Electronic supplementary information (ESI) for

1,1′-Binaphthyl-Based Imidazolium Chemosensors for Highly Selective Recognition of Tryptophan in Aqueous Solutions

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I. General remarks of optical spectroscopic studies

The studies on the binding properties of (*R*)-**1** were carried out in H_2O (10 mM HEPES buffer, pH 7.4) and the other receptors were performed in CH_3OH/H_2O system (1:1, 10 mM HEPES buffer, pH 7.4). Amino acids were also dissolved in a HEPES buffer solution (10 mM HEPES buffer, pH 7.4). Methanol was either HPLC or spectroscopic grade and water was distilled for twice. All solutions were prepared using volumetric syringes, pipettes, and volumetric flasks. The stock solutions of fluorophores and amino acids were freshly prepared and used for each measurement. Each time a 3 mL of receptor was filled in a quartz cell of 1 cm of optical path length, and the stock solution of amino acid was added into a quartz cell dropwise using a micro-syringe. The volume of amino acid stock solution added was less than 100 μL to remain the concentration of receptor unchanged. Absorption spectra were detected on a HITACHI U-2910 absorption spectrophotometer. Fluorescent emission spectra were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer.

II. Binding studies of (*R*)-1-5 with α-amino acids

i). Fluorescence spectra of (*R*)-3, (*R*)-4, and (*R*)-5 with various α-amino acids

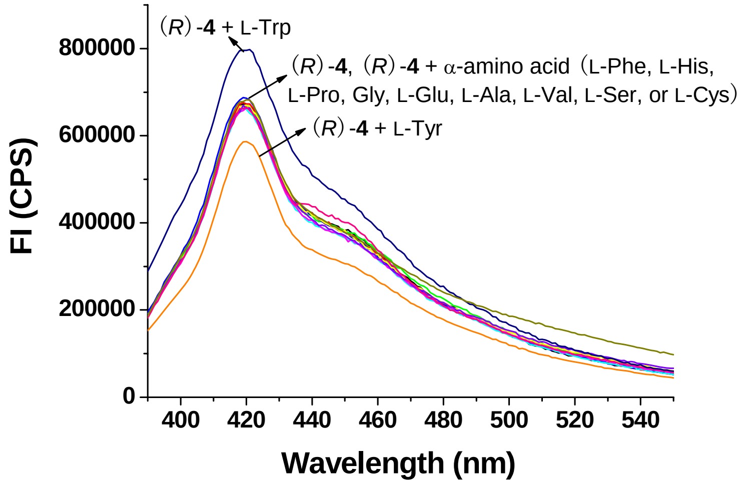


Fig. S1 Changes in fluorescence intensity of (*R*)-**4** (1 μM) upon addition of 200 equiv of various natural amino acids in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) with excitation at 369 nm (excitation and emission slit: 5 nm).

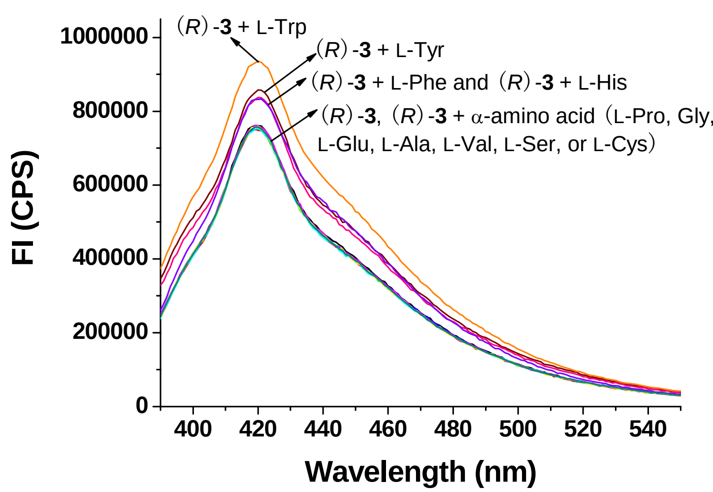


Fig. S2 Changes in fluorescence intensity of (*R*)-**3** (1 μM) upon addition of 200 equiv of various natural amino acids in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) with excitation at 369 nm (excitation and emission slit: 5 nm).

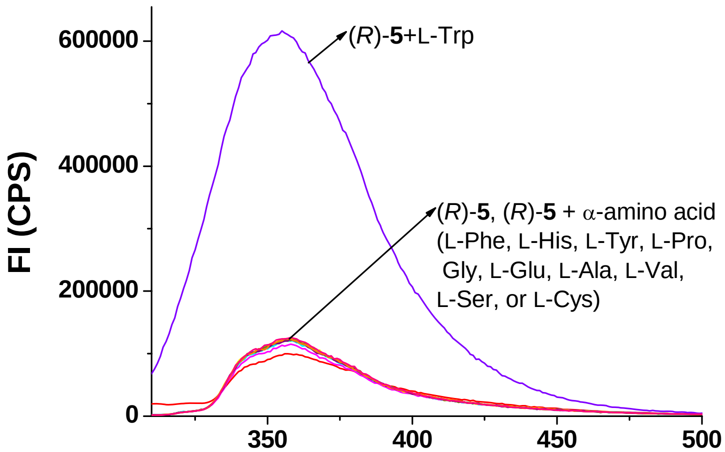
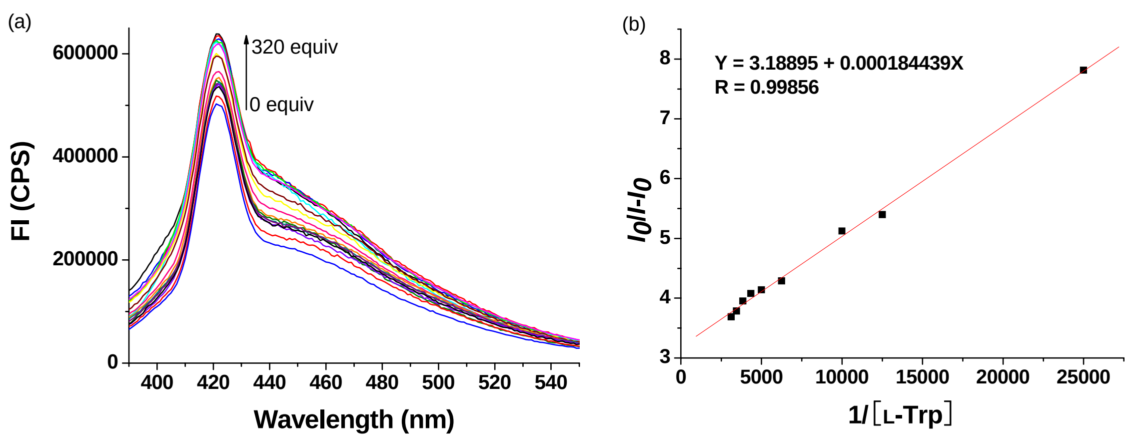


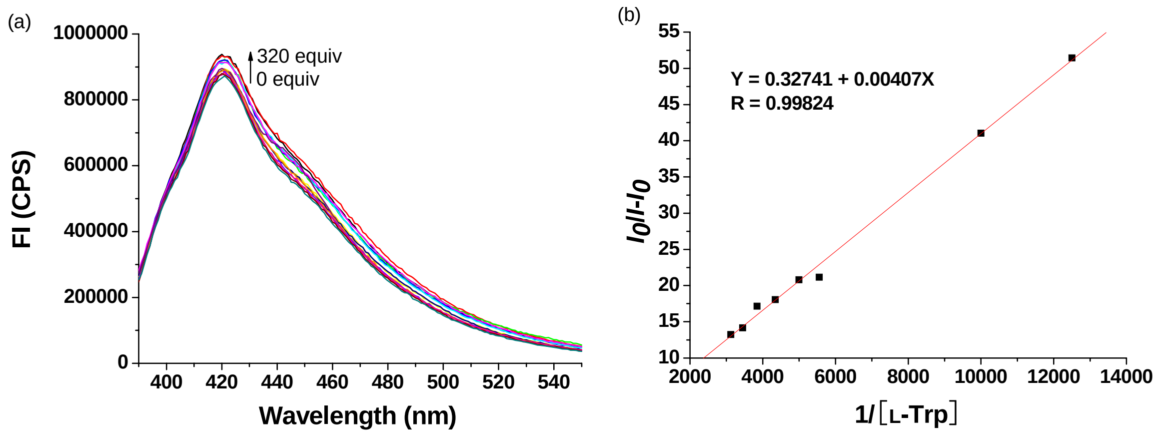
Fig. S3 Changes in fluorescence intensity of (*R*)-**5** (1 μ M) upon addition of 200 equiv of various natural amino acids in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) with excitation at 292 nm (excitation and emission slit: 1 nm).

ii). Binding studies of (*R*)-1-5 with L-Trp



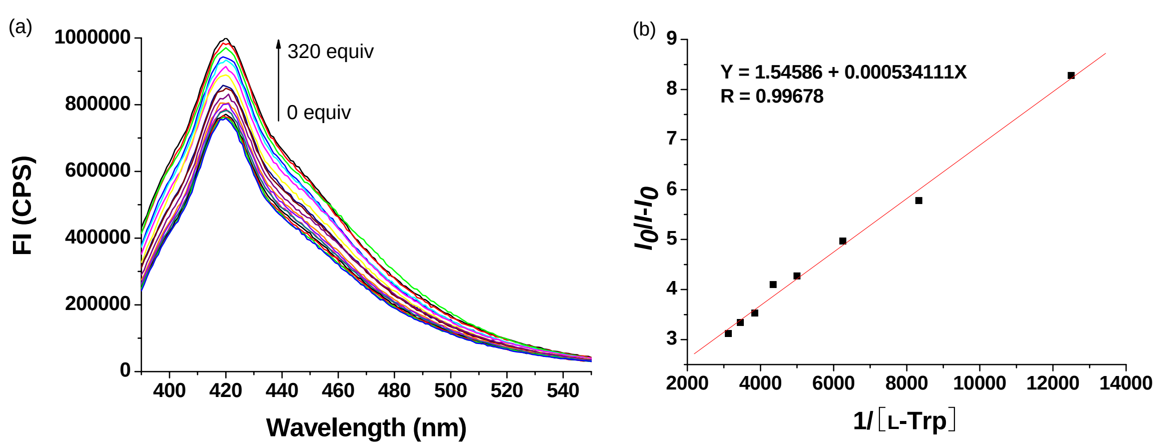
$$K = (1.73 \pm 0.01) \times 10^4\ M^{-1}$$

Fig. S4 (a) Fluorescent titration spectra of (*R*)-**1** (1 μ M) upon addition of L-Trp in H_2O (10 mM HEPES buffer, pH 7.4) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**1** at 422 nm with L-Trp.



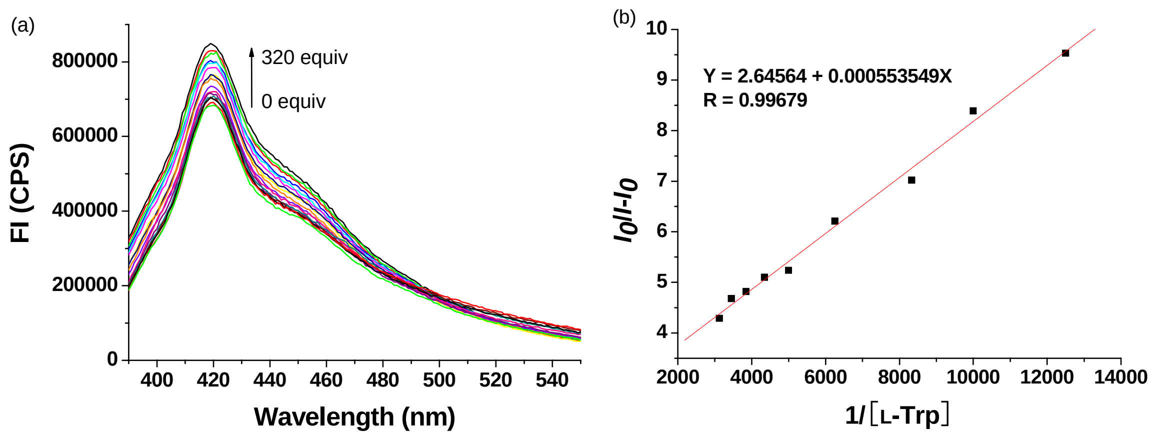
$K = (8.04 \pm 1.62) \times 10\ M^{-1}$

Fig. S5 (a) Fluorescent titration spectra of (*R*)-**2** (1 μM) upon addition of L-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**2** at 421 nm with L-Trp.



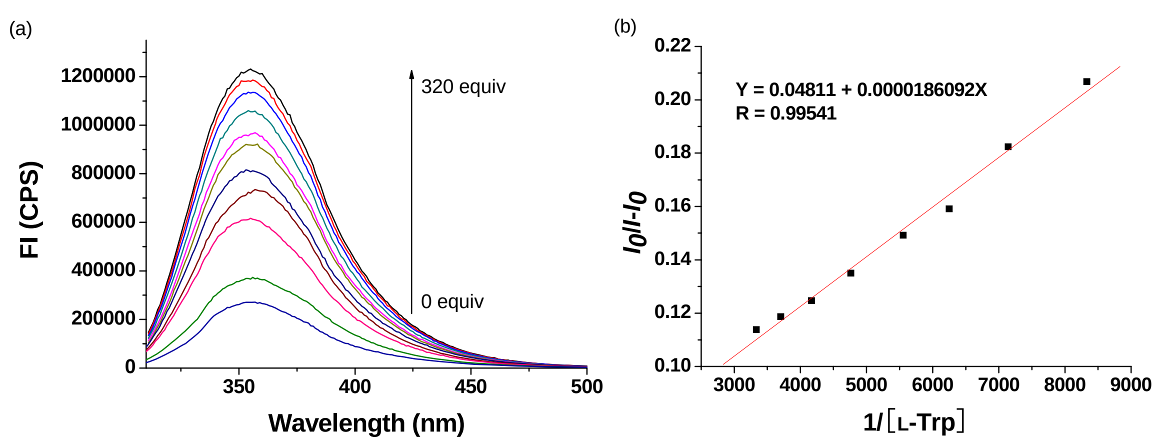
$K = (2.89 \pm 0.12) \times 10^3\ M^{-1}$

Fig. S6 (a) Fluorescent titration spectra of (*R*)-**3** (1 μM) upon addition of L-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**3** at 420 nm with L-Trp.



