Pattern-Based Recognition for the Rapid Determination of Identity, Concentration, and Enantiomeric Excess of Subtly Different Threo Diols

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Supporting Information

EXPERIMENTAL SECTION

Synthesis

Host-**2**: Boronic acid host-**2** was synthesized by reductive amination according to a published procedure.[1]

Complex **7**: Host **2** (0.5 mmol, 178.6 mg) and (*S,S*)-hydrobenzoin (0.5 mmol, 107.1 mg) were dissolved in $CHCl_3$ (2.5 mL) and stirred with 1 g $MgSO_4$ suspension at room temperature for 30 min. $MgSO_4$ was removed by vacuum filtration and the filtrate was concentrated. The crude product was dissolved in $CHCl_3$ (5 mL) and concentrated again in order to azeotropically remove the condensed water. The product was purified by crystallization by diffusing methanol into the concentrated $CHCl_3$ solution. The crystals from the CH_3OH solution were submitted for x-ray crystallographic analysis.

Host (*S*,*S*)-**2** [2-(((2*S*,5*S*)-2,5-diphenylpyrrolidin-1yl)methyl)phenylboronic acid]: mp 118 - 128 °C. ^{1}H NMR (600 MHz, CD_3OD) δ 7.29 (m, 10H), 7.13 (m, 3H), 6.81 (b, 1H), 4.39 (m, 1H), 3.57 (d, J = 13.6 Hz, 1H), 3.26 (d, J = 13.7 Hz, 1H),) 2.58 (m, 2H), 2.17 (m, 2H) ppm. ^{13}C NMR (150 MHz, DMSO) δ 141.79, 133.72, 130.05, 129.24, 128.65, 127.40, 67.89, 55.66, 33.04, 30.65 ppm. HRMS (M+H) calc: 358.1934; found: 358.1973

Host (*R*,*R*)-**2** [2-(((2*R*,5*R*)-2,5-diphenylpyrrolidin-1yl)methyl)phenylboronic acid]: mp 98 - 117 °C. ^{1}H NMR (600 MHz, CD_3OD) δ 7.29 (m, 10H), 7.14 (m, 3H), 6.81 (b, 1H), 4.39 (m, 1H), 3.57 (d, J = 13.6 Hz, 1H), 3.29 (d, J = 13.7 Hz, 1H),) 2.58 (m, 2H), 2.17 (m, 2H) ppm. ^{13}C NMR (150 MHz, DMSO) δ 141.73, 133.45, 130.06, 129.24, 128.67, 127.41, 67.89, 55.46, 33.02, 30.65 ppm. HRMS (M+H) calc: 358.1934; found: 358.1973.

Complex **7**: mp 162-169°C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (m, 2H), δ 7.52 (m, 1H), δ 7.37 (m, 6H), δ 7.27 (m, 12H), δ 7.12 (m, 4H), δ 4.37 (m, 2H), δ 3.80 (d, J = 16.1 Hz, 1H), δ 3.74 (d, J = 16.2 Hz, 1H), δ 2.61 (m, 2H), δ 2.03 (m, 2H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.16, 143.83, 140.29, 135.87, 131.33, 128.61, 128.12, 128.09, 128.05, 128.01, 126.73, 125.80, 125.40, 86.52, 65.19, 50.55, 33.14 ppm. HRMS (M+H) calc: 536.2716; found: 536.2755.

UV-vis Titrations:

UV-vis titrations were performed on a Beckman DU-640 UV-vis spectrophotometer. Stock solutions of the hosts, indicators, and diols were made in 10 mM buffer solution pH 7.4 (Hunig's base and *para*-toluenesulfonic acid) in 100% spectral grade degassed methanol. All measurements were taken at 25°C.

The ideal host and indicator combinations for enantiomeric discrimination were determined by generating 1:1 binding isotherms via UV-vis titration between the host and the indicator (**Figure S1-S6**). During the titration, the solution was allowed to equilibrate for 3 min after each addition, and the

absorbance spectra was recorded until the change in absorbance from one reading to the next was < 0.03. The binding constants (K_{HI}) between the host and the indicators were determined from a 1:1 binding isotherm (**Table 1**).

The binding constant between the host and the guest K_{HG} was determined by measuring the change in absorbance of the host:indicator solution with the addition of the guest. ML was the selected indicator for this analysis. The optimum ratio of host-**2** (440 μM) to ML (75 μM) (~ 90% saturation) was used as determined by the host:indicator binding isotherm.

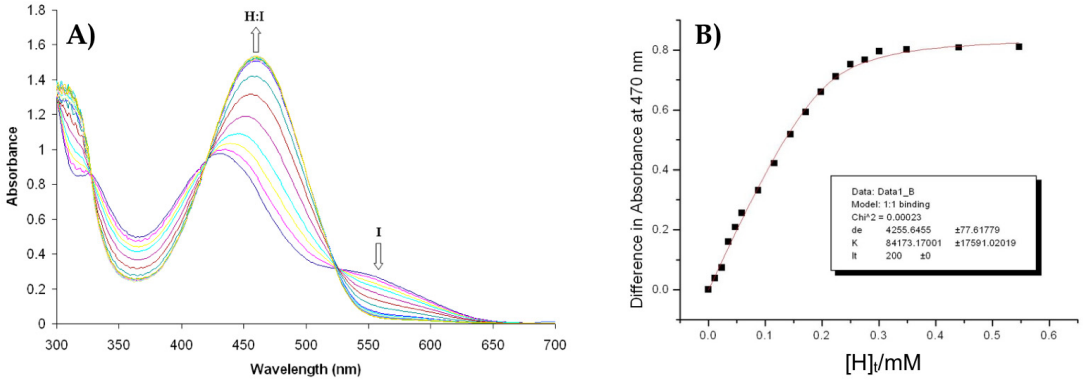


Figure S1: A) UV-visible titration of host (*S,S*)-**2** with A (200 μM), Host:Indicator complex (H:I), free indicator (I) **B)** 1:1 binding isotherm (plot of the difference in absorbance at 470 nm with the addition of the host). Stock solutions were prepared in 100% degassed spectral grade MeOH, using 10 mM *para*-toluenesulfonic acid and Hunig's base buffer, pH 7.4. Association constant: K_{HI}; difference in molar absorptivity between the H:I complex and free I: de; total indicator concentration: It. The solid line is the calculated curve resulting from iterative data fitting to a 1:1 binding isotherm. All measurements were taken at 25ºC.[2]

