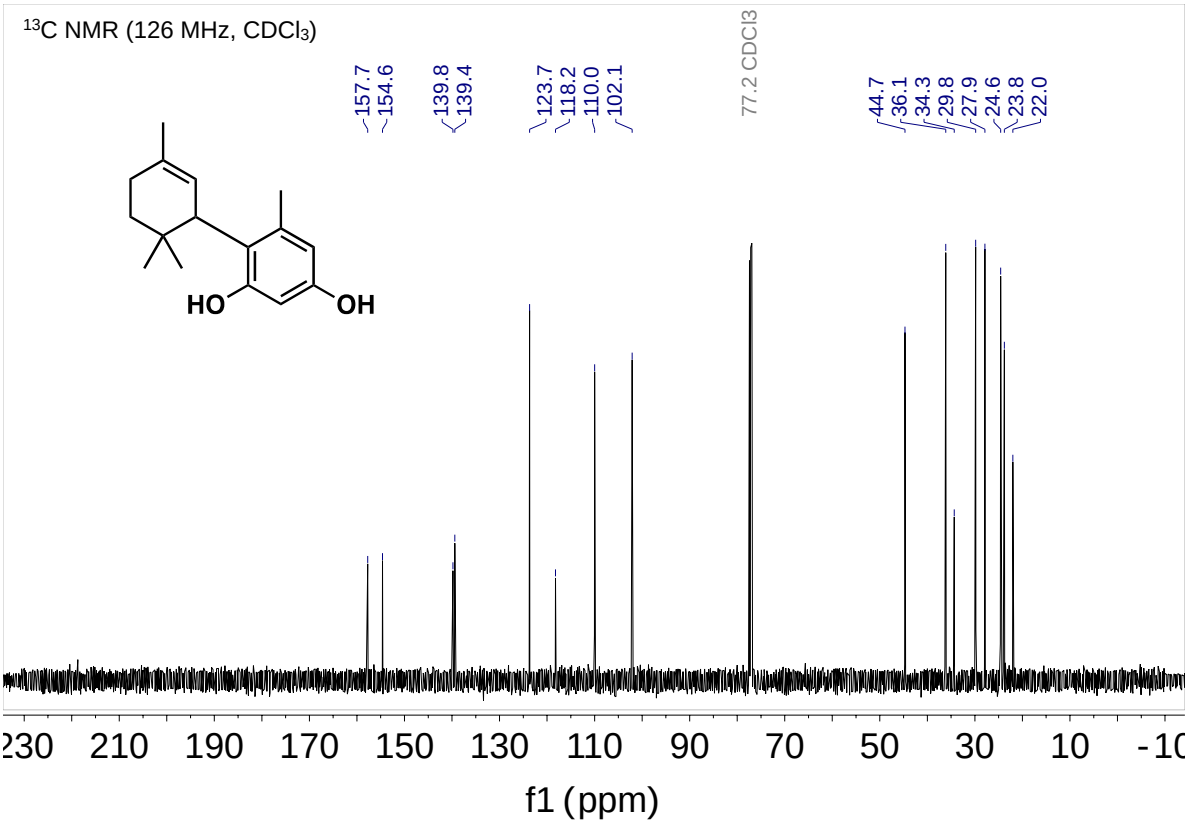


Synthesis of **(±)-6ae** from orcinol and **(±)-10e**:

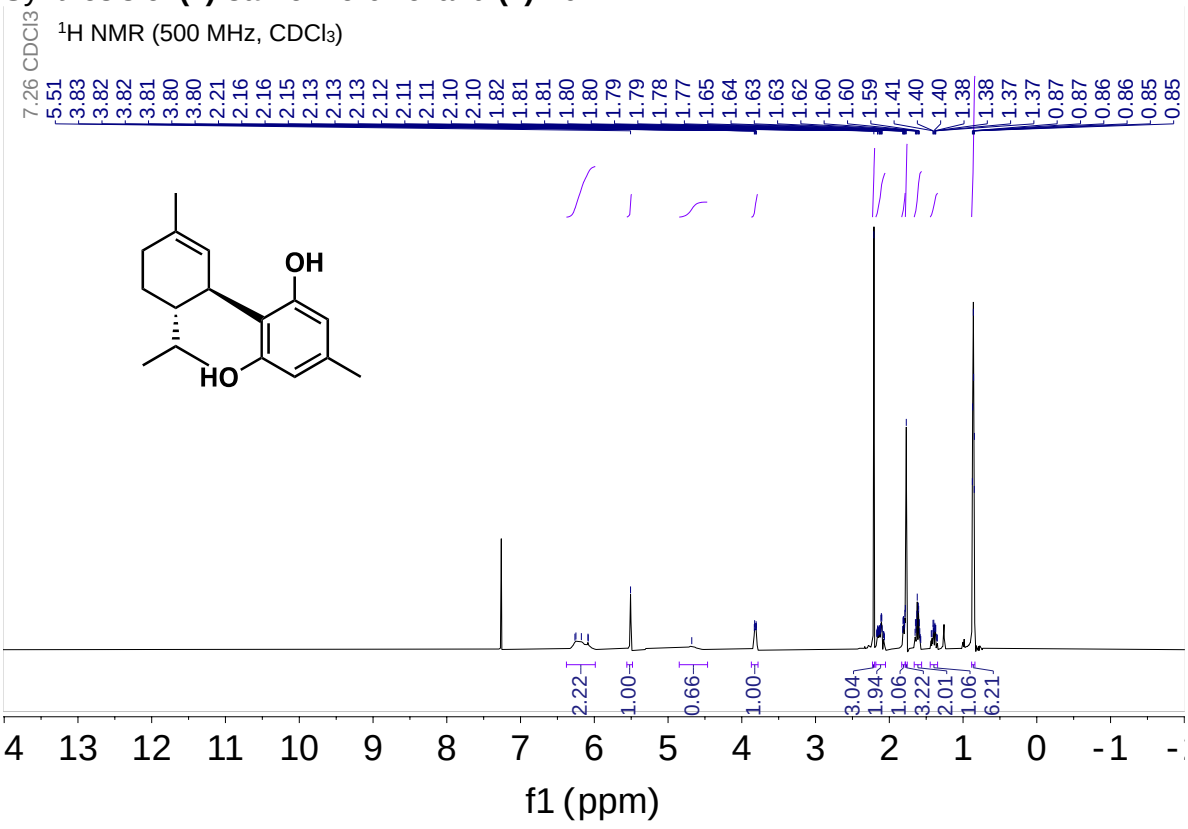
^{1}H NMR (500 MHz, $CDCl_3$)

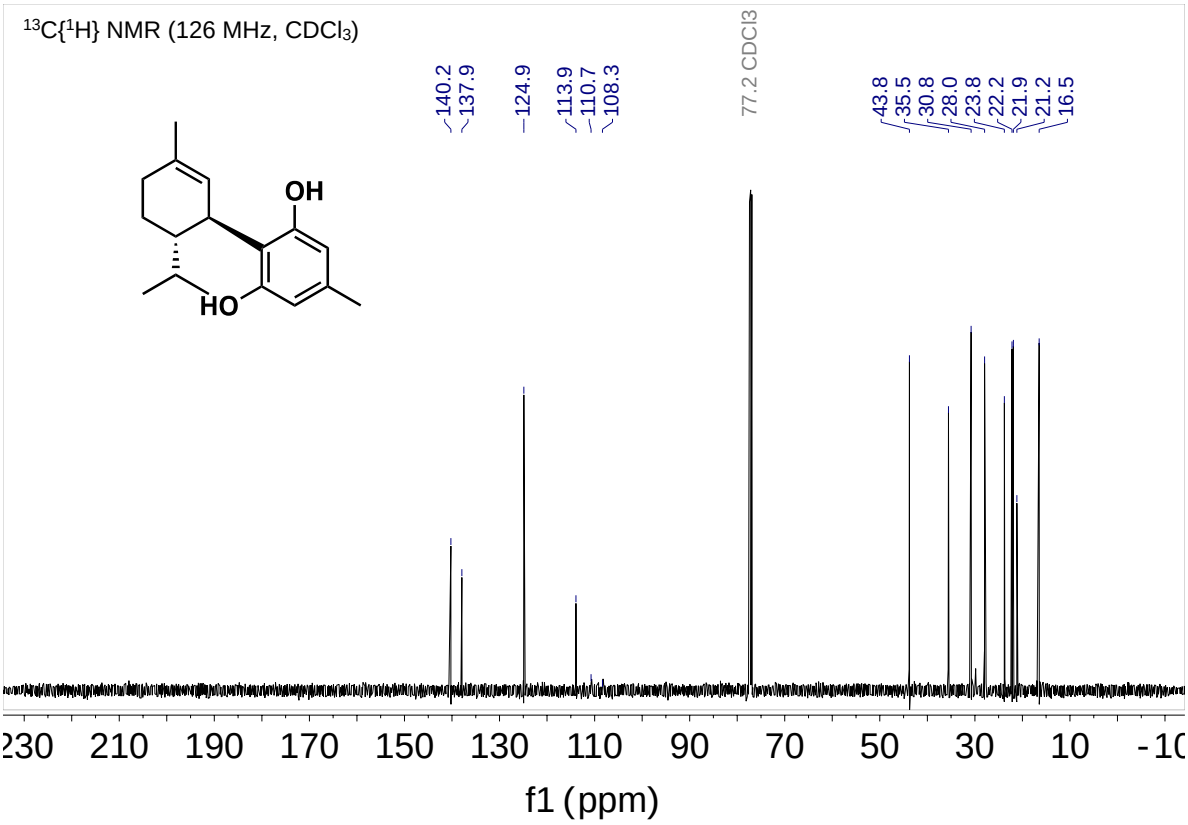


^{13}C NMR (126 MHz, $CDCl_3$)

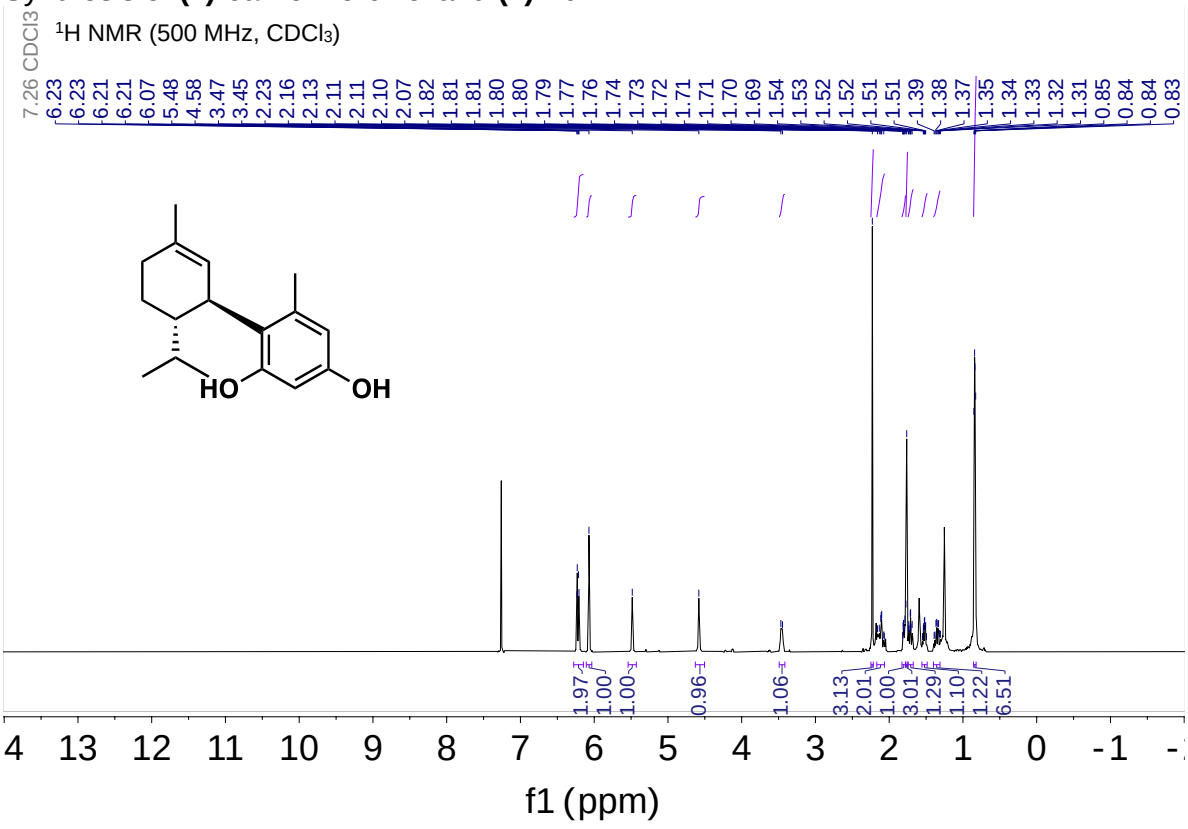


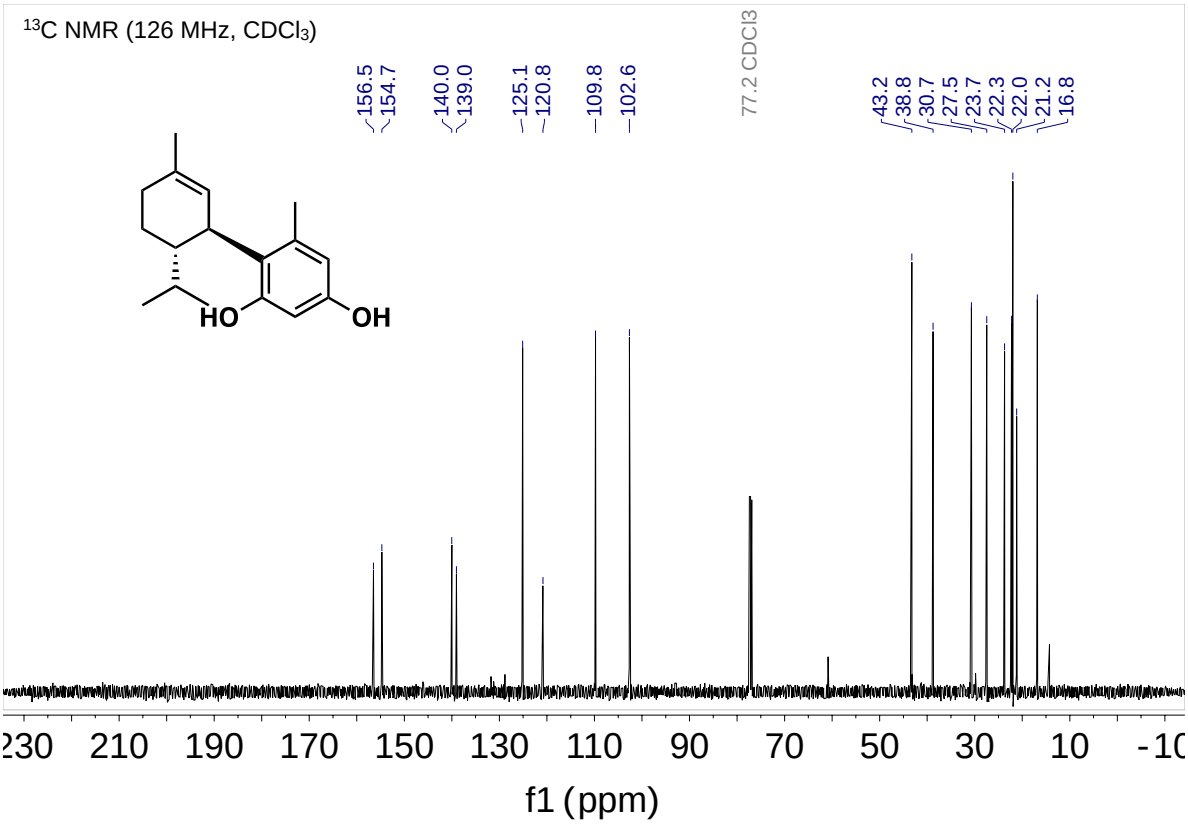
Synthesis of **(±)-3a** from orcinol and **(±)-10**:



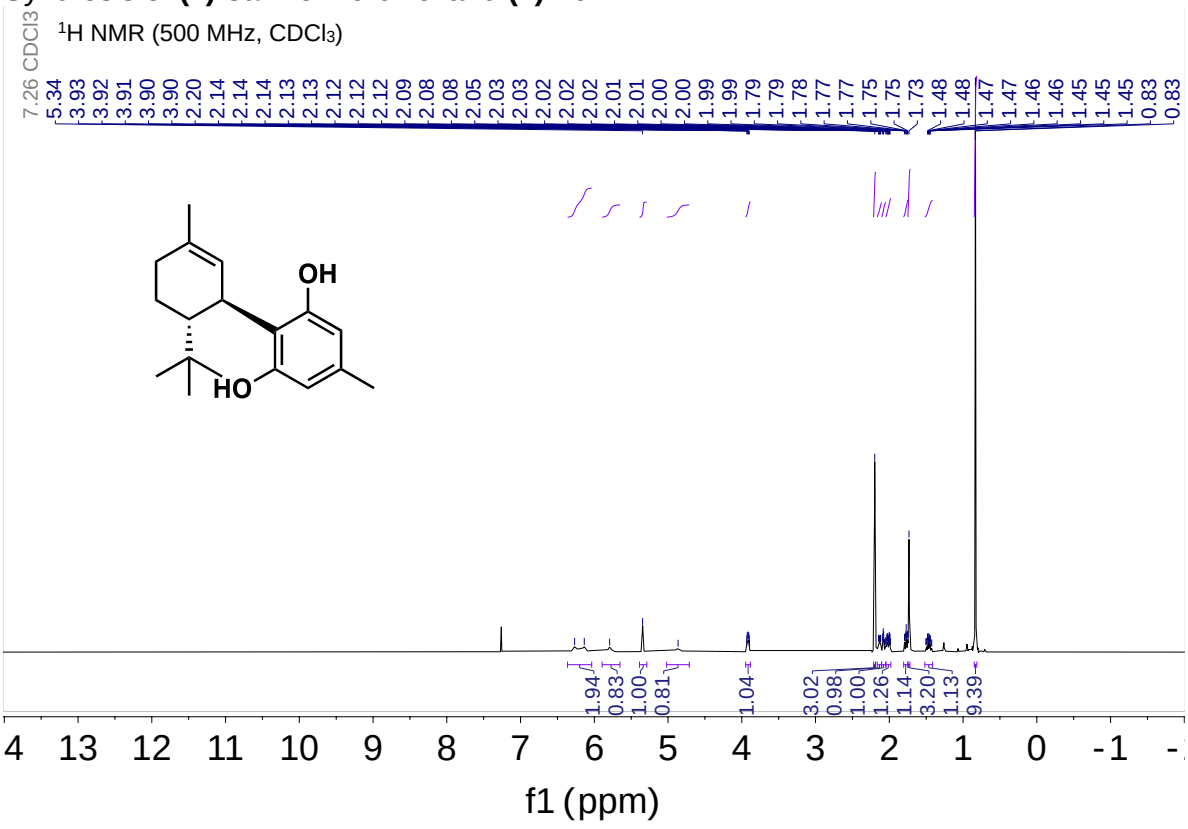


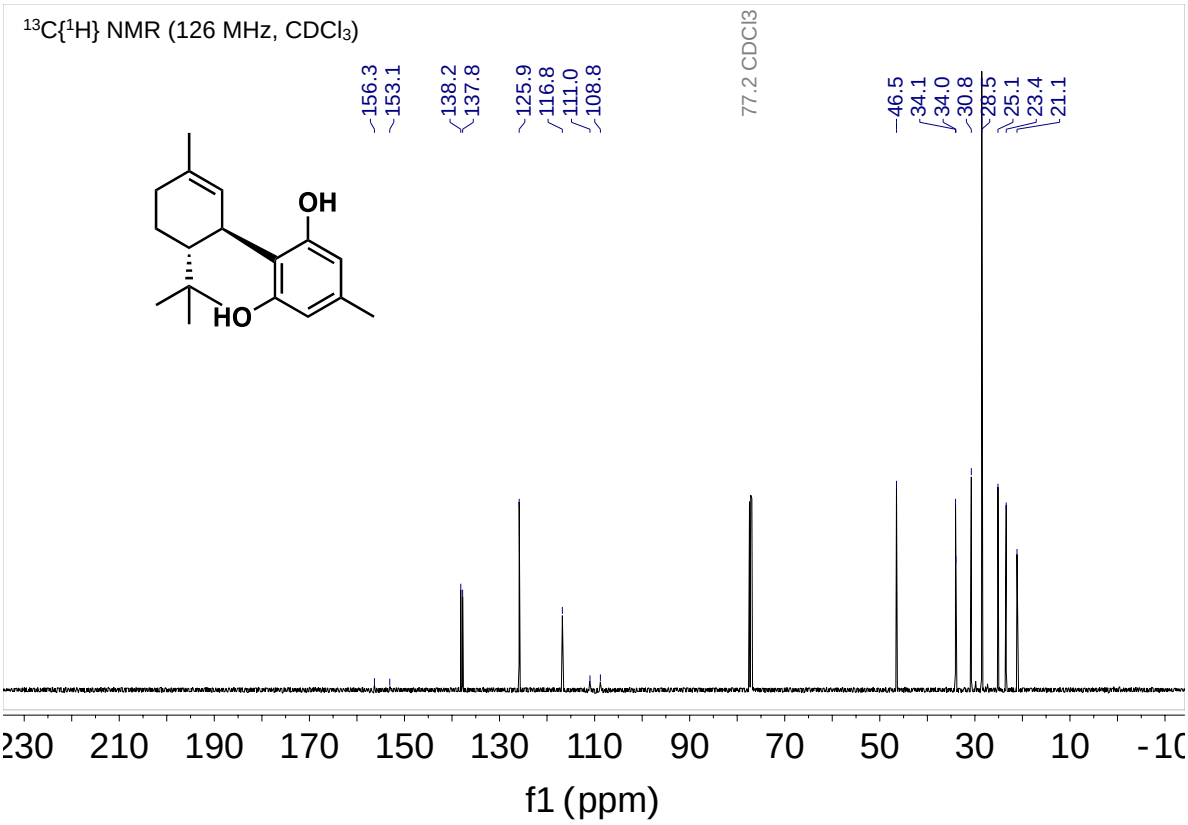
Synthesis of **(±)-6a** from orcinol and **(±)-10**:





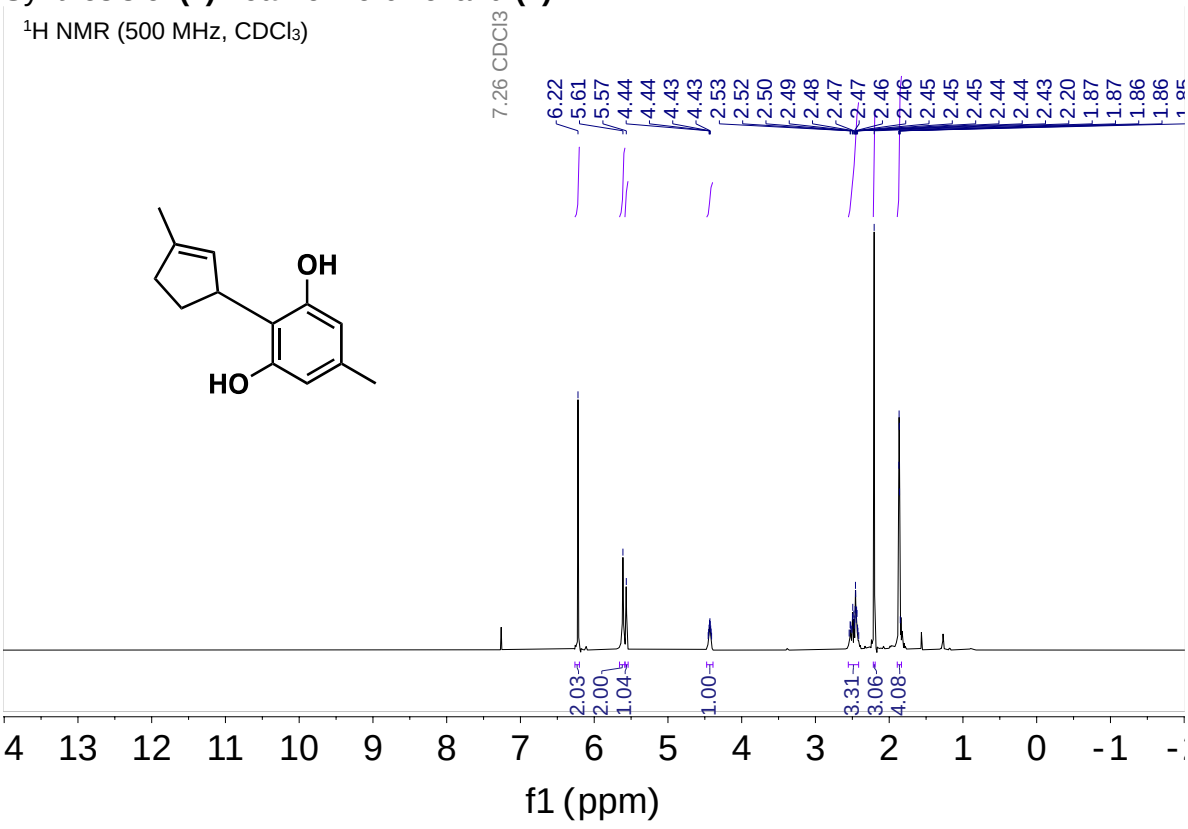
Synthesis of **(±)-3af** from orcinol and **(±)-10f**:



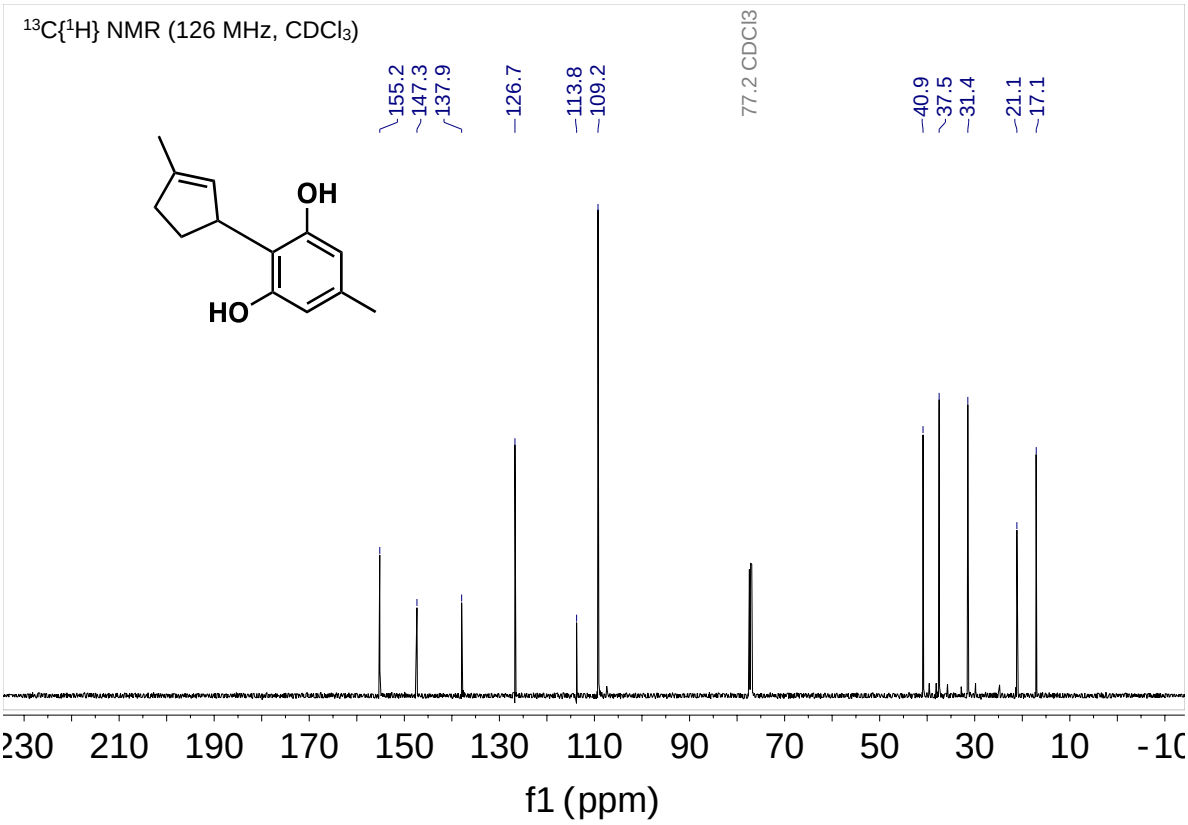


Synthesis of **(±)-19a** from orcinol and **(±)-17**:

^{1}H NMR (500 MHz, $CDCl_3$)

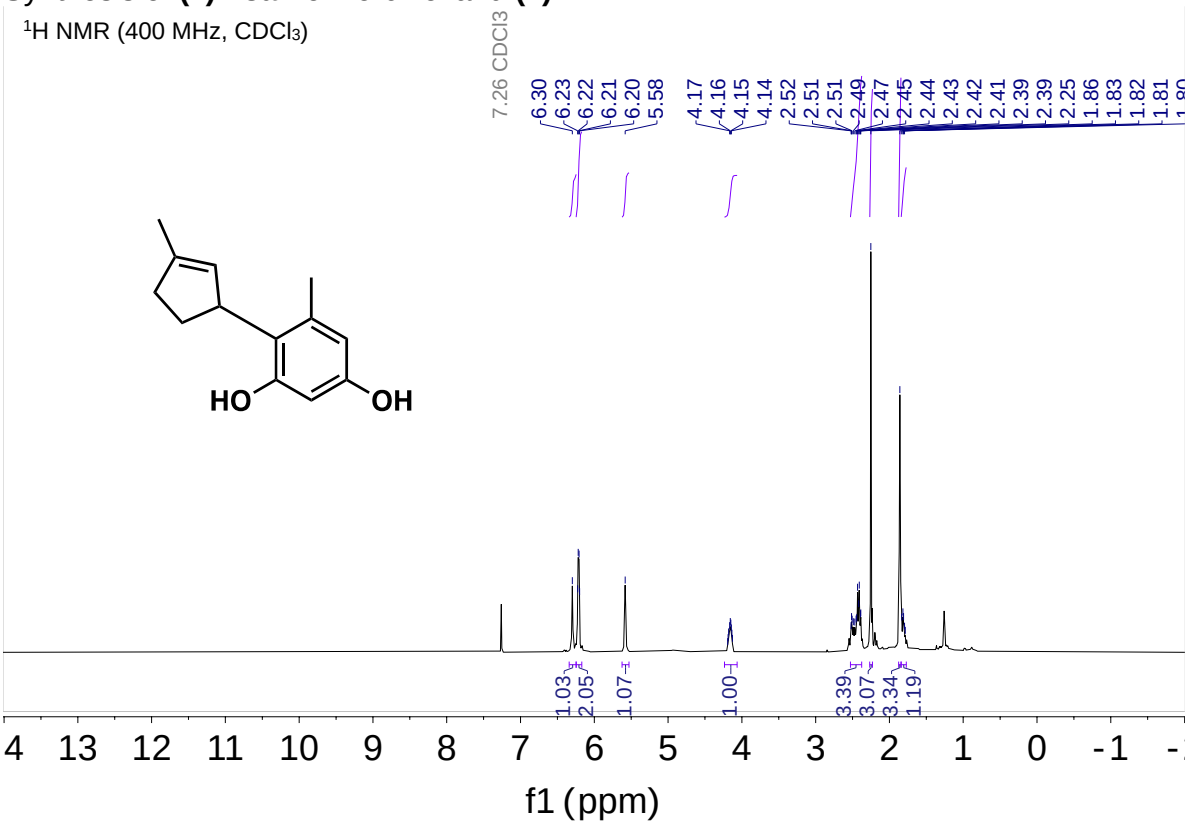


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$)

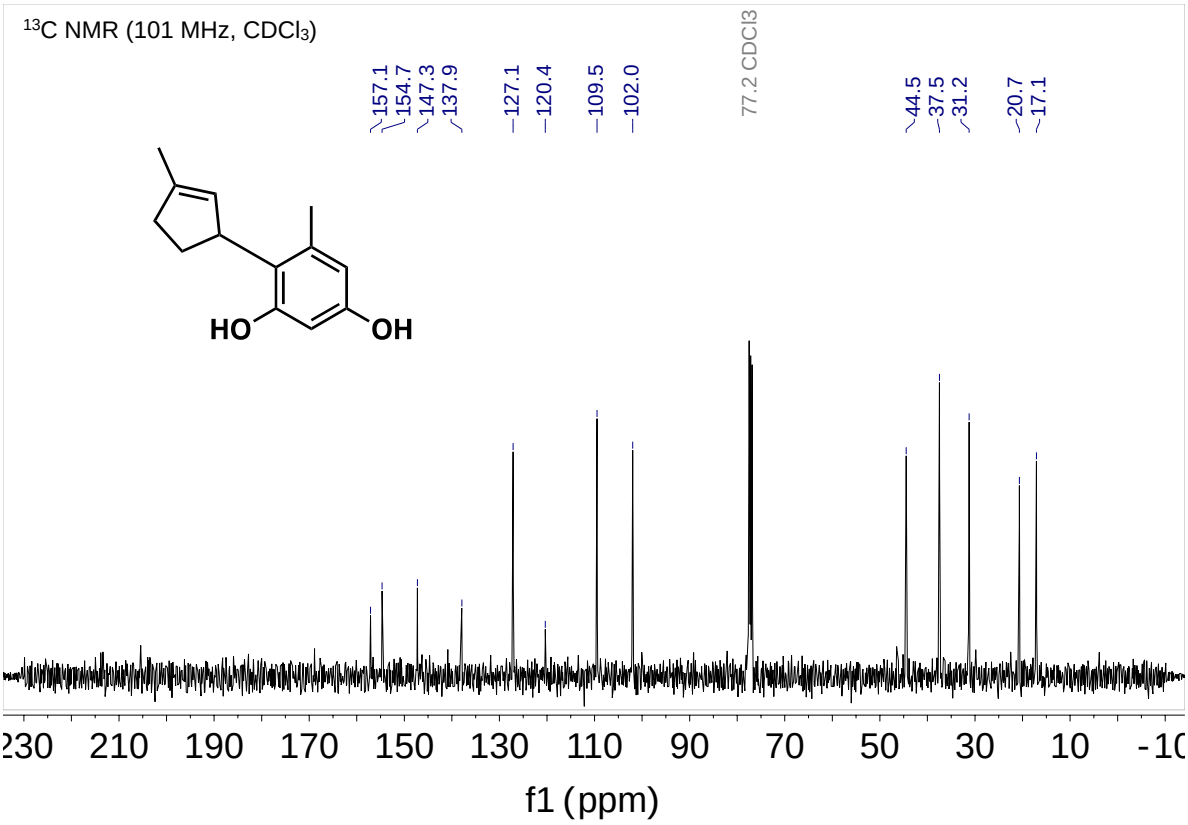


Synthesis of **(±)-18a** from orcinol and **(±)-17**:

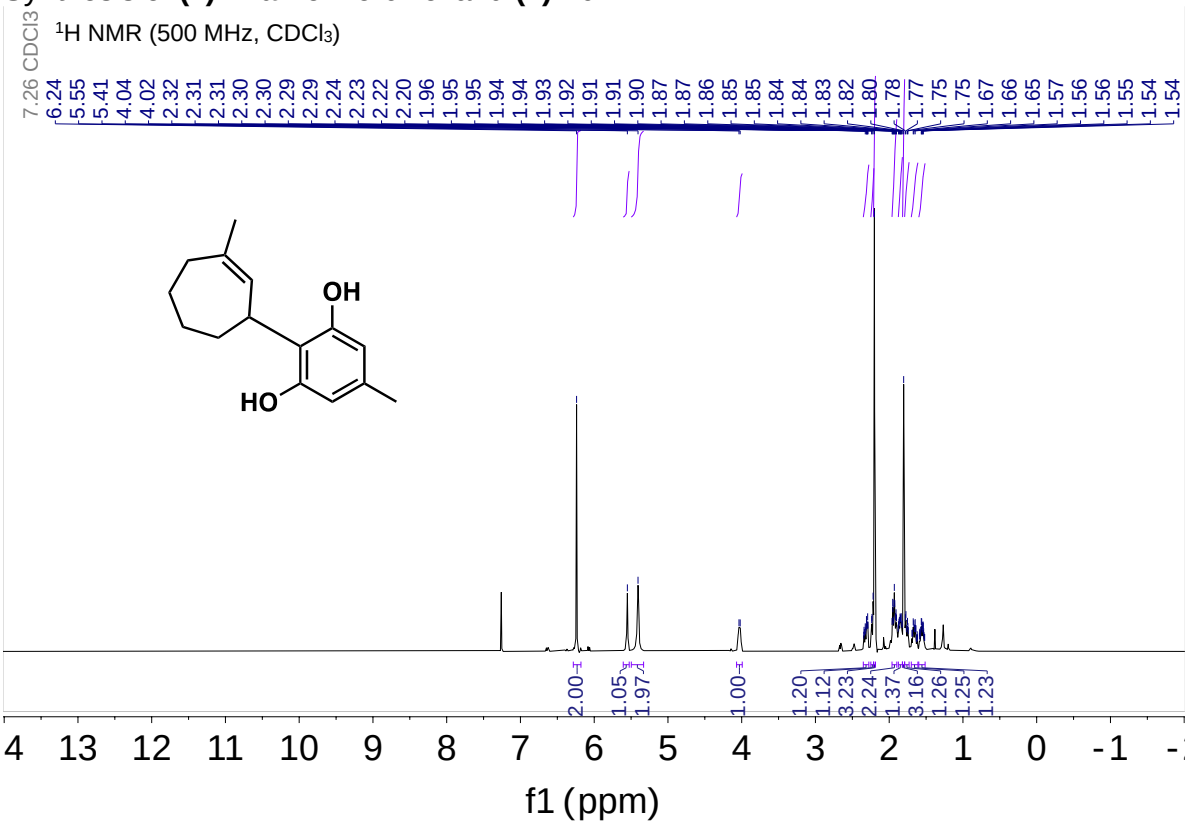
^{1}H NMR (400 MHz, $CDCl_3$)

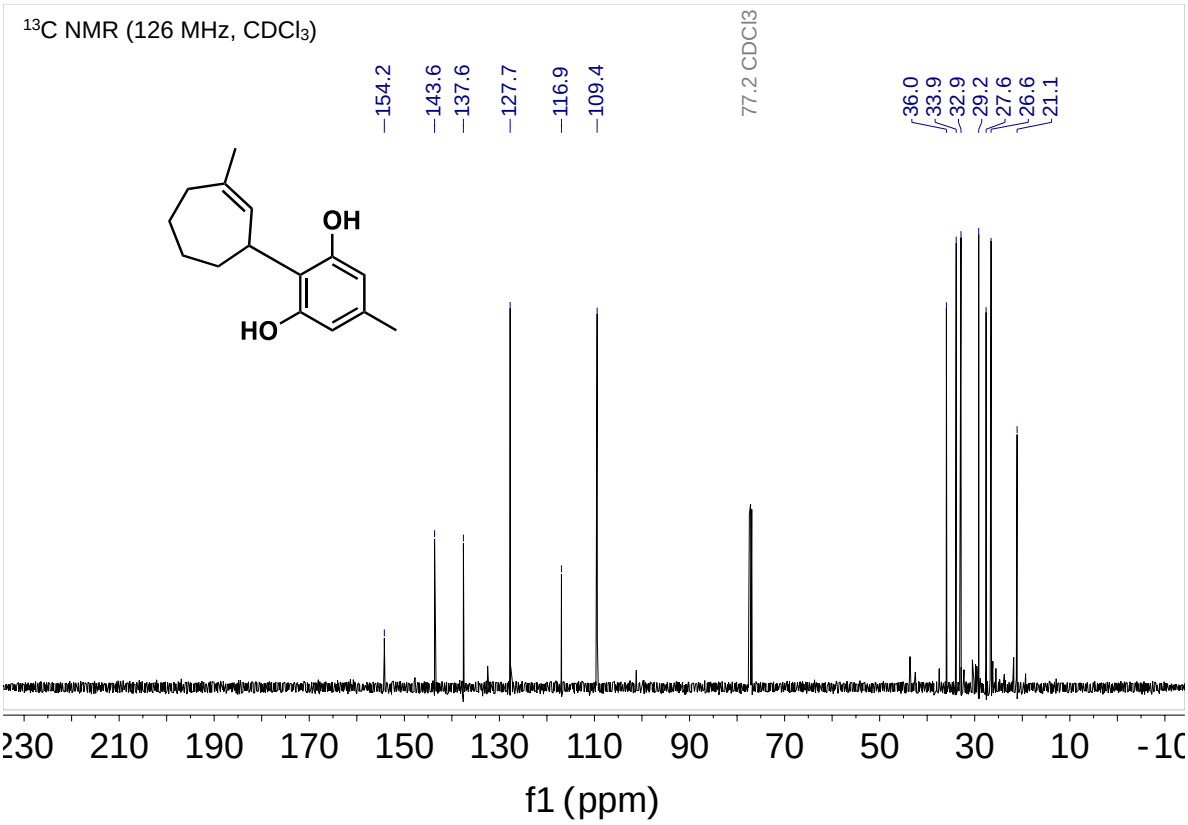


^{13}C NMR (101 MHz, $CDCl_3$)

