Electronic Supplementary Information for the manuscript entitled:

Questioning the γ-gauche effect: stereoassignment of 1,3-disubstituted-tetrahydro-β-carbolines using ^{1}H-^{1}H coupling constants

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Table S1. ^{13}C NMR chemical shifts ($CDCl_3$) of C-1 and C-3 for **7a-ae** and **8a-ae**.

	C-3 [ppm]			C-1 [ppm]		
	7	**8**	**Δ_{7-8}**	**7**	**8**	**Δ_{7-8}**
a 2',4'-Cl_2	52.34[c]	56.7[b]	-4.3	51.3[b]	53.9[b]	-2.6
b H	52.7[b]	57.0[b]	-4.3	55.1[b]	58.8[b]	-3.8
c[e] 2'-Cl	52.23	56.8	-4.58	51.8	54.4	-2.6
d[e] 4'-Cl	52.5	56.9	-4.4	54.3	58.1	-3.8
e[e,g] 2'-Cl, 4'-Me	52.0	56.7	-4.7	51.4	53.9	-2.5
f[e] 2'-Me, 4'-Cl	52.6	57.0	-4.4	51.4	53.5	-2.1
g[e] 2',4'-F_2	52.4[b]	56.8[b]	-4.4	47.8[b]	50.6[b]	-2.8
h[e] 2'-F,4'-Cl	52.6	56.8	-4.3	47.9[a]	50.6[a]	-2.7
I 2'-Cl,4'-F	52.30[c]	56.7[b]	-4.4	51.2[b]	53.8[b]	-2.6
j[e,g] 2'-Cl,4'-Br	52.2	56.6	-4.4	51.2	53.9	-2.7
k 2'-Br,4'-Cl	52.36[c]	56.7[b]	-4.3	53.7[b]	56.6[b]	-2.9
l 2',4'-Br_2	52.1[c]	56.57[c]	-4.5	53.7[b]	56.57[c]	-2.8
m 2'-I,4'-F	52.46[c]	56.8[b]	-4.3	58.0[b]	61.6[b]	-3.6
n 2'-F,4'-I	52.5[c]	56.8[b]	-4.3	48.0[b]	50.7[b]	-2.7
o 2'-Br,4'-I	52.36[c]	56.7[b]	-4.3	53.9[b]	56.8[b]	-2.9
p 2'-Cl,4'-OMe	52.2[c]	56.9[b]	-4.7	51.3[b]	53.9[b]	-2.6
q 2'-OMe,4'-Cl	52.29[c]	57.0[b]	-4.7	48.8[b]	51.3[b]	-2.5
r 2'-Cl,4'-CO_2Me	52.30[c]	56.7[b]	-4.4	51.6[b]	54.3[b]	-2.7
s[e,g] 2',4'-$(CF_3)_2$	53.0	56.6	-3.6	49.8	53.4	-3.6
t[e,g] 2',4'-Me_2	52.4	57.0	-4.6	51.4	53.5	-2.1
u[e] 2',4'-$(OMe)_2$	51.9	57.0	-5.1	49.0	51.5	-2.5
v 3',4'-Cl_2	52.5[c]	56.8[b]	-4.3	53.9[b]	57.9[b]	-4.0
w[e] 3',4'-$(OMe)_2$	53.0	57.1	-4.1	54.8	58.7	-3.9
x 2',6'-F_2,4'-Cl	53.9[b]	57.3[b]	-3.4	44.6[b]	48.0[b]	-3.4
y 2',3',4'-F_3	52.39[c]	56.7[b]	-4.3	47.9[b]	50.5[b]	-2.6
z[e,g] 2'-Br,4'-F,5'-OMe	53.1	56.7	-3.6	53.5	56.4	-2.9
aa Bu	52.7	56.6	-3.9	50.4	52.9	-2.5
ab Cy	53.5	56.6	-3.1	55.4	57.8	-2.4
ac $CHEt_2$	54.1	56.6	-2.5	51.0	54.6	-3.6
ad *t*-Bu	54.4	56.5	-2.1	59.4	62.6	-3.2
ae *i*-Bu	52.5	56.6	-4.1	48.2	50.7	-2.5
Average	52.6	56.8	-4.1	51.7	54.6	-2.9
St. deviation	0.6	0.2	0.6	3.2	3.4	0.5

Signals identified via: [a]JCF, [b]HSQC, [c](C)DEPT and HSQC, [d]HMBC and HSQC. [e]Sample is unavailable. [g]Sample and NMR data unavailable. [h]If the values are identical, only one of them is shown. [e,g]Shifts were assigned based on the pattern seen in proven compounds, unless stated otherwise.

Table S2. ^{13}C NMR chemical shifts ($CDCl_3$) of C=O and C1' for **7a-ae** and **8a-ae**.

		C=O [ppm]			C-1' [ppm]		
		7	**8**	**Δ_{7-8}**	**7**	**8**	**Δ_{7-8}**
a[a]	2',4'-Cl_2	173.8	173.1	0.8	137.9	137.4	0.5
b[a]	H	174.3	173.3	1.0	142.1	140.8	1.3
c[d]	2'-Cl	173.9	173.2	0.7	–	–	–
d[d]	4'-Cl	174.1	173.2	0.9	–	–	–
e[d,e]	2'-Cl, 4'-Me	173.7	173.1	0.6	–	–	–
f[d]	2'-Me, 4'-Cl	174.3	173.3	1.0	–	–	–
g[b,d]	2',4'-F_2	173.9	173.2	0.7	125.2	124.0	1.2
h[c,d]	2'-F,4'-Cl	173.9	173.1	0.8	128.0	126.7	1.3
i[a,b]	2'-Cl,4'-F	173.4	173.1	0.3	135.3	134.7	0.6
j[d,e]	2'-Cl,4'-Br	173.7	172.9	0.8	–	–	–
k[a]	2'-Br,4'-Cl	173.8	173.1	0.8	139.5	139.2	0.3
l[a]	2',4'-Br_2	173.7	173.0	0.7	139.9	139.5	0.4
m[a,b]	2'-I,4'-F	173.9	173.1	0.8	139.8	139.5	0.3
n[b]	2'-F,4'-I	173.9	173.1	0.8	129.2	128.0	1.2
o[a]	2'-Br,4'-I	173.8	173.0	0.8	140.7	140.4	0.3
p[a]	2'-Cl,4'-OMe	173.9	173.2	0.7	131.2	130.5	0.7
q[a]	2'-OMe,4'-Cl	174.1	173.4	0.7	128.8	127.9	0.9
r[a]	2'-Cl,4'-CO_2Me	173.8	173.1	0.7	144.1	143.7	0.4
s[d,e]	2',4'-$(CF_3)_2$	173.8	172.8	1.0	–	–	–
t[d,e]	2',4'-Me_2	174.2	173.3	0.9	–	–	–
u[d]	2',4'-$(OMe)_2$	174.0	173.5	0.5	–	–	–
v[a]	3',4'-Cl_2	174.1	173.1	1.0	142.4	141.2	1.2
w[d]	3',4'-$(OMe)_2$	174.4	173.3	1.1	–	–	–
x[b]	2',6'-F_2,4'-Cl	174.1	173.2	1.0	116.7	114.8	1.9
y[b]	2',3',4'-F_3	173.8	173.1	0.7	126.7	125.6	1.1
z[d,e]	2'-Br,4'-F,5'-OMe	173.9	172.9	1.0	–	–	–
aa[a]	Bu	174.4	173.9	0.5	35.5	34.7	0.8
ab[b]	Cy	174.7	174.0	0.7	43.3	42.5	0.8
ac[b]	$CHEt_2$	174.7	174.1	0.6	46.7	46.1	0.6
ad[a]	*t*-Bu	175.1	174.0	1.1	36.8	35.7	1.1
ae[b]	*i*-Bu	174.4	173.9	0.5	44.5	44.5	0.0
Average		174.0	173.3	0.8	–	–	–
St. deviation		0.4	0.3	0.2	–	–	–
Average a-z		173.9	173.1	0.8	134.2	133.4	0.9
St. deviation a-z		0.2	0.2	0.2	7.8	8.2	0.5
Average aa-ae		174.7	174.0	0.7	41.4	40.7	0.7
St. deviation aa-ae		0.3	0.1	0.2	4.9	5.2	0.4

Carbonyl shifts assigned based on a characteristic δ [ppm] since both are isolated in their area. C1' signals identified via: [a]HMBC, [b]HSQC and J_{CF}, [c]J_{CF}. [d]Archival sample was unavailable. [e] Sample and 2D NMR data unavailable.

Table S3. ^{1}H NMR chemical shifts ($CDCl_3$) of H-3, H-4α, and H-4β for **7a**-**ae** and **8a**-**ae**.

		δ H-3 [ppm]			δ H-4α [ppm]			δ H-4β [ppm]		
		7	**8**	**Δ_{7-8}**	**7**	**8**	**Δ_{7-8}**	**7**	**8**	**Δ_{7-8}**
a	2',4'-Cl_2	3.84	3.99	-0.15	3.26	3.25	0.01	3.10	3.02	0.08
b	H	3.98	3.99	-0.01	3.28	3.24	0.04	3.14	3.02	0.12
c	2'-Cl	3.86	4.00	-0.14	3.27	3.25	0.02	3.09	3.04	0.05
d	4'-Cl	3.91	3.95	-0.04	3.26	3.24	0.02	3.11	3.01	0.10
e	2'-Cl, 4'-Me	3.81	3.96	-0.15	3.22	3.21	0.01	3.04	3.00	0.04
f	2'-Me, 4'-Cl	3.89	3.96	-0.07	3.25	3.24	0.01	3.11	2.99	0.12
g	2',4'-F_2	3.89	3.97	-0.08	3.24	3.24	0.00	3.07	3.01	0.06
h	2'-F,4'-Cl	3.90	3.98	-0.08	3.25	3.23	0.02	3.08	3.00	0.08
i	2'-Cl,4'-F	3.85	4.00	-0.15	3.26	3.24	0.02	3.09	3.02	0.07
j	2'-Cl,4'-Br	3.84	3.99	-0.15	3.26	3.24	0.02	3.10	3.01	0.09
k	2'-Br,4'-Cl	3.85	4.00	-0.15	3.26	3.24	0.02	3.10	3.02	0.08
l	2',4'-Br_2	3.82	3.98	-0.16	3.25	3.25	0.00	3.08	3.03	0.05
m	2'-I,4'-F	3.88	4.01	-0.13	3.26	3.24	0.02	3.12	3.02	0.10
n	2'-F,4'-I	3.89	3.97	-0.08	3.24	3.23	0.01	3.08	2.99	0.09
o	2'-Br,4'-I	3.85	3.99	-0.14	3.25	3.24	0.01	3.10	3.01	0.09
p	2'-Cl,4'-OMe	3.85	4.00	-0.15	3.25	3.23	0.02	3.08	3.01	0.07
q	2'-OMe,4'-Cl	3.82	3.97	-0.15	3.22	3.21	0.01	3.03	2.98	0.05
r	2'-Cl,4'-CO_2Me	3.85	4.01	-0.16	3.27	3.25	0.02	3.10	3.03	0.07
s	2',4'-$(CF_3)_2$	4.00	4.02	-0.02	3.30	3.30	0.00	3.23	3.09	0.14
t	2',4'-Me_2	3.90	3.93	-0.03	3.22	3.20	0.02	3.08	2.97	0.11
u	2',4'-$(OMe)_2$	3.80	3.96	-0.16	3.21	3.21	0.00	3.14	3.00	0.14
v	3',4'-Cl_2	3.94	3.95	-0.01	3.27	3.23	0.04	3.14	3.00	0.14
w	3',4'-$(OMe)_2$	4.00	3.96	0.04	3.27	3.23	0.04	3.15	3.02	0.13
x	2',6'-F_2,4'-Cl	4.12	3.97	0.15	3.28	3.23	0.05	3.15	2.97	0.18
y	2',3',4'-F_3	3.89	3.97	-0.08	3.24	3.24	0.00	3.06	3.00	0.06
z	2'-Br,4'-F,5'-OMe	3.99	4.00	-0.01	3.29	3.24	0.05	3.20	3.03	0.17
aa	Bu	3.99	3.80	0.19	3.12	3.13	-0.01	2.99	2.82	0.17
ab	Cy	4.02	3.74	0.28	3.10	3.11	-0.01	3.00	2.78	0.22
ac	$CHEt_2$	4.05	3.74	0.31	3.12	3.12	0.00	3.12	2.78	0.34
ad	*t*-Bu	4.09	3.68	0.41	3.11	3.14	-0.03	3.08	2.77	0.31
ae	*i*-Bu	3.99	3.80	0.19	3.13	3.14	-0.01	3.00	2.83	0.17
Average		3.91	3.94	-0.03	3.23	3.22	0.01	3.10	2.98	0.12
St. deviation		0.09	0.09	0.16	0.06	0.04	0.02	0.05	0.08	0.07
Average a-z		3.89	3.98	-0.09	3.26	3.24	0.02	3.11	3.01	0.10
St. deviation a-z		0.07	0.02	0.08	0.02	0.02	0.01	0.04	0.02	0.04
Average aa-ae		4.03	3.75	0.28	3.12	3.13	-0.01	3.04	2.80	0.24
St. deviation aa-ae		0.04	0.05	0.09	0.01	0.01	0.01	0.06	0.03	0.08

Table S4. J_{HH} [Hz] values ($CDCl_3$) for H-3, H-4α, and H-4β for **7a-ae** and **8a-ae**.

		7	**8**	**7**	**8**	**7**	**8**	**7**	**8**	**7**	**8**
		$^2J_{4\alpha\text{-}4\beta}$	$^2J_{4\alpha\text{-}4\beta}$	$^3J_{4\alpha\text{-}3}$	$^3J_{4\alpha\text{-}3}$	$^3J_{4\beta\text{-}3}$	$^3J_{4\beta\text{-}3}$	$^5J_{4\alpha\text{-}1}$	$^5J_{4\alpha\text{-}1}$	$^5J_{4\beta\text{-}1}$	$^5J_{4\beta\text{-}1}$
a	2',4'-Cl_2	15.4	15.1	5.0	4.1	7.8	11.0	1.2	1.9	1.5	2.5
b	H	15.4	15.2	5.4	4.3	6.8	11.2	1.4	1.9	1.6	2.6
c	2'-Cl	15.3	15.1	4.9	4.1	8.1	11.0	1.1	1.8	1.5	2.5
d	4'-Cl	15.5	15.2	5.4	4.2	7.0	11.2	1.3	1.9	1.6	2.6
e	2'-Cl, 4'-Me	15.0	15.0	5.0	4.0	8.0	11.0	1.0	2.0	1.5	2.5
f	2'-Me, 4'-Cl	15.4	15.1	5.3	4.2	7.0	11.1	1.3	1.9	1.6	2.6
g	2',4'-F_2	15.4	15.1	5.0	4.2	7.9	11.1	1.1	1.8	1.5	2.5
h	2'-F,4'-Cl	15.4	15.1	5.1	4.2	7.7	11.1	1.1	1.9	1.4	2.5
i	2'-Cl,4'-F	15.4	15.1	5.0	4.1	7.8	11.0	1.2	1.8	1.5	2.5
j	2'-Cl,4'-Br	15.4	15.1	5.0	4.1	7.7	11.0	1.2	1.9	1.6	2.5
k	2'-Br,4'-Cl	15.4	15.1	5.0	4.1	7.6	11.0	1.2	1.8	1.5	2.5
l	2',4'-Br_2	15.4	15.1	4.9	4.1	8.0	11.0	1.1	1.9	1.5	2.5
m	2'-I,4'-F	15.4	15.1	5.2	4.1	7.1	11.1	1.3	1.8	1.6	2.5
n	2'-F,4'-I	15.4	15.1	5.1	4.2	7.8	11.1	1.1	1.9	1.6	2.5
o	2'-Br,4'-I	15.3	15.1	5.1	4.1	7.6	11.0	1.2	1.8	1.5	2.5
p	2'-Cl,4'-OMe	15.3	15.1	4.9	4.2	8.1	11.0	1.1	1.9	1.5	2.6
q	2'-OMe,4'-Cl	15.2	15.1	4.8	4.2	8.7	11.0	0.9	1.9	1.5	2.6
r	2'-Cl,4'-CO_2Me	15.4	15.1	5.0	4.1	7.8	11.0	1.2	1.8	1.5	2.5
s[a]	2',4'-$(CF_3)_2$	15.5	15.1	5.5	4.0	5.5	11.1	1.5	1.8	1.5	2.4
t	2',4'-Me_2	15.0	15.0	5.0	4.0	7.0	11.0	1.5	1.5	1.5	2.0
u	2',4'-$(OMe)_2$	15.2	15.0	4.7	4.2	9.4	11.0	0.8	1.9	1.3	2.6
v[b]	3',4'-Cl_2	15.5	15.1	5.5	4.1	6.4	11.2	1.4	1.8	1.6	2.5
w[b]	3',4'-$(OMe)_2$	15.5	15.1	5.6	4.3	6.3	11.2	1.5	1.9	1.6	2.6
x[b]	2',6'-F_2,4'-Cl	15.4	15.3	5.4	4.4	6.0	11.2	1.6	1.9	1.8	2.6
y	2',3',4'-F_3	15.4	15.2	5.0	4.1	7.9	11.1	1.1	1.9	1.6	2.5
z[b]	2'-Br,4'-F,5'-OMe	15.4	15.0	5.5	4.1	5.7	11.1	1.6	1.8	1.6	2.5
aa	Bu	15.3	15.1	5.3	4.2	7.3	11.2	1.2	1.9	1.5	2.6
ab	Cy	15.3	14.9	5.3	4.1	6.9	11.2	1.3	1.8	1.5	2.6
ac[a]	$CHEt_2$	–	15.0	5.4	4.1	5.4	11.2	1.7	1.9	1.7	2.6
ad[b]	*t*-Bu	15.0	14.6	5.1	3.6	5.3	11.2	1.5	1.5	1.6	2.4
ae	*i*-Bu	15.4	15.0	5.3	4.2	7.4	11.2	1.2	1.9	1.5	2.6
Average		15.3	15.1	5.2	4.1	7.3	11.1	1.3	1.8	1.5	2.5
St. deviation		0.1	0.1	0.2	0.1	1.0	0.1	0.2	0.1	0.1	0.1
Average a-z		15.4	15.1	5.1	4.1	7.4	11.1	1.2	1.9	1.5	2.5
St. deviation a-z		0.1	0.1	0.2	0.1	0.9	0.1	0.2	0.1	0.1	0.1
Average aa-ae		15.3	14.9	5.3	4.0	6.5	11.2	1.4	1.8	1.6	2.6
St. deviation aa-ae		0.2	0.2	0.1	0.3	1.0	0.0	0.2	0.2	0.1	0.1

[a]H-3 signal in the *trans* diastereomer is a triplet, [b]H-3 signal in the *trans* diastereomer is an apparent triplet.

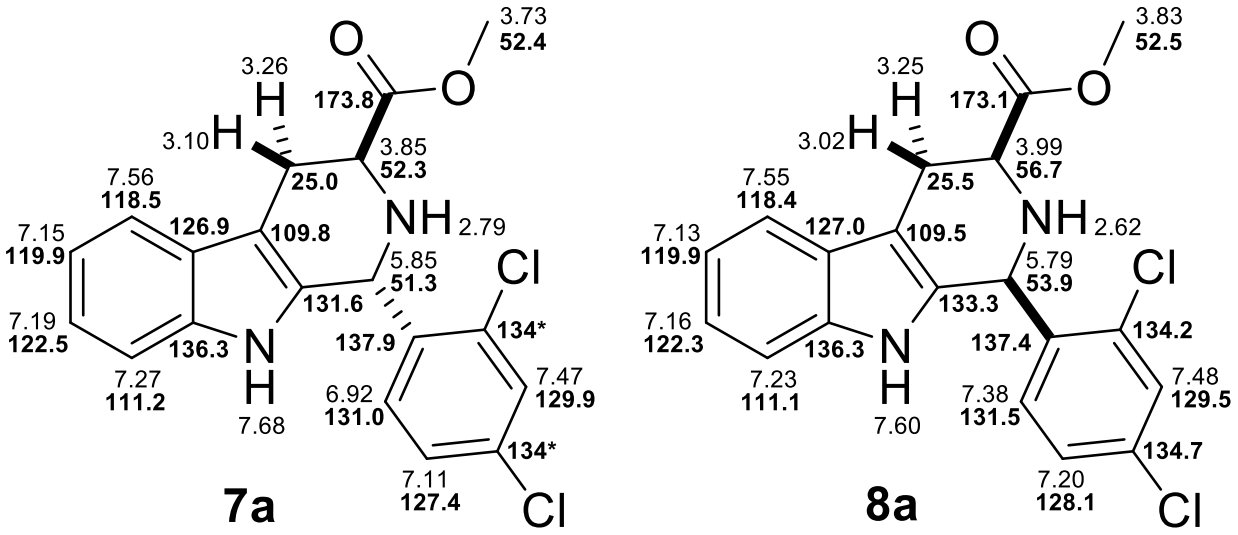


Figure S1. Full ^{1}H and ^{13}C NMR (bold) assignment of structures **7a** and **8a**. Signals marked * are indistinguishable.

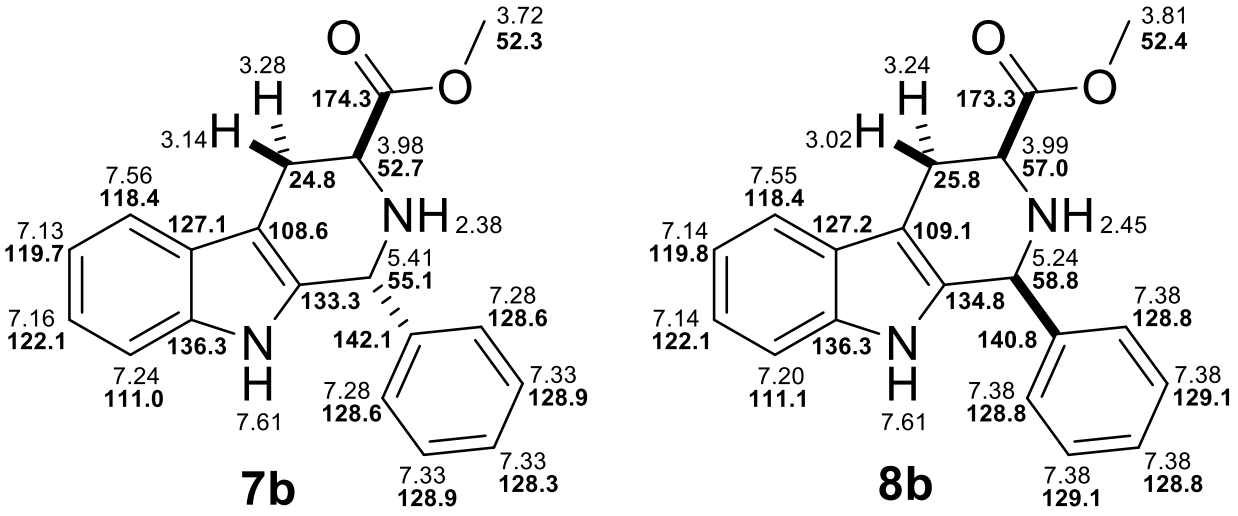
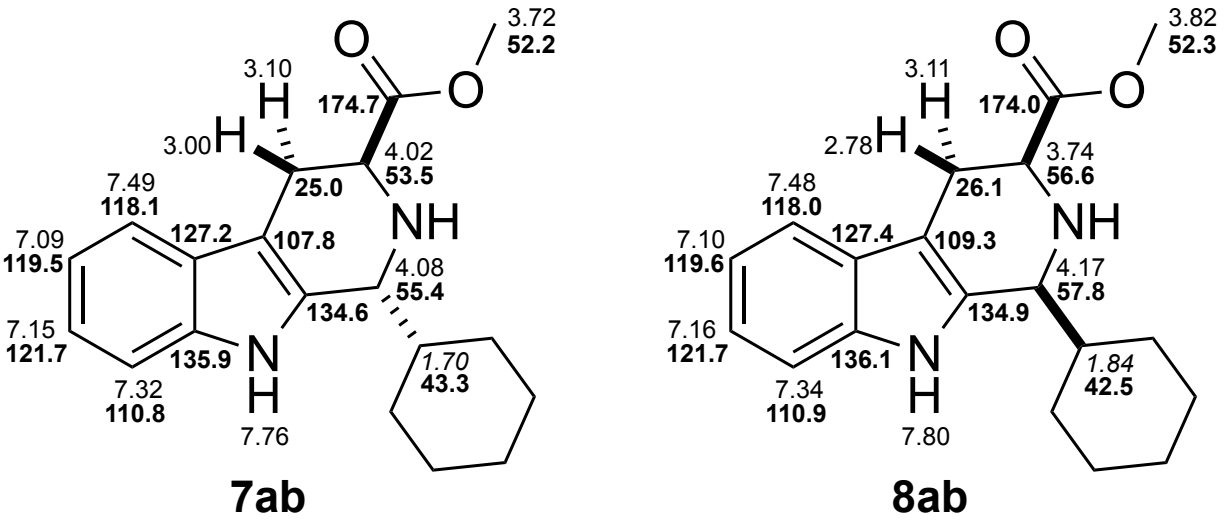


Figure S2. Full ^{1}H and ^{13}C NMR (bold) assignment of structures **7b** and **8b**.



1.87-1.78 (m, 4H), 1.76-1.65 (m, 4H), 1.37-1.10 (m, 6H)
30.4, 28.6, 26.7, 26.53, 26.48

1.89-1.68 (m, 6H), 1.51-1.17 (m, 6H)
29.9, 27.04, 26.97, 26.7, 26.5

Figure S3. Full ^{1}H and ^{13}C NMR (bold) assignment of **7ab** and **8ab**. Unassigned resonances corresponding to cyclohexyl ring are reported under the structures. The underlined unassigned ^{13}C resonances show HMBC correlation to H-1.

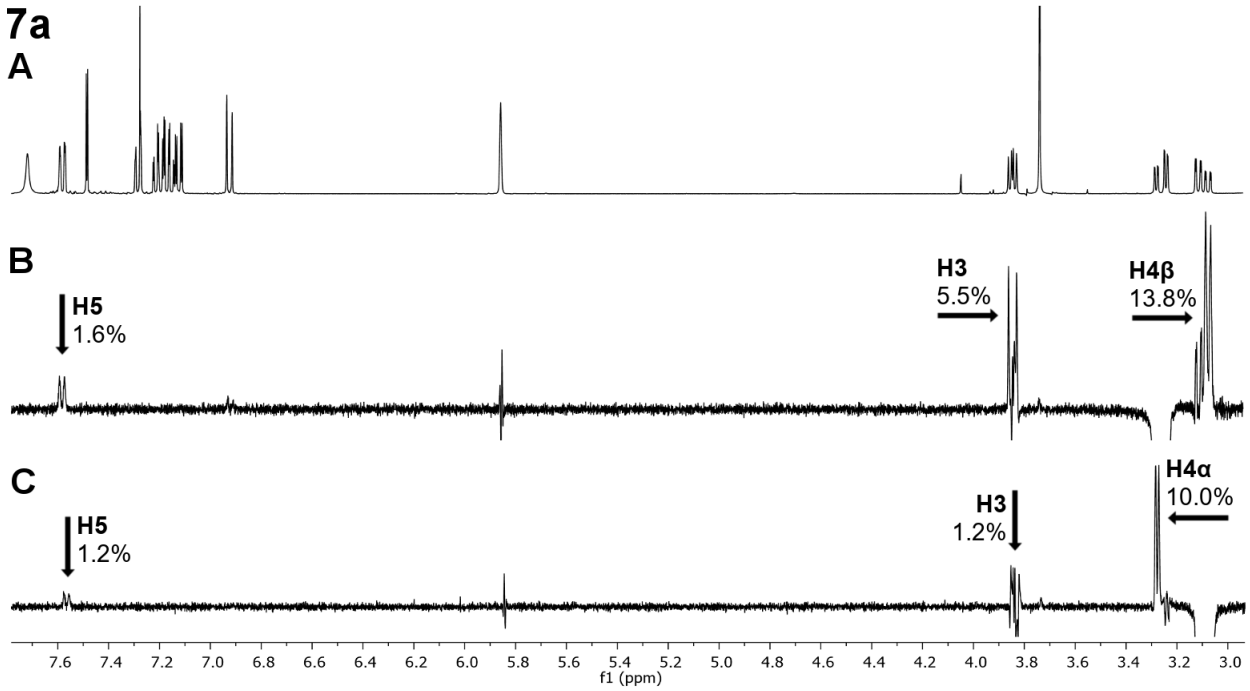


Figure S4. A) ^{1}H NMR spectrum of **7a** ($CDCl_3$); B) 1D NOE ^{1}H NMR spectrum of **7a** resulting from irradiation of H4α; C) 1D NOE ^{1}H NMR spectrum of **7a** resulting from irradiation of H4β

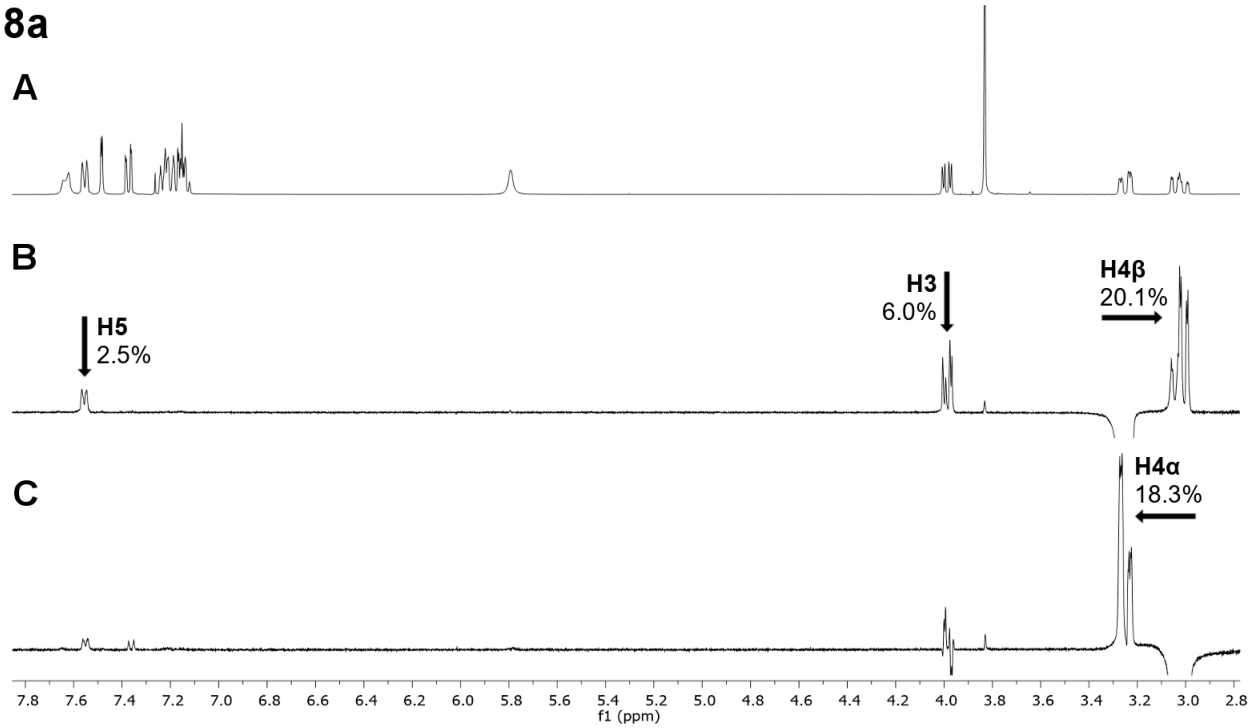


Figure S5. A) ^{1}H NMR spectrum of **8a** ($CDCl_3$); B) 1D NOE ^{1}H NMR spectrum of **8a** resulting from irradiation of H4α; C) 1D NOE ^{1}H NMR spectrum of **8a** resulting from irradiation of H4β.

Table S5. Selected 1D NOE correlations observed in **7a**/**8a** upon irradiation of H1, H3, H4α, and H4β.