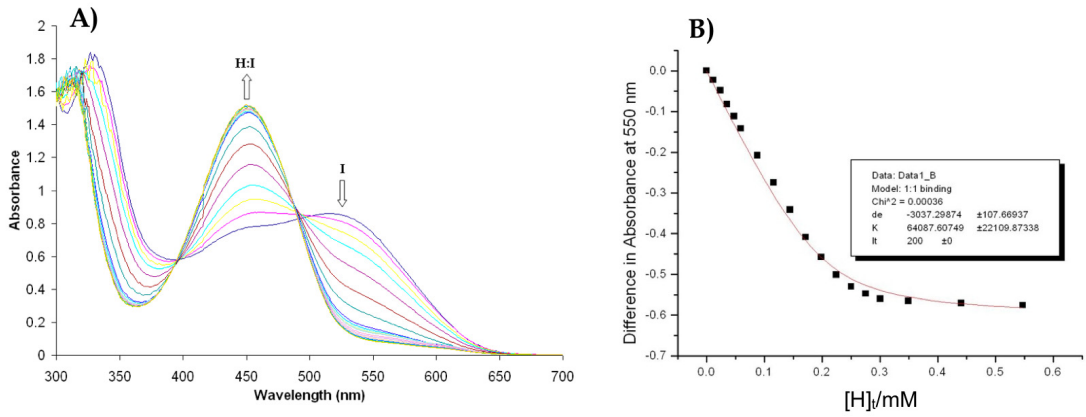


Figure S2: A) UV-visible titration of host (*S,S*)-**2** with AC (200 μM), Host:Indicator complex (H:I), free indicator (I) **B)** 1:1 binding isotherm (plot of the difference in absorbance at 550 nm with the addition of the host). Stock solutions were prepared in 100% degassed spectral grade MeOH, using 10 mM *para*-toluenesulfonic acid and Hunig's base buffer, pH 7.4. Association constant: K_{HI}; difference in molar absorptivity between the H:I complex and free I: de; total indicator concentration: It. The solid line is the calculated curve resulting from iterative data fitting to a 1:1 binding isotherm. All measurements were taken at 25ºC.[2]

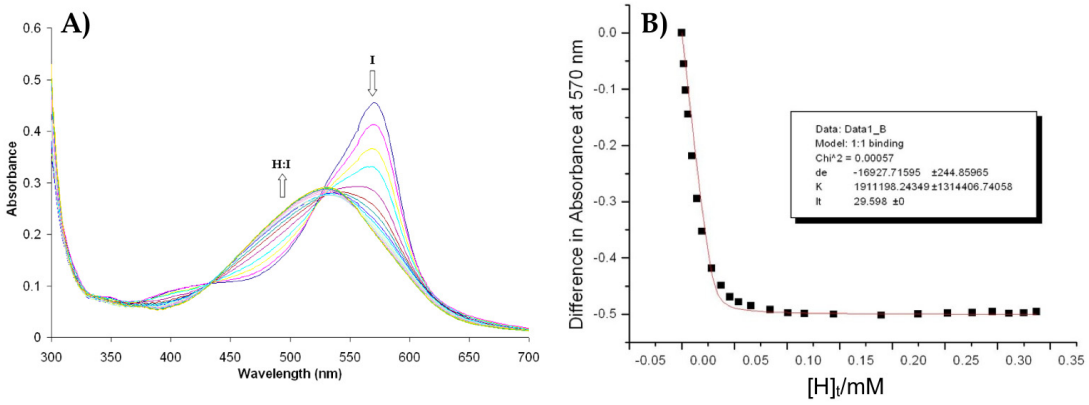


Figure S3: A) UV-visible titration of host (*S,S*)-**2** with BPG (29.59 μM), Host/Indicator complex (H:I), free indicator (I) **B)** 1:1 binding isotherm (plot of the difference in absorbance at 570 nm with the addition of the host). Stock solutions were prepared in 100% degassed spectral grade MeOH, using 10

mM *para*-toluenesulfonic acid and Hunig's base buffer, pH 7.4. Association constant: K_{HI}; difference in molar absorptivity between the H:I complex and free I: de; total indicator concentration: It. The solid line is the calculated curve resulting from iterative data fitting to a 1:1 binding isotherm. All measurements were taken at 25ºC.[2]

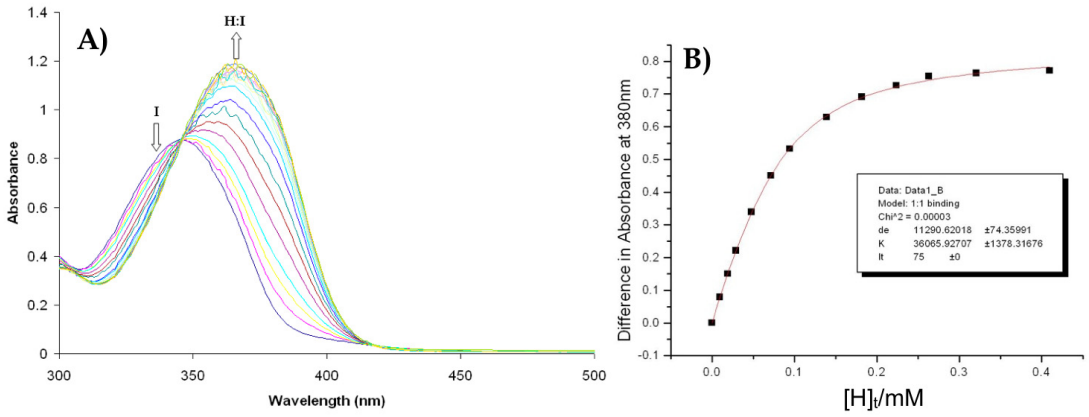


Figure S4: A) UV-visible titration of host (*S,S*)-**2** with ML (75 μM), Host:Indicator complex (H:I), free indicator (I) **B)** 1:1 binding isotherm (plot of the difference in absorbance at 380 nm with the addition of the host). Stock solutions were prepared in 100% degassed spectral grade MeOH, using 10 mM *para*-toluenesulfonic acid and Hunig's base buffer, pH 7.4. Association constant: K_{HI}; difference in molar absorptivity between the H:I complex and free I: de; total indicator concentration: It. The solid line is the calculated curve resulting from iterative data fitting to a 1:1 binding isotherm. All measurements were taken at 25ºC.[2]

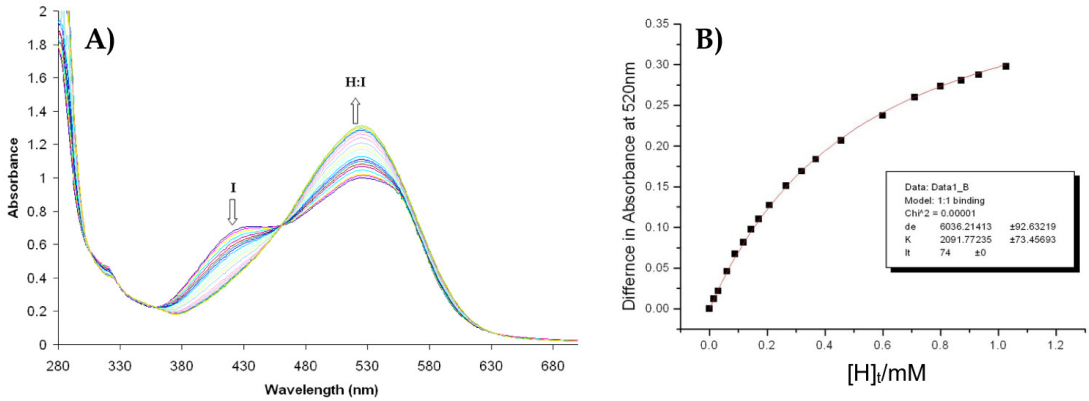


Figure S5: A) UV-visible titration of host (*S,S*)-2 with PG (74 μM), Host:Indicator complex (H:I), free indicator (I) B) 1:1 binding isotherm (plot of the difference in absorbance at 520 nm with the addition of the host). Stock solutions were prepared in 100% degassed spectral grade MeOH, using 10 mM *para*-toluenesulfonic acid and Hunig's base buffer, pH 7.4. Association constant: K_{HI}; difference in molar absorptivity between the H:I complex and free I: de; total indicator concentration: It. The solid line is the calculated curve resulting from iterative data fitting to a 1:1 binding isotherm. All measurements were taken at 25ºC.[2]

