# Electronic Supplementary Information

## Cationic Half-Sandwich Quinolinophaneoxazoline-Based ($\eta^6$-*p*-Cymene)ruthenium(II) Complexes Exhibiting Different Chirality Types: Synthesis, and Structural Determination by Complementary Spectroscopic Methods

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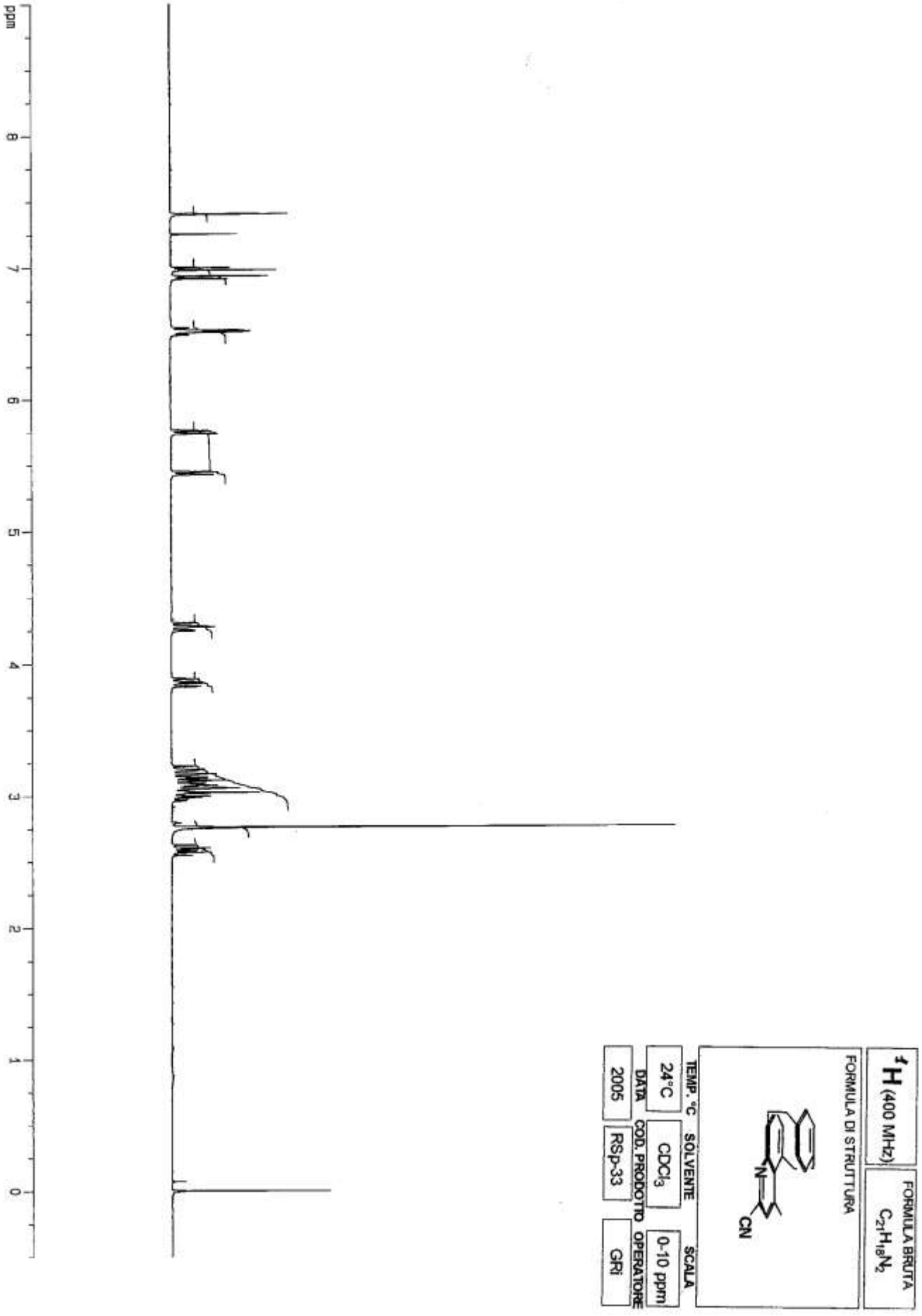
[c] Dipartimento di Chimica e Biologia, Università di Salerno, via Ponte Don Melillo Fisciano, 84084 (SA), Italy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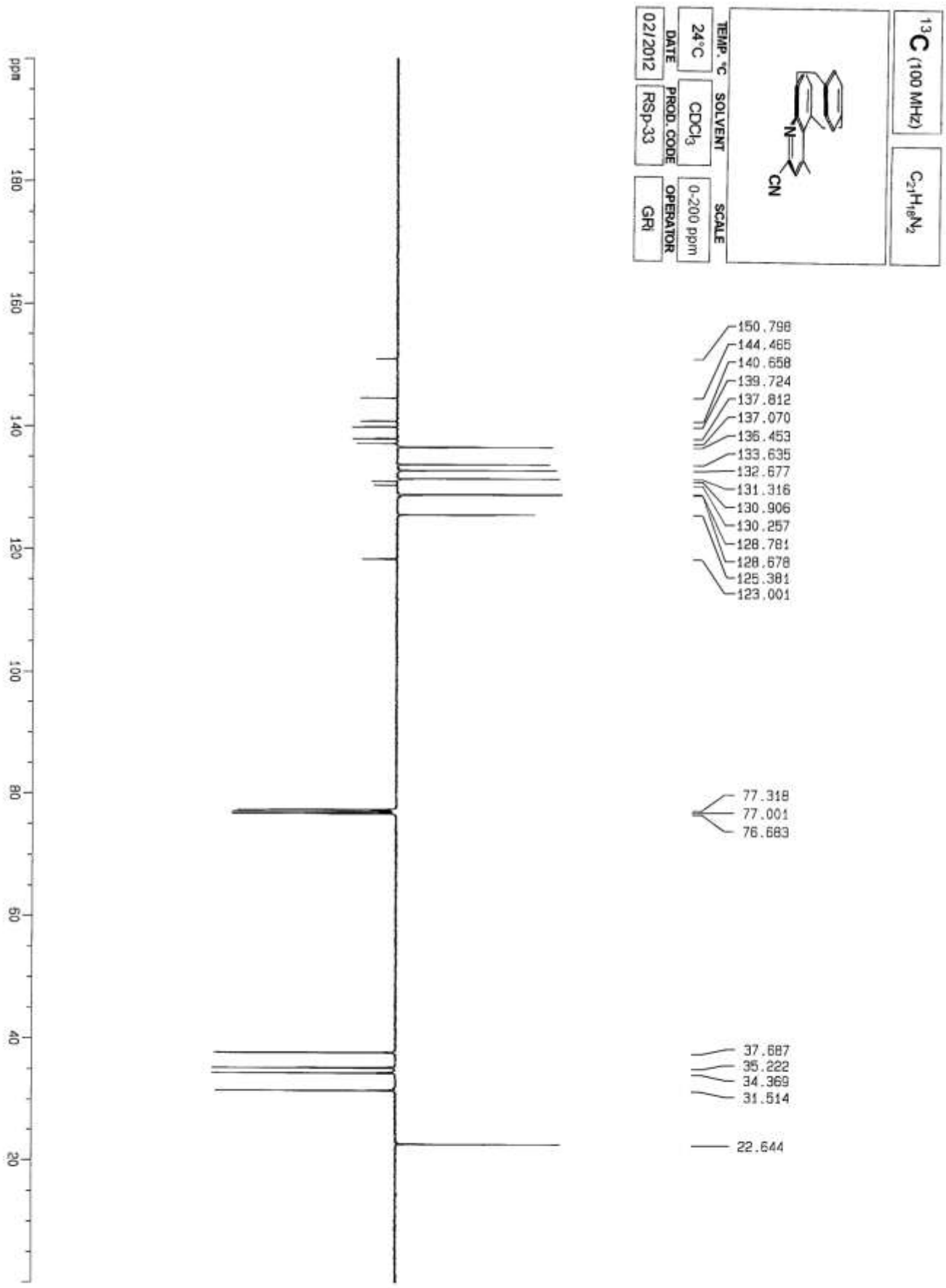
1
2
3
4
5
6
7
8
$^1$H (400 MHz)
FORMULA BRUTA
$C_{21}H_{18}N_2$
FORMULA DI STRUTTURA
CN
N
TEMP. °C
24°C
SOLVENTE
$CDCl_3$
SCALA
0-10 ppm
DATA
2005
COD. PRODOTTO
RSp-33
OPERATORE
GRi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$C_{21}H_{16}N_2$
TEMP. °C
24°C
SOLVENT
$CDCl_3$
SCALE
0-200 ppm
DATE
02/2012
PROD. CODE
RSp-33
OPERATOR
GR
CN
150.798
144.465
140.658
139.724
137.812
137.070
136.453
133.635
132.677
131.316
130.906
130.257
128.781
128.678
125.381
123.001
77.318
77.001
76.683
37.687
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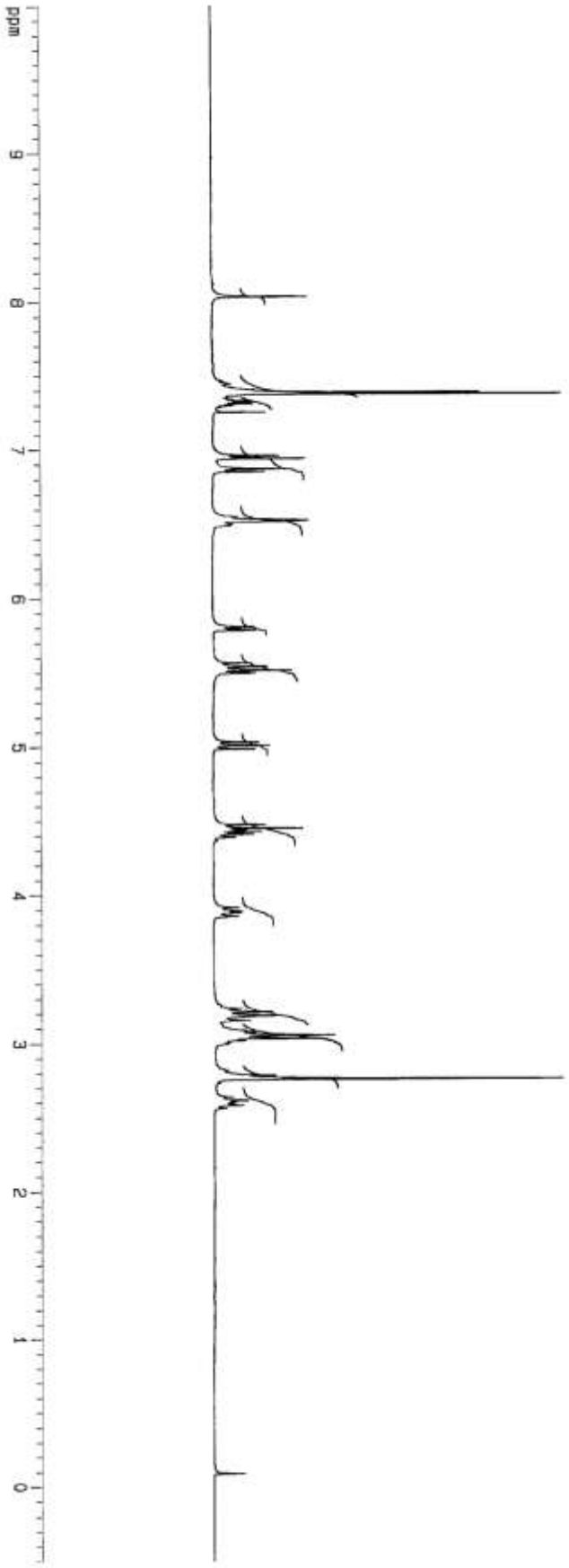
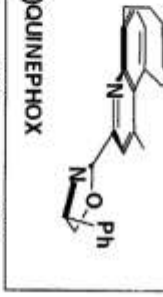
34.369
31.514
22.644
ppm
180
160
140
120
100
80
60
40
20




$^1$H (400 MHz)

$C_{29}H_{26}N_2O$




(*R*$_p$,*R*)QUINEPHOX

TEMP. °C: 24°C

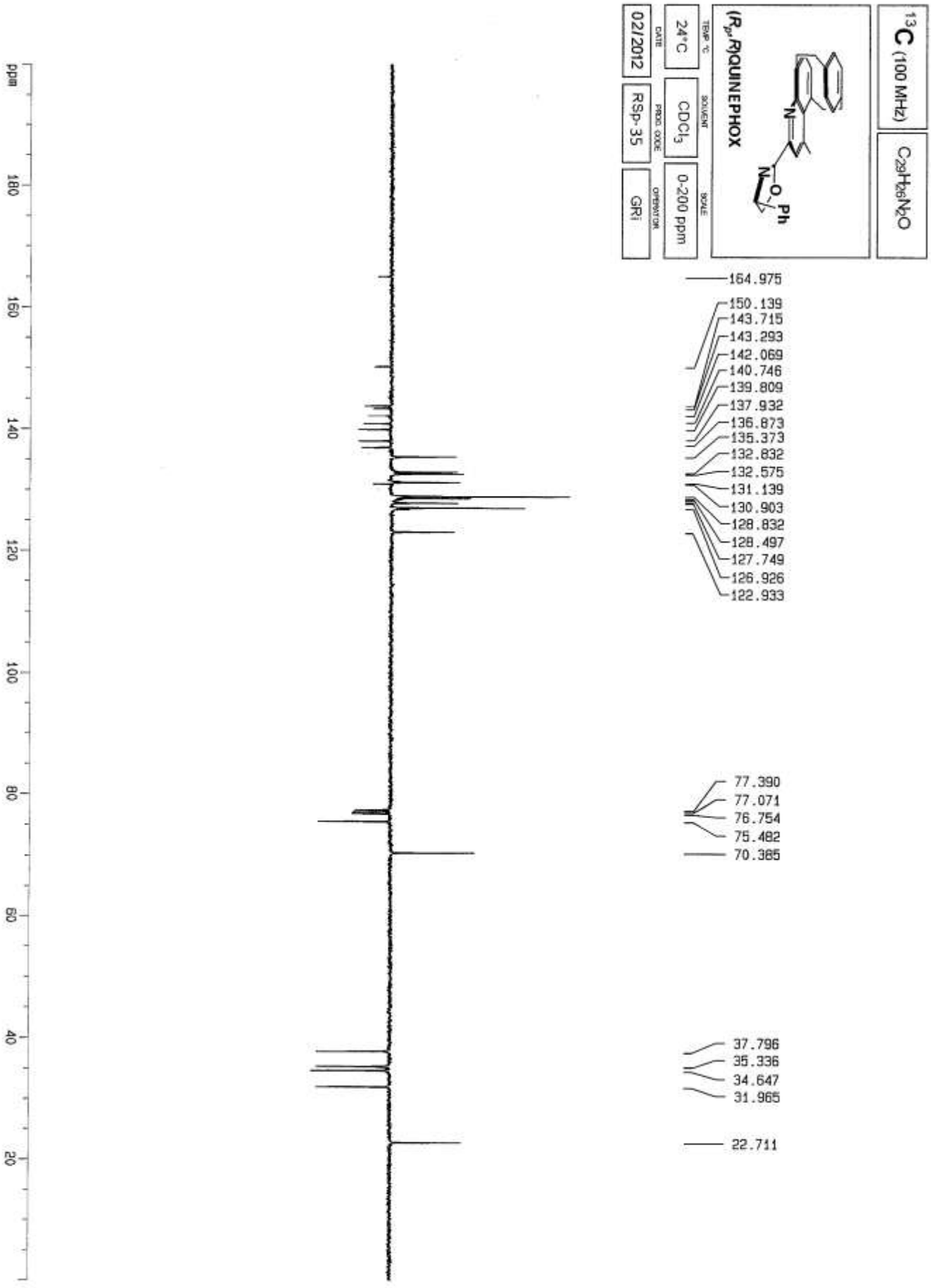
SOLVENT: $CHCl_3$

SCALE: 0-10 ppm

OPERATOR: GRi

02/2012

RSp-34


$^{13}C$ (100 MHz)
$C_{29}H_{26}N_2O$
$(R_p,R)$QUINEPHOX
Ph
TEMP °C
24°C
SOLVENT
$CDCl_3$
SCALE
0-200 ppm
DATE
02/2012
PROG. CODE
RSp-35
OPERATOR
GRi
164.975
150.139
143.715
143.293
142.069
140.746
139.809
137.932
136.873
135.373
132.832
132.575
131.139
130.903
128.832
128.497
127.749
126.926
122.933
77.390
77.071
76.754
75.482
70.365
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35.336
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22.711
ppm
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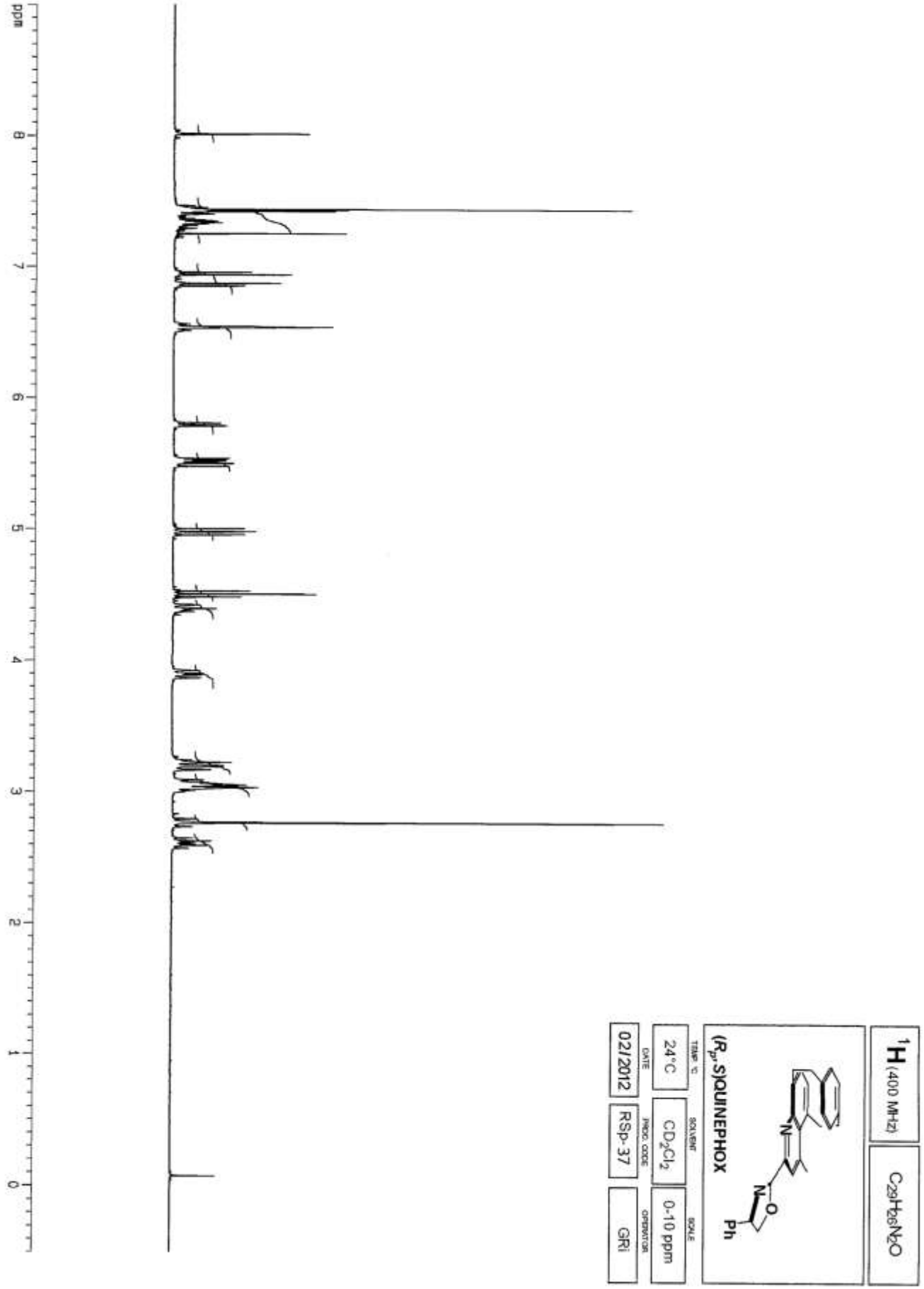
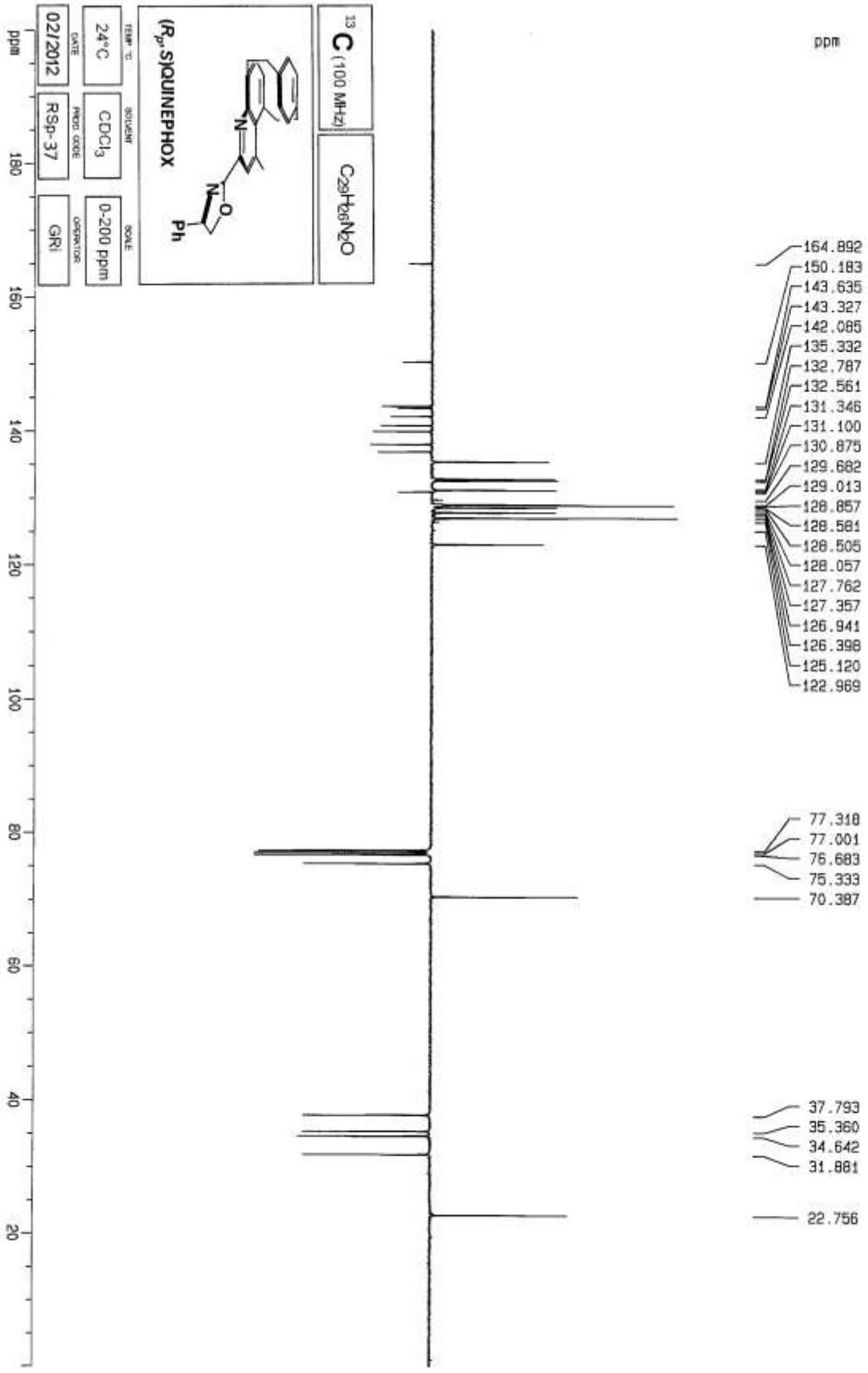
160
140
120
100
80
60
40
20


ppm
0
1
2
3
4
5
6
7
8
$^1$H (400 MHz)
$C_{29}H_{26}N_2O$
($R_{ax}$,S)QUINEPHOX
Ph
N
O
N
SCALE
0-10 ppm
SOLVENT
$CD_2Cl_2$
TEMP. °C
24°C
OPERATOR
GRi
PROG. CODE
RSp-37
DATE
02/2012