Irradiated proton	Observed NOE in 7a [%]				Observed NOE in 8a [%]			
	H1	**H3**	**H4α**	**H4β**	**H1**	**H3**	**H4α**	**H4β**
H-1	–	–	–	–	–	4.3	–	–
H-3	–	–	3.5	–	3.4	–	3.0	–
H-4α	–	5.5	–	13.8	–	6.0	–	20.1
H-4β	–	1.2	10.0	–	–	–	18.3	–

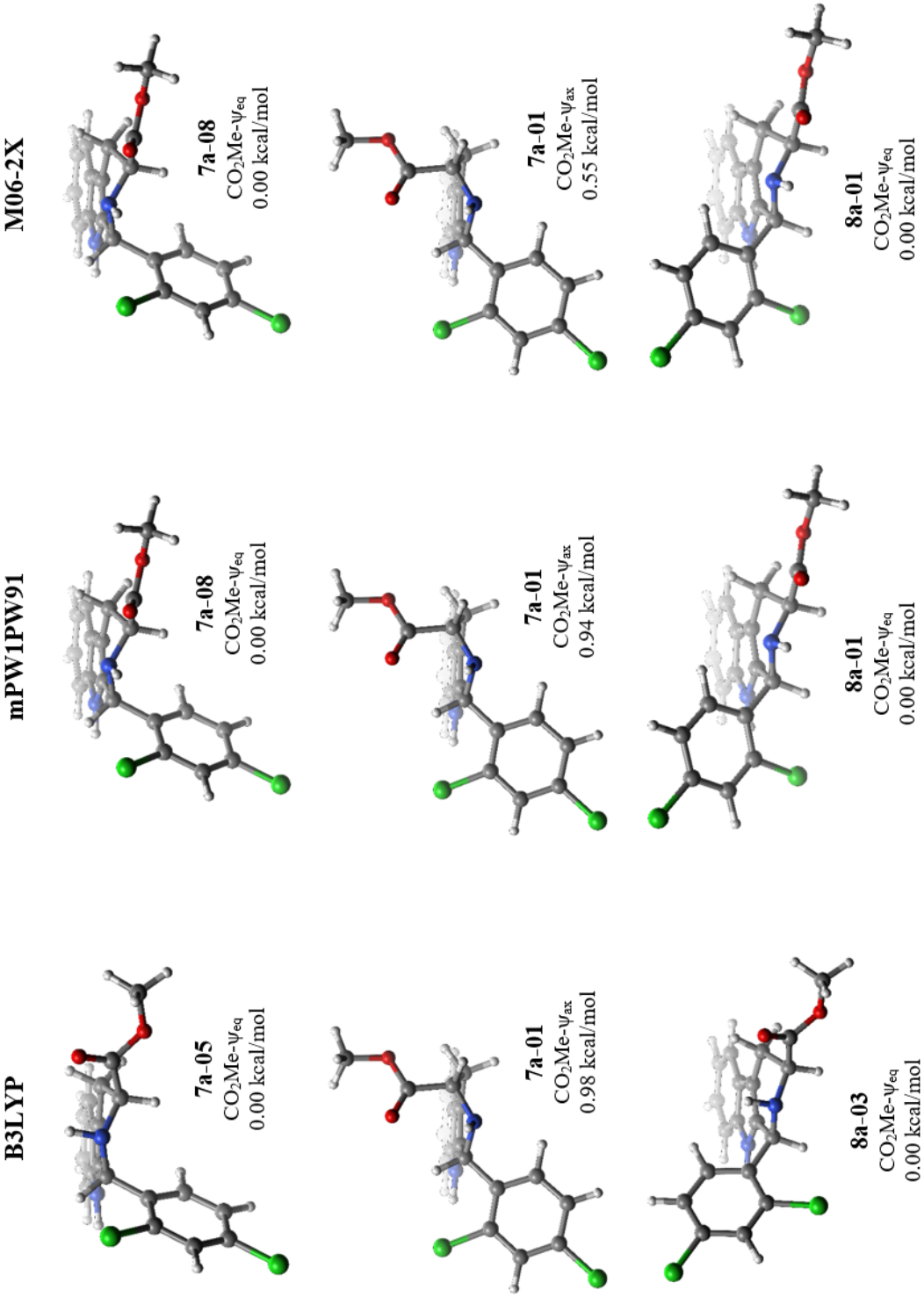


Figure S6. The lowest ΔG (298 K) ψ_{eq}- and ψ_{ax}- conformers of **7a** and the global minimum of **8a**. Geometries were obtained by B3LYP/6-31G(d) optimization; free energies were calculated from single point energies using either the B3LYP/6-311+G(2d,p), mPW1PW91/6-311+G(2d,p), or M06-2X/def2-TZVP, all SCRF=(PCM,solvent=chloroform). Free energy correction was obtained from the B3LYP/6-31G(d) frequencies.

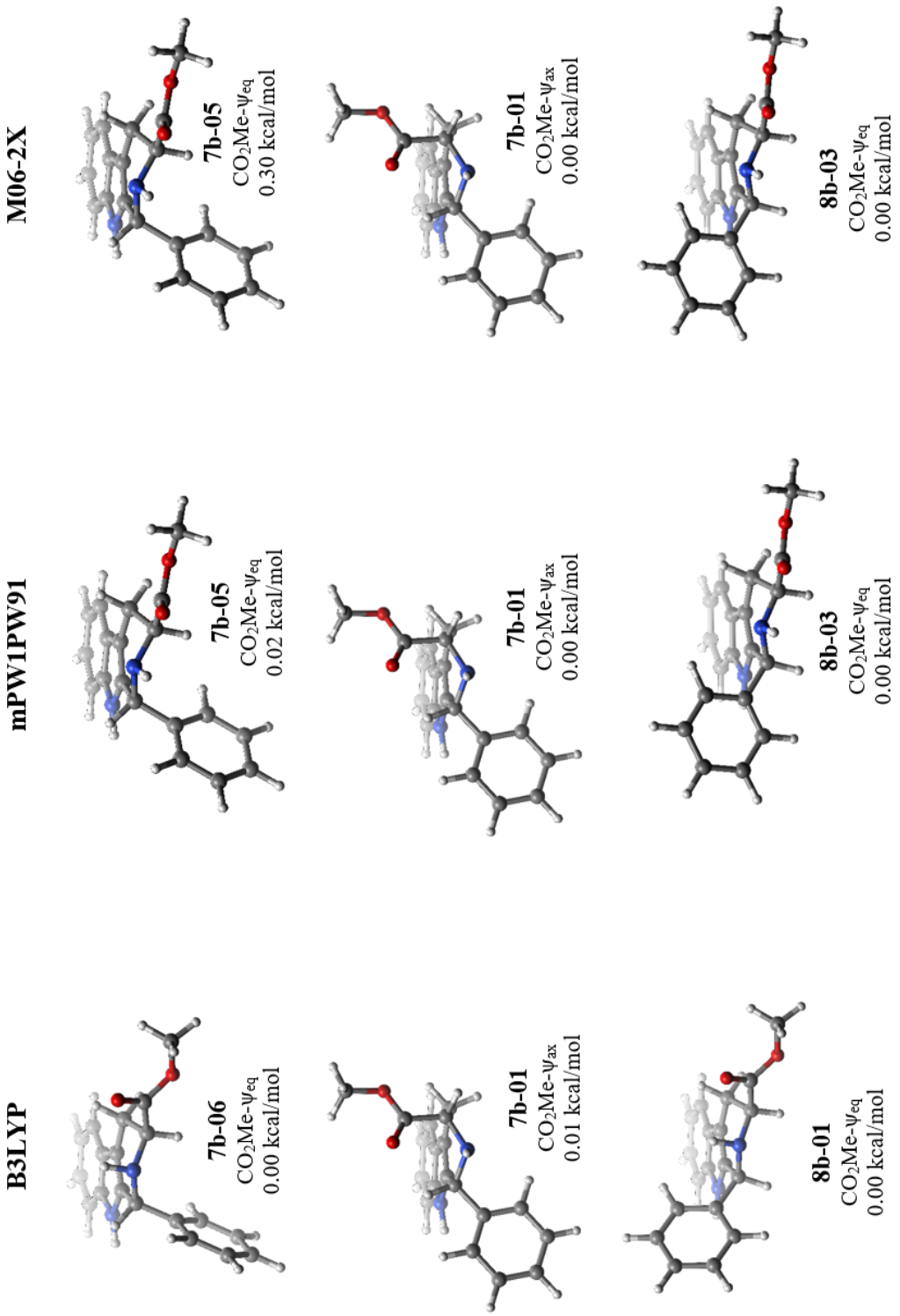


Figure S7. The lowest ΔG (298 K) ψ_{eq}- and ψ_{ax}- conformers of **7b** and the global minimum of **8b**. Geometries were obtained by B3LYP/6-31G(d) optimization; free energies were calculated from single point energies using either the B3LYP/6-311+G(2d,p), mPW1PW91/6-311+G(2d,p), or M06-2X/def2-TZVP, all SCRF=(PCM,solvent=chloroform). Free energy correction was obtained from the B3LYP/6-31G(d) frequencies.

Table S6. Calculated energies of **7a** at MMFF94 and B3LYP/6-31G(d) levels of theory.

	Structural features				MMFF94	B3LYP/6-31G(d), vacuum				
	CO_2Me	2'-Cl	H2	H-bond (H2 to X)	Energy [kJ/mol]	e0 [Hartree]	ZPVE [Hartree]	G_{corr} [a] [Hartree]	G(298) [Hartree]	ΔG(298) [kcal/mol]
7a-1	ψ_{ax}	*exo*	*eq*	C=O	237.34	-1914.01436080	0.317204	0.264808	-1913.7495528	0.00
7a-2	ψ_{ax}	*exo*	*eq*	OCH_3	243.65	-1914.01270533	0.317049	0.264372	-1913.74833333	1.04
7a-3	ψ_{ax}	*endo*	*eq*	C=O	252.89	-1914.00942053	0.316971	0.264333	-1913.74508753	3.10
7a-4	ψ_{ax}	*endo*	*ax*	none[b]	254.24	-1914.00669434	0.317024	0.264215	-1913.74247934	4.81
7a-5	ψ_{eq}	*exo*	*ax*	C=O	254.63	-1914.01118957	0.316725	0.263415	-1913.74777457	1.99
7a-6	ψ_{eq}	*exo*	*eq*	OCH_3	255.98	-1914.01103429	0.316673	0.263891	-1913.74714329	2.09
7a-7	ψ_{ax}	*exo*	*ax*	none[b]	256.20	-1914.00796854	0.316920	0.263858	-1913.74411054	4.01
7a-8	ψ_{eq}	*exo*	*eq*	C=O	256.61	-1914.01209044	0.316635	0.263982	-1913.74810844	1.42
7a-9	ψ_{eq}	*exo*	*ax*	OCH_3	257.95	-1914.00962662	0.316815	0.263635	-1913.74599162	2.97
7a-10	ψ_{ax}	*endo*	*ax*	none[c]	260.51	-1914.00459481	0.317006	0.264311	-1913.74028381	6.13
7a-11	ψ_{ax}	*endo*	*eq*	OCH_3	262.72	-1914.00718234	0.316897	0.264267	-1913.74291534	4.50
7a-12	ψ_{ax}	*exo*	*ax*	none[c]	264.81	-1914.00688677	0.316952	0.263775	-1913.74311177	4.69
7a-13	ψ_{eq}	*endo*	*ax*	C=O	272.33	-1914.00582376	0.316682	0.264074	-1913.74174976	5.36
7a-14	ψ_{eq}	*endo*	*eq*	C=O	276.11	-1914.00427431	0.316387	0.263246	-1913.74102831	6.33
7a-15	ψ_{eq}	*endo*	*eq*	OCH_3	277.22	-1914.00290824	0.316454	0.263129	-1913.73977924	7.19
7a-16	ψ_{eq}	*endo*	*ax*	OCH_3	277.82	-1914.00227563	0.316509	0.263098	-1913.73917763	7.58

[a] Calculated at 298 K. [b] C=O is oriented towards N2 but H-bond is not geometrically possible. [c] OCH_3 is oriented towards N2 but H-bond is not geometrically possible.

Table S7. Calculated energies of **7a** at B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 1**), mPW1PW91/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 2**), and M06-2X/def2-TZVP//B3LYP/6-31G(d) (**Method 3**), all with SCRF=(PCM, solvent=chloroform).

	Method 1		Method 2		Method 3	
	e_0 [Hartree]	G(298) [Hartree]	e_0 [Hartree]	G(298) [Hartree]	e_0 [Hartree]	G(298) [Hartree]
7a-1	-1914.37029604	-1914.10548804	-1914.14966185	-1913.88485385	-1914.01318382	-1913.74837582
7a-2	-1914.36936006	-1914.10498806	-1914.14866297	-1913.88429097	-1914.01189123	-1913.74751923
7a-3	-1914.36790766	-1914.10357466	-1914.14733659	-1913.88300359	-1914.01129940	-1913.7469664
7a-4	-1914.36562128	-1914.10140628	-1914.14491549	-1913.88070049	-1914.00864481	-1913.74442981
7a-5	-1914.37046055	-1914.10704555	-1914.14961148	-1913.88619648	-1914.01195294	-1913.74853794
7a-6	-1914.36976928	-1914.10587828	-1914.14909618	-1913.88520518	-1914.01219656	-1913.74830556
7a-7	-1914.36688658	-1914.10302858	-1914.14618278	-1913.88232478	-1914.00956577	-1913.74570777
7a-8	-1914.37078946	-1914.10680746	-1914.15033222	-1913.88635022	-1914.01323651	-1913.74925451
7a-9	-1914.36922485	-1914.10558985	-1914.14831487	-1913.88467987	-1914.01090188	-1913.74726688
7a-10	-1914.36455952	-1914.10024852	-1914.14396943	-1913.87965843	-1914.00741454	-1913.74310354
7a-11	-1914.36652171	-1914.10225471	-1914.14587465	-1913.88160765	-1914.00960845	-1913.74534145
7a-12	-1914.36639500	-1914.10262000	-1914.14583808	-1913.88206308	-1914.00894024	-1913.74516524
7a-13	-1914.36519480	-1914.10112080	-1914.14424588	-1913.88017188	-1914.00682103	-1913.74274703
7a-14	-1914.36401716	-1914.10077116	-1914.14315101	-1913.87990501	-1914.00574076	-1913.74249476
7a-15	-1914.36273918	-1914.09961018	-1914.14157422	-1913.87844522	-1914.00434922	-1913.74122022
7a-16	-1914.36263186	-1914.09953386	-1914.14138970	-1913.87829170	-1914.00397433	-1913.74087633
	ΔG(298) [kcal/mol]	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**
7a-1	0.98	9.9%	0.94	10.2%	0.55	14.4%
7a-2	1.29	7.2%	1.29	7.2%	1.09	8.4%
7a-3	2.18	3.0%	2.10	3.2%	1.44	5.9%
7a-4	3.54	0.8%	3.55	0.8%	3.03	1.2%
7a-5	0.00	26.3%	0.10	23.7%	0.45	15.9%
7a-6	0.73	12.6%	0.72	12.7%	0.60	13.7%
7a-7	2.52	2.1%	2.53	2.1%	2.23	2.7%
7a-8	0.15	22.6%	0.00	26.1%	0.00	24.9%
7a-9	0.91	10.5%	1.05	9.2%	1.25	7.2%
7a-10	4.27	0.4%	4.20	0.4%	3.86	0.5%
7a-11	3.01	1.3%	2.98	1.3%	2.46	2.1%
7a-12	2.78	1.6%	2.69	1.8%	2.57	1.9%
7a-13	3.72	0.6%	3.88	0.5%	4.08	0.4%
7a-14	3.94	0.5%	4.04	0.5%	4.24	0.4%
7a-15	4.67	0.2%	4.96	0.2%	5.04	0.2%
7a-16	4.71	0.2%	5.06	0.2%	5.26	0.1%

Table S8. Calculated energies of **7b** at MMFF94 and B3LYP/6-31G(d) levels of theory.

	Structural features			MMFF94	B3LYP/6-31G(d), vacuum				
	CO_2Me	H2	H-bond (H2 to X)	Energy [kJ/mol]	e0 [Hartree]	ZPVE [Hartree]	G_{corr} [a] [Hartree]	G(298) [Hartree]	ΔG(298) [kcal/mol]
7b-1	ψ_{ax}	*eq*	C=O	282.54	-994.825578974	0.336524	0.287502	-994.538076974	0.00
7b-2	ψ_{ax}	*eq*	OCH_3	289.74	-994.823944440	0.336427	0.287525	-994.536419440	1.04
7b-3	ψ_{ax}	*ax*	none[b]	292.86	-994.821156197	0.336384	0.287347	-994.533809197	2.68
7b-4	ψ_{eq}	*eq*	OCH_3	295.43	-994.821855495	0.336085	0.287207	-994.534648495	2.15
7b-5	ψ_{eq}	*eq*	C=O	295.65	-994.823088326	0.335979	0.287010	-994.536078326	1.25
7b-6	ψ_{eq}	*ax*	C=O	296.65	-994.822366886	0.336118	0.286375	-994.535991886	1.31
7b-7	ψ_{ax}	*ax*	none[c]	297.48	-994.819721433	0.336393	0.287380	-994.532341433	3.60
7b-8	ψ_{eq}	*ax*	OCH_3	301.06	-994.820741727	0.336125	0.286397	-994.534344727	2.34

[a] Calculated at 298 K. [b] C=O is oriented towards N2 but H-bond is not geometrically possible. [c] OCH_3 is oriented towards N2 but H-bond is not geometrically possible.

Table S9. Calculated energies of **7b** at B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 1**), mPW1PW91/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 2**), and M06-2X/def2-TZVP//B3LYP/6-31G(d) (**Method 3**), all with SCRF=(PCM, solvent=chloroform).

	Method 1		**Method 2**		**Method 3**	
	e_0 [Hartree]	**G(298) [Hartree]**	**e_0 [Hartree]**	**G(298) [Hartree]**	**e_0 [Hartree]**	**G(298) [Hartree]**
7b-1	-995.124145275	-994.836643275	-994.885390029	-994.597888029	-994.808015506	-994.520513506
7b-2	-995.123143164	-994.835618164	-994.884347134	-994.596822134	-994.806852067	-994.519327067
7b-3	-995.121060656	-994.833713656	-994.882227215	-994.594880215	-994.804934854	-994.517587854
7b-4	-995.122386525	-994.835179525	-994.883436878	-994.596229878	-994.805716591	-994.518509591
7b-5	-995.123558562	-994.836548562	-994.884865213	-994.597855213	-994.807044518	-994.520034518
7b-6	-995.123039313	-994.836664313	-994.884166772	-994.597791772	-994.806319801	-994.519944801
7b-7	-995.120364677	-994.832984677	-994.881664652	-994.594284652	-994.804021854	-994.516641854
7b-8	-995.121743096	-994.835346096	-994.882813198	-994.596416198	-994.805156824	-994.518759824
	ΔG(298) [kcal/mol]	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**
7b-1	0.01	21.8%	0.00	22.5%	0.00	26.5%
7b-2	0.66	11.5%	0.67	11.5%	0.74	12.6%
7b-3	1.85	3.5%	1.89	3.4%	1.84	4.2%
7b-4	0.93	8.7%	1.04	8.0%	1.26	7.5%
7b-5	0.07	20.6%	0.02	22.1%	0.30	19.6%
7b-6	0.00	22.1%	0.06	21.2%	0.36	18.5%
7b-7	2.13	2.2%	2.26	2.3%	2.43	2.3%
7b-8	0.83	9.7%	0.92	8.9%	1.10	8.8%

Table S10. Calculated energies of **8a** at MMFF94 and B3LYP/6-31G(d) levels of theory.

	Structural features				MMFF94	B3LYP/6-31G(d), vacuum				
	CO_2Me	2'-Cl	H2	H-bond (H2 to X)	Energy [kJ/mol]	e0 [Hartree]	ZPVE [Hartree]	G_{corr}[a] [Hartree]	G(298) [Hartree]	ΔG(298) [kcal/mol]
8a-1	ψ_{eq}	*exo*	*eq*	C=O	245.12	-1914.01456172	0.316708	0.264065	-1913.75049672	0.00
8a-2	ψ_{eq}	*exo*	*eq*	OCH_3	245.59	-1914.01294988	0.316692	0.263776	-1913.74917388	0.83
8a-3	ψ_{eq}	*exo*	*ax*	C=O	250.02	-1914.01130588	0.316766	0.263040	-1913.74826588	1.40
8a-4	ψ_{ax}	*exo*	*eq*	OCH_3	253.85	-1914.00865712	0.316741	0.264333	-1913.74432412	3.87
8a-5	ψ_{eq}	*exo*	*ax*	OCH_3	254.02	-1914.00985971	0.316841	0.263552	-1913.74630771	2.63
8a-6	ψ_{eq}	*endo*	*ax*	C=O	254.77	-1914.00844097	0.316665	0.263177	-1913.74526397	3.28
8a-7	ψ_{eq}	*endo*	*ax*	OCH_3	256.56	-1914.00728927	0.316802	0.263695	-1913.74359427	4.33
8a-8	ψ_{ax}	*exo*	*eq*	C=O	258.34	-1914.00673342	0.316767	0.263866	-1913.74286742	4.79
8a-9	ψ_{ax}	*exo*	*ax*	none[c]	261.41	-1914.00511940	0.316734	0.264326	-1913.74079340	6.09
8a-10	ψ_{eq}	*endo*	*eq*	C=O	264.78	-1914.00857821	0.316494	0.263896	-1913.74468221	3.65
8a-11	ψ_{eq}	*endo*	*eq*	OCH_3	265.29	-1914.00725406	0.316492	0.263649	-1913.74360506	4.32
8a-12	ψ_{ax}	*exo*	*ax*	none[b]	272.62	-1914.00141662	0.316749	0.264237	-1913.73717962	8.36
8a-13	ψ_{ax}	*endo*	*eq*	C=O	277.59	-1913.99970041	0.316840	0.264779	-1913.73492141	9.77
8a-14	ψ_{ax}	*endo*	*eq*	OCH_3	282.12	-1913.99920233	0.316777	0.264989	-1913.73421333	10.22

[a] Calculated at 298 K. [b] C=O is oriented towards N2 but H-bond is not geometrically possible. [c] OCH_3 is oriented towards N2 but H-bond is not geometrically possible.

Table S11. Calculated energies of **8a** at B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 1**), mPW1PW91/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 2**), and M06-2X/def2-TZVP//B3LYP/6-31G(d) (**Method 3**), all with SCRF=(PCM, solvent=chloroform).

	Method 1		**Method 2**		**Method 3**	
	e_0 [Hartree]	**G(298) [Hartree]**	**e_0 [Hartree]**	**G(298) [Hartree]**	**e_0 [Hartree]**	**G(298) [Hartree]**
8a-1	-1914.37124126	-1914.10717626	-1914.15049755	-1913.88643255	-1914.01302460	-1913.74895960
8a-2	-1914.36989820	-1914.10612220	-1914.14888337	-1913.88510737	-1914.01156644	-1913.74779044
8a-3	-1914.37047890	-1914.10743890	-1914.14935969	-1913.88631969	-1914.01118126	-1913.74814126
8a-4	-1914.36621981	-1914.10188681	-1914.14589369	-1913.88156069	-1914.01210700	-1913.74777400
8a-5	-1914.36935580	-1914.10580380	-1914.14819240	-1913.88464040	-1914.01023058	-1913.74667858
8a-6	-1914.36846112	-1914.10528412	-1914.14743271	-1913.88425571	-1914.0101486	-1913.74697160
8a-7	-1914.36752967	-1914.10383467	-1914.14644047	-1913.88274547	-1914.00914825	-1913.74545325
8a-8	-1914.36485810	-1914.10099210	-1914.14449099	-1913.88062499	-1914.01007648	-1913.74621048
8a-9	-1914.36411026	-1914.09978426	-1914.14384254	-1913.87951654	-1914.00945487	-1913.74512887
8a-10	-1914.36825899	-1914.10436299	-1914.14759393	-1913.88369793	-1914.01051805	-1913.74662205
8a-11	-1914.36716693	-1914.10351793	-1914.14624157	-1913.88259257	-1914.00930004	-1913.74565104
8a-12	-1914.36165907	-1914.09742207	-1914.14116815	-1913.87693115	-1914.00664588	-1913.74240888
8a-13	-1914.35865601	-1914.09387701	-1914.13801560	-1913.87323660	-1914.00390664	-1913.73912764
8a-14	-1914.35871373	-1914.09372473	-1914.13805779	-1913.87306879	-1914.00421326	-1913.73922426
	ΔG(298) [kcal/mol]	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**
8a-1	0.16	25.7%	0.00	29.4%	0.00	26.1%
8a-2	0.83	13.3%	0.83	12.8%	0.73	12.5%
8a-3	0.00	30.3%	0.07	27.4%	0.51	15.6%
8a-4	3.48	0.9%	3.06	1.4%	0.74	12.4%
8a-5	1.03	10.9%	1.12	9.5%	1.43	6.2%
8a-6	1.35	7.8%	1.37	7.5%	1.25	7.5%
8a-7	2.26	3.2%	2.31	2.9%	2.20	2.9%
8a-8	4.05	0.5%	3.64	0.8%	1.73	4.6%
8a-9	4.80	0.2%	4.34	0.4%	2.40	2.4%
8a-10	1.93	4.4%	1.72	5.3%	1.47	6.0%
8a-11	2.46	2.6%	2.41	2.6%	2.08	3.3%
8a-12	6.29	0.1%	5.96	0.1%	4.11	0.4%
8a-13	8.51	0.0%	8.28	0.0%	6.17	0.1%
8a-14	8.61	0.0%	8.39	0.0%	6.11	0.1%

Table S12. Calculated energies of **8b** at MMFF94 and B3LYP/6-31G(d) levels of theory.

	Structural features			MMFF94	B3LYP/6-31G(d), vacuum				
	CO_2Me	H2	H-bond (H2 to X)	Energy [kJ/mol]	e0 [Hartree]	ZPVE [Hartree]	G_{corr} [a] [Hartree]	G(298) [Hartree]	ΔG(298) [kcal/mol]
8b-1	ψ_{eq}	*ax*	C=O	291.03	-994.823809034	0.336080	0.286129	-994.537680034	0.73
8b-2	ψ_{eq}	*eq*	OCH_3	291.46	-994.824456311	0.336034	0.286823	-994.537633311	0.76
8b-3	ψ_{eq}	*eq*	C=O	291.87	-994.825784125	0.336026	0.286945	-994.538839125	0.00
8b-4	ψ_{eq}	*ax*	OCH_3	293.71	-994.822507772	0.336175	0.286669	-994.535838772	1.88
8b-5	ψ_{ax}	*eq*	OCH_3	295.00	-994.819243218	0.336164	0.287649	-994.531594218	4.55
8b-6	ψ_{ax}	*eq*	C=O	301.90	-994.817316664	0.336256	0.287156	-994.530160664	5.45
8b-7	ψ_{ax}	*ax*	none[c]	304.78	-994.815792636	0.336267	0.288082	-994.527710636	6.42
8b-8	ψ_{ax}	*ax*	none[b]	315.26	-994.812854690	0.336270	0.287749	-994.52510569	8.27

[a] Calculated at 298 K. [b] C=O is oriented towards N2 but H-bond is not geometrically possible. [c] OCH_3 is oriented towards N2 but H-bond is not geometrically possible.

Table S13. Calculated energies of **8b** at B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 1**), mPW1PW91/6-311+G(2d,p)// B3LYP/6-31G(d) (**Method 2**), and M06-2X/def2-TZVP//B3LYP/6-31G(d) (**Method 3**), all with SCRF=(PCM, solvent=chloroform).

	Method 1		**Method 2**		**Method 3**	
	e_0 [Hartree]	**G(298) [Hartree]**	**e_0 [Hartree]**	**G(298) [Hartree]**	**e_0 [Hartree]**	**G(298) [Hartree]**
8b-1	-995.124312659	-994.838183659	-994.885065648	-994.598936648	-994.806461995	-994.520332995
8b-2	-995.123982150	-994.837159150	-994.884864392	-994.598041392	-994.80670119	-994.51987819
8b-3	-995.125082968	-994.838137968	-994.886229910	-994.599284910	-994.807950115	-994.521005115
8b-4	-995.123213232	-994.836544232	-994.883953279	-994.597284279	-994.805695866	-994.519026866
8b-5	-995.118342782	-994.830693782	-994.879675706	-994.592026706	-994.804884848	-994.517235848
8b-6	-995.116968010	-994.829812010	-994.878223751	-994.591067751	-994.802598341	-994.515442341
8b-7	-995.116184082	-994.828102082	-994.877885019	-994.589803019	-994.803579255	-994.515497255
8b-8	-995.113689095	-994.825940095	-994.875248592	-994.587499592	-994.800781284	-994.513032284
	ΔG(298) [kcal/mol]	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**	**ΔG(298) [kcal/mol]**	**Boltzmann distribution**
8b-1	0.00	34.8%	0.22	31.3%	0.42	25.2%
8b-2	0.64	18.3%	0.78	17.9%	0.71	19.0%
8b-3	0.03	33.8%	0.00	39.0%	0.00	38.5%
8b-4	1.03	12.4%	1.26	11.1%	1.24	11.1%
8b-5	4.70	0.3%	4.55	0.4%	2.37	3.6%
8b-6	5.25	0.2%	5.16	0.2%	3.49	1.2%
8b-7	5.74	0.1%	5.95	0.1%	3.46	1.2%
8b-8	7.30	0.0%	7.40	0.0%	5.00	0.3%

Table S14. Boltzmann distribution of conformer ensembles of **7a**, **8a**, **7b**, **8b** [%] See Tables S7, S9, S11, S13 for the Boltzmann weights of individual conformers.

	7a			**8a**			**7b**			**8b**		
Method	**M1**	**M2**	**M3**	**M1**	**M2**	**M3**	**M1**	**M2**	**M3**	**M1**	**M2**	**M3**
3-CO_2Me-ψ_{ax}	26.3	26.9	37.2	1.8	2.6	19.9	39.0	39.8	45.6	0.6	0.8	6.3
3-CO_2Me-ψ_{eq}	73.7	73.1	62.8	98.2	97.4	80.1	61.0	60.2	54.4	99.4	99.2	93.7
2'-Cl_{exo}	93.0	93.0	89.1	82.0	81.7	80.2	–	–	–	–	–	–
2'-Cl_{endo}	7.0	7.0	10.9	18.0	18.3	19.8	–	–	–	–	–	–
H-2_{ax}	42.6	38.6	30.0	52.5	47.8	35.0	37.4	35.9	33.9	47.4	42.5	37.8
H-2_{eq}	57.4	61.4	70.0	47.5	52.2	65.0	62.6	64.1	66.1	52.6	57.5	62.2
H-bonding[a]	95.1	95.0	93.7	99.7	99.5	97.2	94.3	94.2	93.5	99.9	99.9	98.5
H-bond to C=O	62.9	64.2	61.9	68.9	70.3	59.9	64.5	65.8	64.6	68.8	70.5	64.8
H-bond to OMe	32.2	30.7	31.7	30.8	29.3	37.3	29.8	28.4	28.9	31.1	29.4	33.7
No H-bond[a]	4.9	5.0	6.3	0.3	0.5	2.8	5.7	5.8	6.5	0.1	0.1	1.5

Methods used for determination of conformer energies:
M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM, solvent=chloroform),
M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM, solvent=chloroform),
M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF=(PCM, solvent=chloroform).
[a]H-bonding assumed for H-2···O distance ranging between 2.3 Å and 2.7 Å. For those conformers described as "No H-bonding", this distance was ≥ 3.7 Å.