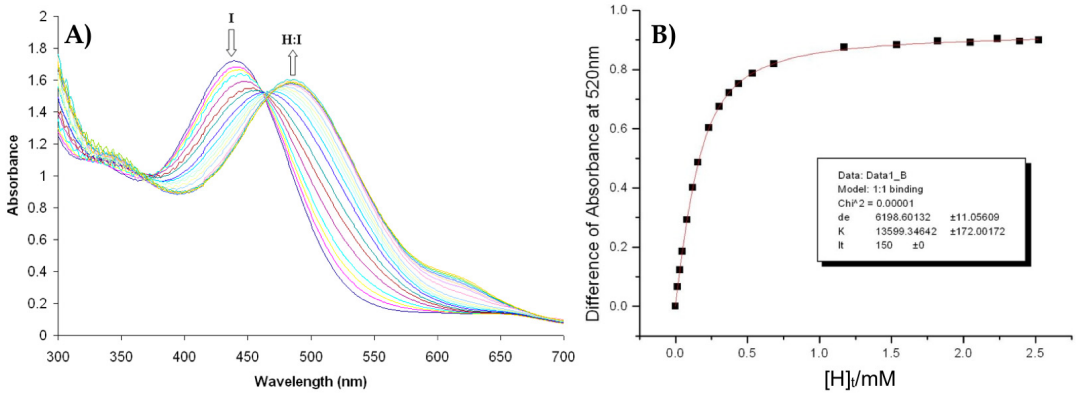


Figure S6: A) UV-visible titration of host (*S,S*)-**2** with PV (150 μM), Host:Indicator complex (H:I), free indicator (I) **B)** 1:1 binding isotherm (plot of the difference in absorbance at 520 nm with the addition of the host). Stock solutions were prepared in 100% degassed spectral grade MeOH, using 10 mM *para*-toluenesulfonic acid and Hunig's base buffer, pH 7.4. Association constant: K_{HI}; difference in molar absorptivity between the H:I complex and free I: de; total indicator concentration: It. The solid line is the calculated curve resulting from iterative data fitting to a 1:1 binding isotherm. All measurements were taken at 25ºC.[2]

NMR Analysis of the Enantiomeric Purity of 4:[3]

2-Formylphenylboronic acid (14.9 mg, 0.1 mole) and (*R*)-α methylbenzylamine (12.7 μL, 0.1 mole) were dissolved in $CDCl_3$ (1 mL), in a dry glass vial equipped with a few 4 Å molecular sieves. (18.02 mg, 0.1 mole) of the diol (3,4 dihydroxy-4-phenyl-butane-2-one) obtained from the asymmetric dihydroxylation reactions was added to the solution. The mixture was allowed to stand with occasional shaking for 5 min. ^{1}H NMR of the resulting solution was recorded (**Figure S7**).

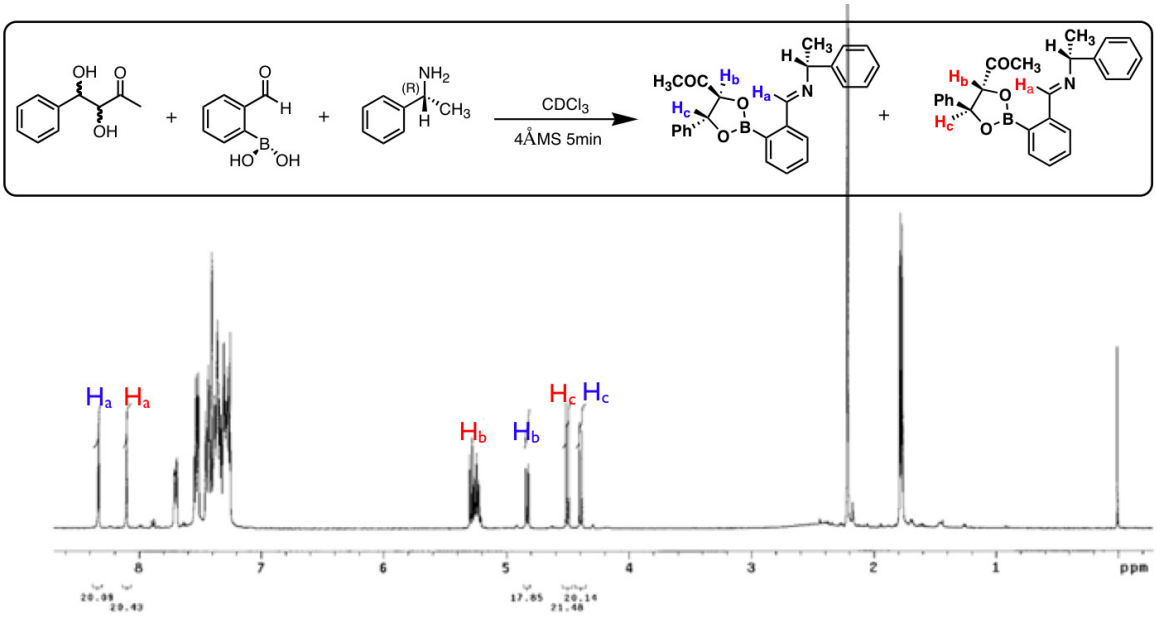


Figure S7: ^{1}H NMR 300 MHz on a Varian Mercury 300 spectrometer in $CDCl_3$ of the racemic mixture of **4** after derivatization.

96-well Plate Analysis:

Arrays were made by mixing host, indicator, and guest stock solutions within a Costar EIA/RIA polystyrene 96-well flat bottom plate. BioTek Precision™ microplate pipetting system was used to add stock solution to the 96-well plate. Each well contained a total solution volume of 300 µL. After making the plate, it was sealed with a UC-500 sealing film to prevent solvent evaporation. The absorbance spectra of the 96-well plate were recorded on a BioTek Synergy™ 4 multi-detection microplate reader.

Table S1: Concentration of the hosts and the indicators used in the 96-well plate.

Indicator	Host (*S*,*S*)-**1**	Host (*S*,*S*)-**2**
A (200 μM)	300 μM	400 μM
AC (200 μM)	446 μM	300 μM
BPG (60 μM)	180 μM	200 μM
ML (125 μM)	380 μM	340 μM
PG (150 μM)	546 μM	300 μM
PV (150 μM)	680 μM	300 μM

Table S2: The UV-vis data used for principal component analysis. **3a**: (*R*,*R*)-Hydrobenzoin, **3b**: (*S*,*S*)-Hydrobenzoin, **4a**: (3*S*,4*R*)-3,4-Dihydroxy-4-phenyl-butane-2-one, **4b**: (3*R*,4*S*)-3,4-Dihydroxy-4-phenyl-butane-2-one, **5a**: Methyl-(2*S*,3*R*)-2,3-dihydroxy-3-phenyl-propionate, **5b**: Methyl-(2*R*,3*S*)-2,3-dihydroxy-3-phenyl-propionate, **6a**: Diethyl-D-tartrate, **6b**: Diethyl-L-tartrate.