$^{13}$C (100 MHz)
$C_{29}H_{26}N_2O$
($R_{pr}$,S)QUINEPHOX
Ph
N
O
N
SOLVENT
$CDCl_3$
TEMP °C
24°C
SCALE
0-200 ppm
DATE
02/2012
PROTO CODE
RSp-37
OPERATOR
GRi
ppm
164.892
150.183
143.635
143.327
142.085
135.332
132.787
132.561
131.346
131.100
130.875
129.682
129.013
128.857
128.581
128.505
128.057
127.762
127.357
126.941
126.398
125.120
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77.001
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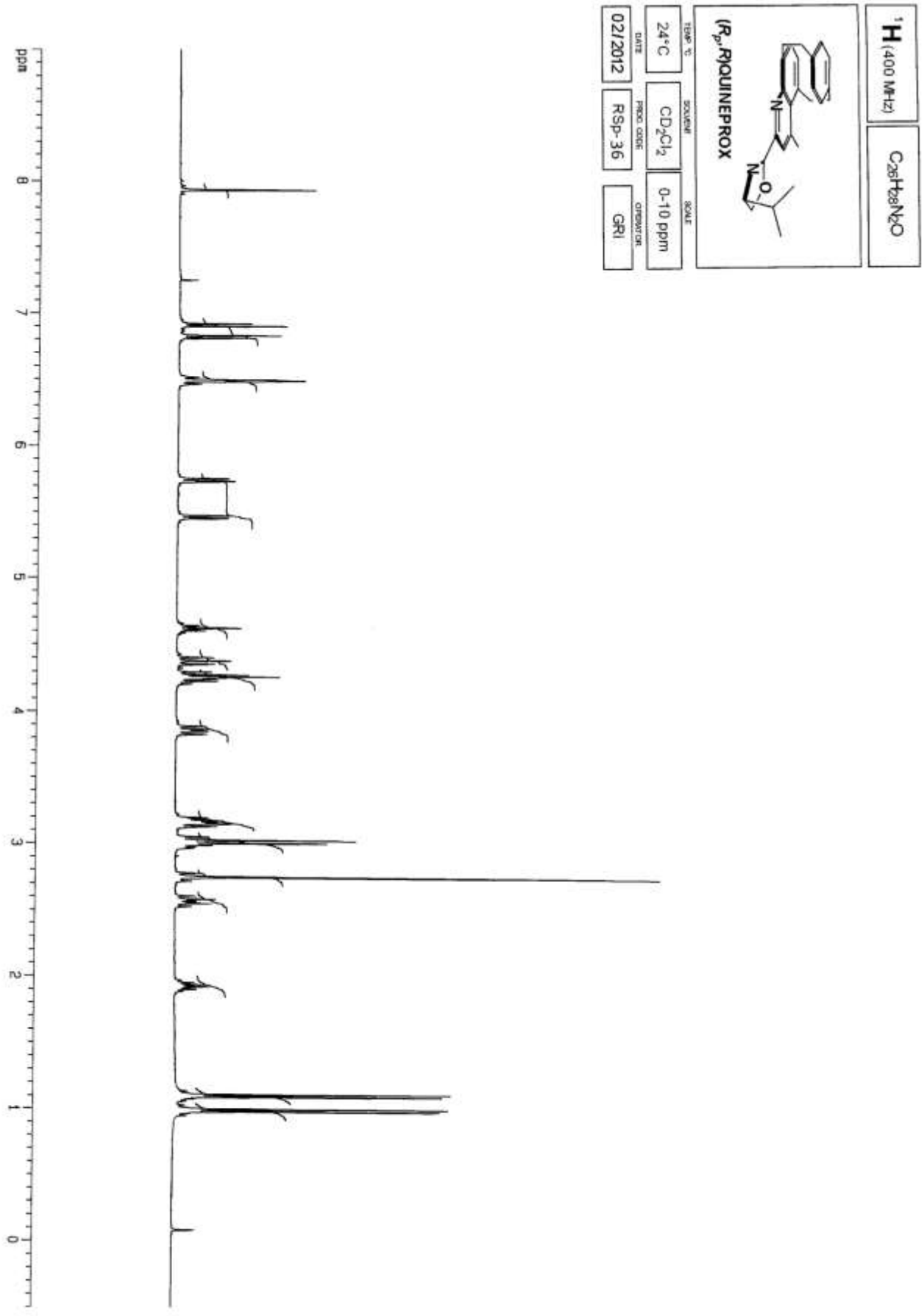
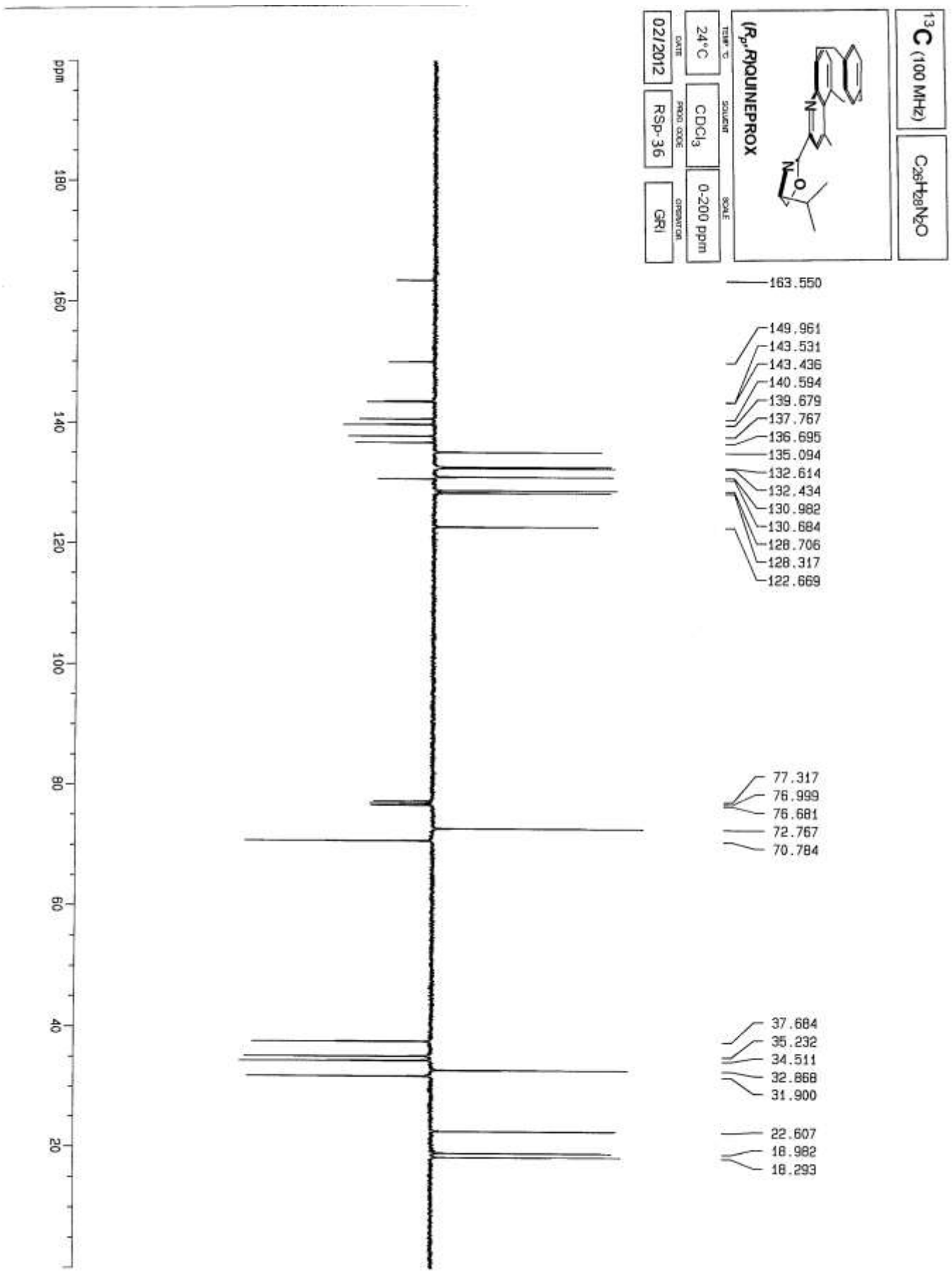
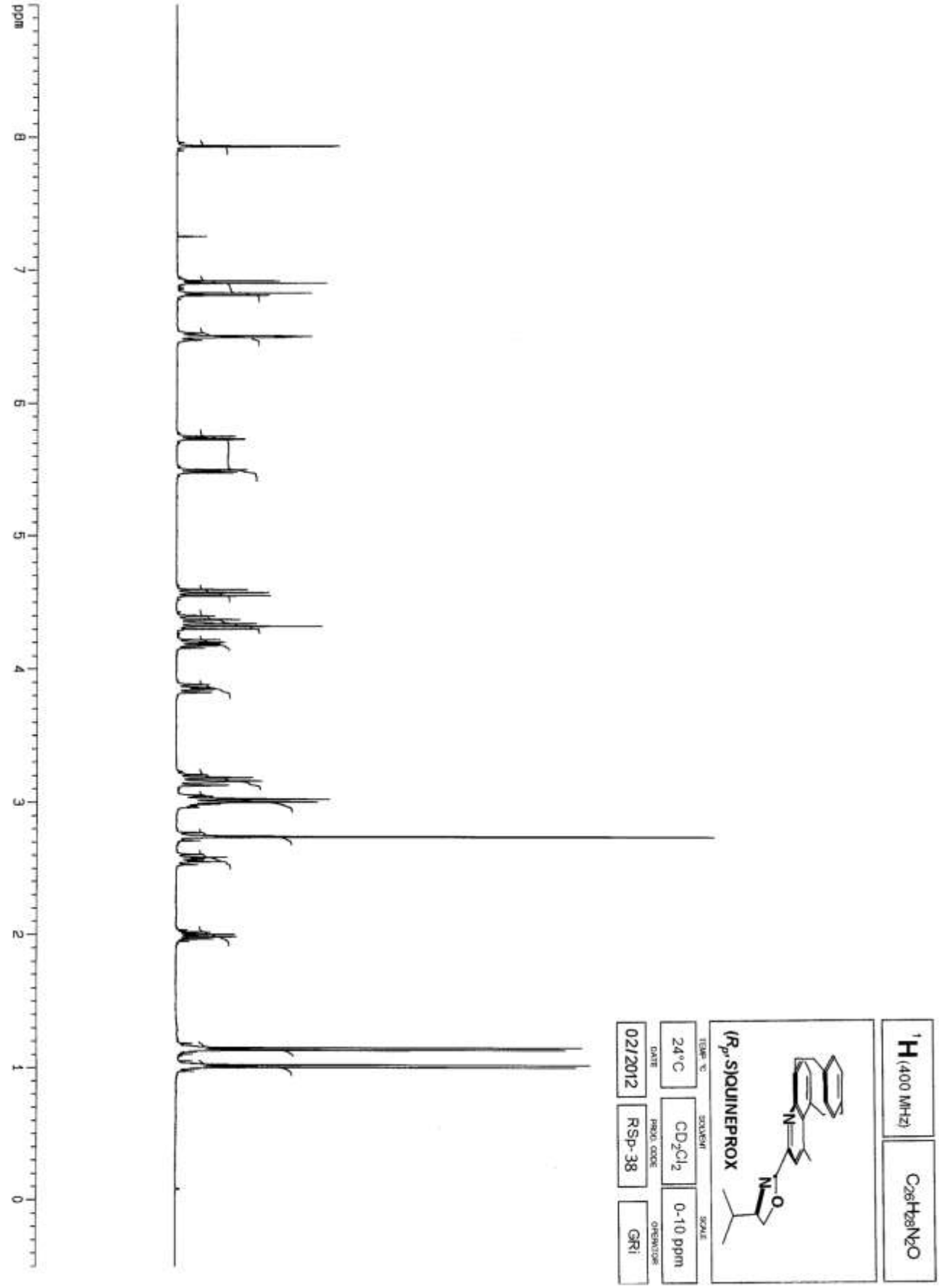
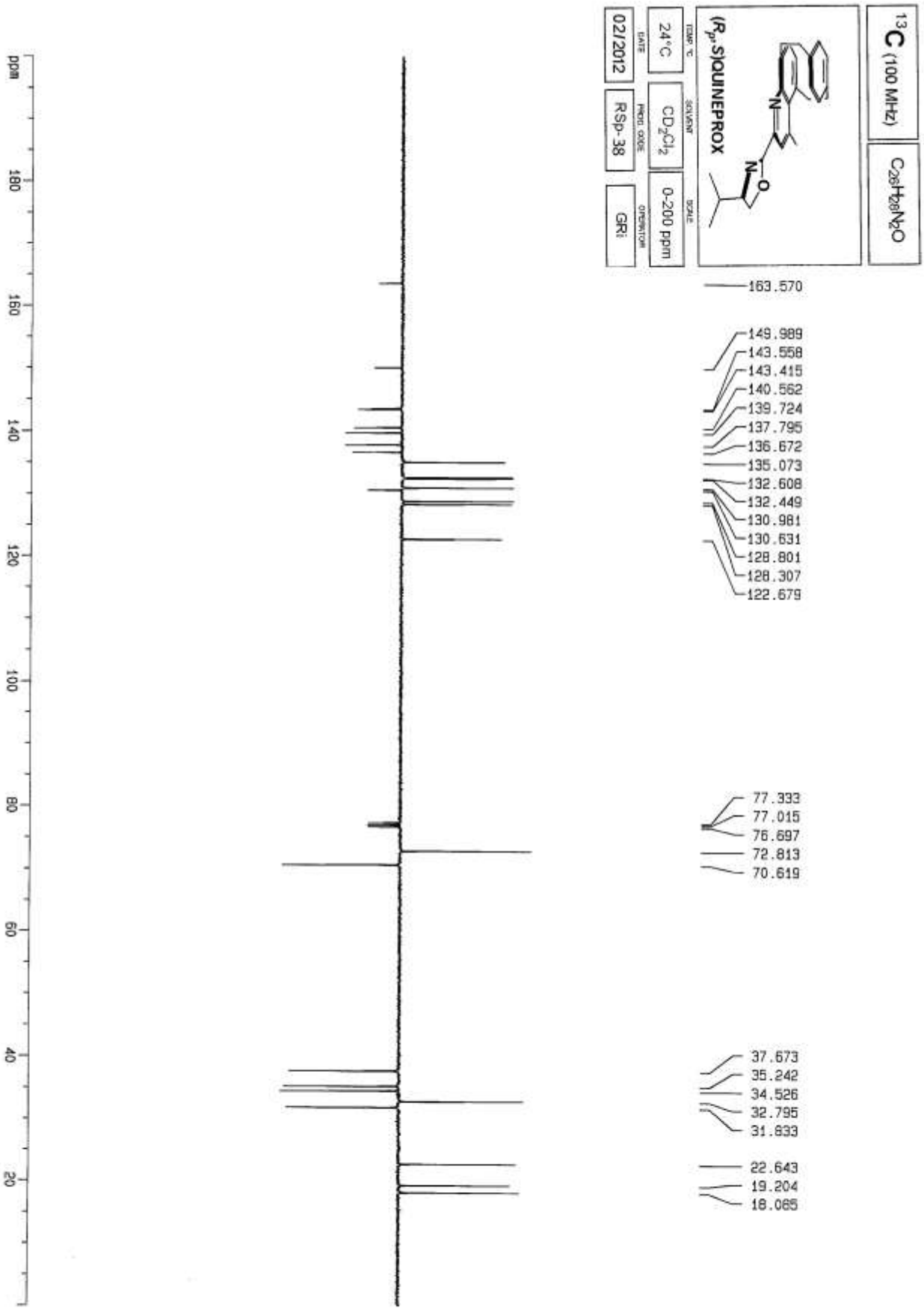
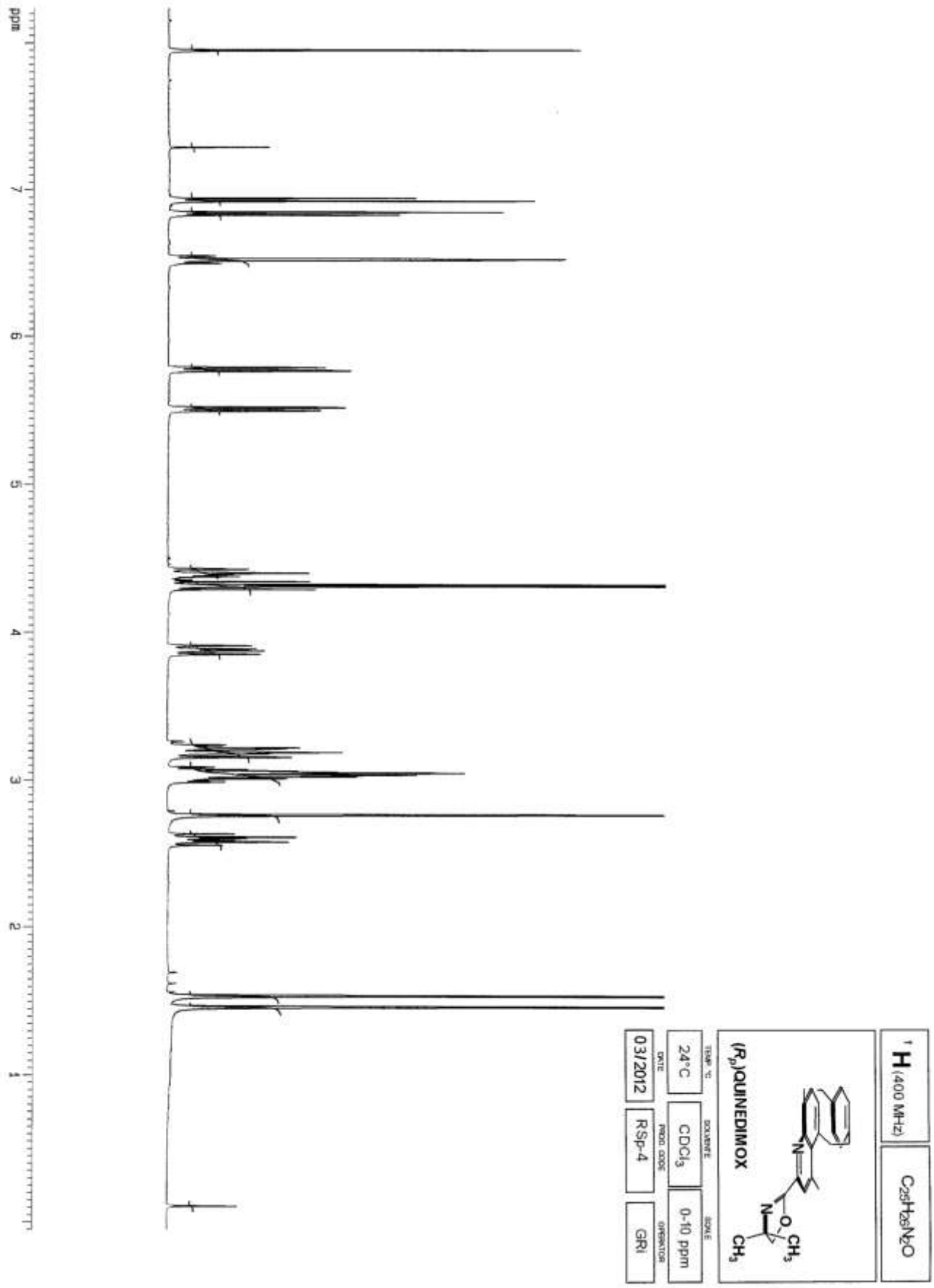
34.642
31.881
22.756

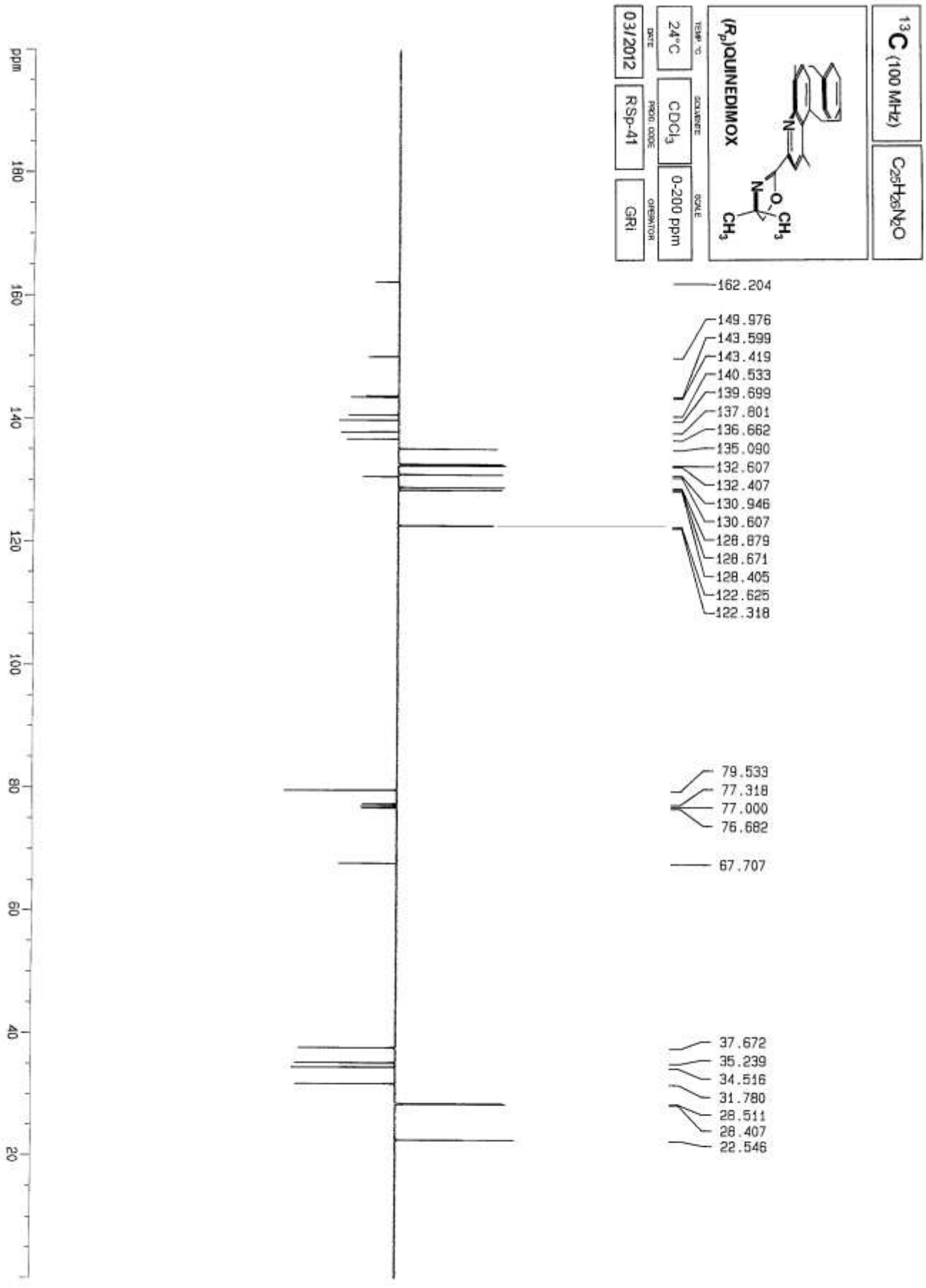

$^1$H (400 MHz)
$C_{26}H_{28}N_2O$
(Rp,R)QUINEPROX
TEMP °C
24°C
SOLVENT
$CD_2Cl_2$
SCALE
0-10 ppm
DATE
02/2012
PROC. CODE
RSp-36
OPERATOR
GRI
ppm
0
1
2
3
4
5
6
7
8


$^{13}$C (100 MHz)
$C_{26}H_{28}N_2O$
(Rp,R)QUINEPROX
24°C
CDCl3
0-200 ppm
02/2012
RSp-36
GRI
163.550
149.961
143.531
143.436
140.594
139.679
137.767
136.695
135.094
132.614
132.434
130.982
130.684
128.706
128.317
122.669
77.317
76.999
76.681
72.767
70.784
37.684
35.232
34.511
32.868
31.900
22.607
18.982
18.293
ppm
180
160
140
120
100
80
60
40
20


ppm
0
1
2
3
4
5
6
7
8
$^1$H (400 MHz)
$C_{26}H_{28}N_2O$
$(R_p,S)$QUINEPROX
N
N
O
SCALE
0-10 ppm
SOLVENT
$CD_2Cl_2$
TEMP. °C
24°C
DATE
02/2012
PROG. CODE
RSp-38
OPERATOR
GRi


$^{13}$C (100 MHz)
$C_{26}H_{28}N_2O$
$(R_{ax},S)$QUINEPROX
DATE 02/2012
TEMP. °C 24°C
SOLVENT $CD_2Cl_2$
SCALE 0-200 ppm
PROG. CODE RSp-38
OPERATOR GRi
163.570
149.989
143.558
143.415
140.562
139.724
137.795
136.672
135.073
132.608
132.449
130.981
130.631
128.801
128.307
122.679
77.333
77.015
76.697
72.813
70.619
37.673
35.242
34.526
32.795
31.833
22.643
19.204
18.065
ppm
180
160
140
120
100
80
60
40
20


ppm
1
2
3
4
5
6
7
$^1$H (400 MHz)
$C_{25}H_{26}N_2O$
$(R_p)$QUINEDIMOX
N
N
O
$CH_3$
$CH_3$
TEMP °C
24°C
SOLVENTE
$CDCl_3$
SCALE
0-10 ppm
DATE
03/2012
PROG. CODE
RSp-4
OPERATOR
GRI


$^{13}$C (100 MHz)
$C_{25}H_{26}N_2O$
$(R_p)$QUINEDIMOX
24°C
$CDCl_3$
0-200 ppm
03/2012
RSp-41
GRi
162.204
149.976
143.599
143.419
140.533
139.699
137.801
136.662
135.090
132.607
132.407
130.946
130.607
128.879
128.671
128.405
122.625
122.318
79.533
77.318
77.000
76.682
67.707
37.672
35.239
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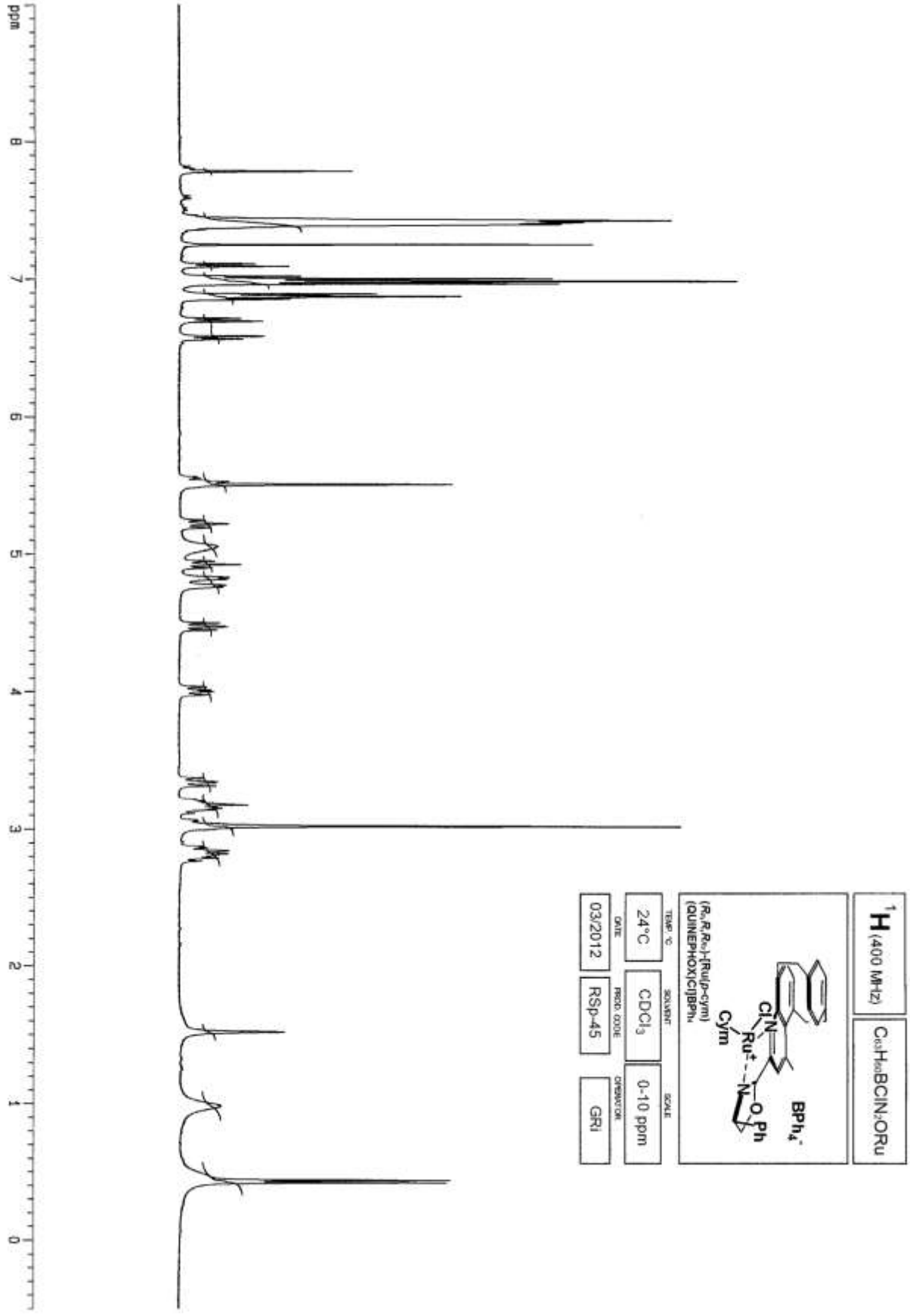
28.511
28.407
22.546
ppm
180
160
140
120
100
80
60
40
20


ppm
0
1
2
3
4
5
6
7
8
$^1$H (400 MHz)
$C_{61}H_{60}BClN_2ORu$
$BPh_4^-$
Cym
Cl
N
Ru
N
O
Ph
(R,R,R$_{Ru}$)-[Ru(p-cym)(QUINEPHOX)Cl]BPh$_4$
TEMP. °C
24°C
SOLVENT
$CDCl_3$
SCALE
0-10 ppm
DATE
03/2012
PROD. CODE
RSp-45
OPERATOR
GRi

# [($R_p$,$R$,$R_{Ru}$)-[Ru($\eta^6$-*p*-cymene)(QUIPHANEPHOX)Cl]$^+$$BPh_4^-$ (6a)

$[\alpha]_D^{20}$ = +298 (c = 0.1, $CHCl_3$)

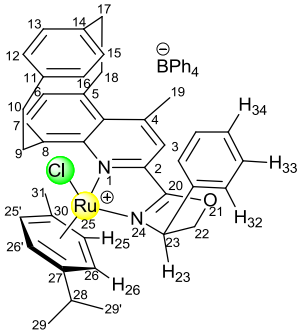
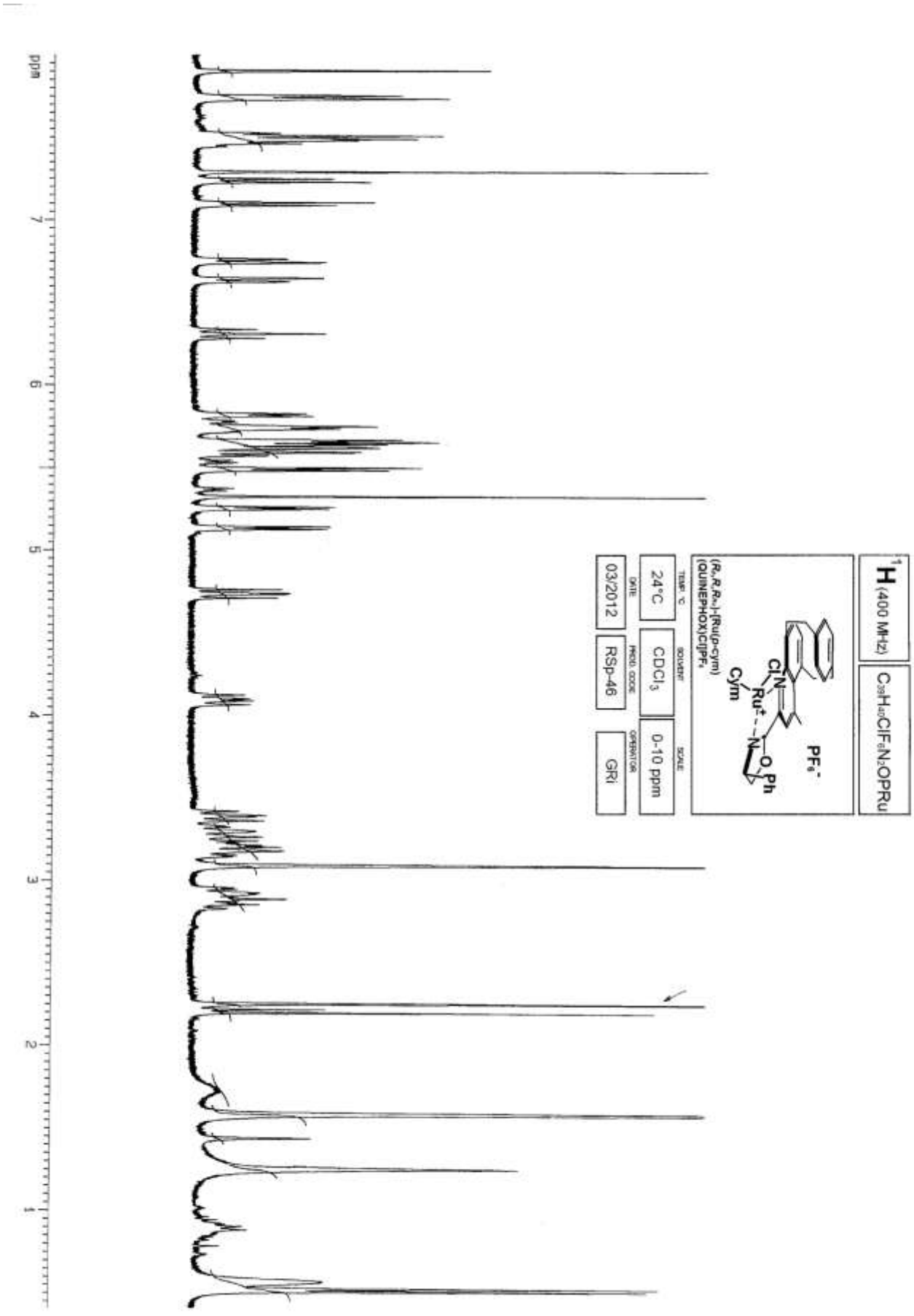


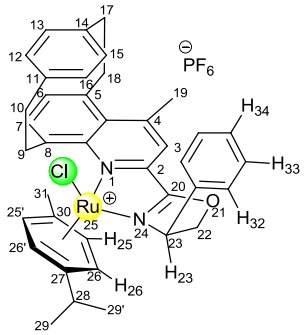

**Table S1.** Chemical shift values assigned to the protons of complex **($R_p$,$R$,$R_{Ru}$)-6a** in $CDCl_3$

| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.84 | H-22t (*t*) | 4.92 |
| H-6 ($d_{AB}$) | 7.07 | H-23 (*t*) | 5.22 |
| H-7 ($d_{AB}$) | 7.16 | H-25 (broad) | 5.05 |
| H-9a (*dt*) | 3.09 | H-25’ (*d*) | 4.77 |
| H-9s (*m*) | 5.59 | H-26 (*d*) | 5.05 |
| H-10a (*m*) | 2.87 | H-26’ | 4.82 |
| H-10s (*m*) | 3.22 | H-28 (*broad*) | 1.5 |
| H-12 ($dd_{AB}$) | 6.61 | H-29 (*d*) | 0.43 |
| H-13 ($dd_{AB}$) | 6.74 | H-29’(*broad*) | 0.44 |
| H-15 (*dd*) | 5.56 | H-31 (*broad*) | 1.5 |
| H-16 (*dd*) | 5.56 | H-32 (*o*) | 7.4 |
| H-17a (*dt*) | 3.34 | H-33 (*m*) | 7.4 |
| H-17s (*dd*) | 2.84 | H-34 (*p*) | 7.4 |
| H-18a (*dd*) | 3.2 | $BPh_4$ *o* (8 H) | 7.4 |
| H-18s (*ddd*) | 4.00 | BPh4 *m* (8 H) | 7.0 |
| H-19 (*s*) | 3.02 | $BPh_4$ *p* (*t*, 4 H) | 6.90 |
| H-22c (*dd*) | 4.47 | | |


ppm
7
6
5
4
3
2
1
$^1$H (400 MHz)
$C_{38}H_{40}ClF_6N_2OPRu$
$PF_6^-$
Cl
N
Ru
Cym
O
Ph
(R$_a$,R,R$_{Ru}$)-[Ru(p-cym)(QUINEPHOX)Cl]PF$_6$
TEMP. °C
24°C
SOLVENT
$CDCl_3$
SCALE
0-10 ppm
DATE
03/2012
PROBE CODE
RSp-46
OPERATOR
GRi

# [($R_p$,$R$,$R_{Ru}$)-[Ru($\eta^6$-*p*-cymene)(QUIPHANEPHOX)Cl]$^+$$PF_6^-$ (6b)

**Table S2.** Chemical shift values assigned to the protons of complex **($R_p$,$R$,$R_{Ru}$)-6b** in $CDCl_3$.




| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.90 | H-19 (*s*) | 3.09 |
| H-6 ($d_{AB}$) | 7.08 | H-22c (*dd*) | 4.73 |
| H-7 ($d_{AB}$) | 7.23 | H-22t (*dd*) | 5.60 |
| H-9a (*m*) | 3.2 | H-23 (*t*) | 6.30 |
| H-9s (*m*) | 5.73 | H-25 (*d*) | 5.25 |
| H-10a (*m*) | 2.92 | H-25’ (*d*) | 5.79 |
| H-10s (*m*) | 3.30 | H-26 (*d*) | 5.13 |
| H-12 ($dd_{AB}$) | 6.63 | H-26’ (*d*) | 5.73 |
| H-13 ($dd_{AB}$) | 6.75 | H-28 (*broad*) | 1.7 |
| H-15 $(dd)_{AB}$ | 5.58 | H-29 (*d*) | 0.51 |
| H-16 $(dd)_{AB}$ | 5.66 | H-29’(*broad*) | 0.56 |
| H-17a (*m*) | 3.38 | H-31 (*broad s*) | 1.25 |
| H-17s (*dd*) | 2.88 | H-32 (*o*) | 7.73 |
| H-18a (*dd*) | 3.20 | H-33 (*m*) | 7.5 |
| H-18s (*dt*) | 4.09 | H-34 (*p*) | 7.50 |

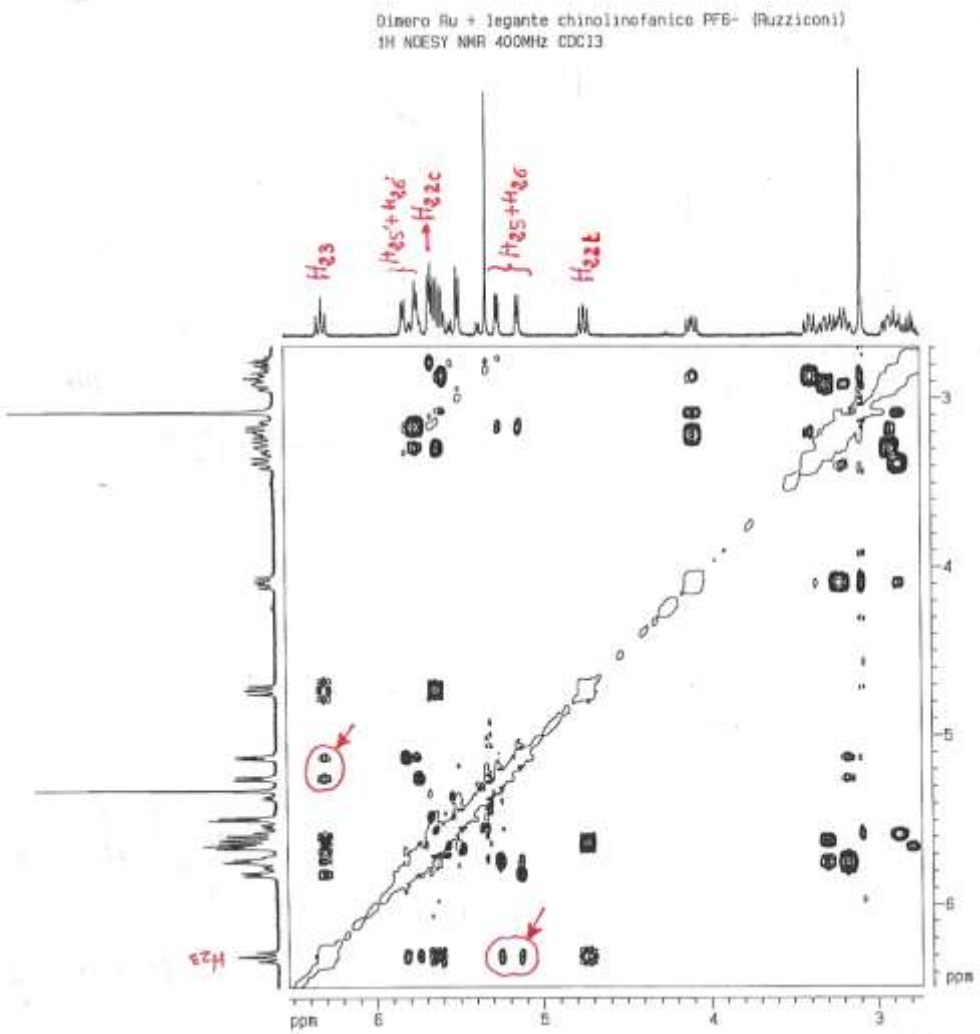
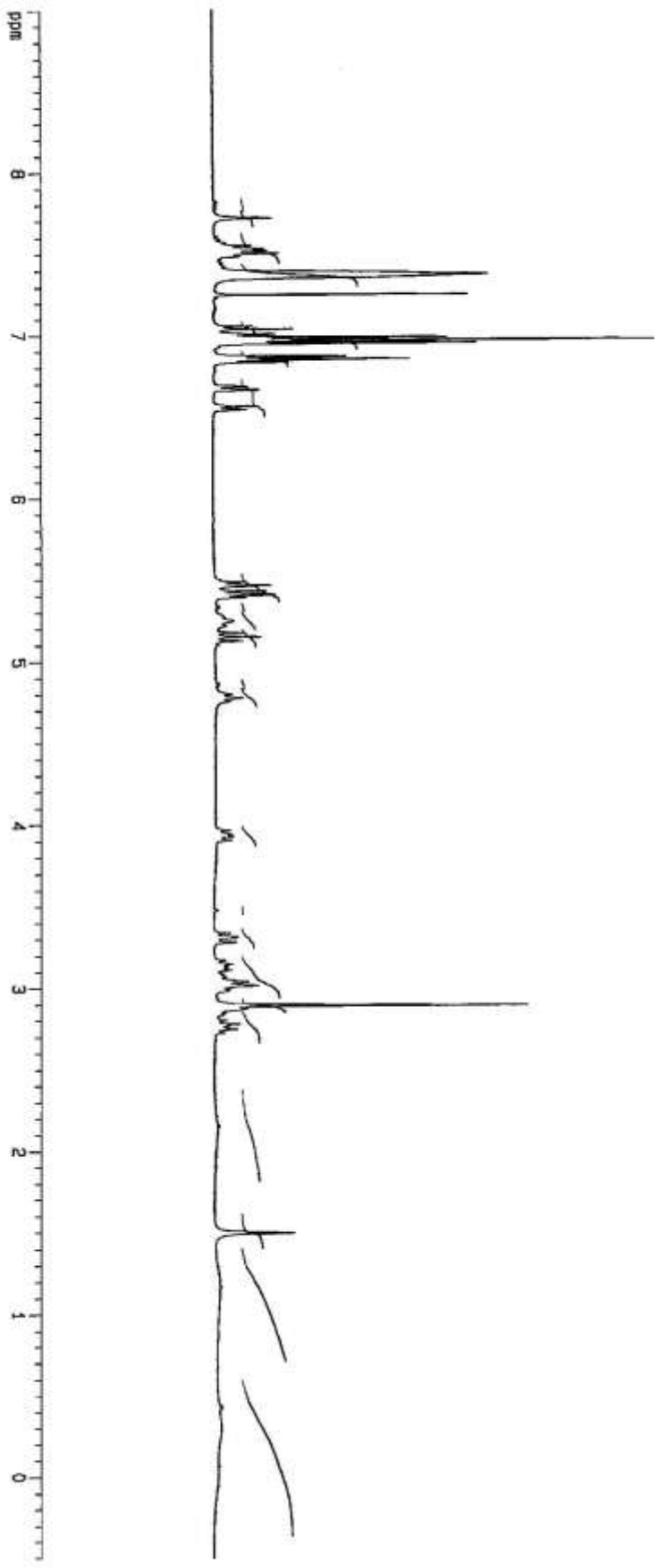
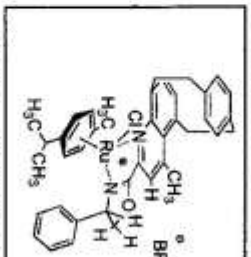



**Figure S1**. A section of the $^{1}$H-NOESY diagram (400.13MHz, 293 K,$CDCl_3$) for complex **6b** showing the NOE correlations of the *p*-cymene aromatic protons H-27 and H-28 with H-23 of the oxazoline ring.




$^1H$ (400 MHz) | $C_{53}H_{60}BClN_2Ru$



| Solvente | Cod. Prodotto | Cod. Spettro |
|---|---|---|
| $CDCl_3$ | RSp 50 | GRi 31/1 |

| Data | Operatore |
|---|---|
| 27/04/2012 | SSp |

# [($R_p$,$S$,$R_{Ru}$)-[Ru($\eta^6$-*p*-cymene)(QUIPHANEPHOX)Cl]$^+$$BPh_4$ (7a)

$[\alpha]_D^{20}$ = +514 (c = 0.081, $CHCl_3$)

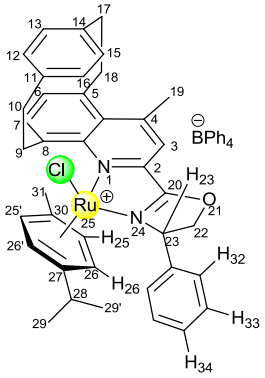
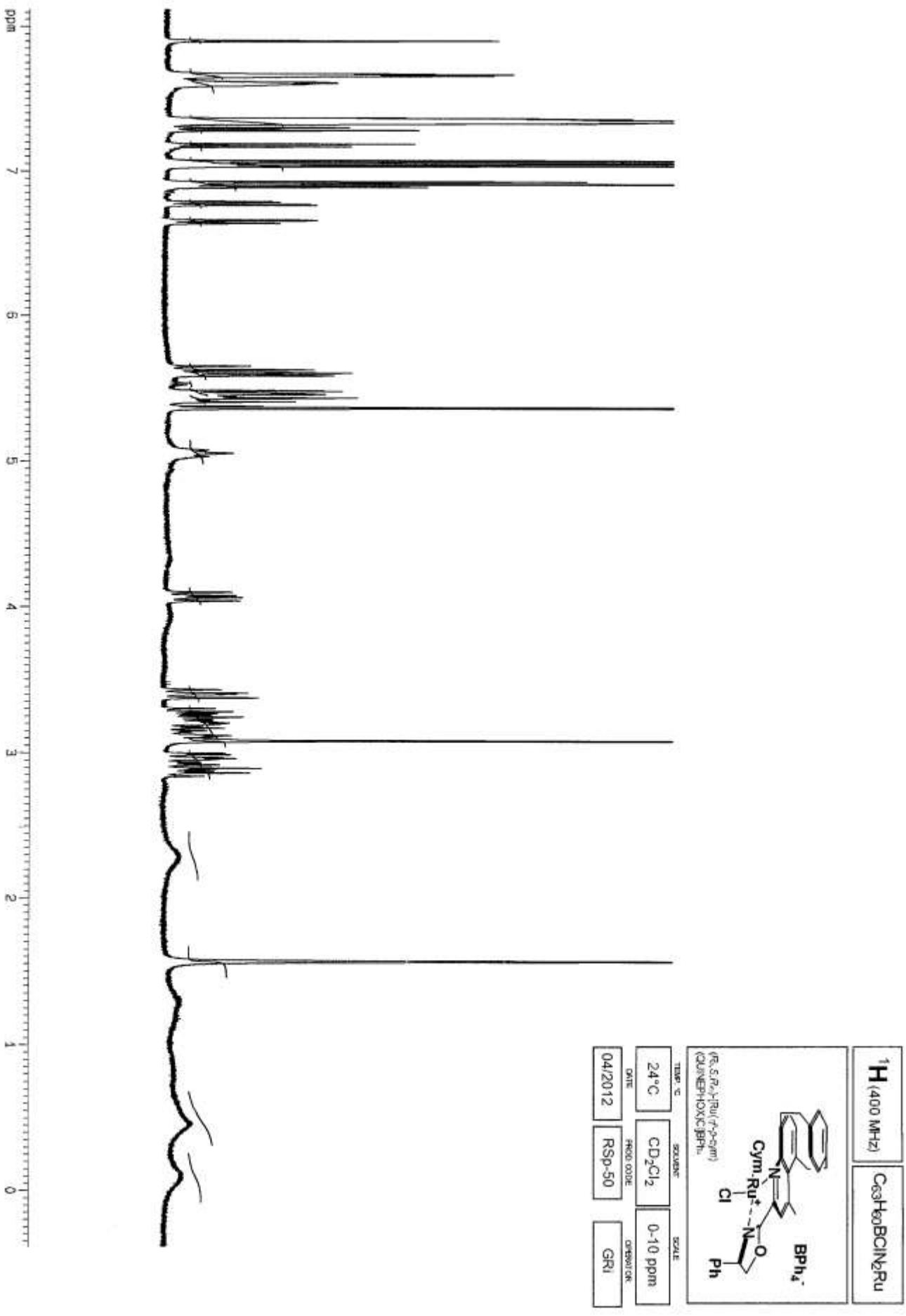



**Table S3.** Chemical shift values assigned to the protons of complex **($R_p$,$S$,$R_{Ru}$)-7a** in $CDCl_3$.

| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.75 | H-22t (*t*) | 4.93 |
| H-6 ($d_{AB}$) | 7.03 | H-23 (*t*) | 5.52 |
| H-7 ($d_{AB}$) | 7.08 | H-25 (*very broad*) | *n.d.* |
| H-9a (*dt*) | 3.07 | H-25’ (*very broad*) | *n.d.* |
| H-9s (*m*) | 5.31 | H-26 (*very broad*) | *n.d.* |
| H-10a (*m*) | 2.90 | H-26’ (*very broad*) | *n.d.* |
| H-10s (*m*) | 3.05 | H-28 (*very broad*) | ~ 2.0 |
| H-12 ($dd_{AB}$) | 6.58 | H-29 (*very broad*) | 0.4 |
| H-13 ($dd_{AB}$) | 6.70 | H-29’ (*very broad*) | 0.4 |
| H-15 (*dd*) | 5.50 | H-31 (*very broad*) | ~ 1.2 |
| H-16 (*dd*) | 5.43 | H-32 (*o*) | 7.4 |
| H-17a (*dt*) | 3.34 | H-33 (*m*) | 7.4 |
| H-17s (*dd*) | 2.80 | H-34 (*p*) | 7.4 |
| H-18a (*dd*) | 3.17 | $BPh_4$ *o* (m, 8 H) | 7.39 |
| H-18s (*ddd*) | 3.97 | $BPh_4$ *m* (t, 8 H) | 6.96 |
| H-19 (*s*) | 2.93 | $BPh_4$ *p* (t, 4 H) | 6.85 |
| H-22c (*t*) | 5.27 | | |


ppm
0
1
2
3
4
5
6
7
$^1$H (400 MHz)
$C_{63}H_{60}BClN_2Ru$
Cym-Ru$^+$
Cl
Ph
$BPh_4^-$
24°C
$CD_2Cl_2$
0-10 ppm
04/2012
RSp-50
GRI

## **[($R_p$,S,$R_{Ru}$)-[Ru($\eta^6$-*p*-cym)(QUIPHANEPHOX)Cl]$^+$BPh$_4$** ($CD_2Cl_2$) (**7a**)

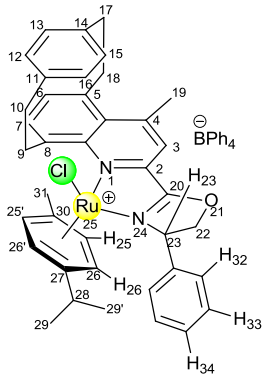



**Table S4.** Chemical shift values assigned to the protons of complex **($R_p$,S,$R_{Ru}$)-7a** in $CD_2Cl_2$.

| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.90 | H-22c (*dd*) | 5.42 |
| H-6 ($d_{AB}$) | 7.17 | H-23 (*dd*) | 5.62 |
| H-7 ($d_{AB}$) | 7.28 | H-25 (*very broad*) | 3.9 |
| H-9a (*dt*) | 3.18 | H-25' (*very broad*) | ~4.3 |
| H-9s (*m*) | 5.43 | H-26 (*very broad*) | ~5.1 |
| H-10a (*m*) | 2.96 | H-26' | n.d. |
| H-10s (*m*) | 3.10 | H-28 (*very broad*) | 1.3 |
| H-12 ($dd_{AB}$) | 6.65 | H-29 (*very broad*) | 0.1 |
| H-13 ($dd_{AB}$) | 6.77 | H-29' (*very broad*) | 0.4 |
| H-15 (*dd*) | 5.59 | H-31 (*very broad*) | 2.3 |
| H-16 (*dd*) | 5.47 | H-32 *o* (*m*) | 7.6 |
| H-17a (*dt*) | 3.40 | H-33 *m* (*m*) | 7.7 |
| H-17s (*dd*) | 2.88 | H-34 *p* (*m*) | 7.7 |
| H-18a (*dd*) | 3.26 | $BPh_4$ *o* (*8 H*) | 7.3 |
| H-18s (*ddd*) | 4.06 | $BPh_4$ *m* (*8 H*) | 7.05 |
| H-19 (*s*) | 3.07 | $BPh_4$ *p* (*t, 4 H*) | 6.9 |
| H-22t (*dd*) | 5.05 | | |

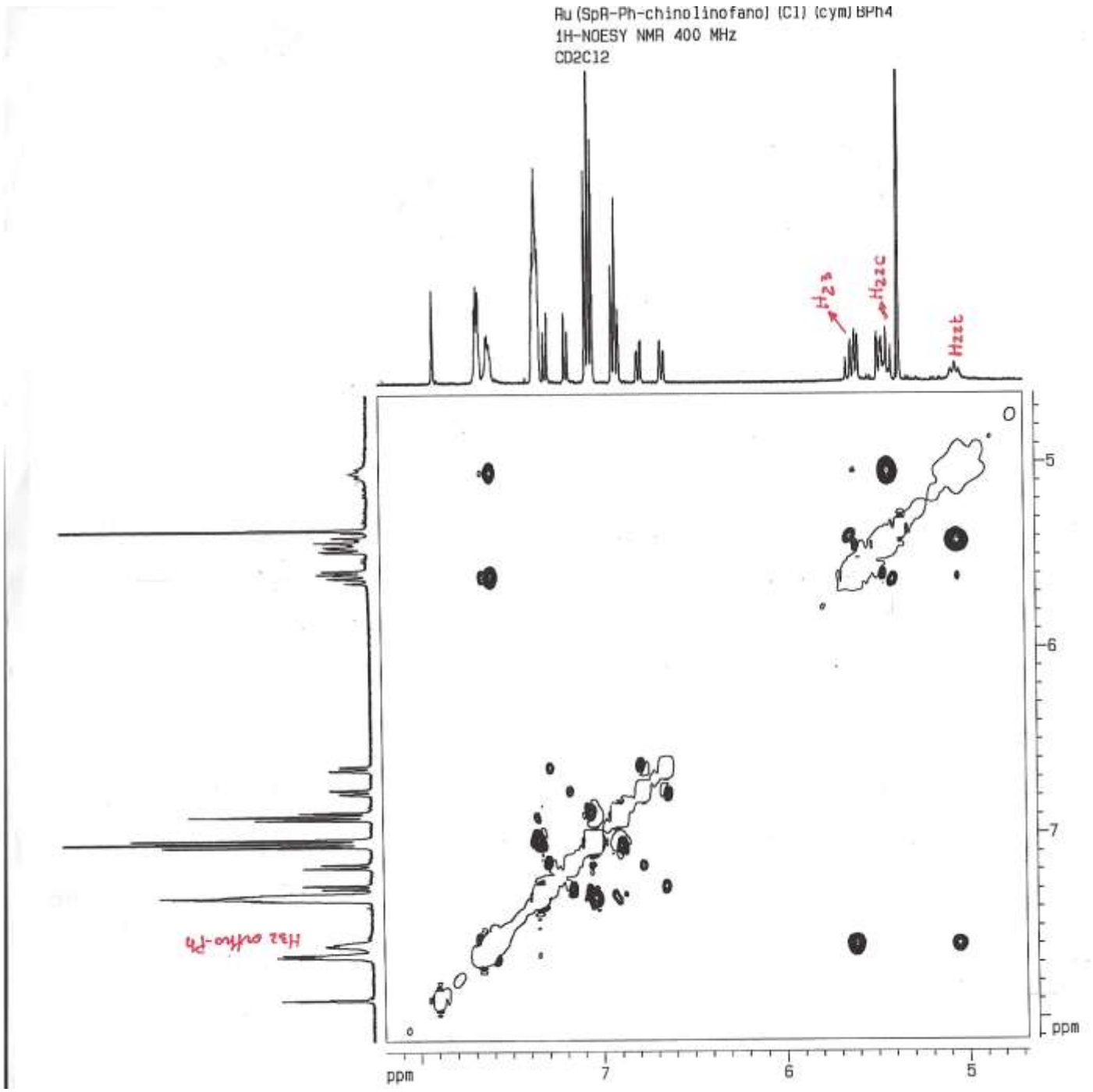
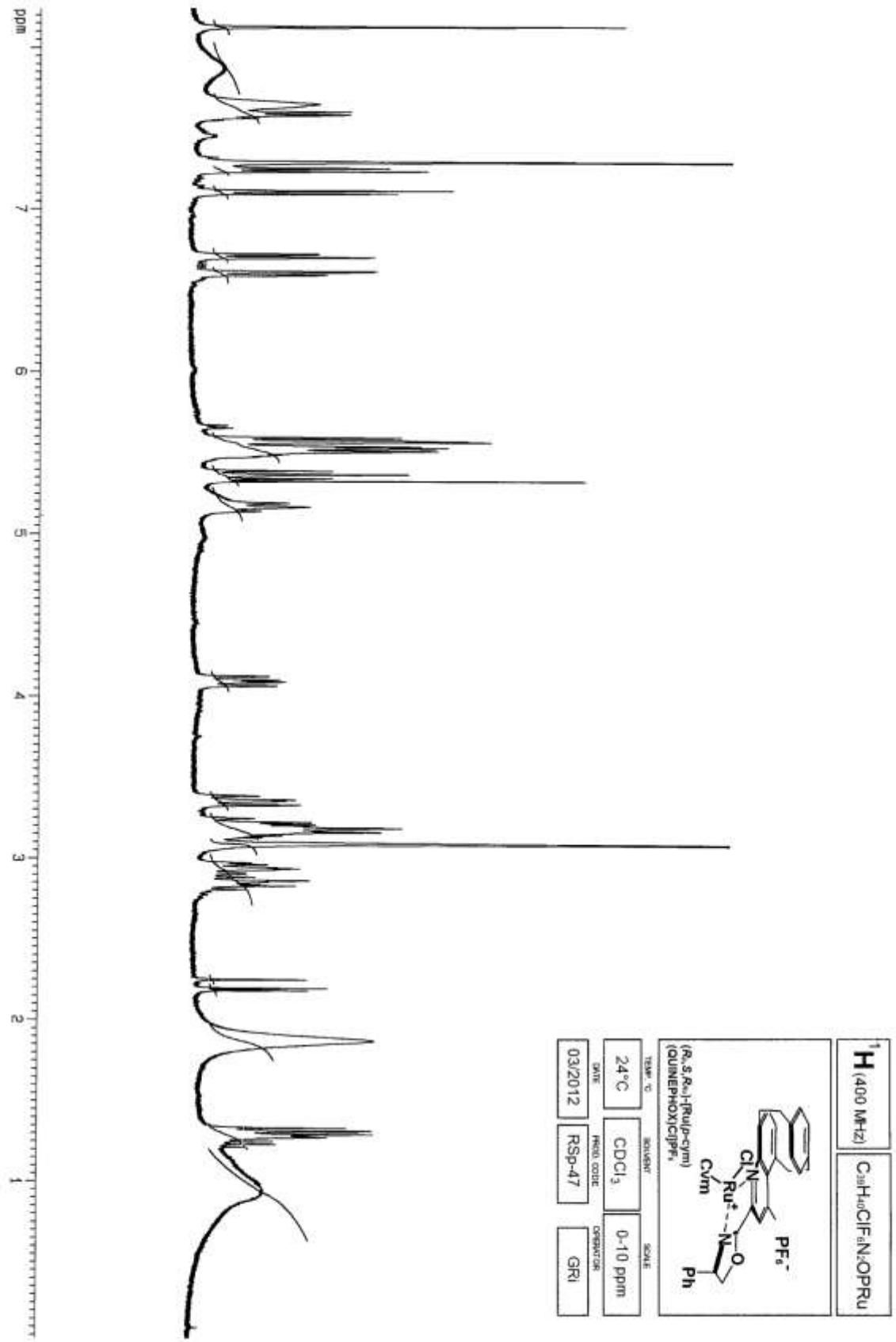



**Figure S2**. A section of the $^{1}$H-NOESY (400.13MHz, 293 K,$CDCl_3$) for complex **7a** showing NOE between aromatic protons H-24 of the phenyl ring and both H-23 and H-22t. No NOE correlation is observed involving either *p*-cymene or $BPh_4$ aromatic protons.


ppm
7
6
5
4
3
2
1
$^1$H (400 MHz)
$C_{38}H_{40}ClF_6N_2OPRu$
PF6-
Cl
Ru
Cym
N
O
Ph
(R,S,RRu)-[(Ru(p-cym)(QUINEPHOX)Cl]PF6
SOLVENT
CDCl3
SCALE
0-10 ppm
TEMP. °C
24°C
DATE
03/2012
PROG. CODE
RSp-47
OPERATOR
GRi

# [($R_p$,$S$,$R_{Ru}$)-[Ru($\eta^6$-*p*-cymene)(QUIPHANEPHOX)Cl]$^+$$PF_6^-$ (7b)

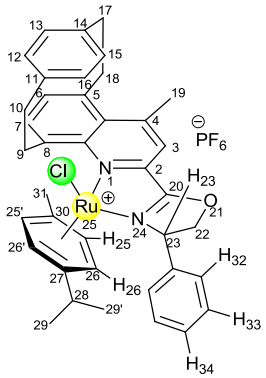
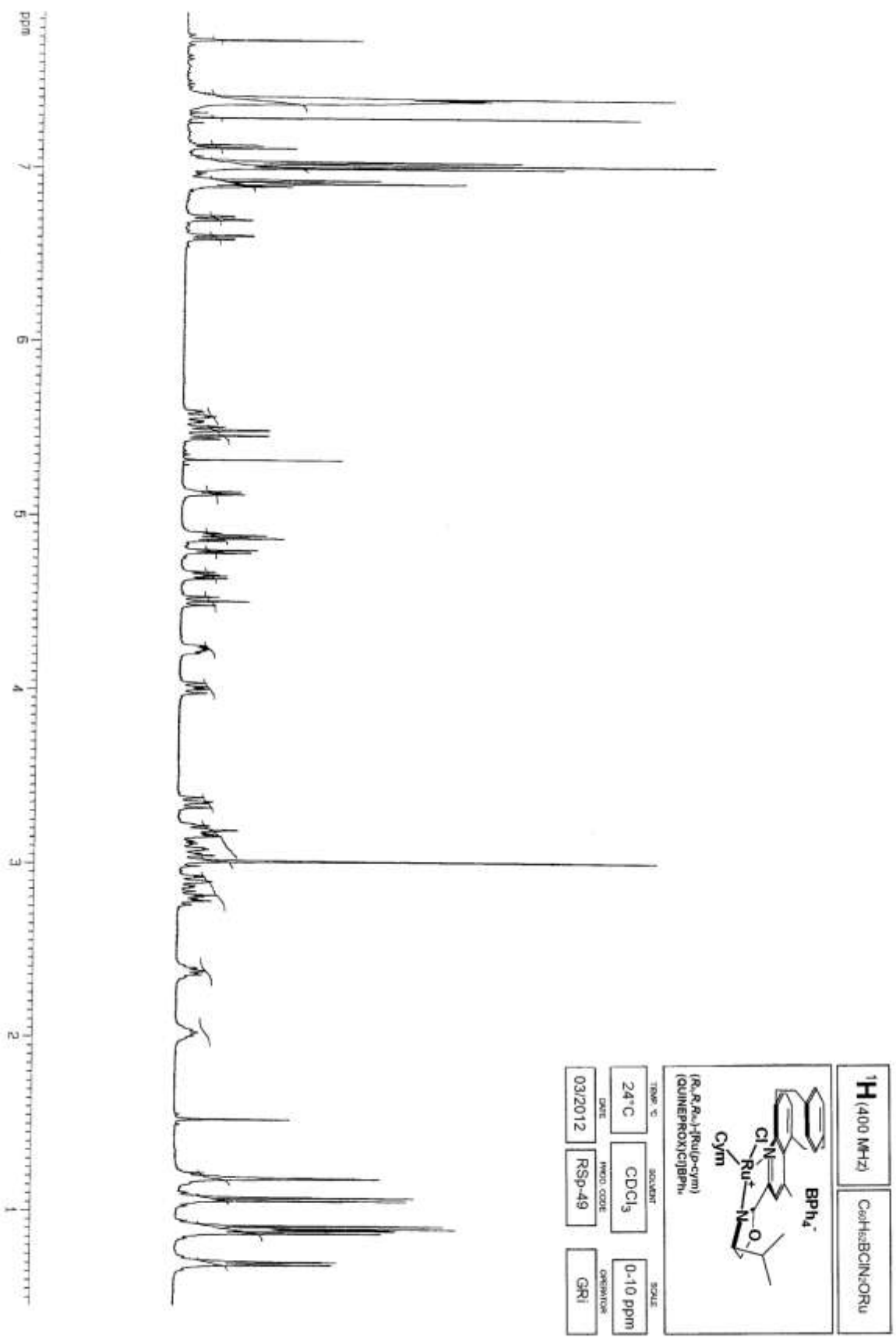



**Table S5.** Chemical shift values assigned to the protons of complex (**$R_p$,$S$,$R_{Ru}$)-7b.**

| | | | |
|---|---|---|---|
| H-3 (*s*) | 8.12 | H-19 (*s*) | 3.09 |
| H-6 ($d_{AB}$) | 7.10 | H-22c (*t*) | 5.36 |
| H-7 ($d_{AB}$) | 7.23 | H-22t (*t*) | 5.16 |
| H-9a (*dt*) | 3.16 | H-23 (*t*) | 5.56 |
| H-9s (*m*) | 5.49 | H-25 (*very broad*) | ~4.9 |
| H-10a (*m*) | 2.93 | H-25’ | ~4.9 |
| H-10s (*m*) | 3.18 | H-26 (*very broad*) | ~5.2 |
| H-12 ($dd_{AB}$) | 6.60 | H-26’ | ~5.2 |
| H-13 ($dd_{AB}$) | 6.71 | H-28 | n.d. |
| H-15 (*dd*) | 5.58 | H-29 (*b*) | 1.0 |
| H-16 (*dd*) | 5.51 | H-29’(*d*) | 1.0 |
| H-17a (*dt*) | 3.36 | H-31 | 1.87 |
| H-17s (*dd*) | 2.84 | H-32 (*very broad*) | 7.8 |
| H-18a (*dd*) | 3.21 | H-33 (*broad*) | 7.6 |
| H-18s (*ddd*) | 4.09 | H-34 (*broad*) | 7.5 |


ppm
1
2
3
4
5
6
7
$^1$H (400 MHz)
$C_{60}H_{52}BClN_2ORu$
$BPh_4^-$
Cl
N
Ru
N
O
Cym
(R,R,R$_{Ru}$)-[Ru(p-cym)(QUINEPROX)Cl]BPh$_4$
TEMP °C
24°C
SOLVENT
$CDCl_3$
SCALE
0-10 ppm
DATE
03/2012
PROG. CODE
RSp-49
OPERATOR
GRI

## [(*R*$_p$,*R*,*R*$_{Ru}$)-[Ru($\eta^6$-*p*-cym)(QUIPHANEPROX)Cl]$^+$BPh$_4$ (8)

$[\alpha]_D^{20}$ = +221 (c = 0.069, $CHCl_3$)

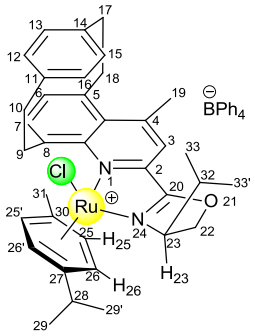



**Table S6.** Chemical shift values assigned to the protons of complex **(*R*$_p$,*R*,*R*$_{Ru}$)-8** in $CDCl_3$.

| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.73 | H-22t (*t*) | 4. 50 |
| H-6 ($d_{AB}$) | 7.02 | H-23 (*ddd*) | 4.22 |
| H-7 ($d_{AB}$) | 7.13 | H-25 (*d*) | 4.79 |
| H-9a (*m*) | 3.06 | H-25’ (*d*) | 4.88 |
| H-9s (*m*) | 5.57 | H-26 (*d*) | 5.12 |
| H-10a (*m*) | 2.90 | H-26’ (*d*) | 4.86 |
| H-10s (*m*) | 3.19 | H-28 (*sept*) | 2.00 |
| H-12 ($dd_{AB}$) | 6.60 | H-29 (*d*) | 069 |
| H-13 ($dd_{AB}$) | 6.71 | H-29’ (*d*) | 0.88 |
| H-15 $(dd)_{AB}$ | 5.50 | H-31 (*s*) | 1.18 |
| H-16 $(dd)_{AB}$ | 5.45 | H-32 (*sept d*) | 2.37 |
| H-17a (*dd*) | 3.34 | H-33 (*d*) | 1.07 |
| H-17s (*dt*) | 2.79 | H-33’ (*d*) | 0.90 |
| H-18a (*m*) | 3.15 | $BPh_4$ *o* (*8 H*) | 7.38 |
| H-18s (*dd*) | 4.00 | $BPh_4$ *m* (*t*, *8 H*) | 7.03 |
| H-19 (*s*) | 3.01 | $BPh_4$ *p* (*t*, *4 H*) | 6.91 |
| H-22c (*dd*) | 4.65 | | |

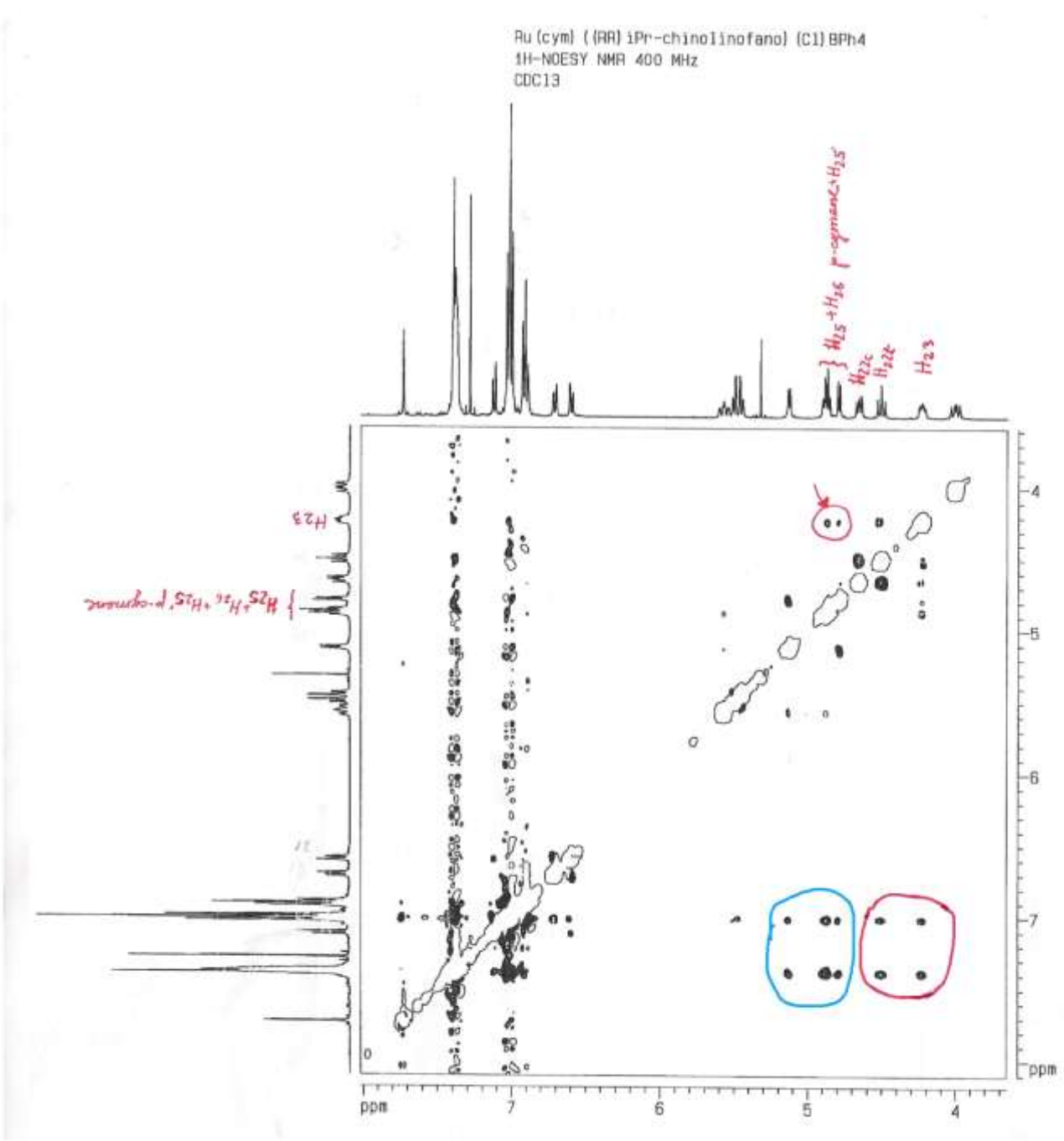
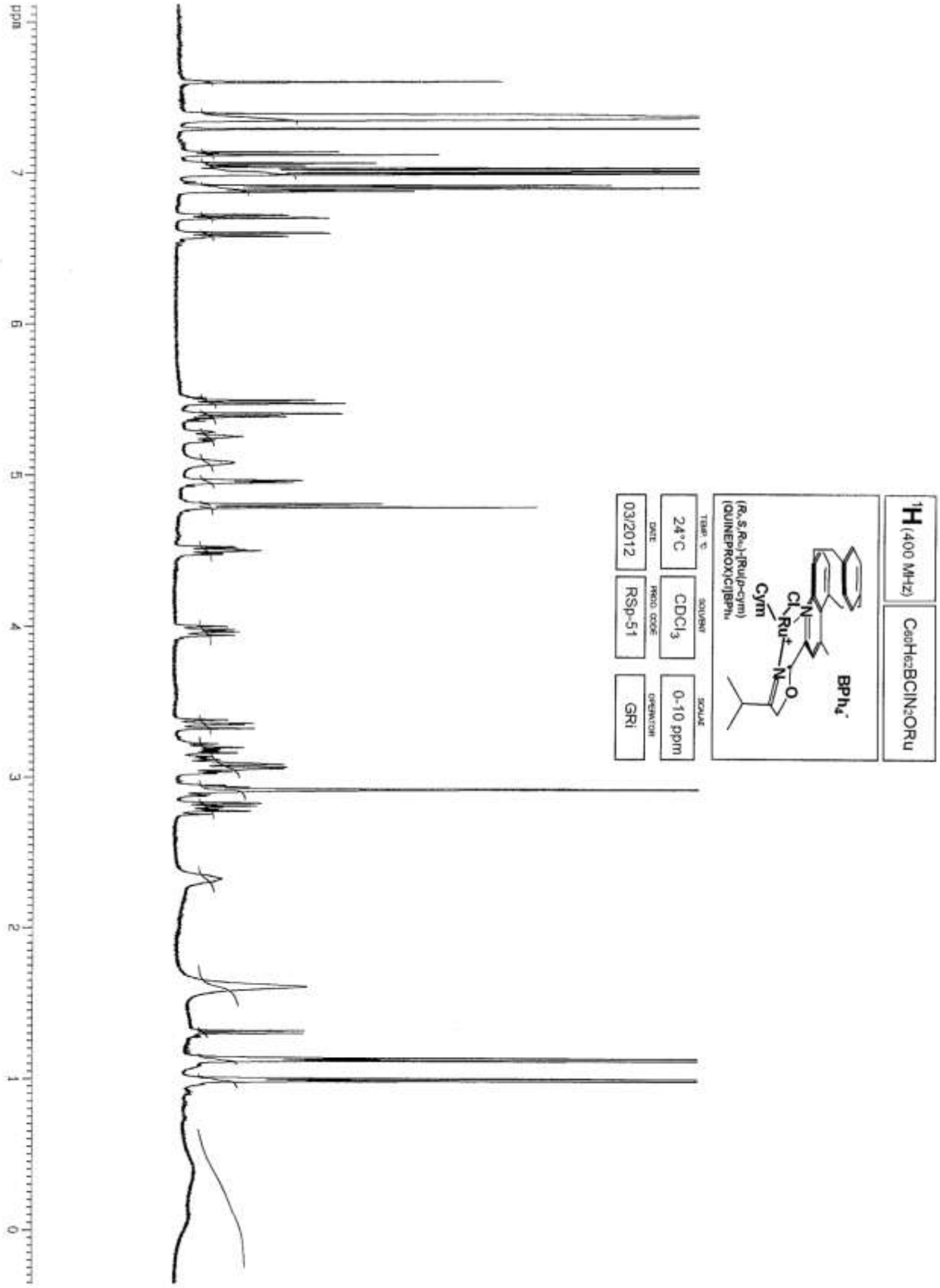



**Figure S3**. The section of the $^{1}$H-NOESY diagram (400.13MHz, 293 K, $CDCl_3$) for complex **($R_p$,R,$R_{Ru}$)-8** showing the NOE correlation between the protons H-23 and the aromatic protons H-27 and H-28 of *p*-cymene ligand. A significant NOE correlation of the aromatic *o*- and *p*-protons of tetraphenylborate anion with H-23, H-22t (red circled) as well as with the aromatic protons of *p*-cymene ligand (bleu circled) is also noticeable.


$^1$H (400 MHz)
$C_{60}H_{62}BClN_2ORu$
Cym
Cl
Ru
N
O
$BPh_4^-$
$(R_a,S,R_{ax})$-[Ru(p-cym)(QUINEPROX)Cl][$BPh_4$]
TEMP. °C
24°C
SOLVENT
$CDCl_3$
SCALE
0-10 ppm
DATE
03/2012
PROG. CODE
RSp-51
OPERATOR
GRi
ppm
0
1
2
3
4
5
6
7

## [($R_p$,$S$,$R_{Ru}$)-[Ru($\eta^6$-p-cymene)(QUIPHANEPROX)Cl]$^+$$BPh_4$ (9)

$[\alpha]_D^{20}$ = +575 (c = 0.105, $CHCl_3$)

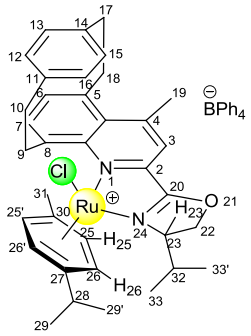



**Table S7.** Chemical shift values assigned to the protons of complex (***R*$_p$,*S*,*R*$_{Ru}$**)-**9**.

| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.59 | H-22c (*dd*) | 4.78 |
| H-6 ($d_{AB}$) | 7.05 | H-23 (*ddd*) | 4.49 |
| H-7 ($d_{AB}$) | 7.12 | H-25 (*broad s*) | 5.07 |
| H-9a (*m*) | 3.08 | H-25’ | n.d. |
| H-9s (*m*) | 5.25 | H-26 (*d*) | 4.95 |
| H-10a (*m*) | 2.92 | H-26’ | n.d. |
| H-10s (*m*) | 3.06 | H-28 (*very broad*) | 1.3? |
| H-12 ($dd_{AB}$) | 6.59 | H-29 (*very broad*) | ~0.1 |
| H-13 ($dd_{AB}$) | 6.70 | H-29’ (*very broad*) | ~0.4 |
| H-15 (*dd*) | 5.48 | H-31 (*broad*) | 1.60 |
| H-16 (*dd*) | 5.39 | H-32 (*broad*) | 2.32 |
| H-17a (*dd*) | 3.35 | H-33 (*d*) | 1.12 |
| H-17s (*dd*) | 2.79 | H-33’ (*d*) | 0.99 |
| H-18a (*dt*) | 3.17 | $BPh_4$ *o* (*8 H*) | 7.01 |
| H-18s (*dd*) | 3.96 | $BPh_4$ *m* (*t, 8 H*) | 7.4 |
| H-19 (*s*) | 2.91 | $BPh_4$ *p* (*t, 4 H*) | 6.90 |
| H-22t (*d*) | 4.79 | | |