Table S15. Calculated (B3LYP/6-31G(d,p)u+1s//B3LYP/6-31G(d)) ^{1}H-^{1}H coupling constants for all conformers of **7a**, **8a**, **7b**, **8b**.[a]

	7a-01	**7a-02**	**7a-03**	**7a-04**	**7a-05**	**7a-06**	**7a-07**	**7a-08**
$^{3}J_{4\beta\text{-}3}$ [Hz]	1.8	1.5	1.6	1.0	10.7	10.8	1.0	11.0
$^{3}J_{4\alpha\text{-}3}$ [Hz]	5.7	5.9	6.0	7.0	4.2	3.9	6.8	3.7
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	-15.1	-15.0	-15.2	-16.0	-15.3	-15.9	-16.0	-15.0
$^{5}J_{4\beta\text{-}1}$ [Hz]	1.8	2.0	1.8	2.1	2.0	1.7	2.0	1.7
$^{5}J_{4\alpha\text{-}1}$ [Hz]	2.9	2.9	3.2	3.3	0.5	0.5	3.0	0.5
	7a-09	**7a-10**	**7a-11**	**7a-12**	**7a-13**	**7a-14**	**7a-15**	**7a-16**
$^{3}J_{4\beta\text{-}3}$ [Hz]	10.8	1.0	1.5	1.0	10.6	10.7	10.5	10.6
$^{3}J_{4\alpha\text{-}3}$ [Hz]	4.2	6.5	6.0	6.4	3.6	3.5	3.6	3.2
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	-15.5	-15.7	-15.1	-15.7	-14.3	-14.8	-15.7	-14.4
$^{5}J_{4\beta\text{-}1}$ [Hz]	2.0	2.2	1.9	2.2	2.7	2.4	2.5	2.8
$^{5}J_{4\alpha\text{-}1}$ [Hz]	0.5	3.3	3.2	3.1	0.9	0.8	0.8	0.9
	8a-01	**8a-02**	**8a-03**	**8a-04**	**8a-05**	**8a-06**	**8a-07**	**8a-08**
$^{3}J_{4\beta\text{-}3}$ [Hz]	10.9	10.7	10.5	0.9	10.7	10.7	10.8	1.0
$^{3}J_{4\alpha\text{-}3}$ [Hz]	3.5	3.6	4.1	6.7	4.0	4.2	4.1	6.8
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	-14.7	-15.6	-15.1	-15.4	-15.3	-15.1	-15.2	-15.8
$^{5}J_{4\beta\text{-}1}$ [Hz]	2.9	3.0	3.1	0.6	3.1	3.2	3.3	0.6
$^{5}J_{4\alpha\text{-}1}$ [Hz]	2.0	1.9	2.1	2.0	2.1	2.2	2.2	2.0
	8a-09	**8a-10**	**8a-11**	**8a-12**	**8a-13**	**8a-14**		
$^{3}J_{4\beta\text{-}3}$ [Hz]	0.6	10.8	10.7	0.6	1.2	1.1		
$^{3}J_{4\alpha\text{-}3}$ [Hz]	6.5	3.5	3.8	6.7	7.0	7.0		
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	-16.0	-14.7	-15.6	-16.3	-15.8	-15.5		
$^{5}J_{4\beta\text{-}1}$ [Hz]	0.7	3.1	3.2	0.6	0.9	1.0		
$^{5}J_{4\alpha\text{-}1}$ [Hz]	2.3	1.9	1.9	2.2	2.8	2.8		
	7b-01	**7b-02**	**7b-03**	**7b-04**	**7b-05**	**7b-06**	**7b-07**	**7b-08**
$^{3}J_{4\beta\text{-}3}$ [Hz]	1.5	1.3	1.0	10.7	10.9	10.8	1.0	1.5
$^{3}J_{4\alpha\text{-}3}$ [Hz]	6.2	6.2	6.9	3.7	3.6	4.6	6.4	6.2
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	-15.3	-15.1	-15.9	-15.7	-14.8	-15.5	-15.6	-15.3
$^{5}J_{4\beta\text{-}1}$ [Hz]	1.9	2.1	2.1	1.8	1.8	1.8	2.3	1.9
$^{5}J_{4\alpha\text{-}1}$ [Hz]	3.1	3.1	3.1	0.5	0.5	0.5	3.1	3.1
	8b-01	**8b-02**	**8b-03**	**8b-04**	**8b-05**	**8b-06**	**8b-07**	**8b-08**
$^{3}J_{4\beta\text{-}3}$ [Hz]	10.6	10.7	11.0	10.7	1.1	1.3	0.6	0.5
$^{3}J_{4\alpha\text{-}3}$ [Hz]	4.1	3.9	3.7	4.0	6.4	6.2	6.6	6.9
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	-15.0	-15.6	-14.7	-15.2	-15.2	-15.5	-16.0	-16.5
$^{5}J_{4\beta\text{-}1}$ [Hz]	3.1	3.1	3.0	3.1	0.7	0.6	0.6	0.5
$^{5}J_{4\alpha\text{-}1}$ [Hz]	2.2	2.0	2.0	2.2	2.3	2.4	2.1	1.9

[a]Only Fermi contact terms (major contributor to J_{HH}) were included to calculate J_{HH}; values have been scaled by 0.9117 as recommended. To perform these calculations in Gaussian09, the following route was used: #n B3LYP/6-31G(d,p) nmr=(fconly,readatoms) iop(3/10=1100000)
specifying the desired H atoms at the end of the molecule specification (e.g. atom=16,25,40,41 for **7a**, preceded by a blank line; route recommended by the CHESHIRE Chemical Shift Repository http://cheshirenmr.info/Recommendations.htm).

Table S16. Observed and Calculated Boltzmann weighted average ^{1}H-^{1}H coupling constants for **7a**, **8a**, **7b**, **8b**, and RMSD values, based on Tables S7, S9, S11, S13, and S15.

		Boltzmann distribution based on:					
7a	**Observed**	**M1**		**M2**		**M3**	
		$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**
$^{3}J_{4\beta\text{-}3}$ [Hz]	7.8	8.4	0.6	8.3	0.5	7.4	0.4
$^{3}J_{4\alpha\text{-}3}$ [Hz]	5.0	4.5	0.5	4.5	0.5	4.7	0.3
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	15.4	15.3	0.1	15.3	0.1	15.3	0.1
$^{5}J_{4\beta\text{-}1}$ [Hz]	1.5	1.9	0.4	1.9	0.4	1.9	0.4
$^{5}J_{4\alpha\text{-}1}$ [Hz]	1.2	1.2	0.0	1.2	0.0	1.4	0.2

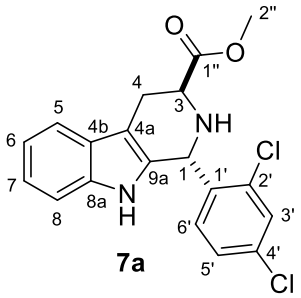
8a	**Observed**	**M1**		**M2**		**M3**	
		$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**
$^{3}J_{4\beta\text{-}3}$ [Hz]	11.0	10.5	0.5	10.5	0.5	8.8	2.2
$^{3}J_{4\alpha\text{-}3}$ [Hz]	4.1	3.9	0.2	3.9	0.2	4.4	0.3
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	15.1	15.1	0.0	15.1	0.0	15.2	0.1
$^{5}J_{4\beta\text{-}1}$ [Hz]	2.5	3.0	0.5	3.0	0.5	2.6	0.1
$^{5}J_{4\alpha\text{-}1}$ [Hz]	1.9	2.1	0.2	2.0	0.1	2.0	0.1

7b	**Observed**	**M1**		**M2**		**M3**	
		$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**
$^{3}J_{4\beta\text{-}3}$ [Hz]	6.8	6.2	0.6	6.2	0.6	5.7	1.1
$^{3}J_{4\alpha\text{-}3}$ [Hz]	5.4	5.1	0.3	5.1	0.3	5.2	0.2
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	15.4	15.3	0.1	15.3	0.1	15.3	0.1
$^{5}J_{4\beta\text{-}1}$ [Hz]	1.6	1.9	0.3	1.9	0.3	1.9	0.3
$^{5}J_{4\alpha\text{-}1}$ [Hz]	1.4	1.8	0.4	1.8	0.4	1.9	0.5

8b	**Observed**	**M1**		**M2**		**M3**	
		$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**	$\|J_{HH}\|$	**Error**
$^{3}J_{4\beta\text{-}3}$ [Hz]	11.2	10.7	0.5	10.7	0.5	10.2	1.0
$^{3}J_{4\alpha\text{-}3}$ [Hz]	4.3	4.0	0.3	3.9	0.4	4.1	0.2
$^{2}J_{4\alpha\text{-}4\beta}$ [Hz]	15.2	15.0	0.2	15.0	0.2	15.1	0.1
$^{5}J_{4\beta\text{-}1}$ [Hz]	2.6	3.0	0.4	3.0	0.4	2.9	0.3
$^{5}J_{4\alpha\text{-}1}$ [Hz]	1.9	2.1	0.2	2.1	0.2	2.1	0.2

RMSD [Hz]	0.4	0.4	0.6
MAD [Hz]	0.3	0.3	0.4

M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform),
M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform),
M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF(PCM=chloroform).

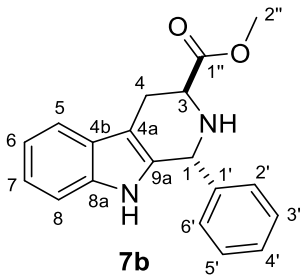


7a

Table S17. Calculated Boltzmann weighted average ^{13}C NMR compared to experimentally obtained chemical shifts in compound **7a**. ^{13}C NMR shifts were calculated by B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (method **M1**) and mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (methods **M2**, and **M3**).

Carbon	^{13}C NMR Chemical shifts [ppm]						
	Exp.	M1	M2	M3	$\Delta_{M1-Exp.}$	$\Delta_{M2-Exp.}$	$\Delta_{M3-Exp.}$
1	51.3	53.6	52.9	53.1	2.3	1.6	1.8
3	52.3	54.5	53.4	53.9	2.2	1.1	1.6
4	25.0	27.5	26.8	26.5	2.5	1.8	1.5
4a	109.8	111.0	110.5	110.1	1.2	0.7	0.3
4b	126.9	126.9	126.2	126.1	0.0	-0.7	-0.8
5	118.5	116.7	117.4	117.3	-1.8	-1.1	-1.2
6	119.9	118.2	118.5	118.4	-1.7	-1.4	-1.5
7	122.5	120.6	121.0	120.9	-1.9	-1.5	-1.6
8	111.2	108.8	109.4	109.4	-2.4	-1.8	-1.8
8a	136.3	135.4	134.7	134.7	-0.9	-1.6	-1.6
9a	131.6	131.8	131.4	131.5	0.2	-0.2	-0.1
1'	137.9	140.2	139.2	139.3	2.3	1.3	1.4
2'	134.0	142.3	141.2	141.1	8.3	7.2	7.1
3'	129.9	129.7	129.8	129.8	-0.2	-0.1	-0.1
4'	134.0	141.4	140.4	140.4	7.4	6.4	6.4
5'	127.4	126.1	126.3	126.4	-1.3	-1.1	-1.0
6'	131.0	130.3	130.7	131.0	-0.7	-0.3	0.0
1''	173.8	176.0	175.3	175.4	2.2	1.5	1.6
2''	52.4	51.5	51.5	51.5	-0.9	-0.9	-0.9

Methods used for determination of conformer energies:
M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform),
M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)
M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)

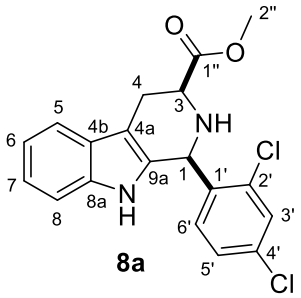


7b

Table S18. Calculated Boltzmann weighted average ^{13}C NMR compared to experimentally obtained chemical shifts in compound **7b**. ^{13}C NMR shifts were calculated by B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (method **M1**) and mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (methods **M2**, and **M3**).

Carbon	^{13}C NMR Chemical shifts [ppm]						
	Exp.	M1	M2	M3	$\Delta_{M1-Exp.}$	$\Delta_{M2-Exp.}$	$\Delta_{M3-Exp.}$
1	55.1	57.6	56.6	56.5	2.5	1.5	1.4
3	52.7	55.0	54.0	54.3	2.3	1.3	1.6
4	24.8	27.0	26.4	26.2	2.2	1.6	1.4
4a	108.6	109.1	108.7	108.4	0.5	0.1	-0.2
4b	127.1	127.6	126.8	126.8	0.5	-0.3	-0.3
5	118.4	116.5	117.2	117.2	-1.9	-1.2	-1.2
6	119.7	118.2	118.5	118.4	-1.5	-1.2	-1.3
7	122.1	120.2	120.6	120.5	-1.9	-1.5	-1.6
8	111.0	109.0	109.6	109.5	-2.0	-1.4	-1.5
8a	136.3	135.7	134.8	134.8	-0.6	-1.5	-1.5
9a	133.3	134.2	133.7	133.8	0.9	0.4	0.5
1'	142.1	144.9	143.8	143.8	2.8	1.7	1.7
2'	128.6	129.2	129.4	129.3	0.6	0.8	0.7
3'	128.9	127.8	128.1	128.1	-1.1	-0.8	-0.8
4'	128.3	126.8	127.3	127.3	-1.5	-1.0	-1.0
5'	128.9	127.4	127.8	127.8	-1.5	-1.1	-1.1
6'	128.6	127.2	127.5	127.6	-1.4	-1.1	-1.0
1''	174.3	176.4	175.8	175.9	2.1	1.5	1.6
2''	52.3	51.3	51.3	51.3	-1.0	-1.0	-1.0

Methods used for determination of conformer energies:
M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform),
M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)
M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)

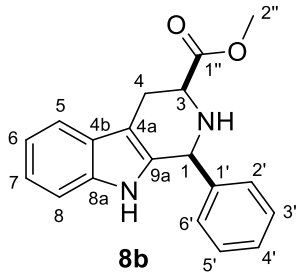


8a

Table S19. Calculated Boltzmann weighted average ^{13}C NMR compared to experimentally obtained chemical shifts in compound **8a**. ^{13}C NMR shifts were calculated by B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (method **M1**) and mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (methods **M2**, and **M3**).

Carbon	^{13}C NMR Chemical shifts [ppm]						
	Exp.	M1	M2	M3	$\Delta_{M1-Exp.}$	$\Delta_{M2-Exp.}$	$\Delta_{M3-Exp.}$
1	53.9	56.6	55.8	55.6	2.7	1.9	1.7
3	56.7	58.9	57.5	56.8	2.2	0.8	0.1
4	25.5	27.7	26.9	26.1	2.2	1.4	0.6
4a	109.5	109.8	109.1	109.1	0.3	-0.4	-0.4
4b	127	127.2	126.5	126.4	0.2	-0.5	-0.6
5	118.4	116.8	117.6	117.6	-1.6	-0.8	-0.8
6	119.9	118.3	118.5	118.4	-1.6	-1.4	-1.5
7	122.3	120.5	120.9	120.8	-1.8	-1.4	-1.5
8	111.1	109.1	109.7	109.6	-2.0	-1.4	-1.5
8a	136.3	134.7	134	134.1	-1.6	-2.3	-2.2
9a	133.3	133.5	133	132.6	0.2	-0.3	-0.7
1'	137.4	139.5	138.6	138.8	2.1	1.2	1.4
2'	134.2	142.2	141.1	141.0	8.0	6.9	6.8
3'	129.5	129.5	129.6	129.6	0.0	0.1	0.1
4'	134.7	141.8	140.9	140.8	7.1	6.2	6.1
5'	128.1	127	127.2	127.1	-1.1	-0.9	-1.0
6'	131.5	131.1	131.4	131.6	-0.4	-0.1	0.1
1''	173.1	175.5	174.9	175.1	2.4	1.8	2.0
2''	52.5	51.6	51.7	51.5	-0.9	-0.8	-1.0

Methods used for determination of conformer energies:
M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform),
M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)
M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)



8b

Table S20. Calculated Boltzmann weighted average ^{13}C NMR compared to experimentally obtained chemical shifts in compound **8b**. ^{13}C NMR shifts were calculated by B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (method **M1**) and mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform) (methods **M2**, and **M3**).

Carbon	^{13}C NMR Chemical shifts [ppm]						
	Exp.	**M1**	**M2**	**M3**	$\Delta_{M1-Exp.}$	$\Delta_{M2-Exp.}$	$\Delta_{M3-Exp.}$
1	58.8	60.9	59.8	59.7	2.1	1.0	0.9
3	57	59.2	57.8	57.6	2.2	0.8	0.6
4	25.8	27.8	27	26.7	2.0	1.2	0.9
4a	109.1	109	108.4	108.4	-0.1	-0.7	-0.7
4b	127.2	127.9	127.1	127.1	0.7	-0.1	-0.1
5	118.4	117	117.7	117.6	-1.4	-0.7	-0.8
6	119.8	118.3	118.6	118.5	-1.5	-1.2	-1.3
7	122.1	120	120.4	120.4	-2.1	-1.7	-1.7
8	111.1	108.9	109.5	109.5	-2.2	-1.6	-1.6
8a	136.3	135.3	134.6	134.6	-1.0	-1.7	-1.7
9a	134.8	135.8	135.3	135.2	1.0	0.5	0.4
1'	140.8	143.2	142.2	142.3	2.4	1.4	1.5
2'	128.8	128.7	128.8	128.7	-0.1	0.0	-0.1
3'	129.1	127.4	127.7	127.8	-1.7	-1.4	-1.3
4'	128.8	127.6	128	128	-1.2	-0.8	-0.8
5'	129.1	128.2	128.5	128.5	-0.9	-0.6	-0.6
6'	128.8	127.7	128.1	128.1	-1.1	-0.7	-0.7
1''	173.3	175.7	175.1	175.1	2.4	1.8	1.8
2''	52.4	51.5	51.5	51.5	-0.9	-0.9	-0.9

Methods used for determination of conformer energies:
M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform),
M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)
M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF=(PCM,solvent=chloroform)

Table S21. Predicted ^{13}C NMR shifts in C-1 and C-3 for conformers of compound **7a**, grouped according to conformer ensembles B and C.

		Ensemble B								Weighted average
		7a-5	**7a-6**	**7a-8**	**7a-9**	**7a-13**	**7a-14**	**7a-15**	**7a-16**	
Method 1	Boltzmann distribution [%]	26.3	12.6	22.6	10.5	0.6	0.5	0.2	0.2	–
	δ C1 [ppm]	52.4	54.6	54.3	53.0	57.3	59.9	60.3	57.7	53.6
	δ C3 [ppm]	52.8	52.5	52.4	55.7	55.3	54.8	55.9	58.2	53.1
Method 2	Boltzmann distribution [%]	23.7	12.7	26.1	9.2	0.5	0.5	0.2	0.2	–
	δ C1 [ppm]	51.5	53.8	53.5	52.2	56.3	58.7	59.1	56.7	52.8
	δ C3 [ppm]	51.6	51.6	51.5	54.3	54.2	53.8	54.9	56.8	52.0
Method 3	Boltzmann distribution [%]	15.9	13.7	24.9	7.2	0.4	0.4	0.2	0.1	–
	δ C1 [ppm]	51.5	53.8	53.5	52.2	56.3	58.7	59.1	56.7	53.0
	δ C3 [ppm]	51.6	51.6	51.5	54.3	54.2	53.8	54.9	56.8	51.9
		Ensemble C								**Weighted average**
		7a-1	**7a-2**	**7a-3**	**7a-4**	**7a-7**	**7a-10**	**7a-11**	**7a-12**	
Method 1	Boltzmann distribution [%]	9.9	7.2	3.0	0.8	2.1	0.4	1.3	1.6	–
	δ C1 [ppm]	52.1	53.1	58.2	57.7	53.2	58.8	59.4	53.1	53.8
	δ C3 [ppm]	58.3	58.8	58.0	57.3	57.3	59.1	58.7	58.8	58.3
Method 2	Boltzmann distribution [%]	10.2	7.2	3.2	0.8	2.1	0.4	1.3	1.8	–
	δ C1 [ppm]	51.4	52.4	57.2	56.6	52.4	57.7	58.3	52.3	53.1
	δ C3 [ppm]	57.1	57.7	56.9	56.1	56.1	57.8	57.6	57.6	57.2
Method 3	Boltzmann distribution [%]	14.4	8.4	5.9	1.2	2.7	0.5	2.1	1.9	–
	δ C1 [ppm]	51.4	52.4	57.2	56.6	52.4	57.7	58.3	52.3	53.3
	δ C3 [ppm]	57.1	57.7	56.9	56.1	56.1	57.8	57.6	57.6	57.2

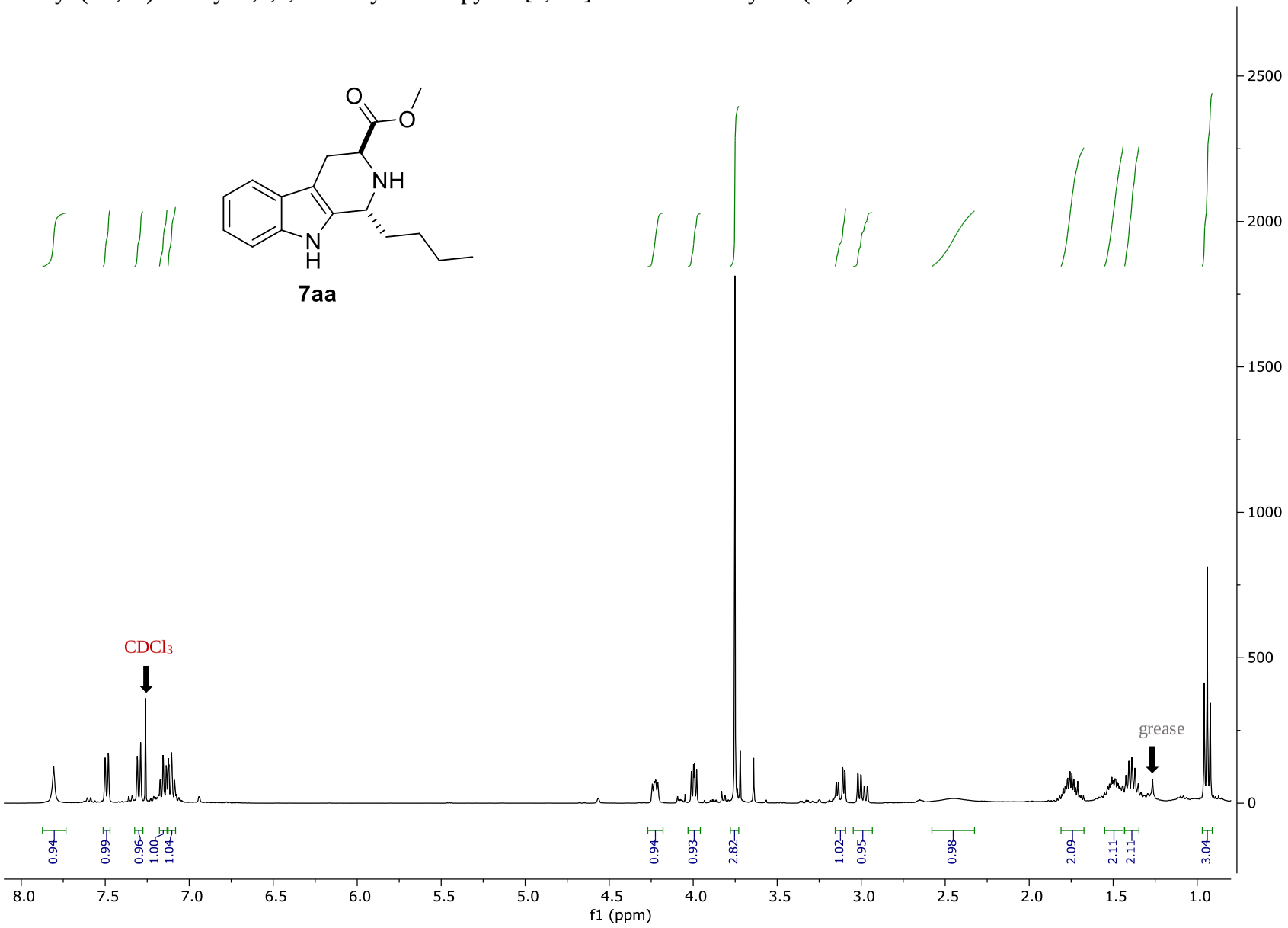
Methods used for calculation of conformer energies: M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform), M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform), M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF=(PCM=chloroform).
Methods used for ^{13}C NMR shift calculation: M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform), M2 and M3 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform).

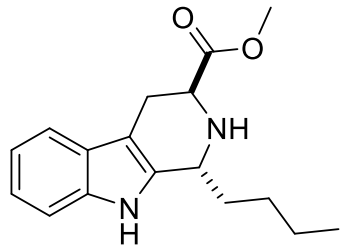
Table S22. Predicted ^{13}C NMR shifts in C-1 and C-3 for calculated conformers of compound **7b**, grouped according to conformer ensemble B and C.

		Ensemble B				Weighted average
		7b-4	**7b-5**	**7b-6**	**7b-8**	
Method 1	Boltzmann distribution [%]	8.7	20.6	22.1	9.7	–
	δ C1 [ppm]	59.5	59.0	56.5	57.1	57.9
	δ C3 [ppm]	52.7	52.1	52.8	55.6	53.0
Method 2	Boltzmann distribution [%]	8.0	22.1	21.2	8.9	–
	δ C1 [ppm]	58.4	57.9	55.5	56.0	56.8
	δ C3 [ppm]	51.9	51.4	51.7	54.2	52.0
Method 3	Boltzmann distribution [%]	7.5	19.6	18.5	8.8	–
	δ C1 [ppm]	58.4	57.9	55.5	56.0	56.8
	δ C3 [ppm]	51.9	51.3	51.7	54.2	52.0
		Ensemble C				**Weighted average**
		7b-1	**7b-2**	**7b-3**	**7b-7**	
Method 1	Boltzmann distribution [%]	21.8	11.5	3.5	2.2	–
	δ C1 [ppm]	56.9	57.7	56.6	56.7	57.1
	δ C3 [ppm]	58.0	58.8	57.3	58.7	58.2
Method 2	Boltzmann distribution [%]	22.5	11.5	3.4	2.3	–
	δ C1 [ppm]	56.0	56.7	55.6	55.8	56.2
	δ C3 [ppm]	56.8	57.7	56.1	57.6	57.0
Method 3	Boltzmann distribution [%]	26.5	12.6	4.2	2.3	–
	δ C1 [ppm]	56.0	56.7	55.6	55.8	56.1
	δ C3 [ppm]	56.8	57.7	56.1	57.6	57.0

Methods used for calculation of conformer energies: M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform), M2 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform), M3 – M06-2X/def2-TZVP//B3LYP/6-31G(d), SCRF(PCM=chloroform).
Methods used for ^{13}C NMR shift calculation: M1 – B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform), M2 and M3 – mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d), SCRF(PCM=chloroform).

Methyl (1*R*,3*S*)-1-butyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**7aa**)

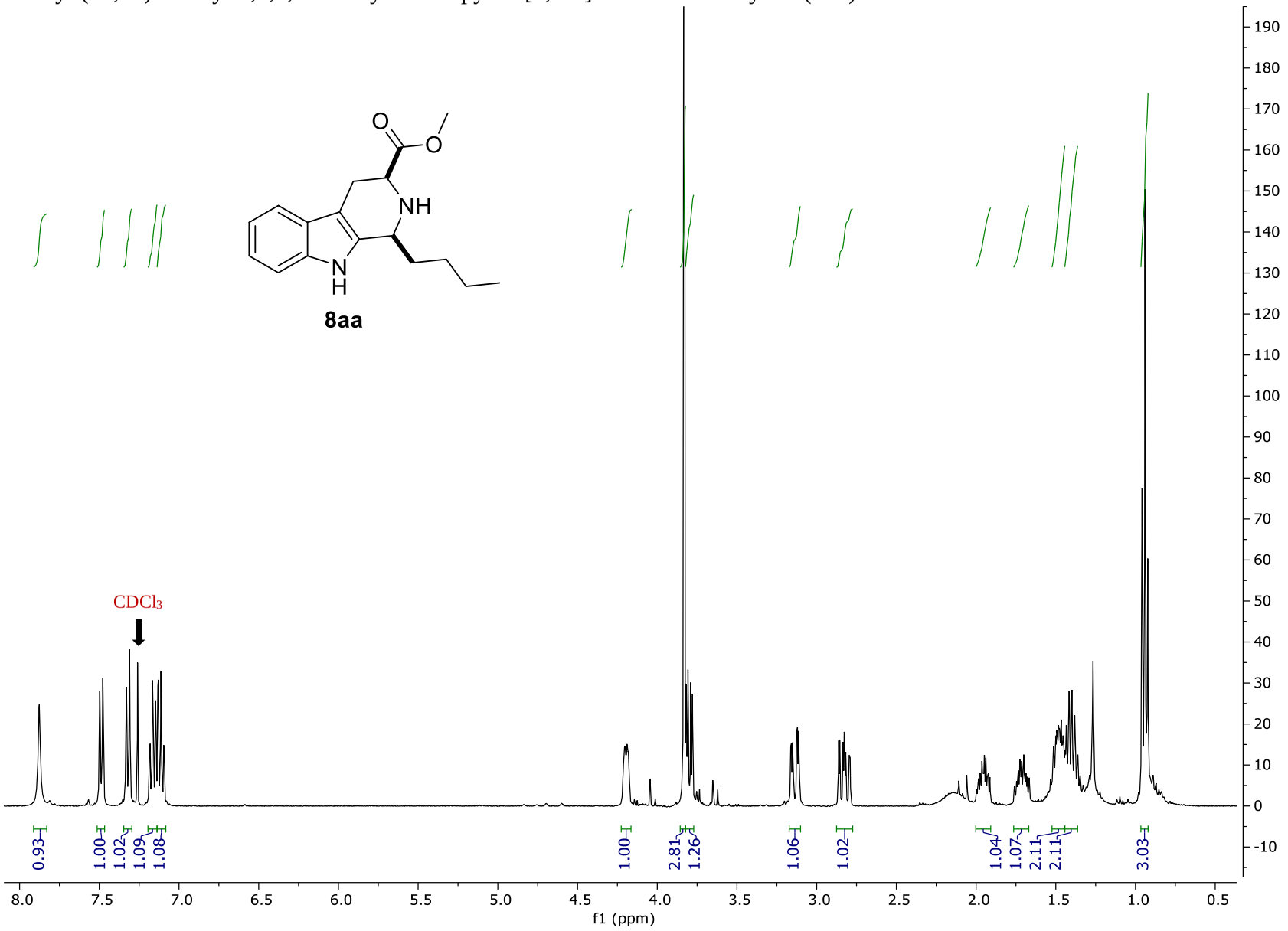


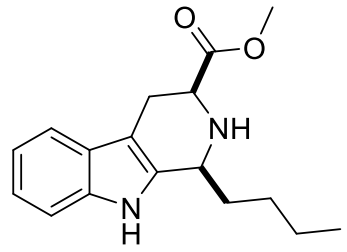

O
O
NH
N
H

7aa

CDCl3
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Methyl (1*S*,3*S*)-1-butyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**8aa**)