Diols	Absorbance of Host (*R*,*R*)-**2** and ML			Absorbance of Host (*S*,*S*)-**1** and PV			Absorbance of Host (*S*,*S*)-**2** and PV		
	362 nm	366 nm	374 nm	496 nm	500 nm	516 nm	496 nm	500 nm	516 nm
3a	1.091	0.997	0.754	0.780	0.736	0.565	0.923	0.885	0.721
3a	1.085	0.992	0.751	0.780	0.735	0.565	0.920	0.882	0.719
3a	1.091	0.996	0.753	0.785	0.741	0.568	0.923	0.886	0.722
3a	1.095	1.001	0.756	0.788	0.744	0.571	0.925	0.888	0.722
3b	1.304	1.255	1.083	0.702	0.653	0.476	0.724	0.676	0.498
3b	1.282	1.232	1.061	0.701	0.653	0.476	0.733	0.685	0.505
3b	1.306	1.256	1.085	0.704	0.656	0.478	0.735	0.687	0.507
3b	1.306	1.257	1.088	0.707	0.658	0.480	0.722	0.674	0.497
6a	1.361	1.323	1.171	0.996	0.964	0.812	1.073	1.043	0.889
6a	1.360	1.322	1.170	0.992	0.960	0.809	1.076	1.047	0.892

6a	1.355	1.317	1.165	0.990	0.959	0.807	1.077	1.047	0.893
6a	1.357	1.32	1.168	0.995	0.963	0.811	1.082	1.053	0.898
6b	1.418	1.393	1.262	0.960	0.926	0.770	0.982	0.947	0.786
6b	1.426	1.401	1.269	0.953	0.919	0.765	0.983	0.949	0.788
6b	1.427	1.402	1.271	0.959	0.925	0.769	0.985	0.950	0.788
6b	1.432	1.407	1.276	0.960	0.926	0.770	0.991	0.955	0.793
4a	1.365	1.329	1.18	0.845	0.803	0.633	0.87	0.828	0.653
4a	1.357	1.321	1.172	0.845	0.803	0.633	0.875	0.832	0.657
4a	1.392	1.356	1.203	0.846	0.804	0.634	0.873	0.830	0.654
4a	1.394	1.356	1.202	0.847	0.805	0.635	0.870	0.827	0.651
4b	1.260	1.191	0.985	0.910	0.871	0.707	1.015	0.981	0.817
4b	1.258	1.191	0.987	0.910	0.872	0.708	1.018	0.983	0.819
4b	1.258	1.191	0.986	0.912	0.873	0.709	1.012	0.977	0.814
4b	1.256	1.188	0.984	0.906	0.867	0.704	1.011	0.976	0.813
5a	1.202	1.124	0.902	0.882	0.843	0.679	1.009	0.974	0.812
5a	1.193	1.113	0.892	0.881	0.842	0.678	1.005	0.970	0.811
5a	1.196	1.118	0.896	0.882	0.843	0.678	1.013	0.979	0.816
5a	1.197	1.118	0.897	0.883	0.843	0.679	1.008	0.973	0.812
5b	1.370	1.333	1.183	0.827	0.784	0.613	0.809	0.764	0.586
5b	1.388	1.350	1.198	0.828	0.785	0.614	0.809	0.764	0.586
5b	1.378	1.341	1.191	0.823	0.779	0.610	0.809	0.764	0.585
5b	1.394	1.357	1.204	0.824	0.781	0.611	0.804	0.758	0.581

Table S3: UV-vis data for Training Artificial Neural Network and Principal Component Analysis

Absorbance with Host (*S*,*S*)-**2** & PV				Absorbance with Host (*R*,*R*)-**2** & ML					Absorbance with Host (*S*,*S*)-**1** & BPG					$[G]_t$mM	%**5a**
512nm	514nm	516nm	518nm	376nm	378nm	380nm	382nm	384nm	570nm	572nm	574nm	576nm	578nm		
0.922	0.903	0.881	0.860	0.936	0.893	0.843	0.792	0.737	1.035	1.024	1.008	0.985	0.956	2.00	100
0.898	0.879	0.858	0.838	0.940	0.896	0.845	0.794	0.738	1.032	1.021	1.005	0.982	0.954	2.00	100
0.881	0.862	0.842	0.822	0.952	0.908	0.856	0.805	0.747	1.031	1.020	1.004	0.981	0.953	2.00	100
0.892	0.872	0.851	0.830	1.023	0.978	0.925	0.870	0.810	1.115	1.104	1.087	1.063	1.032	2.00	80

