SUPPORTING INFORMATION

Bypassing the stereoselectivity issue: transformations of Kinugasa adducts from chiral alkynes and non-chiral acyclic nitrones

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1. HPLC with *on-line* ECD analyses

The analysis of compounds **8–12, 22, 23** and **27** were performed using a Jasco analytical HPLC system equipped with PU-2089 *Plus* pump containing an inner degasser, column oven, a 20 μL sample loop, and MD-2010 high resolution diode array UV–VIS detector (195–600 nm) with various analytical columns at 20 °C; the mobile phase was *i*-PrOH/hexane (the exact chromatographic conditions are given below). In all cases, the concentration of injected samples was *ca.* 1 mg/mL. ECD detection was obtained at one fixed wavelength by setting the flow cell attachment in the sample chamber of ECD Jasco J-815 spectropolarimeter, and then introducing an eluant from HPLC. The signal was processed by Chrom*NAV* Jasco software. The *on-line* ECD spectra were recorded in the range 200–450 nm at room temperature. Solutions with about maximum ECD absorption (manual 'stop-flow') were trapped in the flow cell having a ca. 0.1 cm path length and then *on-line* ECD spectra under following conditions were recorded: 100 nm/min scanning speed, a step size of 0.2 nm, a bandwidth of 2 nm, a response time of 0.5 s, and an accumulation of 5 scans. The spectra were background corrected using the same mobile phase. The experimental ECD signal was not corrected for the concentration.

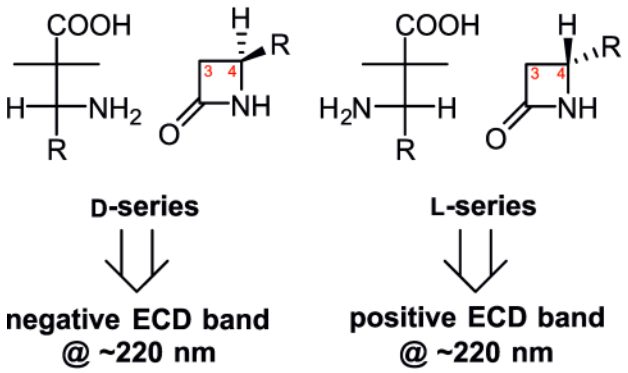
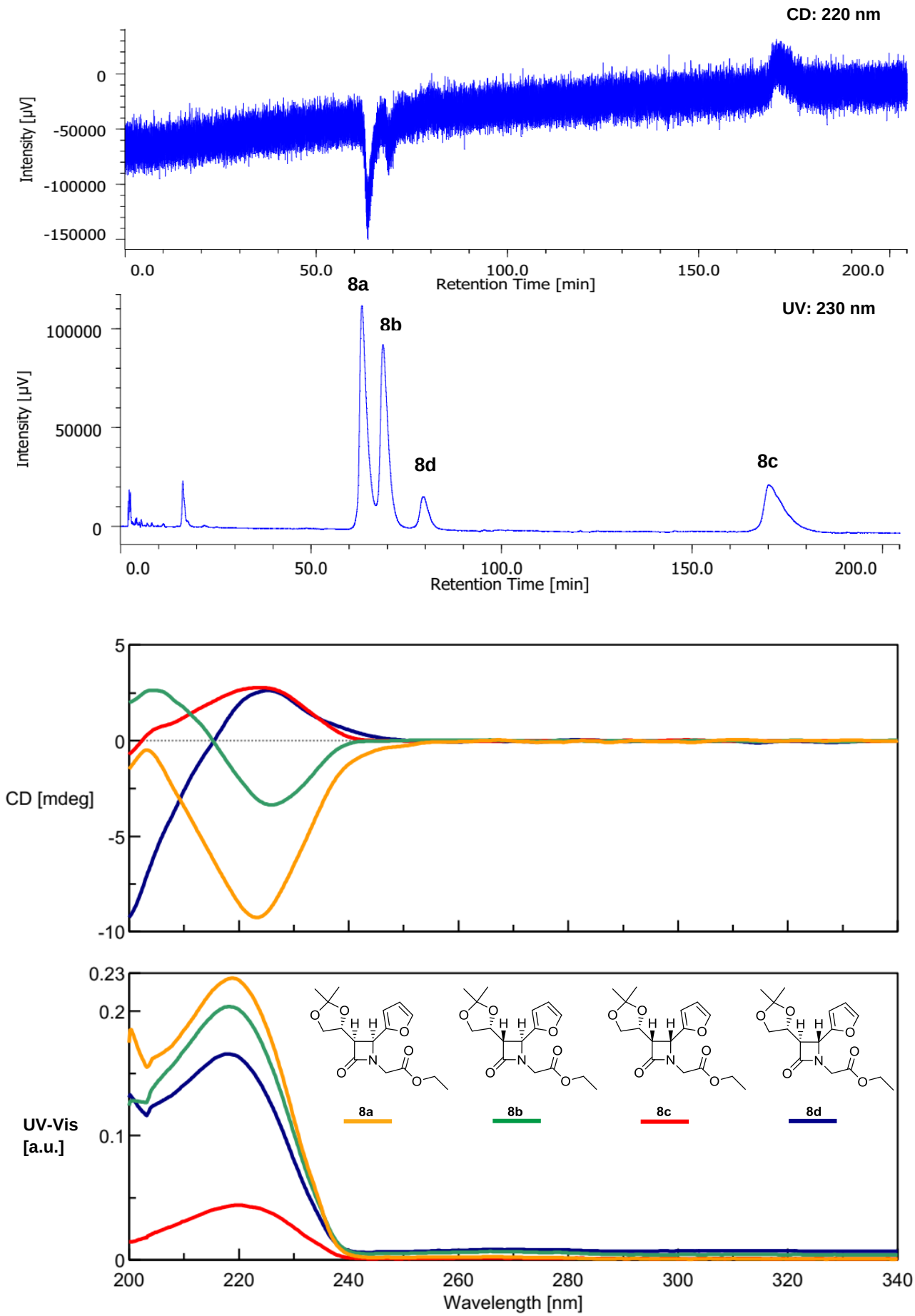
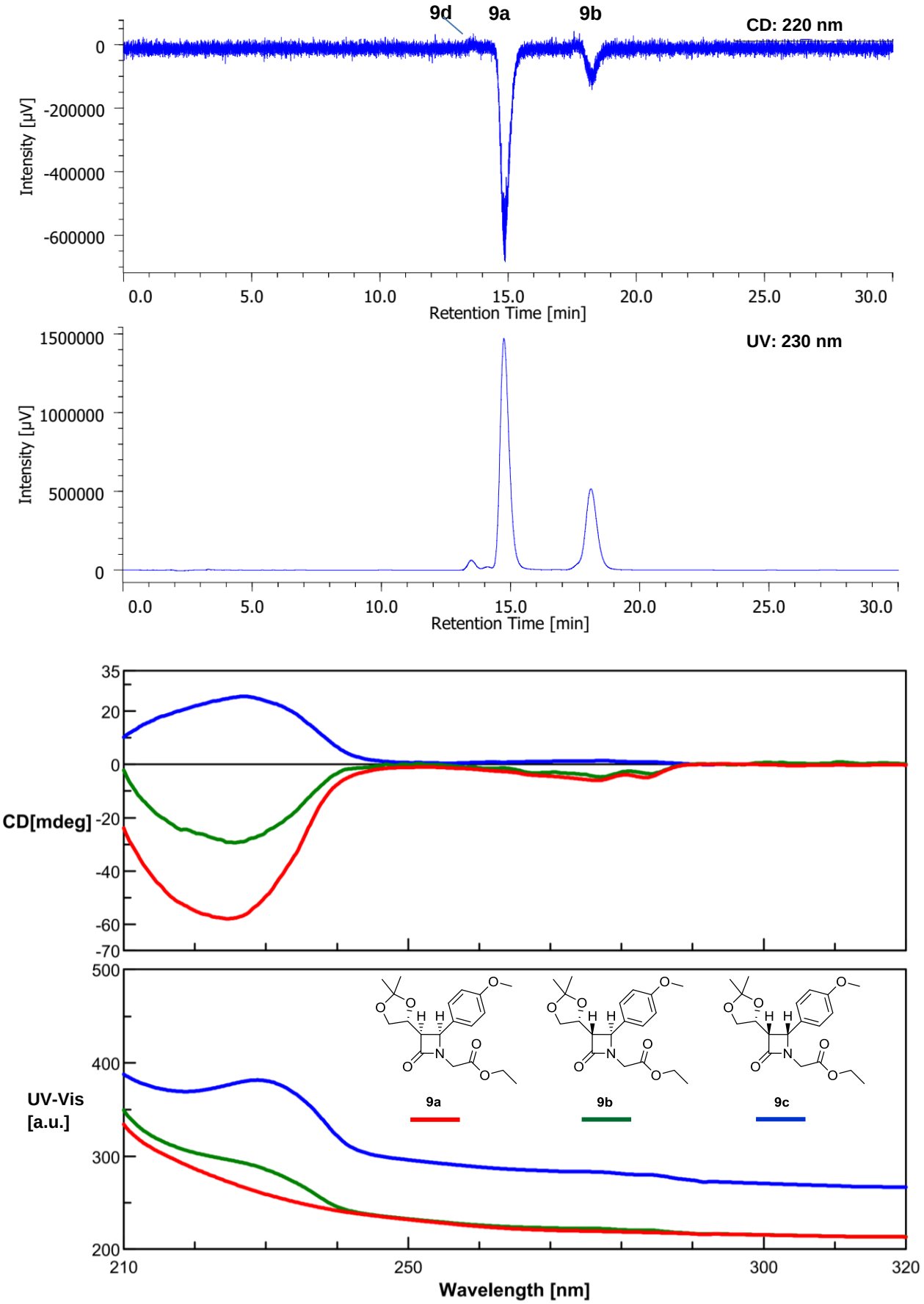


Figure S1. Definition of D- and L-series for β-lactams with reference to the helicity rule for the diagnostic n–π* ECD band.

separation conditions: Lichrospher® Si60/5 µm, *i*-PrOH/Hexane 1/99, 1 mL/min

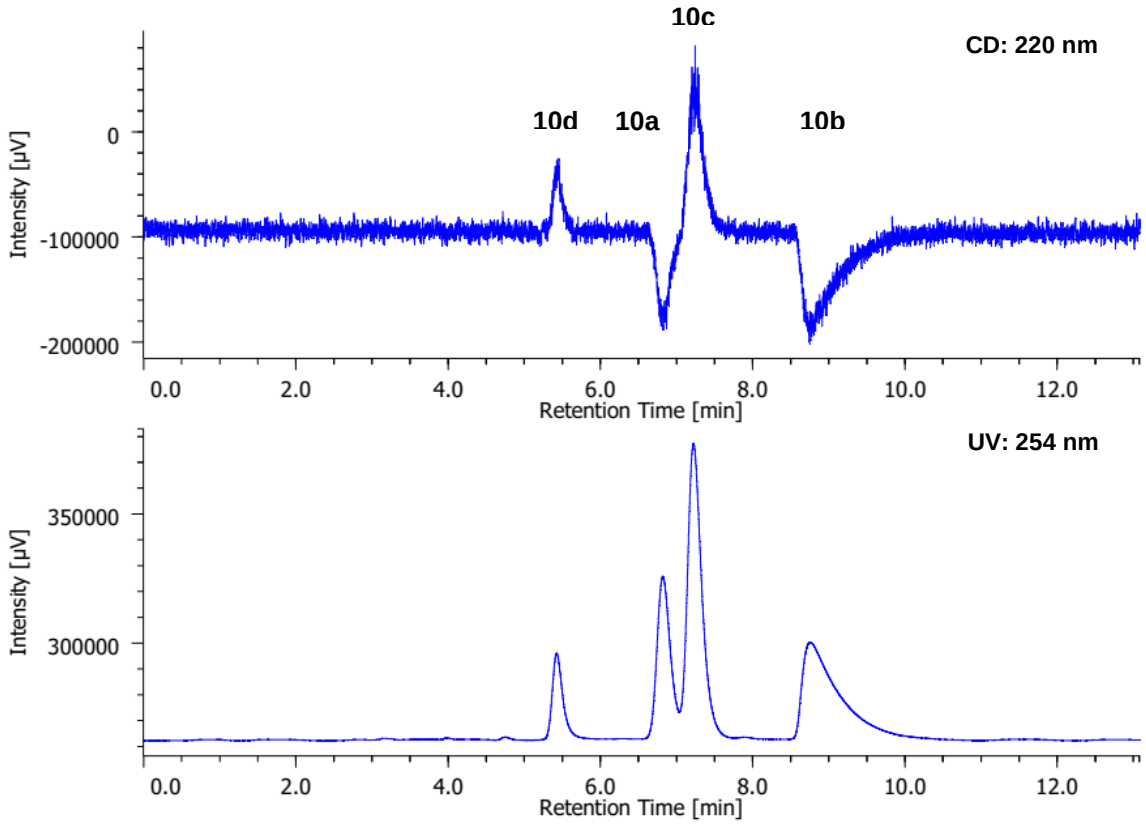


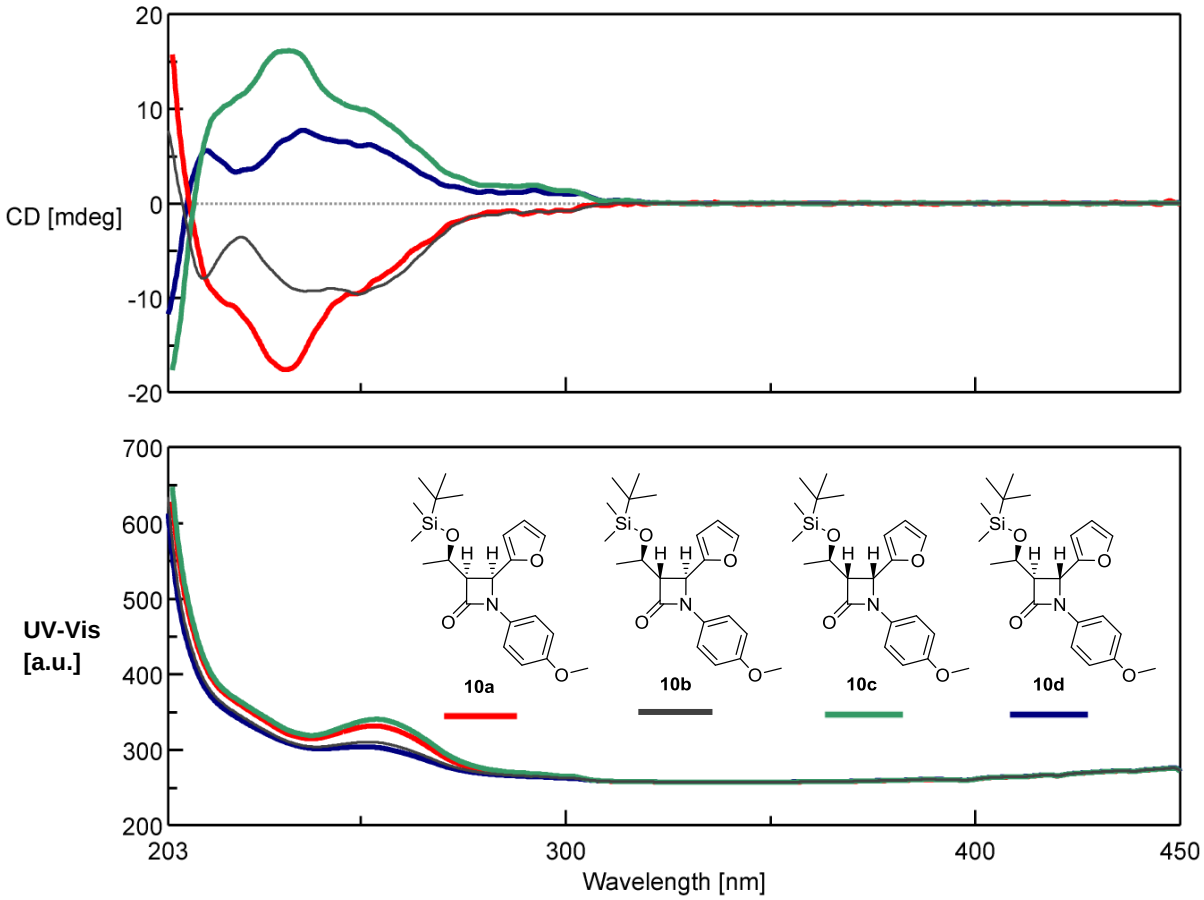
separation conditions: Daicel Chiralpak® AD-H, *i*-PrOH/Hexane 13/87, 1 mL/min



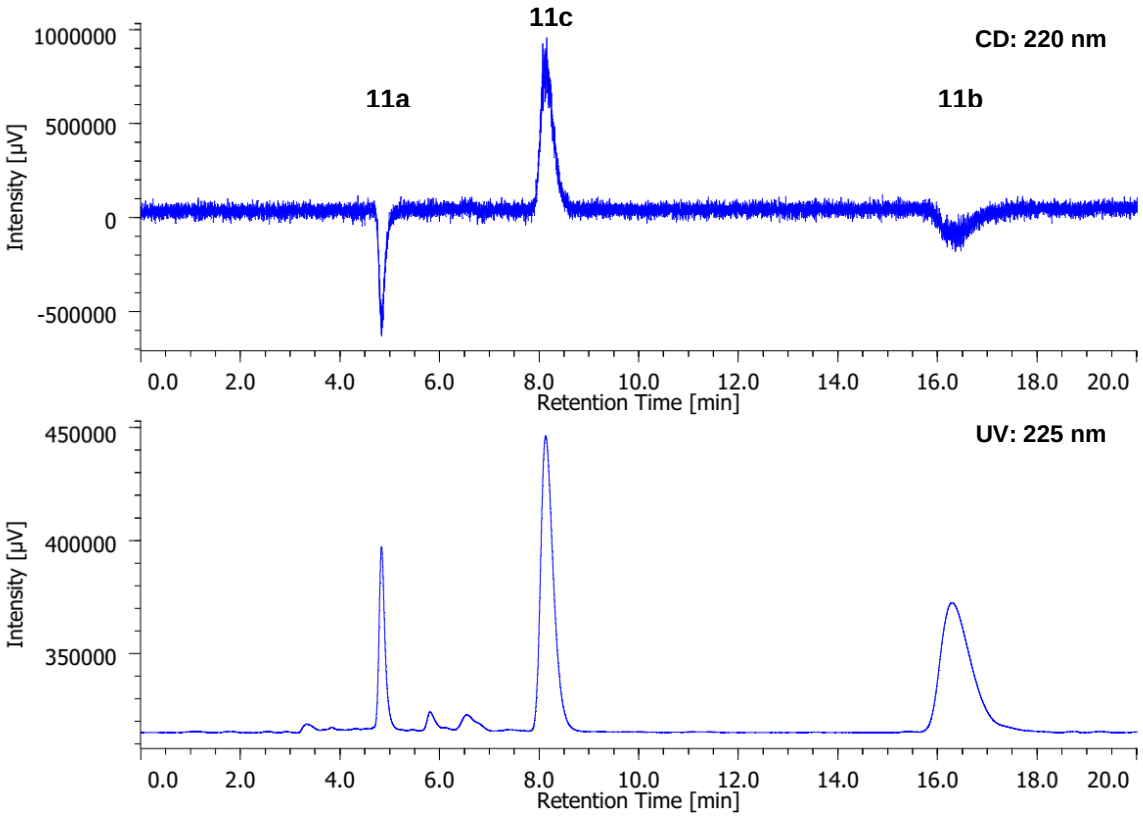
ECD and UV spectra of pure **9c** *(blue) were obtained apart from HPLC-ECD analysis, normalized and imposed on the figure.*

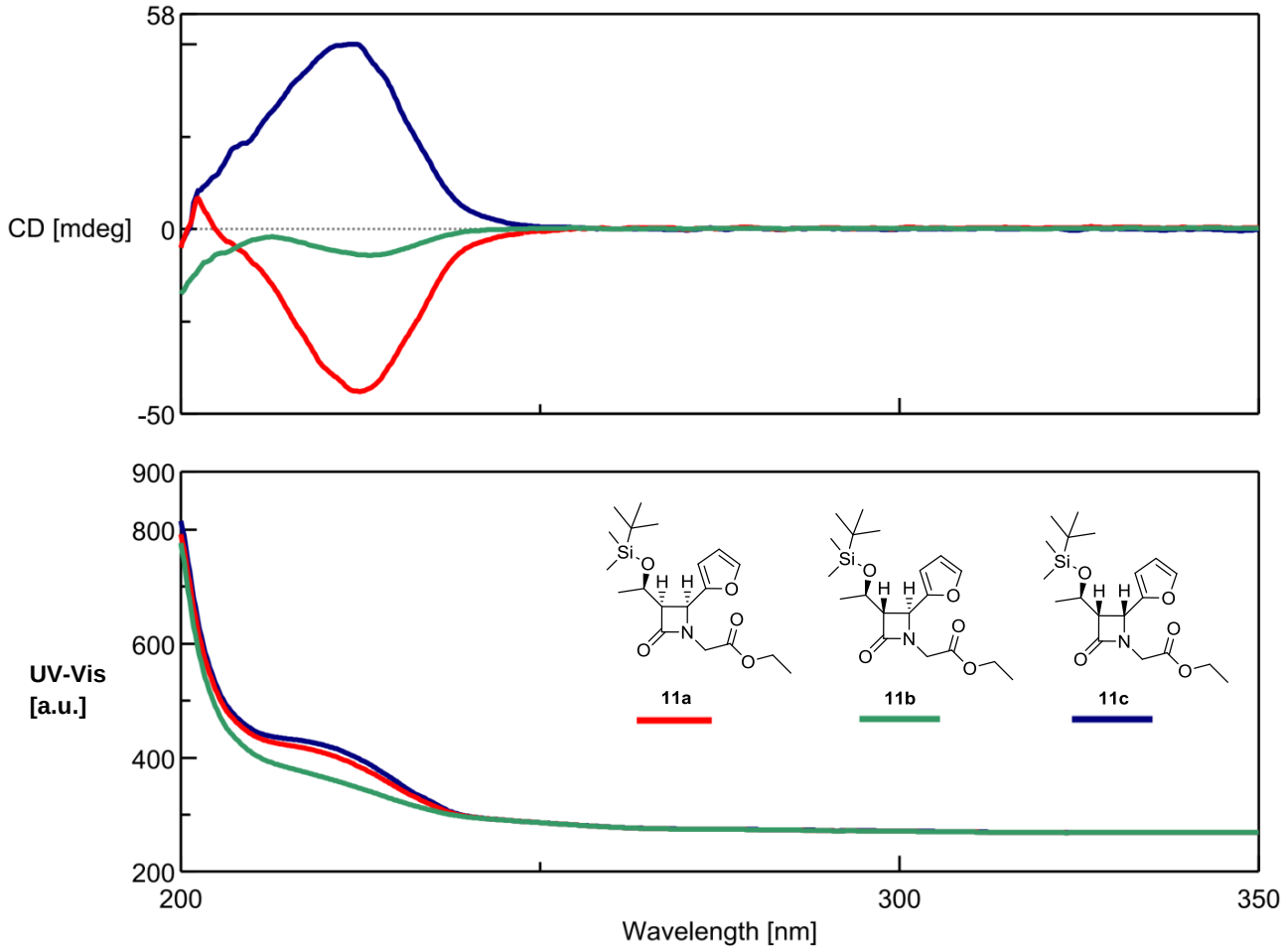
separation conditions: Daicel Chiralcel® OD-H, *i*-PrOH/Hexane 10/90, 1 mL/min



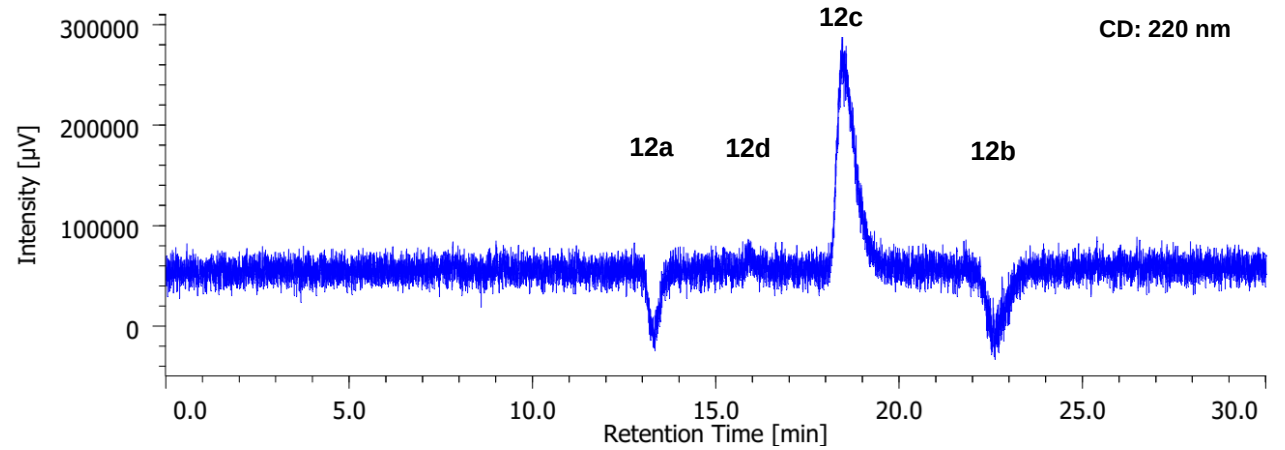


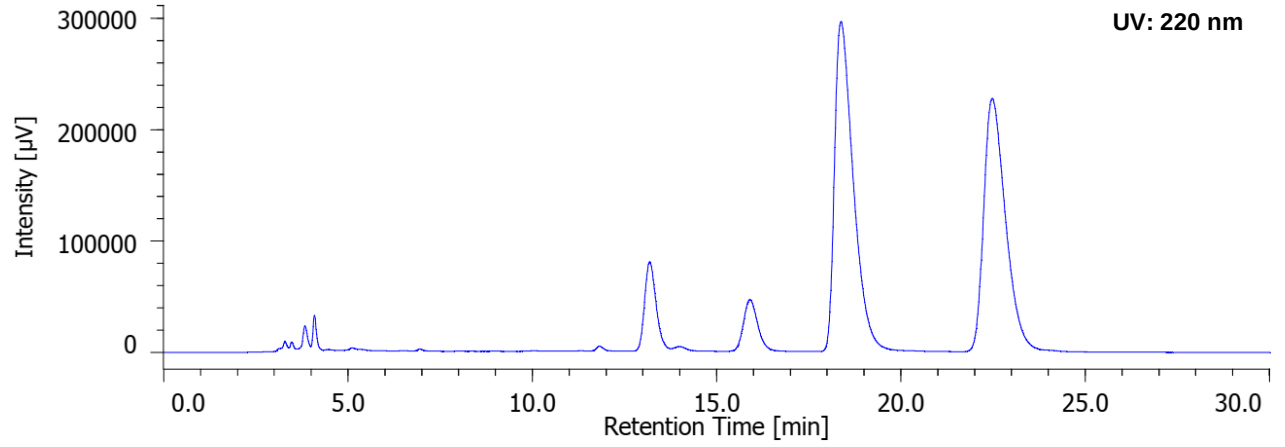
separation conditions: Daicel Chiralcel® AS-H, *i*-PrOH/Hexane 5/95, 1 mL/min

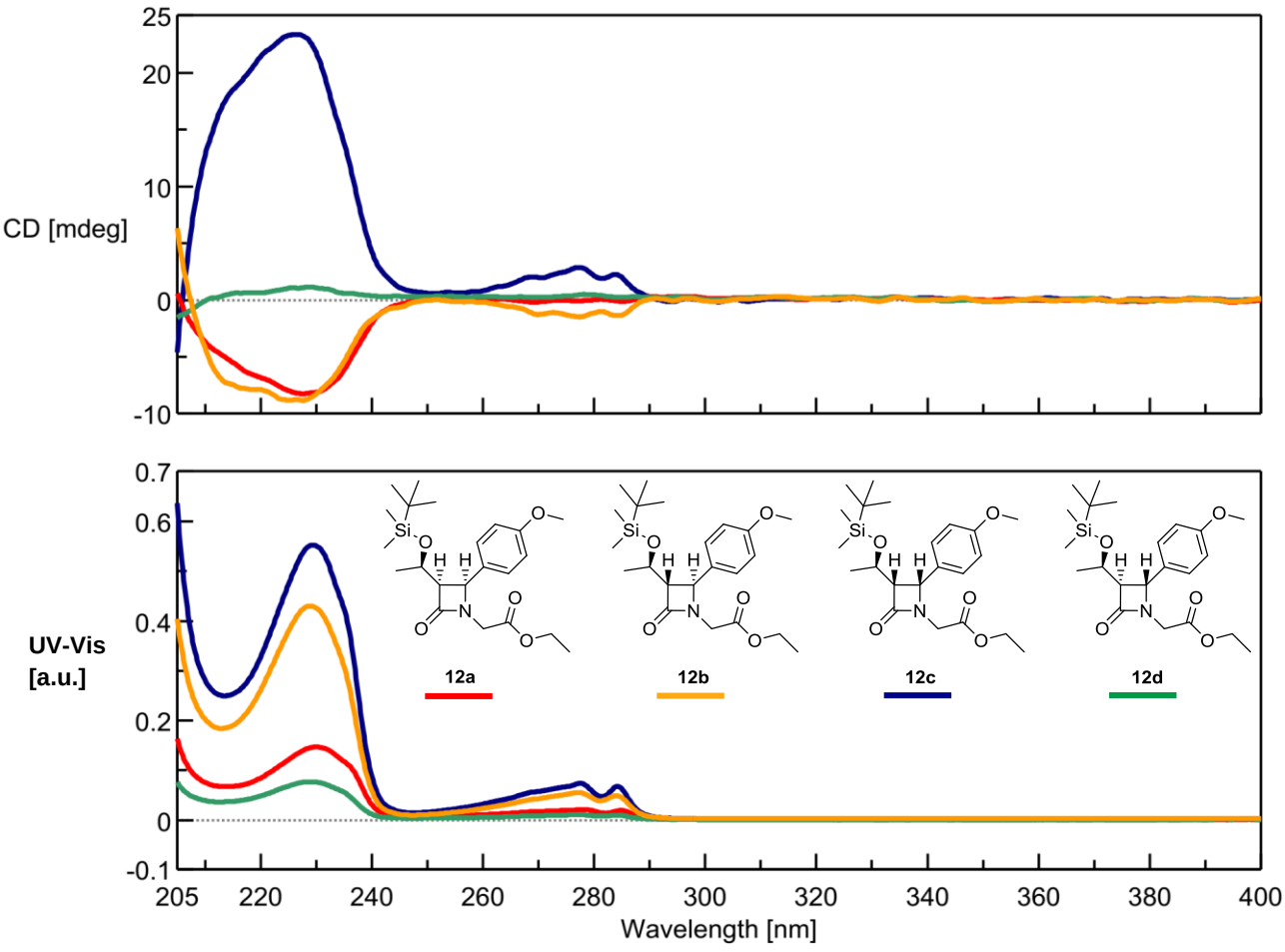




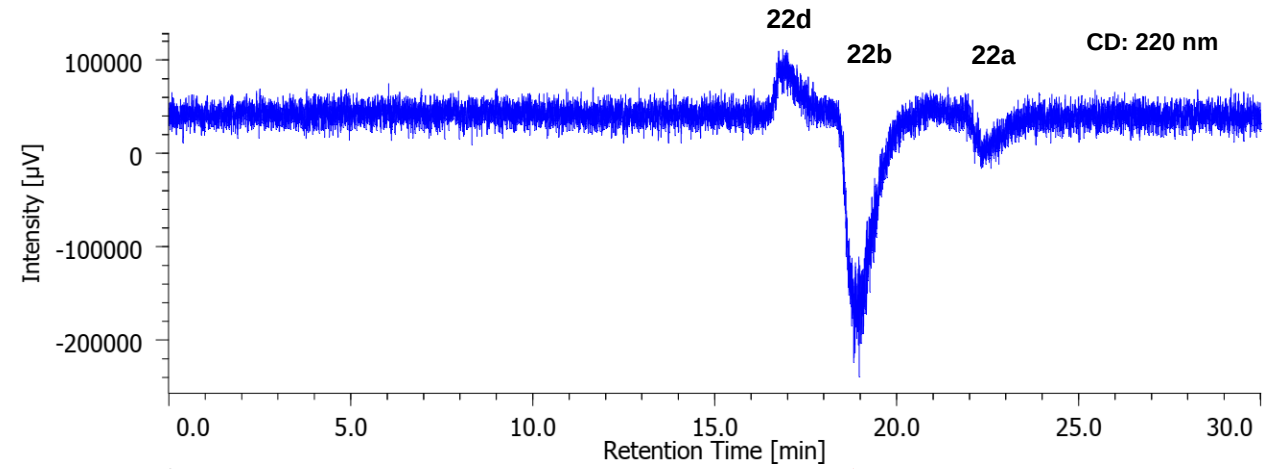
separation conditions: Daicel Chiralpak® AD-H, *i*-PrOH/Hexane 2/98, 1 mL/min

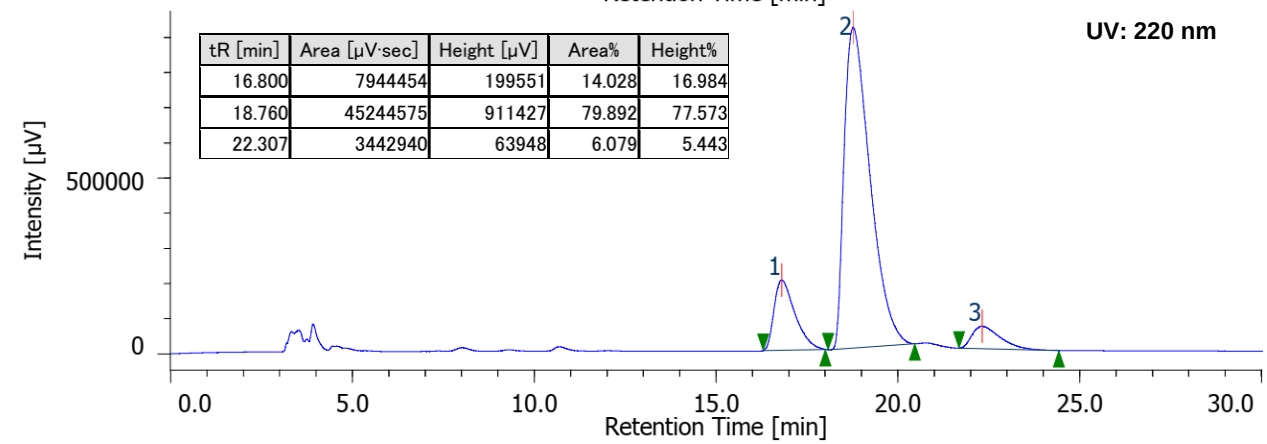




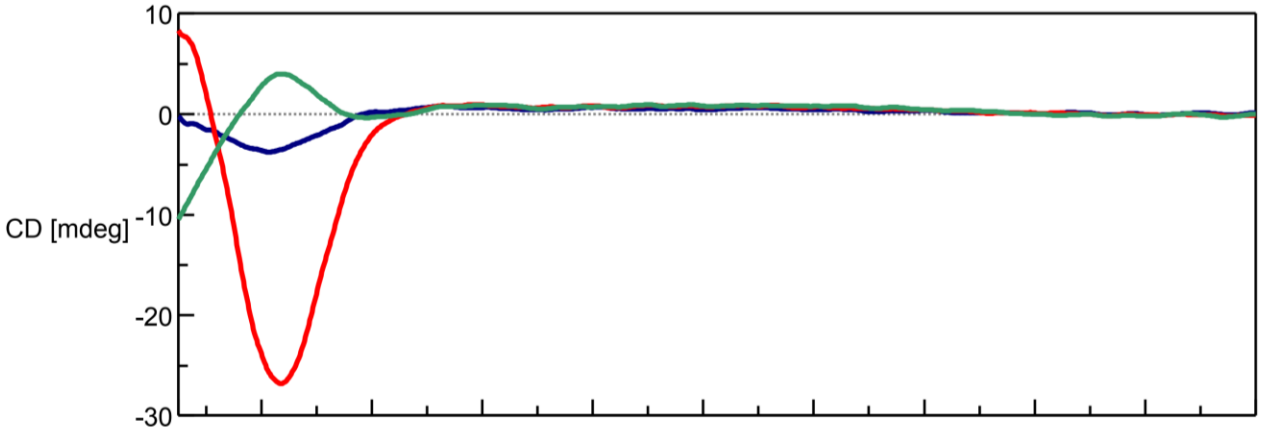


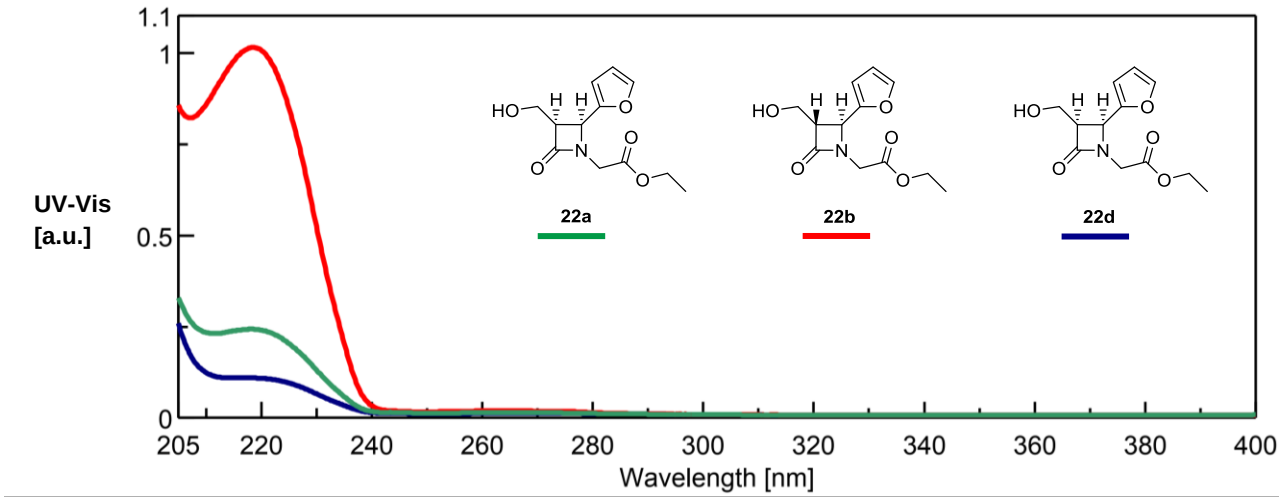
separation conditions: Daicel Chiralcel® OJ-H, *i*-PrOH/Hexane 10/90, 1 mL/min



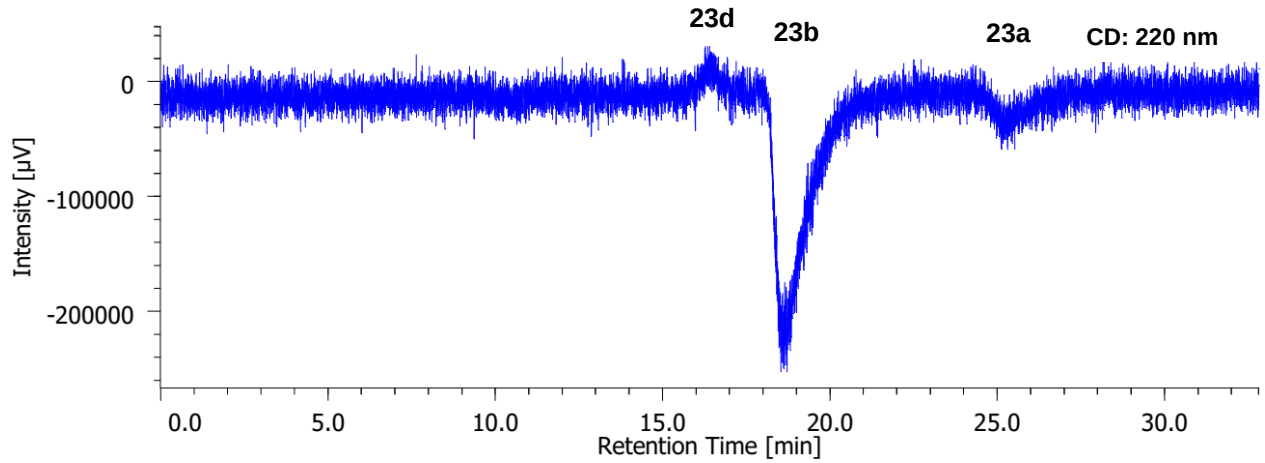


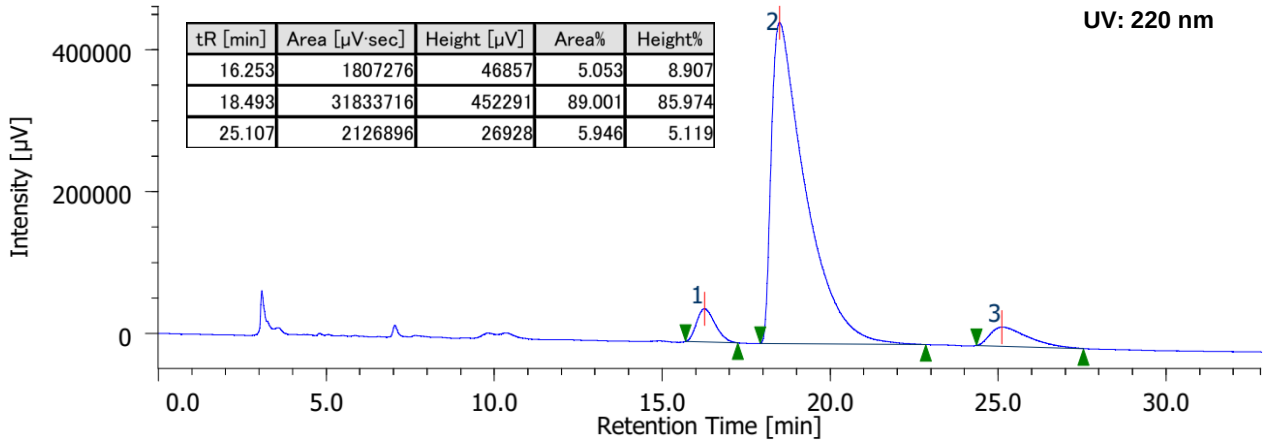
tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
16.800	7944454	199551	14.028	16.984
18.760	45244575	911427	79.892	77.573
22.307	3442940	63948	6.079	5.443





separation conditions: Daicel Chiralcel® OD-H, *i*-PrOH/Hexane 15/85, 1 mL/min





tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%
16.253	1807276	46857	5.053	8.907
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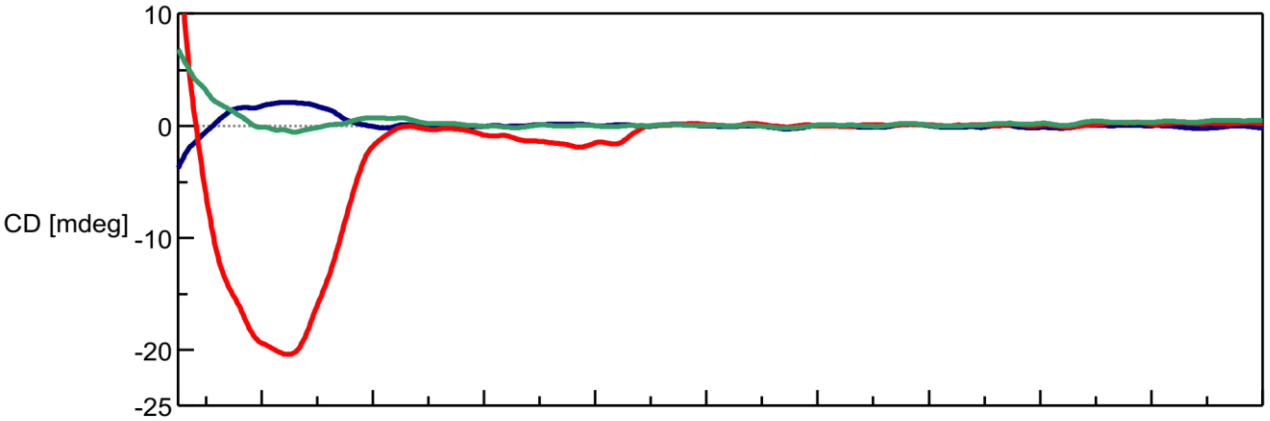
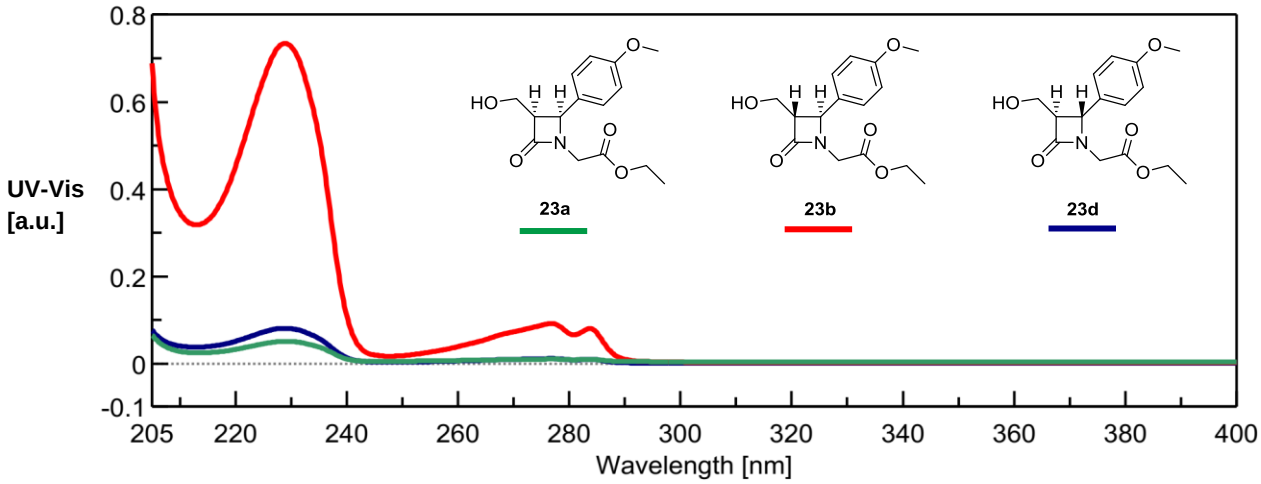
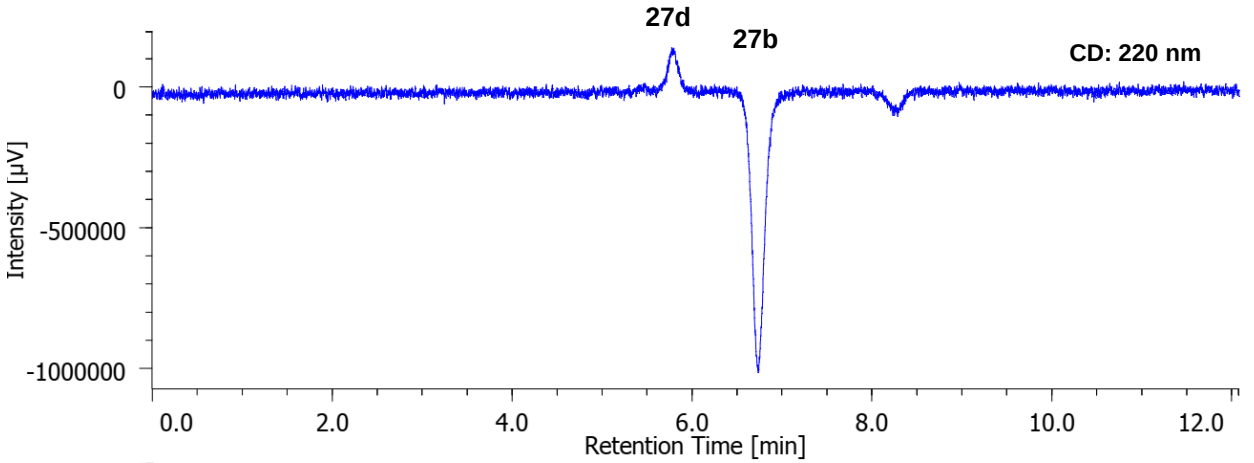
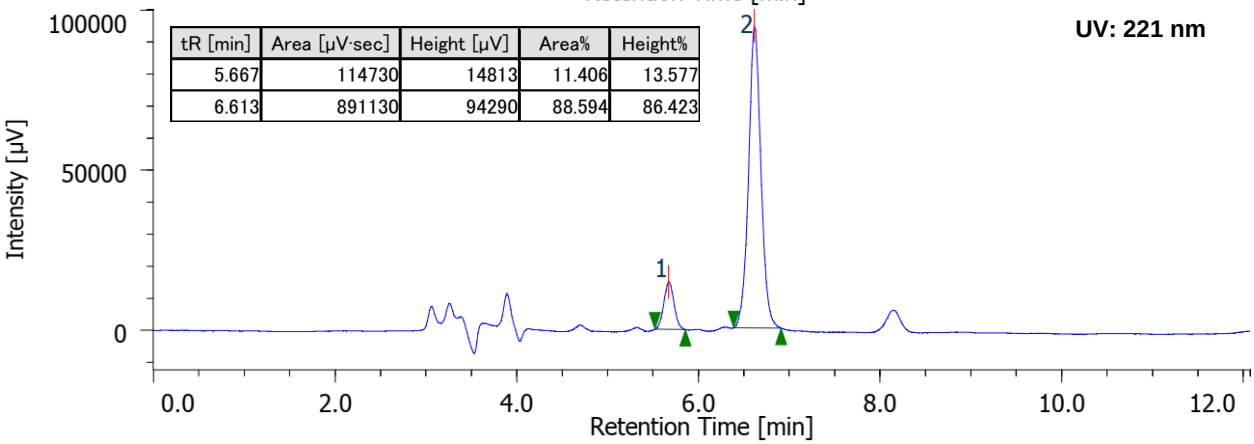
25.107	2126896	26928	5.946	5.119



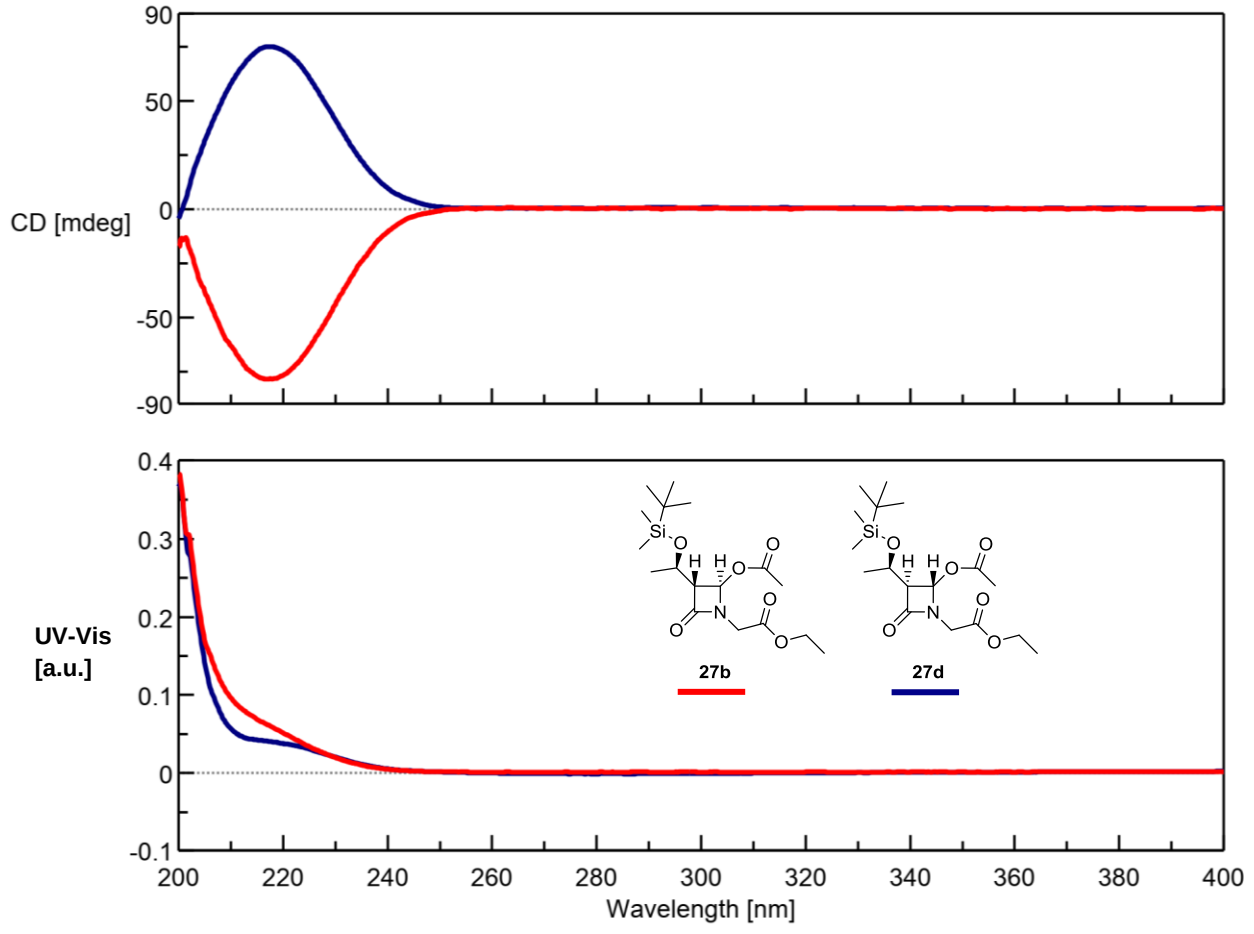


separation conditions: Daicel Chiralpak® IA, *i*-PrOH/Hexane 5/95, 1 mL/min

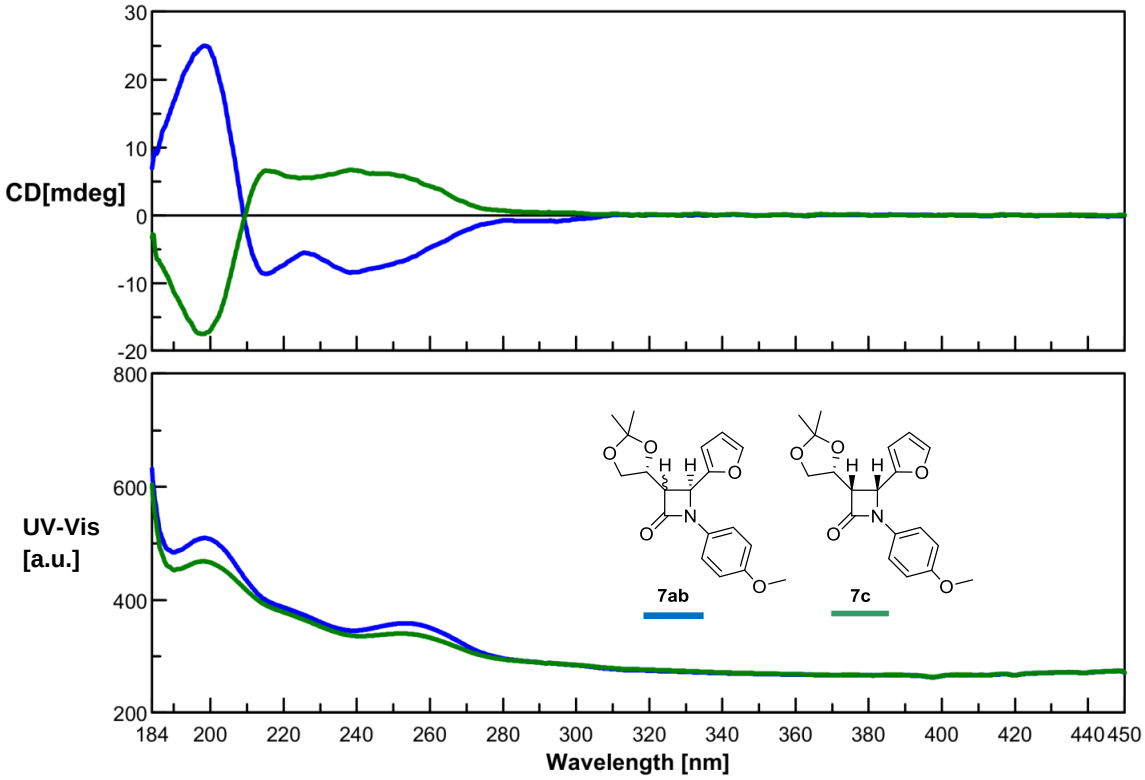


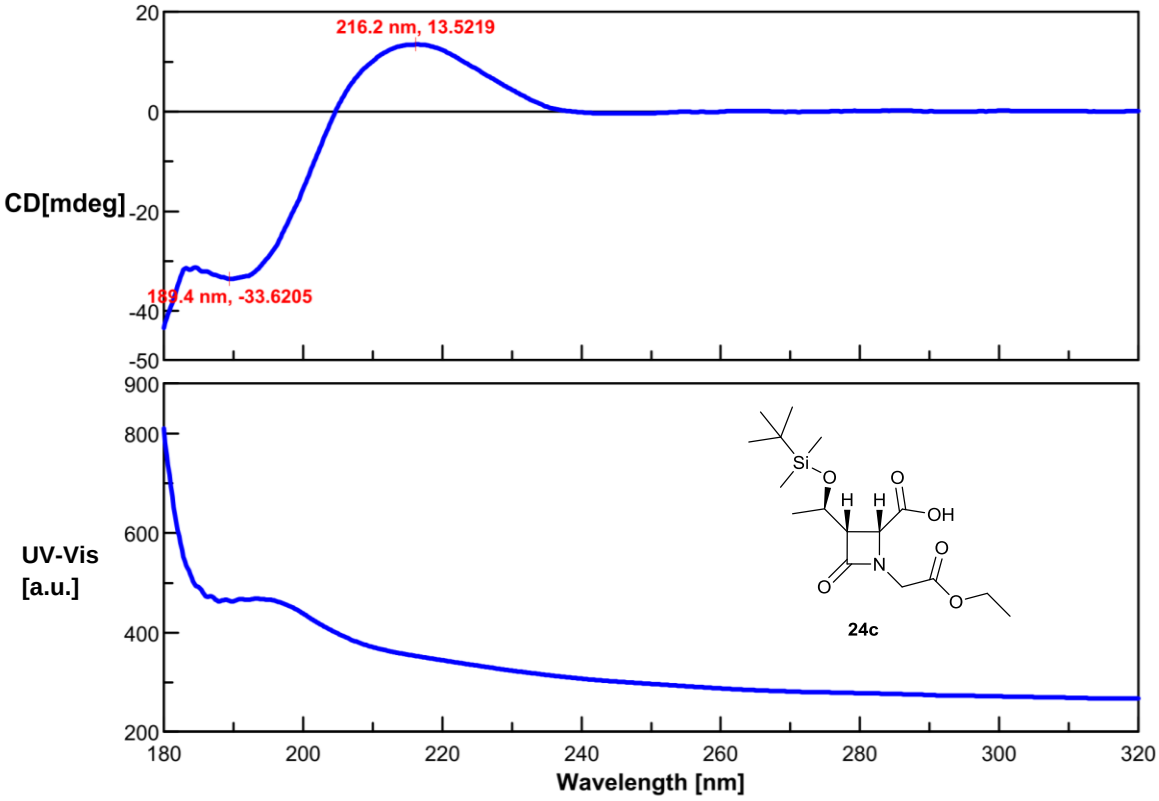


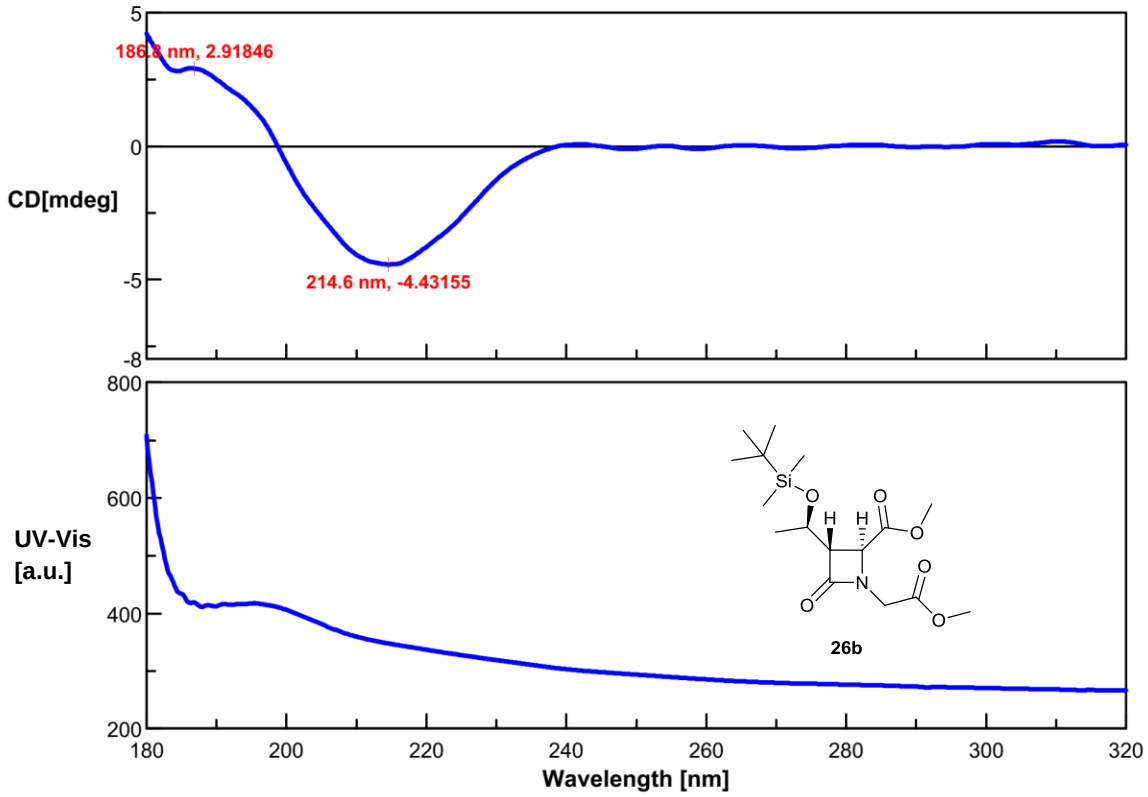
tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%
5.667	114730	14813	11.406	13.577
6.613	891130	94290	88.594	86.423

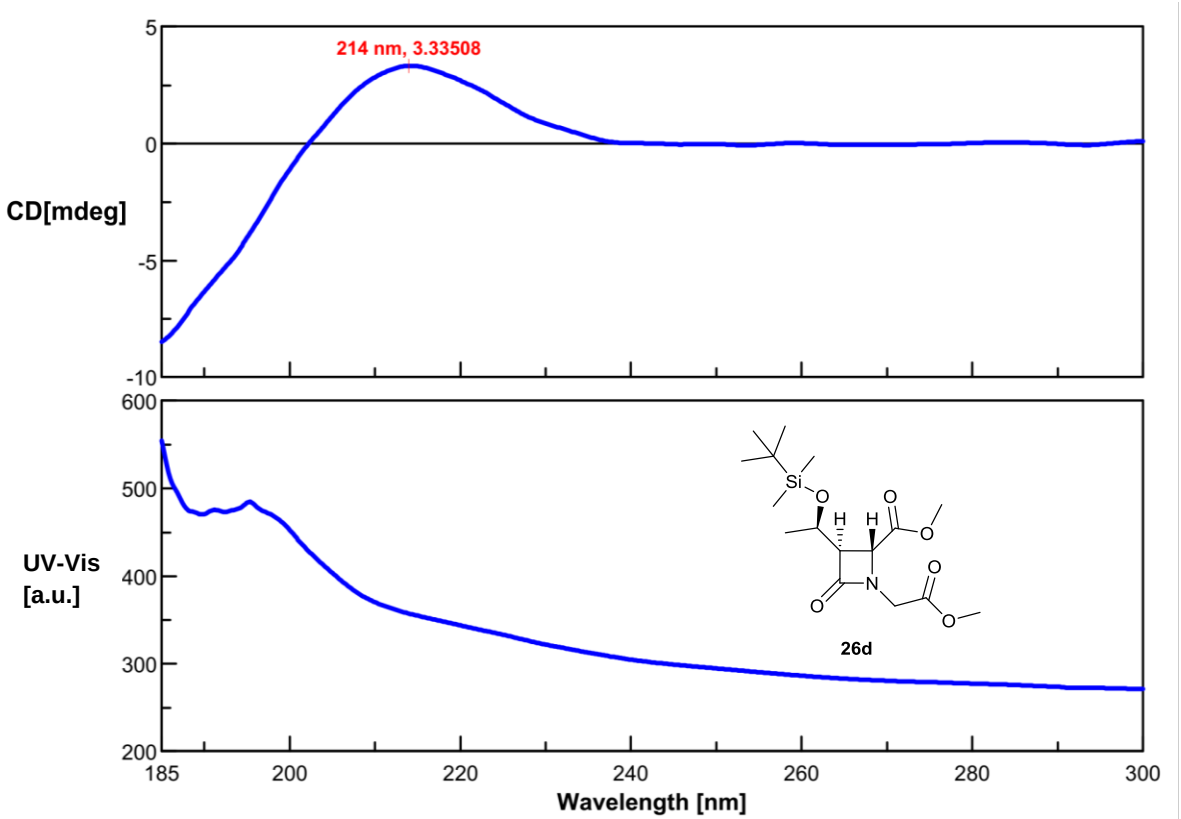


2. Separate ECD analyses





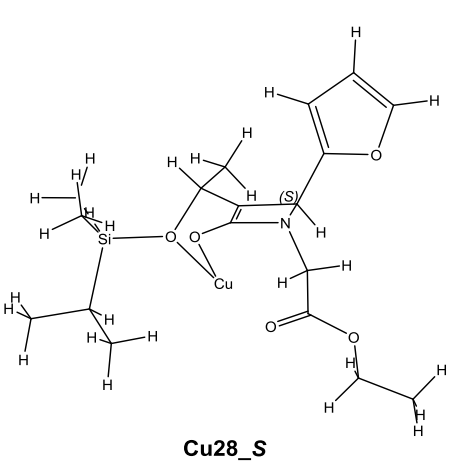

186.8 nm, 2.91846
214.6 nm, -4.43155
CD[mdeg]
UV-Vis
[a.u.]
Wavelength [nm]
26b


214 nm, 3.33508
CD[mdeg]
UV-Vis
[a.u.]
Wavelength [nm]
26d

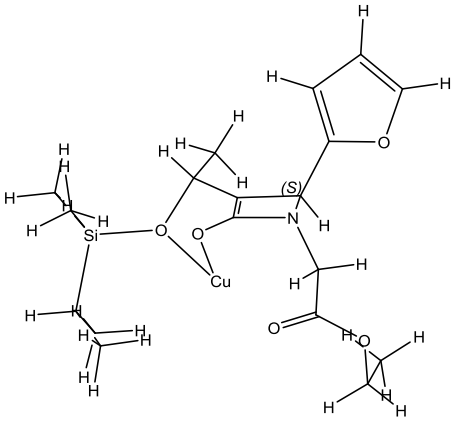
3. Theoretical computations

3.1. Predicting the structure of Cu (I) enolates of 11

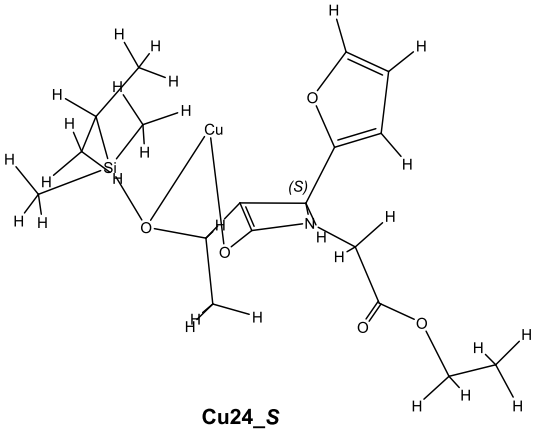
A conformational search was carried out using Spartan'14 (Wave function, Inc. Irvine, CA). Then, the obtained conformers within 3 kcal mol^{-1} were submitted for DFT re-optimization at B3LYP/6-31G(d) level of theory using the Gaussian09 package.[2] Conformers found in the range of 1 kcal mol^{-1} are presented below. Their relative free energies (ΔE) and contributions and are given in Table S1.