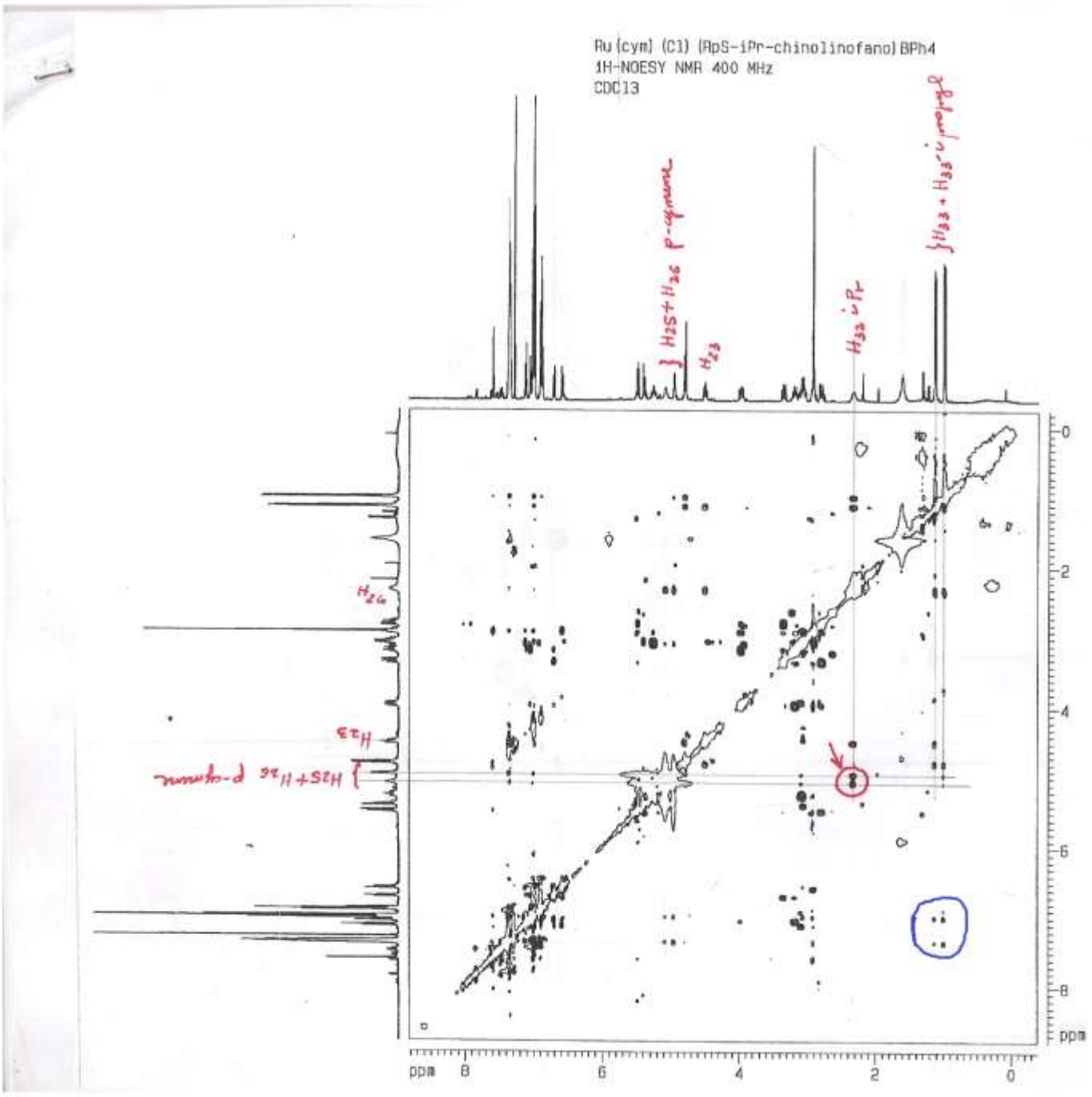
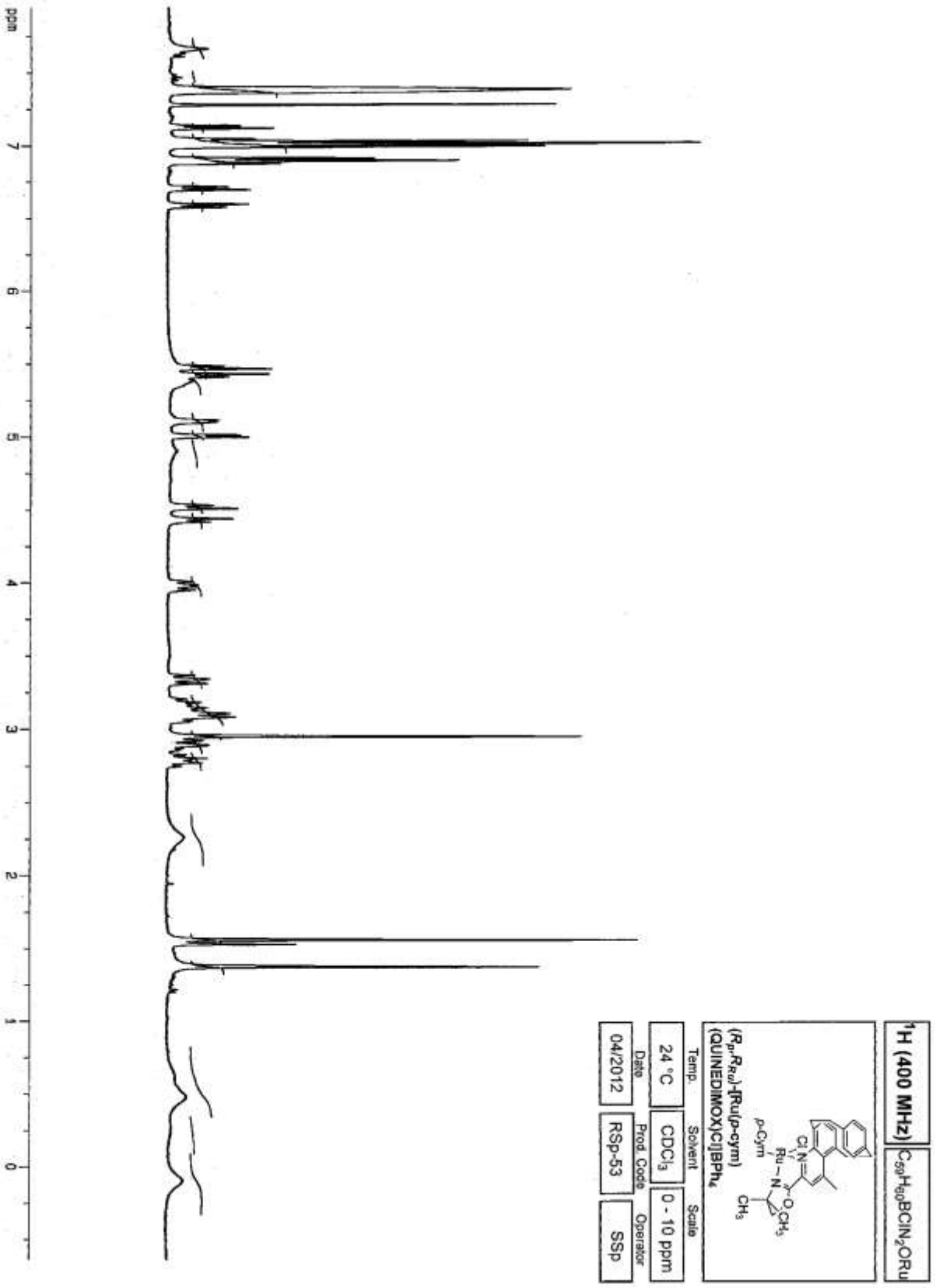



**Figure S4**. The section of the $^{1}$H-NOESY diagram (400.13 MHz, 293 K,$CDCl_3$) of the complex $(R_p,S,R_{Ru})$**-9** showing the NOE correlations between aromatic protons H-27 and H-28 of *p*-cymene and H-24 of the isopropyl group in the oxazoline ring. Significant NOE contacts of the *ortho*- and *para*- aromatic protons of tetraphenylborate anion with H-25, H-26 of the isopropyl group in the oxazoline ring is also noticeable (bleu circled).


ppm
0
1
2
3
4
5
6
7
$^1$H (400 MHz)
$C_{59}H_{60}BClN_2ORu$
$(R_{Ir},R_{Ru})$-[Ru(p-cym)(QUINEDIMOX)Cl]BPh$_4$
Temp.
24 °C
Solvent
$CDCl_3$
Scale
0 - 10 ppm
Date
04/2012
Prod. Code
RSp-53
Operator
SSp

## [($R_p$,$R_{Ru}$)-[Ru($\eta^6$-*p*-cymene)(QUIPHANEDIMOX)Cl]$^+$$BPh_4$ (10)

$[\alpha]_D^{20}$ = +357 (c = 0.0.086, $CHCl_3$)

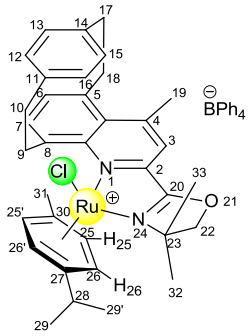



**Table S8.** Chemical shift values assigned to the protons of complex **[($R_p$,$R_{Ru}$)-10.**

| | | | |
|---|---|---|---|
| H-3 (*s*) | 7.66 | H-22c ($d_{AB}$) | 4.51 |
| H-6 ($d_{AB}$) | 7.03 | H-22t ($d_{AB}$) | 4.42 |
| H-7 ($d_{AB}$) | 7.12 | H-25 (*bd*) | 5.10 |
| H-9a (*dt*) | 3.12 | H-25'(*d*) | 5.00 |
| H-9s (*m*) | 5.38 | H-26 (*very broad*) | 5.5 |
| H-10a (*m*) | 2.90 | H-26'(*very broad*) | 4.9 |
| H-10s (*m*) | 3.10 | H-28 (broad) | 2.26 |
| H-12 ($dd_{AB}$) | 6.58 | H-29 (*very broad*) | 0.5 |
| H-13 ($dd_{AB}$) | 6.70 | H-29' (*very broad*) | -0.1? |
| H-15 (*dd*) | 5.47 | H-31 | n.d. |
| H-16 (*dd*) | 5.41 | H-32 (*s*) | 1.58 |
| H-17a (*dd*) | 3.35 | H-33 (*s*) | 1.38 |
| H-17s (*dt*) | 2.80 | $BPh_4$ *o* (*8 H*) | 7.38 |
| H-18a (*dt*) | 3.18 | $BPh_4$ *m* (*t, 8 H*) | 7.00 |
| H-18s (*dd*) | 4.00 | $BPh_4$ *p* (*t, 4 H*) | 6.89 |
| H-19 (*s*) | 2.99 | | |

# Electronic Circular Dichroism Section

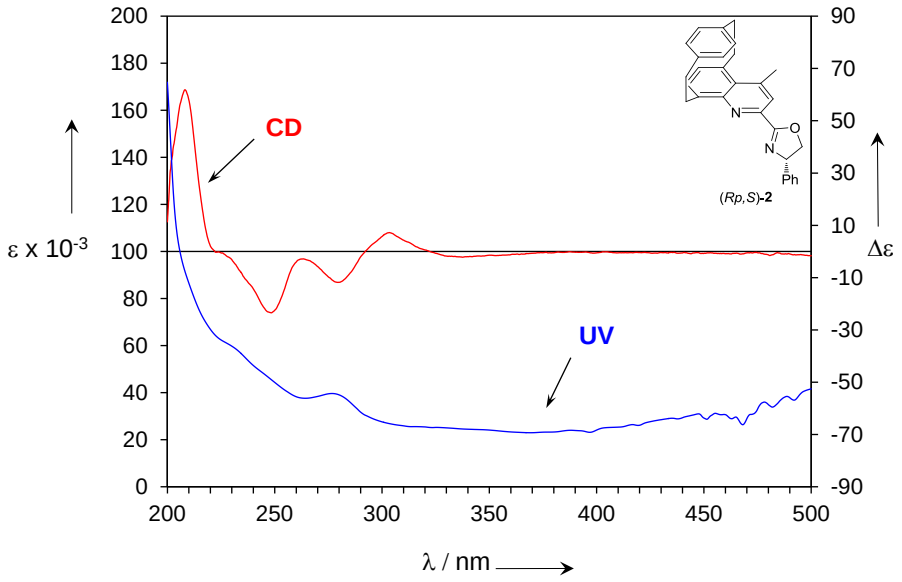



**Figure S5.** ECD spectrum (THF) of ligand ($R_p$,$S$)-**2**.

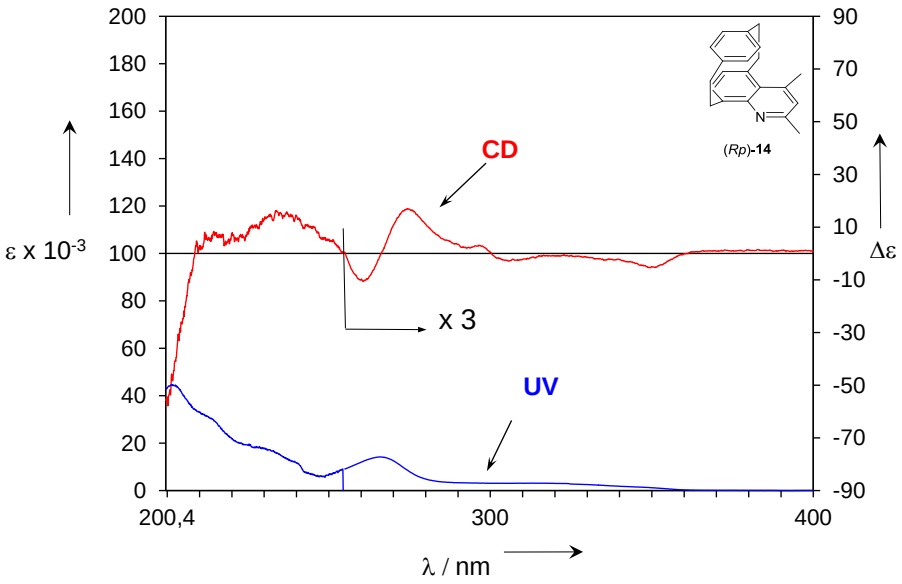



**Figure S6.** ECD spectrum (THF) of compound ($R_p$)-**14**.

Absorption and ECD spectra were recorded at room temperature on a JASCO J815 spectropolarimeter, using 0.1 mm cells and concentrations of about $1 \times 10^{-3}$ M in tetrahydrofurane (THF). During the measurement, the instrument was thoroughly purged with nitrogen.

# Theoretical Section

A preliminary search of the most stable conformations has been performed at the molecular mechanics (MM) level using Spartan02, profiling the strain energy for full rotations in turn of the *p*-cymene isopropyl group and *p*-cymene itself in **6**-**10** and the phenyl and isopropyl moieties at the oxazoline ring in **6-9**. Then, MM conformations have been optimized at the quantum mechanical (QM) density functional theory (DFT) level using the B97-D density functional in combination with the SV(P) basis set, as implemented within Gaussian 09. Solvent effects were not included. Chiroptical properties were calculated for the QM equilibrium geometries at the time-dependent density functional theory (TD-DFT) level, combining the B3LYP density functional with the SV(P) basis set. Rotational strengths were obtained for the first 100 electronic transitions.

A series of Tables follows with optimized QM geometries at B97-D/SV(P) level plus corresponding pictures of the complexes examined in the paper.

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C | 4.313832 | 0.911750 | 0.982575 | H | -2.765852 | 2.131827 | -3.224328 | |
| C | 2.279236 | -1.148668 | 0.950564 | C | -3.090742 | 1.701419 | -1.076895 | |
| C | 3.033360 | 1.195002 | 0.373553 | N | 0.718333 | 0.431421 | -0.059264 | |
| C | 4.392375 | -0.223109 | 1.787561 | N | -1.800609 | 1.076981 | -0.702387 | |
| C | 3.412059 | -1.237039 | 1.751634 | Ru | -1.230238 | -0.498428 | 0.499999 | |
| C | 1.974876 | 0.162284 | 0.421941 | Cl | -1.037179 | -1.743467 | -1.577241 | |
| H | 5.330247 | -0.430865 | 2.316983 | C | -2.111037 | 0.379785 | 2.349799 | |
| H | 3.646641 | -2.199677 | 2.224011 | C | -1.691072 | -2.431521 | 1.686078 | |
| C | 1.682395 | -2.449059 | 0.444869 | C | -0.897574 | -0.291459 | 2.679725 | |
| H | 0.608739 | -2.376502 | 0.255060 | C | -3.112057 | -0.386032 | 1.646550 | |
| H | 1.840062 | -3.214109 | 1.226946 | C | -2.897805 | -1.739754 | 1.281287 | |
| C | 5.653201 | 1.542652 | 0.597625 | C | -0.712255 | -1.688772 | 2.390474 | |
| H | 6.398352 | 1.160720 | 1.317236 | H | -0.072109 | 0.267565 | 3.130476 | |
| H | 5.680921 | 2.638444 | 0.693440 | H | -4.012949 | 0.117618 | 1.282531 | |
| C | 6.151912 | 1.143831 | -0.866746 | H | -3.628074 | -2.247262 | 0.643781 | |
| H | 7.248776 | 1.012823 | -0.814513 | H | 0.241251 | -2.158685 | 2.642122 | |
| H | 5.957451 | 1.979345 | -1.564491 | C | -1.475332 | -3.854973 | 1.263695 | |
| C | 2.329793 | -2.985420 | -0.921296 | H | -0.508624 | -4.244442 | 1.622410 | |
| H | 1.532665 | -2.947938 | -1.683359 | H | -1.498363 | -3.910273 | 0.158024 | |
| H | 2.610384 | -4.043044 | -0.764603 | H | -2.289390 | -4.493364 | 1.657813 | |
| C | 3.517580 | -2.170832 | -1.364845 | C | -2.344111 | 1.843271 | 2.667991 | |
| C | 5.454437 | -0.103140 | -1.362801 | H | -3.129681 | 2.196200 | 1.970733 | |
| C | 4.800350 | -2.391156 | -0.821045 | C | -1.092251 | 2.711172 | 2.452430 | |
| C | 3.310025 | -0.997654 | -2.116521 | H | -1.341568 | 3.778272 | 2.596656 | |
| C | 4.272460 | 0.020726 | -2.119177 | H | -0.683749 | 2.573761 | 1.435714 | |
| C | 5.759506 | -1.368211 | -0.818386 | H | -0.297803 | 2.458075 | 3.179833 | |
| H | 5.008149 | -3.331606 | -0.293050 | C | -2.891972 | 1.976753 | 4.106075 | |
| H | 2.336870 | -0.836991 | -2.598842 | H | -3.128172 | 3.034054 | 4.328760 | |
| H | 4.045880 | 0.978216 | -2.606352 | H | -2.138666 | 1.628316 | 4.838715 | |
| H | 6.706044 | -1.512406 | -0.280074 | H | -3.810587 | 1.376467 | 4.244654 | |
| C | 2.748524 | 2.414162 | -0.333247 | C | -4.206996 | 0.739157 | -1.412313 | |
| C | 1.525949 | 2.521718 | -0.990945 | C | -6.312275 | -1.035128 | -2.011360 | |
| H | 1.277375 | 3.413492 | -1.575188 | C | -5.458637 | 0.879027 | -0.779160 | |
| C | 0.535342 | 1.546281 | -0.799694 | C | -4.018849 | -0.285600 | -2.359929 | |
| C | 3.660497 | 3.616870 | -0.381425 | C | -5.066937 | -1.172470 | -2.651343 | |
| H | 4.564989 | 3.424243 | -0.985545 | C | -6.510293 | -0.003950 | -1.076577 | |
| H | 3.991827 | 3.902346 | 0.632704 | H | -5.610032 | 1.687132 | -0.049753 | |
| H | 3.135273 | 4.477554 | -0.830081 | H | -3.043789 | -0.414035 | -2.841208 | |
| C | -0.840562 | 1.784325 | -1.214989 | H | -4.908039 | -1.976854 | -3.380053 | |
| O | -1.188925 | 2.788163 | -2.021311 | H | -7.481979 | 0.114532 | -0.581488 | |
| C | -2.631884 | 2.621242 | -2.241918 | H | -7.129585 | -1.728912 | -2.244620 | |
| H | -3.097137 | 3.619237 | -2.239634 | H | -3.406338 | 2.317523 | -0.209102 | |

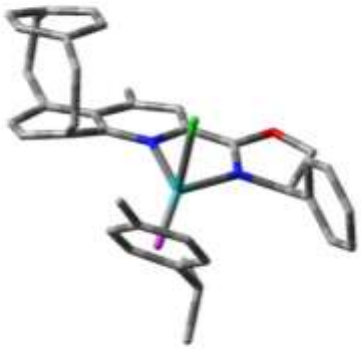


**Table S9**. Structure and Cartesian coordinates of ($R_p$,*R*,$R_M$)-**6a**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -4.321705 | 1.260018 | 0.566122 | H | 2.552877 | -3.181313 | 2.945357 |
| C | -2.263754 | 0.729756 | -1.372055 | C | 2.868000 | -1.264824 | 1.829284 |
| C | -3.112966 | 0.593842 | 0.993055 | N | -0.848067 | -0.175459 | 0.345049 |
| C | -4.304238 | 1.873783 | -0.687524 | N | 1.629024 | -0.736692 | 1.232648 |
| C | -3.311778 | 1.592327 | -1.653831 | Ru | 1.297410 | 0.700025 | -0.221950 |
| C | -2.045171 | 0.391006 | 0.007464 | Cl | 0.575624 | 2.113131 | 1.627361 |
| H | -5.189452 | 2.437652 | -1.006595 | C | 2.820647 | 2.270213 | -0.627270 |
| H | -3.478406 | 1.917305 | -2.688880 | C | 1.855637 | 0.239231 | -2.465461 |
| C | -1.597060 | -0.066782 | -2.464667 | C | 1.684583 | 2.526924 | -1.481913 |
| H | -0.604863 | -0.376646 | -2.118990 | C | 3.421650 | 0.978722 | -0.693877 |
| H | -1.475384 | 0.563968 | -3.363373 | C | 2.950832 | -0.021640 | -1.604689 |
| C | -5.699424 | 1.089665 | 1.203035 | C | 1.201338 | 1.524189 | -2.351079 |
| H | -6.375599 | 1.800296 | 0.696227 | H | 1.145831 | 3.474095 | -1.381787 |
| H | -5.736501 | 1.349234 | 2.271853 | H | 4.234122 | 0.729929 | -0.009017 |
| C | -6.312146 | -0.375905 | 1.014793 | H | 3.422558 | -1.008231 | -1.613729 |
| H | -7.396115 | -0.257525 | 0.830588 | H | 0.302986 | 1.719469 | -2.941531 |
| H | -6.203354 | -0.945590 | 1.956126 | C | 1.461543 | -0.791370 | -3.491981 |
| C | -2.398860 | -1.393923 | -2.897196 | H | 0.522371 | -0.534580 | -4.004942 |
| H | -1.705408 | -2.249677 | -2.799781 | H | 1.361834 | -1.791735 | -3.032519 |
| H | -2.662730 | -1.299991 | -3.966277 | H | 2.262319 | -0.856433 | -4.255263 |
| C | -3.641554 | -1.6212Ru | -2.069656 | C | 3.348786 | 3.359597 | 0.279909 |
| C | -5.627775 | -1.121693 | -0.109810 | H | 2.470232 | 3.948432 | 0.600804 |
| C | -4.859130 | -1.002322 | -2.422929 | C | 4.282323 | 4.265995 | -0.557071 |
| C | -3.547803 | -2.206553 | -0.791842 | H | 5.168697 | 3.699884 | -0.903808 |
| C | -4.532673 | -1.961399 | 0.174878 | H | 4.632736 | 5.112733 | 0.061952 |
| C | -5.842198 | -0.755390 | -1.454622 | H | 3.764885 | 4.675855 | -1.444957 |
| H | -4.984863 | -0.600080 | -3.437043 | C | 4.047642 | 2.835171 | 1.543055 |
| H | -2.636827 | -2.752210 | -0.511578 | H | 4.321055 | 3.684891 | 2.194130 |
| H | -4.382502 | -2.318467 | 1.201942 | H | 4.983657 | 2.295114 | 1.298075 |
| H | -6.725318 | -0.158516 | -1.718838 | H | 3.367542 | 2.171431 | 2.106445 |
| C | -2.909691 | 0.042933 | 2.305938 | H | 3.467411 | -0.411257 | 2.196207 |
| C | -1.754159 | -0.700359 | 2.533640 | C | 3.679381 | -2.057270 | 0.821818 |
| H | -1.562593 | -1.151576 | 3.512479 | C | 5.144992 | -3.465005 | -1.132089 |
| C | -0.737037 | -0.734670 | 1.563778 | C | 5.041143 | -1.773837 | 0.615647 |
| C | -3.834864 | 0.260552 | 3.478276 | C | 3.058683 | -3.067305 | 0.058435 |
| H | -4.791261 | -0.278667 | 3.354151 | C | 3.786547 | -3.766939 | -0.915977 |
| H | -4.069458 | 1.333254 | 3.597519 | C | 5.773586 | -2.472897 | -0.360203 |
| H | -3.364883 | -0.097830 | 4.410288 | H | 5.528947 | -0.995010 | 1.217435 |
| C | 0.609262 | -1.173506 | 1.909114 | H | 1.994616 | -3.289052 | 0.213126 |
| O | 0.857597 | -1.970366 | 2.945815 | H | 3.296510 | -4.548467 | -1.510030 |
| C | 2.311938 | -2.107816 | 3.029839 | H | 6.834514 | -2.242748 | -0.517491 |
| H | 2.629562 | -1.722477 | 4.013679 | H | 5.713979 | -4.009461 | -1.895722 |

