Supporting Information for

Human carbonic anhydrase II as host protein for the creation of a biocompatible artificial metathesase

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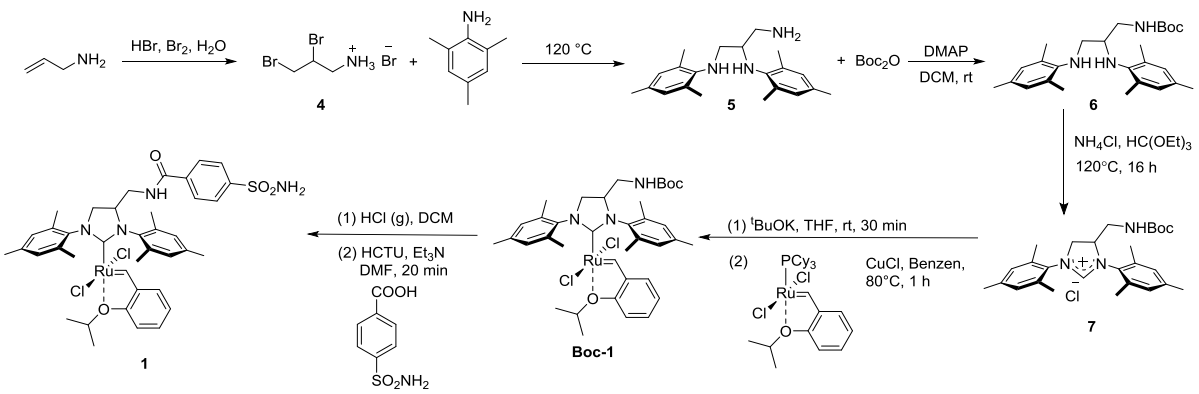
General aspects

Materials and reagents were purchased from the highest commercially available grade and used without further purification.

^{1}H and ^{13}C spectra were recorded on a Bruker 400 MHz, 500 MHz and 600 MHz. Chemical shifts are reported in ppm (parts per million). Signals are quoted as s (singlet), d (doublet), t (triplet), brs (broad) and m (multiplet). Electron Spray Ionization Mass Spectra (ESI-MS) were recorded on a Bruker FTMS 4.7T bioAPEX II. Analysis of the catalytic runs was performed on an Agilent 1100 reverse phase HPLC. High performance liquid chromatography was performed on Agilent 1100 Series with UV-Vis detection.

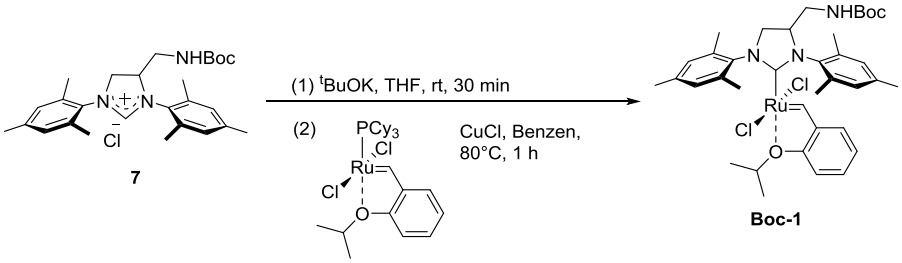
hCA II was expressed in 1 L shaking-flasks in an Infors HT Ecotron shaker and culture growth was monitored by UV-Vis at 600 nm with a Varian Cary 50 Scan. The protein was purified via sulphonamide affinity chromatography by using AKTA prime (Amersham Pharmacia Biotech, Software: PrimeView 5.0). The competitive displacement assays were performed using a Tecan Safire spectrophotometer using NUNC 96-well plates. The data were analyzed with Prism 5.0 software.

Catalyst synthesis



Compound **4**, **5**, **6**, **7**, **Boc-1** were prepared according to the reported procedures.[1]

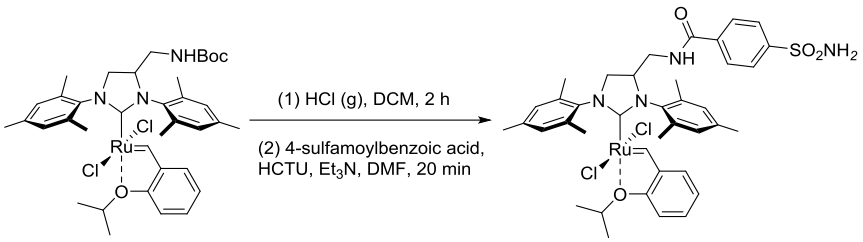
Boc-1



A suspension of ^{t}BuOK (112 mg, 0.99 mmol) was added to the imidazolinium salt **7** (471 mg, 0.99 mmol) in dry and degassed THF (15 ml). The mixture was stirred 30 min at room temperature. The yellow solution was transferred into a flask containing Hoveyda-Grubbs 1st generation (500 mg, 0.83 mmol) in benzene (75 ml) and stirred at 80 °C. After 1 hour, CuCl (99 mg, 0.99 mmol) was slowly added to the solution and stirred for an additional hour at 80 °C. The solvent was evaporated and purification was performed by chromatography (10% EtOAc in cyclohexane) to yield 221 mg (29%) of product **Boc-1** as a green powder.

^{1}H NMR (400 MHz, CD_2Cl_2): δ 16.33 (s, 1H), 7.49-7.45 (m, 1H), 7.01-6.98 (m, 4H), 6.87-6.80 (m, 2H), 6.76 (d, J = 8 Hz, 1H), 4.85-4.79 (m, 1H), 4.48-4.41 (m, 1H), 4.18 (t, J = 12 Hz, 1H), 3.86 (dd, J = 9.2 Hz, 6.8 Hz, 1H), 3.38-3.25 (m, 2H), 2.34 (s, 14 H), 1.35 (s, 4H), 1.30 (s, 9H), 1.18-1.16 (m, 6 H).

^{13}C NMR (100 Hz, CD_2Cl_2): δ 296.6, 214.5, 156.4, 152.4, 145.5, 139.4, 138.9, 130.5, 130.0, 129.7, 122.7, 122.6, 113.3, 79.9, 75.6, 64.3, 55.8, 43.2, 32.3, 30.1, 29.8, 28.4, 27.3, 23.1, 21.4, 21.4, 21.2, 21.2, 21.2, 18.5, 14.3.



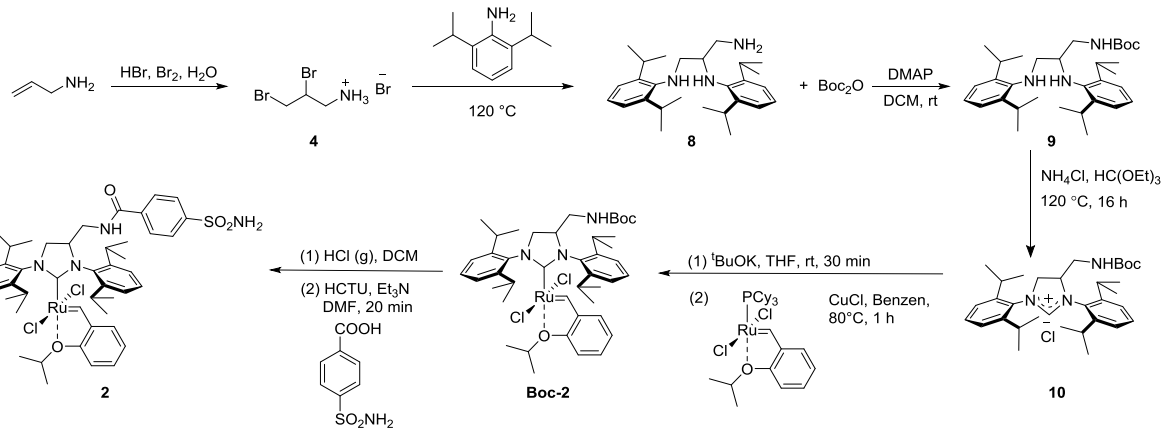
Boc-1 (45.3 mg, 0.06 mmol, 1 eq.) was dissolved in CH_2Cl_2 (2 mL). Gaseous HCl (H_2SO_4 added drop-wise to NH_4Cl) was bubbled through the solution and the mixture was stirred for 2 h at room temperature. The deprotection was monitored by thin-layer chromatography (TLC) (cyclohexane/ EtOAc 8:1). After consumption of the starting material, the solvent was evaporated under N_2 and the resulting mixture was dissolved in DMF (1 mL). In another flask, 4-sulfamoylbenzoic acid (12.1 mg, 0.06 mmol, 1 eq.) and the coupling agent HCTU (27.3 mg, 0.066 mmol, 1.1 eq.) were vigorously stirred in 1 mL of DMF for 20 min. To this latter flask, the deprotected complex in DMF was added, followed by Et_3N (84.3 µL, 0.6 mmol, 10 eq.). The resulting mixture was stirred for 20 min at room temperature. The solvent was removed under vacuum. Purification by chromatography (50% EtOAc in cyclohexane) yielded 8 mg (16%) of catalyst **1** as a green powder.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 16.37 (s, 1H), 7.39-7.88 (m, 4H), 7.58-7.55 (m, 1H), 7.14 (s, 1H), 7.09 (br, 2H), 6.96 (s, 1H), 6.92-6.91 (m, 2H), 6.87 (d, J = 8.6 Hz, 1H), 4.97-4.94 (m, 3H), 4.67 (br, 1H), 4.34 (t, J = 11.0 Hz, 1H), 3.95-3.92 (m, 1H), 3.63 (br, 1H), 2.88 (br, 2H), 2.46-2.40 (m, 14H), 1.43-1.27 (m, 10H).

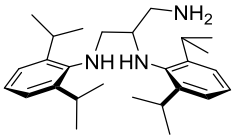
^{13}C NMR (150 Hz, CD_2Cl_2): δ 297.2, 211.0, 166.8, 152.5, 145.2, 137.8, 130.7, 130.4, 130.4, 130.0, 128.6, 126.8, 122.7, 113.3, 75.6, 64.0, 55.7, 55.7, 32.0, 29.9, 21.4, 21.1, 19.1.

HRMS (ESI, pos.) *m/z*: $[M\text{-}Cl]^+$ calcd for $C_{39}H_{46}ClN_4O_4RuS$, 803.1971; found: 803.1969.

Compound **8**, **9**, **10**, **Boc-2** were prepared using the same procedures as described for compound **5**, **6**, **7**, **Boc-1**.[1]



N^1, N^2-bis(2,6-diisopropylphenyl)propane-1,2,3-triamine (8)



8

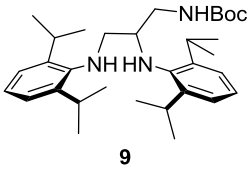
Compound **8** (yield 253 mg, 18 %) was prepared from the same procedure of compound **5**.[1]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02-6.88 (m, 6H), 3.38-3.04 (m, 9H), 3.01-2.93 (m, 3H), 2.85 (dd, J = 12.0 Hz, 5.2 Hz, 1H), 1.17-1.04 (m, 24H).

^{13}C NMR (100 Hz, $CDCl_3$): δ 142.7, 142.6, 141.9, 140.4, 124.0, 123.7, 123.6, 123.5, 59.9, 54.3, 53.4, 44.0, 27.9, 27.7, 24.3, 24.2, 24.1.

HRMS (ESI, pos.) *m/z*: $[M+H]^+$ calcd for $C_{27}H_{44}N_3$, 410.3536; found: 410.3529.

tert-butyl (2,3-bis((2,6-diisopropylphenyl)amino)propyl)carbamate (9)



9

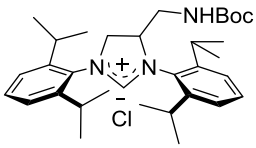
Compound **9** (yield 49 mg, 36 %) was prepared from the same procedure of compound **6**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.03-6.93(m, 6H), 4.96 (br, 1H), 3.45-3.13 (m, 9H), 3.02 (dd, J = 11.7 Hz, 4.8 Hz, 1H), 2.82 (m, 1H), 1.38-1.36 (m, 10H), 1.18-1.11 (m, 17H), 1.06 (d, J = 6.8 Hz, 6H).

^{13}C NMR (100 Hz, $CDCl_3$): δ 156.4, 146.7, 143.3, 142.6, 141.5, 140.9, 123.7, 123.6, 123.5, 123.4, 85.1, 79.4, 60.2, 53.7, 43.1, 28.4, 27.9, 27.5, 27.4, 26.9, 24.3, 24.1, 24.0.

HRMS (ESI, pos.) *m/z*: $[M+H]^+$ calcd for $C_{32}H_{52}N_3O_2$, 510.4059; found: 510.4054.

***tert*-butyl ((1,3-bis(2,6-diisopropylphenyl)imidazolidin-4-yl)methyl)carbamate, chloride salt (10)**



10

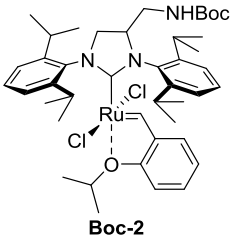
Compound **10** (yield 212 mg, 89 %) was prepared from the same procedure of compound **7**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.54-7.46 (m, 3H), 7.32-7.26 (m, 3H), 5.45-5.36 (m, 1H), 5.09 (dd, J = 12.9 Hz, 9.4 Hz, 1H), 4.62 (t, J = 12.1 Hz, 1H), 3.91-3.84 (m, 1H), 3.46-3.41 (m, 1H), 3.23-3.13 (m, 1H), 3.09-2.89 (m, 3H), 1.53 (d, J = 6.8 Hz, 3H), 1.48 (d, J = 6.8 Hz, 3H), 1.40 (dd, J = 6.7 Hz, 0.9 Hz, 6H), 1.36 (s, 9H), 1.26-1.19 (m, 12H).

^{13}C NMR (100 Hz, $CDCl_3$): δ 157.6, 156.7, 146.7, 146.6, 146.3, 145.8, 131.6, 129.1, 127.6, 125.6, 125.2, 125.1, 124.8, 79.2, 65.2, 58.3, 41.4, 29.5, 29.2, 29.1, 29.1, 28.3, 26.0, 25.5, 25.3, 25.2, 23.9, 23.8, 23.7, 23.2.

HRMS (ESI, pos.) *m/z*: $[M-Cl]^+$ calcd for $C_{33}H_{50}N_3O_2$, 520.3903; found: 520.3893.

Boc-2



Boc-2

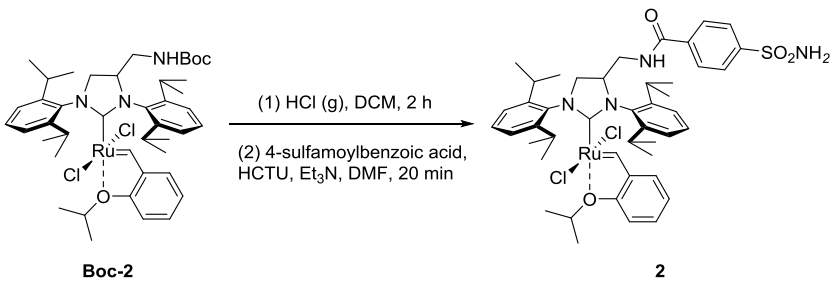
Boc-2 was prepared from the same procedure of compound **Boc-1**.

A suspension of ^{t}BuOK (67.3 mg, 0.6 mmol) was added to the imidazolinium salt **10** (334 mg, 0.6 mmol) in dry and degassed THF (10 ml). The mixture was stirred 30 min at room temperature. The yellow solution was transferred into a flask containing Hoveyda-Grubbs 1st generation (303 mg, 0.50 mmol) in benzene (40 ml) and stirred at 80 °C. After 1 hour, CuCl (59.4 mg, 0.6 mmol) was slowly added to the solution and stirred for an additional hour at 80°C. The solvent was evaporated the crude was purified by flash chromatography (10% EtOAc in cyclohexane) yields 107 mg (21%) of product **Boc-2** as a green powder.

^{1}H NMR (400 MHz, CD_2Cl_2): δ 16.12 (s, 1H), 7.57-7.53 (m, 1H), 7.44-7.33 (m, 4H), 7.28-7.23 (m, 2H), 6.80-6.73 (m, 3H), 4.88-4.79 (m, 1H), 4.36-4.19 (m, 3H), 3.53-3.43 (m, 1H), 3.27-3.14 (m, 4H), 1.39-1.10 (m, 39H),

^{13}C NMR (100 Hz, CD_2Cl_2): δ 288.9, 216.6, 164.8, 156.2, 152.7, 149.6, 144.0, 142.6, 137.4, 130.2, 130.1, 129.8, 126.0, 125.6, 124.4, 124.2, 123.8, 122.7, 122.6, 113.4, 79.9, 75.6, 66.6, 58.6, 56.6, 48.2, 43.0, 32.3, 30.1, 29.8, 29.3, 28.6, 28.4, 28.2, 27.2, 26.0, 24.6, 24.1, 23.3, 23.1, 22.1, 21.8, 14.3.

HRMS (ESI, pos.) *m/z*: $[M\text{-}Cl]^+$ calcd for $C_{43}H_{61}ClN_3O_3Ru$, 804.3444; found: 804.3430.



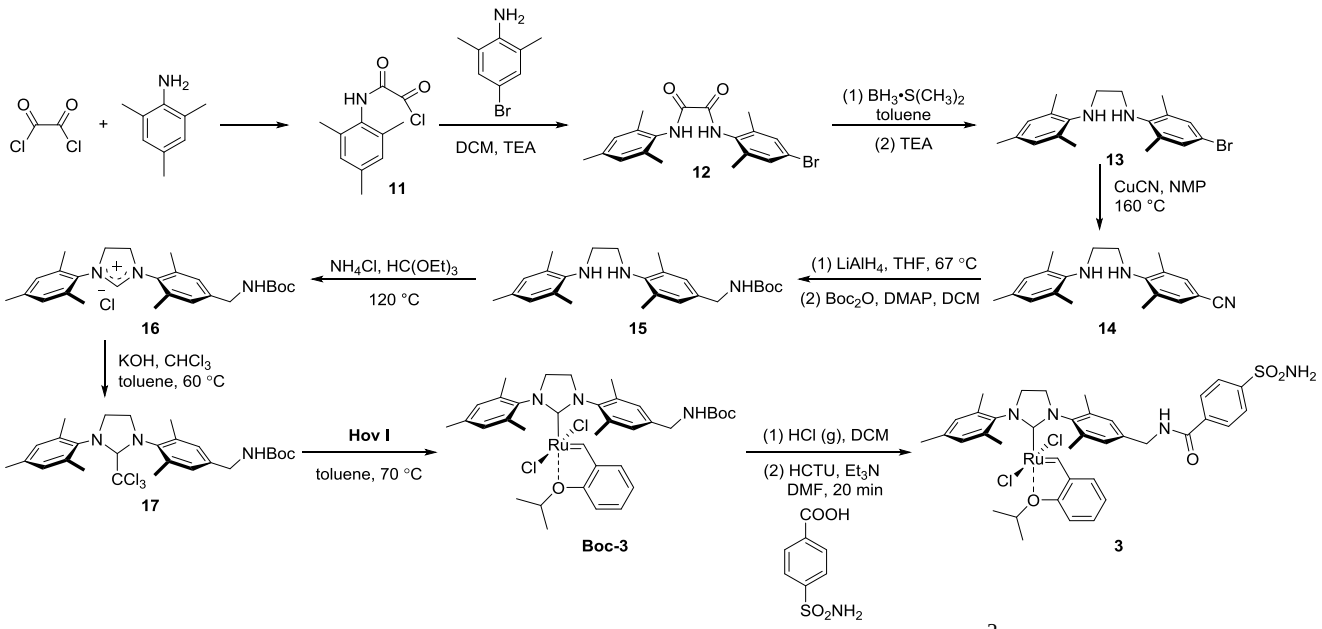
Boc-2 **2**

Catalyst **2** was synthesized according to the preparation procedure used for catalyst **1**. Yield: 13.3 mg, 25%.

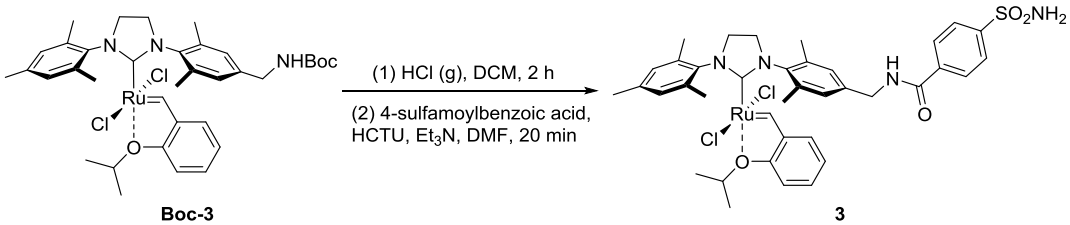
^{1}H NMR (400 MHz, CD_2Cl_2): δ 16.1 (s, 1H), 7.90-7.81 (m, 3H), 7.60-7.15 (m, 7H), 6.83-6.57 (m, 4H), 4.94-4.85 (m, 3H), 4.51-4.33 (m, 2H), 3.79-3.34 (m, 4H), 3.22 (br, 1H), 1.35-0.75 (m, 30H).

^{13}C NMR (100 Hz, CD_2Cl_2): δ 289.3, 217.5, 166.5, 152.9, 145.7, 144.1, 137.6, 130.6, 130.6, 130.3, 128.7, 127.1, 126.0, 123.0, 122.8, 113.8, 75.9, 41.6, 35.2, 32.5, 32.2, 30.3, 29.6, 27.5, 25.8, 23.2, 22.4, 21.9, 21.0, 19.1, 14.5, 11.8.

HRMS (ESI, pos.) *m/z*: $[M\text{-}Cl]^+$ calcd for $C_{45}H_{58}ClN_4O_4RuS$, 887.2910; found: 887.2915.



Compounds **11**-**17**, **Boc-3** were synthesized according to literature protocols.[2]



Catalyst **3** was synthesized according to the preparation procedure of catalyst **1**. Yield: 17.4 mg, 21%.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 16.50 (s, 1H), 7.81-7.75 (m, 4H), 7.49-7.46 (m, 2H), 7.24 (s, 2H), 7.06 (s, 2H), 6.91 (d, J = 7.5 Hz, 1H), 6.76 (d, J = 8.3 Hz, 1H), 5.49 (br, 2H), 4.82-4.75 (m, 1H), 4.62-4.61 (m, 2H), 4.12-4.07 (m, 4H), 2.43-2.38 (m, 15H), 1.16 (d, J = 6.2 Hz, 6H).