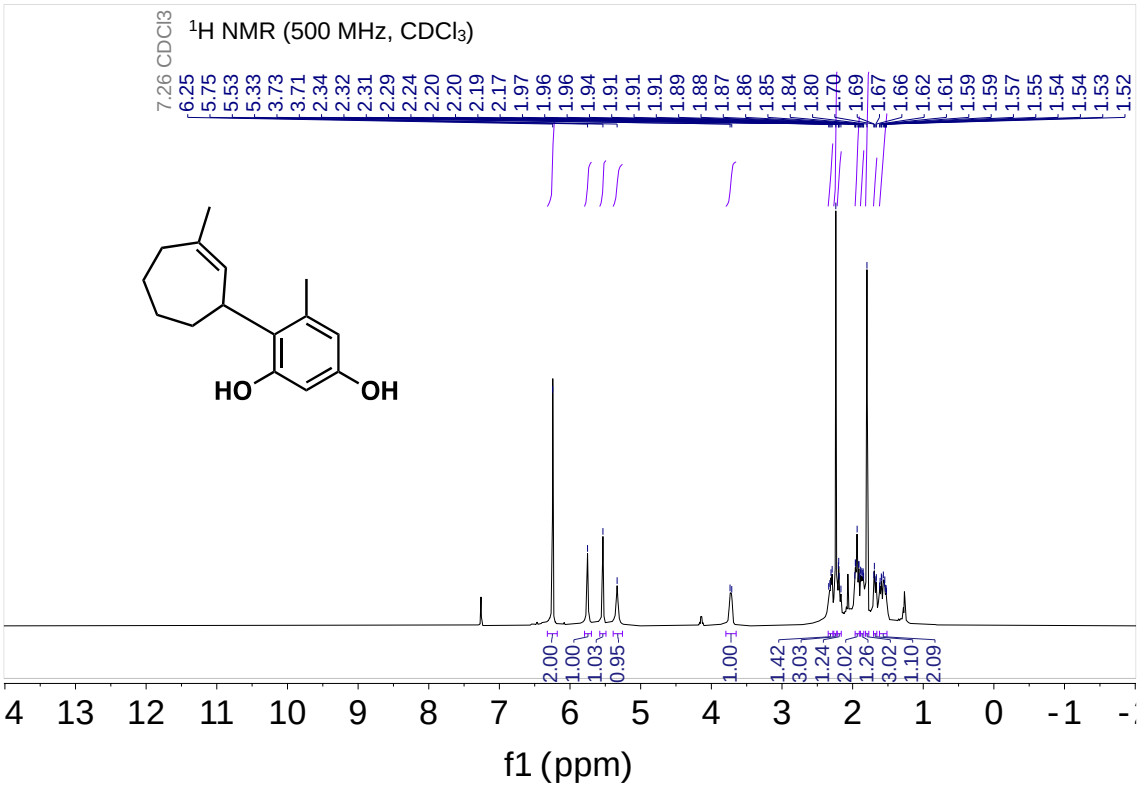


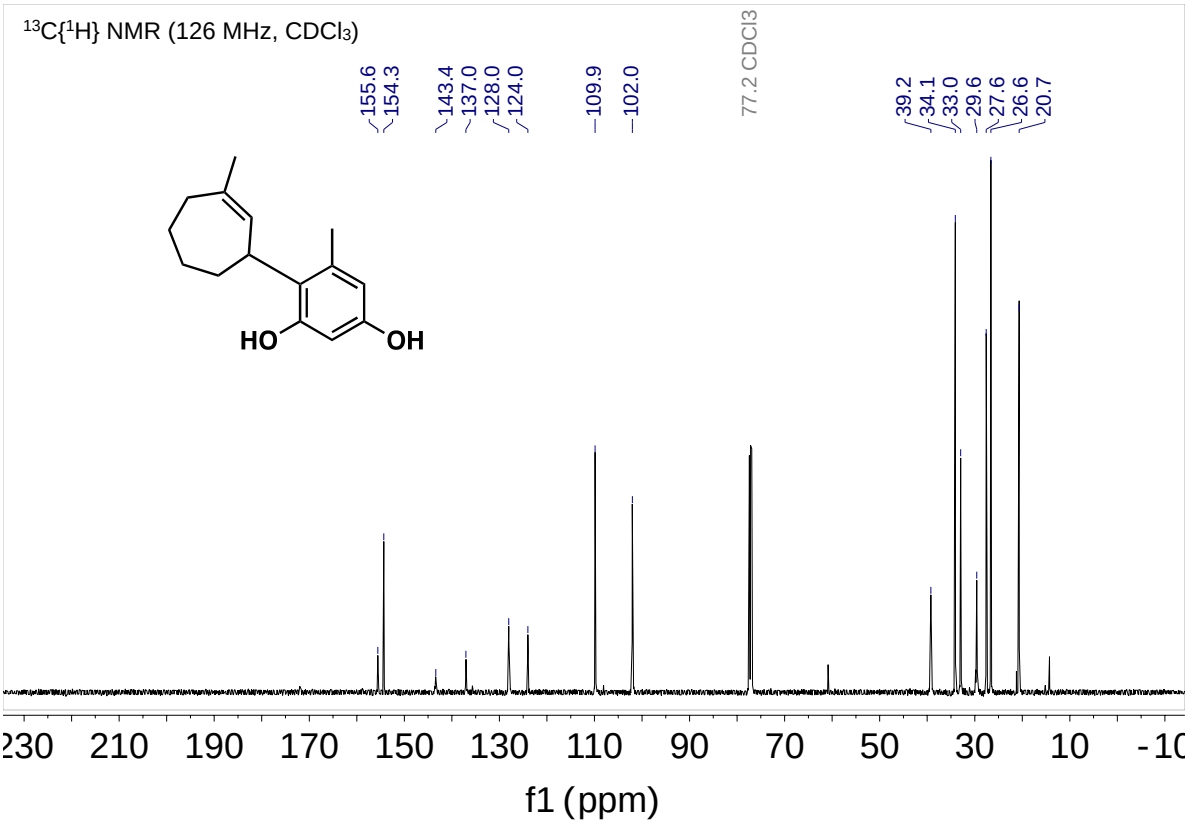
Synthesis of **(±)-22a** from orcinol and **(±)-20**:



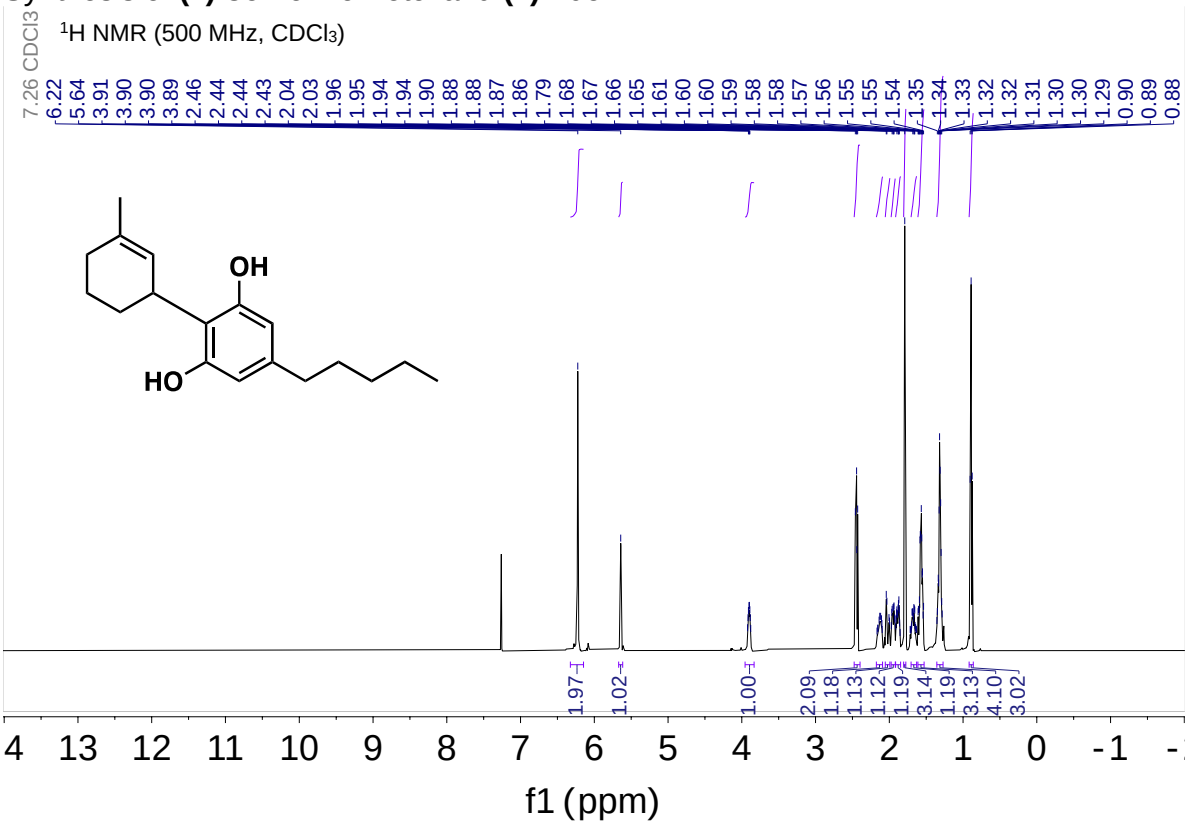


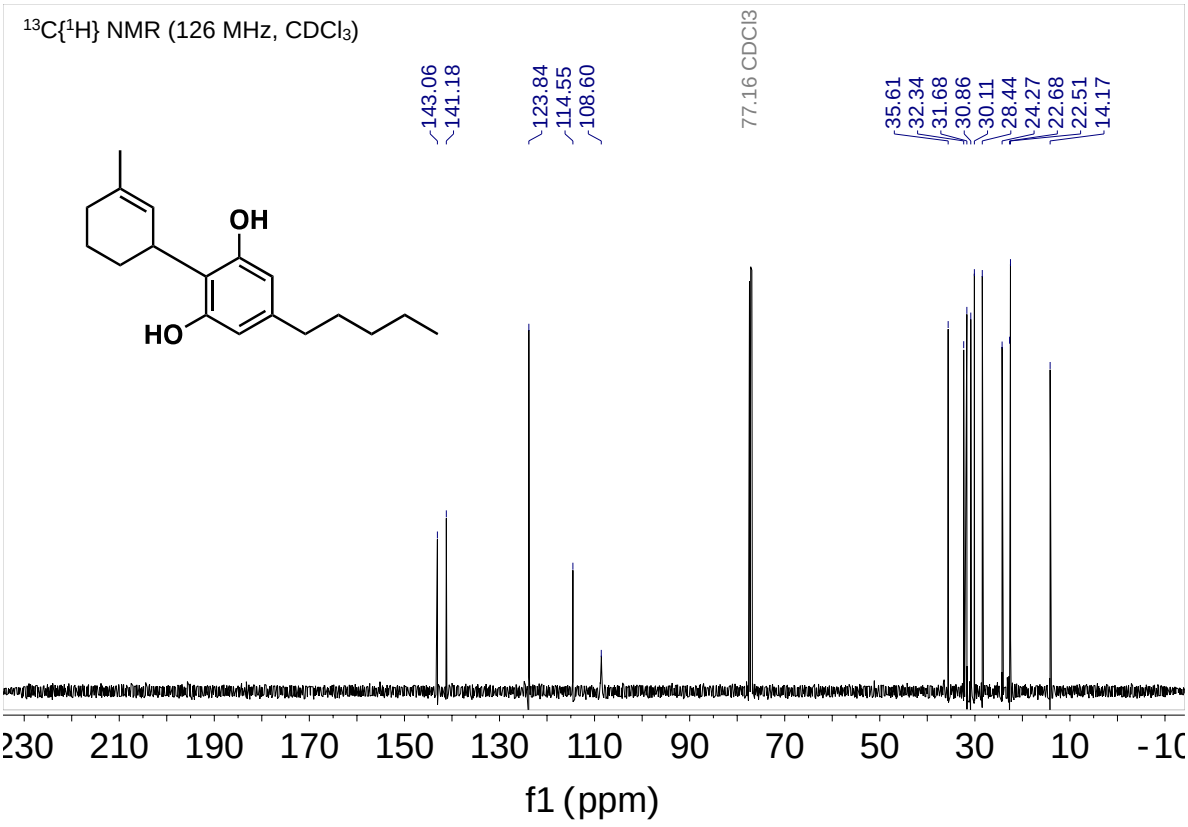
Synthesis of **(±)-21a** from orcinol and **(±)-20**:



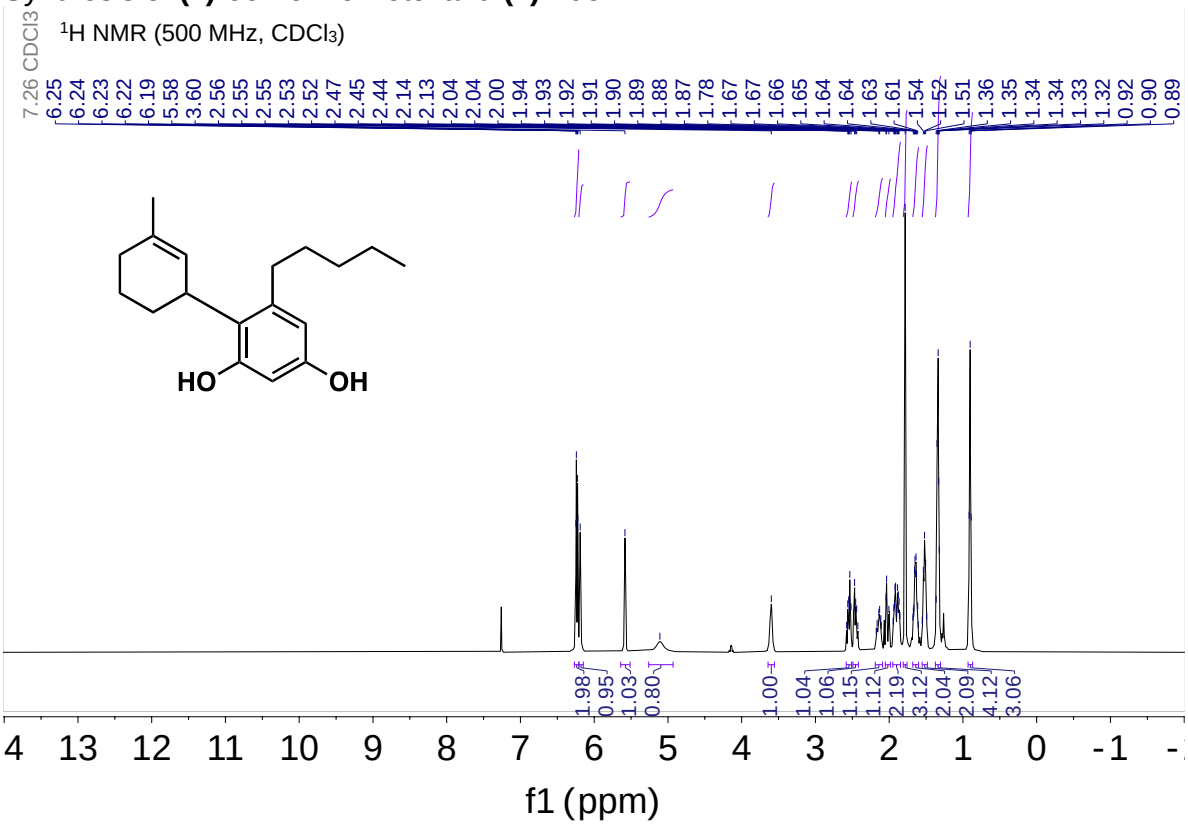


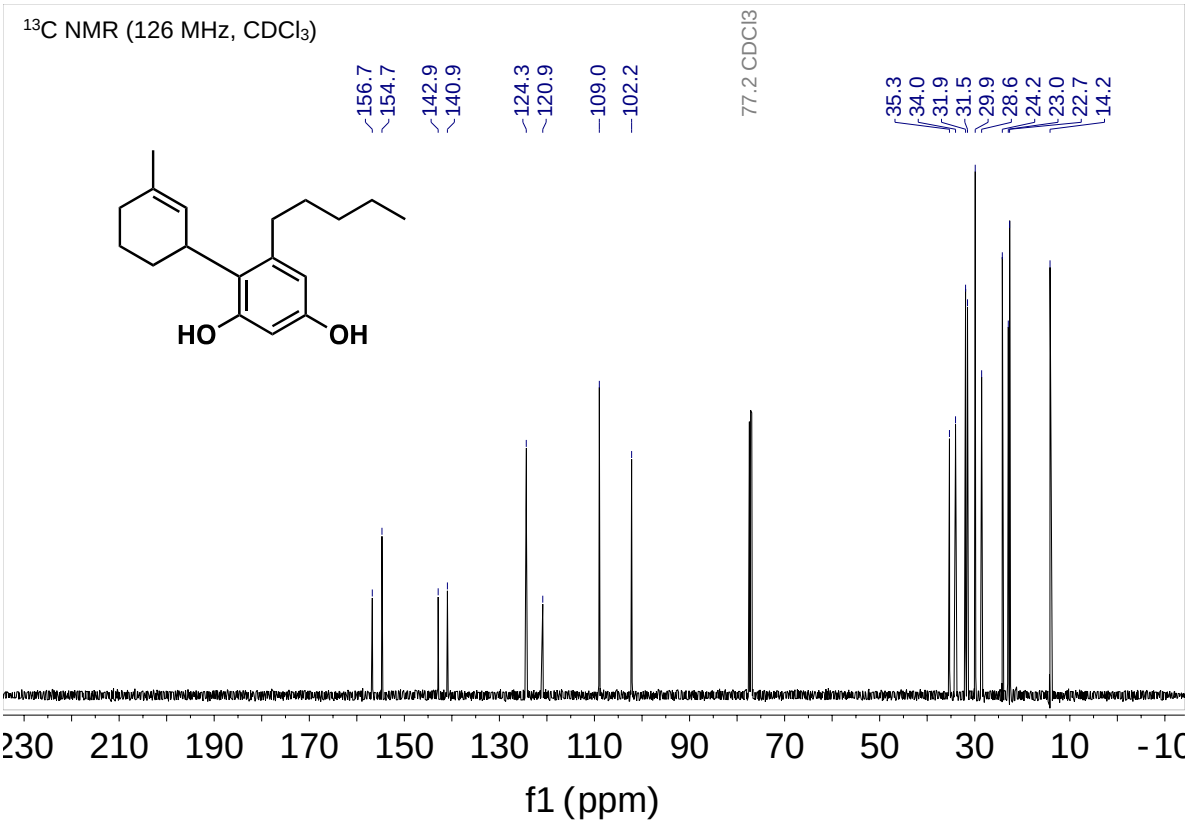
Synthesis of **(±)-3c** from olivetol and **(±)-10c**:



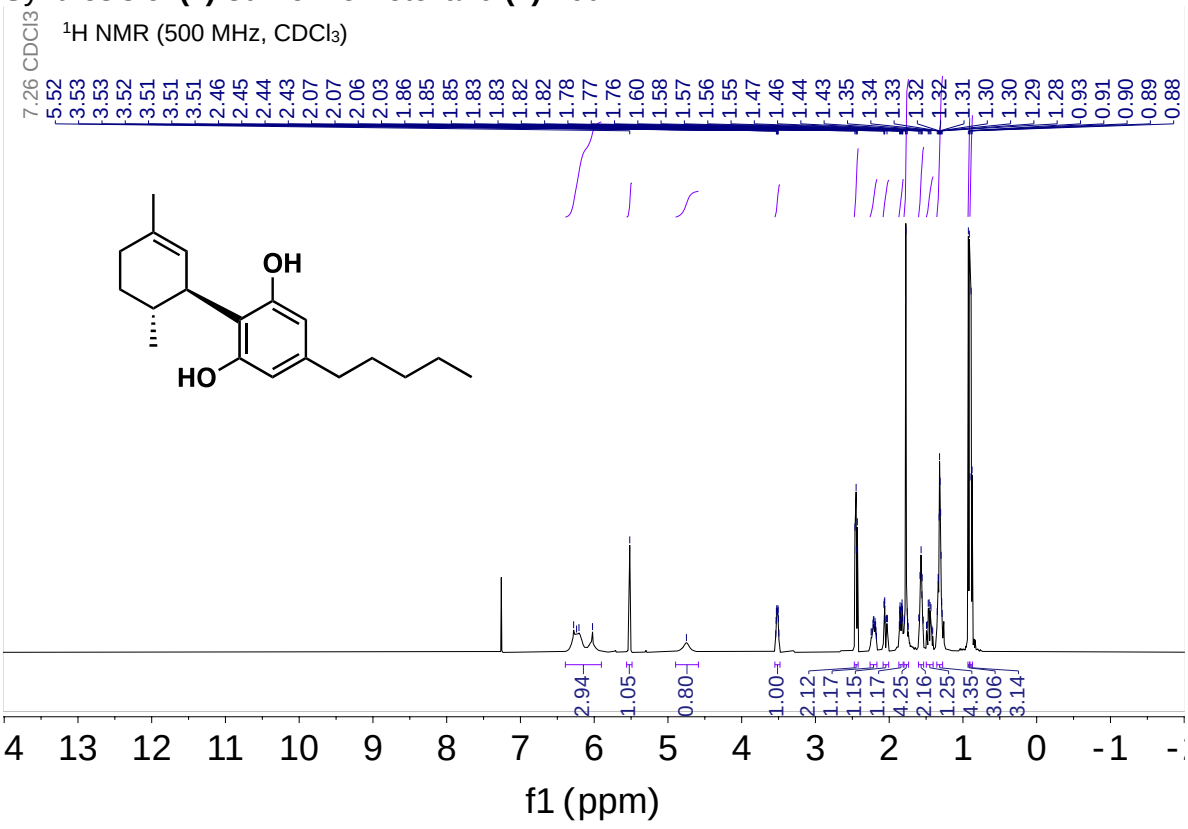


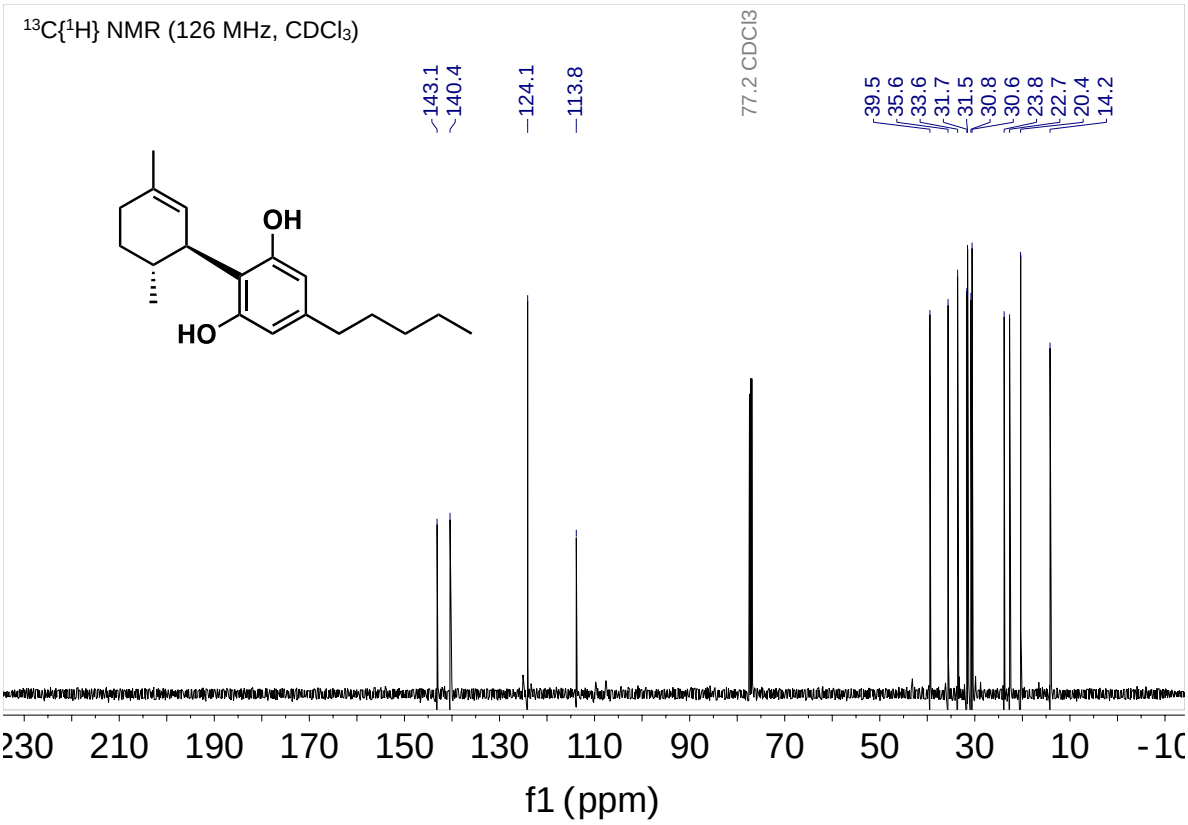
Synthesis of **(±)-6c** from olivetol and **(±)-10c**:



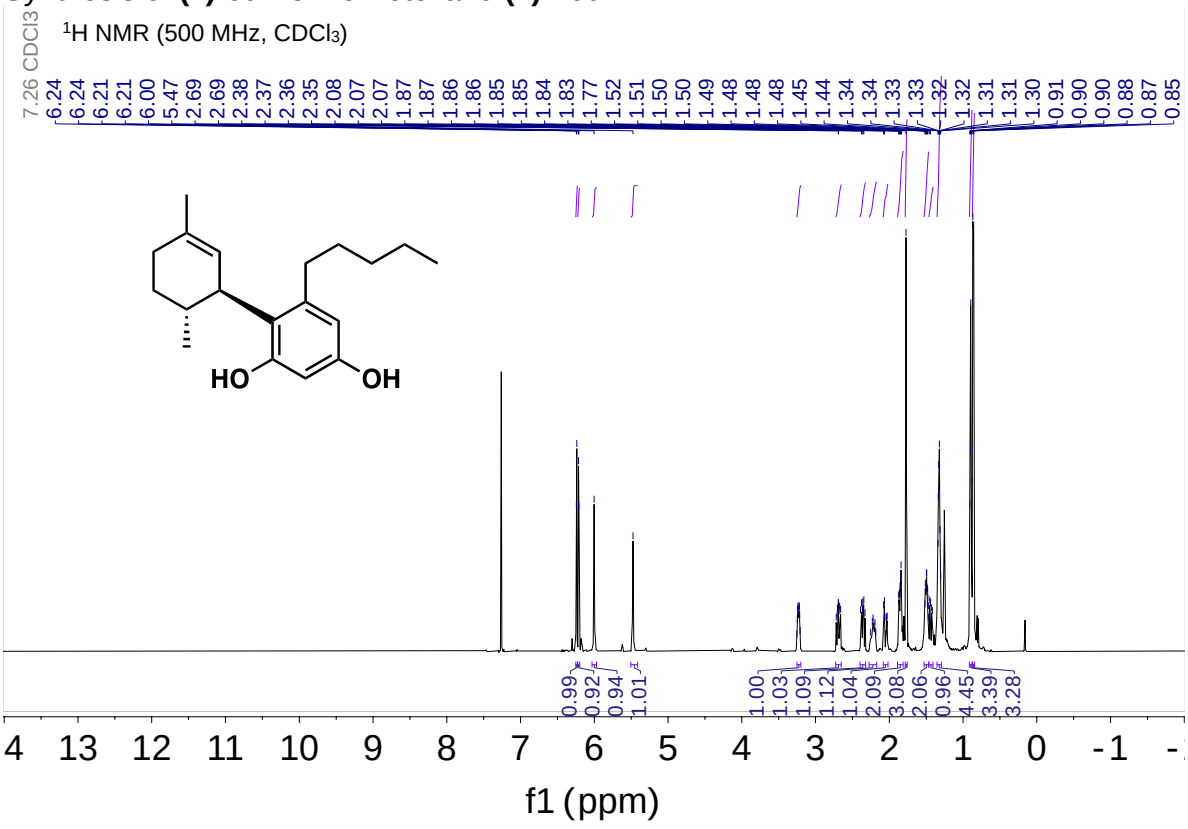


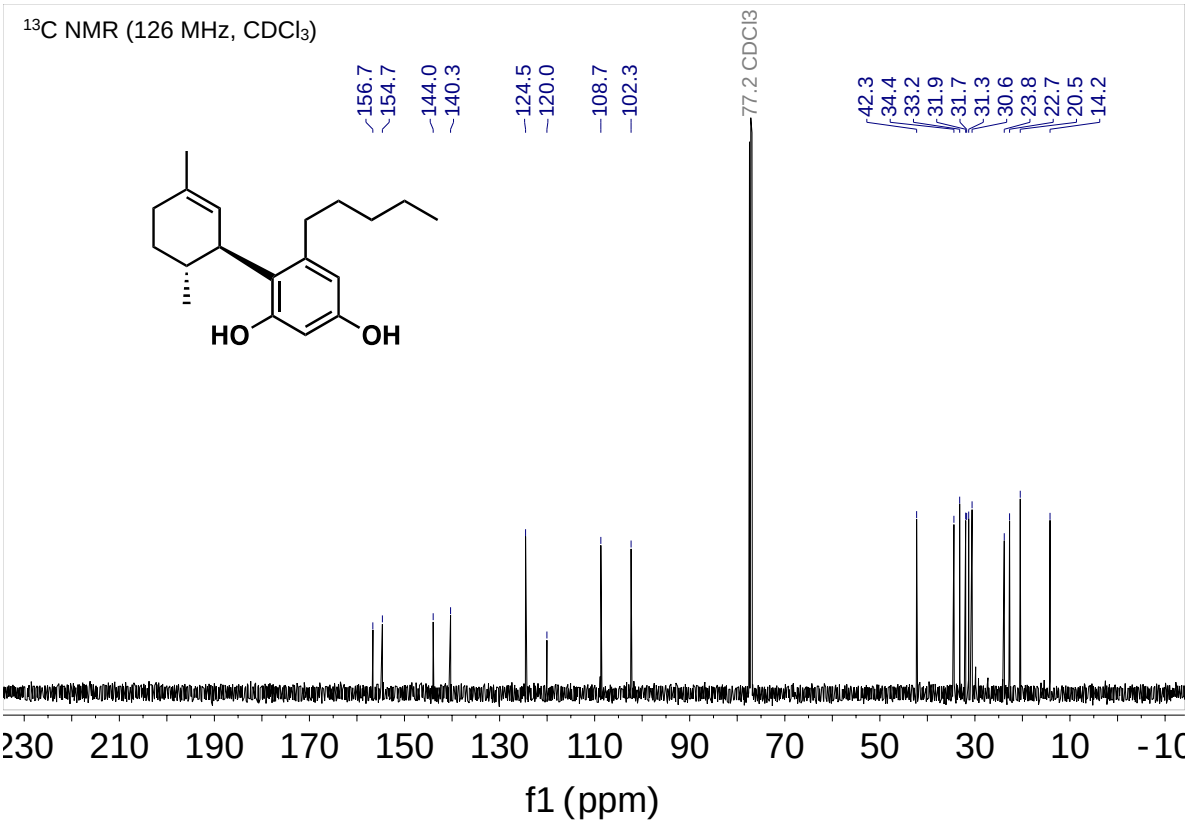
Synthesis of **(±)-3d** from olivetol and **(±)-10d**:



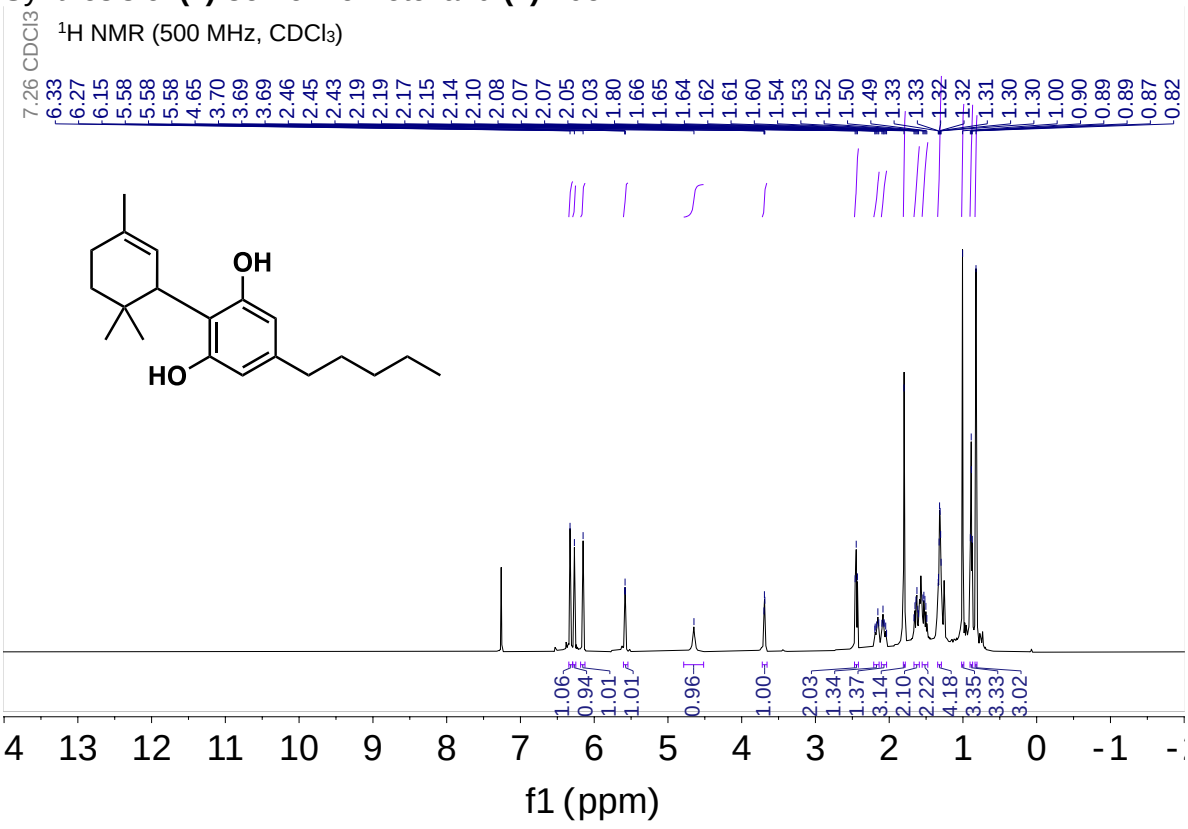


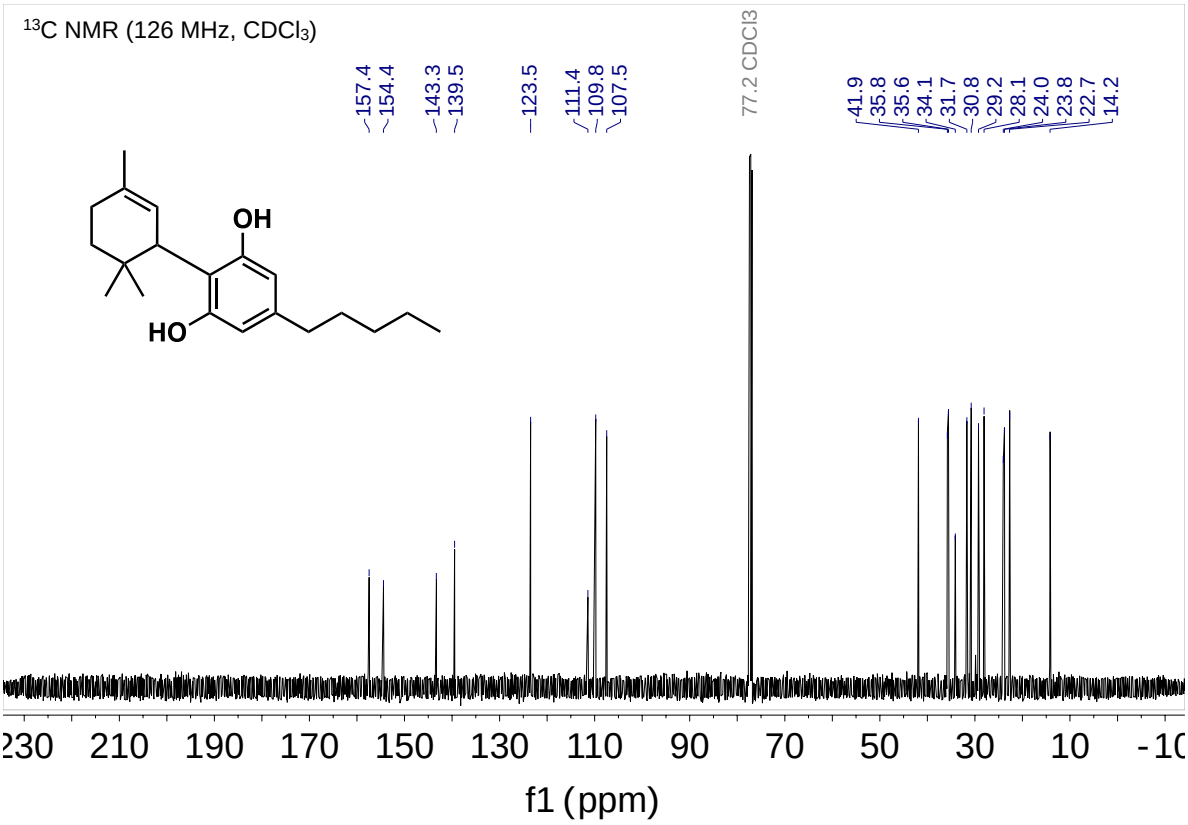
Synthesis of **(±)-6d** from olivetol and **(±)-10d**:



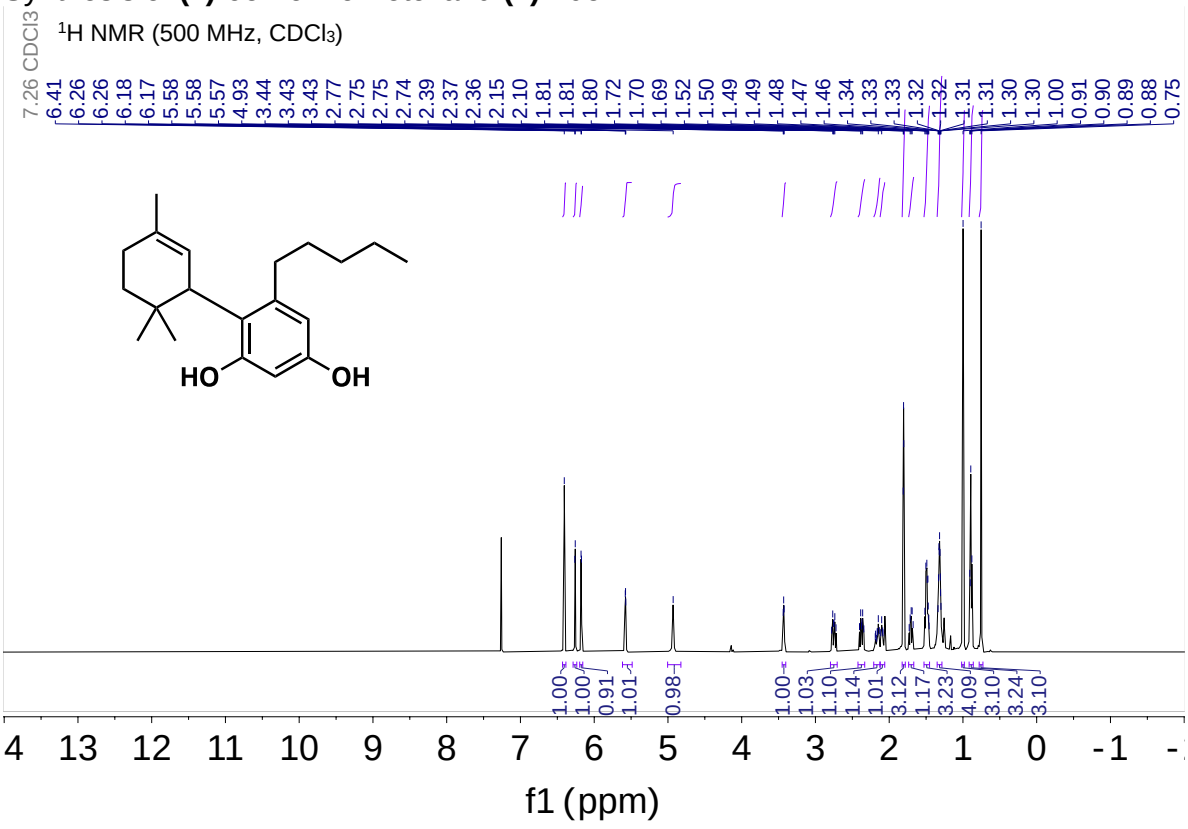


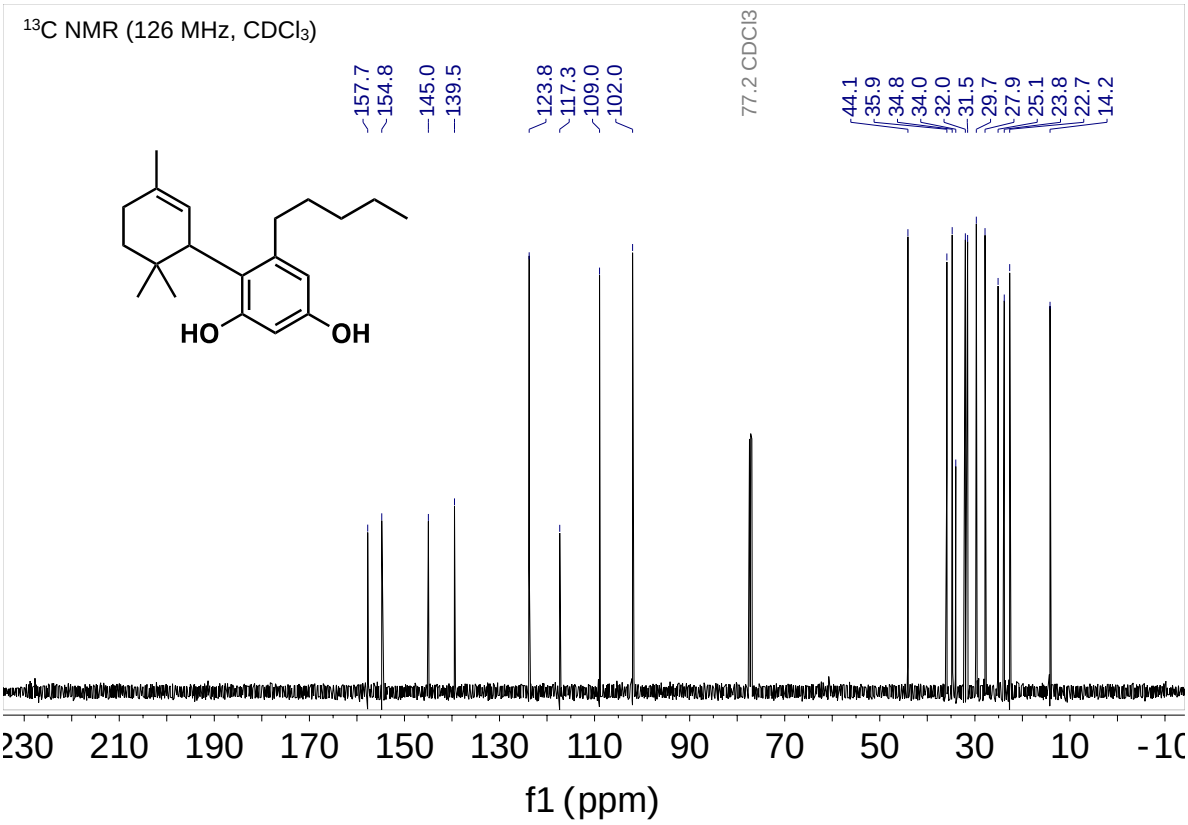
Synthesis of **(±)-3e** from olivetol and **(±)-10e**:



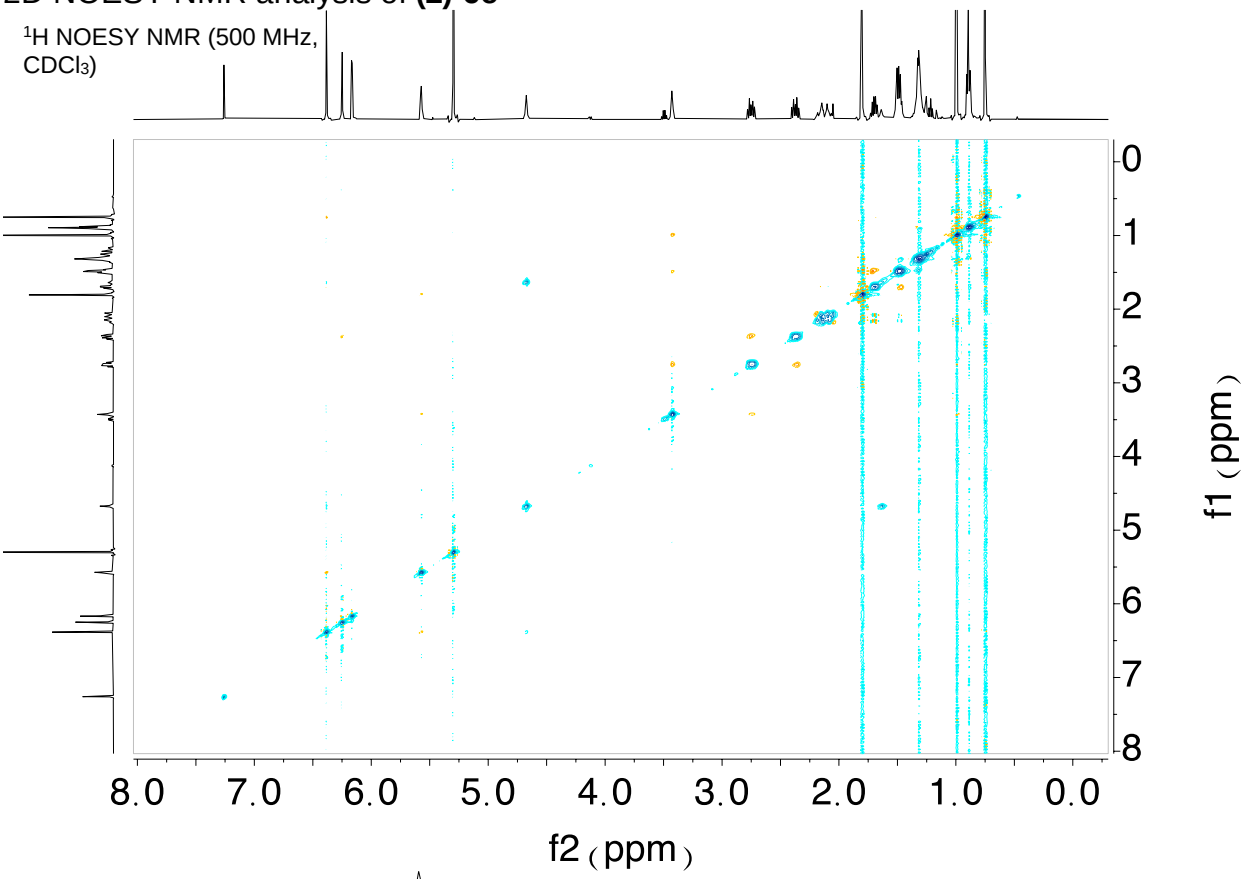


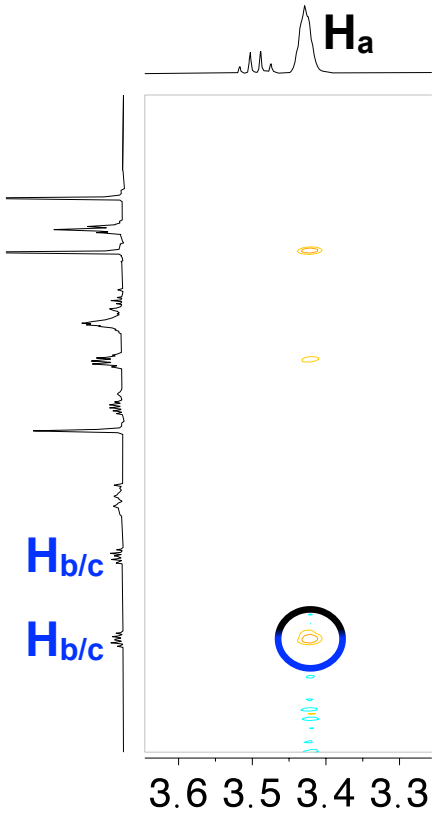
Synthesis of **(±)-6e** from olivetol and **(±)-10e**:

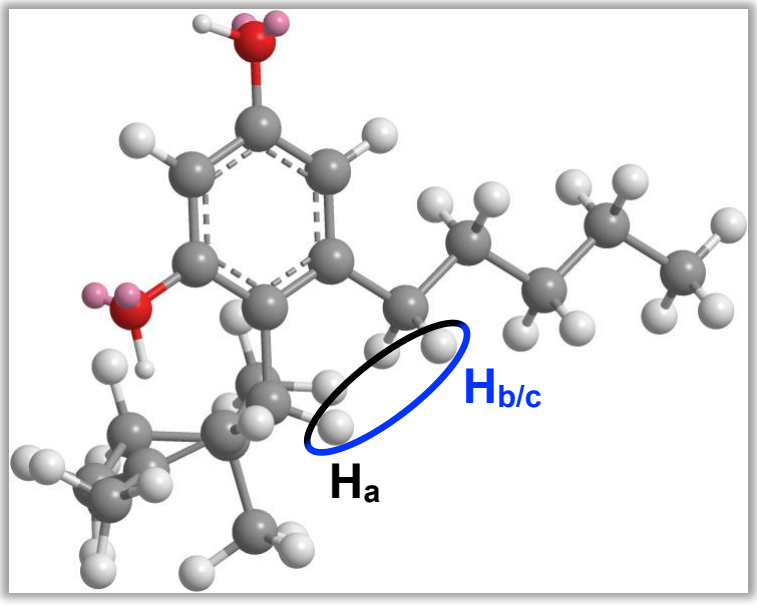




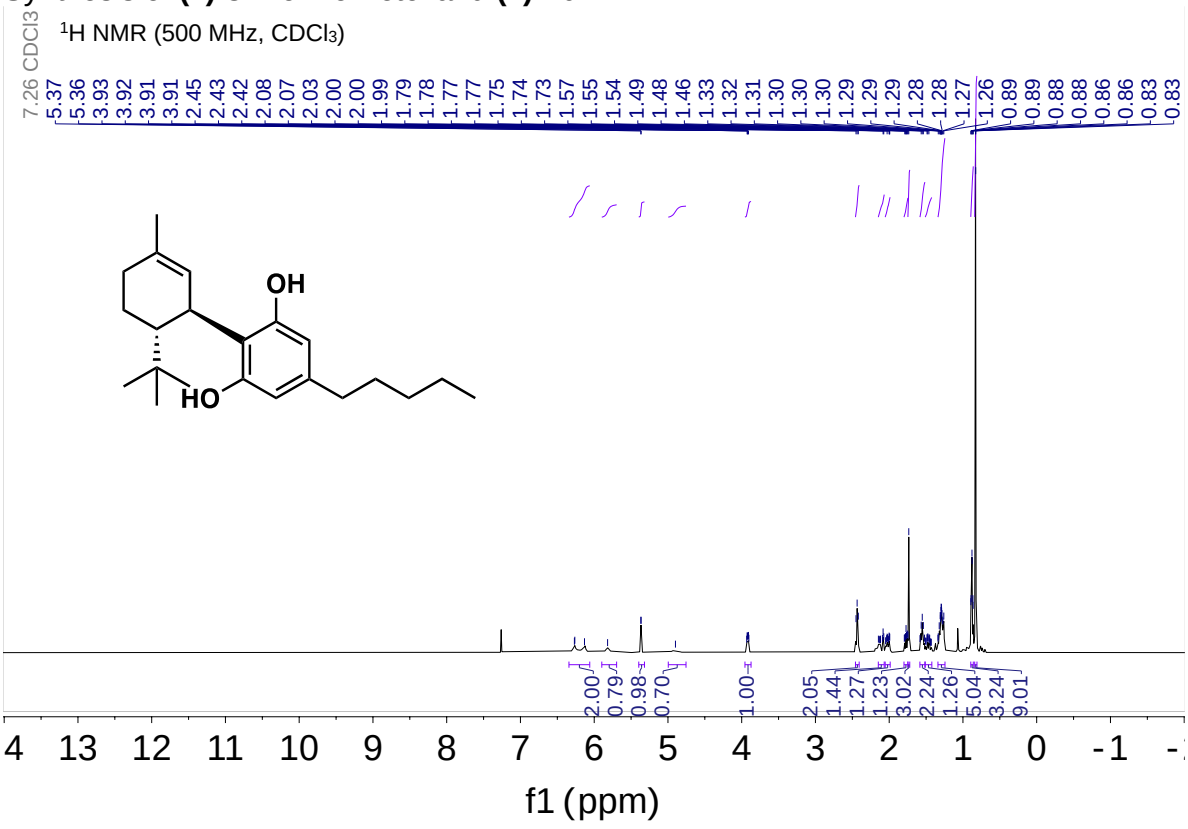
2D NOESY NMR analysis of **(±)-6e**

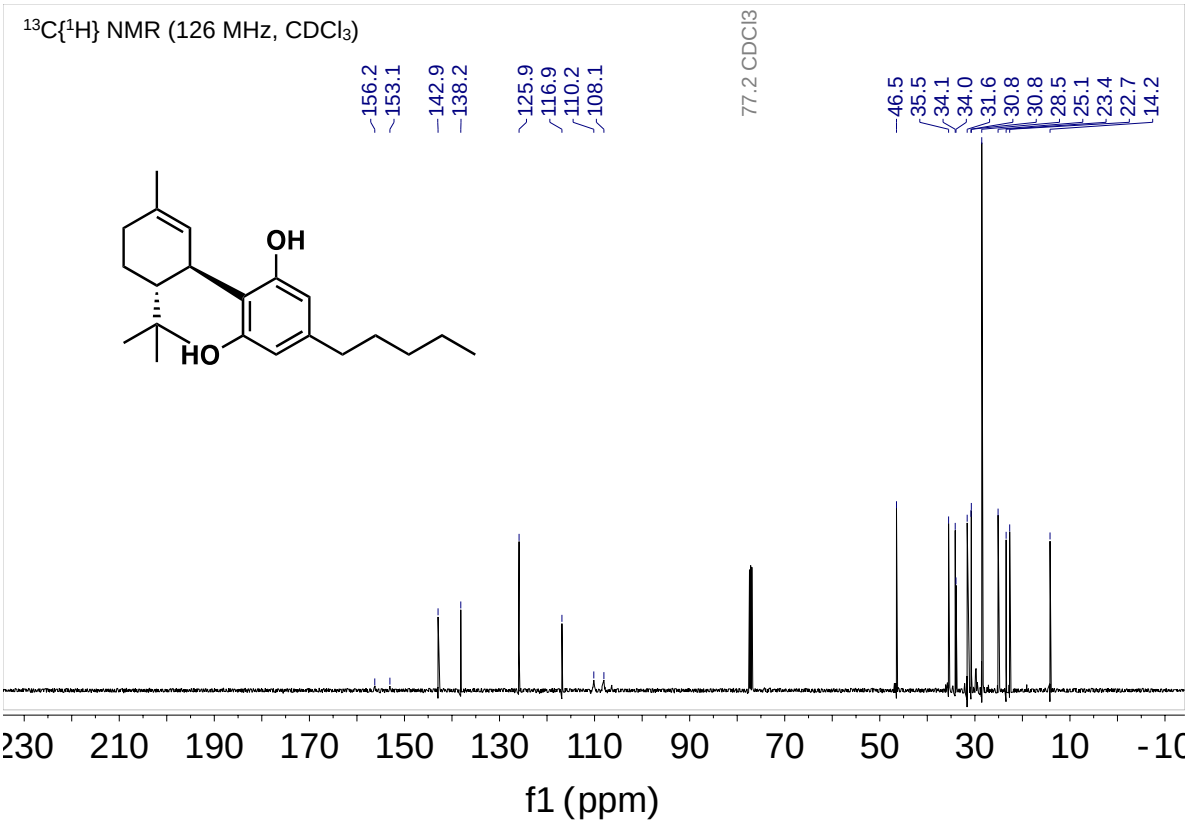




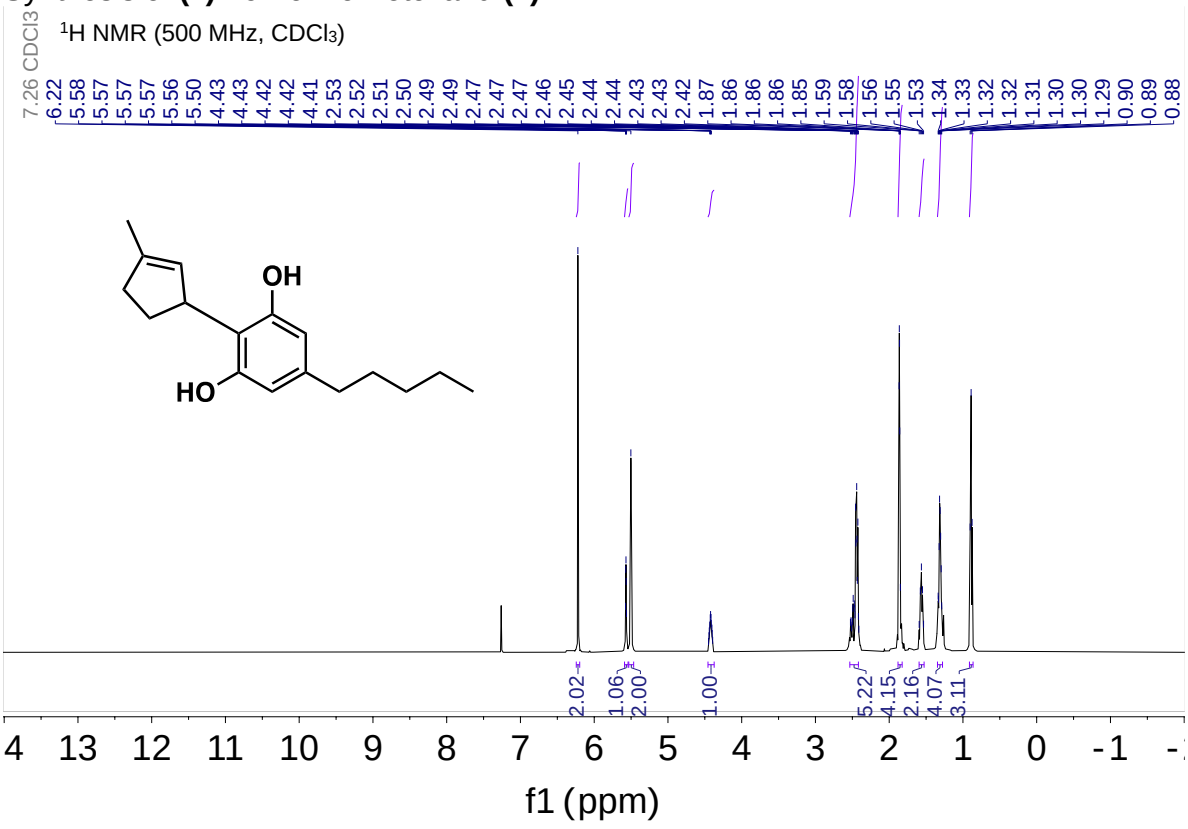


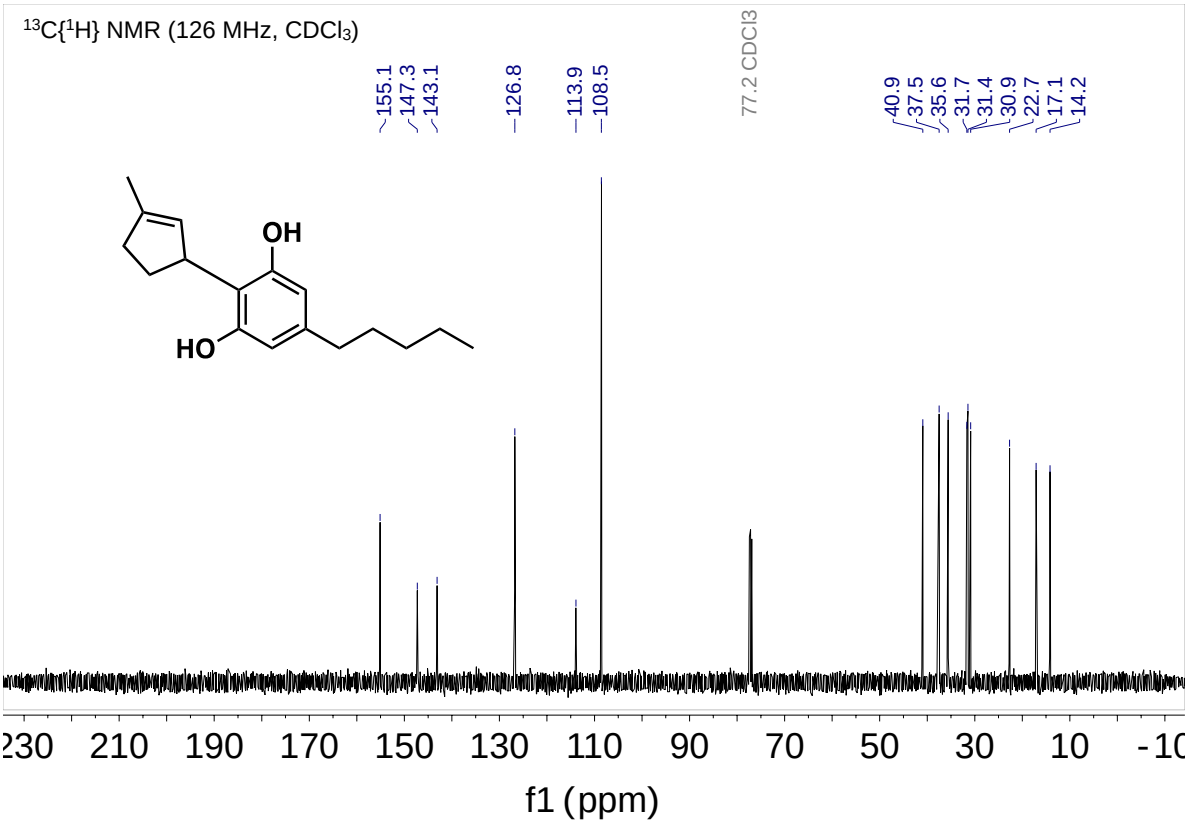
Synthesis of **(±)-3f** from olivetol and **(±)-10f**:





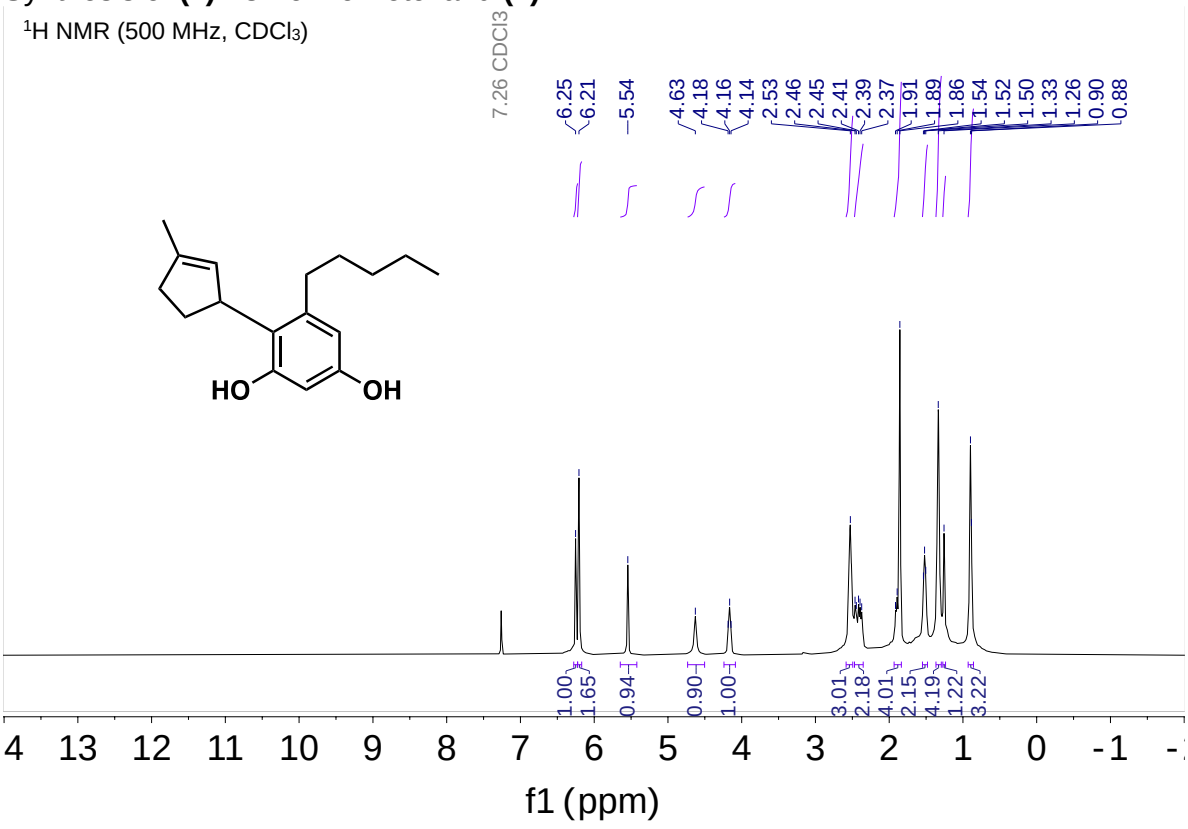
Synthesis of **(±)-19** from olivetol and **(±)-17**:



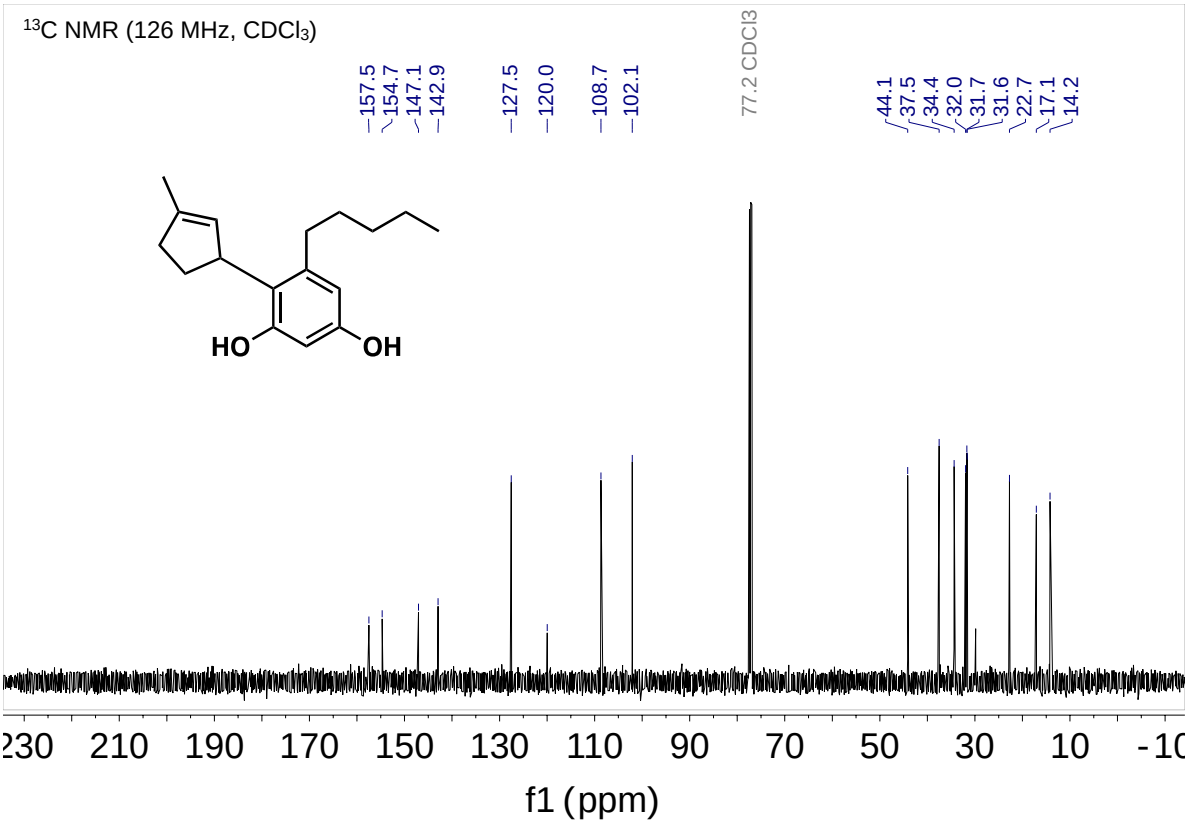


Synthesis of **(±)-18** from olivetol and **(±)-17**:

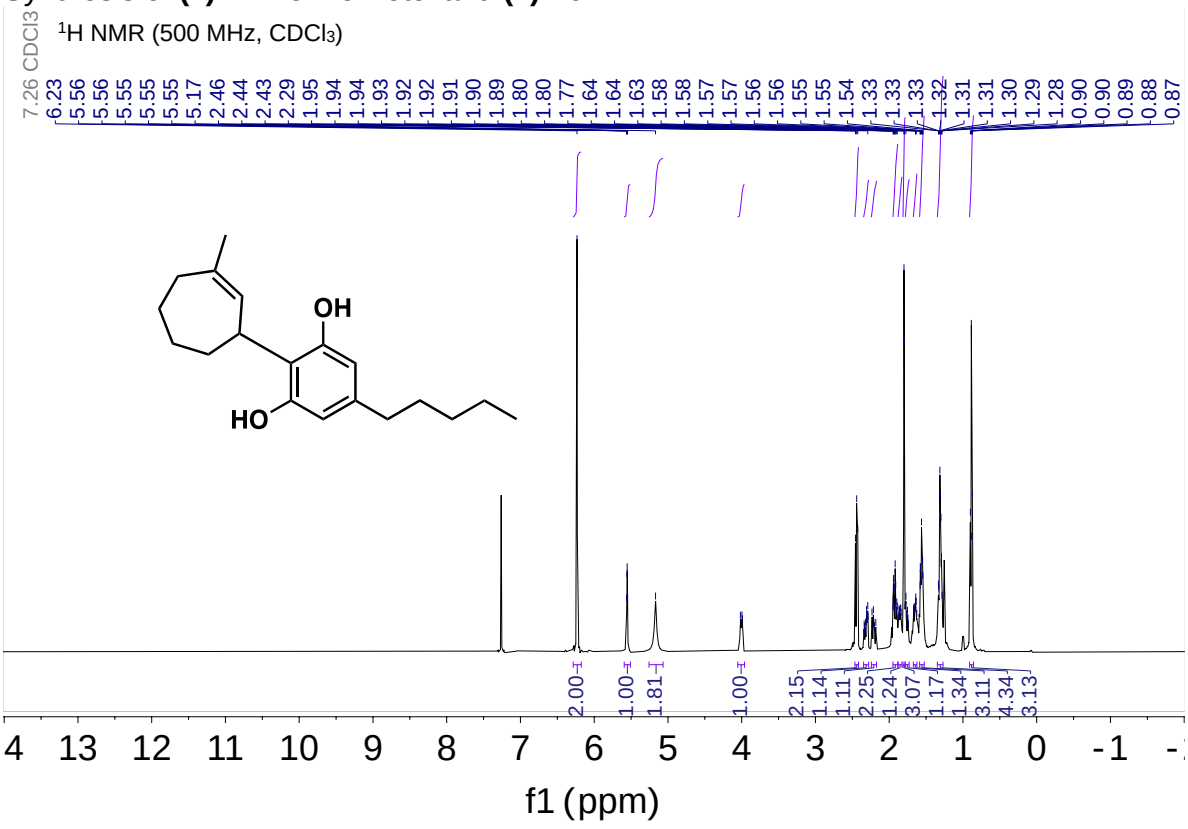
^{1}H NMR (500 MHz, $CDCl_3$)

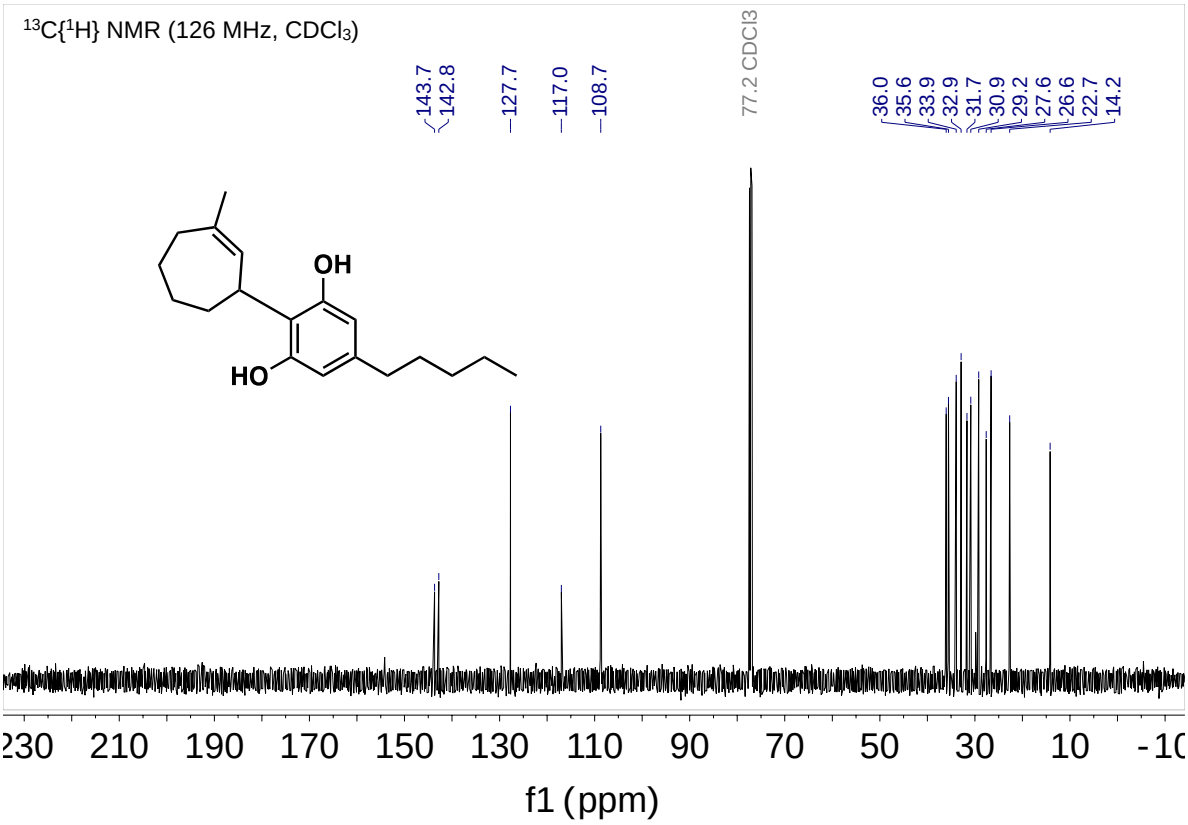


^{13}C NMR (126 MHz, $CDCl_3$)

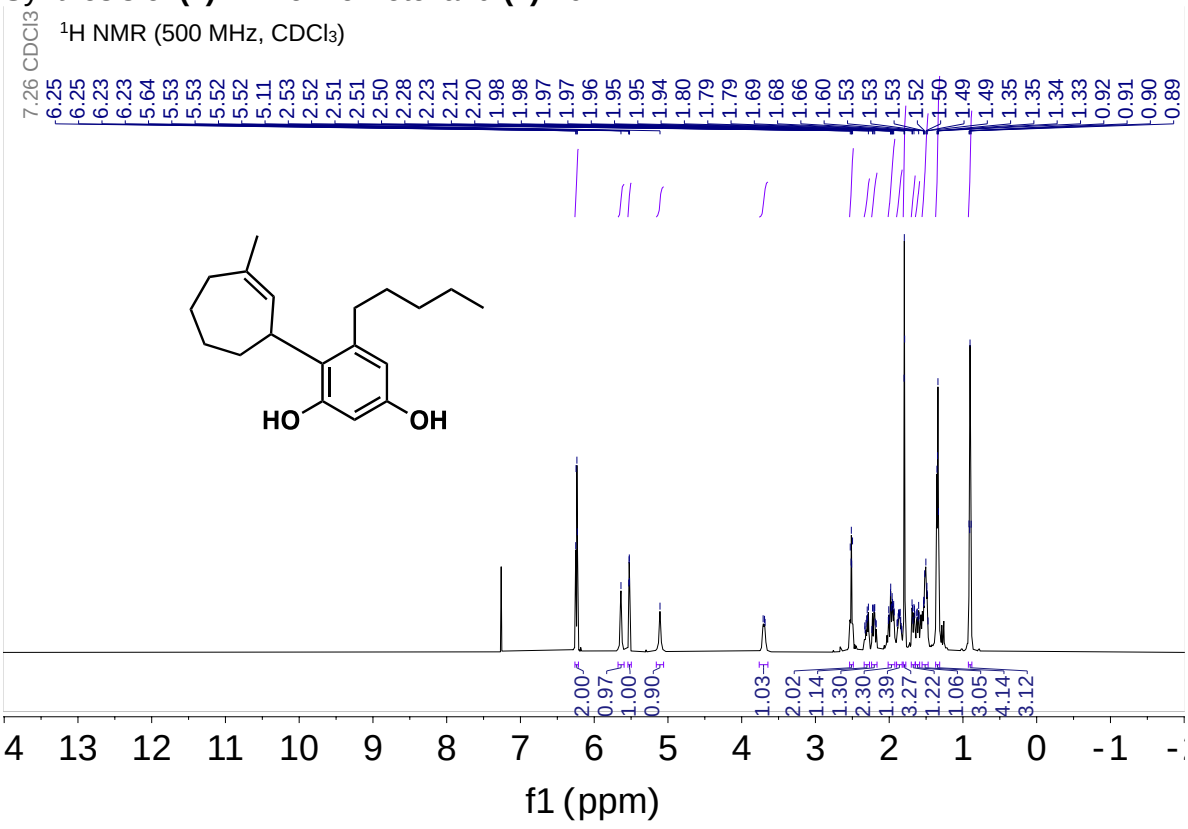


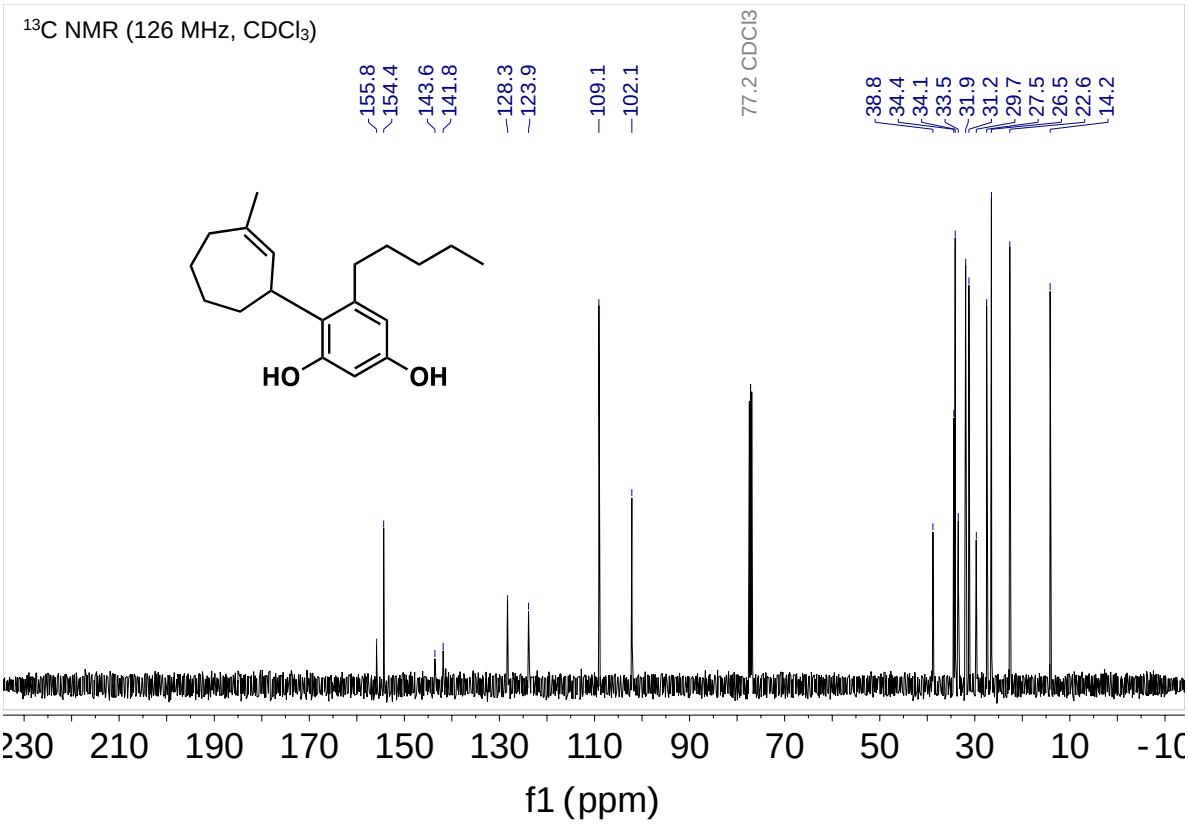
Synthesis of **(±)-22** from olivetol and **(±)-20**:



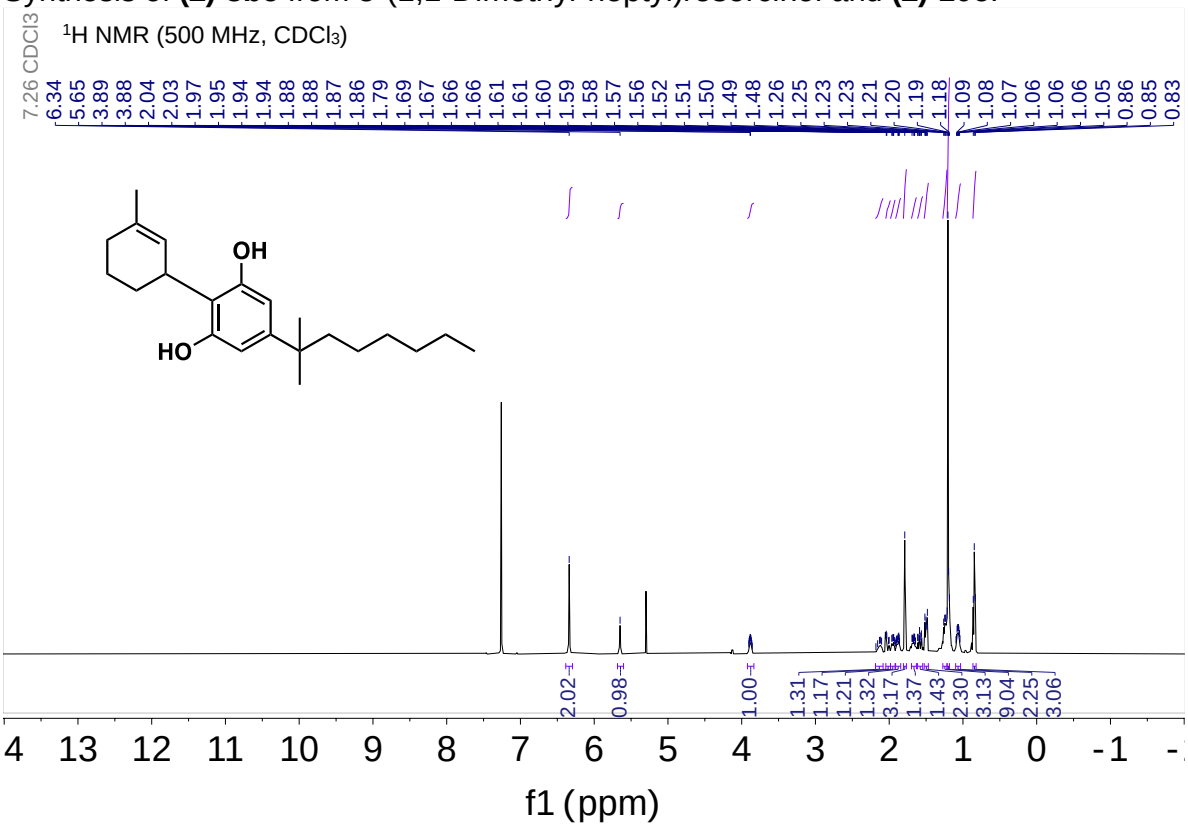


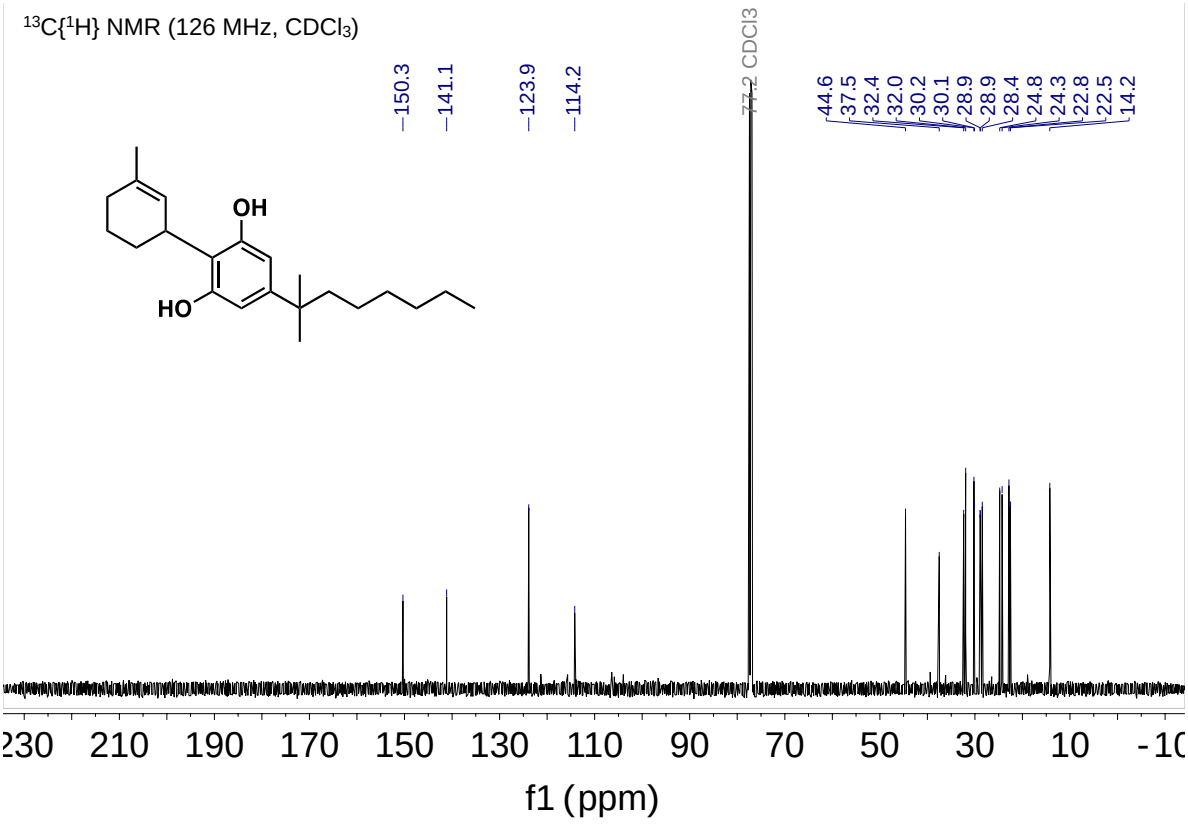
Synthesis of **(±)-21** from olivetol and **(±)-20**:



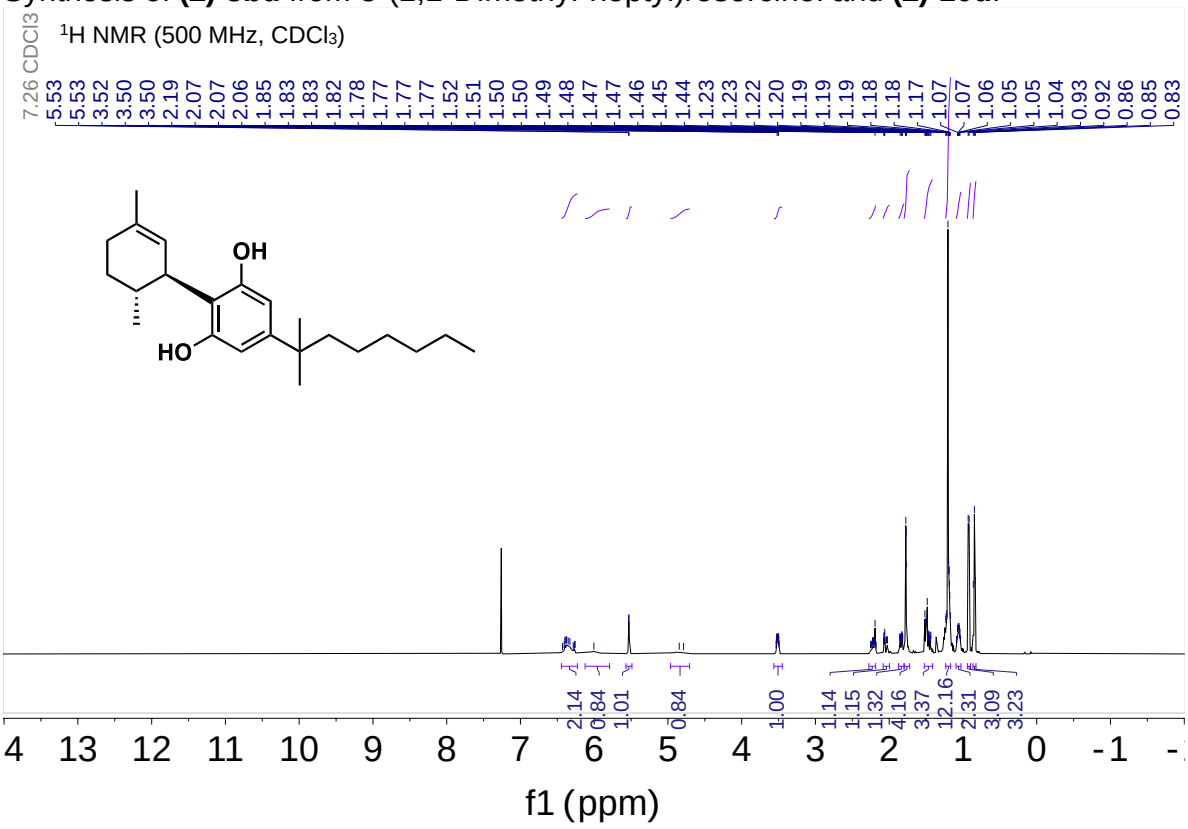


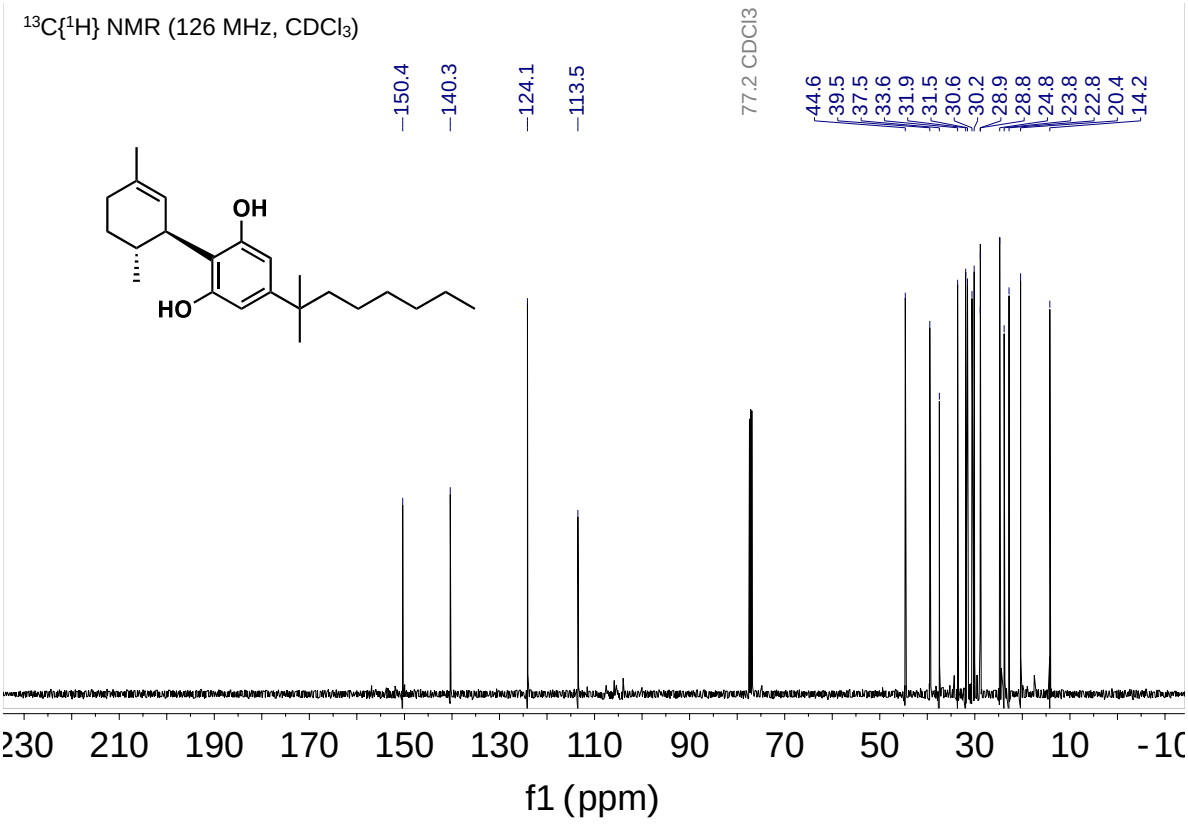
Synthesis of **(±)-3bc** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10c**:





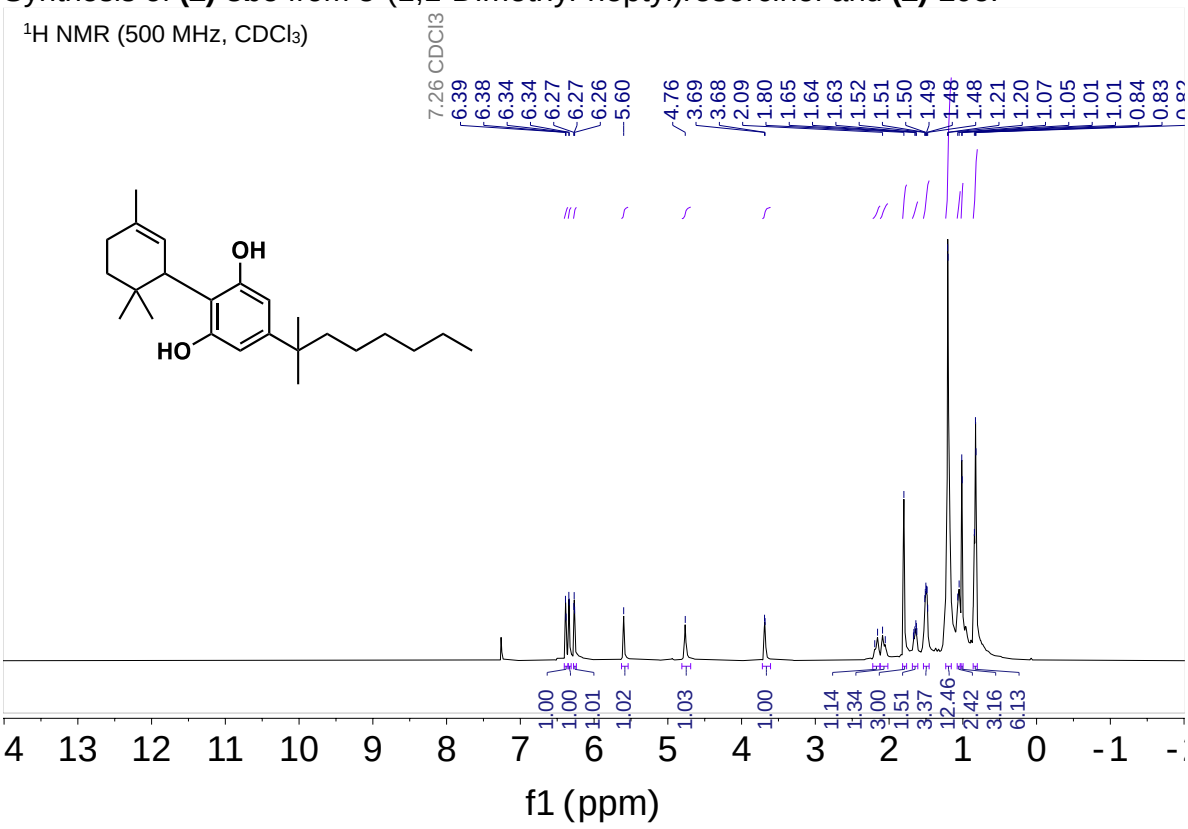
Synthesis of **(±)-3bd** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10d**:



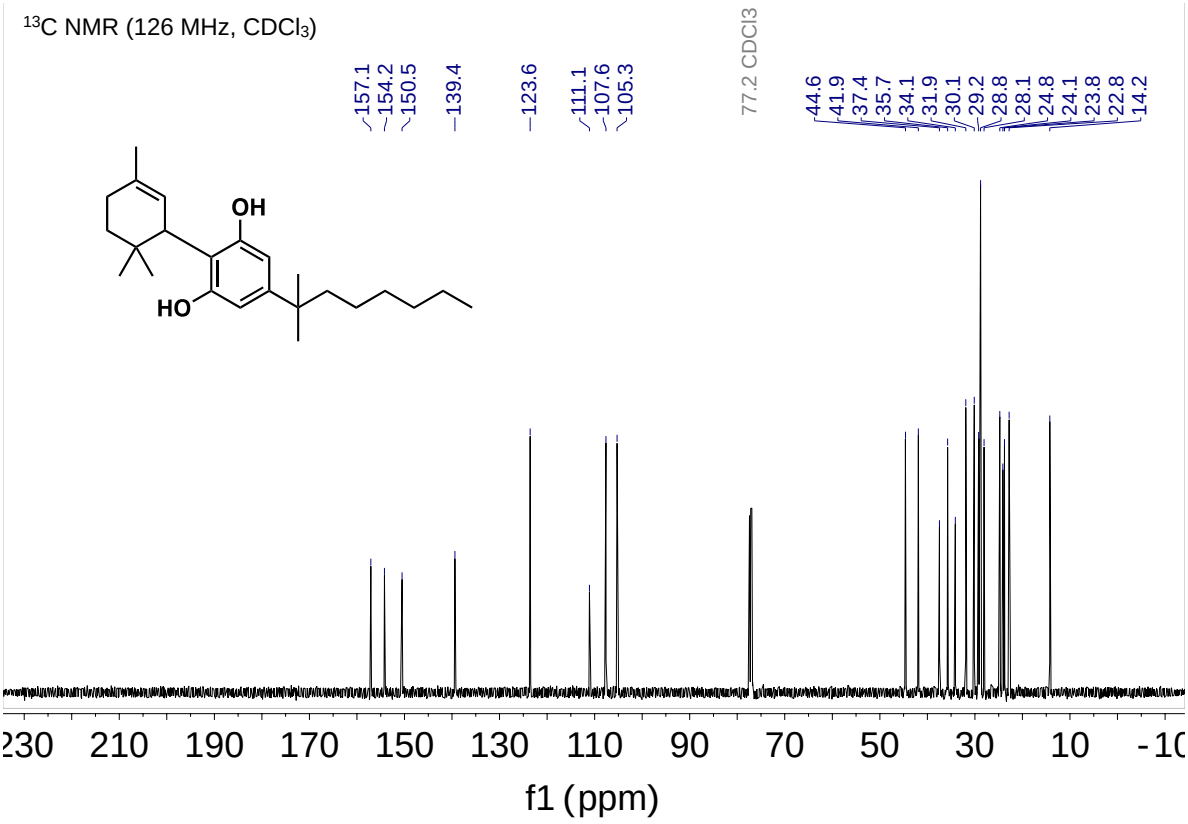


Synthesis of **(±)-3be** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10e**:

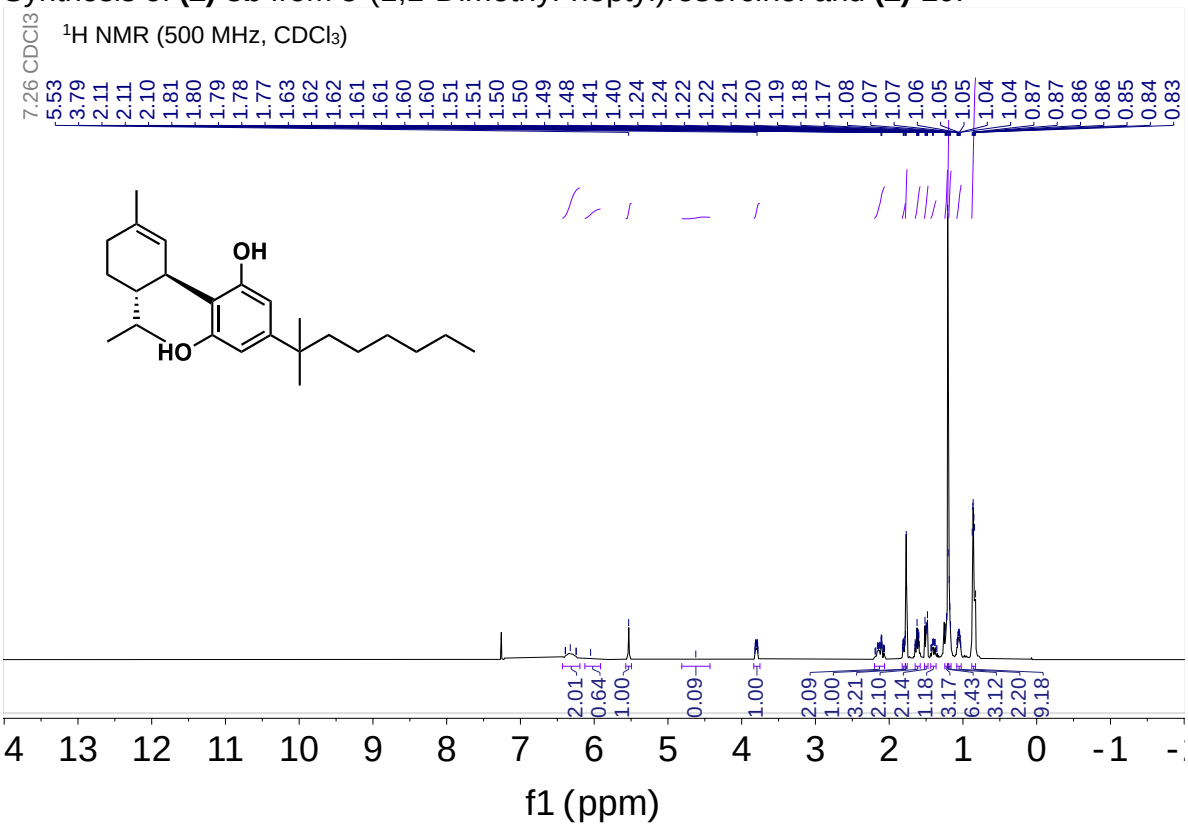
^{1}H NMR (500 MHz, $CDCl_3$)

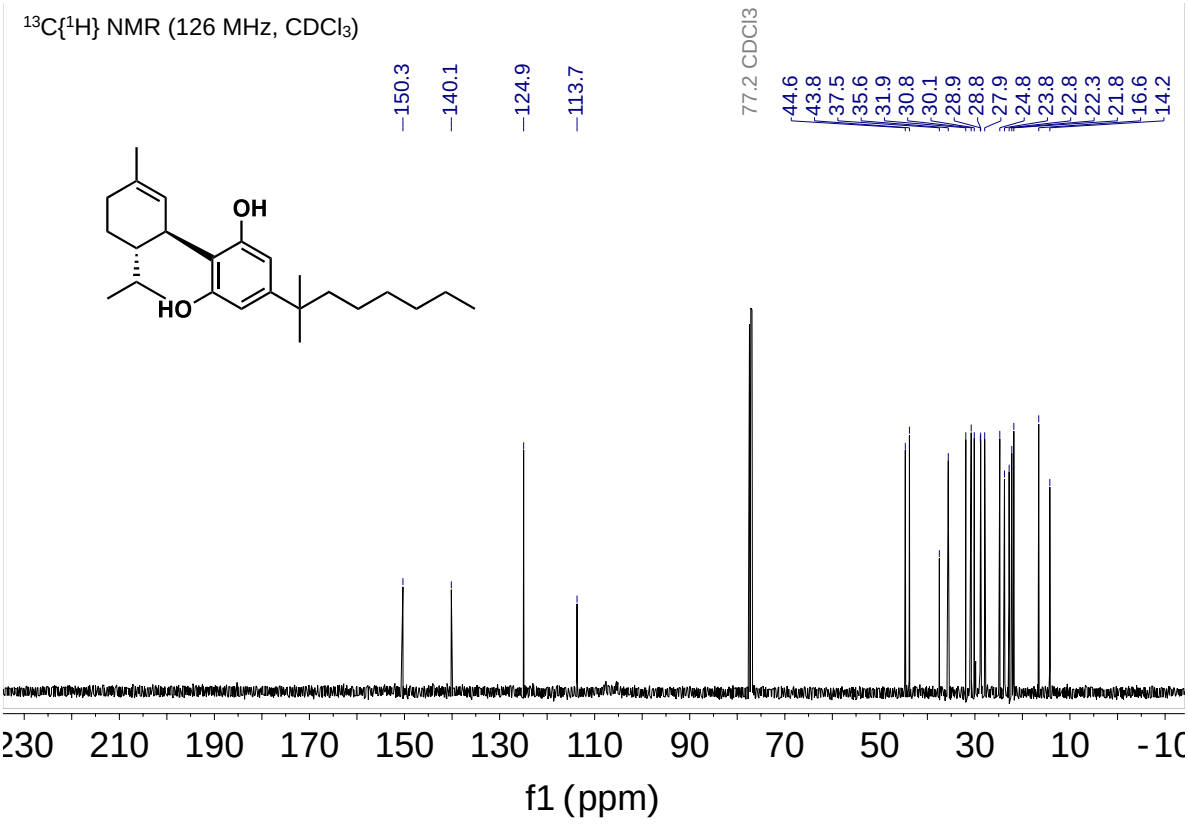


^{13}C NMR (126 MHz, $CDCl_3$)

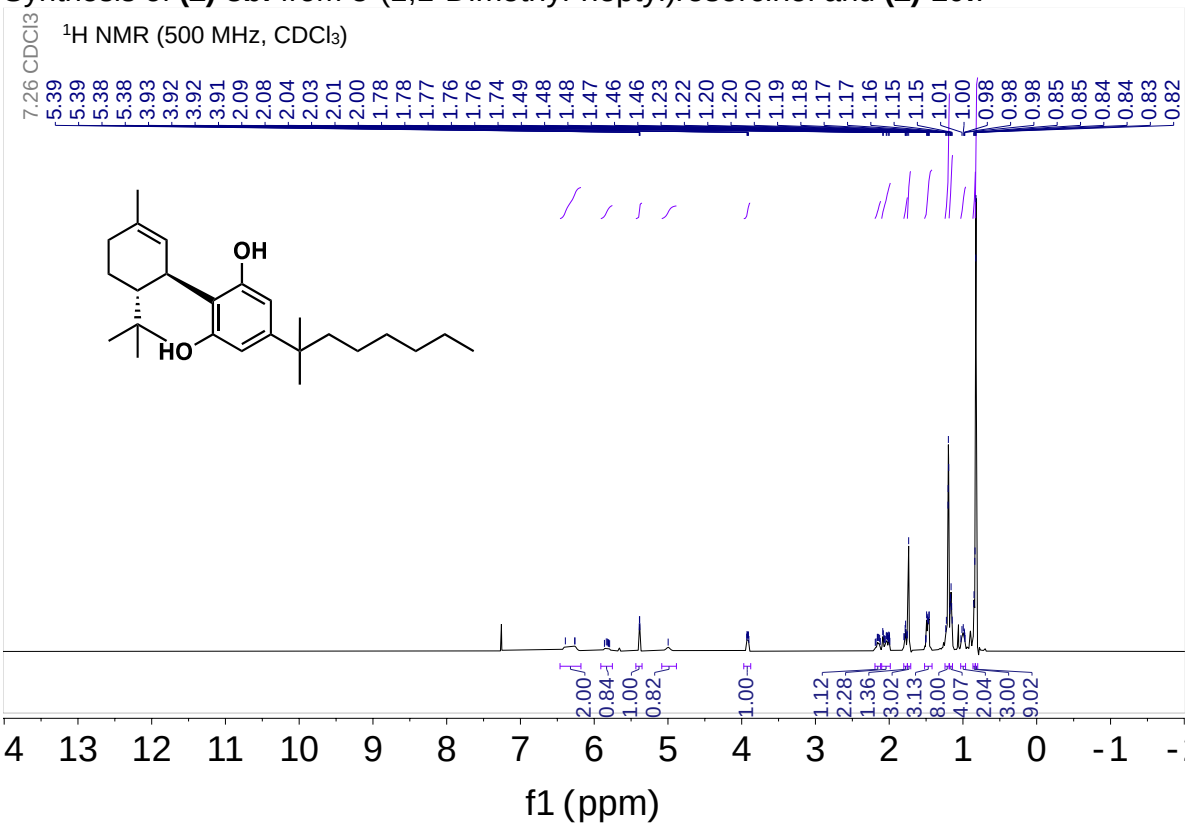


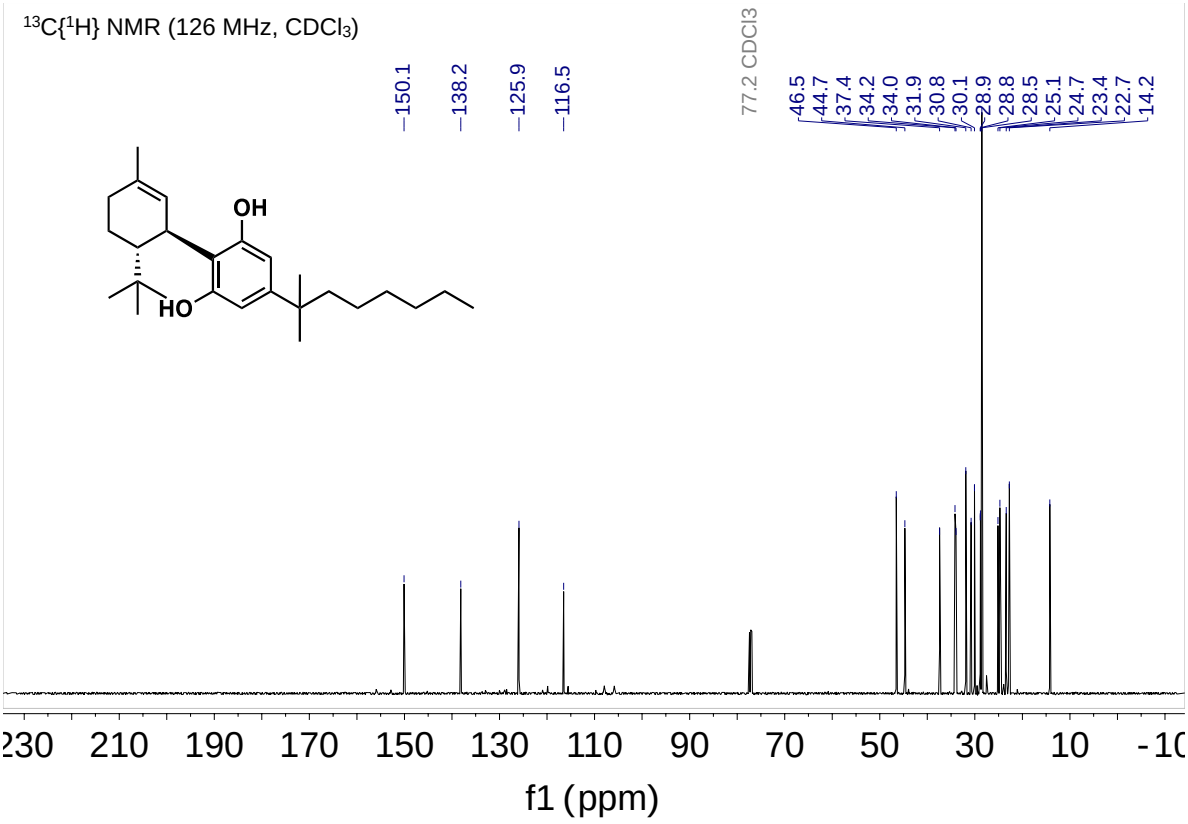
Synthesis of **(±)-3b** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10**:



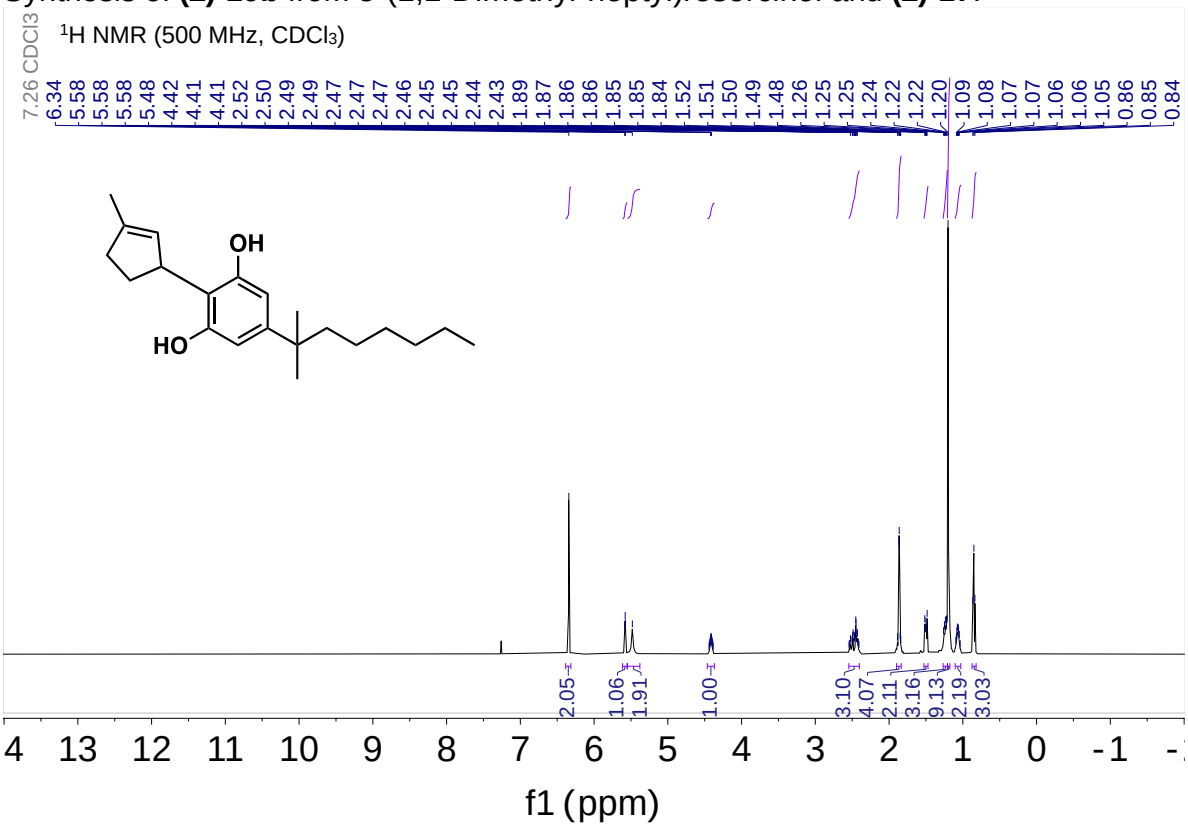


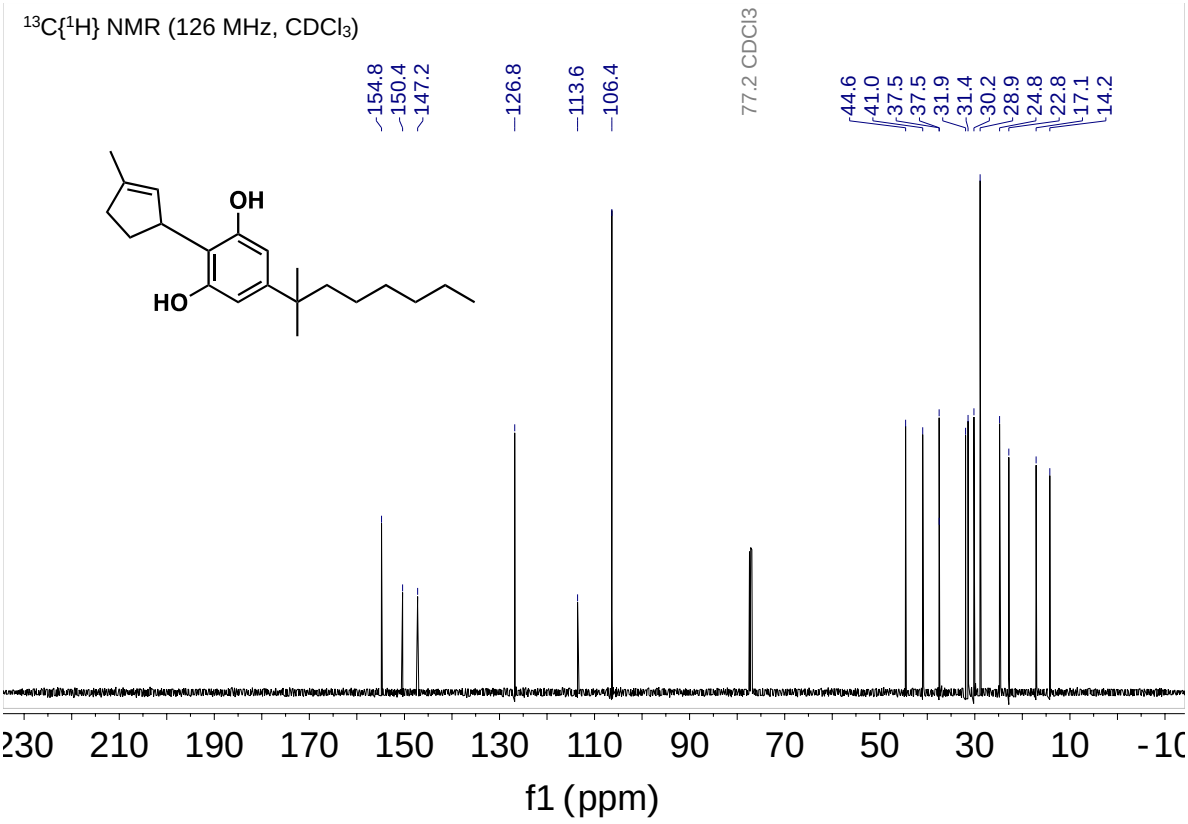
Synthesis of **(±)-3bf** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-10f**:





Synthesis of **(±)-19b** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-17**:





Synthesis of **(±)-22b** from 5-(1,1-Dimethyl-heptyl)resorcinol and **(±)-20**: