Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Machine Learning for Predicting Product Distributions in Catalytic Regioselective Reactions

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1. Alkenes Used in Machine Learning

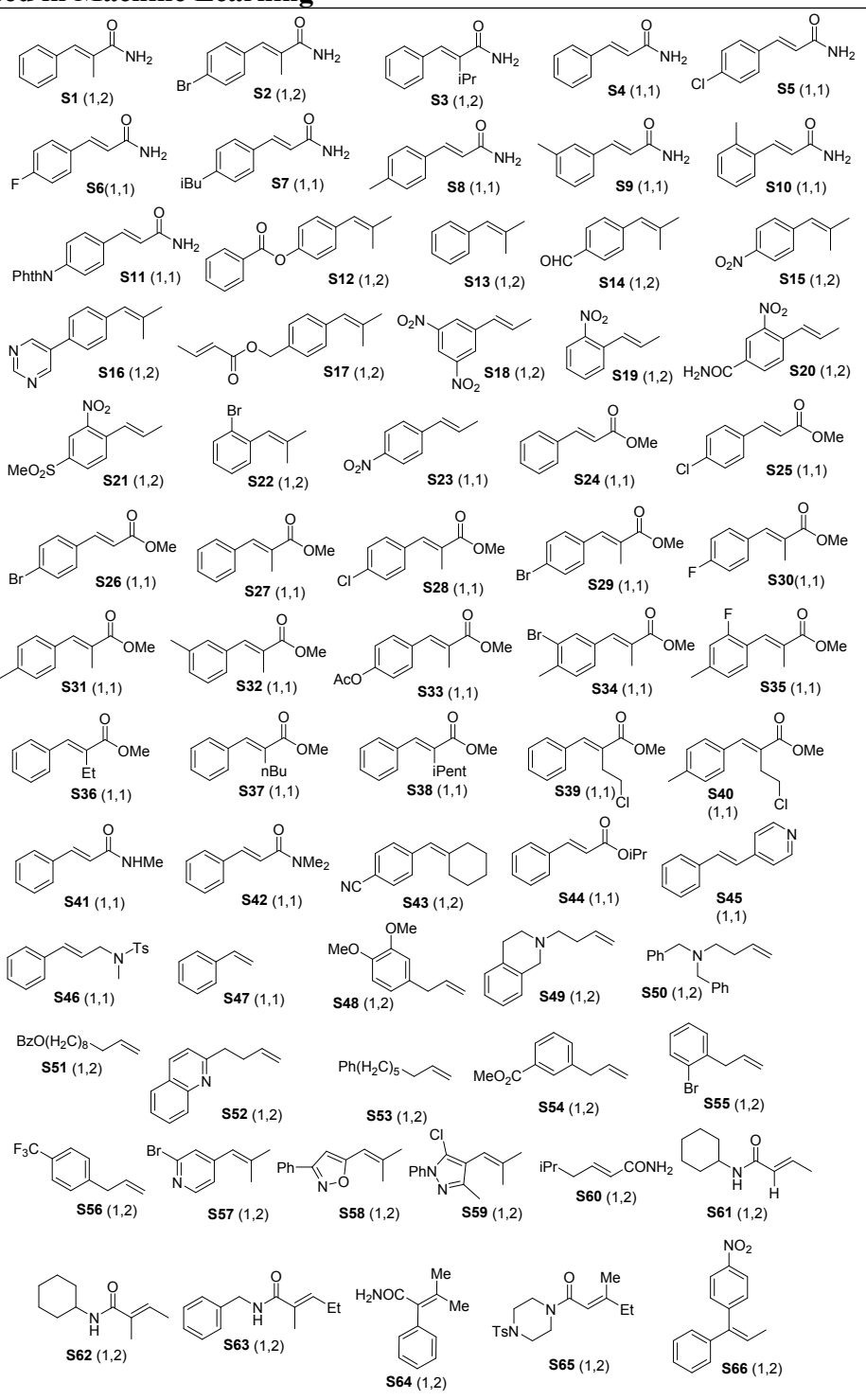

Fig S1. Alkenes **S1**-**S66** and the corresponding regioisomer (1,1-difluoro- or 1,2-difluoro-) formed in the difluorination reaction. The regioselectivity as noted with these substrates form the dataset for machine learning study.

2. Additional Details on Machine Learning Approaches

2. 1. Neural Network

Five NN models are built using different sets of substrates as shown in Table S1. For example, substrates **S1**, **S3**, **S4**, **S24**, **S27**, **S39**, **S41**, **S42**, and **S43** are taken as the test set and the remaining 38 substrates are used for model building in NN model-1. Quality of each model is tested with a test set which is not exposed to the NN during training. To render sufficient generality to our NN models, we have performed a 5-fold cross validation by keeping 20% samples each time in the test set for five such independent NN training. In each case, we have also checked whether the results could be regarded converged by increasing the number of NN form 100 to 500. Average of the predicted outcome remained unchanged even after increasing the number of NN beyond 100.

It would be desirable to apply what was learnt through ML models using a set of known examples to predict the regiochemical outcome for new substrates. To this end, an expanded set of 84 styrenyl family of substrates is considered whose experimental outcome is not known yet. A database consisting of all 63 parameters of 47 styrenyl substrates is considered to build the NN model. To the trained NN model, 63 parameters of each of the external 84 substrates are fed in to predict the outcome (See Tables S4 and S5 for the expanded substrate set and the corresponding predictions on the regioselectivity).

2. 2. Ranking of Parameters

The NN model does not readily provide much chemical insight on how and to what extent each of the parameters impact the reaction outcome. To partly address this issue, all the 63 parameters of the substrates (**S1-S47**) are first ranked using a wrapper-based random forest classifier,[1] which revealed 25 parameters as the most important ones. Following the standard practice, normalization of the data for random forest classification was carried out by subtracting the respective mean and dividing by the standard deviation for each parameter set.

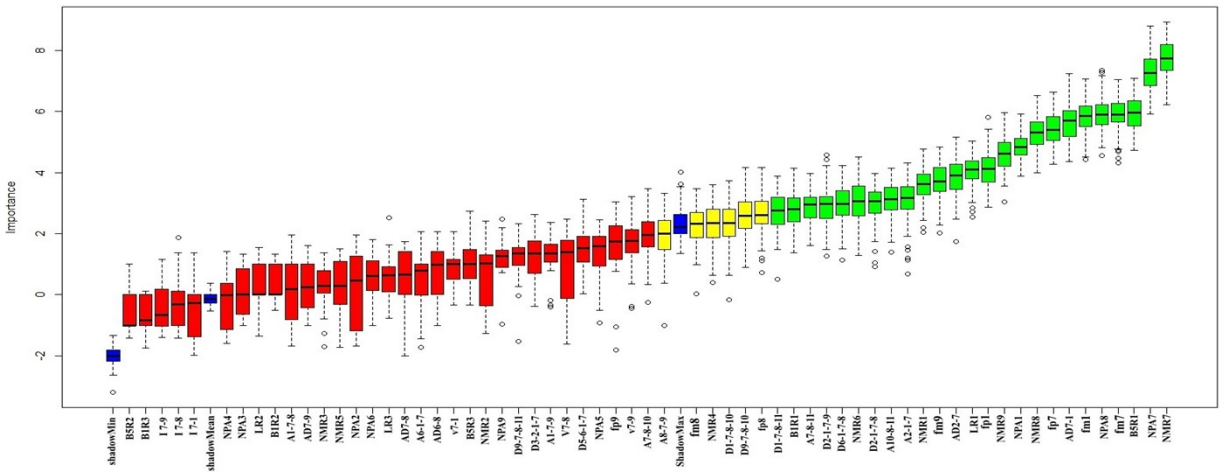

Fig S2. Ranking of parameters (shown in X-axis) on the basis of their relative importance (Y-axis) determined using random forest classification. Maximum and minimum importance is indicated by the upper and lower bars of each box over all iterations.

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(1) Kursa, M. B; Rudnicki, W. R. Feature selection with the Boruta package. *J. Stat. Software*, **2010,** 36, 1-13.

2. 3. Neural Network (NN) Modeling for Styrenyl Derivatives (S1-S47)

The exclusive regioselective products form the binary outputs '0' and '1' respectively for 1,2- and 1,1- difluorinated products. As we are dealing with classification problem, the output values must be discrete in nature, i.e., it should be '0' or '1'. In line with the standard procedure, predictions > 0.5 are considered as '1' whereas < 0.5 are taken as '0' in the NN prediction.

Table S1. Different Model Building and Test Sets from Substrates **S1-S47** for the Five-fold Cross Validation of NN with the Corresponding Predicted Outcome

Neural Network Model No.	Model building set	Test set	No. of correct prediction	No. of incorrect prediction
1	**S44, S18, S9, S36, S38, S32, S37, S15, S46, S22, S10, S19, S20, S2, S26, S14, S5, S25, S17, S6, S30, S7, S8, S40, S12, S16, S31, S34, S35, S23, S11, S33, S21, S45, S13, S47, S28, S29**	**S3, S4, S1, S41, S42, S43, S24, S27, S39**	9	0
2	**S3, S4, S1, S41, S42, S43, S24, S27, S39, S22, S10, S19, S20, S2, S26, S14, S5, S25, S17, S6, S30, S7, S8, S40, S12, S16, S31, S34, S35, S23, S11, S33, S21, S45, S13, S47, S28, S29**	**S44, S18, S9, S36, S38 S32, S37, S15, S46**	8	1
3	**S3, S4, S1, S41, S42, S43, S24, S27, S39, S44, S18, S9, S36, S38 S32, S37, S15, S46, S17, S6, S30, S7, S8, S40, S12, S16, S31, S34, S35, S23, S11, S33, S21, S45, S13, S47, S28, S29**	**S22, S10, S19, S20, S2, S26, S14, S5, S25**	8	1
4	**S3, S4, S1, S41, S42, S43, S24, S27, S39, S44, S18, S9, S36, S38 S32, S37, S15, S46, S22, S10, S19, S20, S2, S26, S14, S5, S25, S35, S23, S11, S33, S21, S45, S13, S47, S28, S29**	**S17, S6, S30, S7, S8, S40, S12, S16, S31, S34**	9	1
5	**S3, S4, S1, S41, S42, S43, S24, S27, S39, S44, S18, S9, S36, S38 S32, S37, S15, S46, S22, S10, S19, S20, S2, S26, S14, S5, S25, S17, S6, S30, S7, S8, S40, S12, S16, S31, S34**	**S35, S23, S11, S33, S21, S45, S13, S47, S28, S29**	9	1

Table S2. Comparison of Experimental and Predicted Regioselectivity Obtained Using Neural Network Models for 47 Styrenyl Substrates (**S1-S47**) Using 63 Parameters. Blue and Red Circles

Respectively Correspond to the 1,1- and 1,2- Difluorinated Regioisomeric Products. It can be Noted that Only 4 Predictions Out of 47 did not Match with the Experimental Regioisomer

substrate	expt.	pred.		substrate	expt.	pred.		substrate	expt.	pred.
S1	🔴	🔴		**S17**	🔴	🔴		**S33**	🔵	🔵
S2	🔴	🔵		**S18**	🔴	🔵		**S34**	🔵	🔵
S3	🔴	🔴		**S19**	🔴	🔴		**S35**	🔵	🔵
S4	🔵	🔵		**S20**	🔴	🔴		**S36**	🔵	🔵
S5	🔵	🔵		**S21**	🔴	🔴		**S37**	🔵	🔵
S6	🔵	🔵		**S22**	🔴	🔴		**S38**	🔵	🔵
S7	🔵	🔵		**S23**	🔵	🔴		**S39**	🔵	🔵
S8	🔵	🔵		**S24**	🔵	🔵		**S40**	🔵	🔵
S9	🔵	🔵		**S25**	🔵	🔵		**S41**	🔵	🔵
S10	🔵	🔵		**S26**	🔵	🔵		**S42**	🔵	🔵
S11	🔵	🔵		**S27**	🔵	🔵		**S43**	🔴	🔴
S12	🔴	🔵		**S28**	🔵	🔵		**S44**	🔵	🔵
S13	🔴	🔴		**S29**	🔵	🔵		**S45**	🔵	🔵
S14	🔴	🔴		**S30**	🔵	🔵		**S46**	🔵	🔵
S15	🔴	🔴		**S31**	🔵	🔵		**S47**	🔵	🔵
S16	🔴	🔴		**S32**	🔵	🔵				

2.4. Neural Network Code

```
net = feedforwardnet(10);
rng default
%number of networks
numNN = 100;
nets = cell(1, numNN);
for i = 1:numNN
  fprintf('Training %d/%d\n', i, numNN)
  nets{i} = train(net, X1, Y1);
end
perfs = zeros(1, numNN);
y2Total = 0;
for i = 1:numNN
  neti = nets{i};
  y2 = neti(X2);
  y2Total = y2Total + y2;
end
y2AverageOutput = y2Total / numNN;
```

2. 5. Decision Tree, Logistic Regression and Ensemble Tree Based Random Forest

We have applied other ML tools such as Decision Tree (DT), Logistic Regression (LR) and Ensemble Tree Based Random Forest to the styrenyl family of alkenes (**S1-S47**). Note that the test set is not exposed to the algorithm while training. In this case, to deal with exclusive regioselective product formation, the output values are taken as '0' for 1,2 and '1' for 1,1 selectivity. The accuracy using decision tree, logistic regression and Ensemble Tree Based Random Forest turn out to be respectively 77%, 62% and 77% which are much lower than the accuracy of NN (92%) (Table S3).

Table S3. Comparison of the Percentage of Successful Predictions Obtained through Neural Network, Decision Tree, Logistic Regression and Ensemble Tree Based Random Forest Models for the Experimentally Known Styrenyl Family of Substrates (**S1-S47**) (same cross-validation sets are used for NN, DT and LR)

Neural Network	Decision Tree	Logistic Regression	Random Forest
92	77	62	77

Note that the DT algorithm used here and the decision tree classification described in the main text are employed for different purposes. Here, DT is trained and then used for prediction. However, the analysis mentioned in the main text involves the construction of a decision tree using 25 high ranked parameters obtained through random forest classifier parameter ranking where all the samples were used while building the DT. This analysis helps to classify substrates based on the important parameters and correlates to the reaction outcome.

2. 6. Decision Tree Code

```
dt=fitctree(X,Y);
%Y1 is the external cross-validation set
Y4= predict(dt,Y1);
```

2. 7. Logistic Regression Code

```
lr= fitglm(X,Y,'Distribution','binomial');
%Y1 is the external cross-validation set
Y3= predict(lr,Y1);
```

2. 8. Ensemble Tree Based Random Forest Code

```
rf=fitcensembletree(X,Y);
%Y1 is the external cross-validation set
Y5= predict(rf,Y1);
```

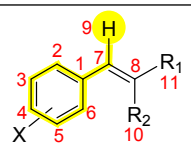
3. "IQ Test" of Trained NN and DT Models

It would be desirable to apply what was learnt through ML models using a set of known examples to predict the regiochemical outcome for new substrates. To this end, an expanded set of 84 substrates (**P1-P84**, as shown in Table S4) is considered whose experimental outcome is not known yet. The dataset consisting of all 63 parameters of 47 known styrenyl family of substrates (**S1-S47**) is generated for the NN and DT model building. The trained models (NN, DT) are then implemented on a new dataset of 63 parameters derived from a totally external set of 84 substrates to predict the regiochemical outcome (Table S5). We considered the average

over 500 different NN models for predicting the outcome for these 84 new substrates. The (1,1):(1,2) difluoro product distribution for the expanded set as predicted by the ML methods is compared with the experimentally known substrates having similar R_1 and R_2 substitutions. For example, (1,1):(1,2) product distribution is 100:0 in the experimentally known substrates with R_1 = COOMe and R_2 = H or Me. NN predicts the same product distribution (100:0) for substrates with similar R_1 and R_2 substitution in the expanded set. However, DT predicts a distribution of 65.4:34.6 for (1,1):(1,2) product (Table S6).

Table S4. Details of the Expanded Substrate Library from the Styrenyl Group of Alkenes (Experimentally Unknown) Considered for External Prdictions

P =



	R1	R2	X		R1	R2	X
P1	$CONH_2$	Me	3-CF_3	**P43**	COOMe	H	3,5-Me
P2	$CONH_2$	Me	3,5-CF_3	**P44**	COOMe	H	3,4- -$(CH)_4$-
P3	$CONH_2$	Me	3,5-Me	**P45**	COOMe	H	2-Br
P4	$CONH_2$	Me	3,4- -(CH)-	**P46**	COOMe	H	2-CF_3
P5	$CONH_2$	Me	2-F, 3-Cl	**P47**	COOMe	H	2-F, 3-Cl
P6	$CONH_2$	Me	2-F, 4-Br	**P48**	COOMe	H	4-CBr_3
P7	CONHMe	Me	4-Br	**P49**	COOMe	H	4-CF_3
P8	CONMe2	Me	4-*t*Bu	**P50**	COOMe	H	4-COOMe
P9	$CONH_2$	Me	4-CBr_3	**P51**	COOMe	H	4-$CONMe_2$
P10	$CONH_2$	Me	4-CF_3	**P52**	COOMe	H	4-OAc
P11	$CONH_2$	Me	4-COOMe	**P53**	COOMe	H	4-OMe
P12	$CONH_2$	Me	4-$CONMe_2$	**P54**	COOMe	Me	3,5-CF_3
P13	$CONH_2$	Me	4-Me	**P55**	COOMe	Me	3,5-Me
P14	$CONH_2$	Me	4-Oac	**P56**	COOMe	Me	3,4-(-$(CH)_4$-)
P15	$CONH_2$	Me	4-Ome	**P57**	COOMe	Me	2-Br
P16	$CONH_2$	Me	4-(4-pyridyl)	**P58**	COOMe	Me	2-CF3
P17	$CONH_2$	Me	4-*t*Bu	**P59**	COOMe	Me	2-F, 3-Cl
P18	Me	H	3,5-CF_3	**P60**	COOMe	Me	2-F, 4-Cl
P19	Me	H	3,4-(-$(CH)_4$-)	**P61**	COOMe	Me	4-CBr_3
P20	Me	H	2-Br	**P62**	COOMe	Me	4-CF_3
P21	Me	H	2-CF3	**P63**	COOMe	Me	4-COOMe
P22	Me	H	2-COOMe	**P64**	COOMe	Me	4-$CONMe_3$
P23	Me	H	2-F, 3-Cl	**P65**	COOMe	Me	4-OAc
P24	Me	H	4-CBr3	**P66**	COOMe	Me	4-OMe
P25	Me	H	4-CF3	**P67**	COOMe	Me	4-*t*Bu
P26	Me	H	4-$CONMe_2$	**P68**	$CONH_2$	H	3-CF3
P27	Me	H	4-OAc	**P69**	$CONH_2$	H	3,5-CF_3
P28	Me	H	4-OMe	**P70**	$CONH_2$	H	3,5-Me
P29	Me	H	4-*t*Bu	**P71**	$CONH_2$	H	3,4-(-$(CH)_4$-)
P30	Me	Me	4-OMe	**P72**	$CONH_2$	H	2-F, 3-Cl
P31	Me	Me	3,5-CF3	**P73**	$CONH_2$	H	2-F, 4-Br

P32	Me	Me	3,5-Me	**P74**	CONHMe	H	4-Br
P33	Me	Me	3,4-(-$(CH)_4$-)	**P75**	$CONMe_2$	H	4-*t*Bu
P34	Me	Me	2-CF_3	**P76**	$CONH_2$	H	4-CBr_3
P35	Me	Me	4-CBr3	**P77**	$CONH_2$	H	4-CF_3
P36	Me	Me	4-CF3	**P78**	$CONH_2$	H	4-COOMe
P37	Me	Me	4-COOMe	**P79**	$CONH_2$	H	4-$CONMe_2$
P38	Me	Me	4-OAc	**P80**	$CONH_2$	H	4-Me
P39	Me	Me	4-OMe	**P81**	$CONH_2$	H	4-OAc
P40	Me	Me	4-*t*Bu	**P82**	$CONH_2$	H	4-OMe
P41	NO_2	Me	H	**P83**	$CONH_2$	H	4-(4-pyridyl)
P42	COOMe	H	3,5-CF_3	**P84**	$CONH_2$	H	4-*t*Bu

Table S5. Predicted Regioselectivity of the Expanded Substrate Library (as Listed in Table S4) using Neural Network (NN) and Decision Tree (DT). Red and Blue Circles Respectively Correspond to the 1,2- and 1,1- Difluoro Regioisomeric Products

Substrate	NN	DT	Substrate	NN	DT
P1	🔴	🔴	**P43**	🔵	🔵
P2	🔴	🔴	**P44**	🔵	🔵
P3	🔴	🔴	**P45**	🔵	🔵
P4	🔵	🔴	**P46**	🔵	🔵
P5	🔴	🔴	**P47**	🔵	🔵
P6	🔴	🔴	**P48**	🔵	🔵
P7	🔴	🔴	**P49**	🔵	🔵
P8	🔴	🔴	**P50**	🔵	🔵
P9	🔴	🔴	**P51**	🔵	🔵
P10	🔴	🔴	**P52**	🔵	🔵
P11	🔴	🔴	**P53**	🔵	🔴
P12	🔵	🔴	**P54**	🔵	🔴
P13	🔴	🔴	**P55**	🔵	🔵
P14	🔴	🔴	**P56**	🔵	🔵
P15	🔵	🔵	**P57**	🔵	🔴
P16	🔴	🔴	**P58**	🔵	🔴
P17	🔴	🔴	**P59**	🔵	🔴
P18	🔵	🔴	**P60**	🔵	🔴
P19	🔵	🔵	**P61**	🔵	🔴
P20	🔵	🔵	**P62**	🔵	🔴
P21	🔴	🔴	**P63**	🔵	🔴
P22	🔴	🔵	**P64**	🔵	🔵
P23	🔵	🔴	**P65**	🔵	🔵
P24	🔵	🔵	**P66**	🔵	🔵
P25	🔵	🔵	**P67**	🔵	🔵
P26	🔵	🔵	**P68**	🔵	🔵
P27	🔴	🔵	**P69**	🔵	🔵
P28	🔵	🔵	**P70**	🔵	🔵
P29	🔵	🔵	**P71**	🔵	🔵

P30	●	●		**P72**	●	●
P31	●	●		**P73**	●	●
P32	●	●		**P74**	●	●
P33	●	●		**P75**	●	●
P34	●	●		**P76**	●	●
P35	●	●		**P77**	●	●
P36	●	●		**P78**	●	●
P37	●	●		**P79**	●	●
P38	●	●		**P80**	●	●
P39	●	●		**P81**	●	●
P40	●	●		**P82**	●	●
P41	●	●		**P83**	●	●
P42	●	●		**P84**	●	●

Table S6. Comparison of the Predicted Product Regioslectivity for New Substrates with the Closely Related Experimental Outcome of the Substrates with Similar R_1 and R_2 Substituents

		block-A		block-B		block-C		block-D	
	substituents	R_1 = $CONH_2$ R_2 = Me or iPr		R_1 = COOMe R_2 = H or Me		R1 = Me R2 = H or Me		R_1 = $CONH_2$ R_2 = H	
Entry	Regio-	1,1	1,2	1,1	1,2	1,1	1,2	1,1	1,2
1	Expt. Set	0	100	100	0	14.3	85.7	100	0
2	NN	17.7	82.3	100	0	41.7	58.3	100	0
3	DT	5.9	94.1	65.4	34.6	37.5	62.5	100	0

The data shown in this table should be read as follows. Any alkene in block-A (R_1 = $CONH_2$, R_2 = Me or iPr substitution pattern), only 1,2-difluro product is formed under hypercoordinate iodine catalyzed difluorination reaction (number of experimentally known examples of this type are 3). In the case of alkenes listed in block-B (12) and block-D (8), only 1,1-difluoro product is formed in the experimentally known examples. The numbers shown in parentheses are the number of experimentally known examples. Some of the alkenes (14.3 %) in block-C gives 1,1-regioisomer whereas some others (85.7 %) give 1,2-regioisomer. The total number of experimentally known examples, with R1= Me; R2=Me/H substutions, are 12.

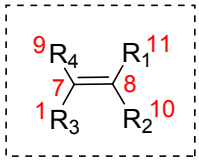
4. Diverse Set of Alkenes

Further, a more general and diverse set of alkenes (**S1-S65**) are considered to demonstrate the general applicability of the trained NN model. Here, all four substituents (R_1, R_2, R_3 and R_4) of the alkene are varied (Figs. 1b and 3a). For this diverse set of alkenes, we have collected parameters in two different ways; (a) important parameters from the alkene carbons (C7 and C8) as well as that from the substituents R_1, R_2, R_3 and R_4. The total number of such parameters in this set turns out to be 41 (Table S7), (b) all geometric and electronic parameters only from the alkene carbons leading to a total of 11 parameters (AD7-8, v7-8, I7-8, NPA7, NPA8, NMR7, NMR8, fp7, fp8, fm7 and fm8). The NN model built using these latter set of parameters would be more general and widely applicable to any olefin. The NN model is built (Table S8) following identical procedure described above except that an 8-fold cross validation is used here due to the presence of different number of samples.

4.1. Parameter Set for Alkenes (S1-S66)

Table S7. Parameter Set for Alkenes **S1-S66**

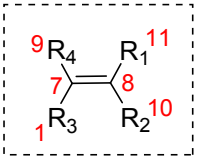
a) 41 parameters from alkene carbons and substituents



Geometric Parameters	Atoms or substituents
Sterimol: B1	R_1, R_2, R_3, R_4
B5	R_1, R_2, R_3, R_4
L	R_1, R_2, R_3, R_4
Distance between atoms (AD)	1-7, 7-8, 7-9, 8-10, 8-11
Bond angle (A)	1-7-9, 1-7-8, 8-7-9, 7-8-11, 7-8-10, 10-8-11
Dihedral angle (D)	1-7-8-11, 9-7-8-11, 1-7-8-10, 9-7-8-10

Electronic Parameters	Atoms
NPA charge (NPA)	7, 8
NMR chemical shift (NMR)	7, 8
Vibrational frequency (v)	7-8
Vibrational intensity (I)	7-8
Electrophilic Fukui index (fp)	7, 8
Nucleophilic Fukui index (fm)	7, 8

b) 11 alkene-only parameters



Geometric Parameters	Atoms
Distance between atoms (AD)	7-8
Electronic Parameters	**Atoms**
NPA charge (NPA)	7, 8
NMR chemical shift (NMR)	7, 8

Electronic Parameters	Atoms
Vibrational frequency (v)	7-8
Vibrational intensity (I)	7-8
Electrophilic Fukui index (fp)	7, 8
Nucleophilic Fukui index (fm)	7, 8

4.2. Neural Network (NN) Modeling for All Alkenes (S1-S66)

Table S8. Different Model Building and Test Sets for Substrates **S1-S66** using 11 Parameters for Eight-fold Cross Validation of NN with the Corresponding Predicted Outcome

Neural Network Model No.	Model building set	Test set	No. of correct Prediction	No. of incorrect Prediction
1	**S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S66**	**S1, S2, S3, S12, S4, S5, S6, S7, S47**	6	3
2	**S1, S2, S3, S12, S4, S5, S6, S7, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S13, S14, S15, S16, S8, S9, S10, S11**	8	0
3	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S17, S18, S19, S20, S23, S24, S25, S26**	7	1
4	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S21, S22, S43, S48, S27, S28, S29, S30**	8	0
5	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S49, S50, S51, S52, S31, S32, S33, S34**	8	0
6	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29,**	**S53, S54, S55, S56, S35, S36, S37, S38**	8	0

	S30, S49, S50, S51, S52, S31, S32, S33, S34, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66			
7	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S57, S58, S59, S60, S65, S39, S40, S41, S42**	7	2
8	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S47**	**S61, S62, S63, S64, S44, S45, S46, S66**	7	1

Table S9. Comparison of Experimental and Predicted Regioselectivity Obtained Using Neural Network Models for Alkenes **S1-S66** Using 11 Alkene-only Parameters. Blue and Red Circles Respectively Correspond to the 1,1- and 1,2-Difluorinated Regioisomeric Products

substrate	expt.	pred.	substrate	expt.	pred.	substrate	expt.	pred.
S1	🔴	🔵	**S23**	🔵	🔴	**S45**	🔵	🔵
S2	🔴	🔵	**S24**	🔵	🔵	**S46**	🔵	🔵
S3	🔴	🔵	**S25**	🔵	🔵	**S47**	🔵	🔵
S4	🔵	🔵	**S26**	🔵	🔵	**S48**	🔴	🔴
S5	🔵	🔵	**S27**	🔵	🔵	**S49**	🔴	🔴
S6	🔵	🔵	**S28**	🔵	🔵	**S50**	🔴	🔴
S7	🔵	🔵	**S29**	🔵	🔵	**S51**	🔴	🔴
S8	🔵	🔵	**S30**	🔵	🔵	**S52**	🔴	🔴
S9	🔵	🔵	**S31**	🔵	🔵	**S53**	🔴	🔴
S10	🔵	🔵	**S32**	🔵	🔵	**S54**	🔴	🔴
S11	🔵	🔵	**S33**	🔵	🔵	**S55**	🔴	🔴
S12	🔴	🔴	**S34**	🔵	🔵	**S56**	🔴	🔴
S13	🔴	🔴	**S35**	🔵	🔵	**S57**	🔴	🔴
S14	🔴	🔴	**S36**	🔵	🔵	**S58**	🔴	🔴
S15	🔴	🔴	**S37**	🔵	🔵	**S59**	🔴	🔴
S16	🔴	🔴	**S38**	🔵	🔵	**S60**	🔴	🔴
S17	🔴	🔴	**S39**	🔵	🔵	**S61**	🔴	🔴
S18	🔴	🔴	**S40**	🔵	🔵	**S62**	🔴	🔴
S19	🔴	🔴	**S41**	🔵	🔵	**S63**	🔴	🔴
S20	🔴	🔴	**S42**	🔵	🔴	**S64**	🔴	🔵

S21	🔴	🔴		**S43**	🔴	🔴		**S65**	🔴	🔵
S22	🔴	🔴		**S44**	🔵	🔵		**S66**	🔵	🔵

Table S10. Comparison of Experimental and Predicted Regioselectivity Obtained Using Neural Network Models for Alkenes **S1-S66** Using 41 Parameters. Blue and Red Circles Respectively Correspond to the 1,1- and 1,2-Difluorinated Regioisomeric Products

substrate	expt.	pred.		substrate	expt.	pred.		substrate	expt.	pred.
S1	🔴	🔵		**S23**	🔵	🔴		**S45**	🔵	🔵
S2	🔴	🔵		**S24**	🔵	🔵		**S46**	🔵	🔵
S3	🔴	🔴		**S25**	🔵	🔵		**S47**	🔵	🔵
S4	🔵	🔵		**S26**	🔵	🔵		**S48**	🔴	🔴
S5	🔵	🔵		**S27**	🔵	🔵		**S49**	🔴	🔴
S6	🔵	🔵		**S28**	🔵	🔵		**S50**	🔴	🔴
S7	🔵	🔵		**S29**	🔵	🔵		**S51**	🔴	🔴
S8	🔵	🔵		**S30**	🔵	🔵		**S52**	🔴	🔴
S9	🔵	🔵		**S31**	🔵	🔵		**S53**	🔴	🔴
S10	🔵	🔵		**S32**	🔵	🔵		**S54**	🔴	🔴
S11	🔵	🔵		**S33**	🔵	🔵		**S55**	🔴	🔴
S12	🔴	🔵		**S34**	🔵	🔵		**S56**	🔴	🔴
S13	🔴	🔴		**S35**	🔵	🔵		**S57**	🔴	🔴
S14	🔴	🔴		**S36**	🔵	🔵		**S58**	🔴	🔴
S15	🔴	🔴		**S37**	🔵	🔴		**S59**	🔴	🔴
S16	🔴	🔴		**S38**	🔵	🔵		**S60**	🔴	🔴
S17	🔴	🔴		**S39**	🔵	🔵		**S61**	🔴	🔵
S18	🔴	🔴		**S40**	🔵	🔵		**S62**	🔴	🔵
S19	🔴	🔴		**S41**	🔵	🔵		**S63**	🔴	🔵
S20	🔴	🔴		**S42**	🔵	🔵		**S64**	🔴	🔴
S21	🔴	🔴		**S43**	🔴	🔴		**S65**	🔴	🔵
S22	🔴	🔴		**S44**	🔵	🔵		**S66**	🔵	🔴

Table S11. Different Model Building and Test Sets formed from Substrates **S1-S66** Using 41 parameters for the Eight-fold Cross Validation of NN with the Corresponding Predicted Outcome

Neural Network Model No.	Model building set	Test set	No. of correct Prediction	No. of incorrect Prediction
1	**S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46,**	**S1, S2, S3, S12, S4, S5, S6, S7, S47**	6	3

	S66			
2	**S1, S2, S3, S12, S4, S5, S6, S7, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S13, S14, S15, S16, S8, S9, S10, S11**	8	0
3	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S17, S18, S19, S20, S23, S24, S25, S26**	7	1
4	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S21, S22, S43, S48, S27, S28, S29, S30**	8	0
5	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S49, S50, S51, S52, S31, S32, S33, S34**	8	0
6	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S57, S58, S59, S60, S65, S39, S40, S41, S42, S61, S62, S63, S64, S44, S45, S46, S47, S66**	**S53, S54, S55, S56, S35, S36, S37, S38**	7	1
7	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27,**	**S57, S58, S59, S60, S65, S39, S40, S41, S42**	8	1

	S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S61, S62, S63, S64, S44, S45, S46, S47, S66			
8	**S1, S2, S3, S12, S4, S5, S6, S7, S13, S14, S15, S16, S8, S9, S10, S11, S17, S18, S19, S20, S23, S24, S25, S26, S21, S22, S43, S48, S27, S28, S29, S30, S49, S50, S51, S52, S31, S32, S33, S34, S53, S54, S55, S56, S35, S36, S37, S38, S57, S58, S59, S60, S65, S39, S40, S41, S42, S47**	**S61, S62, S63, S64, S44, S45, S46, S66**	4	4

Table S12. Comparison between the Percentage Accuracy of Neural Network, Decision Tree, Logistic Regression and Ensemble Tree Based Random Forest Models Obtained Using 11 Parameters for Experimentally Known Substrates (**S1-S66**) (same test sets as shown in Table S11 are used for NN, DT and LR)

Neural Network	Decision Tree	Logistic Regression	Random Forest
90	80	80	83

5. Comparison of Different Models

Table S13. Comparison of the Percentage Accuracy of Predictions Obtained Using Different Datasets for Different Models [a]

entry No.	Dataset	Neural Network	Decision Tree	Logistic Regression	Random Forest
1	47x63	92	77	62	77
2	47x11	89	81	81	89
3	66x41	85	81	74	77
4	66x11	90	80	80	83

[a] Logistic Regression and Random Forest perform better with low dimensional data (entries 2 and 4). NN performs well with both low and high dimensional data.

6. Check for Covariance

Table S14. The Correlation Coefficients Calculated for Angles, Distances and Dihedrals

	A (6-1-7)	*A (2-1-7)*	*A (1-7-9)*	*A (1-7-8)*	*A (8-7-9)*	*A (7-8-11)*	*A (7-8-10)*	*A (10-8-11)*	*D (6-1-7-8)*	*D(2-1-7-9)*	*D (2-1-7-8)*	*D (5-6-1-7)*	*D (3-2-1-7)*	*D (1-7-8-11)*	*D (9-7-8-11)*	*D (1-7-8-10)*	*D (9-7-8-10)*	*L (7-8)*	*L (7-1)*	*L (6-8)*	*L (2-7)*	*L (7-9)*
A(6-1-7)	1.0																					
A(2-1-7)	-0.8	1.0																				
A(1-7-9)	-0.4	0.4	1.0																			
A(1-7-8)	0.4	-0.6	-0.5	1.0																		
A(8-7-9)	-0.2	0.4	-0.1	-0.8	1.0																	
A(7-8-11)	-0.3	0.4	0.0	-0.7	0.9	1.0																
A(7-8-10)	0.3	-0.4	-0.3	0.8	-0.7	-0.9	1.0															
A(10-8-11)	0.2	-0.3	0.6	0.2	-0.6	-0.6	0.1	1.0														
D(6-1-7-8)	-0.4	0.4	-0.2	0.2	-0.1	-0.2	0.4	-0.3	1.0													
D(2-1-7-9)	-0.4	0.4	-0.2	0.2	-0.1	-0.1	0.4	-0.3	1.0	1.0												
D(2-1-7-8)	0.4	-0.4	0.2	-0.2	0.1	0.1	-0.4	0.3	-1.0	-1.0	1.0											
D(5-6-1-7)	-0.2	-0.2	-0.1	0.3	-0.3	-0.1	0.1	0.1	-0.3	-0.3	0.3	1.0										
D(3-2-1-7)	0.1	-0.5	-0.3	0.6	-0.5	-0.3	0.3	0.1	-0.2	-0.2	0.2	0.8	1.0									
D(1-7-8-11)	0.2	-0.4	0.0	-0.1	0.1	0.3	-0.4	0.1	-0.7	-0.7	0.7	0.6	0.4	1.0								
D(9-7-8-11)	0.0	0.1	-0.3	0.4	-0.2	-0.5	0.7	-0.2	0.8	0.7	-0.7	-0.4	-0.3	-0.9	1.0							
D(1-7-8-10)	-0.1	0.2	-0.1	0.3	-0.2	-0.5	0.7	-0.1	0.7	0.7	-0.7	-0.4	-0.2	-0.8	0.9	1.0						
D(9-7-8-10)	0.0	-0.1	0.2	-0.4	0.3	0.5	-0.7	0.1	-0.7	-0.6	0.7	0.4	0.2	0.7	-0.9	-1.0	1.0					
AD(7-8)	0.2	-0.3	-0.4	0.7	-0.6	-0.7	0.9	0.0	0.5	0.5	-0.5	0.0	0.2	-0.5	0.7	0.7	-0.8	1.0				
AD(7-1)	-0.4	0.4	-0.4	-0.1	0.4	0.2	0.1	-0.6	0.6	0.6	-0.6	-0.3	-0.3	-0.4	0.5	0.5	-0.5	0.1	1.0			
AD(6-8)	-0.3	0.1	-0.4	0.5	-0.3	-0.2	0.4	-0.2	0.9	0.9	-0.9	-0.1	0.1	-0.5	0.6	0.5	-0.5	0.5	0.4	1.0		
AD(2-7)	-0.8	1.0	0.3	-0.6	0.4	0.4	-0.3	-0.4	0.5	0.5	-0.5	-0.2	-0.5	-0.4	0.2	0.3	-0.2	-0.2	0.6	0.2	1.0	
AD(7-9)	0.2	-0.5	-0.5	0.5	-0.2	0.0	0.1	-0.2	0.0	0.0	0.0	0.4	0.6	0.3	-0.2	-0.3	0.2	0.0	0.0	0.3	-0.4	1.0

Covariance matrix has been constructed to find how much angles, distances and dihedrals vary together and the corresponding correlation coefficients are tablulated in Table S14).[2] Parameters with a correlation coefficient ≥ (±) 0.9 imply that they are highly correlated (Table S15). Based on this analysis, four strongly dependent parameters (A(2-17), D(6-1-7-8), D(2-1-7-9), and D(1-7-8-10)) are removed from each of the pairs to avoid the redundancy and a new NN model is built. Same model building and test sets are used as given in Table S1. Accuracy of the new NN model is found to be 92% which is same as the previous model.

Table S15. Parameters with a Correlation Coefficient ≥ (±) 0.9

parameters	correlation coefficient
L(2-7) – A(2-1-7)	1.0
D(2-1-7-9) – D(6-1-7-8)	1.0
D (2-1-7-8) – D(6-1-7-8)	-1.0
D (2-1-7-8-) – D(2-1-7-9)	-1.0
AD(6-8) – D(6-1-7-8)	0.9
AD(6-8) – D(2-1-7-9)	0.9
AD(6-8) – D(2-1-7-8)	-0.9
D(9-7-8-10) – D(1-7-8-10)	-1.0

7. Check for Overfitting: Least Absolute Shrinkage and Selection Operator (LASSO) Method

In an additional effort, new NN models were built with parameters selected through the application of least absolute shrinkage and selection operator (LASSO) method,[3] which is a recommended method to prevent overfitting.

Initially, we employed LASSO on 63 parameter set of 47 styrenyl alkene substrates, to identify that 13 parameters are more important (Tablse S16). Similarly, application of LASSO on the 11 alkene-only parameters of 66 general alkene set resulted in 8 important parameters. New NN model is built using these selected parameters following the same approach shown in Tables S1 and S8 for styrenyl and general alkene sets respectively. Similar predicted accuracies in both cases (92 and 94 for styrenyl alkenes, 90 and 86 for general alkene with and without LASSO) which implies that there is no overfitting in the previous NN models.

2) Rice, J. A. *Mathematical Statistics and Data Analysis*; Thomson Higher Education, 10 Davis Drive, Belmont, USA 2007.

3) Tibshirani, R. Regression Shrinkage and Selection via the Lasso. *J. R. Stat. Soc. Ser. B* **1996**, *58*, 267−288.

Table S16. Comparison of Percentage Accuracy of Predictions Using Different NN Models

(**a**) Styrenyl alkene (**S1-S47**) set
13 parameters selected through LASSO: v(7-1), NPA8, NMR5, NMR6, NMR7, D(6-1-7-8), L(7-1), L(2-7), fp(7), fm(7), fp(8), LR1, LR3 Accuracy of previous NN model formed with 63 parameters: 92% Accuracy of new NN model formed with 13 parameters: 94%
(**b**) General alkene (**S1-S66**) set
8 parameters selected through LASSO: I(7-8), NMR7, NMR8, AD(7-8), fp(7), fm(7), fp(8), fm(8) Accuracy of previous NN model formed with 11 parameters: 90% Accuracy of new NN model formed with 8 parameters: 86%

8. Details of the Dataset

Dataset used in this study are given in Tables S17-S20 for the experimentally known substrates (**S1-S66**) (Figure S1) and experimentally unknown expanded set (**P1**-**P84**) (Table S4).

Table S17. Dataset for Experimentally Known Alkenes (**S1-S47**)

	ν(7-1)	**I(7-1)**	**ν(7-8)**	**I(7-8)**	**ν(7-9)**	**I(7-9)**	**NPA1**	**NPA2**	**NPA3**
S1	1548.8700	28.4900	1740.8700	154.8200	3204.2500	0.1700	-0.0896	-0.2280	-0.2529
S2	1255.7900	29.5900	1742.9100	143.0200	3197.8700	0.0000	-0.0854	-0.2107	-0.2589
S3	1255.4200	3.4600	1745.9700	61.6900	3172.2100	20.1500	-0.0870	-0.2366	-0.2508
S4	1289.5000	136.0300	1740.9300	271.1000	3205.6100	3.4200	-0.0988	-0.2223	-0.2535
S5	1285.5700	121.7700	1743.2500	252.5600	3208.3200	7.0300	-0.0959	-0.2062	-0.2625
S6	1287.1900	163.1300	1741.0100	242.1100	3207.3700	0.2500	-0.1137	-0.2044	-0.3239
S7	1276.1100	150.4300	1740.0500	323.3300	3185.1200	2.5100	-0.1071	-0.2144	-0.2493
S8	1287.9900	146.7300	1738.5900	311.4500	3204.9300	5.8300	-0.1088	-0.2143	-0.2530
S9	1299.8000	147.7300	1745.8700	294.6000	3186.6300	1.6200	-0.0927	-0.2207	-0.0370
S10	1283.0800	92.2800	1739.0500	230.6800	3219.6200	3.9600	-0.0930	-0.0079	-0.2516
S11	1289.4500	154.4900	1743.4400	263.5800	3191.3800	1.6500	-0.0951	-0.2128	-0.2447
S12	1238.8400	44.6200	1741.3600	10.8000	3192.7100	10.6400	-0.0944	-0.2211	-0.2778
S13	1266.7100	2.8900	1765.2800	38.6100	3167.0100	27.8500	-0.0744	-0.2391	-0.2536
S14	1272.3500	49.1700	1758.7500	83.3900	3168.2500	25.6400	-0.0410	-0.2366	-0.2024
S15	1272.8800	3.0300	1745.3300	123.7700	3169.2400	20.1600	-0.0322	-0.2290	-0.2225
S16	1271.2400	1.9800	1761.1700	62.9200	3169.5400	31.6700	-0.0648	-0.2291	-0.2297
S17	1272.6800	4.9800	1736.1200	33.5000	3163.5900	32.5000	-0.0733	-0.2306	-0.2382
S18	1336.9600	14.0700	1767.4000	161.6300	3190.6200	28.2800	-0.0481	-0.1822	0.0578
S19	1321.1500	19.0900	1757.2500	27.8600	3204.2200	9.6900	-0.0453	0.0607	-0.2249
S20	1321.3100	22.2300	1752.5100	21.4600	3217.0600	9.7500	-0.0290	0.0647	-0.1844
S21	1250.8900	9.9000	1764.5400	72.4300	3205.7500	11.0400	-0.0244	-0.2117	-0.2002
S22	1263.0700	5.0200	1762.5500	50.4800	3194.7900	11.6400	-0.0813	-0.1134	-0.2602
S23	1256.6800	5.4500	1759.1500	81.5700	3187.5500	18.3200	-0.0379	-0.2311	-0.2190
S24	1551.8500	30.6900	1739.0400	361.5600	3198.5900	1.5200	-0.1036	-0.2187	-0.2537
S25	1260.2200	608.6200	1742.2500	341.4500	3210.4600	0.0600	-0.1007	-0.2028	-0.2625
S26	1261.3800	582.5700	1742.9800	342.8100	3210.5200	2.9900	-0.0991	-0.2026	-0.2592
S27	1253.9200	219.4500	1743.6600	130.8000	3209.8700	1.0800	-0.0936	-0.2256	-0.2529

S28	1254.9300	212.6200	1745.8100	119.8300	3206.9200	0.3000	-0.0909	-0.2086	-0.2621
S29	1255.4500	189.5400	1746.5500	119.8800	3203.4900	0.3500	-0.0893	-0.2084	-0.2588
S30	1338.1700	378.3800	1743.3500	127.3000	3208.4600	1.4000	-0.1088	-0.2071	-0.3225
S31	1253.3300	177.1200	1740.3100	164.8000	3206.7200	4.9500	-0.1041	-0.2182	-0.2488
S32	1205.8700	31.4000	1745.4700	134.6100	3191.6900	4.0800	-0.0872	-0.2248	-0.0363
S33	1248.4000	50.9900	1742.6900	129.1900	3199.3900	0.3900	-0.1000	-0.2120	-0.2791
S34	1244.5300	151.9600	1748.1400	129.7700	3196.1400	0.4700	-0.0845	-0.2280	-0.1209
S35	1220.8400	19.6700	1744.4300	149.1700	3202.7300	1.2400	-0.1665	0.4664	-0.3209
S36	1258.2900	14.3600	1748.1000	20.7000	3199.6900	4.3600	-0.0888	-0.2305	-0.2518
S37	1255.9100	267.7100	1745.7800	96.9400	3186.2200	0.2100	-0.0897	-0.2303	-0.2516
S38	1256.7700	255.4800	1746.2300	95.1500	3201.4600	0.2000	-0.0897	-0.2299	-0.2517
S39	1253.0100	261.0900	1739.7300	167.2400	3205.2900	0.1400	-0.0976	-0.2212	-0.2521
S40	1250.3400	271.5100	1732.0600	202.1300	3187.1800	0.2500	-0.1083	-0.2138	-0.2480
S41	1550.8700	4.2900	1739.9700	247.4000	3199.0100	0.5200	-0.0977	-0.2231	-0.2535
S42	1311.4300	3.3400	1727.6800	291.1100	3189.7000	1.6200	-0.0983	-0.2226	-0.2537
S43	1560.6100	27.3900	1753.8000	87.3400	3167.0900	19.1200	-0.0376	-0.2336	-0.1947
S44	1324.5500	9.5200	1738.3200	357.9100	3201.3600	0.6200	-0.1027	-0.2194	-0.2538
S45	1238.3500	12.1300	1744.5800	46.0800	3203.9200	25.2300	-0.0915	-0.2283	-0.2529
S46	1245.9300	12.5500	1761.1800	2.3700	3173.6000	14.8200	-0.0856	-0.2340	-0.2524
S47	1244.2000	3.5200	1742.7900	9.2000	3170.7600	16.8100	-0.0897	-0.2349	-0.2530

	NPA4	**NPA5**	**NPA6**	**NPA7**	**NPA8**	**NPA9**	**NMR1**	**NMR2**	**NMR3**
S1	-0.2507	-0.2522	-0.2375	-0.1860	-0.1188	0.2673	47.5074	53.6883	56.1781
S2	-0.1335	-0.2581	-0.2204	-0.1901	-0.1126	0.2699	47.7499	51.7540	53.0080
S3	-0.2544	-0.2534	-0.2347	-0.2277	-0.0855	0.2554	47.6131	56.2626	56.6283
S4	-0.2447	-0.2522	-0.2233	-0.1724	-0.3397	0.2613	50.3179	51.4335	55.6449
S5	-0.0533	-0.2613	-0.2066	-0.1761	-0.3334	0.2638	50.8843	50.1502	55.8899
S6	0.4394	-0.3208	-0.2047	-0.1721	-0.3421	0.2625	54.4777	49.0282	70.0186
S7	-0.0246	-0.2477	-0.2157	-0.1708	-0.3443	0.2607	52.6043	51.0974	55.2569
S8	-0.0262	-0.2472	-0.2166	-0.1703	-0.3452	0.2607	53.2860	51.4513	54.9477
S9	-0.2399	-0.2464	-0.2328	-0.1713	-0.3406	0.2608	50.3045	50.5370	43.5538
S10	-0.2400	-0.2620	-0.2205	-0.1750	-0.3380	0.2620	50.3808	44.6533	53.6080
S11	0.1468	-0.2436	-0.2134	-0.1750	-0.3359	0.2628	51.1959	50.7912	58.8267
S12	0.2980	-0.2767	-0.2191	-0.2519	-0.4342	0.2494	50.2423	53.4839	61.5942
S13	-0.2612	-0.2526	-0.2462	-0.2769	0.0155	0.2462	45.3562	56.0175	56.5244
S14	-0.1944	-0.2062	-0.2470	-0.2850	0.0310	0.2505	37.9738	55.0884	58.5080
S15	0.0329	-0.2199	-0.2376	-0.2891	0.0393	0.2532	35.7654	54.3601	61.1257
S16	-0.0792	-0.2284	-0.2371	-0.2805	0.0227	0.2479	43.9508	54.2123	57.5937
S17	-0.0803	-0.2396	-0.2387	-0.2777	0.0175	0.2464	45.2547	55.1272	57.0454
S18	-0.2112	0.0579	-0.1771	-0.2813	-0.1607	0.2543	41.4608	54.4347	36.6086
S19	-0.2493	-0.2168	-0.2301	-0.2716	-0.1822	0.2594	49.0266	37.7853	59.2436
S20	-0.1539	-0.1951	-0.2246	-0.2761	-0.1724	0.2623	45.5713	37.2294	57.4625
S21	-0.3481	-0.2064	0.0756	-0.2857	-0.1546	0.2622	44.0431	52.2450	52.7685
S22	-0.2449	-0.2505	-0.2283	-0.2825	0.0259	0.2529	45.2860	48.5559	52.4436
S23	0.0327	-0.2208	-0.2289	-0.2789	-0.1641	0.2487	38.3991	54.5650	60.3488
S24	-0.2403	-0.2518	-0.2192	-0.1533	-0.3584	0.2624	50.7724	51.0397	55.6666
S25	-0.0504	-0.2607	-0.2026	-0.1572	-0.3523	0.2648	51.4145	49.7356	55.9256
S26	-0.1282	-0.2575	-0.2025	-0.1577	-0.3514	0.2649	51.0106	49.6324	52.4330
S27	-0.2475	-0.2519	-0.2337	-0.1705	-0.1349	0.2672	48.1853	53.3819	56.1096
S28	-0.0548	-0.2610	-0.2171	-0.1746	-0.1291	0.2695	48.8757	51.6574	56.2473
S29	-0.1317	-0.2577	-0.2167	-0.1751	-0.1285	0.2697	48.4677	51.4969	52.9308

S30	0.4368	-0.3218	-0.2155	-0.1705	-0.1358	0.2679	52.5997	50.5781	69.9914
S31	-0.0289	-0.2505	-0.2257	-0.1683	-0.1389	0.2660	51.2950	53.1679	55.2739
S32	-0.2426	-0.2459	-0.2434	-0.1689	-0.1361	0.2668	48.2149	53.0396	44.1439
S33	0.3050	-0.2787	-0.2206	-0.1714	-0.1341	0.2678	51.0419	52.0117	61.3265
S34	-0.0416	-0.2312	-0.2259	-0.1738	-0.1294	0.2696	48.5320	50.0562	46.9866
S35	-0.0121	-0.2670	-0.2100	-0.1783	-0.1301	0.2728	64.0539	25.9737	69.9487
S36	-0.2508	-0.2507	-0.2390	-0.1743	-0.1309	0.2694	47.4080	55.2082	56.0129
S37	-0.2513	-0.2509	-0.2392	-0.1651	-0.1317	0.2688	47.4397	55.1691	55.9640
S38	-0.2511	-0.2510	-0.2389	-0.1667	-0.1299	0.2683	47.5034	54.8175	56.1089
S39	-0.2426	-0.2500	-0.2286	-0.1487	-0.1465	0.2706	49.2707	52.3273	55.4126
S40	-0.0236	-0.2488	-0.2199	-0.1469	-0.1509	0.2694	52.5176	52.2943	54.4697
S41	-0.2456	-0.2522	-0.2241	-0.1763	-0.3325	0.2609	50.1570	51.6593	55.7507
S42	-0.2452	-0.2523	-0.2239	-0.1667	-0.3386	0.2615	49.5828	51.5917	55.6577
S43	-0.2054	-0.1929	-0.2421	-0.2794	0.0302	0.2522	38.8208	54.7668	50.9880
S44	-0.2411	-0.2519	-0.2198	-0.1568	-0.3536	0.2619	50.6707	51.1501	55.7206
S45	-0.2490	-0.2510	-0.2283	-0.1954	-0.2374	0.2475	49.0442	52.5694	55.5975
S46	-0.2544	-0.2509	-0.2343	-0.2363	-0.2252	0.2496	48.0596	55.3936	55.7538
S47	-0.2550	-0.2516	-0.2331	-0.2514	-0.4355	0.2482	47.8350	54.5994	56.0607

	NMR4	**NMR5**	**NMR6**	**NMR7**	**NMR8**	**NMR9**	**A(6-1-7)**	**A(2-1-7)**	**A(1-7-9)**
S1	56.4062	57.0727	55.0338	44.7883	53.5902	23.2733	122.8606	118.6113	115.8108
S2	48.6165	53.8002	53.4007	46.3820	52.3521	23.3198	122.9969	118.6519	115.7094
S3	56.8293	56.4200	55.7311	56.4018	33.9129	24.5389	118.8952	122.5829	115.0897
S4	54.0890	56.0340	60.2456	40.3849	65.8062	23.5637	122.8774	118.5103	116.1394
S5	43.9817	56.0701	58.7114	41.9504	64.7798	23.6318	122.9871	118.5420	116.0996
S6	23.1080	69.6883	57.6103	41.5276	66.4505	23.6079	122.9267	118.5101	116.0699
S7	36.5437	53.6590	60.5918	40.2477	66.8507	23.5617	123.1833	118.6441	116.0420
S8	41.3539	55.0675	60.4237	40.4526	67.0970	23.6284	123.1317	118.7413	116.0860
S9	53.2491	56.1585	63.4653	40.2771	66.1387	23.6127	123.0036	118.2594	116.1252
S10	54.6231	58.4974	58.8606	42.5815	63.9477	22.9908	120.7503	119.9197	117.5968
S11	50.9922	58.9760	59.5052	41.1413	64.9187	23.4717	123.0726	118.5585	116.0271
S12	35.7518	64.2908	60.8233	47.9183	71.3503	24.4233	122.9541	118.7616	114.5712
S13	58.9838	57.3937	55.4299	58.4550	45.0928	24.7084	122.6994	119.1561	114.7360
S14	50.9657	50.4668	54.9984	59.0403	40.5600	24.6378	122.7636	118.7300	114.6003
S15	40.4459	61.8450	54.6468	59.9354	38.1176	24.6115	122.9174	118.6257	114.5461
S16	51.2351	58.0694	54.4288	59.1404	42.9092	24.6115	123.2006	118.9896	114.5235
S17	49.2357	57.7872	55.8494	58.7373	44.4079	24.6883	123.1115	118.9851	114.5377
S18	68.7618	36.5082	60.4939	57.2522	48.8050	24.4903	123.2722	118.6116	114.7840
S19	56.6254	49.0853	54.6989	55.6155	50.5807	24.3752	120.1057	124.2086	117.3521
S20	50.7771	52.6561	54.5382	56.2127	47.8959	24.3243	120.1193	124.3280	117.4222
S21	43.2037	60.1360	34.2139	60.5616	41.3374	24.5471	125.0142	118.5944	115.4275
S22	57.0664	57.9064	51.7599	59.8324	43.2643	24.7292	121.3726	122.0847	115.4646
S23	39.8606	60.8455	61.5796	55.1906	49.7559	24.6950	123.1809	118.3929	115.0087
S24	53.0048	55.8410	59.5743	35.6235	68.9263	23.3449	122.6530	118.5963	115.9856
S25	42.8334	55.9083	58.0797	37.2876	67.8733	23.4221	122.8165	118.5517	115.9552
S26	45.3405	52.5771	58.0165	37.2872	67.7848	23.4302	122.8591	118.5563	115.9339
S27	55.6314	56.9182	54.7573	40.9280	55.0687	23.1403	122.8344	118.5388	115.5811
S28	45.1225	57.0579	53.2785	42.5887	53.9033	23.2029	122.9551	118.5606	115.5217
S29	47.7509	53.6394	53.1394	42.6498	53.7020	23.1952	122.9515	118.6029	115.4903

S30	24.1139	70.8883	52.3523	41.9645	55.4378	23.1771	122.9834	118.4629	115.5136
S31	42.9380	56.0203	54.9355	40.9699	56.0473	23.1915	123.3006	118.6027	115.4563
S32	54.8064	56.9443	57.9121	40.7487	55.3838	23.1895	122.8997	118.3357	115.6055
S33	34.8772	65.4422	53.2578	41.9088	54.9922	23.1571	123.1560	118.3847	115.4227
S34	43.8020	53.1669	55.8262	42.8206	54.0020	23.2721	123.5688	118.1567	115.5714
S35	39.6523	60.9360	53.1223	48.4925	54.4445	23.0328	124.4599	119.2553	116.0274
S36	56.2261	56.5280	55.5235	42.4086	47.5833	23.1906	122.6844	118.5908	114.9475
S37	55.9469	56.5438	55.6534	40.2626	48.6924	23.1636	122.4563	118.7854	115.7622
S38	56.0992	56.5552	55.6465	40.4986	48.7034	23.1545	122.7460	118.5138	115.5509
S39	54.4297	55.9393	56.1783	37.5665	56.2077	23.1413	124.0695	117.4199	114.8677
S40	41.4970	55.1088	56.0984	37.7469	57.1033	23.2100	124.4615	117.5929	114.8266
S41	54.2588	56.1039	60.3931	41.9782	65.2494	23.5803	122.7808	118.6343	116.1793
S42	54.1622	55.9319	60.3111	39.0623	69.1466	23.5162	122.9672	118.4690	116.1006
S43	75.0370	51.3941	54.7129	61.6017	33.0138	24.7299	122.7501	118.8171	114.3862
S44	53.1555	55.8978	59.5751	36.3665	67.1354	23.3837	122.6704	118.6078	116.0320
S45	55.2191	55.8619	61.3590	50.9412	59.7409	23.5376	123.3304	118.2943	114.3634
S46	56.1331	56.0080	60.9152	47.4137	57.9184	24.4363	122.4422	119.0678	115.5417
S47	56.5352	56.2138	62.4768	47.0747	71.2234	24.4356	122.7984	118.8300	114.7163

	A(1-7-8)	**A(8-7-9)**	**A(7-8-11)**	**A(7-8-10)**	**A(10-8-11)**	**D(6-1-7-8)**	**D(2-1-7-9)**	**D(2-1-7-8)**	**D(5-6-1-7)**
S1	128.3145	115.8586	115.3722	125.8900	118.7185	37.2148	33.2290	145.2364	179.1259
S2	128.2708	116.0073	115.2840	125.9617	118.7351	36.6819	32.6061	146.0469	178.6890
S3	127.7942	117.1160	122.2203	122.8442	114.9350	149.1056	147.4308	32.6295	179.8384
S4	127.2696	116.5910	119.3852	122.5669	118.0478	0.0789	0.0721	179.9190	179.9947
S5	127.2058	116.6947	119.2813	122.6822	118.0365	0.0360	0.0330	179.9668	179.9977
S6	127.3704	116.5597	119.3219	122.6282	118.0499	0.0016	0.0053	179.9973	179.9941
S7	127.4416	116.5155	119.3936	122.6179	117.9877	3.1403	2.6755	176.9728	179.8910
S8	127.3990	116.5150	119.4094	122.5636	118.0269	0.0200	0.0230	179.9811	179.9974
S9	127.2724	116.6025	119.5516	122.5504	117.8979	0.0227	0.0212	179.9773	179.9984
S10	126.2490	116.1507	119.5372	122.3935	118.0635	21.1688	20.1312	159.1620	179.4402
S11	127.2883	116.6844	119.2706	122.6465	118.0828	2.0531	1.8863	177.9465	179.5514
S12	126.7066	118.7222	120.5944	122.7483	116.6573	0.1124	0.2699	179.7831	179.8205
S13	127.9085	117.3348	120.4251	125.1140	114.4495	39.3881	35.4437	142.8438	179.6180
S14	127.9144	117.4505	120.2620	125.2561	114.4669	37.7582	33.2181	144.5586	179.7271
S15	127.8966	117.5154	120.1515	125.3263	114.5062	37.2944	32.4273	145.1388	179.5559
S16	128.1418	117.3110	120.3013	125.2322	114.4541	37.2701	32.8952	145.2695	179.2384
S17	128.1863	117.2573	120.3393	125.1628	114.4865	38.0022	33.8727	144.4980	179.4306
S18	126.3251	118.8904	123.7444	120.2337	116.0218	2.8700	2.4847	177.2755	179.8666
S19	123.5725	119.0754	124.0667	119.4978	116.4255	33.4386	29.8439	150.1338	178.4039
S20	123.3682	119.2082	124.0276	119.4589	116.5016	32.3348	28.7460	150.8288	178.5028
S21	124.6651	119.7135	124.2491	119.5248	116.2198	36.4483	34.7087	140.1950	173.3605
S22	126.8083	117.7248	120.2883	125.1421	114.5574	44.9028	41.5353	137.8986	178.6873
S23	126.4510	118.5403	123.9370	120.0274	116.0356	0.0400	0.0334	179.9594	179.9951
S24	126.8687	117.1457	119.4303	123.5289	117.0408	0.0142	0.0131	179.9856	179.9991
S25	126.8240	117.2208	119.3165	123.6426	117.0409	0.0034	0.0029	179.9968	180.0000
S26	126.8264	117.2397	119.3419	123.6680	116.9901	0.0022	0.0041	179.9986	179.9993
S27	128.0508	116.3552	115.3178	126.7017	117.9676	35.9626	32.2407	146.3927	179.1897
S28	127.9811	116.4851	115.2184	126.7785	117.9903	35.4874	31.6798	146.9976	179.1036
S29	128.0188	116.4823	115.1991	126.8042	117.9854	35.3285	31.5362	147.3559	178.6806

S30	128.1101	116.3631	115.2640	126.6775	118.0440	35.2177	31.4685	147.1492	179.2856
S31	128.3042	116.2282	115.2998	126.6452	118.0421	34.4513	30.5433	148.1756	178.9243
S32	128.0916	116.2851	115.2603	126.7691	117.9519	36.9301	33.1982	145.1993	179.4425
S33	128.2444	116.3209	115.2121	126.7449	118.0326	34.6029	30.6454	148.0345	179.2376
S34	128.0343	116.3814	115.1208	126.8468	118.0205	35.8534	32.0127	146.6237	178.9418
S35	127.3389	116.6330	115.2650	126.5798	118.1463	36.3635	32.3180	147.3597	177.6313
S36	127.5635	117.4692	119.1264	126.8550	113.9511	46.9457	42.4165	135.9093	178.8099
S37	127.7718	116.4417	115.1245	126.6760	118.0233	48.0156	43.6045	134.5230	179.0427
S38	128.0447	116.3772	115.1769	126.9348	117.7400	46.6479	41.9713	136.0442	178.8890
S39	129.4735	115.5957	115.3311	126.6547	117.9850	34.2636	29.4036	147.5438	179.7481
S40	129.5749	115.5376	115.5065	126.3940	118.0800	32.0567	27.4738	149.5256	179.8536
S41	127.1793	116.6414	119.4981	122.4957	118.0062	0.0330	0.0319	179.9674	179.9985
S42	126.9619	116.9358	118.9090	121.3801	119.7109	5.0001	4.5956	174.9192	179.5456
S43	128.2096	117.3850	120.1541	125.8006	113.9838	41.2788	36.7312	141.6176	179.1446
S44	126.8352	117.1327	119.5755	123.4354	116.9891	0.0155	0.0145	179.9844	179.9990
S45	126.4695	119.1671	125.2384	120.0370	114.7245	0.0027	0.0077	179.9972	179.9993
S46	126.1145	118.3378	122.9371	121.2446	115.8173	16.2905	15.3225	163.7707	178.9252
S47	126.5765	118.7050	120.6546	122.6602	116.6843	7.1184	6.4695	172.9785	179.6603

	D(3-2-1-7)	**D(1-7-8-11)**	**D(9-7-8-11)**	**D(1-7-8-10)**	**D(9-7-8-10)**	**AD(7-8)**	**AD(7-1)**	**AD(6-8)**	**AD(2-7)**
S1	179.7895	177.7885	3.7468	3.8369	174.6278	1.3429	1.4721	3.1495	2.4725
S2	179.3392	177.6803	3.6700	3.9464	174.7033	1.3427	1.4714	3.1477	2.4719
S3	179.9542	176.5472	3.5141	3.1858	176.7528	1.3406	1.4772	3.7035	2.5259
S4	179.9938	179.9974	0.0115	0.0022	179.9933	1.3378	1.4685	3.0425	2.4664
S5	179.9985	179.9997	0.0001	0.0047	179.9951	1.3375	1.4679	3.0425	2.4659
S6	179.9949	179.9960	0.0066	0.0016	179.9958	1.3379	1.4673	3.0446	2.4658
S7	179.8538	179.8311	0.1842	0.1619	179.4850	1.3382	1.4670	3.0508	2.4675
S8	179.9991	179.9982	0.0059	0.0052	179.9989	1.3385	1.4668	3.0495	2.4664
S9	179.9979	179.9988	0.0027	0.0020	179.9966	1.3376	1.4687	3.0443	2.4641
S10	179.4171	179.3597	1.3382	1.5303	177.7719	1.3383	1.4705	3.0106	2.4953
S11	179.7189	179.9897	0.1578	0.1099	179.7220	1.3377	1.4675	3.0458	2.4658
S12	179.9081	179.9588	0.0138	0.0702	179.9848	1.3344	1.4754	3.0376	2.4758
S13	179.7891	178.7224	3.0284	2.5791	175.6700	1.3429	1.4770	3.1534	2.4838
S14	179.9045	179.0222	3.2558	2.4658	175.2561	1.3438	1.4734	3.1454	2.4795
S15	179.7652	179.2294	3.2669	2.3042	175.1994	1.3442	1.4722	3.1460	2.4752
S16	179.5170	178.8074	3.0719	2.5471	175.5736	1.3434	1.4747	3.1560	2.4800
S17	179.1704	178.4661	3.2013	2.8329	175.4997	1.3432	1.4760	3.1582	2.4823
S18	179.9043	179.9371	0.3115	0.1994	179.5520	1.3368	1.4717	3.0349	2.4697
S19	176.7693	177.9391	2.0836	3.2503	176.7270	1.3365	1.4760	2.9965	2.5457
S20	177.1658	178.1647	2.2678	3.1374	176.4301	1.3372	1.4741	2.9869	2.5466
S21	175.2914	177.3915	2.6916	1.6591	176.3590	1.3358	1.4730	3.1180	2.4735
S22	178.4830	177.7818	2.7956	3.5606	175.8621	1.3422	1.4756	3.1355	2.5184
S23	179.9954	179.9967	0.0041	0.0016	179.9910	1.3381	1.4709	3.0370	2.4696
S24	179.9989	179.9992	0.0005	0.0001	179.9987	1.3396	1.4670	3.0299	2.4662
S25	180.0000	179.9999	0.0003	0.0003	180.0000	1.3391	1.4665	3.0313	2.4647
S26	179.9997	179.9996	0.0023	0.0027	180.0000	1.3391	1.4666	3.0322	2.4648
S27	179.9183	177.6424	3.7332	3.6974	174.9270	1.3446	1.4710	3.1393	2.4706
S28	179.7947	177.6876	3.6459	3.6473	175.0191	1.3443	1.4704	3.1372	2.4699
S29	179.3925	177.3934	3.7239	3.8616	175.0211	1.3443	1.4704	3.1371	2.4704
S30	179.9810	177.7531	3.6392	3.6659	174.9418	1.3447	1.4701	3.1395	2.4692
S31	179.6907	177.5683	3.7211	3.7754	174.9351	1.3452	1.4695	3.1444	2.4710

S32	179.7735	178.2420	3.3697	3.3716	175.0167	1.3446	1.4712	3.1440	2.4688
S33	179.7147	177.6500	3.6802	3.5572	175.1125	1.3448	1.4700	3.1419	2.4686
S34	179.7411	177.7940	3.5790	3.4929	175.1340	1.3440	1.4704	3.1500	2.4633
S35	178.1413	176.2874	4.0365	4.8199	174.8562	1.3443	1.4671	3.1538	2.4720
S36	179.4939	178.1448	3.5660	5.0360	173.2532	1.3442	1.4773	3.1833	2.4758
S37	179.7532	179.1052	2.7783	5.8495	172.2670	1.3437	1.4760	3.1866	2.4770
S38	179.5735	179.1446	2.8540	5.4158	172.5856	1.3435	1.4758	3.1893	2.4734
S39	179.5097	179.5415	2.6124	1.5581	175.3710	1.3455	1.4704	3.1807	2.4563
S40	179.1217	179.7934	2.8115	1.4389	175.5429	1.3463	1.4686	3.1797	2.4582
S41	179.9980	179.9996	0.0003	0.0040	179.9953	1.3379	1.4686	3.0390	2.4681
S42	179.4740	179.8717	0.6171	0.0616	179.4497	1.3390	1.4687	3.0410	2.4665
S43	179.2921	178.3411	3.3526	4.6877	173.6186	1.3434	1.4753	3.1676	2.4792
S44	179.9986	179.9995	0.0016	0.0003	179.9985	1.3394	1.4674	3.0299	2.4667
S45	179.9980	179.9952	0.0002	0.0084	179.9967	1.3420	1.4697	3.0403	2.4654
S46	178.9081	177.8126	3.1169	1.8125	177.2580	1.3365	1.4737	3.0326	2.4781
S47	179.6237	179.9760	0.5476	0.3267	179.1016	1.3343	1.4760	3.0360	2.4765

	AD(7-9)	**fp(1)**	**fm(1)**	**fp(7)**	**fm(7)**	**fp(8)**	**fm(8)**	**fp(9)**	**fm(9)**
S1	1.0888	-0.0373	-0.0982	-0.1420	-0.0534	-0.1434	-0.2207	-0.0371	-0.0349
S2	1.0886	-0.0529	-0.0910	-0.1209	-0.0548	-0.1436	-0.2121	-0.0361	-0.0337
S3	1.0907	-0.0789	-0.0905	-0.0918	-0.0739	-0.1661	-0.2043	-0.0466	-0.0410
S4	1.0896	-0.0302	-0.1182	-0.1408	-0.0226	-0.1597	-0.2456	-0.0369	-0.0313
S5	1.0893	-0.0418	-0.1119	-0.1251	-0.0243	-0.1604	-0.2374	-0.0356	-0.0303
S6	1.0895	-0.0248	-0.1275	-0.1474	-0.0158	-0.1617	-0.2413	-0.0381	-0.0310
S7	1.0897	-0.0245	-0.1420	-0.1439	0.0027	-0.1574	-0.2189	-0.0369	-0.0290
S8	1.0897	-0.0232	-0.1423	-0.1466	0.0026	-0.1573	-0.2222	-0.0372	-0.0292
S9	1.0898	-0.0303	-0.1294	-0.1406	-0.0074	-0.1585	-0.2235	-0.0368	-0.0301
S10	1.0884	-0.0287	-0.1461	-0.1505	-0.0035	-0.1592	-0.2188	-0.0347	-0.0297
S11	1.0896	-0.0176	-0.1262	0.0068	-0.0037	-0.0143	-0.2116	-0.0031	-0.0279
S12	1.0892	-0.0215	-0.0990	0.0060	-0.0573	-0.0186	-0.2623	-0.0038	-0.0352
S13	1.0902	-0.1297	-0.0327	-0.0332	-0.1582	-0.1538	-0.2228	-0.0417	-0.0412
S14	1.0898	-0.1409	0.0050	0.0229	-0.1970	-0.0839	-0.2257	-0.0246	-0.0397
S15	1.0894	-0.1197	0.0351	0.0256	-0.2458	-0.0648	-0.2352	-0.0198	-0.0398
S16	1.0899	-0.1085	-0.0454	0.0152	-0.1244	-0.0689	-0.2007	-0.0200	-0.0380
S17	1.0902	-0.1338	-0.0380	-0.0237	-0.1475	-0.1470	-0.2175	-0.0393	-0.0407
S18	1.0890	-0.0072	0.0171	0.0182	-0.2184	-0.0401	-0.2593	-0.0135	-0.0394
S19	1.0865	-0.0844	0.0016	0.0336	-0.1839	-0.0622	-0.2545	-0.0095	-0.0363
S20	1.0861	-0.0992	0.0174	0.0329	-0.2017	-0.0703	-0.2540	-0.0116	-0.0353
S21	1.0885	-0.1049	0.0416	0.0159	-0.2536	-0.0654	-0.2497	-0.0271	-0.0414
S22	1.0884	-0.1534	-0.0175	-0.0074	-0.1770	-0.1442	-0.2237	-0.0365	-0.0365
S23	1.0896	-0.1180	0.0039	0.0210	-0.1806	-0.0902	-0.2485	-0.0174	-0.0382
S24	1.0896	-0.0137	-0.1375	-0.1629	-0.0034	-0.1399	-0.2362	-0.0386	-0.0310
S25	1.0892	-0.0245	-0.1307	-0.1479	-0.0049	-0.1424	-0.2266	-0.0373	-0.0299
S26	1.0892	-0.0255	-0.1281	-0.1472	-0.0060	-0.1430	-0.2250	-0.0376	-0.0299
S27	1.0888	-0.0183	-0.1167	-0.1654	-0.0327	-0.1258	-0.2101	-0.0377	-0.0346
S28	1.0886	-0.0315	-0.1103	-0.1467	-0.0340	-0.1280	-0.2025	-0.0366	-0.0334
S29	1.0886	-0.0325	-0.1074	-0.1457	-0.0354	-0.1286	-0.2015	-0.0369	-0.0334
S30	1.0887	-0.0123	-0.1280	-0.1735	-0.0232	-0.1268	-0.2045	-0.0383	-0.0344
S31	1.0889	-0.0116	-0.1461	-0.1701	-0.0007	-0.1237	-0.1856	-0.0374	-0.0325
S32	1.0889	-0.0182	-0.1345	-0.1657	-0.0103	-0.1244	-0.1873	-0.0379	-0.0336
S33	1.0887	-0.0202	-0.1237	-0.1605	-0.0235	-0.1267	-0.2027	-0.0375	-0.0340
S34	1.0886	-0.0249	-0.1199	-0.1558	-0.0216	-0.1282	-0.1908	-0.0370	-0.0327
S35	1.0877	-0.0150	-0.1441	-0.1625	-0.0111	-0.1277	-0.1897	-0.0353	-0.0330

S36	1.0879	-0.0117	-0.1443	-0.1817	-0.0158	-0.1246	-0.1828	-0.0405	-0.0366
S37	1.0893	-0.0111	-0.1365	-0.1843	-0.0217	-0.1280	-0.1865	-0.0395	-0.0362
S38	1.0892	-0.0128	-0.1304	-0.1804	-0.0264	-0.1279	-0.1905	-0.0392	-0.0358
S39	1.0891	-0.0098	-0.1397	-0.1758	-0.0060	-0.1282	-0.2059	-0.0379	-0.0327
S40	1.0893	-0.0037	-0.1633	-0.1792	0.0184	-0.1258	-0.1825	-0.0378	-0.0306
S41	1.0896	-0.0313	-0.1113	-0.1379	-0.0298	-0.1603	-0.2423	-0.0364	-0.0311
S42	1.0892	-0.0252	-0.0086	-0.1449	-0.0821	-0.1595	-0.0570	-0.0365	-0.0186
S43	1.0902	-0.1593	0.0185	0.0188	-0.2176	-0.1069	-0.2290	-0.0316	-0.0387
S44	1.0895	-0.0150	-0.1338	-0.1604	-0.0067	-0.1398	-0.2378	-0.0382	-0.0311
S45	1.0888	-0.0006	-0.0512	-0.1458	-0.0874	-0.0927	-0.1993	-0.0311	-0.0312
S46	1.0906	-0.0804	-0.0975	-0.0832	-0.0633	-0.1929	-0.2324	-0.0387	-0.0363
S47	1.0894	-0.0880	-0.0960	-0.0723	-0.0623	-0.2281	-0.2679	-0.0377	-0.0360

	L-R1	**B1-R1**	**B5-R1**	**L-R2**	**B1-R2**	**B5-R2**	**L-R3**	**B1-R3**	**B5-R3**
S1	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	6.2800	3.1100	3.1100
S2	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.1000	1.9000	3.1600
S3	4.0400	1.5000	3.0600	4.0500	1.8800	3.1800	6.2800	3.1100	3.1100
S4	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
S5	4.0500	1.5000	3.0600	2.0600	1.0000	1.0000	7.7600	1.5000	3.2600
S6	4.0500	1.5000	3.0600	2.0600	1.0000	1.0000	6.9100	1.5000	3.2400
S7	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	9.5300	1.8000	4.1900
S8	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	7.2800	1.5300	3.1600
S9	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.3500	1.6100	4.2900
S10	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.3500	1.5800	4.3800
S11	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	12.1800	1.6900	4.6100
S12	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000	12.5200	1.5100	4.2000
S13	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	6.2800	3.1100	3.1100
S14	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	7.7900	1.5000	3.1600
S15	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	7.6200	1.5000	3.1600
S16	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	10.5100	1.8000	3.5600
S17	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	11.9100	1.8900	5.9800
S18	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.9000	1.5000	4.9000
S19	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.3400	1.5200	4.8500
S20	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	8.4700	1.5900	4.8100
S21	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	8.8400	2.4500	4.8100
S22	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	6.3700	1.6300	4.8300
S23	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	7.6300	1.5000	3.2400
S24	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
S25	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	7.7600	1.5000	3.2600
S26	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	8.0600	1.5000	3.2400
S27	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.2800	3.1100	3.1100
S28	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	7.7600	1.5000	3.2600
S29	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	8.0900	1.7200	3.3600
S30	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.9200	1.5000	3.3600
S31	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	7.2800	1.5400	3.3500
S32	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.3400	1.6100	4.5600
S33	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	9.2800	1.5100	3.8700
S34	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	7.3000	1.7000	5.0500
S35	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	7.3000	1.6600	3.7100
S36	4.8800	1.6200	3.4200	4.0700	1.5500	3.1600	6.2800	3.1100	3.1100
S37	4.8800	1.6200	3.4200	6.3800	1.5600	4.4600	6.2800	3.1100	3.1100
S38	4.8800	1.6200	3.4200	6.4600	1.5800	4.6900	6.2800	3.1100	3.1100
S39	4.8800	1.6200	3.4200	5.6000	1.5400	3.2200	6.2800	3.1100	3.1100

S40	4.8800	1.6200	3.4200	5.6100	1.5400	3.2100	7.2800	1.6700	3.3900
S41	4.9900	1.6300	3.4000	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
S42	5.0400	1.5200	4.2000	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
S43	4.0800	1.5100	4.4700	4.0700	1.5100	4.4700	8.3200	1.5200	3.3600
S44	6.0800	2.0100	3.5700	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
S45	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000	5.7800	1.5000	3.1900
S46	8.4200	2.7400	6.1200	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
S47	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100

Table S18. 11 Alkene Parameters for S1-S66

	υ(7-8)	**I(7-8)**	**NPA7**	**NPA8**	**NMR7**
S1	1740.87	154.82	-0.186	-0.1188	44.7883
S2	1742.91	143.02	-0.19009	-0.1126	46.382
S3	1745.97	61.69	-0.22772	-0.0855	56.4018
S4	1740.93	271.1	-0.17239	-0.3397	40.3849
S5	1743.25	252.56	-0.17608	-0.3334	41.9504
S6	1741.01	242.11	-0.17206	-0.3421	41.5276
S7	1740.05	323.33	-0.17076	-0.3443	40.2477
S8	1738.59	311.45	-0.17033	-0.3452	40.4526
S9	1745.87	294.6	-0.17127	-0.3406	40.2771
S10	1739.05	230.68	-0.17502	-0.338	42.5815
S11	1743.44	263.58	-0.17497	-0.3359	41.1413
S12	1741.36	10.8	-0.25189	-0.4342	47.9183
S13	1765.28	38.61	-0.27687	0.0155	58.455
S14	1758.75	83.39	-0.28502	0.03095	59.0403
S15	1745.33	123.77	-0.28909	0.03927	59.9354
S16	1761.17	62.92	-0.28049	0.02267	59.1404
S17	1736.12	33.5	-0.27774	0.01753	58.7373
S18	1767.4	161.63	-0.28132	-0.1607	57.2522
S19	1757.25	27.86	-0.27163	-0.1822	55.6155
S20	1752.51	21.46	-0.27611	-0.1724	56.2127
S21	1764.54	72.43	-0.28574	-0.1546	60.5616
S22	1762.55	50.48	-0.2825	0.02592	59.8324
S23	1759.15	81.57	-0.27888	-0.1641	55.1906
S24	1739.04	361.56	-0.15333	-0.3584	35.6235
S25	1742.25	341.45	-0.15718	-0.3523	37.2876
S26	1742.98	342.81	-0.15766	-0.3514	37.2872
S27	1743.66	130.8	-0.17049	-0.1349	40.928

S28	1745.81	119.83	-0.17463	-0.1291	42.5887
S29	1746.55	119.88	-0.17508	-0.1285	42.6498
S30	1743.35	127.3	-0.17051	-0.1358	41.9645
S31	1740.31	164.8	-0.16834	-0.1389	40.9699
S32	1745.47	134.61	-0.16894	-0.1361	40.7487
S33	1742.69	129.19	-0.17141	-0.1341	41.9088
S34	1748.14	129.77	-0.17378	-0.1294	42.8206
S35	1744.43	149.17	-0.17832	-0.1301	48.4925
S36	1748.1	20.7	-0.17427	-0.1309	42.4086
S37	1745.78	96.94	-0.16513	-0.1317	40.2626
S38	1746.23	95.15	-0.16665	-0.1299	40.4986
S39	1739.73	167.24	-0.14868	-0.1465	37.5665
S40	1732.06	202.13	-0.14692	-0.1509	37.7469
S41	1739.97	247.4	-0.17634	-0.3325	41.9782
S42	1727.68	291.11	-0.16674	-0.3386	39.0623
S43	1753.8	87.34	-0.27941	0.03016	61.6017
S44	1738.32	357.91	-0.15678	-0.3536	36.3665
S45	1744.58	46.08	-0.19542	-0.2374	50.9412
S46	1761.18	2.37	-0.2363	-0.2252	47.4137
S47	1742.8	9.2	-0.251	-0.435	47.075
S48	1747.93	17.11	-0.22333	-0.4679	44.6589
S49	1750.72	21.65	-0.22763	-0.4678	45.7798
S50	1758.68	16.36	-0.22858	-0.465	46.9966
S51	1760.08	17.37	-0.22353	-0.4714	43.8785
S52	1761.47	17.62	-0.22483	-0.4691	43.9784
S53	1759.14	17.67	-0.22356	-0.4713	43.7572
S54	1748.34	13.98	-0.2265	-0.4636	45.6629
S55	1757.65	14.61	-0.2228	-0.461	47.7126
S56	1753.27	12.51	-0.2272	-0.4622	46.135
S57	1755.27	112.64	-0.29296	0.04718	61.9924
S58	1754.07	137.54	-0.33963	0.06398	73.4552
S59	1769.25	14.06	-0.28676	0.02569	71.5454
S60	1757.69	171.04	-0.14959	-0.3675	37.4093
S61	1754.87	198.46	-0.14626	-0.3682	40.4158
S62	1792.3	167.83	-0.15785	-0.151	47.0916
S63	1784.94	155.77	-0.15403	-0.1475	39.6086

S64	1728.75	104.23	0.08241	-0.1816	31.9335
S65	1746.83	182.76	0.0654	-0.3789	23.6994
S66	1736.3	102.08	-0.08006	-0.1658	40.324

	NMR8	**AD(7-8)**	**fp(7)**	**fm(7)**	**fp(8)**	**fm(8)**
S1	53.5902	1.34293	-0.142	-0.0534	-0.1434	-0.2207
S2	52.3521	1.34268	-0.1209	-0.0548	-0.1436	-0.2121
S3	33.9129	1.34065	-0.0918	-0.0739	-0.1661	-0.2043
S4	65.8062	1.33781	-0.1408	-0.0226	-0.1597	-0.2456
S5	64.7798	1.33754	-0.1251	-0.0243	-0.1604	-0.2374
S6	66.4505	1.33792	-0.1474	-0.0158	-0.1617	-0.2413
S7	66.8507	1.33818	-0.1439	0.0027	-0.1574	-0.2189
S8	67.097	1.33847	-0.1466	0.0026	-0.1573	-0.2222
S9	66.1387	1.33761	-0.1406	-0.0074	-0.1585	-0.2235
S10	63.9477	1.33827	-0.1505	-0.0035	-0.1592	-0.2188
S11	64.9187	1.3377	0.0068	-0.0037	-0.0143	-0.2116
S12	71.3503	1.33436	0.006	-0.0573	-0.0186	-0.2623
S13	45.0928	1.34288	-0.0332	-0.1582	-0.1538	-0.2228
S14	40.56	1.34384	0.0229	-0.197	-0.0839	-0.2257
S15	38.1176	1.34415	0.0256	-0.2458	-0.0648	-0.2352
S16	42.9092	1.34342	0.0152	-0.1244	-0.0689	-0.2007
S17	44.4079	1.34321	-0.0237	-0.1475	-0.147	-0.2175
S18	48.805	1.33683	0.0182	-0.2184	-0.0401	-0.2593
S19	50.5807	1.33652	0.0336	-0.1839	-0.0622	-0.2545
S20	47.8959	1.33722	0.0329	-0.2017	-0.0703	-0.254
S21	41.3374	1.33583	0.0159	-0.2536	-0.0654	-0.2497
S22	43.2643	1.3422	-0.0074	-0.177	-0.1442	-0.2237
S23	49.7559	1.33809	0.021	-0.1806	-0.0902	-0.2485
S24	68.9263	1.33964	-0.1629	-0.0034	-0.1399	-0.2362
S25	67.8733	1.33912	-0.1479	-0.0049	-0.1424	-0.2266
S26	67.7848	1.33912	-0.1472	-0.006	-0.143	-0.225
S27	55.0687	1.3446	-0.1654	-0.0327	-0.1258	-0.2101
S28	53.9033	1.34428	-0.1467	-0.034	-0.128	-0.2025

S29	53.702	1.34425	-0.1457	-0.0354	-0.1286	-0.2015
S30	55.4378	1.34467	-0.1735	-0.0232	-0.1268	-0.2045
S31	56.0473	1.34523	-0.1701	-0.0007	-0.1237	-0.1856
S32	55.3838	1.34463	-0.1657	-0.0103	-0.1244	-0.1873
S33	54.9922	1.34477	-0.1605	-0.0235	-0.1267	-0.2027
S34	54.002	1.34405	-0.1558	-0.0216	-0.1282	-0.1908
S35	54.4445	1.34426	-0.1625	-0.0111	-0.1277	-0.1897
S36	47.5833	1.34417	-0.1817	-0.0158	-0.1246	-0.1828
S37	48.6924	1.34368	-0.1843	-0.0217	-0.128	-0.1865
S38	48.7034	1.34353	-0.1804	-0.0264	-0.1279	-0.1905
S39	56.2077	1.34545	-0.1758	-0.006	-0.1282	-0.2059
S40	57.1033	1.34629	-0.1792	0.0184	-0.1258	-0.1825
S41	65.2494	1.33788	-0.1379	-0.0298	-0.1603	-0.2423
S42	69.1466	1.33903	-0.1449	-0.0821	-0.1595	-0.057
S43	33.0138	1.3434	0.0188	-0.2176	-0.1069	-0.229
S44	67.1354	1.33939	-0.1604	-0.0067	-0.1398	-0.2378
S45	59.7409	1.34199	-0.1458	-0.0874	-0.0927	-0.1993
S46	57.9184	1.3365	-0.0832	-0.0633	-0.1929	-0.2324
S47	71.223	1.3343	0.072	-0.062	-0.228	-0.2679
S48	68.9467	1.3307	0.0054	0.0169	-0.0325	-0.0329
S49	68.2651	1.33106	0.0025	0.0164	-0.0046	-0.0481
S50	68.4841	1.33051	0.0029	0.0146	-0.0048	-0.0244
S51	70.611	1.33069	0.0007	0.0003	-0.0007	-0.0005
S52	69.2533	1.33056	0.0063	0.0049	-0.0105	-0.008
S53	70.6487	1.33069	0.0014	0.0015	-0.0017	-0.0029
S54	67.258	1.3305	0.0114	0.0187	-0.0237	-0.0566
S55	68.9843	1.32978	0.0058	0.0165	-0.062	-0.0455
S56	67.047	1.33043	0.0125	0.0138	-0.0405	-0.0678
S57	35.6871	1.34417	-0.0005	-0.3035	-0.1517	-0.2458
S58	32.2307	1.34435	0.004	-0.1548	-0.115	-0.215
S59	40.4603	1.34177	0.0075	-0.1146	-0.0091	-0.1918
S60	58.2072	1.33409	-0.2884	-0.1348	-0.1537	-0.0388
S61	59.3623	1.33354	-0.2856	-0.0803	-0.1462	0.0222
S62	55.718	1.33947	-0.2773	-0.0652	-0.1281	0.0193
S63	56.6391	1.33994	-0.2736	-0.0167	-0.12	0.0063
S64	50.813	1.35089	-0.208	-0.1899	-0.0872	-0.1715

S65	65.9239	1.34214	-0.0044	-0.0628	0.0036	0.0231
S66	52.2428	1.34541	0.0178	-0.1302	-0.05	-0.2299

Table S19. Dataset (41 Parameters) for Experimentally Known Substrates (**S1-S66**)

	υ(7-8)	**I(7-8)**	**NPA7**	**NPA8**	**NPA9**	**NMR7**	**NMR8**
S1	1740.87	154.82	-0.186	-0.11876	0.26734	44.7883	53.5902
S2	1742.91	143.02	-0.19009	-0.11255	0.26991	46.382	52.3521
S3	1745.97	61.69	-0.22772	-0.08551	0.25544	56.4018	33.9129
S4	1740.93	271.1	-0.17239	-0.33967	0.26131	40.3849	65.8062
S5	1743.25	252.56	-0.17608	-0.33342	0.26382	41.9504	64.7798
S6	1741.01	242.11	-0.17206	-0.34205	0.2625	41.5276	66.4505
S7	1740.05	323.33	-0.17076	-0.34434	0.26068	40.2477	66.8507
S8	1738.59	311.45	-0.17033	-0.34524	0.26065	40.4526	67.097
S9	1745.87	294.6	-0.17127	-0.34057	0.26077	40.2771	66.1387
S10	1739.05	230.68	-0.17502	-0.33798	0.26199	42.5815	63.9477
S11	1743.44	263.58	-0.17497	-0.3359	0.26282	41.1413	64.9187
S12	1741.36	10.8	-0.25189	-0.43417	0.24941	47.9183	71.3503
S13	1765.28	38.61	-0.27687	0.0155	0.24616	58.455	45.0928
S14	1758.75	83.39	-0.28502	0.03095	0.25054	59.0403	40.56
S15	1745.33	123.77	-0.28909	0.03927	0.2532	59.9354	38.1176
S16	1761.17	62.92	-0.28049	0.02267	0.24789	59.1404	42.9092
S17	1736.12	33.5	-0.27774	0.01753	0.24643	58.7373	44.4079
S18	1767.4	161.63	-0.28132	-0.16069	0.25428	57.2522	48.805
S19	1757.25	27.86	-0.27163	-0.18223	0.25938	55.6155	50.5807
S20	1752.51	21.46	-0.27611	-0.17239	0.26228	56.2127	47.8959
S21	1764.54	72.43	-0.28574	-0.15457	0.26218	60.5616	41.3374
S22	1762.55	50.48	-0.2825	0.02592	0.2529	59.8324	43.2643
S23	1759.15	81.57	-0.27888	-0.16412	0.24865	55.1906	49.7559
S24	1739.04	361.56	-0.15333	-0.35839	0.26235	35.6235	68.9263
S25	1742.25	341.45	-0.15718	-0.35227	0.2648	37.2876	67.8733
S26	1742.98	342.81	-0.15766	-0.35143	0.26494	37.2872	67.7848
S27	1743.66	130.8	-0.17049	-0.13486	0.26719	40.928	55.0687
S28	1745.81	119.83	-0.17463	-0.12913	0.26947	42.5887	53.9033
S29	1746.55	119.88	-0.17508	-0.12848	0.26965	42.6498	53.702
S30	1743.35	127.3	-0.17051	-0.13575	0.26787	41.9645	55.4378
S31	1740.31	164.8	-0.16834	-0.13885	0.26601	40.9699	56.0473
S32	1745.47	134.61	-0.16894	-0.13612	0.2668	40.7487	55.3838
S33	1742.69	129.19	-0.17141	-0.13406	0.2678	41.9088	54.9922
S34	1748.14	129.77	-0.17378	-0.12936	0.26961	42.8206	54.002
S35	1744.43	149.17	-0.17832	-0.13013	0.27284	48.4925	54.4445
S36	1748.1	20.7	-0.17427	-0.13086	0.26938	42.4086	47.5833
S37	1745.78	96.94	-0.16513	-0.13172	0.26882	40.2626	48.6924
S38	1746.23	95.15	-0.16665	-0.12987	0.2683	40.4986	48.7034
S39	1739.73	167.24	-0.14868	-0.14651	0.27061	37.5665	56.2077
S40	1732.06	202.13	-0.14692	-0.15086	0.26935	37.7469	57.1033
S41	1739.97	247.4	-0.17634	-0.3325	0.26093	41.9782	65.2494
S42	1727.68	291.11	-0.16674	-0.33859	0.26148	39.0623	69.1466
S43	1753.8	87.34	-0.27941	0.03016	0.25217	61.6017	33.0138
S44	1738.32	357.91	-0.15678	-0.35355	0.26192	36.3665	67.1354
S45	1744.58	46.08	-0.19542	-0.23742	0.24747	50.9412	59.7409
S46	1761.18	2.37	-0.2363	-0.2252	0.24961	47.4137	57.9184

S47	1742.79	9.2	-0.25141	-0.43545	0.24822	47.0747	71.2234
S48	1747.93	17.11	-0.22333	-0.46786	0.24145	44.6589	68.9467
S49	1750.72	21.65	-0.22763	-0.4678	0.23768	45.7798	68.2651
S50	1758.68	16.36	-0.22858	-0.46502	0.2385	46.9966	68.4841
S51	1760.08	17.37	-0.22353	-0.47142	0.23559	43.8785	70.611
S52	1761.47	17.62	-0.22483	-0.46907	0.23617	43.9784	69.2533
S53	1759.14	17.67	-0.22356	-0.47125	0.23566	43.7572	70.6487
S54	1748.34	13.98	-0.2265	-0.46355	0.24292	45.6629	67.258
S55	1757.65	14.61	-0.2228	-0.46103	0.24052	47.7126	68.9843
S56	1753.27	12.51	-0.2272	-0.46217	0.24358	46.135	67.047
S57	1755.27	112.64	-0.29296	0.04718	0.25565	61.9924	35.6871
S58	1754.07	137.54	-0.33963	0.06398	0.26689	73.4552	32.2307
S59	1769.25	14.06	-0.28676	0.02569	0.25263	71.5454	40.4603
S60	1757.69	171.04	-0.14959	-0.36745	0.25127	37.4093	58.2072
S61	1754.87	198.46	-0.14626	-0.36816	0.25	40.4158	59.3623
S62	1792.3	167.83	-0.15785	-0.15097	0.2539	47.0916	55.718
S63	1784.94	155.77	-0.15403	-0.14746	0.25366	39.6086	56.6391
S64	1728.75	104.23	0.08241	-0.1816	-0.72685	31.9335	50.813
S65	1746.83	182.76	0.0654	-0.3789	-0.50918	23.6994	65.9239
S66	1736.3	102.08	-0.08006	-0.16577	-0.029	40.324	52.2428

	NMR9	**A(1-7-9)**	**A(1-7-8)**	**A(8-7-9)**	**A(7-8-11)**	**A(7-8-10)**	**A(10-8-11)**
S1	23.2733	115.810759	128.3145133	115.858595	115.372246	125.889975	118.718535
S2	23.3198	115.709438	128.2708207	116.00728	115.283956	125.961682	118.735086
S3	24.5389	115.08971	127.7942207	117.116044	122.220313	122.844231	114.934968
S4	23.5637	116.139391	127.2695934	116.591015	119.385236	122.566946	118.047818
S5	23.6318	116.099556	127.2057517	116.694692	119.281337	122.682157	118.036505
S6	23.6079	116.069942	127.370378	116.55968	119.321908	122.628235	118.049857
S7	23.5617	116.042028	127.4416135	116.515498	119.393579	122.617886	117.987741
S8	23.6284	116.086003	127.3990172	116.514979	119.40945	122.563626	118.026923
S9	23.6127	116.125155	127.2723786	116.602466	119.551648	122.550439	117.897913
S10	22.9908	117.596775	126.2490275	116.150726	119.537245	122.393519	118.063482
S11	23.4717	116.027089	127.2883146	116.684401	119.270592	122.646547	118.082756
S12	24.4233	114.571173	126.7065595	118.722247	120.594408	122.748319	116.657266
S13	24.7084	114.736004	127.9085167	117.334836	120.425093	125.113969	114.449483
S14	24.6378	114.600252	127.9143924	117.450486	120.261958	125.256143	114.466926
S15	24.6115	114.546127	127.8966099	117.515422	120.15154	125.326327	114.506219
S16	24.6115	114.523484	128.1418479	117.310996	120.301281	125.232229	114.454086
S17	24.6883	114.537729	128.1863214	117.257315	120.339333	125.162783	114.486467
S18	24.4903	114.784018	126.3251356	118.890427	123.744411	120.233665	116.021794
S19	24.3752	117.352118	123.5724721	119.075406	124.066743	119.497819	116.425498
S20	24.3243	117.422175	123.3682351	119.20825	124.027591	119.458857	116.501621
S21	24.5471	115.427458	124.6651336	119.713495	124.249128	119.524775	116.219791
S22	24.7292	115.464627	126.8082818	117.724807	120.288302	125.142098	114.557392
S23	24.695	115.008737	126.4509717	118.540291	123.936981	120.027415	116.035604
S24	23.3449	115.985559	126.8687195	117.145721	119.430263	123.528904	117.040833
S25	23.4221	115.95525	126.8239973	117.220753	119.316507	123.64259	117.040903
S26	23.4302	115.93392	126.826365	117.239715	119.341903	123.667971	116.990126
S27	23.1403	115.58107	128.0507629	116.355249	115.317811	126.701734	117.967602
S28	23.2029	115.521662	127.981144	116.485061	115.218434	126.778489	117.990315
S29	23.1952	115.49033	128.0188157	116.482345	115.199133	126.804205	117.985384
S30	23.1771	115.513571	128.1101409	116.363074	115.26397	126.677545	118.044044
S31	23.1915	115.456325	128.3041618	116.228201	115.299767	126.645201	118.042081

S32	23.1895	115.605508	128.0916218	116.285133	115.260311	126.769138	117.951917
S33	23.1571	115.422664	128.2443704	116.320929	115.212052	126.744867	118.032634
S34	23.2721	115.571401	128.0342851	116.381444	115.120764	126.846842	118.020531
S35	23.0328	116.027368	127.3388765	116.633031	115.265019	126.579826	118.146343
S36	23.1906	114.947519	127.5634673	117.469201	119.126354	126.854976	113.95114
S37	23.1636	115.762185	127.7718319	116.441654	115.124467	126.675989	118.023288
S38	23.1545	115.550881	128.0446564	116.377204	115.176869	126.934815	117.739959
S39	23.1413	114.867723	129.4734529	115.595675	115.331066	126.654743	117.985049
S40	23.21	114.826624	129.574887	115.537572	115.506526	126.393985	118.080032
S41	23.5803	116.179324	127.1792642	116.641412	119.49811	122.495698	118.006192
S42	23.5162	116.100583	126.9619176	116.935845	118.909034	121.380061	119.710872
S43	24.7299	114.38624	128.2095619	117.385021	120.154107	125.800644	113.983799
S44	23.3837	116.032022	126.8352314	117.132747	119.575524	123.435401	116.989075
S45	23.5376	114.363356	126.4695055	119.167138	125.238447	120.037035	114.724518
S46	24.4363	115.541738	126.1145381	118.337782	122.93707	121.244621	115.817331
S47	24.4356	114.716325	126.5764548	118.705009	120.654606	122.660189	116.684334
S48	25.0894	115.94208	124.3151545	119.730144	121.676239	121.200024	117.123184
S49	25.0887	116.188934	124.5625937	119.225769	121.824088	121.18227	116.993135
S50	25.3545	115.9735	124.7653518	119.25268	121.674541	121.309676	117.014491
S51	24.9991	115.763193	125.0317967	119.193503	121.665987	121.341722	116.991994
S52	24.8382	115.940787	124.8259084	119.227528	121.668896	121.302543	117.028319
S53	25.0398	115.818888	124.9577819	119.215788	121.71773	121.299701	116.982267
S54	25.0526	115.995152	124.2068499	119.790877	121.631346	121.23173	117.13553
S55	24.8161	116.245972	123.8742653	119.876491	121.569445	121.326561	117.103648
S56	25.0498	116.009963	124.1831528	119.80244	121.626456	121.239264	117.133652
S57	24.8645	114.411644	127.7626288	117.788895	120.073313	125.450153	114.465437
S58	24.5303	114.337435	126.0685515	119.594005	120.452995	123.291505	116.255499
S59	25.0719	115.419082	126.441304	118.132558	120.784377	124.171044	115.038281
S60	23.8643	118.034445	124.8284985	117.136714	120.471778	121.213583	118.314261
S61	24.0828	117.695692	125.0885758	117.215699	120.49253	121.276318	118.230573
S62	24.0562	116.065952	128.1577833	115.776238	115.90589	125.331788	118.761843
S63	23.814	115.751269	128.1595058	116.068185	115.908791	125.231865	118.859003
S64	172.4911	112.66407	122.6605862	124.673589	120.81588	122.615983	116.568136
S65	169.5775	115.712516	119.7186488	124.561704	124.897584	118.562659	116.492875
S66	33.0092	116.974525	120.4730574	122.551838	128.000347	116.744853	115.239665

	D(1-7-8-11)	**D(9-7-8-11)**	**D(1-7-8-10)**	**D(9-7-8-10)**	**AD(7-8)**	**AD(7-1)**	**AD(7-9)**
S1	177.7885	3.7468	3.8369	174.6278	1.3429	1.4721	1.0888
S2	177.6803	3.6700	3.9464	174.7033	1.3427	1.4714	1.0886
S3	176.5472	3.5141	3.1858	176.7528	1.3406	1.4772	1.0907
S4	179.9974	0.0115	0.0022	179.9933	1.3378	1.4685	1.0896
S5	179.9997	0.0001	0.0047	179.9951	1.3375	1.4679	1.0893
S6	179.9960	0.0066	0.0016	179.9958	1.3379	1.4673	1.0895
S7	179.8311	0.1842	0.1619	179.4850	1.3382	1.4670	1.0897
S8	179.9982	0.0059	0.0052	179.9989	1.3385	1.4668	1.0897
S9	179.9988	0.0027	0.0020	179.9966	1.3376	1.4687	1.0898
S10	179.3597	1.3382	1.5303	177.7719	1.3383	1.4705	1.0884
S11	179.9897	0.1578	0.1099	179.7220	1.3377	1.4675	1.0896
S12	179.9588	0.0138	0.0702	179.9848	1.3344	1.4754	1.0892
S13	178.7224	3.0284	2.5791	175.6700	1.3429	1.4770	1.0902
S14	179.0222	3.2558	2.4658	175.2561	1.3438	1.4734	1.0898
S15	179.2294	3.2669	2.3042	175.1994	1.3442	1.4722	1.0894
S16	178.8074	3.0719	2.5471	175.5736	1.3434	1.4747	1.0899
S17	178.4661	3.2013	2.8329	175.4997	1.3432	1.4760	1.0902
S18	179.9371	0.3115	0.1994	179.5520	1.3368	1.4717	1.0890
S19	177.9391	2.0836	3.2503	176.7270	1.3365	1.4760	1.0865
S20	178.1647	2.2678	3.1374	176.4301	1.3372	1.4741	1.0861

S21	177.3915	2.6916	1.6591	176.3590	1.3358	1.4730	1.0885
S22	177.7818	2.7956	3.5606	175.8621	1.3422	1.4756	1.0884
S23	179.9967	0.0041	0.0016	179.9910	1.3381	1.4709	1.0896
S24	179.9992	0.0005	0.0001	179.9987	1.3396	1.4670	1.0896
S25	179.9999	0.0003	0.0003	180.0000	1.3391	1.4665	1.0892
S26	179.9996	0.0023	0.0027	180.0000	1.3391	1.4666	1.0892
S27	177.6424	3.7332	3.6974	174.9270	1.3446	1.4710	1.0888
S28	177.6876	3.6459	3.6473	175.0191	1.3443	1.4704	1.0886
S29	177.3934	3.7239	3.8616	175.0211	1.3443	1.4704	1.0886
S30	177.7531	3.6392	3.6659	174.9418	1.3447	1.4701	1.0887
S31	177.5683	3.7211	3.7754	174.9351	1.3452	1.4695	1.0889
S32	178.2420	3.3697	3.3716	175.0167	1.3446	1.4712	1.0889
S33	177.6500	3.6802	3.5572	175.1125	1.3448	1.4700	1.0887
S34	177.7940	3.5790	3.4929	175.1340	1.3440	1.4704	1.0886
S35	176.2874	4.0365	4.8199	174.8562	1.3443	1.4671	1.0877
S36	178.1448	3.5660	5.0360	173.2532	1.3442	1.4773	1.0879
S37	179.1052	2.7783	5.8495	172.2670	1.3437	1.4760	1.0893
S38	179.1446	2.8540	5.4158	172.5856	1.3435	1.4758	1.0892
S39	179.5415	2.6124	1.5581	175.3710	1.3455	1.4704	1.0891
S40	179.7934	2.8115	1.4389	175.5429	1.3463	1.4686	1.0893
S41	179.9996	0.0003	0.0040	179.9953	1.3379	1.4686	1.0896
S42	179.8717	0.6171	0.0616	179.4497	1.3390	1.4687	1.0892
S43	178.3411	3.3526	4.6877	173.6186	1.3434	1.4753	1.0902
S44	179.9995	0.0016	0.0003	179.9985	1.3394	1.4674	1.0895
S45	179.9952	0.0002	0.0084	179.9967	1.3420	1.4697	1.0888
S46	177.8126	3.1169	1.8125	177.2580	1.3365	1.4737	1.0906
S47	179.9760	0.5476	0.3267	179.1016	1.3343	1.4760	1.0894
S48	179.3716	0.7182	0.9070	97.1084	1.3307	1.5048	1.0901
S49	178.7266	0.5289	1.5404	20.0197	1.3311	1.5006	1.0910
S50	179.5078	0.6110	0.9180	38.9977	1.3305	1.5014	1.0910
S51	179.1462	0.4351	1.0580	48.6381	1.3307	1.5010	1.0912
S52	179.5008	0.4123	0.6835	5.7260	1.3306	1.5010	1.0912
S53	179.3462	0.3890	0.8600	33.1536	1.3307	1.5009	1.0912
S54	179.7729	0.7838	0.6689	48.8929	1.3305	1.5046	1.0899
S55	179.7798	0.4633	0.4406	68.3028	1.3298	1.5074	1.0898
S56	179.8134	0.6119	0.4829	45.0576	1.3304	1.5049	1.0899
S57	179.2024	3.1418	2.0790	175.5768	1.3442	1.4711	1.0889
S58	179.9645	0.0728	0.0436	2.4020	1.3444	1.4512	1.0869
S59	178.2335	2.7811	2.7256	129.0623	1.3418	1.4684	1.0901
S60	179.9315	0.1492	0.2959	14.2772	1.3341	1.4972	1.0903
S61	179.7282	0.2036	0.0100	22.5019	1.3335	1.4932	1.0897
S62	179.9041	0.0328	0.1599	1.4071	1.3395	1.4941	1.0887
S63	179.0893	0.8427	0.6948	52.0092	1.3399	1.4977	1.0896
S64	175.2911	4.1911	4.7162	175.8017	1.3509	1.5064	1.5067
S65	177.3708	3.6438	0.0457	178.9397	1.3421	1.5052	1.5093
S66	175.3640	4.3504	3.1429	177.1427	1.3454	1.4912	1.4889

	AD(8-10)	**AD(8-11)**	**fp(7)**	**fm(7)**	**fp(8)**	**fm(8)**	**fp(9)**
S1	1.5048	1.5090	-0.1420	-0.0534	-0.1434	-0.2207	-0.0371
S2	1.5043	1.5100	-0.1209	-0.0548	-0.1436	-0.2121	-0.0361
S3	1.5081	1.5166	-0.0918	-0.0739	-0.1661	-0.2043	-0.0466
S4	1.0873	1.4908	-0.1408	-0.0226	-0.1597	-0.2456	-0.0369
S5	1.0872	1.4915	-0.1251	-0.0243	-0.1604	-0.2374	-0.0356
S6	1.0872	1.4905	-0.1474	-0.0158	-0.1617	-0.2413	-0.0381
S7	1.0870	1.4898	-0.1439	0.0027	-0.1574	-0.2189	-0.0369
S8	1.0872	1.4899	-0.1466	0.0026	-0.1573	-0.2222	-0.0372
S9	1.0867	1.4903	-0.1406	-0.0074	-0.1585	-0.2235	-0.0368
S10	1.0875	1.4909	-0.1505	-0.0035	-0.1592	-0.2188	-0.0347
S11	1.0871	1.4912	0.0068	-0.0037	-0.0143	-0.2116	-0.0031
S12	1.0865	1.0851	0.0060	-0.0573	-0.0186	-0.2623	-0.0038
S13	1.5055	1.5048	-0.0332	-0.1582	-0.1538	-0.2228	-0.0417

S14	1.5051	1.5041	0.0229	-0.1970	-0.0839	-0.2257	-0.0246
S15	1.5047	1.5037	0.0256	-0.2458	-0.0648	-0.2352	-0.0198
S16	1.5051	1.5045	0.0152	-0.1244	-0.0689	-0.2007	-0.0200
S17	1.5053	1.5046	-0.0237	-0.1475	-0.1470	-0.2175	-0.0393
S18	1.0894	1.4948	0.0182	-0.2184	-0.0401	-0.2593	-0.0135
S19	1.0899	1.4958	0.0336	-0.1839	-0.0622	-0.2545	-0.0095
S20	1.0898	1.4950	0.0329	-0.2017	-0.0703	-0.2540	-0.0116
S21	1.0908	1.4936	0.0159	-0.2536	-0.0654	-0.2497	-0.0271
S22	1.5046	1.5042	-0.0074	-0.1770	-0.1442	-0.2237	-0.0365
S23	1.0893	1.4950	0.0210	-0.1806	-0.0902	-0.2485	-0.0174
S24	1.0849	1.4778	-0.1629	-0.0034	-0.1399	-0.2362	-0.0386
S25	1.0849	1.4787	-0.1479	-0.0049	-0.1424	-0.2266	-0.0373
S26	1.0849	1.4787	-0.1472	-0.0060	-0.1430	-0.2250	-0.0376
S27	1.5030	1.4961	-0.1654	-0.0327	-0.1258	-0.2101	-0.0377
S28	1.5026	1.4971	-0.1467	-0.0340	-0.1280	-0.2025	-0.0366
S29	1.5026	1.4971	-0.1457	-0.0354	-0.1286	-0.2015	-0.0369
S30	1.5030	1.4960	-0.1735	-0.0232	-0.1268	-0.2045	-0.0383
S31	1.5031	1.4953	-0.1701	-0.0007	-0.1237	-0.1856	-0.0374
S32	1.5028	1.4961	-0.1657	-0.0103	-0.1244	-0.1873	-0.0379
S33	1.5029	1.4962	-0.1605	-0.0235	-0.1267	-0.2027	-0.0375
S34	1.5024	1.4970	-0.1558	-0.0216	-0.1282	-0.1908	-0.0370
S35	1.5024	1.4962	-0.1625	-0.0111	-0.1277	-0.1897	-0.0353
S36	1.5073	1.4956	-0.1817	-0.0158	-0.1246	-0.1828	-0.0405
S37	1.5069	1.4986	-0.1843	-0.0217	-0.1280	-0.1865	-0.0395
S38	1.5068	1.4992	-0.1804	-0.0264	-0.1279	-0.1905	-0.0392
S39	1.5076	1.4966	-0.1758	-0.0060	-0.1282	-0.2059	-0.0379
S40	1.5075	1.4951	-0.1792	0.0184	-0.1258	-0.1825	-0.0378
S41	1.0876	1.4897	-0.1379	-0.0298	-0.1603	-0.2423	-0.0364
S42	1.0838	1.4927	-0.1449	-0.0821	-0.1595	-0.0570	-0.0365
S43	1.5096	1.5106	0.0188	-0.2176	-0.1069	-0.2290	-0.0316
S44	1.0849	1.4813	-0.1604	-0.0067	-0.1398	-0.2378	-0.0382
S45	1.0882	1.4691	-0.1458	-0.0874	-0.0927	-0.1993	-0.0311
S46	1.0893	1.4981	-0.0832	-0.0633	-0.1929	-0.2324	-0.0387
S47	1.0865	1.0852	-0.0723	-0.0623	-0.2281	-0.2679	-0.0377
S48	1.0880	1.0860	0.0054	0.0169	-0.0325	-0.0329	-0.0068
S49	1.0881	1.0860	0.0025	0.0164	-0.0046	-0.0481	-0.0022
S50	1.0880	1.0861	0.0029	0.0146	-0.0048	-0.0244	-0.0026
S51	1.0880	1.0862	0.0007	0.0003	-0.0007	-0.0005	-0.0001
S52	1.0880	1.0861	0.0063	0.0049	-0.0105	-0.0080	-0.0035
S53	1.0880	1.0862	0.0014	0.0015	-0.0017	-0.0029	-0.0005
S54	1.0879	1.0860	0.0114	0.0187	-0.0237	-0.0566	-0.0053
S55	1.0878	1.0859	0.0058	0.0165	-0.0620	-0.0455	-0.0111
S56	1.0879	1.0860	0.0125	0.0138	-0.0405	-0.0678	-0.0114
S57	1.5050	1.5034	-0.0005	-0.3035	-0.1517	-0.2458	-0.0392
S58	1.5048	1.5003	0.0040	-0.1548	-0.1150	-0.2150	-0.0237
S59	1.5025	1.5036	0.0075	-0.1146	-0.0091	-0.1918	-0.0054
S60	1.0888	1.4913	-0.2884	-0.1348	-0.1537	-0.0388	-0.0509
S61	1.0888	1.4906	-0.2856	-0.0803	-0.1462	0.0222	-0.0528
S62	1.5052	1.5084	-0.2773	-0.0652	-0.1281	0.0193	-0.0481
S63	1.5056	1.5075	-0.2736	-0.0167	-0.1200	0.0063	-0.0463
S64	1.4935	1.5065	-0.2080	-0.1899	-0.0872	-0.1715	0.0235
S65	1.0874	1.4909	-0.0044	-0.0628	0.0036	0.0231	0.0003
S66	1.0892	1.4977	0.0178	-0.1302	-0.0500	-0.2299	-0.1190

	fm(9)	L-R1	B1-R1	B5-R1	L-R2	B1-R2	B5-R2
S1	-0.0349	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400
S2	-0.0337	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400
S3	-0.0410	4.0400	1.5000	3.0600	4.0500	1.8800	3.1800
S4	-0.0313	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S5	-0.0303	4.0500	1.5000	3.0600	2.0600	1.0000	1.0000
S6	-0.0310	4.0500	1.5000	3.0600	2.0600	1.0000	1.0000
S7	-0.0290	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S8	-0.0292	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S9	-0.0301	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S10	-0.0297	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S11	-0.0279	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S12	-0.0352	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S13	-0.0412	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S14	-0.0397	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S15	-0.0398	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S16	-0.0380	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S17	-0.0407	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S18	-0.0394	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S19	-0.0363	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S20	-0.0353	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S21	-0.0414	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S22	-0.0365	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S23	-0.0382	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S24	-0.0310	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000
S25	-0.0299	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000
S26	-0.0299	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000
S27	-0.0346	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S28	-0.0334	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S29	-0.0334	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S30	-0.0344	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S31	-0.0325	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S32	-0.0336	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S33	-0.0340	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S34	-0.0327	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S35	-0.0330	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400
S36	-0.0366	4.8800	1.6200	3.4200	4.0700	1.5500	3.1600
S37	-0.0362	4.8800	1.6200	3.4200	6.3800	1.5600	4.4600
S38	-0.0358	4.8800	1.6200	3.4200	6.4600	1.5800	4.6900
S39	-0.0327	4.8800	1.6200	3.4200	5.6000	1.5400	3.2200
S40	-0.0306	4.8800	1.6200	3.4200	5.6100	1.5400	3.2100
S41	-0.0311	4.9900	1.6300	3.4000	2.0600	1.0000	1.0000
S42	-0.0186	5.0400	1.5200	4.2000	2.0600	1.0000	1.0000
S43	-0.0387	4.0800	1.5100	4.4700	4.0700	1.5100	4.4700
S44	-0.0311	6.0800	2.0100	3.5700	2.0600	1.0000	1.0000
S45	-0.0312	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S46	-0.0363	8.4200	2.7400	6.1200	2.0600	1.0000	1.0000
S47	-0.0360	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S48	-0.0105	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S49	-0.0130	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S50	-0.0085	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S51	0.0000	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000

S52	-0.0028	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S53	-0.0006	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S54	-0.0163	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S55	-0.0071	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S56	-0.0182	2.0600	1.0000	1.0000	2.0600	1.0000	1.0000
S57	-0.0403	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S58	-0.0388	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S59	-0.0464	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S60	-0.0184	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000
S61	-0.0121	8.0000	1.6800	5.1400	2.0600	1.0000	1.0000
S62	-0.0083	8.0000	1.6800	5.1400	3.0000	1.5200	2.0400
S63	-0.0023	7.0000	1.5000	6.3600	3.0000	1.5200	2.0400
S64	0.0288	4.0400	1.5000	3.0600	6.2800	3.1100	3.1100
S65	0.0050	6.7800	1.6000	10.5800	2.0600	1.0000	1.0000
S66	0.0350	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000