$$K = (4.78 \pm 0.07) \times 10^3\ M^{-1}$$

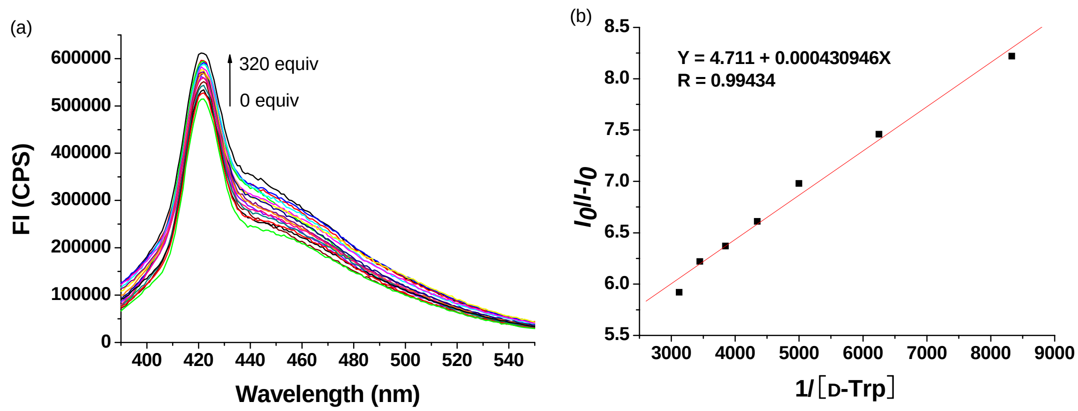
Fig. S7 (a) Fluorescent titration spectra of (*R*)-**4** (1 μM) upon addition of L-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**4** at 420 nm with L-Trp.



$$K = (2.59 \pm 0.12) \times 10^3\ M^{-1}$$

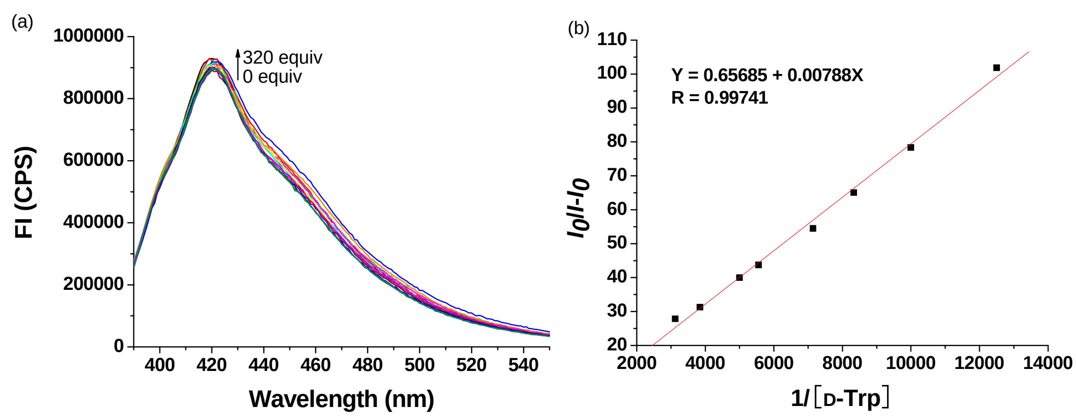
Fig. S8 (a) Fluorescent titration spectra of (*R*)-**5** (1 μM) upon addition of L-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 292 nm, slits = 1.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**5** at 358 nm with L-Trp.

iii). Binding studies of (R)-1-5 with D-Trp



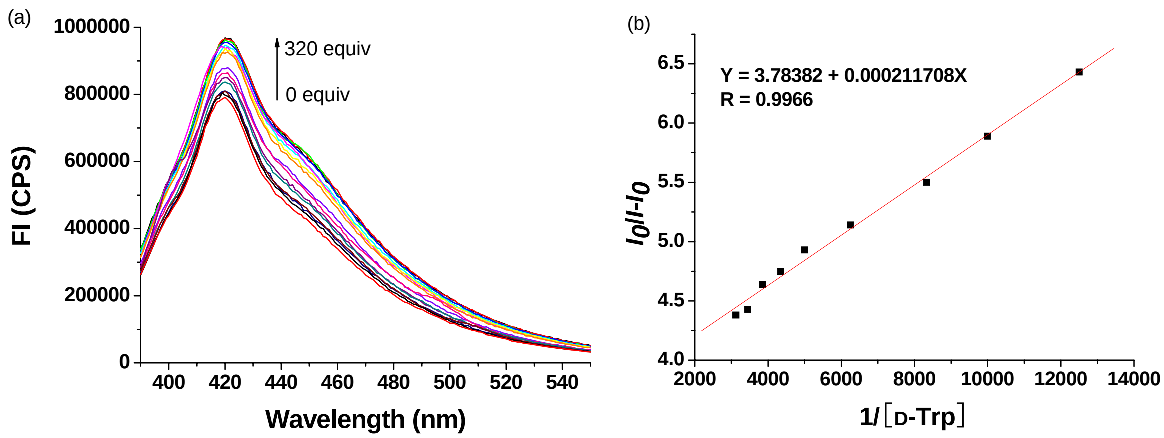
$$K = (1.09\pm0.03)\times10^{4}\ M^{-1}$$

Fig. S9 (a) Fluorescent titration spectra of (*R*)-**1** (1 μM) upon addition of D-Trp in H_2O (10 mM HEPES buffer, pH 7.4) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**1** at 422 nm with D-Trp.



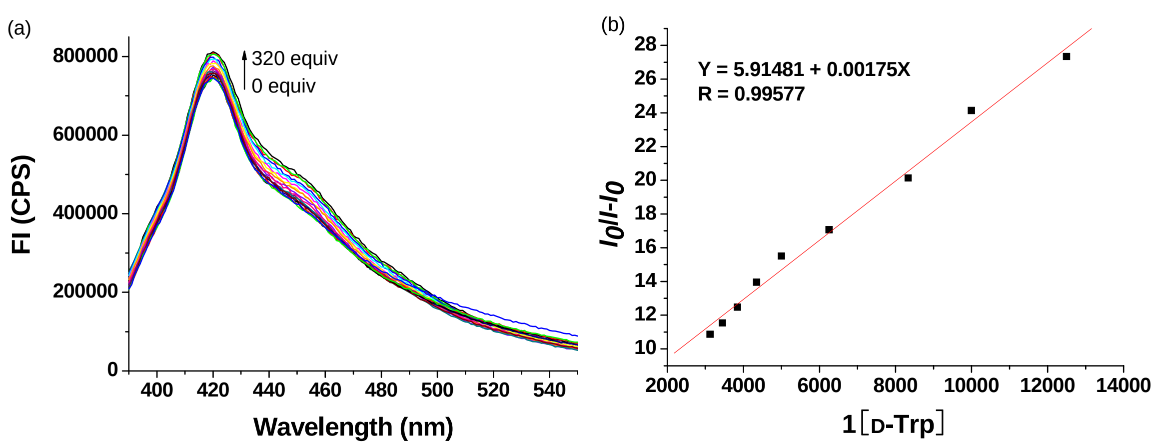
$$K = (8.34\pm2.20)\times10\ M^{-1}$$

Fig. S10 (a) Fluorescent titration spectra of (*R*)-**2** (1 μM) upon addition of D-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**2** at 421 nm with D-Trp.



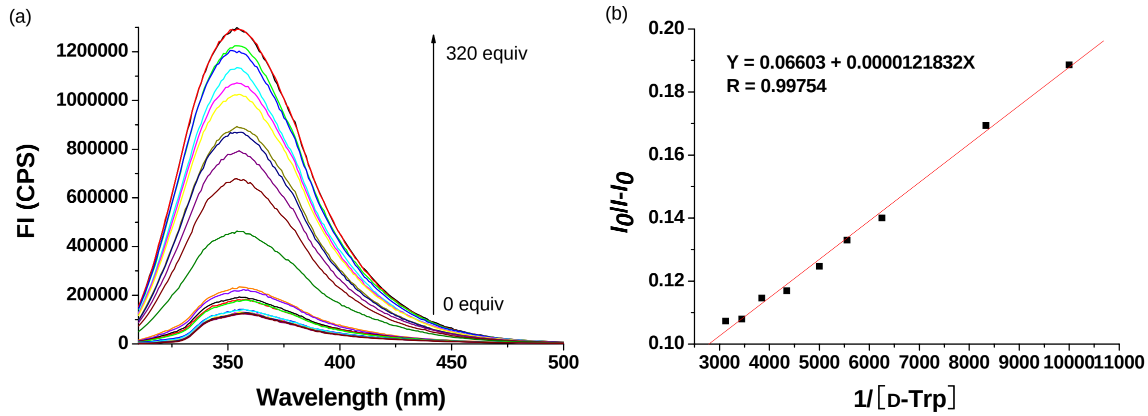
K = (1.79±0.03)×10^{4} M^{-1}

Fig. S11 (a) Fluorescent titration spectra of (*R*)-**3** (1 μM) upon addition of D-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**3** at 420 nm with D-Trp.



K = (3.38±0.13)×10^{3} M^{-1}

Fig. S12 (a) Fluorescent titration spectra of (*R*)-**4** (1 μM) upon addition of D-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 369 nm, slits = 5.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**4** at 420 nm with D-Trp.



K = (5.42±0.02)×10^3 M^{-1}

Fig. S13 (a) Fluorescent titration spectra of (*R*)-**5** (1 μM) upon addition of D-Trp in HEPES buffered (10 mM, pH 7.4) CH_3OH/H_2O (1:1, v/v) (λ_{exc} = 292 nm, slits = 1.0 nm). (b) Benesi-Hildebrand plot of emission spectra of (*R*)-**5** at 358 nm with D-Trp.

iv). Fluorescence intensity changes of (*R*)-1-5 with addition of the two enantiomers of tryptophan

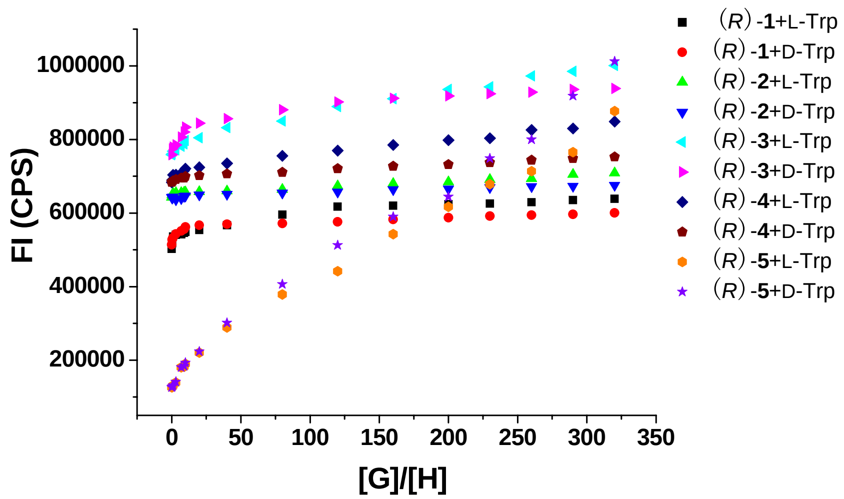


Fig. S14 Fluorescence intensity changes of receptors (*R*)-**1**, (*R*)-**2**, (*R*)-**3**, (*R*)-**4** and (*R*)-**5** (1 μM) with addition of the two enantiomers of Trp in HEPES buffer solution at pH 7.4. ((*R*)-**1**, (*R*)-**2**, (*R*)-**3**, (*R*)-**4**: λ_{exc} = 369 nm, slits = 5.0 nm; (*R*)-**5**: λ_{exc} = 292 nm, slits = 1.0 nm)

III. Copies of the ESI-MS spectra of the complexes (*R*)-1-L-Trp, (*R*)-2-L-Trp, (*R*)-3-L-Trp, (*R*)-4-L-Trp and (*R*)-5-L-Trp

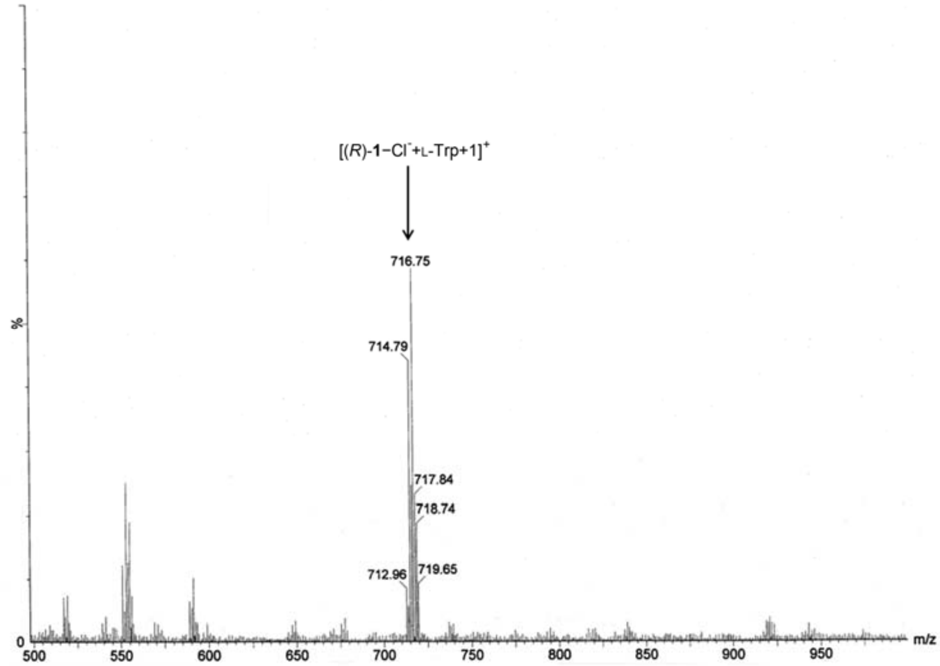


Fig. S15 The ESI-MS of (*R*)-**1**-L-Trp complex.

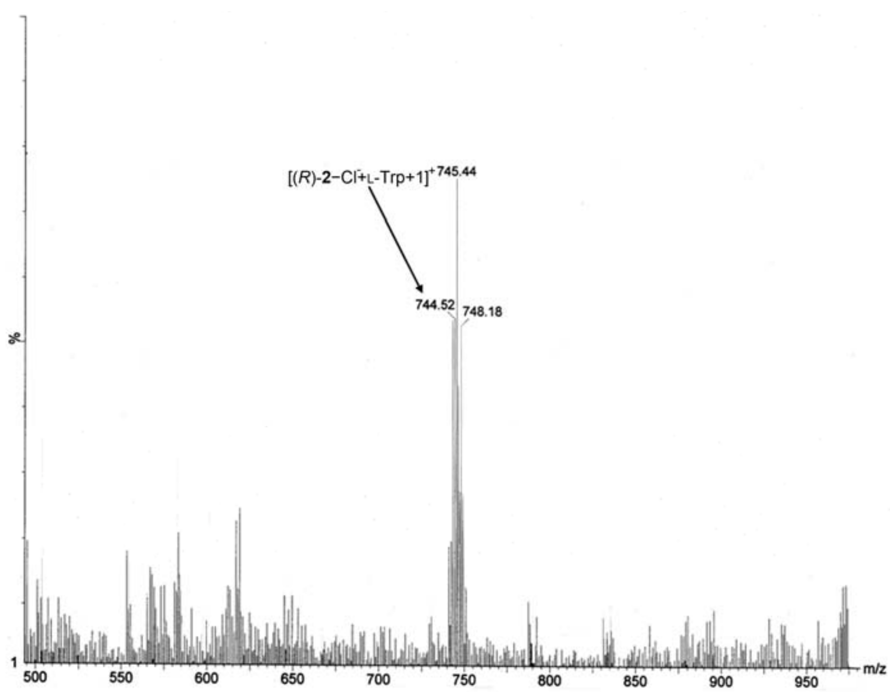


Fig. S16 The ESI-MS of (*R*)-**2**-L-Trp complex.