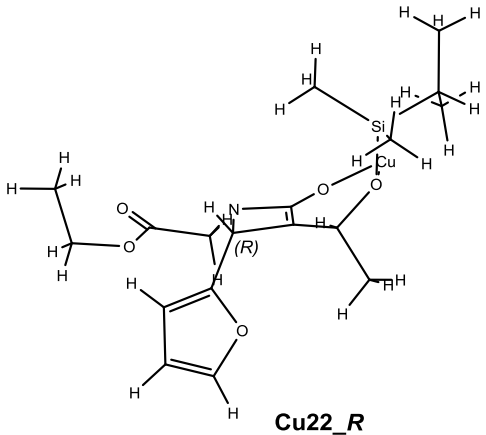
Cu28_*S*



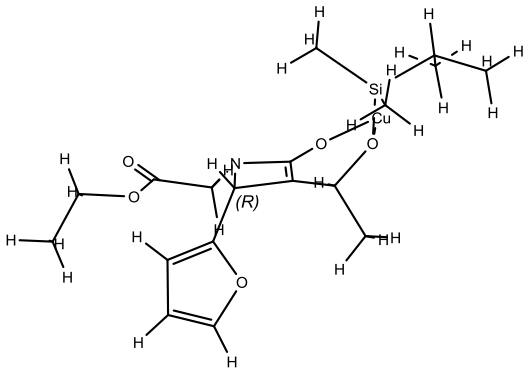
Cu9_*S*



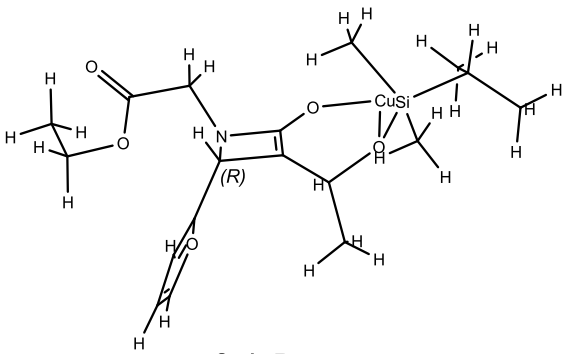
Cu24_*S*



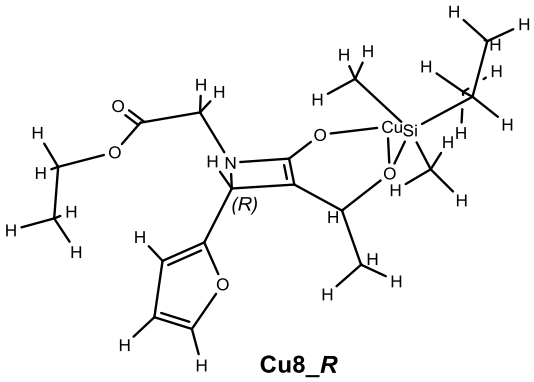
Cu22_*R*



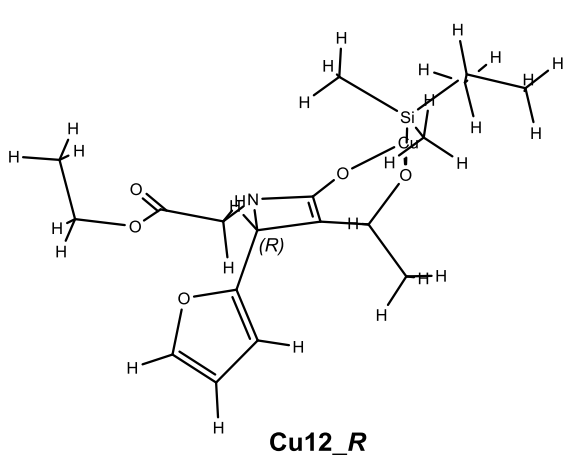
Cu24_*R*



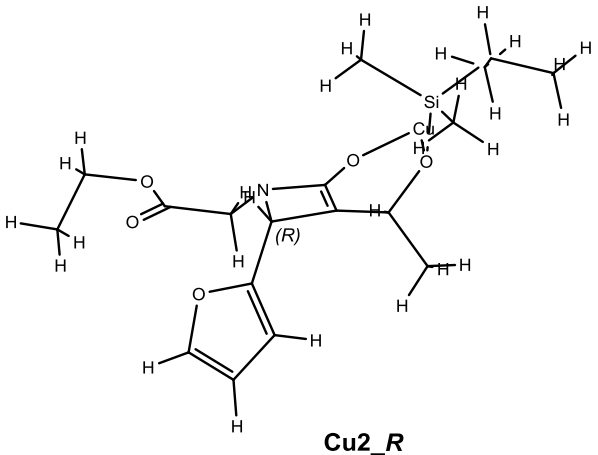
Cu1_*R*



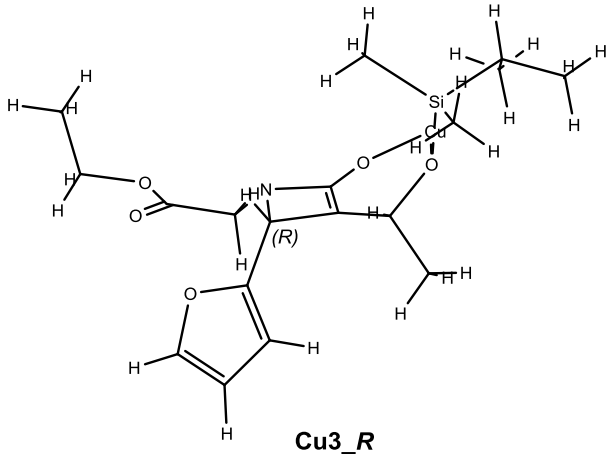
Cu8_*R*



Cu12_*R*



Cu2_*R*



Cu3_*R*

Table S1. Conformers found in the range of 1 kcal mol^{-1} and their relative free energies (Δ*E*) and contributions

C-4 (*S*) Conformers	ΔE/ kcal mol^{-1}	% Contribution	C-4 (*R*) Conformers	ΔE/ kcal mol^{-1}	% Contribution
Cu28_*S*	0	54.2	**Cu22_*R***	0	26.7
Cu9_*S*	0.4	27.3	**Cu24_*R***	0.15	20.6
Cu24_*S*	0.64	18.5	**Cu1_*R***	0.31	15.7
			Cu8_*R*	0.4	13.7
			Cu12_*R*	0.51	11.3
			Cu2_*R*	0.79	7.0
			Cu3_*R*	0.99	5.0

3.2. Conformational search and TDDFT calculations of ECD and UV spectra of selected compounds

In the first step, a conformational search was carried out using the MMFF94s method implemented to Conflex program.[1] Then, the obtained conformers within 5 kcal mol^{-1} were submitted for DFT re-optimization at ωB97X-D/6-311+G(d,p) level of theory using the Gaussian09 package.[2] Finally, the selected group of conformers with population ≥ 3% were used for computations of ECD spectra using CAM-B3LYP/def2-TZVP level. Conformers found and their relative free energies (Δ*E*) are given in Tables S2–S4. Based on comparison experimental and computed UV spectra, ECD spectra were shifted by *ca.* 8-10 nm in relation to the experimental ones. All spectra are presented with a half-width in the range of 0.30-0.35 eV at 1/e of peak height.

Table S2. Calculated at ωB97XD/6-311+G(d,p) level of theory relative energies ΔE (kcal/mol) and conformer distribution (>3%) at 25 °C for compounds **11a**, **11b** and **11c**.

		ΔE / kcal mol^{-1}	Pop. / %
Compound **11a**	**#1**	0	21.40
	#2	0	21.24
	#3	0.06	19.21
	#4	0.30	12.79
	#5	0.62	7.54
	#6	0.64	7.29
	#7	0.79	5.64
	#8	0.88	4.87
Compound **11b**	**#1**	0	25.49
	#2	0.42	12.57
	#3	0.55	10.06
	#4	0.63	8.79
	#5	0.67	8.19
	#6	0.72	7.54
	#7	0.77	6.89
	#8	1.02	4.58
	#9	1.04	4.39
	#10	1.08	4.14
	#11	1.10	3.99
	#12	1.20	3.38
Compound **11c**	**#1**	0	22.58
	#2	0.08	19.87
	#3	0.08	19.81
	#4	0.58	8.40
	#5	0.65	7.59
	#6	0.86	5.25
	#7	0.90	4.97
	#8	0.96	4.44
	#9	1.18	3.06

Table S3. Calculated at ωB97XD/6-311+G(d,p) level of theory relative energies ΔE (kcal/mol) and conformer distribution (>3%) at 25 °C for compound **26b**.

		ΔE / kcal mol^{-1}	Pop. / %
Compound **26b**	#1	0	56.49
	#2	0.76	15.75
	#3	1.06	9.40
	#4	1.21	7.32
	#5	1.37	5.57
	#6	1.56	4.06
	#7	2.25	1.26

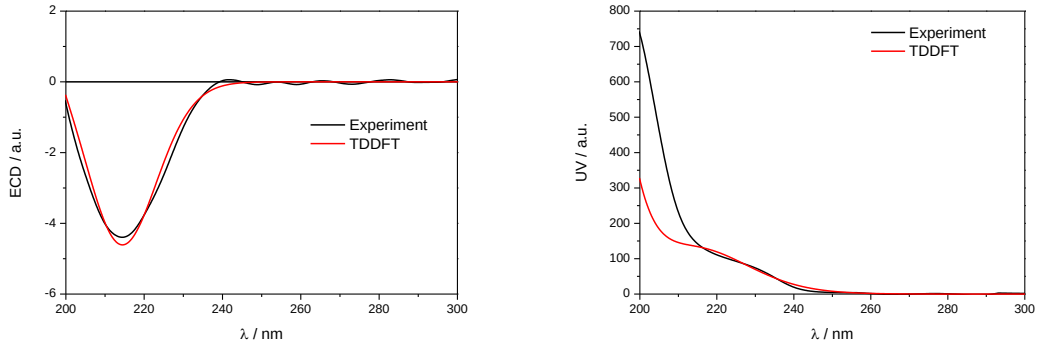


Figure S2. Comparison of experimental (recorded in acetonitrile) and theoretical ECD (left) and UV (right) spectra calculated at CAM-B3LYP/def2-TZVP level of theory for **26b**.

Table S4. Calculated at ωB97XD/6-311+G(d,p) level of theory relative energies ΔE (kcal/mol) and conformer distribution (>3%) at 25 °C for compound **26d**.

		ΔE / kcal mol^{-1}	Pop. / %
Compound **26d**	**#1**	0	41.51
	#2	0.47	18.90
	#3	0.6	14.97
	#4	1.06	6.93
	#5	1.27	4.84
	#6	1.47	3.46
	#7	1.49	3.32
	#8	1.53	3.13
	#9	1.57	2.94

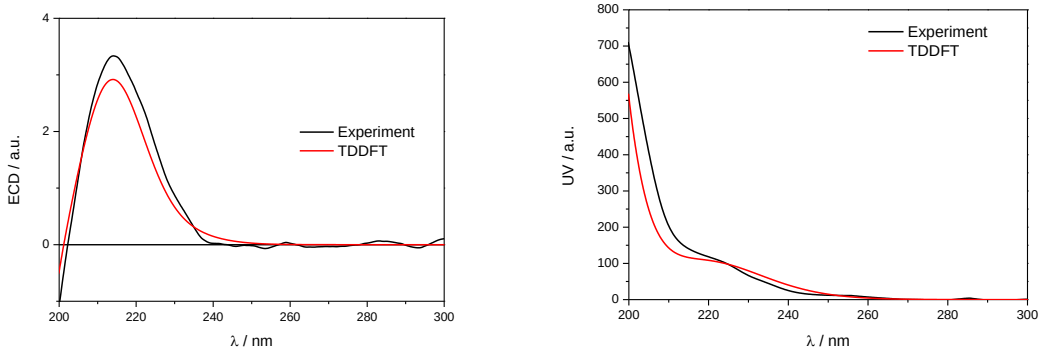


Figure S3. Comparison of experimental (recorded in acetonitrile) and theoretical ECD (left) and UV (right) spectra calculated at CAM-B3LYP/def2-TZVP level of theory for **26d**.

3.3. Cartesian coordinates, number of imaginary frequencies, and total energies of computed conformers

C-4(*S*) conformers of Cu (I) enolate of 11

Conformer Cu28_*S*
No. of imaginary frequencies = 0
Total energy = -3063.4638394

C	-0.326100	1.000900	-0.226400
C	-0.417200	0.421900	-1.529800
N	-1.853900	0.237900	-1.434700
C	-1.836800	0.861400	-0.050200
C	0.805800	1.680600	0.449400
O	1.811700	0.570100	0.695500
Cu	0.501900	-0.899500	0.126600
O	0.316400	0.073600	-2.463300
C	-2.665700	2.092900	0.063100
C	-2.360700	-1.115800	-1.651900
C	-2.701800	-3.762800	0.974400
C	-4.003300	-4.466500	1.305100
C	-2.502100	3.386800	-0.341000
C	-3.695700	4.089000	0.026800
C	-4.500100	3.173300	0.632700
O	-3.891700	1.953400	0.665800
H	-2.192000	0.145200	0.708800
C	0.469200	2.319700	1.786400
H	1.322800	2.400100	-0.200000
Si	3.441700	0.680200	0.178100
C	4.335300	1.973500	1.225300
C	4.138200	-1.055200	0.521900
C	5.665200	-1.124000	0.327400
C	3.427000	-2.139700	-0.306500
C	3.489200	1.125000	-1.650600
C	-1.961200	-2.101100	-0.564900
O	-0.811700	-2.237800	-0.107400
O	-2.981900	-2.813800	-0.089500
H	-3.449500	-1.125200	-1.749400
H	-1.919200	-1.450500	-2.599100
H	-2.299900	-3.212800	1.831200
H	-1.930700	-4.456400	0.626000
H	-3.834600	-5.193600	2.106600
H	-4.392500	-4.999700	0.432200
H	-4.760700	-3.751600	1.641200
H	-1.637700	3.782300	-0.855200
H	-3.919100	5.134400	-0.136400
H	-5.480500	3.221400	1.081900
H	-0.255100	3.128900	1.645400

H	0.028600	1.578500	2.461500
H	1.366700	2.727500	2.261200
H	4.342600	1.697300	2.286300
H	3.857800	2.956900	1.139700
H	5.376600	2.090400	0.900600
H	3.926600	-1.251500	1.585200
H	6.044100	-2.128400	0.558700
H	6.196600	-0.416000	0.973800
H	5.948800	-0.905200	-0.710200
H	3.638100	-2.036100	-1.377600
H	3.728700	-3.149500	0.000500
H	2.335000	-2.069300	-0.186500
H	4.401700	0.741900	-2.124900
H	2.620600	0.704100	-2.171900
H	3.476200	2.210300	-1.807700

Conformer Cu9_*S*
No. of imaginary frequencies = 0
Total energy = -3063.4631943

C	-0.422200	0.959800	-0.271300
C	-0.484900	0.430100	-1.596600
N	-1.885800	0.069800	-1.471600
C	-1.898500	0.630200	-0.060500
C	0.643600	1.733000	0.409600
O	1.769600	0.729100	0.596100
Cu	0.632700	-0.848900	-0.028900
O	0.255100	0.214900	-2.564700
C	-2.864400	1.746600	0.132500
C	-2.236700	-1.322700	-1.739000
C	-2.217100	-4.154100	0.719900
C	-2.375800	-3.595400	2.125000
C	-2.871800	3.065900	-0.219200
C	-4.127000	3.602900	0.215900
C	-4.793400	2.573000	0.805700
O	-4.042300	1.435600	0.766300
H	-2.141300	-0.155400	0.673500
C	0.272500	2.282800	1.776500
H	1.067000	2.525600	-0.221800
Si	3.366000	1.006800	0.044500
C	4.203700	2.290000	1.148200
C	4.215100	-0.686300	0.211400
C	3.627500	-1.717900	-0.768700
C	4.187900	-1.224900	1.654800
C	3.324000	1.581600	-1.747200
C	-1.692000	-2.307900	-0.715500

O	-0.524400	-2.323400	-0.285500
O	-2.608300	-3.173600	-0.280900
H	-3.319400	-1.456800	-1.808300
H	-1.790800	-1.561200	-2.713100
H	-1.190400	-4.468500	0.521100
H	-2.894800	-4.991900	0.542500
H	-3.400500	-3.249500	2.292800
H	-1.689500	-2.760900	2.296200
H	-2.151600	-4.378100	2.858500
H	-2.080200	3.583400	-0.742200
H	-4.479800	4.619100	0.105700
H	-5.755700	2.483900	1.286800
H	-0.536000	3.015200	1.681000
H	-0.072100	1.474800	2.430500
H	1.133000	2.765800	2.249400
H	5.248600	2.435400	0.844700
H	4.199000	1.990200	2.202000
H	3.706800	3.265000	1.076300
H	5.268200	-0.515200	-0.065600
H	2.545900	-1.833700	-0.591800
H	4.085700	-2.707100	-0.639200
H	3.748400	-1.418600	-1.815100
H	3.158700	-1.409200	1.988400
H	4.732000	-2.175900	1.729600
H	4.644000	-0.526400	2.365800
H	3.195100	2.667700	-1.826800
H	4.262600	1.329700	-2.257300
H	2.495000	1.107900	-2.287300

Conformer Cu24_*S*
No. of imaginary frequencies = 0
Total energy = -3063.4628250

C	0.231900	-0.280400	0.101500
C	-0.582000	-0.885100	-1.029400
N	-1.664000	-0.044800	-0.782700
C	-1.084400	0.500000	0.465300
C	0.775400	-1.223900	1.182600
O	2.097100	-1.707200	0.877400
Cu	1.554000	0.788400	-0.719400
O	-0.441900	-1.748900	-1.875900
C	-1.022400	1.984800	0.554800
C	-3.006700	-0.107200	-1.270300
C	-6.233200	-1.560900	-0.125700
C	-6.859400	-0.649100	0.918400
C	-1.678100	2.903400	1.320000

C	-1.205500	4.200200	0.926600
C	-0.294100	3.985700	-0.057300
O	-0.160900	2.643900	-0.298100
H	-1.604400	0.117900	1.351300
C	-0.079900	-2.468800	1.424500
H	0.830800	-0.645200	2.118000
Si	3.539700	-0.880600	0.810300
C	4.834000	-2.171300	1.270600
C	4.041000	-0.255800	-0.947700
C	3.610700	1.162800	-1.385900
C	3.704600	-1.297700	-2.032600
C	3.606200	0.541800	2.057200
C	-3.963300	-0.863800	-0.346100
O	-3.664300	-1.376200	0.710700
O	-5.202900	-0.871800	-0.877900
H	-3.422900	0.893500	-1.448100
H	-2.983800	-0.621000	-2.238300
H	-5.795600	-2.450100	0.334400
H	-6.960800	-1.864200	-0.882300
H	-7.255600	0.260300	0.454700
H	-6.122800	-0.369200	1.676800
H	-7.685400	-1.168500	1.417800
H	-2.416700	2.680600	2.078000
H	-1.507700	5.158700	1.325500
H	0.324600	4.632700	-0.660200
H	-1.117300	-2.199100	1.651300
H	-0.078200	-3.095200	0.527700
H	0.322500	-3.052200	2.259500
H	4.797800	-3.030300	0.591400
H	4.646200	-2.548100	2.282400
H	5.851700	-1.763000	1.245400
H	5.139700	-0.209400	-0.864500
H	4.240900	1.526100	-2.208800
H	3.683500	1.924200	-0.598500
H	2.611700	1.199900	-1.924200
H	2.622000	-1.453000	-2.113800
H	4.080100	-0.988300	-3.017700
H	4.153600	-2.269200	-1.800000
H	3.476300	0.155800	3.075400
H	4.579800	1.047700	2.019900
H	2.832000	1.300700	1.895200

C-4(*R*) Conformers of Cu (I) enolate of 11

Conformer Cu22_*R*
No. of imaginary frequencies = 0
Total energy = -3063.447216

C	-0.125700	0.807200	-0.089800
C	0.221800	-0.390300	-0.657200
N	1.458500	-0.538400	0.042700
C	1.203300	0.833700	0.655000
C	-1.362100	1.627100	-0.091200
O	-2.540300	0.736600	-0.242900
Cu	-2.100400	-1.064500	-1.367200
O	-0.275100	-1.267800	-1.478600
C	2.668000	-0.844600	-0.687200
C	6.085200	-1.904400	0.284100
C	6.050500	-3.309400	0.867600
C	-1.459800	2.642900	-1.231300
H	-1.461900	2.168400	0.862500
Si	-3.532300	0.247000	1.038500
C	-4.333200	1.733300	1.871600
C	-4.830500	-0.802800	0.106500
C	-5.572700	-1.798300	1.015800
C	-4.175900	-1.525800	-1.082600
C	-2.558400	-0.782600	2.275500
C	3.826100	-1.146600	0.249600
O	3.835800	-0.974700	1.448000
O	4.881600	-1.612700	-0.461500
H	2.473300	-1.727100	-1.305700
H	2.994900	-0.046900	-1.377700
H	6.204100	-1.154200	1.070000
H	6.891100	-1.794900	-0.446500
H	5.249900	-3.397000	1.607300
H	7.003200	-3.532600	1.362100
H	5.888400	-4.053500	0.080700
H	-0.604900	3.324700	-1.186300
H	-1.423100	2.123900	-2.195300
H	-2.388100	3.224200	-1.172700
H	-3.593600	2.368900	2.372000
H	-5.053200	1.411800	2.634500
H	-4.869300	2.351200	1.142400
H	-5.568500	-0.097300	-0.302900
H	-6.343200	-2.347000	0.458600
H	-6.072900	-1.290700	1.849100
H	-4.887500	-2.539800	1.444000
H	-4.869300	-2.161800	-1.642500
H	-3.801800	-0.793700	-1.841300
H	-3.380700	-2.232300	-0.742100

H	-1.755200	-0.188800	2.726600
H	-3.199700	-1.144000	3.088600
H	-2.082500	-1.651900	1.807400
C	2.185600	1.908800	0.340900
O	2.169100	2.471300	-0.914000
C	3.157000	3.411000	-0.949000
H	3.262600	3.943300	-1.882400
C	3.805000	3.468600	0.246100
H	4.627200	4.122600	0.502500
C	3.174700	2.490600	1.082700
H	3.431200	2.232900	2.100800
H	1.163600	0.732600	1.746900

Conformer Cu24_*R*
No. of imaginary frequencies = 0
Total energy = -3063.446975

C	-0.125100	0.615200	-0.108900
C	0.179100	-0.659600	-0.508400
N	1.425200	-0.744300	0.185900
C	1.217100	0.705400	0.606800
C	-1.339100	1.461600	-0.206300
O	-2.543700	0.593000	-0.203800
Cu	-2.175700	-1.368000	-1.050200
O	-0.358700	-1.628200	-1.189300
C	2.611600	-1.180700	-0.515000
C	6.043800	-2.122200	0.520300
C	6.909700	-0.871200	0.484600
C	-1.436600	2.302600	-1.480800
H	-1.402900	2.138400	0.659600
Si	-3.533300	0.329400	1.143700
C	-4.219500	1.954600	1.799800
C	-4.890600	-0.787000	0.386000
C	-4.257800	-1.718100	-0.663300
C	-6.074500	-0.012000	-0.219400
C	-2.602900	-0.596200	2.492100
C	3.786000	-1.365100	0.431900
O	3.819800	-1.038100	1.597000
O	4.822400	-1.935500	-0.230000
H	2.386600	-2.140000	-0.993000
H	2.937400	-0.500300	-1.321800
H	6.538700	-2.965400	0.031400
H	5.789200	-2.397200	1.546900
H	7.134600	-0.582900	-0.547500
H	7.856400	-1.056100	1.005700
H	6.400800	-0.039100	0.979400
H	-0.563800	2.959100	-1.551600

H	-1.434700	1.648100	-2.359200
H	-2.348000	2.912800	-1.490700
H	-3.426700	2.587000	2.215700
H	-4.943800	1.773100	2.603800
H	-4.725500	2.524300	1.012900
H	-5.271800	-1.422400	1.199300
H	-4.961500	-2.442300	-1.085600
H	-3.447700	-2.352500	-0.225200
H	-3.907000	-1.129600	-1.547000
H	-6.817200	-0.696400	-0.650300
H	-6.585900	0.596800	0.533900
H	-5.744800	0.660300	-1.021300
H	-3.265200	-0.832700	3.334600
H	-2.173000	-1.536100	2.127200
H	-1.771200	0.002100	2.881100
C	2.221600	1.700100	0.136600
O	2.205500	2.080400	-1.184600
C	3.213900	2.982200	-1.358600
H	3.322400	3.374800	-2.358500
C	3.874600	3.192600	-0.187800
H	4.713200	3.857300	-0.031600
C	3.230700	2.357500	0.782600
H	3.489600	2.241700	1.825900
H	1.193100	0.755700	1.702700

Conformer Cu1_*R*
No. of imaginary frequencies = 0
Total energy = -3063.446719

C	-0.062000	0.503900	0.088600
C	0.362800	-0.706600	-0.398200
N	1.735300	-0.549400	-0.028600
C	1.359200	0.761900	0.600600
C	-1.247400	1.353300	-0.204500
O	-2.435500	0.474000	-0.287800
Cu	-1.961900	-1.529600	-0.930800
O	-0.130500	-1.755100	-0.983400
C	2.359000	-1.589800	0.772800
C	5.917200	-0.944700	-0.153700
C	6.602200	-2.277600	-0.416600
C	-1.190400	2.120800	-1.526900
H	-1.410600	2.078200	0.606600
Si	-3.576900	0.320400	0.956100
C	-4.345900	1.988100	1.365400
C	-4.825800	-0.892600	0.163300
C	-4.069000	-1.895000	-0.725500

C	-5.954000	-0.208600	-0.629300
C	-2.800300	-0.454200	2.484600
C	3.867300	-1.454000	0.933500
O	4.449800	-1.704100	1.968800
O	4.476700	-1.074400	-0.206700
H	1.942700	-1.672300	1.789200
H	2.163700	-2.539800	0.259000
H	6.199700	-0.540000	0.821100
H	6.151000	-0.213700	-0.931600
H	6.373300	-2.990500	0.380500
H	7.689000	-2.137700	-0.451400
H	6.278500	-2.699300	-1.373900
H	-0.325200	2.791400	-1.523500
H	-1.075000	1.420700	-2.361500
H	-2.098300	2.716400	-1.683100
H	-3.612500	2.672000	1.807800
H	-5.159800	1.871600	2.091900
H	-4.758100	2.469900	0.472300
H	-5.278500	-1.462900	0.988200
H	-4.705300	-2.688700	-1.129200
H	-3.279300	-2.449600	-0.155200
H	-3.657300	-1.383400	-1.627800
H	-6.634200	-0.949400	-1.069900
H	-6.553100	0.450200	0.008400
H	-5.554800	0.398700	-1.451300
H	-1.974100	0.159800	2.859900
H	-3.537300	-0.555300	3.291400
H	-2.389200	-1.449200	2.278300
C	2.133500	1.914800	0.052100
O	1.823400	3.144300	0.579900
C	2.597000	4.066300	-0.071400
H	2.468800	5.090700	0.243900
C	3.385100	3.453500	-0.994400
H	4.097900	3.934500	-1.650600
C	3.082700	2.051700	-0.916200
H	3.507900	1.241300	-1.488500
H	1.457800	0.729200	1.696800

Conformer Cu8_*R*
No. of imaginary frequencies = 0
Total energy = -3063.446586

C	0.006700	0.488200	-0.103500
C	0.241000	-0.718400	-0.713500
N	1.609400	-0.833200	-0.318100
C	1.423200	0.454700	0.468000

C	-1.055300	1.512700	-0.288300
O	-2.365900	0.818600	-0.349800
Cu	-2.190500	-1.138400	-1.230900
O	-0.412200	-1.605400	-1.399200
C	2.009500	-2.066300	0.355600
C	5.508200	-1.142400	1.216300
C	6.161400	-0.568500	-0.032000
C	-0.964200	2.333500	-1.576300
H	-1.073900	2.206100	0.565400
Si	-3.428400	0.674100	0.961100
C	-3.995600	2.370300	1.548400
C	-4.862400	-0.300800	0.156500
C	-5.733200	-1.052000	1.179600
C	-4.314700	-1.260900	-0.913000
C	-2.633100	-0.297500	2.362600
C	3.519300	-2.216100	0.458500
O	4.150500	-3.168400	0.054400
O	4.065800	-1.156900	1.095300
H	1.580000	-2.150800	1.372100
H	1.637900	-2.902400	-0.239600
H	5.853700	-2.160000	1.415300
H	5.699200	-0.516100	2.091500
H	5.968400	-1.211400	-0.895400
H	7.246500	-0.504200	0.113200
H	5.777000	0.434000	-0.243300
H	-0.008100	2.863500	-1.607100
H	-1.005700	1.667300	-2.445000
H	-1.782400	3.060700	-1.645700
H	-3.170000	2.952500	1.973600
H	-4.762400	2.277900	2.327700
H	-4.424000	2.948700	0.722100
H	-5.497400	0.435700	-0.357300
H	-6.573100	-1.560100	0.688300
H	-6.157200	-0.372300	1.928400
H	-5.156800	-1.815700	1.715600
H	-5.085800	-1.886100	-1.374900
H	-3.864800	-0.697100	-1.764700
H	-3.601200	-2.002000	-0.472000
H	-3.313200	-0.394200	3.217700
H	-2.338000	-1.305500	2.049400
H	-1.724300	0.204200	2.713000
C	2.391200	1.542000	0.156200
O	2.457400	2.000900	-1.132700
C	3.394100	2.991000	-1.164200
H	3.562700	3.445000	-2.129100
C	3.921800	3.188200	0.074800

H	4.679500	3.910800	0.345500
C	3.266300	2.245200	0.934100
H	3.432000	2.097500	1.992400
H	1.488700	0.256300	1.546700

Conformer Cu12_*R*
No. of imaginary frequencies = 0
Total energy = -3063.446407

C	-0.153700	0.814800	-0.240500
C	0.223400	-0.425400	-0.694000
N	1.470500	-0.468500	-0.006400
C	1.176400	0.944300	0.491100
C	-1.451300	1.535200	-0.194300
O	-2.564500	0.551300	-0.179400
Cu	-2.081100	-1.312900	-1.166200
O	-0.259300	-1.392000	-1.416600
C	2.678800	-0.824800	-0.713000
C	6.103600	-1.815400	0.300100
C	6.084600	-3.222200	0.880100
C	-1.729200	2.455000	-1.384800
H	-1.513800	2.136600	0.725500
Si	-3.447900	0.122900	1.200200
C	-4.238200	1.638400	1.987900
C	-4.742200	-1.070900	0.449600
C	-4.094100	-1.878300	-0.688900
C	-6.025600	-0.376300	-0.039800
C	-2.358600	-0.783200	2.437800
C	3.833300	-1.093600	0.239500
O	3.826000	-0.916700	1.436000
O	4.905200	-1.542200	-0.460300
H	2.474600	-1.735700	-1.285900
H	3.014700	-0.065100	-1.440600
H	6.199400	-1.065400	1.089400
H	6.917300	-1.690800	-0.419300
H	5.276100	-3.324700	1.609300
H	7.034400	-3.430900	1.386700
H	5.945100	-3.967100	0.089600
H	-0.951100	3.223500	-1.440400
H	-1.706200	1.879300	-2.316700
H	-2.705400	2.946500	-1.293000
H	-3.483300	2.315500	2.403800
H	-4.899200	1.345200	2.813200
H	-4.834400	2.203800	1.263600
H	-5.015100	-1.784200	1.241600
H	-4.756400	-2.636600	-1.118400

H	-3.208400	-2.462200	-0.336000
H	-3.848600	-1.210000	-1.551700
H	-6.728500	-1.101400	-0.470800
H	-6.542900	0.138000	0.777100
H	-5.807400	0.368600	-0.815300
H	-1.568300	-0.129000	2.823300
H	-2.946500	-1.133700	3.295600
H	-1.860700	-1.652500	1.993000
C	2.099700	2.022100	0.038900
O	3.061200	2.426600	0.933000
C	3.810000	3.384300	0.320700
H	4.606400	3.807500	0.914300
C	3.360400	3.604600	-0.945400
H	3.762800	4.310800	-1.658700
C	2.247200	2.721000	-1.128200
H	1.627500	2.614300	-2.006700
H	1.150000	0.938000	1.587900

Conformer Cu2_*R*
No. of imaginary frequencies = 0
Total energy = -3063.445954

C	-0.028500	0.650500	-0.312900
C	0.164000	-0.607600	-0.827900
N	1.453100	-0.814700	-0.254400
C	1.363700	0.604300	0.302600
C	-1.221200	1.519500	-0.140100
O	-2.442900	0.678800	-0.104900
Cu	-2.263800	-1.191000	-1.186100
O	-0.481700	-1.487200	-1.533000
C	2.545000	-1.272500	-1.086600
C	4.867800	-1.874000	1.776600
C	5.867500	-0.727500	1.819100
C	-1.450700	2.541300	-1.255500
H	-1.152800	2.064800	0.814100
Si	-3.313500	0.310200	1.299800
C	-3.856400	1.879100	2.185800
C	-4.788100	-0.668900	0.572600
C	-4.306400	-1.505200	-0.626000
C	-5.988300	0.208900	0.175000
C	-2.298500	-0.786300	2.443500
C	3.790500	-1.719900	-0.334600
O	4.759200	-2.188400	-0.896400
O	3.703800	-1.521600	0.994800
H	2.184000	-2.134800	-1.657200
H	2.883000	-0.527800	-1.827800

H	5.316900	-2.777400	1.356500
H	4.469000	-2.093900	2.770300
H	5.384100	0.189100	2.171400
H	6.283200	-0.546100	0.823900
H	6.691800	-0.974300	2.498500
H	-0.584900	3.208500	-1.322100
H	-1.559900	2.027700	-2.217100
H	-2.347600	3.144200	-1.068900
H	-4.407000	2.549500	1.517200
H	-2.999300	2.432900	2.585900
H	-4.509600	1.637700	3.033700
H	-5.117200	-1.373400	1.351100
H	-5.082300	-2.152400	-1.046900
H	-3.489800	-2.214100	-0.340600
H	-4.016300	-0.839100	-1.476700
H	-6.800400	-0.398400	-0.246000
H	-6.394700	0.750900	1.035500
H	-5.708300	0.951300	-0.582800
H	-1.406200	-0.262100	2.804600
H	-2.884100	-1.088000	3.321200
H	-1.950300	-1.696600	1.941900
C	2.364400	1.588800	-0.195800
O	3.438100	1.850300	0.623700
C	4.236600	2.744400	-0.024700
H	5.123200	3.054100	0.507700
C	3.709600	3.061300	-1.238700
H	4.128300	3.745300	-1.964100
C	2.492600	2.313100	-1.349000
H	1.794000	2.309400	-2.173100
H	1.425500	0.562300	1.397800

Conformer Cu3_*R*
No. of imaginary frequencies = 0
Total energy = -3063.445637

C	-0.031300	0.782900	-0.206000
C	0.223600	-0.363600	-0.916400
N	1.523400	-0.596100	-0.375800
C	1.362100	0.708000	0.403500
C	-1.265800	1.552900	0.095100
O	-2.444100	0.657400	-0.010200
Cu	-2.172000	-1.000800	-1.378000
O	-0.378400	-1.148900	-1.758400
C	2.632400	-0.853400	-1.270500
C	5.055600	-1.642500	1.457600
C	5.049200	-3.134900	1.754400

C	-1.548400	2.725400	-0.846000
H	-1.222900	1.942900	1.124000
Si	-3.286400	0.020900	1.313600
C	-3.906700	1.394600	2.440200
C	-4.712000	-0.902900	0.432300
C	-4.193600	-1.508000	-0.884200
C	-5.957700	-0.035500	0.177700
C	-2.209000	-1.192000	2.266800
C	3.901500	-1.357000	-0.599100
O	4.854000	-1.774300	-1.225100
O	3.863800	-1.244800	0.743000
H	2.312600	-1.622800	-1.980200
H	2.929100	0.023700	-1.872400
H	5.029300	-1.050200	2.375700
H	5.931700	-1.361600	0.867700
H	5.092500	-3.710100	0.825300
H	4.145500	-3.418000	2.304000
H	5.921600	-3.398400	2.364100
H	-0.717300	3.437100	-0.800800
H	-1.633100	2.365900	-1.877500
H	-2.474300	3.245600	-0.572100
H	-4.494000	2.134800	1.886100
H	-3.078400	1.920300	2.929000
H	-4.543500	0.985200	3.234400
H	-5.000500	-1.740200	1.085200
H	-4.937600	-2.116500	-1.407900
H	-3.341100	-2.211400	-0.714400
H	-3.941100	-0.698800	-1.614300
H	-6.740000	-0.608100	-0.337600
H	-6.386400	0.339900	1.113000
H	-5.720200	0.832300	-0.450300
H	-1.345900	-0.686800	2.715300
H	-2.774700	-1.666400	3.078800
H	-1.812900	-1.986200	1.623400
C	2.311900	1.809200	0.081400
O	3.365000	1.989700	0.946800
C	4.119800	3.014200	0.460800
H	4.985800	3.279200	1.048600
C	3.585000	3.494600	-0.695000
H	3.972400	4.305600	-1.296300
C	2.408900	2.713700	-0.940400
H	1.716400	2.807000	-1.764400
H	1.427000	0.491200	1.477600

Compound 11a

Conformer #1

No. of imaginary frequencies = 0

Total energy = -1463.0933109

C	-0.036637	0.269461	-1.048794
C	0.415912	-0.853723	-0.104038
N	1.625197	-0.249422	0.103956
C	1.398475	0.863832	-0.818752
O	-0.036234	-1.885409	0.318432
C	1.581141	2.214957	-0.232023
H	2.020607	0.796102	-1.714438
C	-1.270883	1.065990	-0.635089
H	-0.175869	-0.096377	-2.069097
C	2.233576	3.315748	-0.683888
C	2.033323	4.336681	0.299592
C	1.283475	3.769878	1.273375
O	1.002394	2.481307	0.967537
C	2.801778	-0.701175	0.773120
C	3.886377	-1.152996	-0.191731
O	4.957136	-1.575616	0.480886
C	6.072309	-2.036190	-0.306133
O	3.801164	-1.123732	-1.390228
C	7.155457	-2.475111	0.650856
C	-1.487921	2.289819	-1.514496
O	-2.374125	0.195724	-0.751368
Si	-3.493056	-0.117107	0.457582
C	-2.614598	-0.471964	2.072372
C	-4.589659	1.392598	0.666458
C	-4.463244	-1.612642	-0.168632
C	-3.528214	-2.831167	-0.233505
C	-5.631045	-1.912103	0.784968
C	-5.015607	-1.320036	-1.572697
H	-1.143659	1.392930	0.405160
H	2.785275	3.388330	-1.608035
H	2.403364	5.349247	0.283616
H	0.890880	4.129162	2.209904
H	3.213596	0.081095	1.419242
H	2.526310	-1.541783	1.414840
H	6.402597	-1.220054	-0.953129
H	5.732848	-2.854877	-0.944699
H	8.019541	-2.832086	0.085480
H	6.804056	-3.286472	1.291335
H	7.476895	-1.645497	1.283834
H	-2.398886	2.807786	-1.206008
H	-0.649786	2.988270	-1.442694
H	-1.605963	1.982762	-2.557272
H	-3.333651	-0.766314	2.843524

H	-1.888092	-1.277902	1.944102
H	-2.082406	0.409261	2.444427
H	-5.331258	1.241232	1.456840
H	-5.121715	1.630733	-0.258833
H	-3.990632	2.266797	0.942556
H	-4.063856	-3.693519	-0.650958
H	-2.652196	-2.636233	-0.857178
H	-3.163328	-3.115901	0.757780
H	-6.182905	-2.794902	0.438608
H	-6.342347	-1.081010	0.835375
H	-5.285081	-2.124160	1.802231
H	-5.571764	-2.189129	-1.946793
H	-5.702769	-0.467187	-1.571943
H	-4.210161	-1.104207	-2.279475

Conformer #2

No. of imaginary frequencies = 0

Total energy = -1463.0933038

C	0.057652	0.277740	-0.996907
C	0.499522	-0.783521	0.021282
N	1.680759	-0.132707	0.251756
C	1.468435	0.918929	-0.744126
O	0.059848	-1.808135	0.472972
C	1.598939	2.306661	-0.234275
H	2.127742	0.811973	-1.609036
C	-1.209765	1.062827	-0.670664
H	-0.033859	-0.143319	-2.001159
C	2.245985	3.392665	-0.727805
C	1.983519	4.467315	0.180847
C	1.205976	3.944067	1.157363
O	0.965317	2.632741	0.921928
C	2.847238	-0.531516	0.970631
C	3.949749	-1.044656	0.057948
O	5.009611	-1.413252	0.778865
C	6.140673	-1.947896	0.061864
O	3.881317	-1.096042	-1.141237
C	5.950961	-3.418796	-0.248286
C	-1.422477	2.234032	-1.619957
O	-2.287097	0.159839	-0.781059
Si	-3.439775	-0.121985	0.403614
C	-2.610308	-0.377184	2.062565
C	-4.577343	1.368586	0.500834
C	-4.353180	-1.669284	-0.181152
C	-3.386580	-2.864528	-0.164600
C	-5.540531	-1.956718	0.751833
C	-4.871368	-1.454117	-1.611992

H	-1.129439	1.445844	0.354985
H	2.833745	3.421239	-1.631921
H	2.332417	5.485442	0.116351
H	0.767400	4.351030	2.053098
H	3.243984	0.295626	1.568016
H	2.565045	-1.327764	1.663900
H	6.983251	-1.785259	0.733591
H	6.286255	-1.364965	-0.849142
H	6.851730	-3.808951	-0.728978
H	5.109605	-3.567116	-0.926999
H	5.776119	-3.987862	0.667288
H	-2.355564	2.744664	-1.371104
H	-0.603441	2.955560	-1.555463
H	-1.495520	1.870886	-2.648738
H	-3.349589	-0.646828	2.823546
H	-1.864881	-1.173558	1.999753
H	-2.107509	0.532215	2.406633
H	-5.342534	1.237454	1.272115
H	-5.081890	1.548536	-0.452579
H	-4.008501	2.269527	0.753807
H	-3.888999	-3.758920	-0.555095
H	-2.499250	-2.675547	-0.773909
H	-3.041646	-3.093607	0.847989
H	-6.060941	-2.867136	0.429105
H	-6.272735	-1.142411	0.746222
H	-5.219002	-2.116176	1.786544
H	-5.392528	-2.354091	-1.962701
H	-5.581027	-0.621854	-1.668618
H	-4.051440	-1.246722	-2.304543

Conformer #3

No. of imaginary frequencies = 0

Total energy = -1463.0932091

C	0.013977	0.154193	-0.993177
C	0.365039	-0.950511	0.014387
N	1.601093	-0.410335	0.240682
C	1.474742	0.670659	-0.737985
O	-0.163531	-1.933311	0.463705
C	1.723313	2.034175	-0.207199
H	2.120562	0.522969	-1.606929
C	-1.182353	1.040327	-0.657307
H	-0.114384	-0.247538	-2.001317
C	2.460359	3.068356	-0.685574
C	2.293024	4.146802	0.240922
C	1.475338	3.676667	1.211609
O	1.122469	2.394722	0.956259

C	2.724848	-0.900307	0.970984
C	3.816584	-1.449191	0.066794
O	4.837250	-1.897967	0.799126
C	5.971958	-2.433265	0.089039
O	3.771177	-1.467839	-1.134368
C	6.911960	-1.331909	-0.357597
C	-1.293841	2.237205	-1.591793
O	-2.331957	0.233453	-0.780480
Si	-3.509697	0.032373	0.395839
C	-2.712493	-0.306783	2.055456
C	-4.524625	1.608172	0.506323
C	-4.540984	-1.429632	-0.211698
C	-3.673177	-2.698495	-0.205488
C	-5.752634	-1.632251	0.712302
C	-5.032633	-1.156731	-1.642082
H	-1.071663	1.402085	0.373304
H	3.046412	3.060932	-1.591213
H	2.727795	5.132193	0.191370
H	1.074913	4.105339	2.115052
H	3.157733	-0.117381	1.602397
H	2.378843	-1.698015	1.632975
H	5.611520	-3.017138	-0.759345
H	6.447953	-3.098438	0.809015
H	7.793253	-1.773567	-0.829661
H	7.242271	-0.735036	0.495411
H	6.426490	-0.679172	-1.084986
H	-2.181694	2.820691	-1.337715
H	-0.417882	2.887175	-1.517020
H	-1.394505	1.894513	-2.625247
H	-3.475203	-0.525672	2.809581
H	-2.031829	-1.158695	1.986920
H	-2.141611	0.556211	2.412624
H	-5.302691	1.528689	1.271777
H	-5.007235	1.840393	-0.447136
H	-3.887164	2.457294	0.774464
H	-4.243401	-3.545123	-0.609097
H	-2.770299	-2.573927	-0.808478
H	-3.352936	-2.966408	0.805675
H	-6.342599	-2.493936	0.375728
H	-6.417104	-0.761784	0.713743
H	-5.450614	-1.829711	1.746339
H	-5.621931	-2.008052	-2.006145
H	-5.673458	-0.269939	-1.691603
H	-4.195099	-1.007175	-2.328442

Conformer #4

No. of imaginary frequencies = 0

Total energy = -1463.0928257

C	-0.373127	0.102040	0.782710
C	-0.575833	-0.821298	-0.425474
N	-1.729323	-0.170883	-0.787650
C	-1.768730	0.703286	0.383459
O	-0.023925	-1.773307	-0.908283
C	-1.890192	2.144006	0.040875
H	-2.548587	0.426407	1.098954
C	0.854404	1.007573	0.759859
H	-0.401841	-0.454038	1.722709
C	-1.570360	2.866923	-1.061680
C	-1.903772	4.226223	-0.757914
C	-2.400470	4.216548	0.500881
O	-2.404213	2.955702	0.998293
C	-2.782436	-0.589404	-1.662472
C	-3.821083	-1.517047	-1.043667
O	-3.519465	-1.853623	0.209891
C	-4.415947	-2.768678	0.867494
O	-4.793853	-1.895458	-1.638517
C	-3.871998	-3.011688	2.255679
C	0.875091	1.978431	1.931955
O	1.989251	0.174593	0.810602
Si	3.254925	0.201367	-0.290100
C	2.580681	0.185696	-2.037961
C	4.247884	1.771646	-0.024255
C	4.261821	-1.348770	0.097877
C	3.428399	-2.594794	-0.243089
C	5.552918	-1.350987	-0.736587
C	4.621759	-1.370028	1.591936
H	0.838034	1.585336	-0.175535
H	-1.148213	2.475133	-1.973666
H	-1.792182	5.088821	-1.395165
H	-2.784868	4.982589	1.153024
H	-3.310894	0.277671	-2.066589
H	-2.339388	-1.124052	-2.506233
H	-4.465192	-3.687691	0.279319
H	-5.414769	-2.326417	0.886172
H	-4.520880	-3.712461	2.786124
H	-3.831547	-2.082241	2.828017
H	-2.868095	-3.438425	2.209476
H	1.776796	2.593077	1.885117
H	0.004325	2.638419	1.921545
H	0.888332	1.422770	2.873456
H	3.397770	0.122728	-2.763615
H	1.916276	-0.668831	-2.186987

H	2.020325	1.099188	-2.261985
H	5.073762	1.847133	-0.738191
H	4.665933	1.813018	0.985433
H	3.615180	2.654998	-0.160729
H	3.978726	-3.502076	0.037322
H	2.469622	-2.598027	0.281449
H	3.212169	-2.657144	-1.313777
H	6.129144	-2.262597	-0.535178
H	6.196646	-0.497906	-0.498034
H	5.346016	-1.329134	-1.811906
H	5.201638	-2.271885	1.825985
H	5.230780	-0.505890	1.878064
H	3.724879	-1.372747	2.216731

Conformer #5

No. of imaginary frequencies = 0

Total energy = -1463.0923275

C	-0.342022	0.084000	0.756355
C	-0.586494	-0.770264	-0.495521
N	-1.777553	-0.142100	-0.746735
C	-1.766108	0.676410	0.466436
O	-0.029836	-1.668154	-1.069711
C	-1.966318	2.131119	0.253112
H	-2.499904	0.339784	1.204874
C	0.882709	0.994864	0.748041
H	-0.321632	-0.529253	1.660926
C	-2.757361	3.036710	0.882489
C	-2.494165	4.301152	0.265173
C	-1.571124	4.058524	-0.694458
O	-1.241696	2.745743	-0.716228
C	-2.848204	-0.493192	-1.626579
C	-3.903170	-1.422289	-1.039844
O	-3.593994	-1.831983	0.190972
C	-4.507737	-2.755399	0.811306
O	-4.895871	-1.742732	-1.636041
C	-3.956851	-3.084338	2.178998
C	0.897194	1.952109	1.931911
O	2.013440	0.154932	0.802947
Si	3.297670	0.186984	-0.276071
C	2.659995	0.215369	-2.035792
C	4.310014	1.735417	0.043041
C	4.274033	-1.385522	0.103547
C	3.414858	-2.611892	-0.244273
C	5.564816	-1.410105	-0.730850
C	4.633355	-1.423315	1.597378
H	0.876998	1.578434	-0.181788

H	-3.440735	2.827503	1.690594
H	-2.938256	5.254962	0.500536
H	-1.076022	4.681348	-1.420555
H	-3.360526	0.402399	-1.987806
H	-2.424720	-0.998599	-2.498154
H	-4.588099	-3.641676	0.178000
H	-5.494505	-2.289330	0.864221
H	-4.618692	-3.794772	2.679773
H	-3.886083	-2.187460	2.798537
H	-2.964972	-3.533713	2.099991
H	1.805261	2.558549	1.903288
H	0.032332	2.620927	1.917686
H	0.893784	1.386656	2.867863
H	3.491540	0.160260	-2.745583
H	1.989272	-0.628077	-2.215777
H	2.110711	1.137383	-2.251184
H	5.157882	1.806669	-0.645156
H	4.698436	1.755115	1.065128
H	3.696790	2.631463	-0.099511
H	3.949229	-3.532553	0.023360
H	2.460727	-2.601275	0.288623
H	3.188385	-2.659118	-1.313465
H	6.125241	-2.331712	-0.530041
H	6.223455	-0.568528	-0.491801
H	5.357874	-1.383772	-1.805934
H	5.190016	-2.340771	1.827423
H	5.264197	-0.576329	1.887317
H	3.736640	-1.406190	2.222394

Conformer #6

No. of imaginary frequencies = 0

Total energy = -1463.0922957

C	0.105936	0.911623	-1.530031
C	0.286640	-0.605308	-1.697409
N	1.645997	-0.477904	-1.772830
C	1.671566	0.979464	-1.616864
O	-0.424777	-1.572239	-1.761905
C	2.483356	1.512577	-0.492038
H	2.017880	1.486650	-2.523337
C	-0.616106	1.373242	-0.266285
H	-0.381279	1.366189	-2.396376
C	3.496248	2.416166	-0.473985
C	3.898013	2.549442	0.892513
C	3.099341	1.712283	1.594328
O	2.236170	1.075351	0.769649
C	2.696617	-1.448643	-1.860405

C	3.361124	-1.760110	-0.524557
O	2.459715	-1.866210	0.444853
C	2.954135	-2.051945	1.779693
O	4.546816	-1.905955	-0.382625
C	1.791543	-1.838262	2.720650
C	-0.517577	2.879582	-0.066023
O	-1.966797	0.999871	-0.417050
Si	-2.865953	0.128341	0.699601
C	-1.858881	-1.308175	1.353755
C	-3.319506	1.264777	2.123653
C	-4.392125	-0.444813	-0.254914
C	-3.968615	-1.469851	-1.319303
C	-5.396045	-1.094322	0.711235
C	-5.054950	0.759545	-0.942197
H	-0.169426	0.865426	0.597521
H	3.907569	2.923482	-1.332546
H	4.678450	3.176623	1.292002
H	3.023752	1.462038	2.639612
H	2.257198	-2.374466	-2.243960
H	3.475743	-1.121559	-2.551158
H	3.761892	-1.337001	1.954147
H	3.372025	-3.058536	1.862840
H	2.120445	-1.975229	3.753716
H	0.986702	-2.546566	2.514951
H	1.394377	-0.827028	2.608605
H	-1.072518	3.169941	0.828923
H	0.520423	3.203327	0.049257
H	-0.957556	3.397703	-0.922509
H	-2.484790	-1.964064	1.967482
H	-1.440739	-1.892879	0.530696
H	-1.032728	-0.965741	1.983727
H	-3.894385	0.734544	2.889152
H	-3.913316	2.117051	1.781533
H	-2.417249	1.656952	2.604632
H	-4.837310	-1.766661	-1.920997
H	-3.206323	-1.066803	-1.990677
H	-3.553677	-2.375529	-0.866946
H	-6.271208	-1.455706	0.156974
H	-5.755830	-0.386580	1.465299
H	-4.964764	-1.955330	1.233124
H	-5.939133	0.432215	-1.503963
H	-5.386745	1.511748	-0.218474
H	-4.369413	1.244157	-1.642131

Conformer #7

No. of imaginary frequencies = 0

Total energy = -1463.0920538

C	0.293815	0.205367	-0.846179
C	0.622446	-0.718994	0.334834
N	1.794421	-0.056573	0.585145
C	1.701514	0.840923	-0.566775
O	0.126341	-1.676641	0.866827
C	1.846501	2.285398	-0.259376
H	2.420609	0.589803	-1.352110
C	-0.967318	1.057345	-0.729444
H	0.263597	-0.345015	-1.789982
C	2.572660	3.267363	-0.851286
C	2.278745	4.473150	-0.137924
C	1.404707	4.123233	0.834439
O	1.133765	2.798225	0.775843
C	2.905690	-0.407116	1.412500
C	3.979746	-1.261761	0.752451
O	3.671621	-1.591458	-0.503236
C	4.586368	-2.467654	-1.192529
O	4.986601	-1.588567	1.321616
C	4.320981	-3.917085	-0.840567
C	-1.068675	2.092911	-1.840875
O	-2.062458	0.172814	-0.802862
Si	-3.304855	0.073535	0.320052
C	-2.602757	0.014161	2.054402
C	-4.395242	1.591493	0.143188
C	-4.224737	-1.513810	-0.131557
C	-3.300097	-2.719196	0.103633
C	-5.481681	-1.653375	0.742244
C	-4.636629	-1.469769	-1.611585
H	-0.950329	1.574702	0.238625
H	3.232930	3.145480	-1.695674
H	2.671608	5.460227	-0.321499
H	0.911276	4.671450	1.619440
H	3.392382	0.490325	1.803800
H	2.531408	-0.972162	2.269783
H	5.608061	-2.176163	-0.943463
H	4.400140	-2.271512	-2.248434
H	4.972379	-4.562094	-1.435746
H	3.283262	-4.182359	-1.052896
H	4.527343	-4.103206	0.214549
H	-1.999720	2.654542	-1.736268
H	-0.232704	2.797028	-1.810038
H	-1.077994	1.594793	-2.814287
H	-3.403470	-0.127703	2.787235
H	-1.888505	-0.806753	2.152589
H	-2.087718	0.944664	2.313436

H	-5.219440	1.576879	0.862949
H	-4.821589	1.662292	-0.861365
H	-3.816973	2.503217	0.326564
H	-3.802622	-3.644023	-0.207755
H	-2.367304	-2.628973	-0.458661
H	-3.033078	-2.826362	1.159058
H	-6.007883	-2.584794	0.498673
H	-6.185103	-0.829371	0.582862
H	-5.236839	-1.688339	1.809096
H	-5.160459	-2.394903	-1.884060
H	-5.314351	-0.635685	-1.822368
H	-3.765084	-1.369971	-2.263867

Conformer #8

No. of imaginary frequencies = 0

Total energy = -1463.0919155

C	-0.241662	0.045581	0.802947
C	-0.470458	-0.899394	-0.385787
N	-1.682355	-0.326999	-0.663561
C	-1.679213	0.586926	0.478229
O	0.111983	-1.812150	-0.908718
C	-1.906532	2.015825	0.147922
H	-2.403900	0.300240	1.246111
C	0.963395	0.979024	0.723749
H	-0.205187	-0.500713	1.748931
C	-2.710289	2.956261	0.705876
C	-2.475516	4.169116	-0.017359
C	-1.554855	3.863999	-0.961302
O	-1.200596	2.560095	-0.875909
C	-2.731924	-0.725437	-1.547328
C	-3.856651	-1.533939	-0.915629
O	-3.588914	-1.886838	0.343152
C	-4.588778	-2.664602	1.030532
O	-4.862541	-1.817788	-1.509178
C	-5.656002	-1.773131	1.632635
C	0.963296	2.016410	1.838171
O	2.111961	0.168712	0.829451
Si	3.393741	0.160967	-0.252939
C	2.752748	0.061860	-2.008971
C	4.369903	1.750056	-0.037309
C	4.407103	-1.360914	0.223218
C	3.577954	-2.626602	-0.048271
C	5.699291	-1.406145	-0.608190
C	4.765231	-1.297846	1.716493
H	0.941110	1.496237	-0.244307
H	-3.384223	2.802840	1.534179