	L-R3	**B1-R3**	**B5-R3**	**L-R4**	**B1-R4**	**B5-R4**
S1	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S2	8.1000	1.9000	3.1600	2.0600	1.0000	1.0000
S3	6.2800	3.1100	x	2.0600	1.0000	1.0000
S4	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S5	7.7600	1.5000	3.2600	2.0600	1.0000	1.0000
S6	6.9100	1.5000	3.2400	2.0600	1.0000	1.0000
S7	9.5300	1.8000	4.1900	2.0600	1.0000	1.0000
S8	7.2800	1.5300	3.1600	2.0600	1.0000	1.0000
S9	6.3500	1.6100	4.2900	2.0600	1.0000	1.0000
S10	6.3500	1.5800	4.3800	2.0600	1.0000	1.0000
S11	12.1800	1.6900	4.6100	2.0600	1.0000	1.0000
S12	12.5200	1.5100	4.2000	2.0600	1.0000	1.0000
S13	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S14	7.7900	1.5000	3.1600	2.0600	1.0000	1.0000
S15	7.6200	1.5000	3.1600	2.0600	1.0000	1.0000
S16	10.5100	1.8000	3.5600	2.0600	1.0000	1.0000
S17	11.9100	1.8900	5.9800	2.0600	1.0000	1.0000
S18	6.9000	1.5000	4.9000	2.0600	1.0000	1.0000
S19	6.3400	1.5200	4.8500	2.0600	1.0000	1.0000
S20	8.4700	1.5900	4.8100	2.0600	1.0000	1.0000
S21	8.8400	2.4500	4.8100	2.0600	1.0000	1.0000
S22	6.3700	1.6300	4.8300	2.0600	1.0000	1.0000
S23	7.6300	1.5000	3.2400	2.0600	1.0000	1.0000
S24	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S25	7.7600	1.5000	3.2600	2.0600	1.0000	1.0000
S26	8.0600	1.5000	3.2400	2.0600	1.0000	1.0000
S27	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S28	7.7600	1.5000	3.2600	2.0600	1.0000	1.0000
S29	8.0900	1.7200	3.3600	2.0600	1.0000	1.0000
S30	6.9200	1.5000	3.3600	2.0600	1.0000	1.0000
S31	7.2800	1.5400	3.3500	2.0600	1.0000	1.0000
S32	6.3400	1.6100	4.5600	2.0600	1.0000	1.0000
S33	9.2800	1.5100	3.8700	2.0600	1.0000	1.0000
S34	7.3000	1.7000	5.0500	2.0600	1.0000	1.0000
S35	7.3000	1.6600	3.7100	2.0600	1.0000	1.0000
S36	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000

S37	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S38	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S39	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S40	7.2800	1.6700	3.3900	2.0600	1.0000	1.0000
S41	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S42	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S43	8.3200	1.5200	3.3600	2.0600	1.0000	1.0000
S44	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S45	5.7800	1.5000	3.1900	2.0600	1.0000	1.0000
S46	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S47	6.2800	3.1100	3.1100	2.0600	1.0000	1.0000
S48	6.1000	1.5200	7.9400	2.0600	1.0000	1.0000
S49	10.4700	1.5400	4.5000	2.0600	1.0000	1.0000
S50	10.3000	2.0000	7.7900	2.0600	1.0000	1.0000
S51	15.9200	1.5400	13.3100	2.0600	1.0000	1.0000
S52	10.4800	1.8800	4.8800	2.0600	1.0000	1.0000
S53	12.6500	1.5500	6.1200	2.0600	1.0000	1.0000
S54	8.9400	1.5300	6.1100	2.0600	1.0000	1.0000
S55	4.5100	1.5300	6.0600	2.0600	1.0000	1.0000
S56	5.9100	1.5300	7.7200	2.0600	1.0000	1.0000
S57	6.6100	1.6500	4.5900	2.0600	1.0000	1.0000
S58	9.7400	1.5000	4.5000	2.0600	1.0000	1.0000
S59	9.2900	2.3000	5.0600	2.0600	1.0000	1.0000
S60	5.0200	1.5300	4.4800	2.0600	1.0000	1.0000
S61	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S62	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000
S63	4.1100	1.5200	3.1700	2.0600	1.0000	1.0000
S64	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400
S65	3.0000	1.5200	2.0400	4.1100	1.5200	3.1700
S66	6.2800	3.1100	3.1100	7.6400	1.5100	3.1700

Table S20. Dataset (63 parameters) for Experimentally Unknown Substrates (**P1-P84**)

	υ(7-1)	**I(7-1)**	**υ(7-8)**	**I(7-8)**	**υ(7-9)**	**I(7-9)**	**NPA1**	**NPA2**	**NPA3**
P1	1248.2700	140.8300	1746.9800	138.4700	3214.0000	0.0100	-0.0758	-0.2086	-0.2413
P2	1231.7600	170.6100	1744.8300	109.1200	3200.4500	0.3900	-0.0622	-0.1816	-0.1731
P3	1206.2000	13.5400	1741.2600	155.5400	3186.6500	0.0400	-0.0772	-0.2353	-0.0301
P4	1205.6000	18.9200	1740.4900	171.8700	3197.9400	0.6100	-0.0859	-0.2297	-0.2215
P5	1210.8400	32.2500	1748.4500	133.7600	3203.1200	1.6400	-0.1339	0.4479	-0.1305
P6	1247.6700	25.2200	1747.3200	155.4800	3196.4200	0.4700	-0.1451	-0.2001	-0.2733
P7	1255.8000	44.0400	1739.9600	140.4000	3198.0500	0.0100	-0.0846	-0.2112	-0.2590
P8	1268.5600	26.5300	1735.6400	139.3200	3184.2000	2.8400	-0.0855	-0.2101	-0.2594
P9	1265.0200	14.7100	1746.4100	121.9300	3194.9400	0.1100	-0.0640	-0.2152	-0.2193
P10	1257.5100	132.7900	1744.3200	117.1800	3198.3000	0.0900	-0.0671	-0.2184	-0.2224
P11	1255.9000	69.6900	1741.5200	122.8600	3190.4000	0.0800	-0.0618	-0.2270	-0.2097
P12	1256.4200	70.2600	1743.7600	138.4100	3210.7200	1.1000	-0.0748	-0.2233	-0.2319

P13	1253.8400	21.7900	1738.1800	173.1100	3203.5800	0.8700	-0.1000	-0.2207	-0.2488
P14	1249.0000	47.7100	1741.1300	144.8100	3193.0700	0.0200	-0.0955	-0.2148	-0.2788
P15	1257.2300	41.6300	1735.3500	173.6200	3205.1300	1.9400	-0.1230	-0.2034	-0.3412
P16	1257.3600	45.4200	1739.1700	159.1200	3193.1800	0.0300	-0.0803	-0.2197	-0.2281
P17	1259.6500	46.5800	1738.5800	174.9900	3198.4700	1.2600	-0.0977	-0.2194	-0.2459
P18	1229.9300	120.0000	1764.2900	49.3400	3180.2500	13.9800	-0.0537	-0.1947	-0.1718
P19	1201.0700	2.3900	1767.4300	18.4600	3162.0100	21.6900	-0.0752	-0.2361	-0.2219
P20	1249.5200	6.2500	1763.3500	32.0300	3210.9700	14.3700	-0.0856	-0.1147	-0.2591
P21	1248.8400	14.4700	1766.6000	36.8400	3201.3400	15.0200	-0.0412	-0.1774	-0.2228
P22	1248.7000	34.1400	1760.1700	32.3300	3225.7300	16.3900	-0.0284	-0.1685	-0.2106
P23	1323.6400	16.8300	1768.2600	40.8600	3197.2200	18.5400	-0.1247	0.4366	-0.1289
P24	1256.6700	4.1900	1762.0500	49.6500	3181.5900	21.6800	-0.0558	-0.2257	-0.2150
P25	1329.3800	6.5500	1763.7200	32.3400	3180.8500	19.1700	-0.0581	-0.2300	-0.2207
P26	1250.4800	17.5500	1768.0600	56.8600	3176.7500	20.9000	-0.0642	-0.2358	-0.2300
P27	1239.0300	70.7700	1769.5300	17.1700	3171.8300	20.8300	-0.0859	-0.2261	-0.2787
P28	1248.7100	3.0900	1767.0300	3.7300	3156.4700	18.7900	-0.1117	-0.2164	-0.3421
P29	1256.5100	3.2800	1767.3400	12.1400	3163.8900	24.2800	-0.0875	-0.2306	-0.2457
P30	1271.5300	10.8100	1761.7200	72.8000	3164.7600	26.5600	-0.0593	-0.2345	-0.2320
P31	1250.3800	147.2000	1760.1700	78.2900	3173.1900	17.7900	-0.0485	-0.1918	-0.1740
P32	1377.1800	11.4100	1762.2800	38.5200	3155.3600	13.2900	-0.0624	-0.2468	-0.0309
P33	1208.0300	1.7400	1762.1400	44.3300	3158.8800	44.7200	-0.0707	-0.2348	-0.2233
P34	1261.0300	38.1000	1759.4300	65.2100	3202.2500	14.1000	-0.0373	-0.1765	-0.2235
P35	1273.6200	0.7400	1757.6900	81.3400	3168.8000	25.1400	-0.0501	-0.2242	-0.2172
P36	1270.6000	6.5700	1759.1600	60.8500	3166.5500	24.9100	-0.0523	-0.2285	-0.2232
P37	1271.1800	8.3300	1759.3600	74.4400	3168.2500	23.7800	-0.0466	-0.2374	-0.2100
P38	1258.1700	185.6100	1763.9700	39.8400	3165.4800	31.4600	-0.0800	-0.2251	-0.2785
P39	1270.8500	1.4200	1768.0500	17.5100	3162.6600	21.0900	-0.1066	-0.2163	-0.3410
P40	1271.5100	5.6300	1762.4800	33.7800	3159.0700	39.0500	-0.0820	-0.2303	-0.2463
P41	1257.7100	20.7400	1770.8700	136.5800	3237.1500	5.2000	-0.0994	-0.2187	-0.2512
P42	1252.9600	698.0800	1751.6300	204.8900	3197.6300	0.9200	-0.0760	-0.1769	-0.1721
P43	1197.1400	2.5800	1741.2700	396.4500	3192.4400	1.9400	-0.0916	-0.2211	-0.0317
P44	1199.4800	15.3300	1741.3200	289.7000	3191.7000	4.1600	-0.1014	-0.2254	-0.2217
P45	1259.3600	405.9700	1742.9700	231.5100	3215.0900	1.9600	-0.1079	-0.1053	-0.2588
P46	1239.3000	61.3000	1748.2200	199.0500	3218.2700	3.5800	-0.0633	-0.1614	-0.2224
P47	1235.2000	50.3700	1740.3400	298.6700	3191.1200	0.5500	-0.1497	-0.2023	-0.2530
P48	1331.0700	0.8600	1746.2500	275.0600	3211.7200	3.0100	-0.0801	-0.2073	-0.2174

P49	1325.1300	3.0000	1746.6200	243.1200	3212.5500	2.5700	-0.0818	-0.2106	-0.2217
P50	1323.9800	2.7300	1744.5900	261.2300	3209.5600	0.4400	-0.0772	-0.2184	-0.2096
P51	1325.2700	11.3500	1741.4700	323.3500	3187.9700	1.8000	-0.0894	-0.2149	-0.2321
P52	1325.3200	4.2300	1739.7400	336.3800	3186.1000	1.8800	-0.1098	-0.2061	-0.2802
P53	1257.0000	776.9900	1735.0400	275.7000	3198.0800	0.6800	-0.1366	-0.2027	-0.3018
P54	1239.4300	281.0000	1752.0600	60.8100	3198.4600	0.1800	-0.0662	-0.1794	-0.1729
P55	1207.2800	22.5300	1743.8200	146.2900	3189.4100	0.5000	-0.0814	-0.2317	-0.0302
P56	1210.0800	42.0300	1744.4300	146.3900	3205.8600	1.4000	-0.0902	-0.2290	-0.2213
P57	1251.5200	123.7600	1754.4200	78.1900	3209.9300	1.4100	-0.0981	-0.1090	-0.2583
P58	1248.6300	335.7300	1754.3600	81.5400	3207.3600	2.8800	-0.0551	-0.1656	-0.2221
P59	1337.1400	284.6400	1752.9400	84.2200	3210.6000	1.2200	-0.1377	0.4502	-0.1311
P60	1336.2700	378.6200	1747.7600	104.2000	3202.8200	1.4300	-0.1514	0.4766	-0.3283
P61	1258.0500	161.7000	1747.9600	85.5800	3203.9500	0.2600	-0.0696	-0.2122	-0.2176
P62	1257.2400	303.7600	1748.8900	77.1100	3204.7700	0.1300	-0.0713	-0.2162	-0.2224
P63	1255.1600	293.9000	1745.2100	76.2900	3192.7100	0.2100	-0.0665	-0.2244	-0.2100
P64	1253.7400	278.1900	1745.0600	98.9300	3195.6700	0.3400	-0.0789	-0.2215	-0.2321
P65	1335.6800	429.5400	1742.6700	129.1800	3199.4000	0.3900	-0.1000	-0.2120	-0.2791
P66	1257.5200	285.9300	1736.2800	167.5100	3208.9600	2.6200	-0.1274	-0.2001	-0.3416
P67	1257.8000	227.5600	1740.9800	171.2800	3200.9000	1.7800	-0.1018	-0.2169	-0.2461
P68	1233.0200	125.1900	1746.5700	198.5200	3212.3100	2.4100	-0.0857	-0.2039	-0.2411
P69	1274.0800	129.1300	1751.1300	158.9200	3195.4300	0.5200	-0.0714	-0.1787	-0.1723
P70	1273.9200	32.9500	1739.3200	302.5900	3204.4600	4.2200	-0.0869	-0.2281	-0.0314
P71	1342.1300	42.0200	1745.2700	284.4300	3200.9300	3.0000	-0.0958	-0.2270	-0.2217
P72	1247.5900	24.4900	1746.2100	230.9000	3187.4500	0.2400	-0.1449	-0.2058	-0.2529
P73	1240.9900	16.2300	1741.0700	227.5200	3208.5800	0.6500	-0.1577	-0.1897	-0.2745
P74	1322.7900	4.9400	1742.3600	224.8500	3208.8700	4.9600	-0.0931	-0.2069	-0.2590
P75	1317.1800	8.4100	1725.4900	282.9500	3206.6600	0.6900	-0.0939	-0.2064	-0.2592
P76	1284.1700	105.4200	1743.2600	203.9000	3197.7200	1.4500	-0.0748	-0.2092	-0.2203
P77	1285.1200	85.7400	1746.0700	184.2000	3206.1000	0.0300	-0.0768	-0.2139	-0.2219
P78	1290.5000	120.1700	1744.5100	190.2500	3211.0000	5.6700	-0.0720	-0.2220	-0.2091
P79	1290.1500	109.4700	1743.3300	228.7000	3196.2700	0.5400	-0.0840	-0.2186	-0.2317
P80	1287.9900	146.8700	1738.6100	311.5300	3204.9900	5.8000	-0.1088	-0.2143	-0.2530
P81	1286.5600	209.0000	1741.9100	260.7900	3186.2000	1.3700	-0.1048	-0.2096	-0.2797
P82	1283.4400	298.1500	1733.8200	257.5500	3202.6900	5.1800	-0.1313	-0.1977	-0.3440
P83	1292.1000	88.0000	1744.3500	299.6700	3190.8200	2.0800	-0.0897	-0.2145	-0.2280
P84	1286.1100	162.1700	1738.9600	324.4700	3200.0700	3.1700	-0.1065	-0.2141	-0.2471

	NPA4	NPA5	NPA6	NPA7	NPA8	NPA9	NMR1	NMR2	NMR3
P1	-0.2227	-0.1849	-0.2103	-0.1914	-0.1100	0.2711	45.7567	49.4035	54.8153
P2	-0.1966	-0.1716	-0.1925	-0.1978	-0.1007	0.2746	44.2470	52.8264	51.7276
P3	-0.2447	-0.0296	-0.2436	-0.1827	-0.1214	0.2667	47.6073	56.2170	44.7265
P4	-0.0690	-0.0695	-0.2037	-0.1875	-0.1158	0.2677	49.5165	55.7902	55.7958
P5	-0.2454	-0.2520	-0.2217	-0.2005	-0.1018	0.2774	58.3346	53.9641	61.1732
P6	-0.1254	-0.3246	0.4605	-0.2273	-0.0809	0.2627	60.0017	51.7092	57.8251
P7	-0.1340	-0.2581	-0.2211	-0.1936	-0.1059	0.2696	47.6689	51.7921	53.0124
P8	-0.1338	-0.2580	-0.2185	-0.2019	-0.1014	0.2622	48.2311	50.6798	53.0417
P9	-0.1224	-0.2175	-0.2220	-0.2260	-0.0855	0.2592	44.0864	53.5855	58.4048
P10	-0.1872	-0.2219	-0.2287	-0.1934	-0.1071	0.2713	42.4335	52.6872	57.5831
P11	-0.1815	-0.2023	-0.2372	-0.1936	-0.1072	0.2710	41.2595	53.5876	55.1334
P12	-0.1448	-0.2121	-0.2338	-0.1910	-0.1118	0.2689	44.6728	54.8154	55.8007
P13	-0.0324	-0.2506	-0.2297	-0.1838	-0.1226	0.2663	50.7271	53.5060	55.3383
P14	0.3016	-0.2791	-0.2251	-0.1866	-0.1180	0.2682	50.2499	52.5984	61.3701
P15	0.3380	-0.2984	-0.2205	-0.1811	-0.1293	0.2651	56.7860	51.2745	75.8937
P16	-0.0660	-0.2264	-0.2294	-0.1896	-0.1140	0.2691	45.7919	52.3299	56.7720
P17	-0.0237	-0.2513	-0.2266	-0.1840	-0.1220	0.2663	50.2804	53.4745	56.5373
P18	-0.2069	-0.1717	-0.1909	-0.2753	-0.1742	0.2498	43.9748	54.7418	51.4300
P19	-0.0744	-0.0675	-0.2109	-0.2685	-0.1915	0.2441	48.0119	57.3972	55.7646
P20	-0.2443	-0.2488	-0.2246	-0.2742	-0.1823	0.2507	45.5778	50.3003	52.0508
P21	-0.2516	-0.2302	-0.2323	-0.2842	-0.1781	0.2511	46.3606	58.3136	58.3056
P22	-0.2589	-0.2263	-0.2399	-0.2656	-0.1954	0.2567	41.9012	57.2864	53.4320
P23	-0.2546	-0.2512	-0.2237	-0.2806	-0.1762	0.2553	57.9983	33.4661	60.3199
P24	-0.1326	-0.2188	-0.2255	-0.2745	-0.1756	0.2460	44.1346	54.8182	53.9282
P25	-0.1968	-0.2221	-0.2288	-0.2736	-0.1782	0.2454	42.8483	54.5925	57.2307
P26	-0.1546	-0.2117	-0.2353	-0.2708	-0.1852	0.2441	44.2501	57.6641	55.6161
P27	0.2928	-0.2778	-0.2253	-0.2670	-0.1937	0.2431	44.2501	57.6641	55.6161
P28	0.3282	-0.2955	-0.2211	-0.2619	-0.2074	0.2403	56.1576	54.3700	76.8440
P29	-0.0336	-0.2497	-0.2282	-0.2656	-0.1972	0.2409	50.2294	55.4971	56.8230
P30	-0.1550	-0.2124	-0.2425	-0.2813	0.0235	0.2477	42.4292	57.1315	56.3726
P31	-0.2052	-0.1723	-0.2010	-0.2864	0.0339	0.2534	42.7842	54.9041	52.1422
P32	-0.2544	-0.0302	-0.2510	-0.2745	0.0141	0.2449	45.7284	58.0240	45.3156
P33	-0.0744	-0.0678	-0.2172	-0.2783	0.0199	0.2463	47.5230	56.3937	56.2406
P34	-0.2519	-0.2312	-0.2360	-0.2950	0.0313	0.2541	46.2435	56.8058	58.3107
P35	-0.1327	-0.2184	-0.2341	-0.2844	0.0302	0.2504	41.7346	54.9969	54.8988

P36	-0.1972	-0.2218	-0.2372	-0.2837	0.0280	0.2499	40.3981	54.7619	58.3688
P37	-0.1914	-0.2018	-0.2454	-0.2839	0.0288	0.2495	39.2024	55.4952	55.4072
P38	0.2917	-0.2793	-0.2333	-0.2773	0.0169	0.2472	47.8929	54.6772	61.9664
P39	0.3266	-0.2989	-0.2293	-0.2724	0.0071	0.2439	54.4009	54.4412	76.4022
P40	-0.0347	-0.2513	-0.2364	-0.2755	0.0136	0.2449	48.1365	55.7970	57.1662
P41	-0.2388	-0.2499	-0.2285	-0.1719	0.0887	0.2872	51.3856	52.1331	55.5827
P42	-0.1871	-0.1711	-0.1744	-0.1641	-0.3376	0.2693	48.0717	51.4376	50.3472
P43	-0.2337	-0.0288	-0.2292	-0.1508	-0.3611	0.2613	51.0983	52.7934	43.9640
P44	-0.0631	-0.0713	-0.1799	-0.1549	-0.3547	0.2627	52.9924	54.3994	55.2080
P45	-0.2271	-0.2482	-0.2074	-0.1641	-0.3415	0.2683	49.5578	46.8880	51.3244
P46	-0.2350	-0.2303	-0.2158	-0.1733	-0.3384	0.2696	50.4548	55.3948	57.7476
P47	-0.2351	-0.1316	0.4562	-0.1706	-0.3431	0.2695	61.3067	49.7832	59.5824
P48	-0.1139	-0.2211	-0.2050	-0.1621	-0.3418	0.2661	47.5795	50.6420	53.5683
P49	-0.1781	-0.2232	-0.2100	-0.1610	-0.3436	0.2656	46.2576	50.2017	56.7252
P50	-0.1720	-0.2041	-0.2186	-0.1612	-0.3435	0.2651	45.3239	50.8175	54.5526
P51	-0.1346	-0.2136	-0.2159	-0.1581	-0.3502	0.2640	48.2749	52.7026	55.1753
P52	0.3116	-0.2780	-0.2064	-0.1540	-0.3586	0.2636	53.4462	50.2198	61.2985
P53	0.3488	-0.3388	-0.1937	-0.1488	-0.3733	0.2613	59.5111	49.4484	69.0796
P54	-0.1947	-0.1708	-0.1884	-0.1830	-0.1159	0.2741	45.0790	52.7849	52.0414
P55	-0.2421	-0.0292	-0.2401	-0.1677	-0.1371	0.2663	48.4473	55.7195	44.5200
P56	-0.0673	-0.0700	-0.1983	-0.1718	-0.1321	0.2674	50.2316	56.0175	55.7803
P57	-0.2340	-0.2487	-0.2190	-0.1809	-0.1216	0.2736	47.4406	47.5635	51.9398
P58	-0.2403	-0.2303	-0.2254	-0.1926	-0.1174	0.2748	49.2811	55.0968	57.9378
P59	-0.2421	-0.2516	-0.2180	-0.1861	-0.1172	0.2768	59.0694	31.2424	60.3716
P60	-0.1221	-0.2734	-0.2013	-0.1855	-0.1194	0.2762	61.1520	25.9217	66.7585
P61	-0.1198	-0.2192	-0.2202	-0.1797	-0.1210	0.2711	44.6626	52.6341	54.5641
P62	-0.1842	-0.2217	-0.2248	-0.1785	-0.1229	0.2709	43.2956	52.3783	57.4943
P63	-0.1782	-0.2023	-0.2329	-0.1786	-0.1229	0.2704	42.2410	53.1013	55.0682
P64	-0.1416	-0.2126	-0.2304	-0.1755	-0.1279	0.2689	45.3953	55.0106	56.1998
P65	0.3050	-0.2787	-0.2206	-0.1714	-0.1341	0.2678	51.0387	52.0082	61.3198
P66	0.3419	-0.2980	-0.2165	-0.1653	-0.1464	0.2648	57.3464	50.5043	75.8397
P67	-0.0201	-0.2511	-0.2224	-0.1687	-0.1381	0.2660	50.9428	53.1110	56.4678
P68	-0.2186	-0.1845	-0.1945	-0.1774	-0.3289	0.2646	48.7790	47.5332	54.2900
P69	-0.1927	-0.1718	-0.1773	-0.1830	-0.3187	0.2685	46.9810	50.6069	50.6079
P70	-0.2358	-0.0298	-0.2313	-0.1698	-0.3424	0.2604	50.7583	53.1813	44.0667
P71	-0.0656	-0.0706	-0.1867	-0.1741	-0.3356	0.2619	52.2903	54.5705	55.2347