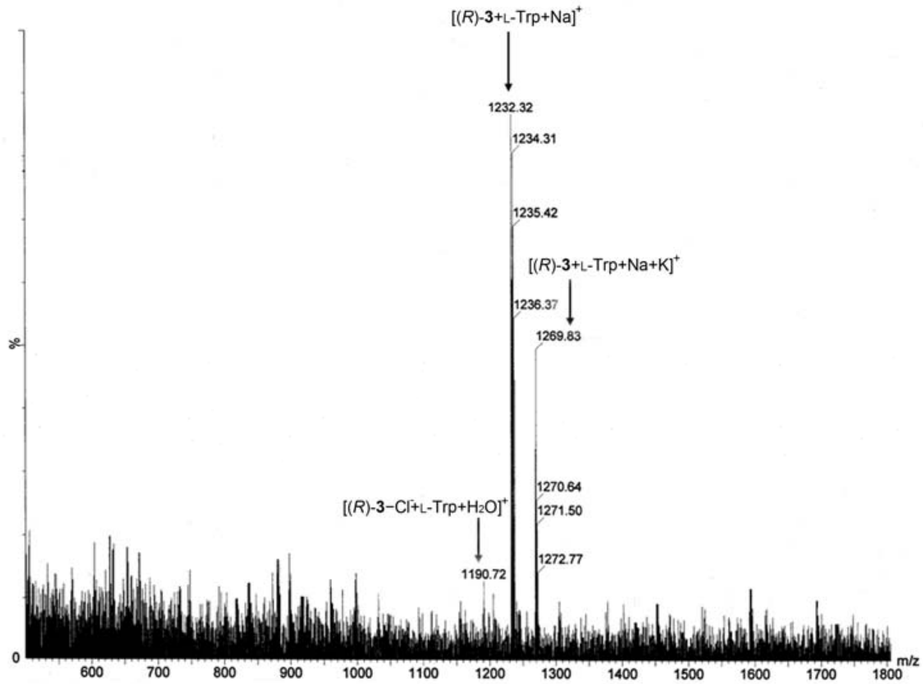


Fig. S17 The ESI-MS of (*R*)-**3**-L-Trp complex.

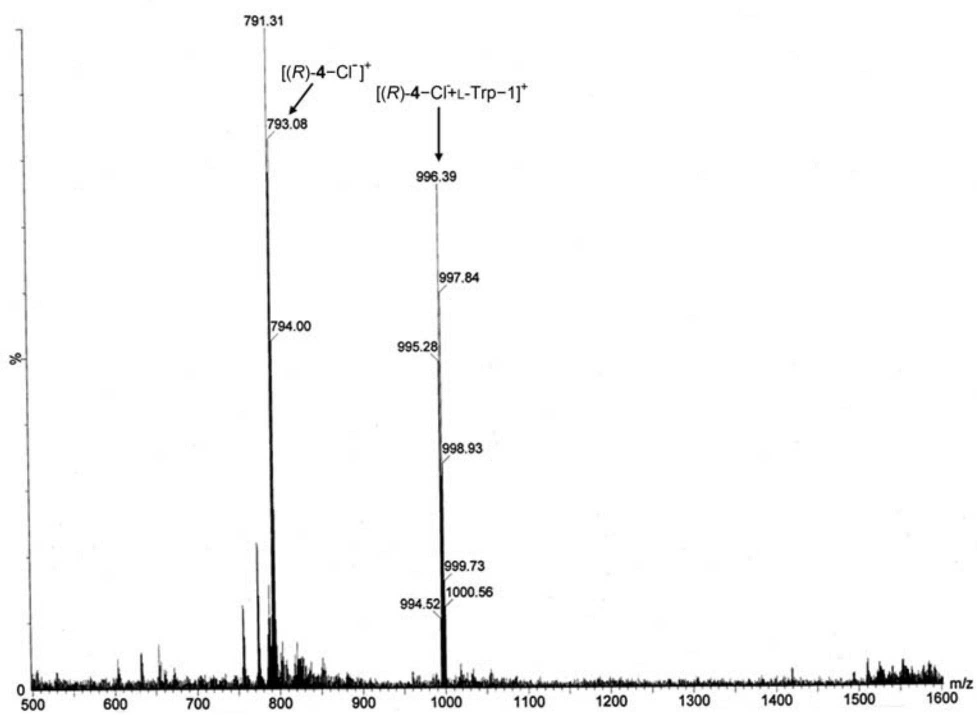


Fig. S18 The ESI-MS of (*R*)-**4**-L-Trp complex.

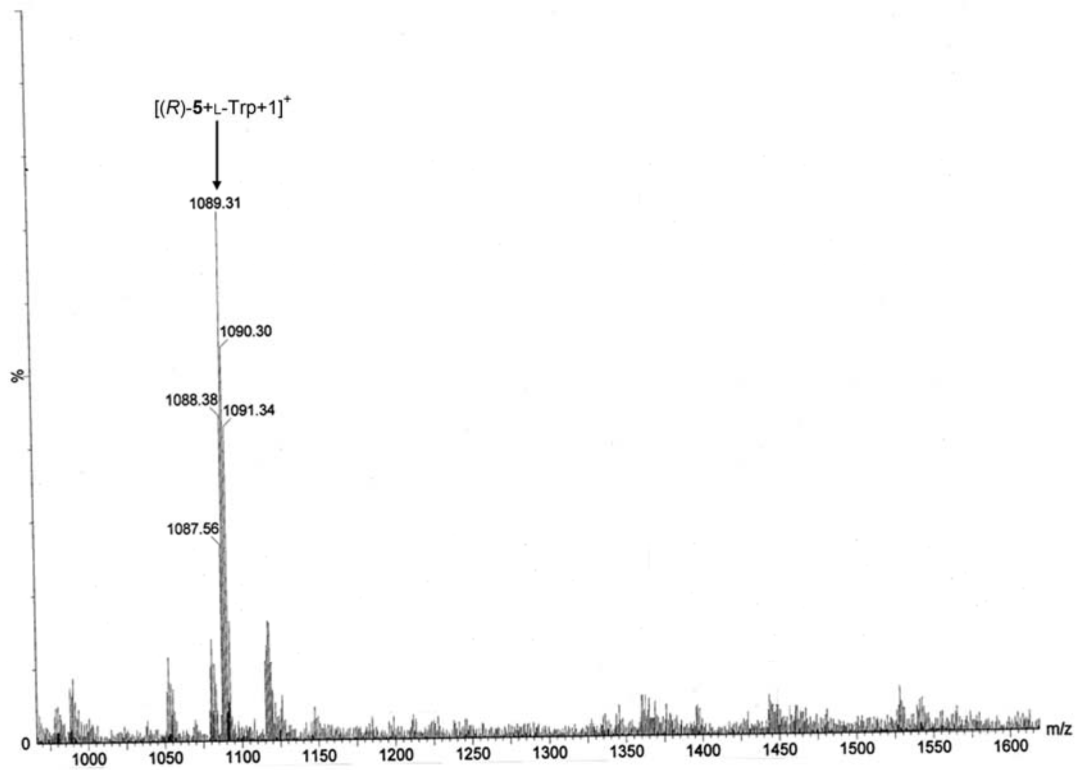


Fig. S19 The ESI-MS of (*R*)-**5**-L-Trp complex.

IV. Optimized geometries of (*R*)-1-L-Trp complex and (*R*)-1-D-Trp complex[1]

i). Standard Orientation of (*R*)-1-L-Trp complex

1	-0.098372	-1.963972	2.828437
1	-2.457734	0.252056	0.474962
6	-2.117220	-1.621060	1.224163
8	-1.697491	-0.435715	0.707671
8	-1.407446	-2.240481	2.020643
6	0.872130	-3.401037	-3.120703
6	1.671843	-4.204914	-2.353889
6	1.199478	-4.769584	-1.150195
6	-0.072881	-4.524303	-0.706218
6	-0.915833	-3.696671	-1.469249
6	-0.436103	-3.155665	-2.669941
1	1.226510	-2.977406	-4.050919
1	2.682079	-4.423074	-2.676331
1	1.856901	-5.413431	-0.581413
1	-0.426944	-4.969919	0.215008
6	-2.285585	-3.236353	-1.313415
7	-1.466457	-2.427023	-3.265632
6	-2.558107	-2.483085	-2.399389
1	-1.321020	-1.623512	-3.926906
1	-3.470942	-1.972011	-2.674371
6	-3.472642	-2.273414	0.772649
6	-3.189132	-3.525433	-0.126822
1	-0.727463	0.279465	-3.657459
8	-1.038672	-0.187898	-4.471224
1	-0.277047	-0.087577	-5.086587
1	-1.152580	-1.335451	5.060223
6	-1.006474	3.938770	-0.745200
6	-1.173008	2.736340	-1.345469
6	-0.119745	1.766190	-1.258017
6	1.001776	1.993095	-0.512431
6	1.166305	3.264441	0.143697
6	0.172802	4.247632	-0.000373
6	2.034026	0.897392	-0.360061
6	3.253714	0.923509	-1.130779
6	4.215150	-0.083214	-0.943919
6	3.943036	-1.135655	-0.014007
6	2.789514	-1.167570	0.690210
6	1.807913	-0.118112	0.532093
1	-1.792301	4.682880	-0.796843
6	-2.509342	2.354280	-1.989452
6	0.342393	5.518578	0.634112
1	4.679080	-1.922678	0.102164
6	2.465673	-2.358439	1.595848
8	0.738770	-0.163509	1.415011
8	-0.313526	0.577567	-1.974350
6	2.317387	3.572556	0.938022

6	3.534856	1.960542	-2.076597
6	5.435545	-0.042426	-1.686882
7	-3.561985	2.250555	-0.943406
6	-4.706936	3.084594	-0.895251
6	-3.471104	1.438592	0.164839
7	-4.581579	1.794487	0.886407
6	-5.343875	2.795612	0.234323
6	-4.980299	1.188823	2.170939
1	-2.427224	1.399934	-2.510983
1	-2.835542	3.111114	-2.704380
1	-4.935050	3.786769	-1.682523
1	-6.255514	3.186893	0.659245
1	-5.152738	1.969939	2.912874
1	-4.179683	0.537243	2.511693
1	-5.891473	0.601046	2.050760
1	0.440991	-0.006545	-1.724189
1	-0.146423	-0.108190	0.950637
6	2.451025	4.783962	1.527532
6	1.445363	5.781107	1.372261
6	5.674577	0.956798	-2.568369
6	4.701001	1.976850	-2.765754
1	-0.433155	6.264026	0.510277
1	3.083147	2.818881	1.057995
1	2.800275	2.739119	-2.229070
1	6.164329	-0.827194	-1.526786
1	3.326589	5.008316	2.124333
1	1.574434	6.743208	1.851608
1	6.600110	0.991054	-3.129046
1	4.905118	2.769485	-3.475445
7	2.109003	-1.970566	2.996423
6	0.845725	-1.804193	3.440274
7	0.919482	-1.396484	4.726175
6	2.277946	-1.288690	5.096458
6	3.007810	-1.638184	4.030704
6	-0.239491	-1.099830	5.604445
1	3.318608	-3.036473	1.658465
1	2.569324	-0.975756	6.088979
1	4.078079	-1.695847	3.890486
1	-0.231305	-0.042791	5.875535
1	-0.177721	-1.711957	6.505404
1	1.608031	-2.916048	1.209991
1	-2.732942	-4.289594	0.497585
1	-4.153969	-3.912498	-0.454986
1	-3.953798	-2.624124	1.689083
7	-4.381279	-1.274803	0.158186
1	-4.068145	-1.119669	-0.811282
1	-5.303152	-1.729579	0.063578

E_{zpe} = −2248.115191 (Hartree)

Number of imaginary frequencies = 0

ii). Standard Orientation of (*R*)-1-D-Trp complex

1	0.248603	-2.283414	2.559045
1	-2.481721	-0.086441	0.413686
6	-1.848572	-1.906201	0.987306
8	-1.632320	-0.583472	0.719689
8	-1.052688	-2.532646	1.682733
6	1.465468	-2.633382	-3.500117
6	2.339950	-3.469707	-2.861099
6	1.921688	-4.277429	-1.781686
6	0.627791	-4.244553	-1.334520
6	-0.293516	-3.388362	-1.965374
6	0.135486	-2.602072	-3.044874
1	1.781179	-2.020838	-4.334047
1	3.370490	-3.522582	-3.188833
1	2.640722	-4.935351	-1.312184
1	0.316853	-4.873171	-0.509342
6	-1.698552	-3.090648	-1.758549
7	-0.956078	-1.874306	-3.513184
6	-2.038877	-2.178716	-2.693307
1	-0.906283	-1.015829	-4.114689
1	-2.994327	-1.701290	-2.867149
6	-3.087005	-2.630140	0.357081
1	-3.708075	-1.884294	-0.149007
6	-2.597985	-3.679594	-0.686167
1	-0.576233	0.886570	-3.730952
8	-0.788790	0.461883	-4.597260
1	0.000641	0.676751	-5.145038
1	-0.832480	-2.237546	4.861166
6	-1.636811	3.748839	-0.163497
6	-1.567158	2.685549	-0.999679
6	-0.362321	1.907578	-1.029987
6	0.679963	2.164449	-0.185723
6	0.599170	3.288316	0.709174
6	-0.552278	4.094224	0.700749
6	1.878378	1.240278	-0.183562
6	3.053011	1.544643	-0.962836
6	4.151258	0.668887	-0.934637
6	4.066186	-0.525593	-0.151309
6	2.956607	-0.816426	0.564193
6	1.835062	0.093555	0.563926
1	-2.538787	4.347871	-0.122335
6	-2.774131	2.241230	-1.832726
6	-0.625786	5.223140	1.576611
1	4.906393	-1.210189	-0.163691
6	2.820422	-2.162616	1.280811
8	0.805291	-0.247360	1.424253
8	-0.322785	0.871792	-1.970096
6	1.662252	3.627365	1.606476
6	3.147312	2.724358	-1.767590
6	5.318408	0.975225	-1.700525
7	-3.897613	1.824671	-0.951228
6	-5.170710	2.447169	-0.965812