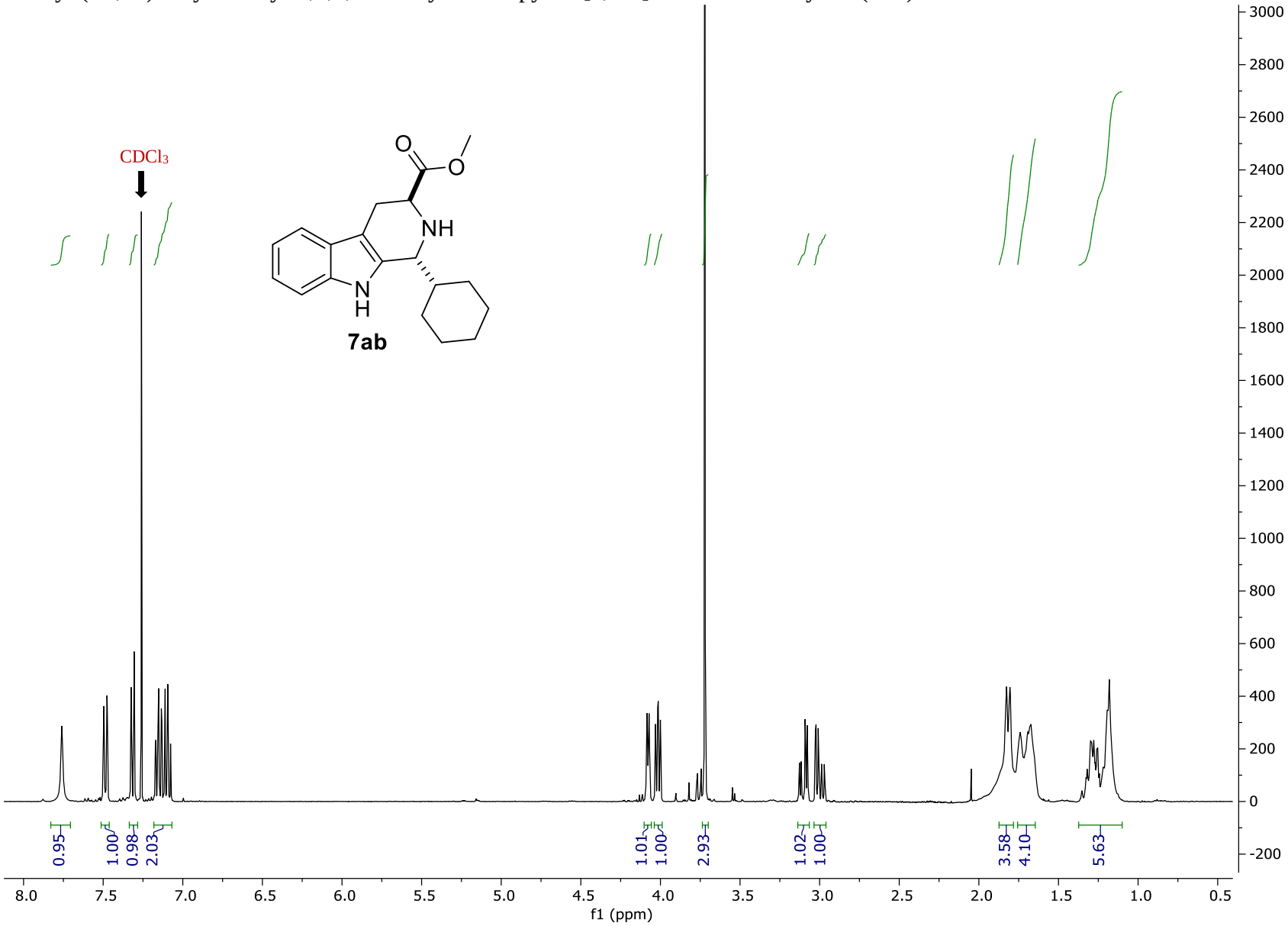



O
O
NH
N
H

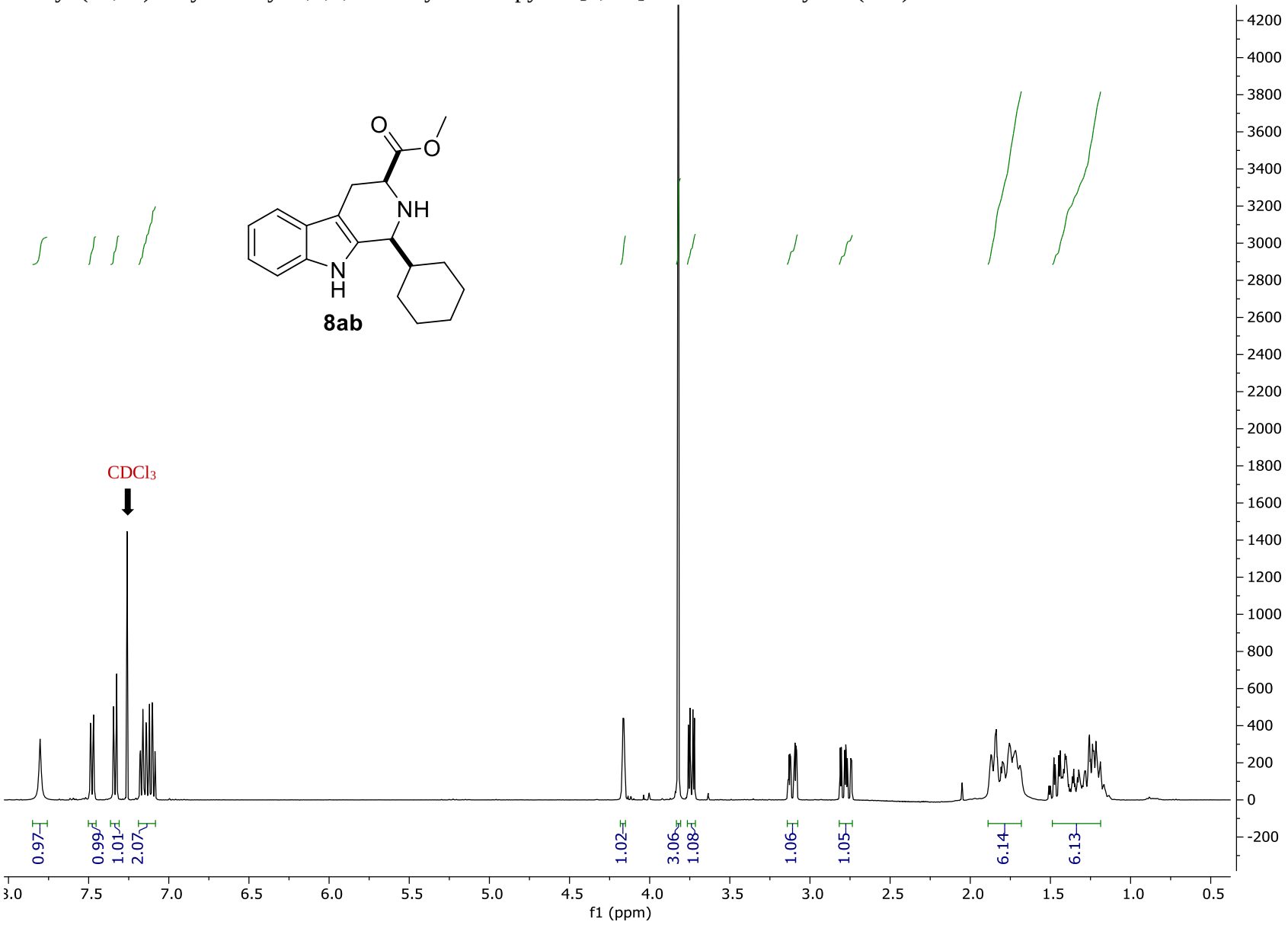
8aa

CDCl3
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

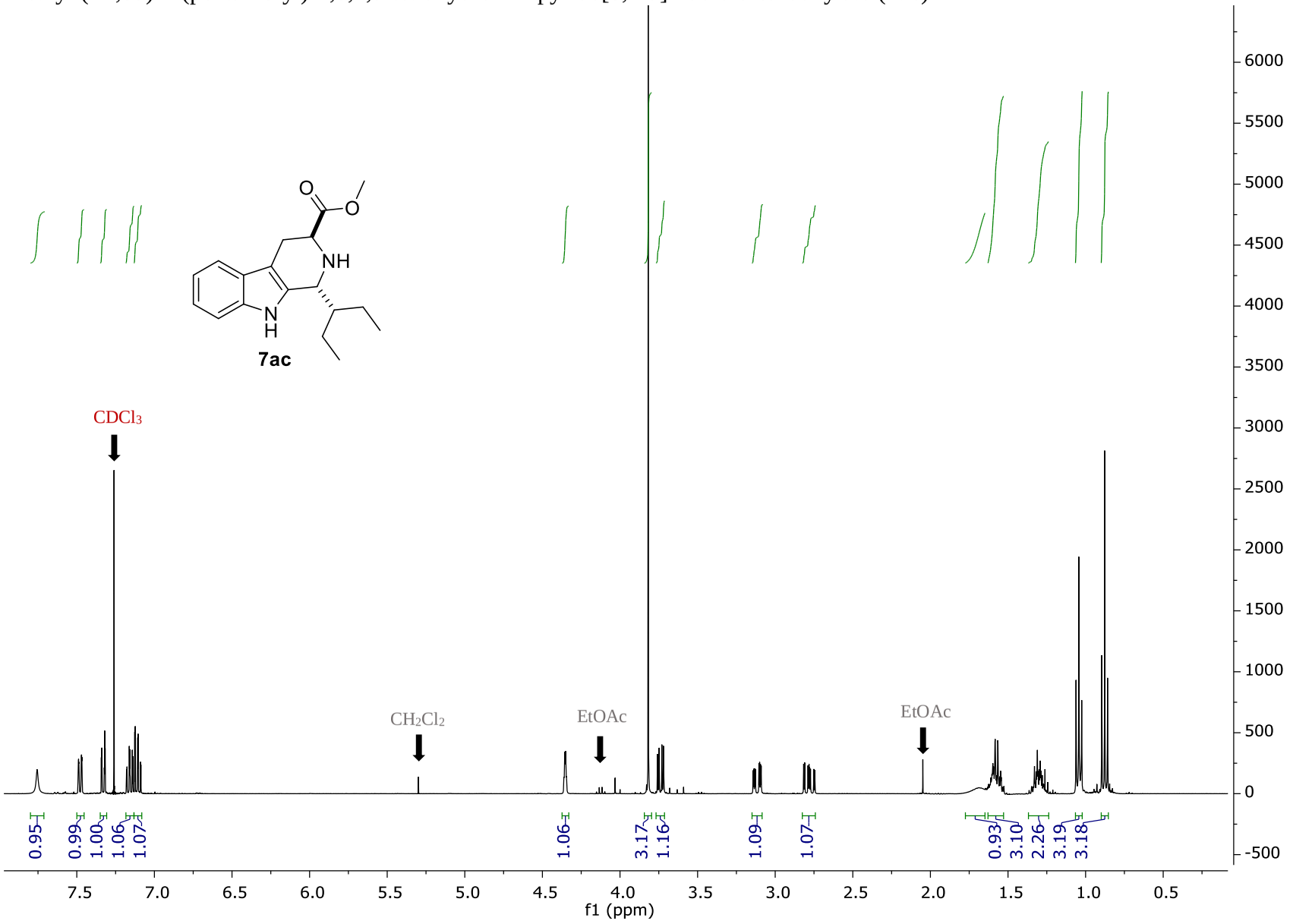
Methyl (1*R*,3*S*)-1-cyclohexyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**7ab**)

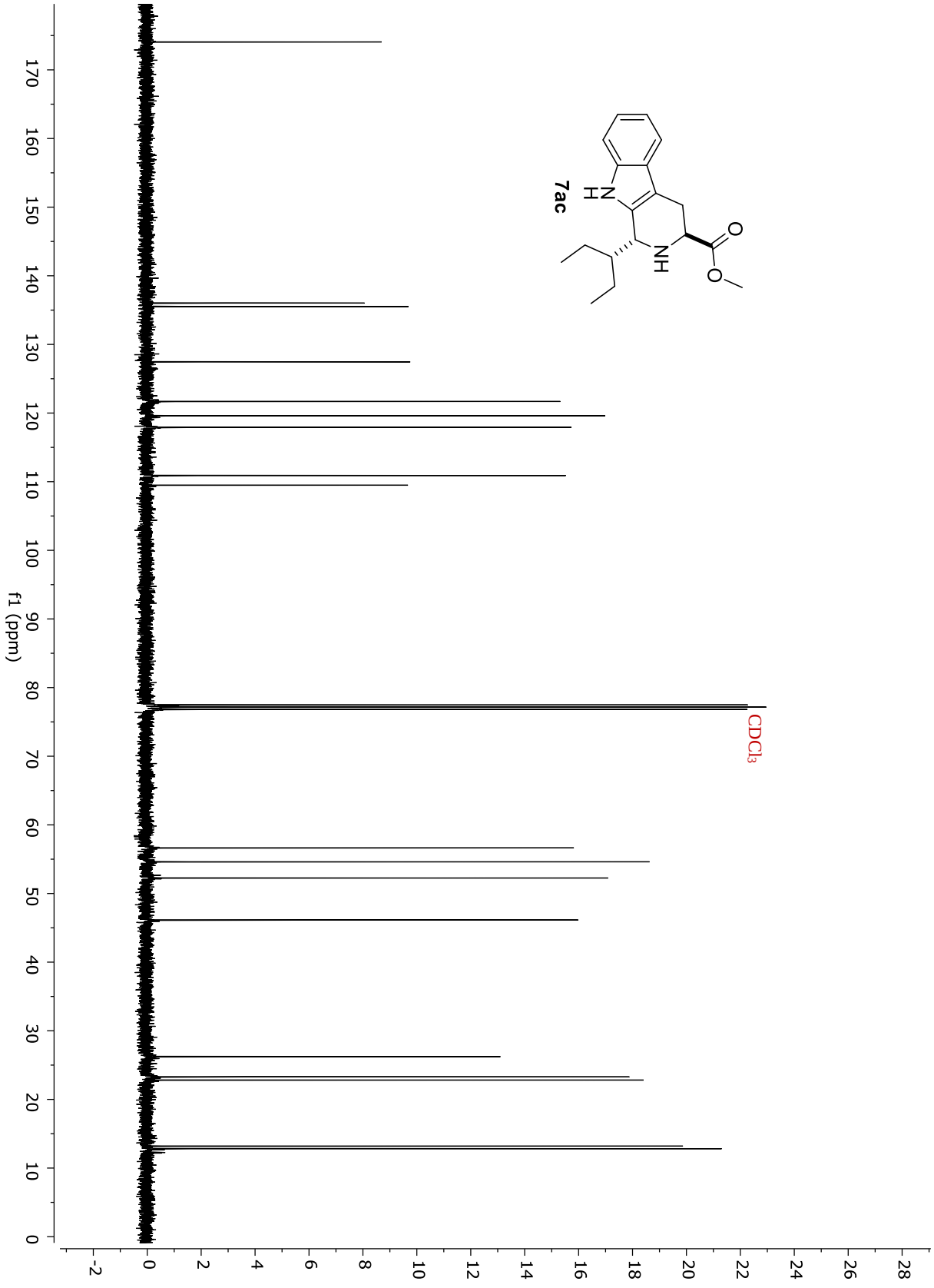


Methyl (1*S*,3*S*)-1-cyclohexyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**8ab**)

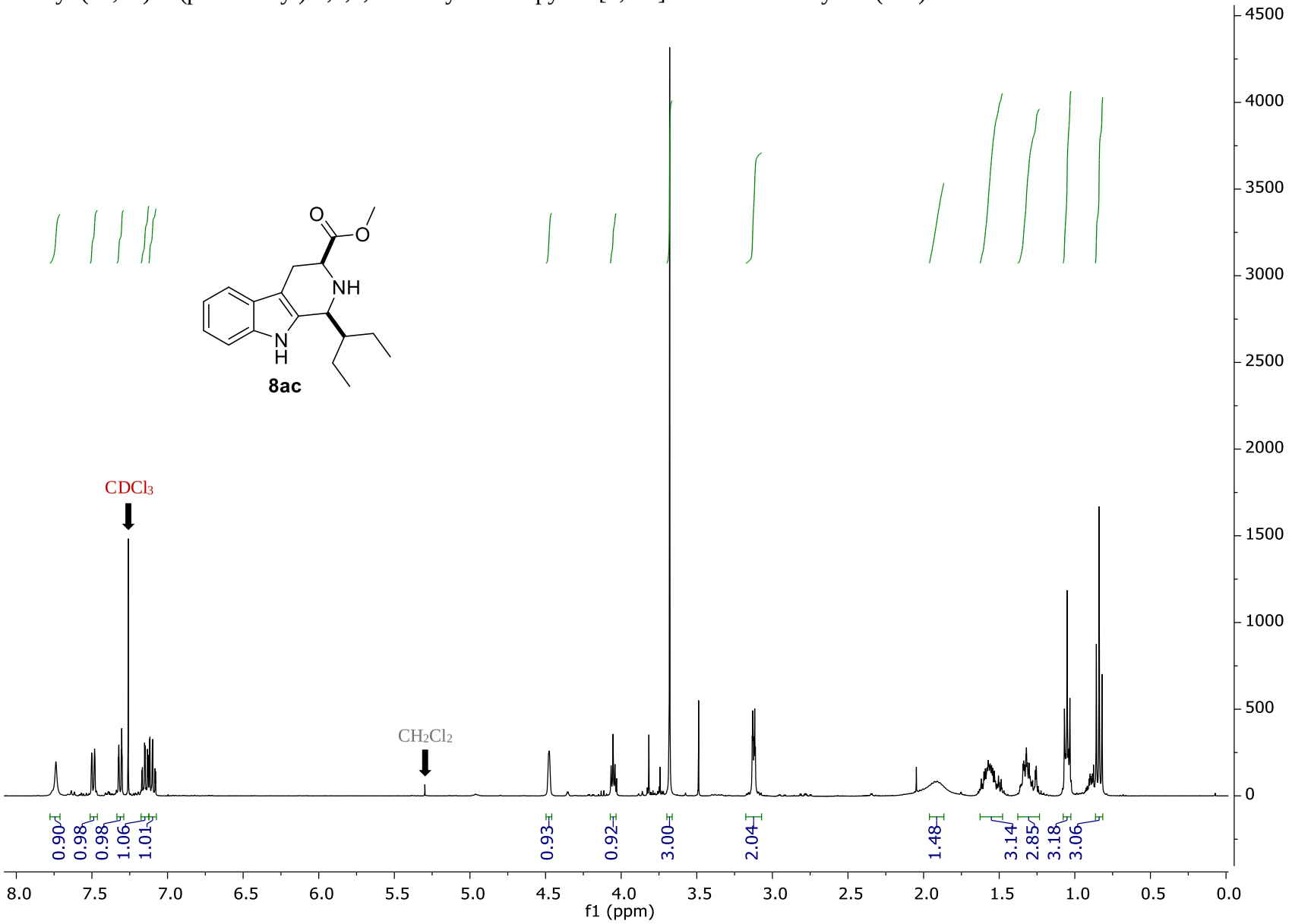


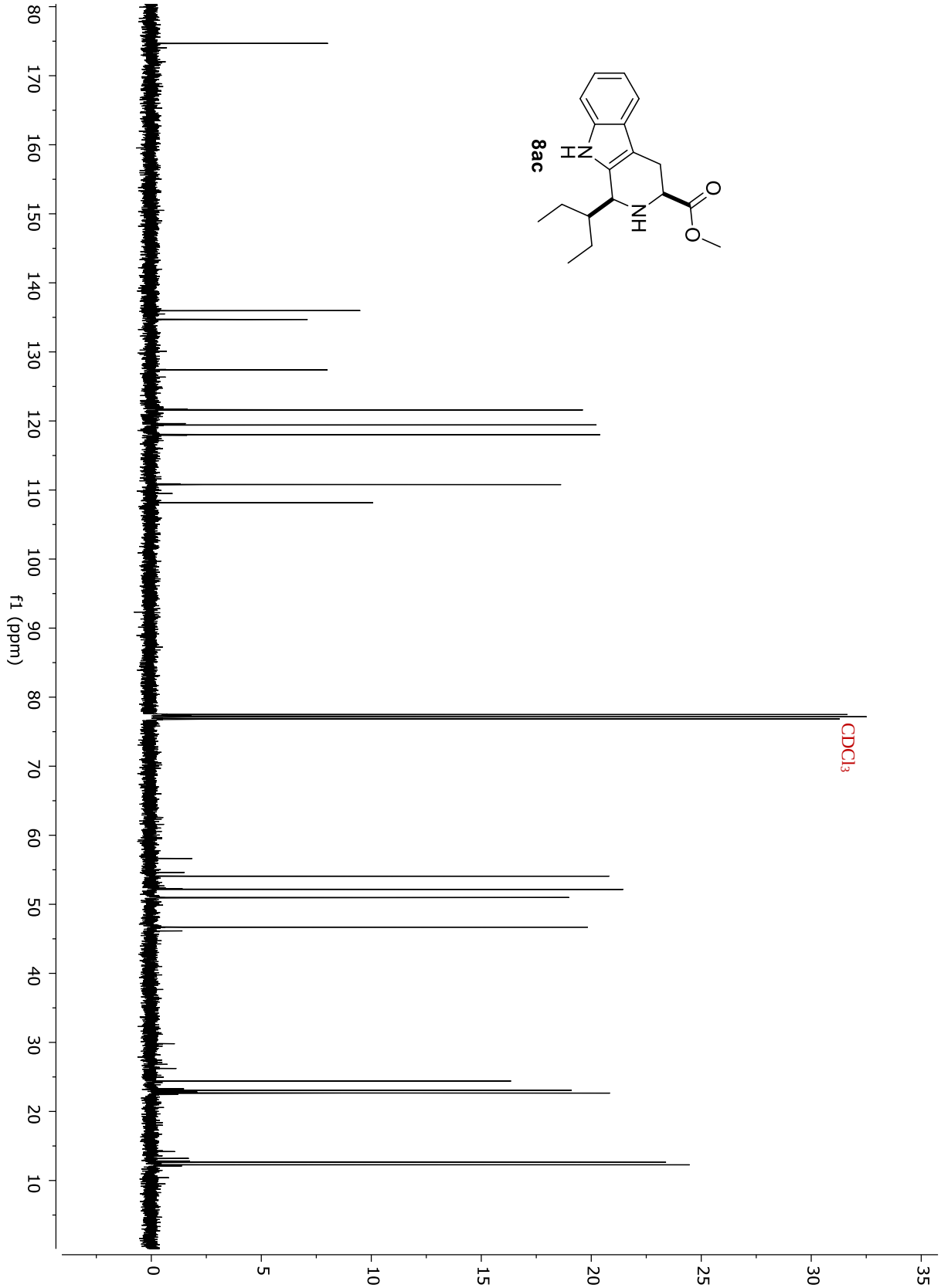
Methyl (1*R*,3*S*)-1-(pentan-3-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**7ac**)



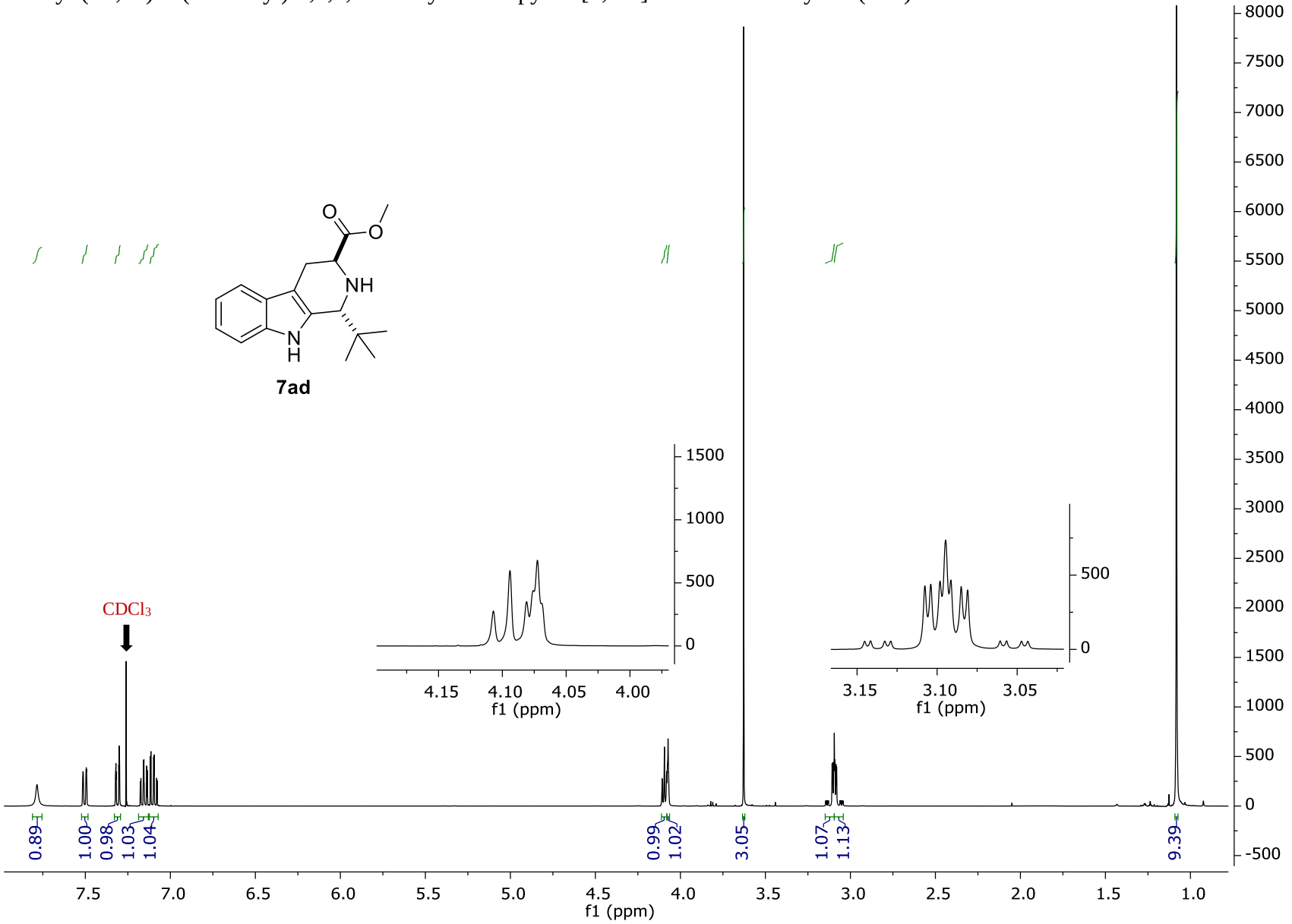

7ac
NH
NH
O
O
CDCl3
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
-2
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28

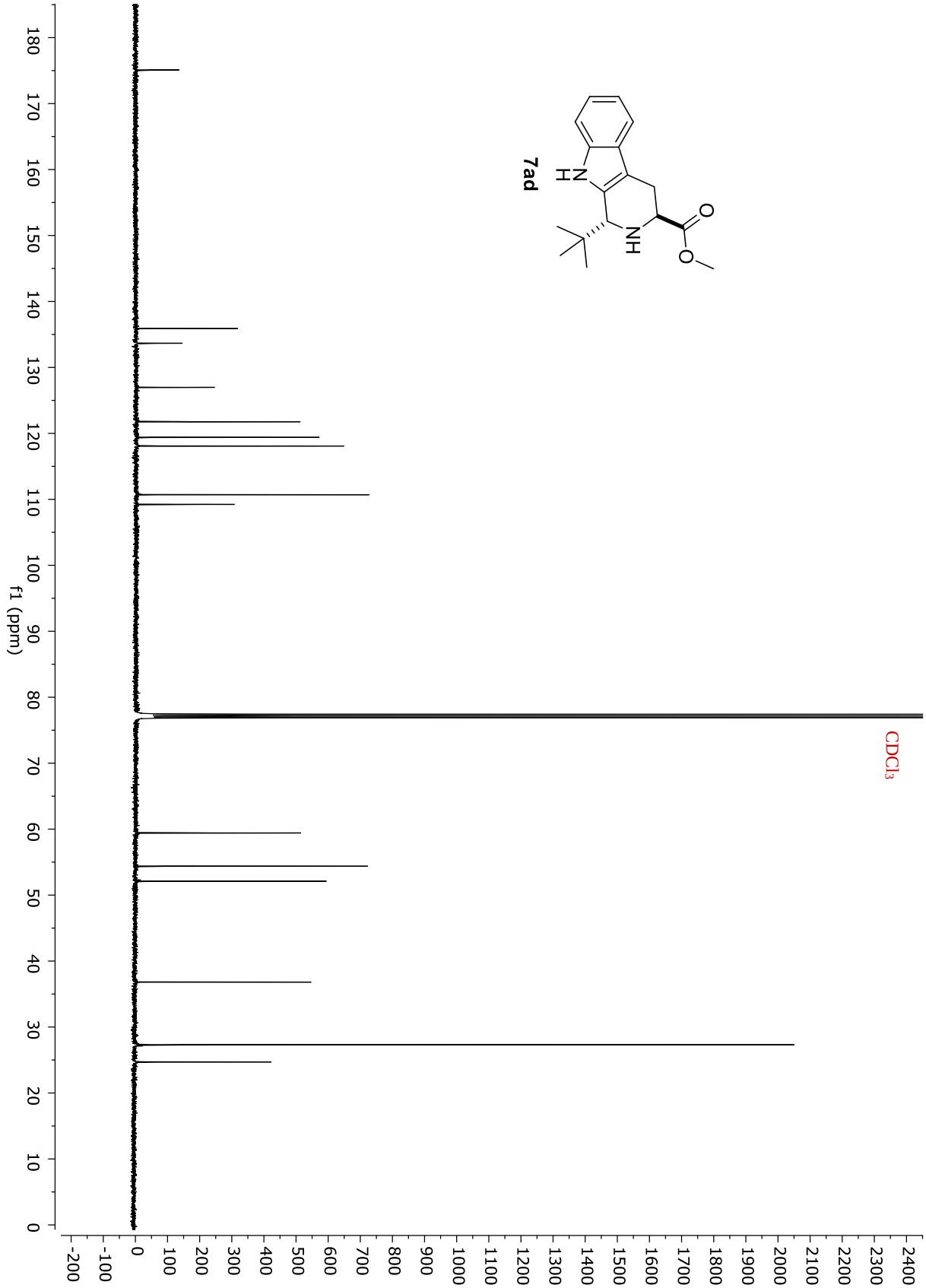
Methyl (1*S*,3*S*)-1-(pentan-3-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**8ac**)



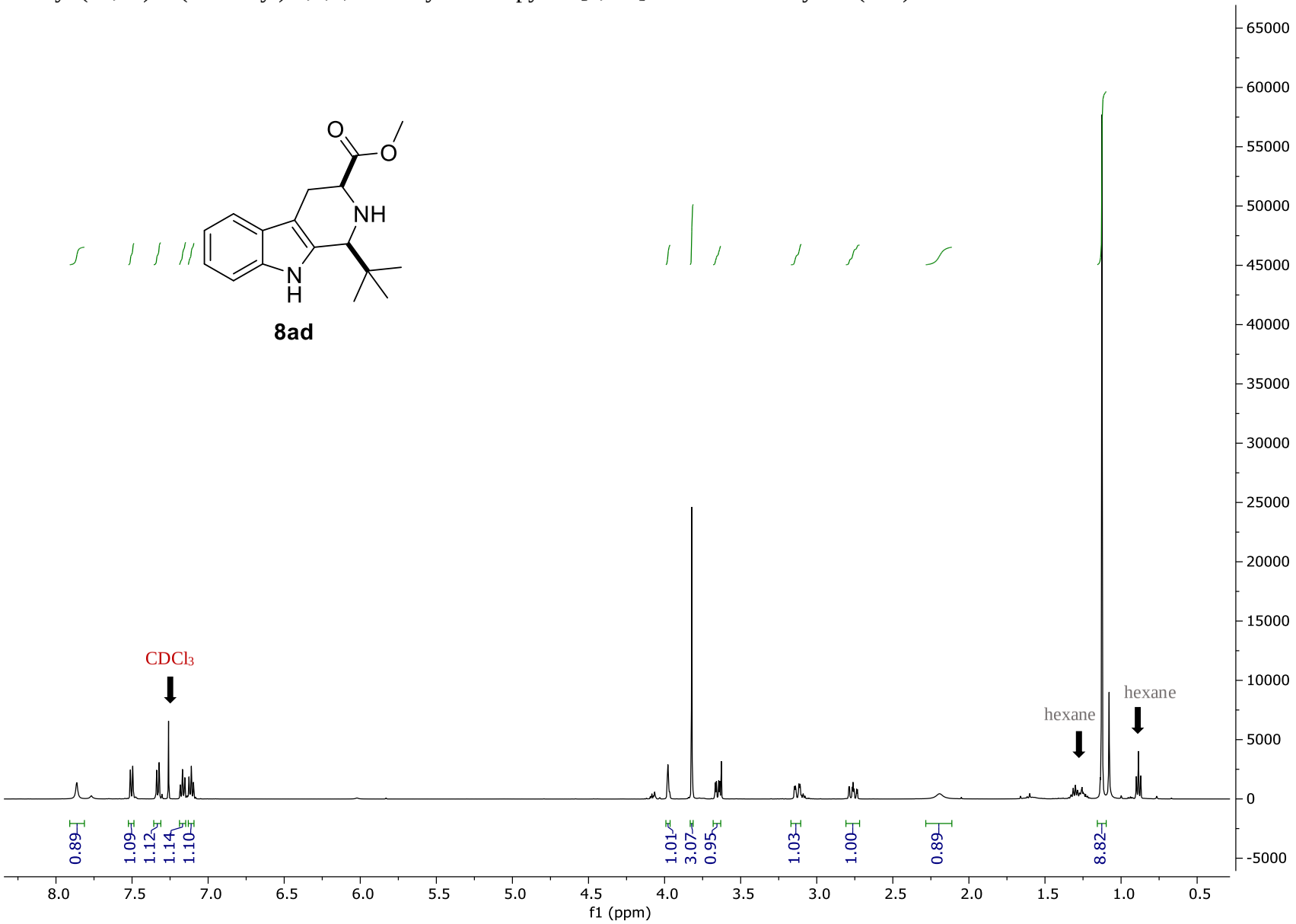

8ac
CDCl3
f1 (ppm)

Methyl (1*R*,3*S*)-1-(*tert*-butyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**7ad**)

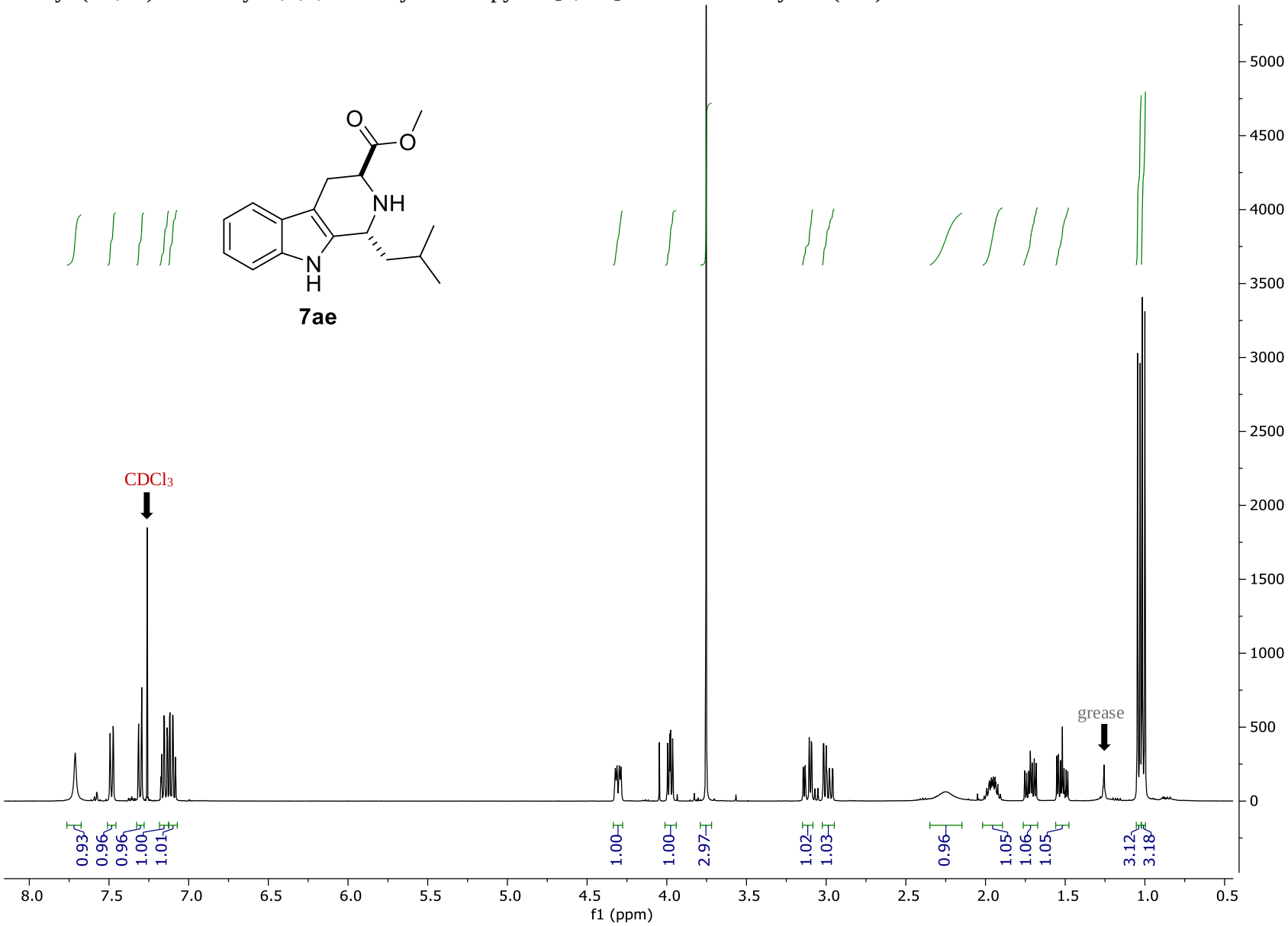



7ad
CDCl3
f1 (ppm)