P72	-0.2393	-0.1317	0.4519	-0.1893	-0.3247	0.2686	60.8196	50.3291	59.7934
P73	-0.1211	-0.3282	0.4777	-0.1889	-0.3271	0.2680	62.5535	47.9956	57.0971
P74	-0.1314	-0.2579	-0.2073	-0.1805	-0.3254	0.2635	50.3466	50.1932	52.5279
P75	-0.1310	-0.2581	-0.2065	-0.1708	-0.3311	0.2641	49.9899	50.0602	52.6071
P76	-0.1179	-0.2172	-0.2109	-0.1805	-0.3238	0.2653	46.8792	52.7544	60.1511
P77	-0.1823	-0.2231	-0.2141	-0.1800	-0.3247	0.2647	45.6021	50.7367	57.2124
P78	-0.1761	-0.2042	-0.2226	-0.1802	-0.3244	0.2642	44.6714	51.2813	54.5262
P79	-0.1391	-0.2135	-0.2201	-0.1771	-0.3312	0.2629	47.5923	53.2299	55.2049
P80	-0.0261	-0.2472	-0.2166	-0.1703	-0.3452	0.2607	53.2877	51.4480	54.9447
P81	0.3074	-0.2785	-0.2104	-0.1728	-0.3398	0.2626	52.9099	50.7214	61.2442
P82	0.3443	-0.2962	-0.2072	-0.1674	-0.3549	0.2601	59.0332	49.4305	76.2827
P83	-0.0604	-0.2273	-0.2153	-0.1763	-0.3337	0.2629	48.7370	50.4962	56.3970
P84	-0.0176	-0.2511	-0.2125	-0.1708	-0.3437	0.2606	52.9851	51.5906	56.2684

	NMR4	**NMR5**	**NMR6**	**NMR7**	**NMR8**	**NMR9**	**A(6-1-7)**	**A(2-1-7)**	**A(1-7-9)**
P1	58.7430	54.0069	57.5401	46.4092	51.6139	23.2162	122.5754	118.9013	115.8505
P2	60.8076	52.0525	53.2604	47.9203	49.4753	23.1764	122.6955	118.8034	115.9682
P3	54.4614	45.4315	57.2417	44.5878	54.3324	23.3059	122.7853	118.3934	115.7623
P4	52.2787	52.4358	54.7738	44.8586	52.9619	23.1454	123.3279	117.8556	115.6502
P5	54.6284	60.4403	31.3927	53.1874	50.2305	23.1741	124.0161	118.6200	116.3883
P6	47.9647	66.3073	27.9633	52.1948	48.6152	23.4513	123.0620	120.3362	115.9611
P7	48.7724	53.8479	53.3960	47.5093	52.2097	23.3297	122.9886	118.6788	115.7283
P8	48.8584	53.7214	54.2436	47.7001	46.1033	23.9374	124.0773	117.8609	114.7062
P9	37.5398	58.7847	54.4874	52.3405	43.9932	23.8200	122.9371	119.0602	114.4010
P10	54.3241	59.8117	54.6580	46.1910	51.0132	23.2043	122.7757	118.5108	115.8359
P11	55.3529	54.4959	54.5882	45.9058	51.2403	23.2027	122.7737	118.5441	115.9137
P12	48.1813	54.2989	54.5178	45.9565	52.1856	23.3036	123.2342	118.3399	115.6139
P13	43.9530	56.2216	55.2581	44.8348	54.5466	23.3173	123.3405	118.6551	115.6682
P14	35.4712	65.6108	53.6115	45.6588	53.5176	23.2804	123.0808	118.5369	115.7430
P15	27.5821	69.9997	53.8092	45.1941	56.1823	23.3668	123.4700	118.8309	115.6577
P16	44.4589	57.6045	53.9687	45.5737	52.4870	23.2140	123.0863	118.7200	115.7449
P17	30.9753	60.8209	55.3702	44.8863	54.2609	23.2603	123.5901	118.7191	115.6202
P18	62.7171	52.1323	60.8768	55.7156	51.5894	24.5600	122.8793	119.0482	115.0751
P19	52.8597	51.7331	62.5946	53.0510	54.7768	24.5121	122.9500	118.5160	115.5133
P20	56.3962	56.7706	56.8586	55.4009	51.2123	24.3762	120.9042	122.6050	116.6902
P21	57.6347	51.7295	57.2799	57.3398	50.3274	24.1586	120.8004	121.8321	117.2270
P22	57.7879	50.8891	56.3227	52.4014	53.2450	23.9440	119.5279	122.8601	117.0272

P23	56.8650	60.7481	61.1532	63.7666	53.1690	24.4546	124.2696	118.8812	115.8062
P24	38.6515	60.6942	64.3393	55.1428	53.1838	24.7852	123.6675	118.7157	114.9556
P25	55.8287	59.2426	62.6023	54.7586	53.8643	24.7599	123.2632	118.4815	114.9210
P26	49.6909	53.8718	61.8715	54.2308	54.9170	24.7189	123.0323	118.8599	115.1399
P27	49.6909	53.8718	61.8715	54.2308	54.9170	24.7189	123.1929	118.7777	114.9452
P28	28.7797	68.7235	61.2201	54.1290	61.4630	24.8982	123.3410	119.2259	114.8260
P29	33.0634	60.1847	63.0806	53.8691	58.9197	24.8601	123.6688	118.9962	114.8640
P30	50.3615	54.8427	55.1122	59.0586	42.6794	24.6413	123.0528	118.8802	114.6205
P31	62.4945	52.6173	55.0026	60.7868	39.5648	24.5866	122.9069	118.9608	114.6150
P32	57.1613	45.9045	57.7703	58.3074	45.5046	24.7801	122.7378	118.8476	114.6540
P33	53.5341	52.3088	56.4635	58.5086	43.6131	24.5701	123.4955	118.0906	114.5359
P34	58.4236	52.6606	52.2013	62.3852	41.5555	24.3358	121.3017	121.3879	115.6986
P35	39.6747	61.4979	57.4179	59.9096	40.4938	24.6749	123.4010	118.9554	114.5603
P36	56.7826	59.9278	55.3714	59.4846	41.2999	24.6335	122.9680	118.7533	114.5879
P37	57.5546	54.6594	55.2801	59.2241	41.3505	24.6531	122.9554	118.8041	114.5506
P38	37.2190	65.3798	54.1817	59.1095	44.5592	24.6747	122.9662	118.9809	114.6458
P39	29.6841	70.5098	54.2716	58.9665	47.7213	24.7914	123.1233	119.4840	114.6973
P40	34.1354	61.2872	56.0747	58.6757	45.5211	24.7127	123.4533	119.2122	114.6314
P41	53.5304	56.1644	54.4843	46.5889	36.2848	22.6730	122.8457	118.1632	116.2768
P42	56.8980	50.8668	58.5724	38.5733	64.5803	23.2316	122.6026	118.5843	115.9661
P43	50.9390	44.2720	62.3117	35.2718	69.1910	23.4174	122.5419	118.4093	115.9502
P44	50.5989	51.9793	58.6179	35.6348	68.6510	23.2445	122.9610	118.0723	115.8769
P45	52.2643	56.2765	55.2141	38.6884	63.6935	22.9188	120.7802	122.1627	117.5280
P46	53.6257	51.2205	55.7802	39.9121	62.7196	22.6693	120.6723	121.4506	118.2565
P47	52.5391	59.5164	29.5957	40.9778	62.4140	23.4976	124.1802	118.7003	114.2530
P48	34.6010	60.4245	60.6421	37.8097	65.7764	23.3754	123.1815	118.5393	115.9502
P49	51.4297	58.8938	59.2604	37.2152	66.0257	23.3253	122.7848	118.2855	115.9536
P50	52.7226	53.5258	59.2590	37.0353	65.8724	23.3395	122.6855	118.4381	116.0588
P51	45.1038	53.7164	59.0173	36.5506	67.1869	23.2655	122.7947	118.5003	116.0026
P52	32.9912	64.0567	57.7779	36.4456	68.8961	23.3387	122.8077	118.5709	115.9419
P53	24.9754	75.3389	57.2760	36.1668	72.5501	23.4802	123.1481	118.9068	115.8173
P54	60.5124	51.7925	52.3821	44.6044	50.9105	23.0548	122.8194	118.6034	115.6455
P55	53.5515	45.2256	57.0483	40.7530	55.6491	23.1658	122.7396	118.3326	115.4538
P56	51.9575	52.4974	53.9594	41.0861	54.2971	23.0043	123.0516	118.0455	115.5820
P57	54.3716	57.4315	51.6084	43.0539	52.7554	23.1386	120.9568	121.8926	116.6721
P58	55.5005	52.2939	52.0349	45.2413	51.9097	22.7783	120.8546	121.3024	116.8861

P59	53.9398	60.9118	53.9949	50.1548	51.7275	23.0614	124.3349	118.2432	116.0115
P60	46.6881	58.3640	51.8552	50.1238	52.1508	23.0516	124.2849	119.0484	115.9765
P61	36.7723	61.1555	55.8893	43.2108	51.7268	23.1298	123.2727	118.5929	115.4815
P62	53.6494	59.6894	54.3703	42.5493	52.2661	23.0891	122.7548	118.4305	115.5702
P63	54.7135	54.4004	54.2934	42.3165	52.3686	23.0967	122.7696	118.4595	115.6173
P64	47.3251	54.4824	54.1653	42.0130	53.6035	23.1609	122.9220	118.4886	115.6094
P65	34.8727	65.4388	53.2582	41.9083	54.9922	23.1571	123.1559	118.3842	115.4206
P66	26.9262	69.7805	53.5421	41.1792	58.1313	23.2322	123.6434	118.5980	115.3055
P67	30.0034	60.6444	54.9892	41.0604	55.7238	23.1326	123.5842	118.6427	115.3955
P68	56.9233	52.9003	62.6478	41.8122	63.7098	23.4944	122.7742	118.6545	116.0554
P69	59.1958	51.6174	59.0429	43.2495	61.3204	23.4300	122.7361	118.6967	116.1713
P70	52.2372	44.5306	62.5843	40.1010	66.1283	23.6517	122.7454	118.3545	116.1236
P71	51.0295	52.0016	59.7302	40.2194	65.0723	23.4151	123.1367	117.9950	116.1440
P72	53.4458	59.9004	29.7859	45.6813	58.8018	23.6764	124.1074	118.9376	114.6322
P73	46.3789	66.0682	24.7215	45.8065	59.2692	23.6870	124.8383	118.9673	114.7684
P74	46.7990	52.8415	58.7758	43.5583	64.0540	23.6635	122.9851	118.6040	116.1527
P75	46.5815	52.8845	58.5863	40.6627	67.8302	23.5656	123.0053	118.5990	116.1580
P76	35.7783	54.2156	59.4452	42.2924	62.6744	23.5362	123.0547	118.8081	116.1389
P77	52.4384	58.6247	59.6951	41.8190	62.9205	23.5257	122.9101	118.3280	116.1181
P78	53.5540	53.5948	59.8816	41.6810	62.6585	23.5431	122.8447	118.4246	116.2477
P79	46.2667	53.7890	59.6006	41.1296	63.9103	23.4851	122.9770	118.4778	116.1503
P80	41.3502	55.0708	60.4288	40.4524	67.0976	23.6286	123.1375	118.7372	116.0855
P81	33.7139	64.2441	58.5021	41.1389	65.8448	23.5549	122.9787	118.5301	116.0825
P82	25.8761	68.3394	58.6055	40.8017	68.9839	23.6567	123.3645	117.9576	117.5443
P83	42.6486	56.7797	59.0471	41.0450	64.6619	23.4573	123.1323	118.5967	116.0625
P84	28.6485	59.7877	60.3892	40.5386	66.8114	23.6049	123.3532	118.8379	116.0859

	A(1-7-8)	**A(8-7-9)**	**A(7-8-11)**	**A(7-8-10)**	**A(10-8-11)**	**D(6-1-7-8)**	**D(2-1-7-9)**	**D(2-1-7-8)**	**D(5-6-1-7)**
P1	127.9427	116.1884	115.3132	125.9624	118.7007	38.8315	35.0644	143.3005	179.6103
P2	127.6510	116.3593	115.1368	126.0704	118.7745	38.0535	34.2097	144.0284	179.9116
P3	128.4349	115.7840	115.3936	125.8887	118.6914	37.9335	33.9403	144.3997	179.0492
P4	128.5560	115.7718	115.2429	125.9375	118.8028	37.4514	32.9877	145.2203	178.7960
P5	127.1695	116.4414	115.1469	125.9585	118.8805	143.6904	140.5543	39.7619	178.1867
P6	127.2754	116.7401	115.3405	125.5243	119.1132	46.6946	41.3875	136.7825	178.5848
P7	128.2595	115.9989	115.2785	125.8587	118.8457	36.8914	32.7520	145.8581	178.6769
P8	129.0111	116.2316	115.0836	126.0020	118.5445	25.8777	21.6254	155.6464	179.7542
P9	127.2892	118.2543	119.2659	126.3343	114.1978	35.2283	29.7342	147.4830	179.0464

P10	127.9941	116.1481	115.2987	125.9606	118.7202	38.3715	34.2518	143.9643	179.2809
P11	128.0134	116.0441	115.2776	125.9951	118.7003	39.0038	34.7350	143.2172	179.5739
P12	128.4949	115.8697	115.1999	126.1032	118.6803	35.8565	31.2892	146.9390	178.9872
P13	128.5746	115.7424	115.3635	125.8515	118.7646	35.8905	31.9480	146.5792	179.0992
P14	128.3429	115.8969	115.3549	125.8843	118.7392	37.2564	33.0684	145.3433	179.3555
P15	128.7114	115.6199	115.4212	125.8080	118.7513	34.1226	30.2060	148.5209	179.1781
P16	128.3171	115.9201	115.2776	125.9861	118.7171	37.1530	33.0137	145.3719	179.1242
P17	128.6194	115.7447	115.3569	125.8475	118.7759	35.6996	31.5285	146.9568	178.9681
P18	126.1457	118.7698	123.9990	119.9456	116.0532	12.3458	10.9445	167.9197	179.4934
P19	125.8437	118.6242	124.2491	119.3736	116.3737	21.5480	19.6756	158.7146	178.7464
P20	124.4602	118.8444	124.1853	119.4245	116.3867	29.1717	27.5992	151.5588	179.4192
P21	124.2219	118.5462	124.1719	119.4581	116.3662	28.7864	27.4675	151.7133	179.3554
P22	123.9574	119.0119	124.1427	119.4120	116.4369	33.2188	30.0969	149.2242	179.2432
P23	125.3183	118.8718	123.9258	119.8411	116.2317	13.5520	12.3633	166.9284	179.7750
P24	126.5916	118.4528	123.9737	119.9546	116.0717	0.0030	0.0054	179.9924	179.9824
P25	126.6654	118.4130	123.9798	119.9865	116.0336	1.3190	1.1976	178.5077	179.6561
P26	126.3604	118.4936	124.0846	119.7427	116.1724	10.8697	9.3080	169.7782	179.8954
P27	126.7320	118.3196	19.2462	124.0406	142.9355	7.7678	7.0610	172.2769	179.7326
P28	127.0119	118.1608	124.0528	119.8516	116.0955	5.9821	5.3741	174.1933	179.7639
P29	126.9522	118.1820	124.0502	119.8835	116.0662	4.4682	3.9179	175.5700	179.7563
P30	128.0473	117.3041	120.3014	125.2494	114.4359	3.0928	33.9545	144.0472	179.8948
P31	127.7233	117.6349	120.1833	125.3108	114.4943	3.2021	32.8153	145.2363	179.2787
P32	128.1262	117.1990	120.4620	125.1735	114.3547	3.2886	34.3625	143.9163	179.0573
P33	128.1877	117.2457	120.3680	125.1350	114.4876	3.2350	33.7271	144.1782	179.5440
P34	126.8295	117.4663	120.1814	125.3554	114.4475	2.9930	39.4302	139.6867	178.9982
P35	127.9727	117.4373	120.2678	125.1981	114.5221	3.2784	32.9015	145.0460	179.1759
P36	127.9658	117.4144	120.2741	125.2260	114.4876	3.1913	33.3411	144.5284	179.2766
P37	128.0098	117.4092	120.2722	125.2452	114.4688	3.1936	32.8796	145.0413	179.5118
P38	128.0542	117.2797	120.3473	125.1806	114.4615	3.0785	34.3802	143.9208	179.3984
P39	128.0973	117.1914	120.4818	124.9941	114.5152	3.1021	34.3567	144.2274	179.4285
P40	128.1649	117.1799	120.4432	125.0777	114.4696	3.1404	33.6882	144.4675	179.4046
P41	126.6770	117.0336	115.7648	130.1136	114.1067	147.8951	31.7553	146.9072	179.3264
P42	126.4266	117.6071	119.2846	123.6917	117.0236	5.2157	4.8701	174.9757	179.8896
P43	126.9928	117.0570	95.2138	119.4430	24.2292	0.2618	0.1424	179.8410	179.9114
P44	127.0206	117.1022	119.4719	123.5292	116.9987	4.3171	3.9281	175.8667	179.9840
P45	125.1174	117.3537	119.3045	123.4790	117.2067	24.6387	23.2981	156.3252	179.8348

P46	124.5479	117.1943	119.4048	123.3888	117.1961	26.2671	25.4681	154.1089	179.5262
P47	129.1755	116.5713	118.2807	124.4718	117.2473	1.8608	1.6031	178.2334	179.9818
P48	126.7257	117.3241	119.2475	123.6996	117.0529	0.0046	0.0043	179.9918	179.9935
P49	126.7439	117.3023	119.2795	123.7097	117.0107	0.3457	0.3897	179.4456	179.6650
P50	126.5929	117.3483	119.3771	123.6137	117.0092	0.0008	0.0007	179.9991	179.9994
P51	126.7599	117.2375	119.3571	123.6119	117.0309	0.5223	0.1148	179.8215	179.7256
P52	126.9243	117.1326	119.3715	123.6127	117.0141	3.2636	2.8617	176.7323	179.4453
P53	127.3046	116.8780	119.4789	123.5606	116.9605	0.0099	0.0069	179.9922	179.9979
P54	127.5497	116.7877	115.0530	127.0321	117.9040	36.3631	32.6483	145.7874	179.8228
P55	128.3264	116.2092	115.2493	126.7933	117.9448	35.8678	32.4650	146.2933	179.2438
P56	128.0493	116.3515	115.2757	126.7061	118.0047	36.4943	32.5048	145.9169	179.1248
P57	126.4001	116.9254	115.3606	126.7143	117.9149	45.8423	43.2137	137.3713	177.6696
P58	126.5239	116.5892	115.1969	127.0279	117.7648	43.0138	40.3180	140.0214	178.2313
P59	127.1181	116.8681	115.1060	126.8973	117.9876	37.2188	33.3488	146.0808	178.0227
P60	127.2068	116.8161	115.1205	126.7941	118.0774	36.7230	32.8216	146.8948	177.5611
P61	127.9194	116.5836	115.1364	126.8861	117.9651	35.5357	31.4755	147.0306	179.2489
P62	127.8080	116.6068	115.1942	126.8607	117.9326	36.8101	32.9706	145.5653	179.1357
P63	127.8338	116.5308	115.1966	126.8457	117.9465	36.4730	32.5317	145.8560	179.3732
P64	127.9588	116.4129	115.2106	126.8559	117.9159	36.9203	33.4391	144.9111	179.9077
P65	128.2469	116.3205	115.2112	126.7473	118.0312	34.5978	30.6346	148.0442	179.2293
P66	128.6585	116.0249	115.2558	126.5803	118.1489	31.9424	28.2138	150.5167	179.3443
P67	128.3785	116.2131	115.2669	126.6673	118.0524	34.0163	30.1347	148.4922	179.1162
P68	127.0676	116.8767	32.1609	122.6020	118.0442	1.4642	1.0635	178.7323	179.8044
P69	126.7063	117.1204	32.2408	122.7178	118.0291	5.2415	4.8283	174.6376	179.5203
P70	127.3413	116.5351	32.0962	122.5416	118.0462	0.0294	0.0831	179.9038	179.8494
P71	127.2611	116.5933	32.0739	122.5206	118.0135	7.4955	6.8047	172.7271	179.7305
P72	129.1863	116.1815	32.6095	123.3646	118.1177	2.2111	1.8889	178.0062	179.8684
P73	129.0860	116.1455	32.6085	123.1800	118.3232	0.0286	0.0003	179.9879	179.9797
P74	127.0898	116.7575	32.0807	122.5970	117.9510	0.0020	0.0002	179.9988	179.9999
P75	126.8004	117.0415	32.4678	121.4473	119.7774	0.4459	0.3111	179.5606	179.9897
P76	126.9395	116.9217	32.2208	122.7094	118.0485	0.0253	0.0233	179.9762	179.9997
P77	127.0935	116.7884	32.2336	122.7385	118.0348	0.2890	0.1295	179.8523	179.8969
P78	126.9323	116.8200	32.1579	122.6197	118.0241	0.0408	0.0361	179.9578	179.9961
P79	127.1162	116.7330	32.1599	122.6131	118.0540	3.9305	3.9380	175.8073	179.6186
P80	127.3957	116.5187	32.0854	122.5575	118.0303	0.0391	0.0355	179.9620	179.9939
P81	127.2803	116.6368	32.1379	122.6217	118.0292	2.6909	2.3811	177.3610	179.5571

P82	125.7064	116.7484	32.4637	122.8145	118.8061	0.3604	0.2339	179.4009	179.5023
P83	127.3185	116.6188	32.2155	122.7321	118.0465	0.0362	0.0156	179.8557	179.6091
P84	127.3713	116.5428	32.0854	122.5650	118.0214	0.0395	0.0317	179.9598	179.9956

