

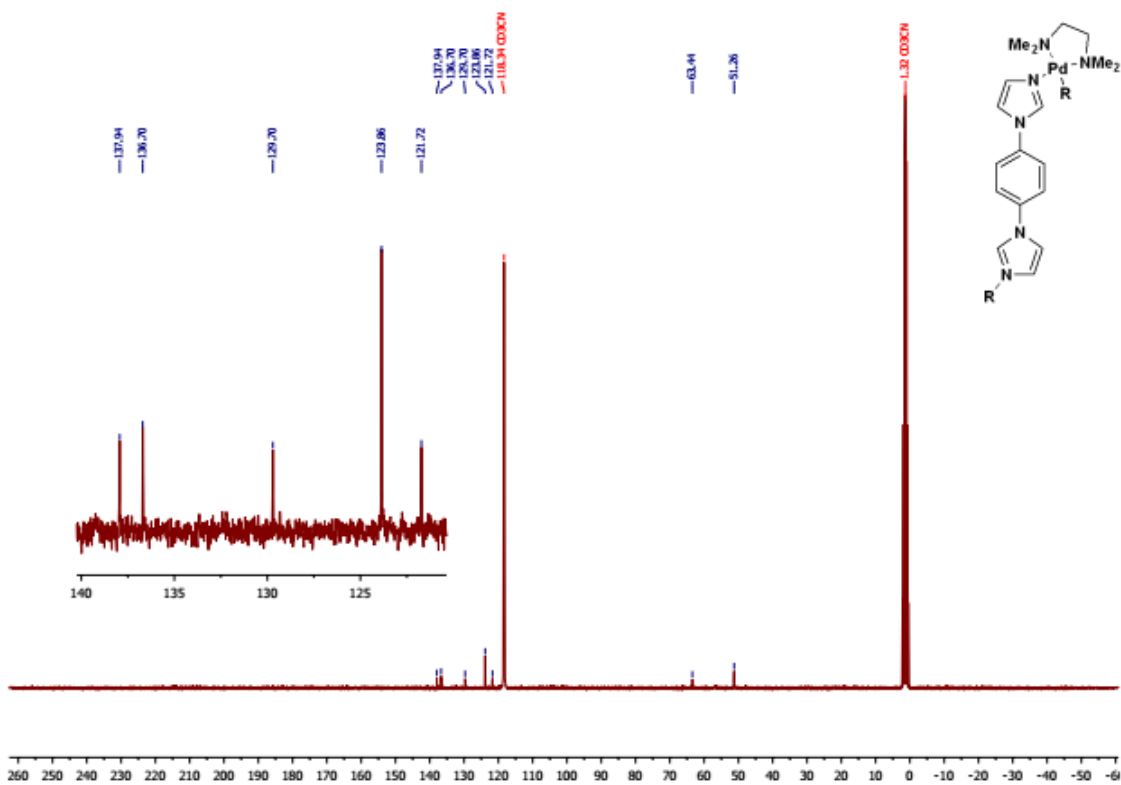
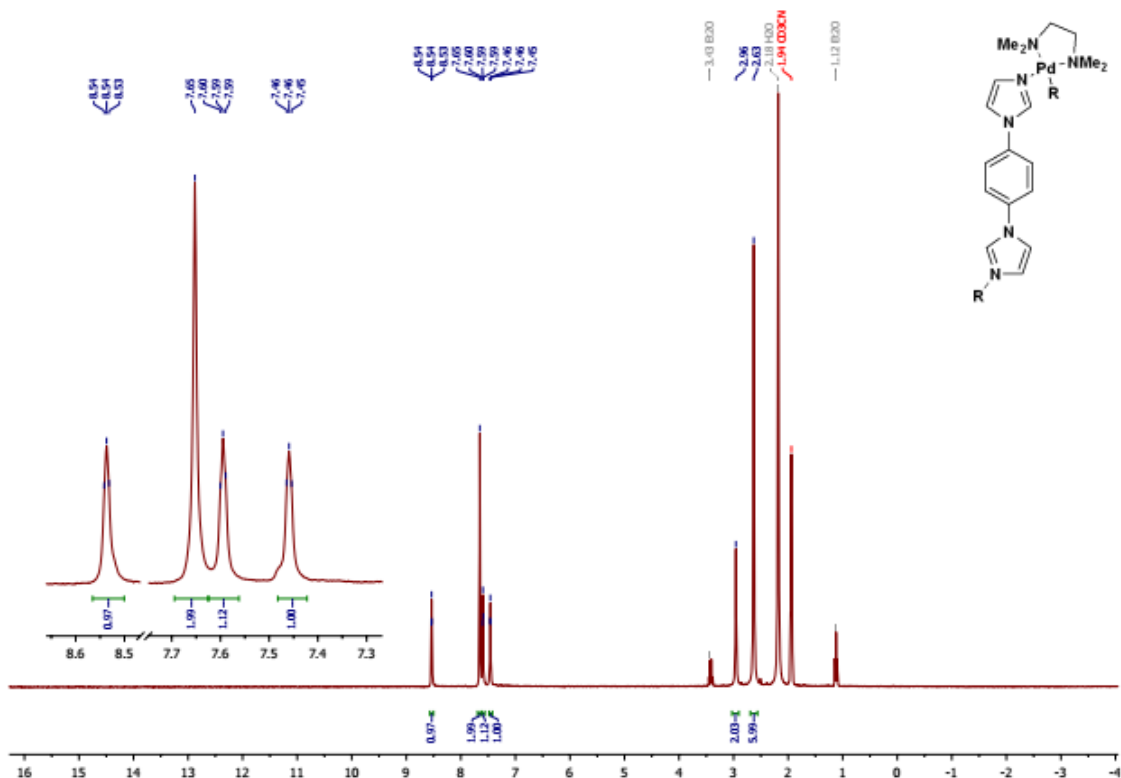
Coordination-driven self-assembly of chiral palladium(II)-based supramolecular triangles structures

Electronic supporting information

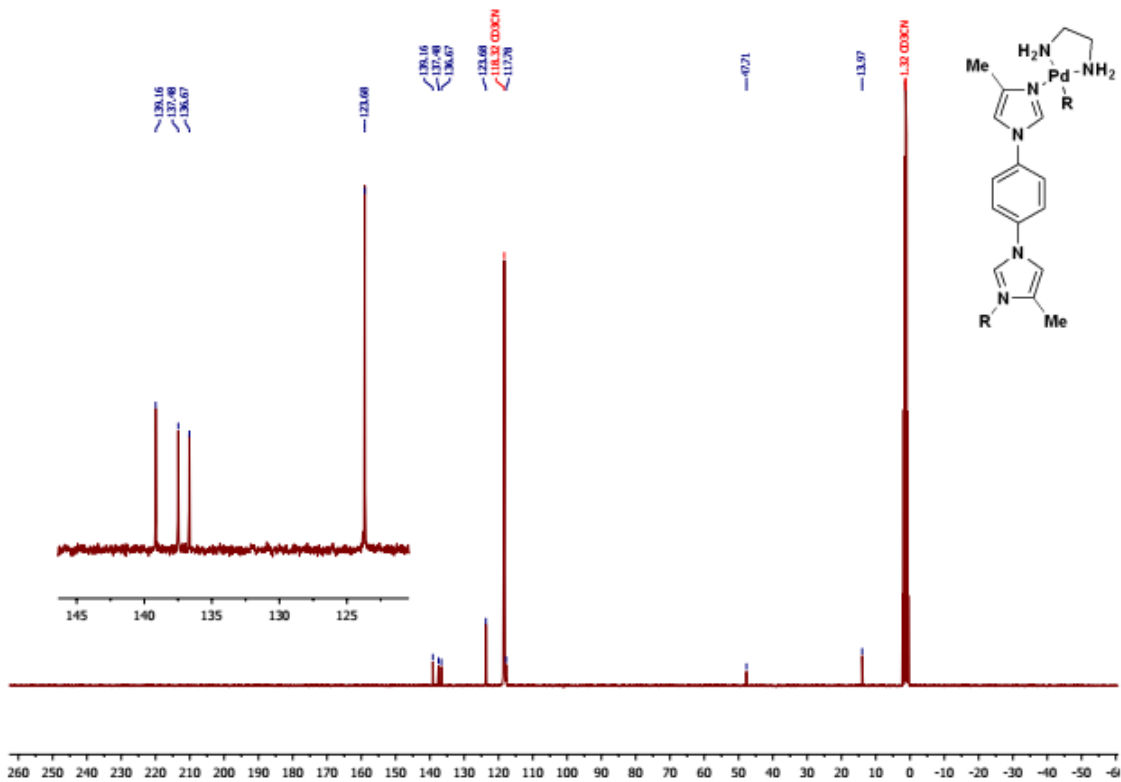
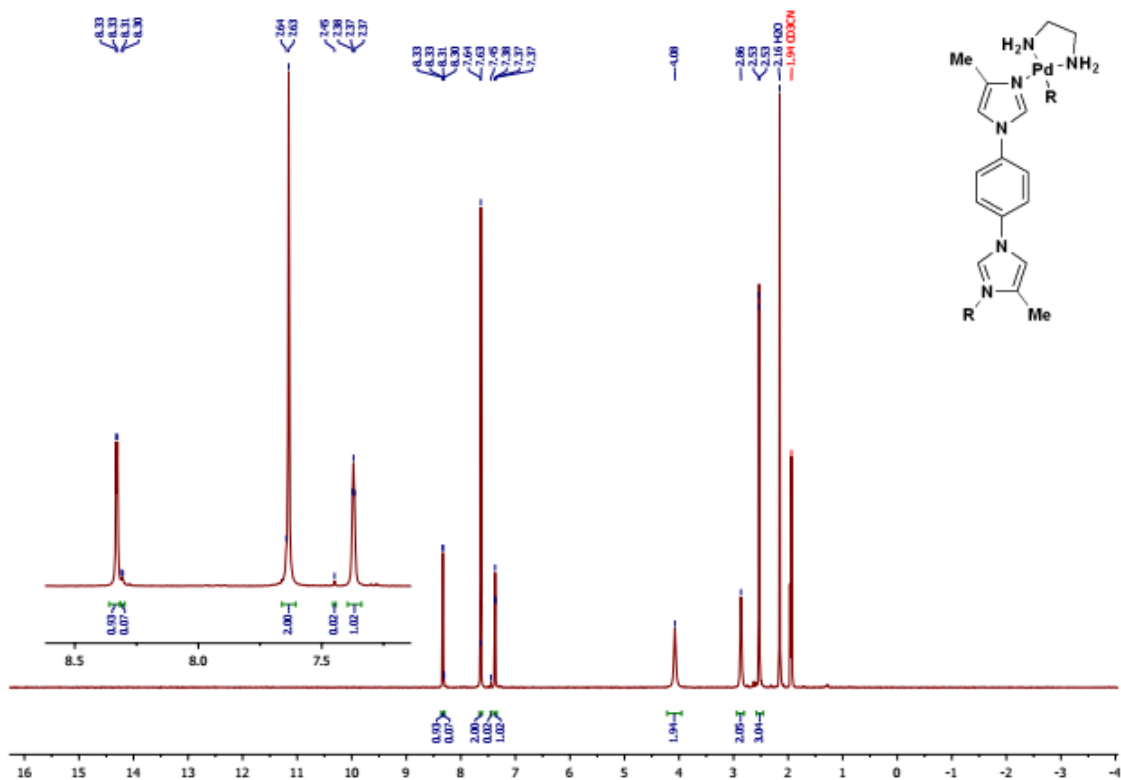
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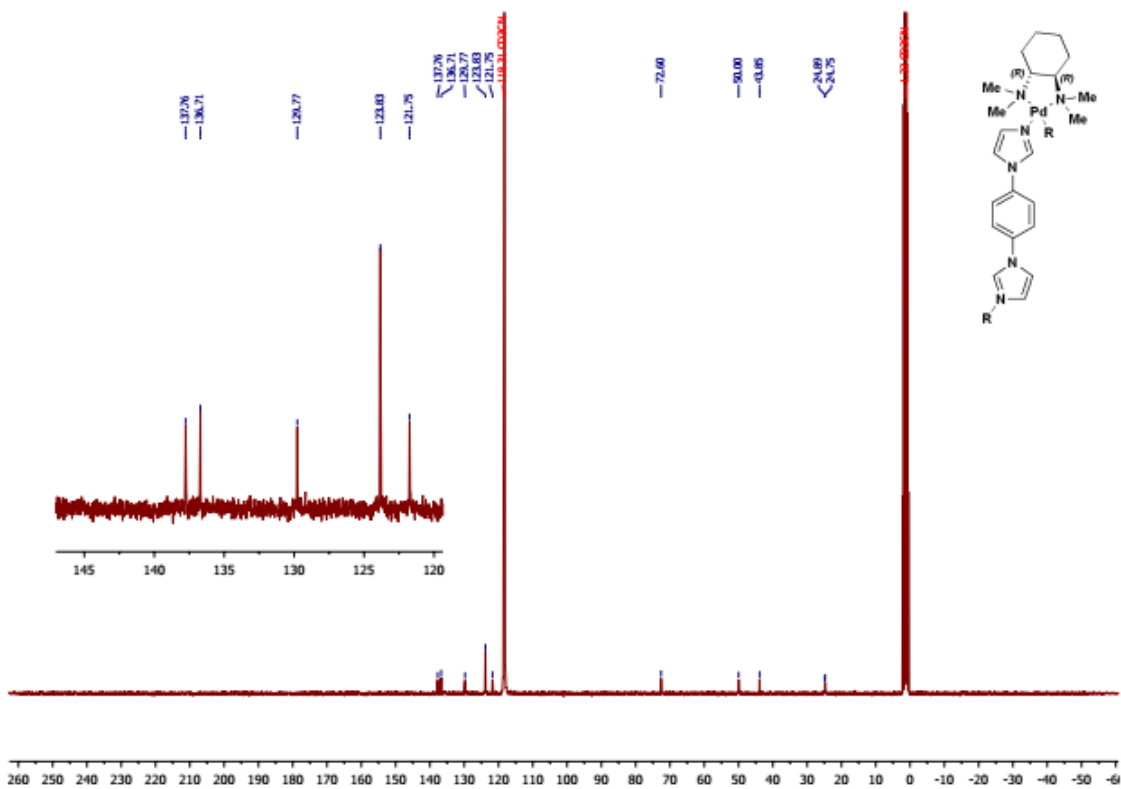
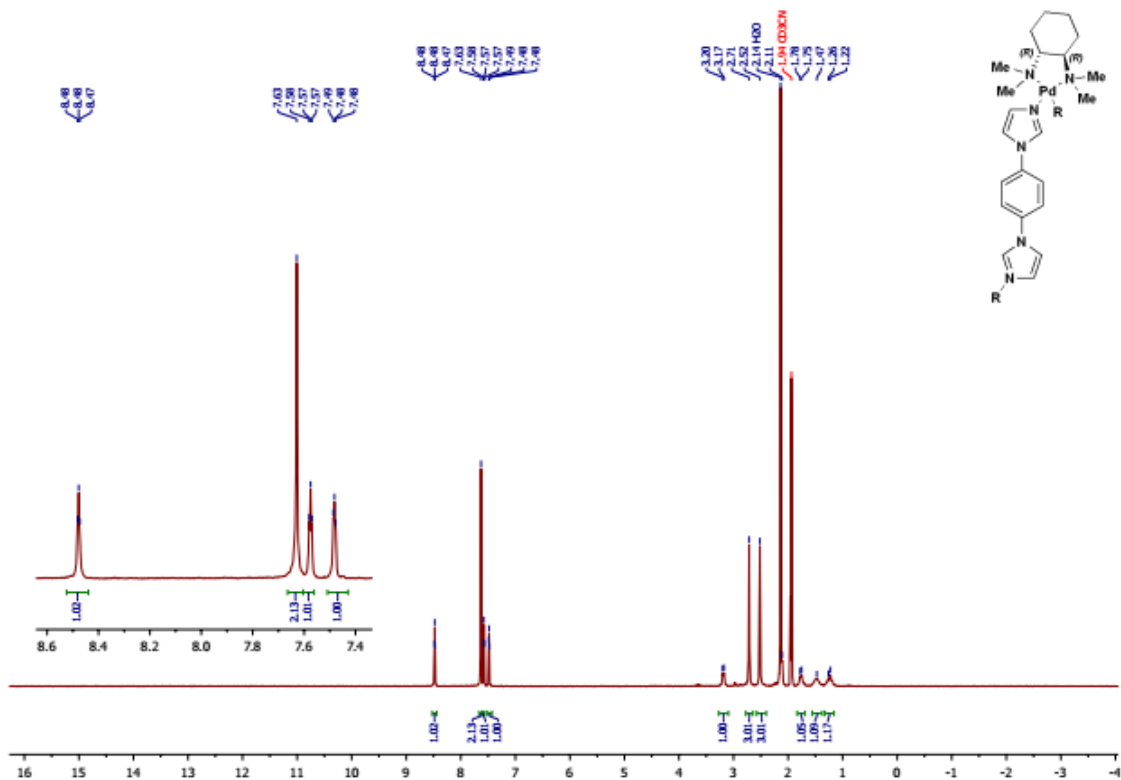
$^1\text{H}/^{13}\text{C}$ NMR spectra of **3**