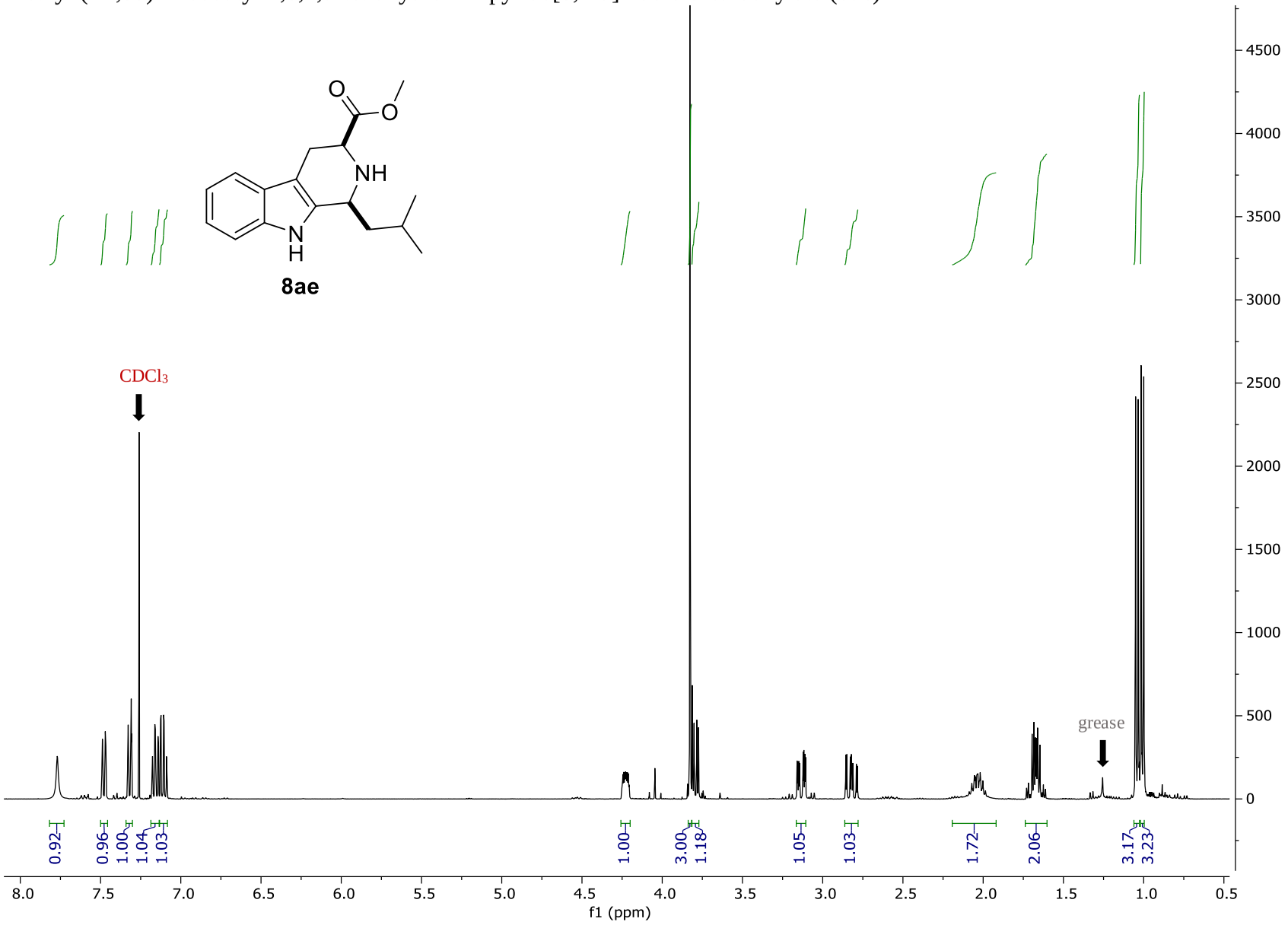
Methyl (1*S*,3*S*)-1-(*tert*-butyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**8ad**)



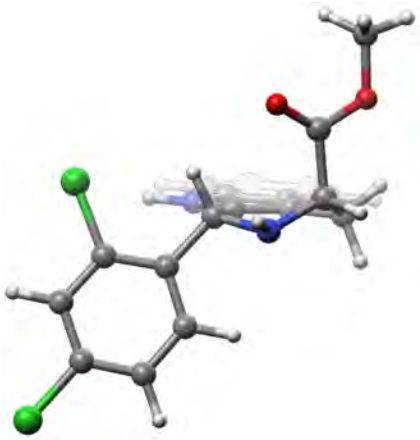
Methyl (1*R*,3*S*)-1-isobutyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**7ae**)



Methyl (1*R*,3*S*)-1-isobutyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (**8ae**)



7a-01



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C	-0.72813900	2.99430800	2.17932800
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N	-2.03854200	-1.19362300	0.71358500
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C	-6.62684000	0.76933500	1.21369300
C	-5.81273600	0.50724100	0.11273500
C	-4.47826800	0.17599900	0.32583700
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H	-6.21844000	0.56030000	-0.89163500
Cl	-8.31707000	1.18134100	0.97356100
H	-6.75391700	0.91525900	3.36362800
Cl	-4.18020300	0.34674500	4.35194800
H	-1.11769100	4.71339000	3.44678400
H	0.85269000	5.94944000	2.57033000
H	2.31730200	4.94573500	0.84615400
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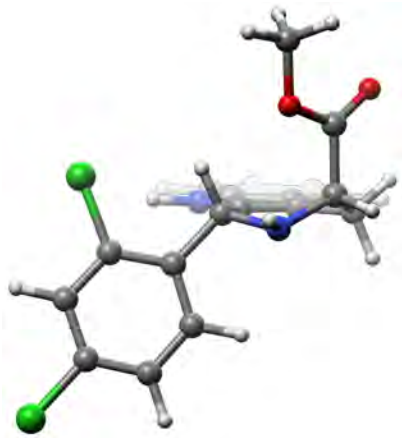

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H	-1.98801600	-2.57098000	0.16917500
C	-1.65438300	-4.20303300	1.53668000
C	-0.83282800	-4.75038500	2.54283000
C	0.31229700	-4.09090400	2.97691000
C	0.61872500	-2.86586700	2.37757300
N	1.67237000	-1.99981300	2.60099100
H	2.39718700	-2.11987300	3.29212300
C	1.54209700	-0.90834800	1.76139700
C	2.49191800	0.25970800	1.73147600
N	2.13399600	1.10682800	0.57805700
C	0.70376500	1.32493500	0.34517900
H	0.63458600	1.99169500	-0.52578400
C	-0.05901700	2.06723800	1.46213000
O	-1.26370200	2.08839800	1.57990100
O	0.77905700	2.76566500	2.26429100
C	0.13804900	3.54290000	3.29228900
H	-0.53313500	4.28263300	2.84842800
H	0.94616600	4.03219600	3.83645000
H	-0.43777100	2.89376900	3.95653100
H	2.59898700	2.00406800	0.69019200
H	2.39822100	0.81377700	2.67799600
C	3.95068600	-0.18772900	1.59669000
C	4.79171700	-0.40430200	2.69509200
C	6.11769700	-0.81654800	2.55592500
C	6.61711000	-1.02664900	1.27429600
C	5.81401300	-0.83499500	0.15075000
C	4.49759000	-0.42045300	0.32680800
H	3.85711600	-0.24778000	-0.53130200
H	6.21418700	-1.00670600	-0.84248600
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H	-1.09869400	-5.70482200	2.98900600
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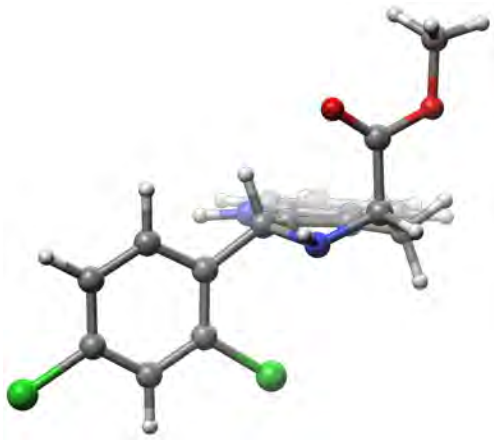

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C	-1.66338600	4.24626200	-1.43475900
C	-0.81806300	4.83672800	-2.39532300
C	0.33700900	4.19475400	-2.83057300
C	0.62881800	2.94443300	-2.27938000
N	1.68300200	2.08243200	-2.52241100
H	2.48508700	2.28453700	-3.09941700
C	1.54691100	0.96977200	-1.71247200
C	2.47069900	-0.21278200	-1.73981000
N	2.13973300	-1.09124000	-0.59900900
C	0.71190600	-1.31874000	-0.37057900
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C	0.04284100	-2.06141900	-1.54285500
O	0.64883700	-2.57685600	-2.46083100
O	-1.29529700	-2.13544900	-1.40388300
C	-1.98950800	-2.86011900	-2.43533400
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H	-3.04331400	-2.82422400	-2.15851100
H	-1.63673400	-3.89374500	-2.48035100
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H	2.30340500	-0.73747400	-2.69544900
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C	4.59694400	0.87185500	-0.69871100
C	5.96605300	1.13946500	-0.74113500
C	6.71980900	0.66917700	-1.81415200
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H	-2.55820200	4.77503700	-1.11765800
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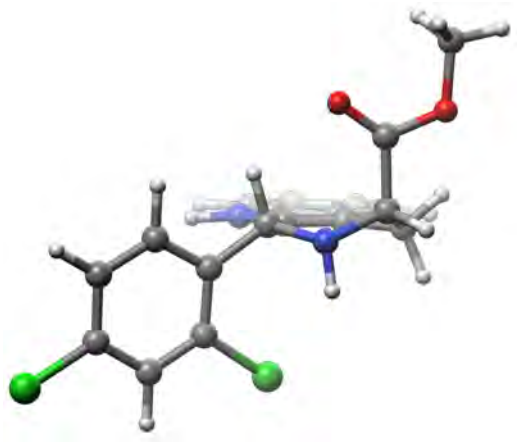
7a-04



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C	0.76094200	2.99720500	-2.16682900	C	6.21011500 -0.14300400 -2.73399200
N	1.82376500	2.13840200	-2.38049100	C	4.83967800 -0.37856200 -2.65559600
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C	1.65213700	1.00530500	-1.60532200	H	6.79600800 -0.53441500 -3.55816600
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N	2.19439600	-1.16144700	-0.55480600	H	6.55125500 1.68040300 0.12318400
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H	0.64168000	-2.00290000	0.52072700	H	1.18207400 4.73421800 -3.39905800
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O	0.62523100	-2.28733700	-2.58806800	H	-2.47097400 4.80949700 -1.10490900
O	-1.15886000	-2.40295900	-1.21273500	H	-1.08169200 -0.15807800 -0.07619000
C	-1.87948800	-3.08012600	-2.25608100	H	0.20002900 0.25310800 1.05211300
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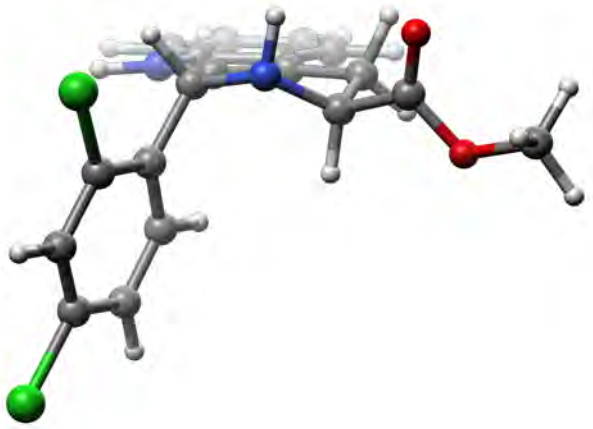
7a-05



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C	-2.34503600	-2.42386200	-0.44326300	H	2.42791100	-1.59575300	2.50465600
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C	-0.58413600	-3.66493400	0.69465300	C	4.53013500	-2.99845100	-1.26280200
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C	0.99069100	-2.08058800	1.00621200	H	4.42867700	-3.43794000	-2.24899000
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N	2.19792800	0.04314300	1.27267200	H	6.90544300	-2.24318400	1.06155100
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H	2.01152500	0.15889400	-0.80086600	H	-0.94448000	-5.77204200	1.07717400
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O	1.51872000	2.53665300	-1.13527600	H	-0.62702700	0.59135200	0.68412600
C	1.44951000	3.97214700	-1.21241600	H	-0.38560200	0.17907700	-1.01208600
H	0.52068400	4.33594400	-0.76532300				

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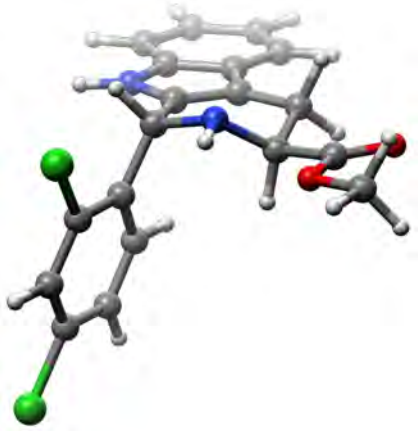

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C	1.89154600	1.66661400	-0.16521600
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C	3.60004000	3.28438300	0.02852300
H	3.59990200	3.50706800	-1.04150800
H	4.61253600	3.32456800	0.43057700
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H	2.94884900	0.11993100	1.56661300
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C	3.04578000	-2.45828500	0.96015100
C	4.34278700	-2.52719000	1.49348200
C	5.38276500	-3.20290200	0.85828100
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C	3.85738200	-3.78550700	-0.93342300
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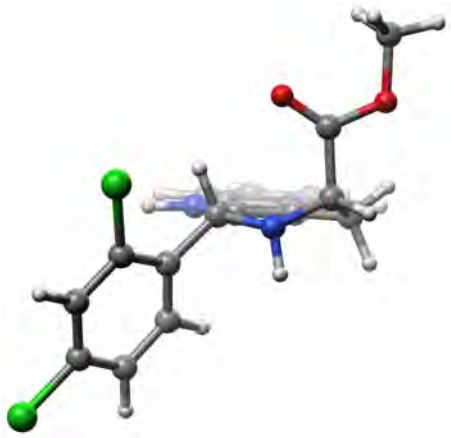
7a-07



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C	2.02307200	3.99927800	1.62823100
C	1.25490400	4.59664100	2.64765200
C	0.05376500	4.03483700	3.06833900
C	-0.36248700	2.85574200	2.44381100
N	-1.48826300	2.08022700	2.65097300
H	-2.23155900	2.28576700	3.30083000
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C	-0.81143200	-1.28815700	0.32699600
H	-0.78812100	-1.94339300	-0.55191400
C	-0.15466300	-2.08100500	1.45827400
O	-0.62263400	-2.30147300	2.55250600
O	1.06334600	-2.52110100	1.06786700
C	1.79519600	-3.26559500	2.05631800
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H	2.73491100	-3.54181800	1.57734200
H	1.23791600	-4.15747300	2.35438200
H	-2.65840600	-0.66264000	-0.21274200
H	-2.38754100	-0.68173200	2.67012600
C	-3.92719300	0.38856800	1.63665100
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C	-6.32155400	0.16152500	2.09200000
C	-6.57230300	1.28664800	1.31110300
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H	-3.41370000	2.05063200	0.38237600
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H	1.60716000	5.51182700	3.11559700
H	2.95715800	4.46440400	1.32514400
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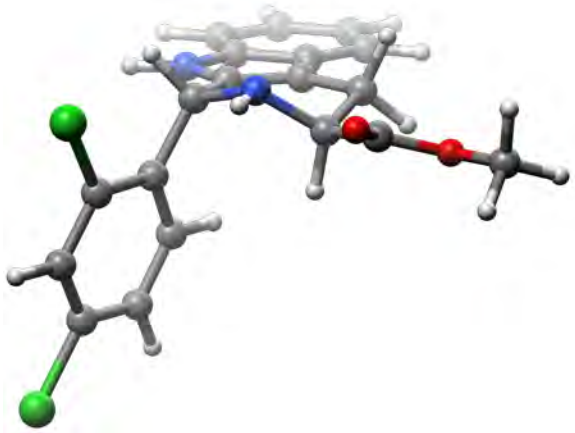
7a-08



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H	-2.80579800	-1.37431600	-0.90372200
C	-3.25607300	-3.44845800	-0.52951100
C	-2.81771700	-4.67093100	0.01823700
C	-1.57193800	-4.78303200	0.62685700
C	-0.77117900	-3.63842300	0.67543300
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H	1.04783000	-4.15743400	1.66190300
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C	1.74387100	1.89462300	0.01463200
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O	0.96448400	2.48106600	-0.91423700
C	1.18590500	3.88987500	-1.10484600
H	0.99209200	4.43573500	-0.17807000
H	0.48506500	4.19197200	-1.88329600
H	2.21615900	4.07595100	-1.41917400
H	2.89847800	0.40006800	1.58817500
H	2.33485800	-1.77542700	2.51672100
C	3.38722400	-2.09824300	0.68056500
C	4.68884400	-2.03487100	1.20317600
C	5.80330200	-2.49014100	0.50118500
C	5.61763000	-3.02184400	-0.77322100
C	4.34765500	-3.10225800	-1.33813800
C	3.25408100	-2.64454100	-0.60460600
H	2.26060900	-2.72113500	-1.03559300
H	4.21485700	-3.51962500	-2.33029100
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H	-1.23569700	-5.72660900	1.04910500
H	-3.46418900	-5.54259100	-0.03526400
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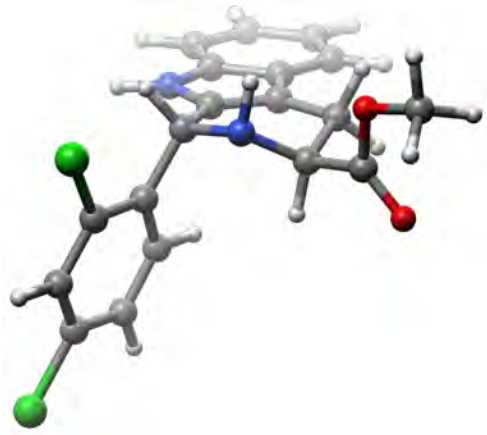
7a-09



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H	-2.74629900	-1.59903200	-0.66977800
C	-3.11907500	-3.60577800	0.02205700
C	-2.63570400	-4.71186500	0.74970300
C	-1.38794700	-4.68181000	1.36373700
C	-0.63109400	-3.51390900	1.23266500
N	0.62120700	-3.19686500	1.72674600
H	1.21542300	-3.81565500	2.25686300
C	0.95419400	-1.91250600	1.32695400
C	2.22939600	-1.19890300	1.68237100
N	2.14893300	0.23372200	1.32930100
C	1.47260300	0.49933900	0.05337600
H	2.03989700	-0.00176500	-0.73666700
C	1.52904700	1.98549200	-0.27105900
O	1.75616600	2.44800200	-1.36605400
O	1.22906000	2.73599400	0.81366800
C	1.23274600	4.15830800	0.60200000
H	2.22072400	4.49217200	0.27507900
H	0.97813300	4.59873300	1.56631100
H	0.49449100	4.43411900	-0.15547300
H	1.66945300	0.74043400	2.06999100
H	2.36652300	-1.22920400	2.77007800
C	3.48010500	-1.82307200	1.05574100
C	4.75552400	-1.62724300	1.60905600
C	5.90614900	-2.16316500	1.03372900
C	5.78403600	-2.91378500	-0.13393400
C	4.54060600	-3.13360900	-0.71923000
C	3.40840100	-2.58916900	-0.11443300
H	2.43467900	-2.76465400	-0.56186600
H	4.45754500	-3.71938300	-1.62799800
Cl	7.22755100	-3.59396600	-0.86641000
H	6.87559100	-1.99704400	1.48776300
Cl	4.96313400	-0.69208500	3.08634500
H	-1.01724900	-5.53570500	1.92505600
H	-3.24824800	-5.60538300	0.83304100
H	-4.09861400	-3.66379900	-0.44449100
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H	-0.35265100	0.02098800	-1.03946800

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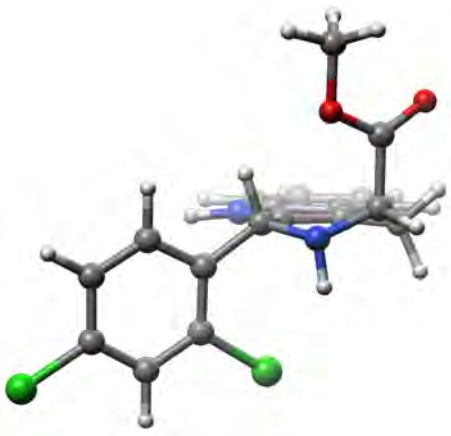

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H	2.17049300	-2.39584500	-0.33588300
C	1.88467900	-4.03694000	-1.70365000
C	1.05307900	-4.63512100	-2.67148800
C	-0.15654400	-4.05494700	-3.03999900
C	-0.51681100	-2.85848600	-2.41431100
N	-1.63347900	-2.05929700	-2.58366900
H	-2.43903200	-2.29254600	-3.14380700
C	-1.55478000	-0.98648700	-1.71156300
C	-2.54312500	0.15038300	-1.65012500
N	-2.26316200	1.04836400	-0.50861700
C	-0.83616800	1.28446800	-0.24698600
H	-0.79704000	1.90006700	0.66195600
C	-0.15252300	2.15411700	-1.31100400
O	1.04501700	2.34233300	-1.33753600
O	-1.00935600	2.72652900	-2.18010800
C	-0.39729500	3.59123300	-3.15322600
H	0.11523500	4.42027800	-2.65863200
H	-1.21676500	3.96030800	-3.77061700
H	0.32584500	3.03814600	-3.75823100
H	-2.65919400	0.63643300	0.33360200
H	-2.40798000	0.76071700	-2.55248800
C	-4.00797200	-0.27917800	-1.66411200
C	-4.60942400	-1.13751500	-0.72821000
C	-5.95516800	-1.49701000	-0.80532100
C	-6.73151100	-0.98941400	-1.84388100
C	-6.18275600	-0.13097600	-2.79277000
C	-4.83635700	0.20861900	-2.68571800
H	-4.40594800	0.88539300	-3.41878400
H	-6.79495600	0.26532700	-3.59519000
Cl	-8.42310600	-1.44230900	-1.94825000
H	-6.38542000	-2.16079600	-0.06514600
Cl	-3.69704500	-1.81057100	0.62065200
H	-0.79544500	-4.51586800	-3.78918000
H	1.36237100	-5.56503000	-3.14089400
H	2.82451100	-4.51541600	-1.44186400
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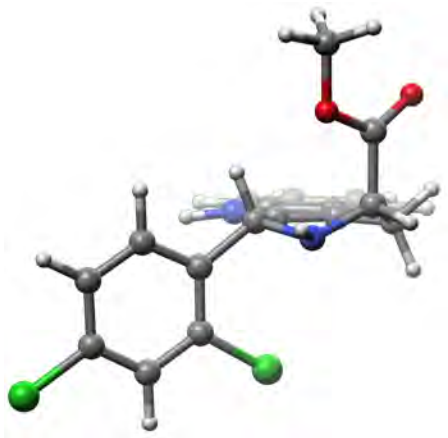
H	-0.18737300	-0.35195600	1.02534900

7a-11



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C	0.34079000	-2.23237400	-1.43752100	H	-2.75442900	1.83194200	-0.59577500
C	1.54588000	-2.85061000	-1.06416500	H	-2.37582800	0.74439200	-2.64028500
H	2.18000500	-2.40538300	-0.30180400	C	-3.95900400	-0.29974300	-1.71395600
C	1.91505900	-4.03954000	-1.68199300	C	-4.54460900	-1.13592100	-0.74579100
C	1.10238200	-4.62832100	-2.67140800	C	-5.89290000	-1.49180000	-0.80619600
C	-0.09367600	-4.03797500	-3.06693300	C	-6.68082700	-1.00866800	-1.84850000
C	-0.46046500	-2.84156400	-2.44517000	C	-6.14321100	-0.17968500	-2.82819500
N	-1.56719500	-2.03411000	-2.63932800	C	-4.79414500	0.15924600	-2.74201200
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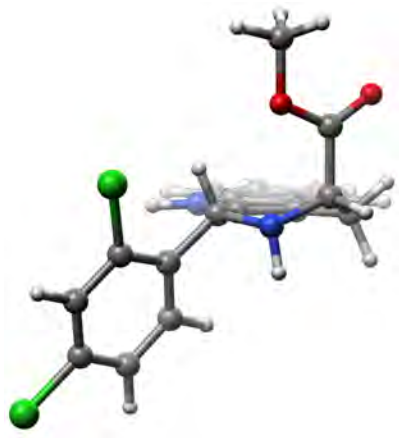
C	-1.49883900	-0.96644800	-1.76159200	H	-6.76297100	0.19423600	-3.63555800
C	-2.49927000	0.15185200	-1.71495300	Cl	-8.37600800	-1.45917400	-1.91922700
N	-2.22158400	0.96948400	-0.52206400	H	-6.31706100	-2.13839200	-0.04744600
C	-0.81221500	1.28170700	-0.27146200	Cl	-3.62181900	-1.79711400	0.58868200
H	-0.79281200	1.90008400	0.63700300	H	-0.71804700	-4.49178100	-3.83248500
C	-0.11133900	2.14743500	-1.33999200	H	1.41567100	-5.55924600	-3.13610900
O	1.08740900	2.26185500	-1.46410600	H	2.84465100	-4.52604000	-1.39930300
O	-1.00283300	2.84035900	-2.09076000	H	1.06518600	0.25023200	-0.02153900
C	-0.42206400	3.73488100	-3.05679900	H	-0.23457500	-0.35564600	1.01192400
H	0.20135000	4.48211400	-2.55912100				

7a-12



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H	-2.38044300	-2.17474400	0.36416300
C	-2.32884000	-3.71245500	1.87385400
C	-1.61198700	-4.29928100	2.93603000
C	-0.37319700	-3.80435100	3.33057700
C	0.13421700	-2.70379400	2.63410500
N	1.31422700	-2.00223800	2.80269600
H	2.04784800	-2.23741300	3.45348500
C	1.38462800	-0.99800100	1.85016000
C	2.48807800	0.02287800	1.75367000
N	2.30772400	0.89173500	0.56648800
C	0.91730200	1.22904000	0.23535100
H	0.96223400	1.81174200	-0.69463400
C	0.25950500	2.18159200	1.24292100
O	-0.92055300	2.45999200	1.20966500
O	1.12180100	2.70796200	2.13110600
C	0.54543600	3.64177200	3.06129300
H	0.12037500	4.49673600	2.52926700
H	1.36868200	3.95748500	3.70225200
H	-0.24190400	3.16176700	3.64823100
H	2.71190100	0.41905400	-0.24019200
H	2.44018300	0.67662200	2.63151000
C	3.88245800	-0.59015900	1.69867300
C	5.00450100	0.01109800	2.28941200
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C	6.44366500	-1.73138100	1.47766500
C	5.35943200	-2.35939900	0.86826000
C	4.09852800	-1.78079300	0.98912000
H	3.24476600	-2.26800500	0.52574300
H	5.49872400	-3.28175300	0.31534700
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Cl	4.86110200	1.51026800	3.19720100
H	0.17646000	-4.25557600	4.15276300
H	-2.03513100	-5.15252200	3.45909300
H	-3.29549500	-4.12274400	1.59484200
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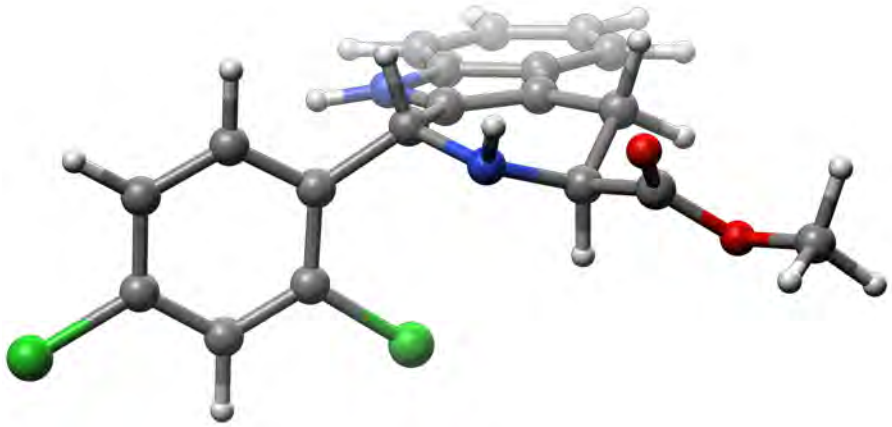
7a-13



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H	-1.82962900	-2.61728800	-0.73978100
C	-1.00439200	-4.60597100	-0.83242700
C	0.13797400	-5.41795100	-0.68281100
C	1.36555500	-4.87488400	-0.31800600
C	1.42477000	-3.49480200	-0.10537400
N	2.48729100	-2.69075100	0.26568500
H	3.44808300	-2.98699900	0.34625600
C	2.05604100	-1.37740100	0.32150100
C	2.90258000	-0.21747800	0.76024800
N	2.28469600	1.06480800	0.39324700
C	1.03923300	1.10111700	-0.36807600
H	1.25658800	0.99233500	-1.43555700
C	0.41920200	2.47363900	-0.15082900
O	0.64205100	3.19250900	0.80211500
O	-0.45500900	2.77386600	-1.12851600
C	-1.14652700	4.02666500	-0.97844800
H	-1.73048000	4.03440800	-0.05433000
H	-1.80034900	4.10388200	-1.84726700
H	-0.43403400	4.85511700	-0.95707400
H	2.20340600	1.68159500	1.19502200
H	2.95046200	-0.25955500	1.86030400
C	4.37005400	-0.31679200	0.31456900
C	4.81411600	-0.26779700	-1.01649100
C	6.16598200	-0.35340600	-1.34897600
C	7.10685400	-0.49597600	-0.33122100
C	6.71475600	-0.55512000	1.00236600
C	5.35577000	-0.46428700	1.29966300
H	5.04519100	-0.50050300	2.34149100
H	7.45262600	-0.66363100	1.78951100
Cl	8.80874800	-0.60337000	-0.74851800
H	6.47580300	-0.31042500	-2.38629000
Cl	3.68672300	-0.10580100	-2.35302100
H	2.24557700	-5.50247000	-0.20242900
H	0.05918500	-6.48795400	-0.85455300
H	-1.94801200	-5.06381400	-1.11651000
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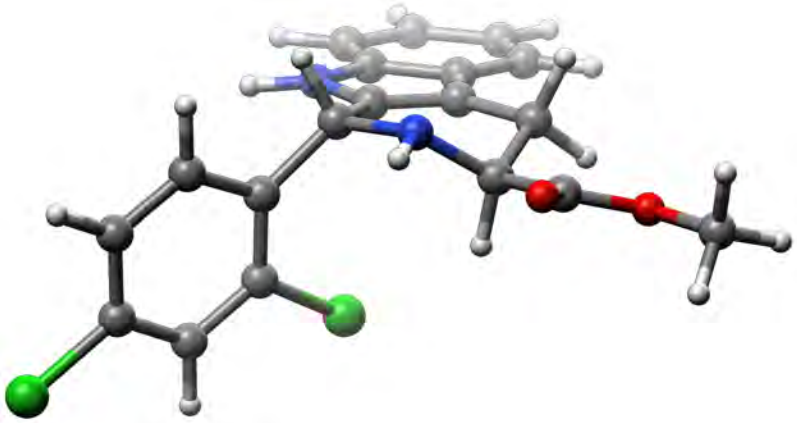
7a-14