H	-2.935990	5.130982	0.141202
H	-1.076732	4.432701	-1.741180
H	-3.186632	0.143783	-2.030208
H	-2.293723	-1.343315	-2.335637
H	-4.030724	-3.199261	1.798773
H	-5.018903	-3.382180	0.330422
H	-6.362539	-2.381888	2.202417
H	-6.209175	-1.249636	0.851168
H	-5.212350	-1.040287	2.310893
H	1.858579	2.637603	1.762181
H	0.084968	2.665128	1.782432
H	0.975634	1.517543	2.811166
H	3.583888	-0.023362	-2.716254
H	2.098397	-0.804543	-2.130893
H	2.185050	0.956877	-2.282602
H	5.215373	1.795995	-0.730593
H	4.758502	1.845372	0.980450
H	3.735896	2.620449	-0.236613
H	4.133549	-3.515903	0.276130
H	2.622717	-2.605893	0.482284
H	3.354978	-2.745288	-1.112664
H	6.280366	-2.300837	-0.351997
H	6.338154	-0.536779	-0.420450
H	5.493413	-1.449629	-1.682947
H	5.343786	-2.185565	2.002394
H	5.374896	-0.419495	1.953752
H	3.867541	-1.264258	2.339407

Compound 11b

Conformer #1
No. of imaginary frequencies = 0
Total energy = -1463.0985297

C	0.708754	0.430158	1.600404
C	2.199296	0.121705	1.791123
N	2.530663	0.771621	0.625576
C	1.143734	1.014982	0.222389
O	2.869418	-0.493512	2.576168
C	0.832462	2.431089	-0.089151
H	0.824396	0.371831	-0.601728
C	-0.214797	-0.775495	1.537484
H	0.315731	1.181359	2.288741
C	1.413080	3.609907	0.245581
C	0.594810	4.633838	-0.334149
C	-0.411760	3.992356	-0.971588
O	-0.277147	2.650426	-0.836269

C	3.685838	0.595112	-0.202662
C	3.692270	-0.672736	-1.050865
O	2.672020	-1.484891	-0.765759
C	2.643567	-2.750510	-1.451970
O	4.540306	-0.905837	-1.868804
C	1.535689	-3.575161	-0.839386
C	-0.398182	-1.426140	2.897745
O	-1.458177	-0.324558	1.034890
Si	-2.288618	-0.981107	-0.260106
C	-1.326671	-0.719608	-1.850728
C	-2.521383	-2.821274	0.025140
C	-3.930806	-0.046313	-0.287310
C	-3.668371	1.447670	-0.539691
C	-4.828695	-0.604799	-1.403137
C	-4.636216	-0.212848	1.068181
H	0.235584	-1.506706	0.848503
H	2.309282	3.730292	0.833296
H	0.741731	5.700730	-0.280157
H	-1.261623	4.325778	-1.543050
H	3.805013	1.446902	-0.875952
H	4.573775	0.554730	0.433224
H	3.618348	-3.228889	-1.338178
H	2.480512	-2.565821	-2.516632
H	1.505031	-4.558113	-1.314971
H	0.563169	-3.100050	-0.984806
H	1.702637	-3.713604	0.230988
H	-1.042117	-2.304449	2.809953
H	0.567124	-1.728994	3.310882
H	-0.870663	-0.720405	3.585994
H	-1.873809	-1.128316	-2.706086
H	-1.154604	0.344965	-2.030187
H	-0.352131	-1.217301	-1.822003
H	-3.003574	-3.297996	-0.833607
H	-3.135544	-3.012108	0.909347
H	-1.558566	-3.319488	0.178287
H	-4.614125	2.003546	-0.514418
H	-3.004110	1.871230	0.218337
H	-3.209664	1.619146	-1.518501
H	-5.783936	-0.066031	-1.424851
H	-5.055613	-1.665366	-1.252232
H	-4.369853	-0.493868	-2.391260
H	-5.584714	0.338677	1.070040
H	-4.868185	-1.261600	1.280591
H	-4.020571	0.169444	1.886614

Conformer #2

No. of imaginary frequencies = 0

Total energy = -1463.0978631

C	0.041634	-0.098402	1.905266
C	1.501864	-0.276538	2.339135
N	1.941091	0.587999	1.366723
C	0.621810	0.708533	0.715099
O	2.097191	-0.926491	3.156876
C	0.113239	2.077242	0.459062
H	0.587239	0.136292	-0.214361
C	-0.741935	-1.345176	1.527705
H	-0.543190	0.510879	2.598514
C	-0.391607	3.062975	1.242904
C	-0.732374	4.141033	0.367108
C	-0.407142	3.725086	-0.879837
O	0.111354	2.476736	-0.841483
C	3.242351	0.693823	0.785873
C	3.490979	-0.379567	-0.266496
O	4.682295	-0.205981	-0.836433
C	5.064933	-1.167110	-1.839632
O	2.721713	-1.260454	-0.546142
C	6.409997	-0.746003	-2.382937
C	-1.104065	-2.180087	2.743684
O	-1.910808	-0.899824	0.869689
Si	-2.460972	-1.294273	-0.659382
C	-1.083310	-1.146174	-1.925016
C	-3.103808	-3.055202	-0.652061
C	-3.831125	-0.029437	-0.980656
C	-3.246998	1.389294	-0.881113
C	-4.421009	-0.242173	-2.383793
C	-4.939270	-0.194127	0.071555
H	-0.120103	-1.947250	0.848319
H	-0.515966	3.023524	2.313547
H	-1.169406	5.090748	0.631202
H	-0.484788	4.177196	-1.854355
H	3.385060	1.678504	0.333071
H	3.992422	0.584156	1.573129
H	4.296119	-1.186341	-2.615180
H	5.101200	-2.155370	-1.375432
H	6.736907	-1.460702	-3.141895
H	7.160136	-0.719240	-1.590192
H	6.352225	0.242516	-2.842944
H	-1.646479	-3.077091	2.436269
H	-0.201384	-2.474896	3.284729
H	-1.745720	-1.601313	3.413418
H	-1.416184	-1.547930	-2.887429
H	-0.788344	-0.104687	-2.081017

H	-0.191559	-1.708275	-1.629900
H	-3.540458	-3.325291	-1.618539
H	-3.868437	-3.192203	0.117345
H	-2.293231	-3.762321	-0.448407
H	-4.037686	2.134892	-1.033086
H	-2.795400	1.571685	0.098022
H	-2.478755	1.568939	-1.639757
H	-5.209611	0.495474	-2.578027
H	-4.869533	-1.235228	-2.493993
H	-3.664171	-0.124402	-3.166477
H	-5.722240	0.559376	-0.082267
H	-5.415064	-1.178243	0.010361
H	-4.546584	-0.069398	1.084464

Conformer #3

No. of imaginary frequencies = 0

Total energy = -1463.0976523

C	0.478149	0.230986	1.909685
C	1.962293	-0.023206	2.209624
N	2.344967	0.612956	1.059360
C	0.972818	0.780988	0.547343
O	2.593876	-0.585098	3.065500
C	0.560098	2.140145	0.124652
H	0.772124	0.083258	-0.268115
C	-0.438423	-0.978549	1.835895
H	0.036512	0.995990	2.552648
C	0.221135	3.278024	0.780880
C	-0.106879	4.241295	-0.224110
C	0.058867	3.612453	-1.411721
O	0.467562	2.337868	-1.218425
C	3.601235	0.612627	0.375451
C	3.787284	-0.473721	-0.676460
O	2.765671	-1.332370	-0.717755
C	2.829652	-2.379381	-1.706842
O	4.759129	-0.530483	-1.380821
C	2.393842	-1.877330	-3.068646
C	-0.731756	-1.556116	3.209402
O	-1.630626	-0.548802	1.209323
Si	-2.359873	-1.191281	-0.150410
C	-1.088025	-1.461825	-1.507598
C	-3.145148	-2.836621	0.282636
C	-3.628979	0.112053	-0.662085
C	-2.919128	1.456419	-0.894537
C	-4.324996	-0.329418	-1.960028
C	-4.677929	0.281528	0.448655
H	0.060959	-1.746483	1.224726

H	0.199440	3.415080	1.850482
H	-0.428359	5.260104	-0.078009
H	-0.070100	3.918352	-2.436419
H	3.771428	1.572609	-0.119273
H	4.394022	0.484226	1.116834
H	2.152754	-3.144822	-1.326379
H	3.844784	-2.778633	-1.732882
H	2.372517	-2.711243	-3.774878
H	3.091439	-1.128084	-3.445571
H	1.392665	-1.444314	-3.017898
H	-1.363416	-2.442930	3.119923
H	0.199547	-1.828000	3.712653
H	-1.260090	-0.817644	3.818127
H	-1.533573	-2.014431	-2.340536
H	-0.710714	-0.512522	-1.898442
H	-0.233344	-2.044495	-1.149732
H	-3.650189	-3.279779	-0.581058
H	-3.877823	-2.725655	1.086408
H	-2.385189	-3.549026	0.619786
H	-3.650603	2.221648	-1.182636
H	-2.406129	1.803060	0.006979
H	-2.176710	1.396857	-1.696794
H	-5.070480	0.416586	-2.261377
H	-4.848779	-1.283891	-1.841090
H	-3.615218	-0.433659	-2.787357
H	-5.404644	1.053408	0.166404
H	-5.234759	-0.644107	0.626433
H	-4.214173	0.584742	1.391489

Conformer #4

No. of imaginary frequencies = 0

Total energy = -1463.097525

C	0.616894	0.252885	1.653884
C	2.105363	-0.018289	1.916147
N	2.483537	0.743529	0.838209
C	1.105347	0.922155	0.346905
O	2.745182	-0.673172	2.695033
C	0.665389	2.308808	0.066361
H	0.921127	0.285248	-0.522991
C	-0.298229	-0.949638	1.496698
H	0.187625	0.958682	2.369008
C	-0.353728	3.072159	0.529208
C	-0.302072	4.299468	-0.208532
C	0.743262	4.180518	-1.058764
O	1.339548	2.971870	-0.910179
C	3.707032	0.680203	0.093863

C	3.829347	-0.503088	-0.860030
O	2.802223	-1.350641	-0.755707
C	2.854653	-2.538093	-1.565502
O	4.756589	-0.649403	-1.609065
C	1.632295	-3.361189	-1.231027
C	-0.497208	-1.689005	2.807611
O	-1.541650	-0.470153	1.016402
Si	-2.300910	-0.911760	-0.407074
C	-1.328678	-0.304854	-1.893935
C	-2.436716	-2.781114	-0.480320
C	-3.990417	-0.067085	-0.313317
C	-3.795206	1.442904	-0.099996
C	-4.765745	-0.303159	-1.619504
C	-4.791655	-0.643561	0.864867
H	0.157780	-1.633682	0.764873
H	-1.064599	2.787568	1.287971
H	-0.955980	5.151503	-0.112876
H	1.177909	4.835044	-1.795562
H	3.847391	1.593612	-0.486856
H	4.539439	0.607838	0.798147
H	3.781181	-3.071166	-1.341609
H	2.880421	-2.245751	-2.618049
H	1.644529	-4.291630	-1.803252
H	0.715925	-2.821103	-1.481127
H	1.613327	-3.610193	-0.167572
H	-1.136988	-2.560778	2.652381
H	0.463884	-2.014757	3.212864
H	-0.981110	-1.031705	3.534865
H	-1.876412	-0.508060	-2.819306
H	-1.149010	0.772725	-1.835342
H	-0.359590	-0.806008	-1.978911
H	-2.910019	-3.108224	-1.411101
H	-3.026131	-3.168827	0.354798
H	-1.448273	-3.249076	-0.434222
H	-4.769072	1.947105	-0.063332
H	-3.276152	1.643231	0.840787
H	-3.215683	1.902098	-0.907409
H	-5.757854	0.160416	-1.555792
H	-4.917533	-1.369227	-1.819855
H	-4.256944	0.135655	-2.483508
H	-5.755424	-0.127154	0.955649
H	-5.004092	-1.708644	0.728305
H	-4.256375	-0.522972	1.811031

Conformer #5

No. of imaginary frequencies = 0

Total energy = -1463.0974593

C	0.171953	0.785908	1.831568
C	1.618423	0.593294	2.307318
N	2.122354	0.961166	1.082811
C	0.795447	1.051275	0.441697
O	2.159428	0.213055	3.310815
C	0.485205	2.334351	-0.231714
H	0.630700	0.216073	-0.243851
C	-0.707614	-0.453408	1.909168
H	-0.331757	1.646692	2.276178
C	-0.410409	3.325438	-0.005517
C	-0.232170	4.277560	-1.061323
C	0.757228	3.787917	-1.842632
O	1.201974	2.603227	-1.356147
C	3.370514	0.587137	0.492909
C	3.325962	-0.824211	-0.079693
O	4.436686	-1.087858	-0.765580
C	4.536879	-2.391443	-1.375210
O	2.414009	-1.595192	0.071444
C	3.785817	-2.445541	-2.690305
C	-1.162762	-0.735569	3.330349
O	-1.818381	-0.228353	1.060728
Si	-2.356952	-1.287069	-0.120219
C	-0.985986	-1.648365	-1.350224
C	-2.892252	-2.893075	0.685542
C	-3.794799	-0.371604	-0.939336
C	-3.294146	0.971656	-1.495257
C	-4.361859	-1.222383	-2.086807
C	-4.897615	-0.109883	0.098284
H	-0.113960	-1.305626	1.545360
H	-1.122902	3.368445	0.802368
H	-0.769223	5.200318	-1.212154
H	1.240019	4.143728	-2.737342
H	3.654127	1.287859	-0.295066
H	4.147638	0.620062	1.260880
H	4.162690	-3.136569	-0.671261
H	5.607114	-2.536570	-1.518978
H	3.936692	-3.422934	-3.155704
H	4.151199	-1.679003	-3.377244
H	2.715412	-2.303860	-2.533046
H	-1.750932	-1.655524	3.364140
H	-0.297921	-0.841452	3.990293
H	-1.786791	0.086258	3.691879
H	-1.311367	-2.408560	-2.067532
H	-0.710425	-0.753524	-1.916076
H	-0.085164	-2.026246	-0.856257

H	-3.286973	-3.598045	-0.052569
H	-3.663710	-2.722363	1.441138
H	-2.042018	-3.376781	1.177233
H	-4.125975	1.524190	-1.950295
H	-2.862230	1.596269	-0.708866
H	-2.531099	0.836650	-2.268620
H	-5.198588	-0.700722	-2.568010
H	-4.741180	-2.186704	-1.732233
H	-3.611105	-1.417644	-2.859565
H	-5.725481	0.445517	-0.360459
H	-5.311111	-1.041933	0.496922
H	-4.521462	0.479440	0.939149

Conformer #6

No. of imaginary frequencies = 0

Total energy = -1463.0973807

C	0.534062	0.520461	1.785387
C	1.983082	0.164900	2.145902
N	2.435705	0.589833	0.923474
C	1.104365	0.851008	0.372141
O	2.552457	-0.335479	3.079310
C	0.916058	2.212506	-0.184731
H	0.804607	0.107003	-0.368642
C	-0.472503	-0.615528	1.852493
H	0.154555	1.400337	2.309532
C	1.469396	3.420763	0.087756
C	0.823895	4.358663	-0.781826
C	-0.064312	3.642969	-1.510149
O	-0.014598	2.334581	-1.163045
C	3.685252	0.358481	0.265312
C	3.749976	-0.877659	-0.622905
O	2.620024	-1.588604	-0.602490
C	2.571696	-2.765347	-1.434658
O	4.724985	-1.159335	-1.265903
C	2.244476	-2.413349	-2.871835
C	-0.805061	-0.992268	3.286478
O	-1.635320	-0.188653	1.168617
Si	-2.414069	-1.040543	-0.042605
C	-1.229491	-1.332506	-1.470271
C	-2.977687	-2.698016	0.629429
C	-3.863925	0.058770	-0.554321
C	-3.337360	1.432976	-0.997885
C	-4.618900	-0.600291	-1.720075
C	-4.820048	0.242435	0.634854
H	-0.029702	-1.489461	1.347632
H	2.236572	3.615968	0.820478

H	1.001812	5.419776	-0.853577
H	-0.772396	3.900941	-2.279609
H	3.957147	1.216051	-0.356520
H	4.460142	0.249568	1.027927
H	1.789805	-3.376913	-0.983381
H	3.526315	-3.288054	-1.358394
H	2.137796	-3.332364	-3.453808
H	3.042919	-1.817857	-3.316799
H	1.304781	-1.859727	-2.931535
H	-1.507934	-1.828412	3.302869
H	0.102199	-1.274605	3.826365
H	-1.268956	-0.142364	3.793755
H	-1.696936	-1.944032	-2.248067
H	-0.912836	-0.387723	-1.921290
H	-0.334731	-1.863744	-1.129980
H	-3.500847	-3.280865	-0.134749
H	-3.652251	-2.571166	1.480415
H	-2.122314	-3.292637	0.966438
H	-4.174594	2.078134	-1.293258
H	-2.791581	1.931061	-0.192499
H	-2.660983	1.354054	-1.854483
H	-5.466148	0.027388	-2.022996
H	-5.022892	-1.580661	-1.446294
H	-3.979951	-0.730551	-2.599645
H	-5.645954	0.908369	0.355144
H	-5.260054	-0.707701	0.954352
H	-4.308781	0.685071	1.494282

Conformer #7

No. of imaginary frequencies = 0

Total energy = -1463.0972952

C	0.245463	-1.657354	-1.166460
C	1.487824	-1.404924	-2.036908
N	2.171165	-0.876562	-0.978827
C	1.027842	-0.919413	-0.054397
O	1.786518	-1.561673	-3.192038
C	1.242694	-1.621798	1.233111
H	0.638835	0.086387	0.127889
C	-1.063141	-1.036501	-1.619648
H	0.102197	-2.719993	-0.955639
C	0.645870	-2.675327	1.840522
C	1.276199	-2.808676	3.120800
C	2.202492	-1.825042	3.186357
O	2.191421	-1.088334	2.048479
C	3.438843	-0.214875	-0.910388
C	3.386794	1.282998	-0.652050

O	2.159921	1.789774	-0.797270
C	1.986274	3.184842	-0.478851
O	4.359750	1.921212	-0.352165
C	1.831968	3.378992	1.016153
C	-1.618485	-1.761013	-2.836080
O	-1.951437	-1.114788	-0.518606
Si	-3.164185	-0.047055	-0.081441
C	-4.106800	0.506066	-1.607087
C	-4.254724	-1.031173	1.070503
C	-2.439651	1.469786	0.813319
C	-1.536819	2.283611	-0.127306
C	-3.593010	2.374007	1.283711
C	-1.629097	1.021651	2.040242
H	-0.875463	0.014841	-1.883288
H	-0.156695	-3.269720	1.434212
H	1.065560	-3.541468	3.883189
H	2.919915	-1.529076	3.933179
H	4.070741	-0.645480	-0.129981
H	3.943594	-0.369344	-1.868243
H	1.081617	3.470006	-1.015604
H	2.834823	3.746468	-0.872071
H	1.600979	4.426254	1.227608
H	2.754197	3.119201	1.538082
H	1.017647	2.761063	1.401544
H	-2.532939	-1.280731	-3.189090
H	-0.882000	-1.756333	-3.643522
H	-1.848749	-2.798137	-2.577595
H	-4.881487	1.233873	-1.348610
H	-3.448860	0.971508	-2.347270
H	-4.597633	-0.346373	-2.085070
H	-5.100055	-0.437692	1.430287
H	-3.690621	-1.381105	1.939156
H	-4.654109	-1.909140	0.555861
H	-1.183938	3.190335	0.380938
H	-0.650709	1.722667	-0.438142
H	-2.066068	2.602533	-1.030926
H	-3.192827	3.243491	1.820078
H	-4.269397	1.852826	1.968113
H	-4.185569	2.754627	0.445810
H	-1.168554	1.889504	2.529656
H	-2.263992	0.528981	2.782878
H	-0.832588	0.320067	1.778088

Conformer #8

No. of imaginary frequencies = 0

Total energy = -1463.0969104

C	0.605179	0.495249	1.590190
C	2.118198	0.309163	1.756485
N	2.379663	0.998342	0.596335
C	0.970817	1.130291	0.214083
O	2.847624	-0.265891	2.519458
C	0.540992	2.519622	-0.075725
H	0.695182	0.472534	-0.613284
C	-0.208190	-0.787777	1.525259
H	0.158363	1.202282	2.292294
C	1.031862	3.738661	0.259015
C	0.122278	4.697915	-0.294624
C	-0.841912	3.982672	-0.919029
O	-0.597287	2.654998	-0.799192
C	3.537156	0.912302	-0.244101
C	3.672294	-0.384419	-1.035924
O	2.614448	-1.186766	-0.885373
C	2.673706	-2.481883	-1.514897
O	4.629410	-0.632020	-1.717760
C	3.394444	-3.477505	-0.630145
C	-0.328728	-1.454810	2.884950
O	-1.488199	-0.451315	1.026640
Si	-2.260511	-1.193160	-0.258751
C	-1.288526	-0.911553	-1.839307
C	-2.373619	-3.037336	0.067686
C	-3.960059	-0.370857	-0.329445
C	-3.792546	1.133157	-0.601304
C	-4.796223	-1.004775	-1.452973
C	-4.679594	-0.564570	1.014869
H	0.305930	-1.473775	0.832728
H	1.926916	3.926262	0.830582
H	0.184622	5.772686	-0.233322
H	-1.727534	4.250788	-1.470305
H	3.545230	1.741092	-0.956461
H	4.435812	1.002371	0.369581
H	3.159152	-2.379668	-2.486564
H	1.628631	-2.757581	-1.661300
H	3.359846	-4.467633	-1.091526
H	2.921538	-3.534577	0.352547
H	4.440837	-3.195595	-0.502538
H	-0.874482	-2.396964	2.794309
H	0.661004	-1.652749	3.303929
H	-0.878627	-0.802635	3.568390
H	-1.785742	-1.381616	-2.693443
H	-1.182396	0.156049	-2.049601
H	-0.284709	-1.342882	-1.768790
H	-2.849517	-3.559112	-0.768131

H	-2.949774	-3.248088	0.972720
H	-1.377241	-3.472072	0.199996
H	-4.773209	1.625582	-0.602135
H	-3.171833	1.611730	0.160681
H	-3.327796	1.320361	-1.574410
H	-5.781876	-0.526230	-1.505501
H	-4.961683	-2.074347	-1.286711
H	-4.323723	-0.883376	-2.433413
H	-5.660732	-0.074074	0.990612
H	-4.849001	-1.623257	1.236680
H	-4.106811	-0.132979	1.839983

Conformer #9

No. of imaginary frequencies = 0

Total energy = -1463.0968697

C	0.611330	0.147058	1.666285
C	2.131976	-0.008714	1.807019
N	2.362357	0.864306	0.774428
C	0.940361	0.964797	0.395861
O	2.879074	-0.656789	2.490785
C	0.377040	2.329507	0.273681
H	0.732370	0.392983	-0.516742
C	-0.213505	-1.108202	1.443699
H	0.174965	0.742926	2.471116
C	-0.508848	3.050630	1.002878
C	-0.693214	4.286975	0.304362
C	0.095680	4.217055	-0.792499
O	0.751318	3.032026	-0.829238
C	3.534336	1.011493	-0.035844
C	3.794734	-0.123692	-1.019826
O	2.912752	-1.116239	-0.894779
C	3.151278	-2.301213	-1.676098
O	4.710590	-0.117713	-1.797270
C	2.211550	-3.368698	-1.166497
C	-0.279359	-1.975981	2.689358
O	-1.496156	-0.663716	1.052567
Si	-2.573037	-1.323810	-0.041177
C	-1.633157	-2.367279	-1.286504
C	-3.811397	-2.391804	0.871938
C	-3.417202	0.153688	-0.874429
C	-2.407732	0.898352	-1.761977
C	-4.590427	-0.335747	-1.738877
C	-3.942176	1.117430	0.201526
H	0.252154	-1.682278	0.628995
H	-0.989687	2.734907	1.914583
H	-1.330427	5.110563	0.584032

H	0.297155	4.894665	-1.605193
H	3.486489	1.945082	-0.599663
H	4.411184	1.067809	0.614027
H	4.198566	-2.586962	-1.559906
H	2.979708	-2.067352	-2.729766
H	2.383057	-4.301001	-1.709709
H	1.169735	-3.076893	-1.312027
H	2.380680	-3.551366	-0.103102
H	-0.840656	-2.891918	2.487380
H	0.728320	-2.243022	3.017727
H	-0.781296	-1.435911	3.496535
H	-2.307334	-2.715954	-2.074740
H	-0.829804	-1.798002	-1.763443
H	-1.194499	-3.252738	-0.816583
H	-4.531342	-2.844695	0.183536
H	-4.369114	-1.805403	1.607392
H	-3.305263	-3.201903	1.405364
H	-2.885684	1.766737	-2.231944
H	-1.561394	1.270318	-1.178454
H	-2.022045	0.262281	-2.565215
H	-5.065776	0.514076	-2.243937
H	-5.360243	-0.831760	-1.139451
H	-4.265402	-1.035350	-2.516694
H	-4.431163	1.979261	-0.269838
H	-4.678557	0.637715	0.854693
H	-3.126905	1.491903	0.825639

Conformer #10

No. of imaginary frequencies = 0

Total energy = -1463.0968142

C	-0.147481	1.306156	0.658162
C	-1.322516	2.234934	0.312312
N	-1.752420	1.390594	-0.670577
C	-0.671931	0.407235	-0.487862
O	-1.736918	3.294292	0.703962
C	-1.089205	-0.971517	-0.128879
H	-0.005017	0.383475	-1.356623
C	1.265765	1.839185	0.511023
H	-0.272439	0.854974	1.645128
C	-0.922138	-1.761258	0.959036
C	-1.593570	-2.993211	0.666244
C	-2.112819	-2.850972	-0.575060
O	-1.805091	-1.630561	-1.077016
C	-2.923229	1.399886	-1.493423
C	-4.041292	0.464503	-1.050162
O	-3.949375	0.144162	0.235854

C	-4.938409	-0.765034	0.747850
O	-4.912358	0.092836	-1.791459
C	-4.592119	-1.040070	2.191768
C	1.595463	2.868216	1.579017
O	2.132739	0.724572	0.604532
Si	3.369789	0.340833	-0.455891
C	2.686205	0.171816	-2.196301
C	4.657699	1.702082	-0.435381
C	4.041973	-1.304189	0.188114
C	2.960049	-2.388435	0.052421
C	5.280461	-1.712110	-0.626041
C	4.430030	-1.156121	1.667883
H	1.355335	2.310999	-0.480750
H	-0.385662	-1.504449	1.858239
H	-1.672627	-3.864359	1.296944
H	-2.692073	-3.493174	-1.217104
H	-3.327286	2.416778	-1.484068
H	-2.680793	1.146398	-2.527695
H	-4.916364	-1.675181	0.143252
H	-5.924871	-0.307931	0.638210
H	-5.324714	-1.729061	2.619267
H	-4.601476	-0.117688	2.776169
H	-3.602104	-1.494208	2.266175
H	2.603660	3.261330	1.429815
H	0.879744	3.693495	1.546398
H	1.549398	2.402839	2.567013
H	3.486289	-0.075557	-2.900922
H	1.933338	-0.618931	-2.256621
H	2.229853	1.104614	-2.542649
H	5.464128	1.495881	-1.145566
H	5.099934	1.819300	0.557658
H	4.210482	2.660939	-0.717006
H	3.316303	-3.332422	0.483440
H	2.038123	-2.108771	0.570502
H	2.709704	-2.582335	-0.995308
H	5.673575	-2.669072	-0.261220
H	6.085553	-0.975106	-0.540638
H	5.050288	-1.839544	-1.689174
H	4.820469	-2.106616	2.052810
H	5.209987	-0.400973	1.810937
H	3.569564	-0.870453	2.278590

Conformer #11

No. of imaginary frequencies = 0

Total energy = -1463.0967806

C	0.590021	0.128825	1.773027

C	2.041699	-0.316645	2.002228
N	2.479570	0.410994	0.928087
C	1.124618	0.765429	0.468988
O	2.617619	-1.042766	2.769137
C	0.854222	2.202837	0.232280
H	0.844478	0.177399	-0.411920
C	-0.467607	-0.945631	1.608094
H	0.264094	0.866098	2.510514
C	-0.003429	3.097243	0.780525
C	0.162370	4.315397	0.044758
C	1.106162	4.061365	-0.890441
O	1.533996	2.778706	-0.795037
C	3.721993	0.337142	0.219674
C	3.802324	-0.730964	-0.863163
O	2.670785	-1.430070	-0.973776
C	2.637918	-2.460597	-1.976304
O	4.778969	-0.904373	-1.540450
C	1.211176	-2.949022	-2.064859
C	-0.759966	-1.656800	2.919543
O	-1.611037	-0.287718	1.101699
Si	-2.870119	-0.911419	0.193875
C	-2.364277	-2.561482	-0.542006
C	-4.358652	-1.142441	1.305121
C	-3.206834	0.374804	-1.156565
C	-1.920662	0.636729	-1.955425
C	-4.301433	-0.140024	-2.104882
C	-3.664939	1.691997	-0.510089
H	-0.103164	-1.678614	0.872368
H	-0.684882	2.905702	1.593816
H	-0.352240	5.250693	0.196320
H	1.566669	4.656768	-1.660928
H	3.948946	1.296234	-0.251431
H	4.517363	0.128039	0.938779
H	3.327463	-3.254376	-1.679339
H	2.990513	-2.042982	-2.921673
H	1.136300	-3.742657	-2.811743
H	0.544687	-2.135358	-2.361921
H	0.872555	-3.346916	-1.105609
H	-1.500009	-2.447933	2.770833
H	0.153947	-2.099793	3.323074
H	-1.158570	-0.946113	3.648611
H	-3.209748	-3.012973	-1.069829
H	-1.542646	-2.459319	-1.255193
H	-2.051443	-3.266359	0.234501
H	-5.239670	-1.457519	0.737530
H	-4.604950	-0.213042	1.825507

H	-4.158738	-1.905997	2.062675
H	-2.118492	1.345129	-2.769425
H	-1.145742	1.073756	-1.320974
H	-1.523042	-0.278134	-2.408451
H	-4.515479	0.609656	-2.876554
H	-5.240356	-0.340670	-1.578230
H	-3.998906	-1.059046	-2.617545
H	-3.818602	2.458625	-1.279924
H	-4.610490	1.572341	0.028141
H	-2.916056	2.071078	0.191553

Conformer #12

No. of imaginary frequencies = 0

Total energy = -1463.096624

C	-0.203534	1.051476	1.697425
C	1.191858	0.836109	2.302542
N	1.803706	1.094607	1.101921
C	0.540677	1.167910	0.345765
O	1.637300	0.517404	3.372742
C	0.336281	2.395923	-0.458914
H	0.400905	0.278144	-0.274562
C	-1.184243	-0.101682	1.832463
H	-0.670370	1.983898	2.023124
C	-0.611352	3.363911	-0.468956
C	-0.275554	4.242256	-1.550527
C	0.847362	3.735653	-2.108818
O	1.231003	2.608262	-1.460918
C	3.103086	0.696715	0.657065
C	3.125289	-0.750207	0.182160
O	4.323464	-1.065663	-0.306412
C	4.484281	-2.411069	-0.796545
O	2.190721	-1.505669	0.235370
C	5.892310	-2.538521	-1.328171
C	-1.677457	-0.237096	3.264739
O	-2.255908	0.168759	0.946767
Si	-3.179743	-0.919121	0.070338
C	-3.454626	-2.479206	1.076956
C	-4.792940	-0.027778	-0.236386
C	-2.323035	-1.347029	-1.572465
C	-1.041977	-2.158410	-1.318413
C	-3.272490	-2.192451	-2.439126
C	-1.977510	-0.055089	-2.330239
H	-0.667852	-1.026930	1.538698
H	-1.455511	3.430857	0.198345
H	-0.801541	5.129760	-1.864160
H	1.471196	4.043998	-2.930985

H	3.448917	1.345305	-0.150883
H	3.807110	0.798036	1.486805
H	3.735736	-2.589216	-1.572166
H	4.290193	-3.106451	0.023284
H	6.044188	-3.546229	-1.722088
H	6.626088	-2.362865	-0.539001
H	6.069862	-1.823473	-2.134062
H	-2.346578	-1.094730	3.359318
H	-0.832906	-0.370428	3.945297
H	-2.225442	0.663708	3.554672
H	-3.994897	-3.229388	0.491583
H	-2.511100	-2.929563	1.399353
H	-4.047648	-2.265615	1.970700
H	-5.480357	-0.636958	-0.830334
H	-4.626697	0.913290	-0.767542
H	-5.282568	0.206641	0.712710
H	-0.544908	-2.385250	-2.270302
H	-0.314116	-1.630650	-0.696946
H	-1.257712	-3.113413	-0.828944
H	-2.784529	-2.451028	-3.387259
H	-4.193894	-1.654575	-2.683016
H	-3.548452	-3.132295	-1.949815
H	-2.877520	0.509106	-2.595133
H	-1.338255	0.609658	-1.744276
H	-1.452069	-0.291122	-3.264311

Compound 11c

Conformer #1
No. of imaginary frequencies = 0
Total energy = -1463.0206855

C	0.186053	1.491201	-0.394991
C	1.443368	2.111050	0.233282
N	2.070683	0.899803	0.266924
C	0.955570	0.130516	-0.292321
O	1.802235	3.209316	0.571565
C	-1.148044	1.671263	0.305177
H	0.078705	1.799942	-1.438332
C	3.390157	0.520432	0.654626
C	4.228480	0.055978	-0.524633
O	5.459924	-0.259292	-0.120839
C	6.369253	-0.729446	-1.134066
O	3.839031	-0.031893	-1.657962
C	7.697928	-0.995287	-0.466643
C	-1.548866	3.140620	0.327279
O	-2.081154	0.884968	-0.411683

Si	-3.540234	0.264984	0.120536
C	-3.311703	-0.546856	1.792578
C	-4.830655	1.621172	0.255201
C	-4.024125	-0.991998	-1.210438
C	-2.901733	-2.028053	-1.375364
C	-5.320275	-1.710239	-0.801047
C	-4.242723	-0.270111	-2.549682
H	-1.062756	1.301383	1.335250
H	3.871027	1.385443	1.117914
H	3.368845	-0.280250	1.402108
H	6.447129	0.032735	-1.912665
H	5.949529	-1.630884	-1.586951
H	8.415038	-1.352239	-1.209700
H	7.599866	-1.756267	0.310268
H	8.095951	-0.084721	-0.014470
H	-2.489949	3.276133	0.864533
H	-0.775110	3.739021	0.813793
H	-1.681619	3.507170	-0.694309
H	-4.262653	-0.941517	2.163532
H	-2.596452	-1.371803	1.739802
H	-2.944372	0.168821	2.534752
H	-5.828482	1.194200	0.397556
H	-4.851123	2.236810	-0.648086
H	-4.632608	2.279322	1.106096
H	-3.174966	-2.761499	-2.144704
H	-1.965498	-1.550455	-1.675500
H	-2.712467	-2.575021	-0.446182
H	-5.605724	-2.440448	-1.568328
H	-6.157278	-1.013284	-0.688743
H	-5.204865	-2.254734	0.141814
H	-4.500704	-0.995080	-3.332039
H	-5.060441	0.455633	-2.492961
H	-3.341174	0.261223	-2.867740
H	1.186510	-0.299637	-1.268938
C	0.475653	-0.961876	0.592264
C	0.228187	-2.273871	0.354414
O	0.302036	-0.692039	1.913803
C	-0.133545	-2.852967	1.612192
H	0.295583	-2.765367	-0.603138
C	-0.066655	-1.847130	2.515637
H	-0.399053	-3.878514	1.813513
H	-0.246929	-1.789381	3.576034

Conformer #2

No. of imaginary frequencies = 0

Total energy = -1463.0200834

C	-0.262996	1.461693	0.327664
C	-1.521724	2.029181	-0.346540
N	-2.113374	0.799868	-0.362756
C	-0.985472	0.075588	0.229771
O	-1.901658	3.107143	-0.724912
C	1.082672	1.669448	-0.342365
H	-0.191570	1.792963	1.367156
C	-3.393102	0.360892	-0.815330
C	-4.251179	-0.181303	0.314538
O	-5.430159	-0.588826	-0.159721
C	-6.370487	-1.128224	0.790695
O	-3.911289	-0.252444	1.465152
C	-7.135148	-0.027035	1.496688
C	1.442139	3.149010	-0.381002
O	2.019105	0.923463	0.411993
Si	3.503865	0.325691	-0.071506
C	3.335136	-0.531350	-1.727930
C	4.765370	1.708275	-0.210913
C	3.982536	-0.886572	1.302092
C	2.882158	-1.947119	1.460576
C	5.307901	-1.579650	0.947029
C	4.143595	-0.127075	2.628666
H	1.034581	1.279714	-1.367428
H	-3.901583	1.212278	-1.274707
H	-3.299286	-0.415681	-1.582714
H	-5.829113	-1.754998	1.501397
H	-7.030124	-1.751926	0.187788
H	-7.882992	-0.469520	2.159811
H	-7.650774	0.610557	0.775298
H	-6.464503	0.586262	2.100522
H	2.390786	3.302000	-0.900054
H	0.662607	3.716472	-0.894738
H	1.542090	3.536355	0.636644
H	4.304016	-0.912535	-2.065247
H	2.637955	-1.371338	-1.672527
H	2.970434	0.157511	-2.496266
H	5.774485	1.301300	-0.330847
H	4.758498	2.341491	0.680321
H	4.565681	2.345400	-1.077365
H	3.148945	-2.652242	2.258130
H	1.924460	-1.486527	1.716682
H	2.737316	-2.523753	0.541392
H	5.588775	-2.285961	1.738043
H	6.129741	-0.863546	0.843973
H	5.234556	-2.146955	0.013402
H	4.395164	-0.826218	3.436227

H	4.945228	0.616728	2.577453
H	3.220550	0.389811	2.906315
H	-1.223290	-0.350928	1.206259
C	-0.454051	-1.011627	-0.631887
C	-0.174989	-2.313729	-0.375311
O	-0.266188	-0.751641	-1.953662
C	0.223011	-2.896359	-1.620441
H	-0.246108	-2.796895	0.586187
C	0.143706	-1.902724	-2.536239
H	0.520020	-3.916244	-1.805961
H	0.340016	-1.851807	-3.594132

Conformer #3

No. of imaginary frequencies = 0

Total energy = -1463.0199438

C	0.200572	1.537445	-0.500425
C	1.424779	2.250393	0.094710
N	2.092118	1.068888	0.235736
C	1.013622	0.217890	-0.274411
O	1.737631	3.384359	0.350542
C	-1.149669	1.728599	0.165446
H	0.099346	1.754658	-1.567185
C	3.408496	0.762764	0.691394
C	4.292234	0.215319	-0.416498
O	5.508377	-0.059002	0.059872
C	6.465832	-0.615336	-0.862875
O	3.944381	0.043467	-1.553936
C	6.284440	-2.112545	-1.011423
C	-1.613252	3.173329	0.028667
O	-2.038330	0.833587	-0.475295
Si	-3.473395	0.196867	0.100112
C	-3.218154	-0.496859	1.820187
C	-4.812856	1.510552	0.151078
C	-3.903308	-1.158245	-1.151233
C	-2.736278	-2.152140	-1.252832
C	-5.168811	-1.905811	-0.701505
C	-4.146936	-0.524207	-2.529878
H	-1.063647	1.473171	1.229767
H	3.855166	1.678331	1.086942
H	3.384999	0.032146	1.507442
H	7.432582	-0.371472	-0.423271
H	6.365496	-0.106202	-1.822764
H	7.064871	-2.510852	-1.664873
H	5.315902	-2.342714	-1.458139
H	6.360575	-2.610131	-0.042157
H	-2.559742	3.327366	0.551128

H	-0.866334	3.855053	0.442112
H	-1.761272	3.415744	-1.027229
H	-4.157565	-0.889548	2.221464
H	-2.482630	-1.305104	1.817848
H	-2.865339	0.274624	2.511862
H	-5.794094	1.056985	0.323634
H	-4.857922	2.065647	-0.789727
H	-4.638532	2.228204	0.957897
H	-2.968022	-2.933784	-1.987707
H	-1.816976	-1.650495	-1.566003
H	-2.536681	-2.644569	-0.295716
H	-5.424069	-2.686516	-1.428734
H	-6.034211	-1.239391	-0.624430
H	-5.030874	-2.394573	0.268519
H	-4.375954	-1.301377	-3.270034
H	-4.991702	0.171928	-2.513831
H	-3.265790	0.022078	-2.878119
H	1.276200	-0.280870	-1.209701
C	0.561260	-0.817548	0.689953
C	0.367467	-2.153089	0.555793
O	0.370166	-0.451355	1.985271
C	0.023376	-2.645331	1.855064
H	0.458908	-2.714827	-0.360289
C	0.045221	-1.569137	2.676102
H	-0.202919	-3.661540	2.135953
H	-0.143091	-1.435021	3.728110

Conformer #4

No. of imaginary frequencies = 0

Total energy = -1463.0199094

C	0.226509	-1.361193	0.181787
C	1.393557	-1.902985	-0.657636
N	2.110355	-0.755273	-0.477864
C	1.119418	-0.088875	0.374881
O	1.644445	-2.918616	-1.253158
C	-1.129002	-1.251090	-0.494360
H	0.115678	-1.912225	1.119175
C	3.453431	-0.411420	-0.814981
C	4.368620	-0.387111	0.398830
O	5.604041	-0.036188	0.039581
C	6.583515	0.040966	1.092735
O	4.030253	-0.633578	1.525227
C	7.887661	0.482646	0.471510
C	-1.678419	-2.633216	-0.817451
O	-1.977625	-0.549439	0.394384
Si	-3.282592	0.436045	0.036217

C	-2.972141	2.087713	0.854546
C	-3.416398	0.643514	-1.823926
C	-4.852301	-0.358336	0.754961
C	-4.707070	-0.483965	2.280093
C	-6.068974	0.524871	0.431106
C	-5.076500	-1.755507	0.159213
H	-1.015292	-0.687102	-1.427426
H	3.826980	-1.151254	-1.527473
H	3.500296	0.566730	-1.305050
H	6.665908	-0.940710	1.564898
H	6.228981	0.747816	1.846598
H	8.655302	0.554226	1.245629
H	7.782208	1.461165	-0.001340
H	8.223495	-0.233776	-0.280802
H	-2.626827	-2.549168	-1.352787
H	-0.971222	-3.191155	-1.435712
H	-1.852045	-3.192267	0.106414
H	-3.840155	2.748186	0.766769
H	-2.750579	1.957109	1.917258
H	-2.117172	2.588000	0.393579
H	-4.241055	1.316728	-2.075966
H	-3.591167	-0.306789	-2.336260
H	-2.498879	1.080359	-2.228720
H	-5.593413	-0.969703	2.707594
H	-3.832838	-1.083808	2.550523
H	-4.606096	0.494374	2.760179
H	-6.978421	0.084615	0.858723
H	-6.229771	0.621106	-0.647634
H	-5.968154	1.531563	0.849151
H	-6.003731	-2.189760	0.554257
H	-5.169451	-1.727605	-0.931837
H	-4.259785	-2.435452	0.413776
H	1.467452	0.019455	1.404468
C	0.702166	1.252181	-0.105429
C	0.751847	2.469890	0.490781
O	0.261943	1.383427	-1.384532
C	0.300799	3.417306	-0.482629
H	1.067683	2.663490	1.503804
C	0.019658	2.699252	-1.594931
H	0.196829	4.484102	-0.365658
H	-0.343665	2.961342	-2.574735

Conformer #5

No. of imaginary frequencies = 0

Total energy = -1463.0184418

C	0.614358	-0.968968	-0.819395

C	1.862442	-0.802563	-1.697480
N	2.310145	0.240160	-0.936544
C	1.197108	0.219329	0.017314
O	2.333899	-1.352541	-2.658400
C	-0.758698	-0.852301	-1.454665
H	0.660788	-1.905808	-0.256922
C	3.567328	0.918406	-0.903276
C	4.563974	0.407102	0.128069
O	4.099247	-0.635144	0.818653
C	4.988461	-1.202886	1.798231
O	5.644745	0.905731	0.292075
C	4.265727	-2.357647	2.451249
C	-0.981332	-1.967757	-2.467509
O	-1.689811	-0.916304	-0.392561
Si	-3.262657	-0.350879	-0.336138
C	-3.327180	1.418467	-0.944792
C	-4.387462	-1.415094	-1.396103
C	-3.728929	-0.483099	1.495114
C	-2.694347	0.271066	2.343833
C	-5.119429	0.130957	1.721878
C	-3.747174	-1.961139	1.915705
H	-0.836062	0.118772	-1.960614
H	4.037820	0.819690	-1.884511
H	3.423208	1.986660	-0.717865
H	5.257251	-0.426208	2.517934
H	5.902301	-1.523502	1.293351
H	4.915962	-2.821904	3.196333
H	3.993478	-3.113952	1.712392
H	3.357305	-2.017442	2.953328
H	-1.953195	-1.858369	-2.953670
H	-0.201283	-1.950458	-3.232110
H	-0.955577	-2.938796	-1.965677
H	-4.361572	1.770158	-1.004636
H	-2.773997	2.088792	-0.282344
H	-2.892879	1.506706	-1.945782
H	-5.440131	-1.202121	-1.184507
H	-4.214353	-2.478790	-1.212776
H	-4.224303	-1.225853	-2.461243
H	-2.949036	0.193843	3.408767
H	-1.692268	-0.141873	2.200824
H	-2.653404	1.334664	2.088049
H	-5.402981	0.042623	2.777943
H	-5.892864	-0.375044	1.134520
H	-5.141679	1.194919	1.464769
H	-3.982221	-2.050094	2.983998
H	-4.502836	-2.530232	1.364917

H	-2.776314	-2.435908	1.746246
H	1.504562	-0.093546	1.018662
C	0.480819	1.514124	0.140612
C	0.115268	2.245246	1.223229
O	0.167848	2.187871	-0.997610
C	-0.471449	3.449608	0.719784
H	0.245982	1.957836	2.254603
C	-0.406036	3.355896	-0.629083
H	-0.878767	4.272176	1.285611
H	-0.714881	4.004864	-1.431393

Conformer #6

No. of imaginary frequencies = 0

Total energy = -1463.0180401

C	0.545903	-1.192776	-0.408855
C	1.800955	-1.292541	-1.288000
N	2.246098	-0.074976	-0.860119
C	1.110893	0.202054	0.023584
O	2.274060	-2.097421	-2.047503
C	-0.823056	-1.298073	-1.054208
H	0.597187	-1.907250	0.417602
C	3.482584	0.610397	-1.061477
C	4.473299	0.532088	0.091588
O	4.043709	-0.248437	1.084727
C	4.930236	-0.424470	2.207982
O	5.519790	1.123425	0.086157
C	5.956974	-1.504302	1.933974
C	-1.029728	-2.680961	-1.657727
O	-1.761579	-1.029217	-0.030212
Si	-3.333978	-0.477154	-0.175363
C	-3.395936	0.998655	-1.326264
C	-4.451482	-1.830487	-0.839844
C	-3.816501	-0.008230	1.594902
C	-2.790012	0.983339	2.163309
C	-5.208812	0.642831	1.600855
C	-3.838400	-1.270231	2.471987
H	-0.904748	-0.540047	-1.843700
H	3.971038	0.179482	-1.939186
H	3.311182	1.670139	-1.272027
H	4.268340	-0.701660	3.028459
H	5.407105	0.531109	2.432255
H	6.556844	-1.671791	2.832137
H	6.626799	-1.206721	1.125803
H	5.468182	-2.443361	1.666060
H	-1.999669	-2.743217	-2.155831
H	-0.244722	-2.901322	-2.384851

H	-0.999298	-3.439724	-0.871074
H	-4.432928	1.299237	-1.505083
H	-2.858450	1.854087	-0.909671
H	-2.950403	0.766641	-2.298667
H	-5.505276	-1.563673	-0.710625
H	-4.277250	-2.777426	-0.321961
H	-4.285658	-1.995541	-1.908434
H	-3.056006	1.253680	3.193374
H	-1.786671	0.549435	2.172695
H	-2.746655	1.907253	1.577796
H	-5.497256	0.905783	2.626240
H	-5.978755	-0.030557	1.209987
H	-5.231257	1.563460	1.008569
H	-4.081709	-1.008276	3.509555
H	-4.589919	-1.989123	2.130315
H	-2.866422	-1.771968	2.471893
H	1.390420	0.229822	1.079996
C	0.392358	1.462067	-0.296988
C	0.011143	2.510632	0.474545
O	0.100040	1.717777	-1.599546
C	-0.563220	3.477470	-0.410999
H	0.127706	2.585389	1.544136
C	-0.476878	2.940523	-1.650481
H	-0.977809	4.440194	-0.158012
H	-0.771024	3.284017	-2.628123

Conformer #7

No. of imaginary frequencies = 0

Total energy = -1463.0176531

C	0.422347	1.407475	-0.662936
C	1.634079	2.208680	-0.162105
N	2.258398	1.072323	0.263710
C	1.181367	0.153516	-0.111529
O	1.965855	3.365209	-0.133808
C	-0.954319	1.753471	-0.126859
H	0.380016	1.394729	-1.755489
C	3.520950	0.851535	0.894677
C	4.509788	0.011463	0.102709
O	4.109454	-0.209872	-1.150978
C	4.962575	-1.031105	-1.971797
O	5.536275	-0.396450	0.576955
C	4.682570	-2.502343	-1.739793
C	-1.365416	3.156776	-0.552345
O	-1.834882	0.771973	-0.640600
Si	-3.319794	0.295307	-0.034326
C	-3.184585	-0.007319	1.808576

C	-4.620631	1.609529	-0.356237
C	-3.719617	-1.296052	-0.980596
C	-2.573743	-2.304132	-0.805779
C	-5.020203	-1.907139	-0.434343
C	-3.891475	-0.980156	-2.474718
H	-0.932406	1.697571	0.969279
H	3.981369	1.827513	1.070916
H	3.398922	0.367710	1.868904
H	6.003691	-0.785939	-1.757216
H	4.723819	-0.732402	-2.992320
H	5.298064	-3.104787	-2.412490
H	3.632714	-2.731932	-1.937077
H	4.922936	-2.783639	-0.713083
H	-2.335164	3.418944	-0.123921
H	-0.624663	3.888217	-0.221333
H	-1.445818	3.209208	-1.641512
H	-4.162086	-0.259824	2.230743
H	-2.493774	-0.824679	2.030414
H	-2.825108	0.885034	2.330687
H	-5.626431	1.209992	-0.192134
H	-4.565656	1.976745	-1.384494
H	-4.496754	2.465202	0.313910
H	-2.799415	-3.231946	-1.347073
H	-1.633531	-1.902241	-1.192717
H	-2.415597	-2.563125	0.246009
H	-5.263742	-2.827285	-0.979924
H	-5.872035	-1.228316	-0.545837
H	-4.932950	-2.168768	0.625220
H	-4.099261	-1.900562	-3.035095
H	-4.725138	-0.293087	-2.651837
H	-2.987425	-0.528539	-2.893352
H	1.475778	-0.542917	-0.900474
C	0.644328	-0.640890	1.023058
C	0.408515	-1.968556	1.167699
O	0.399951	0.001535	2.196071
C	-0.020936	-2.159026	2.519608
H	0.525626	-2.719414	0.402433
C	-0.001582	-0.931976	3.090382
H	-0.297696	-3.084212	2.999368
H	-0.237242	-0.569484	4.076927

Conformer #8

No. of imaginary frequencies = 0

Total energy = -1463.017785

C	0.513215	1.340591	-0.463253
C	1.731947	2.049083	0.147476

N	2.269361	0.861587	0.552994
C	1.188491	0.018807	0.037307
O	2.125443	3.182083	0.245148
C	-0.873021	1.719344	0.023606
H	0.532495	1.403075	-1.554804
C	3.537410	0.531322	1.120473
C	4.548224	-0.073427	0.156332
O	4.137246	-0.025692	-1.112072
C	5.020454	-0.578751	-2.107053
O	5.597701	-0.531633	0.521780
C	4.828552	-2.076644	-2.233324
C	-1.196208	3.163011	-0.338299
O	-1.770471	0.812122	-0.588449
Si	-3.314581	0.396253	-0.095193
C	-3.311049	0.001977	1.735648
C	-4.520385	1.796206	-0.426804
C	-3.746634	-1.125314	-1.137087
C	-2.658278	-2.195381	-0.965444
C	-5.097556	-1.696241	-0.676685
C	-3.836933	-0.729236	-2.619285
H	-0.910817	1.600632	1.114105
H	3.978064	1.446760	1.524219
H	3.422690	-0.169923	1.951967
H	6.049667	-0.330692	-1.843651
H	4.747692	-0.060287	-3.025977
H	5.458323	-2.459944	-3.040077
H	3.788315	-2.314866	-2.467697
H	5.112158	-2.582494	-1.308901
H	-2.172133	3.449808	0.059177
H	-0.438686	3.837533	0.067563
H	-1.220341	3.279565	-1.425250
H	-4.328420	-0.192176	2.088842
H	-2.698933	-0.876956	1.953747
H	-2.916547	0.838158	2.321431
H	-5.553979	1.445933	-0.340668
H	-4.384711	2.208174	-1.430305
H	-4.393041	2.610732	0.292156
H	-2.904124	-3.084257	-1.560814
H	-1.684419	-1.822000	-1.292755
H	-2.556968	-2.511739	0.077616
H	-5.365016	-2.570688	-1.283015
H	-5.908789	-0.968320	-0.781566
H	-5.067672	-2.020286	0.368641
H	-4.061955	-1.610009	-3.234120
H	-4.629416	0.005038	-2.796199
H	-2.895506	-0.301933	-2.976888

H	1.507434	-0.623684	-0.787962
C	0.547417	-0.838944	1.066556
C	0.255588	-2.163262	1.089831
O	0.232092	-0.276035	2.262829
C	-0.287069	-2.435773	2.385904
H	0.406190	-2.860222	0.280605
C	-0.271317	-1.255699	3.048750
H	-0.634137	-3.381323	2.770885
H	-0.571990	-0.959032	4.039666

Conformer #9

No. of imaginary frequencies = 0

Total energy = -1463.017704

C	0.619922	-0.937890	-0.508967
C	1.785249	-0.942679	-1.509119
N	2.347219	0.158647	-0.926627
C	1.352547	0.280088	0.145686
O	2.136285	-1.624245	-2.436397
C	-0.788564	-0.783759	-1.055653
H	0.653873	-1.815880	0.141863
C	3.645518	0.739659	-1.065248
C	4.699110	0.223286	-0.093607
O	4.254572	-0.791435	0.648479
C	5.193676	-1.378234	1.568078
O	5.804585	0.688464	-0.020876
C	4.486774	-2.513982	2.270335
C	-1.173776	-1.993907	-1.894484
O	-1.644913	-0.632750	0.060687
Si	-3.087964	0.208697	0.168434
C	-2.907125	1.471726	1.534088
C	-3.439793	1.060755	-1.465925
C	-4.454062	-1.035529	0.605947
C	-4.110196	-1.719720	1.939173
C	-5.799825	-0.304509	0.743837
C	-4.575292	-2.106691	-0.487853
H	-0.829377	0.113727	-1.683552
H	4.009859	0.536114	-2.075382
H	3.594969	1.825645	-0.949168
H	5.529110	-0.607172	2.265776
H	6.063614	-1.722847	1.004610
H	5.170699	-2.990969	2.976217
H	4.152295	-3.265376	1.552376
H	3.619082	-2.150793	2.825524
H	-2.164897	-1.853425	-2.331917
H	-0.450597	-2.146283	-2.699220
H	-1.195752	-2.892258	-1.270985

H	-3.854247	1.982831	1.731801
H	-2.576254	0.997060	2.461827
H	-2.165593	2.226438	1.261658
H	-4.381340	1.615304	-1.411730
H	-3.518341	0.349925	-2.293425
H	-2.648628	1.775750	-1.709334
H	-4.872084	-2.468832	2.189171
H	-3.142774	-2.228105	1.889106
H	-4.073094	-1.002015	2.764773
H	-6.589433	-1.017411	1.012095
H	-6.101297	0.178161	-0.191645
H	-5.774116	0.460780	1.526002
H	-5.377008	-2.813190	-0.238992
H	-4.814458	-1.670401	-1.463555
H	-3.649460	-2.678433	-0.590357
H	1.766756	0.026770	1.125585
C	0.731062	1.623818	0.251570
C	0.705467	2.522326	1.268258
O	0.149019	2.161098	-0.851935
C	0.055296	3.691749	0.760097
H	1.103717	2.367828	2.258741
C	-0.257058	3.411049	-0.526518
H	-0.149338	4.612780	1.281948
H	-0.744895	3.967600	-1.309349

Compound 26b

Conformer #1
No. of imaginary frequencies = 0
Total energy = -1422.8363536

C	0.523705	0.028672	1.720498
C	1.972434	-0.392035	2.020852
N	2.442300	0.320244	0.952416
C	1.134091	0.724814	0.466089
O	2.524929	-1.094759	2.824195
C	0.934265	2.217427	0.359694
H	0.844078	0.240318	-0.467492
C	-0.460945	-1.095823	1.442487
H	0.113034	0.724829	2.455901
C	3.723016	0.327092	0.321318
C	3.756571	-0.564499	-0.909720
O	4.954503	-0.510586	-1.492378
C	5.119655	-1.307161	-2.669795
O	2.834167	-1.221892	-1.313495
C	-0.797455	-1.875334	2.702855
O	-1.629015	-0.515289	0.898664

Si	-2.365019	-0.971084	-0.534735
C	-1.224362	-0.639437	-1.985279
C	-2.764089	-2.802294	-0.468319
C	-3.925141	0.096337	-0.617937
C	-3.532999	1.582309	-0.617948
C	-4.705500	-0.226127	-1.902347
C	-4.811836	-0.192809	0.603437
O	-0.224340	2.484496	-0.247917
O	1.698802	3.052911	0.763666
C	-0.578184	3.864505	-0.358398
H	0.006141	-1.777467	0.713789
H	4.461314	-0.036764	1.040154
H	4.013275	1.343537	0.040867
H	-3.436070	-3.036207	0.361772
H	-1.851595	-3.392905	-0.338001
H	-5.007772	-1.277785	-1.944593
H	-4.121489	-0.006251	-2.802069
H	-5.152152	-1.233158	0.621637
H	-4.281316	0.005435	1.538732
H	0.161425	4.402064	-0.953917
H	-0.967476	0.421996	-2.043787
H	6.143695	-1.139096	-2.994476
H	4.957248	-2.361460	-2.441881
H	4.415400	-0.993118	-3.441527
H	-1.482937	-2.691291	2.462922
H	0.108046	-2.287880	3.154309
H	-1.285782	-1.217288	3.426488
H	-1.704626	-0.926365	-2.926087
H	-0.294331	-1.212066	-1.908259
H	-3.239257	-3.137722	-1.395202
H	-4.433081	2.209774	-0.649787
H	-2.919344	1.836748	-1.488368
H	-2.964573	1.842857	0.278786
H	-5.619931	0.378151	-1.950332
H	-5.706213	0.442845	0.580733
H	-0.643938	4.321285	0.630240
H	-1.549343	3.877577	-0.847972

Conformer #2

No. of imaginary frequencies = 0

Total energy = -1422.8351491

C	-0.518765	-0.028000	-1.790049
C	-1.959542	-0.527233	-1.994820
N	-2.404334	0.197847	-0.924971
C	-1.097994	0.711383	-0.548858
O	-2.518682	-1.283811	-2.743283

C	-1.005982	2.219489	-0.542312
H	-0.715813	0.310298	0.394017
C	0.503150	-1.110421	-1.479741
H	-0.158635	0.635469	-2.579601
C	-3.655084	0.191715	-0.236089
C	-3.596368	-0.624523	1.044225
O	-4.774210	-0.597853	1.669126
C	-4.854070	-1.332506	2.894275
O	-2.625532	-1.206348	1.450138
C	0.865520	-1.909177	-2.722470
O	1.629310	-0.467056	-0.925720
Si	2.720342	-1.086313	0.182560
C	1.865344	-2.388747	1.226285
C	4.174298	-1.846499	-0.723043
C	3.271529	0.395830	1.227407
C	2.118403	0.847434	2.136871
C	4.478461	0.001463	2.093450
C	3.661849	1.558232	0.300269
O	0.230903	2.609394	-0.232126
O	-1.918061	2.969437	-0.772113
C	0.461699	4.018428	-0.177289
H	0.056170	-1.786601	-0.735381
H	-4.408131	-0.242544	-0.898291
H	-3.972638	1.211457	-0.001736
H	4.704299	-1.098327	-1.319246
H	3.839896	-2.636396	-1.401757
H	5.340770	-0.288621	1.485091
H	4.245828	-0.829950	2.767923
H	4.494609	1.292268	-0.359271
H	2.817499	1.859682	-0.324856
H	-0.187467	4.481890	0.567210
H	0.933974	-2.014711	1.661359
H	-5.865898	-1.179289	3.261972
H	-4.668194	-2.392197	2.713790
H	-4.123859	-0.956227	3.612197
H	1.550519	-2.721187	-2.465807
H	-0.031856	-2.337634	-3.175576
H	1.358501	-1.261255	-3.452097
H	2.515801	-2.702807	2.048735
H	1.627166	-3.282325	0.641212
H	4.889058	-2.289426	-0.022864
H	2.427335	1.715460	2.733976
H	1.816102	0.061146	2.835534
H	1.246315	1.146995	1.550269
H	4.787571	0.848829	2.718150
H	3.980102	2.424084	0.896001

H	0.274942	4.473811	-1.151002
H	1.507071	4.130251	0.102153

Conformer #3

No. of imaginary frequencies = 0

Total energy = -1422.834662

C	0.741914	0.213438	1.638616
C	2.207378	-0.194418	1.867562
N	2.602486	0.435215	0.720031
C	1.264936	0.809439	0.296004
O	2.811206	-0.843782	2.678312
C	1.049624	2.291281	0.099071
H	0.908900	0.259689	-0.576852
C	-0.262158	-0.921495	1.520383
H	0.386501	0.966438	2.346023
C	3.841827	0.399033	0.008364
C	3.911515	-0.605971	-1.132754
O	2.822623	-1.379203	-1.208831
C	2.826749	-2.360874	-2.249538
O	4.848855	-0.686106	-1.878410
C	-0.510211	-1.588634	2.862905
O	-1.462587	-0.379525	1.007083
Si	-2.300054	-0.967299	-0.317932
C	-1.238589	-0.816216	-1.858713
C	-2.715782	-2.773765	-0.034289
C	-3.842979	0.119756	-0.424616
C	-3.425444	1.585957	-0.621182
C	-4.712322	-0.326400	-1.611425
C	-4.650269	-0.004795	0.877130
O	-0.101697	2.506308	-0.543471
O	1.791957	3.158473	0.474082
C	-0.481215	3.873182	-0.720298
H	0.152788	-1.666130	0.821709
H	4.631552	0.139003	0.717587
H	4.083224	1.383994	-0.398758
H	-3.342905	-2.904669	0.851626
H	-1.804205	-3.362147	0.112739
H	-5.045388	-1.364282	-1.507258
H	-4.182657	-0.234323	-2.565379
H	-5.003395	-1.027998	1.040316
H	-4.055378	0.290332	1.745774
H	0.261353	4.401218	-1.320338
H	-0.979789	0.228485	-2.052418
H	1.866210	-2.866618	-2.178604
H	2.938803	-1.882492	-3.223393
H	3.642563	-3.069299	-2.099728