0.890	0.871	0.849	0.829	1.014	0.969	0.916	0.862	0.802	1.051	1.040	1.024	1.001	0.972	2.00	80
0.889	0.870	0.848	0.827	1.019	0.974	0.920	0.866	0.806	1.051	1.041	1.025	1.002	0.973	2.00	80
0.870	0.851	0.829	0.808	1.046	1.001	0.948	0.893	0.831	1.124	1.113	1.096	1.073	1.042	2.00	70
0.868	0.848	0.827	0.806	1.045	1.000	0.947	0.892	0.830	1.125	1.114	1.097	1.073	1.042	2.00	70
0.871	0.852	0.830	0.809	1.041	0.995	0.942	0.887	0.826	1.064	1.054	1.038	1.016	0.986	2.00	70
0.852	0.832	0.811	0.790	1.068	1.023	0.970	0.914	0.853	1.142	1.131	1.115	1.091	1.059	2.00	60
0.849	0.830	0.808	0.788	1.079	1.035	0.981	0.925	0.862	1.138	1.128	1.111	1.087	1.056	2.00	60
0.852	0.832	0.811	0.790	1.054	1.010	0.956	0.901	0.839	1.143	1.132	1.115	1.092	1.06	2.00	60
0.838	0.818	0.797	0.776	1.105	1.061	1.007	0.951	0.888	1.159	1.148	1.131	1.107	1.075	2.00	50
0.836	0.817	0.795	0.774	1.079	1.036	0.983	0.928	0.866	1.162	1.151	1.134	1.110	1.078	2.00	50
0.832	0.812	0.790	0.770	1.083	1.039	0.986	0.931	0.869	1.161	1.150	1.133	1.109	1.077	2.00	50
0.813	0.793	0.771	0.750	1.129	1.085	1.032	0.975	0.911	1.174	1.163	1.146	1.122	1.09	2.00	40
0.811	0.791	0.770	0.749	1.125	1.081	1.028	0.971	0.907	1.167	1.157	1.141	1.117	1.084	2.00	40
0.816	0.796	0.775	0.754	1.131	1.088	1.034	0.977	0.912	1.176	1.165	1.149	1.124	1.092	2.00	40
0.783	0.763	0.742	0.721	1.188	1.146	1.093	1.036	0.969	1.126	1.116	1.100	1.077	1.046	2.00	20
0.783	0.763	0.741	0.721	1.190	1.148	1.095	1.037	0.970	1.160	1.150	1.134	1.110	1.078	2.00	20
0.780	0.760	0.739	0.718	1.190	1.148	1.095	1.037	0.970	1.093	1.084	1.068	1.046	1.016	2.00	20
0.759	0.739	0.717	0.696	1.248	1.208	1.155	1.098	1.028	1.153	1.144	1.128	1.104	1.073	2.00	0
0.757	0.737	0.715	0.694	1.252	1.210	1.158	1.100	1.031	1.188	1.178	1.162	1.137	1.105	2.00	0
0.752	0.732	0.711	0.690	1.254	1.213	1.161	1.103	1.033	1.150	1.140	1.125	1.101	1.07	2.00	0
0.821	0.803	0.782	0.762	0.818	0.770	0.718	0.668	0.616	1.132	1.123	1.108	1.084	1.053	4.00	100
0.851	0.831	0.810	0.790	0.807	0.760	0.708	0.658	0.607	1.185	1.176	1.159	1.135	1.102	4.00	100
0.845	0.826	0.805	0.784	0.820	0.772	0.720	0.670	0.618	1.108	1.099	1.084	1.061	1.031	4.00	100
0.799	0.779	0.758	0.738	0.872	0.823	0.769	0.717	0.663	1.214	1.206	1.189	1.165	1.132	4.00	80
0.792	0.773	0.752	0.732	0.907	0.858	0.805	0.752	0.697	1.207	1.199	1.182	1.158	1.125	4.00	80
0.783	0.763	0.743	0.723	0.882	0.833	0.779	0.727	0.672	1.209	1.200	1.184	1.160	1.126	4.00	80
0.765	0.745	0.724	0.704	0.911	0.863	0.809	0.756	0.699	1.237	1.229	1.213	1.188	1.154	4.00	70
0.767	0.748	0.727	0.707	0.910	0.861	0.808	0.755	0.699	1.228	1.220	1.204	1.180	1.146	4.00	70
0.762	0.743	0.722	0.702	0.888	0.841	0.788	0.735	0.680	1.212	1.203	1.187	1.163	1.13	4.00	70
0.734	0.715	0.694	0.674	0.930	0.882	0.827	0.774	0.717	1.256	1.248	1.232	1.207	1.173	4.00	60
0.739	0.719	0.698	0.678	0.934	0.886	0.832	0.778	0.721	1.247	1.239	1.223	1.199	1.165	4.00	60
0.732	0.712	0.692	0.672	0.935	0.887	0.833	0.780	0.722	1.235	1.227	1.211	1.187	1.153	4.00	60
0.714	0.694	0.673	0.653	0.968	0.920	0.865	0.811	0.753	1.269	1.261	1.245	1.220	1.185	4.00	50
0.713	0.694	0.673	0.653	0.964	0.917	0.863	0.809	0.750	1.265	1.257	1.241	1.216	1.182	4.00	50
0.703	0.683	0.663	0.643	0.956	0.909	0.855	0.802	0.743	1.244	1.237	1.221	1.196	1.162	4.00	50
0.695	0.675	0.654	0.634	1.003	0.955	0.901	0.846	0.786	1.249	1.241	1.226	1.201	1.168	4.00	40
0.694	0.674	0.653	0.633	1.003	0.957	0.902	0.847	0.787	1.279	1.271	1.256	1.231	1.196	4.00	40
0.683	0.663	0.642	0.623	0.992	0.946	0.892	0.837	0.778	1.265	1.258	1.242	1.217	1.183	4.00	40
0.660	0.640	0.619	0.600	1.088	1.042	0.989	0.932	0.869	1.283	1.276	1.260	1.236	1.201	4.00	20
0.659	0.640	0.618	0.599	1.085	1.040	0.986	0.930	0.867	1.278	1.271	1.256	1.231	1.196	4.00	20
0.645	0.625	0.605	0.586	1.078	1.034	0.980	0.925	0.861	1.259	1.252	1.237	1.212	1.178	4.00	20
0.633	0.613	0.592	0.572	1.187	1.144	1.090	1.033	0.966	1.309	1.303	1.287	1.262	1.226	4.00	0
0.637	0.617	0.595	0.576	1.188	1.144	1.091	1.034	0.967	1.300	1.294	1.278	1.253	1.217	4.00	0

0.624	0.604	0.584	0.564	1.166	1.124	1.072	1.016	0.950	1.272	1.265	1.250	1.226	1.192	4.00	0
0.833	0.814	0.793	0.772	0.759	0.711	0.660	0.611	0.562	1.192	1.184	1.168	1.143	1.111	5.00	100
0.837	0.818	0.796	0.776	0.761	0.714	0.662	0.614	0.565	1.152	1.144	1.128	1.105	1.073	5.00	100
0.830	0.811	0.789	0.769	0.771	0.724	0.671	0.622	0.573	1.209	1.200	1.184	1.160	1.126	5.00	100
0.772	0.752	0.731	0.711	0.813	0.766	0.713	0.663	0.612	1.246	1.238	1.222	1.197	1.163	5.00	80
0.777	0.757	0.735	0.715	0.804	0.757	0.705	0.656	0.605	1.247	1.239	1.223	1.198	1.164	5.00	80
0.772	0.752	0.731	0.711	0.838	0.789	0.735	0.684	0.630	1.232	1.224	1.208	1.184	1.15	5.00	80
0.737	0.718	0.697	0.677	0.859	0.810	0.755	0.704	0.649	1.261	1.253	1.238	1.213	1.179	5.00	70
0.729	0.710	0.689	0.669	0.863	0.813	0.759	0.706	0.652	1.268	1.260	1.244	1.220	1.185	5.00	70
0.741	0.721	0.700	0.680	0.862	0.813	0.759	0.706	0.652	1.255	1.247	1.232	1.207	1.173	5.00	70
0.705	0.685	0.664	0.644	0.872	0.824	0.771	0.720	0.665	1.288	1.281	1.265	1.240	1.205	5.00	60
0.706	0.686	0.665	0.645	0.875	0.826	0.773	0.721	0.666	1.282	1.275	1.259	1.234	1.199	5.00	60
0.704	0.685	0.663	0.643	0.891	0.842	0.788	0.735	0.679	1.272	1.264	1.248	1.224	1.189	5.00	60
0.681	0.661	0.640	0.620	0.923	0.875	0.821	0.767	0.709	1.304	1.297	1.282	1.256	1.221	5.00	50
0.685	0.665	0.644	0.624	0.920	0.871	0.816	0.762	0.705	1.300	1.293	1.277	1.252	1.217	5.00	50
0.678	0.659	0.638	0.618	0.903	0.856	0.803	0.750	0.695	1.290	1.283	1.267	1.243	1.207	5.00	50
0.660	0.640	0.619	0.599	0.958	0.910	0.855	0.801	0.743	1.327	1.320	1.304	1.279	1.243	5.00	40
0.659	0.639	0.618	0.598	0.956	0.908	0.854	0.800	0.741	1.316	1.309	1.294	1.268	1.232	5.00	40
0.661	0.641	0.620	0.601	0.943	0.896	0.843	0.790	0.732	1.308	1.302	1.286	1.261	1.225	5.00	40
0.630	0.610	0.589	0.569	1.050	1.004	0.950	0.894	0.832	1.317	1.310	1.295	1.270	1.235	5.00	20
0.627	0.607	0.586	0.566	1.050	1.003	0.950	0.894	0.832	1.306	1.299	1.284	1.259	1.224	5.00	20
0.625	0.605	0.584	0.565	1.014	0.969	0.918	0.864	0.804	1.298	1.291	1.276	1.251	1.216	5.00	20
0.607	0.587	0.566	0.546	1.155	1.111	1.057	1.001	0.935	1.338	1.332	1.317	1.292	1.255	5.00	0
0.607	0.587	0.566	0.547	1.162	1.119	1.065	1.008	0.943	1.331	1.325	1.310	1.285	1.249	5.00	0
0.591	0.571	0.551	0.532	1.157	1.113	1.060	1.003	0.937	1.325	1.319	1.304	1.278	1.243	5.00	0