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H	2.44334500	-1.98559200	0.81876000
C	2.27897800	-4.13194400	0.71100300
C	1.46981800	-5.23826600	0.38287100
C	0.17725200	-5.06745800	-0.10241800
C	-0.28914100	-3.75874100	-0.25262700
N	-1.50490700	-3.28844300	-0.71466700
H	-2.30877900	-3.85928800	-0.92676500
C	-1.50312300	-1.90563300	-0.65052300
C	-2.62721100	-1.03888900	-1.13409800
N	-2.19535800	0.35896100	-1.03557100
C	-1.34629100	0.74578900	0.08781300
H	-1.78849600	0.50814700	1.07231300
C	-1.22674300	2.26414900	0.06358600
O	-2.01192600	3.00496700	-0.49067200
O	-0.17566900	2.69541100	0.78667500
C	-0.03213200	4.12394100	0.87567700
H	0.10186600	4.55737100	-0.11866500
H	0.85286300	4.28981400	1.49027700
H	-0.91494500	4.56889200	1.34214600
H	-2.96216600	1.01441100	-1.14865500
H	-2.74216200	-1.23781600	-2.21152500
C	-4.02888200	-1.34477800	-0.55947300
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C	-5.08861900	-1.34650300	-1.48257900
H	-4.85640900	-1.16985100	-2.53029200
H	-7.20493000	-1.55065600	-1.86757000
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H	-0.44503200	-5.92195600	-0.35612700
H	1.86199900	-6.24359200	0.51018700
H	3.28460100	-4.30194500	1.08598500
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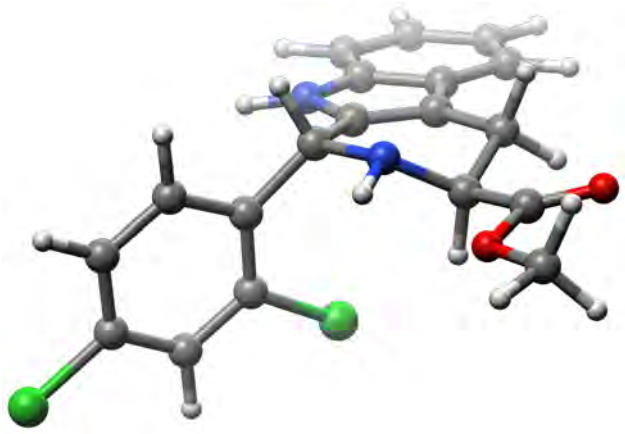
7a-15



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H	2.68157900	-1.68806800	0.75123300
C	2.79627100	-3.83064500	0.54614600
C	2.13709600	-5.01619600	0.16363200
C	0.83348800	-4.99207200	-0.32157600
C	0.20179500	-3.74901500	-0.41572900
N	-1.06536500	-3.41940200	-0.86153600
H	-1.78869100	-4.07899700	-1.10393300
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C	-2.46847200	-1.31853200	-1.18254300
N	-2.26286600	0.12723500	-0.97488300
C	-1.42110300	0.56279000	0.14917300
H	-1.81584000	0.23728300	1.12755400
C	-1.40739300	2.08730400	0.20177100
O	-0.43361000	2.77225200	0.41859600
O	-2.65152700	2.59435200	0.03153100
C	-2.74963300	4.02736800	0.10010700
H	-2.41655500	4.38622500	1.07730400
H	-3.80423600	4.25675600	-0.05486100
H	-2.13614100	4.48992300	-0.67724300
H	-3.15191500	0.61583100	-0.95658900
H	-2.53575100	-1.45099600	-2.27431700
C	-3.81414500	-1.87035800	-0.66828000
C	-4.15431400	-2.20106500	0.65604000
C	-5.42572200	-2.66291100	1.00152600
C	-6.39629300	-2.79636700	0.01220300
C	-6.11034700	-2.48171000	-1.31281100
C	-4.83053300	-2.03087700	-1.62521000
H	-4.60299300	-1.78871700	-2.66071000
H	-6.86757900	-2.58979300	-2.08149100
Cl	-7.99380100	-3.37340300	0.45112900
H	-5.64980100	-2.91396100	2.03135900
Cl	-3.00451200	-2.07445600	1.98147200
H	0.32711200	-5.90739800	-0.61750400
H	2.65603800	-5.96716500	0.24772900
H	3.81532400	-3.88597700	0.91924000
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H	0.57037300	0.22049200	0.90897700

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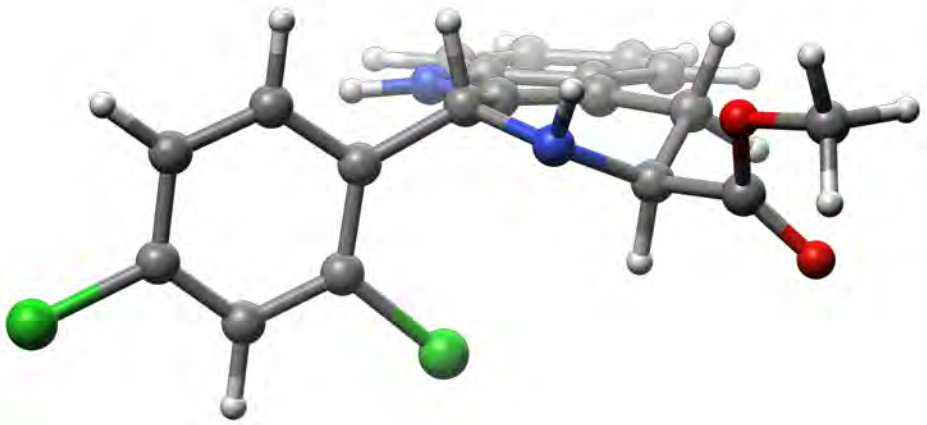

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H	1.99457300	-2.54190500	0.55699300
C	1.31032500	-4.58274500	0.45095900
C	0.23252900	-5.45449600	0.19557300
C	-1.02051600	-4.96669700	-0.16034300
C	-1.17155700	-3.58049500	-0.25567600
N	-2.27877100	-2.82149200	-0.58931700
H	-3.21353900	-3.17485300	-0.72603400
C	-1.94035700	-1.48172200	-0.51792200
C	-2.85431300	-0.34891300	-0.88641600
N	-2.33202300	0.94725600	-0.40719000
C	-1.13278600	0.97397900	0.43775700
H	-1.41128900	0.70227000	1.45861800
C	-0.57092300	2.38552200	0.52846800
O	0.02034100	2.82015600	1.49076100
O	-0.73791500	3.08325800	-0.62094800
C	-0.18801700	4.41234700	-0.62130500
H	-0.64688700	5.01433500	0.16691400
H	-0.41805000	4.82470800	-1.60405100
H	0.89239100	4.37768800	-0.45997700
H	-2.20623700	1.57851500	-1.18967600
H	-2.86679900	-0.30102300	-1.98655900
C	-4.32533400	-0.57794800	-0.50719000
C	-4.82038800	-0.68104300	0.80282600
C	-6.17542000	-0.88045300	1.06843600
C	-7.06753200	-0.98563200	0.00367700
C	-6.62368000	-0.89632800	-1.31201100
C	-5.26391100	-0.69438900	-1.54190200
H	-4.91493600	-0.61636700	-2.56910300
H	-7.32334100	-0.97756300	-2.13640100
Cl	-8.77270500	-1.23575400	0.33679500
H	-6.52445500	-0.95279700	2.09153100
Cl	-3.75788000	-0.57404300	2.19572700
H	-1.85066000	-5.64034700	-0.35712400
H	0.38241100	-6.52755300	0.27742800
H	2.27599400	-4.99834100	0.72562400
H	0.46569000	0.36480000	-0.92796100
H	0.78180500	-0.00931500	0.76897700

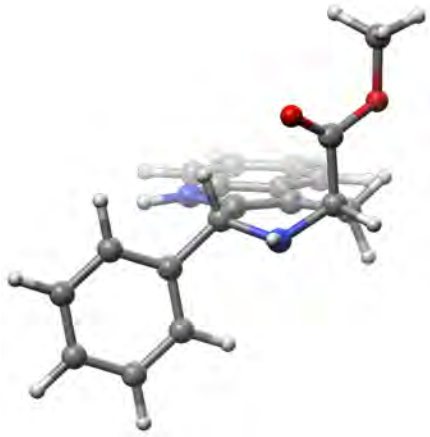
7a Shielding tensors B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	7a-01	**7a-02**	**7a-03**	**7a-04**	**7a-05**	**7a-06**	**7a-07**	**7a-08**
1	127.39	126.30	121.04	121.58	127.11	124.72	126.27	125.04
3	120.96	120.36	121.25	121.97	126.69	126.95	121.97	127.10
4	154.79	155.60	155.44	152.25	151.69	153.85	151.55	152.86
4a	70.56	69.55	69.04	69.11	64.90	64.79	67.04	64.25
4b	49.87	50.05	49.95	49.24	49.15	49.44	49.15	49.18
5	60.24	60.45	60.89	61.03	60.03	59.28	60.60	60.07
6	59.13	59.20	59.12	59.07	57.99	58.68	58.65	58.23
7	56.55	56.66	56.71	56.74	55.54	56.11	56.09	55.72
8	68.26	68.74	68.32	68.32	68.46	67.24	67.94	68.27
8a	40.98	40.12	40.59	41.02	40.69	40.33	40.50	40.25
9a	42.39	43.15	43.76	42.47	44.79	45.70	42.77	44.14
1'	33.62	33.90	36.06	37.29	35.21	36.34	34.98	36.20
2'	35.09	35.30	31.39	33.24	32.40	33.71	31.24	33.61
3'	47.51	47.28	44.68	45.56	46.38	46.35	46.50	46.37
4'	34.66	34.50	33.53	33.22	34.50	33.94	33.72	34.27
5'	49.33	48.95	50.27	49.23	50.58	50.34	49.47	50.62
6'	44.50	44.58	42.96	41.45	46.61	46.04	46.10	46.29
1''	-3.55	-2.20	-3.62	-2.17	-2.85	-0.02	-1.52	-1.32
2''	128.14	127.92	128.27	128.58	128.10	127.99	128.57	127.86
	7a-09	**7a-10**	**7a-11**	**7a-12**	**7a-13**	**7a-14**	**7a-15**	**7a-16**
1	126.45	120.37	119.81	126.37	121.96	119.28	118.85	121.51
3	123.59	120.11	120.45	120.43	124.00	124.55	123.40	121.04
4	152.21	153.92	156.68	152.98	150.37	152.77	154.40	149.85
4a	65.42	67.64	68.07	65.58	68.62	65.61	66.25	67.95
4b	48.99	49.01	49.46	48.63	48.76	48.57	49.02	49.00
5	59.36	60.44	60.34	59.88	60.45	58.48	59.51	60.41
6	57.80	58.81	58.83	58.27	58.08	58.95	58.52	58.34
7	55.53	56.51	56.58	55.72	55.93	56.51	56.52	55.99
8	68.21	68.47	68.52	67.98	67.89	67.87	67.89	68.14
8a	40.81	40.62	40.24	40.45	40.59	40.56	40.09	40.83
9a	44.39	42.97	44.06	43.22	42.65	43.91	44.70	42.86
1'	36.25	37.66	36.49	35.63	34.92	33.51	34.12	35.66
2'	32.29	33.48	31.49	31.99	32.74	33.78	32.67	33.21
3'	46.33	45.24	44.36	46.65	45.22	44.86	45.14	45.06
4'	34.14	33.15	33.43	33.80	34.03	33.65	33.31	33.77
5'	50.53	49.36	50.35	49.34	50.25	49.43	49.32	50.23
6'	46.04	41.82	43.14	46.03	44.49	42.20	42.14	44.34
1''	-0.06	-1.40	-2.49	-1.11	-3.64	-1.62	0.18	-0.39
2''	128.26	128.03	128.10	127.98	127.71	128.03	128.20	127.93

7a Shielding tensors mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	7a-01	**7a-02**	**7a-03**	**7a-04**	**7a-05**	**7a-06**	**7a-07**	**7a-08**
1	132.80	131.75	126.78	127.34	132.65	130.28	131.74	130.57
3	126.85	126.25	127.08	127.90	132.63	132.55	127.89	132.68
4	160.03	160.80	160.66	157.65	157.10	159.10	157.01	158.17
4a	75.86	74.80	74.25	74.46	70.14	69.93	72.23	69.50
4b	55.38	55.49	55.38	54.77	54.71	55.03	54.72	54.77
5	64.32	64.51	64.93	65.09	64.07	63.40	64.61	64.11
6	63.60	63.64	63.58	63.54	62.41	63.11	63.09	62.64
7	60.93	61.00	61.07	61.10	59.84	60.33	60.35	60.01
8	72.39	72.93	72.52	72.49	72.55	71.47	72.09	72.37
8a	46.44	45.65	46.17	46.61	46.26	45.79	46.09	45.76
9a	47.75	48.48	48.99	47.76	50.07	50.89	48.07	49.43
1'	39.48	39.73	42.00	43.19	41.03	41.95	40.88	41.89
2'	40.99	41.16	37.16	38.98	38.38	39.68	37.18	39.57
3'	52.17	51.92	49.40	50.27	51.09	51.09	51.15	51.10
4'	40.51	40.31	39.32	39.01	40.30	39.89	39.48	40.07
5'	53.83	53.49	54.81	53.79	55.06	54.80	54.00	55.06
6'	49.00	49.07	47.35	45.83	50.92	50.47	50.50	50.62
1''	1.91	3.24	1.80	3.33	2.61	5.39	3.96	4.13
2''	132.74	132.55	132.89	133.25	132.76	132.62	133.24	132.50
	7a-09	**7a-10**	**7a-11**	**7a-12**	**7a-13**	**7a-14**	**7a-15**	**7a-16**
1	132.00	126.19	125.64	131.83	127.64	125.16	124.75	127.25
3	129.79	126.10	126.33	126.36	129.91	130.27	129.19	127.15
4	157.65	159.26	161.82	158.42	155.77	158.06	159.66	155.23
4a	70.61	72.98	73.30	70.82	73.80	71.15	71.71	73.24
4b	54.52	54.55	54.92	54.25	54.41	54.20	54.60	54.58
5	63.45	64.48	64.41	63.91	64.52	62.84	63.64	64.50
6	62.26	63.30	63.31	62.76	62.58	63.41	62.97	62.88
7	59.81	60.85	60.92	60.01	60.31	60.85	60.83	60.38
8	72.35	72.61	72.64	72.04	72.02	71.91	71.96	72.21
8a	46.33	46.25	45.86	46.01	46.19	45.82	45.57	46.33
9a	49.73	48.28	49.33	48.52	48.08	49.03	49.83	48.23
1'	41.94	43.63	42.47	41.52	40.76	39.51	40.02	41.44
2'	38.28	39.25	37.31	37.81	38.57	39.52	38.48	38.92
3'	51.07	49.93	49.07	51.32	49.87	49.54	49.84	49.79
4'	40.02	38.97	39.23	39.49	39.75	39.38	39.12	39.49
5'	55.01	53.93	54.91	53.85	54.77	53.87	53.86	54.78
6'	50.41	46.27	47.58	50.45	48.89	46.67	46.68	48.74
1''	5.43	4.06	3.02	4.33	1.87	3.81	5.60	5.13
2''	132.89	132.65	132.70	132.61	132.36	132.65	132.83	132.58

7b-01



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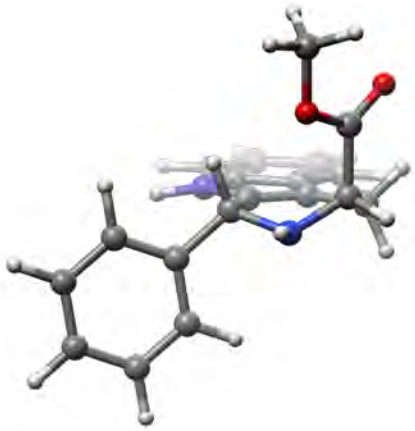
C	1.53770500	-2.96670900	-0.70219900
H	2.17396600	-2.43285000	-0.00061600
C	1.90365400	-4.22399600	-1.16923900
C	1.08749500	-4.92837800	-2.07649100
C	-0.10861500	-4.38830700	-2.53927100
C	-0.47263800	-3.12363400	-2.06956800
N	-1.57793100	-2.34368300	-2.35797900
H	-2.39035000	-2.64124500	-2.87718700
C	-1.50549300	-1.17418600	-1.62408500
C	-2.52566100	-0.07226500	-1.69143100
N	-2.24086600	0.86548700	-0.58457200
C	-0.83456800	1.23235500	-0.41124600
H	-0.79518200	1.95836100	0.41299000
C	-0.26461200	1.98060300	-1.63154500
O	-0.94041300	2.43156300	-2.53376000
O	1.07169000	2.14416100	-1.55395600
C	1.67041100	2.88431800	-2.63265500
H	1.49475400	2.37883100	-3.58559000
H	2.73647700	2.91870800	-2.40701100
H	1.25330100	3.89357400	-2.68224500
H	-2.78659200	1.70844600	-0.74917300
H	-2.42955400	0.42595500	-2.67088500
C	-3.95334000	-0.59902800	-1.58490200
C	-4.76717100	-0.65732900	-2.72136400
C	-6.06206400	-1.17902400	-2.64560300
C	-6.55574700	-1.64168000	-1.42644700
C	-5.75049100	-1.57987600	-0.28461400
C	-4.45831600	-1.06457100	-0.36306200
H	-3.82969400	-1.00359700	0.51981500
H	-6.13270900	-1.93521700	0.66896900
H	-7.56363300	-2.04332700	-1.36243800
H	-6.68416600	-1.21333200	-3.53626400
H	-4.38988100	-0.27963700	-3.66984700
H	-0.73565500	-4.93152700	-3.24178000
H	1.39752600	-5.91046000	-2.42322200
H	2.83285000	-4.67418400	-0.83027400
H	1.06494400	0.24611900	-0.05406100
H	-0.22302000	-0.22871600	1.05107500

7b-02



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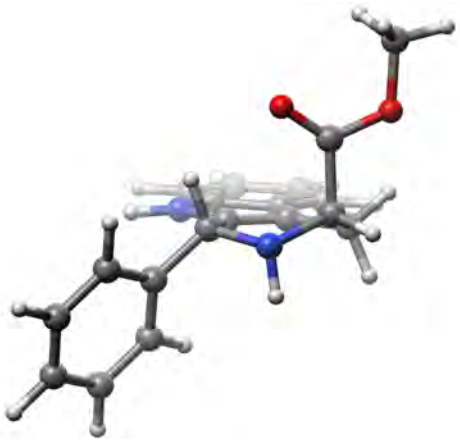
H	2.99164100	-1.27878700	-0.15694100
C	3.45974000	-2.98175700	-1.39290100
C	2.98449100	-3.93848600	-2.31179300
C	1.65633700	-3.94185300	-2.72674500
C	0.81024000	-2.96452600	-2.19622000
N	-0.53078400	-2.71775000	-2.42976700
H	-1.16104100	-3.32514900	-2.93175400
C	-0.93271900	-1.65410400	-1.64161500
C	-2.32643000	-1.08996300	-1.63437700
N	-2.42271100	-0.17673800	-0.48142800
C	-1.30631400	0.75693200	-0.31034700
H	-1.55765800	1.38082400	0.55906800
C	-1.09031600	1.76806200	-1.45638200
O	-0.05985200	2.36505100	-1.67523700
O	-2.23059500	1.97734300	-2.15815100
C	-2.13672200	2.96728900	-3.19753800
H	-1.85852500	3.93744800	-2.77764400
H	-3.12795700	3.01318500	-3.64956700
H	-1.38789900	2.67395600	-3.93765700
H	-3.29428900	0.34121100	-0.55646200
H	-2.48940800	-0.55724500	-2.58964700
C	-3.39322200	-2.17661800	-1.54054600
C	-4.14880400	-2.52136400	-2.66621300
C	-5.10167500	-3.54236800	-2.60084600
C	-5.30993700	-4.22392000	-1.40238900
C	-4.56204900	-3.88104600	-0.27142900
C	-3.60876300	-2.86700200	-0.33992700
H	-3.02964900	-2.58774200	0.53467900
H	-4.72327000	-4.40729800	0.66591600
H	-6.05314400	-5.01488900	-1.34610200
H	-5.68407400	-3.79595500	-3.48285100
H	-3.99940400	-1.97927200	-3.59826000
H	1.29207400	-4.67829100	-3.43868400
H	3.66732800	-4.68611900	-2.70631300
H	4.50419400	-3.00511500	-1.09379300
H	0.84050500	0.69361000	-0.10326500
H	-0.02560800	-0.32895500	1.04754000

7b-03



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C	1.87246200	-2.75488500	-0.70495100
H	2.42702800	-2.16199200	0.01829900
C	2.39772500	-3.94783100	-1.18819400
C	1.68913800	-4.72855900	-2.12308100
C	0.44290900	-4.33039200	-2.59707900
C	-0.08062000	-3.12894400	-2.11192900
N	-1.27097700	-2.48775700	-2.40036800
H	-2.01374700	-2.85739500	-2.97396400
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C	-2.48581200	-0.33422000	-1.72829000
N	-2.33269600	0.72333500	-0.69713100
C	-0.95652600	1.15213400	-0.42856200
H	-1.00629500	1.87853400	0.39198100
C	-0.39897100	1.92264100	-1.62768800
O	-0.91740100	2.04243100	-2.71528600
O	0.78911300	2.48573800	-1.30756800
C	1.42105100	3.23077400	-2.36146300
H	1.62489900	2.58430600	-3.21909800
H	2.35120900	3.60810100	-1.93559000
H	0.78189300	4.05713400	-2.68356400
H	-2.72915700	0.37617100	0.17469200
H	-2.42716900	0.17320400	-2.69861400
C	-3.87380600	-0.94957000	-1.60437200
C	-4.94103700	-0.40570000	-2.33008900
C	-6.22892700	-0.92562700	-2.20046400
C	-6.46734500	-1.99833500	-1.33843500
C	-5.41187200	-2.54533900	-0.60694400
C	-4.12354200	-2.02360300	-0.73931500
H	-3.30245200	-2.45760700	-0.17381200
H	-5.58926800	-3.38089100	0.06524900
H	-7.46965100	-2.40659800	-1.23909800
H	-7.04603600	-0.49416200	-2.77269400
H	-4.75604500	0.43415700	-2.99522300
H	-0.10123200	-4.93218400	-3.32067100
H	2.12371700	-5.65747800	-2.48231000
H	3.36980300	-4.28723500	-0.84056000
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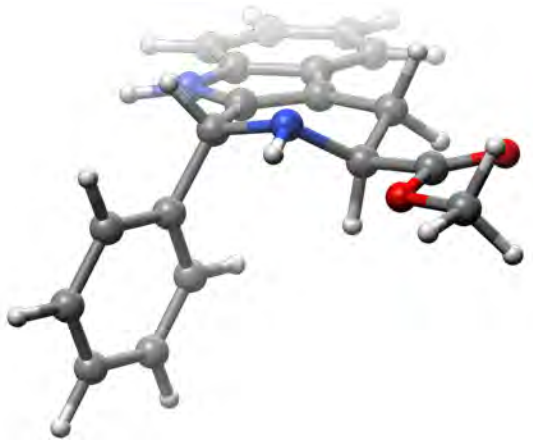
H	-0.20536800	-0.24503100	1.05312300

7b-04



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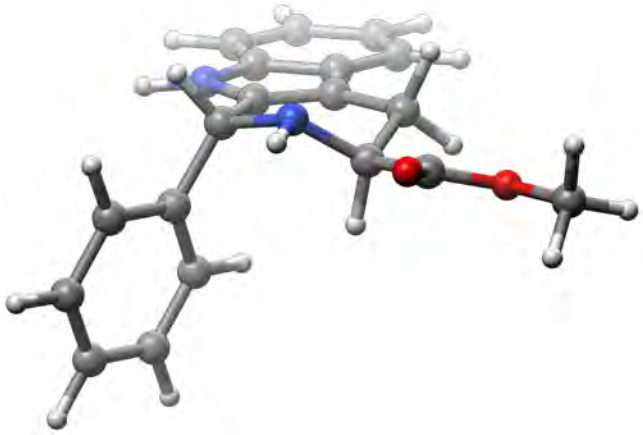
H	-3.08413700	-0.65316900	0.81448400
C	-4.68560200	0.75827600	0.51511600
C	-5.06263800	2.03295900	0.04704500
C	-4.12657000	2.90763100	-0.49548600
C	-2.79876500	2.47599600	-0.55859200
N	-1.67131500	3.11324100	-1.04329200
H	-1.63263700	4.06502400	-1.37408400
C	-0.57725500	2.28053800	-0.87698200
C	0.82180800	2.63362800	-1.28005700
N	1.62953300	1.39159300	-1.21331400
C	1.42029700	0.58765300	-0.00063900
H	1.54922300	1.18701400	0.92331900
C	2.47143200	-0.51355900	0.08438200
O	2.26451200	-1.65024300	0.44530400
O	3.69944800	-0.04900800	-0.24466600
C	4.76596700	-1.00959400	-0.16198600
H	4.85949700	-1.38932900	0.85870800
H	5.66775200	-0.47233400	-0.45678900
H	4.57806900	-1.84783000	-0.83777800
H	2.61454400	1.63512300	-1.28132600
H	0.82530100	2.93136900	-2.33941000
C	1.42134800	3.80090500	-0.48599400
C	2.36662800	4.63044000	-1.10645000
C	2.99166300	5.65965600	-0.40240700
C	2.67613300	5.87809600	0.94025900
C	1.73006600	5.06560600	1.56721400
C	1.10446000	4.03730200	0.85948300
H	0.35283800	3.42383200	1.34831200
H	1.47181700	5.23557300	2.60928600
H	3.15827700	6.68111900	1.49128600
H	3.71881400	6.29409000	-0.90263800
H	2.61241900	4.46786700	-2.15465100
H	-4.41929200	3.88983400	-0.85807700
H	-6.10343800	2.33891700	0.10958900
H	-5.44317200	0.09945000	0.93087800
H	-0.05765100	-0.80195300	-0.74727000
H	-0.19926100	-0.46460600	0.97218800

7b-05



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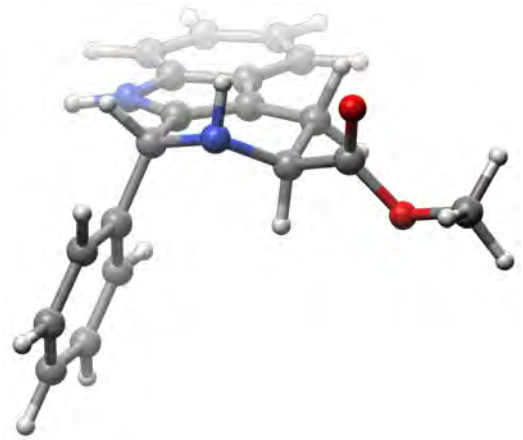
C	2.40179300	-1.17936200	0.07912500
C	3.34856600	-0.27238700	0.58391900
H	3.05207200	0.73659700	0.85951500
C	4.66913000	-0.68211600	0.72628000
C	5.06802700	-1.98656300	0.37225000
C	4.15537200	-2.90723800	-0.13282200
C	2.82871100	-2.49150500	-0.27559000
N	1.72145200	-3.17283800	-0.74632200
H	1.70011900	-4.14589800	-1.01017500
C	0.61843500	-2.33867700	-0.68483000
C	-0.76586500	-2.72932700	-1.11009600
N	-1.56163500	-1.48677100	-1.16712400
C	-1.41557300	-0.61123400	-0.00654400
H	-1.55046800	-1.14844400	0.95464600
C	-2.54235500	0.41230200	-0.04604600
O	-3.58223600	0.26499300	-0.65298800
O	-2.27299600	1.48390400	0.72537300
C	-3.31633900	2.47120700	0.79542600
H	-3.52776500	2.87541100	-0.19781900
H	-2.93546500	3.25129400	1.45498300
H	-4.23118100	2.03343700	1.20344200
H	-2.54720200	-1.69361000	-1.31130900
H	-0.72913800	-3.10924300	-2.14214100
C	-1.39303800	-3.83418400	-0.24934200
C	-2.33136000	-4.69825800	-0.83182900
C	-2.98040800	-5.67145500	-0.07236400
C	-2.69650200	-5.79829800	1.28913000
C	-1.75820200	-4.95042500	1.87944300
C	-1.10853000	-3.97810900	1.11608300
H	-0.36333200	-3.33652000	1.57813800
H	-1.52495500	-5.04870800	2.93658000
H	-3.19792300	-6.55737300	1.88353600
H	-3.70262000	-6.33313800	-0.54353900
H	-2.55442800	-4.60610400	-1.89353400
H	4.46496500	-3.91261400	-0.40710400
H	6.10724600	-2.27947900	0.49461500
H	5.40858700	0.01225400	1.11603300
H	0.07993100	0.74222200	-0.80616600
H	0.16759200	0.53192200	0.94285700

7b-06



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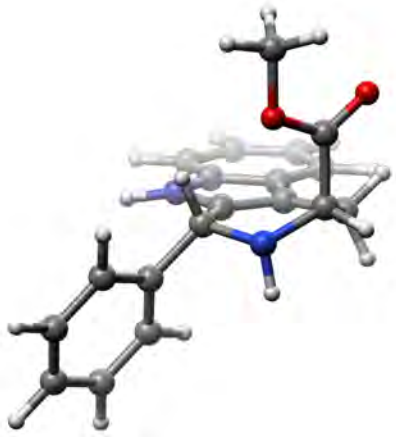
C	-2.45681700	1.04695600	-0.02761900
C	-3.35527900	0.12586400	0.53651700
H	-3.00236800	-0.83583800	0.90040300
C	-4.70123400	0.46137200	0.62426700
C	-5.17286200	1.70431900	0.15670800
C	-4.30901900	2.63659800	-0.40927700
C	-2.95641300	2.29562700	-0.49635900
N	-1.88333600	3.00377500	-1.00644800
H	-1.91898600	3.94838000	-1.35777700
C	-0.73065800	2.24769100	-0.86337000
C	0.64528100	2.66384000	-1.30652000
N	1.55704400	1.50266800	-1.33030600
C	1.42024500	0.62146900	-0.16860300
H	1.65596400	1.20487900	0.72695500
C	2.43422500	-0.50209600	-0.31083800
O	2.75556000	-1.00509600	-1.36635000
O	2.88476600	-0.91783900	0.89012200
C	3.79195000	-2.03347500	0.85556100
H	3.31597700	-2.90143000	0.39157700
H	4.03957200	-2.24092800	1.89686300
H	4.69118400	-1.77657700	0.28978600
H	1.40355300	0.94986100	-2.17191500
H	0.59461800	3.01647700	-2.34710800
C	1.26230400	3.80249500	-0.48182600
C	2.46808900	4.36492900	-0.92559100
C	3.07482000	5.39994500	-0.21904200
C	2.48609700	5.88912200	0.95140900
C	1.29252700	5.33156300	1.40548100
C	0.68359100	4.29354800	0.69228400
H	-0.24366600	3.86303600	1.05851700
H	0.83053200	5.69908000	2.31819400
H	2.95816200	6.69709700	1.50418600
H	4.00818200	5.82569600	-0.57847400
H	2.93470800	3.97032000	-1.82436800
H	-4.67487700	3.59418500	-0.77120400
H	-6.23045600	1.93979500	0.23881500
H	-5.40399700	-0.24389400	1.05957500
H	-0.11247400	-0.84704100	-0.69389900
H	-0.09650600	-0.41250400	1.01283000

7b-07



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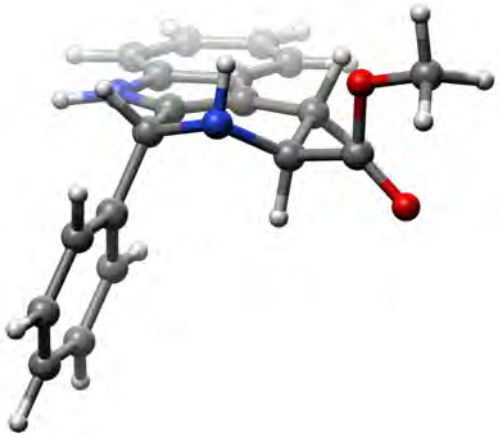
C	1.29021800	-1.92817200	-1.32793800
C	2.62689700	-1.96863200	-0.89778800
H	2.97963100	-1.28224200	-0.13221200
C	3.49130000	-2.89838500	-1.46389100
C	3.04692900	-3.79366000	-2.45734800
C	1.73102500	-3.77421100	-2.90901200
C	0.86569300	-2.83569500	-2.34006600
N	-0.47001600	-2.57931600	-2.59100000
H	-1.07295000	-3.13558200	-3.17787200
C	-0.90377000	-1.56898000	-1.74739800
C	-2.28952700	-0.97967300	-1.75547200
N	-2.45553900	-0.00336500	-0.65237200
C	-1.27552400	0.81315700	-0.34533300
H	-1.54616000	1.41965300	0.52993200
C	-0.95233400	1.84990900	-1.43031700
O	0.06922700	2.50371800	-1.43522000
O	-1.92997500	2.00030900	-2.34514400
C	-1.67559100	3.00275400	-3.34439200
H	-1.55179600	3.98399000	-2.87895300
H	-2.55066100	2.99367200	-3.99485500
H	-0.77090400	2.76213000	-3.90892100
H	-2.71070200	-0.51669600	0.18950700
H	-2.42664400	-0.41944600	-2.69073500
C	-3.40887000	-2.01122600	-1.67574700
C	-4.61929200	-1.77360300	-2.33880400
C	-5.67411900	-2.68116400	-2.24389400
C	-5.53223900	-3.84154300	-1.47959800
C	-4.33201100	-4.08593200	-0.81041600
C	-3.27725700	-3.17609700	-0.90796900
H	-2.34185100	-3.37366500	-0.39020700
H	-4.21371800	-4.98643800	-0.21341400
H	-6.35207200	-4.55124400	-1.40728000
H	-6.60628300	-2.48323800	-2.76654200
H	-4.73242200	-0.86620500	-2.92704600
H	1.39090200	-4.46287900	-3.67839700
H	3.74456400	-4.51097700	-2.88117000
H	4.52700500	-2.93821300	-1.13748500
H	0.86766300	0.66763300	-0.02389100
H	-0.08503400	-0.37128100	1.03224300