H	-1.214940	-2.415102	2.746807
H	0.425039	-1.969449	3.280333
H	-0.939703	-0.866144	3.561918
H	-1.762244	-1.208945	-2.735606
H	-0.307727	-1.383296	-1.754093
H	-3.244420	-3.200100	-0.892155
H	-4.314032	2.229236	-0.653312
H	-2.880090	1.727364	-1.559962
H	-2.783019	1.929355	0.193846
H	-5.611209	0.299009	-1.675849
H	-5.534568	0.643545	0.836743
H	-0.579834	4.367633	0.247245
H	-1.440781	3.844947	-1.231567

Conformer #4

No. of imaginary frequencies = 0

Total energy = -1422.8344266

C	-0.352237	-1.433975	1.199109
C	-1.695527	-1.093978	1.868868
N	-2.248025	-0.743832	0.670392
C	-1.046984	-0.968772	-0.115570
O	-2.129834	-1.082405	2.989990
C	-1.206359	-2.016864	-1.192742
H	-0.612168	-0.060507	-0.537647
C	0.838144	-0.613445	1.672724
H	-0.112557	-2.499924	1.216793
C	-3.509775	-0.162199	0.342328
C	-3.382591	1.304691	-0.029463
O	-4.579012	1.817151	-0.319924
C	-4.600253	3.198026	-0.694276
O	-2.351866	1.922271	-0.070747
C	1.275825	-1.067168	3.058729
O	1.871152	-0.779622	0.724043
Si	3.075140	0.304377	0.296468
C	3.719728	1.185034	1.823535
C	4.402429	-0.764698	-0.468465
C	2.424577	1.574997	-0.960350
C	1.278461	2.406429	-0.361621
C	3.567704	2.527017	-1.353867
C	1.927409	0.847780	-2.219995
O	-0.089775	-2.119987	-1.913842
O	-2.199666	-2.669573	-1.379667
C	-0.093513	-3.104373	-2.950035
H	0.528422	0.441218	1.719823
H	-4.163723	-0.252006	1.213122
H	-3.984950	-0.702117	-0.481986

H	4.002909	-1.331752	-1.313337
H	4.781621	-1.481037	0.265316
H	4.420775	1.991867	-1.783368
H	3.928695	3.110310	-0.500985
H	2.747759	0.339784	-2.737491
H	1.169482	0.094660	-1.989914
H	-0.884136	-2.895691	-3.672425
H	2.929029	1.730326	2.347651
H	-5.645921	3.433351	-0.877649
H	-4.202678	3.816757	0.111292
H	-4.007824	3.356341	-1.596636
H	2.079216	-0.431942	3.435521
H	0.435886	-1.022763	3.756440
H	1.641760	-2.096406	3.010413
H	4.496626	1.906903	1.555431
H	4.158647	0.471106	2.526062
H	5.246293	-0.167885	-0.826528
H	0.953034	3.170312	-1.078831
H	1.584701	2.928383	0.550996
H	0.395743	1.807764	-0.123201
H	3.217410	3.240849	-2.109966
H	1.490775	1.566866	-2.924843
H	-0.244554	-4.098932	-2.527674
H	0.883730	-3.033978	-3.421934

Conformer #5

No. of imaginary frequencies = 0

Total energy = -1422.8341688

C	0.520311	0.677701	1.475729
C	1.972101	0.378778	1.872925
N	2.419196	0.638527	0.601306
C	1.088099	0.818518	0.030057
O	2.548361	0.008472	2.859320
C	0.803538	2.121603	-0.680208
H	0.781346	0.003742	-0.625036
C	-0.480935	-0.450549	1.672656
H	0.133761	1.609213	1.895000
C	3.634939	0.224150	-0.024919
C	3.523440	-1.173719	-0.618965
O	4.646463	-1.501462	-1.257446
C	4.676988	-2.806125	-1.846601
O	2.560173	-1.886602	-0.527467
C	-0.786122	-0.684461	3.142677
O	-1.655093	-0.090133	0.975088
Si	-2.436583	-1.039771	-0.165812
C	-1.314526	-1.338992	-1.636510

C	-2.885167	-2.683402	0.619490
C	-3.963266	-0.032750	-0.643609
C	-3.531918	1.381048	-1.066115
C	-4.687203	-0.718841	-1.813408
C	-4.916145	0.065218	0.558146
O	1.451287	3.154236	-0.136853
O	0.047734	2.213463	-1.612308
C	1.170919	4.436083	-0.704884
H	-0.042064	-1.366349	1.246936
H	4.426239	0.215980	0.728850
H	3.937474	0.926641	-0.805901
H	-3.484497	-2.540506	1.522713
H	-1.984892	-3.240752	0.897722
H	-4.989658	-1.742879	-1.567979
H	-4.063207	-0.756932	-2.711869
H	-5.300833	-0.916138	0.853941
H	-4.421541	0.511447	1.425923
H	1.781601	5.142322	-0.147226
H	-1.042966	-0.396583	-2.121348
H	5.659174	-2.897880	-2.303907
H	4.536715	-3.570465	-1.081170
H	3.893075	-2.900402	-2.599342
H	-1.490099	-1.512955	3.248518
H	0.128701	-0.918569	3.692470
H	-1.240600	0.210708	3.575551
H	-1.814511	-1.972876	-2.375572
H	-0.393741	-1.852138	-1.339930
H	-3.457133	-3.310800	-0.071114
H	-4.409241	1.964157	-1.374377
H	-2.829224	1.366477	-1.904402
H	-3.045754	1.908463	-0.241495
H	-5.597816	-0.163699	-2.070922
H	-5.779959	0.693028	0.304914
H	0.111590	4.674096	-0.596494
H	1.434139	4.451403	-1.763662

Conformer #6

No. of imaginary frequencies = 0

Total energy = -1422.8338704

C	0.660801	1.076890	1.417045
C	1.994453	0.472807	1.893010
N	2.451320	0.374568	0.610360
C	1.245835	0.886737	-0.014919
O	2.474969	0.153192	2.947292
C	1.456477	2.154505	-0.811933
H	0.700185	0.152847	-0.612059

C	-0.578927	0.268275	1.767587
H	0.526463	2.123425	1.700528
C	3.635794	-0.208347	0.062863
C	3.458995	-1.584082	-0.560883
O	2.236882	-2.089999	-0.367391
C	2.016285	-3.400273	-0.899339
O	4.335965	-2.147615	-1.157049
C	-0.900316	0.410925	3.248759
O	-1.636965	0.741171	0.959339
Si	-2.966973	-0.096215	0.382697
C	-3.600016	-1.286988	1.687941
C	-4.230588	1.226086	0.008443
C	-2.513932	-1.055438	-1.198349
C	-1.415552	-2.092346	-0.914187
C	-3.758063	-1.790415	-1.725164
C	-2.019251	-0.074363	-2.273062
O	0.345569	2.481605	-1.473868
O	2.478171	2.787331	-0.843419
C	0.397726	3.690090	-2.236117
H	-0.371547	-0.789285	1.544368
H	4.366128	-0.310446	0.869744
H	4.076400	0.449459	-0.690401
H	-3.827536	1.961168	-0.693105
H	-4.508934	1.755268	0.923733
H	-4.578225	-1.099747	-1.944741
H	-4.125377	-2.537477	-1.014685
H	-2.812607	0.614288	-2.580280
H	-1.178443	0.531339	-1.925536
H	1.174629	3.625856	-2.999375
H	-2.831889	-1.998722	2.005215
H	0.988774	-3.649496	-0.645469
H	2.154422	-3.398389	-1.981572
H	2.709330	-4.112544	-0.449936
H	-1.750246	-0.216848	3.521831
H	-0.037637	0.119019	3.852851
H	-1.151399	1.451363	3.471880
H	-4.447117	-1.863760	1.305051
H	-3.942825	-0.745986	2.574238
H	-5.140255	0.802292	-0.426957
H	-1.179945	-2.650324	-1.830013
H	-1.726230	-2.820750	-0.157589
H	-0.486587	-1.628647	-0.570810
H	-3.518387	-2.316405	-2.657772
H	-1.697860	-0.622083	-3.168315
H	0.603050	4.541040	-1.584977
H	-0.583012	3.788732	-2.695546

Conformer #7

No. of imaginary frequencies = 0

Total energy = -1422.8327667

C	0.665276	0.449250	1.479198
C	2.113124	0.063139	1.815956
N	2.538505	0.410422	0.561284
C	1.208574	0.692079	0.037960
O	2.694222	-0.400538	2.759515
C	0.960199	2.061490	-0.550759
H	0.856636	-0.049719	-0.679506
C	-0.397065	-0.628339	1.616739
H	0.341769	1.363434	1.982143
C	3.777236	0.153900	-0.105238
C	3.811265	-1.093500	-0.978041
O	2.706712	-1.835636	-0.863461
C	2.677993	-3.035405	-1.643002
O	4.741447	-1.368005	-1.685746
C	-0.666700	-0.972742	3.072082
O	-1.567335	-0.133261	1.001186
Si	-2.471157	-0.912702	-0.175637
C	-1.406081	-1.217097	-1.690033
C	-3.068366	-2.556830	0.501413
C	-3.892086	0.278464	-0.536647
C	-3.322510	1.605470	-1.063320
C	-4.829701	-0.331249	-1.591353
C	-4.681330	0.543229	0.755523
O	1.675353	3.013898	0.050278
O	0.176044	2.263096	-1.440927
C	1.434383	4.351703	-0.395330
H	-0.037124	-1.530000	1.095432
H	4.551179	0.034653	0.657557
H	4.069322	1.001009	-0.731440
H	-3.684410	-2.417752	1.393900
H	-2.222875	-3.196176	0.776135
H	-5.276211	-1.271052	-1.249743
H	-4.312236	-0.524512	-2.536828
H	-5.136958	-0.370511	1.150790
H	-4.040411	0.965720	1.534130
H	0.387673	4.618185	-0.240993
H	-1.029754	-0.275589	-2.100392
H	1.706002	-3.485423	-1.454020
H	2.794867	-2.803869	-2.702397
H	3.477391	-3.708489	-1.330525
H	-1.418231	-1.762890	3.134929
H	0.249438	-1.307673	3.564509

H	-1.048391	-0.092719	3.596175
H	-1.975919	-1.728778	-2.471820
H	-0.547556	-1.852328	-1.446470
H	-3.661771	-3.100748	-0.239702
H	-4.137402	2.316197	-1.250659
H	-2.775664	1.474431	-2.001307
H	-2.635151	2.059898	-0.345223
H	-5.652146	0.361751	-1.807151
H	-5.492235	1.256464	0.561391
H	1.676559	4.451433	-1.454387
H	2.083460	4.982135	0.207765

Compound 26d

Conformer #1
No. of imaginary frequencies = 0
Total energy = -1422.8344224

C	0.541212	-0.333567	-1.303813
C	1.961101	-0.646442	-1.804696
N	2.514590	0.170670	-0.860645
C	1.258959	0.550476	-0.238034
C	0.946364	2.026346	-0.322625
H	1.133061	0.194162	0.786003
O	2.445227	-1.338696	-2.659400
C	3.875907	0.481777	-0.552745
C	4.417541	-0.134657	0.726923
O	3.508424	-0.870790	1.373628
O	5.542647	0.037328	1.109462
C	3.956621	-1.500580	2.577379
H	-0.029024	0.256574	-2.023833
C	-0.294166	-1.503156	-0.783363
O	1.579617	2.832460	-0.951142
O	-0.147457	2.314906	0.386387
C	-0.589528	3.673872	0.340455
O	-1.338143	-0.997064	0.023334
C	0.504960	-2.509986	0.028906
Si	-2.879433	-0.574482	-0.479855
C	-2.789073	0.834667	-1.716465
C	-3.700591	-2.058771	-1.277812
C	-3.771133	-0.049158	1.103474
C	-3.605334	-1.139753	2.173470
C	-3.172988	1.267318	1.624807
C	-5.266470	0.155518	0.809993
H	4.019473	1.564060	-0.488345
H	4.497475	0.121734	-1.376024
H	4.301435	-0.753626	3.293688

H	4.770067	-2.194196	2.360725
H	3.093010	-2.035309	2.966460
H	-0.702750	-2.020430	-1.663160
H	-0.845025	3.954619	-0.683001
H	-1.468668	3.714523	0.979450
H	0.188151	4.342814	0.711450
H	-0.165650	-3.291555	0.390001
H	1.285231	-2.969099	-0.582561
H	0.974120	-2.033882	0.893343
H	-3.785342	1.232534	-1.932975
H	-2.175466	1.650323	-1.324072
H	-2.357233	0.507804	-2.667537
H	-4.691321	-1.796368	-1.661020
H	-3.820167	-2.877979	-0.563407
H	-3.115939	-2.434423	-2.123113
H	-4.116832	-0.842770	3.097600
H	-4.037606	-2.093180	1.852495
H	-2.551288	-1.309953	2.406587
H	-3.655542	1.553080	2.567867
H	-3.330477	2.084774	0.913110
H	-2.097886	1.178197	1.802500
H	-5.434757	0.919405	0.043047
H	-5.747963	-0.769008	0.476359
H	-5.785968	0.486660	1.717562

Conformer #2

No. of imaginary frequencies = 0

Total energy =-1422.8336803

C	-0.336821	-0.056445	1.198062
C	-1.627861	-0.570091	1.858594
N	-2.402290	0.076746	0.936976
C	-1.290062	0.618802	0.171756
C	-1.264075	2.128013	0.120185
H	-1.194951	0.212317	-0.838330
O	-1.906040	-1.275172	2.791810
C	-3.811662	0.057141	0.704211
C	-4.174945	-0.741856	-0.534806
O	-5.497497	-0.753038	-0.709380
O	-3.389761	-1.279295	-1.269556
C	-5.975848	-1.469399	-1.851741
H	0.202496	0.660358	1.819677
C	0.622930	-1.104717	0.627405
O	-2.167855	2.844512	0.462980
O	-0.102062	2.570977	-0.368053
C	0.032919	3.990111	-0.480690
O	1.385531	-0.500399	-0.399062

C	-0.077459	-2.325181	0.052262
Si	2.870271	0.257885	-0.270354
C	2.973264	1.378785	-1.759153
C	2.945118	1.253769	1.319354
C	4.244266	-1.054636	-0.305789
C	4.038990	-2.076506	0.824386
C	4.205449	-1.793093	-1.653539
C	5.616073	-0.382708	-0.133666
H	-4.203596	1.072884	0.602093
H	-4.292285	-0.397762	1.573765
H	-7.055671	-1.340931	-1.845414
H	-5.715384	-2.525872	-1.772825
H	-5.545243	-1.058860	-2.766066
H	1.270970	-1.431233	1.451597
H	-0.073434	4.463189	0.496603
H	1.031096	4.157736	-0.879965
H	-0.721662	4.391600	-1.158712
H	0.667804	-2.990591	-0.388170
H	-0.612711	-2.867146	0.835489
H	-0.791561	-2.043916	-0.725920
H	3.926749	1.914087	-1.796385
H	2.865730	0.810296	-2.686362
H	2.163655	2.111471	-1.722356
H	3.916387	1.745522	1.426813
H	2.791629	0.632061	2.206760
H	2.175663	2.031078	1.310497
H	4.853829	-2.811231	0.823338
H	4.028100	-1.603107	1.811879
H	3.103182	-2.630315	0.701626
H	4.955724	-2.593597	-1.669126
H	4.425515	-1.122826	-2.490159
H	3.226632	-2.247771	-1.834402
H	5.806057	0.366917	-0.909132
H	5.712607	0.107319	0.840452
H	6.414738	-1.131916	-0.202045

Conformer #3

No. of imaginary frequencies = 0

Total energy =-1422.8334606

C	-0.215233	-0.383656	0.981322
C	-1.488017	-0.789761	1.741397
N	-2.260360	0.006471	0.945653
C	-1.176659	0.468120	0.094470
C	-0.933964	1.958336	0.155712
H	-1.239051	0.131886	-0.941035
O	-1.756534	-1.520664	2.657260

C	-3.669459	0.232510	0.907911
C	-4.305332	-0.340834	-0.345966
O	-5.622324	-0.125416	-0.339717
O	-3.713881	-0.898342	-1.231139
C	-6.343395	-0.607995	-1.477256
H	0.447413	0.233021	1.592490
C	0.574351	-1.479078	0.270993
O	-1.410033	2.702039	0.973533
O	-0.095785	2.338582	-0.809597
C	0.299249	3.711634	-0.795052
O	1.380735	-0.845434	-0.701601
C	-0.300691	-2.531537	-0.393222
Si	3.047122	-0.802145	-0.817753
C	3.726728	-2.541636	-0.645019
C	3.363664	-0.108482	-2.521750
C	3.790806	0.327699	0.523171
C	3.122590	1.710130	0.465354
C	3.587095	-0.275656	1.922328
C	5.299939	0.489147	0.272172
H	-3.896019	1.301694	0.968813
H	-4.113849	-0.245183	1.784442
H	-7.387202	-0.372292	-1.284131
H	-6.206441	-1.684661	-1.586024
H	-5.998863	-0.109043	-2.384336
H	1.195031	-1.976110	1.029285
H	0.810697	3.948178	0.139685
H	0.976607	3.829548	-1.637758
H	-0.569424	4.362398	-0.905290
H	0.333918	-3.245393	-0.922136
H	-0.885966	-3.072814	0.354357
H	-0.988172	-2.082915	-1.114340
H	4.818328	-2.548267	-0.719551
H	3.459409	-2.994102	0.314418
H	3.335389	-3.184638	-1.438577
H	4.432651	0.005247	-2.722547
H	2.886922	0.868996	-2.633329
H	2.944518	-0.771316	-3.283441
H	3.539870	2.368310	1.237963
H	3.279551	2.196372	-0.502833
H	2.043645	1.642441	0.625432
H	4.018109	0.384041	2.685743
H	4.073634	-1.250880	2.020502
H	2.529231	-0.404229	2.169936
H	5.826716	-0.469963	0.309192
H	5.505366	0.950759	-0.698532
H	5.743343	1.133884	1.041280

Conformer #4

No. of imaginary frequencies = 0

Total energy =-1422.8327343

C	0.541212	-0.333567	-1.303813
C	1.961101	-0.646442	-1.804696
N	2.514590	0.170670	-0.860645
C	1.258959	0.550476	-0.238034
C	0.946364	2.026346	-0.322625
H	1.133061	0.194162	0.786003
O	2.445227	-1.338696	-2.659400
C	3.875907	0.481777	-0.552745
C	4.417541	-0.134657	0.726923
O	3.508424	-0.870790	1.373628
O	5.542647	0.037328	1.109462
C	3.956621	-1.500580	2.577379
H	-0.029024	0.256574	-2.023833
C	-0.294166	-1.503156	-0.783363
O	1.579617	2.832460	-0.951142
O	-0.147457	2.314906	0.386387
C	-0.589528	3.673872	0.340455
O	-1.338143	-0.997064	0.023334
C	0.504960	-2.509986	0.028906
Si	-2.879433	-0.574482	-0.479855
C	-2.789073	0.834667	-1.716465
C	-3.700591	-2.058771	-1.277812
C	-3.771133	-0.049158	1.103474
C	-3.605334	-1.139753	2.173470
C	-3.172988	1.267318	1.624807
C	-5.266470	0.155518	0.809993
H	4.019473	1.564060	-0.488345
H	4.497475	0.121734	-1.376024
H	4.301435	-0.753626	3.293688
H	4.770067	-2.194196	2.360725
H	3.093010	-2.035309	2.966460
H	-0.702750	-2.020430	-1.663160
H	-0.845025	3.954619	-0.683001
H	-1.468668	3.714523	0.979450
H	0.188151	4.342814	0.711450
H	-0.165650	-3.291555	0.390001
H	1.285231	-2.969099	-0.582561
H	0.974120	-2.033882	0.893343
H	-3.785342	1.232534	-1.932975
H	-2.175466	1.650323	-1.324072
H	-2.357233	0.507804	-2.667537
H	-4.691321	-1.796368	-1.661020

H	-3.820167	-2.877979	-0.563407
H	-3.115939	-2.434423	-2.123113
H	-4.116832	-0.842770	3.097600
H	-4.037606	-2.093180	1.852495
H	-2.551288	-1.309953	2.406587
H	-3.655542	1.553080	2.567867
H	-3.330477	2.084774	0.913110
H	-2.097886	1.178197	1.802500
H	-5.434757	0.919405	0.043047
H	-5.747963	-0.769008	0.476359
H	-5.785968	0.486660	1.717562

Conformer #5

No. of imaginary frequencies = 0

Total energy =-1422.8323951

C	0.249379	1.355650	0.379547
C	1.596930	2.087339	0.282974
N	2.086335	1.149922	-0.591149
C	0.870032	0.329605	-0.590486
C	1.054120	-1.075014	-0.044386
H	0.390671	0.266911	-1.571055
O	2.089523	3.080659	0.745059
C	3.400550	0.935470	-1.114411
C	4.283783	-0.012319	-0.313712
O	3.731079	-0.361216	0.847729
O	5.358745	-0.387015	-0.697353
C	4.498172	-1.233934	1.679821
H	0.098621	0.922668	1.369121
C	-1.018339	2.058716	-0.111018
O	0.688571	-1.474348	1.028097
O	1.689063	-1.830571	-0.946985
C	1.958911	-3.179324	-0.556652
O	-1.957542	1.063048	-0.467172
C	-0.787749	2.959550	-1.313225
Si	-3.104828	0.339513	0.520439
C	-2.372441	-0.042762	2.201405
C	-4.558878	1.504093	0.721378
C	-3.581882	-1.236757	-0.413886
C	-4.291165	-0.871506	-1.727585
C	-2.315212	-2.047144	-0.733348
C	-4.522494	-2.087244	0.455019
H	3.913900	1.900375	-1.147813
H	3.352520	0.550926	-2.135452
H	3.845169	-1.491529	2.510425
H	5.393284	-0.723088	2.037610
H	4.793948	-2.126470	1.125770

H	-1.400708	2.674719	0.714723
H	1.024710	-3.710689	-0.369080
H	2.494144	-3.626156	-1.390999
H	2.570468	-3.196389	0.346901
H	-1.736262	3.397070	-1.628886
H	-0.092422	3.765089	-1.065240
H	-0.382342	2.390909	-2.154943
H	-3.126122	-0.499051	2.850782
H	-1.523109	-0.727044	2.125607
H	-2.028787	0.869734	2.699664
H	-5.361884	1.038315	1.301290
H	-4.968242	1.800010	-0.248073
H	-4.258661	2.413918	1.250570
H	-4.524652	-1.780679	-2.296019
H	-5.234881	-0.347280	-1.547424
H	-3.664311	-0.233490	-2.357651
H	-2.582658	-2.975191	-1.254558
H	-1.763975	-2.319293	0.171844
H	-1.641202	-1.480824	-1.382792
H	-4.038363	-2.412310	1.381216
H	-5.436045	-1.545393	0.722533
H	-4.827370	-2.989349	-0.089778

Conformer #6

No. of imaginary frequencies = 0

Total energy =-1422.832079

C	0.452959	-0.778474	-1.253111
C	1.903783	-1.069791	-1.665769
N	2.349116	0.067695	-1.035516
C	1.049408	0.385883	-0.434574
C	0.545060	1.776065	-0.768087
H	1.028844	0.231884	0.646019
O	2.489641	-1.928693	-2.266096
C	3.673756	0.493365	-0.701154
C	4.178046	0.083702	0.675724
O	3.369988	-0.786659	1.283049
O	5.202967	0.499340	1.143917
C	3.801832	-1.256401	2.563395
H	-0.132994	-0.405644	-2.094623
C	-0.336176	-1.818965	-0.458205
O	-0.126051	2.069130	-1.721685
O	0.967641	2.654984	0.145752
C	0.549216	4.010235	-0.044536
O	-1.326970	-1.125156	0.277805
C	0.509196	-2.631042	0.508832
Si	-2.899856	-0.801402	-0.205714

C	-2.928338	-0.214545	-1.984289
C	-3.918179	-2.366190	-0.044046
C	-3.481060	0.549010	0.987503
C	-3.532715	-0.007838	2.418948
C	-2.503525	1.734709	0.942282
C	-4.881276	1.031481	0.575581
H	3.768535	1.579496	-0.770663
H	4.359462	0.060321	-1.434632
H	3.045620	-1.970220	2.882460
H	3.870806	-0.427448	3.269244
H	4.775115	-1.741166	2.479238
H	-0.800652	-2.509219	-1.176214
H	-0.539249	4.075106	-0.002350
H	0.997001	4.571717	0.771967
H	0.897141	4.386299	-1.007625
H	-0.133134	-3.316862	1.064182
H	1.265393	-3.207378	-0.029307
H	1.014448	-1.976434	1.222971
H	-3.957113	-0.024240	-2.305501
H	-2.351089	0.704333	-2.119489
H	-2.517843	-0.973825	-2.658088
H	-4.975293	-2.177839	-0.255413
H	-3.841903	-2.785291	0.962716
H	-3.574602	-3.127717	-0.751168
H	-3.824308	0.781647	3.123072
H	-4.265319	-0.815636	2.512764
H	-2.559362	-0.395650	2.733569
H	-2.845509	2.529849	1.617182
H	-2.424689	2.161997	-0.062532
H	-1.501556	1.434043	1.262838
H	-4.879786	1.481202	-0.422260
H	-5.614138	0.217738	0.578860
H	-5.239312	1.793892	1.278483

Conformer #7

No. of imaginary frequencies = 0

Total energy =-1422.8320409

C	-0.465852	0.029316	1.187795
C	-1.773692	-0.442761	1.846608
N	-2.525138	0.165336	0.880832
C	-1.395574	0.661047	0.111972
C	-1.341807	2.166527	-0.001956
H	-1.282629	0.207858	-0.876162
O	-2.072828	-1.101113	2.806640
C	-3.936036	0.178508	0.644161
C	-4.420175	-0.715485	-0.486026

O	-3.424682	-1.366962	-1.096083
O	-5.576811	-0.811585	-0.793627
C	-3.811459	-2.245786	-2.156355
H	0.060372	0.774970	1.786610
C	0.503928	-1.047715	0.694334
O	-2.199237	2.918628	0.378858
O	-0.204800	2.558985	-0.584525
C	-0.032896	3.970814	-0.736951
O	1.285683	-0.508752	-0.352972
C	-0.186142	-2.300668	0.179588
Si	2.758977	0.278460	-0.245836
C	2.892921	1.260431	-1.827349
C	2.772546	1.413964	1.248691
C	4.148891	-1.011700	-0.118746
C	3.915288	-1.936226	1.086889
C	4.171465	-1.863909	-1.398084
C	5.504047	-0.304676	0.045386
H	-4.280381	1.195352	0.439197
H	-4.433196	-0.156107	1.557733
H	-2.888400	-2.695370	-2.515733
H	-4.302840	-1.687284	-2.954435
H	-4.491663	-3.012684	-1.783795
H	1.135179	-1.326502	1.548274
H	-0.062506	4.465776	0.234811
H	0.942787	4.098626	-1.201198
H	-0.816509	4.383199	-1.374149
H	0.566598	-2.994532	-0.199740
H	-0.747516	-2.790203	0.978626
H	-0.875515	-2.059508	-0.633352
H	3.839460	1.805971	-1.885196
H	2.823073	0.607525	-2.701027
H	2.072225	1.979636	-1.881389
H	3.732058	1.932414	1.334794
H	2.608309	0.871982	2.185140
H	1.990579	2.172599	1.152276
H	4.743950	-2.648868	1.183801
H	3.851410	-1.381556	2.029050
H	2.997777	-2.521660	0.973670
H	4.931360	-2.651174	-1.316270
H	4.414919	-1.265344	-2.281319
H	3.206105	-2.348079	-1.575432
H	5.710537	0.386196	-0.778849
H	5.558227	0.260340	0.981234
H	6.315212	-1.043064	0.062628

Conformer #8

No. of imaginary frequencies = 0

Total energy =-1422.8319844

C	0.207480	1.271486	0.447288
C	1.558496	1.996856	0.518045
N	2.096726	1.163844	-0.428221
C	0.874353	0.374588	-0.621969
C	1.072758	-1.106951	-0.359927
H	0.459117	0.474155	-1.627940
O	2.023057	2.925572	1.122647
C	3.439417	0.980637	-0.878438
C	4.183457	-0.089617	-0.091186
O	5.402389	-0.270114	-0.599916
O	3.745264	-0.684763	0.855151
C	6.209362	-1.262802	0.040613
H	0.016985	0.723741	1.369298
C	-1.039148	2.038476	0.009740
O	1.577452	-1.835552	-1.175803
O	0.657526	-1.497436	0.840754
C	0.938490	-2.856368	1.184851
O	-1.984947	1.093224	-0.455913
C	-0.782911	3.055413	-1.089924
Si	-3.165536	0.321095	0.449410
C	-2.479935	-0.187312	2.119687
C	-4.606916	1.491548	0.698174
C	-3.642640	-1.187787	-0.588929
C	-4.291693	-0.730621	-1.904703
C	-2.383406	-2.009938	-0.906301
C	-4.636471	-2.059326	0.195769
H	3.974692	1.926879	-0.761817
H	3.459984	0.715118	-1.938336
H	7.159562	-1.253244	-0.488046
H	5.735502	-2.242130	-0.040670
H	6.353267	-1.016409	1.093450
H	-1.427103	2.572065	0.888835
H	2.017753	-3.009199	1.219797
H	0.498383	-3.005482	2.168479
H	0.492168	-3.534038	0.455293
H	-1.720715	3.542463	-1.362412
H	-0.074785	3.816600	-0.753489
H	-0.382391	2.571629	-1.984939
H	-3.259396	-0.664740	2.721381
H	-1.649356	-0.890200	2.013124
H	-2.120379	0.678536	2.684823
H	-5.427606	1.005364	1.234713
H	-4.993240	1.851668	-0.259063
H	-4.301880	2.363226	1.285716

H	-4.532398	-1.599618	-2.529942
H	-5.224895	-0.186425	-1.728362
H	-3.623488	-0.081102	-2.477553
H	-2.649067	-2.903275	-1.485095
H	-1.876020	-2.345409	0.003783
H	-1.669346	-1.430132	-1.497369
H	-4.197144	-2.447466	1.120314
H	-5.546556	-1.509575	0.458731
H	-4.941319	-2.922384	-0.408989

Conformer #9

No. of imaginary frequencies = 0

Total energy = -1422.8319249

C	-0.336829	-0.202966	1.014649
C	-1.627670	-0.477328	1.802748
N	-2.358431	0.291712	0.942846
C	-1.259549	0.598478	0.043920
C	-0.930555	2.070286	-0.062512
H	-1.347355	0.151726	-0.947655
O	-1.931721	-1.117087	2.773426
C	-3.756894	0.577585	0.873535
C	-4.519892	-0.153649	-0.220201
O	-3.770762	-1.056661	-0.858759
O	-5.674081	0.065258	-0.469821
C	-4.433815	-1.805975	-1.881139
H	0.343141	0.447266	1.569059
C	0.418426	-1.391129	0.429357
O	-1.285580	2.912867	0.718901
O	-0.164730	2.305048	-1.129239
C	0.309064	3.644957	-1.279675
O	1.264109	-0.894530	-0.588134
C	-0.486115	-2.472956	-0.141797
Si	2.935503	-0.931276	-0.660376
C	3.528950	-2.655800	-0.221165
C	3.333031	-0.502965	-2.432874
C	3.686667	0.346913	0.533348
C	3.039909	1.721539	0.303438
C	3.465874	-0.079034	1.994088
C	5.199034	0.454286	0.272349
H	-3.928154	1.649297	0.741950
H	-4.206221	0.293362	1.828561
H	-4.788095	-1.140743	-2.669931
H	-5.281259	-2.350169	-1.462494
H	-3.688223	-2.497661	-2.266853
H	1.005409	-1.832578	1.246632
H	0.935060	3.921939	-0.429451

H	0.892705	3.647297	-2.197445
H	-0.526622	4.342224	-1.353813
H	0.127868	-3.275772	-0.554955
H	-1.130728	-2.889513	0.635998
H	-1.115734	-2.075452	-0.941302
H	4.621507	-2.705012	-0.191022
H	3.159088	-2.976738	0.757091
H	3.183010	-3.380946	-0.963311
H	4.406755	-0.570676	-2.629620
H	3.003985	0.511187	-2.674531
H	2.820406	-1.190335	-3.110898
H	3.466761	2.462646	0.990813
H	3.204721	2.083020	-0.716655
H	1.960135	1.691556	0.469714
H	3.893892	0.665876	2.676352
H	3.944539	-1.038005	2.214678
H	2.404657	-0.171032	2.244603
H	5.709885	-0.503499	0.416460
H	5.413031	0.801646	-0.743135
H	5.652105	1.172349	0.967107

3.4. HPLC with *on-line* ECD analysis in combination with TDDFT calculations: a representative example

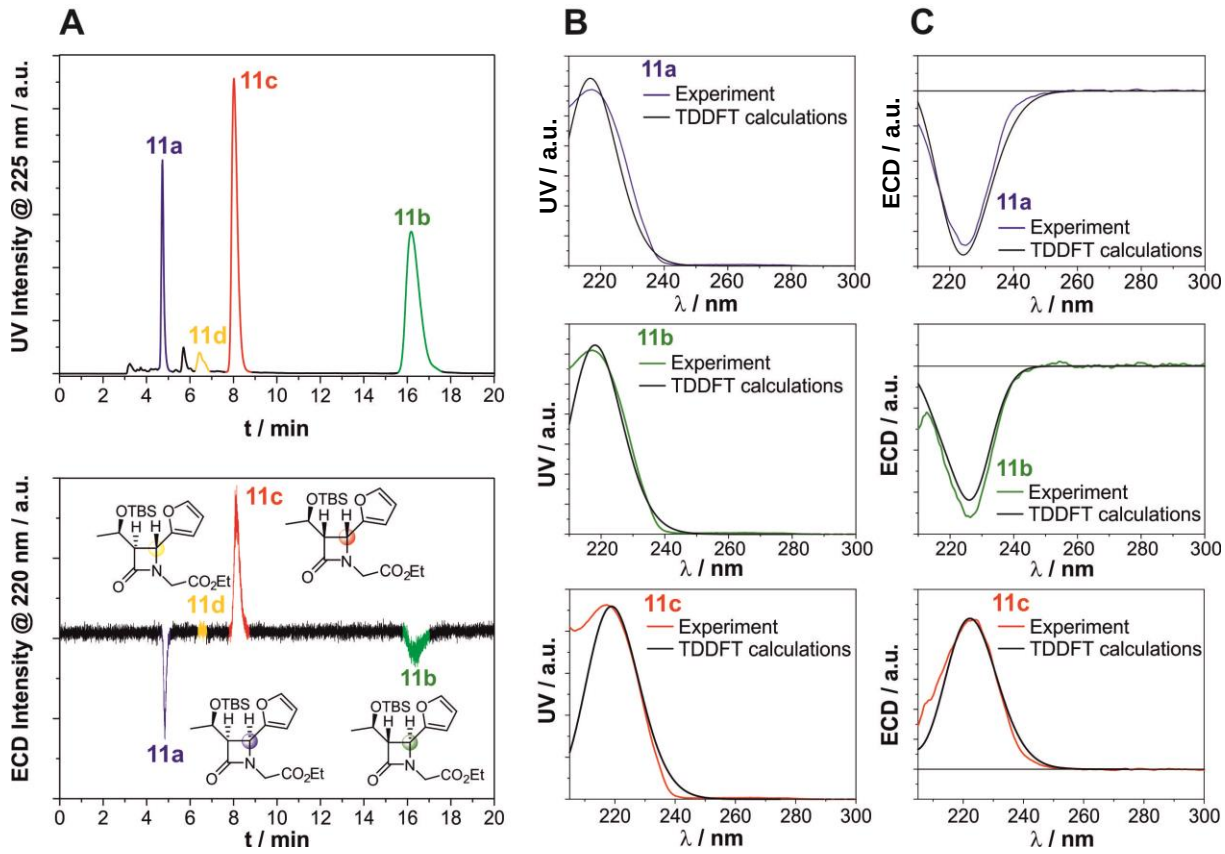


Figure S4. (A) UV (top) and ECD (bottom) chromatogram of **11abcd** mixture on Daicel Chiralcel® AS-H (250 × 4.6 mm, 5 μm) column, eluent *i*-PrOH/hexane = 5/95, flow 1 mL/min, UV detection at 225 nm, ECD detection at 220 nm; **(B)** and **(C)** *on-line* UV and ECD spectra compared to those computed at CAM-B3LYP/def2-TZVP level of theory. Note that using $c \sim 1$ mg/ml it was not possible to record a full ECD spectrum.

4. Crystallographic data

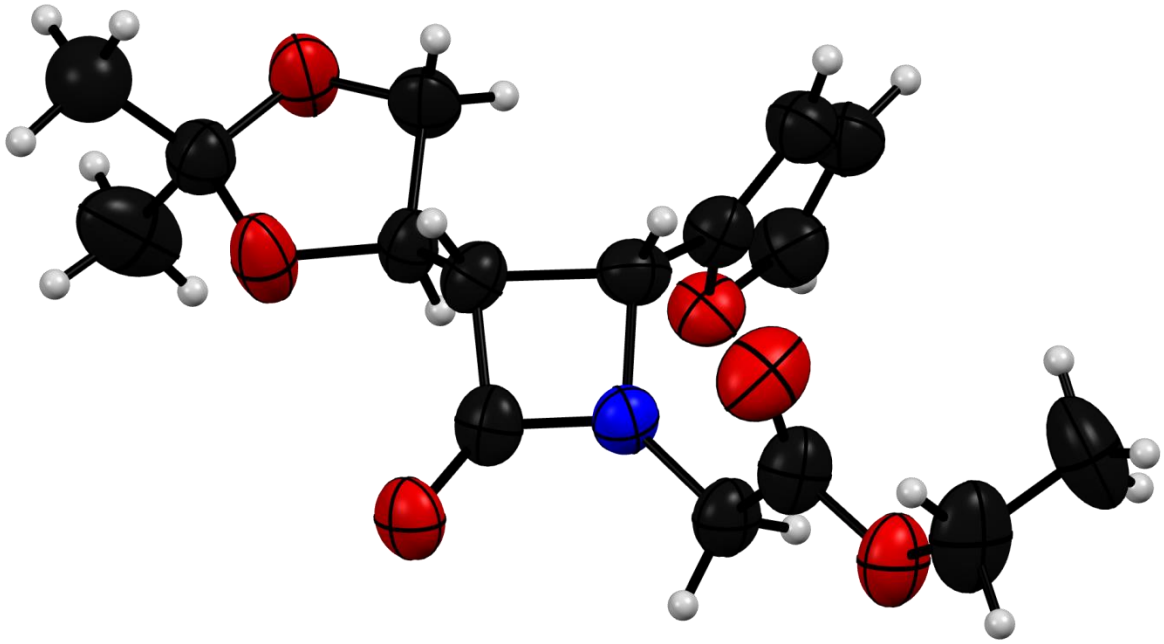


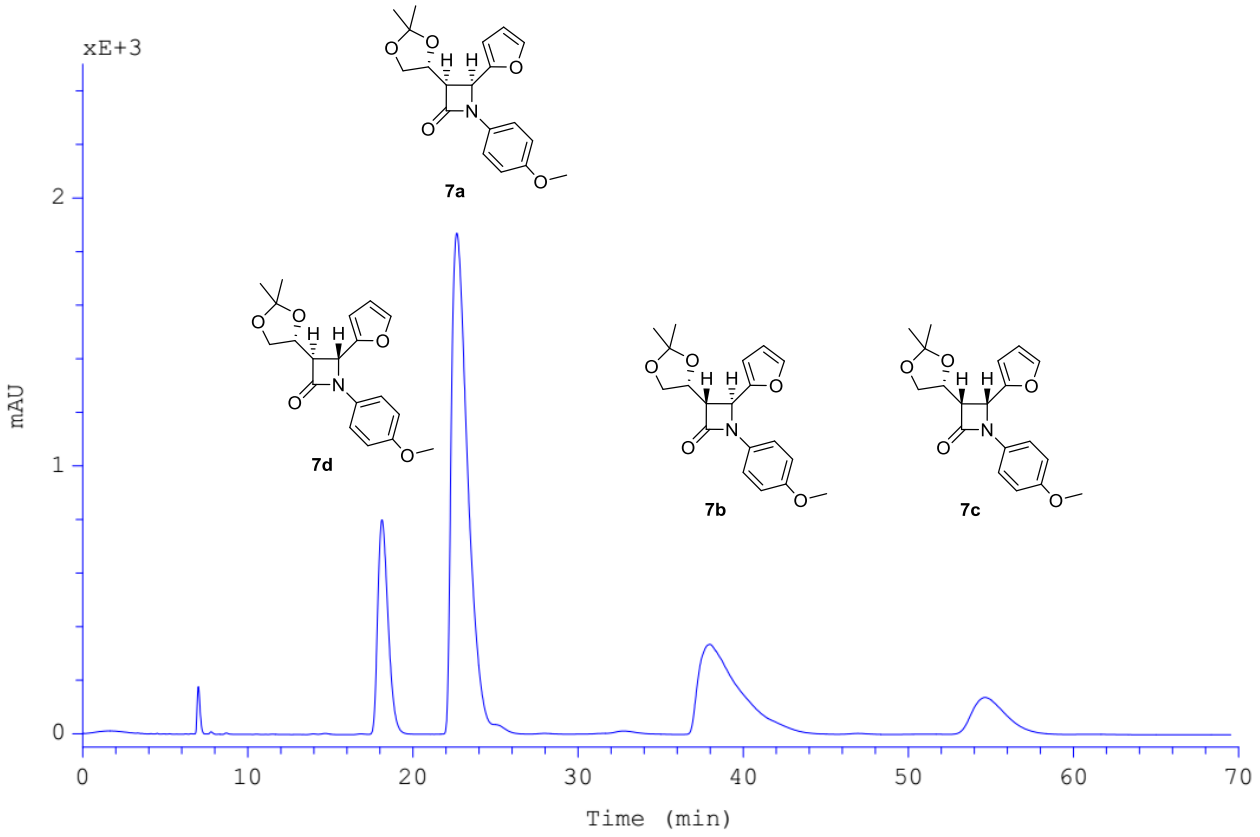
Figure S5. ORTEP plot of **8c**, represented by thermal ellipsoids shown at the 35% probability level.

Colorless crystals suitable for X-ray structural analysis were obtained by slow evaporation of heptane–ether solution of **8c**. Crystal data were obtained on a Bruker APEX II CCD detector employing graphite monochromated Cu-Kα radiation (λ=1.54178 Å) at 296(2) K and operating in the φ-ω scan mode. The structure was solved by direct methods SHELXS-2014[3] and refined with full-matrix least-squares calculations on F^2 using SHELX-2014. [3] All non-hydrogen atoms were refined anisotropically. The hydrogen atom positions were geometrically idealized and allowed to ride on their parent atoms. Crystallographic data for **8c** have been deposited at the Cambridge Crystallographic Data Centre (deposition no. **CCDC 1878740**). Copies of these data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK [fax: (+44) 1223-336-033; or email: deposit@ccdc.cam.ac.uk].

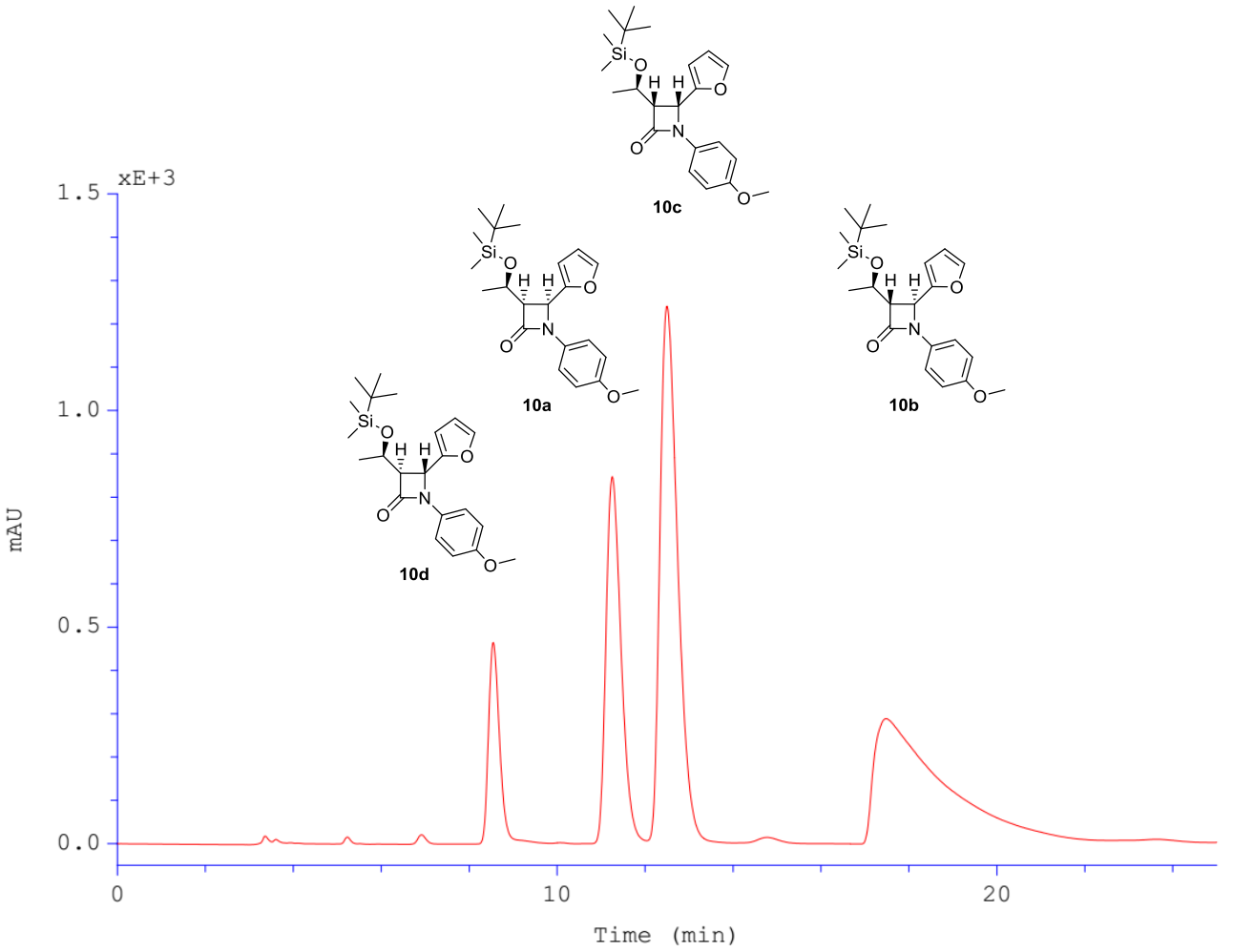
Table S5. Summary of the crystal parameters and refinement metrics for **8c**.

Chemical formula	$C_{16}H_{21}NO_6$	**θ range [°]**	4.88 to 66.58
Formula weight	323.34 g/mol	**Index ranges**	-5<=h<=6, -20<=k<=18, -9<=l<=9
CCDC number	1878740	**Reflections collected**	5201
Crystal appearance	colorless block	**Reflections unique**	1983 [R(int) = 0.0465]
Crystal size [mm]	0.215 x 0.350 x 0.440	**Completeness**	78.4%
Crystal system	monoclinic	**Absorption correction**	numerical
Space group	P 1 2_1 1	**Max and min transmission**	0.8430 and 0.7130
***a* [Å]**	5.4441(3)	**Solution method**	direct methods
***b* [Å]**	18.1287(8)	**Refinement method**	Full-matrix least-squares on F^2
***c* [Å]**	8.5243(4)	**H atom treatment**	geometrically idealized
***α* [°]**	90	**Data/restraints/parameters**	1983 / 1 / 214
***β* [°]**	95.698(3)	**Goodness-of-fit on F^2**	0.873
***γ* [°]**	90	**Final R indices [I>2σ(I)][4]**	1551 data; R1 = 0.0645, wR2 = 0.1458
***V* [Å^3]**	837.14(7)	**R indices (all data)**	R1 = 0.0942, wR2 = 0.1886
Z	2	**Absolute structure parameter**	-0.5(9)
T [K]	296(2)	**Largest diff peak and hole [eÅ^{-3}]**	0.252 and -0.334
***$D_{calc.}$* [gcm^{-3}]**	1.283		
μ [mm^{-1}]	0.824		
F(000)	344		

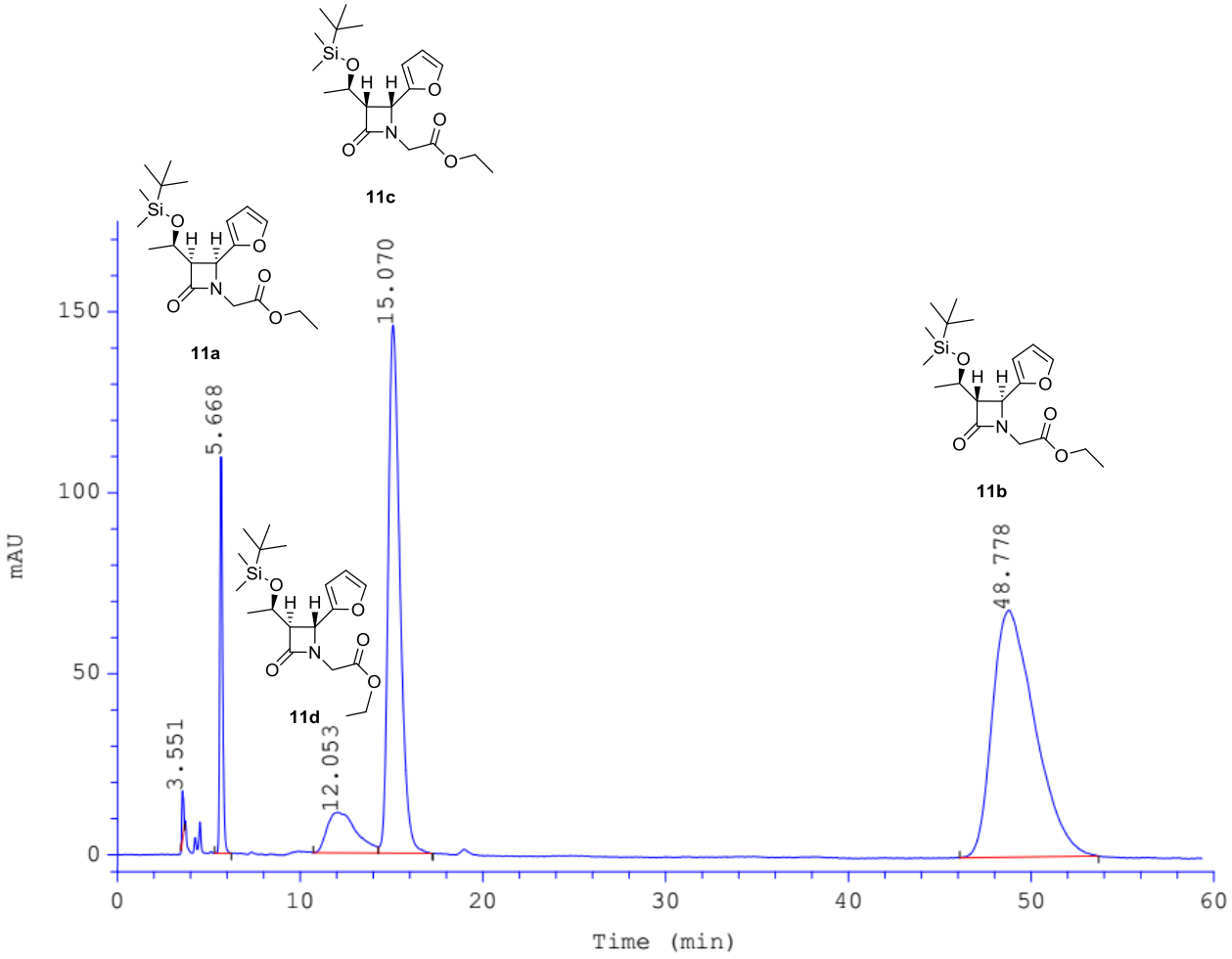
5. HPLC analyses of reference samples



conditions	Daicel Chiralcel® OD-H, *i*-PrOH/Hexane 5/95, 1 mL/min, 254 nm			
product	**7a**	**7b**	**7c**	**7d**
t_R/min	22.6	38.0	54.6	18.1

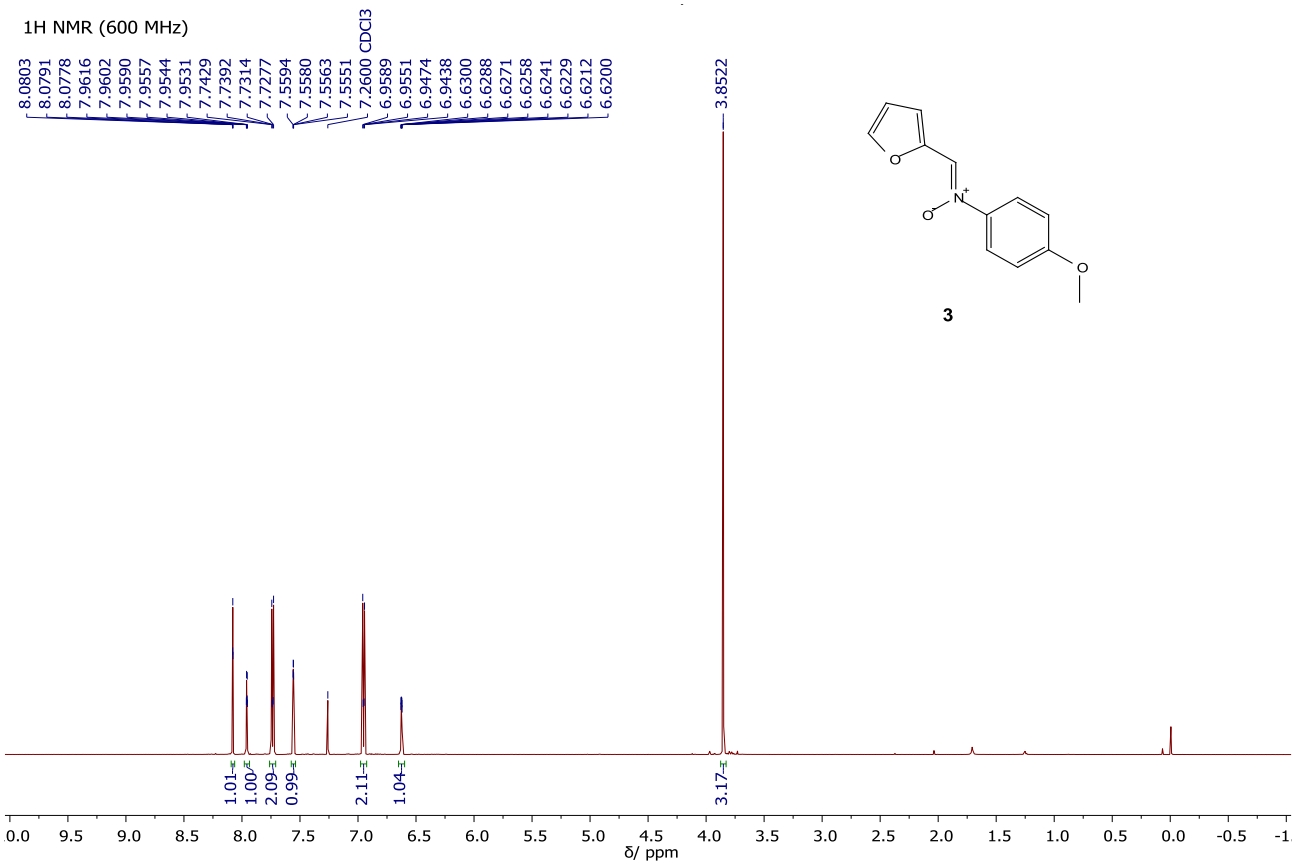


conditions	Daicel Chiralcel® OD-H, *i*-PrOH/Hexane 2/98, 1 mL/min, 254 nm			
product	**10a**	**10b**	**10c**	**10d**
t_R/min	11.5	17.7	12.6	8.3



conditions	Daicel Chiralcel® AS-H, *i*-PrOH/Hexane 5/95, 1 mL/min, 225 nm			
product	**11a**	**11b**	**11c**	**11d**
t_R/min	5.7	48.8	15.1	12.1

6. NMR spectra



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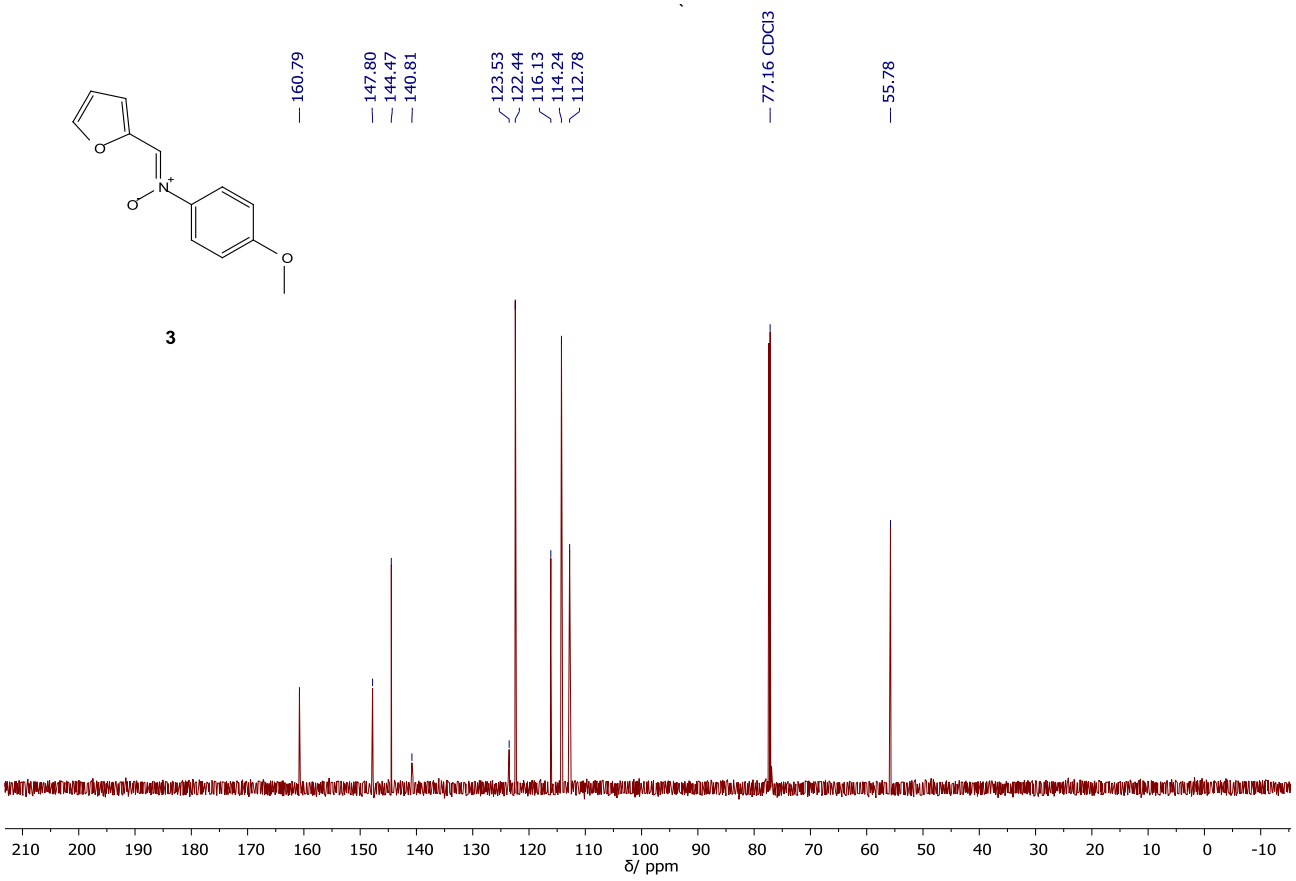
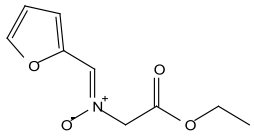
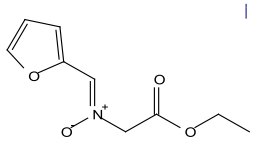


3

1H NMR (400 MHz)

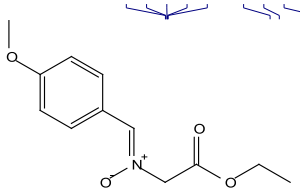


4

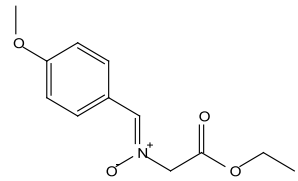


4

1H NMR (500 MHz)