^{13}C NMR (145 Hz, CD_2Cl_2): δ 296.0, 210.9, 166.2, 152.4, 145.5, 145.4, 138.4, 129.7, 122.6, 129.6, 128.7, 128.4, 128.4, 126.9, 129.9, 122.6, 113.2, 75.7, 52.0, 52.0, 44.0, 21.5, 21.4, 19.8.

HRMS (ESI, pos.) *m/z*: $[M\text{-}Cl]^+$ calcd for $C_{38}H_{44}ClN_4O_4RuS$, 789.1815; found: 789.1807.

Binding affinity for the inhibition of hCA II

A competitive displacement assay was performed according the procedure previously described by Zambel.[3]

The stock solutions used were phosphate buffer (0.1 M, pH 7.0), dansylamide stock solution (1000 μM, 800 μM, 100 μM, 10 μM) in DMSO, catalyst 2 stock solution (500 μM, 50 μM, 5 μM) in DMSO, and hCA II isoform stock (0.278 μM) in phosphate buffer (0.1 M, pH 7.0).

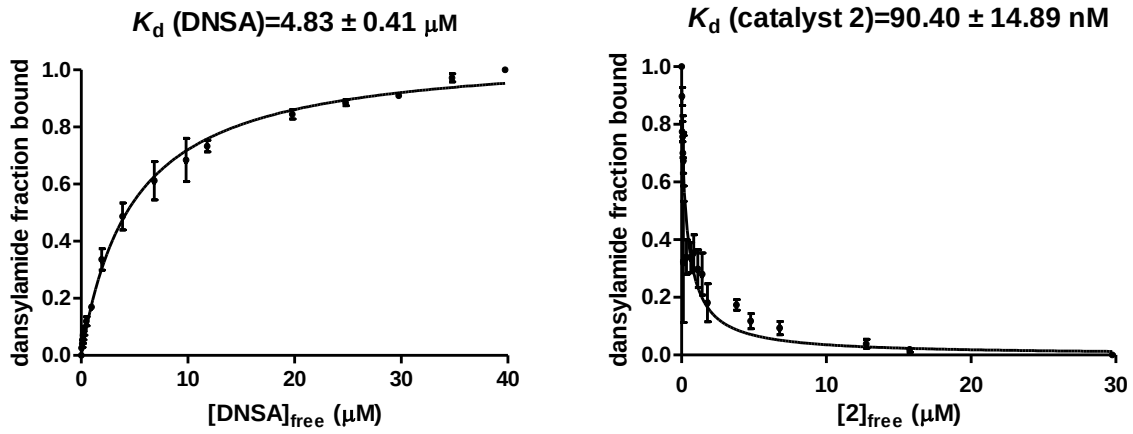
Fluorescence measurements were performed at 29 °C by using TECAN and Nunclon black flat-bottom 96-well plates. The excitation wavelength was set to 280 nm with a fluorescence intensity at 470 nm, and the scan speed was set to 100 nm/min. The K_d value for DNSA was determined by titrating 0.25 μM hCA II (180 μL) with varying concentrations of DNSA (1~20 μL), ranging from 0–40 μM in a total assay volume of 200 μL. The equilibrium dissociation constant for DNSA K_{DNSA} was then determined by fitting the data to equation 1 using Prism 5.0 software.

$$r = \frac{[\mathrm{DNSA}]}{K_{DNSA} + [\mathrm{DNSA}]} \qquad \text{(Eq. 1)}$$

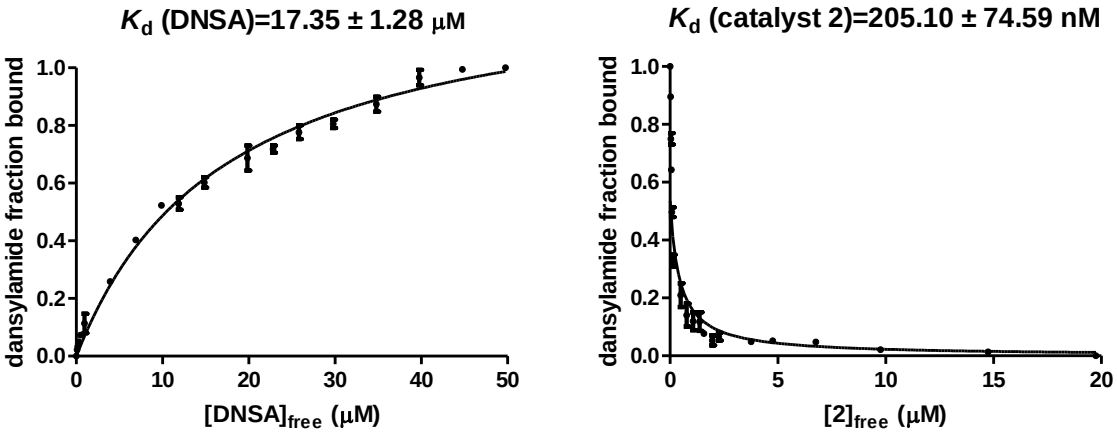
The equilibrium dissociation constants for catalyst **2** were determined by competitive binding with DNSA. A fixed concentration of 20 μM DNSA (5 μL) and 0.25 μM hCA II (180 μL) were then titrated against catalyst **2** from 0–30 μM (1~15 μL). The K_d value of catalyst **2** was then determined by fitting the data to equation 2 with Prism 5.0 software. All the titration experiment were performed in triplicate.

$$r = \frac{1}{1 + (K_{\mathrm{DNSA}}/[\mathrm{DNSA}])(1 + [\mathrm{catalyst}]/K_{\mathrm{d}}(\mathrm{catalyst}))} \qquad \text{(Eq. 2)}$$

Determination of DNSA and catalyst **2** dissociation constants (K_d) for hCA II WT.



Determination of DNSA and catalyst **2** K_d for hCA II mutant L198H.



Protein expression and purification

The plasmid encoding human carbonic anhydrase isozyme II (hCA II) and containing a T7 RNA polymerase promoter and an ampicillin resistance gene (pACA) was a generous gift from Carol Fierke, Michigan University. The construct of this plasmid has a serine residue at position 2 instead of an alanine, with no effect on protein expression or catalytic properties.

An overnight pre-culture (50 mL) was used to inoculate 1 L of induction media (20 g/L tryptone, 10 g/L yeast extract, 5 g/L NaCl, 0.36X M9 salts solution, 0.4%glucose, 60 μM $ZnSO_4$, 100 μg/mL Ampicillin and 34 μg/mL Chloramphenicol). Cells were grown at 37 °C until OD_{600}=0.6-0.8. Protein expression were induced through the addition of IPTG (250 μM final concentration) and $ZnSO_4$ (450 μM final concentration). After 6 to 7 h of incubation at 37 °C at 200 rpm, cells were harvested (4400 rpm, 15 min at 4 °C) and frozen at -20 °C overnight. Cells were lysed by activating the gene encoding T7 lysozyme by three cycles of "freeze/thraw". To the cell pellets, a buffer containing Tris-sulfate (50 mM, pH 8.0), NaCl (50 mM), EDTA (10 mM, pH 8.0), $ZnSO_4$ (0.5 mM), and the protease inhibitors PMSF (10 μg/mL) was added. Cells were resuspended by vigorously shaking at rt for 1 h, followed by adding DNase I (1 μg/L final concentration) for another 1 h shaking until complete digestion

of nucleic acids. The cellular remnants were centrifuged (10,000 rpm, 45 min at 4 °C) and cell debris was discarded. After identification of hCA II by SDS-PAGE, the crude supernatant was dialyzed in buffer (50 mM Tris-sulfate pH 8.0 and 0.5 mM $ZnSO_4$) overnight at 4 °C.

The protein was purified by affinity chromatography. Collected fractions were dialyzed in ddH_2O overnight. The protein was lyophilized and kept at 4 °C as white powder.

General procedure for artificial ring closing metathesase of *N*-tosyldiallylamine

A stock solution (200 μM) of the catalyst was prepared by adding DMSO to an aliquot of the catalyst. A stock solution of *N*-tosyldiallylamine (20 mM) was prepared in a separate vial. A stock solution of protein (13.3 μM) was prepared by using 0.1 M phosphate buffer pH 7.0.

In a small glass reaction vial, protein stock solution (180 μL) and catalyst DMSO stock solution (10 μL) were added and incubated at 37 °C for 20 min. Then substrate *N*-tosyldiallylamine stock solution (10 μL) was added, and the reaction vial was placed in an incubator for 4 h at 37 °C.

Upon completion of the reaction, the mixture was added internal standard 2-phenylethanol (100 μL, 1 mM water solution) and MeOH (700 μL). The solution mixture was transferred to an eppendorf tube and centrifuged at 14'000 rpm for 15 minutes to precipitate the protein. The supernatant (500 μL) was transferred in an HPLC vial with additional 500 μL water and the sample was subjected to RP-HPLC to determine the TON and conversion.

HPLC analysis. Column: XDB-C18, Eclipse by Agilent: 150 x 4.6 mm; 5 μm with guard column. Method: $V_{injected}$: 50 μL. Eluent (Solvent A: H_2O) , (Solvent B: CH_3CN) 10% B at 0 min, 10% B at 5 min; 90% B at 20 min; 10 % B at 30 min. Detection at 210 nm. T_R 12.2 min (internal standard 2-phenylethanol), 14.6 min (product 1-tosyl-2,5-dihydro-1*H*-pyrrole), 16.1 min (substrate *N*-tosyldiallylamine).

Docking simulation results

Both (*R*) and (*S*)-enantiomers of catalyst **2** were docked within hCA II WT by GOLD programme. The following table summarizes the calculation results of the best fitted catalyst within hCA II.

Host protein	Score*	ΔG^{+}	S_{hbond}*	S_{lipo}*	H_{rot}*	ΔE_{clash}*	ΔE_{int}*
(*R*)-**2** ⊂ WT hCA II	32.77	-26.92	1.25	187.00	1.80	-8.55	0.84
(*S*)-**2** ⊂ WT hCA II	40.86	-33.03	1.29	238.03	1.80	-11.51	1.91

* Values dimensionless $^{+}$ Values in $kJ \cdot mol^{-1}$

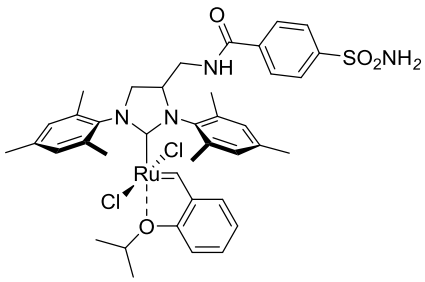
References:

1. (a) M. D'hooghe, I. Kerkaert, M. Rottiers and N. De Kimpe, *Tetrahedron*, 2004, **60**, 3637–3641; (b) J. P. Jordan and R. H. Grubbs, *Angew. Chem. Int. Ed.*, 2007, **46**, 5152 –5155.