7b-08



C	0.00000000	0.00000000	0.00000000
C	-1.00694500	1.00880100	-0.47067000
C	-2.43969900	1.04015900	-0.32644500
C	-3.38429900	0.19492100	0.27958300
H	-3.06717100	-0.71799800	0.77737600
C	-4.72914500	0.54308000	0.23589700
C	-5.15404800	1.72407700	-0.40500000
C	-4.24369200	2.58054700	-1.01602400
C	-2.89218500	2.22719700	-0.97047400
N	-1.77915400	2.86702200	-1.48539200
H	-1.77940900	3.76666100	-1.94107300
C	-0.64757000	2.12894400	-1.17635700
C	0.75928900	2.48527000	-1.57264500
N	1.65372800	1.31837500	-1.39953800
C	1.42723900	0.60649200	-0.13308900
H	1.58181800	1.32250200	0.67928800
C	2.47295800	-0.48231500	0.05625300
O	3.03559000	-0.73302500	1.09820500
O	2.65834900	-1.18911500	-1.08343600
C	3.61250500	-2.26033700	-0.99668300
H	4.59627400	-1.87364400	-0.71855300
H	3.64273500	-2.70779800	-1.99060500
H	3.29646400	-2.99600800	-0.25233800
H	1.49964700	0.66498100	-2.16591400
H	0.78174700	2.71081800	-2.64891200
C	1.33633600	3.70865200	-0.85017900
C	2.55216500	4.23845800	-1.30608000
C	3.12496900	5.34561500	-0.68578200
C	2.49073400	5.94152400	0.40881700
C	1.28604000	5.41845900	0.87442100
C	0.71135100	4.30790600	0.24777400
H	-0.22567100	3.90589800	0.62188100
H	0.78891400	5.86974800	1.72918100
H	2.93645200	6.80545300	0.89471500
H	4.06717400	5.74430300	-1.05294100
H	3.05389700	3.76345200	-2.14527000
H	-4.57366000	3.49061500	-1.51071200
H	-6.21196500	1.97145800	-0.42269600
H	-5.46745000	-0.10331600	0.70258100
H	-0.06283800	-0.92542300	-0.59202500
H	-0.17526600	-0.28676900	1.04527200

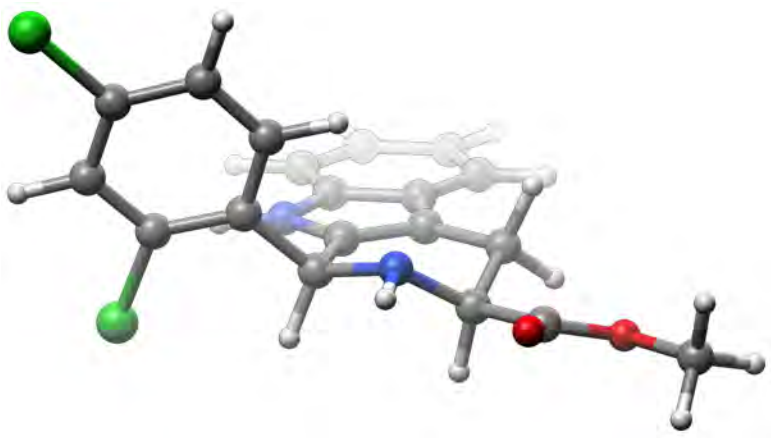
7b Shielding tensors B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	7b-01	**7b-02**	**7b-03**	**7b-04**	**7b-05**	**7b-06**	**7b-07**	**7b-08**
1	122.3475	121.5511	122.7069	119.6161	120.1419	122.755	122.5338	122.175
3	121.2533	120.4276	121.9359	126.7257	127.3429	126.6166	120.5222	123.7218
4	155.3685	156.0723	152.0397	154.1438	153.0938	151.5335	152.8969	152.1903
4a	71.8384	70.1304	68.6232	65.8282	65.3758	66.6313	65.8549	66.4389
4b	49.1992	48.328	48.7876	48.8445	48.6932	48.1878	48.5593	48.3412
5	60.5605	59.936	60.7871	60.0991	59.7792	60.4575	60.4009	60.2128
6	58.6485	59.0539	58.5199	58.4475	58.1558	58.1963	58.9981	58.5605
7	56.713	56.7449	56.3189	56.2739	56.6245	55.9383	56.1866	55.8271
8	68.3444	68.2327	68.0123	68.0532	67.514	68.0986	68.2646	68.0736
8a	40.4074	39.9568	41.0802	39.6633	40.1078	40.2491	40.1538	40.5912
9a	40.3515	40.5757	41.4741	43.3677	42.9563	41.8454	41.5906	41.9793
1'	30.6007	31.324	30.5434	30.973	31.1831	29.7556	32.9739	29.899
2'	48.1048	48.1138	44.5239	47.9987	47.8017	45.3906	45.7357	45.3525
3'	48.8392	49.3104	48.0471	47.6028	47.7613	48.5581	48.8678	48.2141
4'	49.063	49.0079	48.9444	49.1302	49.2594	50.1694	48.6853	50.103
5'	48.0278	48.1371	48.2187	48.832	49.0687	49.7995	48.747	49.5583
6'	47.8521	47.4484	50.5145	49.4939	49.6667	49.9	49.0562	49.6496
1''	-3.4409	-2.5902	-1.6735	-0.3724	-1.5255	-3.4342	-1.491	-0.6233
2''	128.3693	128.0755	128.7087	128.071	128.0803	128.2265	128.1948	128.2969

7b Shielding tensors mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	7b-01	**7b-02**	**7b-03**	**7b-04**	**7b-05**	**7b-06**	**7b-07**	**7b-08**
1	128.0079	127.2749	128.4267	128.5594	125.554	126.0445	128.177	127.9535
3	127.1486	126.2765	127.8764	132.4641	132.2988	132.8862	126.3669	129.8368
4	160.5948	161.2546	157.485	156.9403	159.4594	158.3741	158.2906	157.6138
4a	76.9614	75.4322	73.7343	71.9052	71.0478	70.5736	71.1759	71.714
4b	54.6608	53.9213	54.3041	53.7993	54.4664	54.3095	54.1132	53.9783
5	64.6167	63.985	64.7442	64.3298	63.9627	63.7572	64.4148	64.119
6	63.1199	63.5389	62.9865	62.6456	62.8783	62.5734	63.4854	63.0257
7	61.0757	61.1651	60.6586	60.3032	60.6063	60.8676	60.6253	60.2086
8	72.5197	72.2675	72.1514	72.2421	72.208	71.7386	72.3439	72.1897
8a	46.008	45.5638	46.6914	45.9564	45.3381	45.685	45.7572	46.2331
9a	45.6713	45.9098	46.7037	47.356	48.6639	48.198	46.9352	47.4105
1'	36.5372	37.2917	36.4822	35.5826	36.7399	36.9346	39.0455	35.7134
2'	52.5494	52.6179	49.0568	50.0225	52.5119	52.3365	50.2603	49.9208
3'	53.2421	53.7024	52.4797	52.9278	52.108	52.2578	53.2641	52.5803
4'	53.414	53.3373	53.2925	54.4485	53.5224	53.6572	52.9964	54.3427
5'	52.4362	52.4815	52.631	54.1058	53.1788	53.4293	53.0947	53.8657
6'	52.3442	51.8815	54.8084	54.3645	54.0421	54.1774	53.5245	54.102
1''	1.983	2.8499	3.7839	2.1064	5.0771	3.9087	3.9016	4.8793
2''	132.9791	132.7181	133.3643	132.8904	132.72	132.7085	132.8235	132.9491

8a-01



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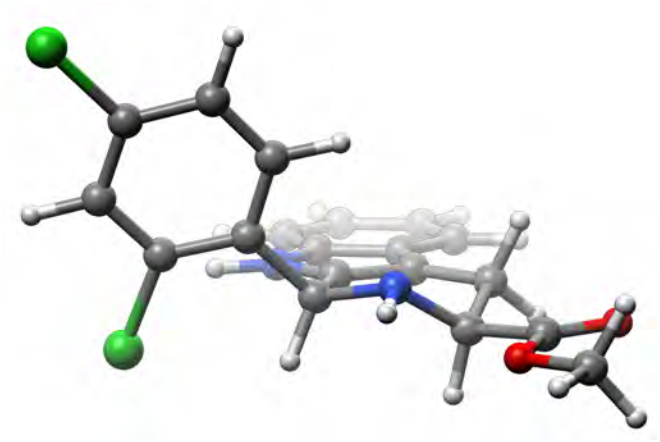
C	0.47780800	2.63160800	0.04233700
C	-0.63483600	3.31409800	-0.47821400
H	-1.49971100	2.76342200	-0.83963800
C	-0.61362400	4.70269800	-0.52624300
C	0.50169300	5.42985400	-0.06326000
C	1.61802900	4.78384800	0.45740700
C	1.59326800	3.38702900	0.50451100
N	2.54059000	2.49026100	0.96094000
H	3.42847700	2.73116800	1.37455100
C	2.05614000	1.20517900	0.80308800
C	2.79624200	-0.04942900	1.19941600
H	2.83955500	-0.09752600	2.30231900
N	2.05463400	-1.18102300	0.63346300
C	0.61128900	-1.12470000	0.85634700
H	0.35928800	-0.90520600	1.91473100
C	0.04069500	-2.51096800	0.58337100
O	0.69629500	-3.53194800	0.58700400
O	-1.29077000	-2.47576700	0.39349400
C	-1.92103500	-3.75416300	0.19375000
H	-1.75776200	-4.40005800	1.06024600
H	-1.51805800	-4.24305400	-0.69672200
H	-2.98212000	-3.53863800	0.06790700
H	2.41700900	-2.06506700	0.98355800
C	4.23441600	-0.06299700	0.67641200
C	5.32512500	0.41596800	1.41266700
C	6.62903800	0.40233000	0.91596500
C	6.84780500	-0.10153300	-0.36267400
C	5.79158400	-0.58121800	-1.13587400
C	4.50426700	-0.55493300	-0.60858700
H	3.66674400	-0.93493700	-1.18356500
H	5.97557400	-0.96912500	-2.13173100
Cl	8.48242600	-0.12870000	-1.00276900
H	7.45021800	0.77559000	1.51574400
Cl	5.10075500	1.09078200	3.03495800
H	2.47747500	5.34579800	0.81395400
H	0.49018500	6.51519900	-0.11376400
H	-1.46867200	5.23996900	-0.92751100
H	0.02371900	-0.29308000	-1.05879700
H	-1.05222500	0.13803400	0.27113100

8a-02



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C	-0.61671300	-1.33675500	0.28488000
C	-0.10249300	-2.66988900	0.11262800
C	1.09800100	-3.20188500	-0.38773400
H	1.87945300	-2.54392500	-0.75947900
C	1.27130400	-4.58053300	-0.40100800
C	0.26547800	-5.44513000	0.07649600
C	-0.93369000	-4.94954900	0.57750800
C	-1.10441900	-3.56219100	0.59036700
N	-2.17038000	-2.79568600	1.02224600
H	-3.01804900	-3.14836200	1.43991100
C	-1.86751700	-1.45946500	0.83344600
C	-2.77140600	-0.31284200	1.20806900
H	-2.81363400	-0.24587400	2.30964600
N	-2.20390300	0.90983800	0.61675900
C	-0.75510900	1.05738900	0.81819900
H	-0.47745300	0.92917200	1.88454600
C	-0.31434200	2.46956400	0.44527100
O	0.70910500	2.74872300	-0.13632600
O	-1.19286700	3.39452300	0.89707600
C	-0.84682500	4.76377600	0.62141300
H	-0.77276600	4.92819900	-0.45647100
H	0.10906200	5.01609200	1.08727300
H	-1.65303000	5.36099200	1.04778800
H	-2.67955400	1.71897100	1.00821000
C	-4.20123200	-0.50896000	0.69892700
C	-5.21398900	-1.10512200	1.46046000
C	-6.51140400	-1.27938900	0.97664000
C	-6.80311900	-0.85021200	-0.31454800
C	-5.82398100	-0.26126700	-1.11357600
C	-4.54158000	-0.10007700	-0.59854700
H	-3.76549300	0.36816200	-1.19425700
H	-6.06320500	0.06507100	-2.11975800
Cl	-8.43114500	-1.05851500	-0.93728100
H	-7.27204300	-1.73911000	1.59595800
Cl	-4.89236500	-1.69358400	3.09936100
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H	0.42910100	-6.51907900	0.05310400
H	2.19564000	-5.00256400	-0.78603200
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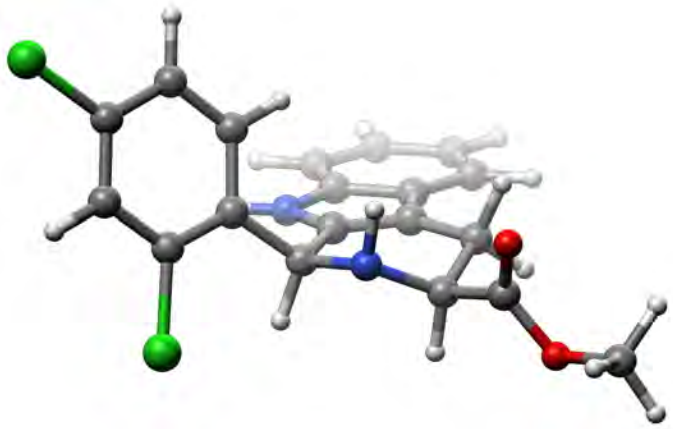

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C	-1.74073900	4.43566500	0.11866300
C	-0.80701800	5.35069200	0.64523400
C	0.45689500	4.93697600	1.05335200
C	0.76644300	3.58020500	0.92280100
N	1.91934200	2.88824800	1.24654700
H	2.77540700	3.30090900	1.58417500
C	1.75699100	1.55428400	0.90908300
C	2.75765800	0.46001200	1.18177500
H	2.79483500	0.29406300	2.26713400
N	2.33818200	-0.81325100	0.56792800
C	0.90191400	-1.08410300	0.66277100
H	0.63712800	-1.15895400	1.72277800
C	0.64343100	-2.42348100	-0.01071100
O	1.19467800	-2.79055100	-1.02652100
O	-0.31678300	-3.12367600	0.62316400
C	-0.67562800	-4.37445200	0.00809100
H	0.18882300	-5.04209600	-0.02966600
H	-1.04357600	-4.21032700	-1.00813300
H	-1.45935400	-4.79500200	0.63840400
H	2.61182500	-0.84559800	-0.41305100
C	4.17062700	0.78891200	0.71587300
C	5.31763400	0.38011800	1.41303400
C	6.60359600	0.65942500	0.94845100
C	6.74963400	1.35515600	-0.24882000
C	5.63867200	1.77170300	-0.97929800
C	4.36861500	1.48355400	-0.48620000
H	3.49560900	1.80990800	-1.04482200
H	5.76526600	2.31088300	-1.91150500
Cl	8.36356100	1.71215600	-0.83842000
H	7.47106400	0.33593100	1.51086300
Cl	5.19381700	-0.50987000	2.92525800
H	1.17460100	5.64373100	1.46209300
H	-1.07899200	6.39872000	0.73606400
H	-2.71964400	4.79322500	-0.18880900
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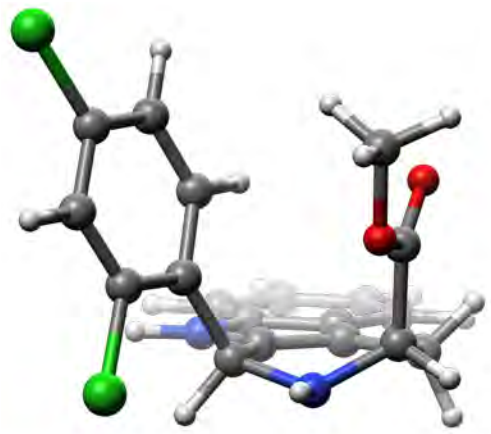

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C	2.62185000	-2.00257600	-0.82439500	H	-2.95994600	-0.11566000	1.59289300
H	2.86706000	-0.99408200	-1.14732700	C	-3.16256900	-2.54931900	0.52740500
C	3.51837700	-3.04504600	-1.02623600	C	-4.42935400	-2.70107800	1.11220800
C	3.21185500	-4.35770000	-0.61468500	C	-5.50508900	-3.27865100	0.44001700
C	2.00351600	-4.65533100	0.00689700	C	-5.31352400	-3.71836100	-0.86781400
C	1.10478600	-3.60400500	0.20877200	C	-4.07731000	-3.58358700	-1.49576000
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C	-1.99091400	-1.90614800	1.29467000	Cl	-6.65699800	-4.45141500	-1.72842000
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O	-1.89045500	-0.09139100	-2.16777200	H	0.29109400	0.34479200	-0.99756600
O	-3.60516800	0.50520300	-0.82199000	H	0.59437200	0.56823200	0.72797400
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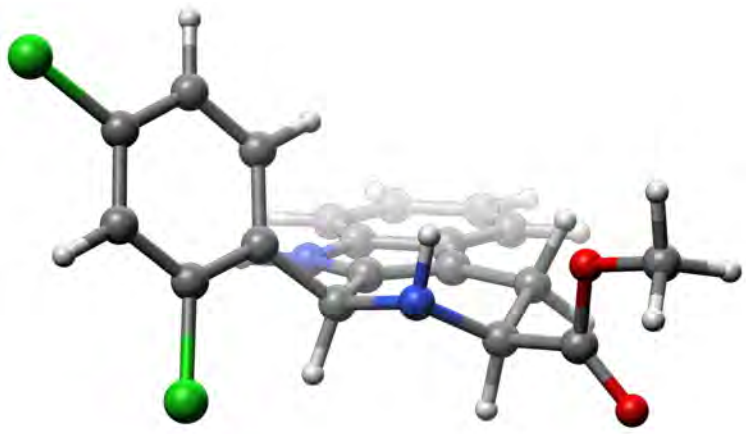

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H	2.46436900	-2.03051600	-0.57896900	C	-4.03372000	-1.41751100	0.56809800
C	2.33337400	-4.15002800	-0.21050200	C	-5.23164000	-1.20001800	1.26603900
C	1.53197100	-5.22467500	0.22486700	C	-6.46540900	-1.61571000	0.76375500
C	0.22073900	-5.02346500	0.64319500	C	-6.50777800	-2.25534800	-0.47250000
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C	-2.68234600	-0.92988600	1.07462400	Cl	-8.05583300	-2.78098500	-1.11022100
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O	-1.52068700	2.53723300	-0.91011500	H	1.00466600	0.26268900	0.35646900
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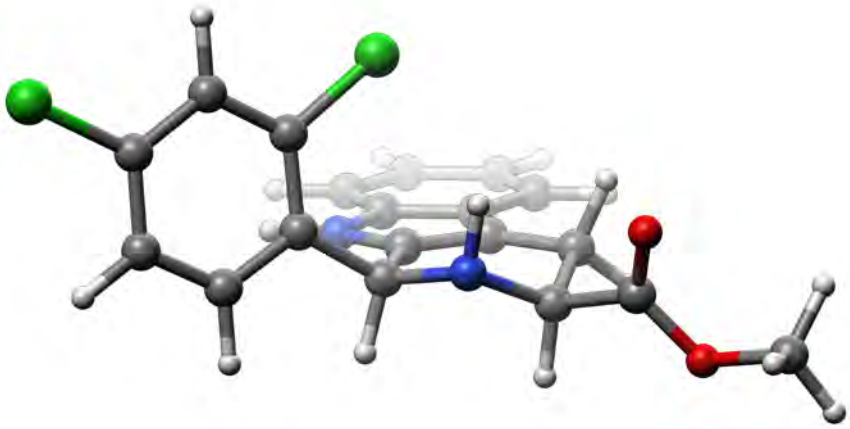

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C	1.03631600	4.64866200	0.25419300
C	-0.04331300	5.44888700	-0.17022100
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C	-1.32454900	3.48420500	-0.60216900
N	-2.36097000	2.65114800	-0.98459300
H	-3.29109700	2.95238000	-1.23243700
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N	-2.21205000	-1.11278700	-0.59939600
C	-0.75257700	-1.16145500	-0.71850900
H	-0.49660800	-1.13059100	-1.78366000
C	-0.28398200	-2.48702200	-0.13842500
O	-0.79966700	-3.04068900	0.80839600
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C	1.38399400	-4.14775400	-0.22970900
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H	1.66330900	-4.00808500	0.81789700
H	2.26415700	-4.35547000	-0.83861200
H	-2.46032900	-1.24104200	0.37982900
C	-4.28643800	0.22612400	-0.78739000
C	-4.79648200	0.45151300	0.50244800
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C	-7.05817700	0.40072900	-0.30717700
C	-6.60029700	0.17237200	-1.60203400
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H	-4.86552300	-0.09816500	-2.82601500
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H	-2.06727000	5.49729100	-0.93296400
H	0.05712100	6.53077200	-0.16053900
H	1.95423400	5.12699200	0.58496300
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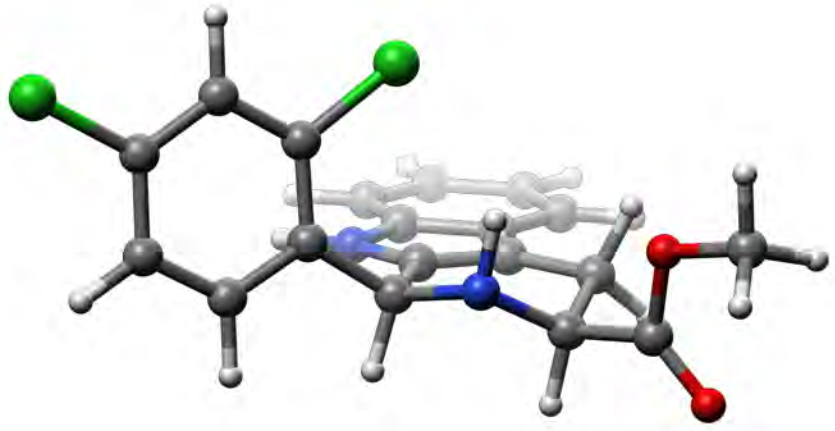

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C	0.94006600	-3.64735500	-0.28489500
N	2.07317000	-2.96721200	-0.69449900
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H	0.71145800	0.88533300	-1.84669200
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H	2.53935300	0.91148900	0.43619900
C	4.25921000	-0.77315700	-0.62332600
C	4.72034100	-0.96971300	0.68935100
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H	1.45887400	-5.75016700	-0.43692600
H	-0.78603100	-6.47771000	0.34320700
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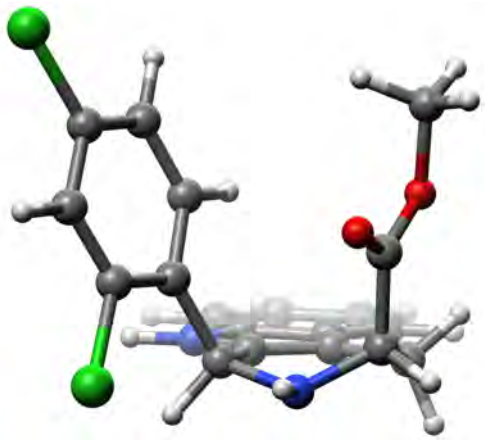

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C	1.80971400	-4.69440500	-0.61471200
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N	-2.06214300	-0.52133600	1.27108700
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C	-4.55742600	-2.60876200	0.64430500
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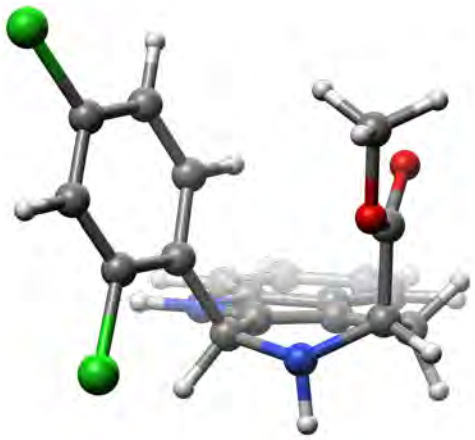

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C	3.50990100	-2.99593900	-1.17138700
C	3.17828300	-4.33390800	-0.87782300
C	1.95151700	-4.66582500	-0.31207400
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N	-2.15677700	-0.49298000	1.26142100
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O	-1.82297000	-0.01299200	-2.17421700
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C	-4.37614900	0.69699300	-2.08588900
H	-4.47827100	-0.31249700	-2.49238600
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H	-1.78784600	-0.21930900	2.16777000
C	-3.22290700	-2.54640300	0.35304500
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C	-4.18385500	-3.43637100	-1.71458900
C	-3.11011900	-2.91333800	-0.99429300
H	-2.15868800	-2.76991000	-1.49639600
H	-4.07025100	-3.70916500	-2.75803400
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Cl	-4.72770800	-2.31768100	2.65261400
H	1.69804800	-5.69846000	-0.08592800
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H	4.47703900	-2.77296800	-1.61359700
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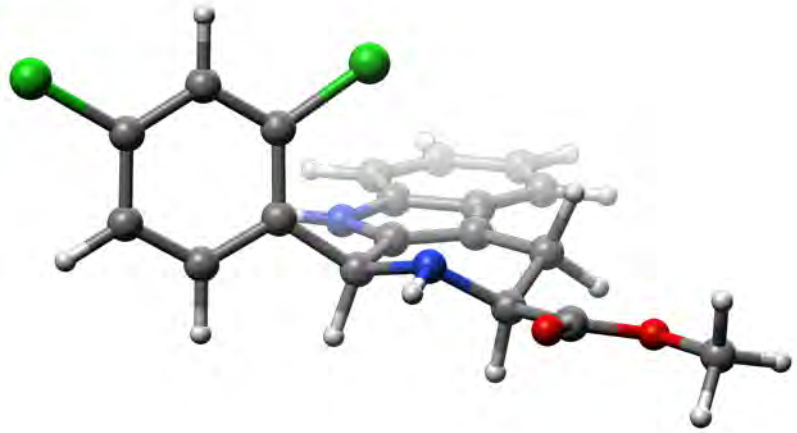
H	0.59231200	0.51582400	0.77073300

8a-10



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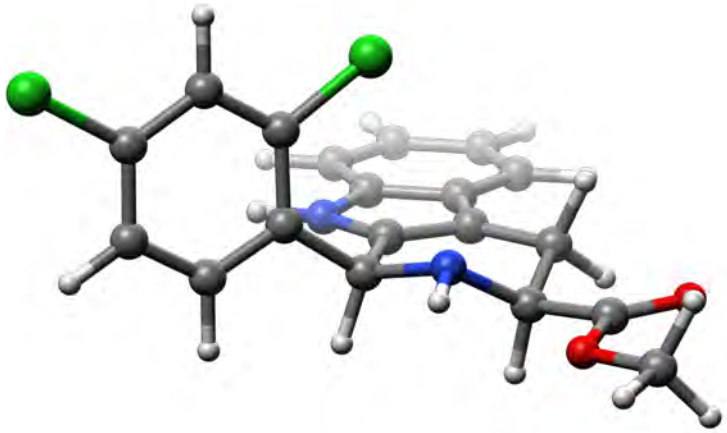
C	-0.19262400	2.66297100	-0.20946000	H	2.54406600	-3.83712100	0.29608500
C	0.99874200	3.25492200	0.24280400	H	-2.64967500	-1.84804300	-0.82750300
H	1.81627500	2.63805500	0.60747700	C	-4.25637400	0.31428800	-0.81010800
C	1.11579400	4.63963700	0.22213300	C	-4.73605100	0.53986500	0.49330000
C	0.06259300	5.45215300	-0.24346800	C	-6.10265400	0.63671300	0.76162800
C	-1.12742200	4.89648500	-0.70243500	C	-7.01495100	0.50834900	-0.28303100
C	-1.24054700	3.50389900	-0.68301100	C	-6.58423600	0.28664600	-1.58750200
N	-2.28053600	2.68408800	-1.08408200	C	-5.21464100	0.19304400	-1.82603800
H	-3.20101100	2.99691500	-1.35286100	H	-4.87094300	0.01304400	-2.84178700
C	-1.92987200	1.36837200	-0.84144200	H	-7.30024300	0.18559300	-2.39540700
C	-2.78301500	0.17786600	-1.18823100	Cl	-8.73193700	0.63176400	0.06062100
H	-2.76959000	0.07738600	-2.29418300	H	-6.44443500	0.81021700	1.77491600
N	-2.18570100	-0.99024000	-0.53861800	Cl	-3.65730300	0.72935800	1.86018300
C	-0.74677900	-1.11128800	-0.76336500	H	-1.93823000	5.52423400	-1.06342800
H	-0.48289900	-1.00271300	-1.83761400	H	0.18152900	6.53220500	-0.24558200
C	-0.33262300	-2.53048700	-0.39409600	H	2.03233200	5.10696100	0.57199200
O	-1.09108700	-3.47728300	-0.37465100	H	-0.04002800	-0.20786500	1.07786400
O	0.98781500	-2.62353500	-0.15241500	H	1.05644400	-0.00262600	-0.28953600
C	1.47112200	-3.94738700	0.13812100				

8a-11



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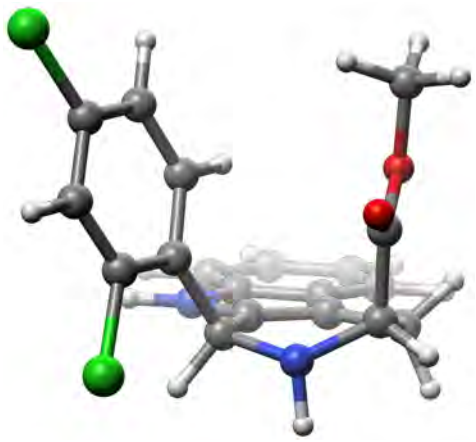
C	0.43926200	-1.39039000	-0.35090600
C	-0.24300200	-2.65418300	-0.25512600
C	-1.51772800	-3.05095900	0.18291500
H	-2.22737000	-2.31443700	0.55120500
C	-1.85659200	-4.39817400	0.14341400
C	-0.94474300	-5.36438100	-0.32693800
C	0.32277800	-5.00286000	-0.77219000
C	0.65916500	-3.64710900	-0.73386400
N	1.82109200	-3.00110100	-1.11800200
H	2.68264800	-3.45550400	-1.37970600
C	1.68471700	-1.64893100	-0.85718300
C	2.71825700	-0.60862800	-1.18689100
H	2.71650200	-0.48364700	-2.28976500
N	2.32990500	0.63858700	-0.51382500
C	0.91984200	0.99865800	-0.72107400
H	0.65407500	0.99076900	-1.79933900
C	0.66902100	2.42684400	-0.24706300
O	-0.31216700	2.80114400	0.35347800
O	1.66909800	3.25374600	-0.63236800
C	1.51385600	4.63183700	-0.24977900
H	1.45417700	4.72076100	0.83780500
H	0.60639100	5.05032300	-0.69247300
H	2.39889000	5.14277000	-0.62961900
H	2.92259500	1.39570800	-0.84391300
C	4.15122900	-0.99035500	-0.82348300
C	4.59393600	-1.31556300	0.47209700
C	5.92731200	-1.64096000	0.72756200
C	6.84320300	-1.64471200	-0.32190800
C	6.44845100	-1.33050500	-1.61875700
C	5.11158500	-1.00882400	-1.84465700
H	4.79693200	-0.75700100	-2.85459400
H	7.16712700	-1.33441400	-2.43062700
Cl	8.51799800	-2.05528500	0.00570100
H	6.24090500	-1.88816400	1.73467500
Cl	3.50518700	-1.34894100	1.84330200
H	1.02413500	-5.74911600	-1.13692900
H	-1.23639500	-6.41097300	-0.34389500
H	-2.83915200	-4.71539200	0.48213800
H	0.05321000	0.17779000	1.08170300
H	-1.03759500	0.18837600	-0.29767900