6	-3.798922	0.865392	0.030842
7	-5.042814	0.920476	0.615216
6	-5.883706	1.883778	0.002784
6	-5.471071	0.109338	1.770142
1	-2.501135	1.406800	-2.479873
1	-3.141646	3.055702	-2.459112
1	-5.419327	3.222823	-1.674133
1	-6.895736	2.054320	0.336764
1	-5.992144	0.739835	2.490783
1	-4.590870	-0.316325	2.246888
1	-6.140968	-0.693917	1.456680
1	0.496370	0.360974	-1.767587
1	-0.088798	-0.110662	1.005131
6	1.565422	4.702984	2.422709
6	0.398596	5.520628	2.408926
6	5.376936	2.100431	-2.451056
6	4.266671	2.991290	-2.482361
1	-1.519615	5.834026	1.556582
1	2.549494	3.009381	1.616605
1	2.307438	3.404998	-1.792600
1	6.153215	0.286238	-1.667654
1	2.376529	4.954740	3.094932
1	0.344008	6.376625	3.069490
1	6.260557	2.333347	-3.031544
1	4.328093	3.888315	-3.086677
7	2.440083	-2.055557	2.724898
6	1.175294	-2.131973	3.189262
7	1.222696	-1.959801	4.527878
6	2.564757	-1.756336	4.916033
6	3.311163	-1.812778	3.806444
6	0.051496	-1.974632	5.440342
1	3.760713	-2.715082	1.239958
1	2.835475	-1.597731	5.950210
1	4.377853	-1.713970	3.662068
1	-0.075989	-0.986981	5.886749
1	0.213874	-2.715687	6.224271
1	2.042609	-2.769642	0.809297
1	-2.069175	-4.460963	-0.145559
1	-3.482489	-4.134921	-1.132077
7	-3.811019	-3.337477	1.450929
1	-4.403480	-2.653946	1.947612

$E_{zpe} = -2248.116016$ (Hartree)

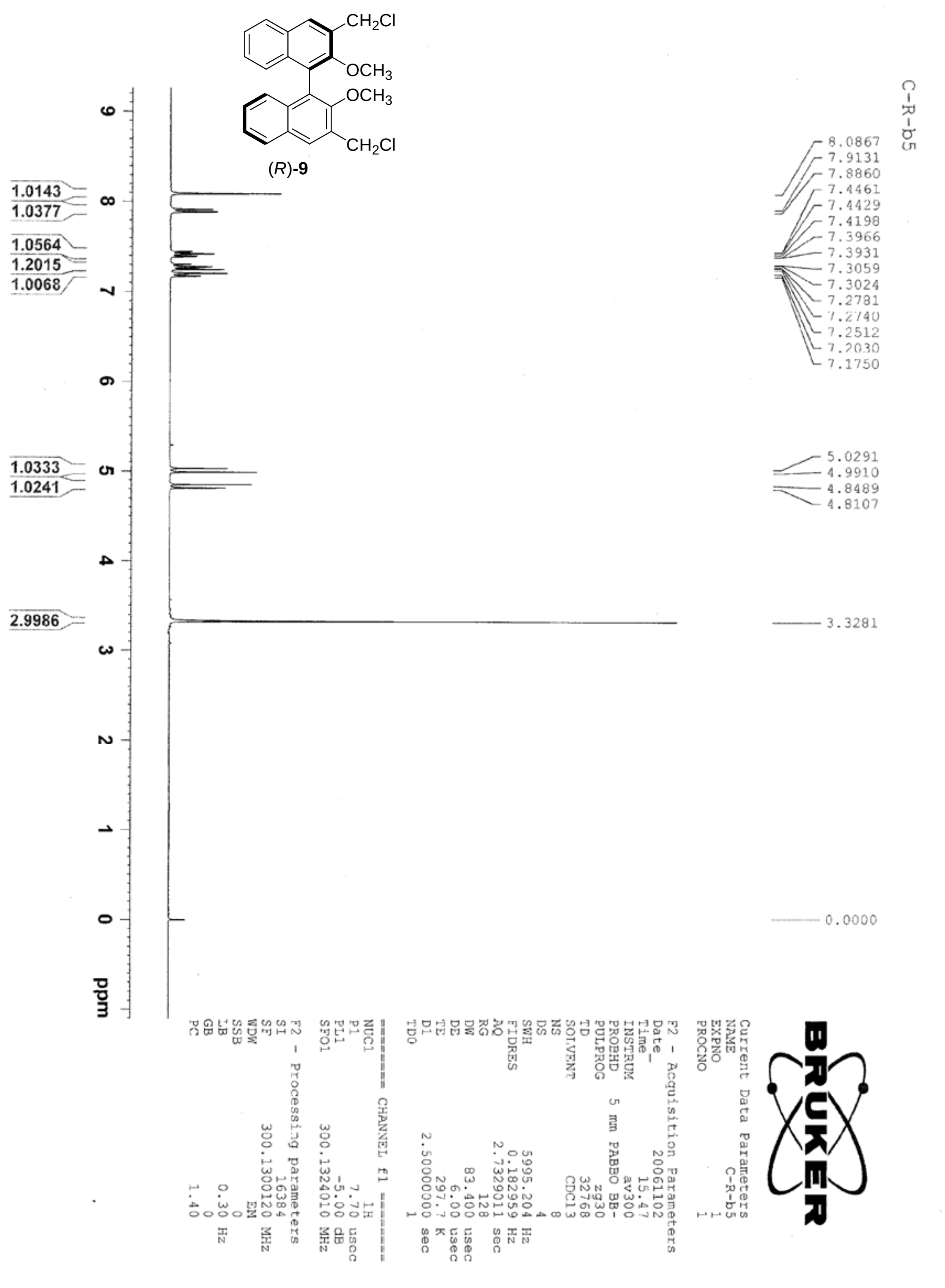
Number of imaginary frequencies = 0

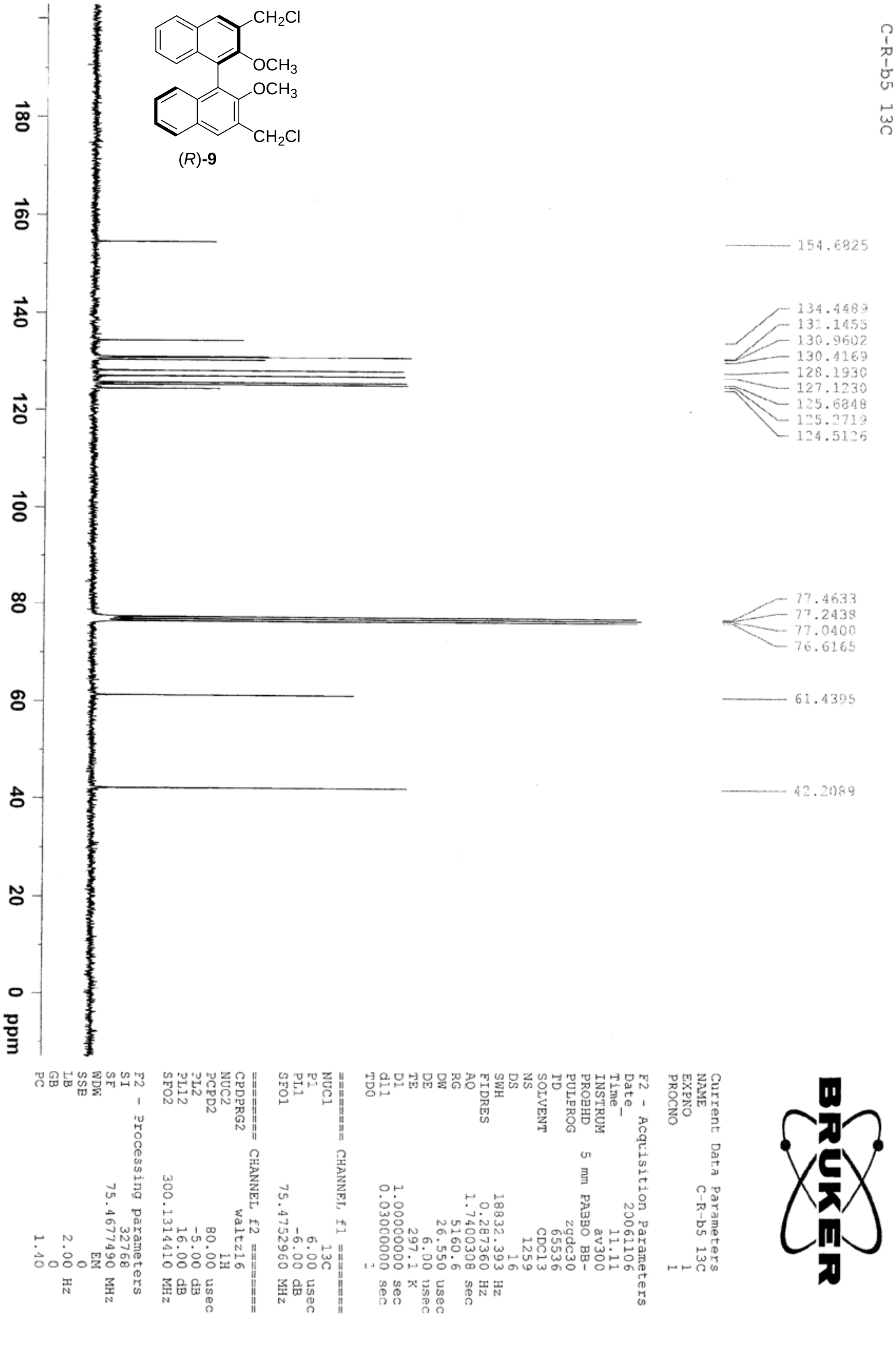
Reference:

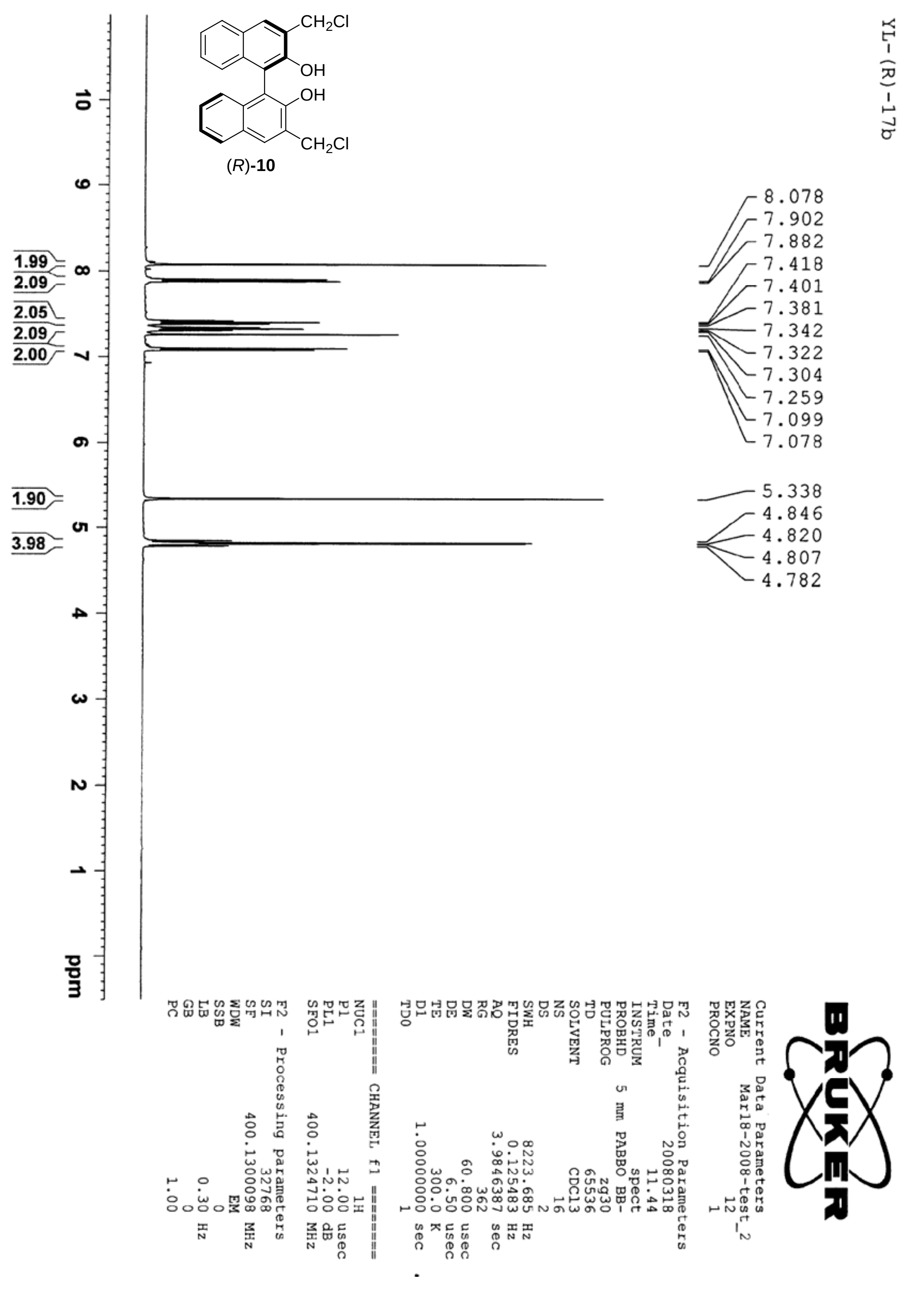
1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, Jr. J. A. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J.

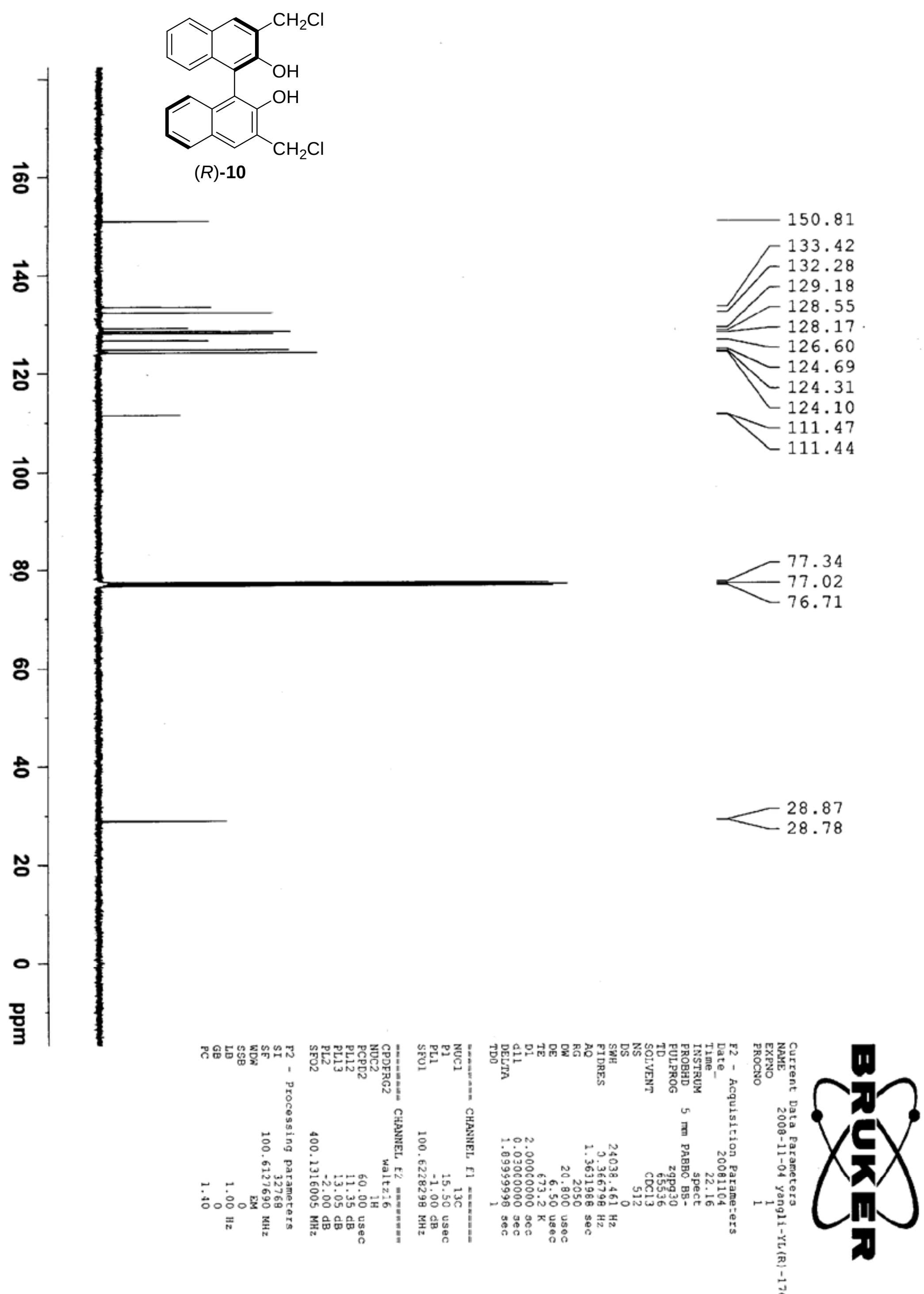
Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian 03, B05; Gaussian, Inc.: Wallingford, CT, 2003.