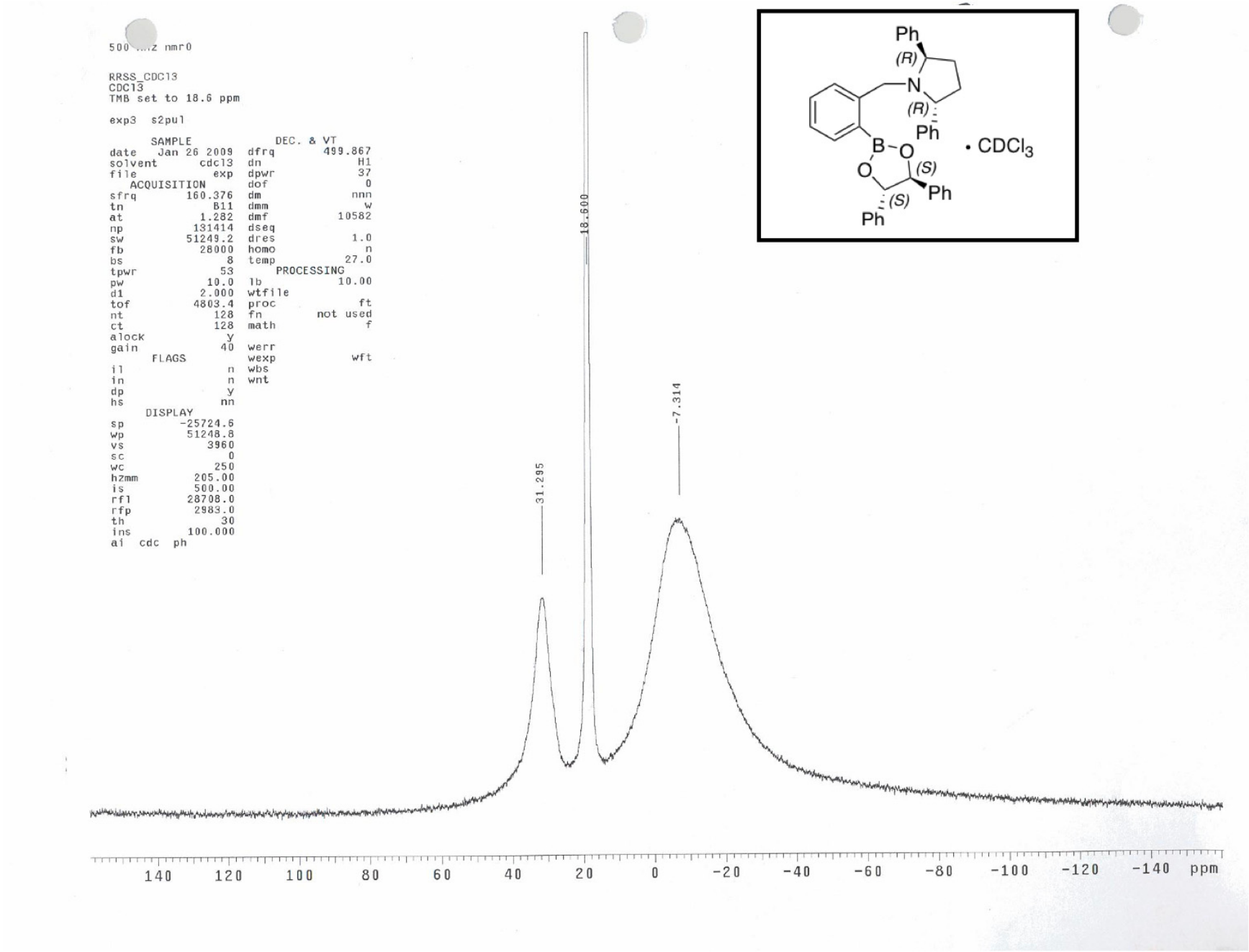
Table S4: UV-vis data of unknown solution for artificial neural network

Absorbance with Host (*S*,*S*)-**2** & PV				Absorbance with Host (*R*,*R*)-**2** & ML					Absorbance with Host (*S*,*S*)-**1** & BPG					$[G]_t$mM	%**5a**
512nm	514nm	516nm	518nm	376nm	378nm	380nm	382nm	384nm	570nm	572nm	574nm	576nm	578nm		
0.882	0.863	0.842	0.822	0.852	0.807	0.756	0.706	0.654	1.120	1.11	1.093	1.070	1.038	3.00	100
0.874	0.856	0.834	0.814	0.848	0.803	0.752	0.703	0.651	1.118	1.107	1.091	1.068	1.037	3.00	100
0.889	0.869	0.848	0.827	0.856	0.811	0.760	0.710	0.658	1.101	1.09	1.074	1.051	1.02	3.00	100
0.824	0.804	0.783	0.763	0.914	0.869	0.817	0.765	0.709	1.160	1.15	1.134	1.110	1.078	3.00	75
0.832	0.813	0.792	0.771	0.908	0.864	0.813	0.763	0.708	1.152	1.142	1.125	1.102	1.070	3.00	75
0.829	0.809	0.788	0.768	0.903	0.858	0.807	0.756	0.702	1.147	1.137	1.121	1.097	1.065	3.00	75
0.800	0.781	0.76	0.739	0.957	0.912	0.858	0.805	0.747	1.174	1.164	1.148	1.124	1.092	3.00	65
0.790	0.770	0.749	0.729	0.981	0.934	0.88	0.826	0.767	1.171	1.161	1.145	1.121	1.089	3.00	65
0.804	0.784	0.763	0.743	0.976	0.930	0.876	0.823	0.764	1.159	1.149	1.133	1.109	1.077	3.00	65
0.769	0.750	0.728	0.708	1.014	0.968	0.914	0.859	0.799	1.198	1.189	1.173	1.149	1.116	3.00	55
0.765	0.745	0.724	0.704	1.020	0.974	0.920	0.866	0.806	1.186	1.176	1.160	1.136	1.104	3.00	55
0.770	0.750	0.729	0.709	1.022	0.976	0.923	0.868	0.808	1.175	1.165	1.149	1.125	1.093	3.00	55
0.756	0.736	0.715	0.695	1.045	0.999	0.946	0.890	0.829	1.206	1.197	1.181	1.157	1.124	3.00	50
0.754	0.735	0.713	0.693	1.039	0.994	0.940	0.885	0.824	1.199	1.190	1.174	1.150	1.117	3.00	50
0.760	0.740	0.719	0.699	1.027	0.982	0.929	0.875	0.815	1.190	1.180	1.164	1.140	1.107	3.00	50