$^1\text{H}/^{13}\text{C}$ NMR spectra of **4**

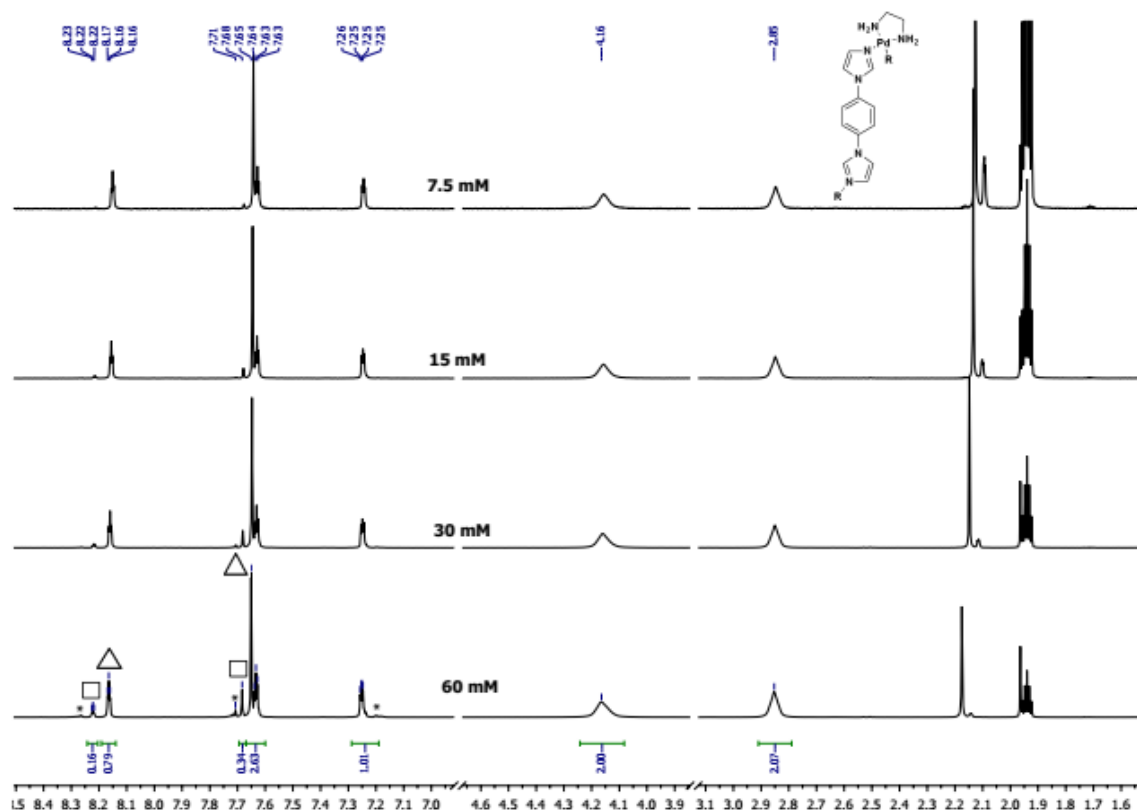


$^1\text{H}/^{13}\text{C}$ NMR spectra of **5**

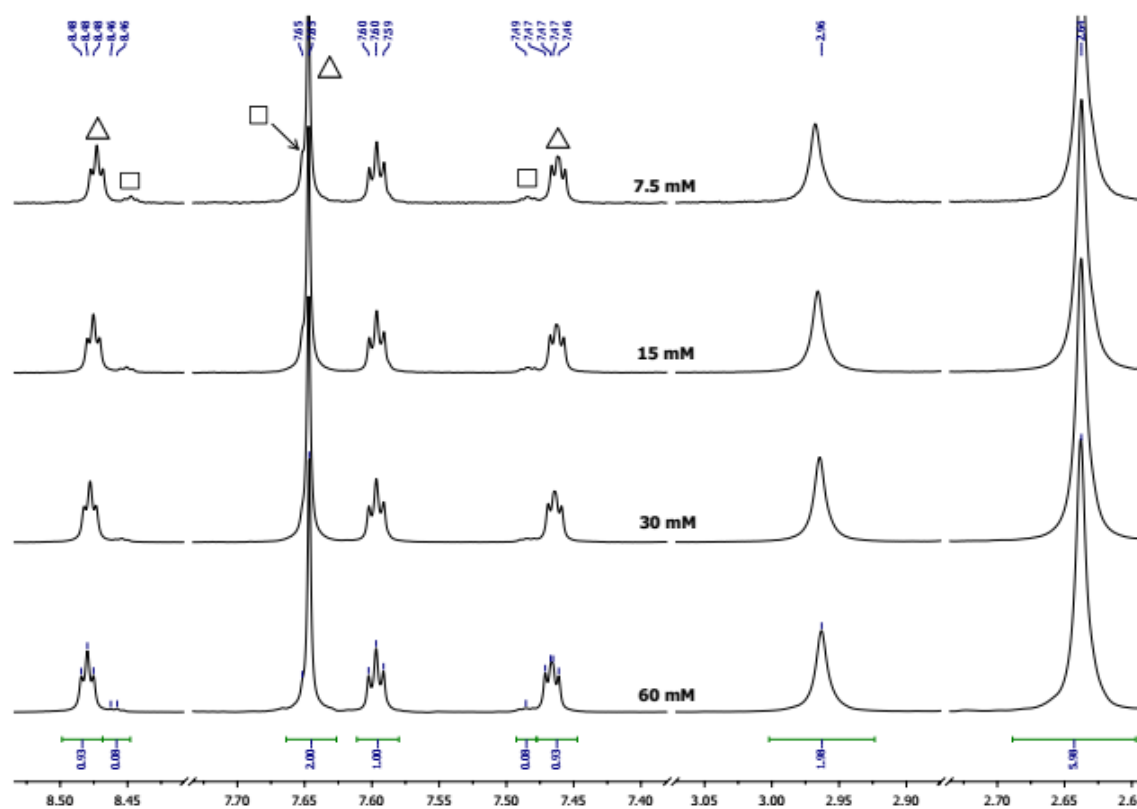


¹H NMR spectra of SCCs 2-4 as a function of concentration

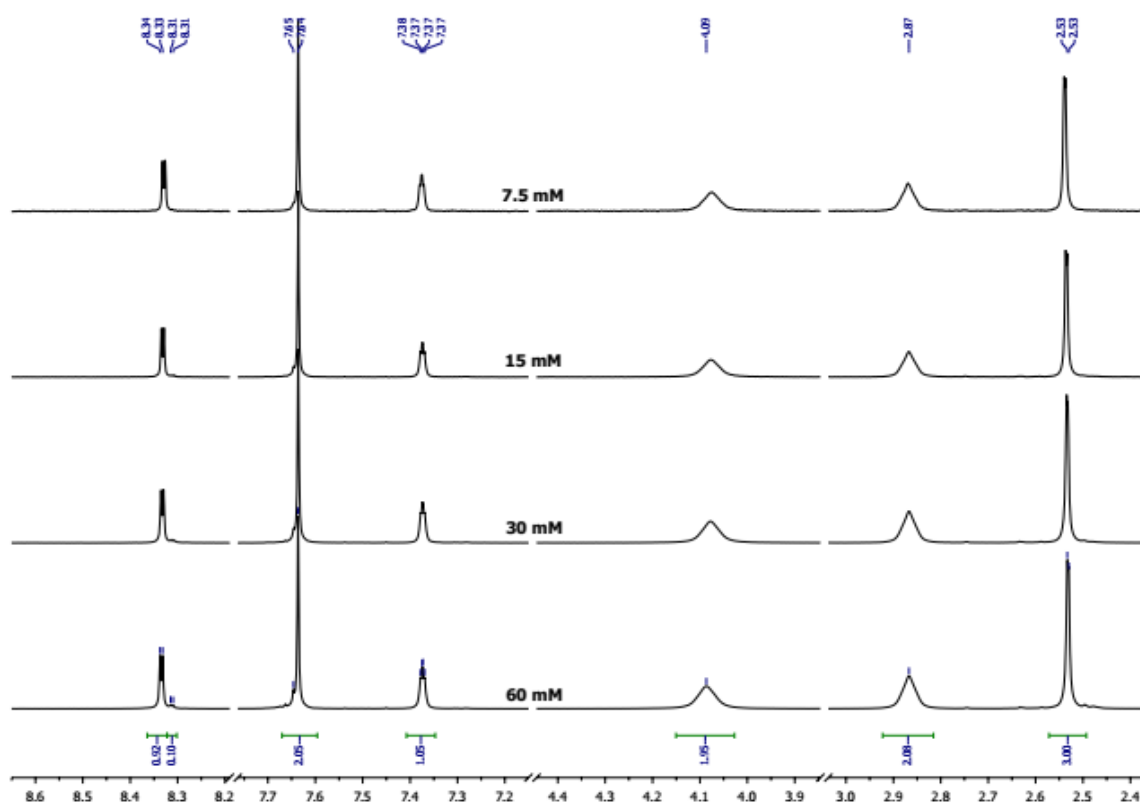
¹H NMR spectra of **2** as a function of its concentration (S1)



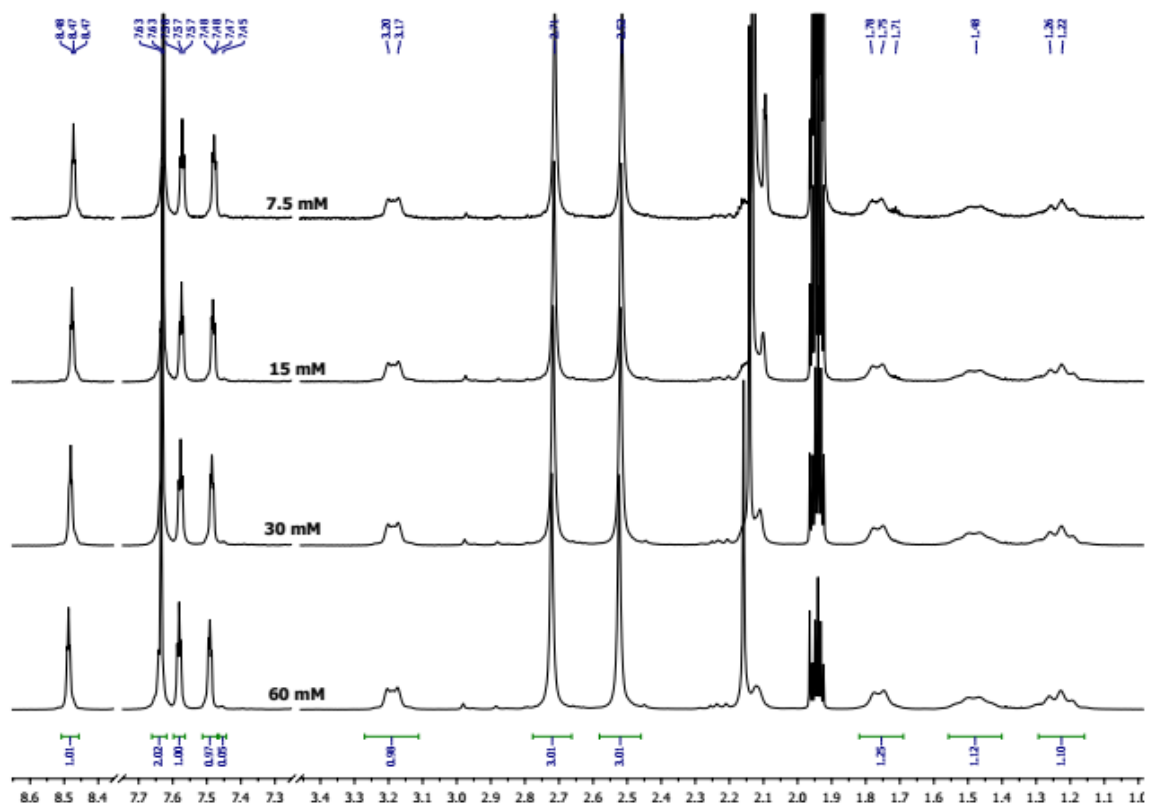
¹H NMR spectra of **3** as a function of its concentration (S2)



^1H NMR spectra of **4** as a function of its concentration (S3)

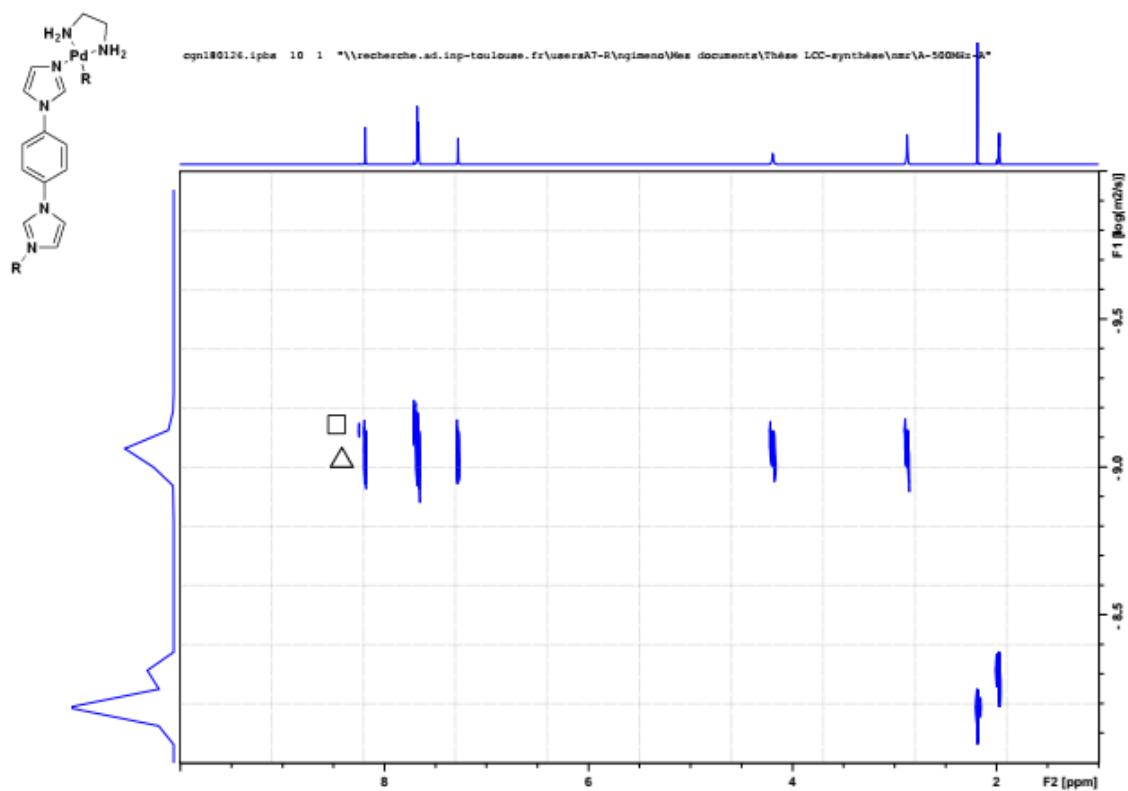


^1H NMR spectra of **5** as a function of its concentration (S4)

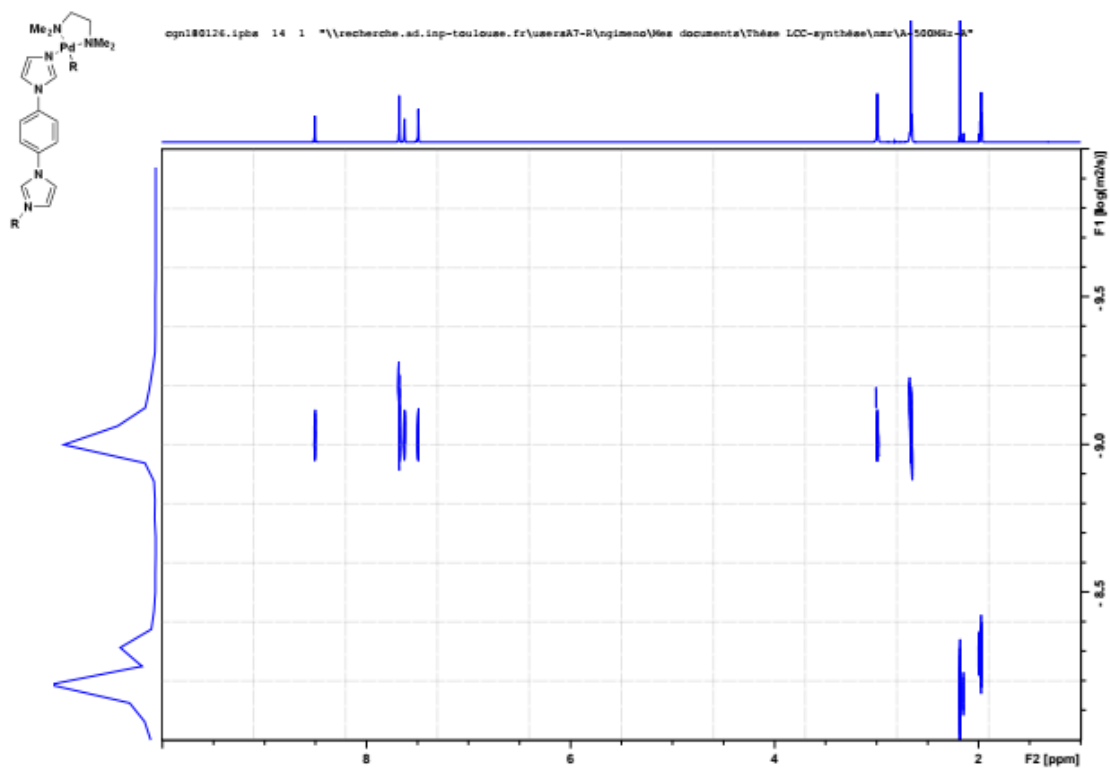


DOSY spectra of SCCs 2-4

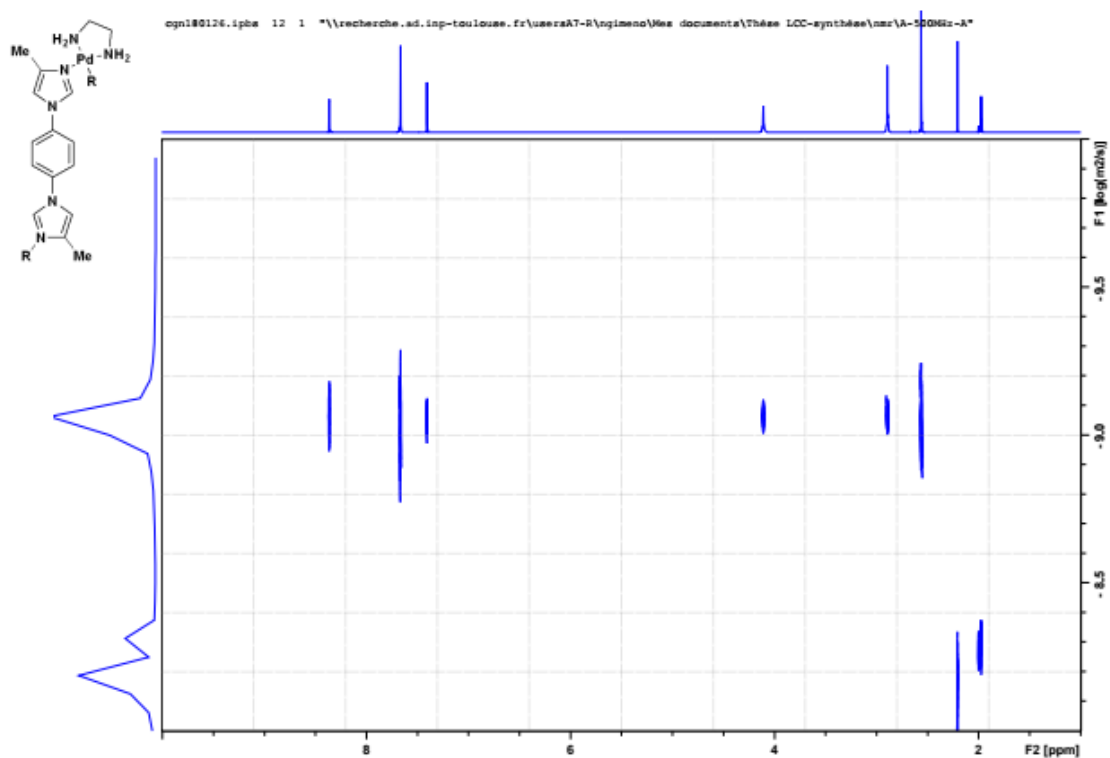
DOSY spectrum of 2 (S5)



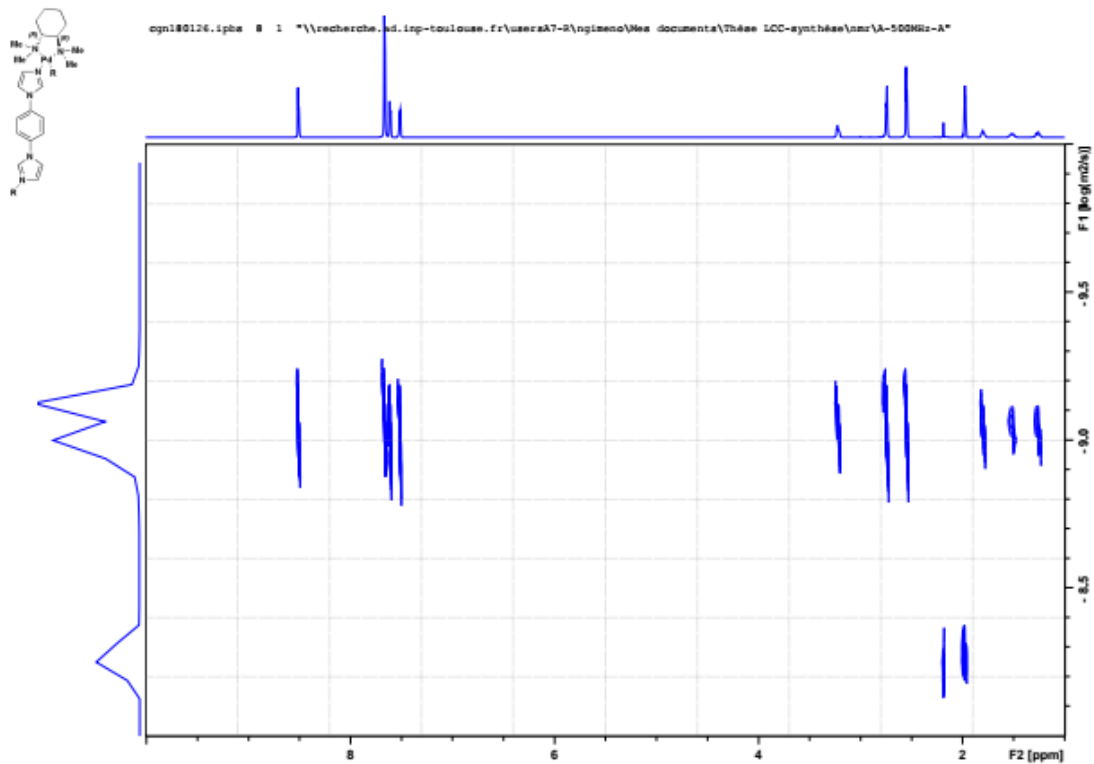
DOSY spectrum of 3 (S6)



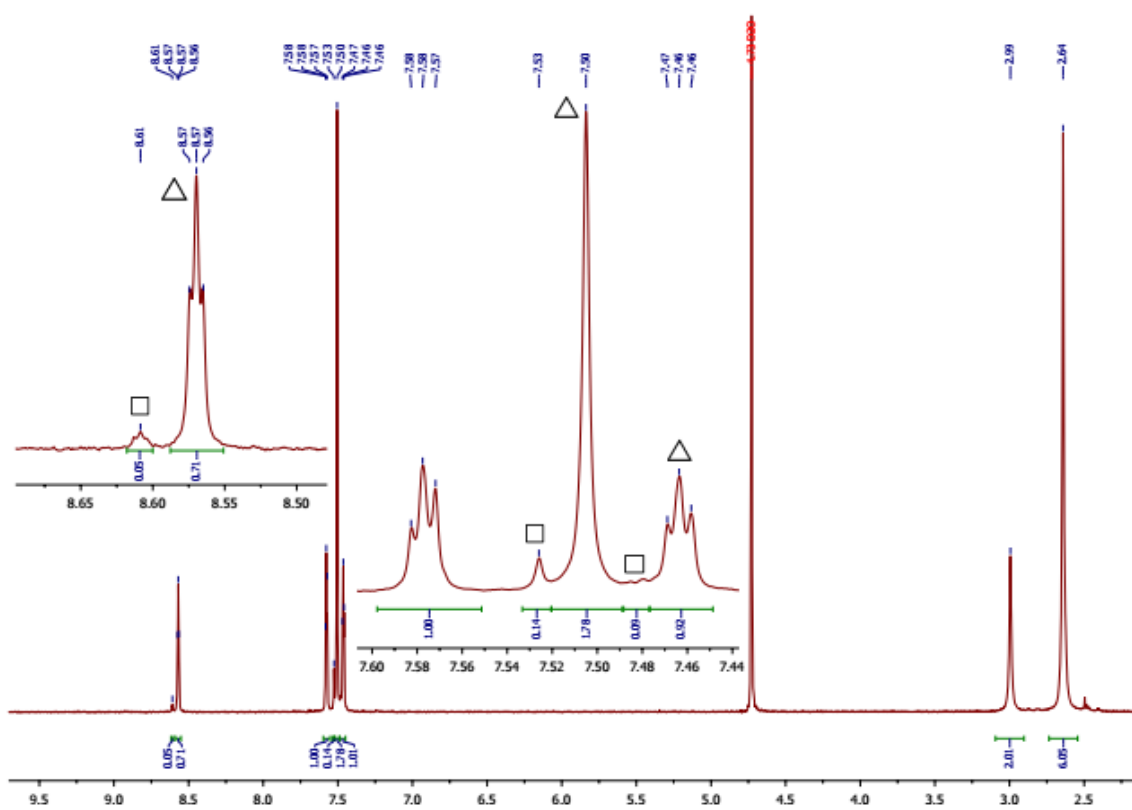
DOSY spectrum of 4 (S7)



DOSY spectrum of 5 (S8)



^1H NMR spectrum of triangle/square **3** in D_2O as the nitrate salts



Diffusion coefficients of triangle/square 3 in D₂O as the nitrate salts (S13)

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SIMFIT RESULTS

Dataset : //recherche.ad.inp-toulouse.fr/usersA7-R/ngimeno/Mes documents/Th
 AREA fit : Diffusion : Variable Gradient :

$I=I[0]*\exp(-D*\text{SQR}(2*\text{PI}*\text{gamma}*\text{Gi}*\text{LD})*(\text{BD}-\text{LD}/3)*1e4)$

16 points for Integral 1, Integral Region from 8.583 to 8.567 ppm

Converged after 68 iterations!

Results Comp. 1

I[0] - 1.534e-002
 Diff Con. - 1.717e-010 m²/s
 Gamma - 4.258e+003 Hz/G
 Little Delta - 2.800m
 Big Delta - 129.900m



RSS - 5.657e-007

SD - 1.880e-004

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	1.555e-002	1.531e-002	-2.327e-004
2	4.592e+000	1.531e-002	1.494e-002	-3.709e-004
3	8.064e+000	1.390e-002	1.415e-002	2.440e-004
4	1.154e+001	1.266e-002	1.300e-002	3.407e-004
5	1.501e+001	1.146e-002	1.159e-002	1.336e-004
6	1.848e+001	9.862e-003	1.003e-002	1.717e-004
7	2.195e+001	8.381e-003	8.427e-003	4.639e-005
8	2.542e+001	7.128e-003	6.869e-003	-2.591e-004
9	2.890e+001	5.574e-003	5.434e-003	-1.401e-004
10	3.237e+001	4.054e-003	4.172e-003	1.180e-004
11	3.584e+001	3.232e-003	3.108e-003	-1.241e-004
12	3.931e+001	2.166e-003	2.247e-003	8.111e-005
13	4.278e+001	1.684e-003	1.577e-003	-1.075e-004
14	4.626e+001	1.042e-003	1.074e-003	3.154e-005
15	4.973e+001	8.106e-004	7.097e-004	-1.009e-004
16	5.320e+001	3.955e-004	4.552e-004	5.973e-005

16 points for Integral 2, Integral Region from 8.554 to 8.525 ppm

Converged after 54 iterations!

Results Comp. 1

I[0] - 1.867e-001
 Diff Con. - 2.008e-010 m²/s
 Gamma - 4.258e+003 Hz/G
 Little Delta - 2.800m
 Big Delta - 129.900m



RSS - 8.675e-006

(1/5)

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SD - 7.363e-004

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	1.861e-001	1.863e-001	2.704e-004
2	4.592e+000	1.804e-001	1.810e-001	6.546e-004
3	8.064e+000	1.689e-001	1.698e-001	9.455e-004
4	1.154e+001	1.540e-001	1.538e-001	-1.392e-004
5	1.501e+001	1.360e-001	1.346e-001	-1.434e-003
6	1.848e+001	1.150e-001	1.136e-001	-1.317e-003
7	2.195e+001	9.369e-002	9.267e-002	-1.018e-003
8	2.542e+001	7.285e-002	7.297e-002	1.173e-004
9	2.890e+001	5.452e-002	5.547e-002	9.535e-004
10	3.237e+001	3.977e-002	4.072e-002	9.488e-004
11	3.584e+001	2.818e-002	2.886e-002	6.809e-004
12	3.931e+001	1.939e-002	1.975e-002	3.677e-004
13	4.278e+001	1.302e-002	1.305e-002	3.676e-005
14	4.626e+001	8.266e-003	8.330e-003	6.400e-005
15	4.973e+001	5.065e-003	5.132e-003	6.683e-005
16	5.320e+001	3.069e-003	3.053e-003	-1.613e-005

16 points for Integral 3, Integral Region from 7.497 to 7.486 ppm

Converged after 64 iterations!

Results Comp. 1

I[0] - 5.218e-002
Diff Con. - 1.911e-010 m2/s
Gamma - 4.258e+003 Hz/G
Little Delta - 2.800m
Big Delta - 129.900m



RSS - 1.394e-005

SD - 9.333e-004

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	5.312e-002	5.209e-002	-1.030e-003
2	4.592e+000	5.207e-002	5.068e-002	-1.386e-003
3	8.064e+000	4.835e-002	4.769e-002	-6.588e-004
4	1.154e+001	4.176e-002	4.341e-002	1.650e-003
5	1.501e+001	3.636e-002	3.822e-002	1.858e-003
6	1.848e+001	3.141e-002	3.254e-002	1.127e-003
7	2.195e+001	2.602e-002	2.680e-002	7.778e-004
8	2.542e+001	2.198e-002	2.134e-002	-6.381e-004
9	2.890e+001	1.728e-002	1.644e-002	-8.363e-004
10	3.237e+001	1.296e-002	1.225e-002	-7.087e-004
11	3.584e+001	9.198e-003	8.831e-003	-3.670e-004
12	3.931e+001	6.424e-003	6.156e-003	-2.686e-004

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13	4.278e+001	4.554e-003	4.150e-003	-4.039e-004
14	4.626e+001	3.190e-003	2.706e-003	-4.838e-004
15	4.973e+001	2.188e-003	1.707e-003	-4.810e-004
16	5.320e+001	1.206e-003	1.041e-003	-1.645e-004

16 points for Integral 4, Integral Region from 7.481 to 7.461 ppm

Converged after 49 iterations!

Results Comp. 1

I[0] - 4.446e-001
Diff Con. - 1.996e-010 m2/s
Gamma - 4.258e+003 Hz/G
Little Delta - 2.800m
Big Delta - 129.900m



RSS - 7.236e-005

SD - 2.127e-003

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	4.434e-001	4.438e-001	3.825e-004
2	4.592e+000	4.297e-001	4.312e-001	1.572e-003
3	8.064e+000	4.015e-001	4.047e-001	3.255e-003
4	1.154e+001	3.670e-001	3.668e-001	-1.368e-004
5	1.501e+001	3.240e-001	3.211e-001	-2.917e-003
6	1.848e+001	2.761e-001	2.714e-001	-4.663e-003
7	2.195e+001	2.249e-001	2.216e-001	-3.268e-003
8	2.542e+001	1.745e-001	1.748e-001	2.340e-004
9	2.890e+001	1.311e-001	1.331e-001	1.995e-003
10	3.237e+001	9.536e-002	9.787e-002	2.510e-003
11	3.584e+001	6.757e-002	6.951e-002	1.942e-003
12	3.931e+001	4.615e-002	4.768e-002	1.530e-003
13	4.278e+001	3.059e-002	3.159e-002	1.004e-003
14	4.626e+001	1.950e-002	2.021e-002	7.161e-004
15	4.973e+001	1.204e-002	1.249e-002	4.490e-004
16	5.320e+001	7.309e-003	7.453e-003	1.443e-004

16 points for Integral 5, Integral Region from 3.010 to 2.916 ppm

Converged after 52 iterations!

Results Comp. 1

I[0] - 4.140e-001
Diff Con. - 1.992e-010 m2/s
Gamma - 4.258e+003 Hz/G
Little Delta - 2.800m
Big Delta - 129.900m



RSS - 2.550e-006

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SD - 3.992e-004

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	4.129e-001	4.132e-001	2.881e-004
2	4.592e+000	4.012e-001	4.016e-001	3.664e-004
3	8.064e+000	3.770e-001	3.769e-001	-4.665e-005
4	1.154e+001	3.423e-001	3.417e-001	-5.386e-004
5	1.501e+001	2.992e-001	2.992e-001	8.430e-006
6	1.848e+001	2.539e-001	2.531e-001	-8.258e-004
7	2.195e+001	2.068e-001	2.067e-001	-1.277e-004
8	2.542e+001	1.625e-001	1.631e-001	5.916e-004
9	2.890e+001	1.238e-001	1.243e-001	4.884e-004
10	3.237e+001	9.093e-002	9.146e-002	5.332e-004
11	3.584e+001	6.534e-002	6.502e-002	-3.260e-004
12	3.931e+001	4.492e-002	4.464e-002	-2.750e-004
13	4.278e+001	2.940e-002	2.960e-002	1.988e-004
14	4.626e+001	1.925e-002	1.896e-002	-2.925e-004
15	4.973e+001	1.213e-002	1.173e-002	-4.022e-004
16	5.320e+001	6.997e-003	7.009e-003	1.113e-005

16 points for Integral 6, Integral Region from 2.634 to 2.594 ppm

Converged after 47 iterations!

Results Comp. 1

I[0] - 1.001e+000
Diff Con. - 2.020e-010 m2/s
Gamma - 4.258e+003 Hz/G
Little Delta - 2.800m
Big Delta - 129.900m



RSS - 4.965e-005

SD - 1.762e-003

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	1.000e+000	9.995e-001	-5.332e-004
2	4.592e+000	9.703e-001	9.709e-001	6.461e-004
3	8.064e+000	9.077e-001	9.105e-001	2.832e-003
4	1.154e+001	8.236e-001	8.243e-001	6.636e-004
5	1.501e+001	7.219e-001	7.204e-001	-1.452e-003
6	1.848e+001	6.120e-001	6.078e-001	-4.190e-003
7	2.195e+001	4.975e-001	4.951e-001	-2.430e-003
8	2.542e+001	3.886e-001	3.893e-001	6.598e-004
9	2.890e+001	2.935e-001	2.955e-001	2.016e-003
10	3.237e+001	2.135e-001	2.165e-001	2.973e-003
11	3.584e+001	1.523e-001	1.532e-001	8.856e-004
12	3.931e+001	1.044e-001	1.046e-001	2.320e-004

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13	4.278e+001	6.931e-002	6.896e-002	-3.559e-004
14	4.626e+001	4.422e-002	4.389e-002	-3.338e-004
15	4.973e+001	2.736e-002	2.696e-002	-3.974e-004
16	5.320e+001	1.658e-002	1.599e-002	-5.875e-004

16 points for Integral 7, Integral Region from 2.594 to 2.581 ppm

Converged after 57 iterations!

Results Comp. 1

I[0] - 9.468e-002

Diff Con. - 1.898e-010 m2/s

Gamma - 4.258e+003 Hz/G

Little Delta - 2.800m

Big Delta - 129.900m

RSS - 1.521e-005

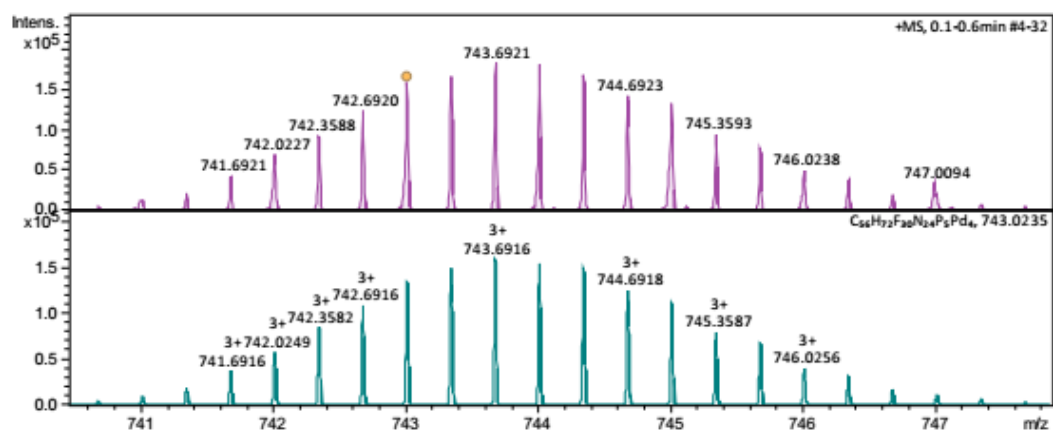
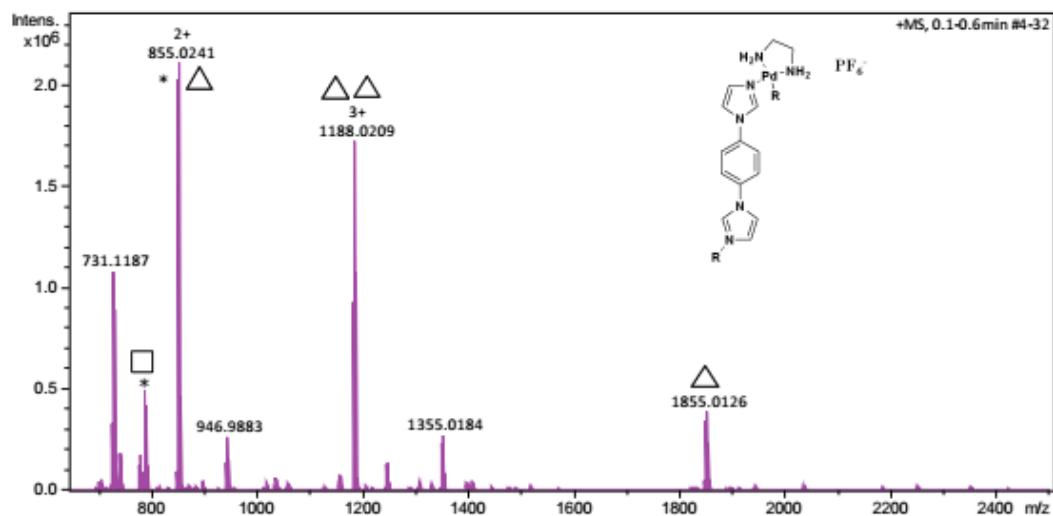
SD - 9.749e-004

Point	Gradient	Expt	Calc	Difference
1	1.120e+000	9.355e-002	9.451e-002	9.626e-004
2	4.592e+000	9.006e-002	9.198e-002	1.917e-003
3	8.064e+000	8.754e-002	8.659e-002	-9.468e-004
4	1.154e+001	8.107e-002	7.886e-002	-2.208e-003
5	1.501e+001	7.109e-002	6.949e-002	-1.599e-003
6	1.848e+001	5.893e-002	5.923e-002	3.067e-004
7	2.195e+001	4.806e-002	4.885e-002	7.837e-004
8	2.542e+001	3.803e-002	3.897e-002	9.416e-004
9	2.890e+001	2.945e-002	3.008e-002	6.288e-004
10	3.237e+001	2.270e-002	2.246e-002	-2.414e-004
11	3.584e+001	1.639e-002	1.622e-002	-1.656e-004
12	3.931e+001	1.172e-002	1.134e-002	-3.803e-004
13	4.278e+001	7.690e-003	7.666e-003	-2.380e-005
14	4.626e+001	4.802e-003	5.014e-003	2.124e-004
15	4.973e+001	3.278e-003	3.173e-003	-1.050e-004
16	5.320e+001	1.908e-003	1.942e-003	3.451e-005

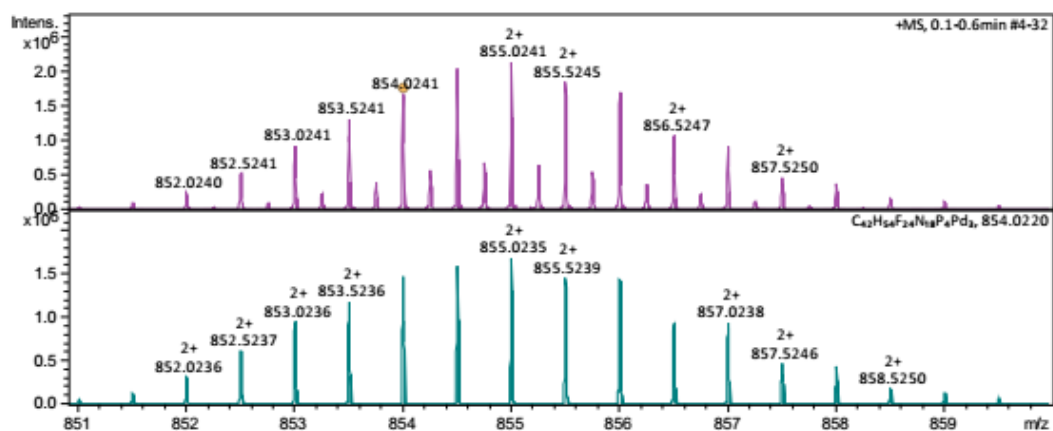
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CSI spectra of SCCs 2-4

CSI mass spectrum of 2 (S9)

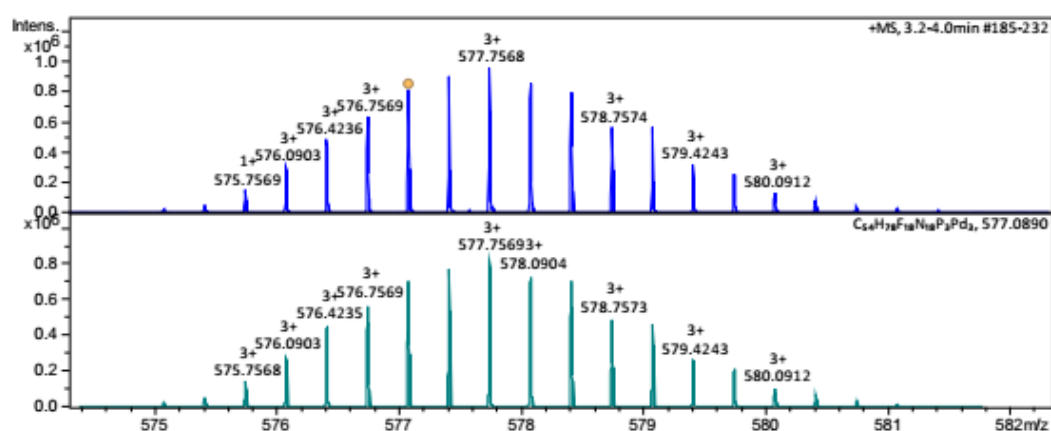
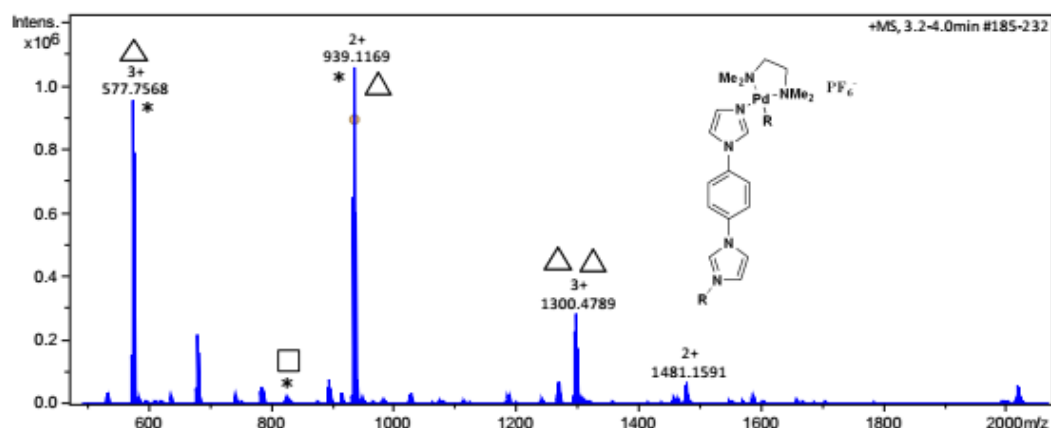


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Adduct	z
743.023476	C ₅₆ H ₇₂ F ₃₀ N ₁₄ P ₅ Pd ₄	743.02346	1.9	25.3	M	3+

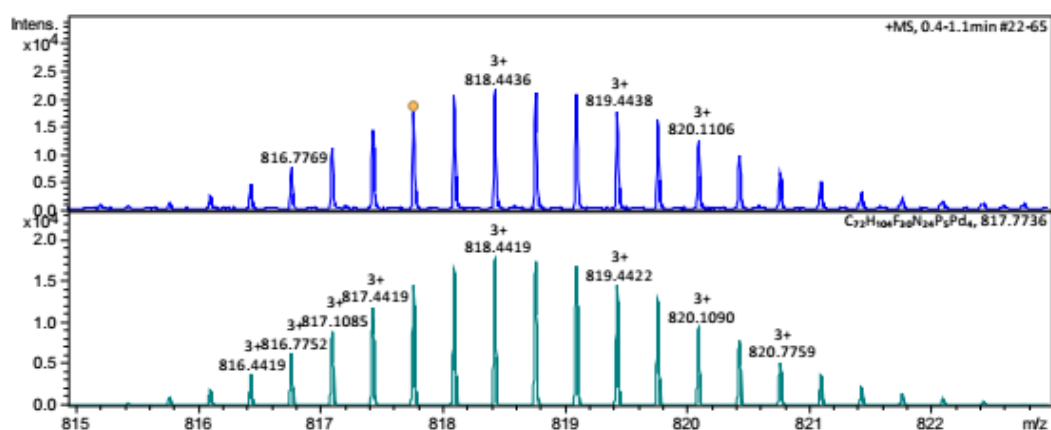


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Adduct	z
854.024074	C ₄₂ H ₅₄ F ₂₄ N ₁₈ P ₄ Pd ₃	854.021984	-0.7	18.3	M	2+

CSI mass spectrum of **3** (S10)

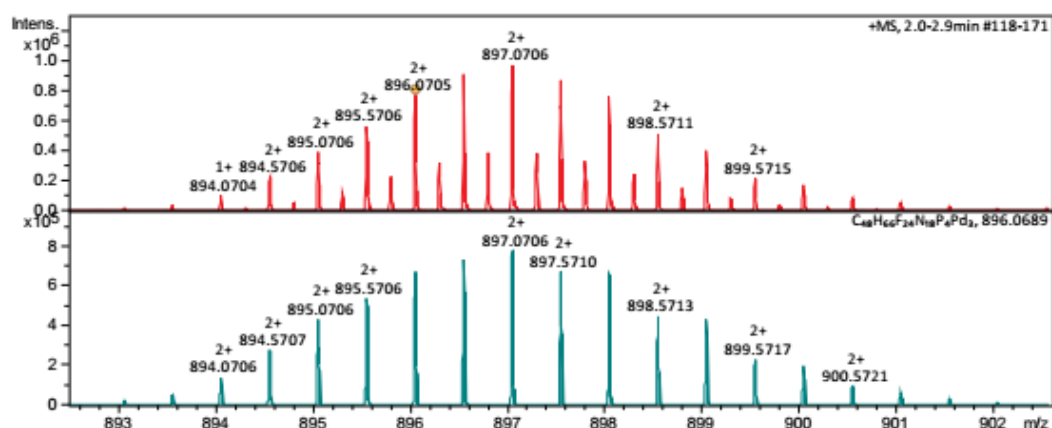
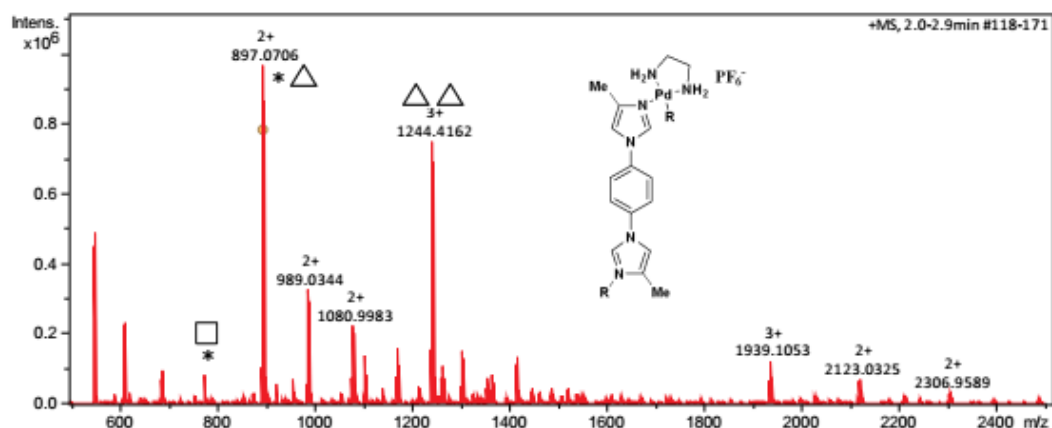


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Score	Adduct	z
577.0902	C54H78F18N18Pd3	577.089	-0.1	17.8	100	M	3+
938.1169	C54H78F24N18Pd4	938.1159	0.8	17.3	100	M	2+

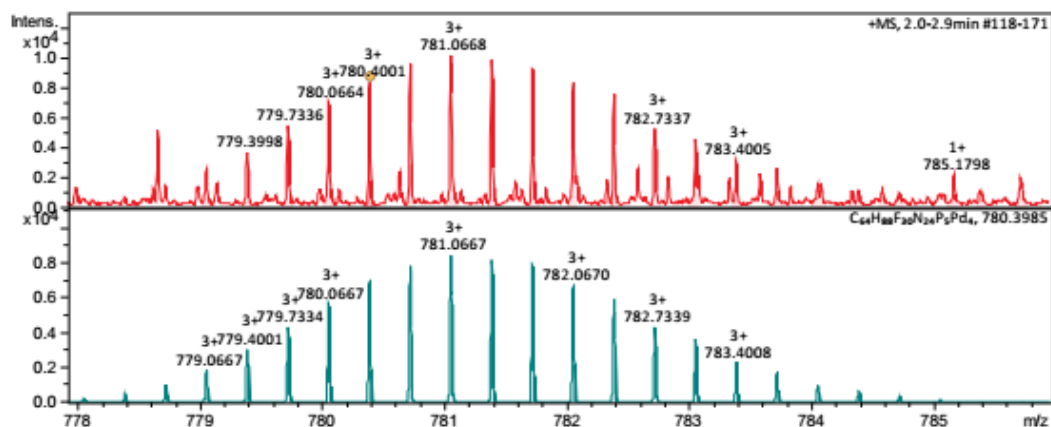


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Score	Adduct	z
817.7768	C72H104F30N24Pd4	817.7736	-2	22.4	100	M	3+

CSI mass spectrum of 4 (S11)

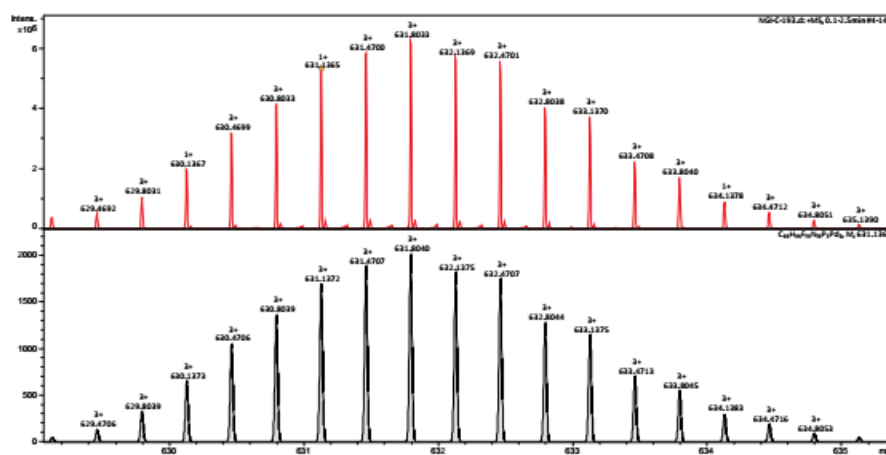
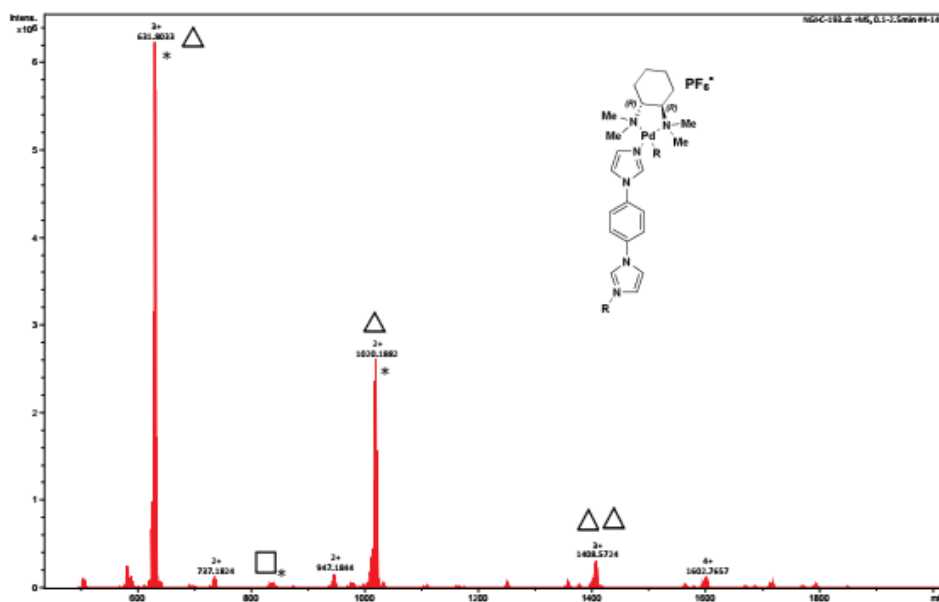


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Score	Adduct	z
896.0705	C48H66F24N18Pd3	896.0689	0	18.4	100	M	2+

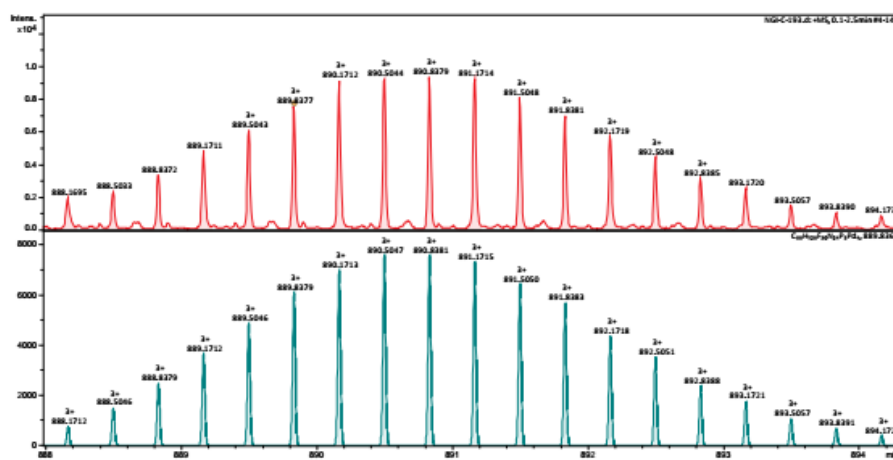


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Score	Adduct	z
780.4001	C64H88F30N24P5Pd4	780.3985	0	26.9	100	M	3+

CSI mass spectrum of 5 (S12)



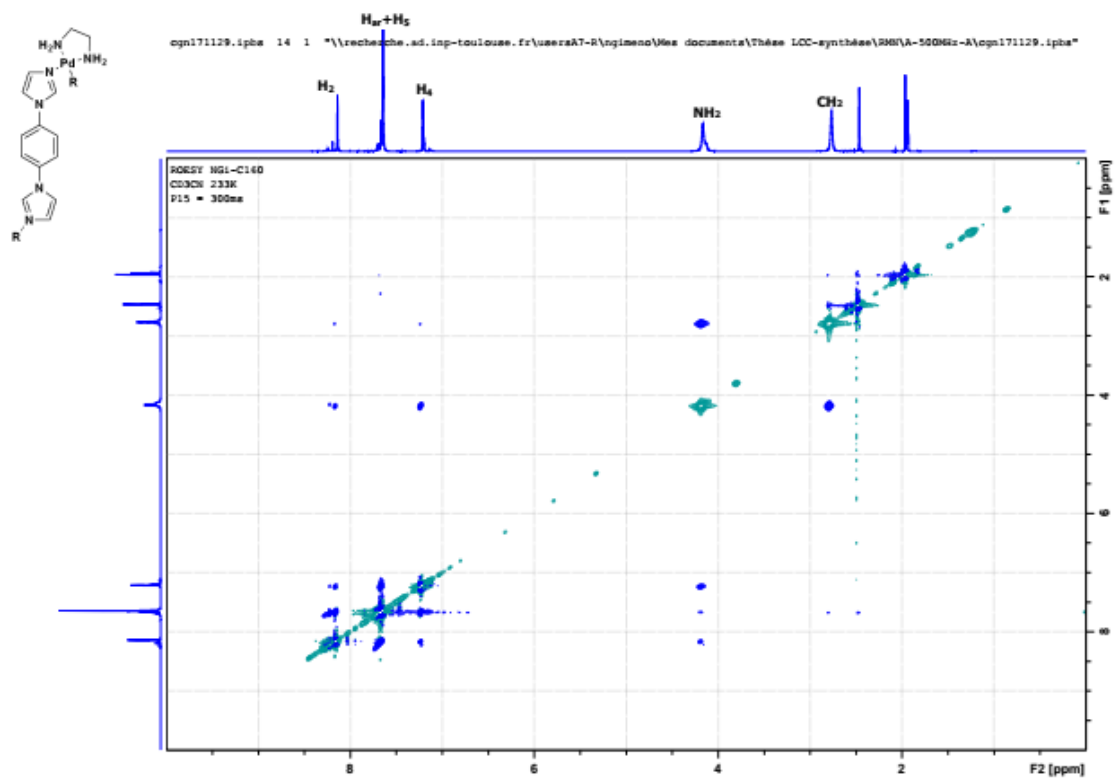
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Score	Adduct	z
631.1365	C66H96F18N18P3Pd3	631.136	1.1	13.7	100	M	1+