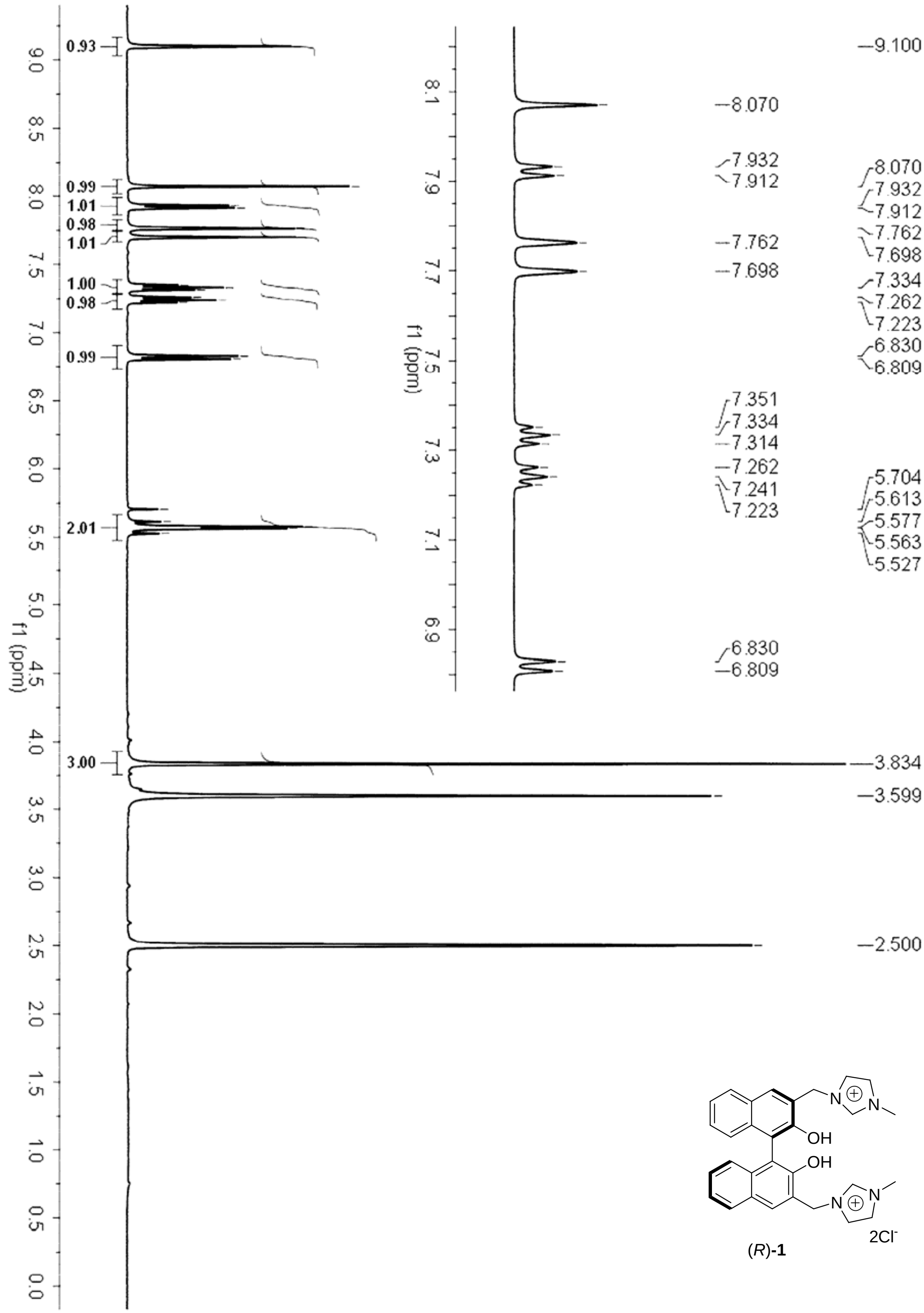
V. Copies of ^{1}H and ^{13}C NMR spectra of (*R*)-1-5, 9, 10, 11 and 16

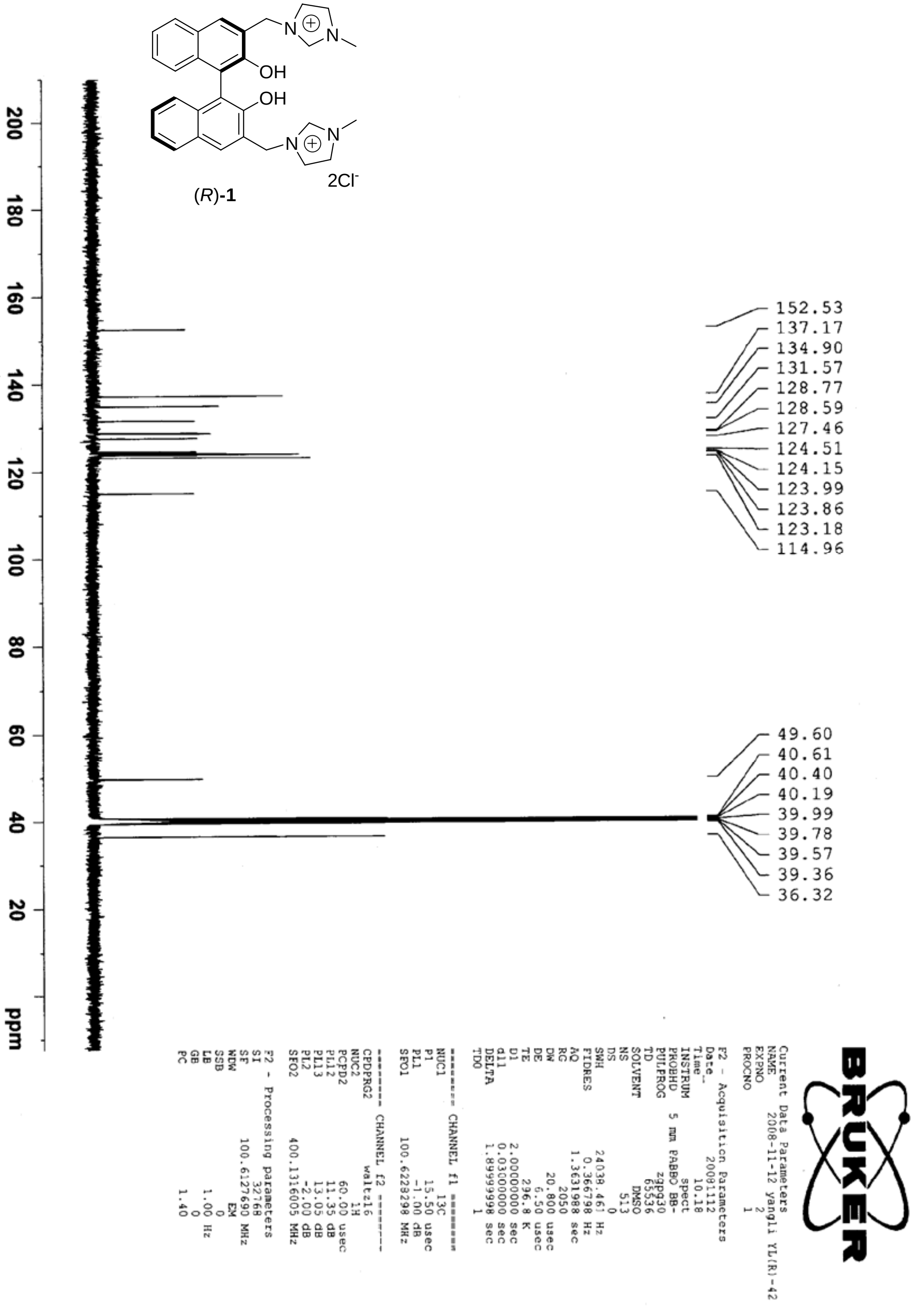


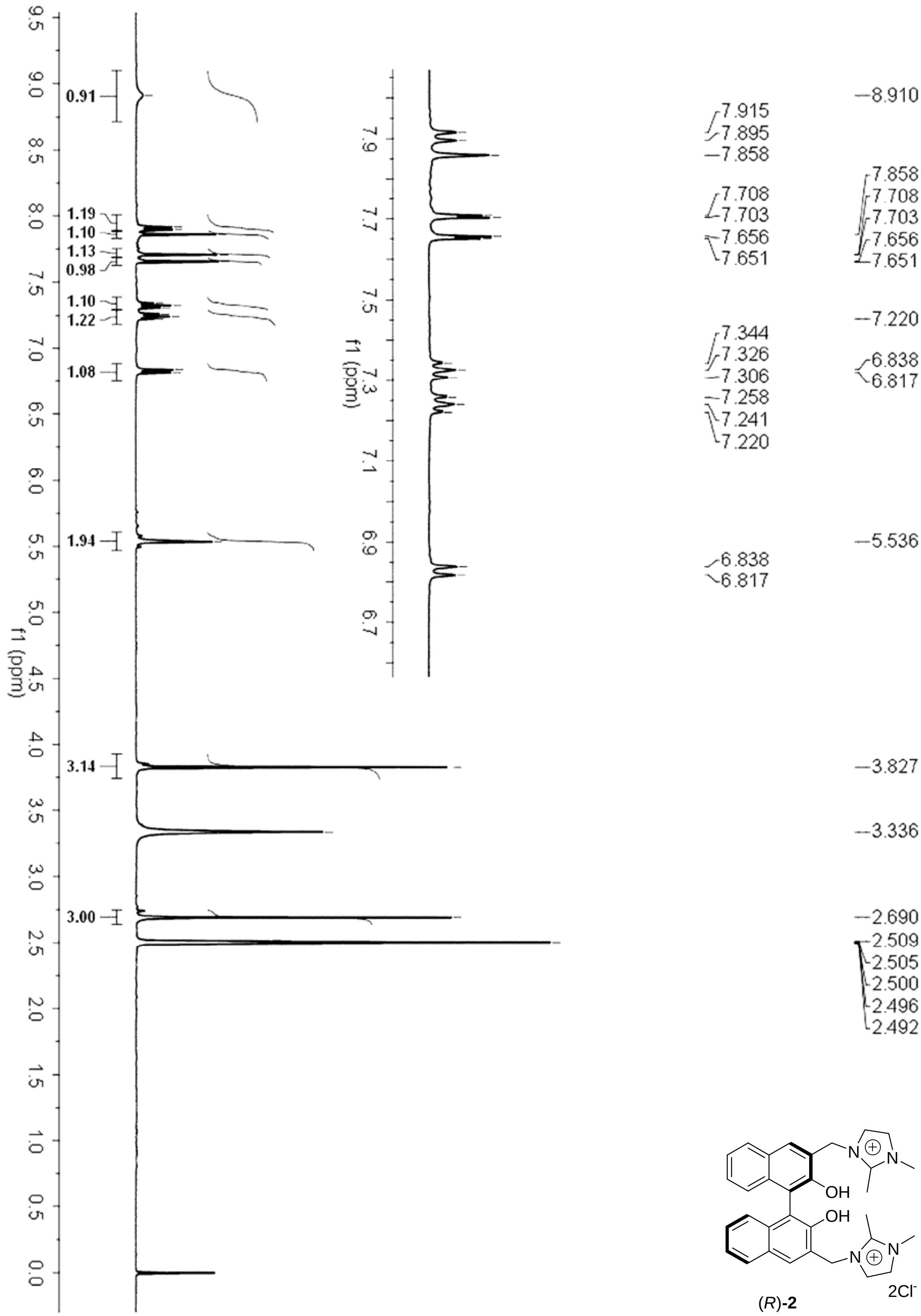

C-R-b5 13C
CH2Cl
OCH3
OCH3
CH2Cl
(R)-9
154.6825
134.4489
131.1455
130.9602
130.4169
128.1930
127.1230
125.6848
125.2719
124.5126
77.4633
77.2438
77.0400
76.6165
61.4395
42.2089
180
160
140
120
100
80
60
40
20
0 ppm
Current Data Parameters
NAME C-R-b5 13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061106
Time 11.11
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1259
DS 16
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5160.6
DW 26.550 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -6.00 dB
SFO1 75.4752960 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 16.00 dB
SFO2 300.1314410 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