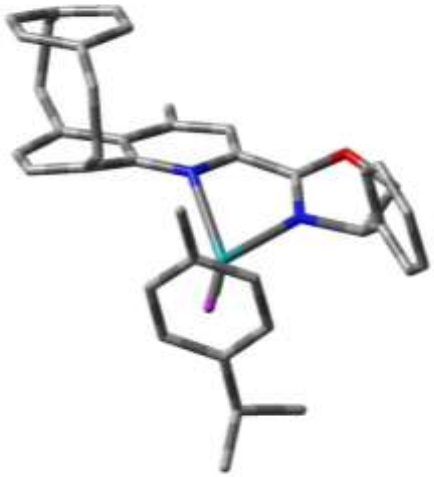


**Table S10**. Structure and Cartesian coordinates of ($R_p$,*R*,$S_M$)-**6a**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.056475 | 0.416280 | 1.397786 | H | -2.729669 | 3.379896 | -2.879756 |
| C | 2.194526 | -1.462803 | 0.230013 | C | -3.007867 | 1.592955 | -1.551366 |
| C | 2.829283 | 0.910974 | 0.814706 | H | -3.043973 | 1.004389 | -2.488113 |
| C | 4.131907 | -0.954357 | 1.643434 | C | -4.290613 | 1.397503 | -0.774931 |
| C | 3.240760 | -1.873766 | 1.046368 | C | -6.612429 | 0.892476 | 0.741272 |
| C | 1.856242 | -0.061656 | 0.288558 | C | -5.315789 | 0.588238 | -1.297066 |
| H | 5.024084 | -1.351446 | 2.143248 | C | -4.441068 | 1.967302 | 0.505790 |
| H | 3.496001 | -2.940728 | 1.079548 | C | -5.594564 | 1.713744 | 1.263393 |
| C | 1.716315 | -2.402556 | -0.860220 | C | -6.475177 | 0.336346 | -0.542345 |
| H | 0.628802 | -2.381223 | -1.005908 | H | -5.193872 | 0.140617 | -2.291675 |
| H | 1.997324 | -3.428128 | -0.557464 | H | -3.640133 | 2.593764 | 0.920541 |
| C | 5.376899 | 1.181085 | 1.473466 | H | -5.703944 | 2.155459 | 2.261754 |
| H | 6.080484 | 0.543303 | 2.036513 | H | -7.270129 | -0.296735 | -0.955498 |
| H | 5.318149 | 2.127142 | 2.032694 | H | -7.514532 | 0.693918 | 1.332959 |
| C | 6.029561 | 1.476481 | 0.041306 | N | 0.639743 | 0.350749 | -0.187924 |
| H | 7.118648 | 1.312389 | 0.140178 | N | -1.828146 | 1.112004 | -0.808468 |
| H | 5.884251 | 2.542049 | -0.215882 | Ru | -1.291159 | -0.757903 | -0.095190 |
| C | 2.357577 | -2.092381 | -2.291795 | Cl | -1.194882 | -1.216375 | -2.474614 |
| H | 1.573417 | -1.616108 | -2.904706 | C | -1.012686 | -1.132924 | 2.103521 |
| H | 2.607436 | -3.065580 | -2.753824 | C | -2.857448 | -2.356128 | 0.215296 |
| C | 3.566772 | -1.191688 | -2.200712 | C | -0.665442 | -2.340206 | 1.386811 |
| C | 5.425633 | 0.608312 | -1.040673 | C | -2.306552 | -0.582754 | 1.884223 |
| C | 4.788979 | -1.662563 | -1.674382 | C | -3.215879 | -1.193754 | 0.952492 |
| C | 3.415141 | 0.199106 | -2.365127 | C | -1.548167 | -2.925618 | 0.454888 |
| C | 4.339465 | 1.088455 | -1.797382 | H | 0.344837 | -2.742247 | 1.502542 |
| C | 5.704723 | -0.774125 | -1.095203 | H | -2.592760 | 0.357579 | 2.362400 |
| H | 4.964987 | -2.744391 | -1.603213 | H | -4.178626 | -0.716458 | 0.755326 |
| H | 2.500451 | 0.585438 | -2.833854 | H | -1.215325 | -3.772718 | -0.153266 |
| H | 4.142179 | 2.168073 | -1.829338 | C | -3.766110 | -2.948843 | -0.821793 |
| H | 6.586410 | -1.168379 | -0.571961 | H | -3.214978 | -3.075266 | -1.772095 |
| C | 2.523489 | 2.308256 | 0.664808 | H | -4.639628 | -2.298542 | -0.997493 |
| C | 1.370887 | 2.657984 | -0.035611 | H | -4.124317 | -3.942424 | -0.486804 |
| H | 1.116436 | 3.707618 | -0.215602 | C | -0.010202 | -0.531207 | 3.065899 |
| C | 0.447075 | 1.669368 | -0.404826 | H | 0.993007 | -0.775094 | 2.670099 |
| C | 3.342494 | 3.433100 | 1.249074 | C | -0.157834 | -1.231217 | 4.437158 |
| H | 4.314404 | 3.540169 | 0.735017 | H | 0.612229 | -0.857014 | 5.137311 |
| H | 3.550615 | 3.256538 | 2.319312 | H | -0.041282 | -2.327442 | 4.345822 |
| H | 2.803748 | 4.391325 | 1.152081 | H | -1.154320 | -1.024900 | 4.872791 |
| C | -0.881059 | 1.990717 | -0.912390 | C | -0.115421 | 0.995128 | 3.200445 |
| O | -1.175897 | 3.146402 | -1.503496 | H | 0.712614 | 1.371997 | 3.827711 |
| C | -2.607907 | 3.077724 | -1.827324 | H | -1.062366 | 1.292811 | 3.690340 |
| H | -3.133778 | 3.787207 | -1.163173 | H | -0.058823 | 1.490828 | 2.215585 |

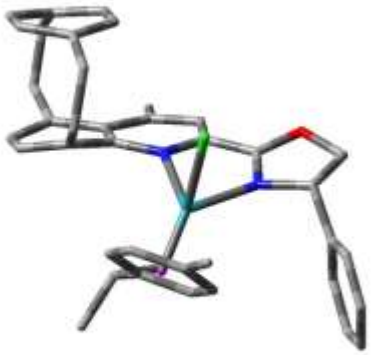


**Table S11**. Structure and Cartesian coordinates of ($R_p$,*S*,$R_M$)-**7a**.

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C | -4.186411 | -0.783590 | 1.298569 | H | 2.750264 | -2.793737 | -3.389095 | |
| C | -2.345999 | 1.320735 | 0.591984 | C | 2.923690 | -1.279125 | -1.739513 | |
| C | -2.959862 | -1.126231 | 0.616424 | H | 3.068058 | -0.542462 | -2.554558 | |
| C | -4.279629 | 0.501884 | 1.836112 | C | 4.170876 | -1.319702 | -0.886623 | |
| C | -3.400618 | 1.546507 | 1.464646 | C | 6.477920 | -1.317386 | 0.729067 | |
| C | -2.002535 | -0.053028 | 0.338262 | C | 5.362879 | -0.733212 | -1.352772 | |
| H | -5.178922 | 0.766128 | 2.405567 | C | 4.142297 | -1.927112 | 0.384892 | |
| H | -3.678831 | 2.577250 | 1.719994 | C | 5.291551 | -1.918896 | 1.190188 | |
| C | -1.841975 | 2.423009 | -0.322759 | C | 6.515343 | -0.730568 | -0.547749 | |
| H | -0.940264 | 2.063741 | -0.837250 | H | 5.386827 | -0.267383 | -2.347133 | |
| H | -1.568514 | 3.324207 | 0.255287 | H | 3.208680 | -2.357093 | 0.765800 | |
| C | -5.495390 | -1.567437 | 1.212796 | H | 5.259314 | -2.380648 | 2.185042 | |
| H | -6.202205 | -1.088054 | 1.912739 | H | 7.439706 | -0.269051 | -0.916331 | |
| H | -5.411758 | -2.615647 | 1.539005 | H | 7.373865 | -1.310886 | 1.362172 | |
| C | -6.161397 | -1.536387 | -0.237911 | N | -0.790821 | -0.317574 | -0.237839 | |
| H | -7.258146 | -1.524502 | -0.095859 | N | 1.698258 | -0.893846 | -1.002697 | |
| H | -5.913272 | -2.466805 | -0.781443 | Ru | 1.221792 | 0.395418 | 0.582609 | |
| C | -2.905206 | 2.881904 | -1.430938 | Cl | 0.899349 | -1.644782 | 1.906654 | |
| H | -2.343558 | 3.049799 | -2.369626 | C | 2.548372 | 2.070272 | -0.094960 | |
| H | -3.335238 | 3.853530 | -1.127297 | C | 1.402891 | 1.555145 | 2.536918 | |
| C | -4.015692 | 1.875059 | -1.620600 | C | 3.247559 | 1.262383 | 0.874317 | |
| C | -5.677867 | -0.342936 | -1.031551 | C | 1.301342 | 2.633519 | 0.291515 | |
| C | -5.258508 | 2.057755 | -0.980360 | C | 0.735672 | 2.365530 | 1.585471 | |
| C | -3.742201 | 0.611365 | -2.179708 | C | 2.674930 | 0.989717 | 2.141511 | |
| C | -4.566445 | -0.483433 | -1.887637 | H | 4.183347 | 0.773548 | 0.592968 | |
| C | -6.086509 | 0.962627 | -0.693806 | H | 0.739712 | 3.232144 | -0.427352 | |
| H | -5.523088 | 3.052123 | -0.596489 | H | -0.264821 | 2.733859 | 1.825754 | |
| H | -2.810439 | 0.453945 | -2.739721 | H | 3.162645 | 0.265855 | 2.801407 | |
| H | -4.267974 | -1.486672 | -2.218298 | C | 0.797416 | 1.218491 | 3.867369 | |
| H | -6.987102 | 1.108967 | -0.082521 | H | 0.888430 | 0.133164 | 4.054568 | |
| C | -2.645253 | -2.437555 | 0.111073 | H | -0.270057 | 1.498115 | 3.899653 | |
| C | -1.518285 | -2.580351 | -0.697182 | H | 1.330832 | 1.761935 | 4.672679 | |
| H | -1.261507 | -3.548744 | -1.138422 | C | 3.133529 | 2.290979 | -1.474907 | |
| C | -0.598420 | -1.524636 | -0.802889 | H | 3.861704 | 1.475050 | -1.636504 | |
| C | -3.425934 | -3.686236 | 0.440214 | C | 3.907725 | 3.627427 | -1.498845 | |
| H | -4.414983 | -3.699078 | -0.051787 | H | 4.388485 | 3.771427 | -2.484489 | |
| H | -3.594509 | -3.762941 | 1.529100 | H | 4.693439 | 3.650273 | -0.720750 | |
| H | -2.873947 | -4.582844 | 0.109875 | H | 3.220644 | 4.477383 | -1.321791 | |
| C | 0.743211 | -1.708825 | -1.346231 | C | 2.072394 | 2.222260 | -2.586798 | |
| O | 1.046309 | -2.697797 | -2.182627 | H | 2.559455 | 2.245131 | -3.578973 | |
| C | 2.505283 | -2.664945 | -2.322863 | H | 1.383092 | 3.087164 | -2.541543 | |
| H | 2.915105 | -3.501909 | -1.728495 | H | 1.470753 | 1.299057 | -2.497407 | |

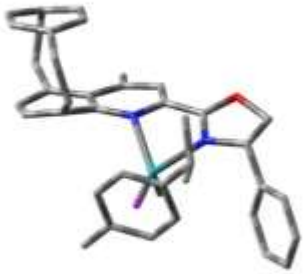


**Table S12**. Structure and Cartesian coordinates of ($R_p$,*S*,$S_M$)-**7a**.

| | | | |
|---|---|---|---|
| C | -3.869515 | -0.566480 | 1.442194 |
| C | -1.972442 | 1.418143 | 0.526299 |
| C | -2.596982 | -1.000628 | 0.910653 |
| C | -3.985733 | 0.780923 | 1.776608 |
| C | -3.070130 | 1.749625 | 1.312422 |
| C | -1.610673 | 0.018912 | 0.494801 |
| H | -4.913630 | 1.130820 | 2.245449 |
| H | -3.341110 | 2.808388 | 1.415158 |
| C | -1.473638 | 2.462077 | -0.453468 |
| H | -0.394379 | 2.406809 | -0.624647 |
| H | -1.696955 | 3.454856 | -0.022228 |
| C | -5.178080 | -1.355106 | 1.385427 |
| H | -5.930437 | -0.755555 | 1.927291 |
| H | -5.145891 | -2.327573 | 1.899956 |
| C | -5.721977 | -1.582578 | -0.098858 |
| H | -6.824472 | -1.504867 | -0.057362 |
| H | -5.481381 | -2.610361 | -0.428317 |
| C | -2.153434 | 2.375651 | -1.903076 |
| H | -1.364327 | 2.063275 | -2.608036 |
| H | -2.476291 | 3.396592 | -2.177712 |
| C | -3.308805 | 1.407409 | -1.947712 |
| C | -5.117851 | -0.587757 | -1.065040 |
| C | -4.581105 | 1.761873 | -1.451265 |
| C | -3.062825 | 0.047884 | -2.222342 |
| C | -3.961029 | -0.937367 | -1.789220 |
| C | -5.476467 | 0.775798 | -1.013972 |
| H | -4.823712 | 2.821917 | -1.296785 |
| H | -2.101280 | -0.241844 | -2.666383 |
| H | -3.696882 | -1.997505 | -1.899905 |
| H | -6.408295 | 1.072030 | -0.513330 |
| C | -2.252350 | -2.383530 | 0.727568 |
| C | -1.044080 | -2.682285 | 0.103538 |
| H | -0.746559 | -3.719521 | -0.080693 |
| C | -0.125879 | -1.661048 | -0.183667 |
| C | -3.080520 | -3.548385 | 1.214491 |
| H | -4.010643 | -3.663325 | 0.629918 |
| H | -3.367220 | -3.414786 | 2.272546 |
| H | -2.509699 | -4.488555 | 1.124272 |
| C | 1.245784 | -1.969514 | -0.567599 |
| O | 1.641689 | -3.195888 | -0.905554 |
| C | 3.107951 | -3.139903 | -0.965488 |
| H | 3.490403 | -3.684518 | -0.083104 |
| H | 3.426963 | -3.646775 | -1.889807 |
| C | 3.443271 | -1.617967 | -0.939641 |
| N | -0.365688 | -0.352189 | 0.054315 |
| N | 2.158327 | -1.051316 | -0.500498 |
| Ru | 1.543531 | 0.806689 | 0.168437 |
| Cl | 1.345918 | 1.396042 | -2.171794 |
| C | 2.507896 | 0.530529 | 2.157937 |
| C | 1.889616 | 3.017271 | 0.752978 |
| C | 1.261258 | 1.197581 | 2.333353 |
| C | 3.442420 | 1.125922 | 1.229297 |
| C | 3.135451 | 2.315001 | 0.519274 |
| C | 0.973408 | 2.440269 | 1.664225 |
| H | 0.481362 | 0.738998 | 2.947642 |
| H | 4.371605 | 0.592648 | 0.999216 |
| H | 3.820987 | 2.680823 | -0.251286 |
| H | -0.010399 | 2.897133 | 1.797955 |
| C | 1.575358 | 4.253273 | -0.036869 |
| H | 0.575503 | 4.647363 | 0.207661 |
| H | 1.615671 | 4.014696 | -1.117060 |
| H | 2.330670 | 5.035637 | 0.171422 |
| C | 2.850662 | -0.776069 | 2.843864 |
| H | 3.515602 | -1.327261 | 2.148723 |
| C | 1.620440 | -1.655057 | 3.121833 |
| H | 1.938829 | -2.642426 | 3.502557 |
| H | 1.020834 | -1.802047 | 2.206189 |
| H | 0.968808 | -1.199647 | 3.891651 |
| C | 3.648022 | -0.486071 | 4.135293 |
| H | 3.961927 | -1.433589 | 4.611524 |
| H | 3.021477 | 0.073549 | 4.856099 |
| H | 4.552632 | 0.115282 | 3.926075 |
| H | 4.206230 | -1.401661 | -0.168669 |
| C | 3.918252 | -1.024650 | -2.288156 |
| H | 3.872112 | 0.073642 | -2.160799 |
| C | 5.372833 | -1.447568 | -2.551219 |
| H | 5.457339 | -2.548220 | -2.653730 |
| H | 6.046647 | -1.128120 | -1.732032 |
| H | 5.739200 | -0.999429 | -3.492785 |
| C | 2.993163 | -1.400389 | -3.455566 |
| H | 1.946159 | -1.125145 | -3.241322 |
| H | 3.051064 | -2.481816 | -3.688502 |
| H | 3.299961 | -0.850026 | -4.363203 |

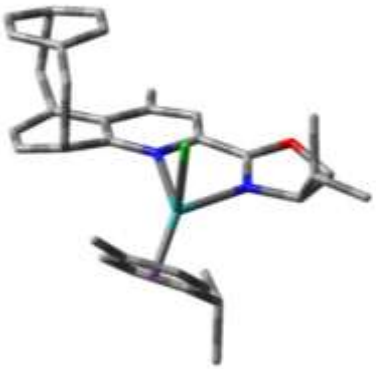


**Table S13**. Structure and Cartesian coordinates of ($R_p$,$R$,$R_M$)-**8**.

| | | | |
|---|---|---|---|
| C | -3.888730 | -0.350175 | -1.631005 |
| C | -2.035036 | -1.539233 | 0.219917 |
| C | -2.724139 | 0.402073 | -1.224698 |
| C | -3.901921 | -1.715043 | -1.338939 |
| C | -3.013236 | -2.296846 | -0.406413 |
| C | -1.753411 | -0.243987 | -0.334689 |
| H | -4.748688 | -2.317625 | -1.689996 |
| H | -3.222930 | -3.311392 | -0.043728 |
| C | -1.535478 | -1.902280 | 1.595741 |
| H | -0.568392 | -1.414228 | 1.760026 |
| H | -1.393296 | -2.995319 | 1.665504 |
| C | -5.226216 | 0.252377 | -2.057899 |
| H | -5.865570 | -0.586453 | -2.384643 |
| H | -5.156128 | 0.931160 | -2.921349 |
| C | -5.990426 | 1.010610 | -0.875665 |
| H | -7.069478 | 0.798456 | -0.991744 |
| H | -5.859338 | 2.102426 | -0.990770 |
| C | -2.515505 | -1.459335 | 2.793538 |
| H | -1.916617 | -0.870333 | 3.512727 |
| H | -2.854974 | -2.373272 | 3.313940 |
| C | -3.704457 | -0.663008 | 2.311836 |
| C | -5.472630 | 0.580873 | 0.479306 |
| C | -4.881334 | -1.317882 | 1.892669 |
| C | -3.564611 | 0.703554 | 2.000315 |
| C | -4.442177 | 1.317708 | 1.096526 |
| C | -5.757735 | -0.703097 | 0.987441 |
| H | -5.048932 | -2.363440 | 2.183935 |
| H | -2.689966 | 1.256444 | 2.368469 |
| H | -4.244626 | 2.345157 | 0.764550 |
| H | -6.598993 | -1.274797 | 0.573329 |
| C | -2.487929 | 1.778788 | -1.567793 |
| C | -1.406381 | 2.425580 | -0.975618 |
| H | -1.196914 | 3.477862 | -1.192148 |
| C | -0.463931 | 1.688637 | -0.237125 |
| C | -3.296134 | 2.561976 | -2.573372 |
| H | -4.310990 | 2.789588 | -2.200433 |
| H | -3.405820 | 1.992997 | -3.513710 |
| H | -2.799019 | 3.520050 | -2.803081 |
| C | 0.854074 | 2.244218 | 0.045847 |
| O | 1.083423 | 3.553194 | 0.010063 |
| C | 2.525920 | 3.727654 | 0.165273 |
| H | 2.903856 | 4.217426 | -0.748167 |
| H | 2.686607 | 4.386656 | 1.035077 |
| C | 3.088206 | 2.284065 | 0.375136 |
| N | -0.596798 | 0.380022 | 0.044795 |
| N | 1.871566 | 1.461689 | 0.252089 |
| Ru | 1.558842 | -0.573194 | -0.066781 |
| Cl | 1.133986 | 0.075422 | -2.376330 |
| C | 3.182106 | -1.851158 | -0.899216 |
| C | 1.888167 | -2.127650 | 1.686637 |
| C | 2.001974 | -2.669838 | -0.745173 |
| C | 3.652751 | -1.143214 | 0.245029 |
| C | 3.014919 | -1.284398 | 1.521606 |
| C | 1.359269 | -2.775671 | 0.508054 |
| H | 1.560556 | -3.137742 | -1.630344 |
| H | 4.494893 | -0.455938 | 0.133768 |
| H | 3.383603 | -0.720296 | 2.383975 |
| H | 0.435746 | -3.354177 | 0.585486 |
| C | 1.334737 | -2.361460 | 3.069450 |
| H | 0.423591 | -2.977923 | 3.054276 |
| H | 1.112552 | -1.407859 | 3.583182 |
| H | 2.098518 | -2.891631 | 3.671966 |
| C | 3.882707 | -1.782831 | -2.238361 |
| H | 3.091656 | -1.860640 | -3.006413 |
| C | 4.813184 | -3.014666 | -2.348786 |
| H | 5.292949 | -3.030810 | -3.344984 |
| H | 4.255362 | -3.961048 | -2.216992 |
| H | 5.609845 | -2.972755 | -1.580837 |
| C | 4.644190 | -0.471851 | -2.481686 |
| H | 5.051359 | -0.467512 | -3.508745 |
| H | 5.502018 | -0.361778 | -1.789167 |
| H | 3.962507 | 0.390999 | -2.375512 |
| H | 3.771052 | 2.009728 | -0.451647 |
| C | 3.833794 | 2.086778 | 1.717730 |
| H | 4.242703 | 1.061576 | 1.694465 |
| C | 5.032847 | 3.046625 | 1.809469 |
| H | 4.704705 | 4.101886 | 1.876677 |
| H | 5.697075 | 2.948789 | 0.928941 |
| H | 5.628534 | 2.829401 | 2.714849 |
| C | 2.890935 | 2.204460 | 2.923584 |
| H | 2.071901 | 1.463590 | 2.856178 |
| H | 2.436683 | 3.213020 | 2.982703 |
| H | 3.444669 | 2.036452 | 3.865702 |

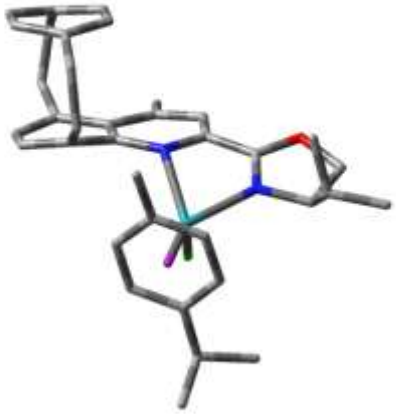


**Table S14**. Structure and Cartesian coordinates of ($R_p$,*R*,$S_M$)-**8**.

| | | | |
|---|---|---|---|
| C | 3.721143 | 0.595291 | 1.385048 |
| C | 1.917716 | -1.425107 | 0.371520 |
| C | 2.472585 | 1.004455 | 0.782528 |
| C | 3.850416 | -0.751911 | 1.721236 |
| C | 2.987161 | -1.740407 | 1.201560 |
| C | 1.528150 | -0.036192 | 0.335637 |
| H | 4.760960 | -1.081343 | 2.236516 |
| H | 3.279935 | -2.793099 | 1.305787 |
| C | 1.465275 | -2.461644 | -0.638152 |
| H | 0.394167 | -2.400505 | -0.856602 |
| H | 1.672571 | -3.459469 | -0.209677 |
| C | 5.014684 | 1.409107 | 1.395680 |
| H | 5.744271 | 0.835195 | 1.993405 |
| H | 4.928826 | 2.388972 | 1.889295 |
| C | 5.645644 | 1.624938 | -0.058535 |
| H | 6.743209 | 1.540254 | 0.047029 |
| H | 5.431682 | 2.653168 | -0.404188 |
| C | 2.201866 | -2.351693 | -2.058793 |
| H | 1.438338 | -2.037544 | -2.791186 |
| H | 2.545561 | -3.366005 | -2.332652 |
| C | 3.349489 | -1.372565 | -2.043746 |
| C | 5.095783 | 0.630532 | -1.057119 |
| C | 4.599287 | -1.720617 | -1.488624 |
| C | 3.107102 | -0.012967 | -2.321593 |
| C | 3.975458 | 0.975907 | -1.838586 |
| C | 5.461727 | -0.730864 | -0.997280 |
| H | 4.843270 | -2.779790 | -1.330467 |
| H | 2.166918 | 0.272863 | -2.811751 |
| H | 3.710225 | 2.034640 | -1.958271 |
| H | 6.369626 | -1.023647 | -0.452684 |
| C | 2.121935 | 2.377042 | 0.534774 |
| C | 0.961985 | 2.637582 | -0.190745 |
| H | 0.675343 | 3.662035 | -0.449580 |
| C | 0.068089 | 1.596214 | -0.481322 |
| C | 2.901340 | 3.567633 | 1.038398 |
| H | 3.865420 | 3.678633 | 0.510649 |
| H | 3.122535 | 3.468467 | 2.115881 |
| H | 2.325364 | 4.496260 | 0.884004 |
| C | -1.271628 | 1.852473 | -0.993786 |
| O | -1.595638 | 2.971236 | -1.636170 |
| C | -2.956326 | 2.749668 | -2.144974 |
| H | -3.537912 | 3.665852 | -1.954523 |
| H | -2.871049 | 2.568775 | -3.230843 |
| C | -3.465432 | 1.502722 | -1.361859 |
| N | 0.297053 | 0.306006 | -0.162173 |
| N | -2.208422 | 0.975613 | -0.810361 |
| Ru | -1.596960 | -0.862557 | -0.067781 |
| Cl | -1.371417 | -1.328853 | -2.436685 |
| C | -1.489098 | -1.084569 | 2.154304 |
| C | -2.964485 | -2.652401 | 0.189393 |
| C | -0.926866 | -2.273723 | 1.557961 |
| C | -2.816355 | -0.730478 | 1.777907 |
| C | -3.543003 | -1.511661 | 0.808810 |
| C | -1.629032 | -3.029891 | 0.594858 |
| H | 0.111562 | -2.528547 | 1.788309 |
| H | -3.263271 | 0.191184 | 2.160309 |
| H | -4.536602 | -1.188505 | 0.483793 |
| H | -1.133494 | -3.864113 | 0.090062 |
| C | -3.669853 | -3.414318 | -0.892899 |
| H | -2.990766 | -3.550116 | -1.754240 |
| H | -4.571541 | -2.878850 | -1.236434 |
| H | -3.970041 | -4.411717 | -0.514700 |
| C | -0.653798 | -0.274470 | 3.124674 |
| H | 0.402507 | -0.439722 | 2.836343 |
| C | -0.849483 | -0.825221 | 4.555110 |
| H | -0.191704 | -0.287507 | 5.263257 |
| H | -0.609798 | -1.903833 | 4.608550 |
| H | -1.898083 | -0.687975 | 4.882536 |
| C | -0.933012 | 1.234845 | 3.053037 |
| H | -0.205977 | 1.782376 | 3.679557 |
| H | -1.943971 | 1.477543 | 3.432002 |
| H | -0.850497 | 1.601615 | 2.014970 |
| H | -3.889247 | 0.748835 | -2.049500 |
| C | -4.490755 | 1.829525 | -0.246752 |
| H | -4.685331 | 0.874662 | 0.274091 |
| C | -5.813199 | 2.308198 | -0.867999 |
| H | -6.572208 | 2.472809 | -0.081459 |
| H | -6.213184 | 1.567936 | -1.587124 |
| H | -5.678953 | 3.268409 | -1.403458 |
| C | -3.938626 | 2.830838 | 0.779909 |
| H | -2.996155 | 2.469397 | 1.230678 |
| H | -4.671438 | 2.990380 | 1.592212 |
| H | -3.741362 | 3.816191 | 0.315732 |