2. A. Kajetanowicz, A, Chatterjee, R, Reuter and T. R. Ward, *Catal. Lett.,* 2014, **144**, 373–379.

3. S. C. Wang and D. B. Zamble, *Biochem. Mol. Biol. Educ.*, 2006, **34**, 364-368.

NMR Spectra:



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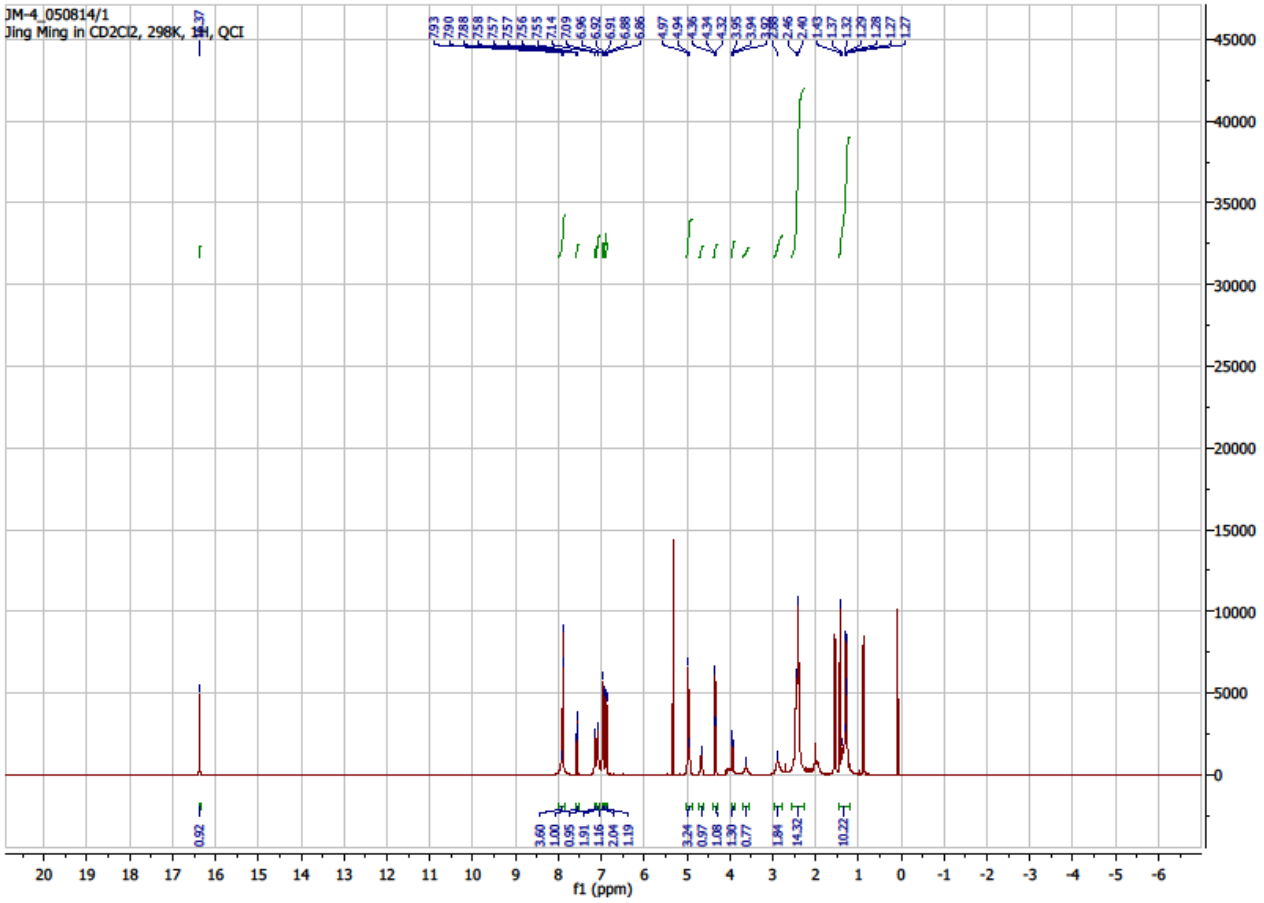

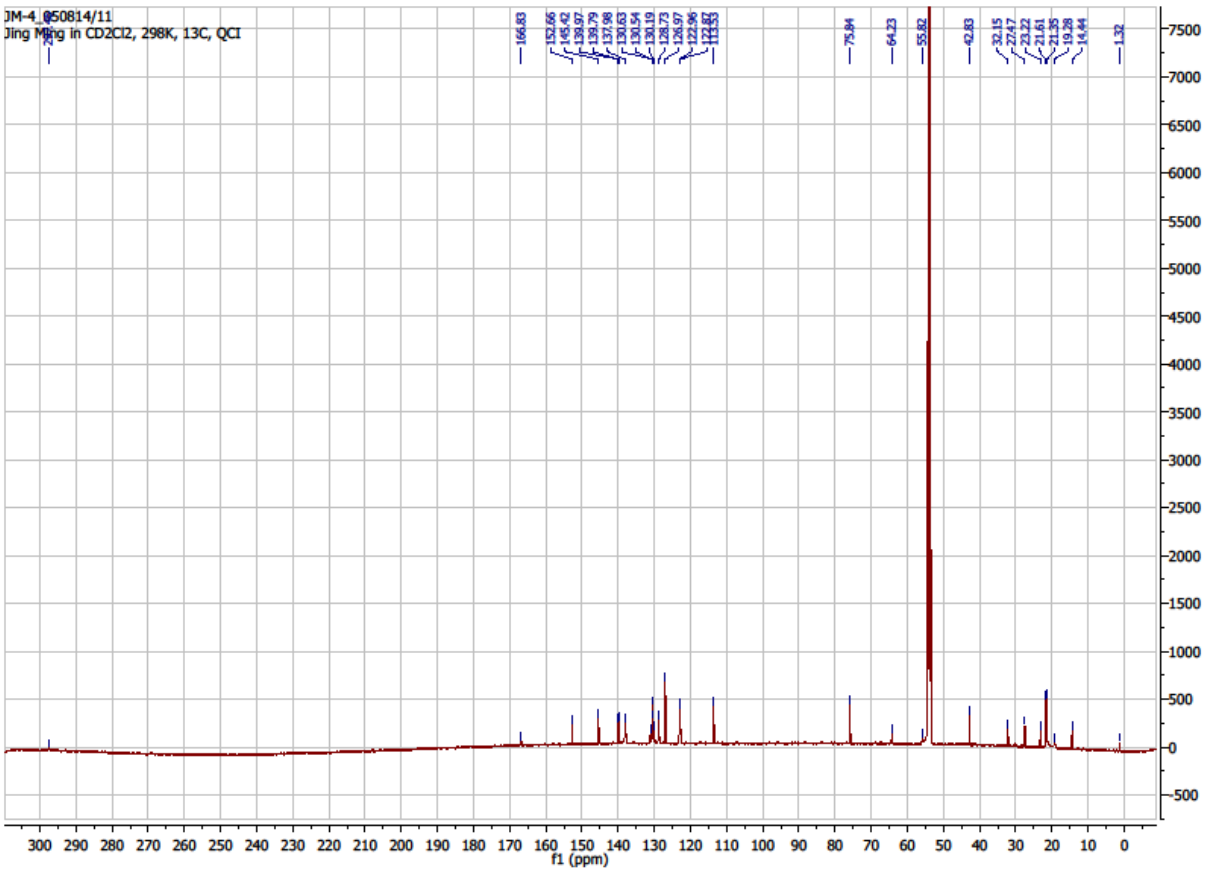
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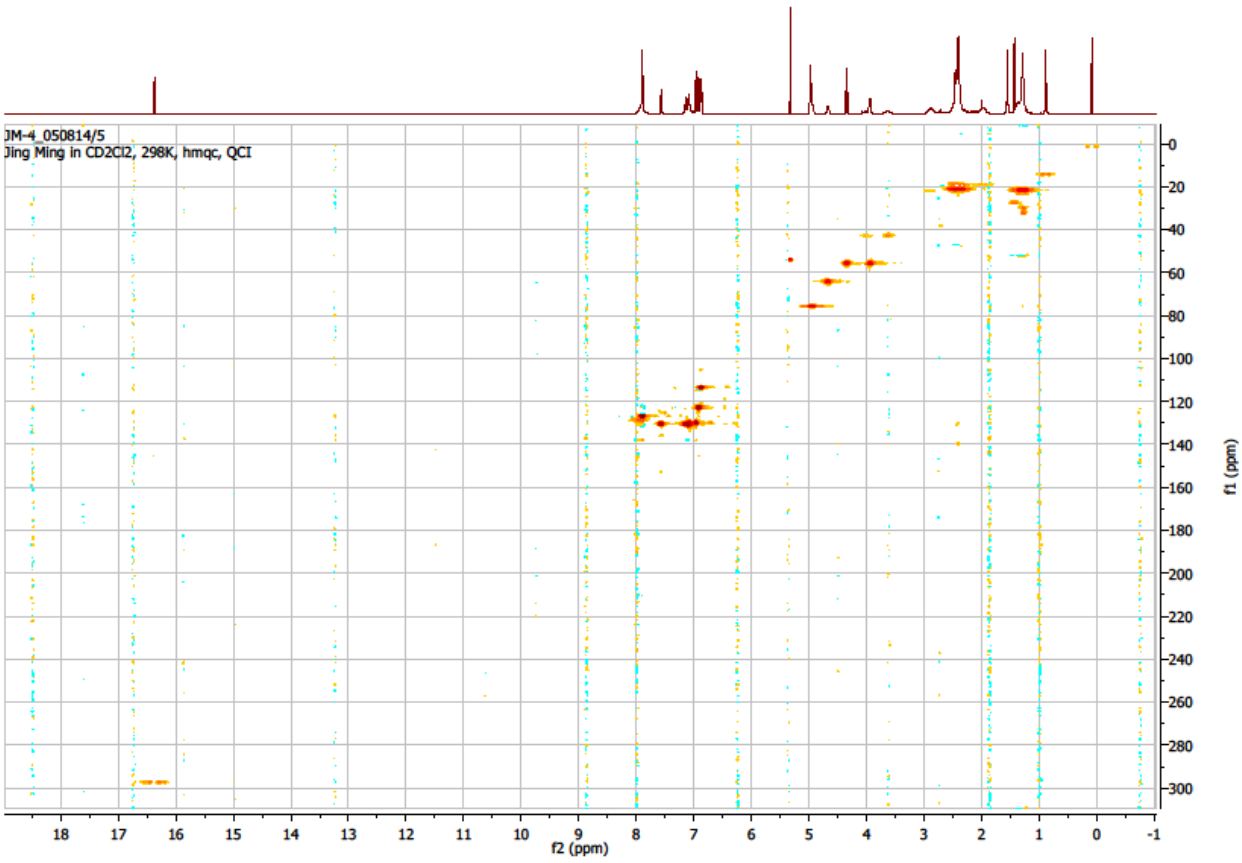
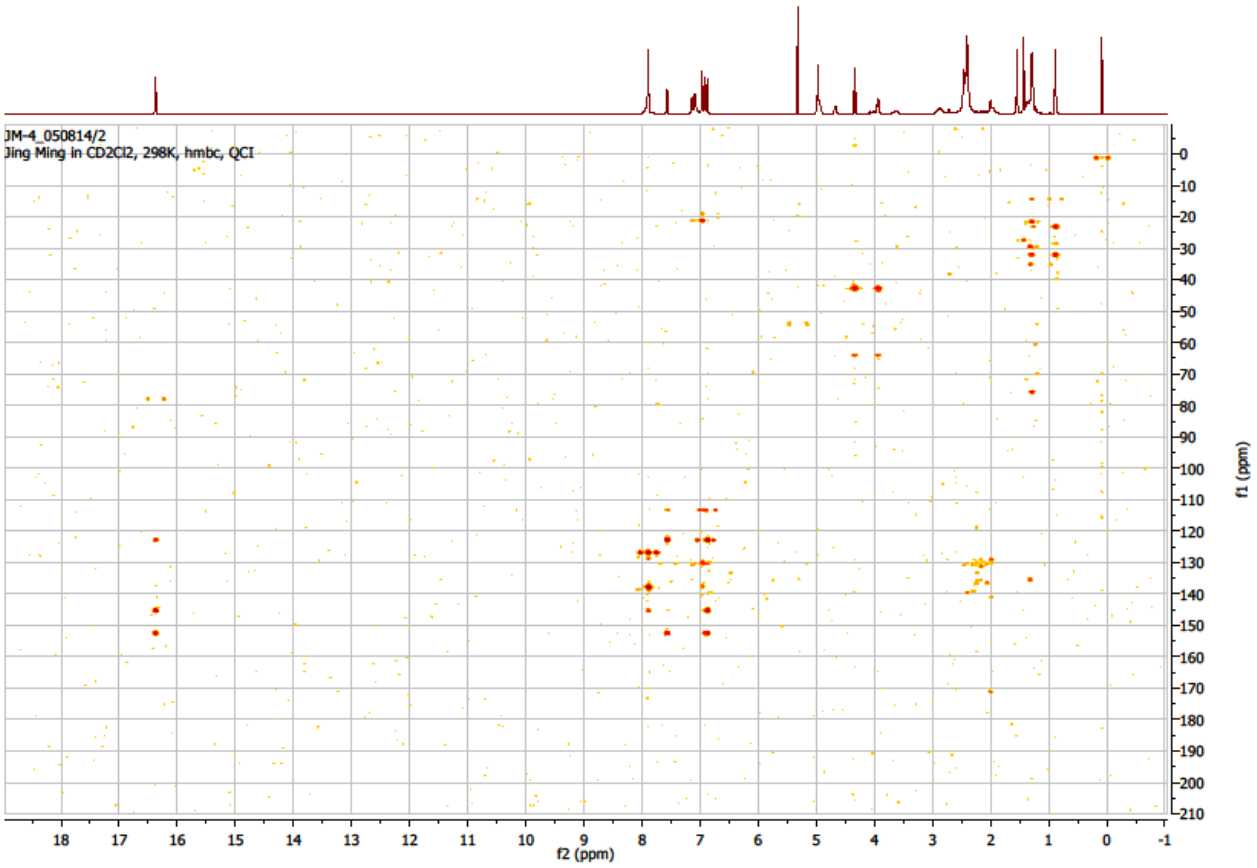
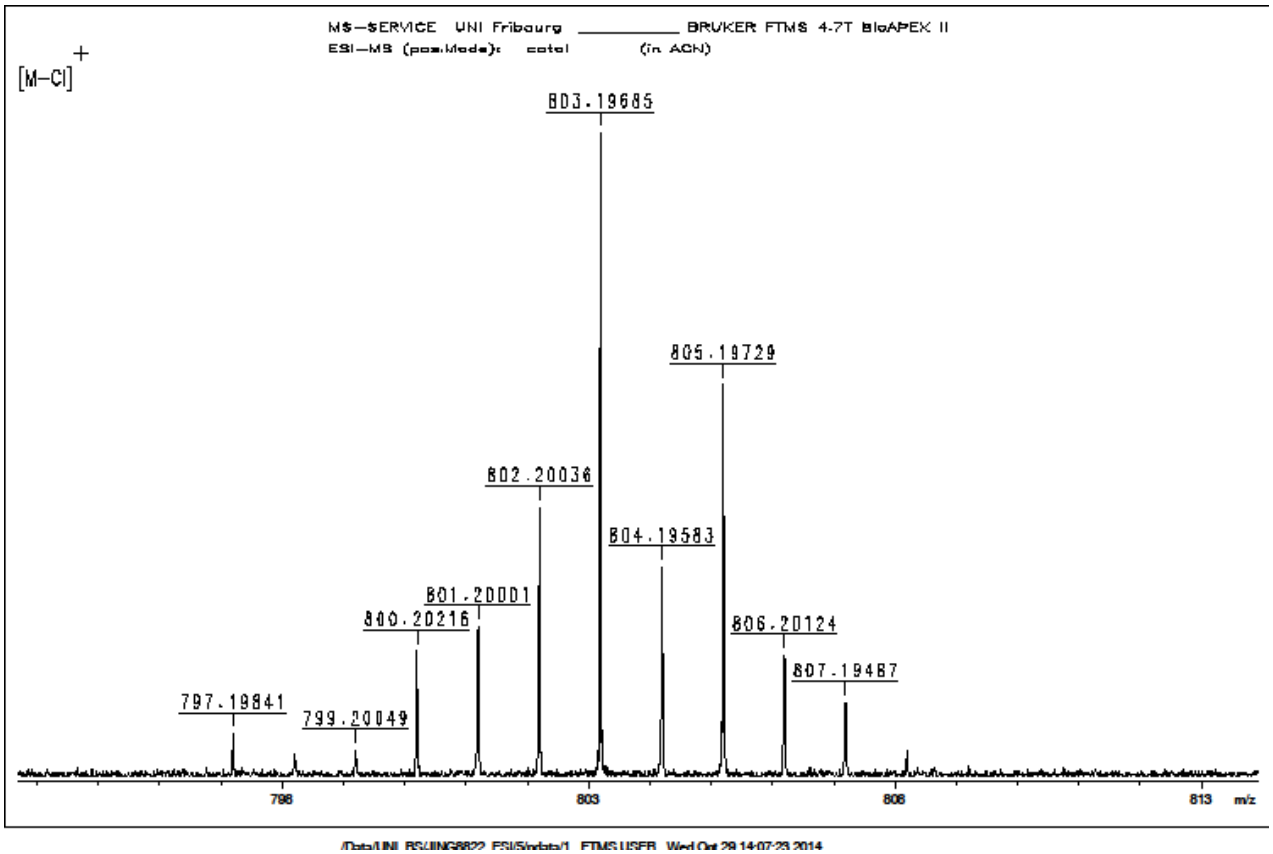
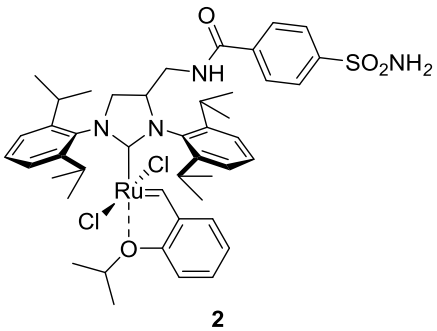
42.83
32.15
27.47
21.22
21.61
21.35
19.28
14.44
1.32
f1 (ppm)

