ELECTRONIC SUPPLEMENTARY INFORMATION

^{31}P NMR spectroscopy and pattern-recognition techniques as tools for the identification and enantiodiscrimination of α-amino acids

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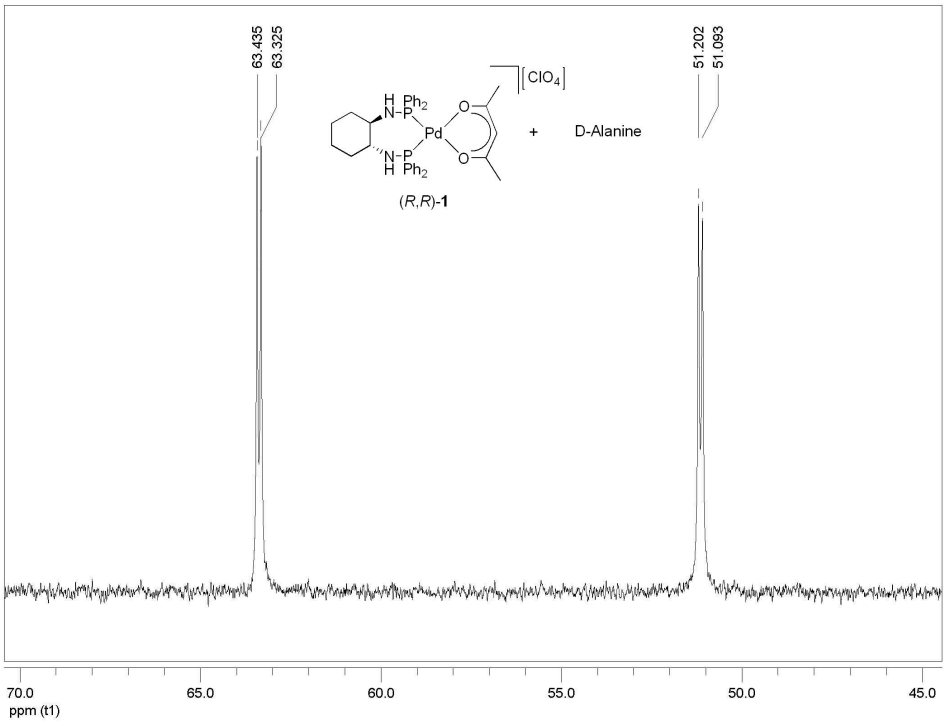


Figure S1. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*-Alanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

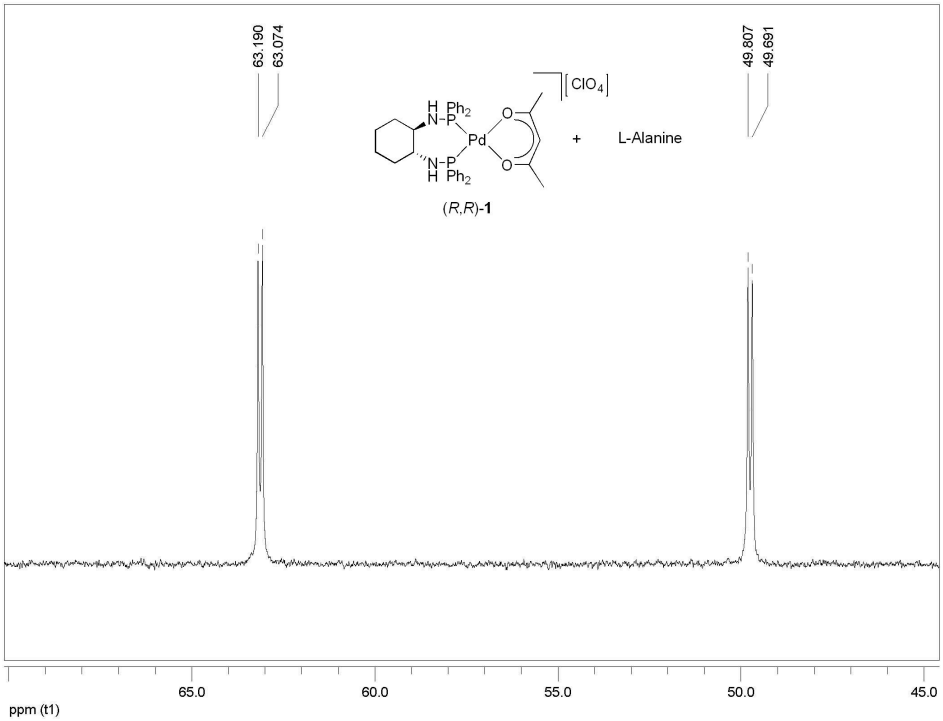


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Alanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

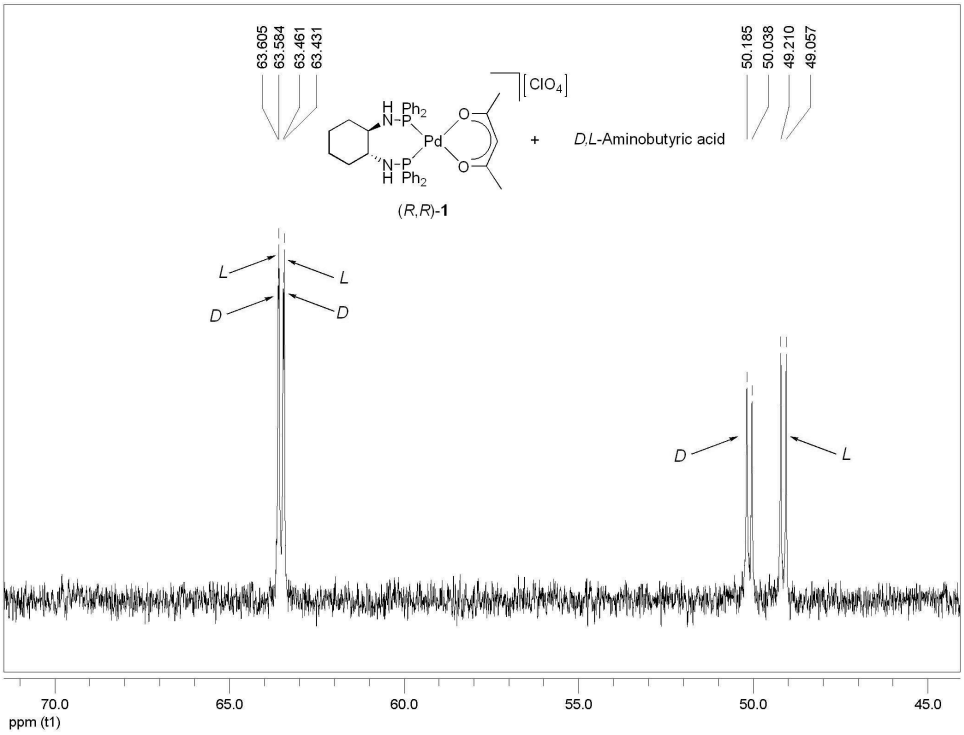


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Aminobutyric acid to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

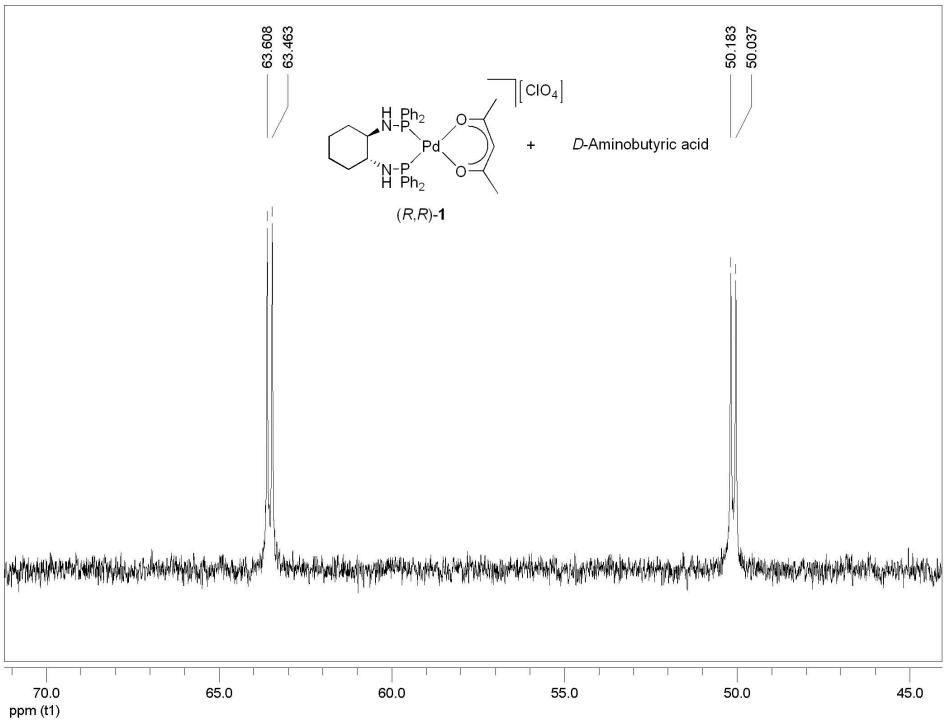


Figure S4. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*-Aminobutyric acid to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

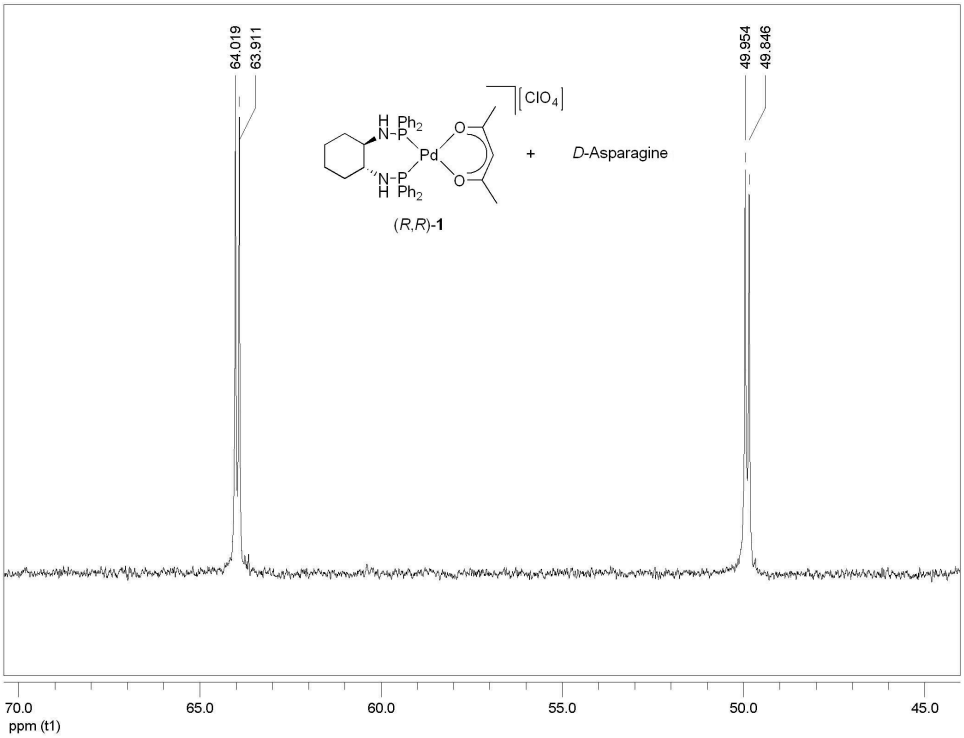


Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*-Asparagine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

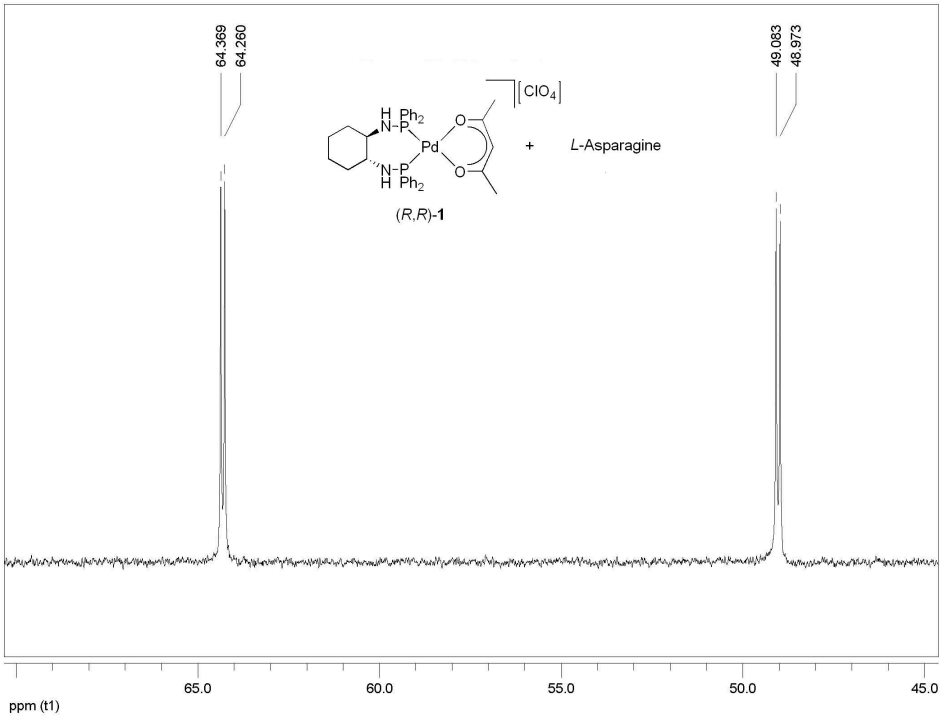


Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Asparagine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

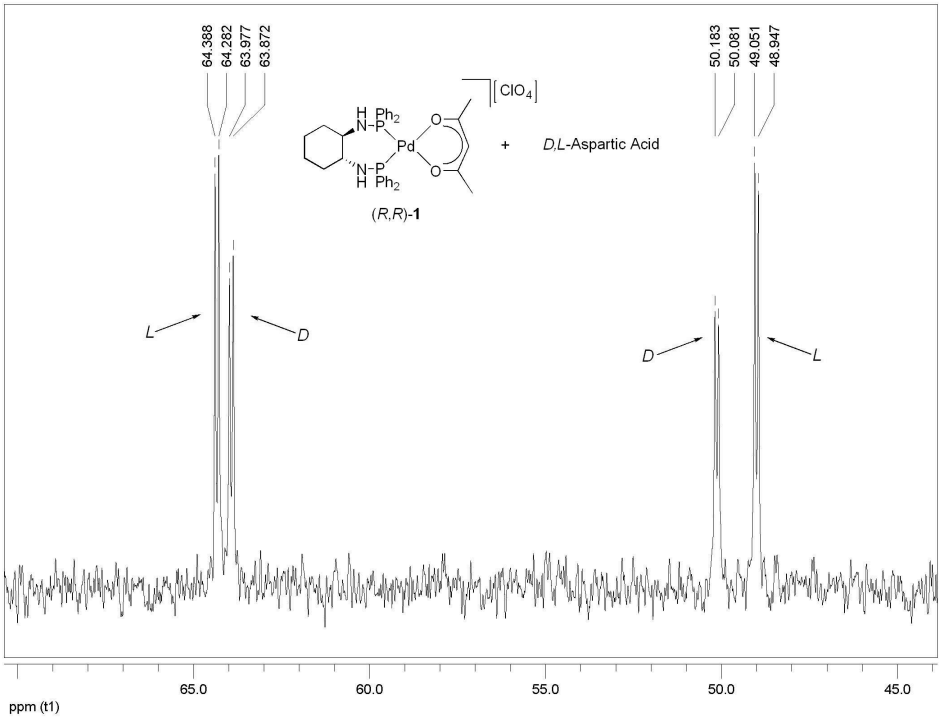


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Aspartic acid to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

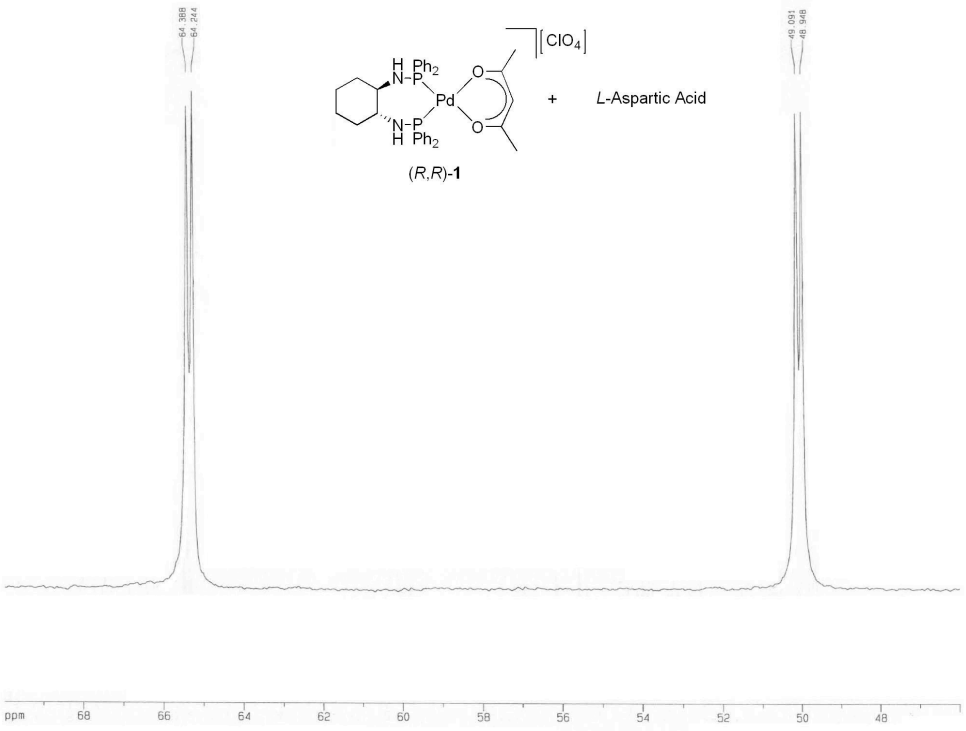


Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Aspartic acid to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

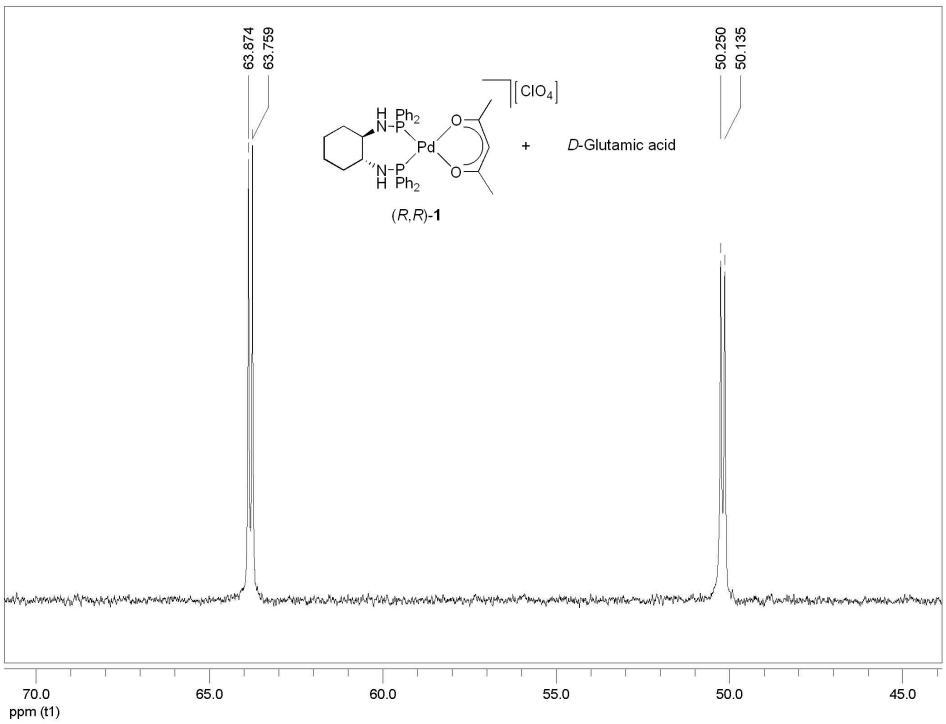


Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*-Glutamic acid to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

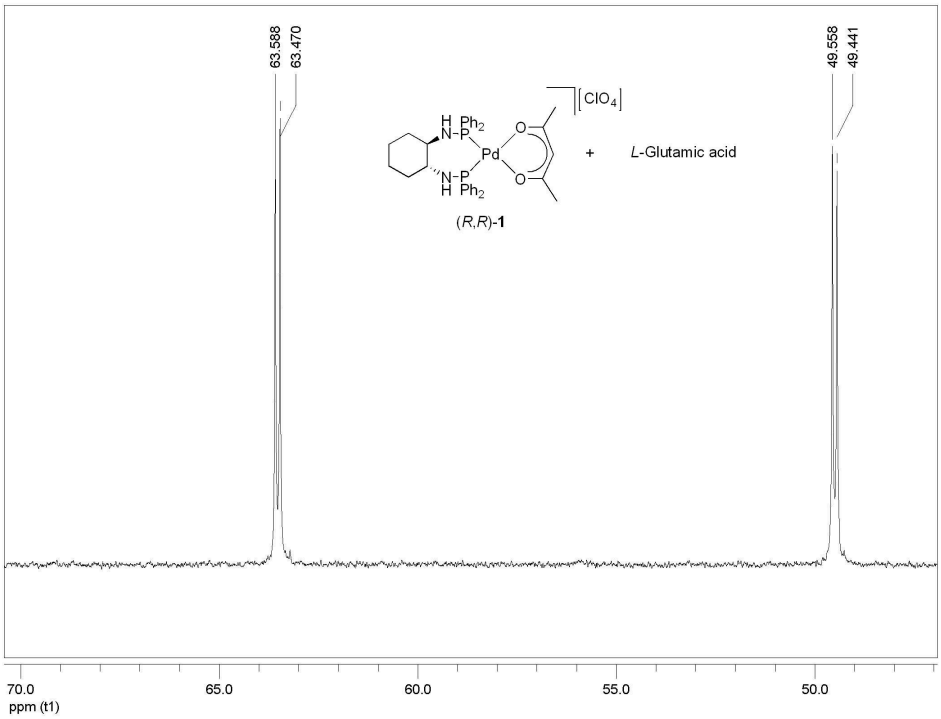


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Glutamic acid to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