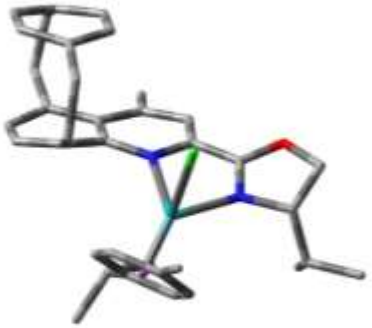


**Table S15**. Structure and Cartesian coordinates of ($R_p$,*S*,$R_M$)-**9**.

| | | | |
|---|---|---|---|
| C | -3.771799 | -1.032702 | 1.435639 |
| C | -1.999729 | 1.174229 | 0.925640 |
| C | -2.573212 | -1.260428 | 0.662248 |
| C | -3.852966 | 0.164378 | 2.148067 |
| C | -3.000797 | 1.259553 | 1.881547 |
| C | -1.645596 | -0.139369 | 0.461028 |
| H | -4.724329 | 0.333017 | 2.792742 |
| H | -3.257108 | 2.239419 | 2.304393 |
| C | -1.535105 | 2.403420 | 0.187257 |
| H | -0.537862 | 2.209555 | -0.217532 |
| H | -1.473856 | 3.255222 | 0.888182 |
| C | -5.077237 | -1.814658 | 1.296986 |
| H | -5.759272 | -1.437808 | 2.079172 |
| H | -4.976161 | -2.895007 | 1.480935 |
| C | -5.798755 | -1.605124 | -0.112965 |
| H | -6.887958 | -1.577258 | 0.076692 |
| H | -5.604731 | -2.478773 | -0.762212 |
| C | -2.480616 | 2.841025 | -1.037379 |
| H | -1.847802 | 2.902396 | -1.941528 |
| H | -2.863004 | 3.856421 | -0.828068 |
| C | -3.626998 | 1.883882 | -1.256660 |
| C | -5.313601 | -0.347450 | -0.800522 |
| C | -4.827830 | 2.028390 | -0.530926 |
| C | -3.421112 | 0.678893 | -1.956126 |
| C | -4.258277 | -0.422674 | -1.731355 |
| C | -5.663733 | 0.925981 | -0.305998 |
| H | -5.045761 | 2.983941 | -0.035552 |
| H | -2.528541 | 0.562653 | -2.585456 |
| H | -4.010654 | -1.390697 | -2.185947 |
| H | -6.525118 | 1.027671 | 0.367510 |
| C | -2.263872 | -2.500525 | 0.004130 |
| C | -1.151666 | -2.537779 | -0.832549 |
| H | -0.883890 | -3.454238 | -1.368385 |
| C | -0.257767 | -1.453065 | -0.861857 |
| C | -3.025839 | -3.788489 | 0.200379 |
| H | -4.026765 | -3.749802 | -0.265950 |
| H | -3.166719 | -3.999653 | 1.275321 |
| H | -2.476387 | -4.632298 | -0.251270 |
| C | 1.081737 | -1.624116 | -1.405149 |
| O | 1.380810 | -2.546076 | -2.319253 |
| C | 2.802551 | -2.353416 | -2.625841 |
| H | 3.273119 | -3.347068 | -2.691179 |
| H | 2.859491 | -1.839497 | -3.602755 |
| C | 3.326679 | -1.482803 | -1.451989 |
| N | -0.462115 | -0.294075 | -0.208816 |
| N | 2.066906 | -0.917530 | -0.937604 |
| Ru | 1.695273 | 0.485367 | 0.527372 |
| Cl | 1.206853 | -1.345009 | 2.036154 |
| C | 2.011053 | 2.659918 | -0.149123 |
| C | 3.263618 | 1.142382 | 1.990965 |
| C | 3.174570 | 1.881728 | -0.390860 |
| C | 1.490038 | 2.676154 | 1.198919 |
| C | 2.086367 | 1.938251 | 2.242722 |
| C | 3.791898 | 1.133366 | 0.664713 |
| H | 3.571166 | 1.807526 | -1.408082 |
| H | 0.578160 | 3.239213 | 1.405357 |
| H | 1.619671 | 1.910914 | 3.232124 |
| H | 4.654342 | 0.496447 | 0.446737 |
| C | 3.899825 | 0.341498 | 3.087982 |
| H | 4.591560 | -0.415475 | 2.680278 |
| H | 3.127533 | -0.173511 | 3.685108 |
| H | 4.472043 | 1.023092 | 3.749184 |
| C | 1.387420 | 3.465109 | -1.276610 |
| H | 0.469771 | 3.936337 | -0.881247 |
| C | 0.996157 | 2.569425 | -2.468313 |
| H | 0.546392 | 3.180079 | -3.272761 |
| H | 0.272788 | 1.793311 | -2.160240 |
| H | 1.883838 | 2.060053 | -2.889204 |
| C | 2.346818 | 4.598234 | -1.705807 |
| H | 1.862284 | 5.230767 | -2.472470 |
| H | 3.276595 | 4.184399 | -2.141072 |
| H | 2.622843 | 5.239489 | -0.848077 |
| H | 3.974057 | -0.667822 | -1.825091 |
| C | 4.082516 | -2.269341 | -0.348478 |
| H | 4.125017 | -1.589665 | 0.522343 |
| C | 5.512731 | -2.577069 | -0.819504 |
| H | 6.075328 | -3.104206 | -0.027407 |
| H | 6.065817 | -1.653671 | -1.082288 |
| H | 5.504876 | -3.233720 | -1.712183 |
| C | 3.340351 | -3.537283 | 0.102452 |
| H | 2.318013 | -3.301980 | 0.444970 |
| H | 3.876777 | -3.994324 | 0.953978 |
| H | 3.298983 | -4.293749 | -0.705097 |

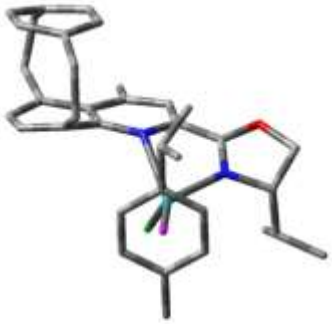


**Table S16**. Structure and Cartesian coordinates of ($R_p$,*S*,$S_M$)-**9**.

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C | -3.620160 | -0.725457 | 1.462996 | C | 2.887294 | -2.873671 | -2.297583 |
| C | -1.739943 | 1.360028 | 0.762336 | H | 3.328096 | -3.638395 | -1.628910 |
| C | -2.417829 | -1.073988 | 0.739599 | H | 3.056745 | -3.148060 | -3.351433 |
| C | -3.655766 | 0.535544 | 2.054862 | C | 3.358033 | -1.426439 | -1.947890 |
| C | -2.750957 | 1.558544 | 1.695965 | N | -0.251914 | -0.314276 | -0.185986 |
| C | -1.437514 | -0.013263 | 0.435966 | N | 2.208073 | -0.972575 | -1.104092 |
| H | -4.525111 | 0.807283 | 2.666169 | Ru | 1.711660 | 0.691691 | 0.087722 |
| H | -2.974180 | 2.583604 | 2.018789 | Cl | 1.450027 | 1.833857 | -2.028045 |
| C | -1.284934 | 2.552664 | -0.056155 | C | 2.512001 | -0.082201 | 2.033958 |
| H | -0.212687 | 2.536362 | -0.282354 | C | 2.293325 | 2.680087 | 1.099915 |
| H | -1.491889 | 3.460300 | 0.540303 | C | 1.342956 | 0.698157 | 2.268143 |
| C | -4.956277 | -1.464079 | 1.382124 | C | 3.567745 | 0.553242 | 1.289266 |
| H | -5.633352 | -0.969288 | 2.100301 | C | 3.460334 | 1.883400 | 0.798444 |
| H | -4.909850 | -2.518552 | 1.694301 | C | 1.255065 | 2.070335 | 1.848856 |
| C | -5.641974 | -1.388380 | -0.059497 | H | 0.467135 | 0.242317 | 2.738189 |
| H | -6.729601 | -1.270473 | 0.102551 | H | 4.447931 | -0.039103 | 1.029920 |
| H | -5.495382 | -2.347790 | -0.589867 | H | 4.248147 | 2.296716 | 0.160816 |
| C | -2.027995 | 2.687413 | -1.467884 | H | 0.333333 | 2.624400 | 2.037462 |
| H | -1.289944 | 2.428764 | -2.246217 | C | 2.165582 | 4.071014 | 0.553379 |
| H | -2.300588 | 3.751556 | -1.593641 | H | 1.209897 | 4.534028 | 0.850493 |
| C | -3.236566 | 1.790596 | -1.576834 | H | 2.214933 | 4.033959 | -0.551812 |
| C | -5.067429 | -0.260025 | -0.887444 | H | 3.000451 | 4.699254 | 0.919353 |
| C | -4.438557 | 2.099077 | -0.904721 | C | 2.658355 | -1.524234 | 2.475400 |
| C | -3.094976 | 0.495568 | -2.112301 | H | 3.235442 | -2.033283 | 1.677272 |
| C | -4.004075 | -0.517078 | -1.774378 | C | 1.313312 | -2.251956 | 2.627968 |
| C | -5.343206 | 1.085019 | -0.561648 | H | 1.484864 | -3.325265 | 2.827011 |
| H | -4.606398 | 3.121764 | -0.541021 | H | 0.699557 | -2.154033 | 1.715281 |
| H | -2.197410 | 0.254386 | -2.697001 | H | 0.735030 | -1.846115 | 3.479831 |
| H | -3.810479 | -1.548826 | -2.096024 | C | 3.486744 | -1.584804 | 3.778358 |
| H | -6.208112 | 1.321345 | 0.072825 | H | 3.657435 | -2.636529 | 4.074898 |
| C | -2.144656 | -2.398371 | 0.252176 | H | 2.948241 | -1.075830 | 4.600753 |
| C | -1.018723 | -2.585759 | -0.545422 | H | 4.470529 | -1.093813 | 3.655845 |
| H | -0.785358 | -3.568028 | -0.968269 | C | 4.680607 | -1.437056 | -1.179049 |
| C | -0.090190 | -1.546065 | -0.709808 | H | 4.583946 | -1.977275 | -0.219413 |
| C | -2.965427 | -3.621046 | 0.583660 | H | 5.454384 | -1.939809 | -1.788101 |
| H | -3.950398 | -3.601412 | 0.083401 | H | 5.019972 | -0.403760 | -0.991962 |
| H | -3.146183 | -3.693134 | 1.670747 | C | 3.469118 | -0.556742 | -3.211349 |
| H | -2.441236 | -4.535293 | 0.256011 | H | 4.276796 | -0.960625 | -3.850980 |
| C | 1.217716 | -1.786119 | -1.309178 | H | 3.698385 | 0.487359 | -2.944516 |
| O | 1.446764 | -2.865441 | -2.057717 | H | 2.519977 | -0.560942 | -3.775074 |

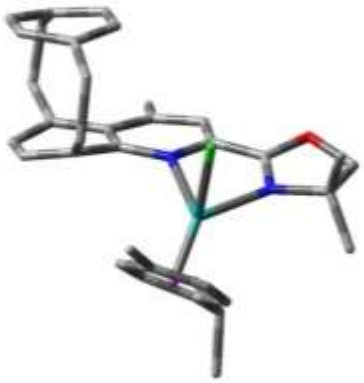


**Table S17**. Structure and Cartesian coordinates of ($R_p$,$R_M$)-**10**.

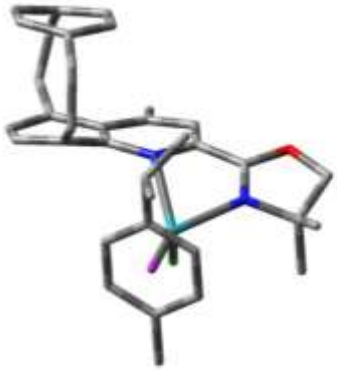
| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C | -3.742040 | -0.637091 | 1.457848 | C | 2.559598 | -2.906642 | -2.578133 |  |
| C | -1.753888 | 1.341573 | 0.818569 | H | 2.914544 | -3.950191 | -2.564250 | |
| C | -2.570498 | -1.034777 | 0.712793 | H | 2.641390 | -2.490134 | -3.600424 | |
| C | -3.711356 | 0.612930 | 2.078887 | C | 3.244798 | -1.998540 | -1.510711 | |
| C | -2.756668 | 1.598694 | 1.742466 | N | -0.367599 | -0.351356 | -0.192059 | |
| C | -1.531183 | -0.031141 | 0.457699 | N | 2.065061 | -1.230609 | -1.015022 | |
| H | -4.566563 | 0.912546 | 2.697022 | Ru | 1.801576 | 0.118059 | 0.569354 | |
| H | -2.926136 | 2.629776 | 2.078349 | Cl | 1.212784 | -1.846166 | 1.881597 | |
| C | -1.169127 | 2.454250 | -0.017931 | C | 2.383590 | 2.297903 | 0.072152 | |
| H | -0.197626 | 2.128016 | -0.400581 | C | 3.263396 | 0.563385 | 2.237278 | |
| H | -1.021650 | 3.353637 | 0.606632 | C | 3.482729 | 1.412288 | -0.093065 | |
| C | -5.115679 | -1.300399 | 1.365180 | C | 1.701447 | 2.262583 | 1.340231 | |
| H | -5.758767 | -0.807379 | 2.115083 | C | 2.116573 | 1.419884 | 2.398708 | |
| H | -5.115741 | -2.369902 | 1.625628 | C | 3.928473 | 0.566860 | 0.975729 | |
| C | -5.816870 | -1.123924 | -0.061147 | H | 3.981209 | 1.361640 | -1.063519 | |
| H | -6.896404 | -0.967992 | 0.121057 | H | 0.812133 | 2.878509 | 1.481918 | |
| H | -5.717453 | -2.059687 | -0.641196 | H | 1.535011 | 1.374006 | 3.324199 | |
| C | -2.066121 | 2.883919 | -1.281331 | H | 4.760382 | -0.124326 | 0.814453 | |
| H | -1.425784 | 2.815748 | -2.180083 | C | 3.727035 | -0.319510 | 3.356463 | |
| H | -2.348633 | 3.944593 | -1.153919 | H | 4.317694 | -1.170933 | 2.978301 | |
| C | -3.299840 | 2.029404 | -1.440653 | H | 2.868085 | -0.713003 | 3.924925 | |
| C | -5.205243 | 0.020431 | -0.839080 | H | 4.366005 | 0.278769 | 4.037774 | |
| C | -4.486728 | 2.350617 | -0.749297 | C | 1.992555 | 3.240530 | -1.051757 | |
| C | -3.209687 | 0.757673 | -2.039100 | H | 1.080734 | 3.776909 | -0.735441 | |
| C | -4.155705 | -0.233202 | -1.744555 | C | 1.680812 | 2.477797 | -2.354100 | |
| C | -5.429720 | 1.357258 | -0.450908 | H | 1.353910 | 3.182304 | -3.140832 | |
| H | -4.613415 | 3.360199 | -0.336115 | H | 0.889554 | 1.723671 | -2.192845 | |
| H | -2.326589 | 0.502871 | -2.640141 | H | 2.579637 | 1.951085 | -2.727482 | |
| H | -4.002842 | -1.254130 | -2.116938 | C | 3.105075 | 4.292150 | -1.263360 | |
| H | -6.282457 | 1.596916 | 0.198270 | H | 2.795286 | 5.017777 | -2.038147 | |
| C | -2.394574 | -2.332146 | 0.116771 | H | 4.042782 | 3.809886 | -1.600627 | |
| C | -1.316807 | -2.515005 | -0.744572 | H | 3.318190 | 4.847078 | -0.330785 | |
| H | -1.159956 | -3.472715 | -1.250683 | C | 3.809602 | -2.831265 | -0.346567 | |
| C | -0.308980 | -1.537635 | -0.823901 | H | 3.033886 | -3.496600 | 0.070630 | |
| C | -3.267533 | -3.530393 | 0.397742 | H | 4.140849 | -2.167210 | 0.467922 | |
| H | -4.265064 | -3.435106 | -0.067922 | H | 4.667809 | -3.432303 | -0.701115 | |
| H | -3.416583 | -3.657824 | 1.484491 | C | 4.318427 | -1.115579 | -2.156034 | |
| H | -2.798644 | -4.447321 | 0.001107 | H | 5.028004 | -1.753980 | -2.714822 | |
| C | 0.993458 | -1.867393 | -1.388095 | H | 4.900518 | -0.569291 | -1.395481 | |
| O | 1.147851 | -2.900008 | -2.216059 | H | 3.865028 | -0.394806 | -2.860414 | |

**Table S18**. Structure and Cartesian coordinates of ($R_p$,$S_M$)-**10**.

## Analysis of the electronic transitions

In order to verify which kind of electronic transitions occur above the 250 nm and which role can be attributed to the Ru atom, we report hereafter a detailed analysis of some of them in terms of molecular orbital composition for ($R_p$,$R$,$R_M$)-**8**. Compound **8** has been chosen as a representative of all complexes. Since length and velocity formalisms provide quite similar results, we focus only on the data computed for the velocity formalism.

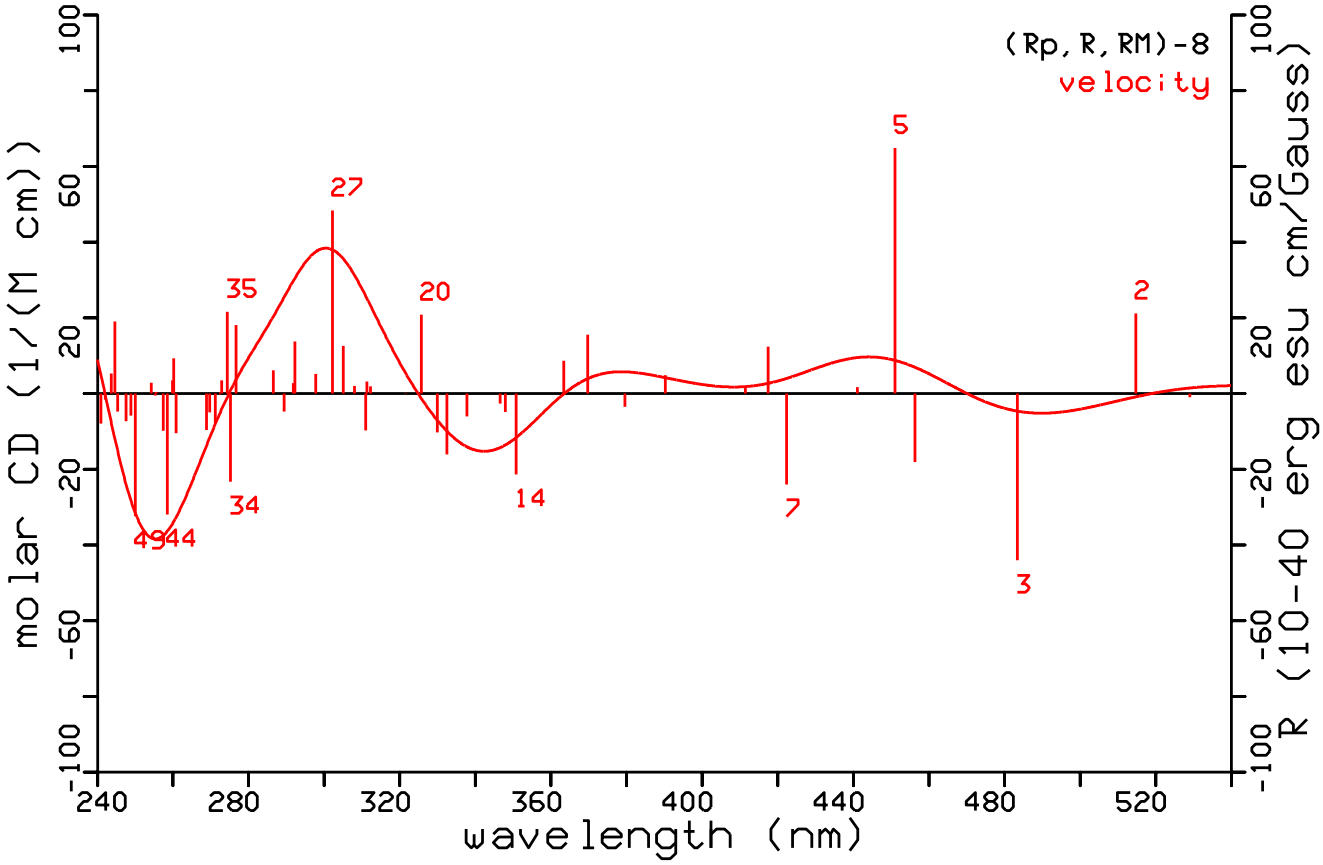



**Figure S7.** Calculated (B3LYP/SV(P)) ECD spectra of ($R_p$,$R$,$R_M$)-**8.** Rotational strengths larger than $20\times10^{-40}$ erg esu cm Gauss$^{-1}$ have been indicated using the enumeration of the calculation.

Apart the HOMO (170), which is localized almost exclusively on the paracyclophane unit, all others highest occupied MOs shown below are delocalized on Ru (d orbitals), Cl (p orbitals) and ligands (π orbitals). With the exception of MO 174, all other relevant occupied orbitals are delocalized on Ru, Cl, p-cymene and the two aromatic parts of quinolinophane. Some of the relevant virtual orbitals are slightly more localized. MO 171, 172 and 175 lack appreciable electron density of the phenyl part of the quinolinophane;

MO 176 lack density on all the quinolinophane and MO 174 lack density on chlorine and the metal. Therefore, Cotton effects above 250 nm are attributable to metal-to-metal (MM) d-d transitions, metal-to-ligand and ligand-to-metal charge transfer, and π–π* transitions.

**Table S19**. Analysis of the most important rotational strengths calculated at B3LYP/SV(P) level above the 250 nm.

| Excited State | Wavelength (nm) | Rotational strength ($10^{-40}$ erg esu cm Gauss$^{-1}$) | Largest contributions |
|---|---|---|---|
| 2 | 515 | 21.3 | 169→171<br>168→171 |
| 3 | 483 | -44.0 | 167→171<br>167→172 |
| 5 | 451 | 64.9 | 168→171<br>169→171 |
| 7 | 422 | -24.0 | 167→171<br>167→172 |
| 14 | 351 | -21.3 | 164→171<br>168→172 |
| 20 | 326 | 20.9 | 168→174 |
| 27 | 302 | 48.4 | 166→174<br>164→172<br>162→171 |
| 34 | 275 | -23.2 | 170→176<br>167→176<br>162→171 |
| 35 | 274 | 21.7 | 170→177<br>162→171<br>170→176 |
| 44 | 258 | -31.9 | 164→174<br>166→175 |
| 49 | 250 | -32.4 | 162→172<br>163→172 |

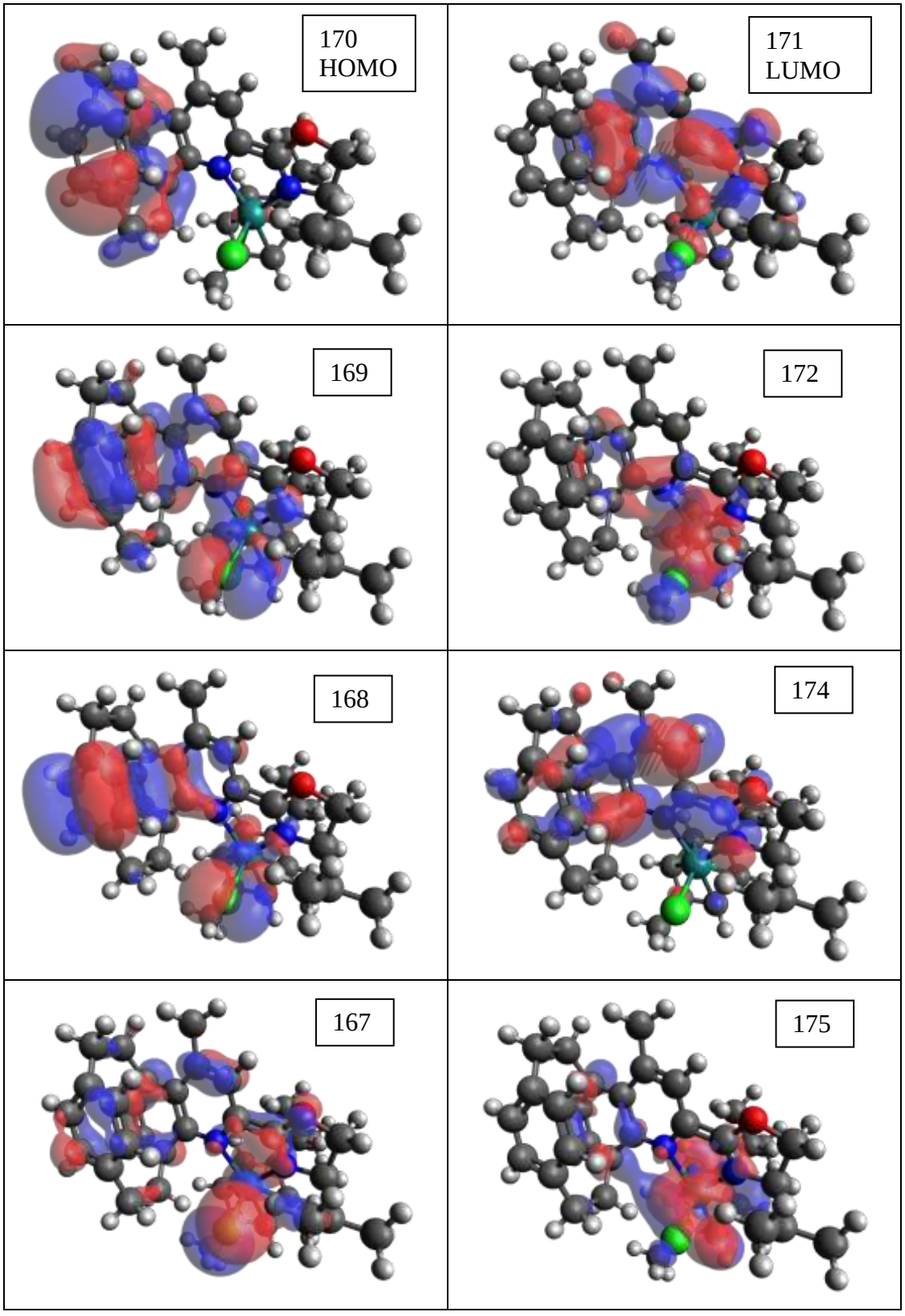



**Figure S8**. Isosurfaces (0.02 a.u.) of some selected MOs.

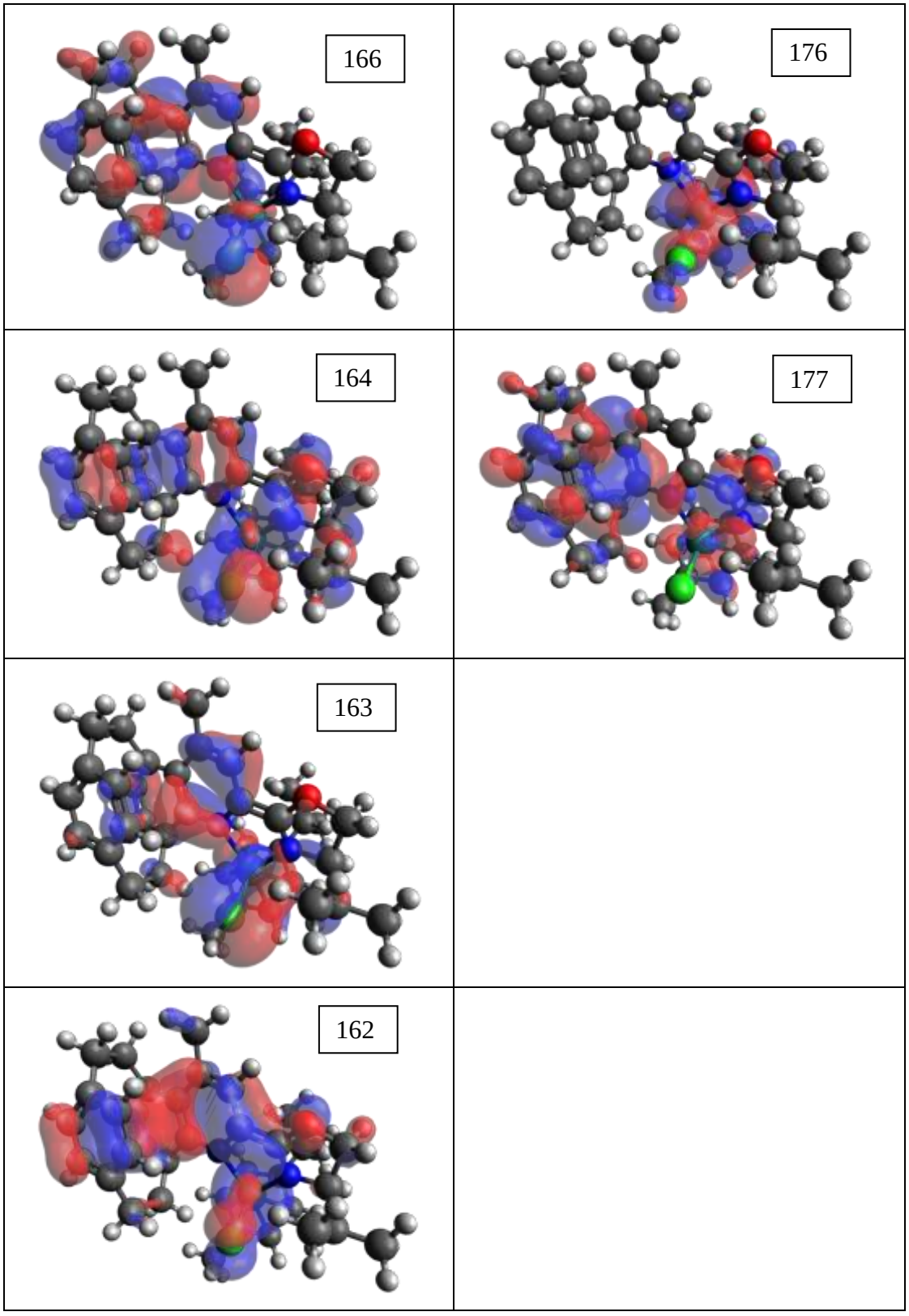



**Figure S9.** Isosurfaces (0.02 a.u.) of some selected MOs.

## Pearson's correlation coefficient (PCC)

Pearson's correlation coefficient *r* has been computed according to the formula

$$r = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n\sum x_i^2 - \left(\sum x_i\right)^2}\sqrt{n\sum y_i^2 - \left(\sum y_i\right)^2}}$$

where $x_i$, $y_i$ (for $i$=1,2,...$n$) are data set points, that is, circular dichroism values, taken from experimental and theoretically predicted spectra of a given complex respectively. In order to find the best resemblance between experimental and theoretical spectra, it is customary to apply a wavelength shift $w_s$ to the predicted data; hence, PCC can be thought as a function of the shift, i.e., $r$=$r$($w_s$).