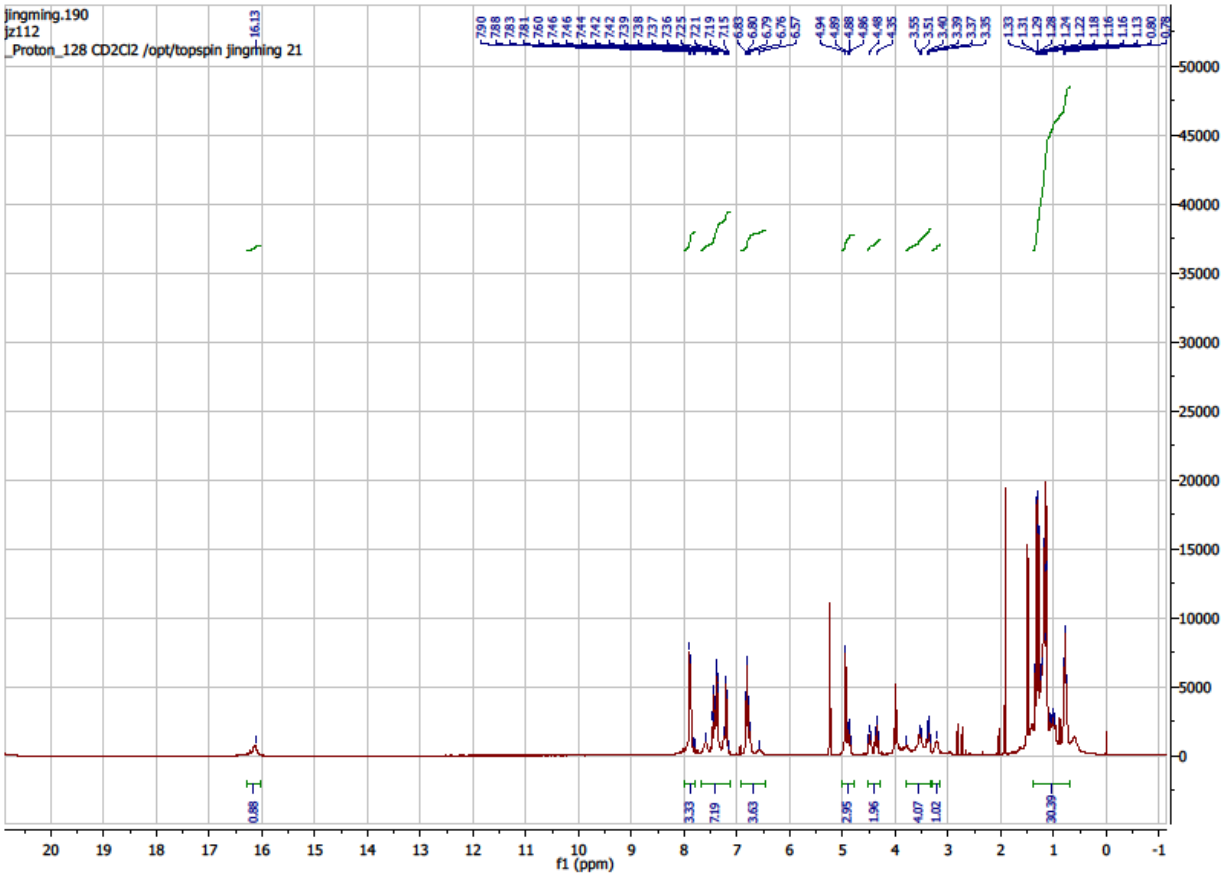

JM-4_050814/5
Jing Ming in CD2Cl2, 298K, hmqc, QCI
f2 (ppm)
f1 (ppm)