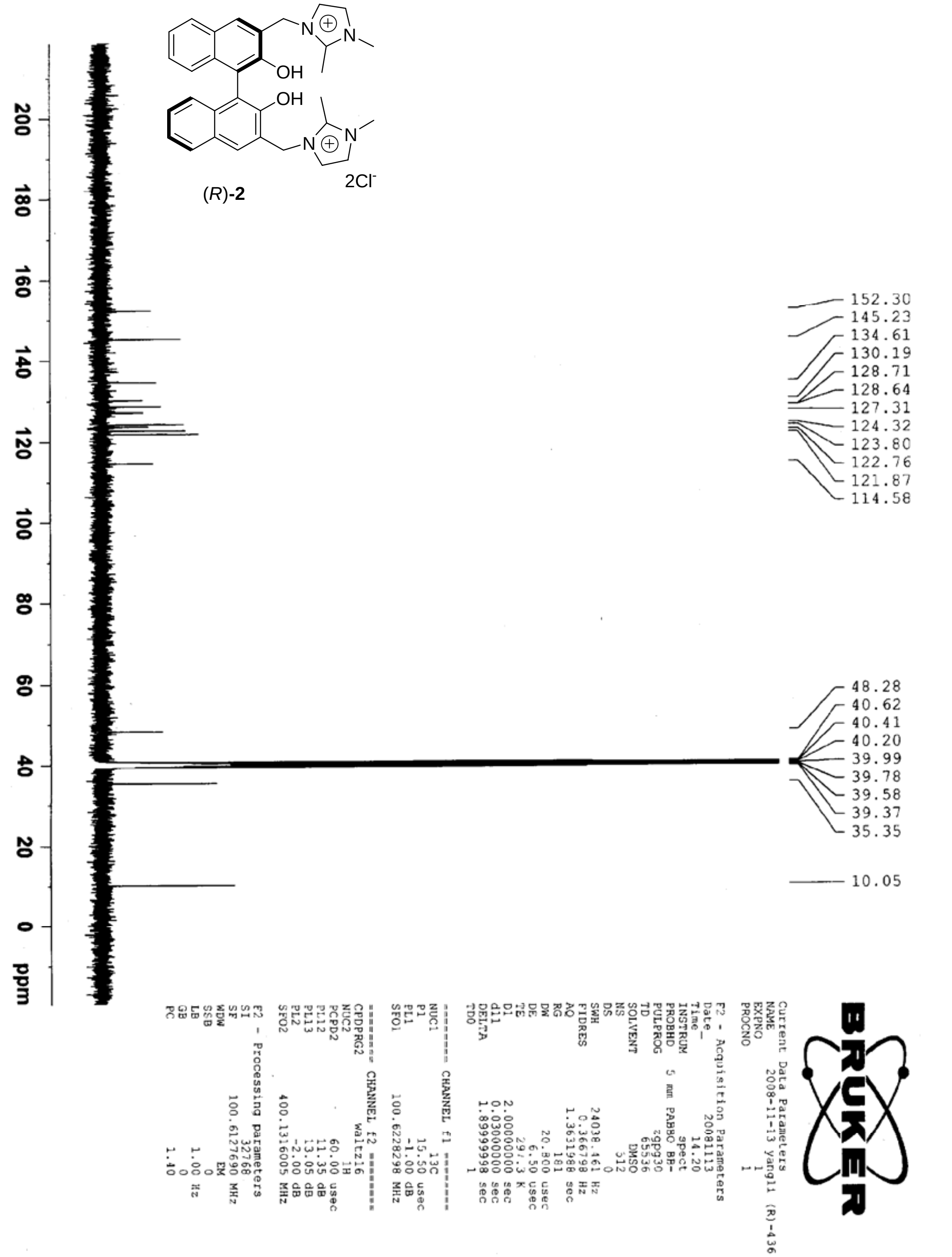

YL-(R)-17b
CH2Cl
OH
OH
CH2Cl
(R)-10
8.078
7.902
7.882
7.418
7.401
7.381
7.342
7.322
7.304
7.259
7.099
7.078
5.338
4.846
4.820
4.807
4.782
1.99
2.09
2.05
2.09
2.00
1.90
3.98
ppm
Current Data Parameters
NAME Mar18-2008-test_2
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080318
Time 11.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

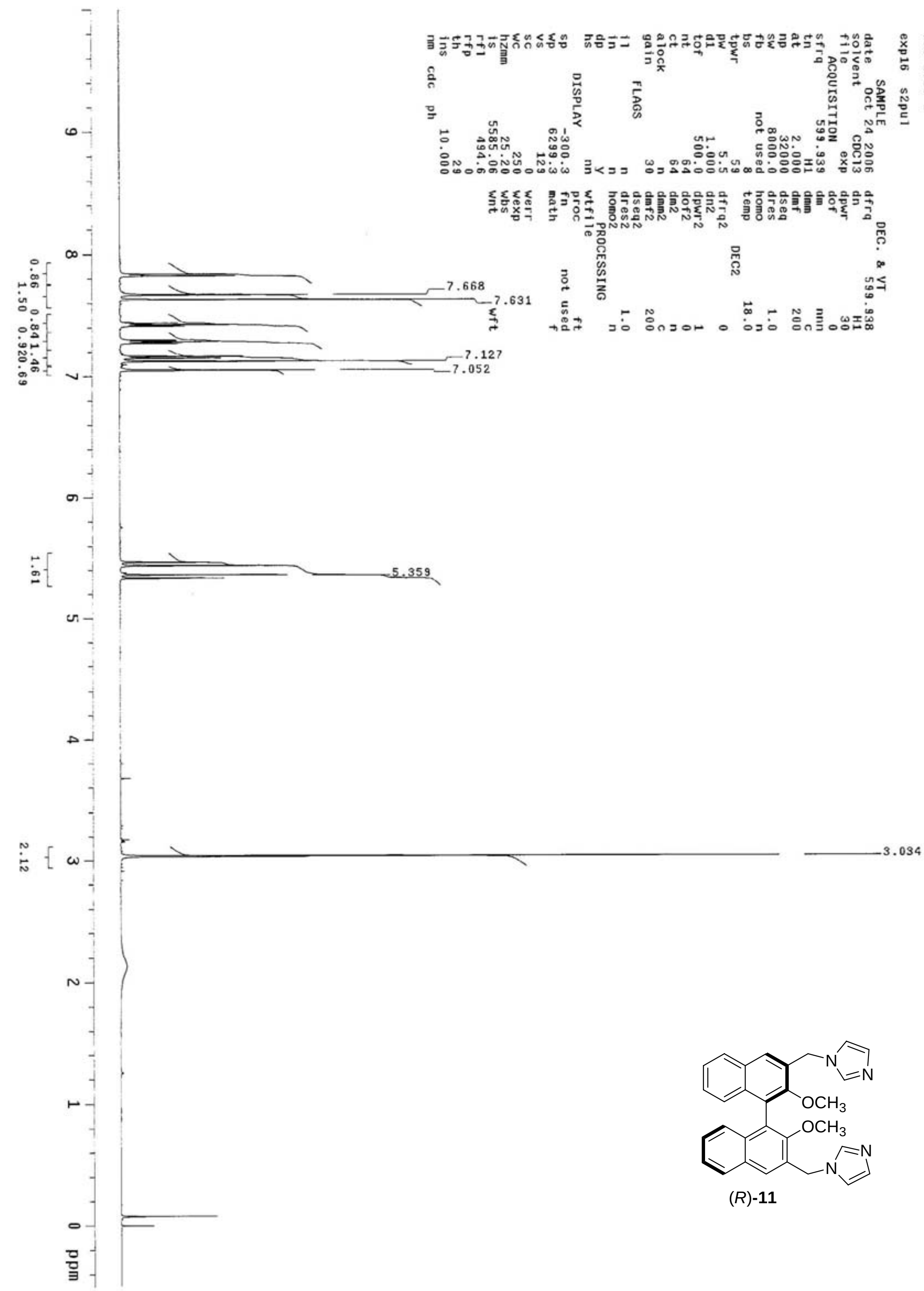

CH2Cl
OH
OH
CH2Cl
(R)-10
150.81
133.42
132.28
129.18
128.55
128.17
126.60
124.69
124.31
124.10
111.47
111.44
77.34
77.02
76.71
28.87
28.78
160
140
120
100
80
60
40
20
0
ppm


9.100
8.070
7.932
7.912
7.762
7.698
7.351
7.334
7.314
7.262
7.241
7.223
6.830
6.809
7.334
7.262
7.223
5.704
5.613
5.577
5.563
5.527
3.834
3.599
2.500
OH
OH
2Cl-
(R)-1

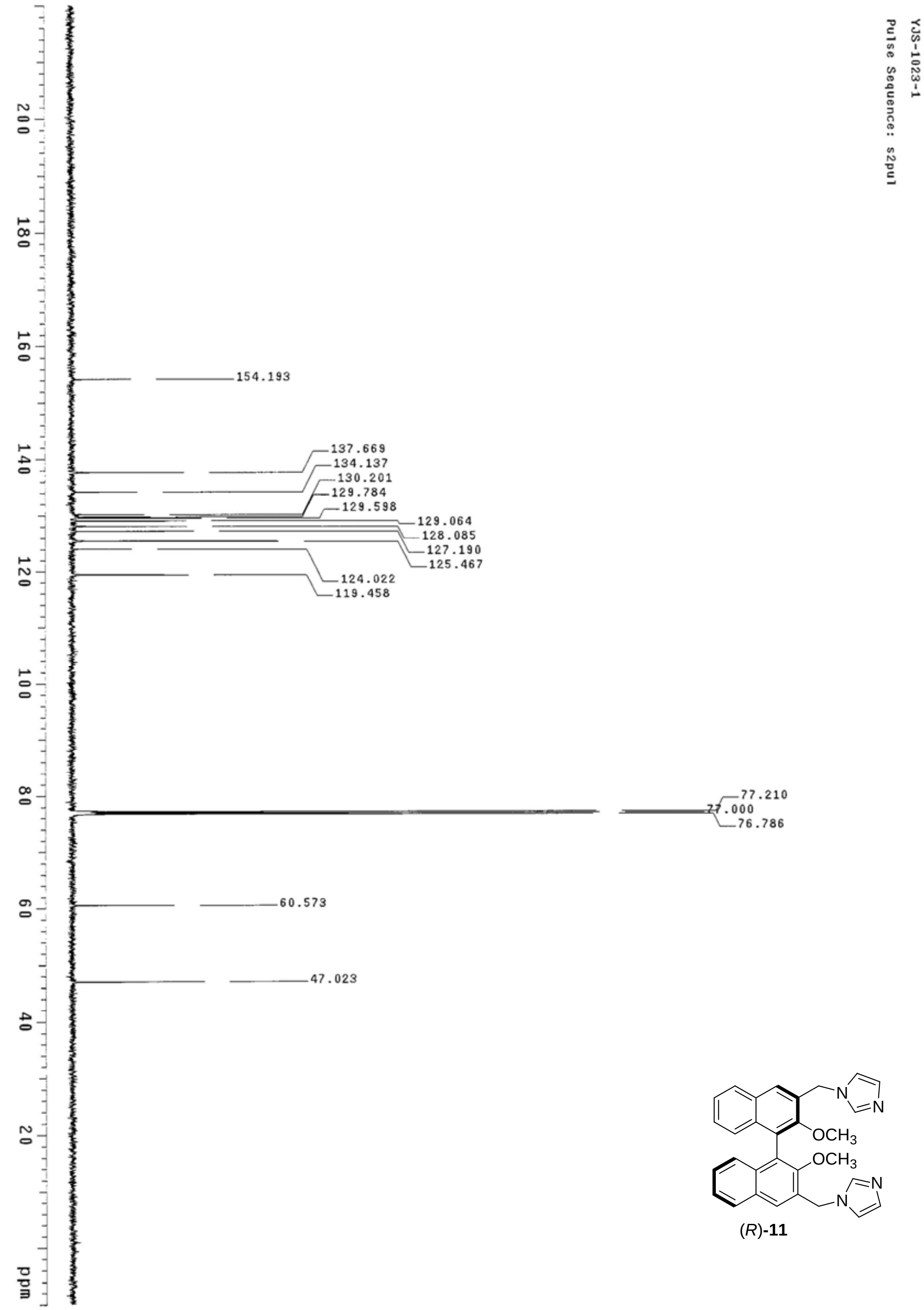

OH
OH
2Cl-
(R)-1
152.53
137.17
134.90
131.57
128.77
128.59
127.46
124.51
124.15
123.99
123.86
123.18
114.96
49.60
40.61
40.40
40.19
39.99
39.78
39.57
39.36
36.32
200
180
160
140
120
100
80
60
40
20
ppm