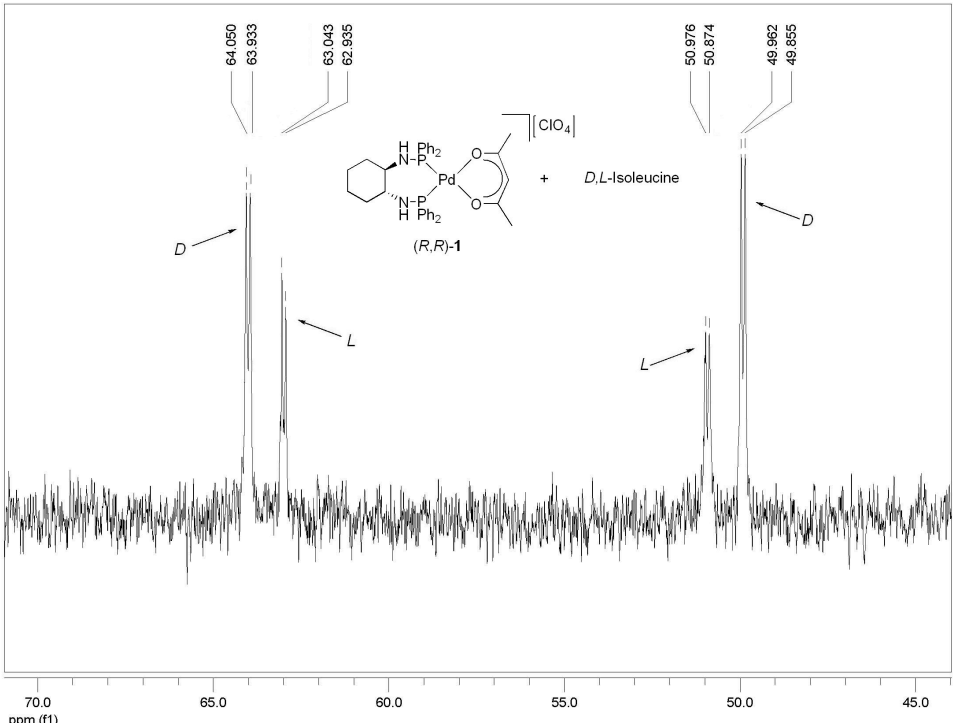


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Isoleucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

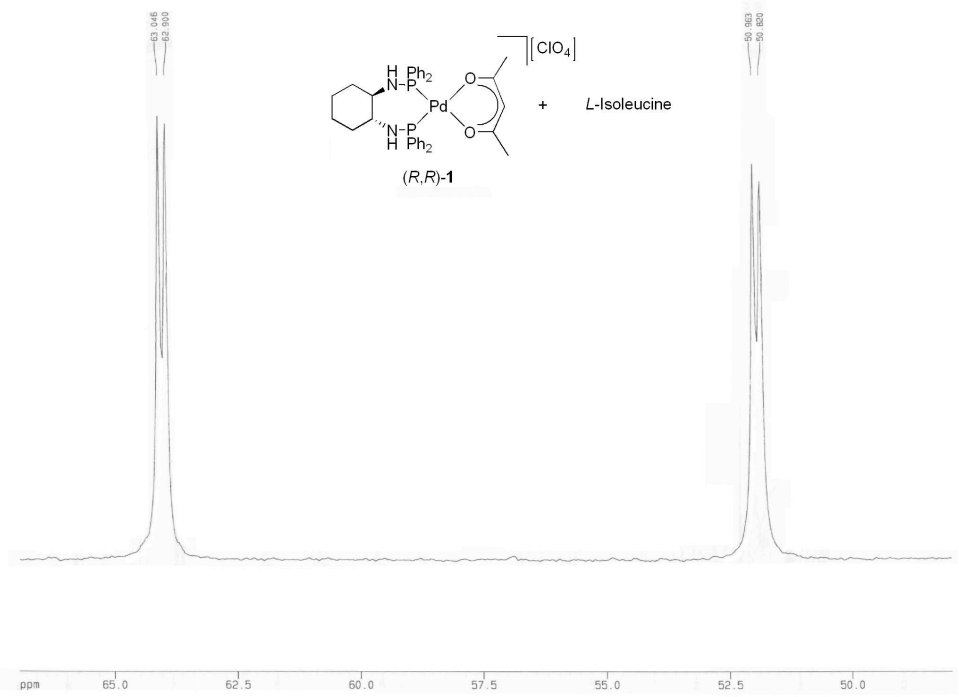


Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Isoleucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

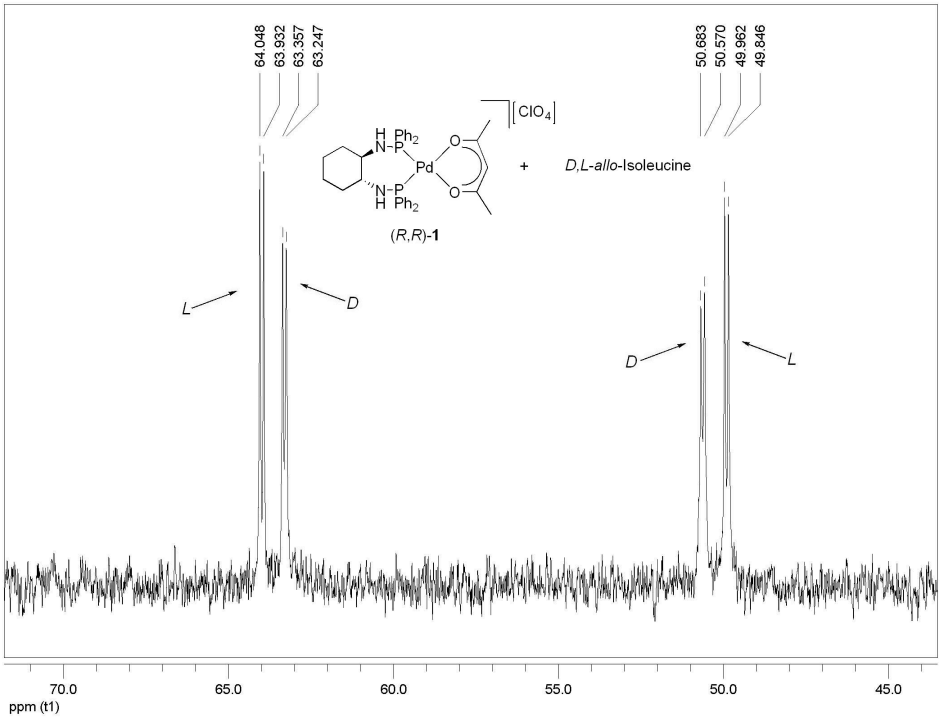


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D,L-allo*-Isoleucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

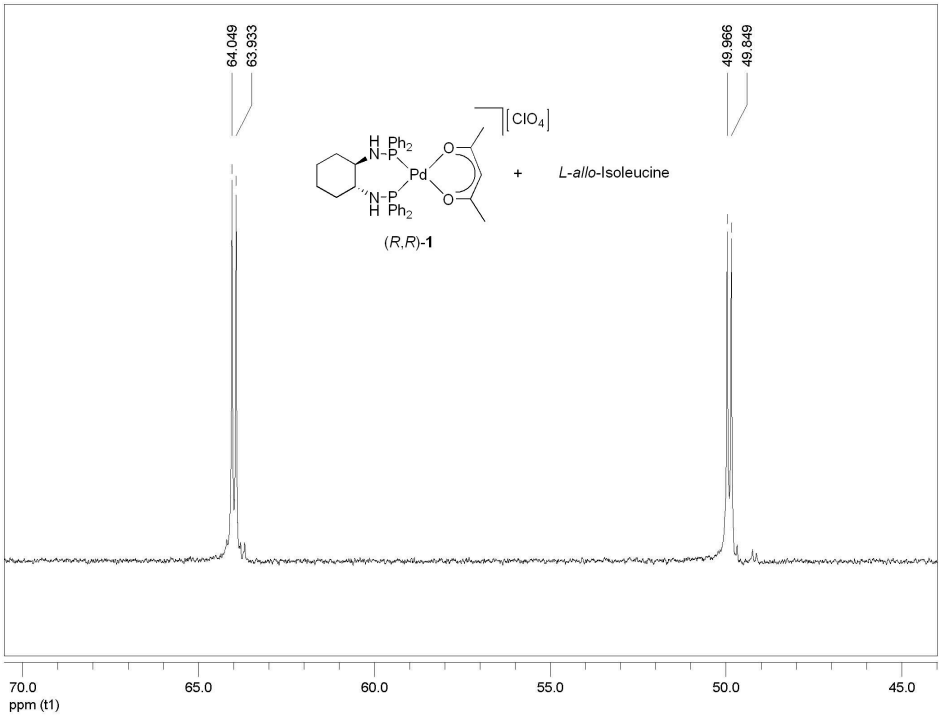


Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L-allo*-Isoleucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

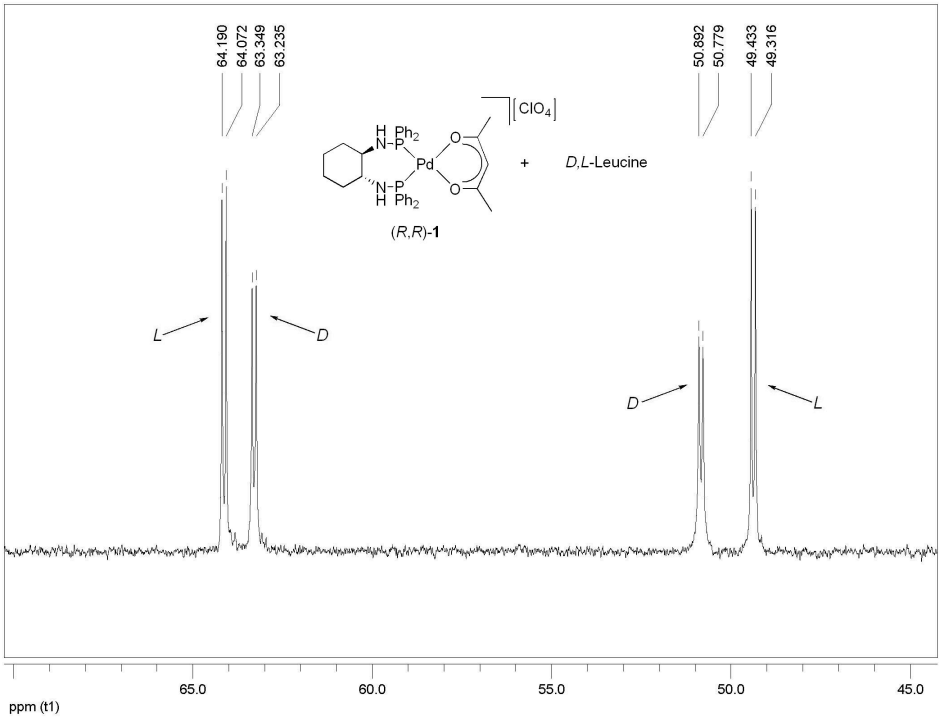


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Leucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

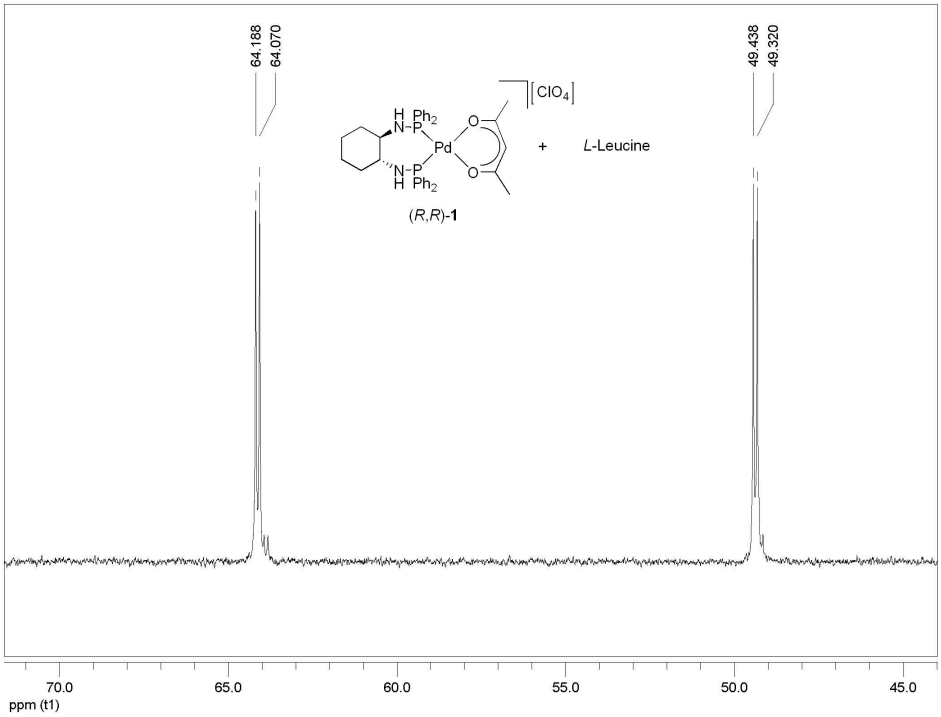


Figure S16. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Leucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

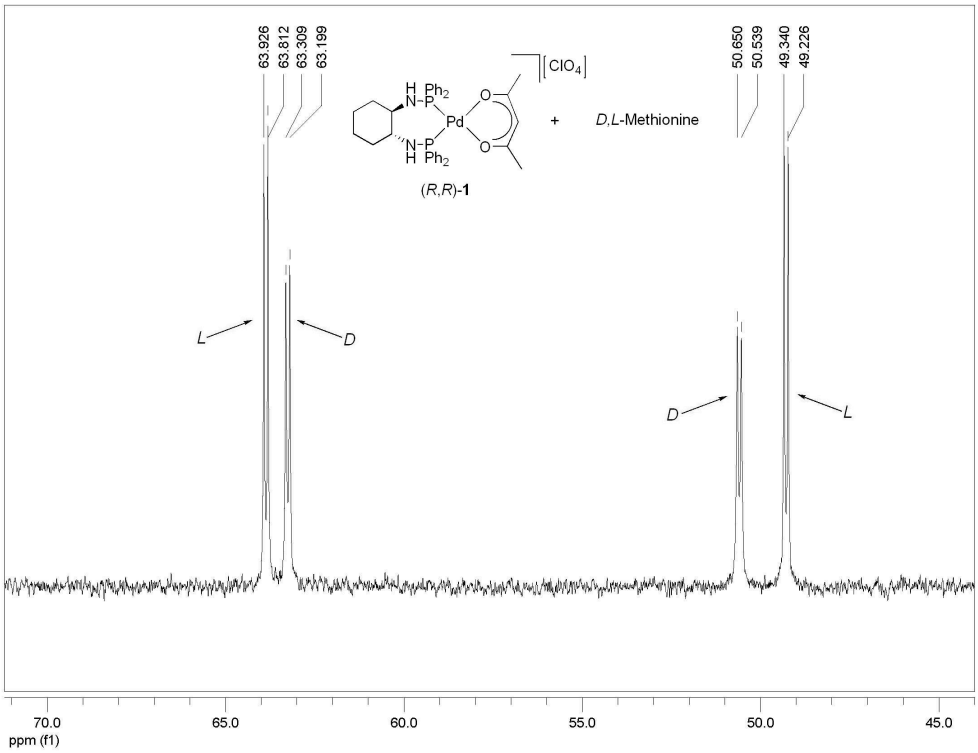


Figure S17. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Methionine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

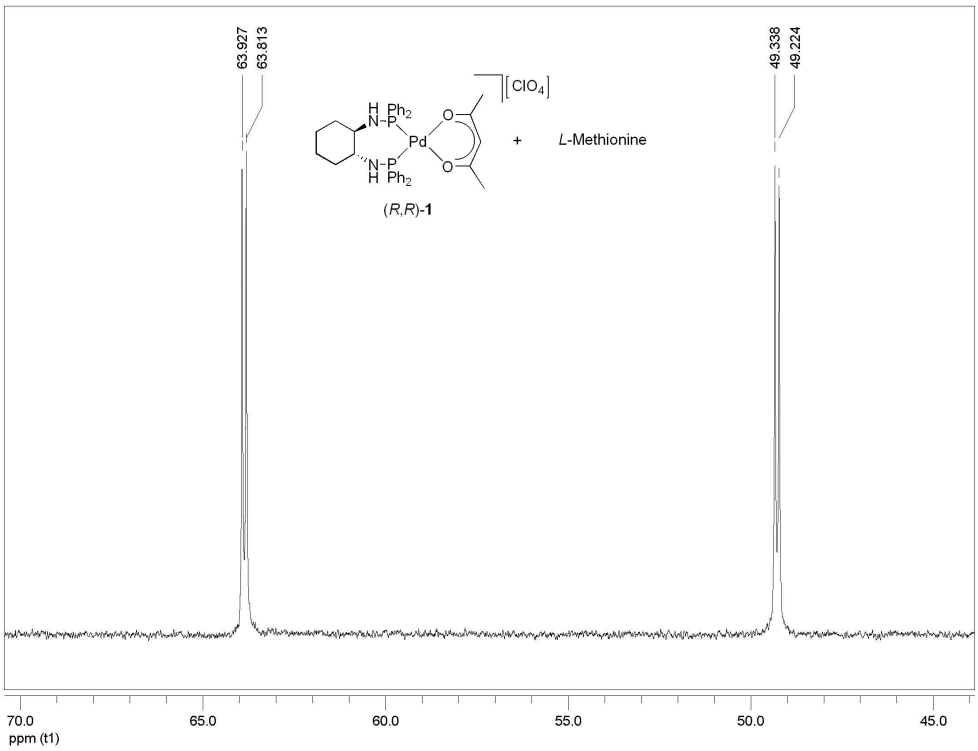


Figure S18. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Methionine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

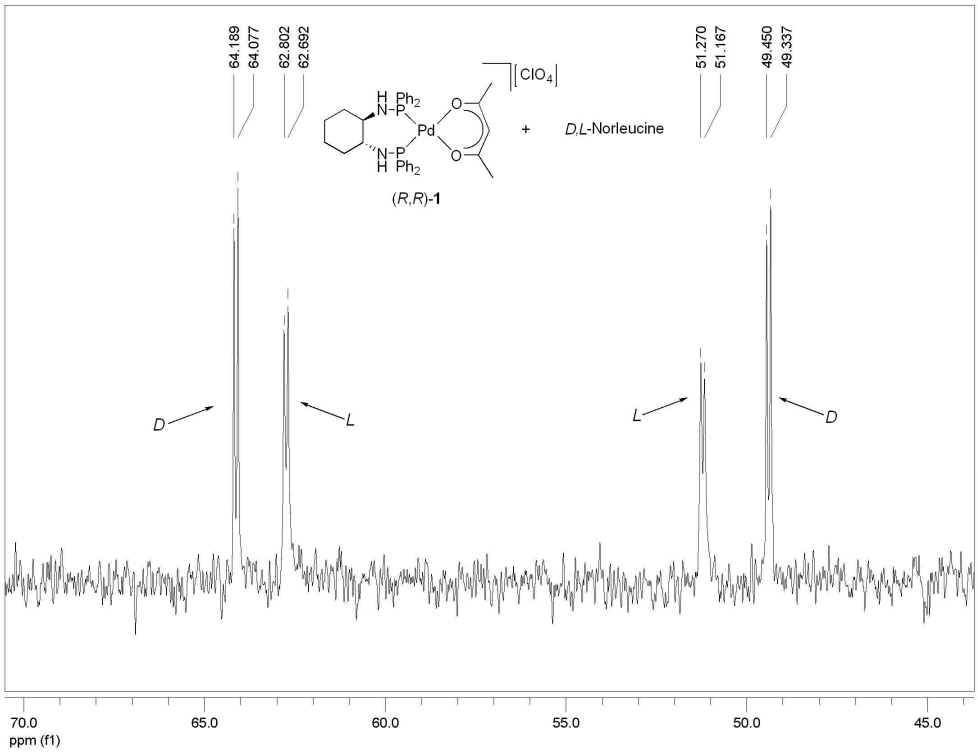


Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Norleucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

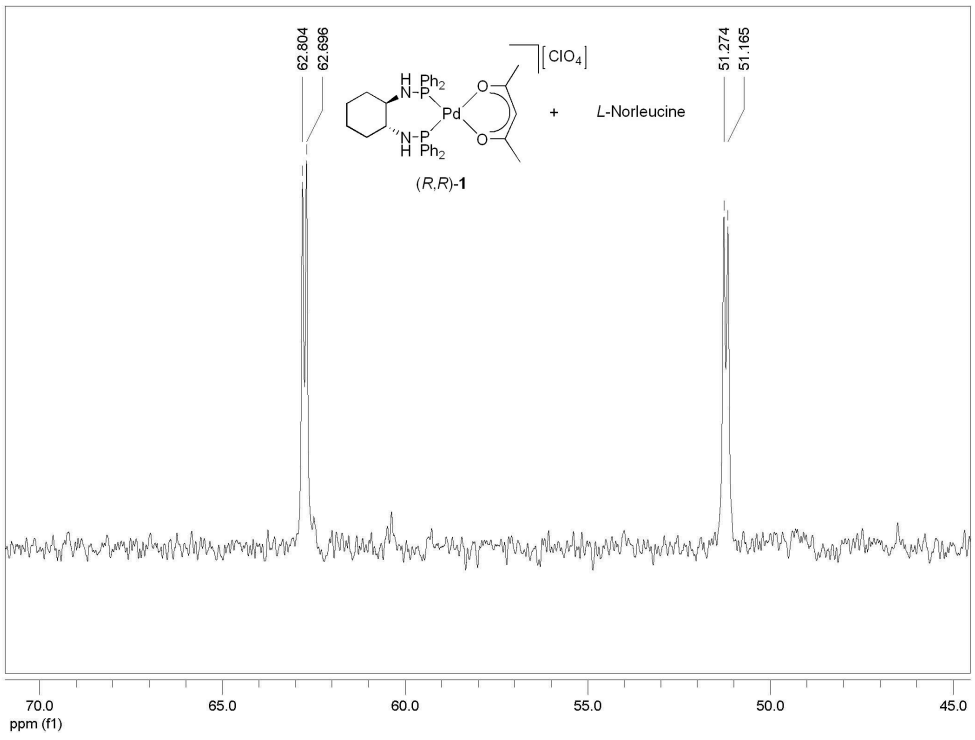


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Norleucine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