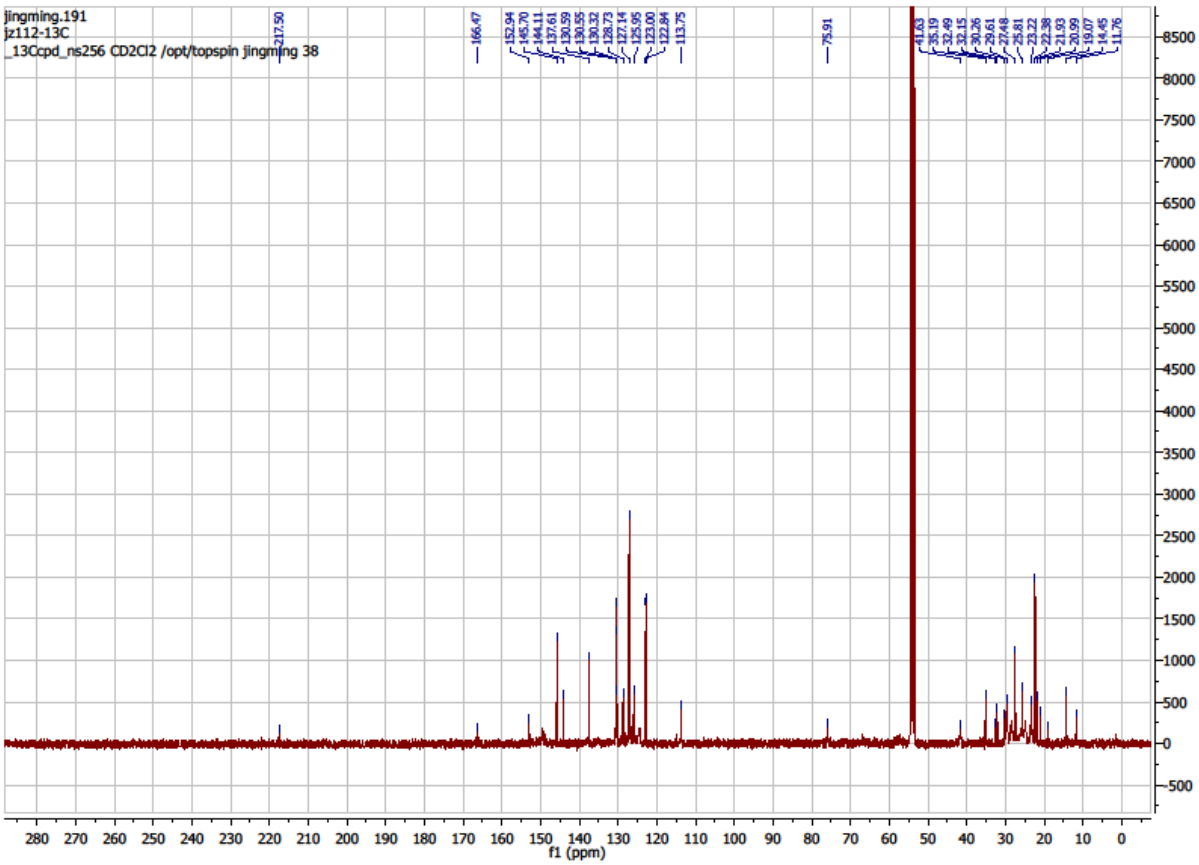

JM-4_050814/2
Jing Ming in CD2Cl2, 298K, hmbc, QCI
f2 (ppm)
f1 (ppm)

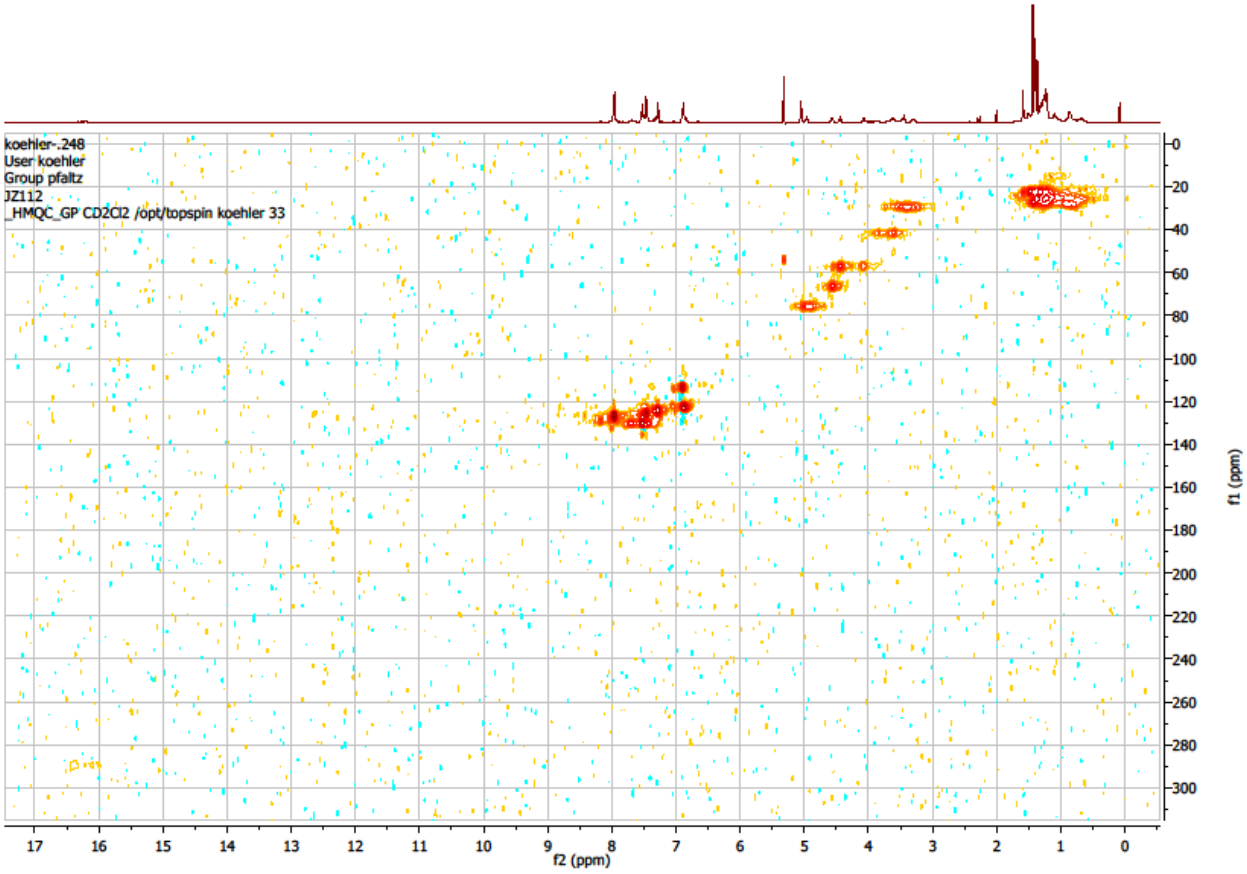

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II
ESI-MS (pos.Mode): cotol (in ACN)
[M-Cl]+
803.19685
805.19729
802.20036
804.19583
801.20001
800.20216
806.20124
807.19487
797.19841
799.20049
m/z