0.737	0.717	0.696	0.676	1.074	1.029	0.976	0.920	0.857	1.22	1.211	1.195	1.171	1.138	3.00	35
0.737	0.717	0.696	0.675	1.070	1.026	0.972	0.917	0.854	1.220	1.210	1.194	1.170	1.137	3.00	35
0.735	0.716	0.695	0.674	1.069	1.025	0.972	0.917	0.855	1.207	1.198	1.181	1.157	1.124	3.00	35
0.731	0.711	0.690	0.669	1.120	1.076	1.022	0.966	0.901	1.206	1.197	1.181	1.158	1.125	3.00	25
0.719	0.699	0.677	0.657	1.119	1.074	1.020	0.964	0.899	1.203	1.195	1.179	1.155	1.122	3.00	25
0.722	0.702	0.681	0.661	1.123	1.079	1.025	0.969	0.905	1.200	1.192	1.176	1.152	1.119	3.00	25
0.693	0.673	0.652	0.631	1.226	1.184	1.131	1.073	1.005	1.236	1.227	1.212	1.187	1.154	3.00	0
0.677	0.658	0.637	0.617	1.220	1.179	1.126	1.068	1.000	1.230	1.221	1.206	1.181	1.148	3.00	0

X-ray Crystal Structure Determination

X-ray Experimental for $C_{37}H_{34}BNO_2$: Crystals grew as colorless prisms by diffusion of methanol into a DCM solution. The data crystal was cut from a larger crystal and had approximate dimensions: 0.33 x 0.25 x 0.17 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 166 frames of data were collected using ω-scans with a scan range of 2° and a counting time of 98 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Data reduction were performed using DENZO-SMN.