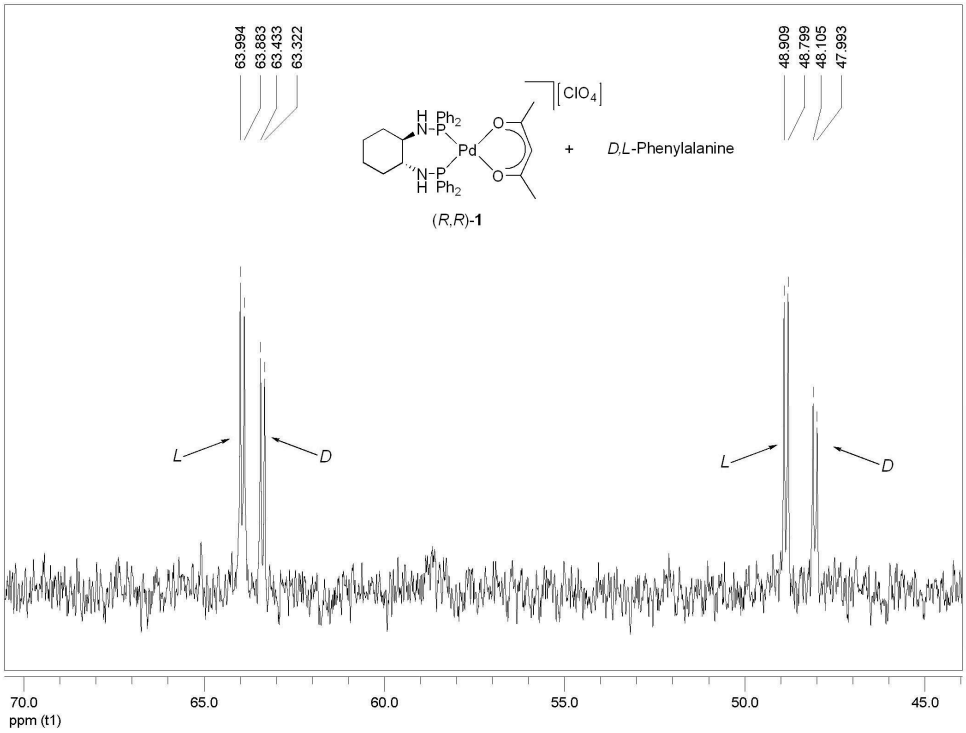


Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Phenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

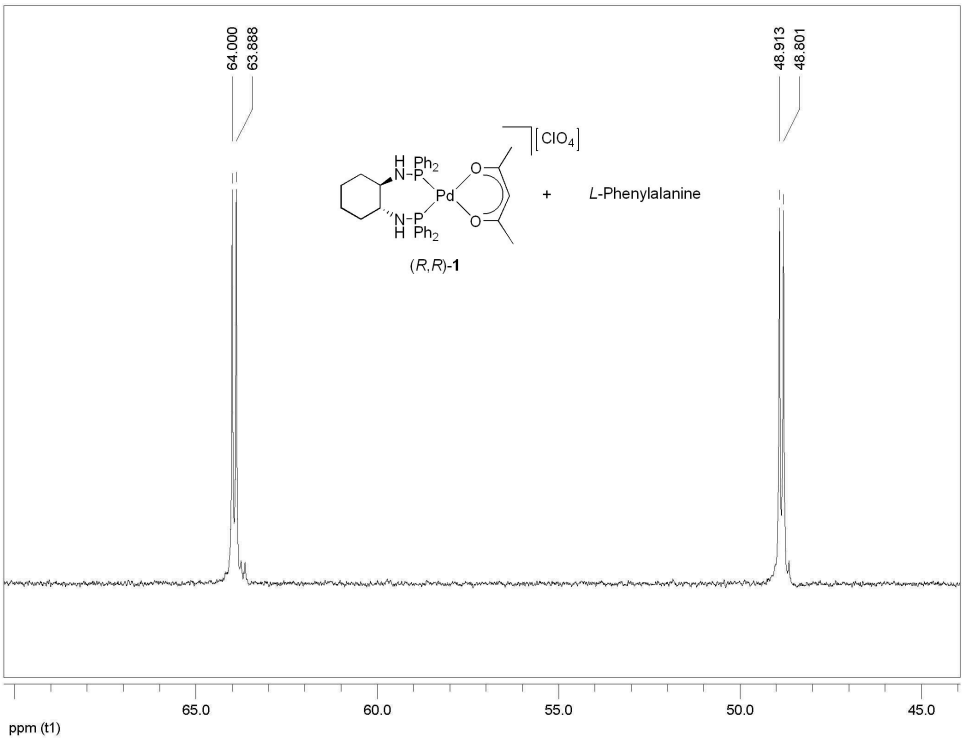


Figure S22. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Phenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

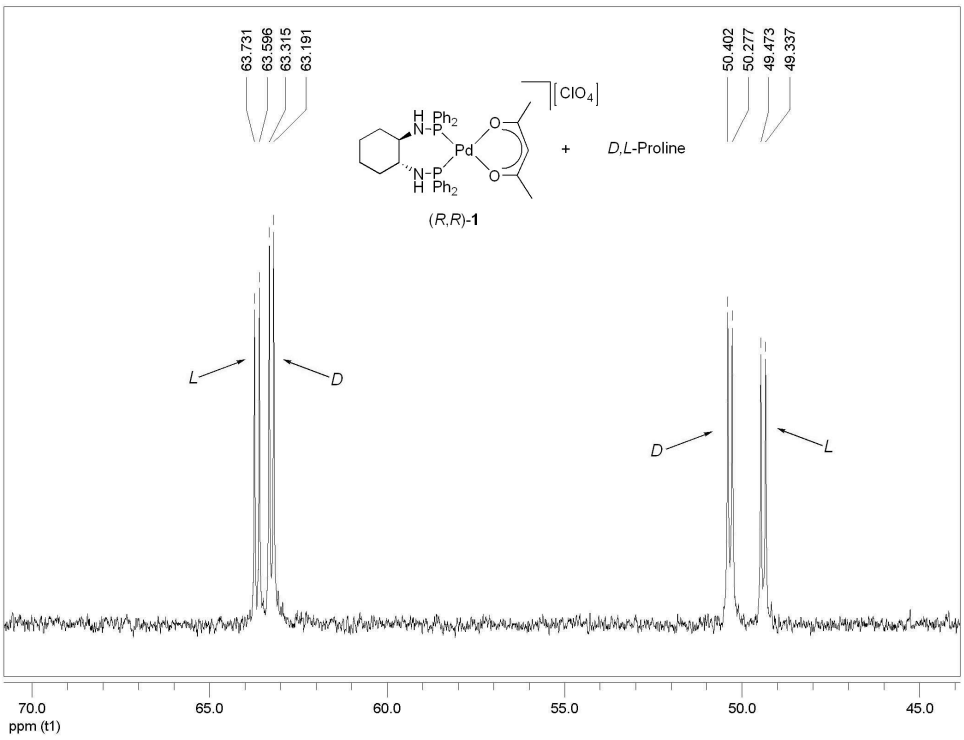


Figure S23. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Proline to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

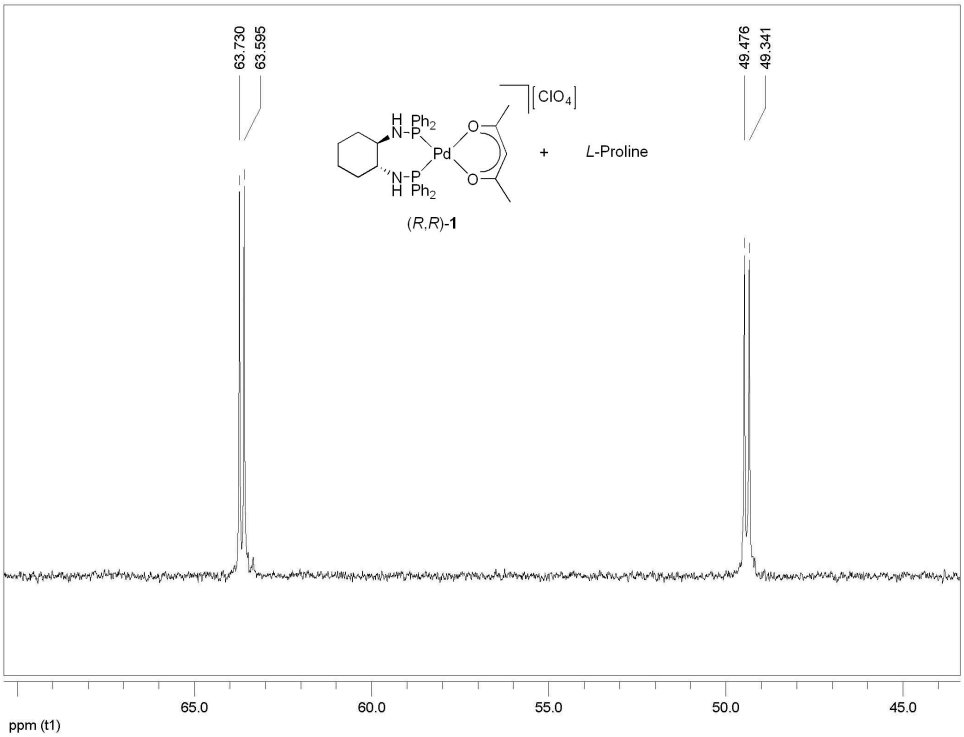


Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Proline to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

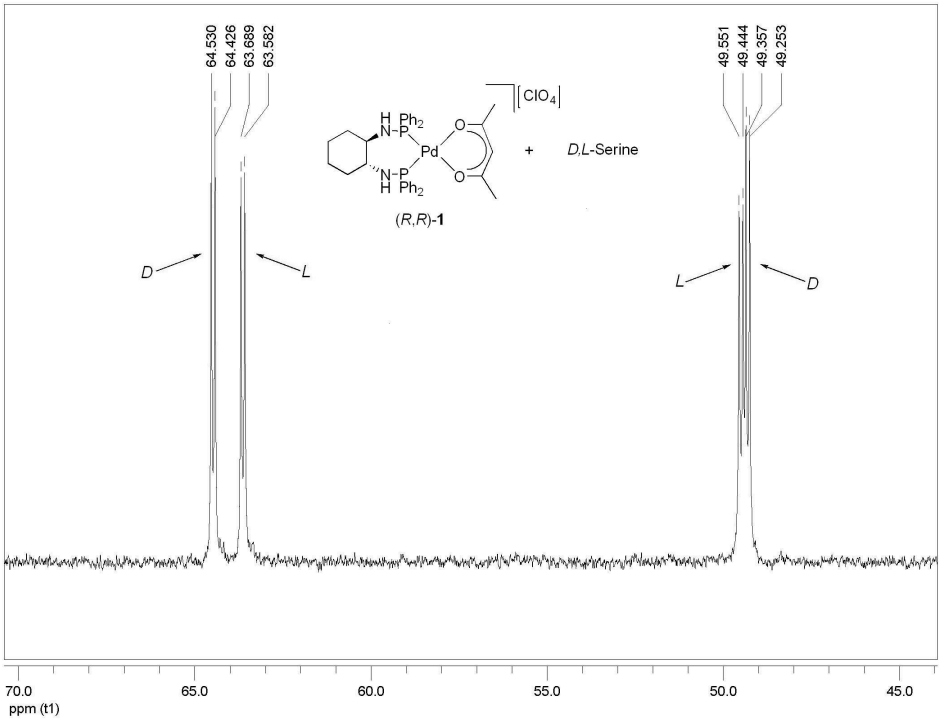


Figure S25. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Serine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

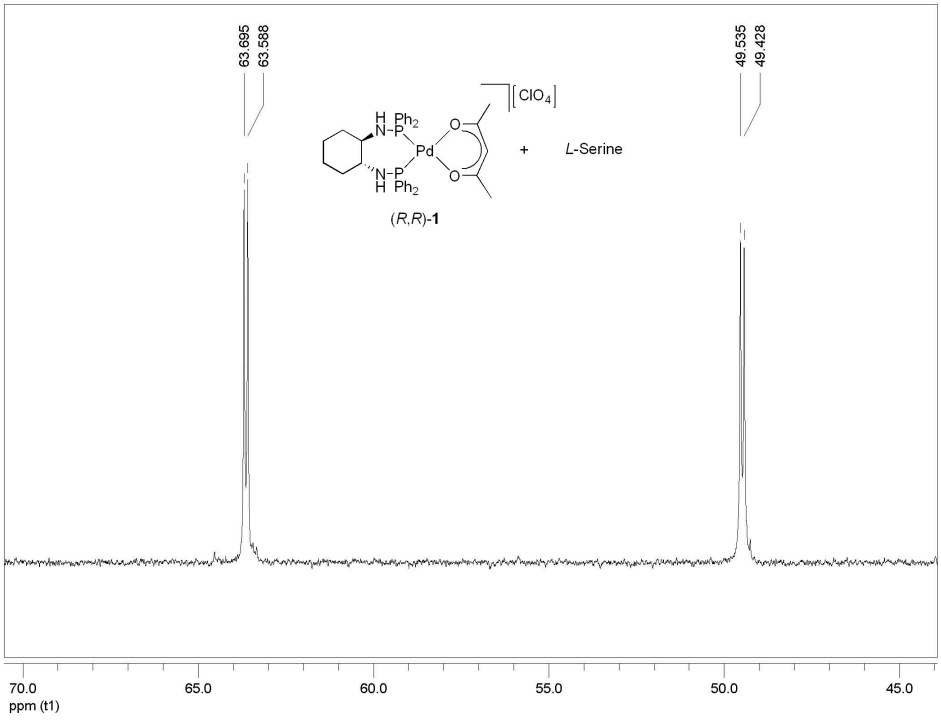


Figure S26. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Serine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

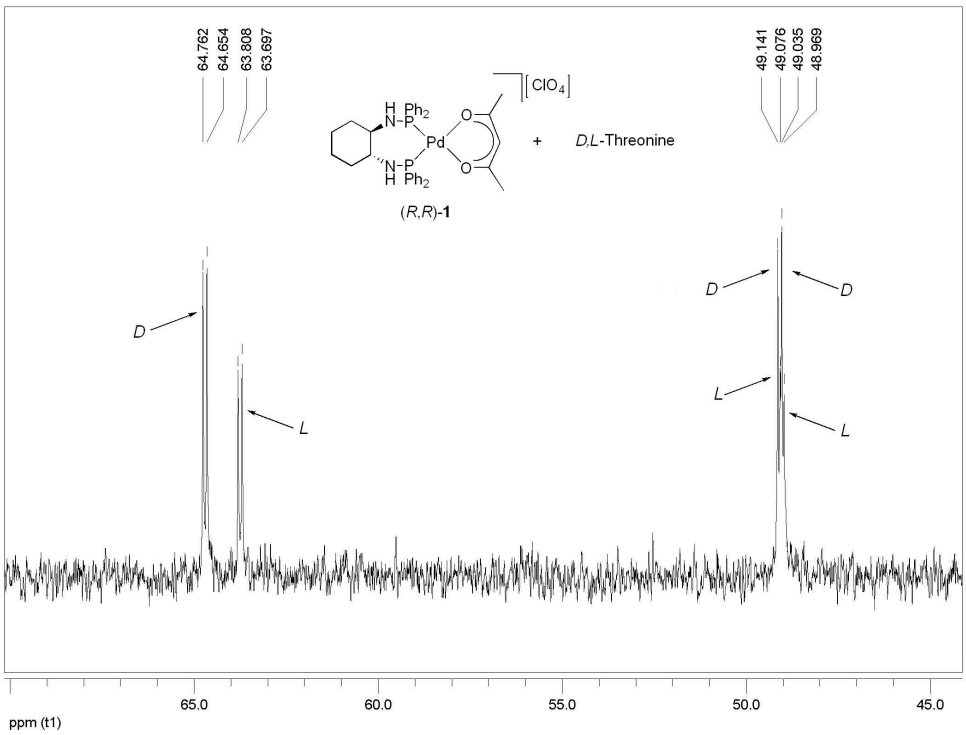


Figure S27. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Threonine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

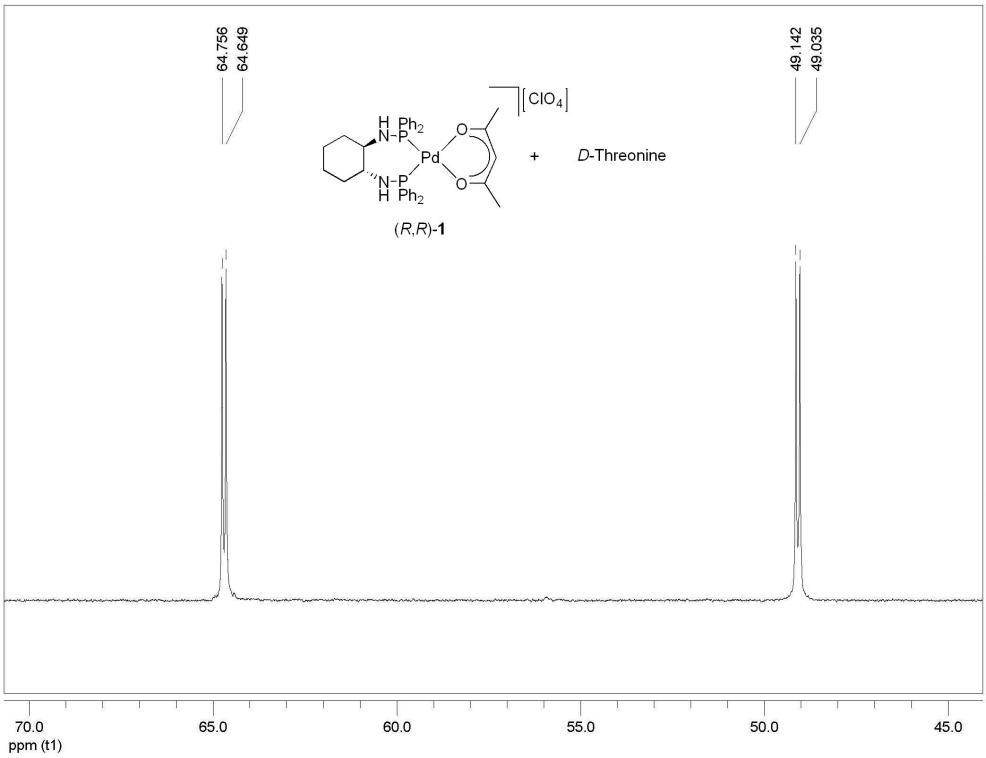


Figure S28. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*-Threonine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

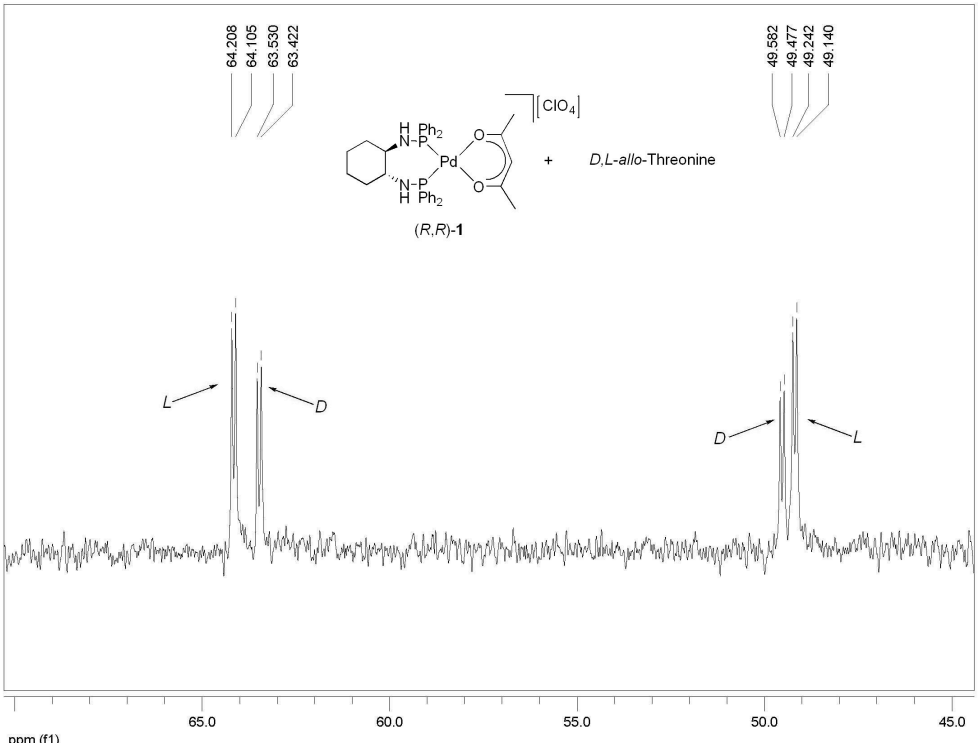


Figure S29. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *DL-allo*-Threonine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

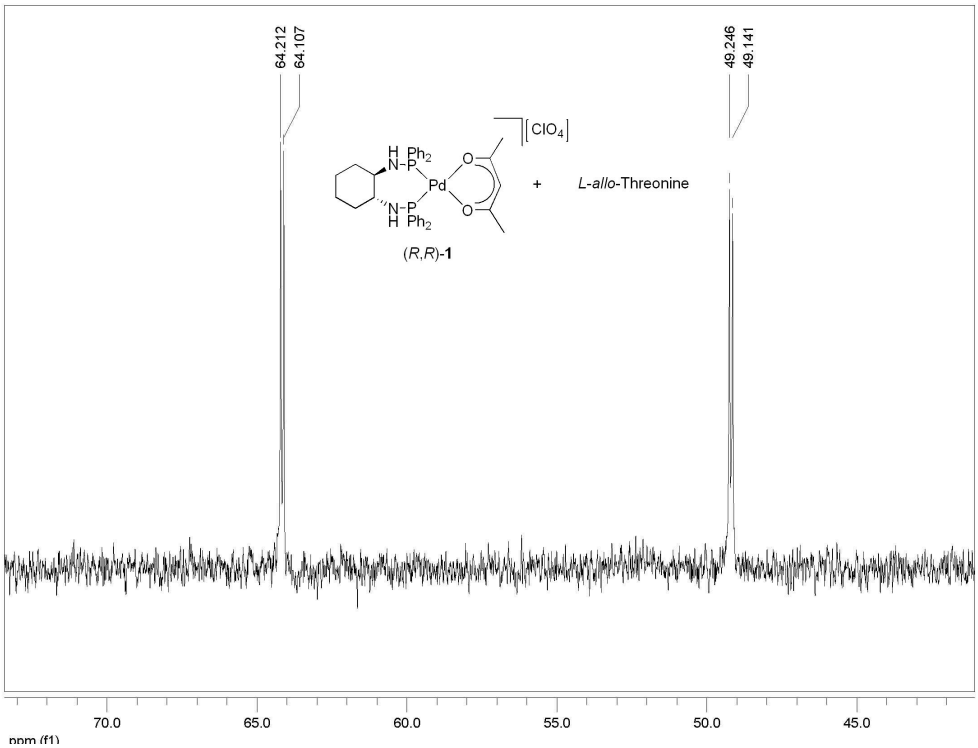


Figure S30. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L-allo*-Threonine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