In the following a series of plots is reported where *r* is analyzed with respect to a varying blue-shift from –50 nm to 50 nm. For each complex four PCC's were determined, that is, for the length and velocity formalism and for both Ru configurations. PCC's are computed summing over the whole range of experimental wavelengths (200 nm - 600 nm) in step of 0.1 nm as collected by the instrument.

It can be observed that: i) length and velocity formalism do not deviate appreciable; ii) the *R* configuration at Ru provides the largest positive correlation in all cases for a moderate negative blue-shift, i.e., a red-shift; iii) for all complexes, the *S* configuration at Ru provides a negative correlation where the PCC for the R configuration is maximum.

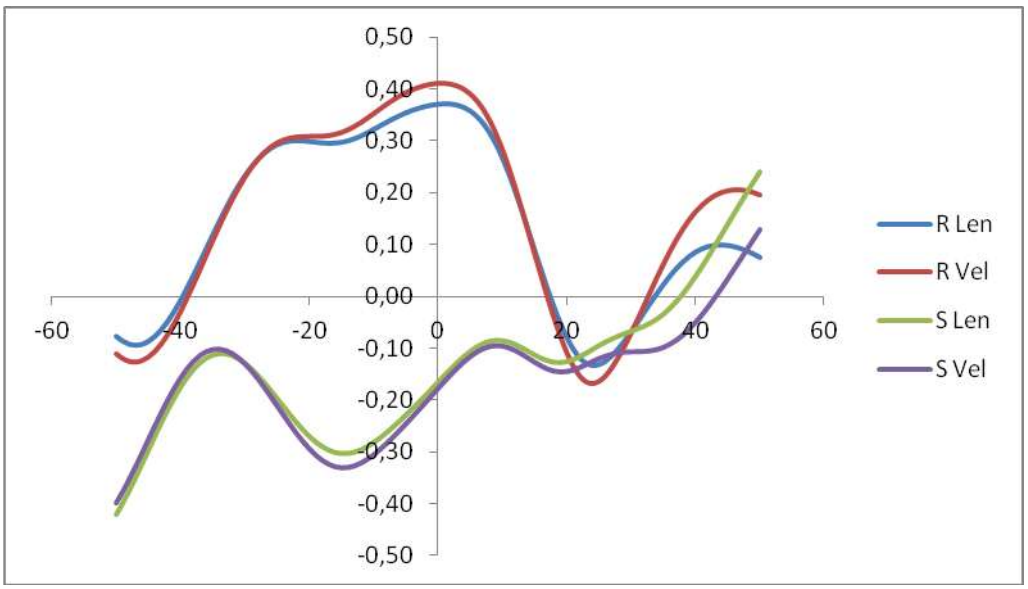



**Figure S10.** PCC's of **7a** as a function of blue-shift.

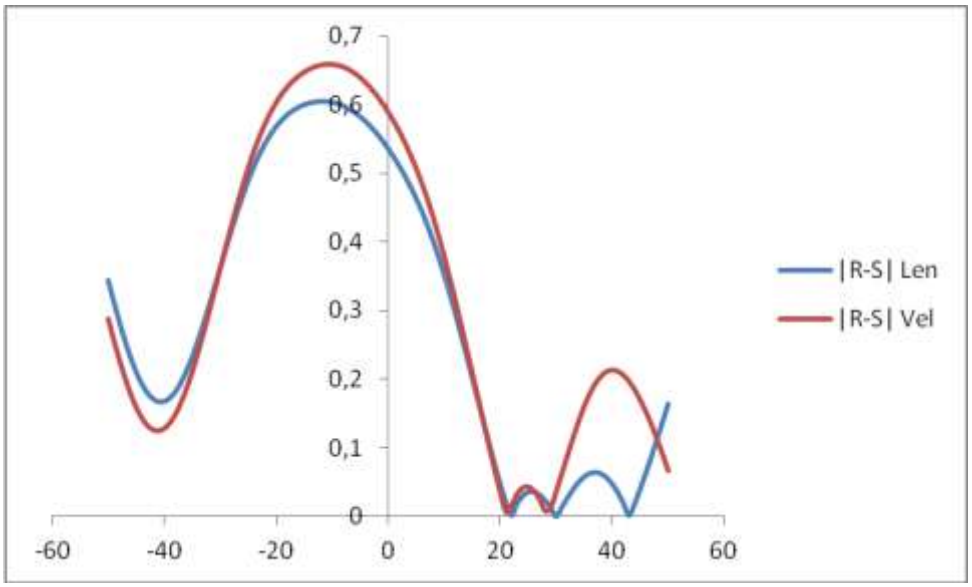



**Figure S11.** PCC's difference between $R_M$ and $S_M$ configuration of **7a** as a function of blue-shift.

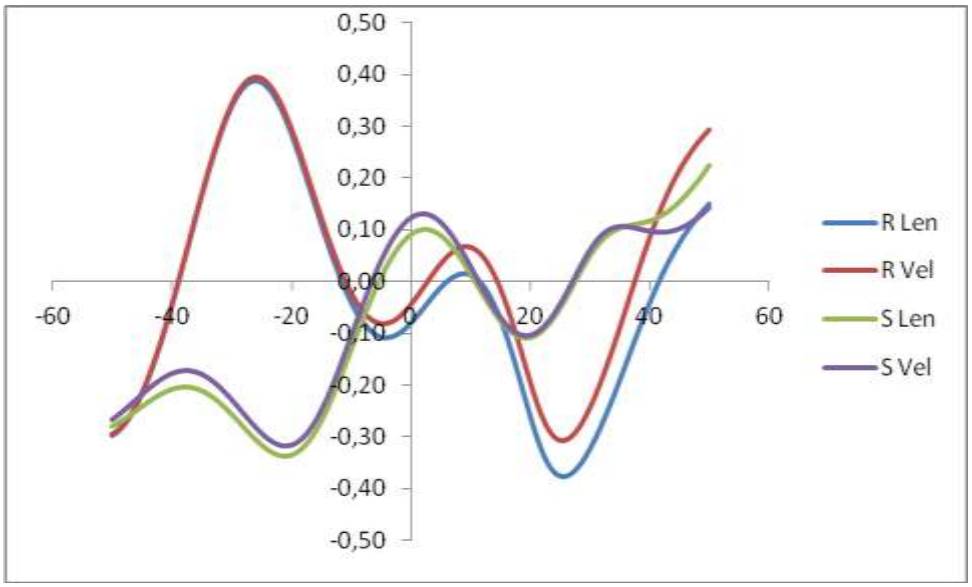



**Figure S12.** PCC's of **6a** as a function of blue-shift.

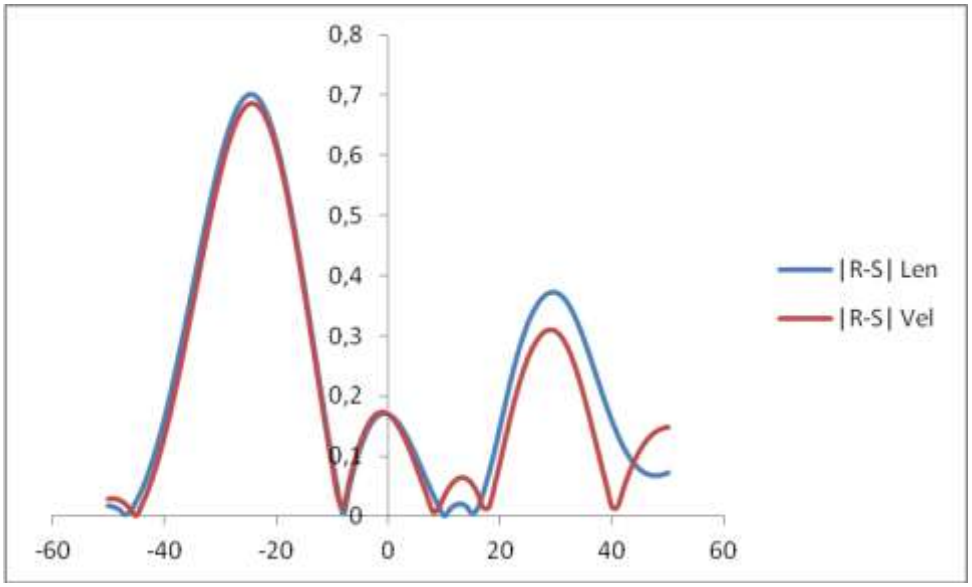



**Figure S13.** PCC's difference between $R_M$ and $S_M$ configuration of **6a** as a function of blue-shift.

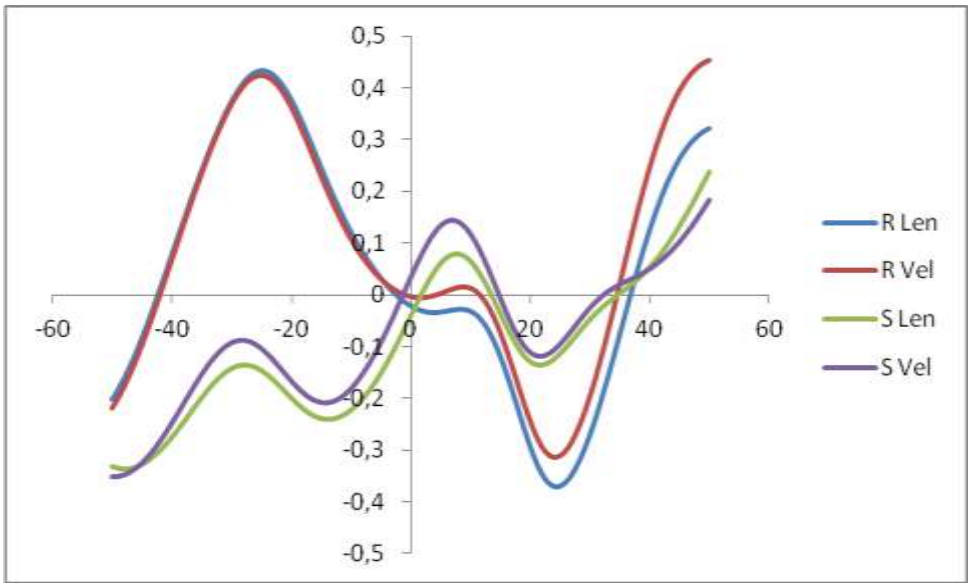



**Figure S14**. PCC's of **8** as a function of blue-shift.

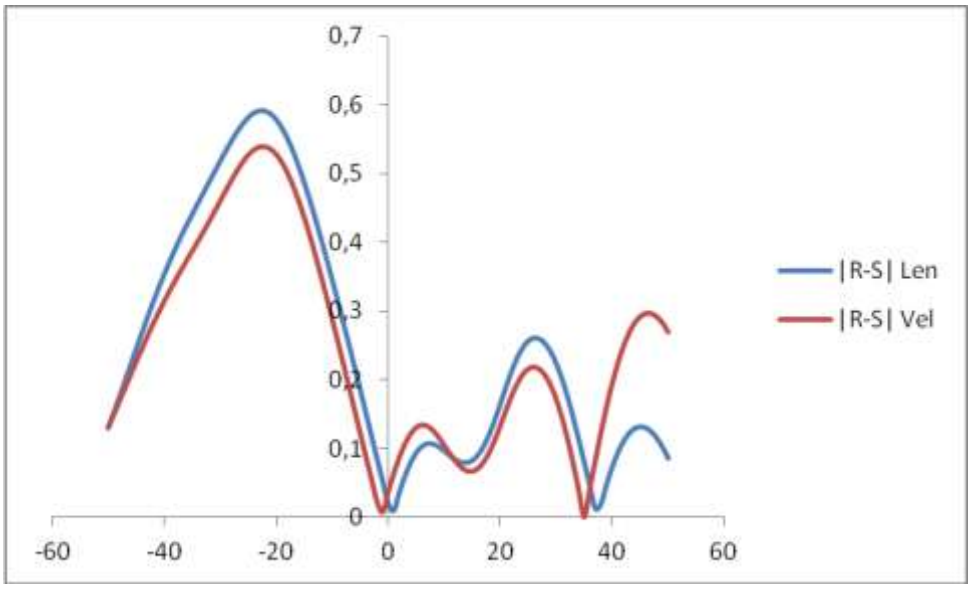



**Figure S15.** PCC's difference between $R_M$ and $S_M$ configuration of **8** as a function of blue-shift.

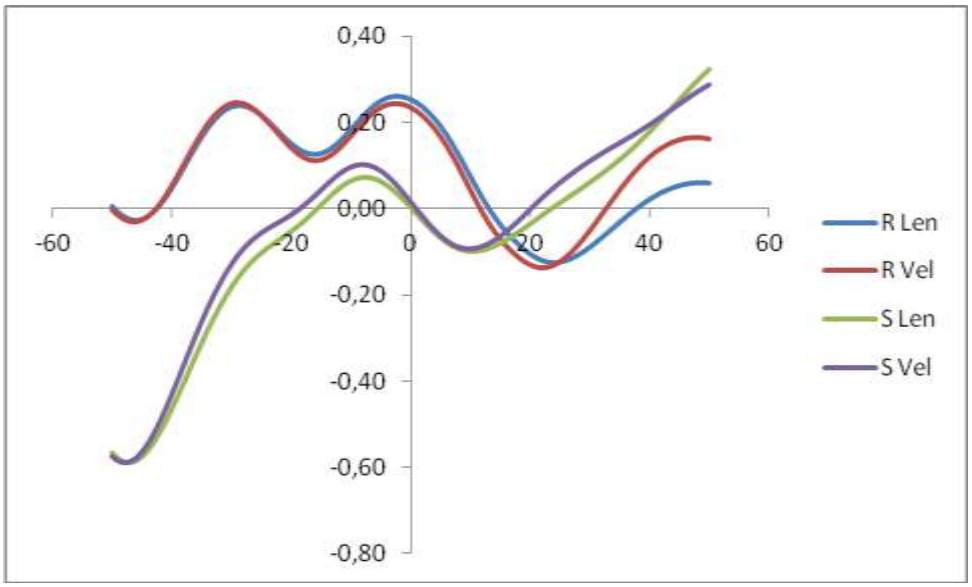



**Figure S16.** PCC's of **9** as a function of blue-shift.

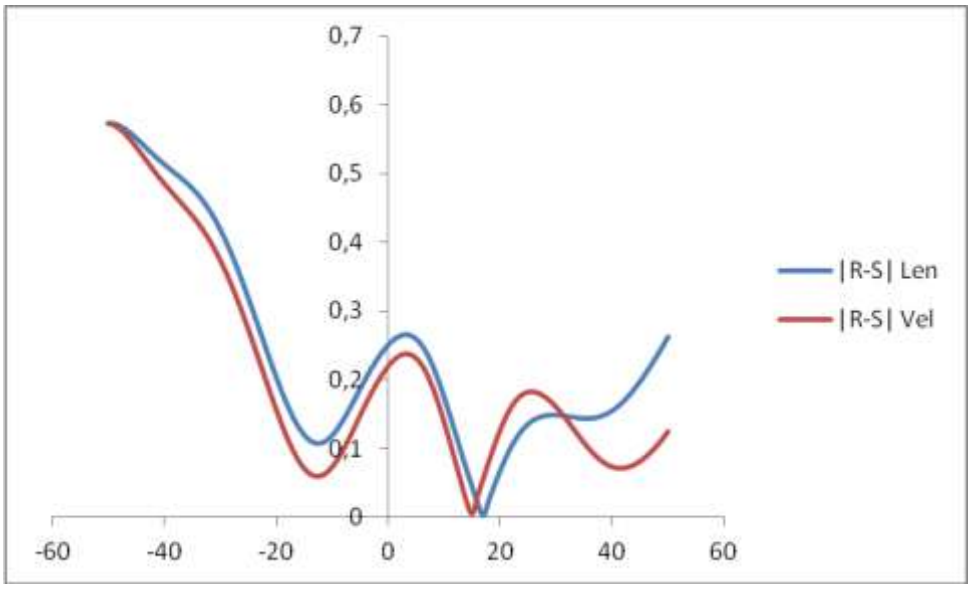



**Figure S17.** PCC's difference between $R_M$ and $S_M$ configuration of **9** as a function of blue-shift.

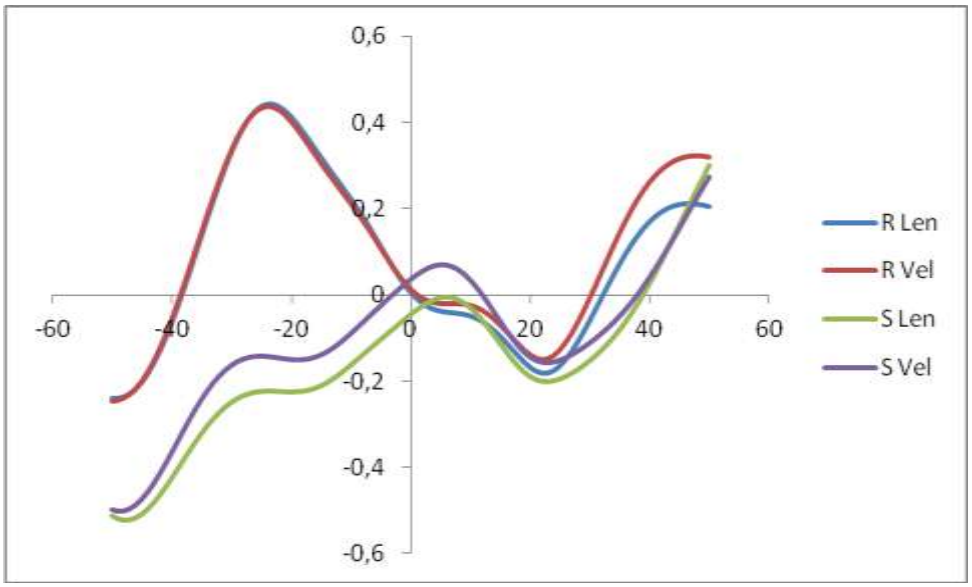



**Figure S18.** PCC's of **10** as a function of blue-shift.

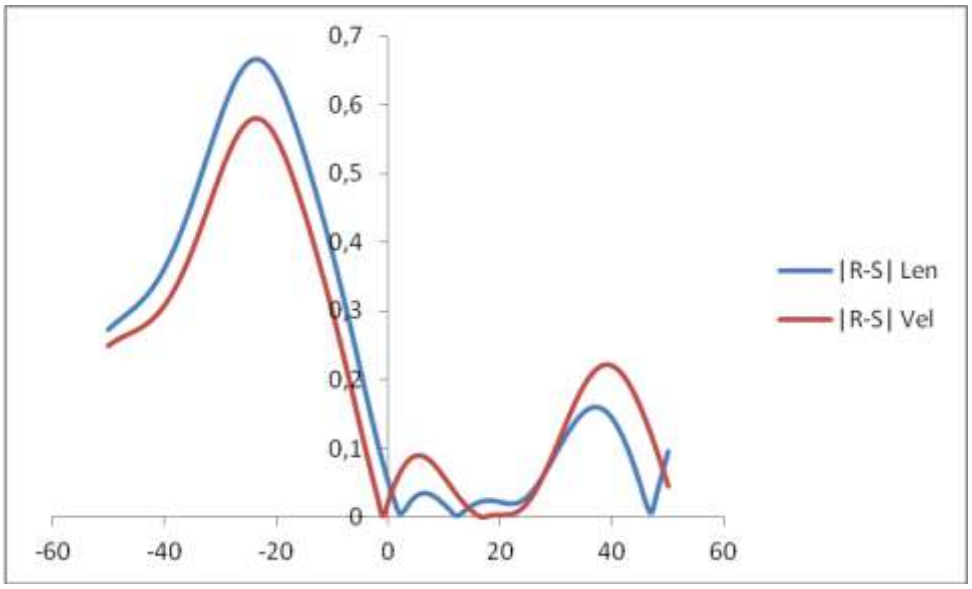



**Figure S19.** PCC's difference between $R_M$ and $S_M$ configuration of **10** as a function of blue-shift.

## X Ray crystallography section

A single crystal of ($R_p$,*S*)-[QUINOPHOX]$^+$ $PF_6^-$ suitable for X-ray diffraction (a red block) with approximate dimensions of 0.18 mm × 0.14 mm × 0.12 mm), was obtained by crystallization from dichloromethane.

Data were collected on a XCALIBUR (Kuma4CCD) diffractometer using Mo-Kα graphite monochromated radiation (λ = 0.71069 Å), ω scans and the frame data were acquired with the CRYSALIS (CCD 171) software.[1] The crystal to detector distance was 65.77 mm.

The structure was solved using direct methods and refined against $|F|^2$.

The Laue symmetry was determined to be 2/m. The dimensions of the cell yield a calculated density to 1.538 g cm$^{-3}$ (*Z* = 2 and FW = 919.15) and the investigation of the observed systematic absences are consistent with the monoclinic space group *P21* (no. 4). The data were collected at room temperature. The lattice parameters are: *a* = 12.3597(9), *b* = 11.3107(8) and *c* = 14.8410(10) Å, β = 106.960(5), and *V* = 1984.5(2) Å$^3$. Data were collected to $2\theta_{max}$ of 56.70° in the index ranges $-17 \leq h \leq 17$, $-13 \leq k \leq 15$, and $-21 \leq l \leq 20$ with a total of 18065 reflections collected of which 0 rejected and 9895 are unique reflections independent *R*(int) = 0.0279, up to a resolution of 0.69 Å.

The frames were then processed using the CRYSALIS (RED 171) software to give the *hkl* file corrected for scan speed, background, and Lorentz and polarization effects. Standard reflections, measured periodically, showed no apparent variation in intensity during data collection, therefore, no correction for crystal decomposition was necessary. The data were corrected for absorption using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.[1]

The structure was solved by the direct method using the Sir97 [2] program and refined by the full-matrix least-squares method on $F^2$ using SHELXL-97 [3] WinGX [4] version. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were added at the calculated positions and refined using a riding model.

The final cycle of full-matrix least-squares refinement against $|F|^2$ was based on 7906 observed reflections [$F_0 > 4\,\sigma\,(F_0)$] and 483 variable parameters and converged with unweighted and weighted agreement factors of $R = 0.0468$ and $R_w = 0.0719$, and GOF = 0.923.

(w=1/[\s^2^(Fo^2^)+(0.0675P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3').

The absolute configuration was determined by the Flack parameter determinate with SHELXL-97. The value obtained was quite definitive, but as a further check it has been also determined correctly, using the TWIN and BASF commands of the program.

Finally the $PF_6^-$ anion is positioned on the opposite side of the paracyclophane moiety. It shows a disorder probably ascribable to its thermal movement, so it is impossible to determine exactly the position of the fluorine atoms. A better determination could be obtained at low temperature, but that it was not possible to perform not having available the necessary instrumentation.

For better resolution, based on experimental evidence, we have hypothesized two conformations of the PF6 with the same probability of existence (0.5). The distance P-Ru is of 5,729 Å. In the crystal unit cell a molecule of dicloromethane (solvent) is present.

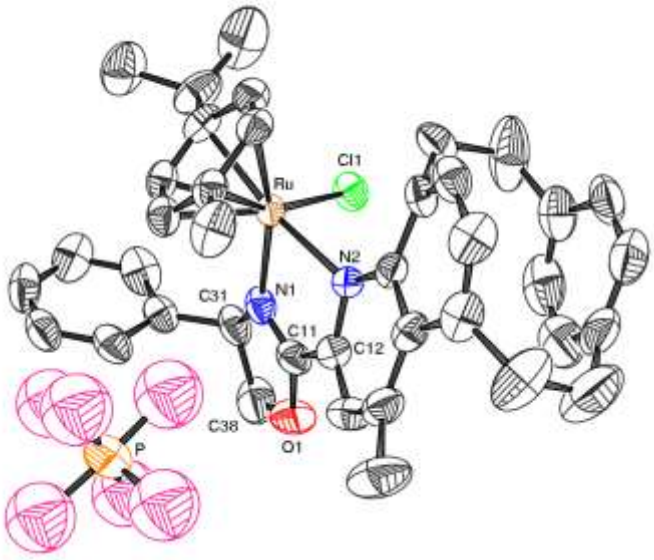



**Figure S20.** Thermal ellipsoid plot of ($S_p$,*R*,$S_{Ru}$)-**7b** complex with significant bond length and angles

**References**

1) CrysAlis RED, Oxford Diffraction Ltd., Version 1.171.33.32 (release 27-01-2009 CrysAlis171 .NET) (compiled Jan 27 2009,14:17:37)

2) A. Altomare, M.C. Burla, M. Camalli, G. Cascarano, c. Giacovazzo, A. Gagliardi, A.G.G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst*. 1999, **32**, 115-119.

3) G.M. Sheldrick SHELXL-97, A program for crystal structure refinement, University of Goettingen, Germany, 1997. Release 92-2

4) L. J. Farrugia, *J. Appl. Cryst* 1999, **32**, 837-838.