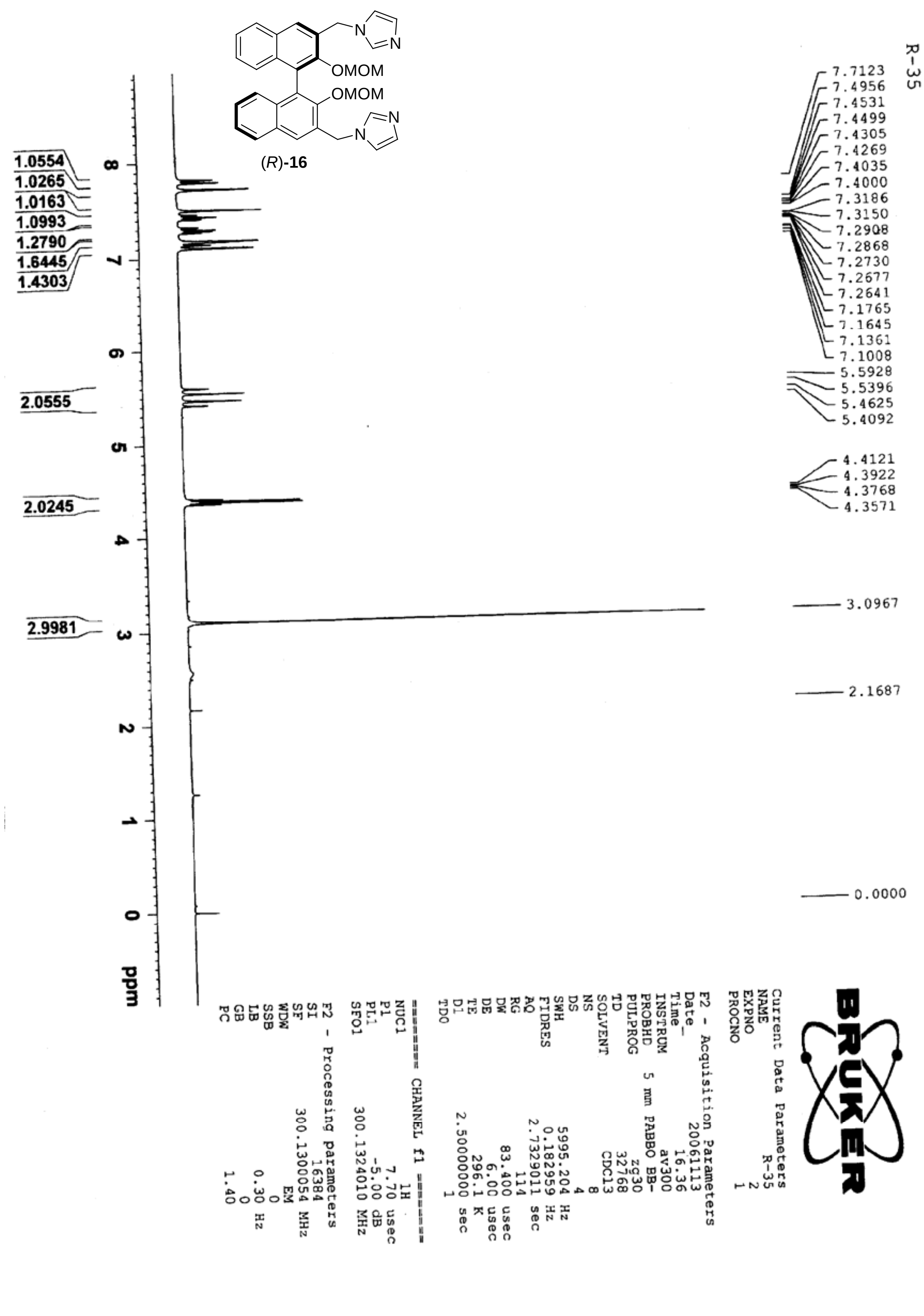

(R)-2
2Cl⁻
OH
OH

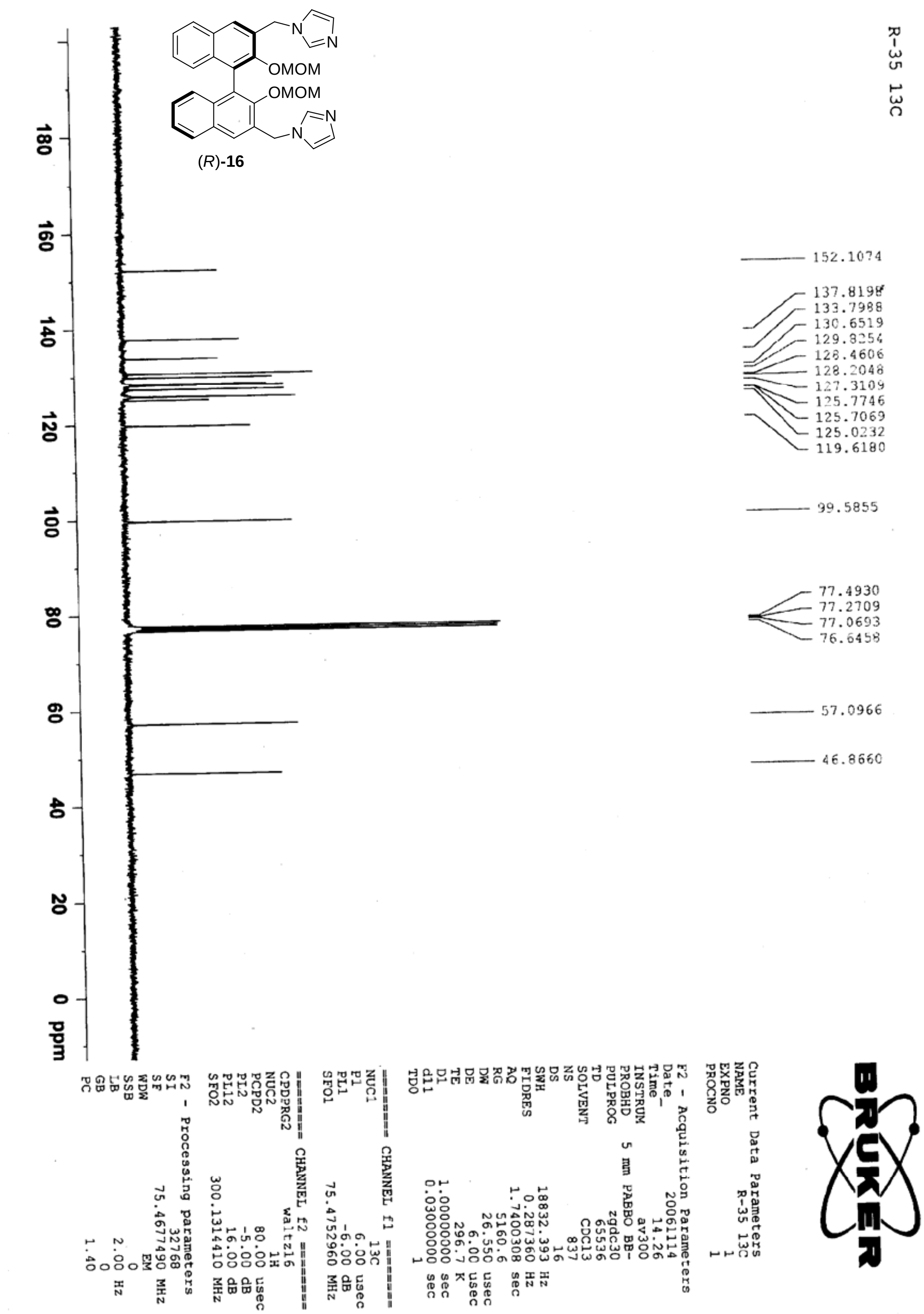

OH
OH
N
N
2Cl⁻
(R)-2
152.30
145.23
134.61
130.19
128.71
128.64
127.31
124.32
123.80
122.76
121.87
114.58
48.28
40.62
40.41
40.20
39.99
39.78
39.58
39.37
35.35
10.05
200
180
160
140
120
100
80
60
40
20
0
ppm



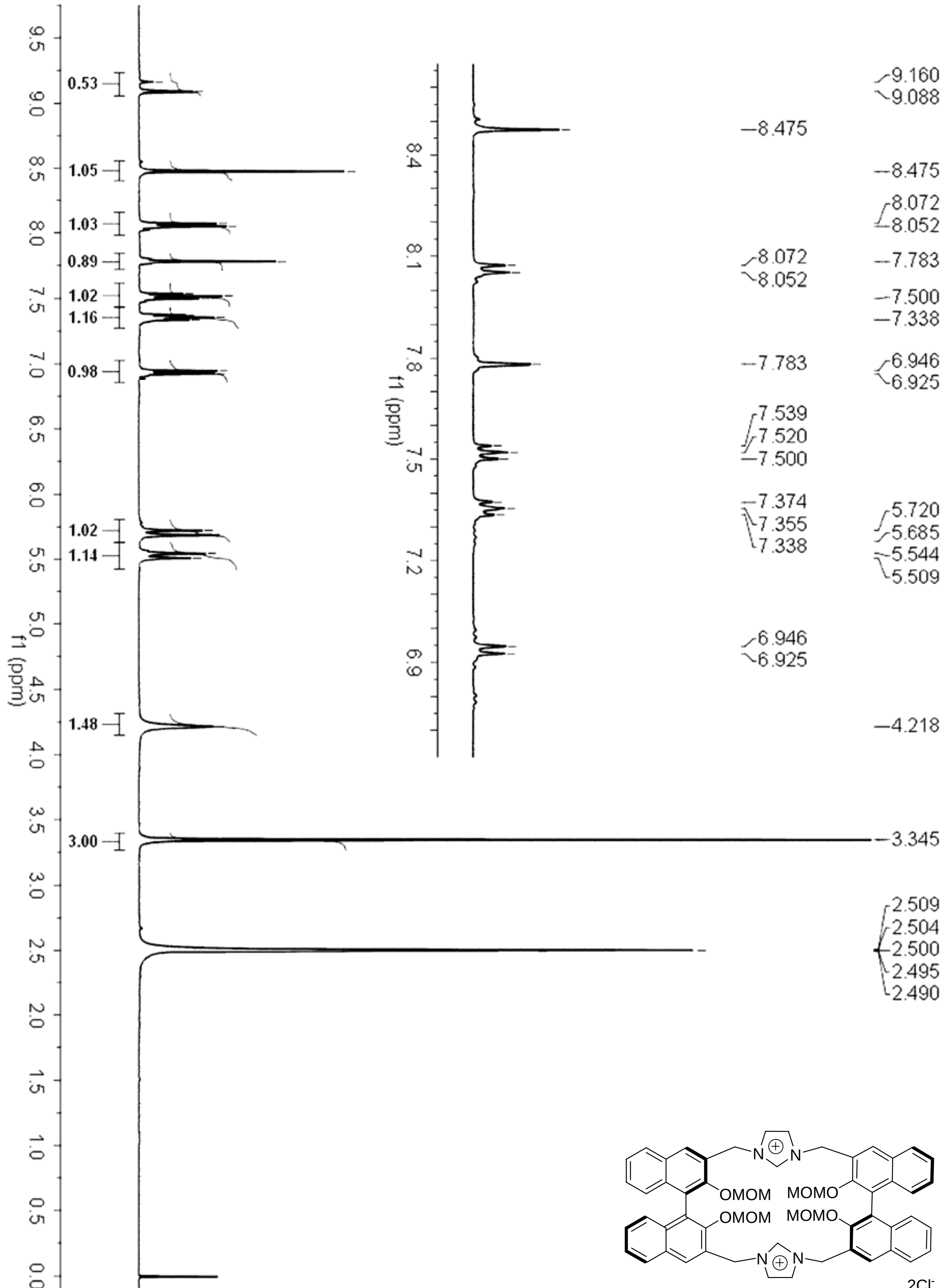
(*R*)-**11**


YJS-1023-1
Pulse Sequence: s2pul
154.193
137.669
134.137
130.201
129.784
129.598
129.064
128.085
127.190
125.467
124.022
119.458
77.210
77.000
76.786
60.573
47.023
200
180
160
140
120
100
80
60
40
20
ppm
OCH3
OCH3
N
N
N
N
(R)-11

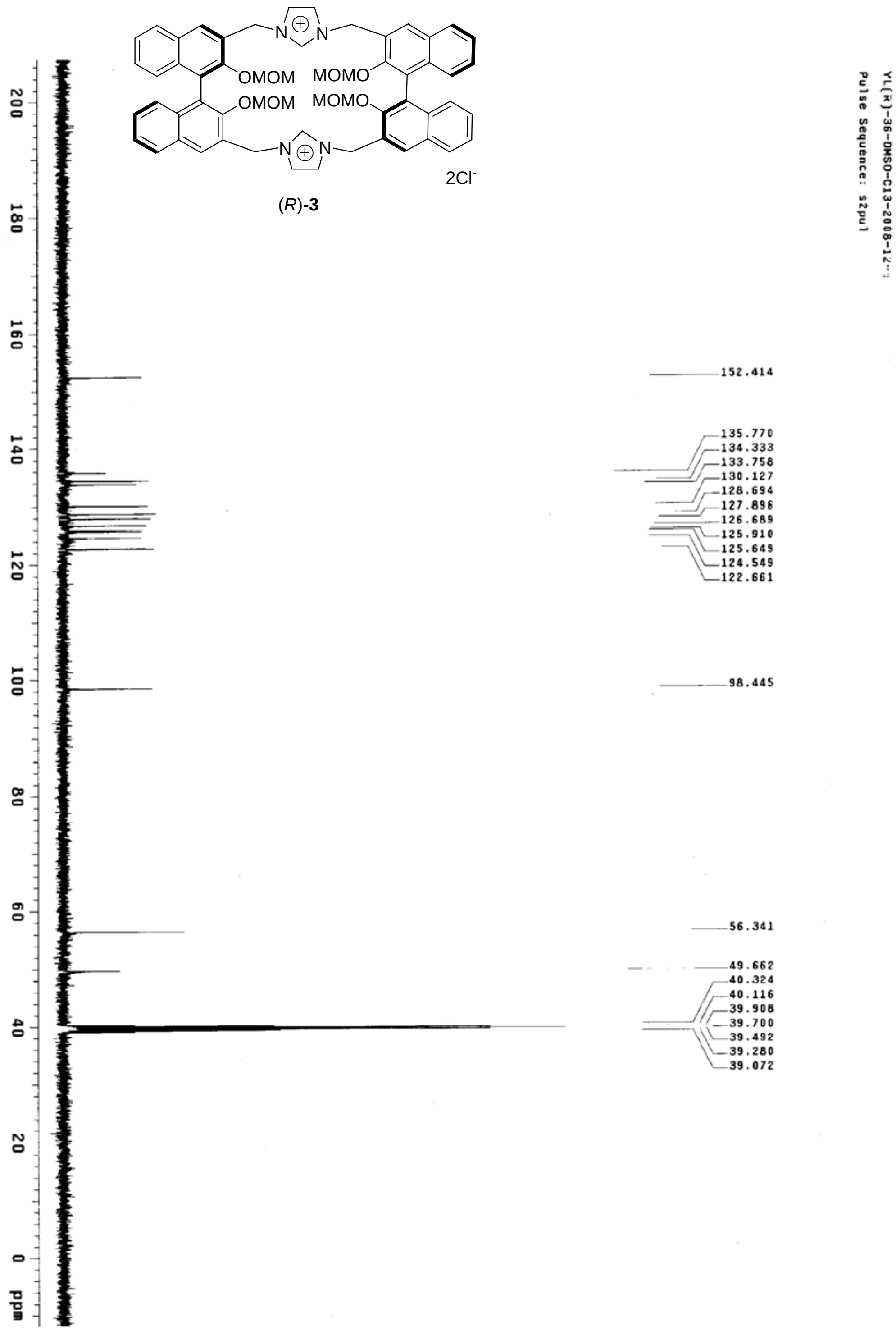

OMOM
OMOM
(R)-16
R-35


R-35 13C
OMOM
OMOM
N
N
N
N
(R)-16
152.1074
137.8198
133.7988
130.6519
129.8254
128.4606
128.2048
127.3109
125.7746
125.7069
125.0232
119.6180
99.5855
77.4930
77.2709
77.0693
76.6458
57.0966
46.8660
180
160
140
120
100
80
60
40
20
0 ppm
BRUKER
Current Data Parameters
NAME R-35 13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061114
Time_ 14.26
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 837
DS 16
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5160.6
DW 26.550 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -6.00 dB
SFO1 75.4752960 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 16.00 dB
SFO2 300.1314410 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

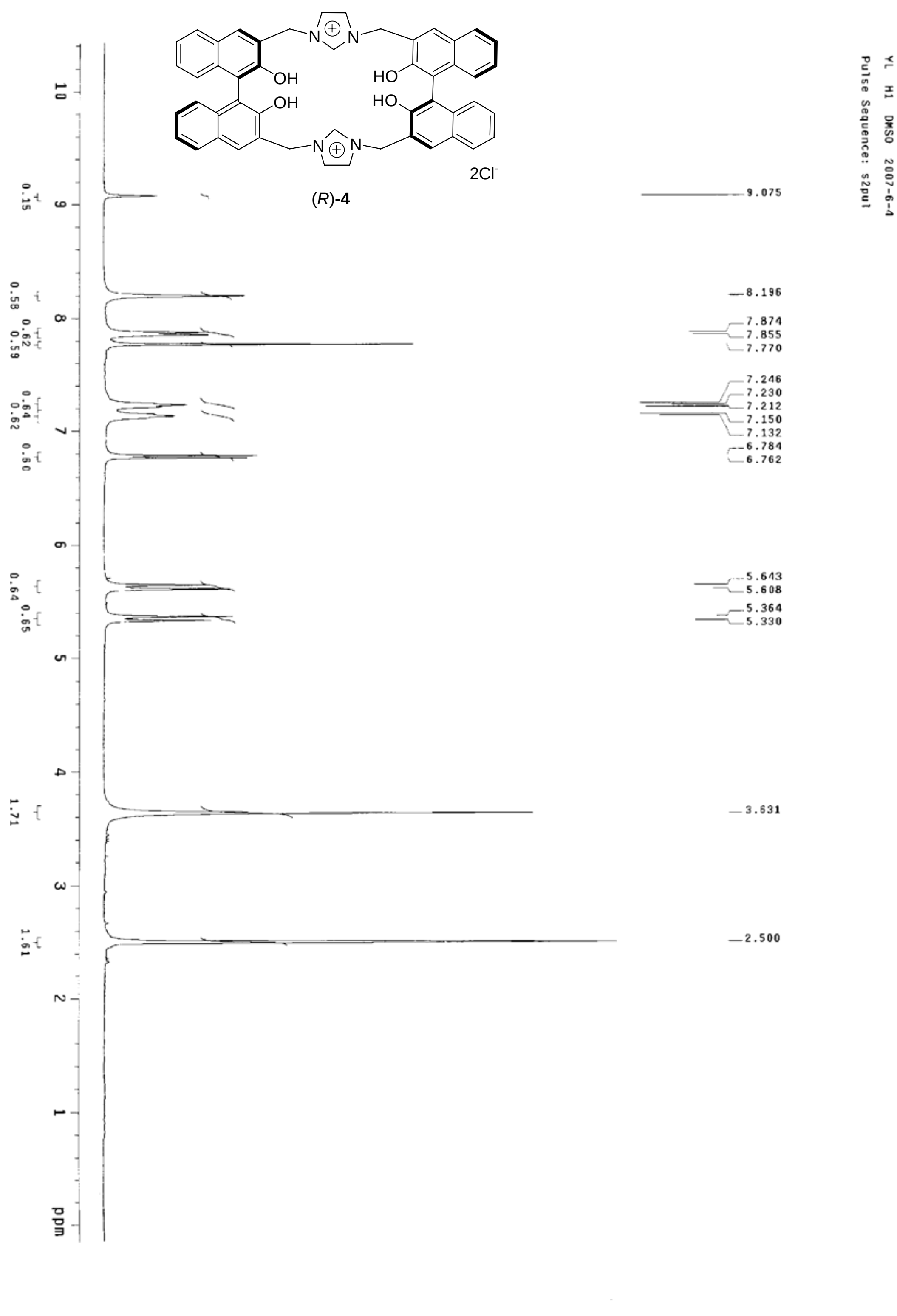
Supplementary Material (ESI) for Organic and Biomolecular Chemistry