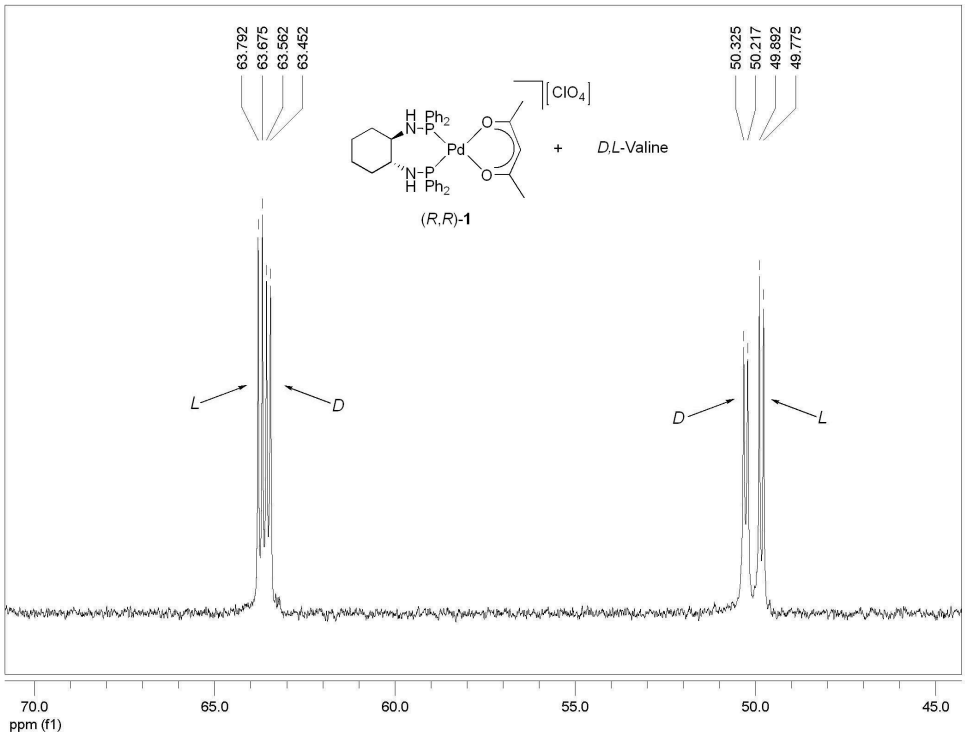


Figure S31. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Valine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

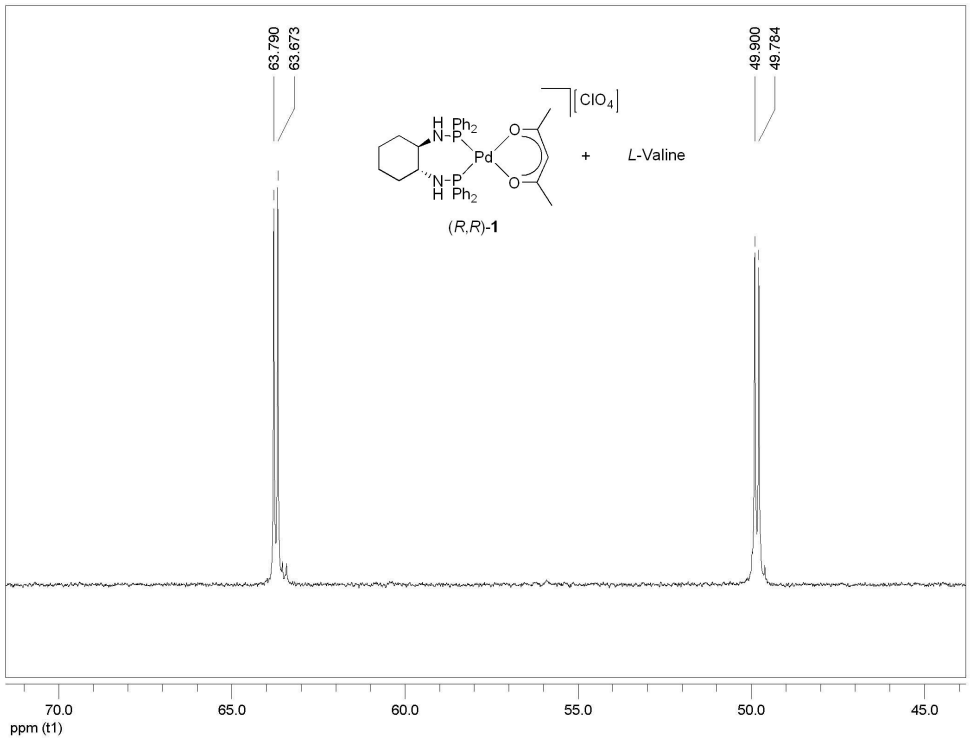


Figure S32. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Valine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

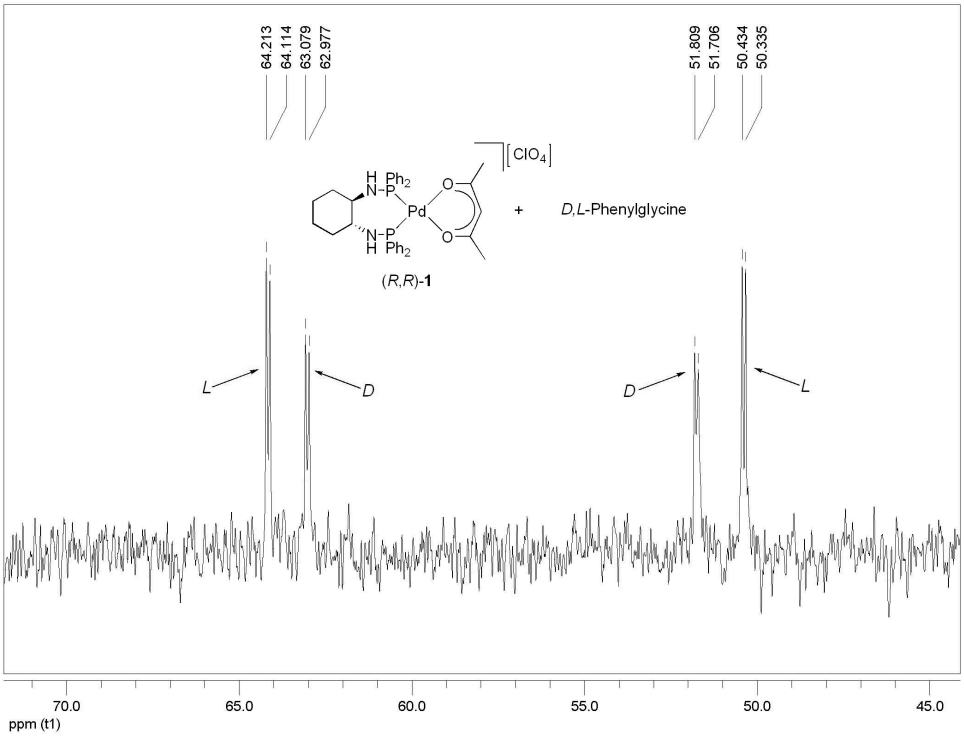


Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Phenylglycine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

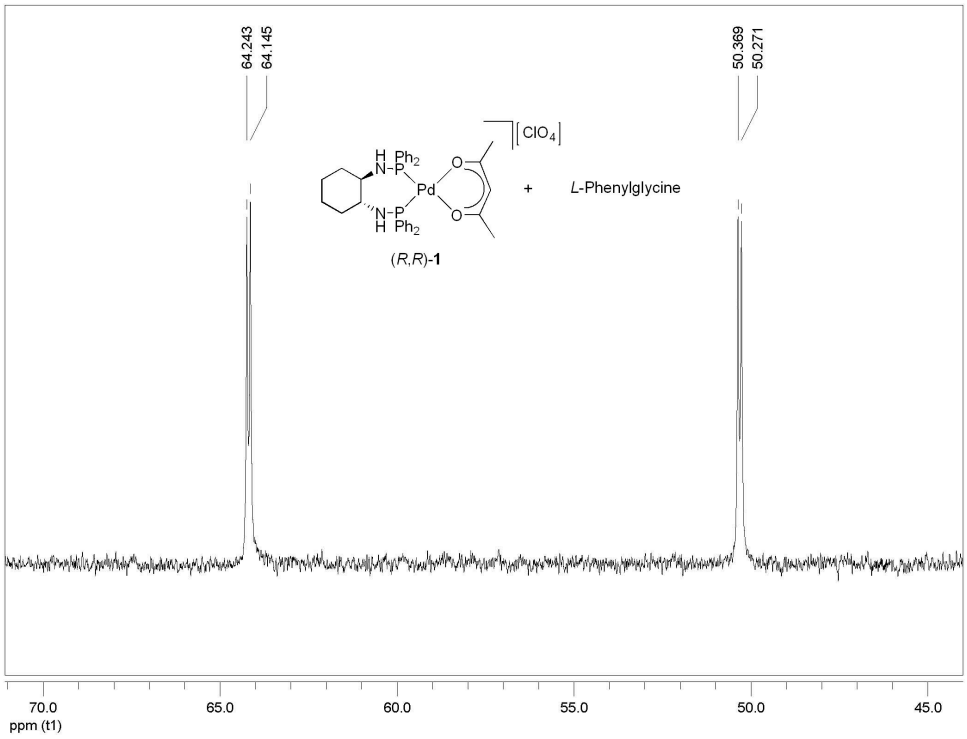


Figure S34. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-Phenylglycine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

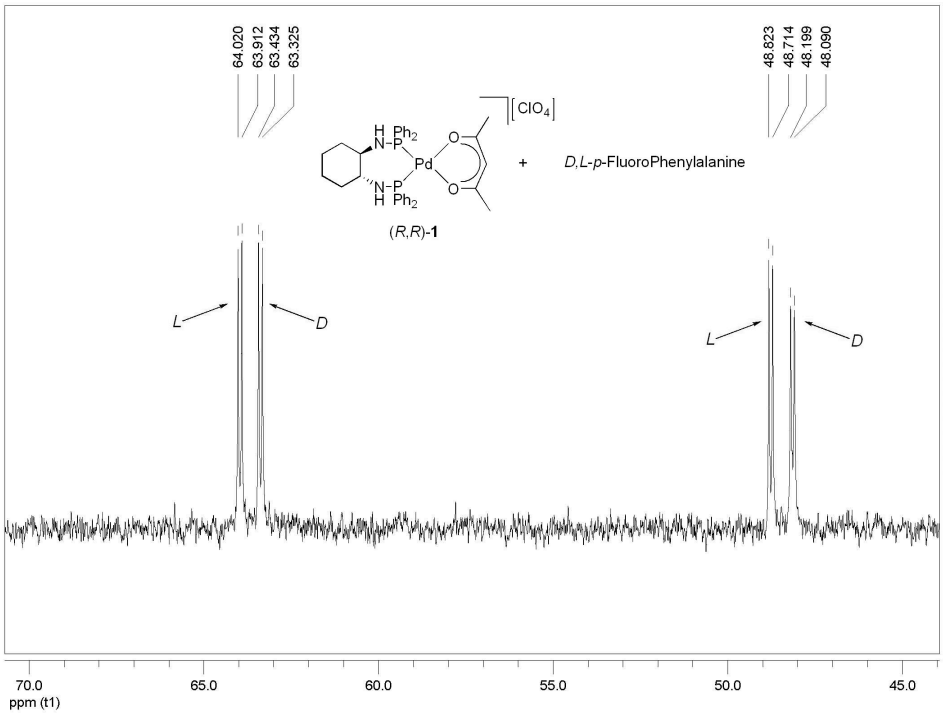


Figure S35. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D,L-p*-FluoroPhenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

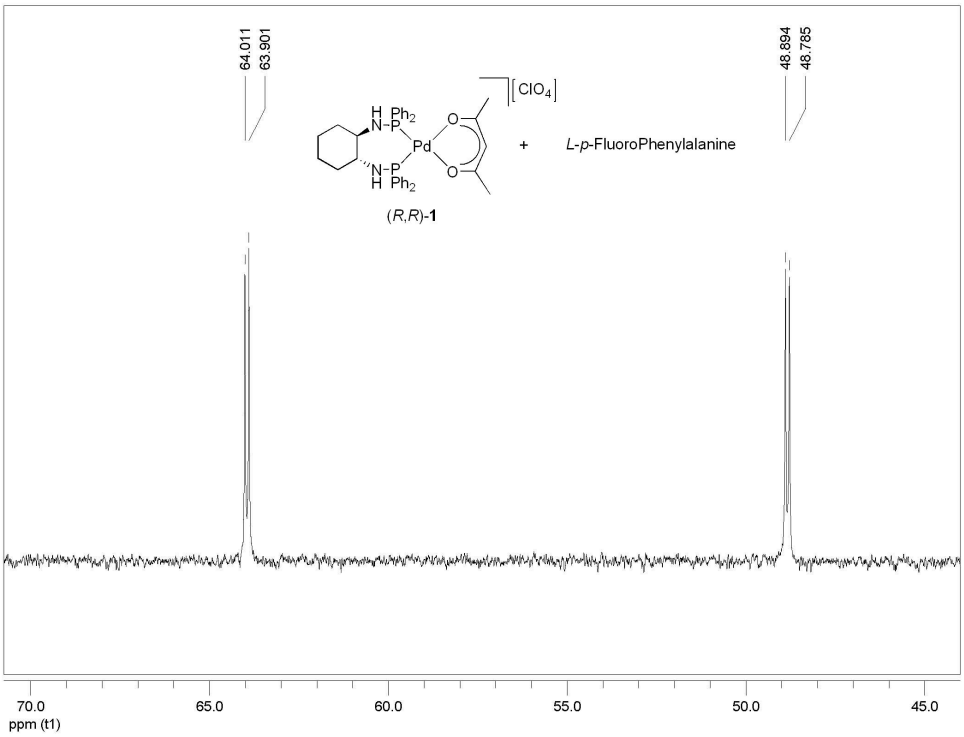


Figure S36. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L-p*-FluoroPhenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

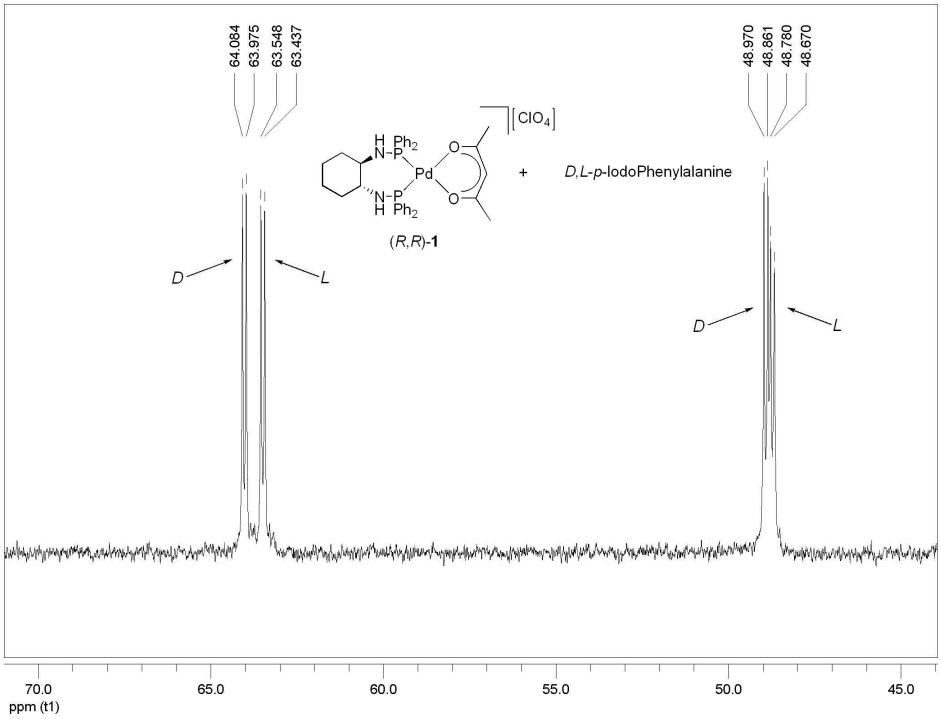


Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-*p*-IodoPhenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

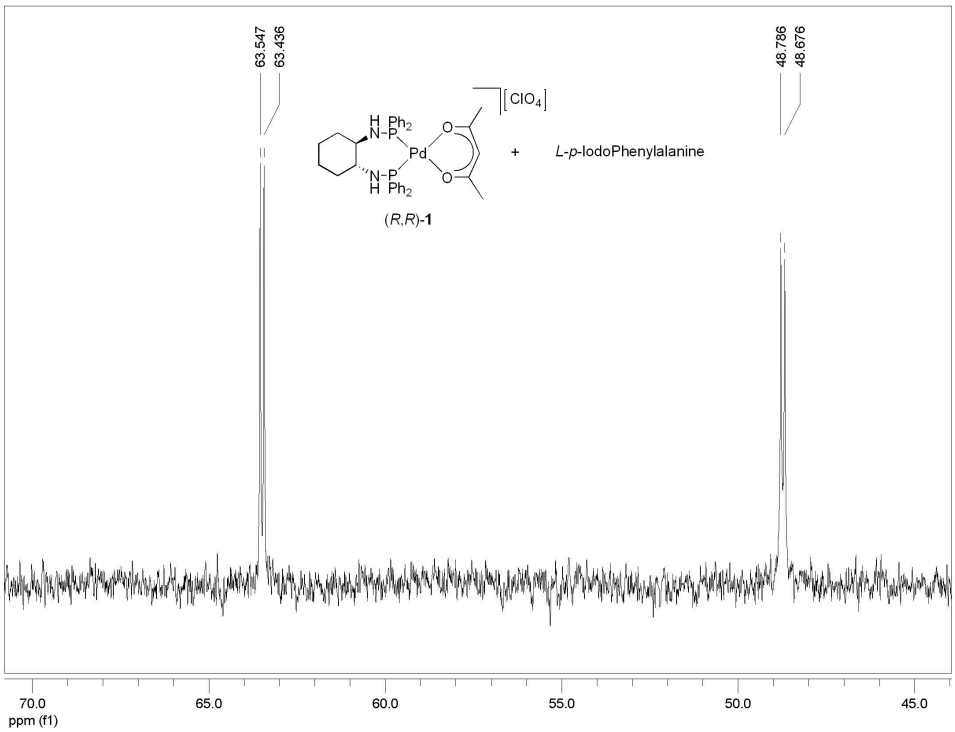


Figure S38. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-*p*-IodoPhenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

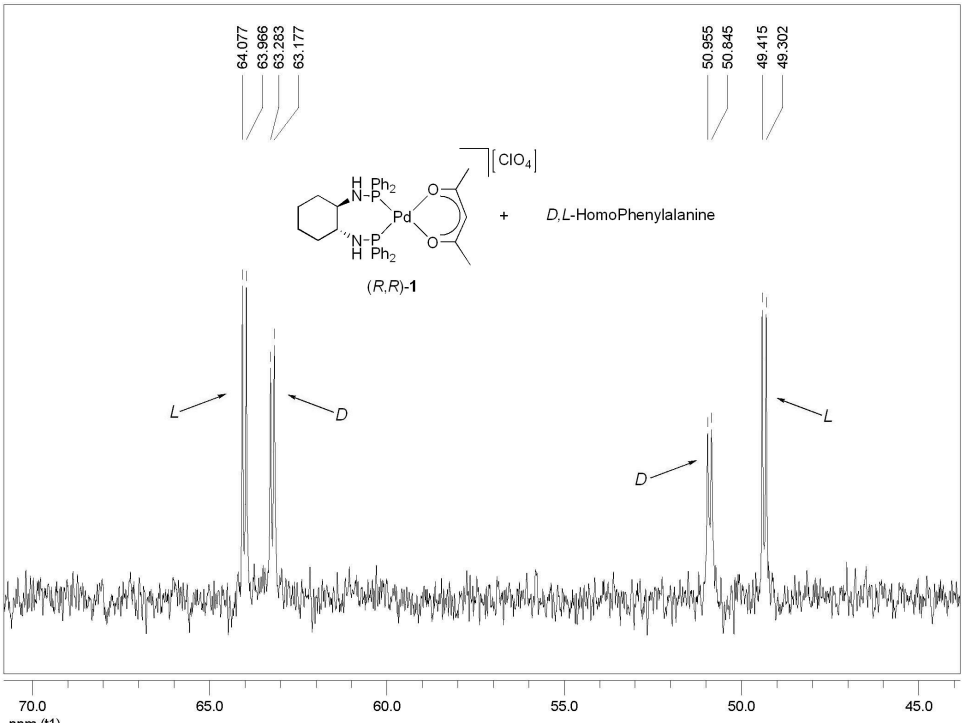


Figure S39. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-HomoPhenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

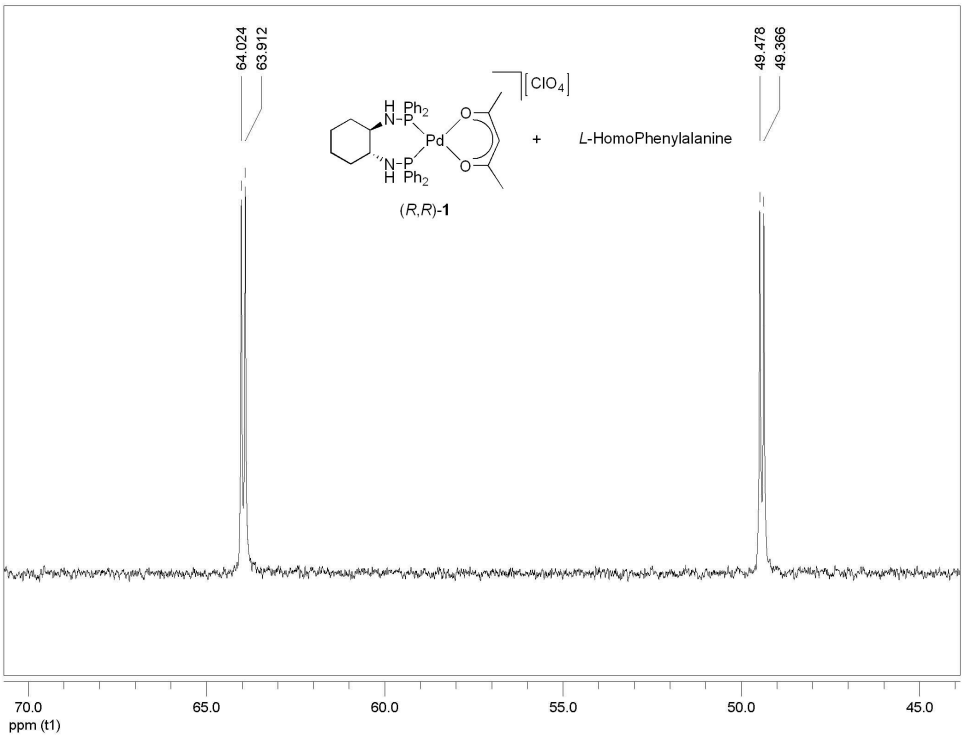


Figure S40. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *L*-HomoPhenylalanine to a solution of (*R*,*R*)-**1** complex in DMSO-d_6.