5



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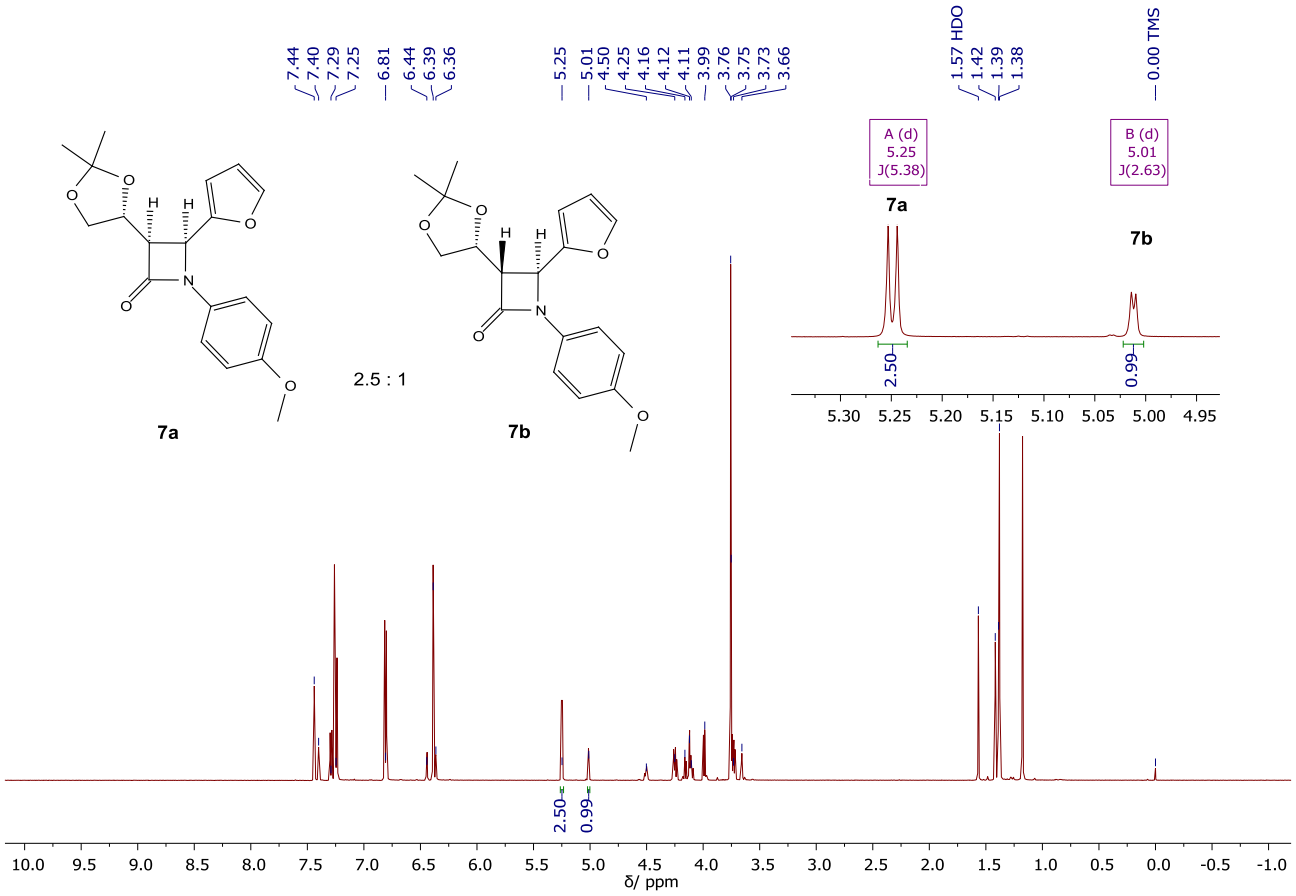
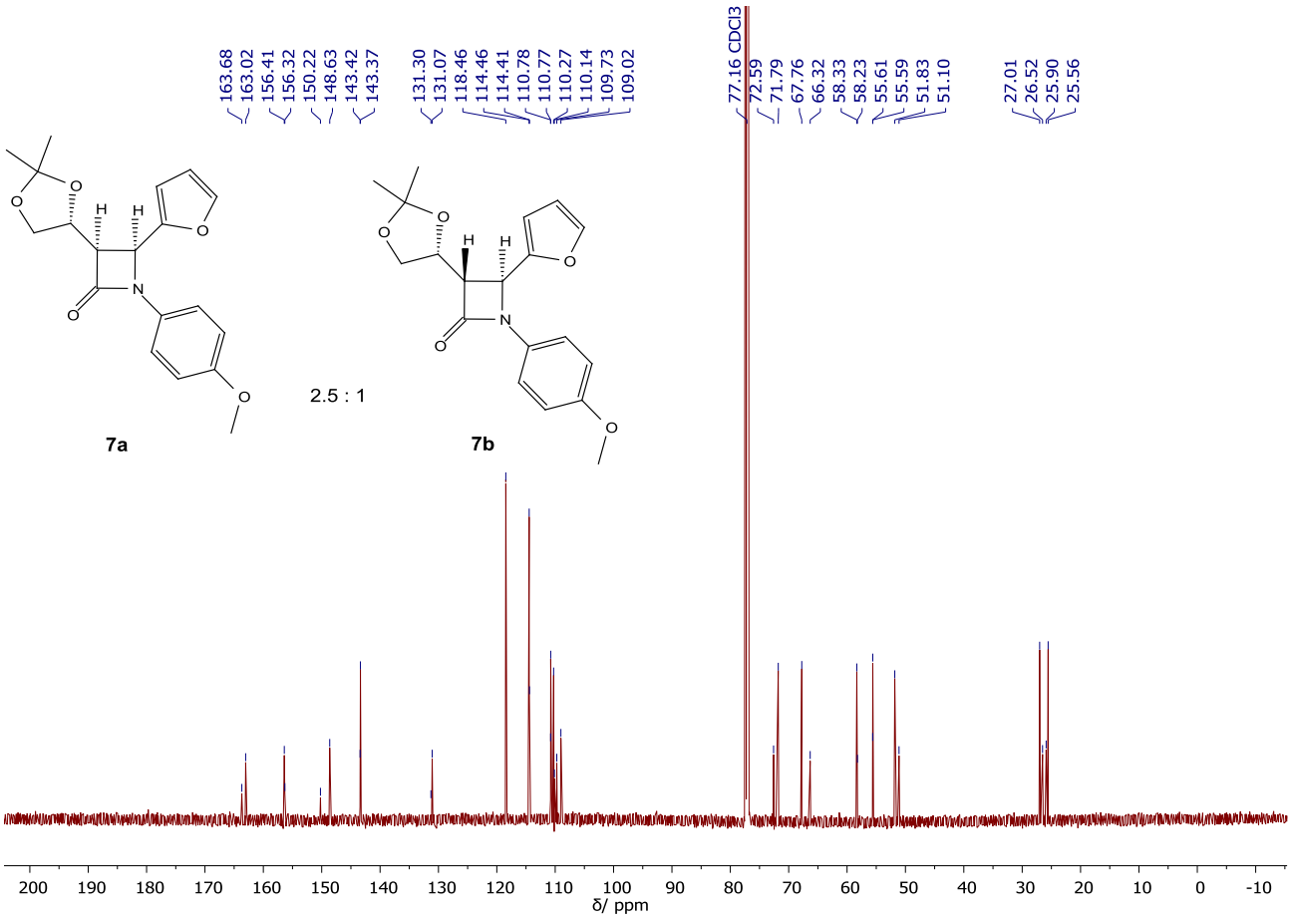
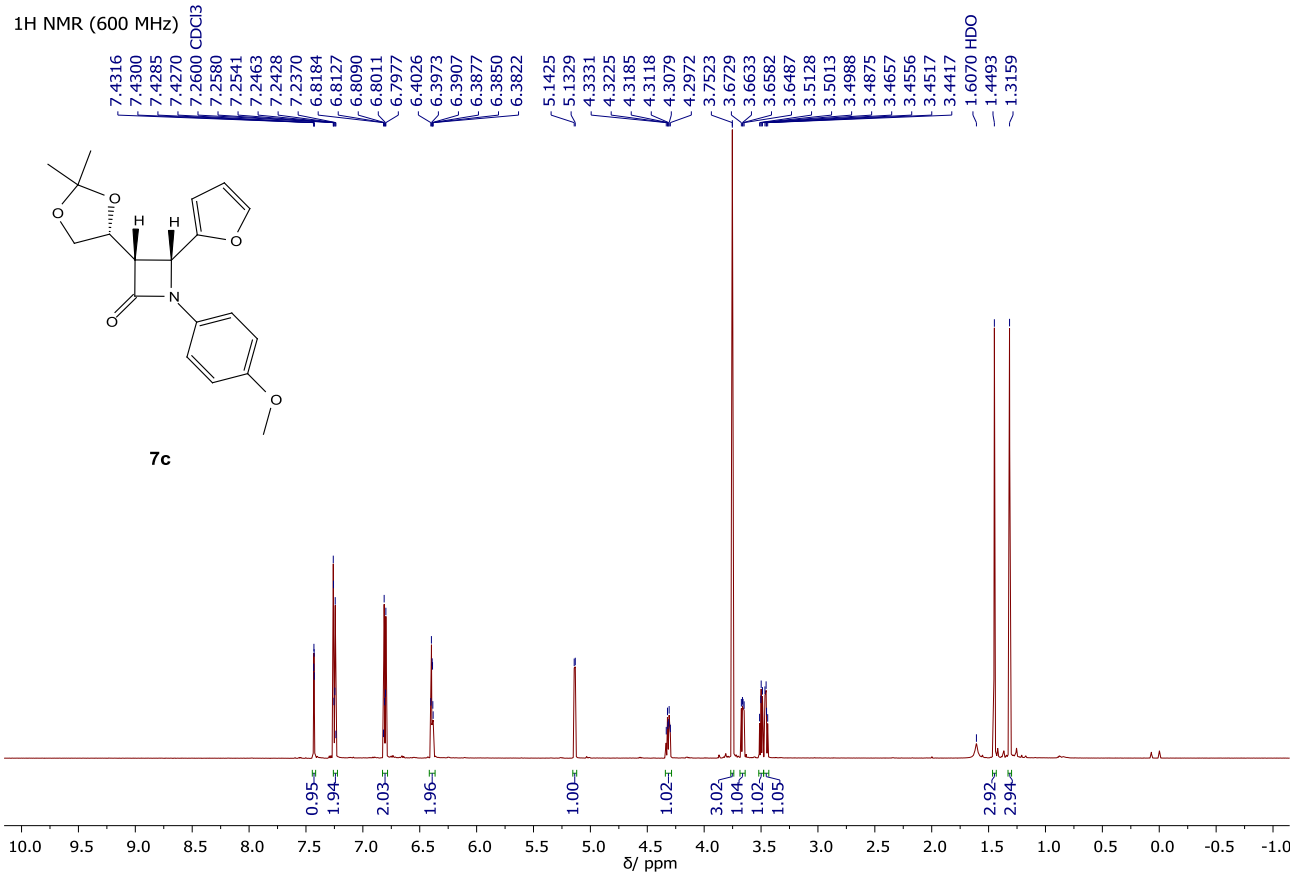
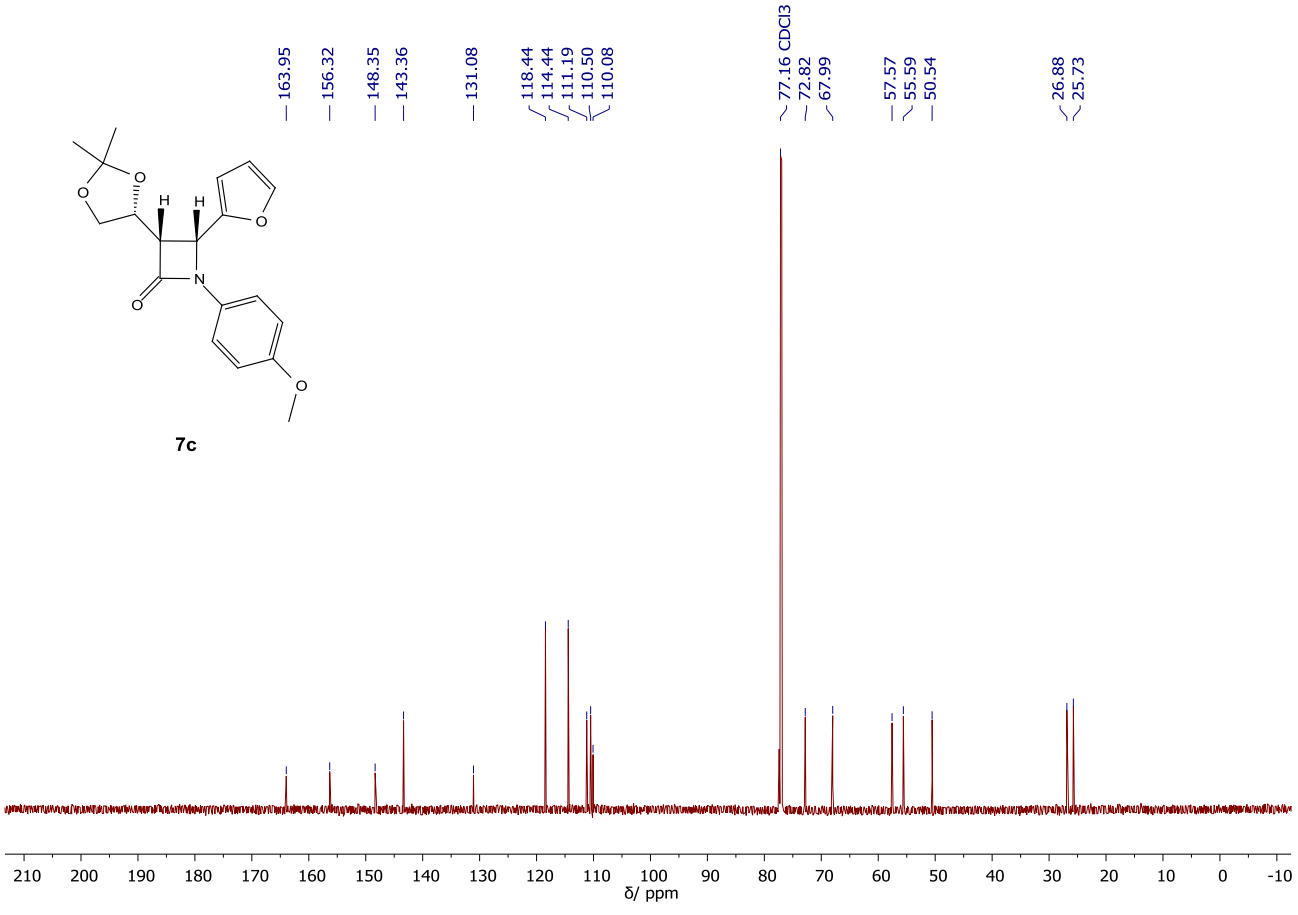

7.44
7.40
7.29
7.25
6.81
6.44
6.39
6.36
5.25
5.01
4.50
4.25
4.16
4.12
4.11
3.99
3.76
3.75
3.73
3.66
1.57 HDO
1.42
1.39
1.38
0.00 TMS
A (d)
5.25
J(5.38)
B (d)
5.01
J(2.63)
7a
7b
2.5 : 1
2.50
0.99
δ/ ppm


163.68
163.02
156.41
156.32
150.22
148.63
143.42
143.37
131.30
131.07
118.46
114.46
114.41
110.78
110.77
110.27
110.14
109.73
109.02
77.16 CDCl3
72.59
71.79
67.76
66.32
58.33
58.23
55.61
55.59
51.83
51.10
27.01
26.52
25.90
25.56
7a
7b
2.5 : 1
δ/ ppm

1H NMR (600 MHz)

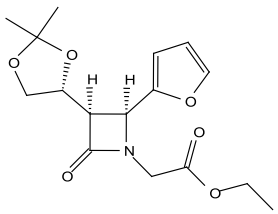


7c

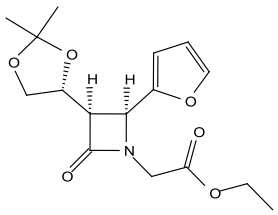


7c

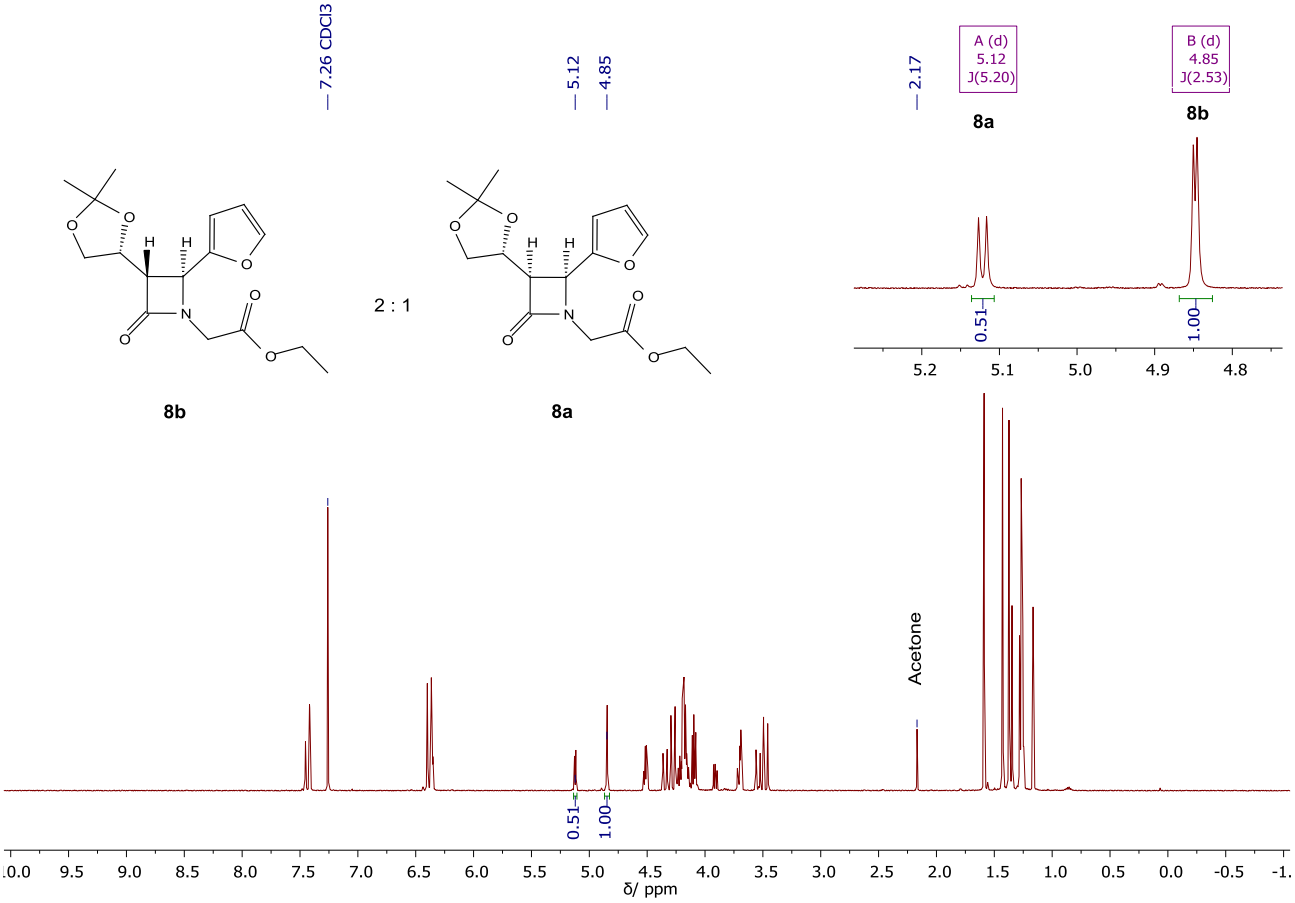
1H NMR (400 MHz)

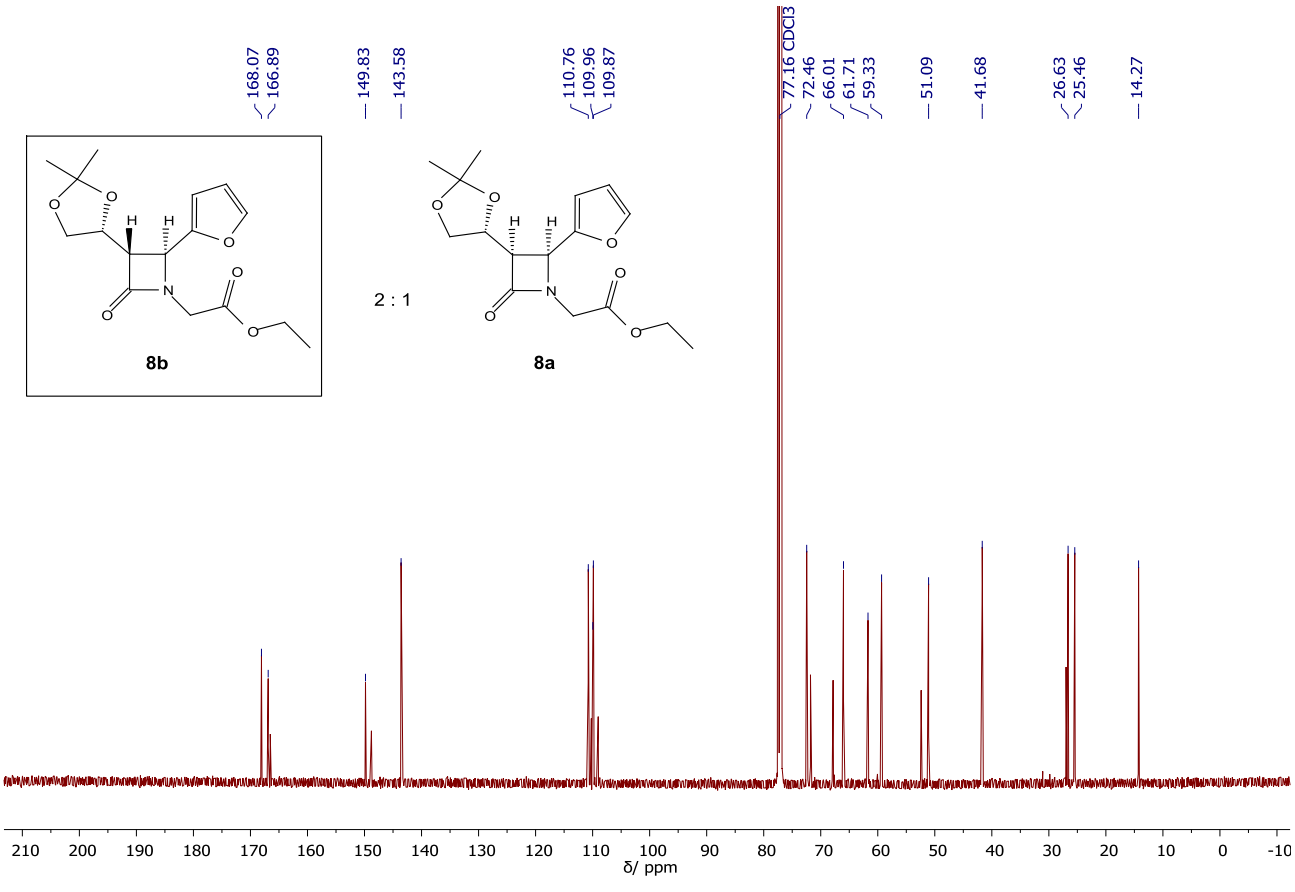


8a

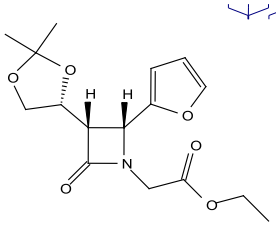


8a

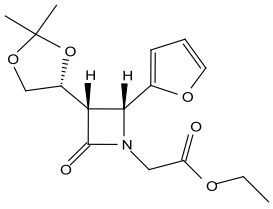

7.26 CDCl3
5.12
4.85
2.17
A (d)
5.12
J(5.20)
B (d)
4.85
J(2.53)
8a
8b
2 : 1
8b
8a
0.51
1.00
Acetone
δ/ ppm


168.07
166.89
149.83
143.58
110.76
109.96
109.87
77.16 CDCl3
72.46
66.01
61.71
59.33
51.09
41.68
26.63
25.46
14.27
8b
2 : 1
8a
δ/ ppm

1H NMR (500 MHz)

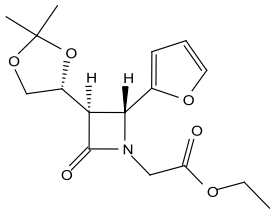


8c

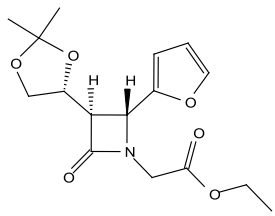


8c

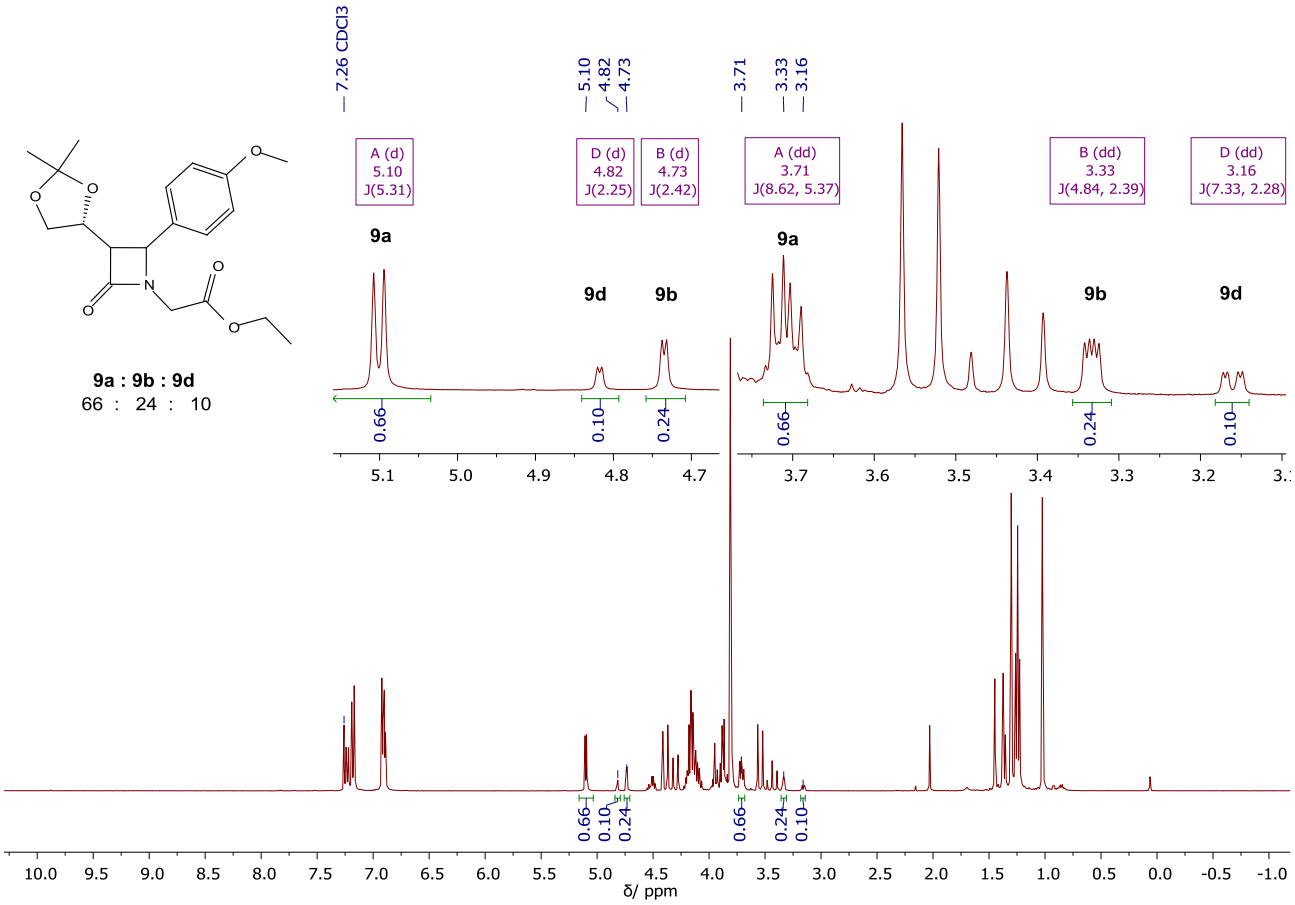
1H NMR (400 MHz)



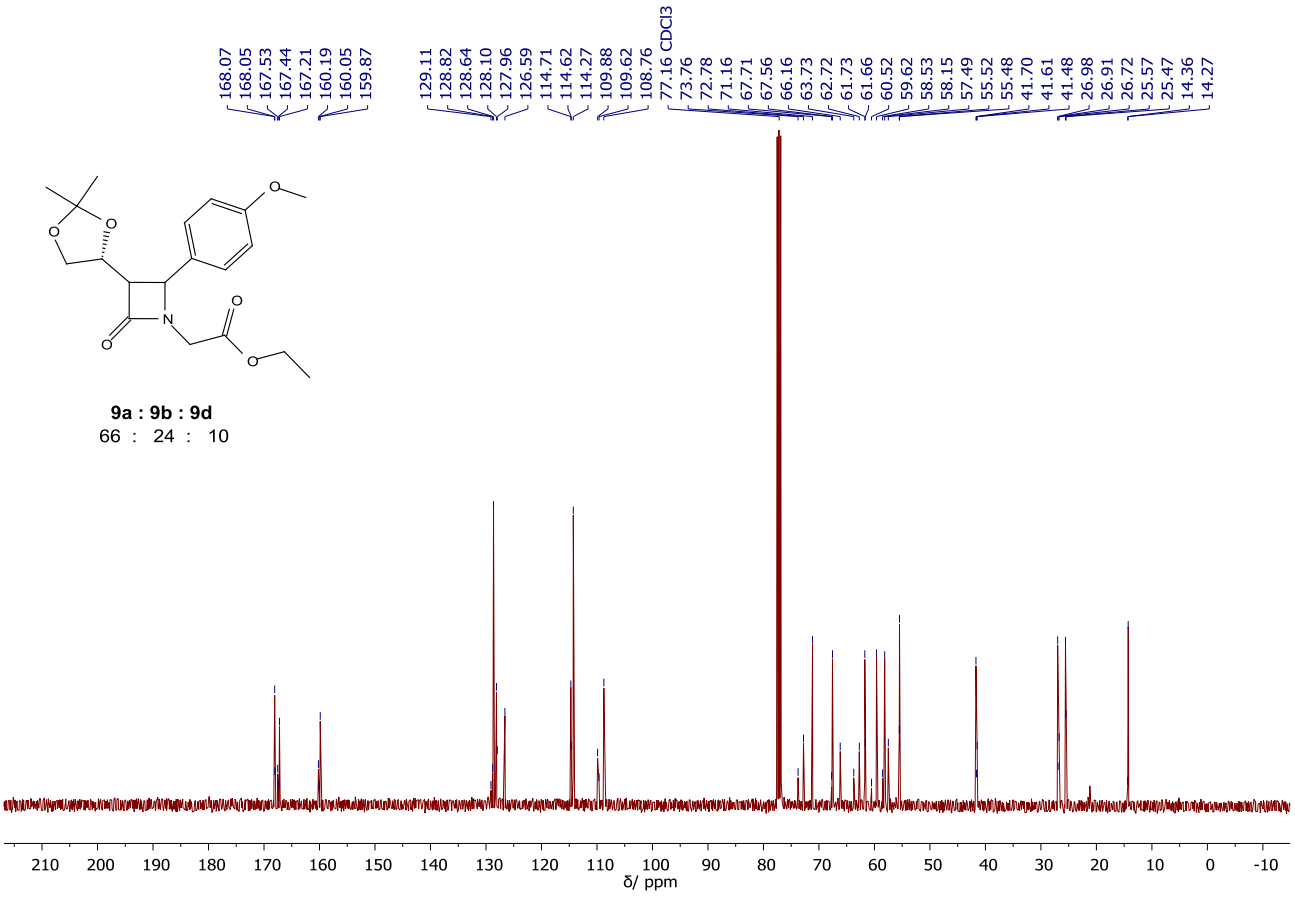
8d



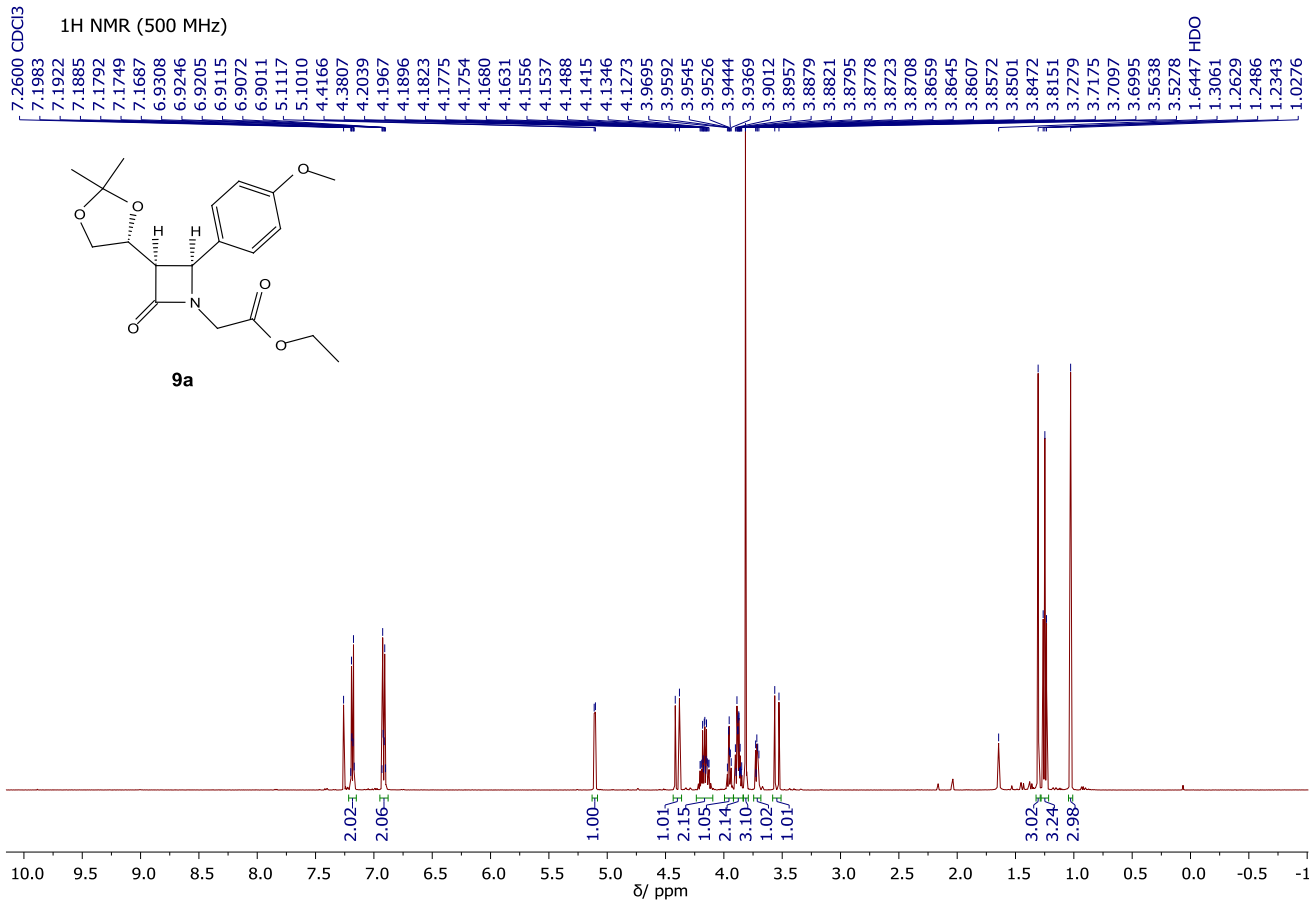
8d

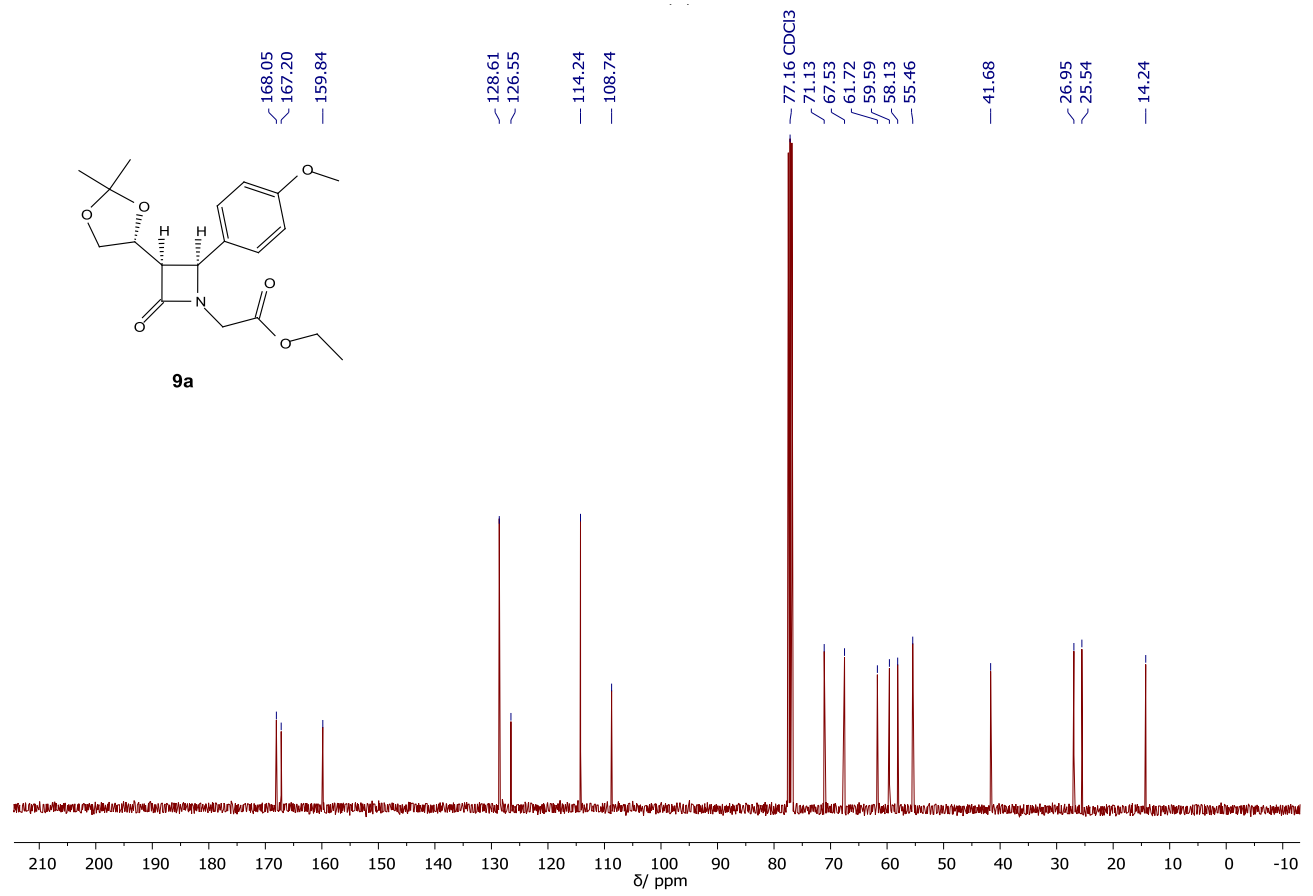


9a : 9b : 9d
66 : 24 : 10

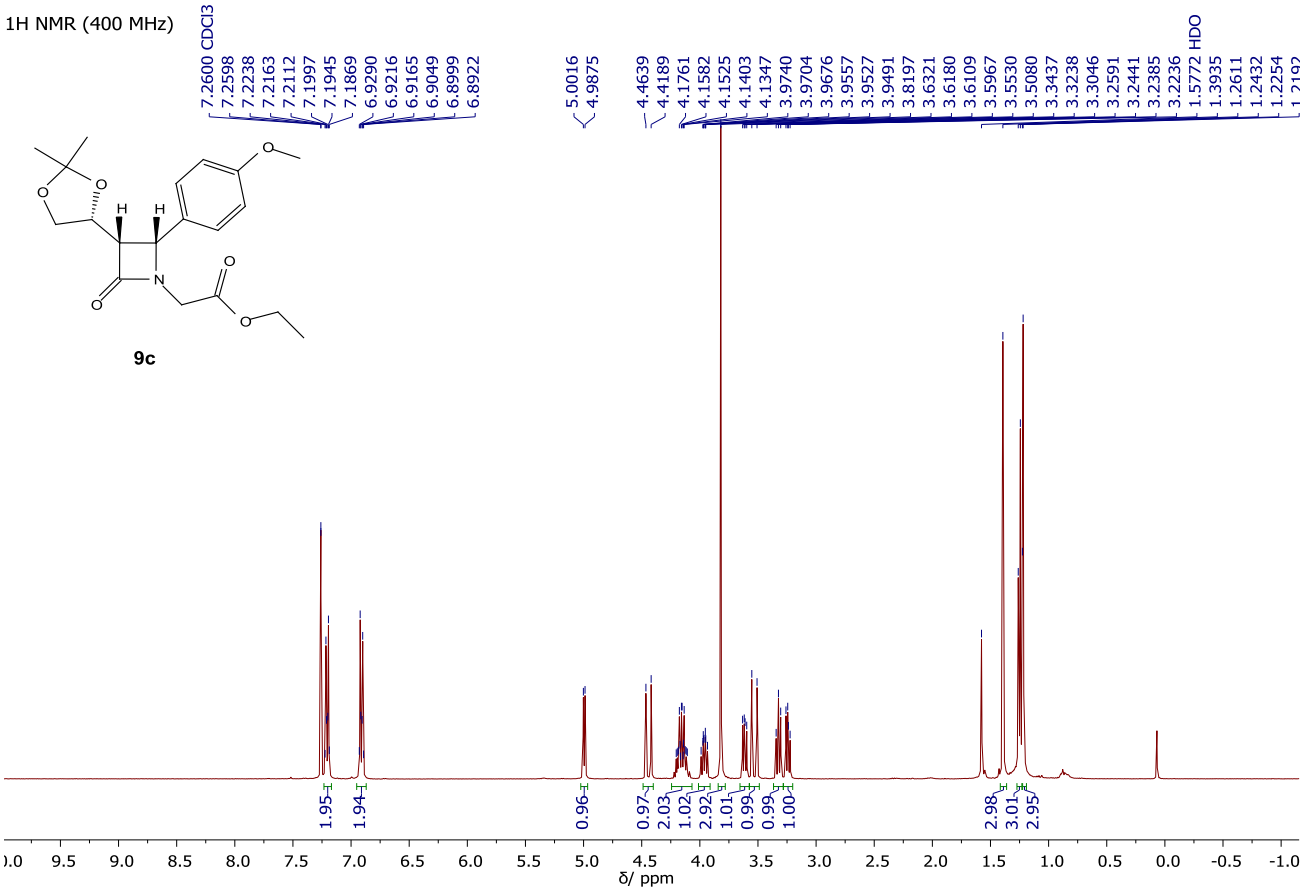


9a : 9b : 9d
66 : 24 : 10

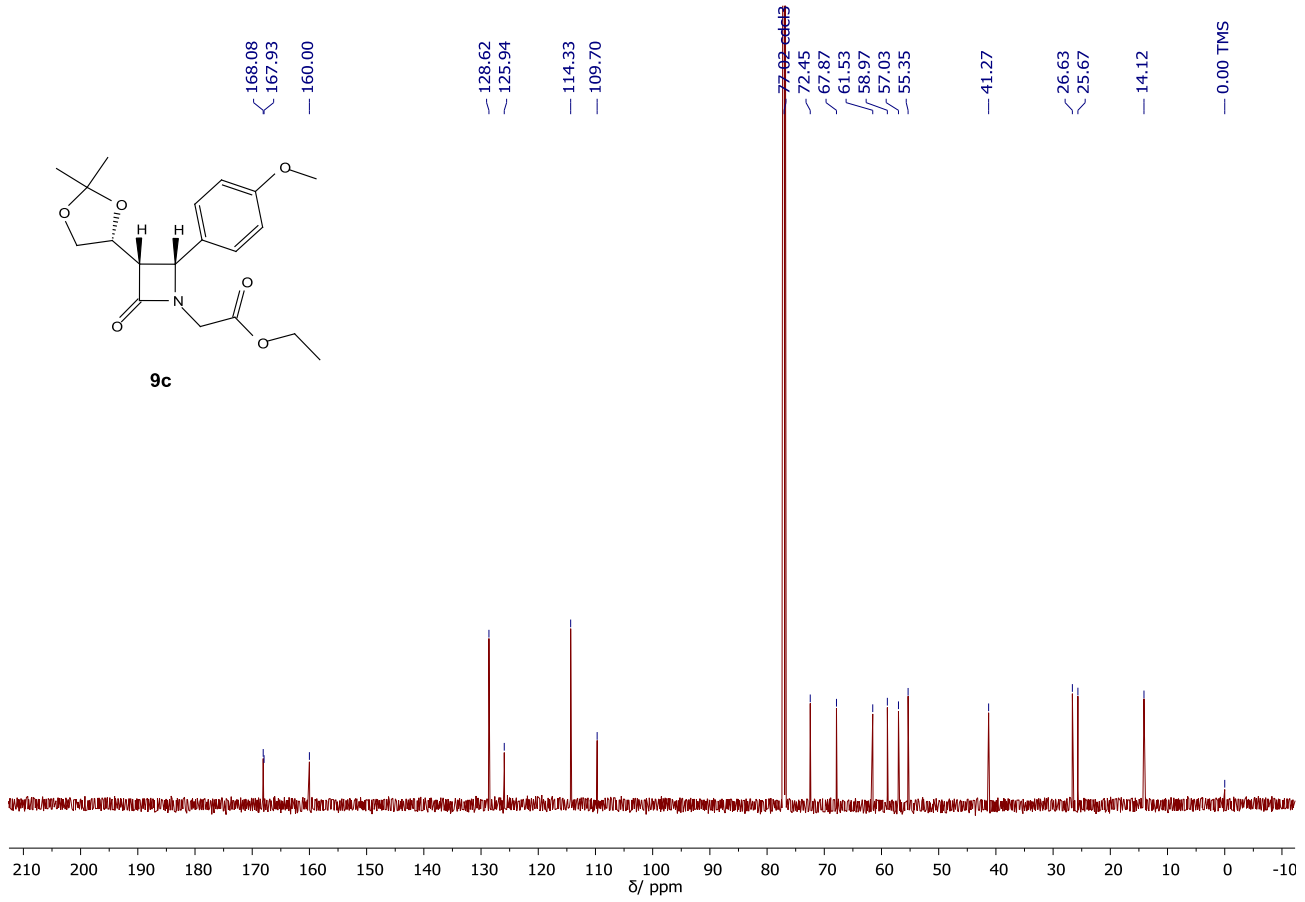

1H NMR (500 MHz)
7.2600 CDCl3
1.6447 HDO
9a
δ/ ppm


168.05
167.20
159.84
128.61
126.55
114.24
108.74
77.16 CDCl3
71.13
67.53
61.72
59.59
58.13
55.46
41.68
26.95
25.54
14.24
9a
δ/ ppm

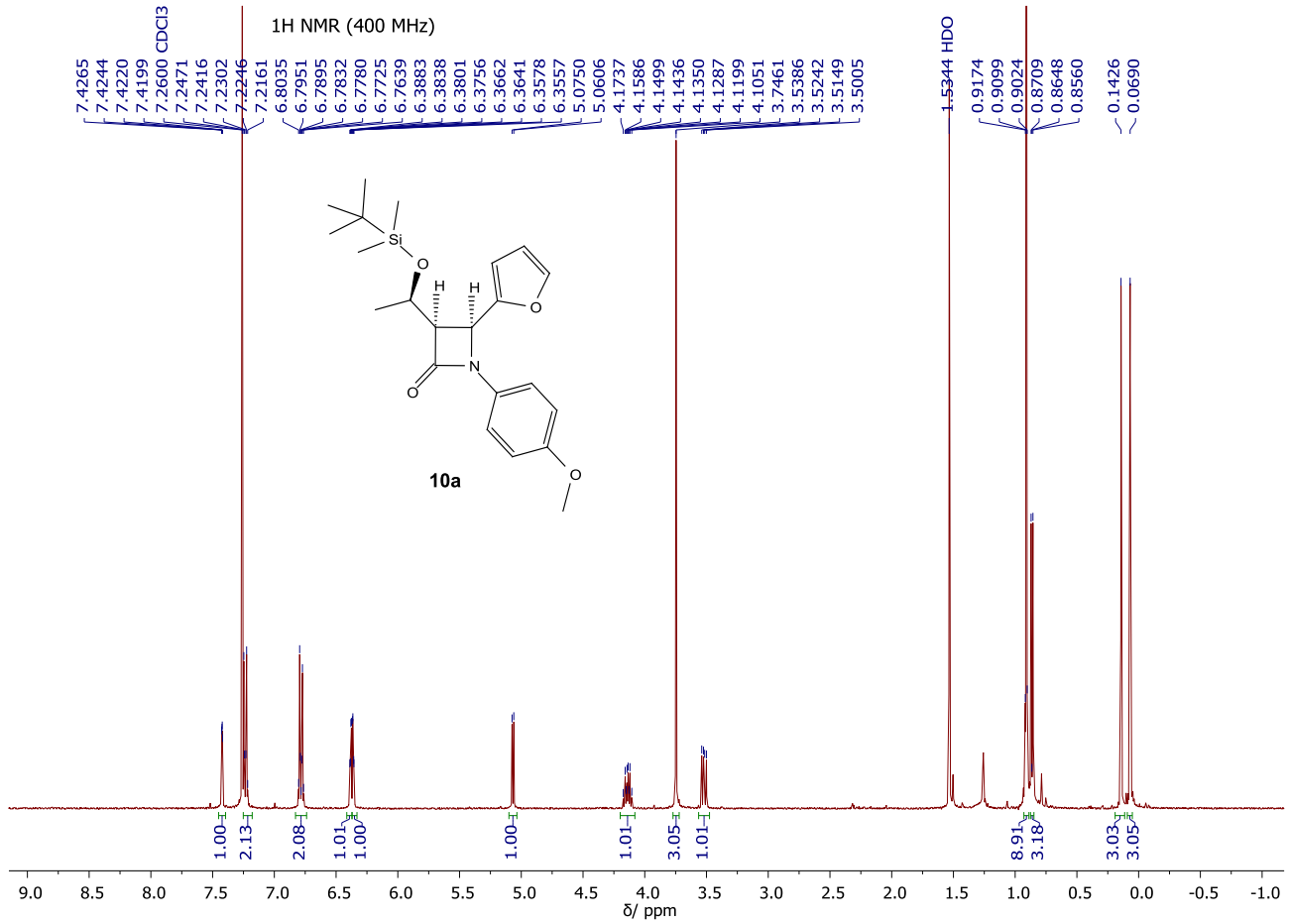
1H NMR (400 MHz)

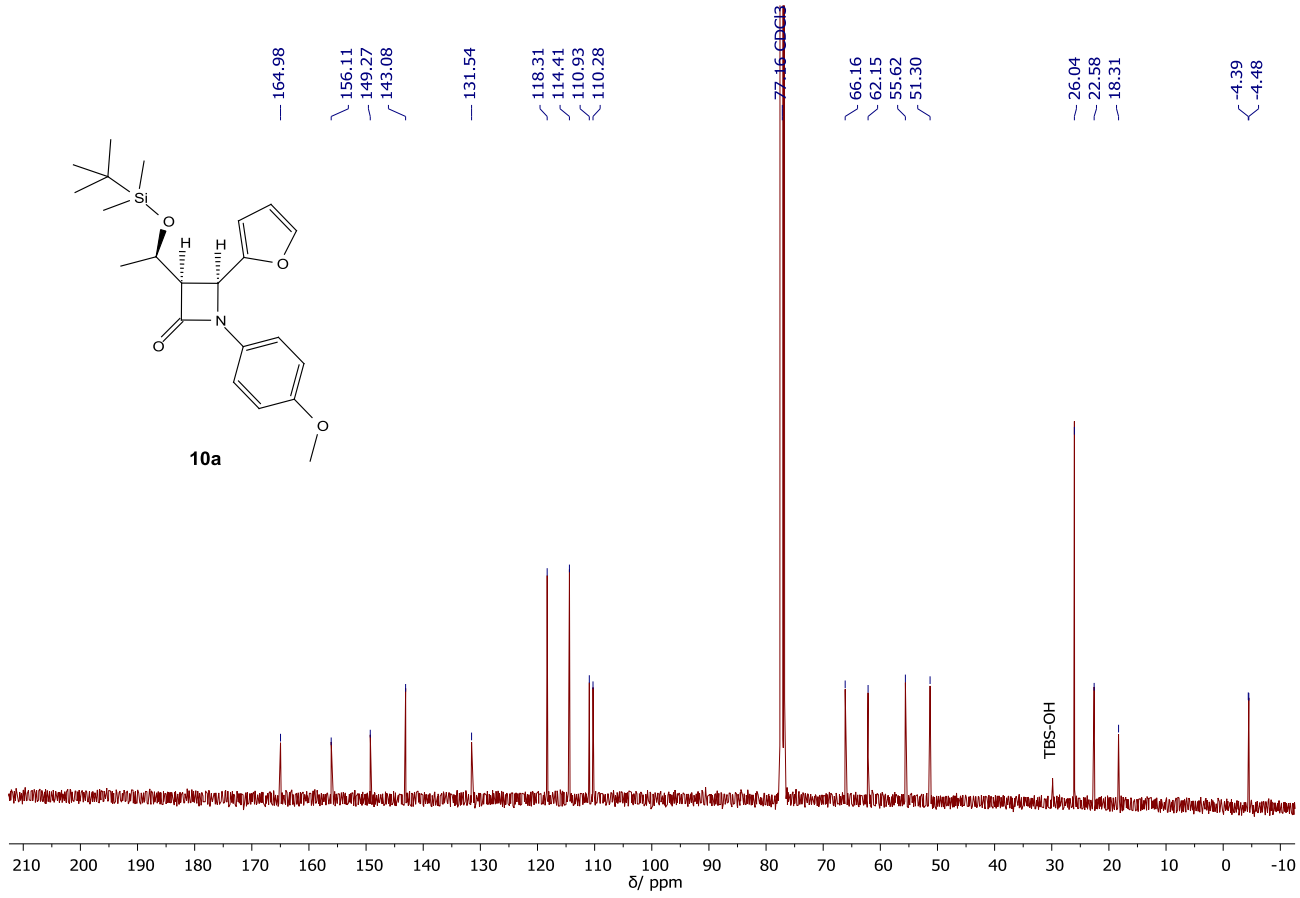


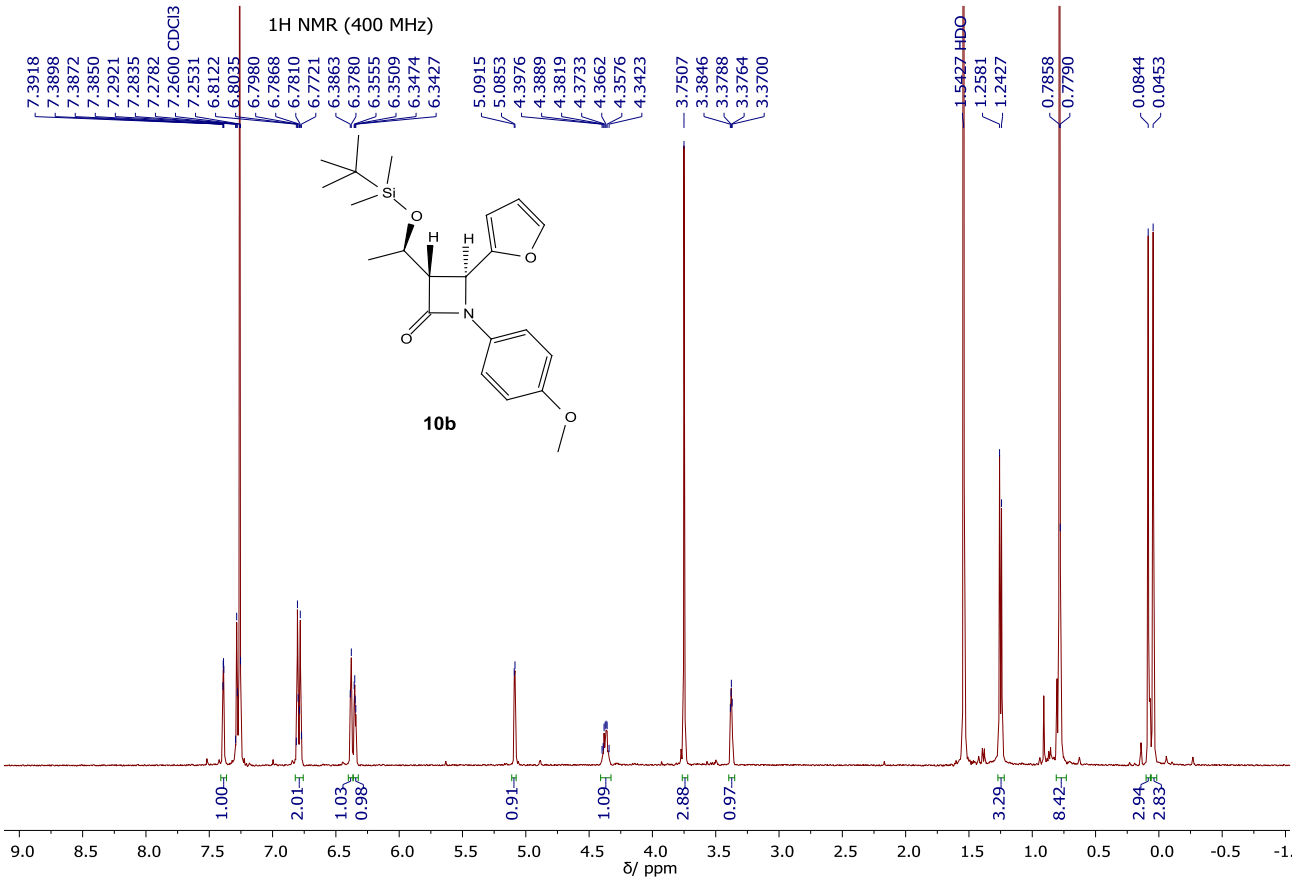
9c

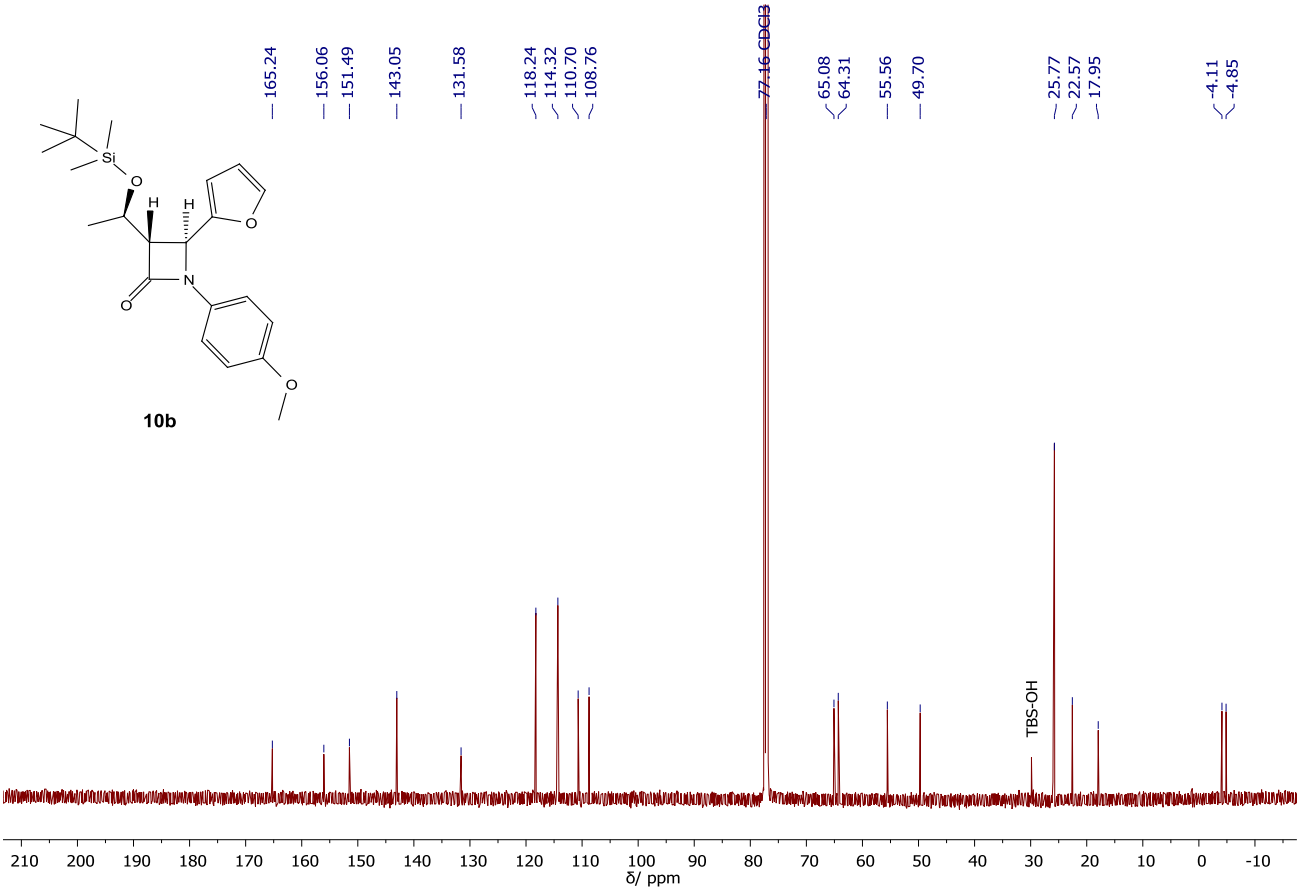


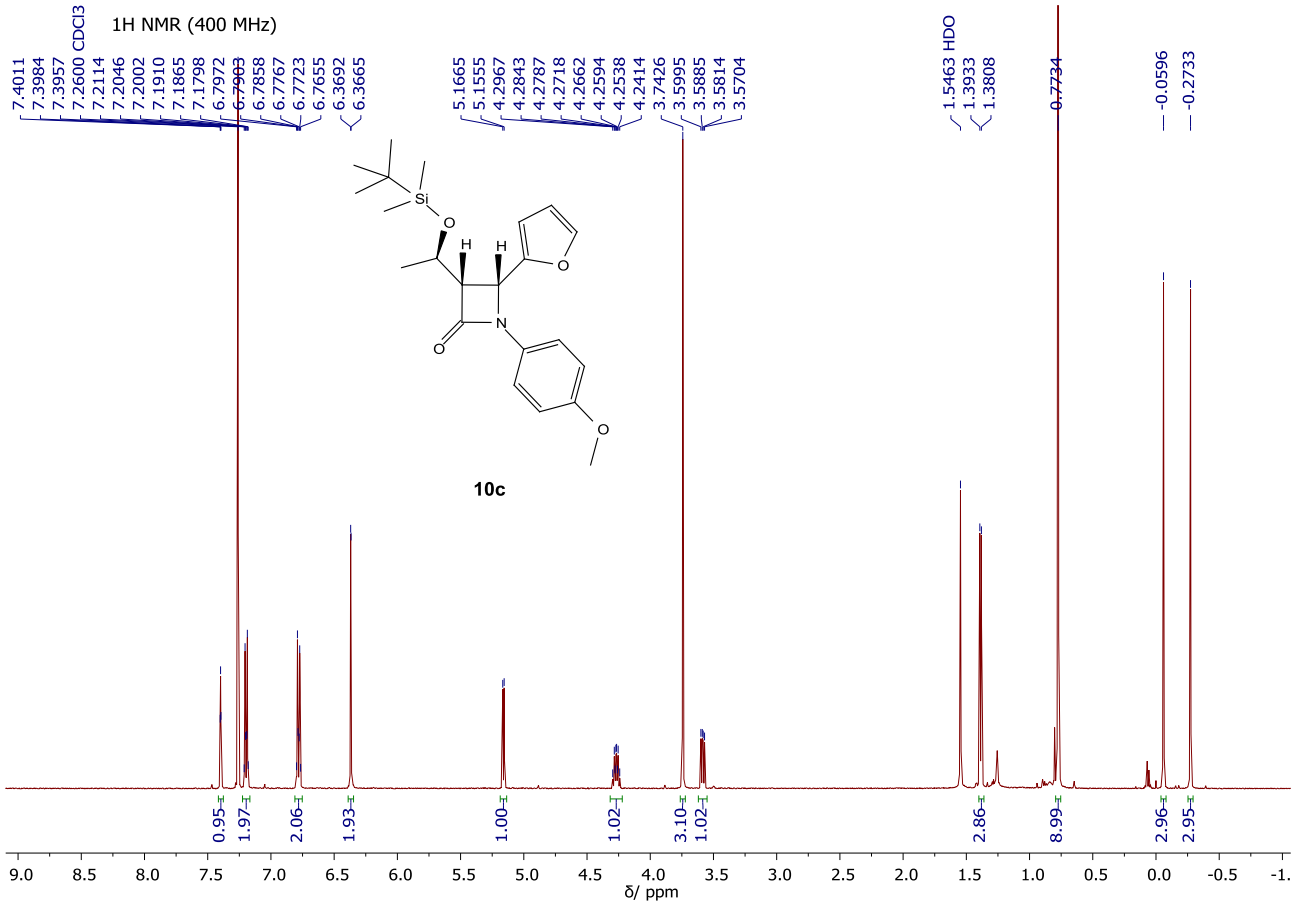
9c


1H NMR (400 MHz)
7.4265
7.4244
7.4220
7.4199
7.2600 CDCl3
7.2471
7.2416
7.2302
7.2246
7.2161
6.8035
6.7951
6.7895
6.7832
6.7780
6.7725
6.7639
6.3883
6.3838
6.3801
6.3756
6.3662
6.3641
6.3578
6.3557
5.0750
5.0606
4.1737
4.1586
4.1499
4.1436
4.1350
4.1287
4.1199
4.1051
3.7461
3.5386
3.5242
3.5149
3.5005
1.5344 HDO
0.9174
0.9099
0.9024
0.8709
0.8648
0.8560
0.1426
0.0690
10a
1.00
2.13
2.08
1.01
1.00
1.00
1.01
3.05
1.01
8.91
3.18
3.03
3.05
δ/ ppm