[4] The structure was solved by direct methods using SIR97[5] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[6] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The absolute configuration was determined from the known configuration of the amine portion of the molecule. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0439*P)^2 + (0.2884*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.0910, with R(F) equal to 0.0424 and a goodness of fit, S, = 1.07. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given in reference 42.[7] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (2.5(7)x10^{-6})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[8] All figures were generated using SHELXTL/PC.[9]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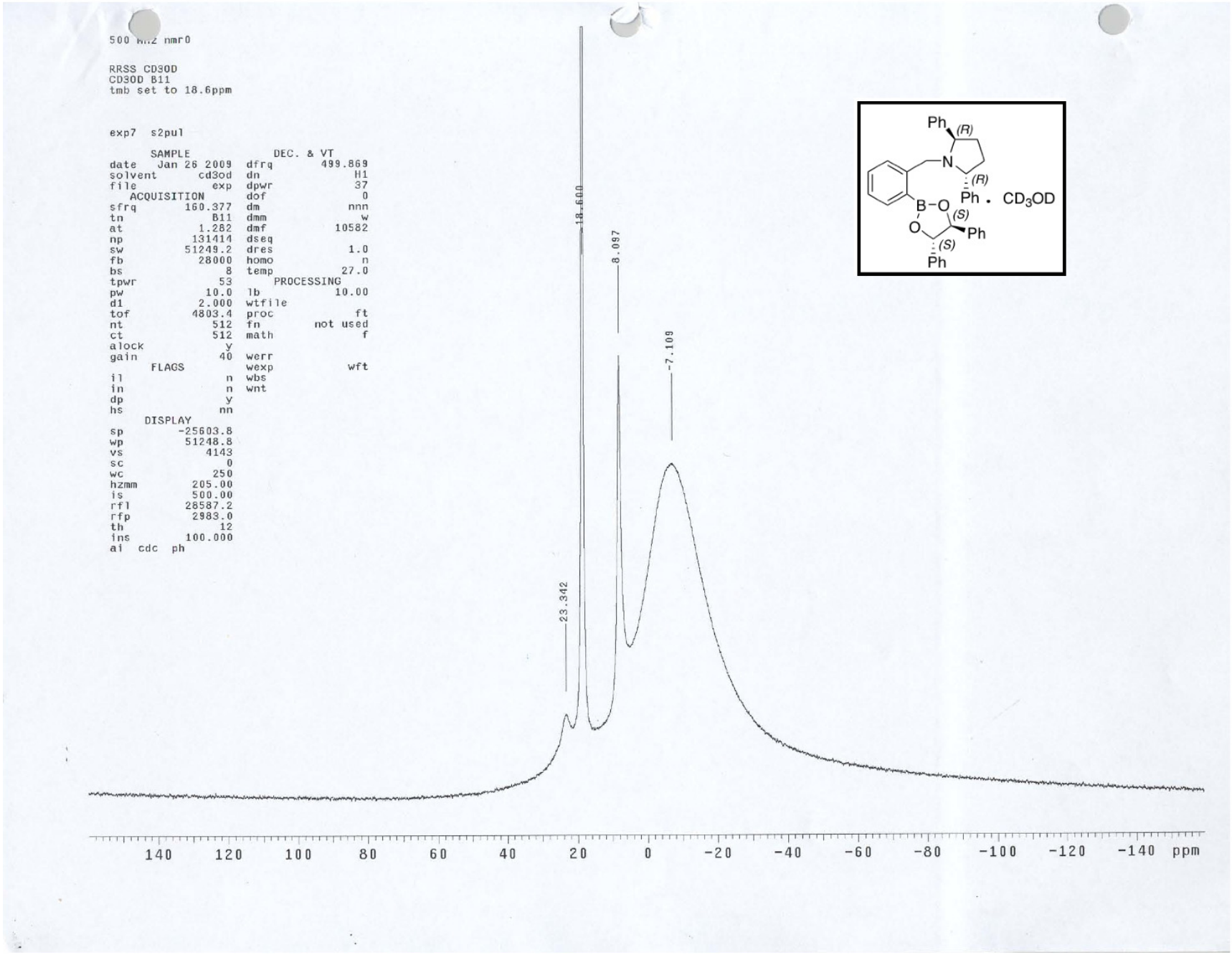
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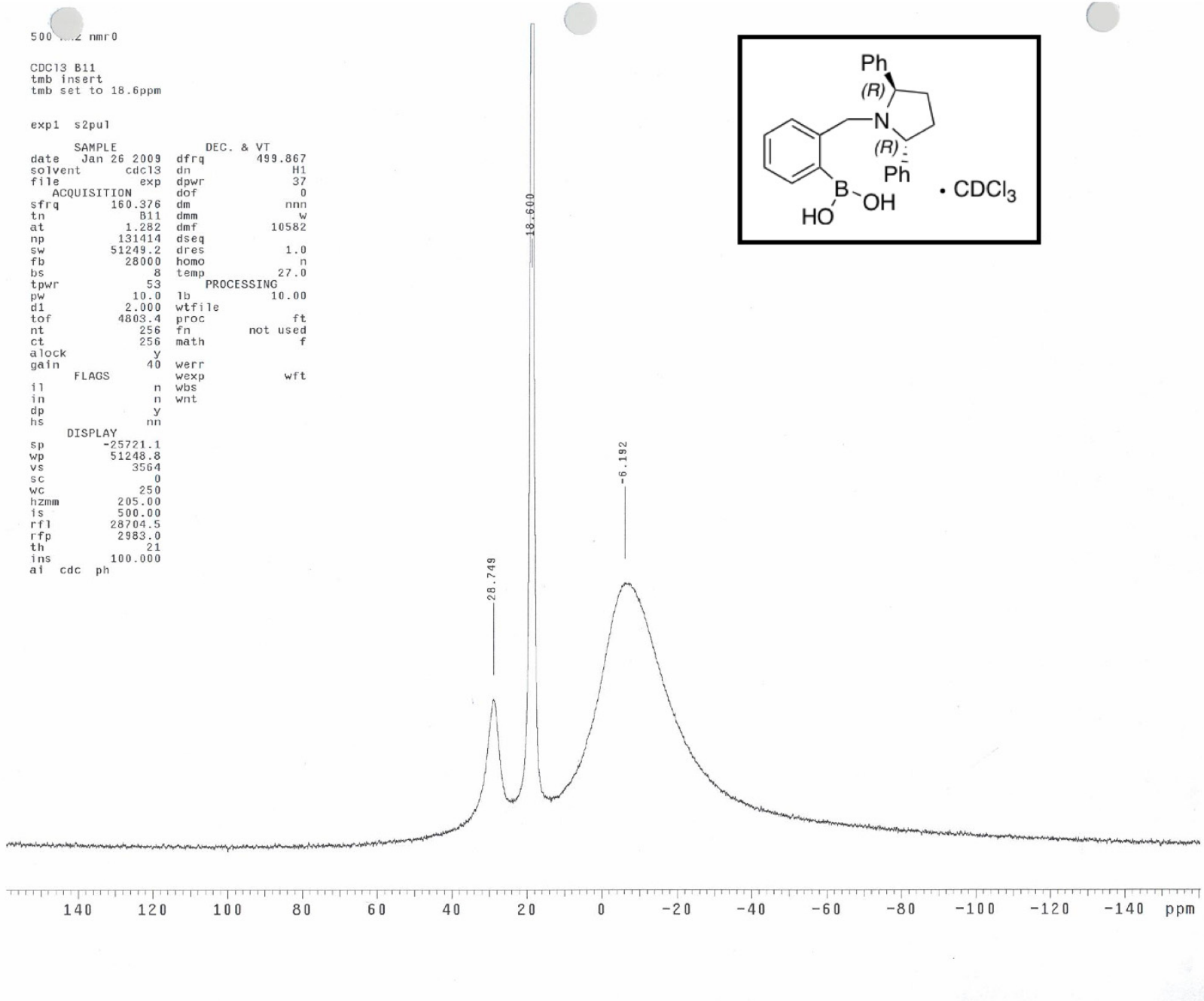
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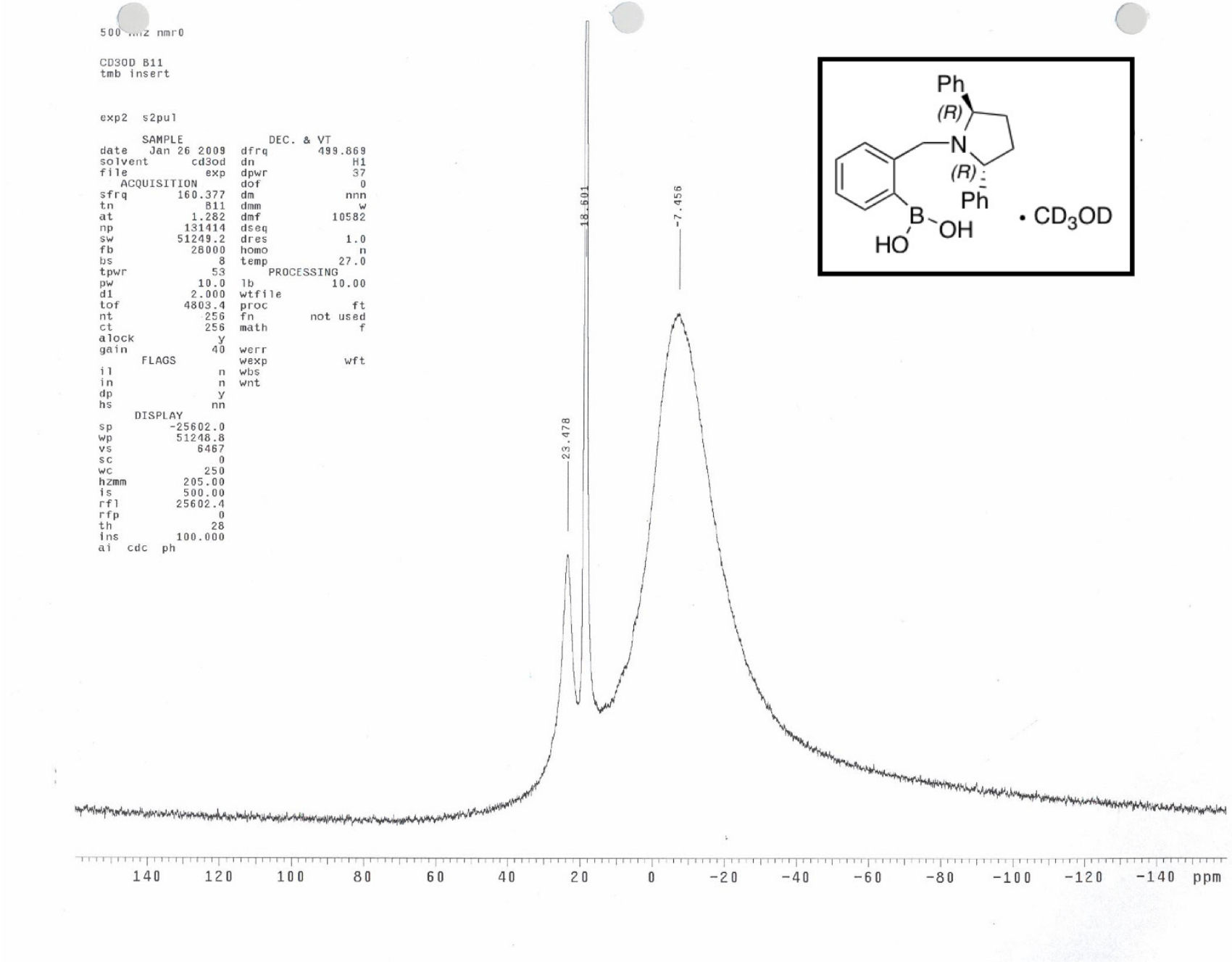
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(7) $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection. $R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$. $S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameter.

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