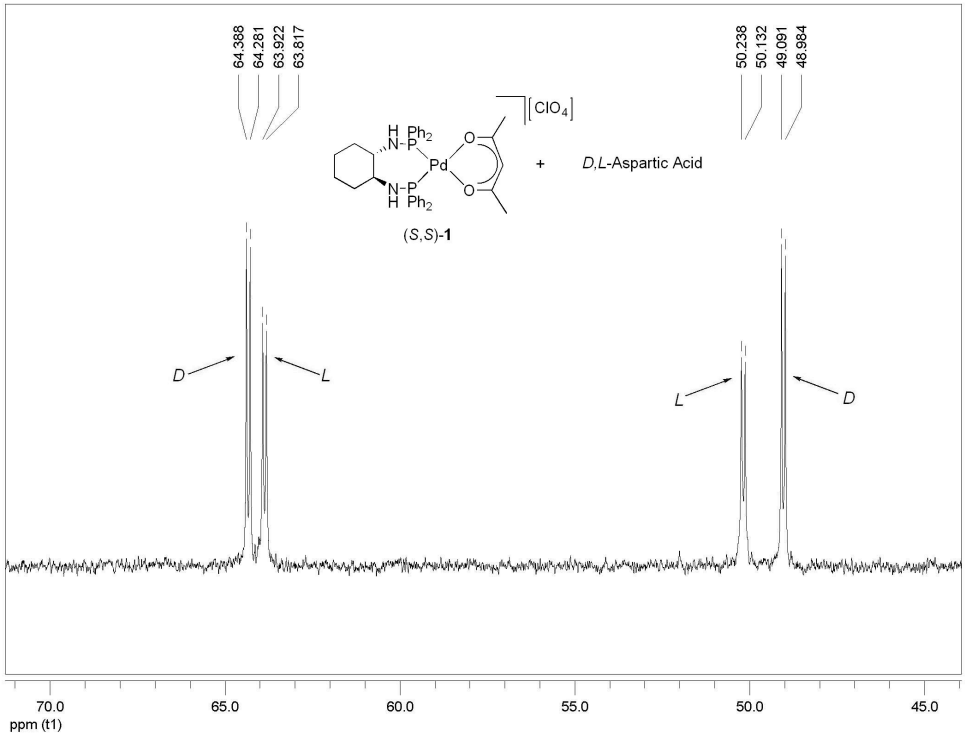


Figure S41. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Aspartic acid to a solution of (*S*,*S*)-**1** complex in DMSO-d_6.

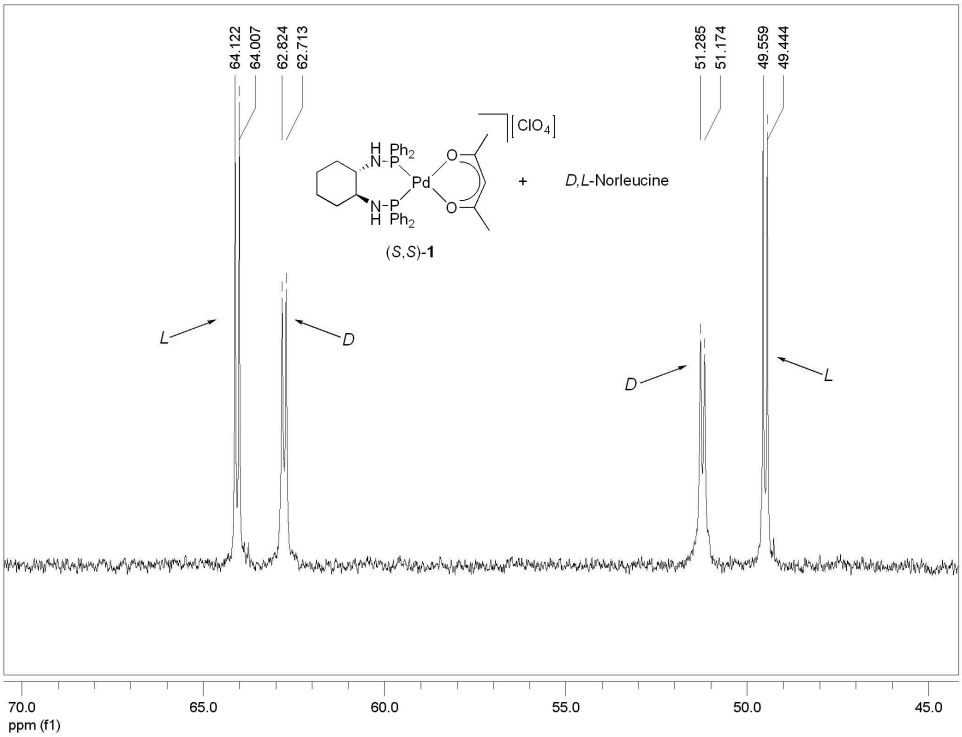


Figure S42. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Norleucine to a solution of (*S*,*S*)-**1** complex in DMSO-d_6.

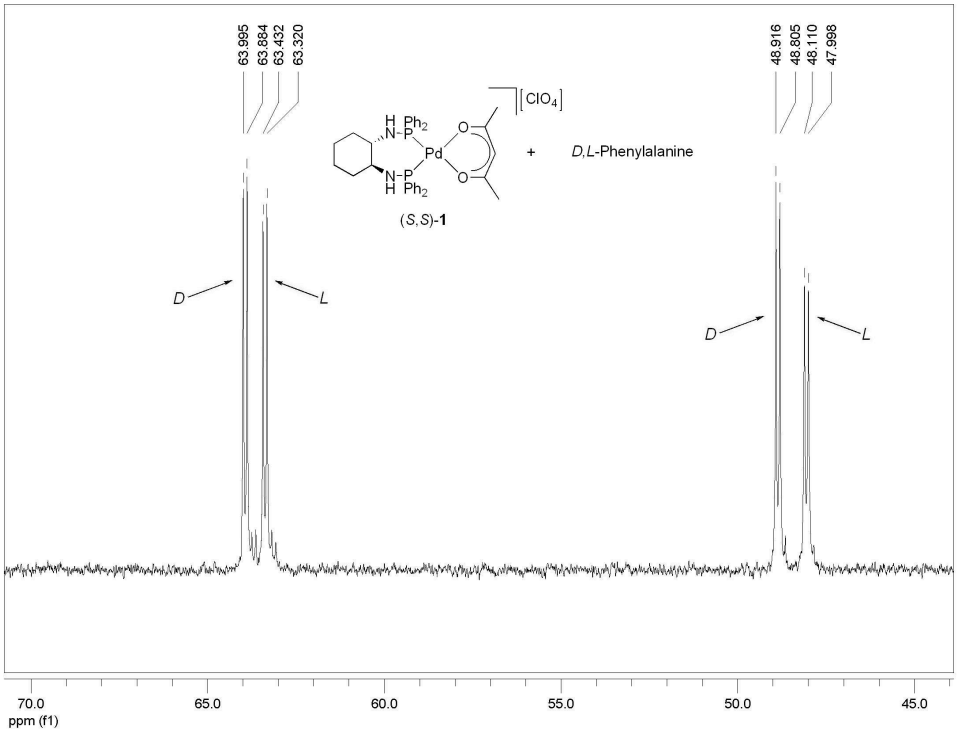


Figure S43. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Phenylalanine to a solution of (*S*,*S*)-**1** complex in DMSO-d_6.

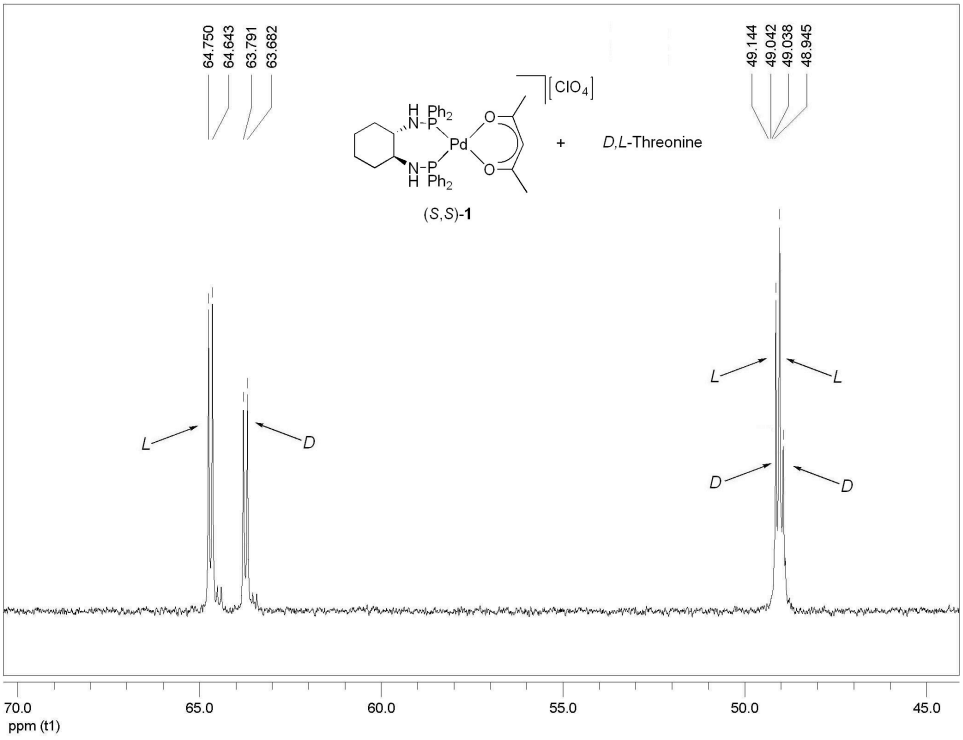


Figure S44. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Threonine to a solution of (*S*,*S*)-**1** complex in DMSO-d_6.

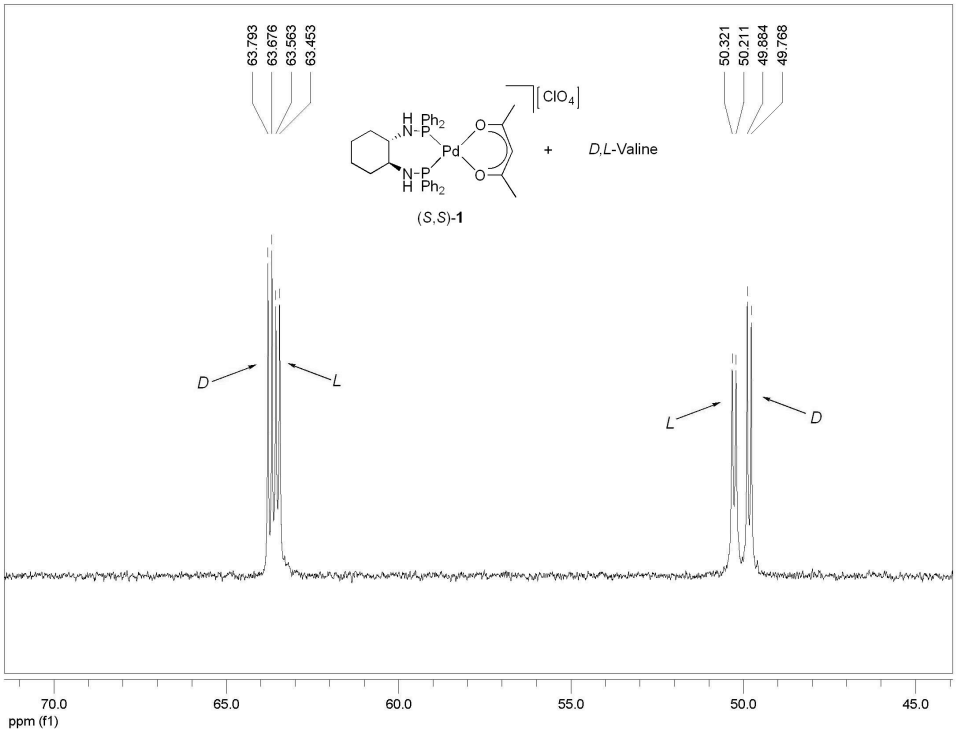


Figure S45. $^{31}P\{^{1}H\}$ NMR spectrum resulting to the addition of *D*,*L*-Valine to a solution of (*S*,*S*)-**1** complex in DMSO-d_6.

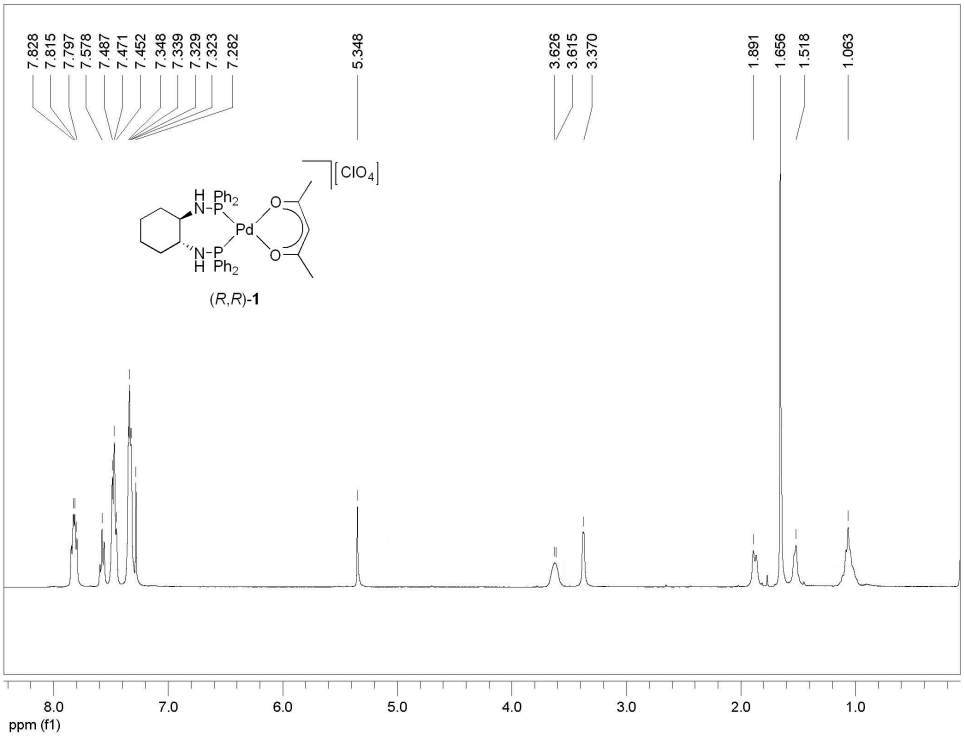


Figure S46. ^{1}H NMR spectrum of (*R*,*R*)-**1** complex in $CDCl_3$.

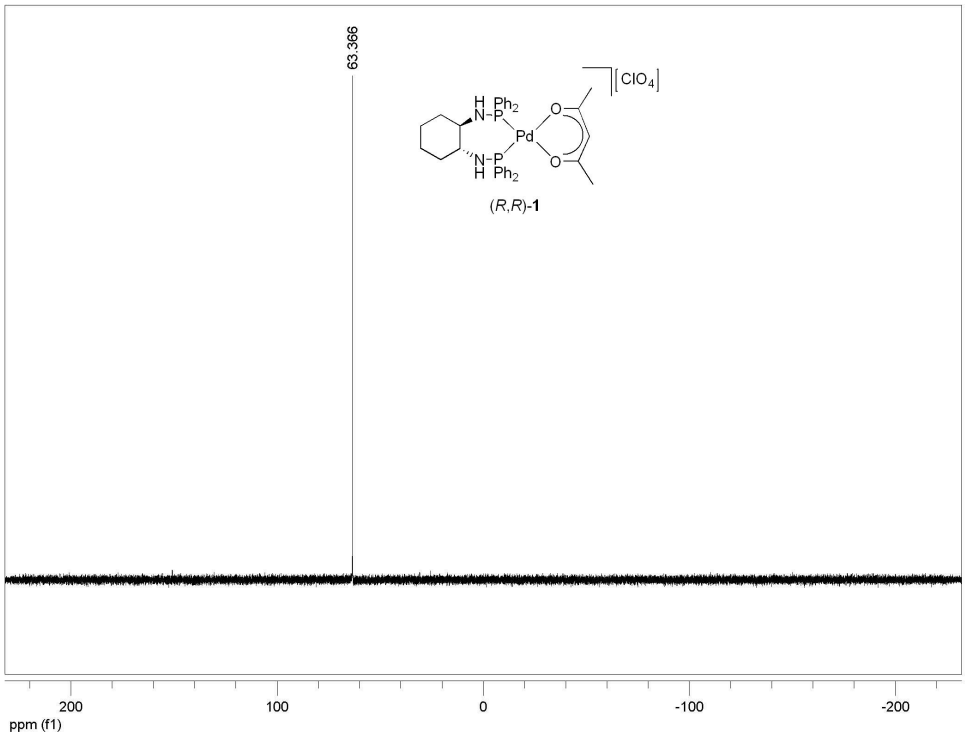


Figure S47. $^{31}P\{^{1}H\}$ NMR spectrum of (*R*,*R*)-**1** complex in $CDCl_3$.

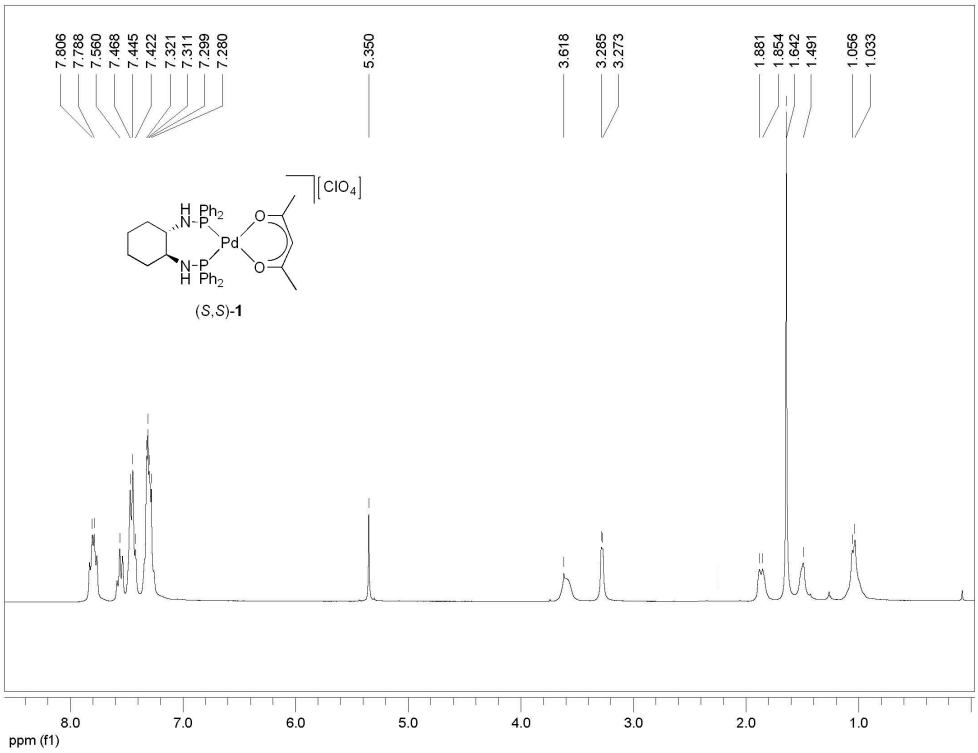


Figure S48. ^{1}H NMR spectrum of (*S*,*S*)-**1** complex in $CDCl_3$.

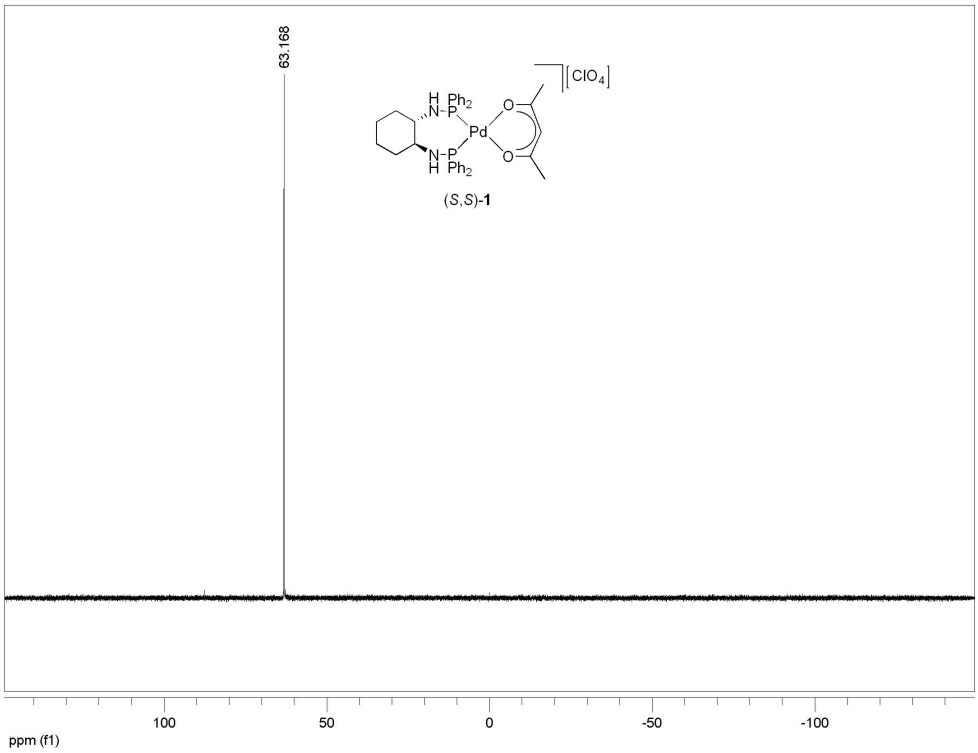


Figure S49. $^{31}P\{^{1}H\}$ NMR spectrum of (*S*,*S*)-**1** complex in $CDCl_3$.