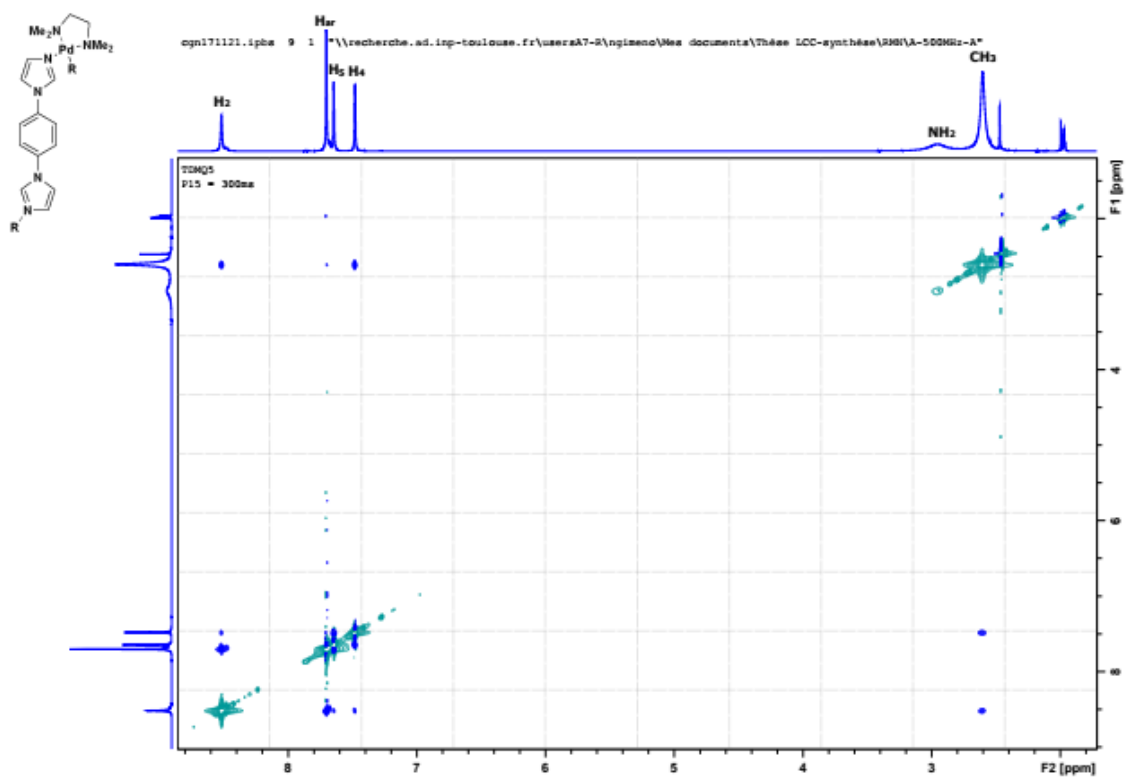
Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	Score	Adduct	z
889.8377	C88H128F30N24P5Pd4	889.8362	0.3	46	100	M	3+

ROESY spectra of SCCs 2-4 at 233K

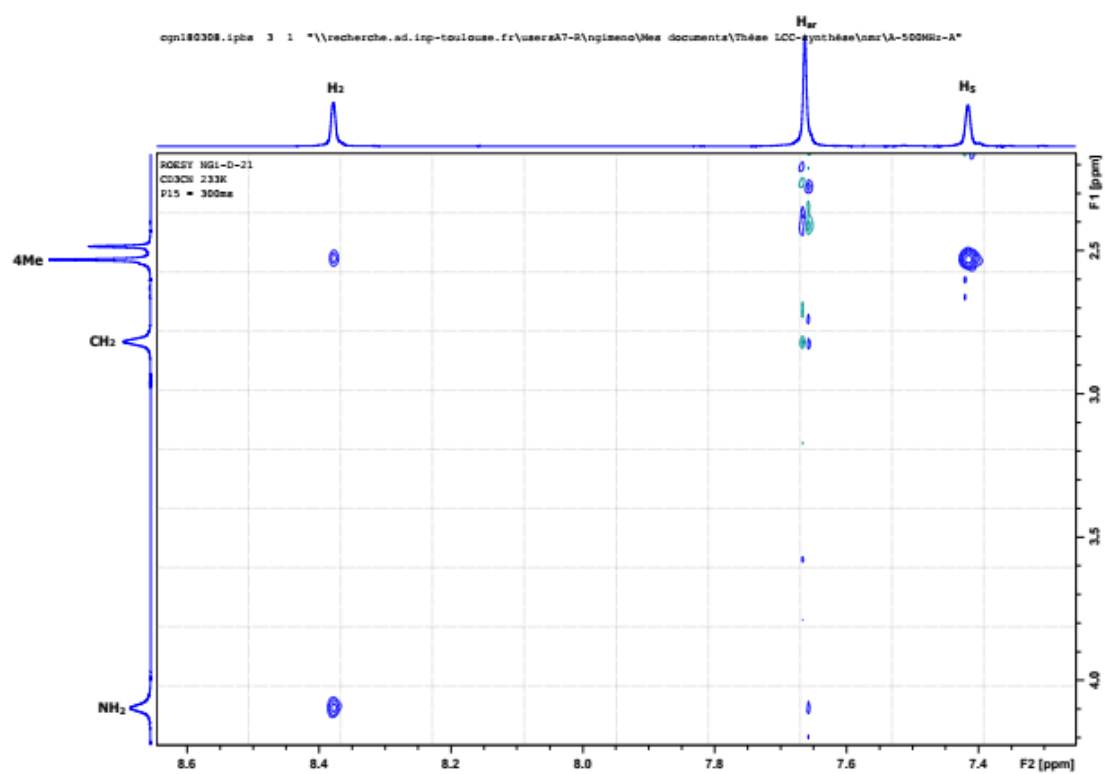
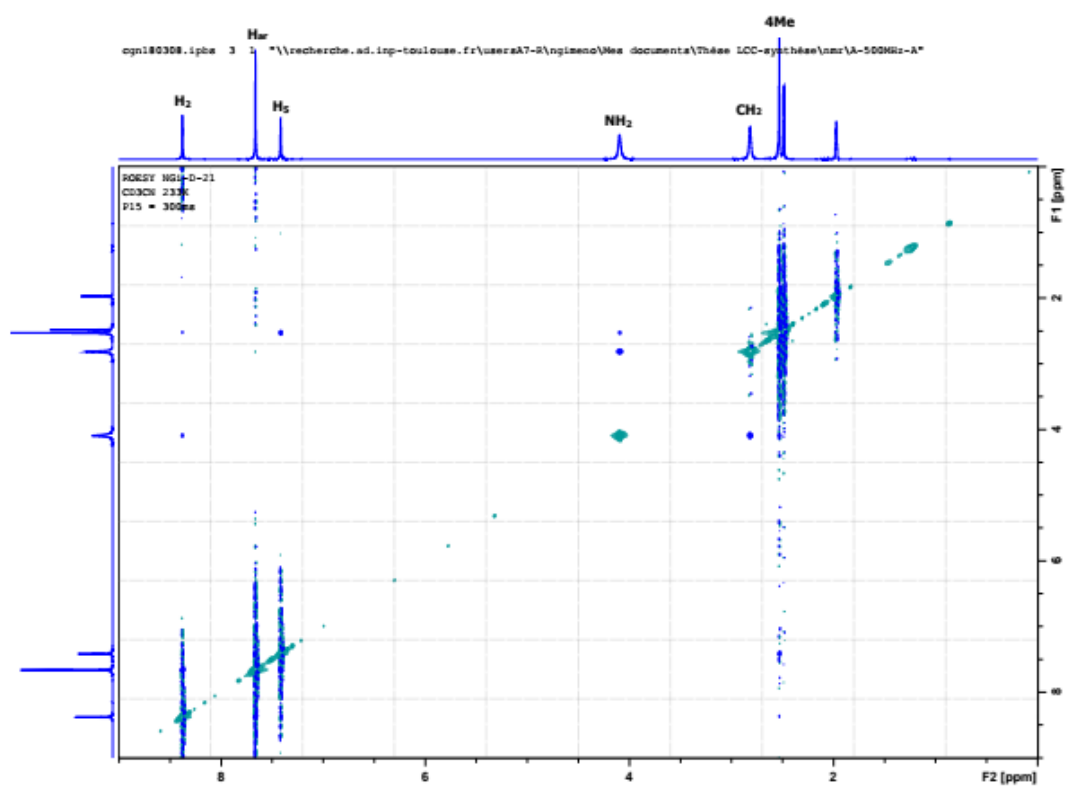
ROESY spectrum of 2 at 233K