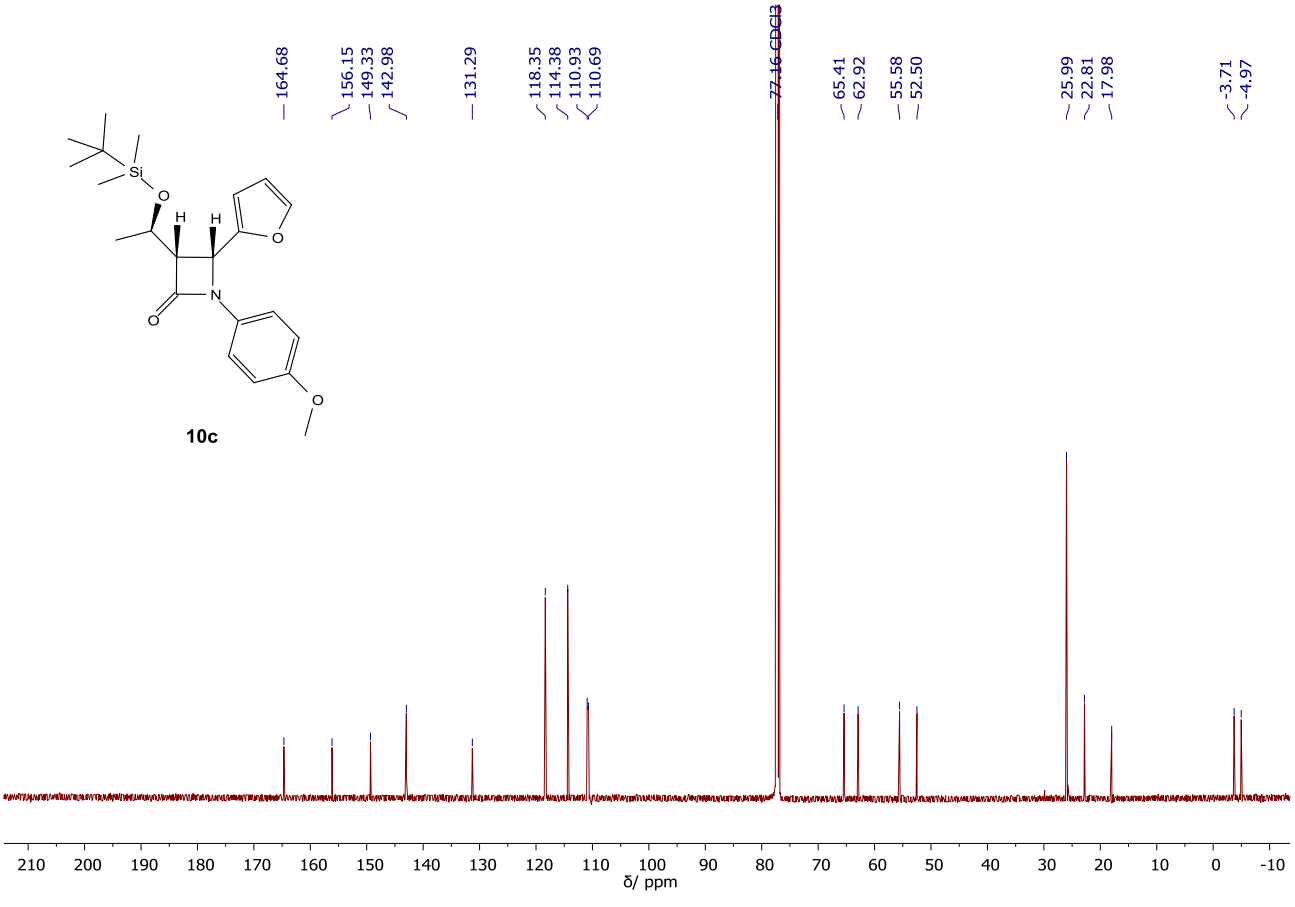

164.98
156.11
149.27
143.08
131.54
118.31
114.41
110.93
110.28
77.16 CDCl3
66.16
62.15
55.62
51.30
26.04
22.58
18.31
-4.39
-4.48
10a
TBS-OH
δ/ ppm


1H NMR (400 MHz)
7.3918
7.3898
7.3872
7.3850
7.2921
7.2835
7.2782
7.2600 CDCl3
7.2531
6.8122
6.8035
6.7980
6.7868
6.7810
6.7721
6.3863
6.3780
6.3555
6.3509
6.3474
6.3427
5.0915
5.0853
4.3976
4.3889
4.3819
4.3733
4.3662
4.3576
4.3423
3.7507
3.3846
3.3788
3.3764
3.3700
1.5427 HDO
1.2581
1.2427
0.7858
0.7790
0.0844
0.0453
1.00
2.01
1.03
0.98
0.91
1.09
2.88
0.97
3.29
8.42
2.94
2.83
δ/ ppm
10b

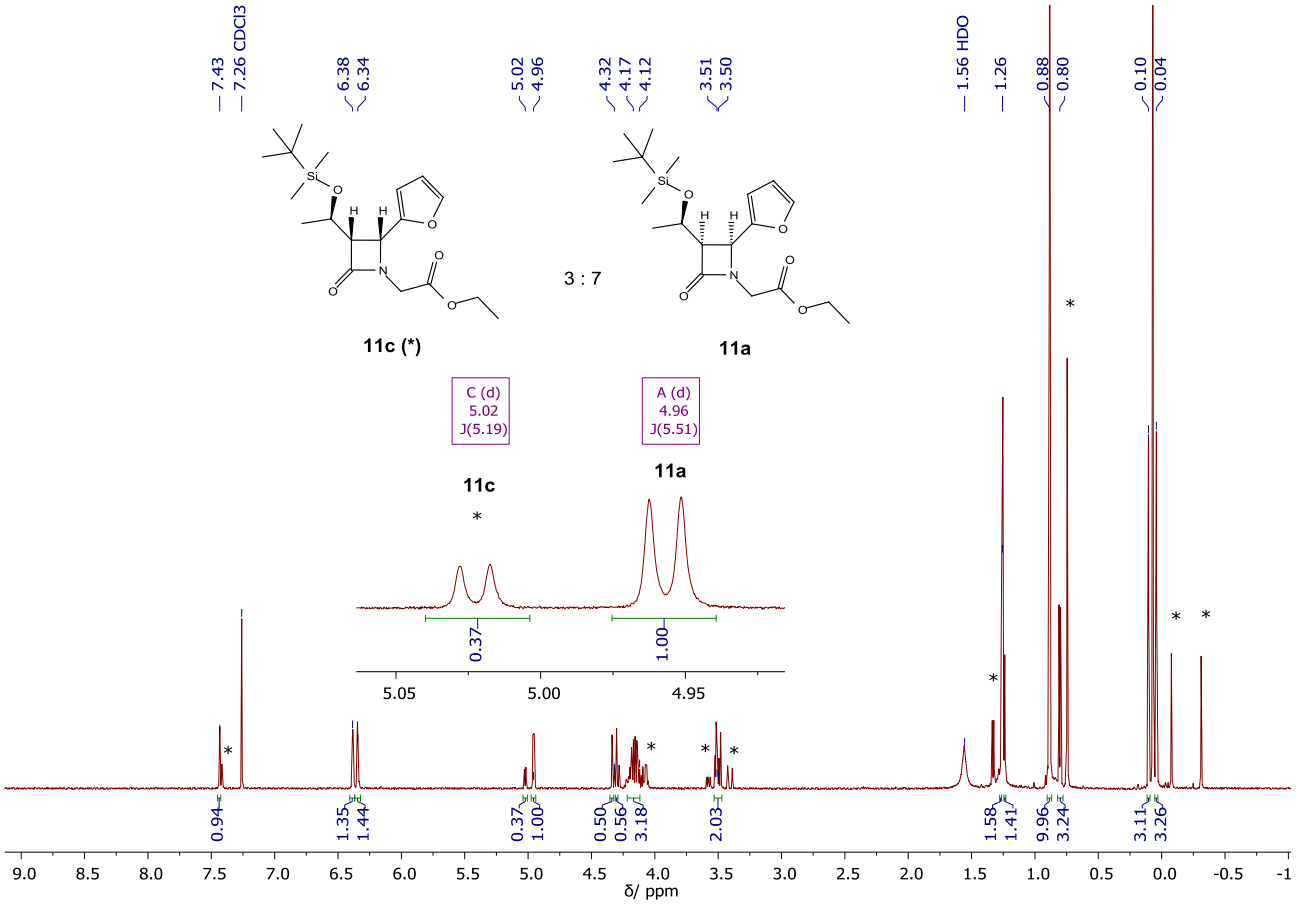

165.24
156.06
151.49
143.05
131.58
118.24
114.32
110.70
108.76
77.16 CDCl3
65.08
64.31
55.56
49.70
25.77
22.57
17.95
-4.11
-4.85
TBS-OH
δ/ ppm
10b

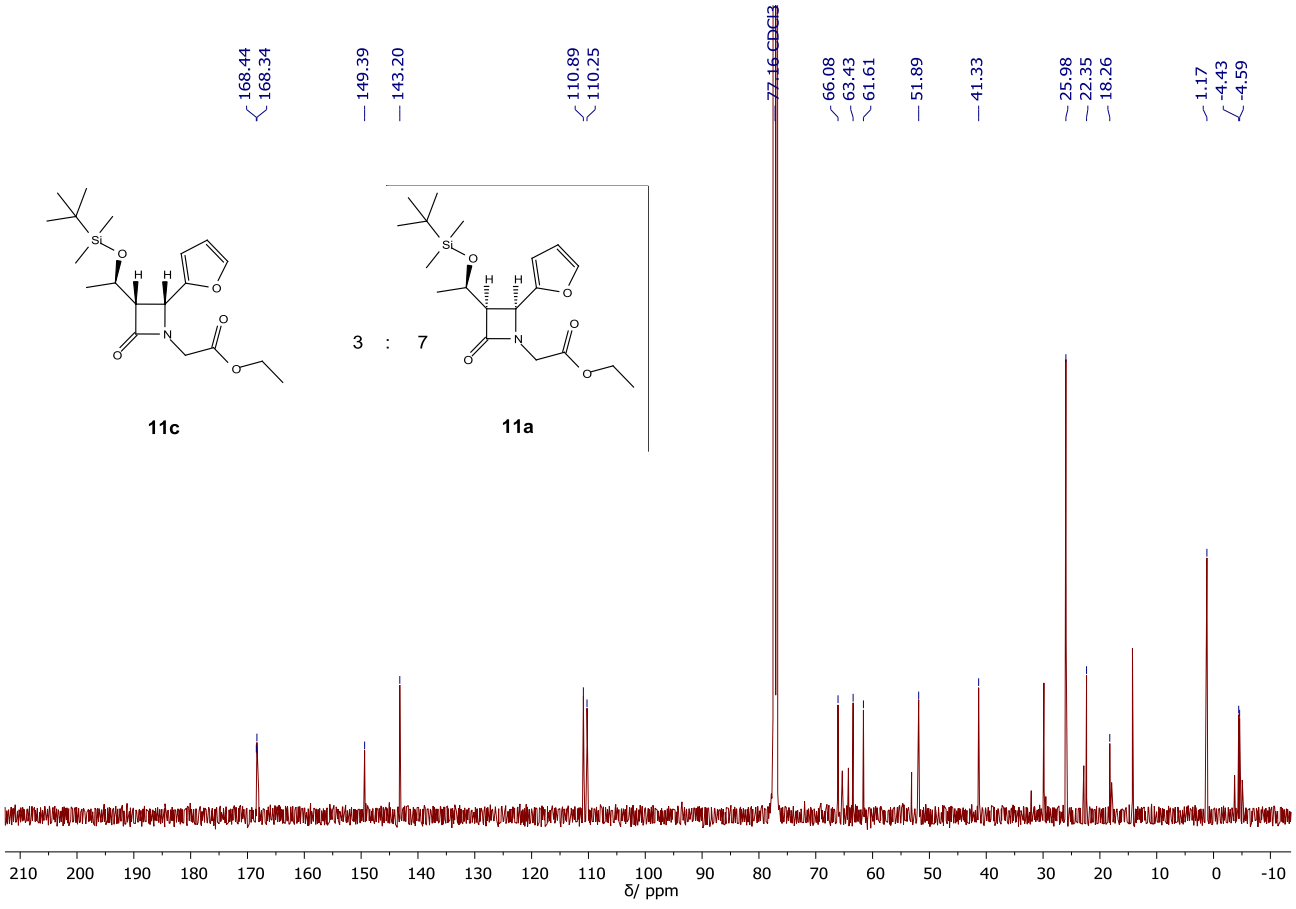

1H NMR (400 MHz)
7.4011
7.3984
7.3957
7.2600 CDCl3
7.2114
7.2046
7.2002
7.1910
7.1865
7.1798
7.7972
6.7903
6.7858
6.7767
6.7723
6.7655
6.3692
6.3665
5.1665
5.1555
4.2967
4.2843
4.2787
4.2718
4.2662
4.2594
4.2538
4.2414
3.7426
3.5995
3.5885
3.5814
3.5704
1.5463 HDO
1.3933
1.3808
0.7734
-0.0596
-0.2733
0.95
1.97
2.06
1.93
1.00
1.02
3.10
1.02
2.86
8.99
2.96
2.95
δ/ ppm

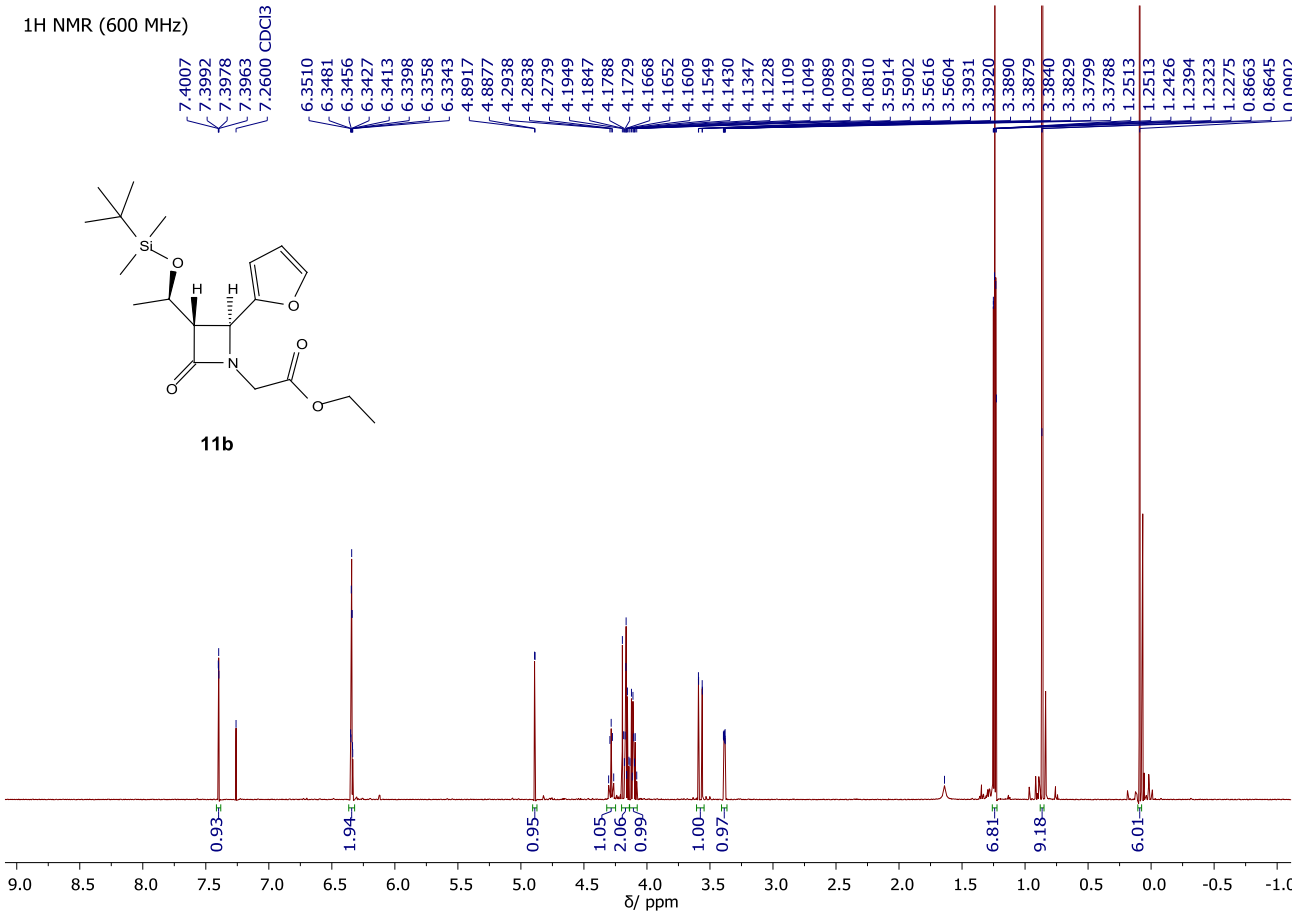
10c

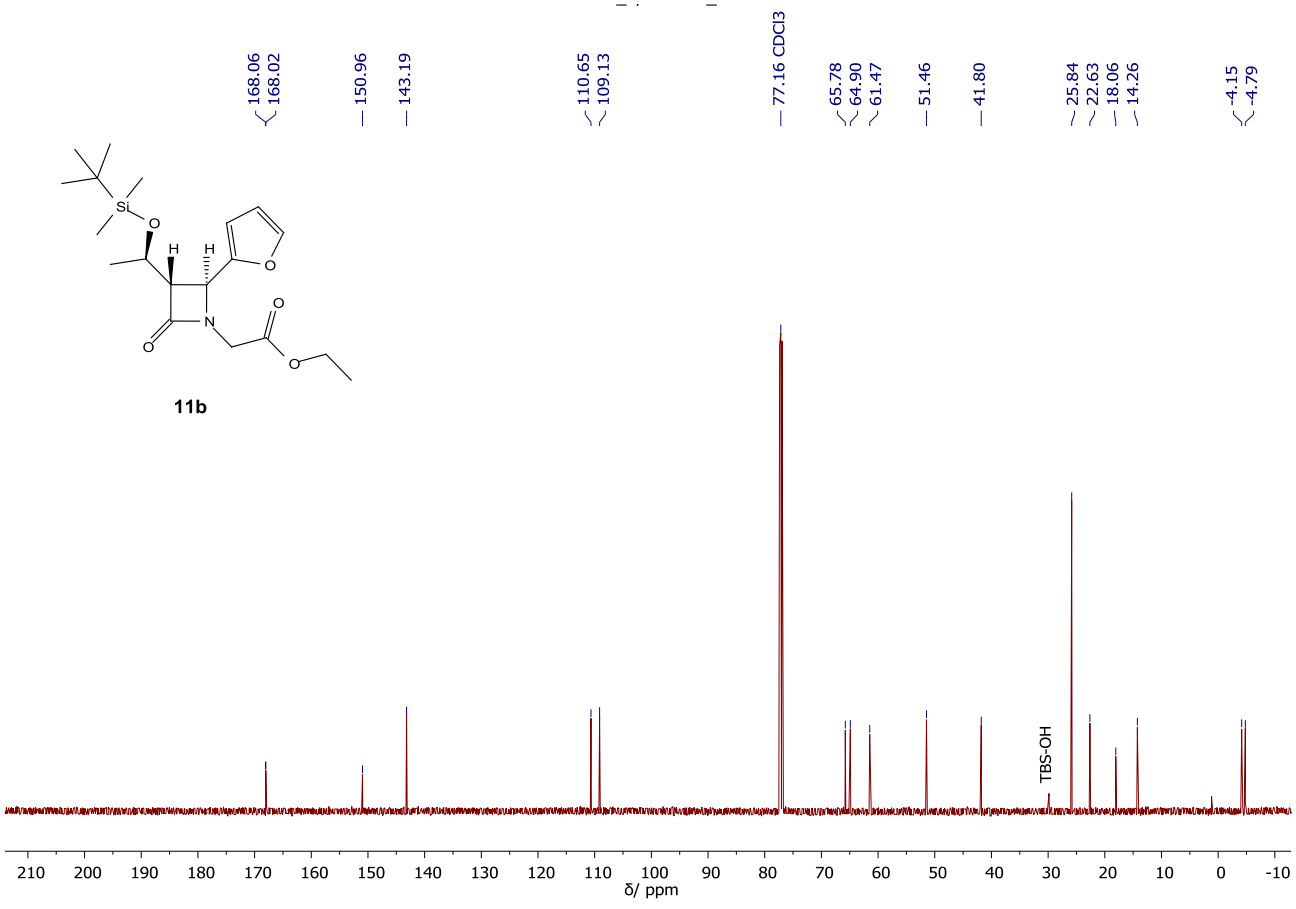

164.68
156.15
149.33
142.98
131.29
118.35
114.38
110.93
110.69
77.16 CDCl3
65.41
62.92
55.58
52.50
25.99
22.81
17.98
-3.71
-4.97
δ/ ppm

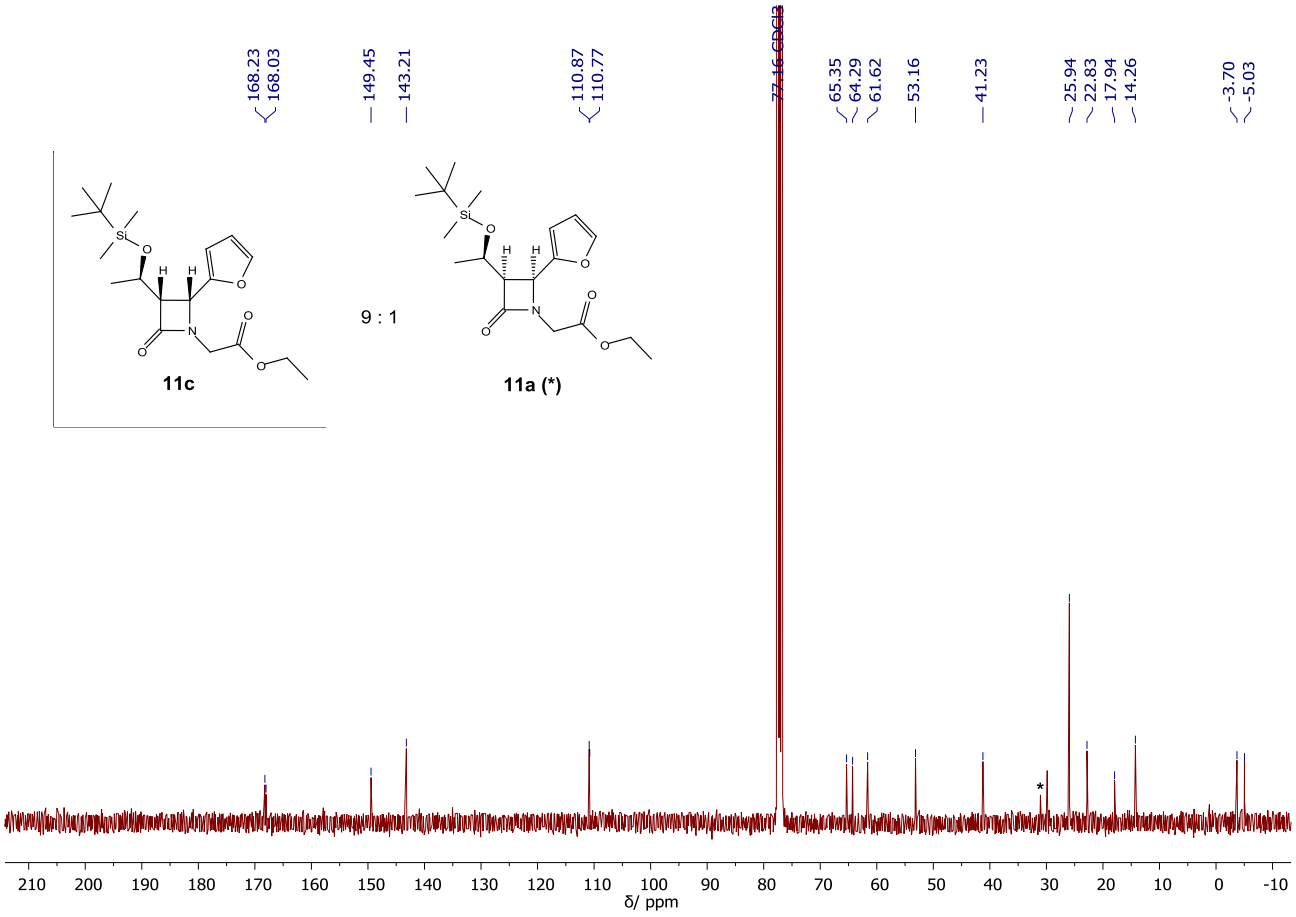
10c

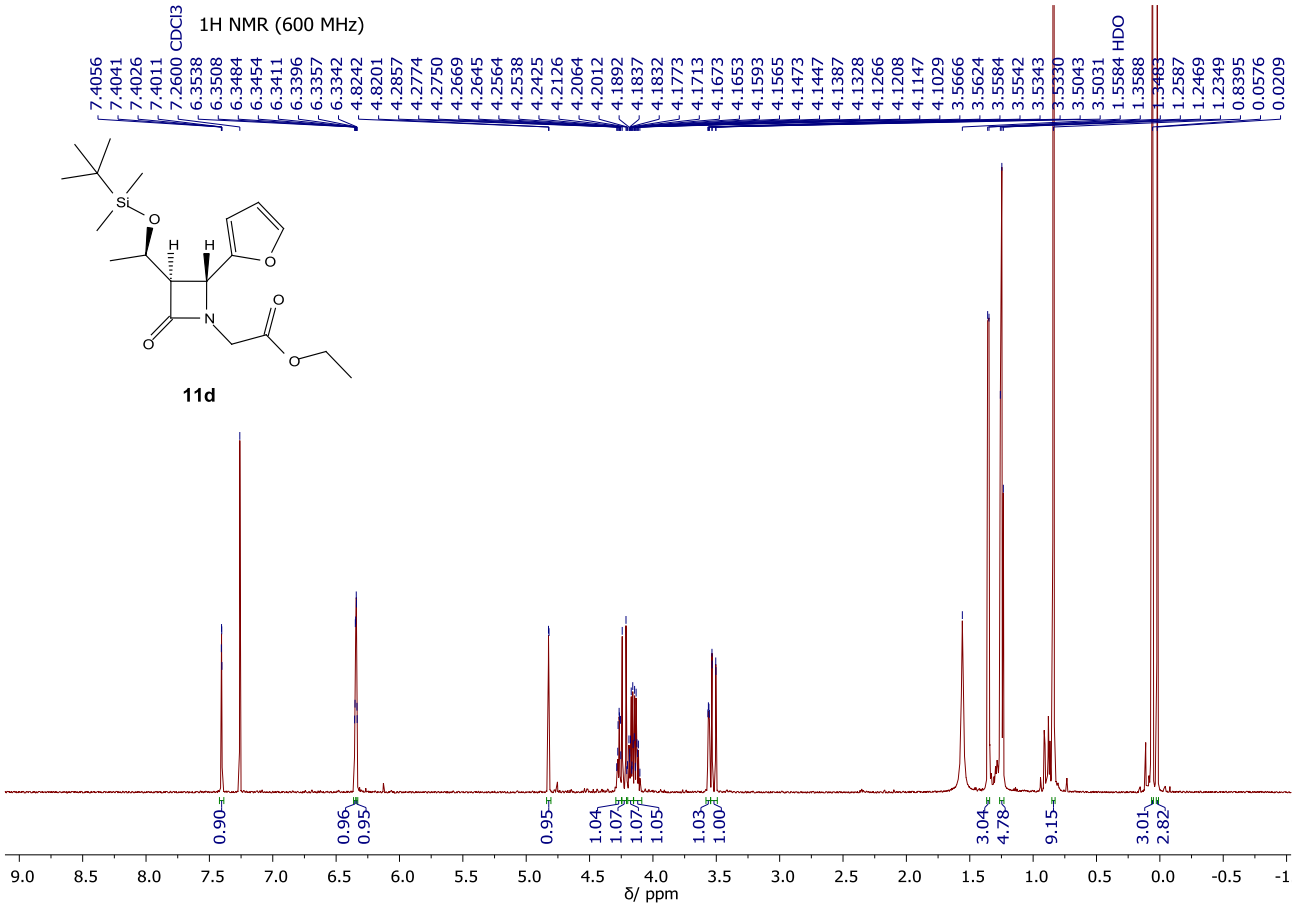

7.43
7.26 CDCl3
6.38
6.34
5.02
4.96
4.32
4.17
4.12
3.51
3.50
1.56 HDO
1.26
0.88
0.80
0.10
0.04
3 : 7
11c (*)
11a
C (d)
5.02
J(5.19)
A (d)
4.96
J(5.51)
11c
11a
0.37
1.00
5.05
5.00
4.95
0.94
1.35
1.44
0.37
1.00
0.50
0.56
3.18
2.03
1.58
1.41
9.96
3.24
3.11
3.26
δ/ ppm


168.44
168.34
149.39
143.20
110.89
110.25
77.16 CDCl3
66.08
63.43
61.61
51.89
41.33
25.98
22.35
18.26
1.17
-4.43
-4.59
3 : 7
11c
11a
δ/ ppm

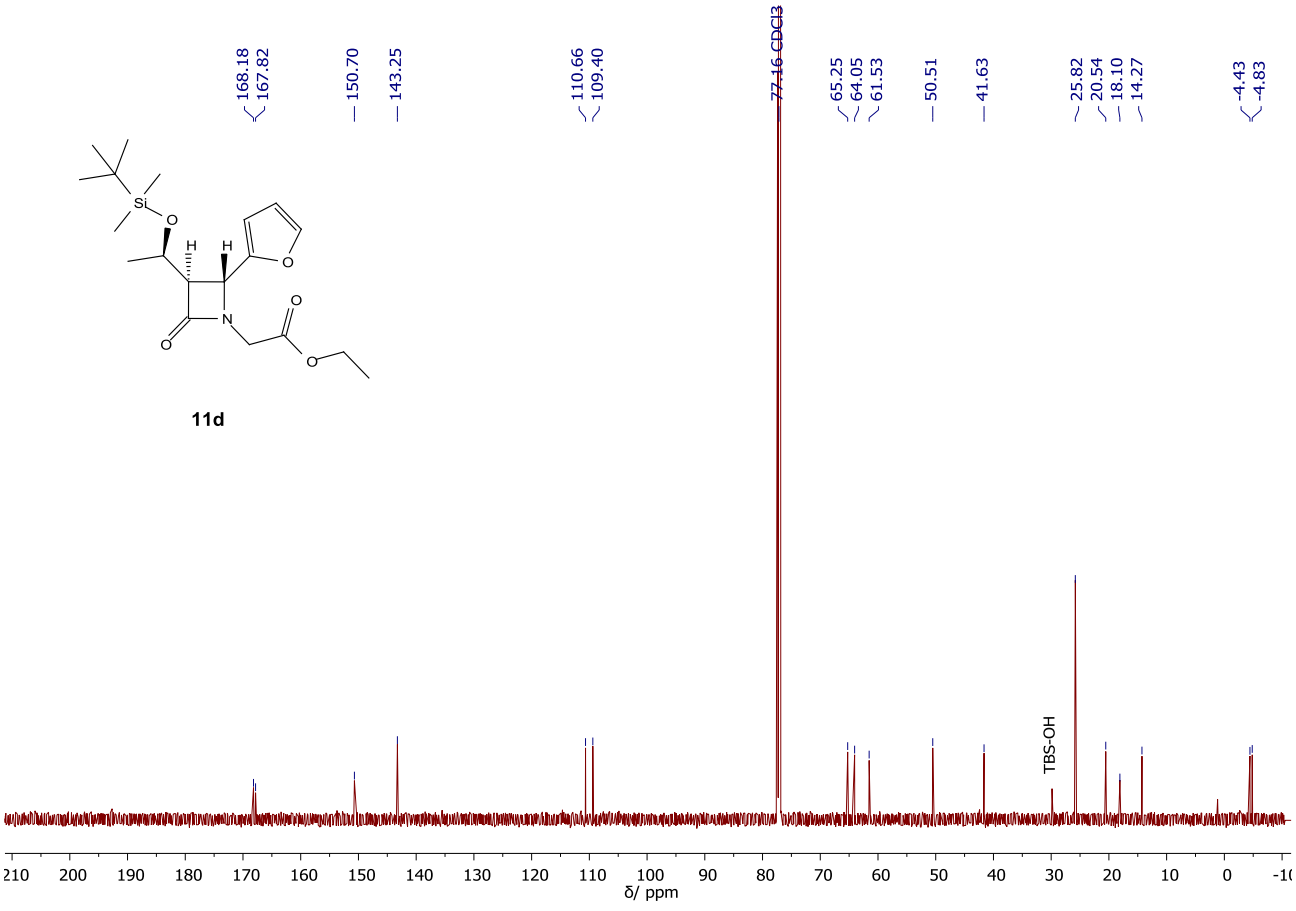

1H NMR (600 MHz)
7.4007
7.3992
7.3978
7.3963
7.2600 CDCl3
6.3510
6.3481
6.3456
6.3427
6.3413
6.3398
6.3358
6.3343
4.8917
4.8877
4.2938
4.2838
4.2739
4.1949
4.1847
4.1788
4.1729
4.1668
4.1652
4.1609
4.1549
4.1430
4.1347
4.1228
4.1109
4.1049
4.0989
4.0929
4.0810
3.5914
3.5902
3.5616
3.5604
3.3931
3.3920
3.3890
3.3879
3.3840
3.3829
3.3799
3.3788
1.2513
1.2513
1.2426
1.2394
1.2323
1.2275
0.8663
0.8645
Si
O
H
H
O
N
O
O
O
11b
0.93
1.94
0.95
1.05
2.06
0.99
1.00
0.97
6.81
9.18
6.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
δ/ ppm


168.06
168.02
150.96
143.19
110.65
109.13
77.16 CDCl3
65.78
64.90
61.47
51.46
41.80
25.84
22.63
18.06
14.26
-4.15
-4.79
Si
O
H
H
O
N
O
O
O
11b
TBS-OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
δ/ ppm

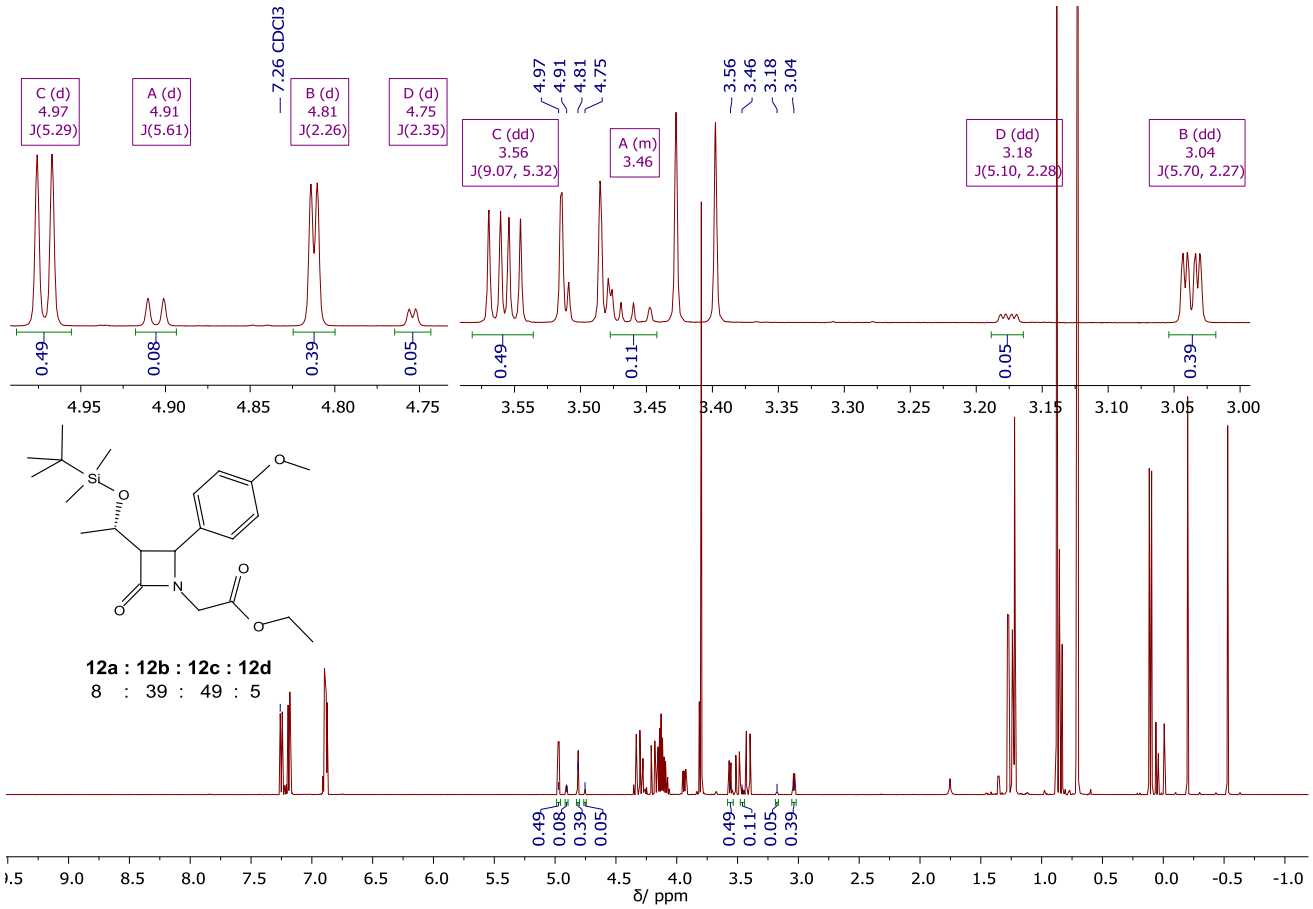

168.23
168.03
149.45
143.21
110.87
110.77
77.16 CDCl3
65.35
64.29
61.62
53.16
41.23
25.94
22.83
17.94
14.26
-3.70
-5.03
9 : 1
11c
11a (*)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
δ/ ppm

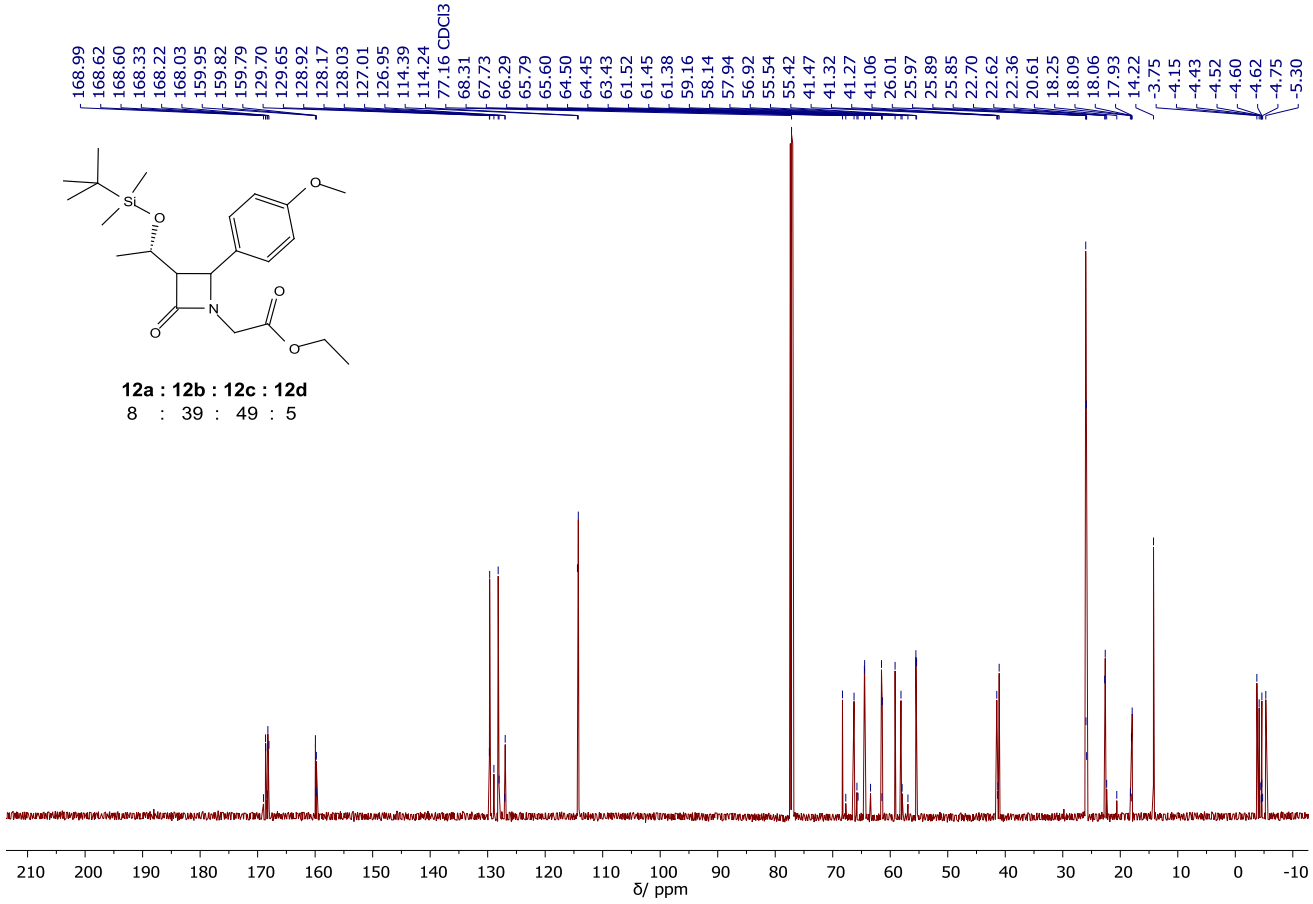

1H NMR (600 MHz)
7.4056
7.4041
7.4026
7.4011
7.2600 CDCl3
6.3538
6.3508
6.3484
6.3454
6.3411
6.3396
6.3357
6.3342
4.8242
4.8201
4.2857
4.2774
4.2750
4.2669
4.2645
4.2564
4.2538
4.2425
4.2126
4.2064
4.2012
4.1892
4.1837
4.1832
4.1773
4.1713
4.1673
4.1653
4.1593
4.1565
4.1473
4.1447
4.1387
4.1328
4.1266
4.1208
4.1147
4.1029
3.5666
3.5624
3.5584
3.5542
3.5343
3.5330
3.5043
3.5031
1.5584 HDO
1.3588
1.3483
1.2587
1.2469
1.2349
0.8395
0.0576
0.0209
0.90
0.96
0.95
0.95
1.04
1.07
1.07
1.05
1.03
1.00
3.04
4.78
9.15
3.01
2.82
δ/ ppm

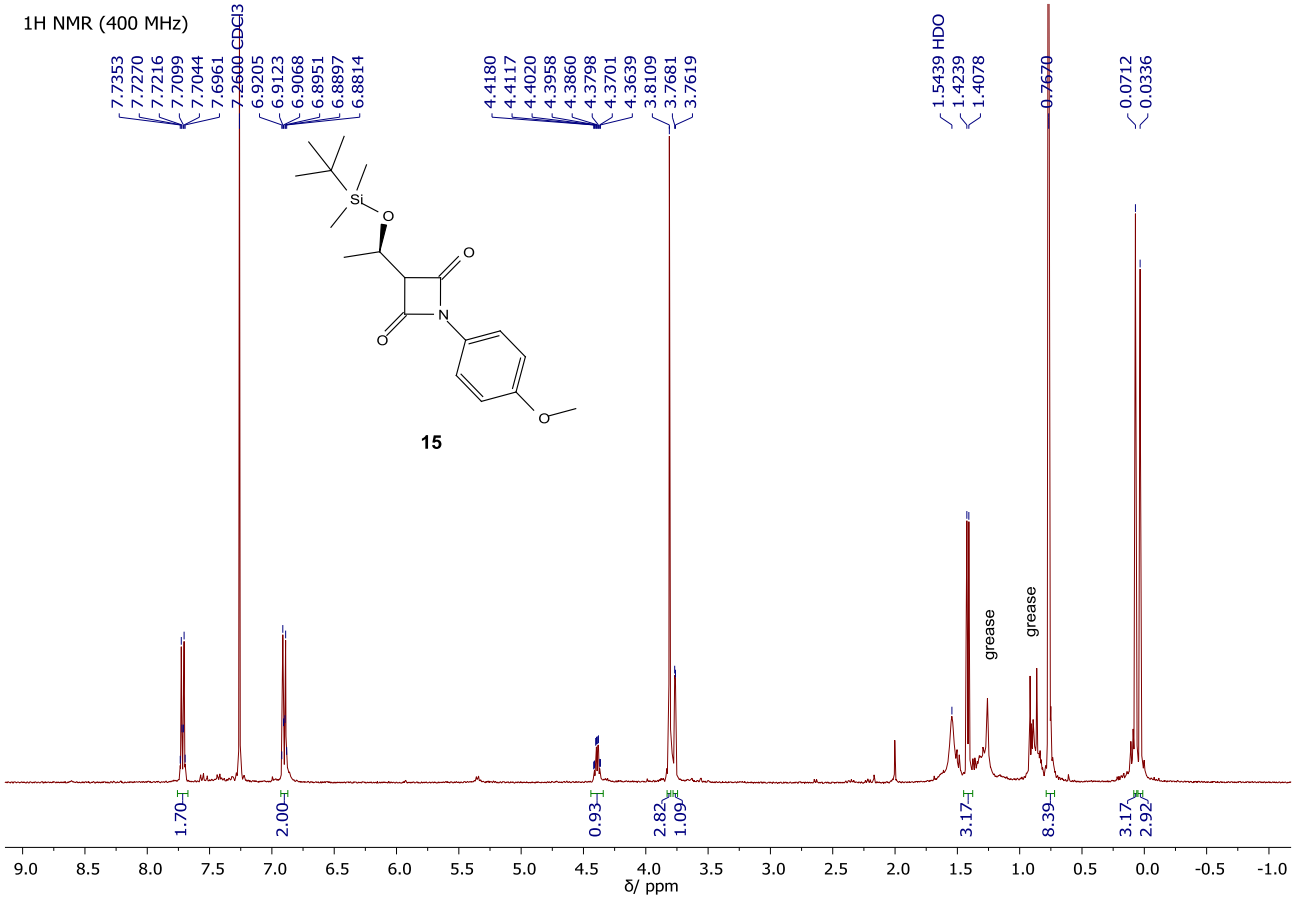
11d


168.18
167.82
150.70
143.25
110.66
109.40
77.16 CDCl3
65.25
64.05
61.53
50.51
41.63
25.82
20.54
18.10
14.27
-4.43
-4.83
TBS-OH
δ/ ppm

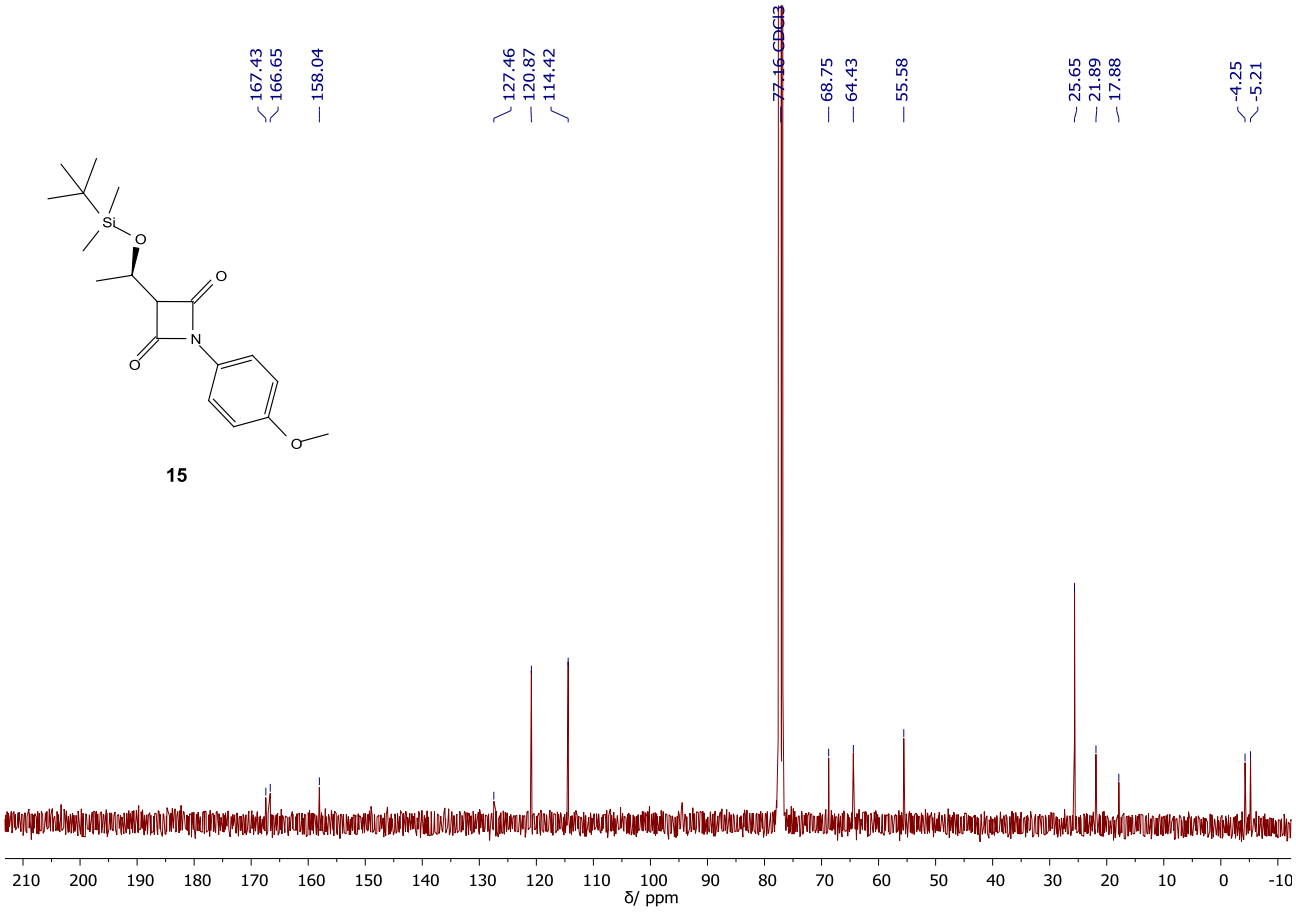
11d


C (d)
4.97
J(5.29)
A (d)
4.91
J(5.61)
7.26 CDCl3
B (d)
4.81
J(2.26)
D (d)
4.75
J(2.35)
4.97
4.91
4.81
4.75
3.56
3.46
3.18
3.04
C (dd)
3.56
J(9.07, 5.32)
A (m)
3.46
D (dd)
3.18
J(5.10, 2.28)
B (dd)
3.04
J(5.70, 2.27)
0.49
0.08
0.39
0.05
0.49
0.11
0.05
0.39
12a : 12b : 12c : 12d
8 : 39 : 49 : 5
δ/ ppm

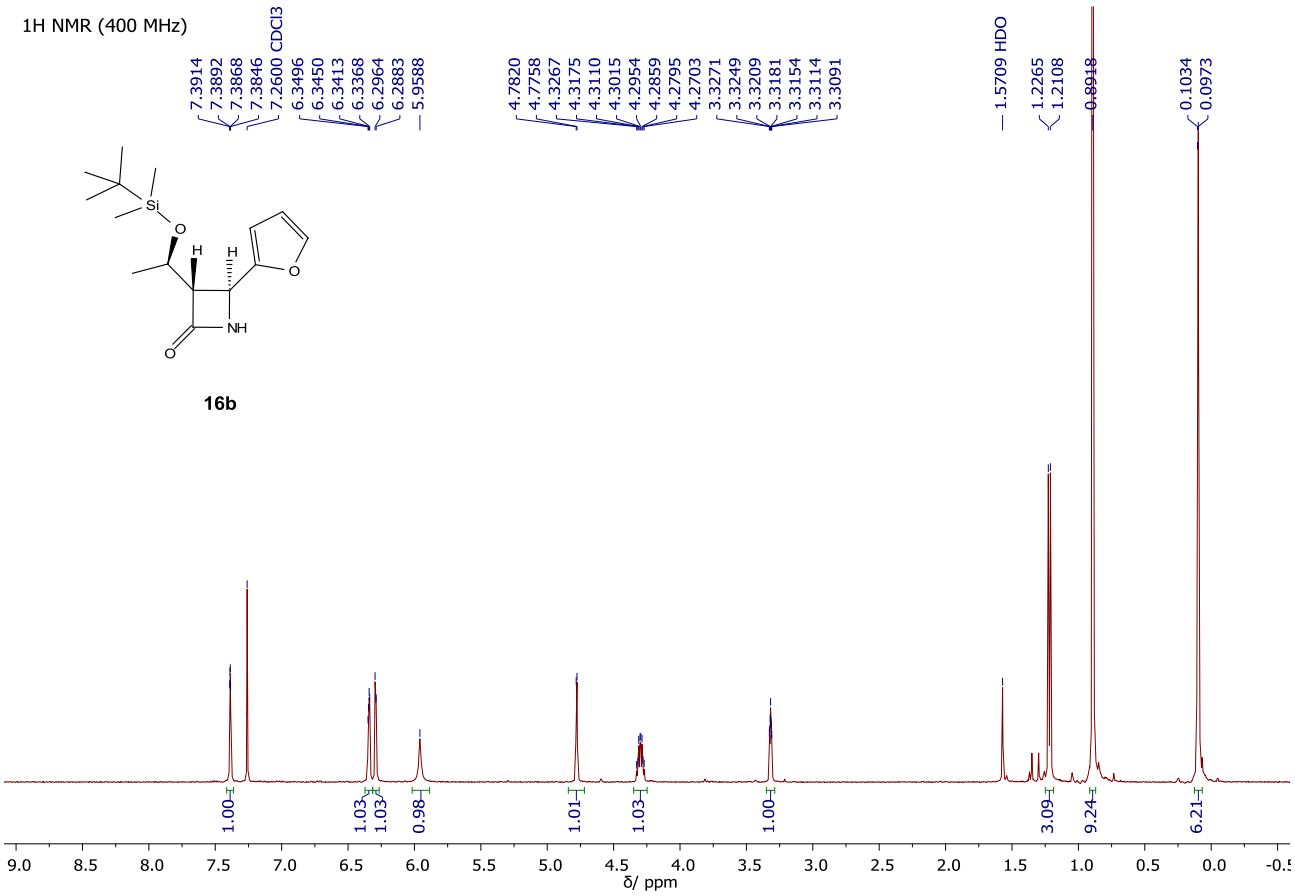

168.99
168.62
168.60
168.33
168.22
168.03
159.95
159.82
159.79
129.70
129.65
128.92
128.17
128.03
127.01
126.95
114.39
114.24
77.16 CDCl3
68.31
67.73
66.29
65.79
65.60
64.50
64.45
63.43
61.52
61.45
61.38
59.16
58.14
57.94
56.92
55.54
55.42
41.47
41.32
41.27
41.06
26.01
25.97
25.89
25.85
22.70
22.62
22.36
20.61
18.25
18.09
18.06
17.93
14.22
-3.75
-4.15
-4.43
-4.52
-4.60
-4.62
-4.75
-5.30
12a : 12b : 12c : 12d
8 : 39 : 49 : 5
δ/ ppm

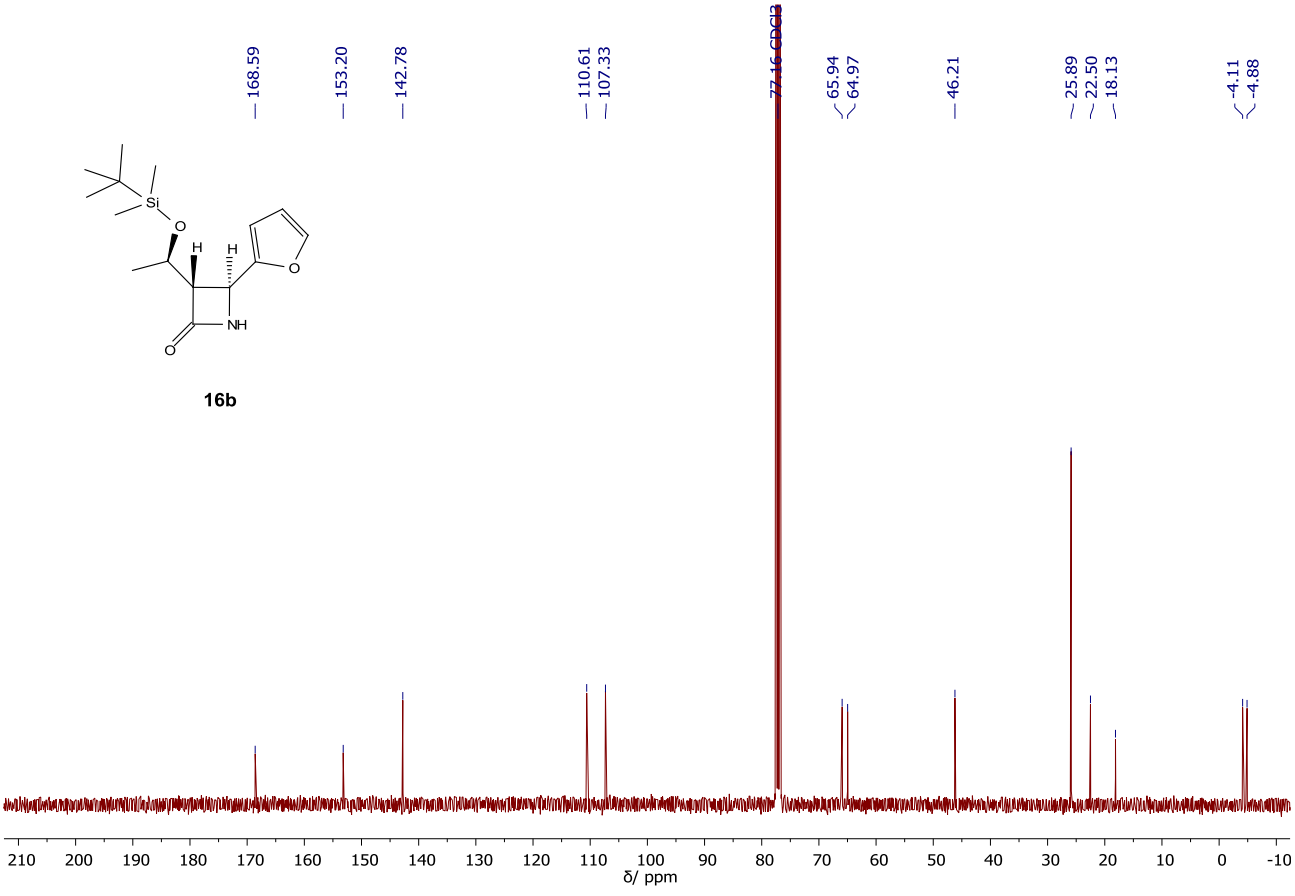

1H NMR (400 MHz)
7.7353
7.7270
7.7216
7.7099
7.7044
7.6961
7.2600 CDCl3
6.9205
6.9123
6.9068
6.8951
6.8897
6.8814
4.4180
4.4117
4.4020
4.3958
4.3860
4.3798
4.3701
4.3639
3.8109
3.7681
3.7619
1.5439 HDO
1.4239
1.4078
0.7670
0.0712
0.0336
grease
grease
1.70
2.00
0.93
2.82
1.09
3.17
8.39
3.17
2.92
δ/ ppm

15

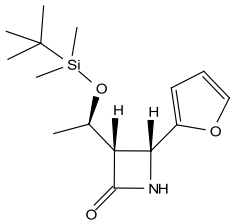

167.43
166.65
158.04
127.46
120.87
114.42
77.16 CDCl3
68.75
64.43
55.58
25.65
21.89
17.88
-4.25
-5.21
δ/ ppm