	D(3-2-1-7)	**D(1-7-8-11)**	**D(9-7-8-11)**	**D(1-7-8-10)**	**D(9-7-8-10)**	**AD(7-8)**	**AD(7-1)**	**AD(6-8)**	**AD(2-7)**
P1	179.8358	178.2227	3.4171	3.5835	174.7766	1.3421	1.4724	3.1427	2.4762
P2	179.8806	178.2012	3.5667	3.3841	174.8480	1.3420	1.4716	3.1347	2.4740
P3	179.9687	178.2479	3.4124	3.6527	174.6870	1.3431	1.4727	3.1525	2.4695
P4	179.4692	178.1183	3.6756	3.4009	174.8052	1.3433	1.4706	3.1483	2.4821
P5	177.8508	176.4428	3.8735	4.9430	174.7407	1.3415	1.4706	3.6684	2.5359
P6	178.8876	178.2957	3.5467	3.4313	174.7263	1.3407	1.4719	3.1731	2.4929
P7	179.3014	177.6642	3.7290	3.8673	174.7395	1.3427	1.4715	3.1484	2.4724
P8	179.7088	177.2998	0.0629	4.4269	172.8100	1.3437	1.4701	3.1430	2.4617
P9	179.6023	179.9754	2.9017	5.5070	171.6159	1.3446	1.4721	3.1246	2.4767
P10	179.8754	178.2986	3.4900	3.3773	174.8341	1.3423	1.4723	3.1461	2.4725
P11	179.8278	178.6202	3.4298	3.3050	174.6450	1.3425	1.4718	3.1501	2.4717
P12	179.5167	178.1974	3.5783	3.3143	174.9101	1.3428	1.4712	3.1535	2.4683
P13	179.8024	177.7385	3.7351	3.9351	174.5912	1.3434	1.4709	3.1557	2.4728
P14	179.7541	178.0622	3.5283	3.6579	174.7516	1.3429	1.4716	3.1531	2.4718
P15	179.9400	177.2650	4.0077	4.3716	174.3557	1.3441	1.4688	3.1554	2.4695
P16	179.9874	177.9084	3.7084	3.7155	174.6677	1.3431	1.4710	3.1523	2.4729
P17	179.6381	177.8877	3.6286	3.7553	174.7284	1.3434	1.4706	3.1589	2.4734
P18	179.4114	179.9303	1.1039	0.4879	178.3385	1.3370	1.4726	3.0349	2.4734
P19	178.8387	179.7558	1.8993	0.9647	177.3801	1.3370	1.4746	3.0384	2.4929
P20	179.8147	178.8194	2.0395	1.8912	177.2499	1.3368	1.4744	3.0105	2.5234
P21	179.7171	179.0520	1.7773	1.6846	177.4861	1.3367	1.4779	3.0039	2.5223
P22	178.0905	178.2519	2.4395	2.8429	176.4657	1.3369	1.4779	2.9929	2.5379
P23	179.8948	179.5746	1.1535	0.8770	178.3949	1.3367	1.4724	3.0470	2.4704
P24	179.9791	179.9798	0.0068	0.0080	179.9946	1.3376	1.4721	3.0462	2.4751
P25	179.6187	179.7727	0.0765	0.1289	179.8250	1.3373	1.4734	3.0431	2.4724
P26	178.9890	179.8446	1.0967	0.3710	178.6877	1.3373	1.4732	3.0408	2.4755
P27	179.5044	9.4514	169.8667	179.9650	0.7169	1.3369	1.4739	3.0471	2.4756
P28	179.7637	179.7807	0.6647	0.3473	179.2073	1.3373	1.4730	3.0552	2.4760
P29	179.7300	179.9032	0.4303	0.0516	179.4214	1.3372	1.4739	3.0566	2.4783
P30	179.0643	178.9516	3.0928	2.4513	175.5043	1.3433	1.4751	3.1552	2.4790
P31	179.3630	178.7974	3.2021	2.5125	175.4879	1.3433	1.4740	3.1419	2.4777
P32	179.1867	178.4702	3.2886	2.7326	175.5086	1.3431	1.4771	3.1526	2.4815

P33	179.6906	178.9083	3.2350	2.2750	175.5817	1.3435	1.4748	3.1518	2.4893
P34	178.8332	177.9038	2.9930	3.6187	175.4845	1.3426	1.4786	3.1257	2.5183
P35	179.4471	178.8250	3.2784	2.5038	175.3928	1.3436	1.4734	3.1537	2.4808
P36	179.3925	178.9912	3.1913	2.3549	175.4626	1.3434	1.4748	3.1517	2.4781
P37	179.6742	178.9367	3.1936	2.4918	175.3779	1.3437	1.4740	3.1502	2.4781
P38	179.7775	178.6590	3.0785	2.5899	175.6726	1.3431	1.4762	3.1552	2.4819
P39	179.6407	178.3441	3.1021	2.8005	175.7533	1.3429	1.4760	3.1606	2.4835
P40	179.6039	178.7441	3.1404	2.4399	175.6755	1.3431	1.4759	3.1625	2.4842
P41	179.8159	177.1486	4.1978	4.3589	174.2947	1.3393	1.4683	3.1066	2.4631
P42	179.8170	179.5665	0.5900	0.5436	179.2999	1.3375	1.4682	3.0206	2.4658
P43	179.9308	179.9936	0.0231	0.0095	179.9738	1.3397	1.4667	3.0309	2.4598
P44	179.9221	179.8169	0.3904	0.3149	179.4778	1.3397	1.4673	3.0280	2.4800
P45	179.7532	178.9121	1.4641	2.2620	177.3619	1.3380	1.4683	2.9991	2.5133
P46	179.4522	179.3072	1.1118	1.8990	177.6820	1.3375	1.4734	2.9937	2.5132
P47	179.9495	179.8721	0.0388	0.0412	179.7921	1.3399	1.4646	3.0991	2.4668
P48	179.9935	179.9930	0.0030	0.0022	179.9982	1.3386	1.4673	3.0342	2.4675
P49	179.6321	179.7701	0.0632	0.1048	179.9381	1.3384	1.4684	3.0300	2.4644
P50	179.9999	179.9980	0.0018	0.0008	179.9991	1.3388	1.4678	3.0260	2.4651
P51	179.3244	179.9428	0.1216	0.0667	179.9977	1.3391	1.4671	3.0307	2.4648
P52	179.6283	179.6529	0.0632	0.1414	179.4483	1.3396	1.4660	3.0333	2.4657
P53	179.9993	179.9971	0.0019	0.0046	179.9944	1.3416	1.4621	3.0428	2.4695
P54	179.8035	178.0751	3.5047	3.1558	175.2644	1.3433	1.4709	3.1273	2.4724
P55	179.9849	177.5905	3.6590	3.7364	175.0140	1.3447	1.4716	3.1418	2.4667
P56	179.8710	177.9300	3.6587	3.4417	174.9697	1.3451	1.4696	3.1307	2.4836
P57	177.7767	176.1313	3.2823	5.0576	175.5288	1.3423	1.4726	3.1224	2.5124
P58	178.5302	176.1528	3.5087	5.0558	175.2827	1.3426	1.4757	3.1090	2.5135
P59	178.4269	176.8644	3.7102	4.2664	175.1590	1.3430	1.4693	3.1525	2.4598
P60	177.9875	176.3360	3.9497	4.7248	174.9896	1.3435	1.4678	3.1498	2.4694
P61	179.8456	177.9873	3.5207	3.3244	175.1676	1.3440	1.4700	3.1387	2.4723
P62	179.8026	177.9144	3.5628	3.4067	175.1161	1.3438	1.4716	3.1360	2.4707
P63	179.9899	177.8881	3.7369	3.3618	175.0132	1.3441	1.4709	3.1363	2.4698
P64	179.6005	178.2013	3.4598	3.3642	174.9747	1.3442	1.4709	3.1429	2.4696
P65	179.7051	177.6495	3.6818	3.5504	175.1184	1.3448	1.4700	3.1419	2.4686
P66	179.8241	177.4557	3.8215	3.9885	174.7343	1.3463	1.4667	3.1492	2.4651
P67	179.8395	177.7964	3.5861	3.5678	175.0497	1.3452	1.4692	3.1479	2.4712
P68	179.9504	179.7150	0.0794	0.0254	179.8198	1.3369	1.4691	3.0355	2.4686

P69	179.4538	179.7956	0.3342	0.2210	179.2404	1.3361	1.4689	3.0297	2.4657
P70	179.9995	179.9931	0.0062	0.0064	179.9804	1.3381	1.4685	3.0407	2.4629
P71	179.6485	179.7542	0.7158	0.4691	179.0609	1.3378	1.4689	3.0389	2.4804
P72	179.9627	179.9355	0.1707	0.1672	179.7265	1.3382	1.4657	3.0979	2.4709
P73	179.9857	179.9899	0.0018	0.0114	179.9767	1.3389	1.4638	3.1089	2.4697
P74	179.9996	179.9983	0.0007	0.0002	179.9992	1.3375	1.4681	3.0404	2.4668
P75	179.9986	179.6148	0.2559	0.2146	179.6560	1.3388	1.4681	3.0361	2.4668
P76	179.9971	179.9924	0.0081	0.0032	179.9963	1.3373	1.4676	3.0399	2.4651
P77	179.8791	179.9993	0.0176	0.0031	179.9848	1.3370	1.4693	3.0396	2.4655
P78	179.9949	179.9957	0.0018	0.0028	179.9967	1.3373	1.4687	3.0359	2.4659
P79	179.5737	179.9904	0.2656	0.3674	179.3766	1.3375	1.4684	3.0427	2.4658
P80	179.9919	179.9947	0.0078	0.0017	179.9992	1.3385	1.4668	3.0495	2.4663
P81	179.7600	179.9171	0.1763	0.1253	179.6156	1.3378	1.4677	3.0440	2.4666
P82	179.4344	179.2962	0.3412	0.3357	179.9732	1.3607	1.4251	3.0085	2.4475
P83	179.7762	179.7054	0.1339	0.1232	179.9626	1.3377	1.4673	3.0472	2.4664
P84	179.9979	179.9920	0.0005	0.0093	179.9992	1.3384	1.4669	3.0507	2.4700

	AD(7-9)	**fp(1)**	**fp(7)**	**fp(8)**	**fp(9)**	**fm(1)**	**fm(7)**	**fm(8)**	**fm(9)**
P1	1.0884	-0.0598	-0.1142	-0.1419	-0.0362	-0.0569	-0.1023	-0.2402	-0.0359
P2	1.0883	-0.0861	-0.0813	-0.1394	-0.0342	-0.0211	-0.1475	-0.2547	-0.0357
P3	1.0890	-0.0338 -	-0.1479	-0.1417	-0.0373	-0.1255	-0.0193	-0.1927	-0.0329
P4	1.0889	-0.0672	-0.0582	-0.1137	-0.0271	-0.0940	0.0247	-0.0855	-0.0214
P5	1.0876	-0.0580	-0.1125	-0.1464	-0.0345	0.0093	0.0303	-0.0404	-0.0148
P6	1.0882	-0.0582	-0.1138	-0.1407	-0.0373	-0.0981	-0.0645	-0.2033	-0.0365
P7	1.0885	-0.0550	-0.1171	-0.1442	-0.0359	-0.0872	-0.0600	-0.2133	-0.0338
P8	1.0888	-0.0671	-0.0993	-0.1520	-0.0353	-0.0633	-0.0814	-0.2204	-0.0352
P9	1.0889	-0.0990	-0.0360	-0.1163	-0.0312	-0.0570	-0.1029	-0.2242	-0.0377
P10	1.0885	-0.0744	-0.0944	-0.1392	-0.0346	-0.0408	-0.1180	-0.2464	-0.0354
P11	1.0886	-0.1010	-0.0438	-0.1168	-0.0289	-0.0557	-0.0948	-0.2330	-0.0344
P12	1.0887	-0.0730	-0.0851	-0.1323	-0.0319	-0.0290	0.0115	-0.0186	-0.0051
P13	1.0889	-0.0292	-0.1482	-0.1420	-0.0368	-0.1319	-0.0158	-0.1945	-0.0330
P14	1.0887	-0.0388	-0.1384	-0.1433	-0.0369	-0.1092	-0.0410	-0.2102	-0.0344
P15	1.0890	-0.0129	-0.1672	-0.1416	-0.0378	-0.1651	0.0216	-0.1568	-0.0293
P16	1.0888	-0.0842	-0.0420	-0.1033	-0.0251	-0.1121	-0.0249	-0.1862	-0.0314
P17	1.0889	-0.0299	-0.1471	-0.1419	-0.0368	-0.1289	-0.0179	-0.1953	-0.0329
P18	1.0895	-0.1307	-0.0193	-0.1732	-0.0321	-0.0066	-0.1807	-0.2552	-0.0391
P19	1.0907	-0.0778	0.0021	-0.1038	-0.0220	-0.0954	-0.0193	-0.1370	-0.0284

P20	1.0878	-0.1262	-0.0344	-0.1889	-0.0319	-0.0520	-0.1223	-0.2330	-0.0318
P21	1.0876	-0.1417	-0.0214	-0.1740	-0.0340	-0.0333	-0.1431	-0.2376	-0.0353
P22	1.0862	-0.1141	0.0205	-0.0965	-0.0195	-0.0195	-0.1534	-0.2497	-0.0354
P23	1.0876	-0.1134	-0.0358	-0.1854	-0.0326	-0.0393	-0.1468	-0.2437	-0.0363
P24	1.0900	-0.1225	0.0026	-0.1319	-0.0241	-0.0267	-0.1428	-0.2407	-0.0381
P25	1.0901	-0.1258	-0.0264	-0.1798	-0.0323	-0.0203	-0.1561	-0.2492	-0.0388
P26	1.0903	-0.1236	-0.0184	-0.1610	-0.0296	-0.0315	0.0083	-0.0268	-0.0061
P27	1.0904	-0.1014	-0.0519	-0.1943	-0.0355	-0.0670	-0.0998	-0.2334	-0.0371
P28	1.0910	-0.0769	-0.0787	-0.2086	-0.0384	-0.1219	-0.0306	-0.1954	-0.0322
P29	1.0908	-0.0929	-0.0587	-0.1965	-0.0358	-0.0826	-0.0786	-0.2228	-0.0359
P30	1.0900	-0.1460	0.0031	-0.1183	-0.0330	-0.0431	0.0012	-0.0399	-0.0105
P31	1.0893	-0.1611	0.0052	-0.1299	-0.0359	0.0235	-0.2414	-0.2388	-0.0411
P32	1.0903	-0.1268	-0.0358	-0.1544	-0.0409	-0.0538	-0.1248	-0.2089	-0.0401
P33	1.0903	-0.0781	0.0165	-0.0703	-0.0201	-0.0886	-0.0326	-0.1331	-0.0318
P34	1.0879	-0.1512	0.0032	-0.1280	-0.0365	0.0052	-0.2079	-0.2300	-0.0384
P35	1.0897	-0.1354	0.0178	-0.0920	-0.0263	0.0045	-0.2018	-0.2284	-0.0406
P36	1.0897	-0.1542	-0.0035	-0.1361	-0.0373	0.0124	-0.2191	-0.2356	-0.0410
P37	1.0898	-0.1485	0.0160	-0.1016	-0.0290	0.0033	-0.1974	-0.2279	-0.0401
P38	1.0900	-0.1304	-0.0299	-0.1529	-0.0406	-0.0414	-0.1457	-0.2176	-0.0408
P39	1.0904	-0.1007	-0.0560	-0.1639	-0.0435	-0.1210	-0.0415	-0.1670	-0.0364
P40	1.0903	-0.1208	-0.0381	-0.1563	-0.0406	-0.0639	-0.1131	-0.2051	-0.0397
P41	1.0865	0.0258	-0.2055	-0.0308	-0.0314	-0.1811	0.0224	-0.1598	-0.0322
P42	1.0890	-0.0500	-0.1177	-0.1466	-0.0350	-0.0786	-0.0636	-0.2704	-0.0336
P43	1.0895	-0.0117	-0.1672	-0.1378	-0.0386	-0.1532	0.0167	-0.2093	-0.0284
P44	1.0895	-0.0309	-0.1169	-0.1324	-0.0324	-0.0910	0.0264	-0.0895	-0.0183
P45	1.0874	-0.0264	-0.1496	-0.1501	-0.0309	-0.1372	-0.0044	-0.2177	-0.0256
P46	1.0874	-0.0380	-0.1392	-0.1475	-0.0346	-0.1253	-0.0154	-0.2214	-0.0302
P47	1.0894	-0.0311	-0.1379	-0.1451	-0.0364	0.0094	0.0266	-0.0451	-0.0155
P48	1.0891	-0.0559	-0.0944	-0.1343	-0.0310	-0.1013	-0.0321	-0.2447	-0.0320
P49	1.0891	-0.0400	-0.1295	-0.1440	-0.0356	-0.0937	-0.0444	-0.2604	-0.0330
P50	1.0892	-0.0562	-0.0972	-0.1339	-0.0310	-0.1038	-0.0291	-0.2467	-0.0315
P51	1.0895	-0.0352	-0.1284	-0.1381	-0.0346	-0.0279	0.0108	-0.0211	-0.0044
P52	1.0896	-0.0148	-0.1598	-0.1404	-0.0385	-0.1434	0.0031	-0.2261	-0.0303
P53	1.0898	0.0045	-0.1793	-0.1339	-0.0403	-0.1777	0.0368	-0.1744	-0.0258
P54	1.0882	-0.0599	-0.1127	-0.1309	-0.0352	-0.0379	-0.1243	-0.2473	-0.0361
P55	1.0890	-0.0148	-0.1716	-0.1243	-0.0378	-0.1396	-0.0035	-0.1832	-0.0323

P56	1.0889	-0.0456	-0.0994	-0.1133	-0.0306	-0.0905	0.0280	-0.0767	-0.0204
P57	1.0881	-0.0330	-0.1442	-0.1335	-0.0326	-0.1176	-0.0290	-0.1905	-0.0313
P58	1.0876	-0.0500	-0.1246	-0.1325	-0.0342	-0.0880	-0.0616	-0.2112	-0.0340
P59	1.0874	-0.0369	-0.1378	-0.1331	-0.0348	-0.0862	-0.0734	-0.2240	-0.0348
P60	1.0875	-0.0375	-0.1356	-0.1321	-0.0348	-0.1069	-0.0457	-0.2043	-0.0337
P61	1.0886	-0.0763	-0.0702	-0.1143	-0.0297	-0.0699	-0.0762	-0.2253	-0.0348
P62	1.0886	-0.0516	-0.1219	-0.1280	-0.0355	-0.0593	-0.0942	-0.2375	-0.0357
P63	1.0886	-0.0776	-0.0738	-0.1151	-0.0303	-0.0738	-0.0717	-0.2241	-0.0345
P64	1.0888	-0.0479	-0.1195	-0.1228	-0.0342	-0.0285	0.0114	-0.0171	-0.0047
P65	1.0888	-0.0202	-0.1605	-0.1267	-0.0375	-0.1237	-0.0235	-0.2028	-0.0340
P66	1.0889	0.0018	-0.1849	-0.1208	-0.0382	-0.1717	0.0294	-0.1526	-0.0285
P67	1.0889	-0.0124	-0.1688	-0.1239	-0.0374	-0.1430	-0.0026	-0.1865	-0.0324
P68	1.0891	-0.0467	-0.1222	-0.1619	-0.0356	-0.0867	-0.0559	-0.2626	-0.0328
P69	1.0890	-0.0663	-0.0975	-0.1613	-0.0334	-0.0573	-0.0893	-0.2778	-0.0334
P70	1.0896	-0.0309	-0.1403	-0.1573	-0.0364	-0.1386	0.0022	-0.2178	-0.0289
P71	1.0896	-0.0482	-0.0865	-0.1409	-0.0298	-0.0959	0.0233	-0.1009	-0.0196
P72	1.0895	-0.0490	-0.1147	-0.1621	-0.0347	0.0095	0.0265	-0.0458	-0.0154
P73	1.0893	-0.0492	-0.1121	-0.1610	-0.0348	-0.1034	-0.0403	-0.2487	-0.0314
P74	1.0892	-0.0440	-0.1213	-0.1616	-0.0355	-0.1036	-0.0321	-0.2322	-0.0303
P75	1.0888	-0.0376	-0.1285	-0.1617	-0.0352	-0.0137	-0.0793	-0.0665	-0.0192
P76	1.0891	-0.0762	-0.0682	-0.1419	-0.0285	-0.0806	-0.0537	-0.2579	-0.0318
P77	1.0892	-0.0584	-0.1057	-0.1594	-0.0338	-0.0734	-0.0673	-0.2681	-0.0329
P78	1.0892	-0.0760	-0.0707	-0.1433	-0.0287	-0.0837	-0.0510	-0.2549	-0.0317
P79	1.0895	-0.0548	-0.1024	-0.1523	-0.0324	-0.0285	0.0110	-0.0220	-0.0044
P80	1.0897	-0.0232	-0.1467	-0.1573	-0.0372	-0.1423	0.0026	-0.2222	-0.0292
P81	1.0897	-0.0312	-0.1377	-0.1600	-0.0367	-0.1247	-0.0154	-0.2368	-0.0306
P82	1.0879	-0.0091	-0.1619	-0.1555	-0.0386	-0.1677	0.0291	-0.1857	-0.0257
P83	1.0895	-0.0621	-0.0743	-0.1341	-0.0270	-0.1246	-0.0038	-0.2093	-0.0274
P84	1.0897	-0.0239	-0.1449	-0.1578	-0.0371	-0.1403	0.0008	-0.2206	-0.0294

	LR1	**B1R1**	**B5R1**	**LR2**	**B1R2**	**B5R2**	**LR3**	**B1R3**	**B5R3**
P1	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	6.9400	1.6100	4.8000
P2	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	6.9800	2.2800	4.9700
P3	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	6.4300	1.7300	4.3600
P4	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.5400	1.5000	4.2500
P5	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	6.3700	1.5400	4.6800
P6	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.1100	1,81	3.7100

P7	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.1000	1.8100	3.2500
P8	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.1000	1.8100	3.2500
P9	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.6200	2.6300	4.0200
P10	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	7.7000	1.8600	3.2500
P11	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	9.2000	1.7100	3.4700
P12	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	9.4600	1.9500	4.2600
P13	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	7.3000	1.5900	3.2600
P14	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	9.3800	1.5400	3.5700
P15	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.4000	1.6200	3.2700
P16	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	10.0900	1.8000	3.2800
P17	4.1500	1.5000	3.0500	3.0000	1.5200	2.0400	8.6000	2.5900	3.4200
P18	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.9800	2.2800	4.9700
P19	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	8.5400	1.5000	4.2500
P20	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.3800	1.6500	4.8300
P21	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.3800	1.7900	4.9100
P22	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.3800	3.1100	3.1100
P23	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	6.3700	1.5400	4.6800
P24	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	8.6200	2.6300	4.0200
P25	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	7.7000	1.8600	3.2500
P26	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	9.4600	1.9500	4.2600
P27	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	9.3800	1.5400	3.5700
P28	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	8.4000	1.6200	3.2700
P29	3.0000	1.5200	2.0400	2.0600	1.0000	1.0000	8.6000	2.5900	3.4200
P30	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	9.4600	1.9500	4.2600
P31	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	6.9400	2.2800	4.9700
P32	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	6.4300	1.7300	4.3600
P33	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	8.5400	1.5000	4.2500
P34	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	6.3800	1.7900	4.9100
P35	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	8.6200	2.6300	4.0200
P36	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	7.7000	1.8600	3.2500
P37	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	9.2000	1.7100	3.4700
P38	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	9.3800	1.5400	3.5700
P39	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	8.4000	1.6200	3.2700
P40	3.0000	1.5200	2.0400	3.0000	1.5200	2.0400	8.6000	2.5900	3.4200
P41	2.2400	1.5000	2.4400	2.0600	1.0000	1.0000	6.2800	3.1100	3.1100
P42	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	6.9400	2.2800	4.9700

P43	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	6.9800	1.7300	4.3600
P44	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	8.5400	1.5000	4.2500
P45	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	6.3800	1.6500	4.8300
P46	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	6.3800	1.7900	4.9100
P47	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	6.3700	1.5400	4.6800
P48	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	8.6200	2.6300	4.0200
P49	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	7.7000	1.8600	3.2500
P50	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	9.2000	1.7100	3.4700
P51	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	9.4600	1.9500	4.2600
P52	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	9.3800	1.5400	3.5700
P53	4.8800	1.6200	3.4200	2.0600	1.0000	1.0000	8.4000	1.6200	3.2700
P54	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.9800	2.2800	4.9700
P55	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.4300	1.7300	4.3600
P56	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	8.5400	1.5000	4.2500
P57	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.3800	1.6500	4.8300
P58	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.3800	1.7900	4.9100
P59	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	6.3700	1.5400	4.6800
P60	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	8.1100	1,81	3.7100
P61	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	8.6200	2.6300	4.0200
P62	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	7.7000	1.8600	3.2500
P63	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	9.2000	1.7100	3.4700
P64	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	9.4600	1.9500	4.2600
P65	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	9.3800	1.5900	3.2600
P66	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	8.4000	1.5400	3.5700
P67	4.8800	1.6200	3.4200	3.0000	1.5200	2.0400	8.6000	1.6200	3.2700
P68	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.9400	1.6100	4.8000
P69	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.9400	2.2800	4.9700
P70	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.9400	1.7300	4.3600
P71	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.9400	1.5000	4.2500
P72	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	6.3700	1.5400	4.6800
P73	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	8.1100	1,81	3.7100
P74	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	8.1000	1.8100	3.2500
P75	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	8.1000	1.8100	3.2500
P76	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	8.6200	2.6300	4.0200
P77	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	7.7000	1.8600	3.2500
P78	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	9.2000	1.7100	3.4700

P79	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	9.4600	1.9500	4.2600
P80	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	7.3000	1.5900	3.2600
P81	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	9.3800	1.5400	3.5700
P82	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	8.4000	1.6200	3.2700
P83	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	10.0900	1.8000	3.2800
P84	4.0400	1.5000	3.0600	2.0600	1.0000	1.0000	8.6000	2.5900	3.4200