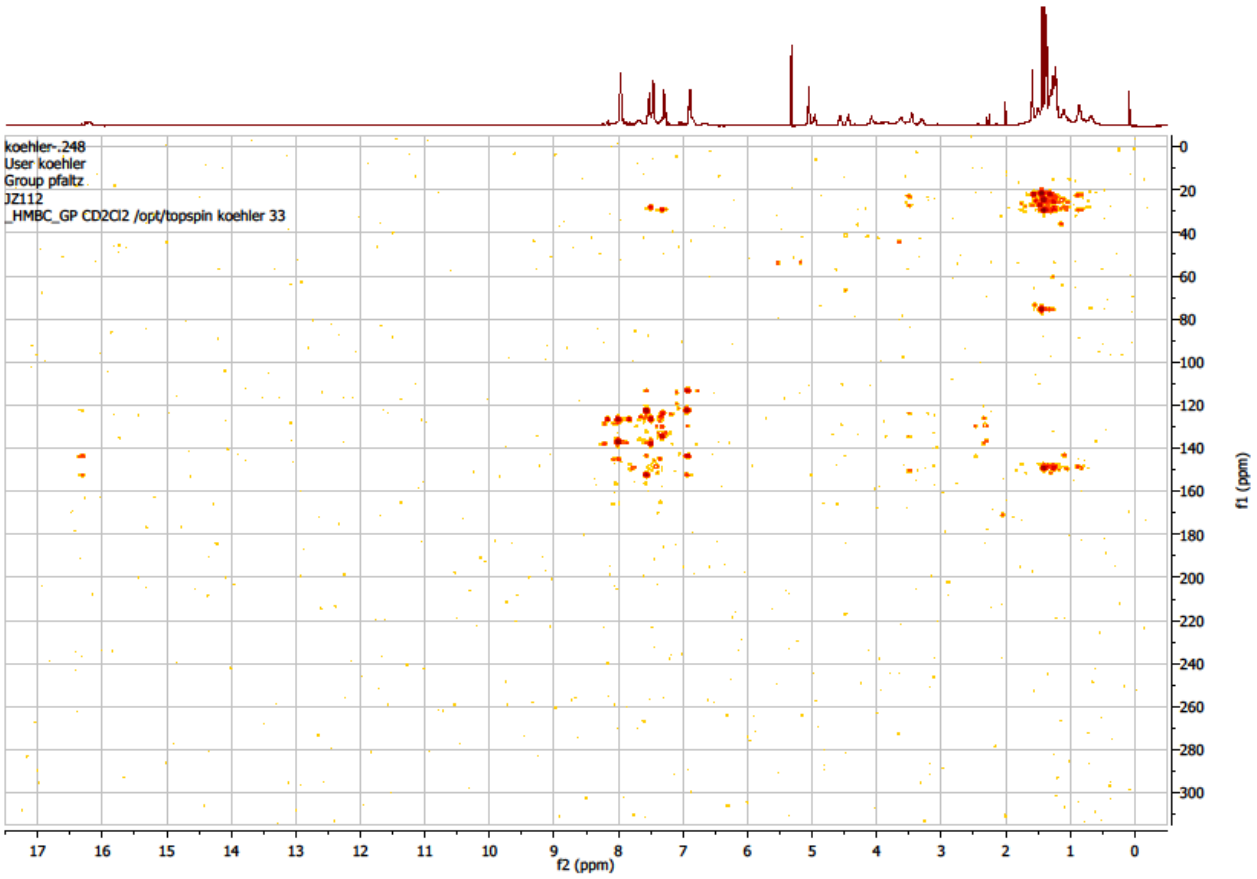

O
NH
SO2NH2
N
N
Cl
Ru
Cl
O

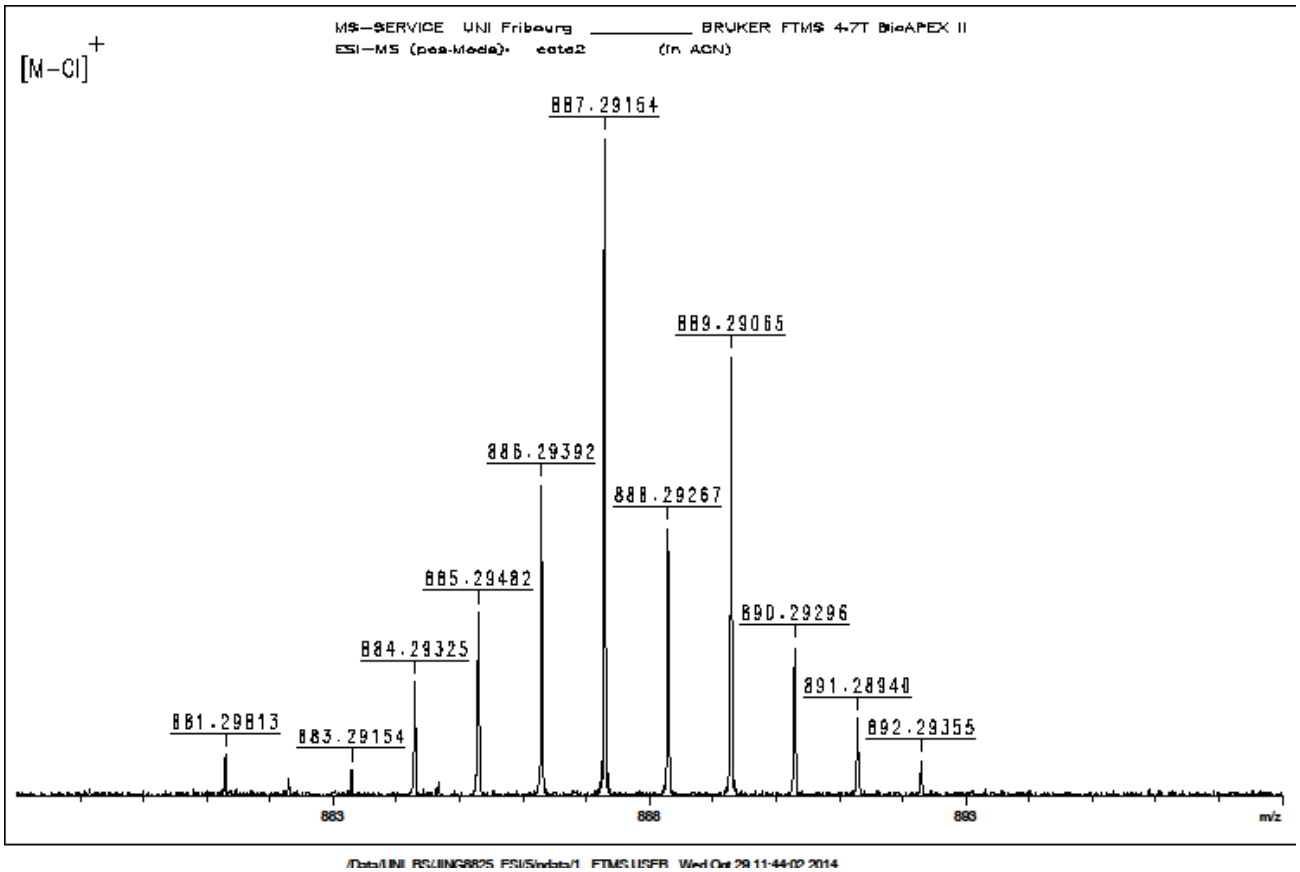
2

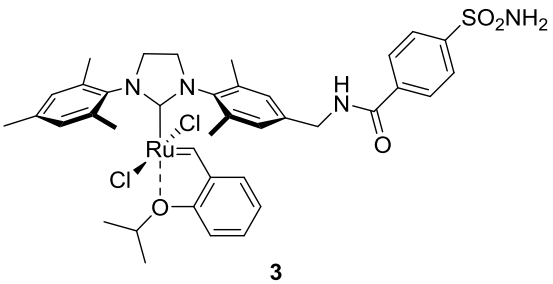

jingming.190
jz112
_Proton_128 CD2Cl2 /opt/topspin jingming 21
f1 (ppm)


jingming.191
jz112-13C
_13Ccpd_ns256 CD2Cl2 /opt/topspin jingming 38
217.50
166.47
152.94
145.70
144.11
137.61
130.59
130.55
130.32
128.73
127.14
125.95
123.00
122.84
113.75
75.91
41.03
35.19
32.49
32.15
30.26
29.61
27.48
25.81
23.22
22.38
21.93
20.99
19.07
14.45
11.76
f1 (ppm)

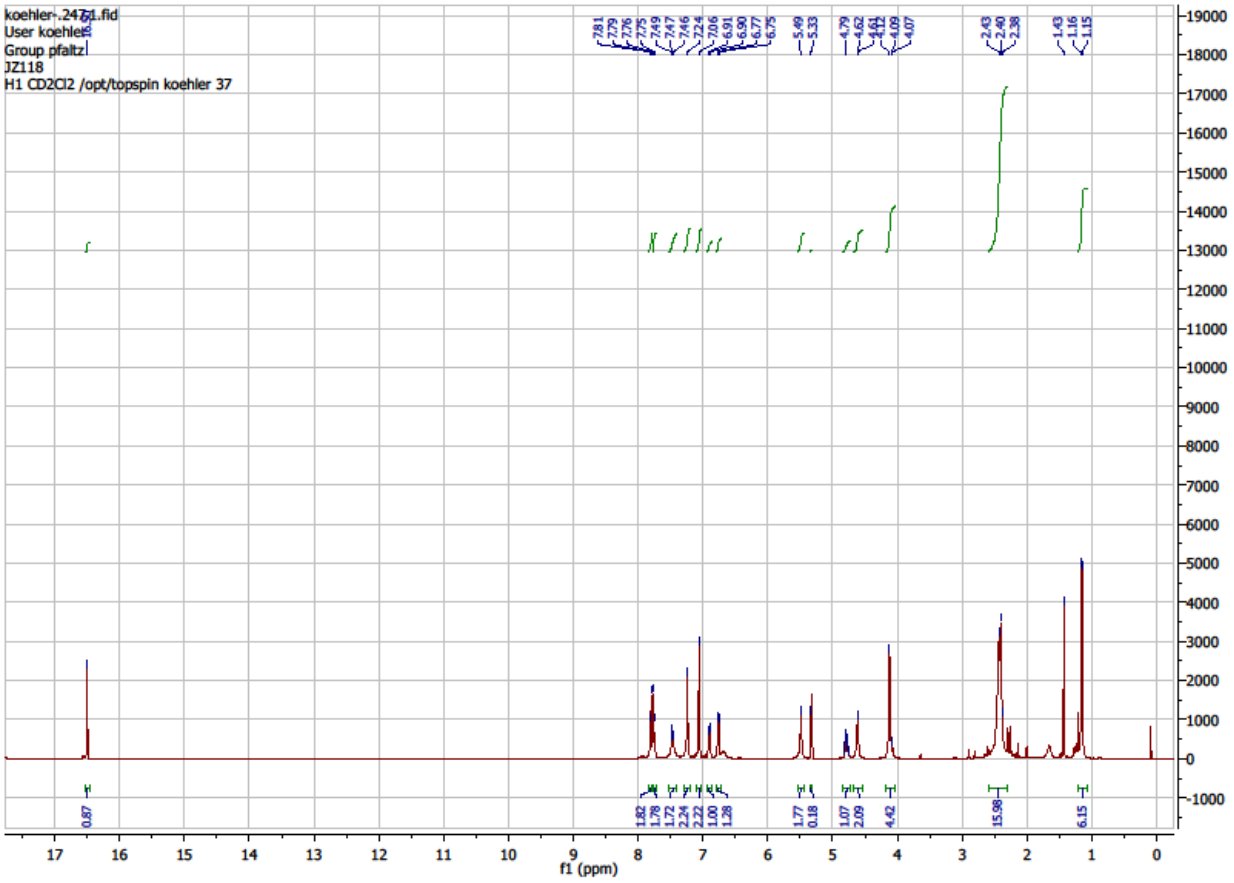

koehler-.248
User koehler
Group pfaltz
JZ112
_HMQC_GP CD2Cl2 /opt/topspin koehler 33
f2 (ppm)
f1 (ppm)

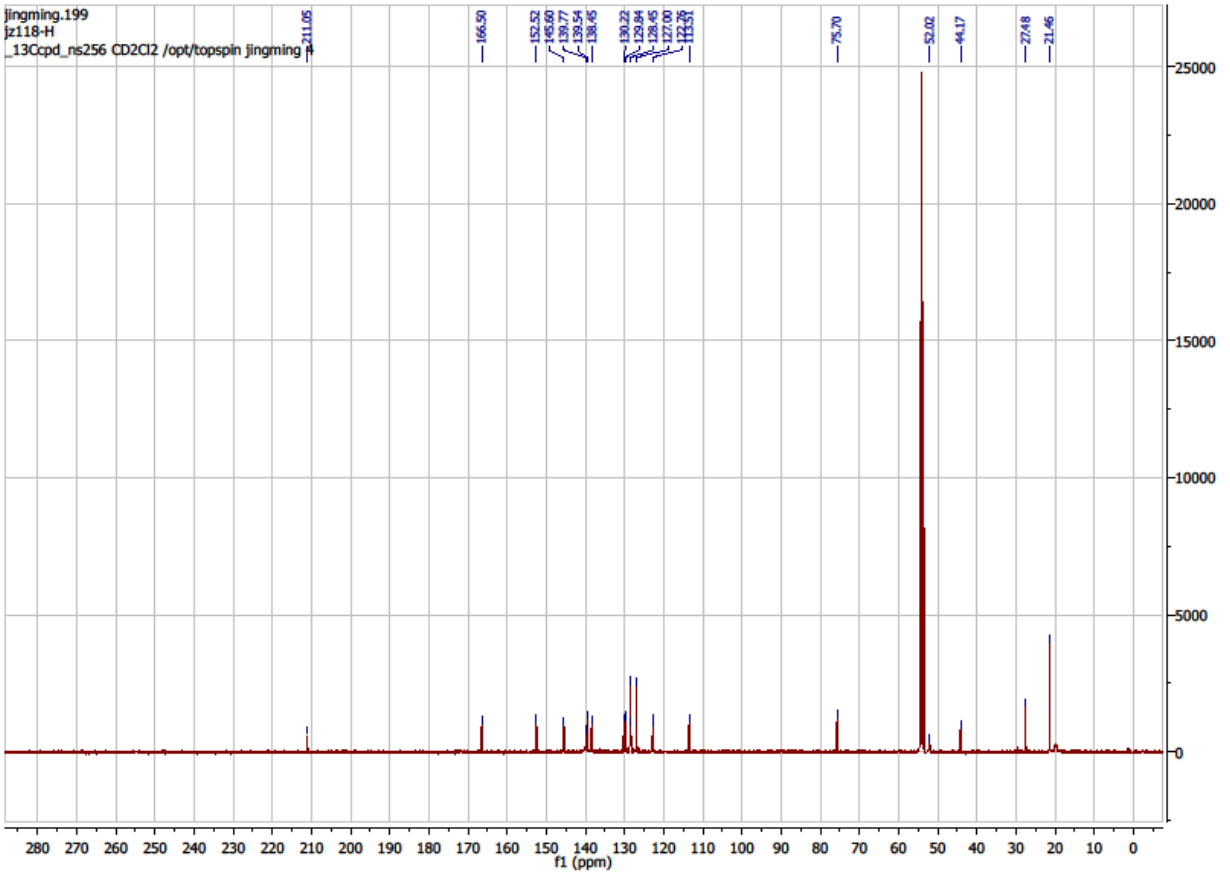

koehler-.248
User koehler
Group pfaltz
JZ112
_HMBC_GP CD2Cl2 /opt/topspin koehler 33
f2 (ppm)
f1 (ppm)