15

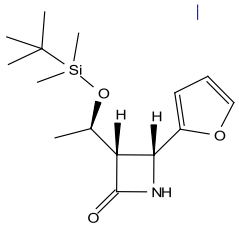

1H NMR (400 MHz)
7.3914
7.3892
7.3868
7.3846
7.2600 CDCl3
6.3496
6.3450
6.3413
6.3368
6.2964
6.2883
5.9588
4.7820
4.7758
4.3267
4.3175
4.3110
4.3015
4.2954
4.2859
4.2795
4.2703
3.3271
3.3249
3.3209
3.3181
3.3154
3.3114
3.3091
1.5709 HDO
1.2265
1.2108
0.8918
0.1034
0.0973
Si
O
H
H
O
NH
O
16b
1.00
1.03
1.03
0.98
1.01
1.03
1.00
3.09
9.24
6.21
δ/ ppm


168.59
153.20
142.78
110.61
107.33
77.16 CDCl3
65.94
64.97
46.21
25.89
22.50
18.13
-4.11
-4.88
Si
O
H
H
O
NH
O
16b
δ/ ppm

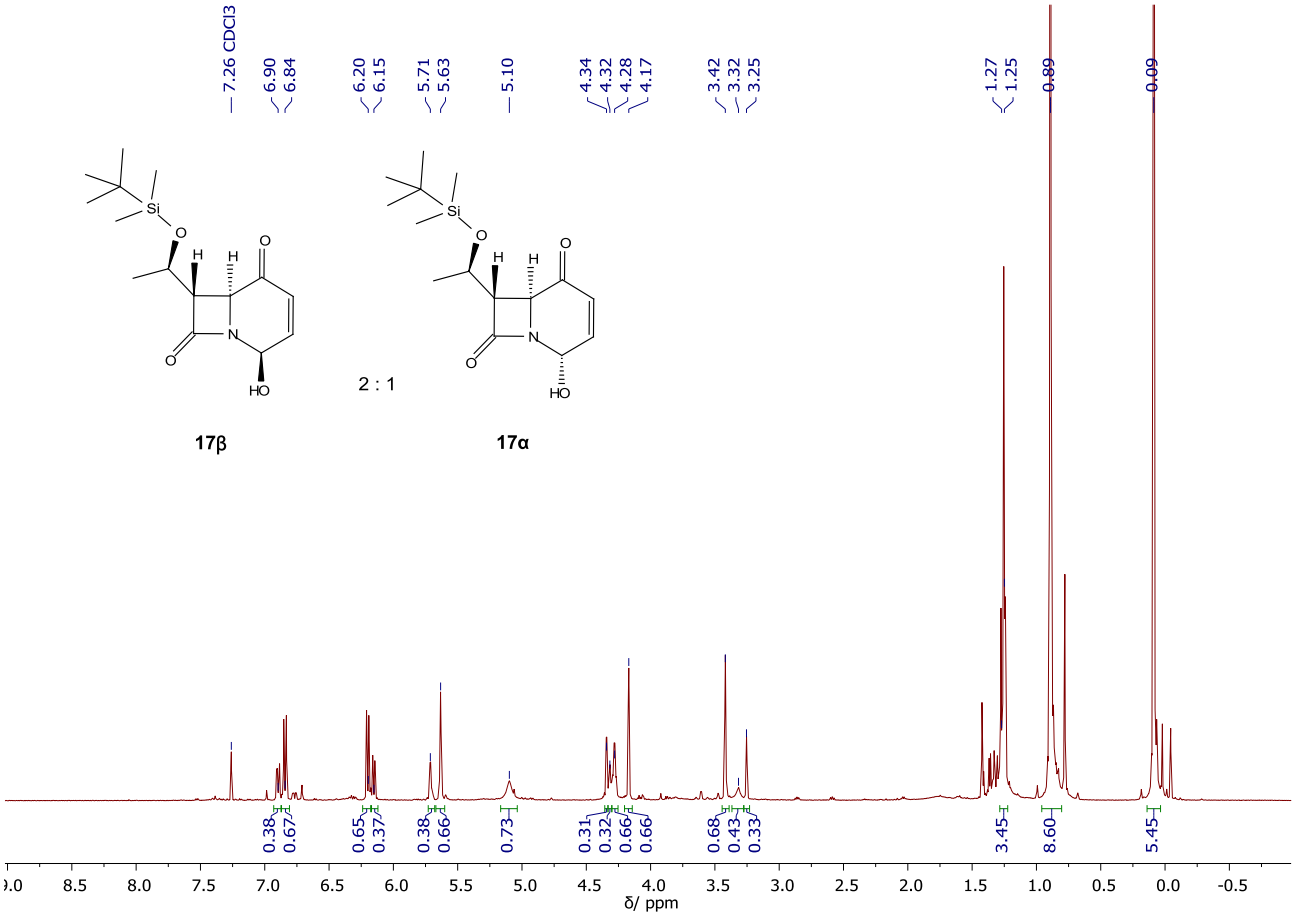
1H NMR (400 MHz)



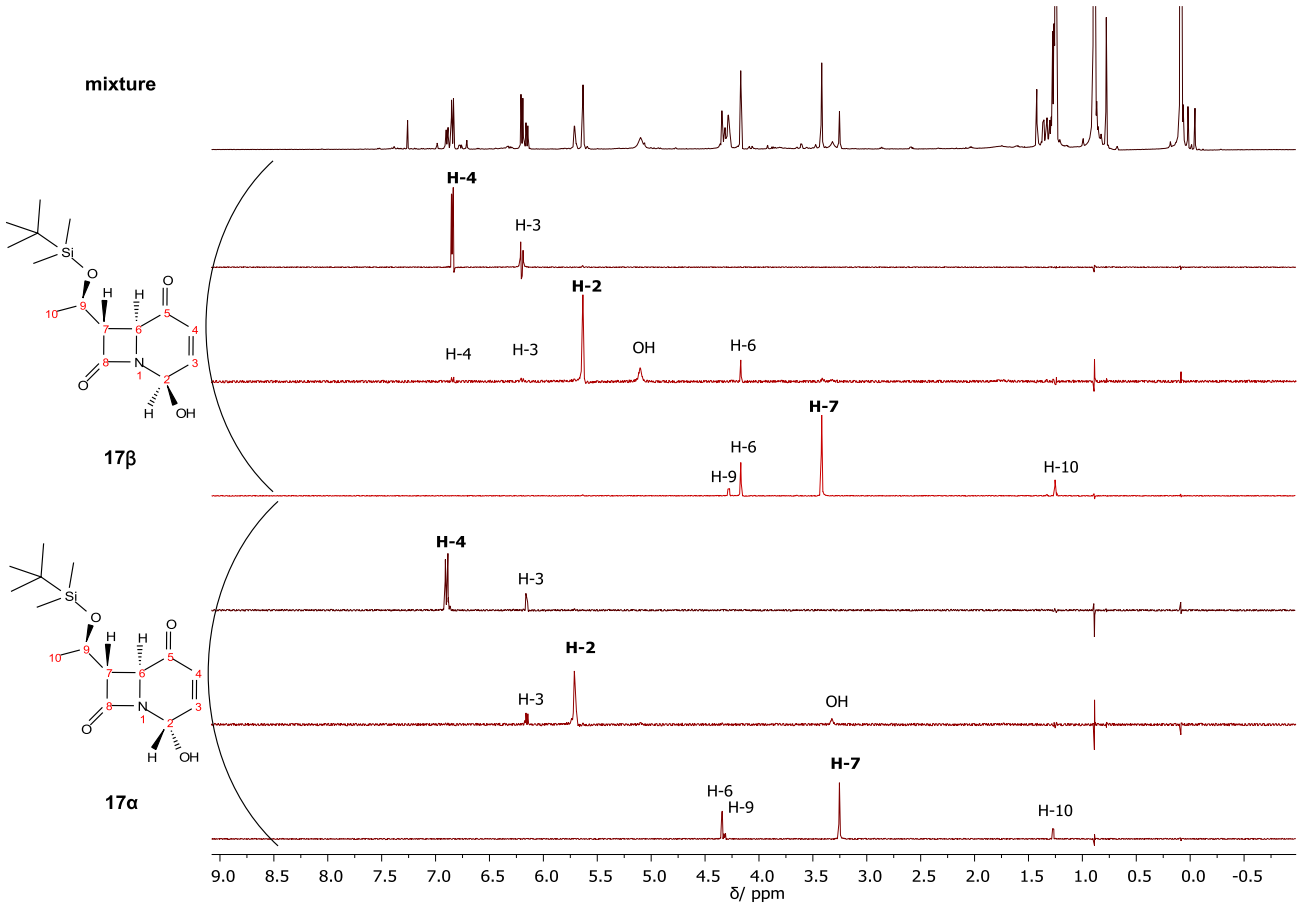
16c



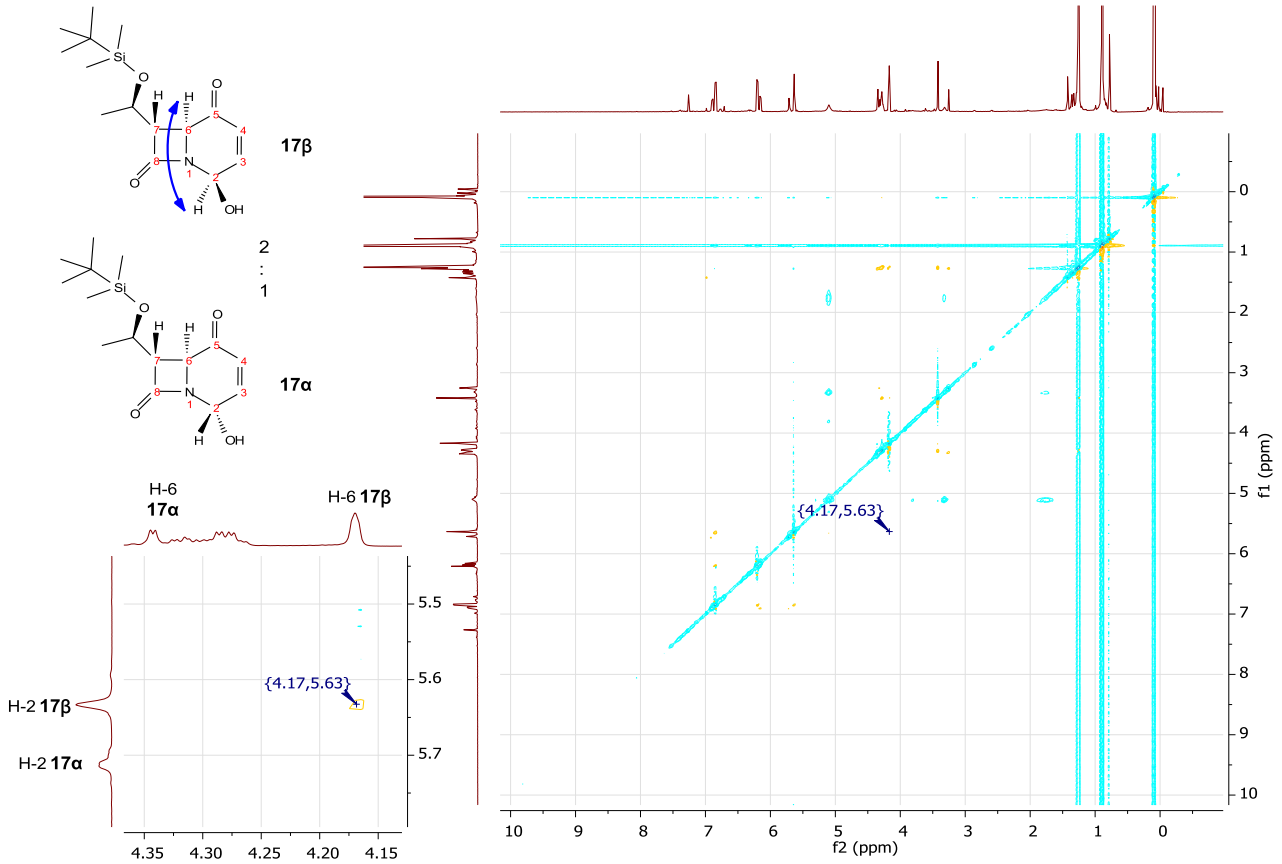
16c

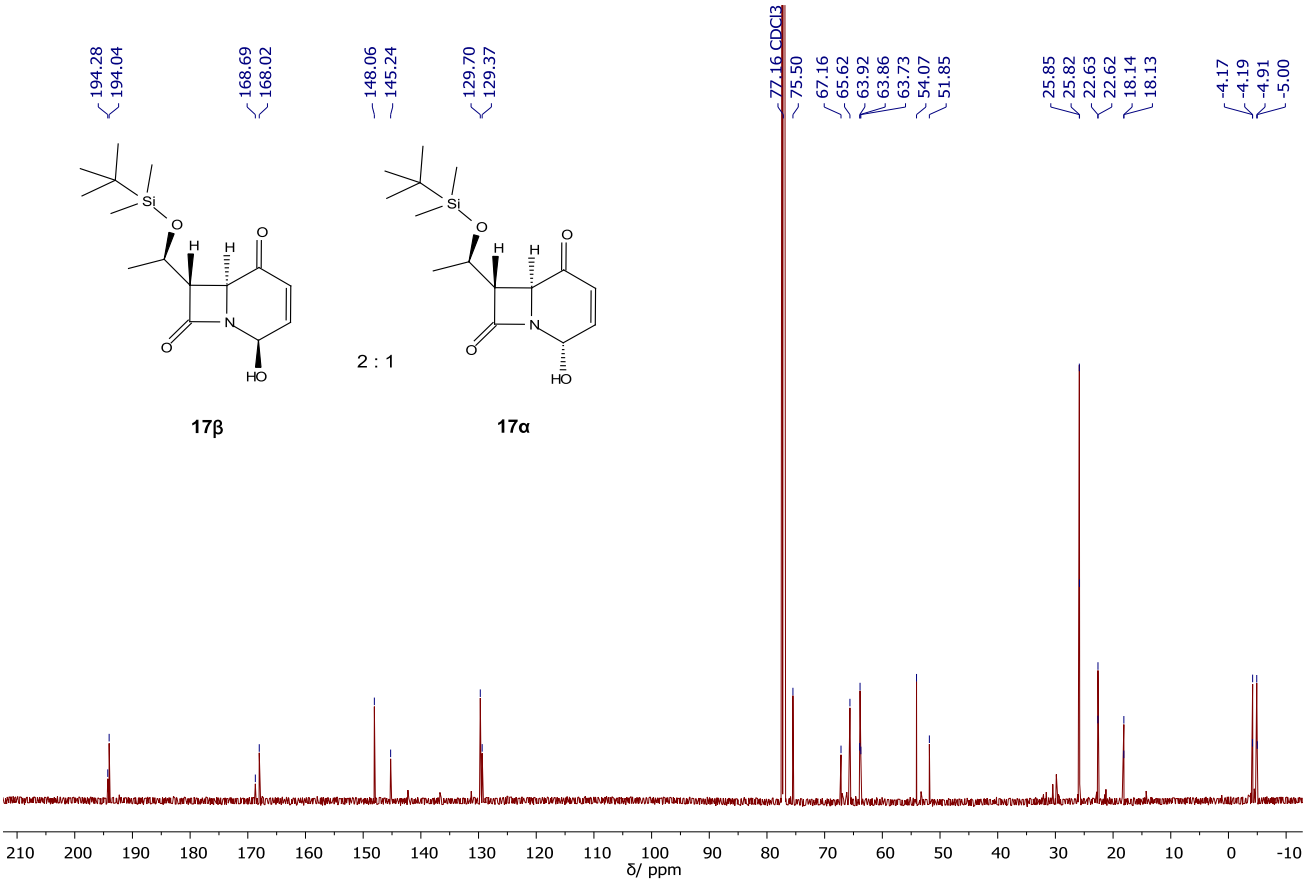


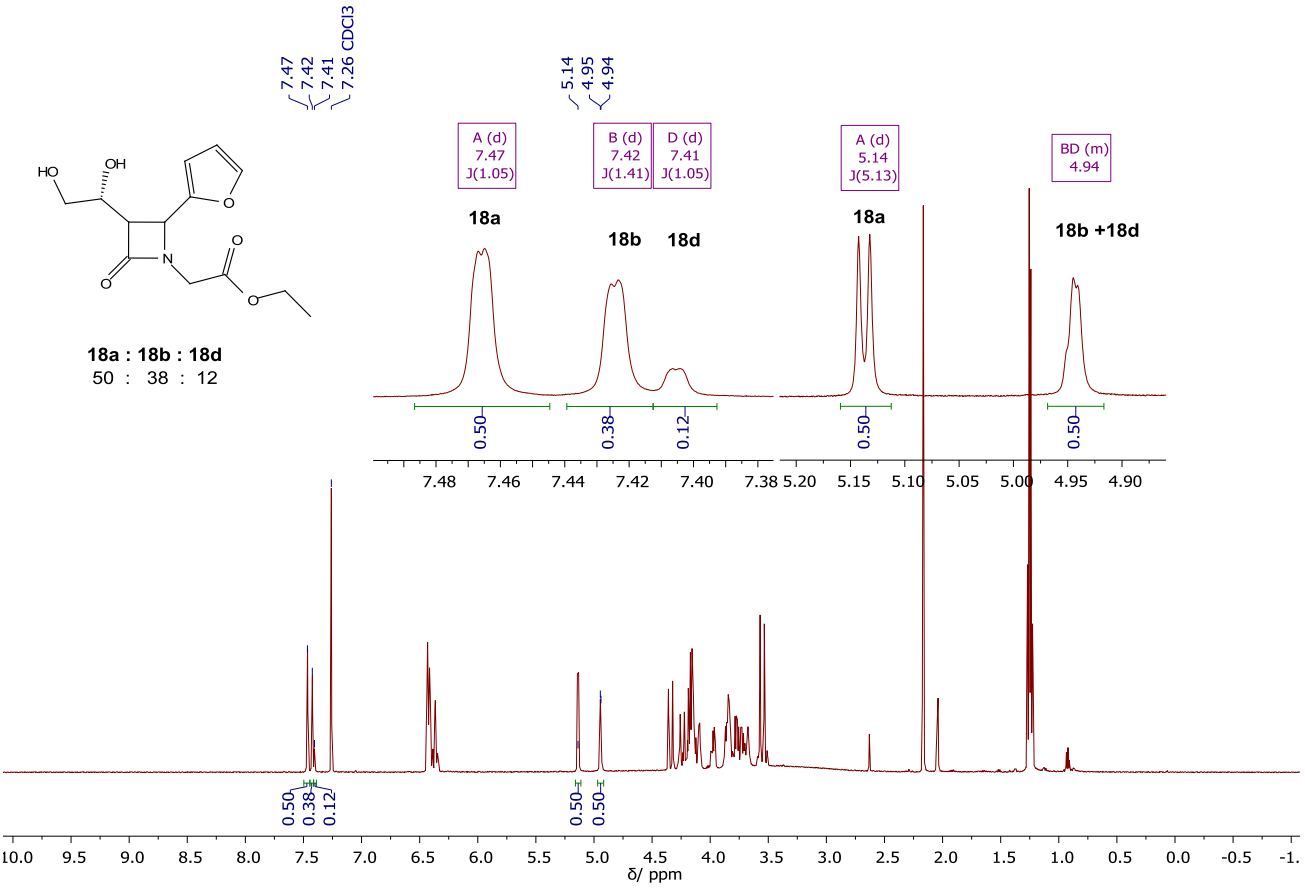
Signals in **17** were assigned using ^{1}H TOCSY experiment:

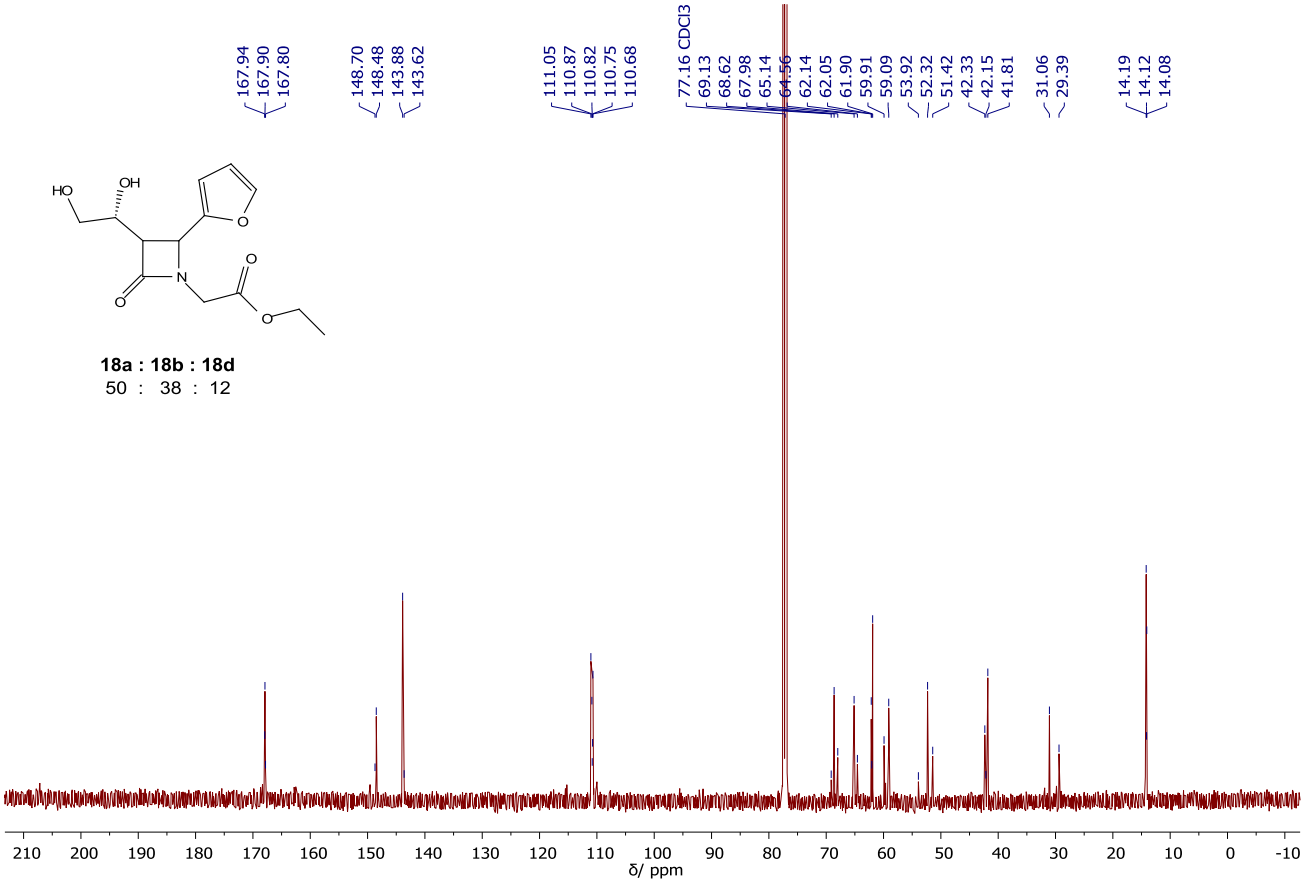


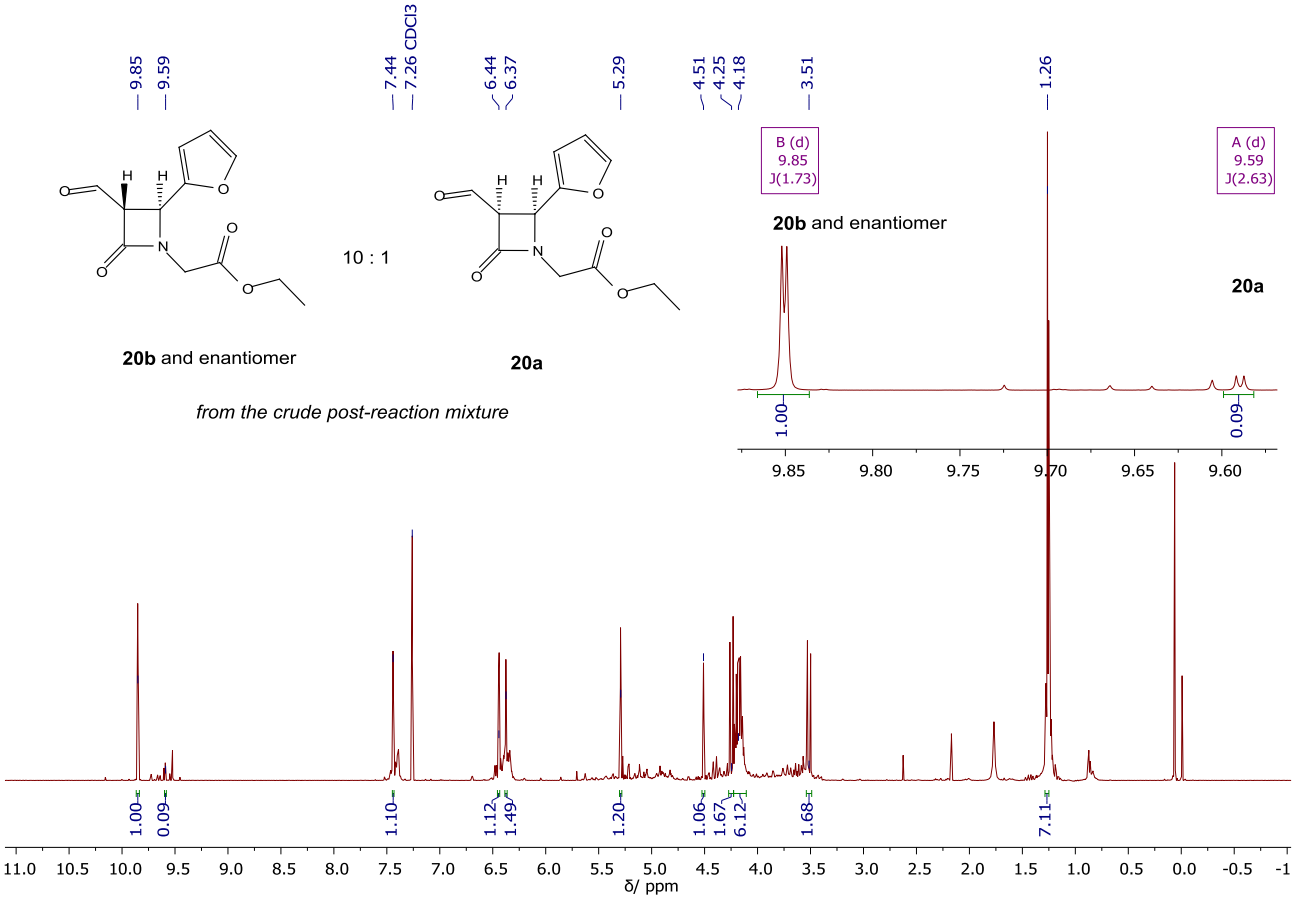
Stereochemistry of **17** was confirmed by ^{1}H–^{1}H NOESY experiment:

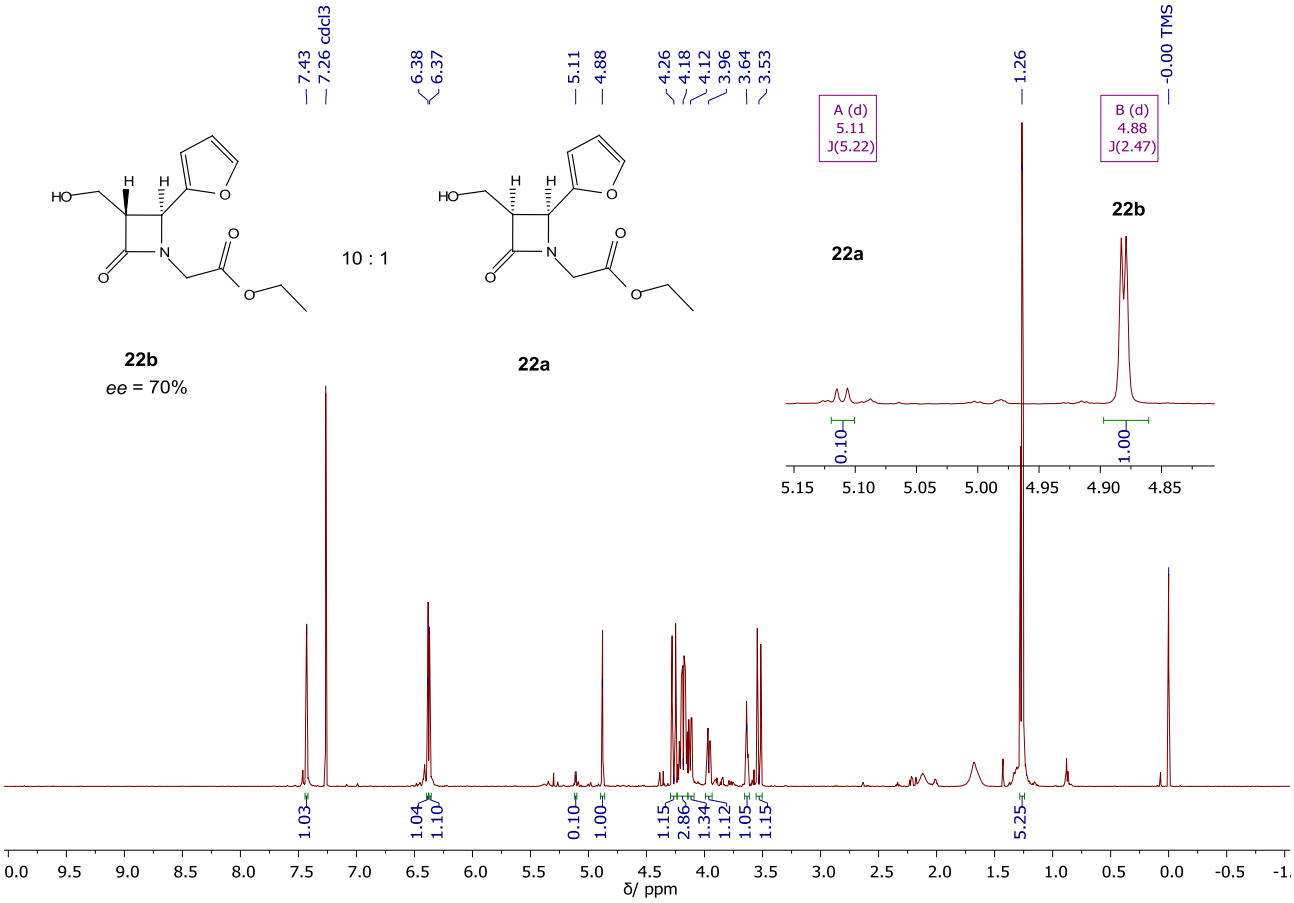


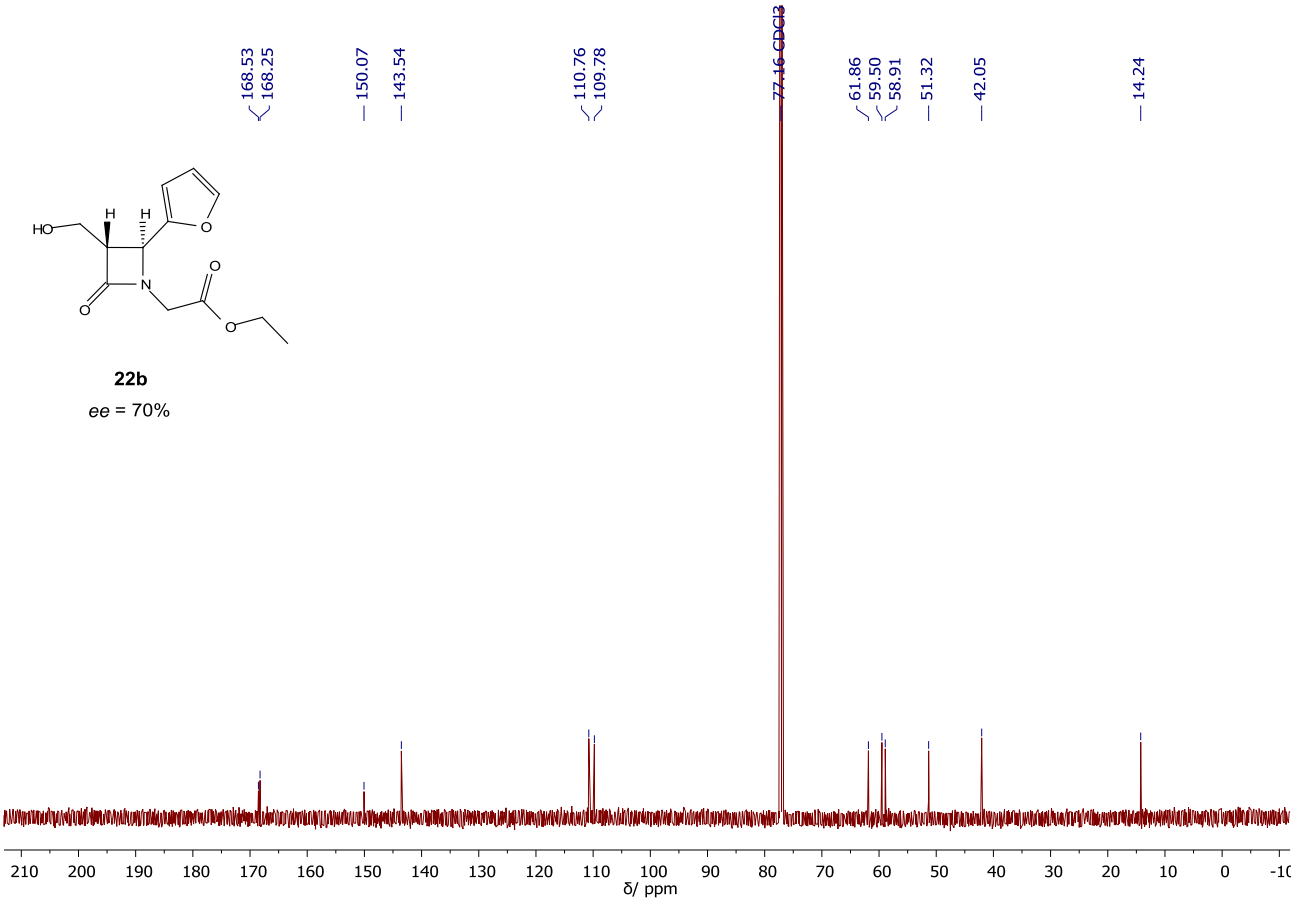


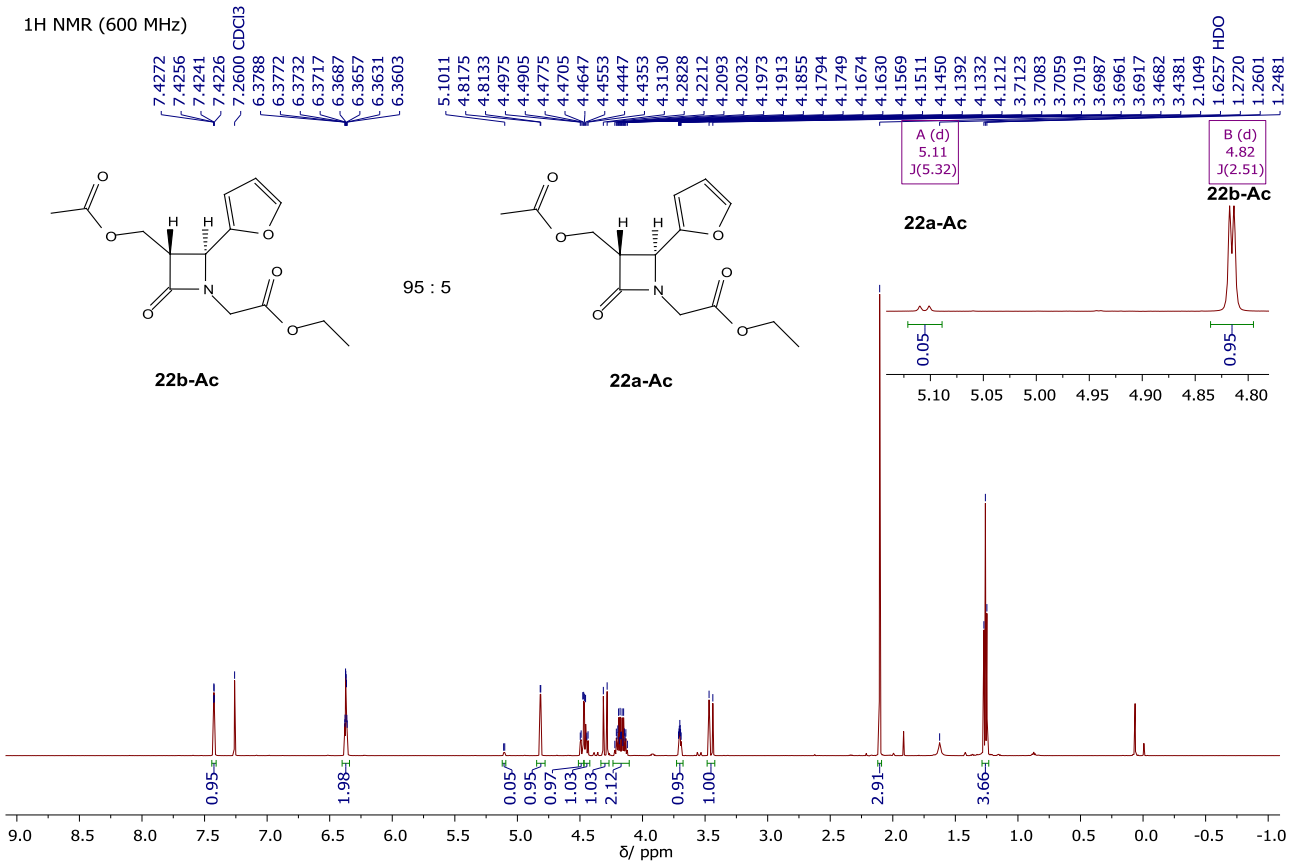

7.47
7.42
7.41
7.26 CDCl3
5.14
4.95
4.94
A (d)
7.47
J(1.05)
B (d)
7.42
J(1.41)
D (d)
7.41
J(1.05)
A (d)
5.14
J(5.13)
BD (m)
4.94
18a
18b
18d
18a
18b +18d
HO
OH
O
N
O
O
O
18a : 18b : 18d
50 : 38 : 12
0.50
0.38
0.12
0.50
0.50
0.50
0.38
0.12
0.50
0.50
7.48 7.46 7.44 7.42 7.40 7.38
5.20 5.15 5.10 5.05 5.00 4.95 4.90
δ/ ppm

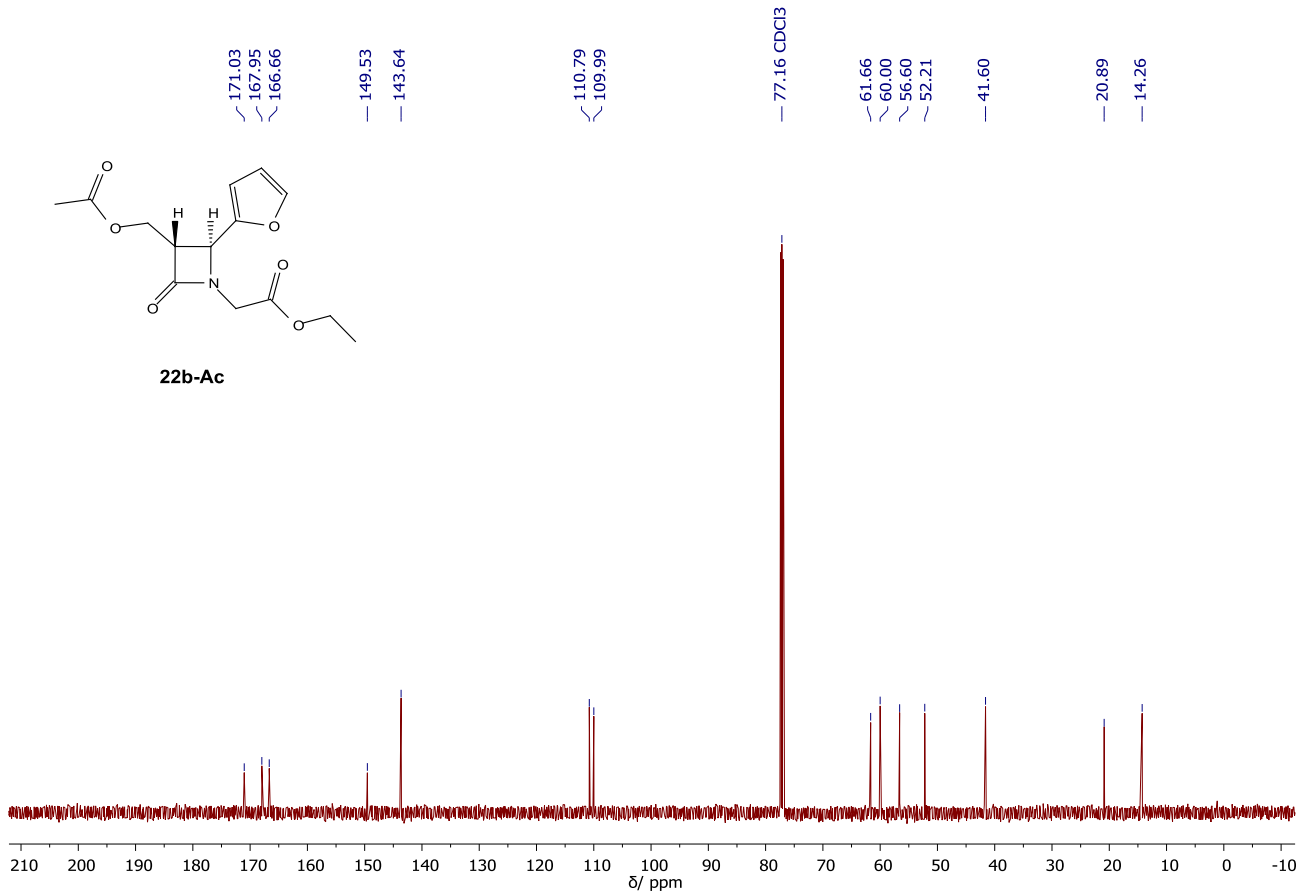

167.94
167.90
167.80
148.70
148.48
143.88
143.62
111.05
110.87
110.82
110.75
110.68
77.16 CDCl3
69.13
68.62
67.98
65.14
64.56
62.14
62.05
61.90
59.91
59.09
53.92
52.32
51.42
42.33
42.15
41.81
31.06
29.39
14.19
14.12
14.08
HO
OH
O
N
O
O
O
18a : 18b : 18d
50 : 38 : 12
δ/ ppm

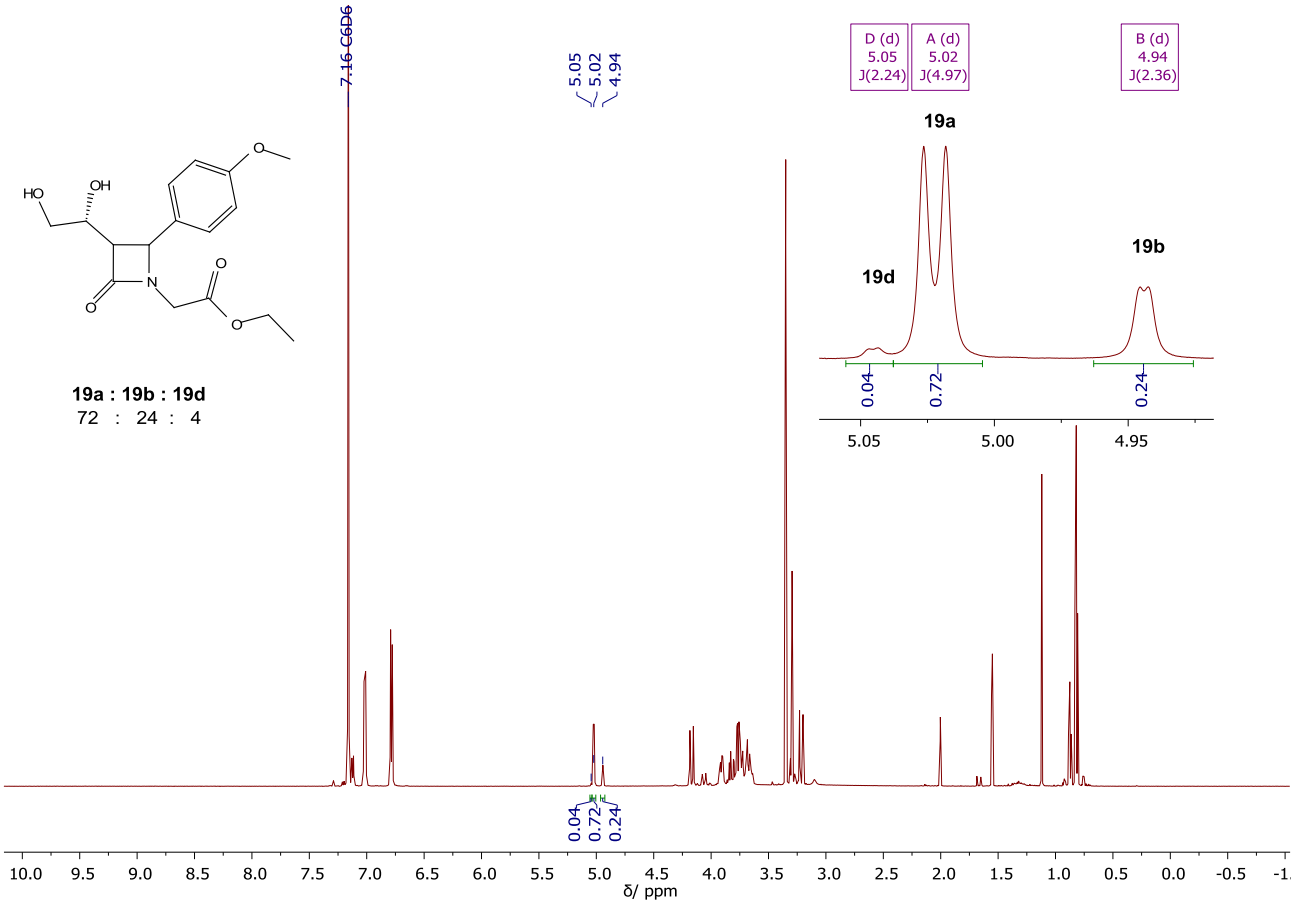

9.85
9.59
7.44
7.26 CDCl3
6.44
6.37
5.29
4.51
4.25
4.18
3.51
1.26
B (d)
9.85
J(1.73)
A (d)
9.59
J(2.63)
20b and enantiomer
20a
10 : 1
20b and enantiomer
20a
from the crude post-reaction mixture
1.00
0.09
1.10
1.12
1.49
1.20
1.06
1.67
6.12
1.68
7.11
δ/ ppm

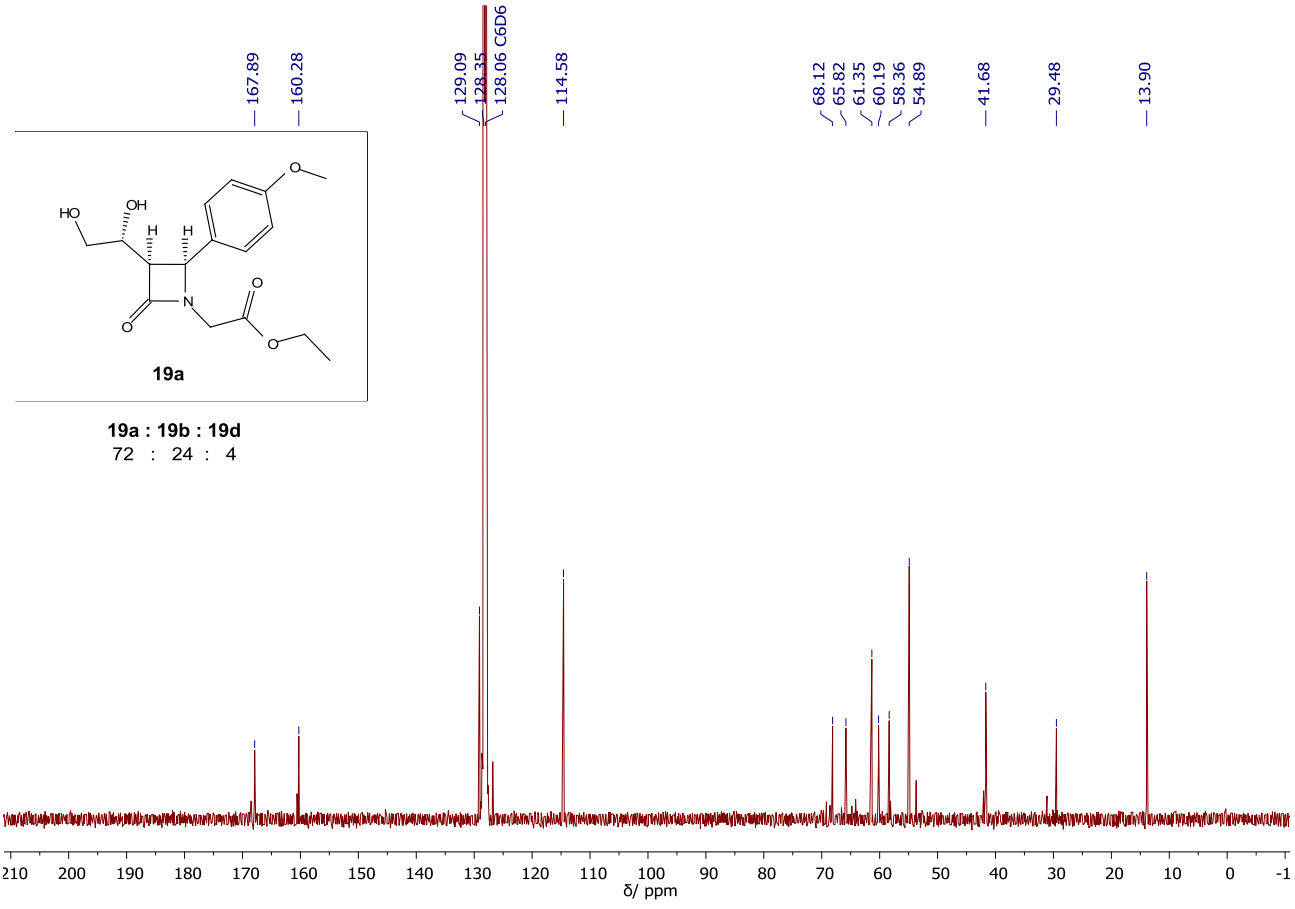

7.43
7.26 cdcl3
6.38
6.37
5.11
4.88
4.26
4.18
4.12
3.96
3.64
3.53
1.26
-0.00 TMS
A (d)
5.11
J(5.22)
B (d)
4.88
J(2.47)
22b
22a
10 : 1
22b
ee = 70%
22a
0.10
1.00
1.03
1.04
1.10
0.10
1.00
1.15
2.86
1.34
1.12
1.05
1.15
5.25
δ/ ppm

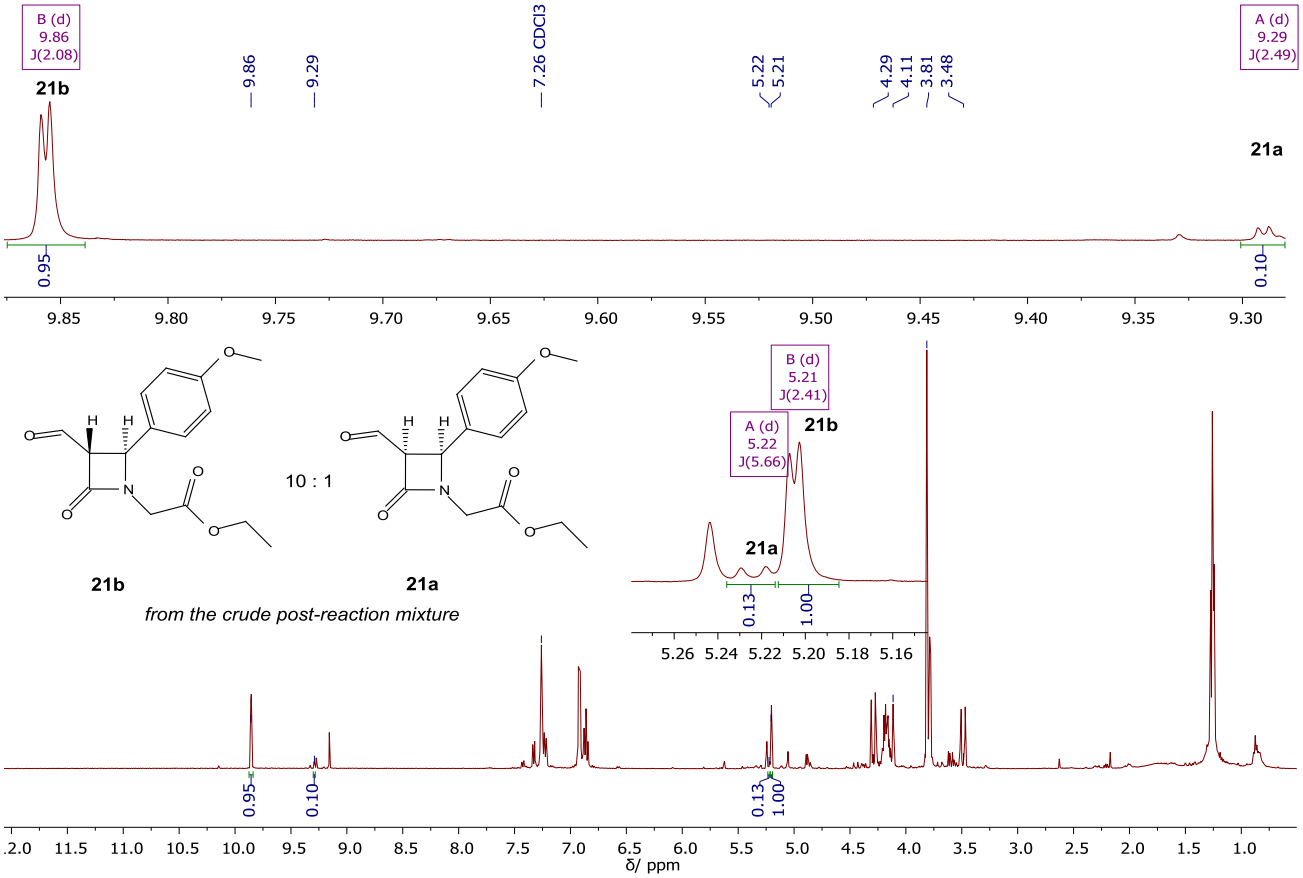

168.53
168.25
150.07
143.54
110.76
109.78
77.16 CDCl3
61.86
59.50
58.91
51.32
42.05
14.24
22b
ee = 70%
δ/ ppm

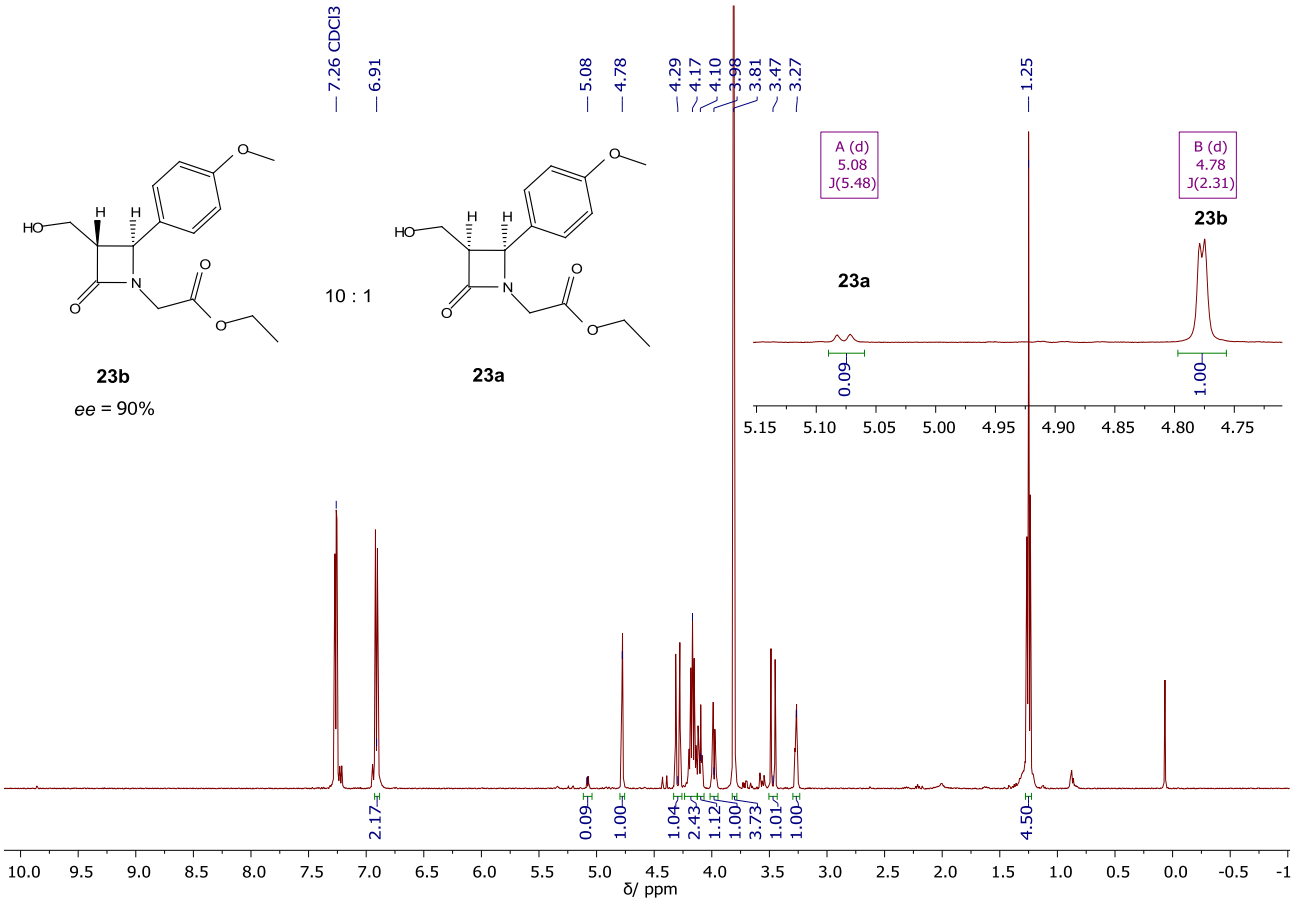

1H NMR (600 MHz)
7.4272
7.4256
7.4241
7.4226
7.2600 CDCl3
6.3788
6.3772
6.3732
6.3717
6.3687
6.3657
6.3631
6.3603
5.1011
4.8175
4.8133
4.4975
4.4905
4.4775
4.4705
4.4647
4.4553
4.4447
4.4353
4.3130
4.2828
4.2212
4.2093
4.2032
4.1973
4.1913
4.1855
4.1794
4.1749
4.1674
4.1630
4.1569
4.1511
4.1450
4.1392
4.1332
4.1212
3.7123
3.7083
3.7059
3.7019
3.6987
3.6961
3.6917
3.6682
3.4381
2.1049
1.6257 HDO
1.2720
1.2601
1.2481
A (d)
5.11
J(5.32)
B (d)
4.82
J(2.51)
22b-Ac
22a-Ac
95 : 5
22b-Ac
22a-Ac
0.05
0.95
5.10
5.05
5.00
4.95
4.90
4.85
4.80
0.95
1.98
0.05
0.95
0.97
1.03
1.03
2.12
0.95
1.00
2.91
3.66
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
δ/ ppm

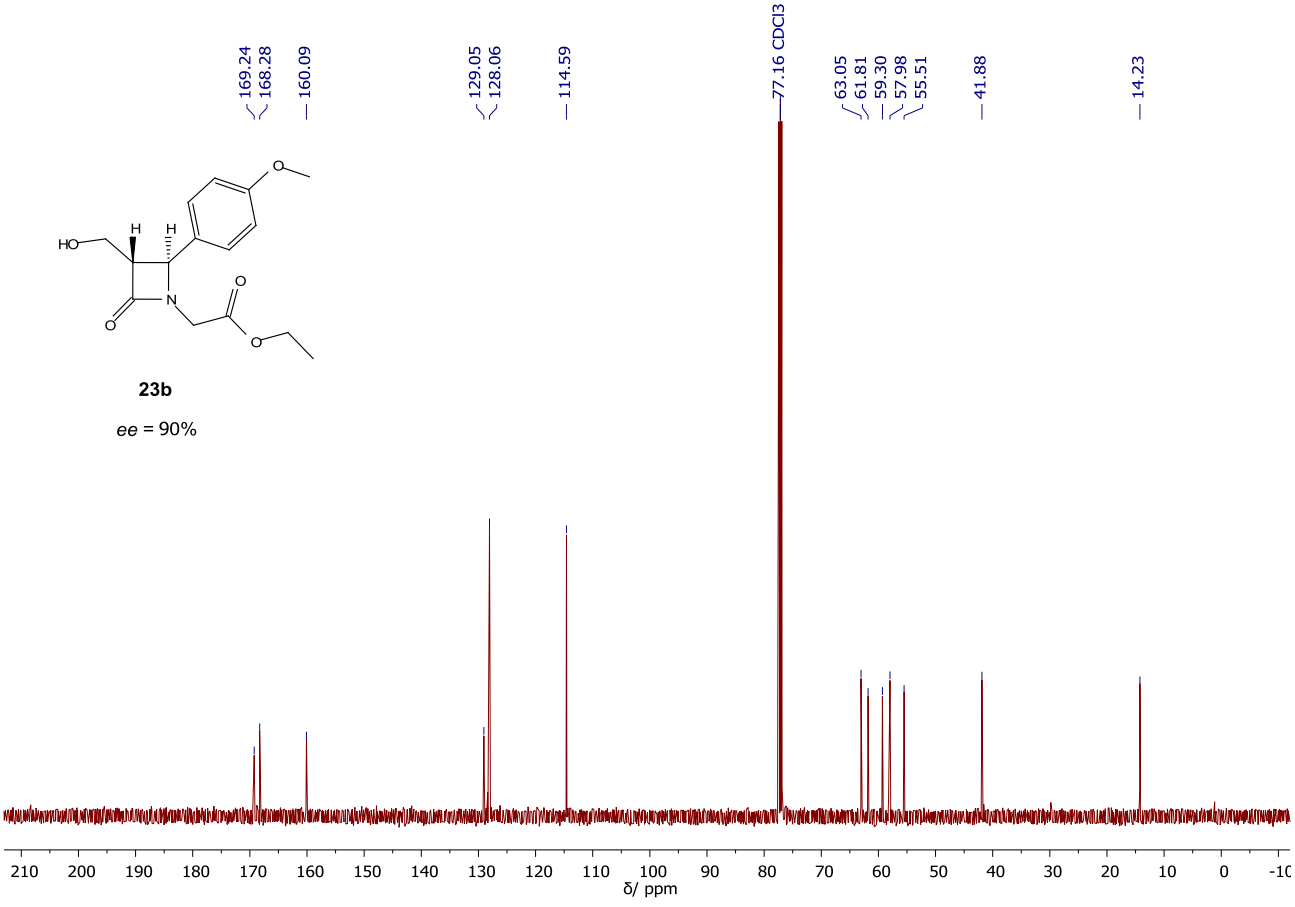

171.03
167.95
166.66
149.53
143.64
110.79
109.99
77.16 CDCl3
61.66
60.00
56.60
52.21
41.60
20.89
14.26
22b-Ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
δ/ ppm