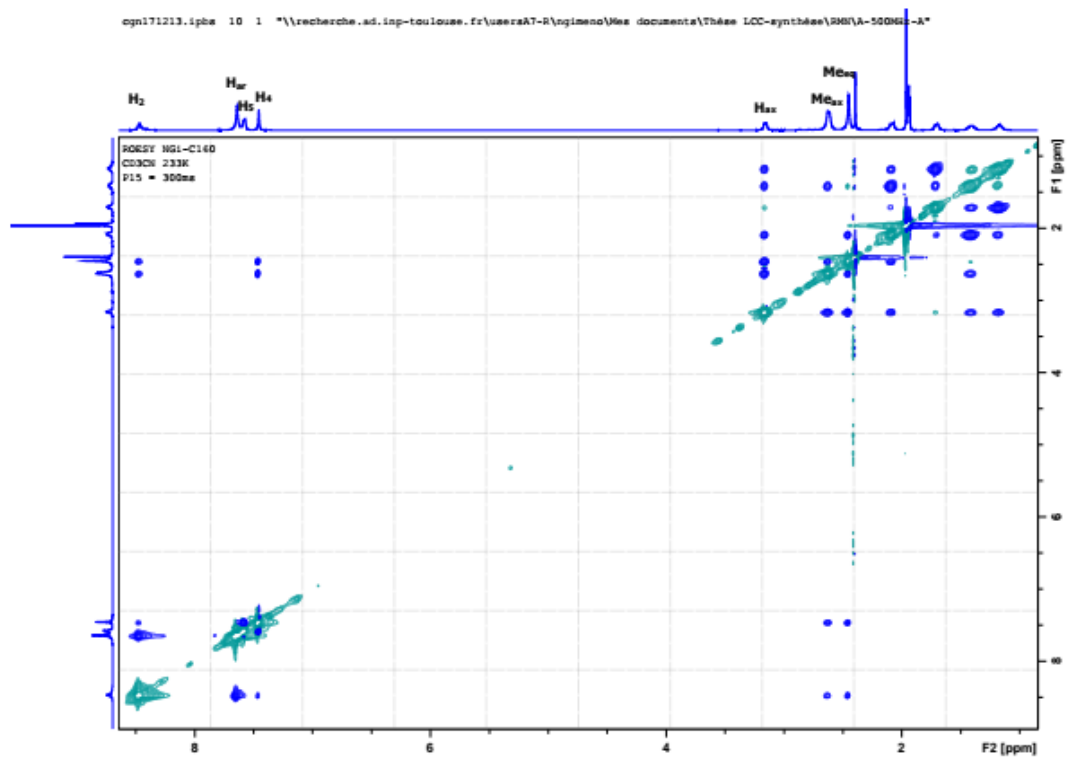
ROESY spectrum of 3 at 233K



ROESY spectrum of 4 at 233K

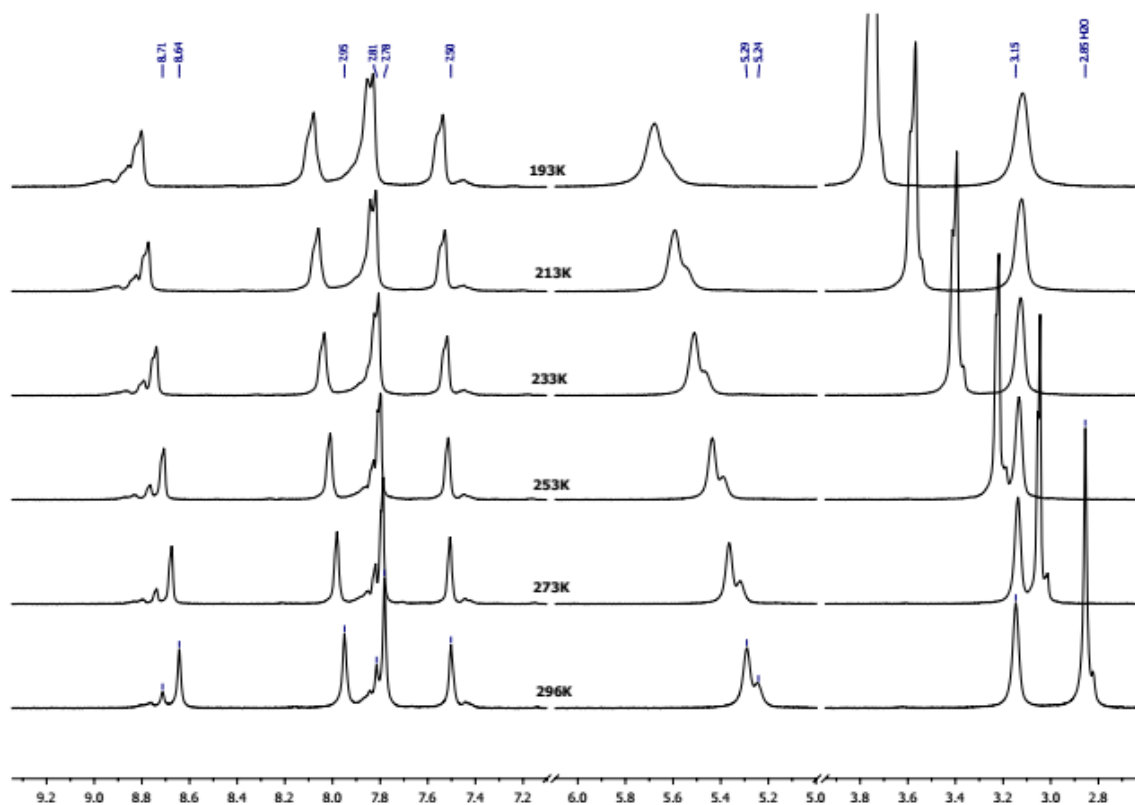


ROESY spectrum of **5** at 233K

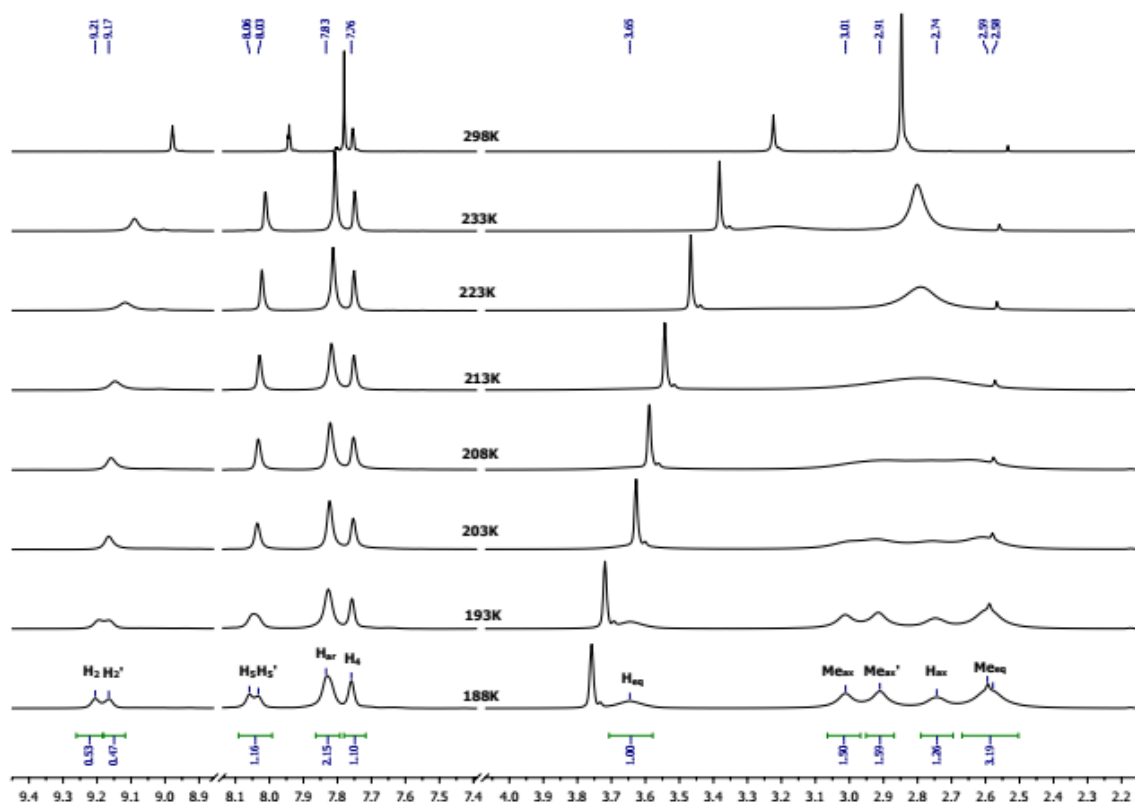


^1H VT-NMR spectra of SCCs 2-4

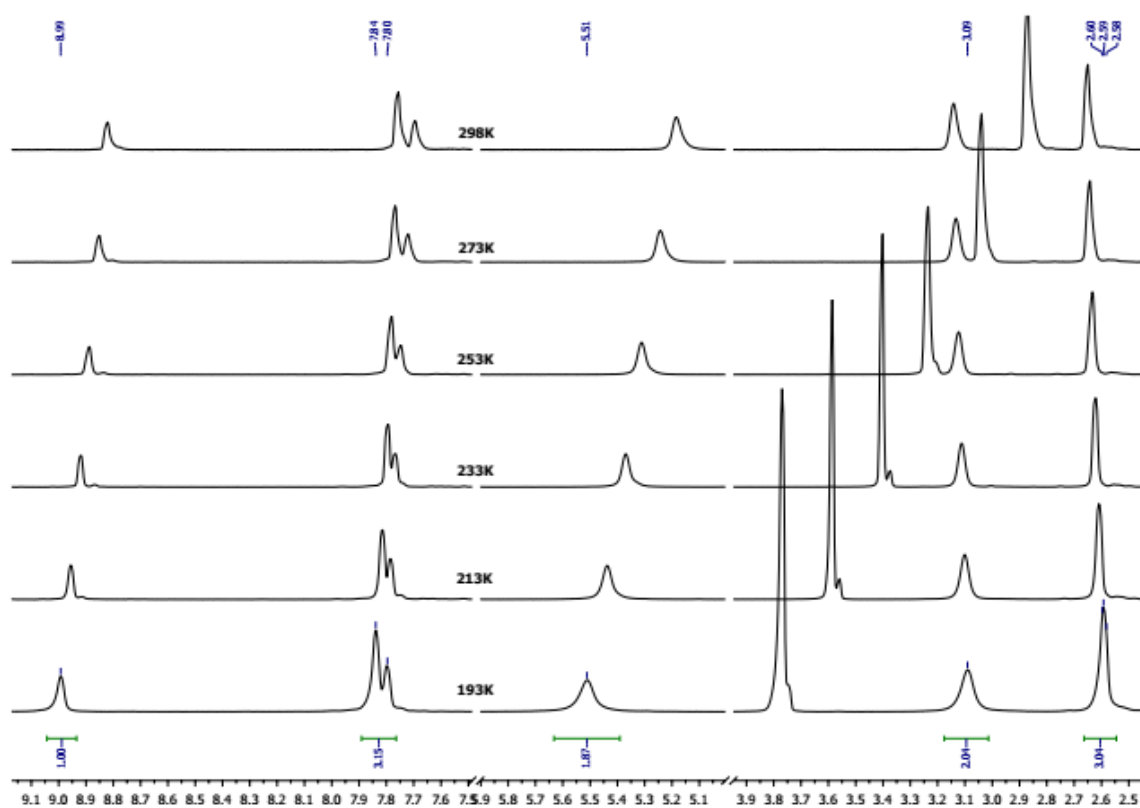
^1H VT-NMR spectra of 2



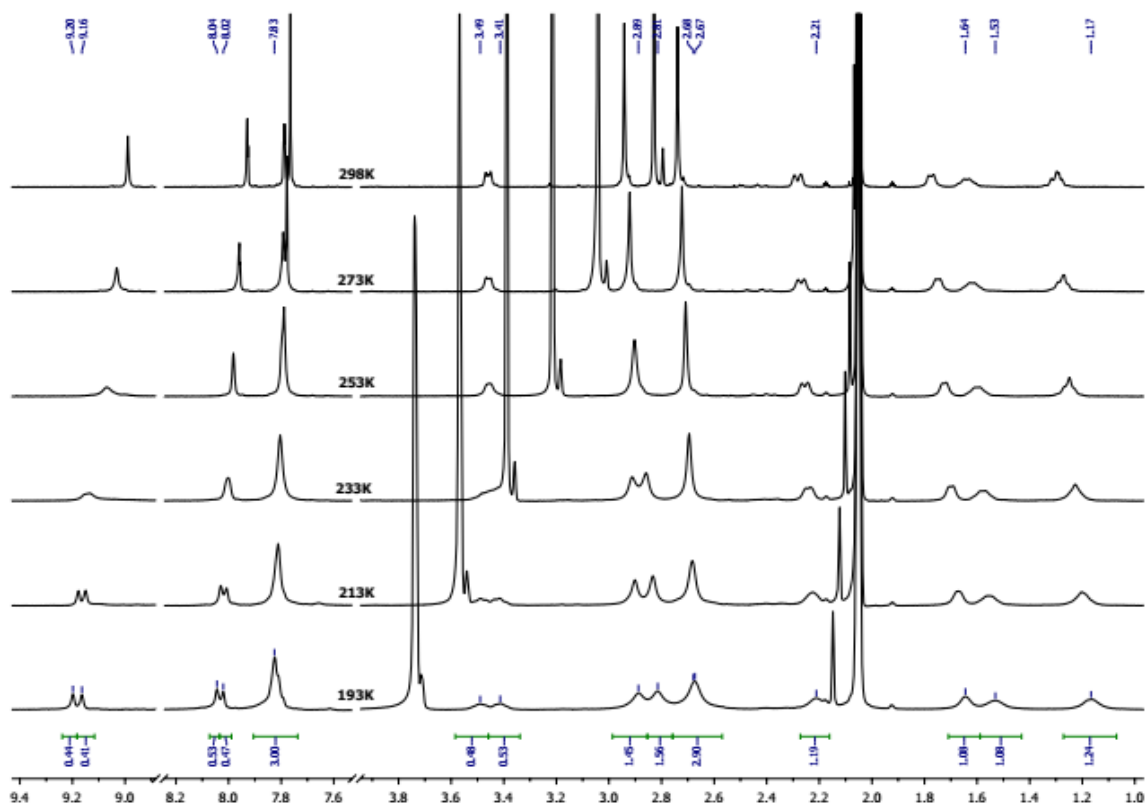
^1H VT-NMR spectra of 3 (S15)



¹H VT-NMR spectra of **4**

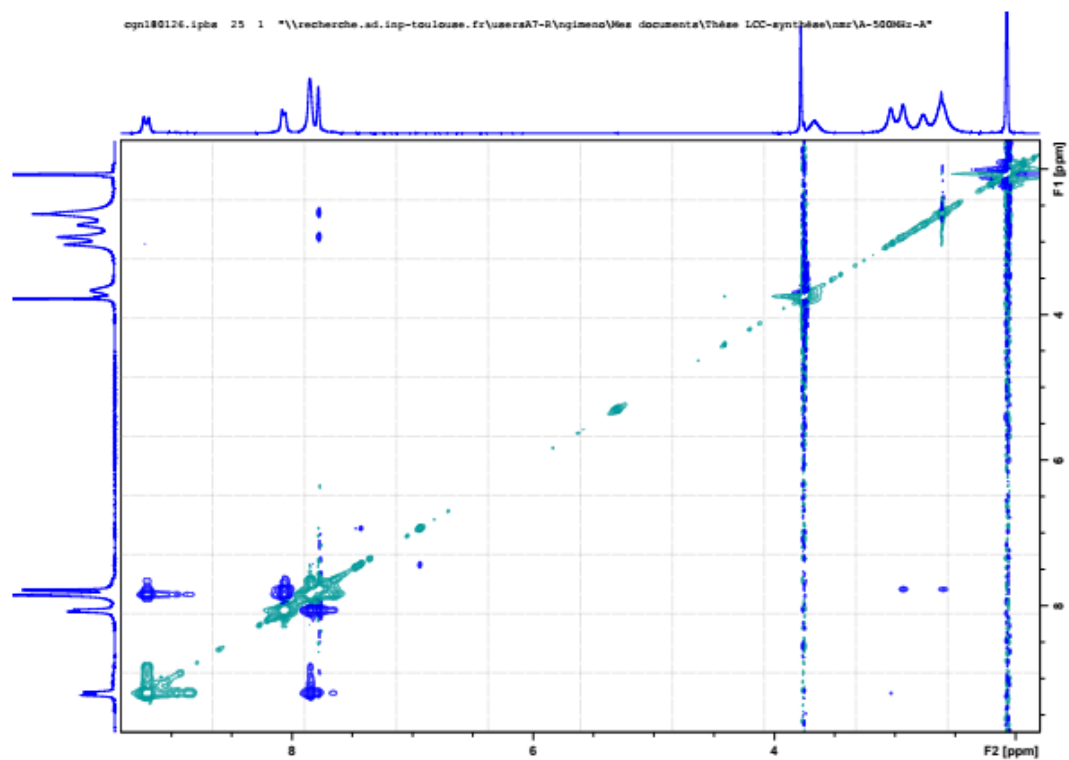


¹H VT-NMR spectra of **5** (S14)



ROESY NMR spectra of SCCs 3 and 5 at low temperatures

ROESY spectrum of **3** at 188K (S16)



ROESY spectrum of **5** at 193K (S17)