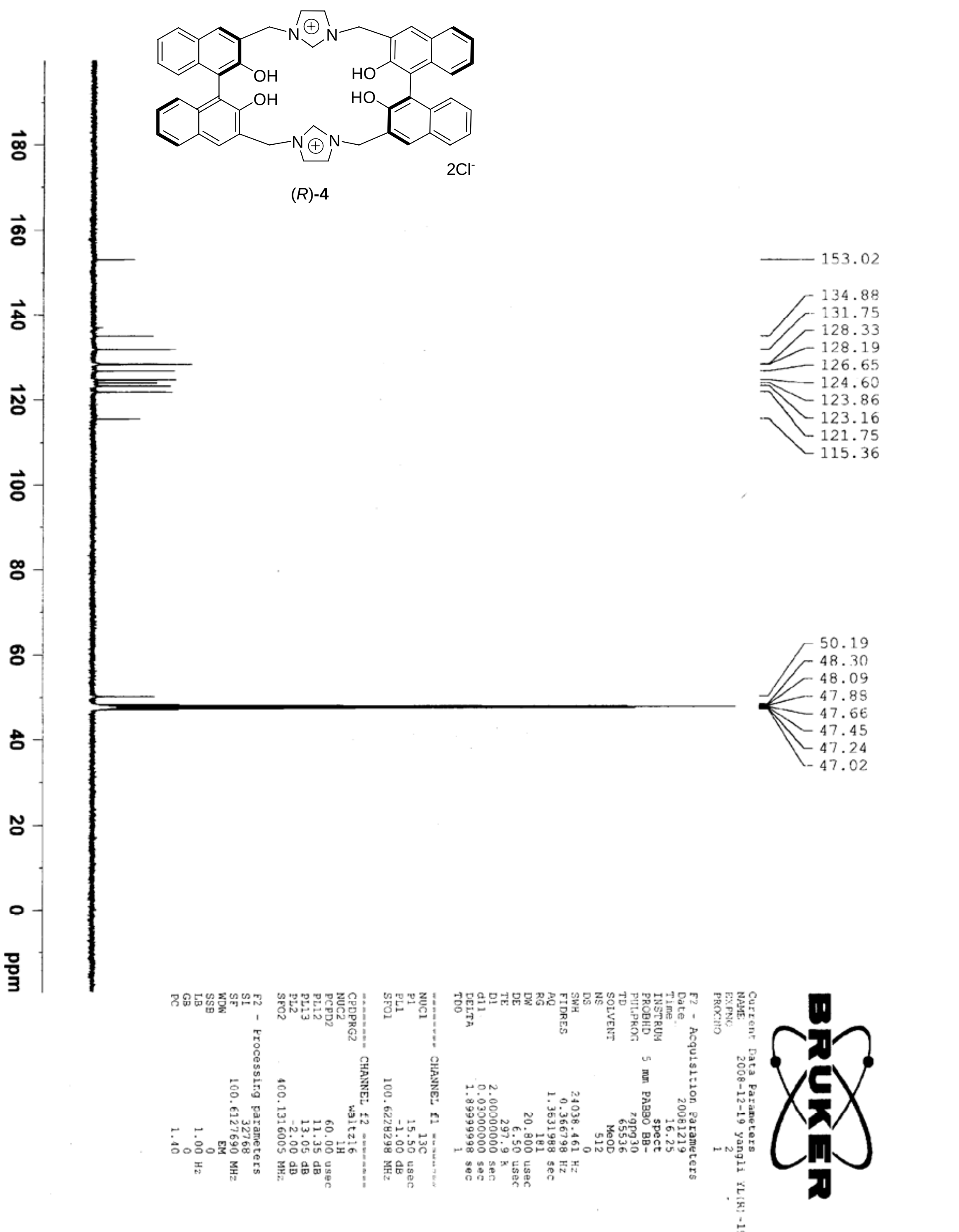


(R)-3

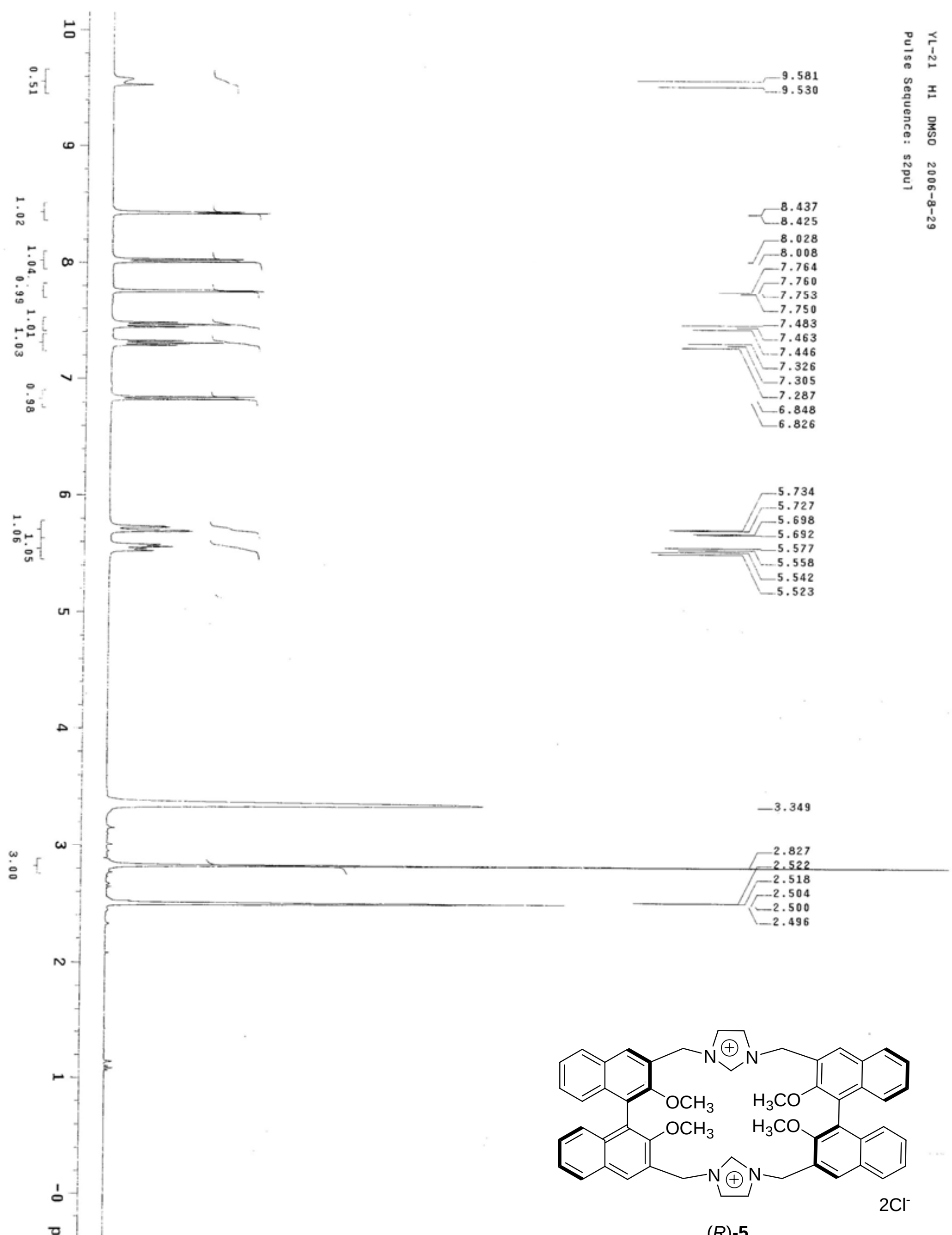

OMOM
MOMO
OMOM
MOMO
2Cl⁻
YL(R)-36-DMSO-C13-2008-12
Pulse Sequence: s2pul
152.414
135.770
134.333
133.758
130.127
128.694
127.896
126.689
125.910
125.649
124.549
122.661
98.445
56.341
49.662
40.324
40.116
39.908
39.700
39.492
39.280
39.072
200
180
160
140
120
100
80
60
40
20
0
ppm

(*R*)-**3**

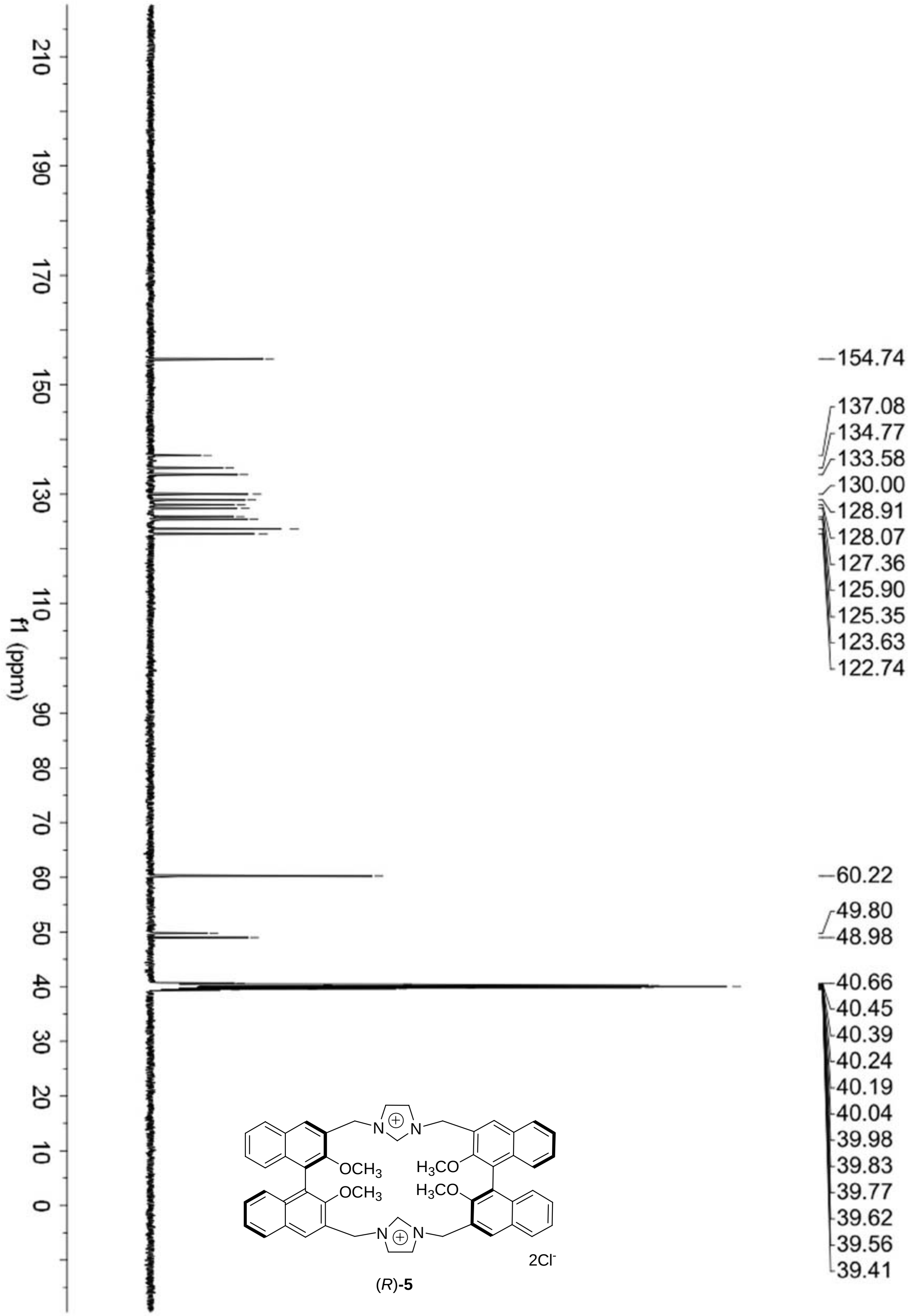

OH
OH
HO
HO
2Cl⁻
(R)-4
YL H1 DMSO 2007-6-4
Pulse Sequence: s2pul
9.075
8.196
7.874
7.855
7.770
7.246
7.230
7.212
7.150
7.132
6.784
6.762
5.643
5.608
5.364
5.330
3.631
2.500
0.15
0.58
0.62
0.59
0.64
0.62
0.60
0.64
0.65
1.71
1.61
ppm



OH
OH
HO
HO
2Cl⁻
(R)-4
153.02
134.88
131.75
128.33
128.19
126.65
124.60
123.86
123.16
121.75
115.36
50.19
48.30
48.09
47.88
47.66
47.45
47.24
47.02
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME 2008-12-19 yangli YL(R)-19
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081219
Time 16.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 15.50 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 11.35 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


YL-21 H1 DMSO 2006-8-29
Pulse Sequence: s2pul
9.581
9.530
8.437
8.425
8.028
8.008
7.764
7.760
7.753
7.750
7.483
7.463
7.446
7.326
7.305
7.287
6.848
6.826
5.734
5.727
5.698
5.692
5.577
5.558
5.542
5.523
3.349
2.827
2.522
2.518
2.504
2.500
2.496
0.51
1.02
1.04
0.99
1.01
1.03
0.98
1.05
1.06
3.00
ppm
OCH3
H3CO
2Cl-

(*R*)-**5**


154.74
137.08
134.77
133.58
130.00
128.91
128.07
127.36
125.90
125.35
123.63
122.74
60.22
49.80
48.98
40.66
40.45
40.39
40.24
40.19
40.04
39.98
39.83
39.77
39.62
39.56
39.41
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
OCH3
H3CO
2Cl-
(R)-5