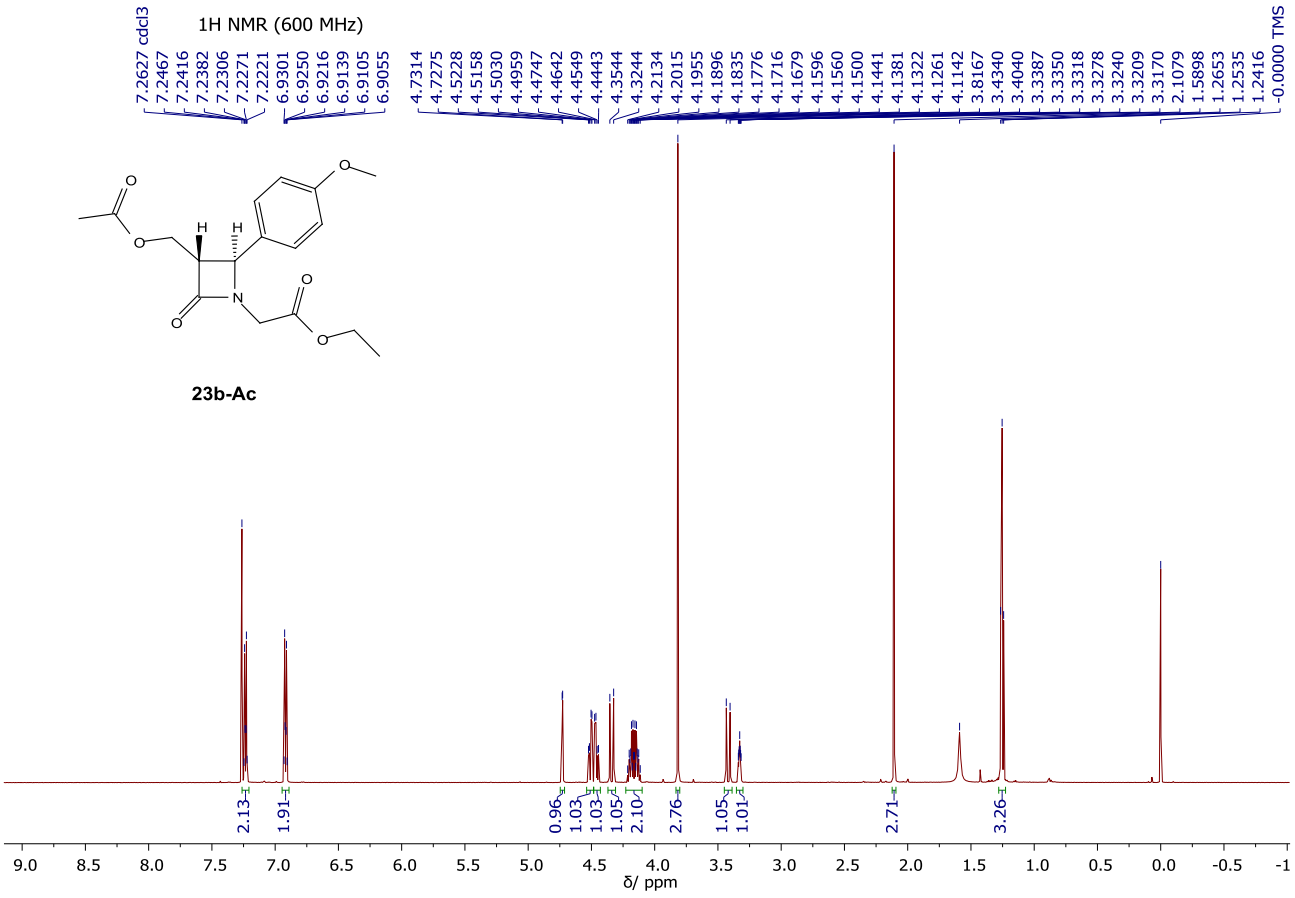

7.16 C6D6
5.05
5.02
4.94
D (d)
5.05
J(2.24)
A (d)
5.02
J(4.97)
B (d)
4.94
J(2.36)
19a
19b
19d
0.04
0.72
0.24
5.05
5.00
4.95
HO
OH
O
N
O
O
O
19a : 19b : 19d
72 : 24 : 4
δ/ ppm

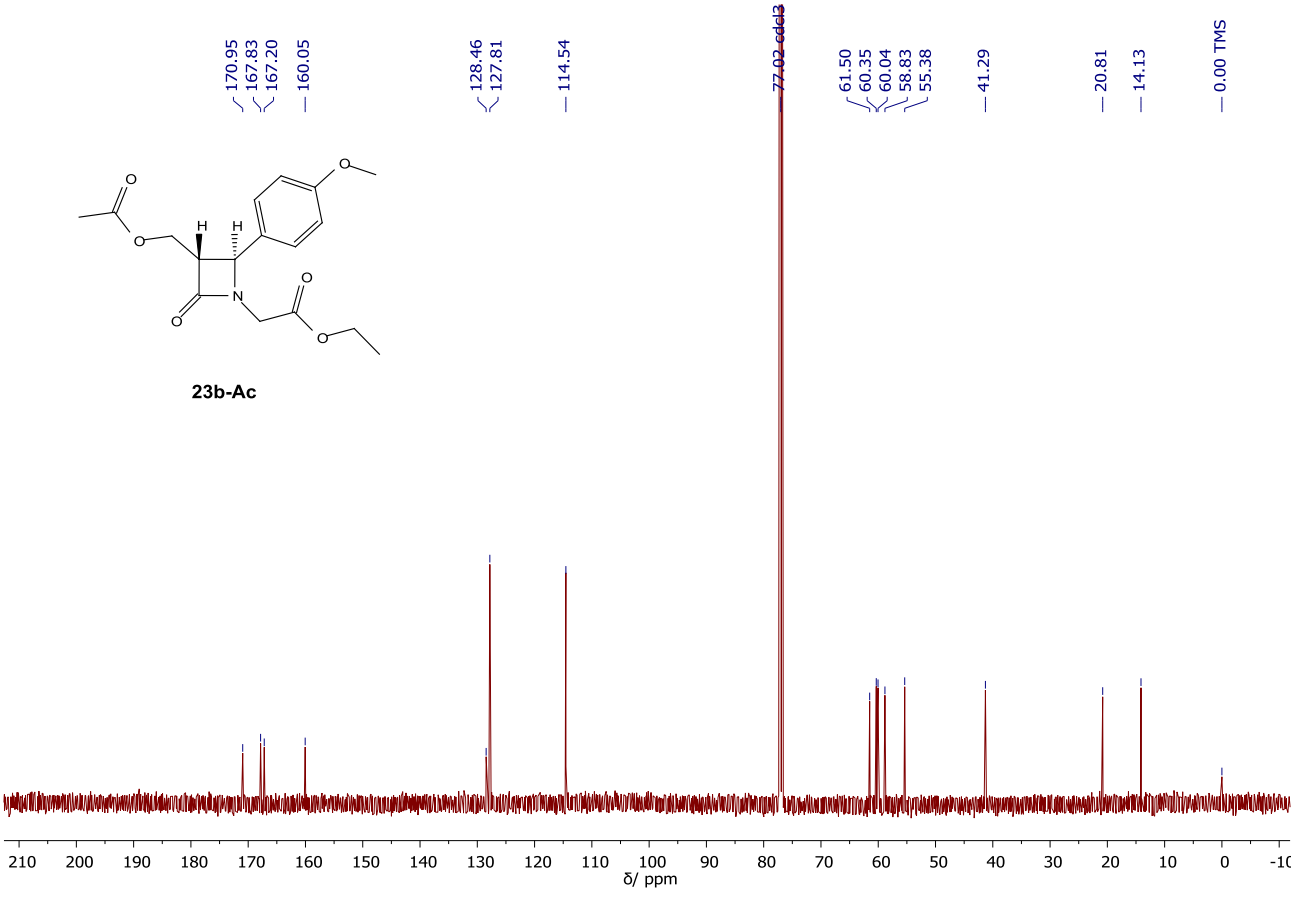

167.89
160.28
129.09
128.35
128.06 C6D6
114.58
68.12
65.82
61.35
60.19
58.36
54.89
41.68
29.48
13.90
HO
OH
H
H
O
N
O
O
O
19a
19a : 19b : 19d
72 : 24 : 4
δ/ ppm

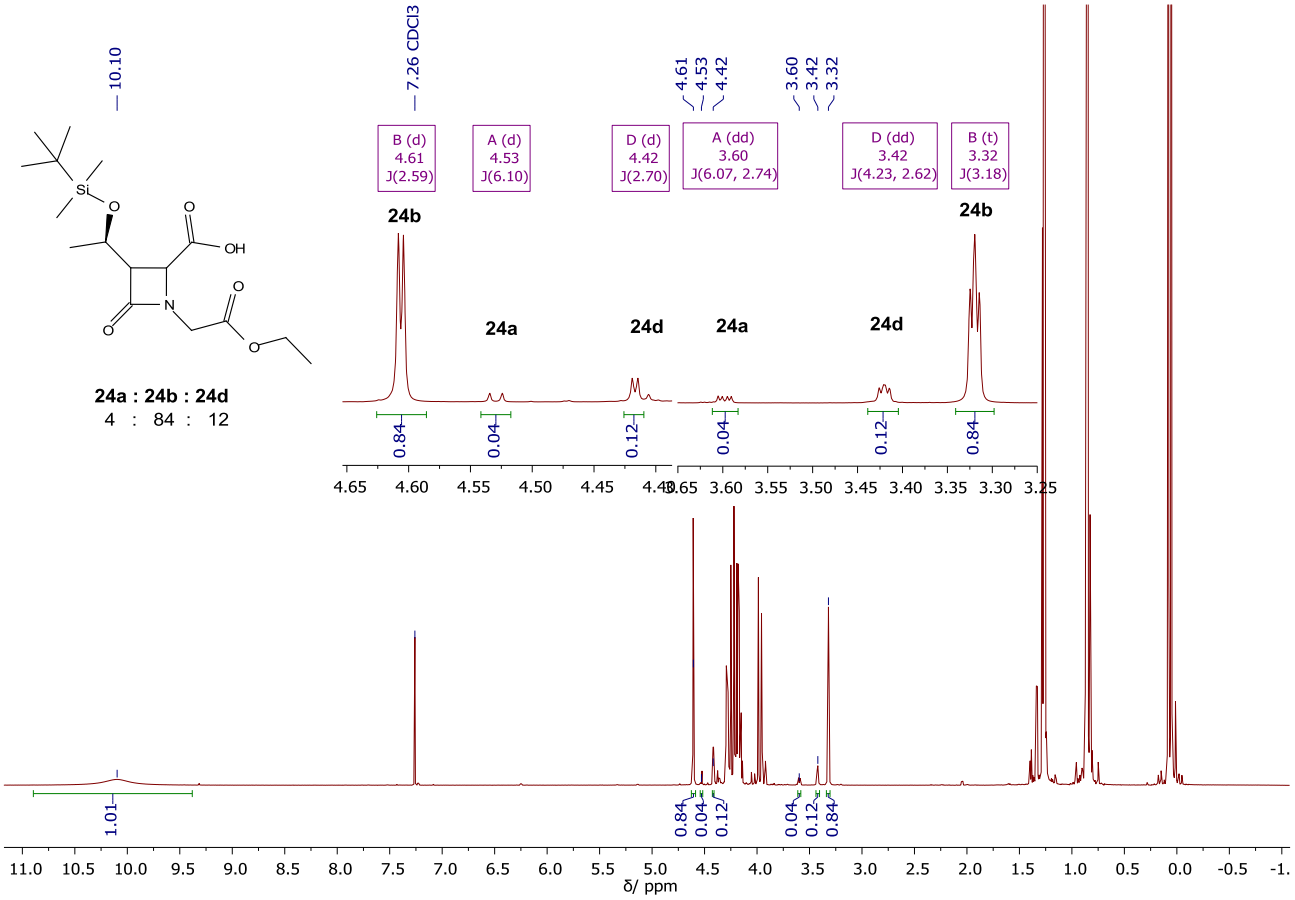

B (d)
9.86
J(2.08)
21b
9.86
9.29
7.26 CDCl3
5.22
5.21
4.29
4.11
3.81
3.48
A (d)
9.29
J(2.49)
21a
0.95
0.10
9.85 9.80 9.75 9.70 9.65 9.60 9.55 9.50 9.45 9.40 9.35 9.30
10 : 1
21b
21a
from the crude post-reaction mixture
B (d)
5.21
J(2.41)
A (d)
5.22
J(5.66)
21b
21a
0.13
1.00
5.26 5.24 5.22 5.20 5.18 5.16
0.95
0.10
0.13
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
δ/ ppm


7.26 CDCl3
6.91
5.08
4.78
4.29
4.17
4.10
3.98
3.81
3.47
3.27
1.25
A (d)
5.08
J(5.48)
B (d)
4.78
J(2.31)
23b
23a
10 : 1
23b
ee = 90%
23a
0.09
1.00
2.17
0.09
1.00
1.04
2.43
1.12
1.00
3.73
1.01
1.00
4.50
δ/ ppm

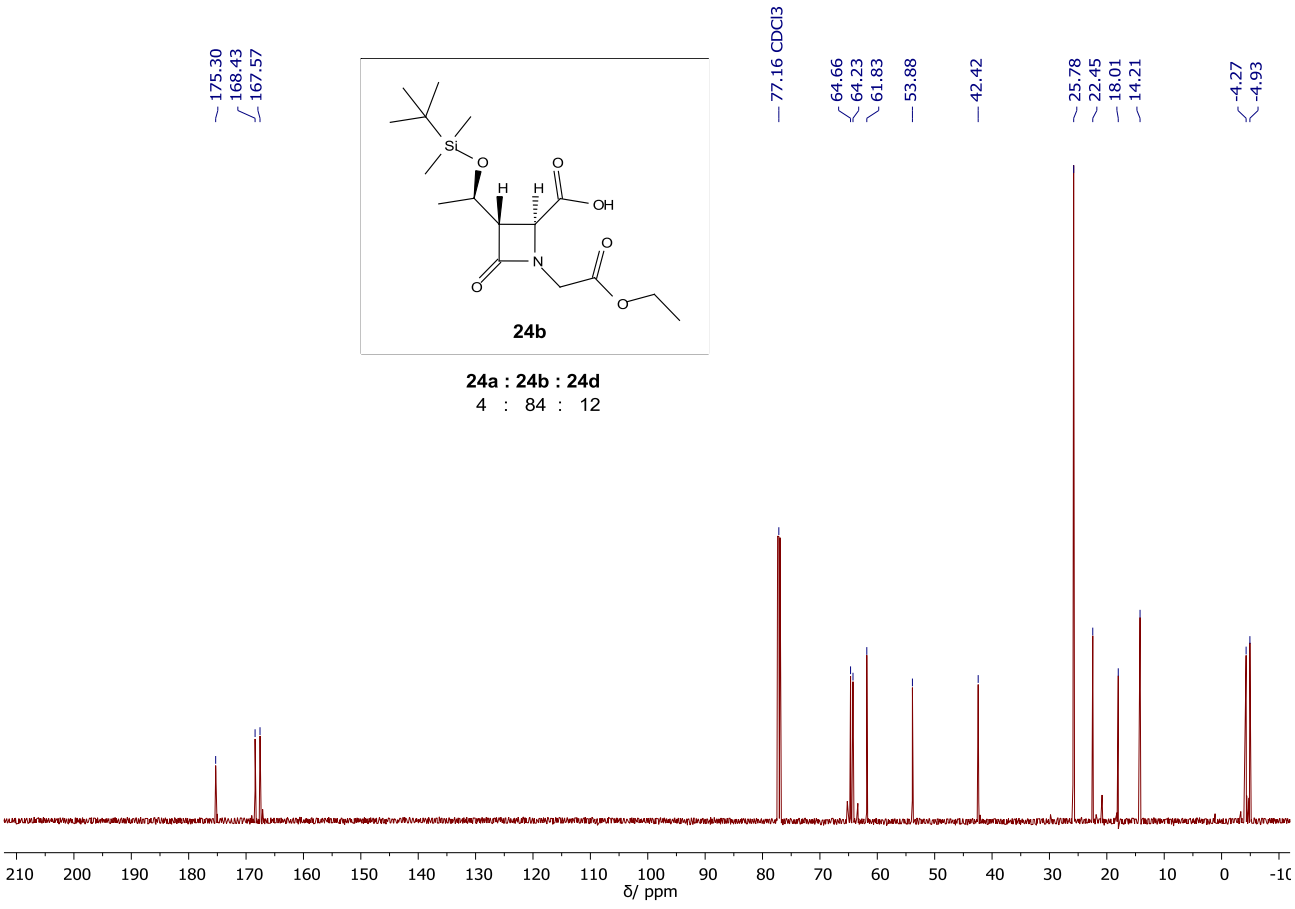

169.24
168.28
160.09
129.05
128.06
114.59
77.16 CDCl3
63.05
61.81
59.30
57.98
55.51
41.88
14.23
23b
ee = 90%
δ/ ppm


1H NMR (600 MHz)
7.2627 cdcl3
7.2467
7.2416
7.2382
7.2306
7.2271
7.2221
6.9301
6.9250
6.9216
6.9139
6.9105
6.9055
4.7314
4.7275
4.5228
4.5158
4.5030
4.4959
4.4747
4.4642
4.4549
4.4443
4.3544
4.3244
4.2134
4.2015
4.1955
4.1896
4.1835
4.1776
4.1716
4.1679
4.1596
4.1560
4.1500
4.1441
4.1381
4.1322
4.1261
4.1142
3.8167
3.4340
3.4040
3.3387
3.3350
3.3318
3.3278
3.3240
3.3209
3.3170
2.1079
1.5898
1.2653
1.2535
1.2416
-0.0000 TMS
23b-Ac
2.13
1.91
0.96
1.03
1.03
1.05
2.10
2.76
1.05
1.01
2.71
3.26
δ/ ppm


170.95
167.83
167.20
160.05
128.46
127.81
114.54
77.02 cdcl3
61.50
60.35
60.04
58.83
55.38
41.29
20.81
14.13
0.00 TMS
23b-Ac
δ/ ppm

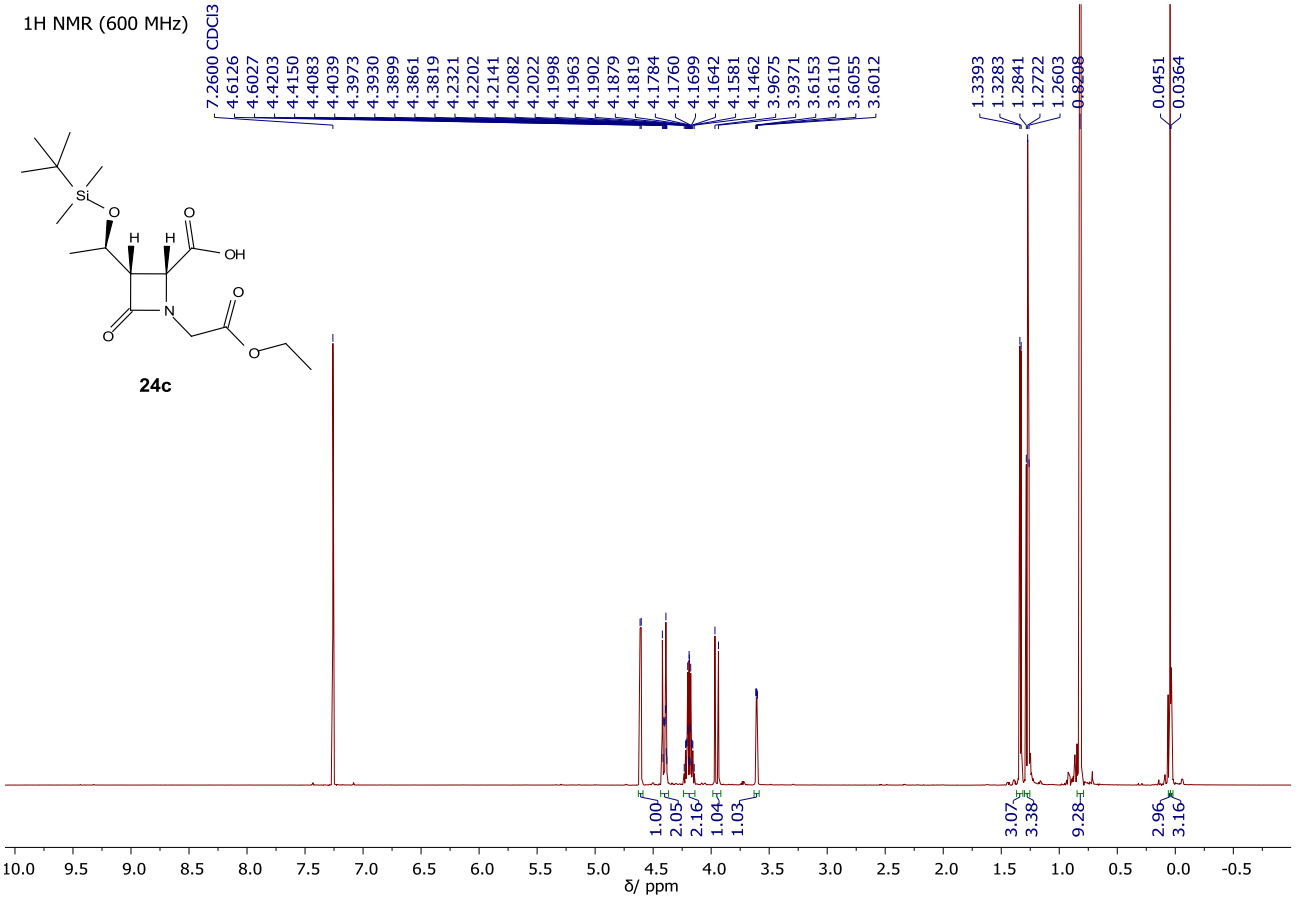


24a : 24b : 24d
4 : 84 : 12

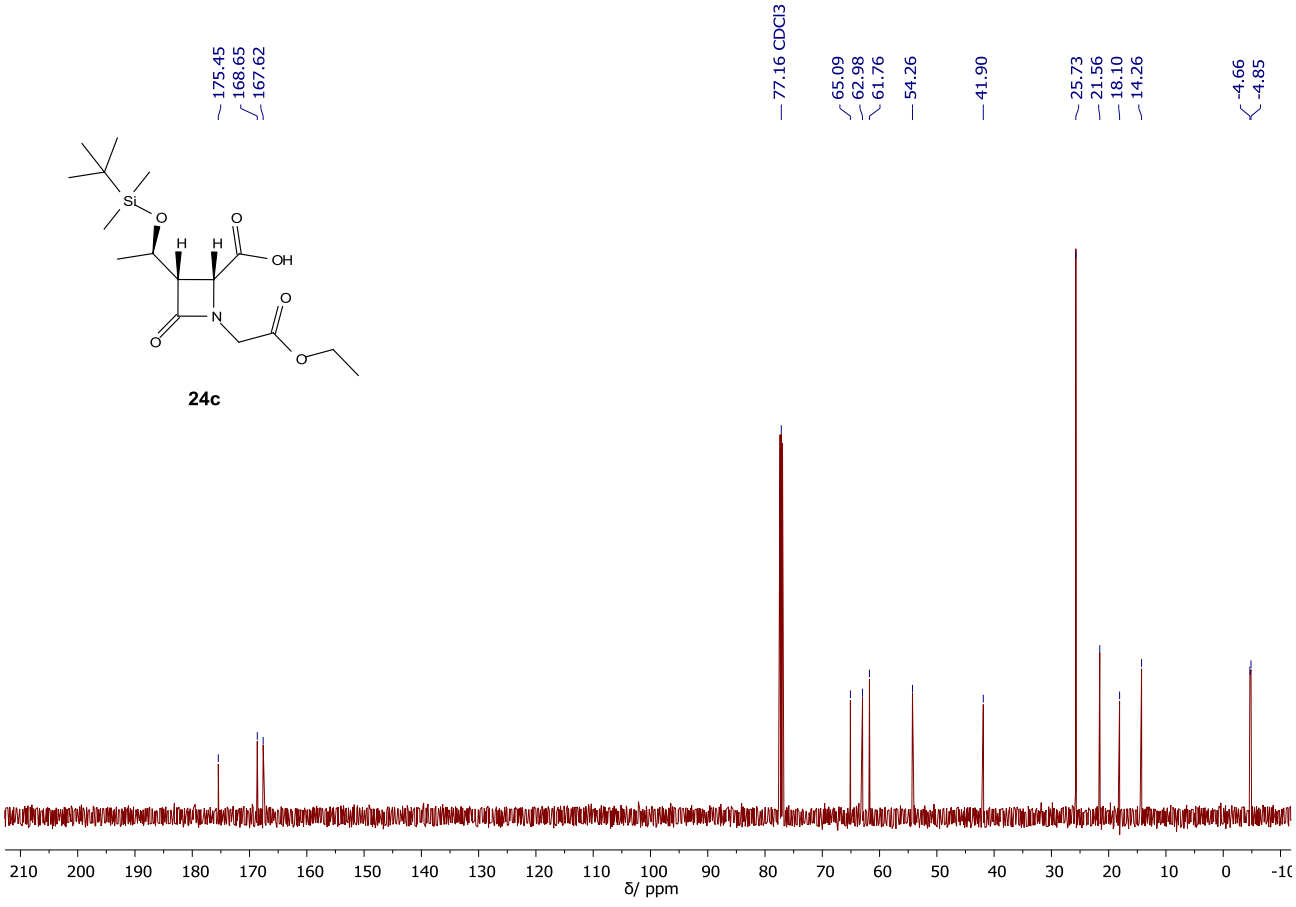


24b

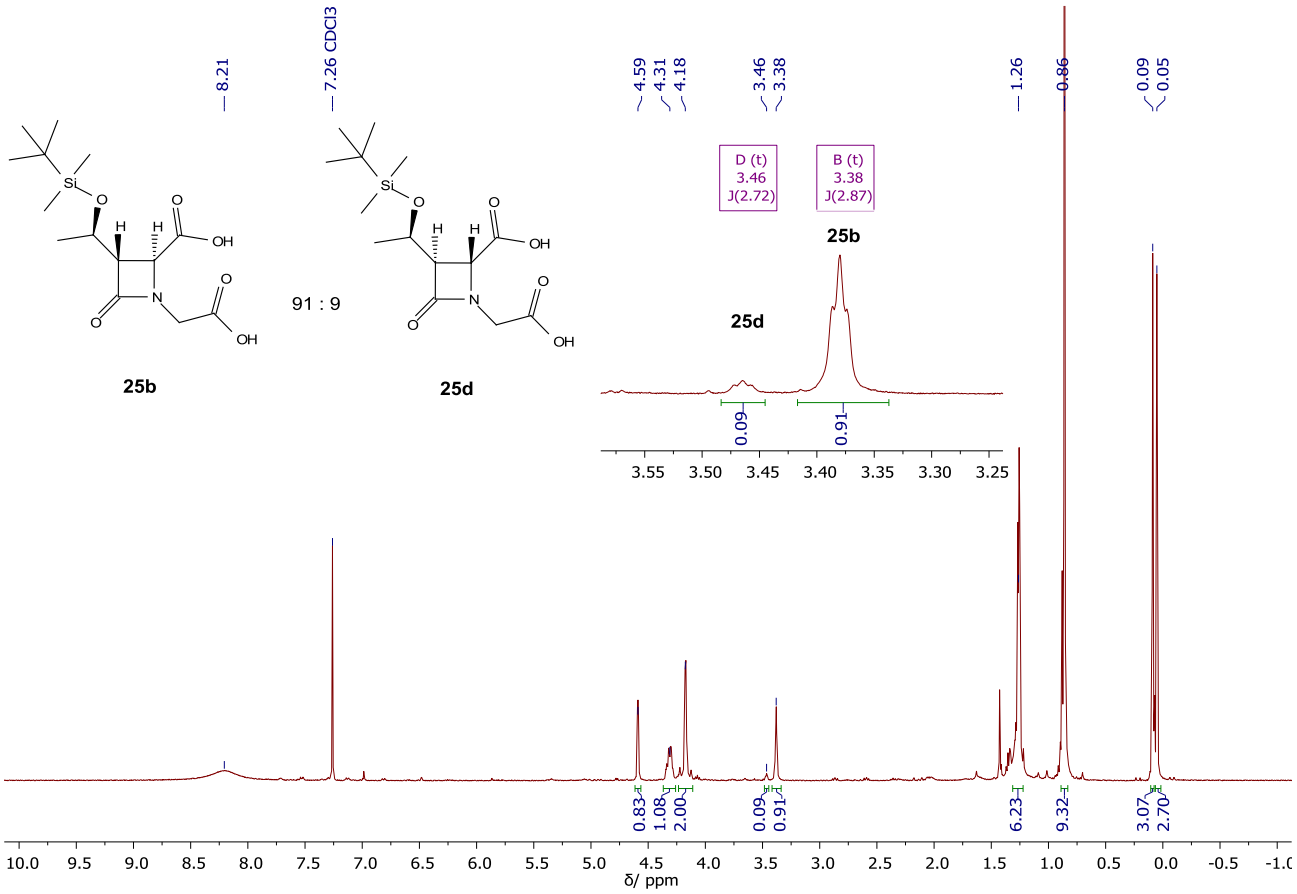
24a : 24b : 24d
4 : 84 : 12

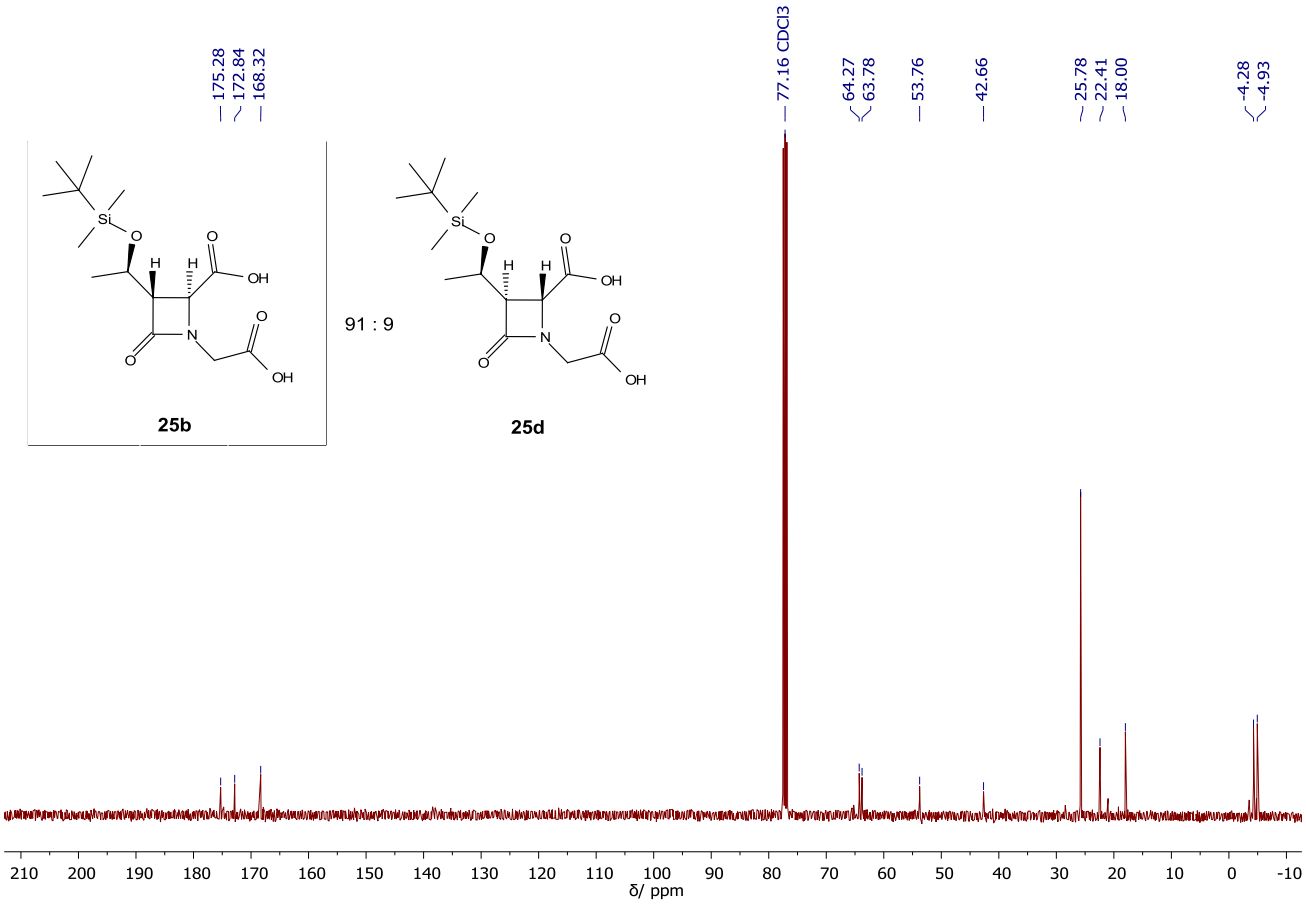

1H NMR (600 MHz)
7.2600 CDCl3
4.6126
4.6027
4.4203
4.4150
4.4083
4.4039
4.3973
4.3930
4.3899
4.3861
4.3819
4.2321
4.2202
4.2141
4.2082
4.2022
4.1998
4.1963
4.1902
4.1879
4.1819
4.1784
4.1760
4.1699
4.1642
4.1581
4.1462
3.9675
3.9371
3.6153
3.6110
3.6055
3.6012
1.3393
1.3283
1.2841
1.2722
1.2603
0.8208
0.0451
0.0364
1.00
2.05
2.16
1.04
1.03
3.07
3.38
9.28
2.96
3.16
δ/ ppm

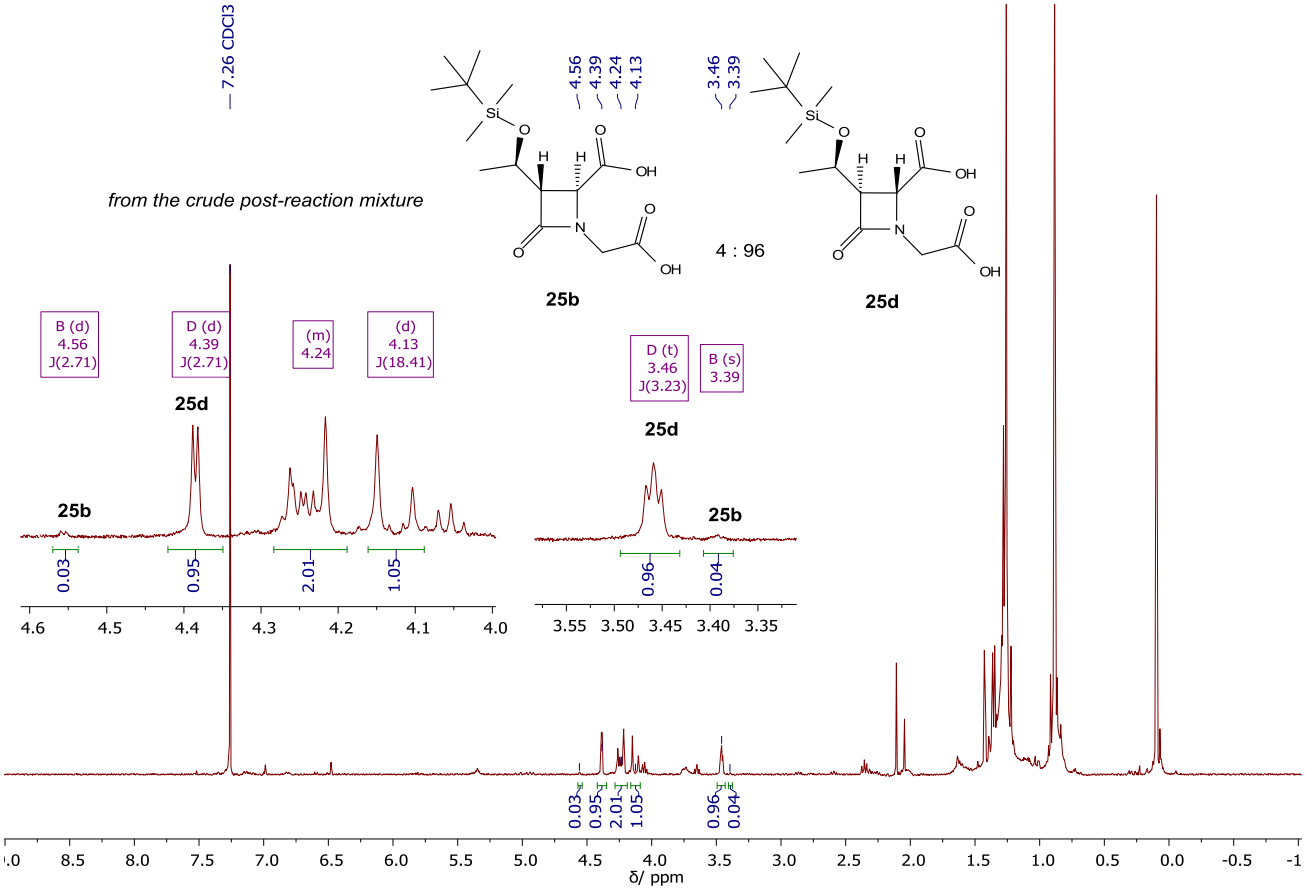
24c


175.45
168.65
167.62
77.16 CDCl3
65.09
62.98
61.76
54.26
41.90
25.73
21.56
18.10
14.26
-4.66
-4.85
δ/ ppm

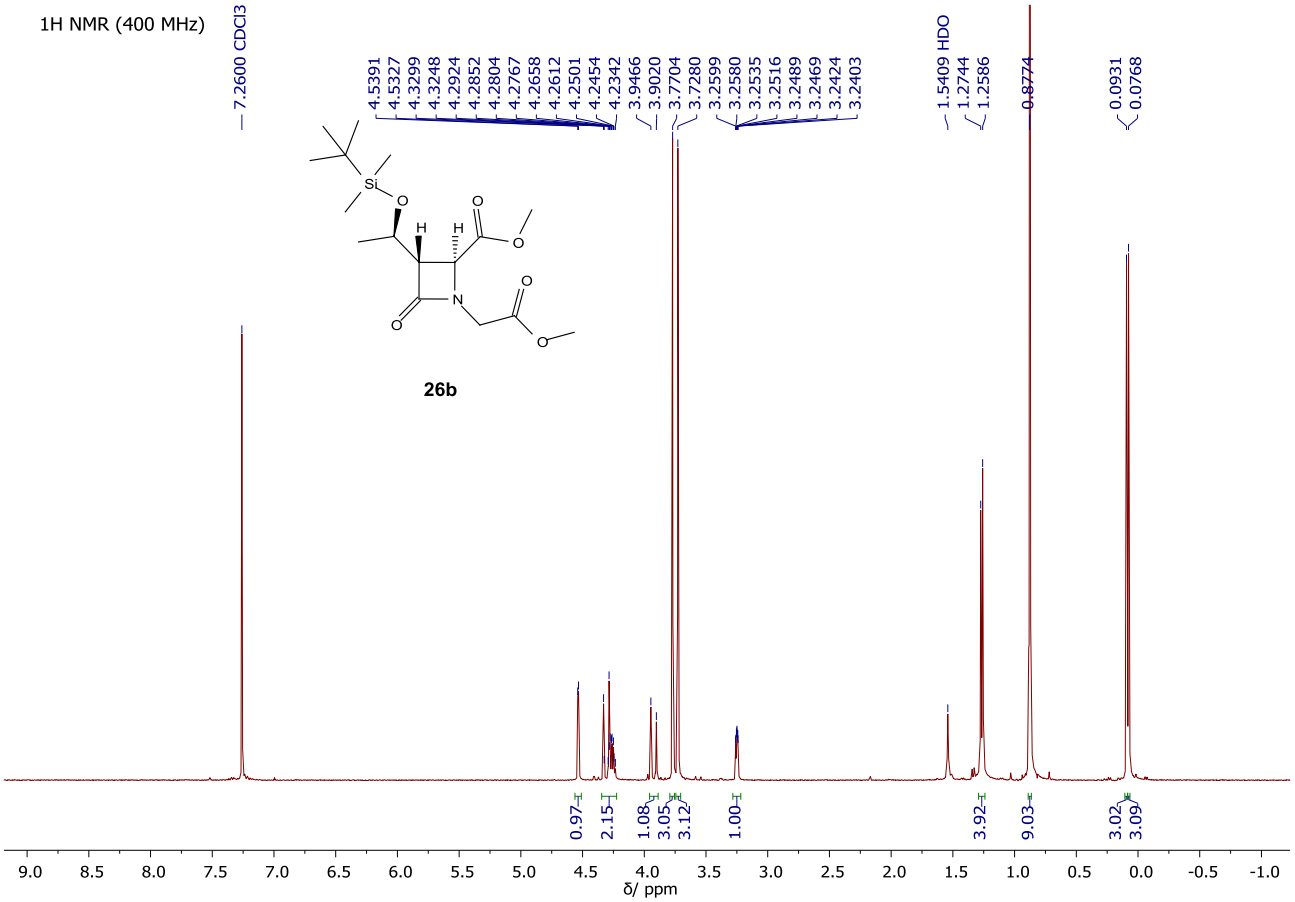
24c


8.21
7.26 CDCl3
4.59
4.31
4.18
3.46
3.38
1.26
0.86
0.09
0.05
D (t)
3.46
J(2.72)
B (t)
3.38
J(2.87)
25b
25d
91 : 9
0.09
0.91
0.83
1.08
2.00
0.09
0.91
6.23
9.32
3.07
2.70
δ/ ppm

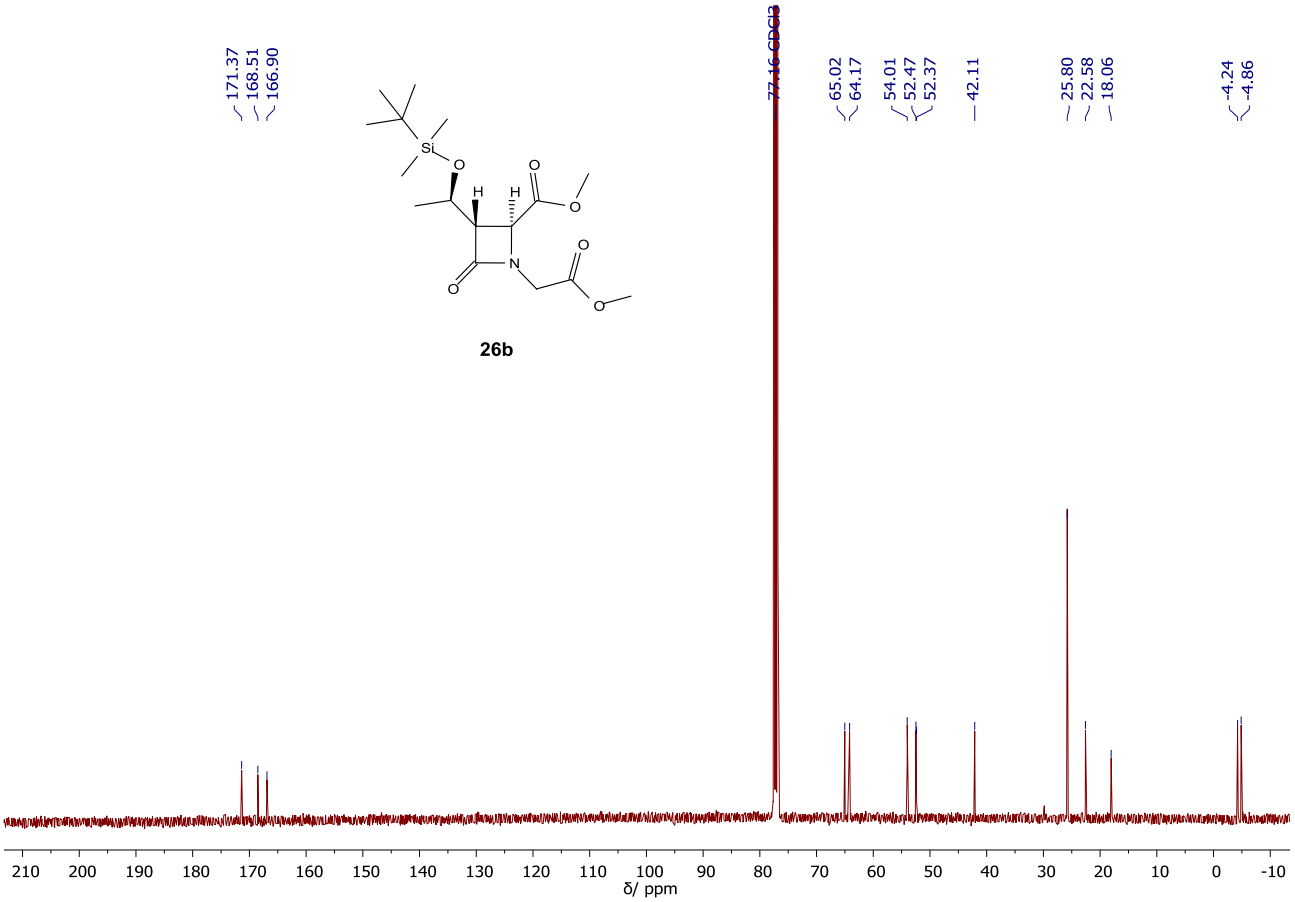

175.28
172.84
168.32
77.16 CDCl3
64.27
63.78
53.76
42.66
25.78
22.41
18.00
-4.28
-4.93
25b
25d
91 : 9
δ/ ppm


7.26 CDCl3
from the crude post-reaction mixture
4.56
4.39
4.24
4.13
3.46
3.39
25b
4 : 96
25d
B (d)
4.56
J(2.71)
D (d)
4.39
J(2.71)
(m)
4.24
(d)
4.13
J(18.41)
D (t)
3.46
J(3.23)
B (s)
3.39
0.03
0.95
2.01
1.05
0.96
0.04
δ/ ppm

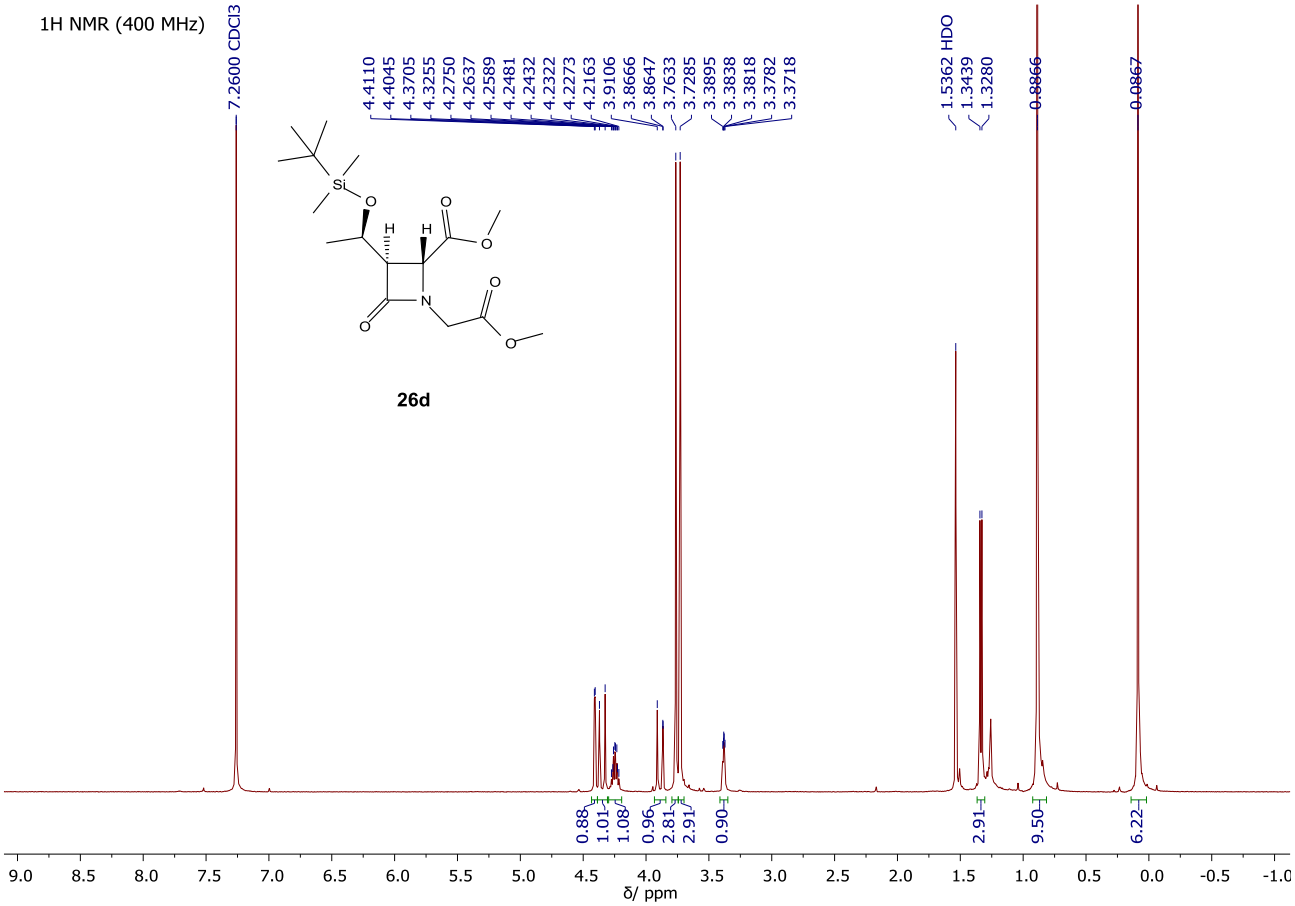
1H NMR (400 MHz)



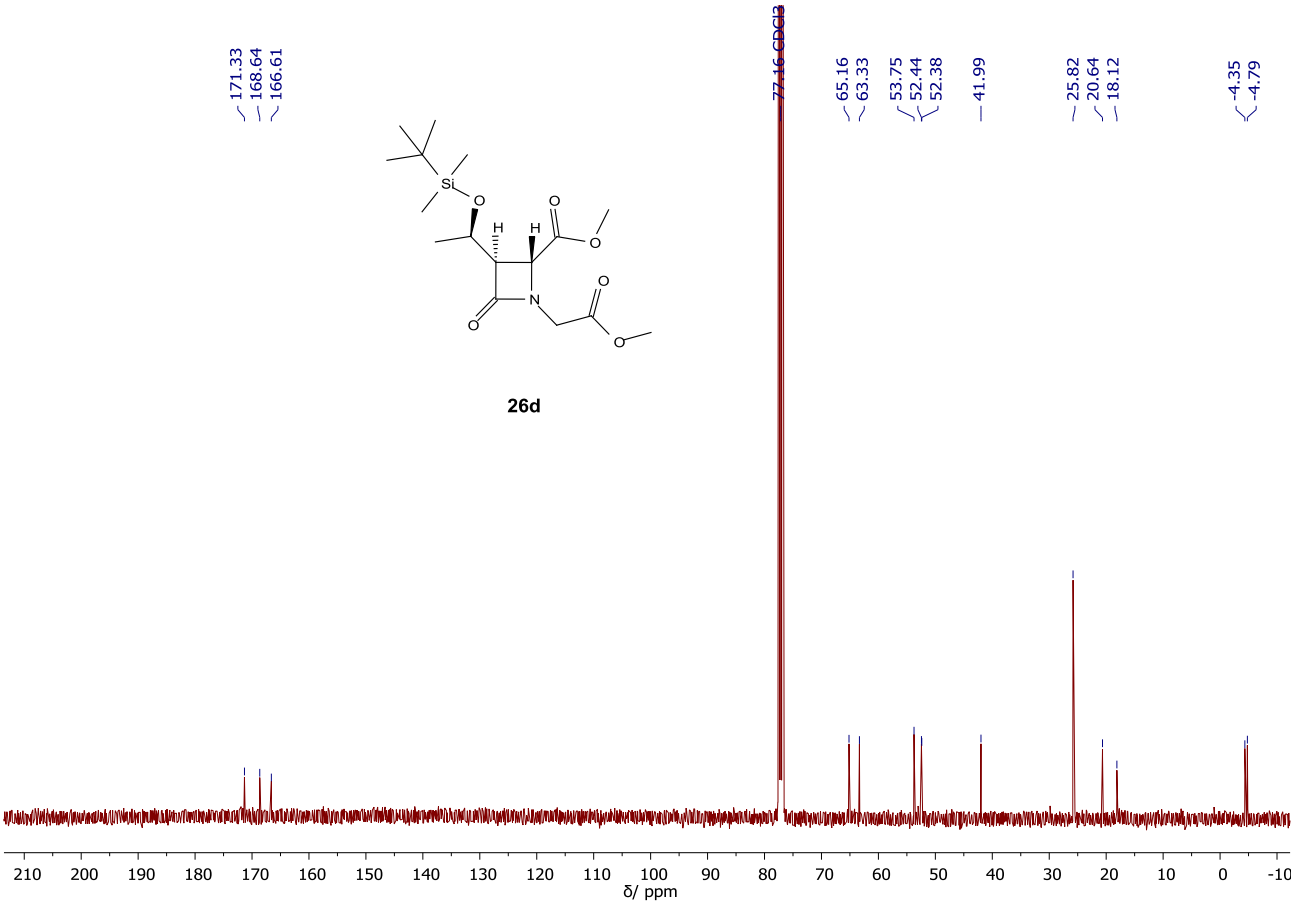
26b



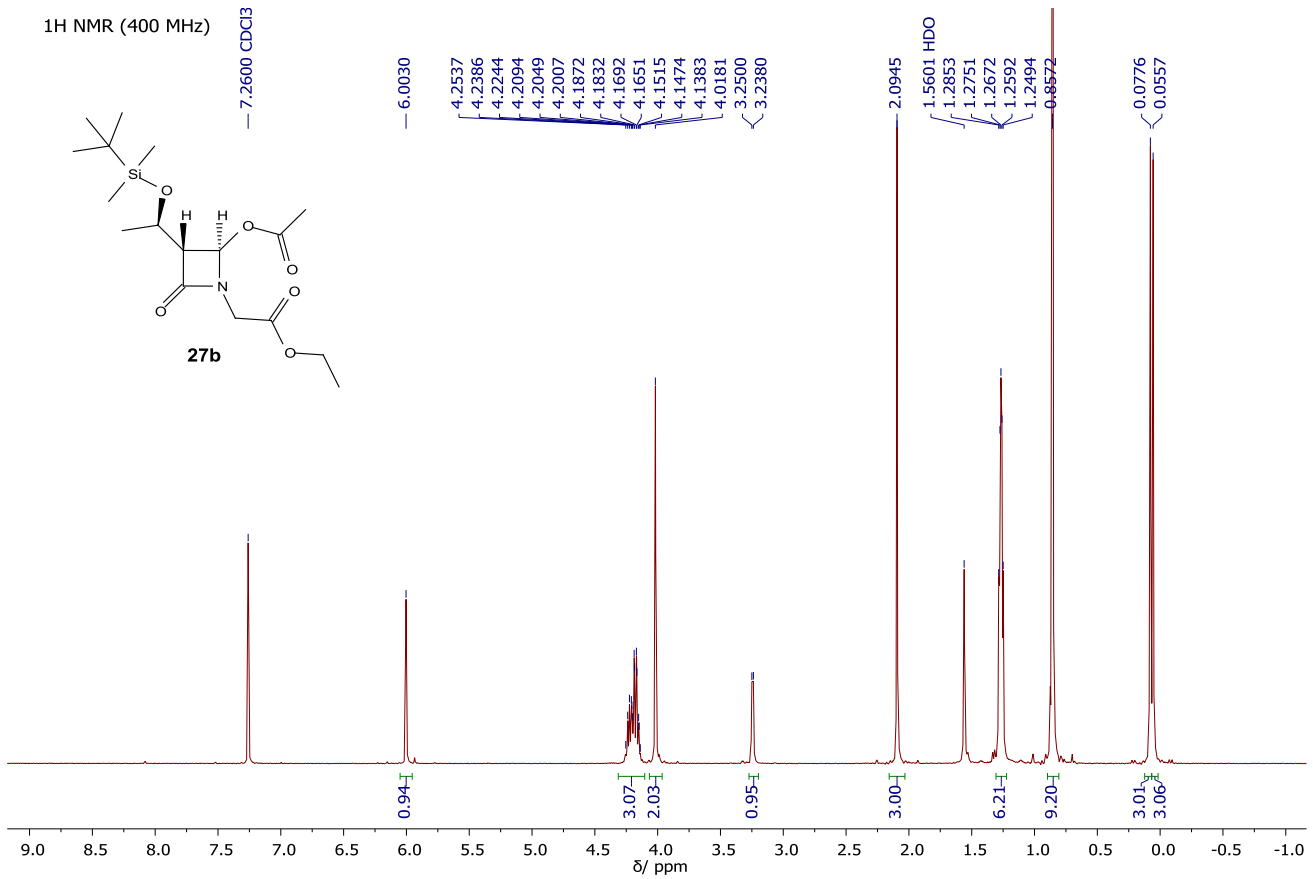
26b

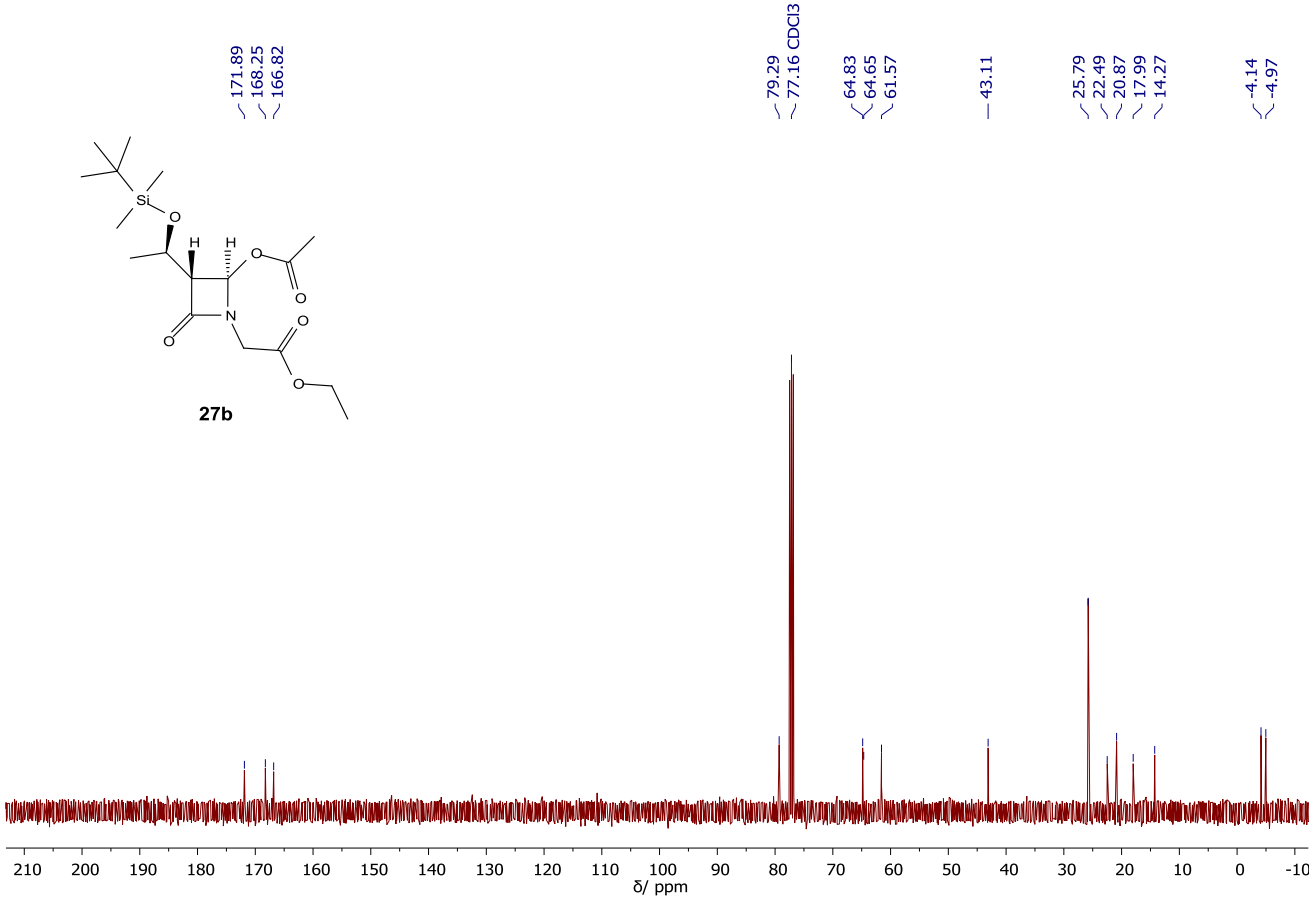

1H NMR (400 MHz)
7.2600 CDCl3
4.4110
4.4045
4.3705
4.3255
4.2750
4.2637
4.2589
4.2481
4.2432
4.2322
4.2273
4.2163
3.9106
3.8666
3.8647
3.7633
3.7285
3.3895
3.3838
3.3818
3.3782
3.3718
1.5362 HDO
1.3439
1.3280
0.8866
0.0867
0.88
1.01
1.08
0.96
2.81
2.91
0.90
2.91
9.50
6.22
δ/ ppm

26d


171.33
168.64
166.61
77.16 CDCl3
65.16
63.33
53.75
52.44
52.38
41.99
25.82
20.64
18.12
-4.35
-4.79
δ/ ppm

26d


1H NMR (400 MHz)
7.2600 CDCl3
6.0030
4.2537
4.2386
4.2244
4.2094
4.2049
4.2007
4.1872
4.1832
4.1692
4.1651
4.1515
4.1474
4.1383
4.0181
3.2500
3.2380
2.0945
1.5601 HDO
1.2853
1.2751
1.2672
1.2592
1.2494
0.8572
0.0776
0.0557
0.94
3.07
2.03
0.95
3.00
6.21
9.20
3.01
3.06
δ/ ppm
27b


171.89
168.25
166.82
79.29
77.16 CDCl3
64.83
64.65
61.57
43.11
25.79
22.49
20.87
17.99
14.27
-4.14
-4.97
δ/ ppm
27b

References

[1] CONFLEX 7, Conflex Corp., Japan, **2012**. H. Goto and E. Osawa, *J. Am. Chem. Soc.*, **1989**, 111, 8950–8951. H. Goto and E. Osawa, *J. Chem. Soc., Perkin Trans. 2*, **1993**, 187–198.

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