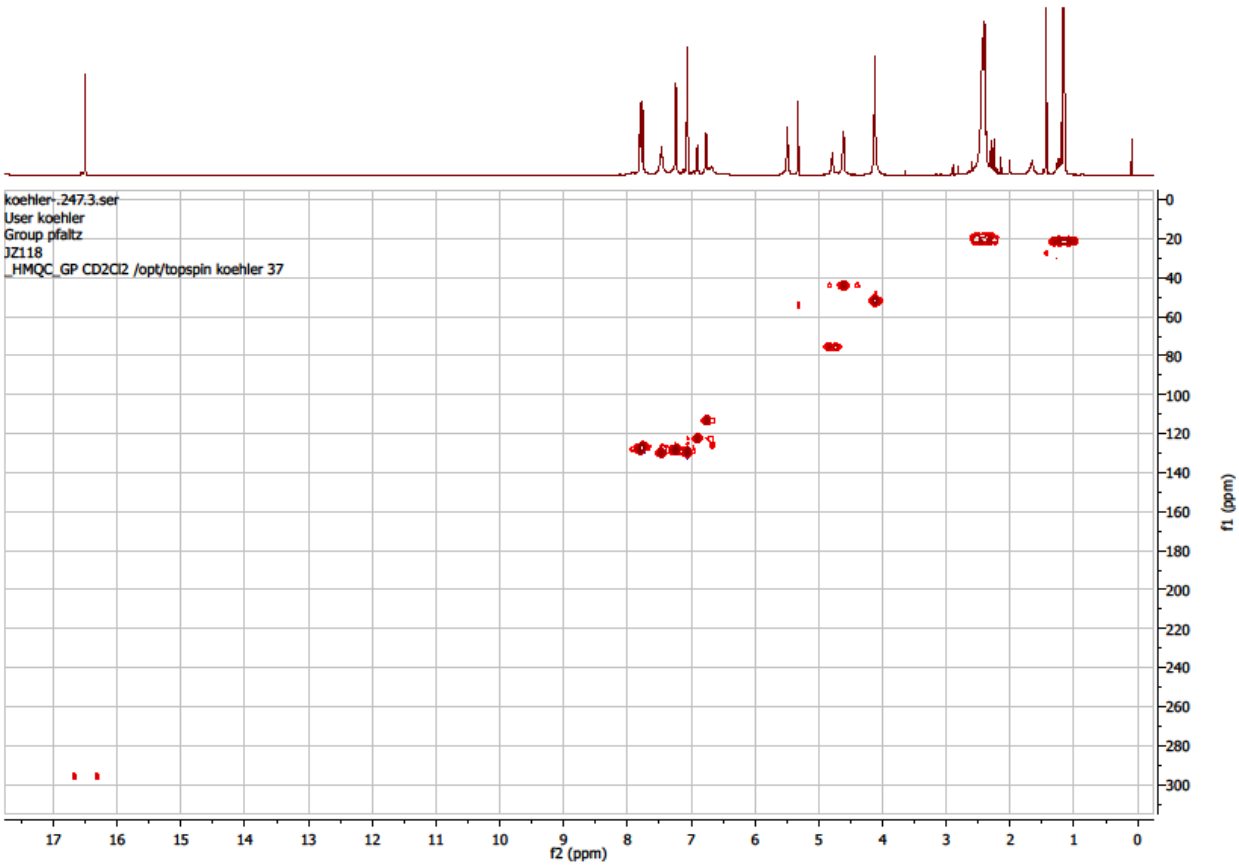

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II
ESI-MS (pos-Mode) cats2 (in AGN)
[M-Cl]+
887.29154
889.29065
886.29392
888.29267
885.29482
890.29296
884.29325
891.28940
881.29813
883.29154
892.29355
883
888
893
m/z

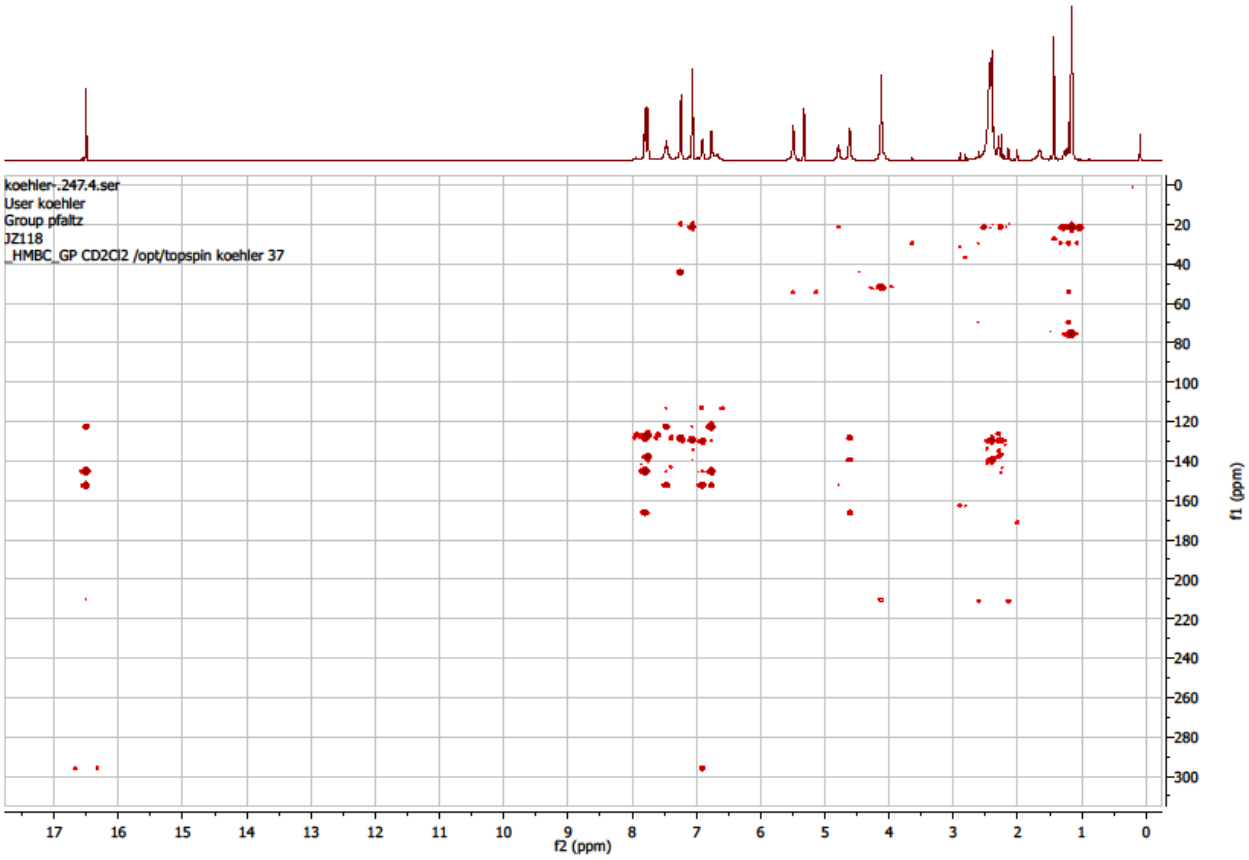

SO2NH2
N
N
H
N
O
Cl
Ru
Cl
O

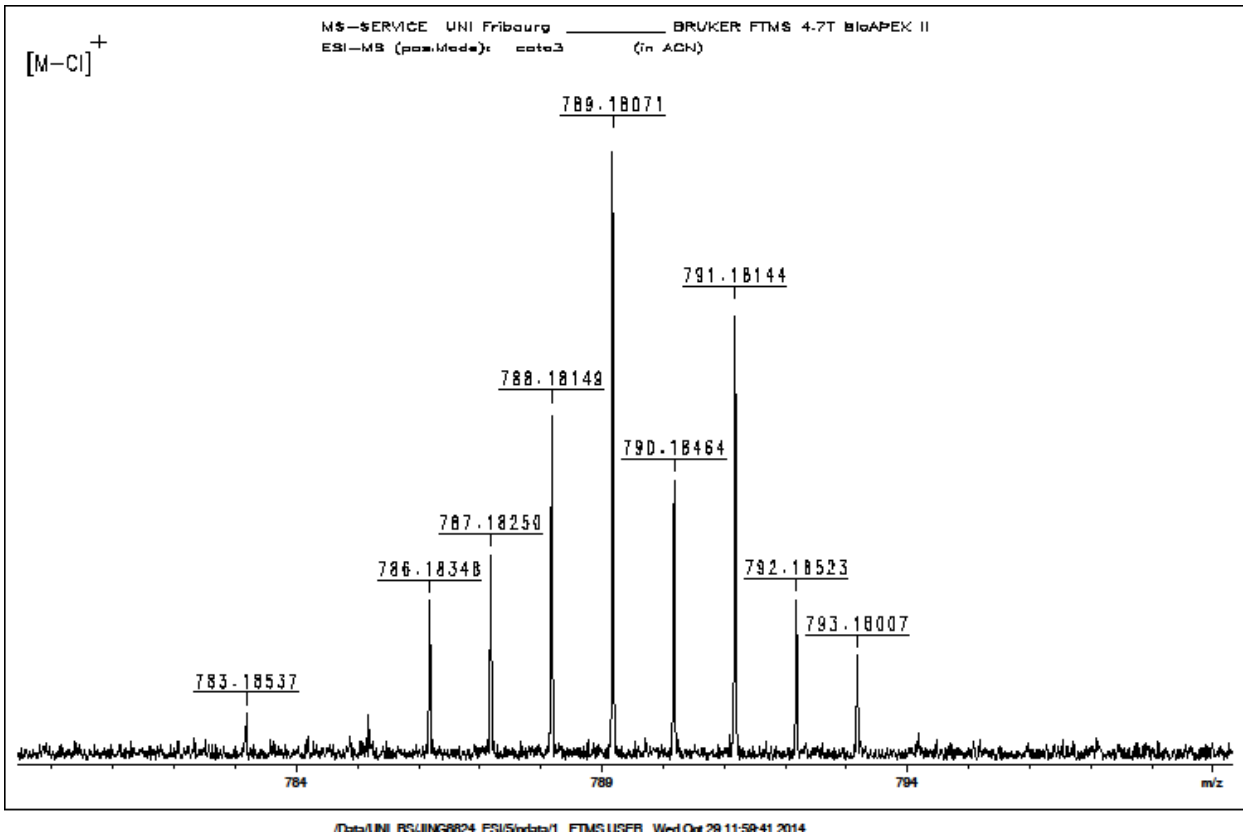
3


koehler-.247z1.fid
User koehler
Group pfaltz
JZ118
H1 CD2Cl2 /opt/topspin koehler 37
f1 (ppm)


jingming.199
jz118-H
_13Ccpd_ns256 CD2Cl2 /opt/topspin jingming
211.05
166.50
152.52
145.69
139.77
139.54
138.45
130.22
129.84
128.45
127.00
75.70
52.02
44.17
27.48
21.46
f1 (ppm)


koehler-.247.3.ser
User koehler
Group pfaltz
JZ118
_HMQC_GP CD2Cl2 /opt/topspin koehler 37
f2 (ppm)
f1 (ppm)


koehler-.247.4.ser
User koehler
Group pfaltz
JZ118
_HMBC_GP CD2Cl2 /opt/topspin koehler 37
f2 (ppm)
f1 (ppm)


MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II
ESI-MS (pos.Mode): cato3 (in ACN)
[M-Cl]+
789.18071
791.18144
788.18149
790.18464
787.18250
786.18348
792.18523
793.18007
783.18537
784
789
794
m/z