8a-12



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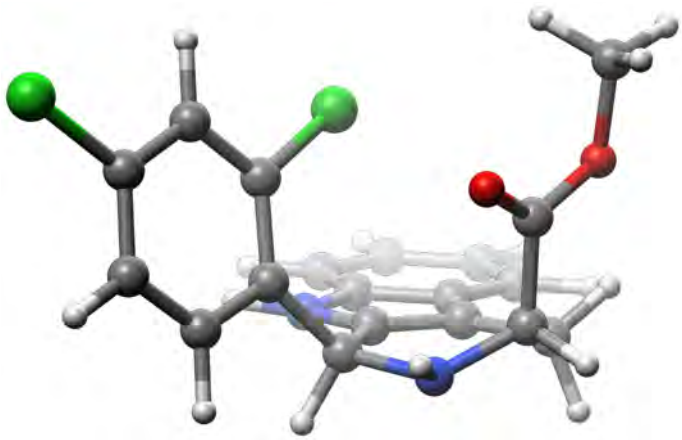
C	1.29936600	-2.29778100	-0.40217900
C	2.56521400	-2.01963900	-0.94440800
H	2.86851800	-0.99368200	-1.13718900
C	3.42346700	-3.07407800	-1.23255400
C	3.04283400	-4.40886500	-0.98799900
C	1.79742400	-4.71696900	-0.45009000
C	0.93728800	-3.65371900	-0.16081400
N	-0.33790700	-3.65125700	0.37415300
H	-0.87748800	-4.47091700	0.60642900
C	-0.78642700	-2.34207300	0.46784100
C	-2.12070800	-1.92634900	1.01878000
H	-2.23687200	-2.34884400	2.02495100
N	-2.18995100	-0.46038400	1.20403700
C	-1.48874400	0.37245600	0.21277100
H	-1.53959400	1.39043500	0.61643900
C	-2.34225900	0.46948600	-1.06720000
O	-3.46603100	0.91406700	-1.08543400
O	-1.68994500	0.05061400	-2.17562800
C	-2.43474400	0.16972800	-3.39964700
H	-2.71955500	1.21046400	-3.57437100
H	-3.33918600	-0.44243600	-3.35442300
H	-1.76562500	-0.18453600	-4.18439900
H	-1.83572400	-0.23002400	2.12776000
C	-3.31121800	-2.43428800	0.19682200
C	-4.59578600	-2.53489200	0.75381700
C	-5.69179900	-2.98468900	0.01992500
C	-5.50238000	-3.34748200	-1.31166600
C	-4.24572600	-3.26916600	-1.90527600
C	-3.16938700	-2.81647200	-1.14294900
H	-2.18822200	-2.74794000	-1.60184100
H	-4.10970600	-3.56051800	-2.94112600
Cl	-6.87489100	-3.92075200	-2.24526400
H	-6.67047700	-3.05090800	0.47957800
Cl	-4.88298000	-2.11058000	2.43747200
H	1.50637000	-5.74715500	-0.26113700
H	3.73429900	-5.21323500	-1.22356300
H	4.40449000	-2.86981700	-1.65269100
H	0.36986800	0.44325800	-0.93074100
H	0.58636200	0.45639100	0.81234400

8a-13



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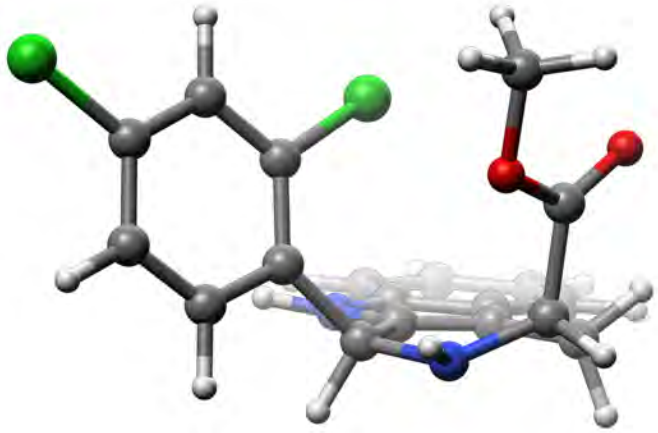
C	1.01183000	-2.27033100	-0.97840000
C	2.32215500	-2.04022600	-1.42947100
H	2.76768200	-1.05195400	-1.34797600
C	3.03938100	-3.09253900	-1.98652700
C	2.47397700	-4.37831400	-2.09999500
C	1.18186700	-4.63956700	-1.65501400
C	0.46476200	-3.57977800	-1.09366900
N	-0.81135700	-3.54543100	-0.56015100
H	-1.49505700	-4.28142500	-0.65301100
C	-1.09581900	-2.24651600	-0.17116700
C	-2.37382100	-1.83402500	0.48560900
H	-2.45164800	-2.41614600	1.41760400
N	-2.26820000	-0.42057600	0.92782200
C	-1.44069000	0.51862300	0.16812600
H	-1.38844700	1.42767200	0.78683500
C	-2.13405100	1.01161800	-1.11599700
O	-3.34121400	1.04378300	-1.23920900
O	-1.27791900	1.50325700	-2.03025800
C	-1.88651300	2.06565600	-3.20745000
H	-2.54420500	2.89601700	-2.93735600
H	-2.46751600	1.30410800	-3.73272500
H	-1.05864500	2.41440400	-3.82527600
H	-3.20442400	-0.03237000	1.00770300
C	-3.68219800	-2.17146400	-0.26036200
C	-3.92468100	-2.17806800	-1.64522800
C	-5.18663700	-2.46222800	-2.17250800
C	-6.24226800	-2.74256900	-1.31138700
C	-6.05215300	-2.75486900	0.06738800
C	-4.78140800	-2.47763100	0.56098300
H	-4.62684600	-2.49662300	1.63751400
H	-6.87431300	-2.98347000	0.73642400
Cl	-7.82572200	-3.09662700	-1.98068400
H	-5.33624900	-2.46035500	-3.24538100
Cl	-2.66661100	-1.86439600	-2.83528200
H	0.74802200	-5.63259700	-1.74092000
H	3.05727200	-5.18144800	-2.54209900
H	4.05251800	-2.92432900	-2.34159800
H	0.51942900	0.61116800	-0.74358900
H	0.52710700	0.14192800	0.95365400

8a-14



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C	0.04126400	-1.47178700	-0.26932500
C	1.08832000	-2.29972500	-0.80869600
C	2.38623500	-2.05309700	-1.28585800
H	2.79087200	-1.04424700	-1.28538200
C	3.14263100	-3.11610500	-1.76493400
C	2.62828800	-4.42807500	-1.77562100
C	1.34884100	-4.70501600	-1.30445300
C	0.59247900	-3.63404600	-0.82104500
N	-0.68223800	-3.60833200	-0.28328900
H	-1.33515500	-4.37683600	-0.30759900
C	-1.01303400	-2.29554000	0.01285800
C	-2.29592800	-1.88623600	0.66254400
H	-2.32488300	-2.38468700	1.64503700
N	-2.24976600	-0.43837100	0.96610300
C	-1.45694500	0.47630300	0.14178700
H	-1.44224300	1.42471900	0.70027600
C	-2.05852400	0.88580000	-1.21746700
O	-1.42809900	1.28426700	-2.17124900
O	-3.41095500	0.86602000	-1.17245300
C	-4.07425700	1.35148800	-2.35242400
H	-3.82401400	0.72568600	-3.21205000
H	-3.77656300	2.38259800	-2.56051000
H	-5.14095100	1.29490400	-2.13312800
H	-3.19313000	-0.08015000	1.07245200
C	-3.60048200	-2.35797200	-0.01413000
C	-3.87981400	-2.46363500	-1.38824400
C	-5.12970700	-2.87591200	-1.85807800
C	-6.13672400	-3.18338100	-0.94852500
C	-5.90917000	-3.09590900	0.42196100
C	-4.65019600	-2.69457300	0.85822800
H	-4.46493900	-2.63819200	1.92853000
H	-6.69298700	-3.34453700	1.12888500
Cl	-7.70554400	-3.69572700	-1.54533900
H	-5.30707700	-2.95501300	-2.92402700
Cl	-2.68446200	-2.10758400	-2.62698700
H	0.95450300	-5.71803000	-1.31134800
H	3.24168000	-5.23935600	-2.15812500
H	4.14660600	-2.93584000	-2.13945600
H	0.47190700	0.56757500	-0.80782800
H	0.53908000	0.24103100	0.92619200

8a Shielding tensors B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	8a-01	**8a-02**	**8a-03**	**8a-04**	**8a-05**	**8a-06**	**8a-07**
1	123.2424	123.0253	124.5188	125.7839	123.9887	118.3157	117.2873
3	120.6582	120.237	121.0327	125.0976	117.8691	120.3565	116.9153
4	153.1466	154.2828	151.9047	157.7095	152.3807	151.974	152.6891
4a	69.5784	68.8268	65.4008	66.6129	64.7392	67.7289	67.4782
4b	49.405	49.2185	48.7247	49.3867	49.1548	48.7507	48.6831
5	59.8227	60.0005	59.7493	59.2373	60.5246	59.6165	60.1879
6	58.5256	58.5199	58.0586	58.7455	58.4956	58.5133	58.3951
7	56.2813	55.9968	55.7327	56.1439	55.7451	56.4153	55.8429
8	67.8026	68.3478	67.736	68.6508	68.1495	67.66	68.5173
8a	42.05	41.278	40.7513	40.38	40.9227	41.3914	41.3588
9a	41.3211	42.2783	43.2326	45.7185	43.1065	42.3987	42.3536
1'	34.8139	34.4731	36.8291	35.783	36.8442	38.0048	38.8832
2'	35.4298	35.141	31.9276	33.2266	31.6184	33.2434	33.5821
3'	47.5548	47.5242	46.523	47.0119	46.4213	45.073	45.3006
4'	34.4679	34.2563	33.6288	33.7608	33.4503	32.8882	32.7891
5'	49.007	48.9461	49.2945	49.9355	49.3487	49.2919	49.261
6'	44.8868	44.9824	46.1672	44.7402	46.3908	41.8092	42.1607
1''	-1.2859	0.6689	-2.6908	-3.3525	0.1707	-2.761	0.0261
2''	127.7413	127.823	127.844	128.7967	128.3385	128.0147	128.167

	8a-08	**8a-09**	**8a-10**	**8a-11**	**8a-12**	**8a-13**	**8a-14**
1	125.8347	126.2946	116.1691	115.7368	126.4183	121.9585	121.2309
3	124.7949	124.4588	119.6681	119.6213	123.5796	122.9416	122.9609
4	157.4084	156.1761	153.5556	154.8891	155.7036	157.5584	157.6768
4a	65.6188	65.078	67.0027	67.2964	64.6966	67.5412	67.4042
4b	49.6801	49.3073	49.1604	48.6084	49.0644	49.0371	48.7703
5	59.9864	59.7294	59.8349	59.468	60.0928	60.3263	60.0828
6	58.8562	58.9164	58.4755	58.1453	58.9223	58.6435	58.7059
7	56.0503	56.0276	56.5384	56.2827	56.1133	55.9621	56.1509
8	67.7665	68.3405	67.8214	68.0891	68.0088	68.4069	68.1103
8a	40.1874	40.3228	41.077	41.0876	40.4593	39.9047	39.806
9a	43.7915	43.8511	42.2329	43.175	43.6012	45.6172	45.4898
1'	33.9853	36.3873	37.6313	37.2255	35.7879	34.6811	34.6238
2'	33.2687	31.8534	31.744	31.07	31.5746	33.1009	33.0535
3'	46.915	46.9431	44.5002	44.569	46.6023	45.1292	45.4992
4'	34.3185	34.3229	33.0949	32.9191	34.5116	34.0089	33.692
5'	50.3916	50.6691	50.2733	50.1607	50.9479	49.3091	49.0341
6'	46.3562	44.4465	43.2847	42.9983	45.9489	42.4235	41.9052
1''	-4.0772	-2.4	-0.9625	0.4737	-0.7391	-3.8693	-2.6819
2''	128.4821	128.5402	127.83	127.9628	128.7929	127.8722	128.2179

8a Shielding tensors mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	8a-01	8a-02	8a-03	8a-04	8a-05	8a-06	8a-07
1	128.8008	128.631	130.0945	131.4085	129.5127	124.2144	123.2759
3	126.6067	126.2065	127.1493	130.9445	124.2869	126.5478	123.41
4	158.4903	159.6111	157.2159	162.8718	157.7357	157.3493	157.9574
4a	74.749	74.1966	70.6775	71.6895	70.0198	73.0284	72.8509
4b	54.8682	54.6736	54.3068	54.9095	54.7157	54.2965	54.2521
5	63.7457	63.9174	63.769	63.3869	64.5419	63.7035	64.2581
6	63.0643	63.0679	62.4931	63.1564	62.9528	63.0558	62.9474
7	60.7119	60.4293	60.0323	60.4268	60.0813	60.7857	60.2752
8	71.8688	72.3443	71.8949	72.7729	72.3147	71.7859	72.5691
8a	47.4256	46.7802	46.2555	45.7969	46.3347	46.8406	46.7972
9a	46.7937	47.6779	48.525	50.9224	48.3821	47.7027	47.711
1'	40.6819	40.3588	42.6578	41.4363	42.66	43.9172	44.6316
2'	41.3231	41.0947	37.7828	39.2194	37.4953	39.0714	39.3459
3'	52.2075	52.2374	51.1903	51.6012	51.1011	49.7861	50.0359
4'	40.1882	40.0079	39.3795	39.6614	39.2647	38.6365	38.5294
5'	53.5334	53.4693	53.8359	54.3839	53.8799	53.8365	53.7751
6'	49.3746	49.4623	50.5383	49.2015	50.781	46.2711	46.5506
1''	4.1243	6.117	2.8214	2.3522	5.6521	2.769	5.527
2''	132.3265	132.4534	132.5321	133.4658	132.952	132.6561	132.8171

	8a-08	8a-09	8a-10	8a-11	8a-12	8a-13	8a-14
1	131.4335	131.8371	122.1166	121.7828	131.9493	127.7972	127.138
3	130.6591	130.3783	125.6938	125.5757	129.6685	128.8829	128.8637
4	162.5668	161.4826	158.9089	160.128	160.9532	162.6862	162.7855
4a	71.0357	70.3839	72.2884	72.616	70.0054	72.8536	72.7086
4b	55.182	54.8015	54.6713	54.2045	54.6503	54.5511	54.2972
5	64.043	63.7982	63.9191	63.5748	64.0966	64.4012	64.1092
6	63.2909	63.3454	63.0337	62.6548	63.3751	63.0846	63.1562
7	60.388	60.354	60.9324	60.6467	60.4437	60.3299	60.5165
8	71.8918	72.4522	71.9329	72.2064	72.1089	72.6017	72.3065
8a	45.6658	45.7925	46.4695	46.5098	45.9663	45.4627	45.4128
9a	49.2525	49.3793	47.5378	48.5063	49.0854	50.6146	50.6326
1'	39.7927	42.0795	43.4512	43.0267	41.4883	40.6651	40.5927
2'	39.2503	37.8459	37.4574	36.8496	37.5878	38.8794	38.8597
3'	51.5772	51.541	49.2051	49.3308	51.2872	49.8859	50.2765
4'	40.1055	40.1325	38.8594	38.7059	40.2671	39.863	39.4926
5'	54.8944	55.1234	54.7891	54.6583	55.4402	53.9269	53.6831
6'	50.7203	48.9345	47.6447	47.4259	50.4072	46.937	46.443
1''	1.6528	3.2853	4.4296	5.8893	4.9145	1.7209	2.934
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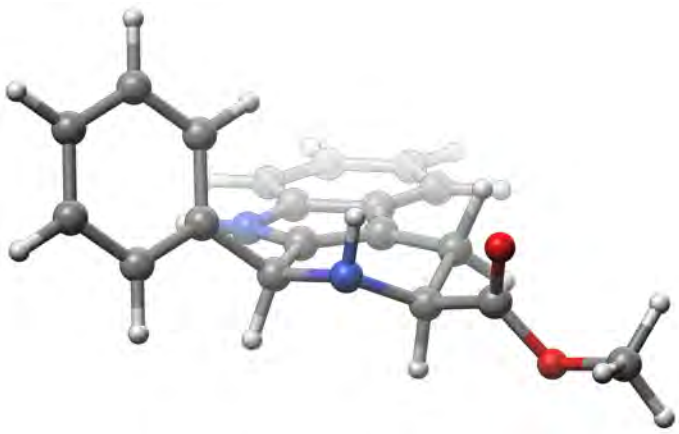

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H	2.78164300	-1.58516400	0.56397900
C	4.71330900	-0.70298500	0.19627800
C	5.42930800	0.42976000	-0.23966400
C	4.77052900	1.57984500	-0.66304800
C	3.37318600	1.57135600	-0.63934800
N	2.46399100	2.54720600	-1.00511600
H	2.69218800	3.50050600	-1.24345300
C	1.18084500	2.08111000	-0.77004300
C	-0.08290800	2.83668500	-1.09207200
H	-0.18205400	2.88618300	-2.18880000
N	-1.27207100	2.12354100	-0.58816800
C	-1.21175500	0.66716000	-0.71903200
H	-1.15748400	0.42128100	-1.78537000
C	-2.49995000	0.09693900	-0.14600700
O	-3.07101000	0.54163900	0.82673000
O	-2.89567700	-1.00586100	-0.81354200
C	-4.06503500	-1.65763700	-0.28704100
H	-4.92521000	-0.98405400	-0.32092900
H	-3.89805200	-1.96894600	0.74752500
H	-4.22996900	-2.52399500	-0.92801900
H	-1.44451500	2.36198700	0.38711100
C	-0.09362100	4.27001400	-0.57373500
C	-0.65170800	5.29351200	-1.34819600
C	-0.70405600	6.60260300	-0.86797800
C	-0.19948500	6.90336700	0.39854400
C	0.35598500	5.88900700	1.18075900
C	0.40944600	4.58105200	0.69691200
H	0.84941300	3.79495100	1.30579700
H	0.75043600	6.11537300	2.16784700
H	-0.23788800	7.92262600	0.77352400
H	-1.13894700	7.38652700	-1.48235000
H	-1.05228200	5.05885500	-2.33158300
H	5.32425000	2.45165600	-1.00238900
H	6.51561700	0.40491600	-0.24758800
H	5.25955700	-1.58564300	0.51779000
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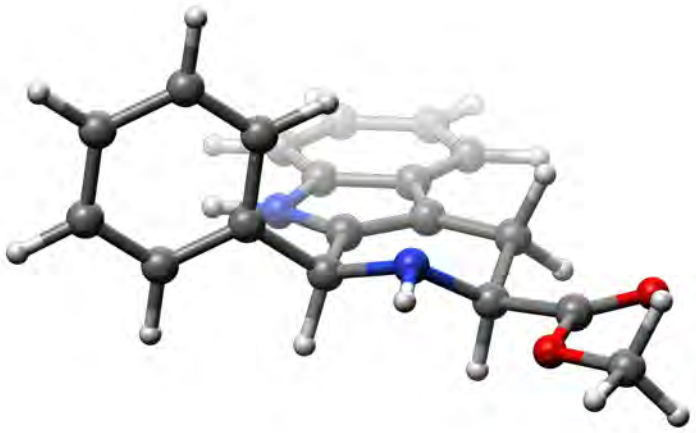

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C	4.76946200	-0.12515800	0.22324000
C	5.34170000	1.10431900	-0.15997200
C	4.54790200	2.17781500	-0.55180200
C	3.16271500	1.99339800	-0.54905200
N	2.14247100	2.86060600	-0.89714300
H	2.24611000	3.84869300	-1.07366300
C	0.93017000	2.22473900	-0.69871500
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H	-0.54457100	2.88292000	-2.08425400
N	-1.42325500	1.98522900	-0.34854400
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H	-1.16771600	0.40388800	-1.76797800
C	-2.50598500	-0.22009100	-0.25571300
O	-2.50332800	-1.31582300	0.25773100
O	-3.63773700	0.44761600	-0.58150500
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H	-4.92804800	-0.39824700	0.82554400
H	-4.93226400	-1.17943700	-0.77372800
H	-5.66255800	0.44947100	-0.57663100
H	-2.34940200	2.29523400	-0.63142500
C	-0.51869000	4.27433300	-0.46596800
C	-0.44956500	5.35374900	-1.35326000
C	-0.50673400	6.66868200	-0.88220200
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C	-0.71490700	5.83919200	1.37626400
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H	-0.45591900	7.49703400	-1.58406200
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H	4.99095700	3.12454300	-0.85060600
H	6.42251700	1.21654000	-0.15162700
H	5.41919600	-0.94385600	0.52072100
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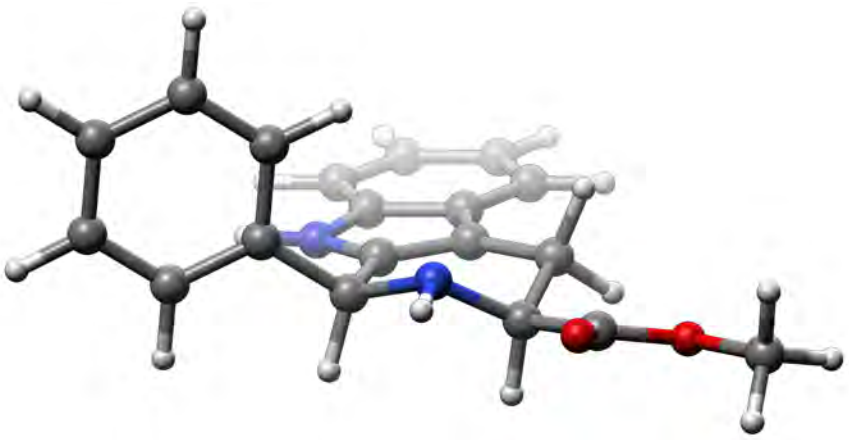

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C	-3.66372000	3.05362100	0.27832900
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C	-3.72173300	0.40358400	-0.52158200
N	-3.46174100	-0.90615700	-0.88360200
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C	0.62716400	-1.22177500	-0.70171500
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O	2.59186200	-2.56301500	-0.23680000
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C	4.18987100	-0.45812000	-0.00034400
H	4.67017500	-1.02758100	-0.80031800
H	4.35153400	-0.97320200	0.94993500
H	4.58451200	0.55727400	0.04020000
H	0.42340400	-3.25123500	-0.59857400
C	-2.25261400	-3.66915400	-0.46631900
C	-2.99796900	-4.46111200	-1.34645000
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H	-5.85833900	0.65419600	-0.81139700
H	-5.79418800	3.03138500	-0.08767800
H	-3.66367400	4.09557400	0.58705900
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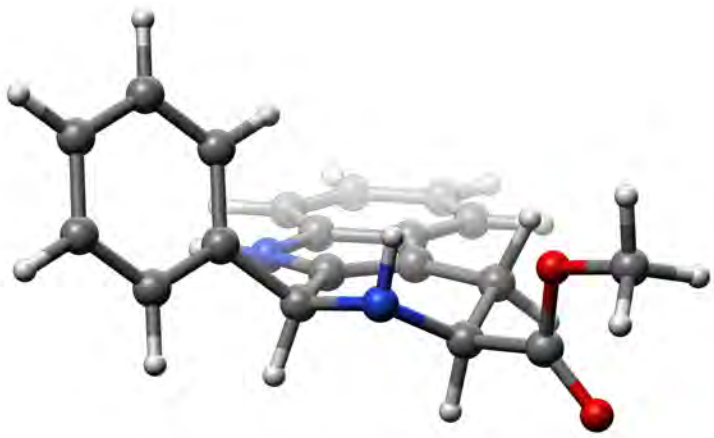
8b-04



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C	3.36554800	0.29261400	0.41861900	H	-2.01938200	1.80474200	0.47021900
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C	2.77839100	2.53707000	-0.32517400	C	-1.42730900	5.72032800	1.42167700
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C	-0.87316800	2.75534100	-0.94322400	H	-2.63257600	7.47276000	1.06220700
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C	-1.31291300	0.33668500	-0.76314700	H	4.39501400	3.97423200	-0.51242000
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O	-2.96071000	-0.42244200	0.76818500	H	0.42313400	-0.93274500	-0.39622200
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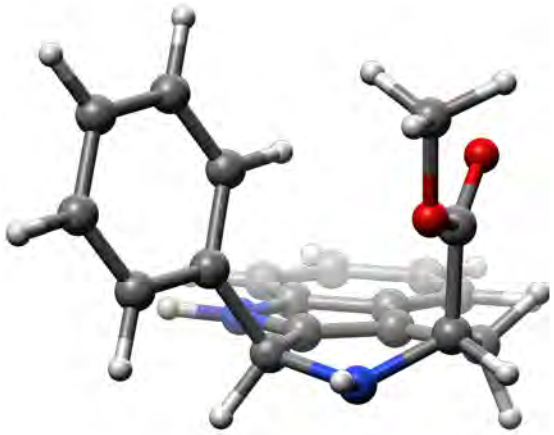

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N	0.61603900	-3.62415000	-0.22654300
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O	-1.75958300	0.09335700	-2.27866700
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H	4.94643100	-1.34921700	-2.03745100
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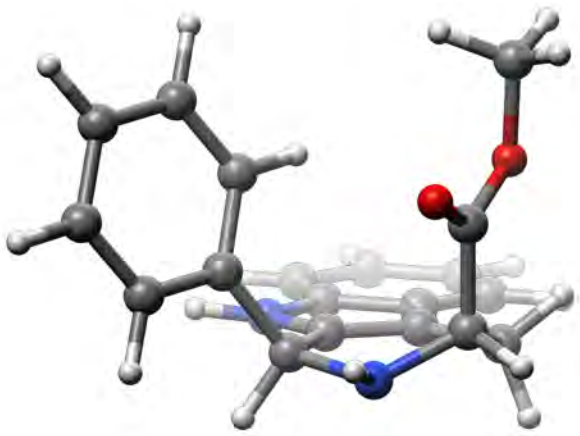

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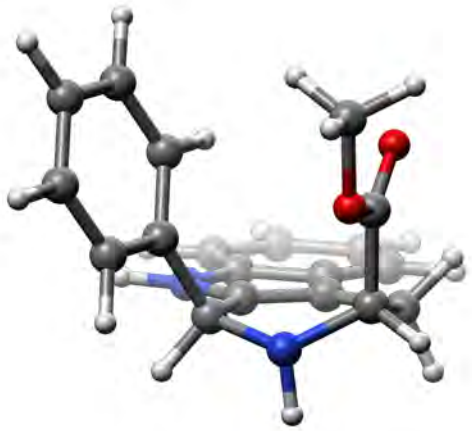

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H	-4.32548200	-1.24624700	-2.44005900
H	-4.29559700	0.52770600	-2.61677500
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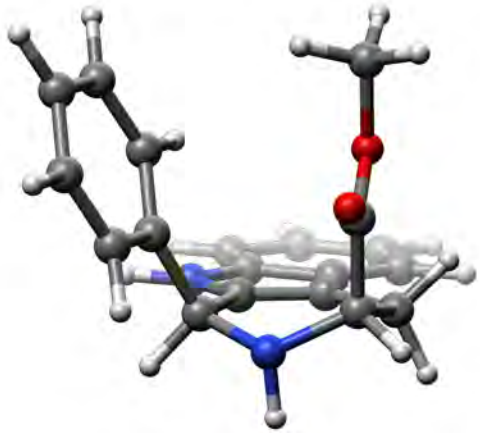
H	5.06703000	-3.77862700	-1.63114800
H	5.01566300	-1.31472000	-1.85993100
H	0.15785700	0.57293600	-0.92009000
H	0.47360800	0.57090500	0.81321900

8b-08



C	0.00000000	0.00000000	0.00000000
C	-0.58084800	-1.37589600	0.13555600
C	-1.87758300	-1.79818900	0.59760600
C	-3.00741200	-1.12909400	1.09736500
H	-3.00679000	-0.04656800	1.19766600
C	-4.12481200	-1.86965700	1.46499700
C	-4.13911100	-3.27346100	1.34272100
C	-3.03727400	-3.96524300	0.84932900
C	-1.91627700	-3.21698000	0.47955500
N	-0.69943800	-3.61990600	-0.03977800
H	-0.41320400	-4.57524300	-0.18886700
C	0.10068500	-2.50386200	-0.23896600
C	1.48479600	-2.52063000	-0.82471400
H	1.46482200	-3.11358600	-1.75209100
N	1.88101900	-1.16021000	-1.25869600
C	1.51217800	-0.06315000	-0.33953900
H	1.79457100	0.85466500	-0.86652300
C	2.45942000	-0.07952600	0.87321100
O	3.63646500	0.19039500	0.80098000
O	1.83391500	-0.39443500	2.02666100
C	2.67890900	-0.43479000	3.18876300
H	3.18612000	0.52352300	3.32691300
H	3.42556500	-1.22578800	3.08338000
H	2.01262400	-0.64404700	4.02627400
H	1.42897000	-0.97038400	-2.15098100
C	2.56584700	-3.15365800	0.06449400
C	3.88084900	-3.20080000	-0.42007000
C	4.89471400	-3.79485400	0.32687800
C	4.61123800	-4.35227300	1.57731400
C	3.30886100	-4.30281100	2.07187800
C	2.29154200	-3.70543300	1.31996800
H	1.28479200	-3.66052900	1.72347100
H	3.07810200	-4.72649700	3.04616600
H	5.40164300	-4.81657300	2.16125400
H	5.90901200	-3.81852800	-0.06282100
H	4.10383300	-2.74379000	-1.37966000
H	-3.05047700	-5.04819700	0.75465400
H	-5.02609700	-3.82682800	1.63903300
H	-5.00295800	-1.36119500	1.85378400
H	-0.15281300	0.58736600	0.91255700
H	-0.51136600	0.54943200	-0.80570800

8b Shielding tensors B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	8b-01	**8b-02**	**8b-03**	**8b-04**	**8b-05**	**8b-06**	**8b-07**	**8b-08**
1	119.7767	116.7167	117.2034	118.7587	120.9346	121.3299	122.8195	123.6806
3	120.8299	119.6897	120.1121	117.4989	124.9719	124.0013	123.9525	122.6274
4	151.5696	154.201	153.2238	152.3809	157.8562	157.8366	156.4641	155.7107
4a	66.6307	69.4623	69.3968	66.3085	66.5976	66.5505	66.3663	67.4106
4b	48.4866	47.7594	48.5007	48.4502	48.7576	49.3057	48.4298	48.2199
5	59.0301	58.6664	60.6549	60.0507	59.2215	59.5067	59.1388	59.3529
6	58.5358	58.7008	57.9704	58.191	58.9695	58.9859	59.0201	59.0033
7	56.4706	56.886	56.4583	56.2697	56.4208	56.4097	56.3884	56.4632
8	67.6033	68.2479	68.6529	67.8316	68.0768	68.264	67.637	67.8087
8a	41.3169	40.6981	39.8707	40.6168	40.204	40.0269	40.9205	41.5086
9a	41.1077	39.3535	38.7588	41.3257	44.3214	43.7245	44.6593	43.5052
1'	32.9148	32.0619	31.8827	32.4868	30.4629	30.0536	32.3461	33.0061
2'	45.6805	49.0096	49.3291	45.2079	48.1062	47.8496	45.151	44.9841
3'	48.7018	49.0245	49.3329	47.2503	47.7609	48.3507	48.6917	49.0691
4'	48.5437	48.6599	48.4589	48.8474	49.2601	49.2213	50.0174	50.2085
5'	48.2249	48.0041	47.6984	48.4579	48.5038	48.9875	49.9351	50.2461
6'	48.96	47.9456	47.6448	50.8589	48.3642	48.9686	48.0688	49.8045
1''	-2.9426	0.1264	-1.5574	-0.0947	-3.4803	-3.8975	-1.4941	0.1212
2''	128.1357	127.9082	127.8355	128.3818	129.0169	128.5566	128.9634	129.1278

8b Shielding tensors mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d) SCRF = (PCM, $CHCl_3$)

	8b-01	**8b-02**	**8b-03**	**8b-04**	**8b-05**	**8b-06**	**8b-07**	**8b-08**
1	125.6949	122.7393	123.1648	124.6905	126.9518	127.2819	128.6799	129.4753
3	127.0067	125.7269	126.1043	123.9514	130.8401	129.9767	129.9018	128.8085
4	157.002	159.5501	158.546	157.7749	162.9761	162.9768	161.6953	160.993
4a	71.8495	74.758	74.6291	71.5913	71.8769	71.8119	71.5675	72.6384
4b	53.9287	53.3765	54.0635	54.0342	54.3464	54.8247	54.0077	53.825
5	63.0851	62.8529	64.6558	64.0441	63.2725	63.7023	63.2178	63.3829
6	63.07	63.1802	62.4827	62.6236	63.4665	63.4372	63.4623	63.4426
7	60.8418	61.2229	60.8362	60.576	60.8067	60.7146	60.7504	60.812
8	71.7287	72.31	72.7105	71.9979	72.1076	72.4378	71.7854	71.9533
8a	46.7232	46.1947	45.5798	46.2294	45.6892	45.5327	46.3896	47.0443
9a	46.4416	44.8257	44.2283	46.6691	49.4593	48.7885	49.7149	48.7025
1'	38.9117	37.9654	37.8286	38.2353	36.3509	36.027	38.1549	38.7511
2'	50.1433	53.4788	53.8095	49.6321	52.6461	52.374	49.8421	49.7377
3'	53.0525	53.4715	53.7511	51.735	52.3231	52.8444	53.1414	53.5085
4'	52.9031	53.0358	52.8756	53.206	53.6335	53.611	54.3714	54.5791
5'	52.6639	52.3986	52.1223	52.8558	52.9005	53.3711	54.3068	54.6726
6'	53.2957	52.3842	52.0542	55.1676	52.9327	53.4384	52.6183	54.2846
1''	2.5772	5.5764	3.8428	5.4047	2.1842	1.7096	4.0984	5.7235
2''	132.7801	132.5492	132.4624	133.0071	133.6777	133.1967	133.6496	133.829