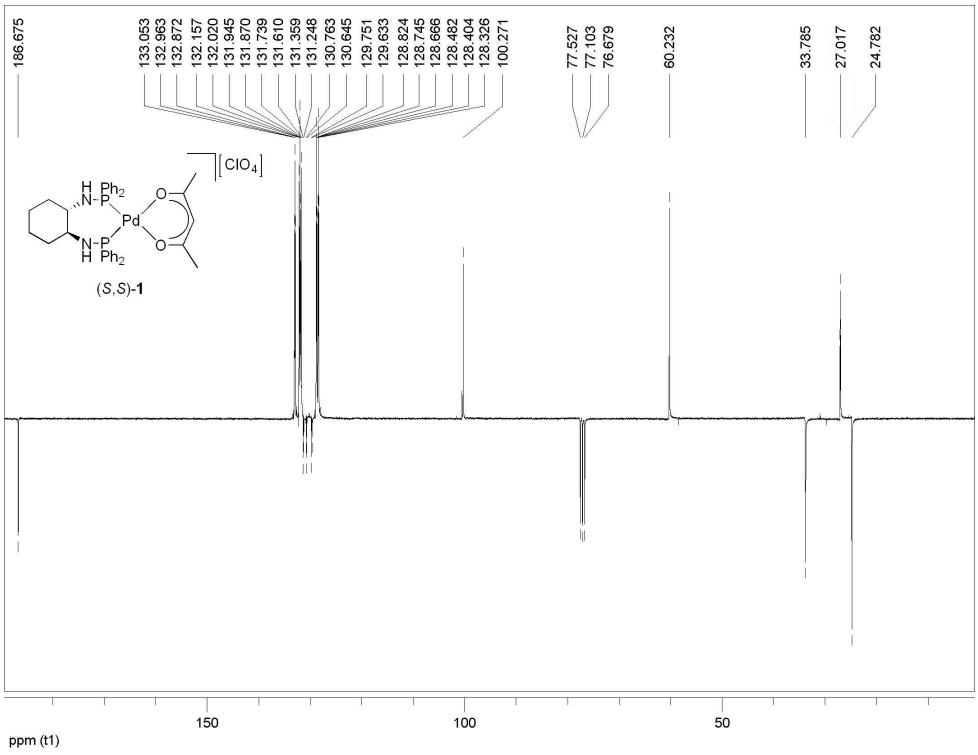


Figure S50. $^{13}C\{^{1}H\}$-APT NMR spectrum of (*S*,*S*)-**1** complex in $CDCl_3$.

2. Supplementary Notes

The ^{1}H, $^{13}C\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectra were recorded in DMSO-d_6 and $CDCl_3$ solutions at 25 ºC on a Bruker Avance-400 spectrometer (δ, ppm; *J*, Hz). The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were referenced using the solvent signal as internal standard, while $^{31}P\{^{1}H\}$ NMR spectra were referenced to H_3PO_4 (85%). Standard Bruker software was used for acquisition and processing routines. Selected spectral parameters for $^{31}P\{^{1}H\}$ NMR spectra were as follows: 202.4 MHz; inverse-gated pulse sequence to avoid NOE effects in the integral (zgig30); 64*K* data points; spectral width 32 KHz; acquisition time 1 s; relaxation delay 2s; 32 scans; exponential multiplication with a line broadening factor of 1 Hz; experimental time 1 min 50 sec. ESI/APCI mass spectra were recorded using an Esquire 3000 ion-trap mass spectrometer (Bruker Daltonic GmbH, Bremen, Germany) equipped with a standard ESI/APCI source. Samples were introduced by direct infusion with a syringe pump. Nitrogen served both as the nebulizer gas and the dry gas. Helium served as a cooling gas for the ion trap and collision gas for MS_n experiments. Elemental analysis were carried out on a Perkin Elmer 2400 series II microanalyser. Reagents were used as purchased from various commercial sources.

(*R*,*R*)-**1** palladium complex.[S1] Mass Spect. (ESI+) [m/z]: 516.3 $[M\text{-}Cl]^+$. $[\alpha]_D^{20}$ -74.3 ($CHCl_3$, *c*= 0.26). ^{1}H NMR ($CDCl_3$): δ 1.06 (m, 4H, CH_2), 1.52 (m, 2H, CH_2), 1.66 (s, 6H, Me- acac), 1.89 (m, 2H, CH_2), 3.37 (m, 2H, C*H*-NH), 3.61 (s broad, 2H, NH), 5.35 (s, 1H, acac), 7.28-7.83 (m, 20H, Ph). $^{31}P\{^{1}H\}$ NMR ($CDCl_3$): δ 63.40.

Linear Discriminant Analysis (LDA): XLSTAT[S2] was the program used to carry out the LDA studies. LDA analysis was used to systematically differentiate and classified the analytes employed. LDA reduced the complexity and size of the training and transformed them into roots that are linear combinations of the response patterns. The

accuracy of this classification method was monitored using a Jackknife analysis to measure of the generalization error. The Jackknife classification matrix is an iterative method in which one sample pattern at a time is omitted from the LDA and treated as an unknown. The unknown pattern is then classified based on the LDA function generated from the remaining sample patterns. This kind of classification is then repeated for each measured data.

3. References

S1. J. Bravo, C. Cativiela, J. E. Chaves, R. Navarro, and E. P. Urriolabeitia, *Inorg. Chem.* 2003, **42**, 1006.

S2. From http://www.xlstat.com.

LDA obtained with the (R,R)-1 complex and both enantiomers of the aa's: Asp, Nle, Phe, Thr and Val

Within-class covariance matrices are assumed to be equal
Prior probabilities are taken into account
Significance level (%): 5

Summary statistics:

Variable	Categories	Frequencies	%
Q1	D-Asp	3	10,000
	D-Nle	3	10,000
	D-Phe	3	10,000
	D-Thr	3	10,000
	D-Val	3	10,000
	L-Asp	3	10,000
	L-Nle	3	10,000
	L-Phe	3	10,000
	L-Thr	3	10,000
	L-Val	3	10,000

Variable	Observations s. with missing cwithout missing			Minimum	Maximum	Mean	Std. deviation
1	30	0	30	47958,000	51183,000	49412,767	868,463
2	30	0	30	48098,000	51287,000	49503,500	865,029
3	30	0	30	62650,000	64697,000	63753,400	523,571
4	30	0	30	62797,000	64953,000	63907,767	557,341

Correlation matrix:

Variables	1	2	3	4
1	**1,000**	0,977	-0,488	-0,420
2	0,977	**1,000**	-0,495	-0,496
3	-0,488	-0,495	**1,000**	0,945
4	-0,420	-0,496	0,945	**1,000**

Discriminant Analysis:

Means by class:

Class \ Variabl	1	2	3	4
D-Asp	50034,333	49818,667	63838,333	64290,667
D-Nle	49385,000	49512,000	64013,000	64139,333
D-Phe	47979,000	48101,333	63316,667	63441,000
D-Thr	48993,000	49122,667	64654,667	64770,667
D-Val	50200,333	50321,333	63453,667	63574,667
L-Asp	48950,667	49068,667	64305,000	64423,667
L-Nle	51153,667	51273,000	62683,000	62807,333
L-Phe	48779,333	48901,333	63876,667	63999,667
L-Thr	48891,333	49023,667	63713,000	63833,000
L-Val	49761,000	49892,333	63680,000	63797,667

Multicolinearity statistics:

Statistic	1	2	3	4
Tolerance	0,001	0,001	0,004	0,003
VIF	707,252	705,671	269,321	306,406

Between-classes covariance matrix:

	1	2	3	4
1	808659,384	784277,512	-238172,649	-215051,283
2	784277,512	771511,710	-240480,630	-228636,944
3	-238172,649	-240480,630	293299,625	295437,425
4	-215051,283	-228636,944	295437,425	308546,964

Within-class covariance matrix for class D-Asp:

	1	2	3	4
1	4692,333	44143,167	185,333	-38736,333
2	44143,167	424944,333	-1793,333	-374035,167
3	185,333	-1793,333	1301,333	1990,667
4	-38736,333	-374035,167	1990,667	329356,333

Within-class covariance matrix for class D-Nle:

	1	2	3	4
1	3637,000	3285,000	-1099,000	-1474,500
2	3285,000	3441,000	-2265,000	-2139,500
3	-1099,000	-2265,000	3748,000	2614,000
4	-1474,500	-2139,500	2614,000	1974,333

Within-class covariance matrix for class D-Phe:

	1	2	3	4
1	343,000	-17,500	94,500	-280,000
2	-17,500	8,333	-3,333	25,000
3	94,500	-3,333	26,333	-75,000
4	-280,000	25,000	-75,000	244,000

Within-class covariance matrix for class D-Thr:

	1	2	3	4
1	1609,000	558,500	30,000	-430,500
2	558,500	630,333	-792,167	-655,667
3	30,000	-792,167	1476,333	922,833
4	-430,500	-655,667	922,833	702,333

Within-class covariance matrix for class D-Val:

	1	2	3	4
1	1070,333	413,833	-37,333	-800,833
2	413,833	160,333	-14,333	-308,333
3	-37,333	-14,333	1,333	28,333
4	-800,833	-308,333	28,333	604,333

Within-class covariance matrix for class L-Asp:

	1	2	3	4
1	9,333	6,333	175,000	171,333
2	6,333	340,333	-584,500	-230,167
3	175,000	-584,500	4753,000	3937,500
4	171,333	-230,167	3937,500	3502,333

Within-class covariance matrix for class L-Nle:

	1	2	3	4
1	1221,333	452,000	1042,000	394,667
2	452,000	183,000	385,500	172,000
3	1042,000	385,500	889,000	336,500
4	394,667	172,000	336,500	170,333

Within-class covariance matrix for class L-Phe:

	1	2	3	4
1	670,333	142,333	259,167	-268,833
2	142,333	46,333	49,167	-46,833
3	259,167	49,167	102,333	-107,667
4	-268,833	-46,833	-107,667	114,333

Within-class covariance matrix for class L-Thr:

	1	2	3	4
1	2354,333	2733,167	-1338,500	-1690,500
2	2733,167	3202,333	-1320,000	-1839,500
3	-1338,500	-1320,000	2623,000	1940,500
4	-1690,500	-1839,500	1940,500	1729,000

Within-class covariance matrix for class L-Val:

	1	2	3	4
1	3793,000	2476,000	-1161,000	-1129,000
2	2476,000	1616,333	-757,000	-736,333
3	-1161,000	-757,000	372,000	358,000
4	-1129,000	-736,333	358,000	345,333

Pooled within-class covariance matrix:

	1	2	3	4
1	1940,000	5419,283	-184,983	-4424,450
2	5419,283	43457,267	-709,500	-37979,450
3	-184,983	-709,500	1529,267	1194,567
4	-4424,450	-37979,450	1194,567	33874,267

Total covariance matrix:

	1	2	3	4
1	754227,702	733926,845	-221874,524	-203271,505
2	733926,845	748274,534	-224385,069	-239061,603
3	-221874,524	-224385,069	274126,731	275886,269
4	-203271,505	-239061,603	275886,269	310629,426

Wilks' Lambda test (Rao's approximation):

Lambda	0,000
F (Observed v	66,077
F (Critical vali	1,597
DF1	36
DF2	65
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Unidimensional test of equality of the means of the classes:

Variable	Lambda	F	DF1	DF2	p-value
1	0,002	1250,504	9	20	< 0,0001
2	0,040	53,260	9	20	< 0,0001
3	0,004	575,373	9	20	< 0,0001
4	0,075	27,326	9	20	< 0,0001

Pillai's trace:

Trace	2,307
F (Observed v	3,027
F (Critical vali	1,564
DF1	36

DF2	80
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Hotelling-Lawley trace:

Trace	1820,311
F (Observed \	803,248
F (Critical vali	1,744
DF1	36
DF2	36
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

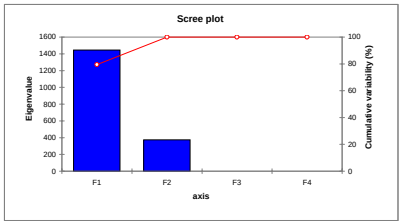
Roy's greatest root:

Root	1445,863
F (Observed \	3213,030
F (Critical vali	2,393
DF1	9
DF2	20
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

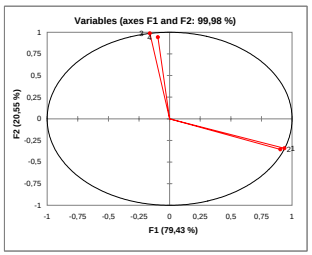
Eigenvalues:

	F1	F2	F3	F4
Eigenvalue	1445,863	374,018	0,409	0,020
Discriminatior	79,429	20,547	0,022	0,001
Cumulative %	79,429	99,976	99,999	100,000



Variables/Factors correlations:

	F1	F2	F3	F4
1	0,939	-0,342	0,024	-0,021
2	0,905	-0,355	0,235	-0,005
3	-0,161	0,986	-0,001	-0,035
4	-0,096	0,942	-0,320	-0,001

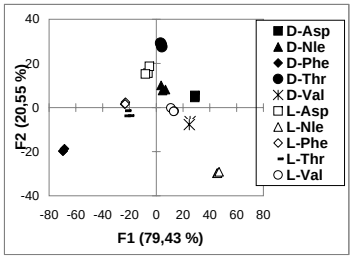


Classification functions:

	D-Asp	D-Nle	DPhe	D-Thr	D-Val	L-Asp	L-Nle	L-Phe	L-Thr	L-Val
Intercept	-8988050,845	-8911941,849	-8587397,146	-8952903,998	-8945979,690	-8889088,852	-8970743,017	-8796331,674	-8788576,069	-8915610,060
1	-14,583	-14,821	-14,854	-15,163	-14,402	-15,025	-13,876	-14,897	-14,811	-14,599
2	168,793	168,070	164,957	168,427	168,411	167,826	168,671	166,959	166,896	168,116
3	-30,369	-29,946	-29,080	-29,688	-30,445	-29,657	-31,045	-29,566	-29,644	-30,177
4	190,313	189,452	185,906	189,817	189,889	189,150	190,249	188,179	188,118	189,531

Prior and posterior classification, membership probabilities, scores and squared distances:

Observation	Prior	Posterior	Pr(D-Asp)	Pr(D-Nle)	Pr(D-Phe)	Pr(D-Thr)	Pr(D-Val)	Pr(L-Asp)	Pr(L-Nle)	Pr(L-Phe)	Pr(L-Thr)	Pr(L-Val)	F1	F2	F3	F4	D²(D-Asp)	D²(D-Nle)	D²(D-Phe)	D²(D-Thr)	D²(D-Val)	D²(L-Asp)	D²(L-Nle)	D²(L-Phe)	D²(L-Thr)	D²(L-Val)
D-Nle	D-Nle	D-Nle	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	4,774	7,739	0,247	1,535	597,902	7,328	6218,168	434,549	641,331	210,185	3095,355	827,356	854,397	145,843
D-Nle	D-Nle	D-Nle	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	3,676	10,037	0,219	-0,508	667,666	9,059	6184,548	341,904	758,903	148,761	3361,461	796,938	849,341	208,540
D-Nle	D-Nle	D-Nle	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	6,852	8,176	0,234	-0,429	502,438	8,294	6551,659	422,847	572,568	250,614	2958,763	951,201	979,194	124,245
L-Nle	L-Nle	L-Nle	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	45,399	-29,750	0,342	1,209	1491,146	3104,220	13251,861	5116,140	927,381	4832,587	6,563	5720,923	5302,498	1905,052
L-Nle	L-Nle	L-Nle	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	45,723	-29,713	0,317	-0,627	1498,275	3127,288	13324,304	5137,879	937,695	4860,970	5,054	5762,001	5343,981	1923,630
L-Nle	L-Nle	L-Nle	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	46,853	-29,142	0,305	-0,702	1498,311	3176,947	13573,936	5167,836	960,694	4927,708	5,940	5883,456	5468,858	1967,831
D-Asp	D-Asp	D-Asp	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	28,912	4,497	0,356	0,878	9,000	589,335	10206,294	1206,352	160,714	1400,033	1455,341	2734,403	2683,032	307,345
D-Asp	D-Asp	D-Asp	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	28,882	5,062	-5,127	0,073	17,924	611,782	10249,905	1207,068	202,542	1411,693	1523,999	2760,346	2715,169	341,650
D-Asp	D-Asp	D-Asp	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	28,811	5,482	0,335	-0,932	8,998	578,130	10234,377	1155,302	183,936	1369,486	1526,758	2729,920	2689,040	316,587
L-Asp	L-Asp	L-Asp	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	-6,197	15,534	0,194	0,886	1348,472	180,106	5196,858	271,043	1498,414	6,827	4760,427	483,043	607,888	633,893
L-Asp	L-Asp	L-Asp	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	-5,115	18,697	0,195	-0,665	1349,930	210,627	5564,912	178,863	1586,026	11,469	4943,176	617,065	771,296	710,272
L-Asp	L-Asp	L-Asp	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	-8,037	15,221	0,165	-0,927	1474,385	221,643	4946,431	319,545	1601,965	9,200	4927,603	415,098	541,120	696,015
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	3,869	28,438	0,389	1,535	1184,131	399,483	7636,468	6,952	1730,406	257,158	5142,348	1448,478	1679,670	958,558
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	4,272	27,551	0,270	-0,834	1121,311	363,597	7609,522	6,234	1648,838	242,409	5004,641	1422,275	1644,885	898,728
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	3,305	29,196	0,304	-0,683	1246,527	430,706	7625,177	5,981	1806,943	261,555	5276,476	1456,877	1697,388	1012,500
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-23,310	-3,836	-0,019	0,560	2807,905	967,850	2354,603	1779,608	2347,106	702,428	5468,214	37,655	6,516	1293,309
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-20,723	-3,714	0,140	0,104	2542,744	824,380	2602,350	1637,779	2104,518	616,418	5122,270	42,380	7,558	1113,906
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,013	0,987	0,000	-22,832	-1,473	0,112	-0,230	2722,142	887,493	2477,546	1606,860	2322,726	595,433	5528,768	16,083	7,397	1252,166
D-Phe	D-Phe	D-Phe	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-68,508	-18,671	-0,254	1,162	10050,612	6170,501	7,059	7452,169	8871,548	5093,893	13234,627	2475,885	2387,391	6871,940
D-Phe	D-Phe	D-Phe	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-69,703	-19,767	-0,282	-0,599	10336,880	6408,712	5,301	7729,929	9121,200	5320,143	13485,994	2630,619	2534,375	7105,827
D-Phe	D-Phe	D-Phe	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-69,453	-19,706	-0,284	-0,676	10284,694	6368,012	5,172	7687,433	9072,467	5284,199	13429,455	2604,899	2508,793	7062,613
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-22,972	2,399	0,068	1,204	2702,692	832,790	2619,685	1399,446	2398,088	478,060	5781,988	6,500	35,426	1276,054
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-23,622	1,589	0,038	-0,660	2774,306	880,230	2524,177	1476,500	2444,393	521,560	5819,799	5,207	28,159	1316,720
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-23,188	1,656	0,040	-0,659	2728,502	854,548	2566,763	1449,269	2403,636	504,843	5763,791	5,047	27,814	1285,957
D-Val	D-Val	D-Val	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	25,310	-6,351	0,298	1,207	151,026	639,127	9112,576	1675,412	7,337	1536,858	971,359	2433,151	2282,593	197,012
D-Val	D-Val	D-Val	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	24,844	-7,864	0,278	-0,839	190,437	668,230	8986,541	1762,266	5,483	1577,106	922,096	2414,334	2250,643	202,771
D-Val	D-Val	D-Val	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	24,723	-7,732	0,286	-0,633	187,759	658,715	8966,518	1747,291	5,131	1562,894	932,709	2399,829	2237,593	197,699
L-Val	L-Val	L-Val	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	10,905	-0,208	0,349	0,695	358,371	117,033	6793,412	873,489	253,259	585,306	2096,293	1176,887	1114,602	8,441
L-Val	L-Val	L-Val	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	13,418	-1,604	0,242	-0,274	290,165	179,176	7150,216	996,880	170,461	726,522	1845,835	1362,159	1281,693	5,777
L-Val	L-Val	L-Val	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	13,136	-1,744	0,241	-0,171	300,746	177,361	7098,844	999,872	175,435	720,477	1856,453	1342,555	1261,239	5,405



Confusion matrix for the estimation sample:

from \ to	D-Asp	D-Nle	D-Phe	D-Thr	D-Val	L-Asp	L-Nle	L-Phe	L-Thr	L-Val	Total	% correct
D-Asp	3	0	0	0	0	0	0	0	0	0	3	100,00%
D-Nle	0	3	0	0	0	0	0	0	0	0	3	100,00%
D-Phe	0	0	3	0	0	0	0	0	0	0	3	100,00%
D-Thr	0	0	0	3	0	0	0	0	0	0	3	100,00%
D-Val	0	0	0	0	3	0	0	0	0	0	3	100,00%
L-Asp	0	0	0	0	0	3	0	0	0	0	3	100,00%
L-Nle	0	0	0	0	0	0	3	0	0	0	3	100,00%
L-Phe	0	0	0	0	0	0	0	3	0	0	3	100,00%
L-Thr	0	0	0	0	0	0	0	0	3	0	3	100,00%
L-Val	0	0	0	0	0	0	0	0	0	3	3	100,00%
Total	3	3	3	3	3	3	3	3	3	3	30	100,00%

LDA obtained with (S,S)-1 complex and both enantiomers of the aa's: Asp, Nle, Phe, Thr and Val

Within-class covariance matrices are assumed to be equal
Prior probabilities are taken into account
Significance level (%): 5

Summary statistics:

Variable	Categories	Frequencies	%
Q1	D-Asp	3	10,000
	D-Nle	3	10,000
	D-Phe	3	10,000
	D-Thr	3	10,000
	D-Val	3	10,000
	L-Asp	3	10,000
	L-Nle	3	10,000
	L-Phe	3	10,000
	L-Thr	3	10,000
	L-Val	3	10,000

Variable	Observations	s. with missing d	without missing	Minimum	Maximum	Mean	Std. deviation
1	30	0	30	47995,000	51174,000	49447,067	866,950
2	30	0	30	48107,000	51284,000	49556,167	867,426
3	30	0	30	62712,000	64644,000	63751,567	507,052
4	30	0	30	62824,000	64751,000	63854,633	512,349

Correlation matrix:

Variables	1	2	3	4
1	**1,000**	1,000	-0,489	-0,458
2	1,000	**1,000**	-0,490	-0,459
3	-0,489	-0,490	**1,000**	0,999
4	-0,458	-0,459	0,999	**1,000**

Discriminant Analysis:

Means by class:

Class \ Variabl	1	2	3	4
D-Asp	48980,333	49087,333	64279,667	64387,000
D-Nle	51163,333	51273,667	62719,000	62830,333
D-Phe	48804,333	48915,000	63884,667	63995,333
D-Thr	48944,333	49042,333	63681,333	63790,667
D-Val	49778,667	49895,667	63673,667	63791,000
L-Asp	50126,000	50231,333	63822,667	63928,000
L-Nle	49423,667	49539,333	64002,333	64118,000
L-Phe	47996,667	48109,333	63357,333	63394,667
L-Thr	49037,000	49142,333	64643,333	64750,000
L-Val	50216,333	50325,333	63451,667	63561,333

Multicolinearity statistics:

Statistic	1	2	3	4
Tolerance	0,463	0,000	0,002	0,002
VIF	2,160	26570,956	575,162	554,123

Between-classes covariance matrix:

	1	2	3	4
1	807144,538	807574,926	-230766,560	-218646,936
2	807574,926	808036,228	-231362,784	-219256,290
3	-230766,560	-231362,784	275816,347	278443,404
4	-218646,936	-219256,290	278443,404	281618,060

Within-class covariance matrix for class D-Asp:

	1	2	3	4
1	82,333	90,833	12,167	15,500
2	90,833	100,333	13,167	17,000
3	12,167	13,167	2,333	2,500
4	15,500	17,000	2,500	3,000

Within-class covariance matrix for class D-Nle:

	1	2	3	4
1	310,333	300,167	-198,000	-193,167
2	300,167	290,333	-191,500	-186,833
3	-198,000	-191,500	127,000	123,500
4	-193,167	-186,833	123,500	120,333

Within-class covariance matrix for class D-Phe:

	1	2	3	4
1	4,333	3,500	-0,333	0,833
2	3,500	3,000	-0,500	0,500
3	-0,333	-0,500	0,333	0,167
4	0,833	0,500	0,167	0,333

Within-class covariance matrix for class D-Thr:

	1	2	3	4
1	121,333	93,333	-43,667	-38,333
2	93,333	72,333	-34,167	-29,833

3	-43,667	-34,167	16,333	14,167
4	-38,333	-29,833	14,167	12,333

Within-class covariance matrix for class D-Val:

	1	2	3	4
1	185,333	188,333	-33,667	-36,000
2	188,333	192,333	-34,667	-36,500
3	-33,667	-34,667	6,333	6,500
4	-36,000	-36,500	6,500	7,000

Within-class covariance matrix for class L-Asp:

	1	2	3	4
1	148,000	151,000	-108,000	-104,000
2	151,000	154,333	-110,833	-107,000
3	-108,000	-110,833	80,333	78,000
4	-104,000	-107,000	78,000	76,000

Within-class covariance matrix for class L-Nle:

	1	2	3	4
1	856,333	849,167	163,667	154,000
2	849,167	842,333	162,833	153,000
3	163,667	162,833	32,333	30,000
4	154,000	153,000	30,000	28,000

Within-class covariance matrix for class L-Phe:

	1	2	3	4
1	2,333	2,667	74,667	-18,667
2	2,667	4,333	37,333	-93,333
3	74,667	37,333	4181,333	2090,667
4	-18,667	-93,333	2090,667	4181,333

Within-class covariance matrix for class L-Thr:

	1	2	3	4
1	31,000	31,500	-3,000	-5,500
2	31,500	32,333	-3,167	-5,500
3	-3,000	-3,167	0,333	0,500
4	-5,500	-5,500	0,500	1,000

Within-class covariance matrix for class L-Val:

	1	2	3	4
1	30,333	27,833	-16,333	-8,167
2	27,833	26,333	-14,333	-7,167
3	-16,333	-14,333	9,333	4,667
4	-8,167	-7,167	4,667	2,333

Pooled within-class covariance matrix:

	1	2	3	4
1	177,167	173,833	-15,250	-23,350
2	173,833	171,800	-17,583	-29,567
3	-15,250	-17,583	445,600	235,067
4	-23,350	-29,567	235,067	443,167

Total covariance matrix:

	1	2	3	4
1	751601,582	751999,989	-214862,143	-203583,940
2	751999,989	752428,075	-215418,856	-204155,557
3	-214862,143	-215418,856	257101,840	259402,525
4	-203583,940	-204155,557	259402,525	262501,757

Wilks' Lambda test (Rao's approximation):

Lambda	0,000
F (Observed v	332,677
F (Critical vali	1,597
DF1	36
DF2	65
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Unidimensional test of equality of the means of the classes:

Variable	Lambda	F	DF1	DF2	p-value
1	0,000	13667,546	9	20	< 0,0001
2	0,000	14110,062	9	20	< 0,0001
3	0,001	1856,932	9	20	< 0,0001
4	0,001	1906,403	9	20	< 0,0001

Pillai's trace:

Trace	3,339
F (Observed v	11,220

F (Critical vali	1,564
DF1	36
DF2	80
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Hotelling-Lawley trace:

Trace	7486,427
F (Observed \	3303,534
F (Critical vali	1,744
DF1	36
DF2	36
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

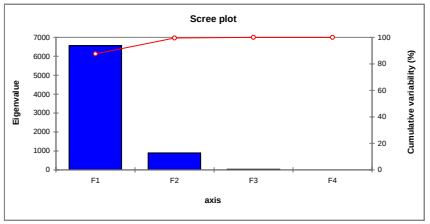
Roy's greatest root:

Root	6557,052
F (Observed \	14571,226
F (Critical vali	2,393
DF1	9
DF2	20
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

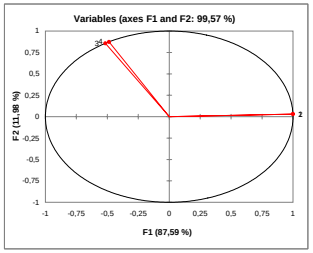
Eigenvalues:

	F1	F2	F3	F4
Eigenvalue	6557,052	896,951	31,835	0,588
Discriminatior	87,586	11,981	0,425	0,008
Cumulative %	87,586	99,567	99,992	100,000



Variables/Factors correlations:

	F1	F2	F3	F4
1	0,999	0,030	-0,017	0,001
2	1,000	0,029	-0,011	0,001
3	-0,516	0,856	-0,030	0,022
4	-0,486	0,873	-0,033	-0,020



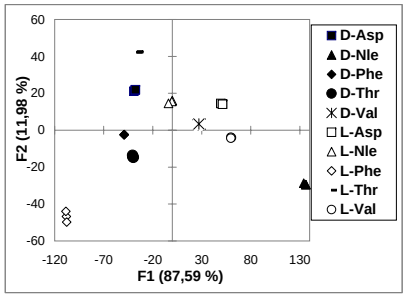
Classification functions:

	D-Asp	D-Nle	D-Phe	D-Thr	D-Val	L-Asp	L-Nle	L-Phe	L-Thr	L-Val
Intercept	-15754030,919	-16150250,315	-15611003,458	-15588775,199	-15903918,019	-16034320,847	-15856265,100	-15215563,748	-15854209,785	-15987296,141
1	-1438,618	-1450,189	-1435,098	-1423,499	-1450,143	-1445,880	-1448,432	-1419,792	-1442,078	-1445,912
2	1774,717	1798,692	1769,971	1758,871	1790,924	1788,632	1787,223	1749,458	1778,700	1789,069
3	91,547	89,296	90,967	90,710	90,637	90,900	91,114	90,332	92,073	90,352

4	139,334	138,005	138,626	138,172	138,946	139,187	139,274	137,046	139,957	138,678

Prior and posterior classification, membership probabilities, scores and squared distances:

Observation	Prior	Posterior	Pr(D-Asp)	Pr(D-Nle)	Pr(D-Phe)	Pr(D-Thr)	Pr(D-Val)	Pr(L-Asp)	Pr(L-Nle)	Pr(L-Phe)	Pr(L-Thr)	Pr(L-Val)	F1	F2	F3	F4	D²(D-Asp)	D²(D-Nle)	D²(D-Phe)	D²(D-Thr)	D²(D-Val)	D²(L-Asp)	D²(L-Nle)	D²(L-Phe)	D²(L-Thr)	D²(L-Val)
D-Nle	D-Nle	D-Nle	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	136,137	-29,480	-1,032	0,051	33016,997	5,271	35095,982	31402,748	13005,170	9230,254	21027,476	59996,270	34741,597	6467,148
D-Nle	D-Nle	D-Nle	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	136,207	-29,440	-1,039	0,101	33037,388	5,357	35119,985	31426,268	13018,018	9238,634	21043,349	60031,959	34759,891	6475,816
D-Nle	D-Nle	D-Nle	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	133,963	-28,671	-0,112	0,087	32182,329	7,431	34247,335	30633,835	12470,134	8798,431	20348,947	58961,658	33885,566	6099,948
L-Nle	L-Nle	L-Nle	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	-0,024	16,019	6,594	-0,266	1553,607	20451,922	2786,660	2801,374	910,225	2678,284	7,386	15662,838	2056,511	4048,242
L-Nle	L-Nle	L-Nle	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	-0,589	15,589	5,707	-0,318	1503,026	20554,507	2708,019	2702,163	931,860	2717,595	5,904	15480,959	2024,768	4087,140
L-Nle	L-Nle	L-Nle	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	-4,011	14,577	6,605	-0,390	1283,017	21420,044	2359,221	2412,103	1108,094	3095,771	11,470	14637,791	1865,319	4486,293
D-Asp	D-Asp	D-Asp	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-39,221	21,072	-1,893	0,033	6,598	33037,629	671,520	1315,285	4813,535	8131,758	1523,868	9386,603	470,161	10457,284
D-Asp	D-Asp	D-Asp	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-37,968	21,679	-1,001	0,046	4,695	32661,946	721,158	1377,415	4655,924	7920,495	1424,522	9636,379	438,773	10240,185
D-Asp	D-Asp	D-Asp	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-37,535	21,916	-0,103	-0,007	6,039	32536,413	738,188	1413,133	4594,944	7852,792	1383,832	9724,412	430,070	10168,090
L-Asp	L-Asp	L-Asp	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	49,477	14,514	-3,746	0,800	7756,829	9313,739	10063,512	8909,057	746,536	6,144	2710,432	28653,633	8061,087	467,333
L-Asp	L-Asp	L-Asp	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	51,268	14,159	-2,880	0,793	8075,393	8973,636	10399,405	9224,389	803,880	5,329	2880,506	29167,956	8387,579	415,664
L-Asp	L-Asp	L-Asp	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	51,219	14,066	-3,764	0,755	8072,013	8978,407	10395,426	9198,547	817,560	5,047	2892,474	29151,374	8386,529	417,773
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-40,464	-13,585	-7,109	-0,906	1282,648	31230,752	285,380	12,308	5059,928	9098,017	2539,676	5788,281	3185,440	10206,013
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-40,333	-14,409	-10,687	-0,870	1397,125	31217,855	383,585	5,460	5183,913	9159,370	2686,625	5834,069	3326,141	10254,824
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-39,747	-14,707	-11,581	-0,908	1434,715	31022,173	424,740	8,218	5148,079	9084,074	2690,567	5919,356	3371,499	10162,773
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-36,357	42,251	-2,324	0,623	438,565	34624,829	2185,920	3267,864	5657,078	8361,173	2013,299	13117,323	4,982	11412,164
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-35,621	42,522	-1,435	0,623	451,590	34409,089	2223,024	3318,753	5569,551	8251,632	1962,631	13263,930	5,029	11293,982
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-35,516	42,342	-2,337	0,682	446,327	34349,887	2216,661	3285,287	5558,472	8220,679	1960,720	13255,041	4,800	11259,653
D-Phe	D-Phe	D-Phe	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-49,317	-2,402	2,131	-0,888	711,858	34864,946	4,706	370,210	5911,639	10310,061	2621,537	5442,946	2210,792	11939,012
D-Phe	D-Phe	D-Phe	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-49,209	-2,518	1,245	-0,925	710,387	34814,850	4,964	345,184	5905,905	10283,486	2623,658	5447,000	2211,861	11911,099
D-Phe	D-Phe	D-Phe	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-49,082	-2,377	2,137	-0,934	705,670	34779,831	4,713	366,706	5875,542	10262,657	2598,328	5472,929	2202,523	11888,090
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-108,132	-46,711	2,550	-2,697	9569,665	59654,643	5441,547	5832,205	20827,595	28981,748	15243,041	17,923	13199,903	30068,986
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-107,760	-49,793	3,420	2,689	9954,749	59596,638	5692,102	6023,324	21042,194	29251,775	15553,900	17,311	13706,637	30221,534
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-108,566	-43,959	1,782	2,860	9258,140	59773,041	5267,336	5712,682	20691,855	28775,413	15012,380	17,258	12767,437	29982,920
D-Val	D-Val	D-Val	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	28,364	3,258	6,951	-0,445	4839,111	12581,476	6079,911	5289,574	6,004	732,203	1046,655	21170,226	5737,382	1109,433
D-Val	D-Val	D-Val	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	26,163	2,902	6,073	-0,461	4550,781	13021,900	5731,218	4951,768	6,511	825,620	928,278	20531,862	5472,679	1235,293
D-Val	D-Val	D-Val	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	27,028	3,345	7,862	-0,518	4675,166	12889,875	5885,563	5142,579	5,473	811,620	968,475	20825,051	5578,217	1211,491
L-Val	L-Val	L-Val	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	60,320	-4,067	-0,665	0,068	10375,656	6278,403	12009,766	10292,790	1213,377	441,747	4258,901	30226,894	11408,459	4,807
L-Val	L-Val	L-Val	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	59,651	-3,793	0,214	0,202	10231,525	6394,197	11859,363	10181,389	1153,076	424,811	4154,549	30020,054	11257,799	5,512
L-Val	L-Val	L-Val	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	59,654	-4,297	-1,562	0,119	10256,872	6368,080	11870,515	10139,271	1187,602	433,518	4199,293	29989,826	11300,557	5,507



Confusion matrix for the estimation sample:

from \ to	D-Asp	D-Nle	D-Phe	D-Thr	D-Val	L-Asp	L-Nle	L-Phe	L-Thr	L-Val	Total	% correct
D-Asp	3	0	0	0	0	0	0	0	0	0	3	100,00%
D-Nle	0	3	0	0	0	0	0	0	0	0	3	100,00%
D-Phe	0	0	3	0	0	0	0	0	0	0	3	100,00%
D-Thr	0	0	0	3	0	0	0	0	0	0	3	100,00%
D-Val	0	0	0	0	3	0	0	0	0	0	3	100,00%
L-Asp	0	0	0	0	0	3	0	0	0	0	3	100,00%
L-Nle	0	0	0	0	0	0	3	0	0	0	3	100,00%
L-Phe	0	0	0	0	0	0	0	3	0	0	3	100,00%
L-Thr	0	0	0	0	0	0	0	0	3	0	3	100,00%
L-Val	0	0	0	0	0	0	0	0	0	3	3	100,00%
Total	3	3	3	3	3	3	3	3	3	3	30	100,00%

LDA obtained with (R,R)-1 complex and both enantiomers of the aa's: Phg, Phe, Phe (I), Phe (F) and Hph

Within-class covariance matrices are assumed to be equal
Prior probabilities are taken into account
Significance level (%): 5

Summary statistics:

Variable	Categories	Frequencies	%
Q1	D-Phe(F)	3	10,000
	D-Hph	3	10,000
	D-Phe(I)	3	10,000
	D-Phe	3	10,000
	D-Phg	3	10,000
	L-Phe(F)	3	10,000
	L-Hph	3	10,000
	L-Phe(I)	3	10,000
	L-Phe	3	10,000
	L-Phg	3	10,000

Variable	Observations	os. with missing da	s. without missing d	Minimum	Maximum	Mean	Std. deviation
P1	30	0	30	47958,000	51713,000	49353,533	1185,602
P2	30	0	30	48098,000	51811,000	49464,433	1181,313
P3	30	0	30	62977,000	64116,000	63599,667	383,510
P4	30	0	30	63078,000	64217,000	63710,600	383,438

Correlation matrix:

Variables	P1	P2	P3	P4
P1	**1,000**	1,000	0,307	0,294
P2	1,000	**1,000**	0,308	0,295
P3	0,307	0,308	**1,000**	1,000
P4	0,294	0,295	1,000	**1,000**

Discriminant Analysis:

Means by class:

Class \ Variabl	P1	P2	P3	P4
D-Phe(F)	48140,667	48250,667	63330,000	63440,667
D-Hph	49403,000	49513,667	63165,333	63274,333
D-Phe(I)	48863,333	48972,667	63977,000	64084,667
D-Phe	47979,000	48101,333	63316,667	63441,000
D-Phg	50333,000	50436,667	62977,667	63079,667
L-Phe(F)	48772,333	48881,333	63903,333	64013,333
L-Hph	50886,000	50996,000	63899,000	64011,333
L-Phe(I)	48671,333	48781,667	63436,000	63546,333
L-Phe	48779,333	48901,333	63876,667	63999,667
L-Phg	51707,333	51809,000	64115,000	64215,000

Multicolinearity statistics:

Statistic	P1	P2	P3	P4
Tolerance	0,710	0,000	0,001	0,001
VIF	1,408	234793,000	1615,798	1602,608

Between-classes covariance matrix:

	P1	P2	P3	P4
P1	1509356,647	1503918,015	149799,938	143699,286
P2	1503918,015	1498523,779	149642,074	143592,464
P3	149799,938	149642,074	157957,457	157889,160
P4	143699,286	143592,464	157889,160	157881,106

Within-class covariance matrix for class D-Phe(F):

	P1	P2	P3	P4
P1	1929,333	1968,333	193,000	255,333
P2	1968,333	2008,333	197,500	260,833
P3	193,000	197,500	21,000	26,500
P4	255,333	260,833	26,500	34,333

Within-class covariance matrix for class D-Hph:

	P1	P2	P3	P4
P1	12,000	8,000	7,000	4,000
P2	8,000	14,333	6,167	8,667
P3	7,000	6,167	4,333	3,333
P4	4,000	8,667	3,333	5,333

Within-class covariance matrix for class D-Phe(I):

	P1	P2	P3	P4
P1	10,333	12,167	3,500	3,667
P2	12,167	14,333	4,000	4,333
P3	3,500	4,000	3,000	1,000
P4	3,667	4,333	1,000	1,333

Within-class covariance matrix for class D-Phe:

	P1	P2	P3	P4
P1	343,000	-17,500	94,500	-280,000
P2	-17,500	8,333	-3,333	25,000
P3	94,500	-3,333	26,333	-75,000

P4	-280,000	25,000	-75,000	244,000

Within-class covariance matrix for class D-Phg:

	P1	P2	P3	P4
P1	103,000	36,000	-1,000	-21,000
P2	36,000	21,333	1,333	-6,667
P3	-1,000	1,333	0,333	0,333
P4	-21,000	-6,667	0,333	4,333

Within-class covariance matrix for class L-Phe(F):

	P1	P2	P3	P4
P1	2552,333	2551,833	-379,167	-291,667
P2	2551,833	2552,333	-379,167	-291,667
P3	-379,167	-379,167	56,333	43,333
P4	-291,667	-291,667	43,333	33,333

Within-class covariance matrix for class L-Hph:

	P1	P2	P3	P4
P1	3,000	0,000	7,500	8,500
P2	0,000	4,000	3,000	1,000
P3	7,500	3,000	21,000	22,000
P4	8,500	1,000	22,000	24,333

Within-class covariance matrix for class L-Phe(I):

	P1	P2	P3	P4
P1	5,333	4,667	-2,000	-0,667
P2	4,667	4,333	-2,000	-0,333
P3	-2,000	-2,000	1,000	0,000
P4	-0,667	-0,333	0,000	0,333

Within-class covariance matrix for class L-Phe:

	P1	P2	P3	P4
P1	670,333	142,333	259,167	-268,833
P2	142,333	46,333	49,167	-46,833
P3	259,167	49,167	102,333	-107,667
P4	-268,833	-46,833	-107,667	114,333

Within-class covariance matrix for class L-Phg:

	P1	P2	P3	P4
P1	24,333	9,000	-0,500	-5,000
P2	9,000	4,000	-1,000	-3,000
P3	-0,500	-1,000	1,000	1,500
P4	-5,000	-3,000	1,500	3,000

Pooled within-class covariance matrix:

	P1	P2	P3	P4
P1	565,300	471,483	18,200	-59,567
P2	471,483	467,767	-12,433	-4,867
P3	18,200	-12,433	23,667	-8,467
P4	-59,567	-4,867	-8,467	46,467

Total covariance matrix:

	P1	P2	P3	P4
P1	1405652,947	1400524,692	139481,460	133747,910
P2	1400524,692	1395499,909	139313,356	133686,179
P3	139481,460	139313,356	147080,161	146994,414
P4	133747,910	133686,179	146994,414	147024,800

Wilks' Lambda test (Rao's approximation):

Lambda	0,000
F (Observed v	276,312
F (Critical vali	1,597
DF1	36
DF2	65
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Unidimensional test of equality of the means of the classes:

Variable	Lambda	F	DF1	DF2	p-value
P1	0,000	8010,030	9	20	< 0,0001
P2	0,000	9610,713	9	20	< 0,0001
P3	0,000	20022,776	9	20	< 0,0001
P4	0,000	10193,185	9	20	< 0,0001

Pillai's trace:

Trace	2,562
F (Observed v	3,959
F (Critical vali	1,564
DF1	36

DF2	80
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Hotelling-Lawley trace:

Trace	23681,414
F (Observed \	10449,894
F (Critical vali	1,744
DF1	36
DF2	36
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

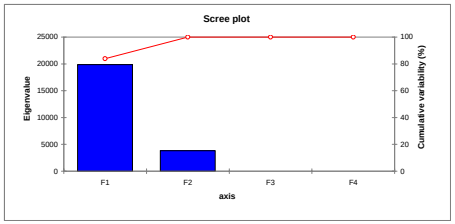
Roy's greatest root:

Root	19855,313
F (Observed \	44122,919
F (Critical vali	2,393
DF1	9
DF2	20
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 10 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

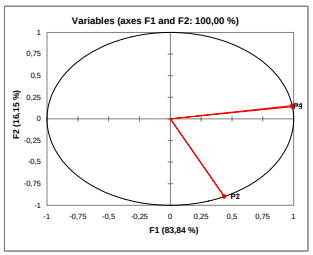
Eigenvalues:

	F1	F2	F3	F4
Eigenvalue	19855,313	3825,190	0,762	0,149
Discriminatior	83,843	16,153	0,003	0,001
Cumulative %	83,843	99,996	99,999	100,000



Variables/Factors correlations:

	F1	F2	F3	F4
P1	0,438	-0,899	0,002	-0,008
P2	0,438	-0,899	-0,003	-0,002
P3	0,990	0,141	0,008	-0,004
P4	0,988	0,154	-0,013	0,009

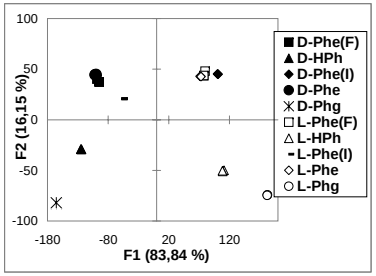


Classification functions:

	D-Phe(F)	D-Hph	D-Phe(I)	D-Phe	D-Phg	L-Phe(F)	L-Hph	L-Phe(I)	L-Phe	L-Phg
Intercept	-181387741,650	-180733760,435	-185151980,180	-181310589,266	-179875084,048	-184724500,786	-185157545,782	-182088668,254	-184605610,823	-186523234,105
P1	380,290	373,808	382,950	380,943	368,752	383,071	375,460	379,159	382,767	373,715
P2	-171,210	-162,125	-171,210	-172,221	-155,282	-171,662	-159,281	-168,710	-171,349	-155,348
P3	3155,638	3154,447	3189,302	3154,212	3150,160	3185,073	3194,842	3163,180	3184,044	3209,230
P4	2409,851	2398,697	2433,255	2410,331	2387,963	2431,057	2424,335	2412,312	2430,218	2429,514

Prior and posterior classification, membership probabilities, scores and squared distances:

Observation	Prior	Posterior	Pr(D-Phe(F))	Pr(D-Hph)	Pr(D-Phen(I))	Pr(D-Phe)	Pr(D-Phg)	Pr(L-Phe(F))	Pr(L-Hph)	Pr(L-Phe(I))	Pr(L-Phe)	Pr(L-Phg)	F1	F2	F3	F4	D²(D-Phe(F))	D²(D-Hph)	D²(D-Phe(I))	D²(D-Phe)	D²(D-Phg)	D²(L-Phe(F))	D²(L-Hph)	D²(L-Phe(I))	D²(L-Phe)	D²(L-Phg)
D-Phe	D-Phe	D-Phe	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-99,752	44,842	-3,142	1,578	78,990	6102,351	40248,282	11,926	20521,453	31794,253	52861,347	2388,436	29681,697	93969,760
D-Phe	D-Phe	D-Phe	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-101,498	44,413	0,098	-0,374	73,911	5943,144	40933,534	6,940	20172,670	32404,324	53508,203	2503,896	30279,370	94842,300
D-Phe	D-Phe	D-Phe	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-100,651	44,434	-0,070	-0,753	65,751	5986,631	40592,520	6,375	20287,161	32100,313	53155,199	2431,457	29986,009	94367,345
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	71,558	42,969	-2,637	2,273	28113,907	43649,839	883,147	29664,261	71845,822	72,957	10168,616	17168,940	12,129	26132,291
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	72,731	42,944	0,192	-0,364	28492,394	44096,007	798,861	30064,520	72383,103	42,233	10069,621	17457,677	6,345	25853,442
L-Phe	L-Phe	L-Phe	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	73,170	42,555	0,187	-0,362	28637,161	44213,386	776,277	30218,327	72494,770	39,136	9965,010	17555,033	6,799	25665,930
D-Phg	D-Phg	D-Phg	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	-165,292	-82,598	0,037	-0,674	19395,300	4528,911	87133,154	20356,914	5,118	75726,969	76544,326	22295,061	72275,318	121102,596
D-Phg	D-Phg	D-Phg	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	-165,094	-82,833	1,693	2,072	19432,795	4541,737	87089,839	20400,541	11,093	75698,836	76463,654	22307,660	72246,740	120973,620
D-Phg	D-Phg	D-Phg	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	-165,454	-81,984	-0,853	-1,449	19272,254	4480,418	87067,879	20223,033	8,234	75652,086	76593,982	22206,362	72200,810	121209,171
L-Phg	L-Phg	L-Phg	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	182,562	-74,313	-0,139	-0,776	90247,626	96326,601	20962,022	94337,682	121065,608	25075,896	5918,589	66657,167	25844,043	5,748
L-Phg	L-Phg	L-Phg	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	182,961	-74,282	0,444	0,290	90463,262	96567,556	21017,795	94556,970	121343,291	25151,874	5977,426	66842,609	25924,141	4,786
L-Phg	L-Phg	L-Phg	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	182,286	-74,696	1,011	0,830	90182,045	96191,274	21006,340	94275,663	120868,193	25111,878	5901,868	66598,586	25874,355	5,616
D-Hph	D-Hph	D-Hph	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-123,855	-29,319	0,545	0,846	5339,016	5,334	56022,857	6005,331	4546,663	46480,932	54899,873	6911,061	43760,660	95956,431
D-Hph	D-Hph	D-Hph	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-124,510	-28,925	0,045	-0,295	5321,413	5,146	56259,818	5976,580	4534,143	46686,419	55219,698	6958,239	43961,141	96393,667
D-Hph	D-Hph	D-Hph	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-125,099	-29,162	0,300	0,538	5388,029	5,010	56560,350	6040,464	4461,306	46962,118	55487,450	7061,546	44227,648	96734,674
L-Hph	L-Hph	L-Hph	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	111,025	-49,837	-1,946	-1,116	50610,034	55906,674	9142,314	53717,966	77420,086	10067,182	8,381	33383,028	10079,774	5740,021
L-Hph	L-Hph	L-Hph	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	109,032	-50,961	-0,075	0,884	49984,165	55012,823	9310,850	53090,624	76245,333	10152,322	8,007	32870,260	10136,080	5968,978
L-Hph	L-Hph	L-Hph	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	108,392	-50,388	-1,705	-0,810	49622,753	54694,646	9198,237	52713,531	75934,711	10006,316	6,224	32579,030	9984,733	6095,347
D-Phe(F)	D-Phe(F)	D-Phe(F)	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-98,387	40,099	0,613	-0,344	14,171	5479,900	39708,641	32,544	19503,060	31318,077	51407,447	2053,789	29212,533	92077,479
D-Phe(F)	D-Phe(F)	D-Phe(F)	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-94,378	37,098	0,423	-0,185	8,424	5298,421	38166,971	101,701	19328,645	29954,428	49222,046	1634,374	27883,168	89162,042
D-Phe(F)	D-Phe(F)	D-Phe(F)	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-95,188	37,340	-0,146	-0,726	6,234	5283,476	38481,672	87,995	19273,028	30231,402	49593,676	1703,247	28151,317	89666,092
L-Phe(F)	L-Phe(F)	L-Phe(F)	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	79,878	47,963	0,972	0,020	31028,708	47714,814	450,568	32604,860	77120,641	15,799	10560,446	19619,088	88,885	25537,381
L-Phe(F)	L-Phe(F)	L-Phe(F)	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	77,806	43,449	0,196	-0,361	30235,443	46196,273	537,711	31848,317	74951,195	7,592	9816,881	18827,723	34,958	24882,880
L-Phe(F)	L-Phe(F)	L-Phe(F)	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	77,815	43,669	-0,295	-0,974	30241,866	46233,831	538,813	31851,411	75012,549	7,548	9856,821	18841,407	36,149	24934,176
D-Phe(I)	D-Phe(I)	D-Phe(I)	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	100,350	45,325	0,613	-0,187	38603,150	56101,418	5,280	40402,625	86895,826	482,299	9253,810	25525,315	789,605	21111,509
D-Phe(I)	D-Phe(I)	D-Phe(I)	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	100,878	45,124	1,586	0,513	38810,085	56310,287	4,904	40618,828	87126,842	507,964	9211,318	25684,256	821,422	20978,312
D-Phe(I)	D-Phe(I)	D-Phe(I)	0,000	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	101,190	44,993	1,181	0,354	38930,200	56430,808	4,796	40742,621	87258,737	520,869	9178,639	25775,822	836,963	20895,166
L-Phe(I)	L-Phe(I)	L-Phe(I)	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-57,381	20,709	0,642	0,059	1800,435	6992,638	25625,080	2447,301	22293,146	19059,843	32907,610	4,785	17361,274	66648,246
L-Phe(I)	L-Phe(I)	L-Phe(I)	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-57,432	20,742	0,239	-0,101	1795,105	6989,064	25640,272	2440,183	22288,781	19071,877	32927,863	4,616	17372,301	66679,050
L-Phe(I)	L-Phe(I)	L-Phe(I)	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	-57,662	20,632	-0,009	-0,407	1781,236	6947,848	25719,256	2425,259	22216,906	19139,753	32988,428	4,794	17436,997	66769,111



Confusion matrix for the estimation sample:

from \ to	D-Phe(F)	D-Hph	D-Phe(I)	D-Phe	D-Phg	L-Phe(F)	L-Hph	L-Phe(I)	L-Phe	L-Phg	Total	% correct
D-Phe(F)	3	0	0	0	0	0	0	0	0	0	3	100,00%
D-Hph	0	3	0	0	0	0	0	0	0	0	3	100,00%
D-Phe(I)	0	0	3	0	0	0	0	0	0	0	3	100,00%
D-Phe	0	0	0	3	0	0	0	0	0	0	3	100,00%
D-Phg	0	0	0	0	3	0	0	0	0	0	3	100,00%
L-Phe(F)	0	0	0	0	0	3	0	0	0	0	3	100,00%
L-Hph	0	0	0	0	0	0	3	0	0	0	3	100,00%
L-Phe(I)	0	0	0	0	0	0	0	3	0	0	3	100,00%
L-Phe	0	0	0	0	0	0	0	0	3	0	3	100,00%
L-Phg	0	0	0	0	0	0	0	0	0	3	3	100,00%
Total	3	3	3	3	3	3	3	3	3	3	30	100,00%

LDA obtained with the (R,R)-1 complex and both enantiomers of the aa's: Ile, alle, Thr and aThr

Within-class covariance matrices are assumed to be equal
Prior probabilities are taken into account
Significance level (%): 5

Summary statistics:

Variable	Categories	Frequencies	%
Q1	D-alle	3	12,500
	D-aThr	3	12,500
	D-Ile	3	12,500
	D-Thr	3	12,500
	L-alle	3	12,500
	L-aThr	3	12,500
	L-alle	3	12,500
	L-Thr	3	12,500

Variable	Observations	s. with missing d	without missing	Minimum	Maximum	Mean	Std. deviation
P1	24	0	24	48858,000	50874,000	49689,875	694,299
P2	24	0	24	48990,000	50992,000	49795,875	693,345
P3	24	0	24	62927,000	64697,000	63753,042	515,752
P4	24	0	24	63037,000	64801,000	63864,958	517,506

Correlation matrix:

Variables	P1	P2	P3	P4
P1	**1,000**	0,998	-0,747	-0,748
P2	0,998	**1,000**	-0,734	-0,735
P3	-0,747	-0,734	**1,000**	1,000
P4	-0,748	-0,735	1,000	**1,000**

Discriminant Analysis:

Means by class:

Class \ Variabl	P1	P2	P3	P4
D-alle	50575,333	50675,000	63249,000	63356,667
D-aThr	49426,000	49473,000	63437,667	63544,667
D-Ile	49806,333	49918,000	63983,667	64098,667
D-Thr	48993,000	49122,667	64654,667	64770,667
L-alle	49848,333	49962,667	63930,333	64046,667
L-aThr	49127,000	49229,333	64111,667	64215,333
L-Ile	50851,667	50962,667	62944,333	63054,000
L-Thr	48891,333	49023,667	63713,000	63833,000

Multicolinearity statistics:

Statistic	P1	P2	P3	P4
Tolerance	0,003	0,003	0,000	0,000
VIF	353,121	337,855	3053,195	3078,453

Between-classes covariance matrix:

	P1	P2	P3	P4
P1	526032,823	523503,252	-292270,486	-293510,149
P2	523503,252	521675,776	-286626,312	-287766,006
P3	-292270,486	-286626,312	290755,950	291813,923
P4	-293510,149	-287766,006	291813,923	292904,236

Within-class covariance matrix for class D-alle:

	P1	P2	P3	P4
P1	25,333	-52,000	8,000	-2,333
P2	-52,000	148,000	-12,000	7,000
P3	8,000	-12,000	3,000	-0,500
P4	-2,333	7,000	-0,500	0,333

Within-class covariance matrix for class D-aThr:

	P1	P2	P3	P4
P1	8917,000	18807,500	-2732,500	-2652,000
P2	18807,500	39679,000	-5756,000	-5584,500
P3	-2732,500	-5756,000	842,333	818,833
P4	-2652,000	-5584,500	818,833	796,333

Within-class covariance matrix for class D-Ile:

	P1	P2	P3	P4
P1	5126,333	4953,000	-1239,333	-1193,833
P2	4953,000	4804,000	-1215,000	-1160,000
P3	-1239,333	-1215,000	316,333	294,833
P4	-1193,833	-1160,000	294,833	280,333

Within-class covariance matrix for class D-Thr:

	P1	P2	P3	P4
P1	1609,000	558,500	30,000	-430,500
P2	558,500	630,333	-792,167	-655,667
P3	30,000	-792,167	1476,333	922,833
P4	-430,500	-655,667	922,833	702,333

Within-class covariance matrix for class L-alle:

	P1	P2	P3	P4
P1	186,333	163,167	-36,667	-56,333
P2	163,167	144,333	-30,833	-48,667
P3	-36,667	-30,833	8,333	11,667
P4	-56,333	-48,667	11,667	17,333

Within-class covariance matrix for class L-aThr:

	P1	P2	P3	P4
P1	721,000	728,000	-405,000	-389,500
P2	728,000	737,333	-403,333	-387,667
P3	-405,000	-403,333	241,333	232,667
P4	-389,500	-387,667	232,667	224,333

Within-class covariance matrix for class L-lle:

	P1	P2	P3	P4
P1	1304,333	1321,333	-827,333	-870,500
P2	1321,333	1429,333	-885,333	-920,000
P3	-827,333	-885,333	549,333	572,000
P4	-870,500	-920,000	572,000	597,000

Within-class covariance matrix for class L-Thr:

	P1	P2	P3	P4
P1	2354,333	2733,167	-1338,500	-1690,500
P2	2733,167	3202,333	-1320,000	-1839,500
P3	-1338,500	-1320,000	2623,000	1940,500
P4	-1690,500	-1839,500	1940,500	1729,000

Pooled within-class covariance matrix:

	P1	P2	P3	P4
P1	2530,458	3651,583	-817,667	-910,688
P2	3651,583	6346,833	-1301,833	-1323,625
P3	-817,667	-1301,833	757,500	599,104
P4	-910,688	-1323,625	599,104	543,375

Total covariance matrix:

	P1	P2	P3	P4
P1	482051,158	480521,462	-267424,473	-268621,049
P2	480521,462	480727,853	-262607,908	-263663,658
P3	-267424,473	-262607,908	265999,781	266855,567
P4	-268621,049	-263663,658	266855,567	267812,303

Wilks' Lambda test (Rao's approximation):

Lambda	0,000
F (Observed	80,280
F (Critical val	1,710
DF1	28
DF2	48
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 8 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Unidimensional test of equality of the means of the classes:

Variable	Lambda	F	DF1	DF2	p-value

P1	0,004	623,641	7	16	< 0,0001
P2	0,009	246,584	7	16	< 0,0001
P3	0,002	1151,509	7	16	< 0,0001
P4	0,001	1617,139	7	16	< 0,0001

Pillai's trace:

Trace	2,506
F (Observed	3,835
F (Critical val	1,652
DF1	28
DF2	64
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 8 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

Hotelling-Lawley trace:

Trace	1871,732
F (Observed	802,171
F (Critical val	1,952
DF1	28
DF2	24
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 8 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

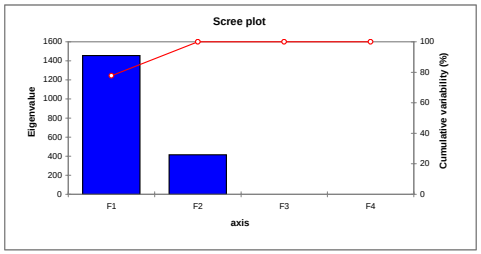
Roy's greatest root:

Root	1456,287
F (Observed	3328,657
F (Critical val	2,657
DF1	7
DF2	16
p-value	< 0,0001
alpha	0,05

Test interpretation:
H0: The means vectors of the 8 classes are equal.
Ha: At least one of the means vector is different from another.
As the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0,01%.

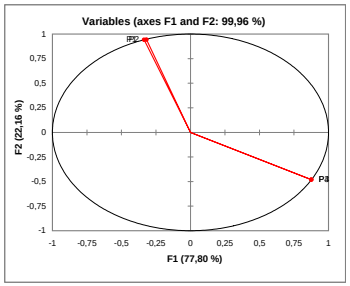
Eigenvalues:

	F1	F2	F3	F4
Eigenvalue	1456,287	414,703	0,569	0,172
Discriminatio	77,804	22,156	0,030	0,009
Cumulative %	77,804	99,960	99,991	100,000



Variables/Factors correlations:

	F1	F2	F3	F4
P1	-0,335	0,941	-0,024	-0,035
P2	-0,319	0,943	-0,074	-0,064
P3	0,876	-0,481	0,036	-0,009
P4	0,876	-0,481	0,022	0,004

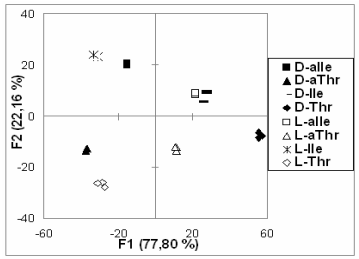


Classification functions:

	D-alle	D-aThr	D-Ile	D-Thr	L-alle	L-aThr	L-Ile	L-Thr
Intercept	-29840448,474	-29592581,172	-30093378,686	-30280274,533	-30072689,358	-29940197,074	-29727596,402	-29612995,262
P1	421,901	419,317	422,738	423,091	422,648	421,120	421,447	418,834
P2	-91,093	-90,323	-91,009	-90,815	-91,004	-90,512	-91,087	-90,020
P3	-731,360	-727,834	-733,966	-735,682	-733,759	-731,670	-730,196	-727,836
P4	1408,171	1402,173	1414,016	1418,209	1413,553	1410,200	1405,584	1402,635

Prior and posterior classification, membership probabilities, scores and squared distances:

Observation	Prior	Posterior	Pr(D-alle)	Pr(D-aThr)	Pr(D-Ile)	Pr(D-Thr)	Pr(L-alle)	Pr(L-aThr)	Pr(L-Ile)	Pr(L-Thr)	F1	F2	F3	F4	D²(D-alle)	D²(D-aThr)	D²(D-Ile)	D²(D-Thr)	D²(L-alle)	D²(L-aThr)	D²(L-Ile)	D²(L-Thr)
D-aThr	D-aThr	D-aThr	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-36,433	-12,887	-0,138	-0,533	1550,207	6,801	4147,150	8564,642	3807,379	2264,516	1370,452	254,785
D-aThr	D-aThr	D-aThr	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-37,258	-13,632	3,367	2,478	1653,060	14,029	4295,822	8744,021	3952,489	2361,013	1454,482	272,929
D-aThr	D-aThr	D-aThr	0,000	1,000	0,000	0,000	0,000	0,000	0,000	0,000	-36,953	-12,876	-0,070	-0,601	1571,966	6,591	4210,432	8660,954	3867,521	2314,114	1374,450	263,415
L-aThr	L-aThr	L-aThr	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	11,246	-12,341	0,622	-0,682	1750,940	2322,467	589,066	2025,330	538,430	4,340	3193,804	1828,341
L-aThr	L-aThr	L-aThr	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	11,468	-13,494	0,720	-0,737	1839,085	2343,511	631,396	2018,176	583,289	4,868	3298,174	1814,746
L-aThr	L-aThr	L-aThr	0,000	0,000	0,000	0,000	0,000	1,000	0,000	0,000	10,594	-12,382	0,672	-0,631	1719,766	2259,999	608,383	2084,354	553,844	4,547	3140,784	1775,396
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	55,383	-8,458	-1,952	1,106	5790,510	8548,145	1228,930	10,013	1441,368	1993,277	8707,361	7446,670
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	55,180	-6,338	0,833	-0,320	5639,857	8526,231	1148,604	7,067	1358,748	1988,068	8536,751	7496,628
D-Thr	D-Thr	D-Thr	0,000	0,000	0,000	1,000	0,000	0,000	0,000	0,000	57,233	-7,741	0,853	-0,734	6009,175	8892,257	1321,376	7,357	1545,431	2157,196	8986,469	7791,328
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	-28,285	-26,119	-2,309	2,255	2328,587	261,289	3953,172	7452,817	3674,926	1752,113	2522,728	11,546
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	-31,211	-26,374	-0,730	-1,116	2428,059	217,312	4281,337	7955,469	3986,485	1982,671	2525,589	10,975
L-Thr	L-Thr	L-Thr	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,000	-27,233	-27,823	-0,335	-1,193	2451,860	317,706	3955,061	7334,503	3685,920	1702,543	2696,164	10,079
D-Ile	D-Ile	D-Ile	0,000	0,000	0,997	0,000	0,003	0,000	0,000	0,000	25,103	9,266	0,156	0,210	1736,089	4348,797	6,559	1236,155	18,437	685,441	3491,193	4221,950
D-Ile	D-Ile	D-Ile	0,000	0,000	0,922	0,000	0,078	0,000	0,000	0,000	23,338	5,399	-0,052	0,125	1696,198	3975,217	11,569	1233,265	16,496	484,011	3419,493	3770,056
D-Ile	D-Ile	D-Ile	0,000	0,000	0,997	0,000	0,003	0,000	0,000	0,000	25,036	8,915	-0,284	0,471	1738,822	4325,755	5,659	1228,839	17,305	669,424	3493,796	4188,748
L-Ile	L-Ile	L-Ile	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-32,431	24,465	-0,115	-0,185	324,477	1439,228	3520,368	8834,779	3167,938	3284,349	4,733	2642,807
L-Ile	L-Ile	L-Ile	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-30,959	23,032	-0,409	-0,078	265,373	1349,485	3309,452	8487,292	2967,270	3054,472	6,151	2489,334
L-Ile	L-Ile	L-Ile	0,000	0,000	0,000	0,000	0,000	0,000	1,000	0,000	-32,975	23,968	-0,583	-0,353	340,061	1399,110	3566,737	8899,933	3211,376	3296,046	4,976	2595,600
D-alle	D-alle	D-alle	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-15,097	19,999	0,069	-0,307	4,201	1577,955	1719,168	5806,267	1476,448	1762,885	308,817	2384,028
D-alle	D-alle	D-alle	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-15,089	19,793	-0,243	-0,196	4,409	1565,226	1713,446	5793,718	1470,871	1749,543	310,532	2364,276
D-alle	D-alle	D-alle	1,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	-15,027	20,568	0,571	0,032	4,590	1617,828	1727,908	5828,318	1485,160	1796,807	307,900	2440,801
L-alle	L-alle	L-alle	0,000	0,000	0,010	0,000	0,990	0,000	0,000	0,000	21,468	8,082	-0,316	0,457	1484,750	3860,760	13,455	1435,349	4,259	547,400	3124,197	3757,765
L-alle	L-alle	L-alle	0,000	0,000	0,009	0,000	0,991	0,000	0,000	0,000	21,461	8,248	-0,227	0,272	1480,019	3866,786	13,524	1440,857	4,174	553,617	3118,075	3768,635
L-alle	L-alle	L-alle	0,000	0,000	0,007	0,000	0,993	0,000	0,000	0,000	21,442	8,732	-0,099	0,261	1467,264	3885,174	14,225	1457,658	4,320	573,544	3101,205	3801,084



Confusion matrix for the estimation sample:

from \ to	D-alle	D-aThr	D-Ile	D-Thr	L-alle	L-aThr	L-Ile	L-Thr	Total	% correct
D-alle	3	0	0	0	0	0	0	0	3	100,00%
D-aThr	0	3	0	0	0	0	0	0	3	100,00%
D-Ile	0	0	3	0	0	0	0	0	3	100,00%
D-Thr	0	0	0	3	0	0	0	0	3	100,00%
L-alle	0	0	0	0	3	0	0	0	3	100,00%
L-aThr	0	0	0	0	0	3	0	0	3	100,00%
L-Ile	0	0	0	0	0	0	3	0	3	100,00%
L-Thr	0	0	0	0	0	0	0	3	3	100,00%
Total	3	3	3	3	3	3	3	3	24	100,00%