Supplementary Information

Machine Learning on a Robotic Platform for the Design of Polymer-Protein Hybrids

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Chemical Space of the Seed Dataset

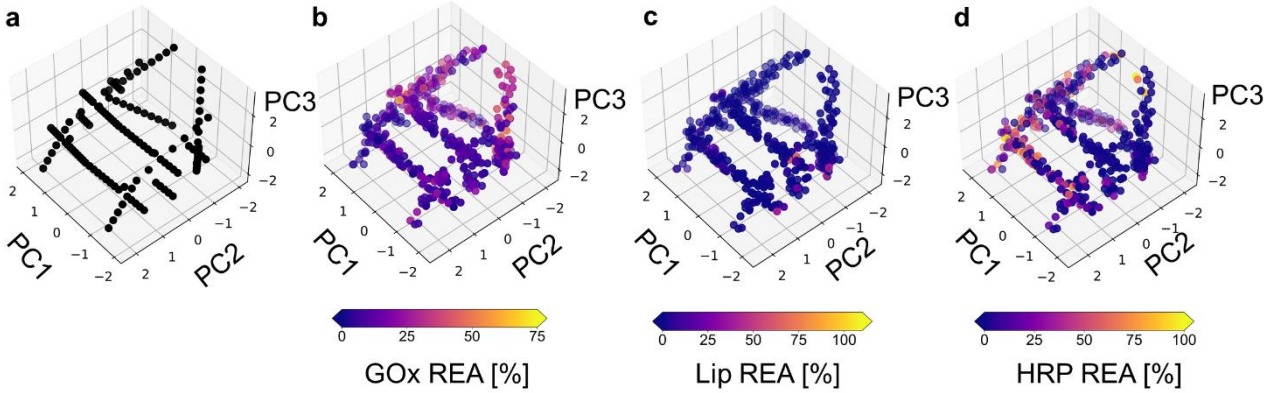

Fig. S1| Principal component analysis (PCA) was performed on the seed dataset. The data is projected onto the first three principal components and shown in panel (**a)**. Panels (**b)**, (**c)**, (**d)** add jitter to the data presented in panel A and are colored with the retained enzyme activities (REAs) measured for GOx, Lip, and HRP, respectively.

The seed dataset, represented using DP-explicit composition vectors, was mean centered and scaled to unit variance before performing principal component analysis (PCA) for dimensionality reduction. The data is projected onto the first three components, capturing 52% variation in the data, and displayed in **Fig. S1a**, revealing the systematic nature of the seed dataset construction. The first principal component (PC1), explaining the greatest source of variance in the seed dataset, is exclusively a linear combination of methyl methacrylate (MMA) and butyl methacrylate (BMA) fractions of incorporation. Increasing PC1 corresponds to increasing MMA and decreasing BMA incorporations; symmetry about PC1 = 0 indicates a number of nearly identical datapoints where the only difference is the reversal in MMA and BMA incorporations. Notably, PC1-3 contain variation from all monomer fractions of incorporations but lack any representation of degree of polymerization. Jitter added to the data shown in **Fig. S1a** is presented in **Fig. S1b-d**, revealing that many seed datapoints are compositionally identical but vary in DP. Interestingly, **Fig. S1b-d** suggest that particular regions of the chemical space are associated with particularly high REAs for each of the enzymes, with very few instances of isolated high-performers. Consistent with the results presented in **Fig. 2d-f** and **Fig. S2a-c**, these regions appear distinct for each of the enzymes, suggesting that distinct chemistries are responsible for their stabilization.

Fig. S2a-c presents the seed dataset again in reduced dimensions, but in this case are hand-crafted to hold chemical significance and are relatively easily interpreted. The ternary plots are colored by the highest measured REA of a PPH formed with a copolymer of composition given by a point in the chemical space; interpolative methods are used to color points between assayed regions. Comparison to **Fig. 2d-f**, which includes data obtained from the active learning campaigns, visually conveys the 1) improvement of REA seen from PPHs formed with copolymers suggested by the active learning, particularly in the case of GOx and Lip, and 2) the fine tuning of the REA – chemical space landscape formed from the initial seed dataset. The appearance of vast regions of the copolymer chemical space viable for HRP stabilization shown in **Fig. S2c** is slightly misleading considering the extent of the space over which interpolation takes place. Notably, the 504 copolymers constituting the seed dataset leave much of the chemical space unsampled, including the region where many of the top performing copolymers for Lip. stabilization come from. Despite this, iterations of active learning identify and exploit this region for polymer design.

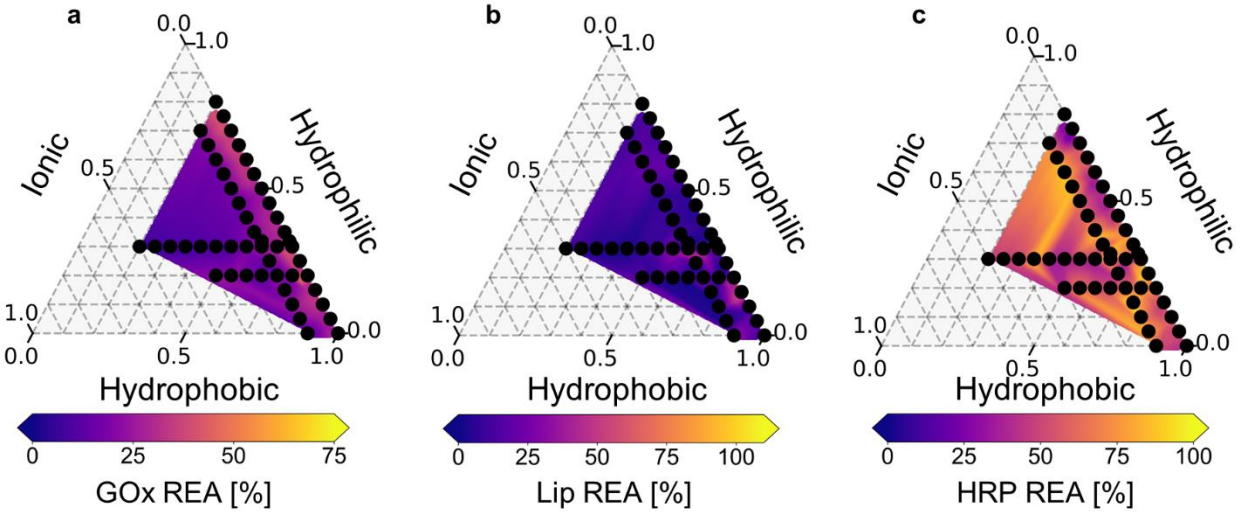

Fig. S2| Ternary plots of copolymers in the seed dataset. Monomers 1-4, 5-6, and 7-8 are grouped together as hydrophobic, hydrophilic, and ionic monomer types, respectively. Points are colored by considering the maximum REA of a copolymer found within a given region in the chemical space, thus accounting for overlaps. Extrapolative coloring is performed with linear barycentric interpolation.

Copolymer Featurization and Initial Modeling

Copolymers were numerically encoded as a weighted average of "fingerprint" vectors representing individual monomers, where the weights are set in proportion to the monomers' fraction of incorporations within the polymer being represented. One-hot encoding (OHE), Morgan fingerprints (MFP), and vectors of chemical descriptors (CD), some computed using density functional theory (DFT), were all probed as potential fingerprints used to represent monomers in the polymer featurization strategy.

The OHE is a $n-$ bit vector, *n* being the number of unique monomer types (8 in this case), where a "1" in a particular bit corresponds to the indication of a particular monomer type. The remaining bits populated with "0". MFP represent monomers as a collection of chemical structures, encoding their presence and absence with "1s" and "0s", respectively. The vector of chemical descriptors includes molecular weight, nuclear repulsion energy, dispersion correction energy, total energy, and dipole magnitude, the latter four being mean quantities computed with DFT for all conformers found using in-house code.

Linear, Gaussian process regression (GPR), and neural network (NN) models were trained to predict REA for each of the three enzymes from polymer representations (**Fig. S3**). Notably, predictive performance is insensitive to the identity of the chemical fingerprint used to encode monomer identity for any given model type and enzyme. It is likely that much of the variation in REA can be explained by variation in composition between copolymers, which is encoded in the featurization strategy regardless of the fingerprint used. Furthermore, any potential performance gain in using chemically informed monomer representations is likely masked by noise in the REA measurements. For this reason, the simple OHE was chosen to represent monomers in the polymer featurization strategy. Using this strategy, polymer representations amounted to 8-dimensional vectors, where each dimension contains the fraction of incorporation of a particular monomer. Representations are then appended with a max-normalized value of the DP, resulting in a final 9-dimensional vector.

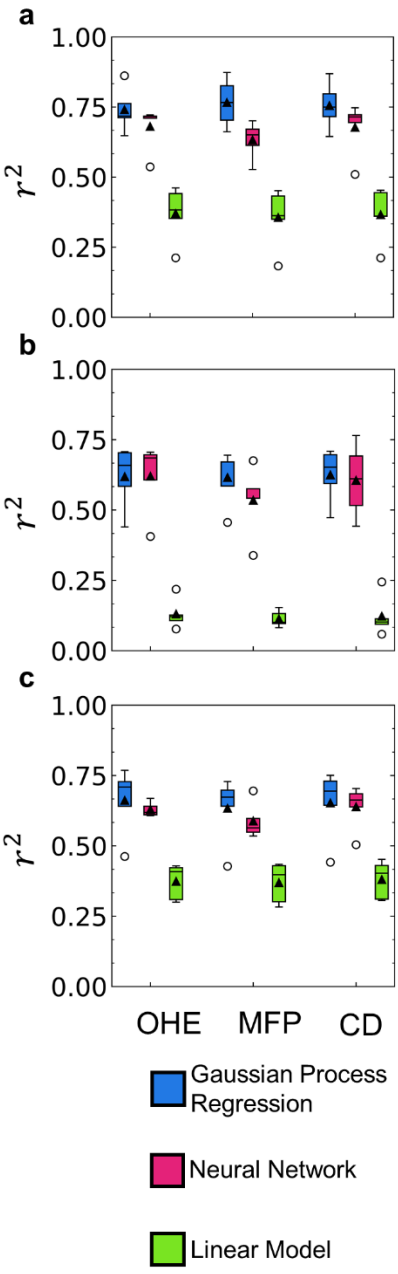

Fig. S3| Boxplots showing the distribution of coefficients of determinations obtained via K = 5 cross validation for Gaussian process regression, neural network, and linear models trained to predict GOx. (a), Lip **(b)**, and HRP **(c)**. REAs from polymer representations employing one-hot encodings (OHE), Morgan fingerprints (MFP), and vectors of chemical descriptors (CD) to represent monomers.

Fig. S3 also shows the relatively high predictive performance of nonlinear GPR and MLP models over the simple linear models for all enzymes and fingerprint types, suggesting a complex relationship between polymer chemistry and enzyme stabilization. The marginal yet consistent success of the GPR model over the NN model can likely be attributed to the relatively limited size of the seed datasets. Due to its demonstrated superior predictive performance and ability to robustly quantify uncertainty in such predictions, GPR was chosen to model PPH REA for all enzymes.

REA Distributions Through Iterations of Design

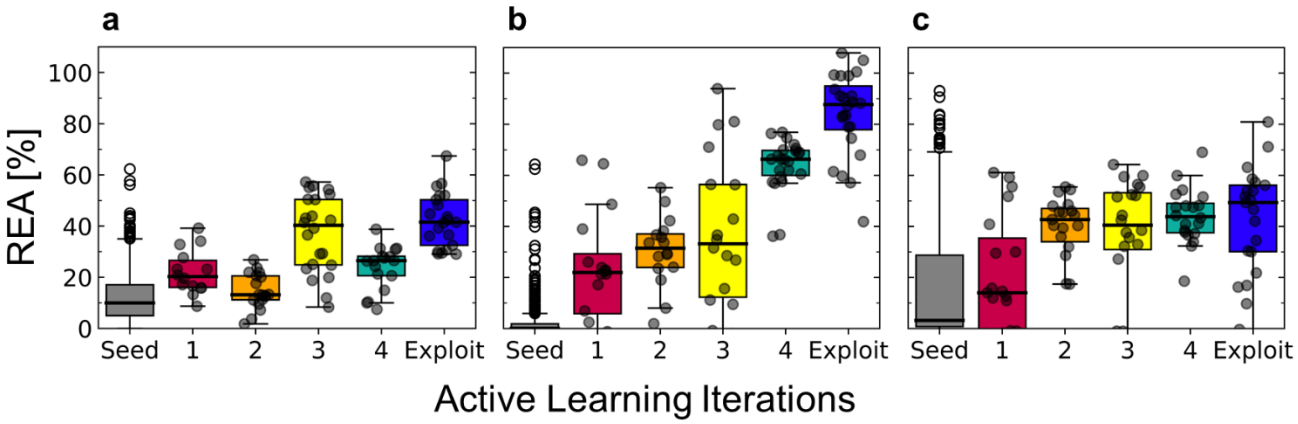

Fig. S4| Boxplots depicting the distribution of copolymer REAs found at progressive stages of the design campaign for (a) GOx, (b) Lip, (c) HRP. Distributions for iterations 1-4 and the exploit stage show the individual polymer performances. Dark lines within the boxes, bounded by the first and third quartiles, demarcate medians. Whiskers are extended to 1.5 × Interquartile Range + (-) Quartile 3 (1).

Fig. S4 depicts general upward trend in median REA of copolymers discovered at iterative stages of the active learning. In all cases, median REAs of polymers constituting the exploit iteration of all design campaigns are greater than those found at any previous iteration of design.

Model Robustness to Noise

Table S1| Measured, remeasured, and predicted REAs for four outlier points within the dataset used to train HRP models

Candidates	397	415	295	439
Measured REA	167%	113%	110%	102%
Re-measured REA	25%	18%	62%	7%
Seed Model Predictions	74%	54%	77%	37%
Iteration 1 Model Predictions	55%	50%	23%	32%
Iteration 2 Model Predictions	69%	51%	42%	39%
Iteration 3 Model Predictions	50%	47%	23%	32%
Iteration 4 Model Predictions	47%	48%	21%	31%
Iteration 5 Model Predictions	52%	51%	25%	34%

Upon completion of the active learning, it was found that none of the polymer candidates identified by the active learning for HRP had REAs above 100%. This result was surprising considering four polymers from the seed dataset were observed to pass this threshold, one even reaching an REA of 167%. Suspected to be outliers, the four polymers were resynthesized and characterized. **Table S1** shows the initial REA measurement used to label the four polymers in model training and their re-measured values. Unsurprisingly, all remeasured REAs were lower than their initial measurements, albeit in larger-than-expected amounts. To better understand potential implications on the active learning, the HRP REA models trained at every iteration we used to predict the REA of these four polymers. In all four cases, the REA predicted by the seed model and all following models is substantially lower than the label it was trained to predict and closer to the remeasured value, indicating the GPR model's robustness to noise. This robustness likely reduced the impact of these erroneous points in guiding the AL through chemical space.

Characterization of EP1:

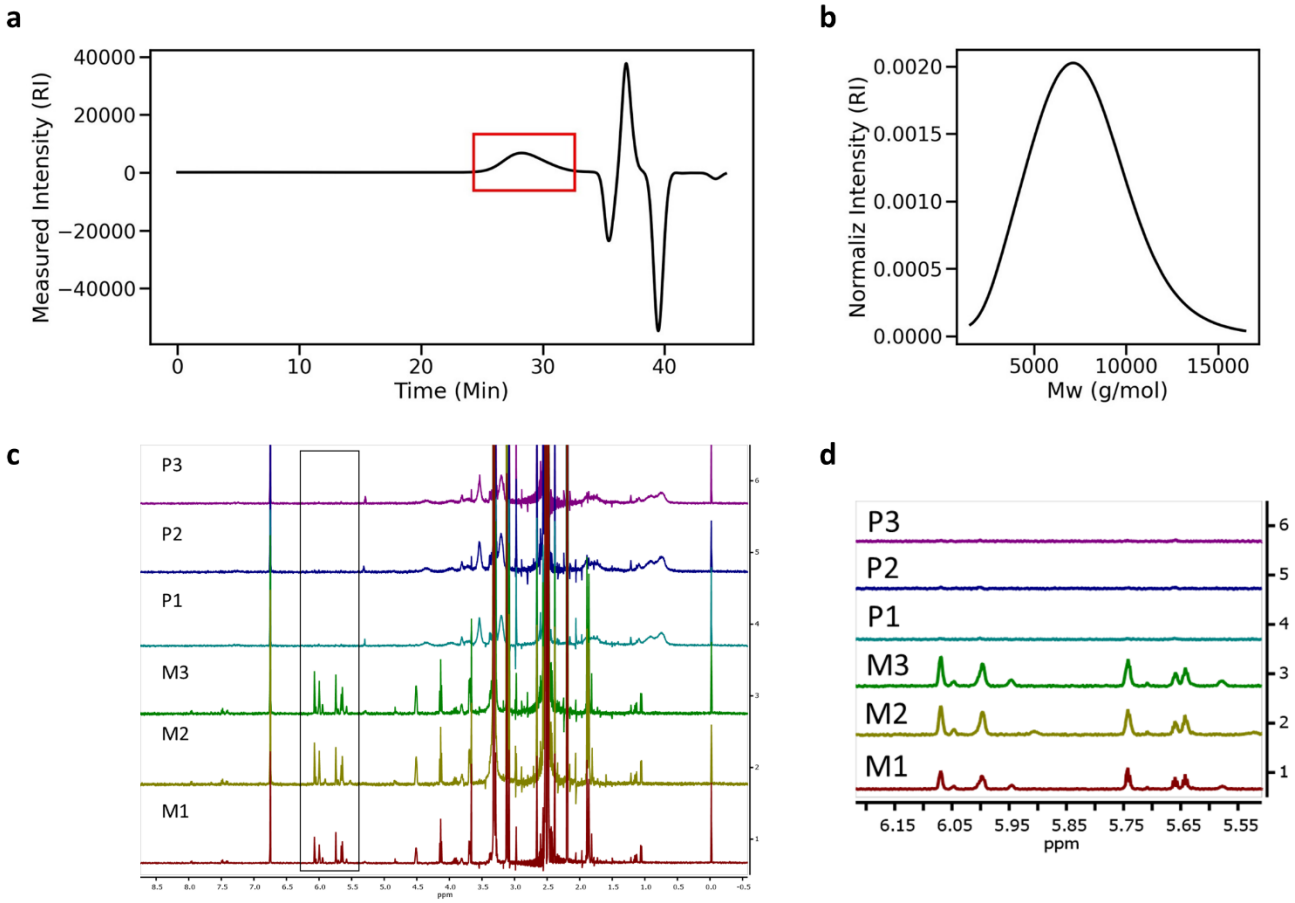

Fig. S5| Characterization of copolymer EP1. a. Size-exclusion chromatography (SEC) trace of copolymer EP1 where signal peak representative of EP1 highlighted in red. **b.** Molecular weight distribution of EP1, as measured by calculation from identified peak region. **c-d.** ^{1}H NMR triplicate polymerizations (M = pre-polymerization, P = post-polymerization) of EP1.

Upon selection of EP1-HRP for further analysis through biophysical characterization, we characterized EP1 by size-exclusion chromatography and ^{1}H NMR. As EP1 is composed of 13% 2-HPMA, 12% SPMA, 53% MMA, and 22% TMAEMA (mol %), with a target DP of 75, EP1's theoretical molecular weight (MW) = 10790 g/mol. While measured MW was lower than anticipated (Measured Mn = 5802 g/mol, Mw = 6866 g/mol) (**Fig. S5a-b**), the use of aqueous GPC calibrated by PEG standards may create discrepancies between expected and measured MW. While polymerization of EP1 demonstrated excellent reaction control ($Đ$ = 1.18), to confirm robust polymerization, further analysis by ^{1}H NMR (**Fig. S5c-d**) triplicate polymerizations (M = pre-polymerization, P = post-polymerization) of EP1 demonstrate >99.9% conversion over 16hr polymerizations as observed from the complete loss of methacrylic peaks at 5.5 - 6.0 ppm and the appearance of peaks at 0.5 - 1.0 ppm indicative of polymer backbone. These results suggest complete polymerization of EP1.

Circular Dichroism (CD) Spectroscopy:

Table S2| Secondary structures of HRP-EP1 during thermal stress.

Sample	Helix	Parallel	Anti-Parallel	Beta Sheet	Random Coil	Total Sum	Condition (°C)
HRP	34.8%	7.9%	8.4%	16.6%	32.3%	100.0%	25
HRP	26.5%	9.8%	10.0%	17.5%	36.3%	100.0%	60
HRP	17.2%	12.5%	12.0%	18.0%	40.3%	100.0%	75
HRP	17.4%	12.3%	12.0%	18.0%	40.2%	100.0%	90
HRP	24.6%	10.2%	10.3%	17.6%	37.1%	100.0%	25 (Refolding)
HRP-EP1	36.8%	7.5%	8.1%	16.4%	31.3%	100.0%	25
HRP-EP1	28.1%	9.4%	9.7%	17.4%	35.5%	100.0%	60
HRP-EP1	19.7%	11.6%	11.4%	18.0%	39.3%	100.0%	75
HRP-EP1	20.3%	11.5%	11.3%	17.9%	39.0%	100.0%	90
HRP-EP1	31.6%	8.5%	8.9%	17.0%	33.8%	100.0%	25 (Refolding)

CD spectra collected were analyzed using CDNN software which uses neural network algorithms to estimate the secondary structure of proteins using data from a trained set of proteins.[2] Utilizing CDNN, the secondary structure of HRP and HRP-EP1 were estimated and wavelength range between 205-260 nm was selected to reduce the error associated from salts present in buffers at lower wavelengths.

Small-Angle X-Ray Scattering (SAXS):

To observe the changes in the physical conformation of HRP, EP1, and HRP-EP1 from pre-heat to post-heat conditions, small-angle X-ray scattering (SAXS) was performed on all samples. To obtain information about molecular size, Guinier analysis, pair distance distribution functions, and Kratky analysis were completed to calculate R_g, *Dmax*, and gauge sample compactness (**Table S3**). First, Guinier analysis was performed to calculate R_g of HRP, EP1, and HRP-EP1 before and after heating. **Fig. S6** shows the lines of best fit for all samples ranging from scattering angles q_{min} = 0.012 $Å^{-1}$ to q_{max} = 0.05 $Å^{-1}$. HRP, EP1, and HRP-EP1 demonstrated single species populations as measured by SAXS with R_g determined by Guinier analysis ranging from 24.6-27.2 Å. Upon exposure to heat, HRP exhibited an increased R_g of 51.9 Å by Guinier analysis with an upward slope at low q indicative of aggregation or denaturation. In contrast, heating did not induce as drastic of a shift in EP1 and HRP-EP1 which post heating exhibited Guinier R_g of 26.0 and 26.9 Å respectively. This evidence is further supported by the pair distance distribution functions and calculated R_g which suggest the development of a highly extended HRP after thermal stress (R_g = 60.6 Å) whereas HRP-EP1 maintains a more conserved size (R_g = 27.7 Å) relative to HRP before thermal stress (R_g = 24.3 Å). This is clear indication of the presence of a single population both before and after heating, indicating that HRP-EP1 maintained much of its conformational integrity after heating similar to that of native HRP. Furthermore, to observe whether the complexation of HRP with EP1 could form a compact structure, we utilized Kratky analysis to qualitatively assess the PPH's compactness in comparison to the native protein. **Fig. S7** shows the Kratky plots in which both HRP and HRP-EP1 demonstrate strong peaks at scattering angles q = 0.065 ($Å^{-1}$) and q = 0.075 ($Å^{-1}$) respectively that is indicative of compactness.

Table S3| Characterization of HRP, EP1, and HRP-EP1 by SAXS. R_g were determined by Guiner analysis, and R^2 was calculated based on the corresponding linear fit. Further, maximum dimension (*Dmax*) was calculated by evaluation of the pairwise distribution function in BioXTAS.

Sample	R_g (Guinier) (Å)	R^2	q_{min} ($Å^{-1}$)	q_{max} ($Å^{-1}$)	R_g (P(r)) (Å)	P(r) *Dmax* (Å)
HRP	25.0 ± 0.4	0.974	0.012	0.05	24.3 ± 0.4	80
HRP Post-Heat	51.9 ± 1.3	0.977	0.012	0.025	60.6 ± 0.2	219
EP1	27.2 ± 0.4	0.983	0.012	0.05	28.9 ± 0.7	118
EP1 Post-Heat	26.0 ± 0.3	0.986	0.012	0.05	28.6 ± 0.4	117
HRP-EP1	24.6 ± 0.2	0.995	0.012	0.05	25.0 ± 0.2	94
HRP-EP1 Post-Heat	26.9 ± 0.1	0.993	0.012	0.05	27.7 ± 0.3	105

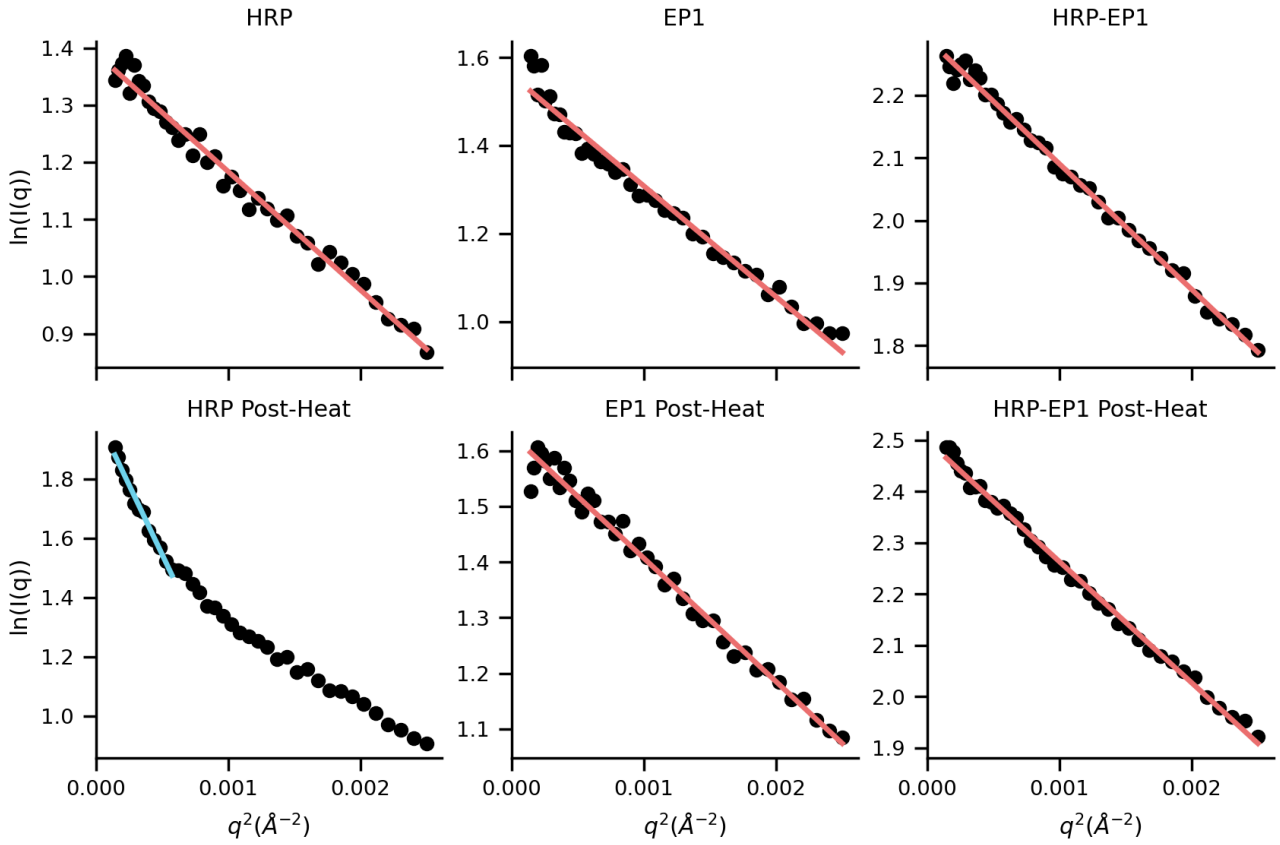

Fig. S6| Guinier analysis of HRP, EP1, and HRP-EP1. Highlighted regions show q-region of best-fit used to determine R_g for each sample.

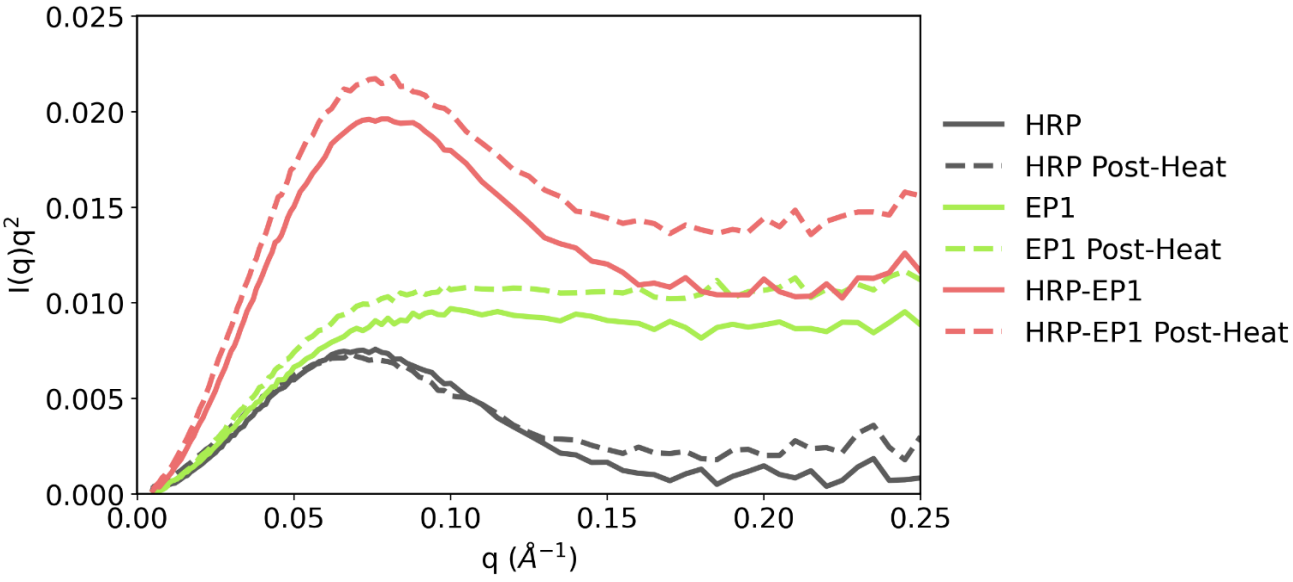

Fig. S7| Kratky plots of HRP, EP1, and HRP-EP1. Kratky analysis suggests both HRP and HRP-EP1 are compact structures.

Dynamic Light Scattering (DLS):

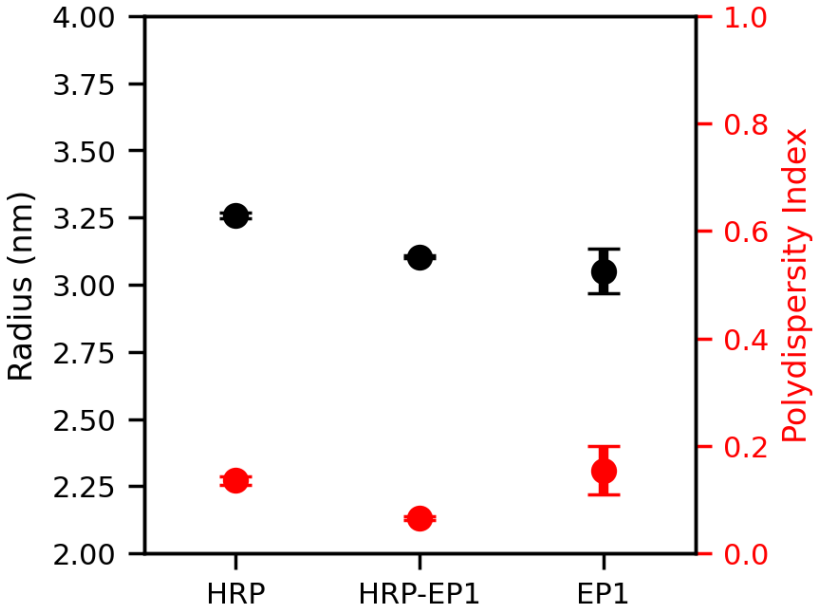

Fig S8| Dynamic light scattering (DLS) data for HRP, EP1, and HRP-EP1.

Table S4. DLS data for HRP, EP1, and HRP-EP1.

Sample	R_h	PD Index
HRP	3.26 +/- 0.011	0.136 +/- 0.002
HRP-EP1	3.10 +/- 0.006	0.066 +/- 0.003
EP1	3.05 +/- 0.082	0.154 +/- 0.045

Quartz Crystal Microbalance with Dissipation (QCM-D):

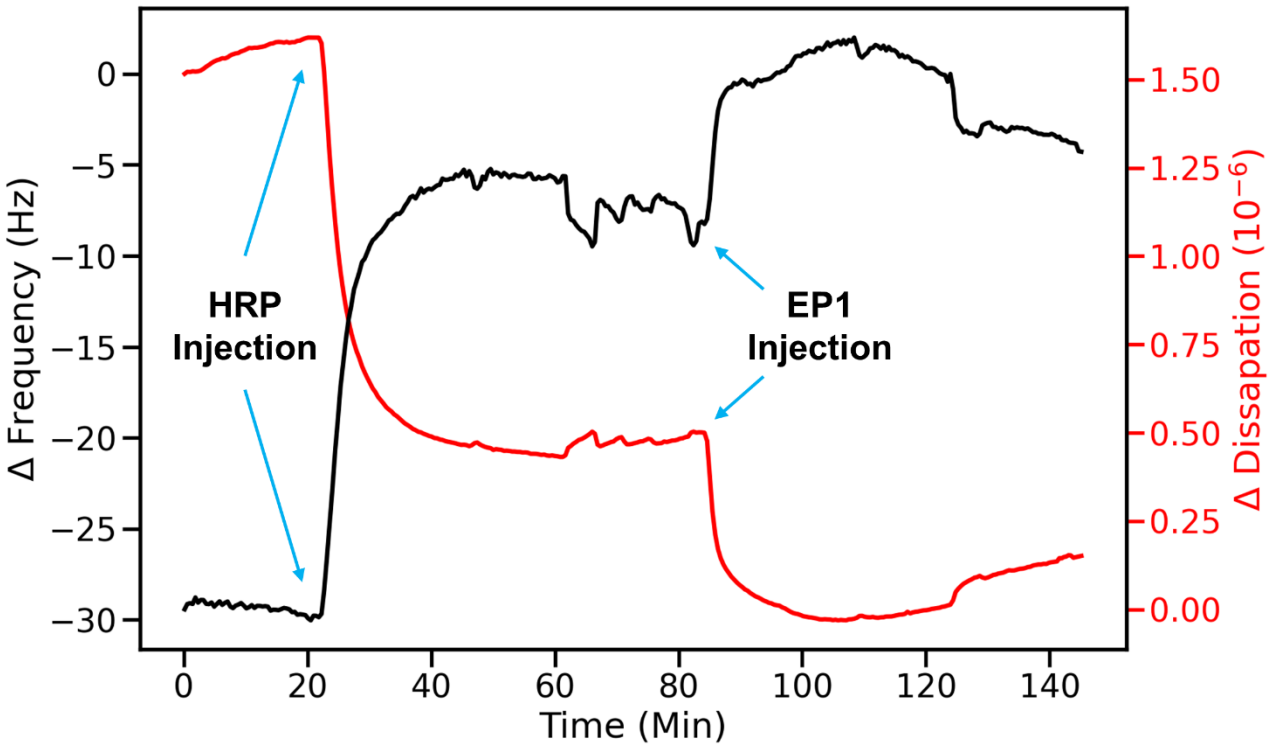

Fig S9| Measured change in frequency and dissipation of HRP and HRP-EP1 by quartz crystal microbalance with dissipation (QCM-D). Direct adsorption of HRP followed by EP1 is observed closely following injection. Washing and injection steps were as follows: NaAc wash (T = 0min), HRP injection (T = 22min), NaAc wash (T = 57min), and EP1 injection (T = 82min).

Penalty Function

Upon application of the diversity filter, it was found that only 19 sufficiently diverse candidates could be identified from the 200 proposed at iteration one of active learning for Lip. Although the acquisition function is varied between each of the proposals by changing the explore-exploit hyperparameter ξ along a logarithmically spaced interval, meaning each of the 200 candidates is a theoretically unique and optimal solution, it is likely that small variations in ξ lead to proximate optima. Accordingly, a penalty function was used to bias against proposing candidates within experimental error of candidates synthesized in the seed database, those found in any previous iteration of active learning, and those previously proposed within a given round of active learning. The form of the penalty function is given by:

$$P(\vec{x}) = 100 \times H\left(d - 0.05\sqrt{2}\right) \times \left(1 - \tanh\left(\frac{d}{\frac{0.05\sqrt{2}}{10} - 1.}\right)\right),\ d = \min(\|\vec{x} - \vec{x}_i\|_2)\ ,\ \vec{x}_i \in \{A\}$$

where $\vec{x}$ is the point in the feature space in question and $\vec{x}_i$ is an element of the set $\{A\}$ of avoided points. The quantity $0.05\sqrt{2}$ is used to penalize polymers that differ by less than 0.05 in the fraction of incorporation of a given monomer type given that the Hamilton MLSTARlet liquid handling robot dispenses reagents to within ~5% error. The geometric distance between feature vectors was computed excluding the bit containing the DP representation; points within the penalty threshold of elements of $\{A\}$ but differing in DP were not penalized. The penalty tends to ~10^2 as points approach the aforementioned penalized points and ~10^{-6} at a distance of 0.07 away from them; the penalty function would not act outside this distance threshold. The penalty is calculated by considering only the closest penalizing-point at a given position in the feature space. Use of a density-based penalty that simultaneously accounted for all elements of $\{A\}$ at all points of the feature space was explored, however, it was found that "optimal candidates" identified with BO with use of this density-based penalty function had extreme sensitivity to the length scale over which the penalty propagated from a given point. Too large of a length scale biased candidates away from optimal regions; too small and not enough diverse candidates would be proposed.

Fig. S10 shows the distribution of pairwise distances less than 0.07 between each unique pair of the 200 candidates produced with and without use of the penalty function at iteration one of active learning for each enzyme. In all three cases, the penalty function aided in biasing proposed candidates away from one another on length-scales in feature space on order with experimental error and ultimately aided in producing diverse candidates at every round of active learning. This was found particularly helpful for Lip (**Fig. S10B**) where a relatively large number of candidates were produced in proximity of one another. While use of the penalty function was less necessary for GOx (**Fig. S10A**) and even less so for HRP

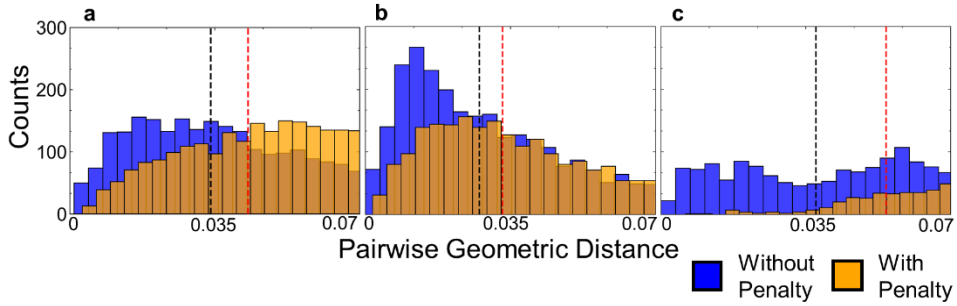

Fig. S10| Distributions of pairwise distances less than 0.07 for the 200 candidates proposed for GOx (a), Lip (b), and HRP (c) at iteration 1 of the active learning. Bars colored blue (orange) belong to the distribution of pairwise distances between candidates without (with) use of the penalty function during active learning; the mean of the distribution is indicated by a black (red) line.

(**Fig. S10C**), it still aided in diversifying the candidates produced at iterations 1-4 of the active learning. For iterations 2-5, the penalty function was adopted to bias optimal candidates away from points in the chemical space observed or predicted to gel.

Classifier Implementation

20 of the 24 iteration-four polymer candidates for GOx stabilization were found to phase separate into liquid and gel phases. Outside of the penalty function, the GPR model and Bayesian Optimization algorithm are agnostic to polymer phase behavior, motivating the development of an additional model that could be used to avoid areas of the chemical space prone to gelling. In the spirit of data-driven / ML lead design this was framed as a classification problem, where a model was trained to predict the binary outcome of "gelling or non-gelling".

Table S5| Hyperparameters tuned during training of the RFC gelation model.

Hyperparameter	Possible Values
Features	[DP,{M1-M8}]
Number of Estimators	[100,200,300]
Max Depth	[None, {10-100} (intervals of 10)
Max Features	[$\sqrt{n_{features}}$, $\log_2(n_{features})$, None]
Minimum Samples at Leaf Node	[1,2,4]
Minimum Samples to Split a Node	[2,4,6]
Probability Threshold for Classification	[0-0.5]

For simplicity, the classifier was trained using the same polymer representations used to train the GPR model, though, investigation of model performance using alternative representations is a worthy future pursuit. Initial investigations of multiple classifiers with minimal hyperparameter tuning suggested that a Random Forrest Classifier (RFC) would perform well for the task and was the basis for further model development. **Table S5** provides details of tuned hyperparameters for the RFC model.

Notably, the available data to train the initial classifier was largely imbalanced, with only 15% of the datapoints corresponding to gelled polymers. To combat this issue and avoid the model learning to only predict a "non-gelling" outcome, it was found imperative to follow three particular strategies in designing the classifier. First was using the balanced accuracy score, defined as the average recall of a classifier for each class, as the metric of interest for model selection. The balanced accuracy score for a model that predicts only "non-gelling" is quite low compared to models that can predict nearly equally as well for either class. Second, it was found important to reweight the class importance to be inversely proportional to its frequency in the dataset during model training. Lastly, as **Table S5** shows, treating the probability threshold for classification as a hyperparameter allowed for models to be more conservative when predicting a sample to be "non-gelling". The latter two strategies facilitated the training and selection of models that maximized the balanced accuracy score. The Tree-structured Parzen Estimator Approach (TPE) was again used to identify model hyperparameters that maximized the mean balanced accuracy scored obtained through K=5 fold-cross validation over the full dataset. The final RFC model was then trained with the entirety of the dataset and using ideal hyperparameters.

Shapely Additive Explanation (SHAP) analysis was used to better understand gelling behavior by looking at how monomer fraction of incorporations in a given polymer affected classifier predictions. As **Fig. S11** shows, PEGMA, DMAEAEMA, and SPMA were largely the most influential features used by the RFC in making a prediction. In line with physical expectation, the classifier learned to associate polymers with relatively more the hydrophilic monomer-type PEGMA with larger probabilities of solubility, and likewise, polymers with relatively less PEGMA with larger probabilities of gelling. In a similar fashion, the classifier associated polymers with larger fraction of incorporations of hydrophobic monomer type DMEAEMA with

larger probabilities of gelling; smaller fractions of incorporations of DMEAEMA had a smaller impact on model predictions, though, were generally associated with higher probabilities of solubility.

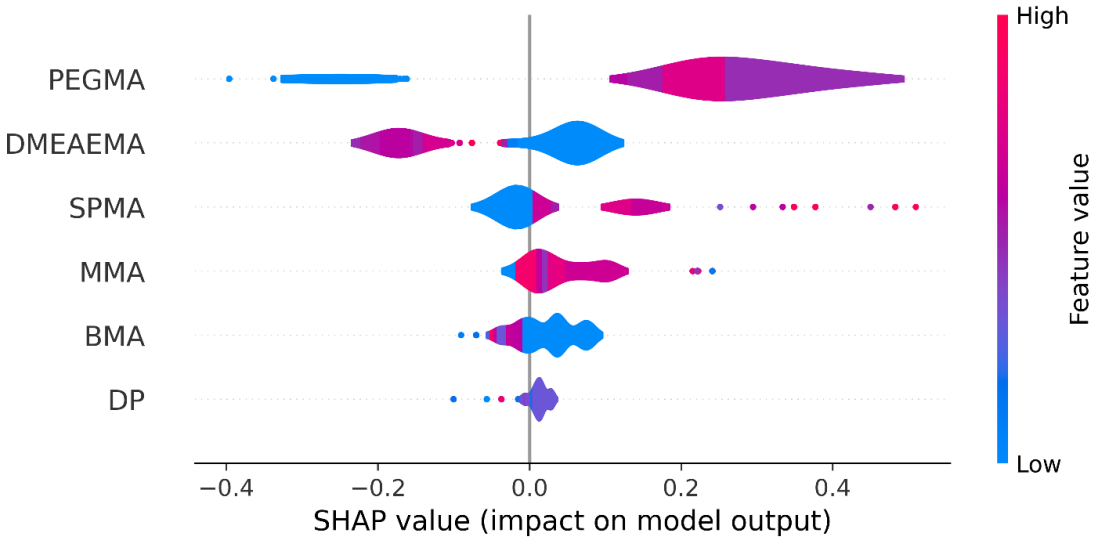

Fig. S11| SHAP summary values for the random forest gelation classifier. The features displayed are those retained from the feature selection during model selection. Negative SHAP values are interpreted as predicted probabilities towards gelation.

Comparing **Fig. S11** and **Fig. 3e**, one finds that feature values associated with predictions of solubility are often associated with predictions of lower REA. For example, large fractions of incorporations of PEGMA are predicted to increase the probability of solubility but are detrimental to predictions on REA. A similar effect can be seen with SPMA. Equally problematic, feature values that are associated with predictions of gelling are associated with higher predictions of GOx REA. For example, larger fractions of incorporation of DMEAEMA lead to larger predictions in REA but are strongly linked to predictions of gelation. Thus, there is an apparent tradeoff between solubility and REA for polymers for GOx stabilization.

The classifier was deployed to avoid proposing gelling polymer candidates for iterations four (a retry) and five of the GOx campaign, albeit in varying capacities. For iteration four, the classifier acted as a screening tool: as each of the 200 candidates were proposed by the BO algorithm, the classifier would predict whether the candidate would gel or not. If the candidate was predicted to gel, a scaling penalty would be added in the region of the feature space of that particular polymer. The acquisition function would then be re-maximized, taking into account the penalty placed in the formerly optimal position in chemical space. This process is continued until an optimal candidate for a given value of ξ is identified that is predicted to not gel. While the classifier was successful in reducing the number of gelling candidates from 20/24 (w/o classifier) to only 7/24 (w/classifier) for iteration four of the active learning, there were two potential shortcomings identified with its use screening tool. Firstly, polymer candidates from iteration four of the GOx campaign, while exhibiting high REAs relative to those from the seed database, were underwhelming compared to many polymers found in iteration three. While use of the classifier was key in identifying many non-gelling, high performing polymers, it is possible that many globally top performing polymers proposed by BO were simultaneously at high-risk for gelling and ultimately rejected by the classifier. This is likely since polymer chemistries responsible for gelation and GOx stabilization were found to be related.

Secondly, a related issue, the Bayesian optimization algorithm was still agnostic to gelling behavior when selecting optimal candidates, outside of small regions in the chemical space where polymers have either

been previously observed or predicted to gel. Accordingly, since the same polymer chemistries were largely responsible for gelation and GOx stabilization, a significant number of candidates suggested by BO were rejected by the classifier and was thus a computationally inefficient approach. An alternative approach considered was to first screen the chemical space and restrict the bounds of the optimization to only consider predicted non-gelling regions as a viable domain. However, due to the high dimensionality of the feature space and their complex interactions, putting definitive bounds on the domain was deemed unreliable. Furthermore, such agnosticism is likely what caused 7/24 polymers to gel despite all being predicted to not gel. A simple Bayes' rule argument, expanded in the following equations and plotted in **Fig. S12**, shows that even the most successful classifier will fail if presented with predominantly gelling polymers:

$$P(T = Gel \,|Pred = Not\ gel)$$

$$= \frac{P(Pred. = Not\ Gel \mid T = Gel)\ P(T = Gel)}{P(Pred. = Not\ Gel \mid T = Gel)\ P(T = Gel) + P(Pred. = Not\ Gel \mid T = Not\ Gel)\ P(T = Not\ Gel)}$$

$$= \frac{FNR * P(T = Gel)}{FNR * P(T = Gel) + TNR\ (1 - P(T = Gel))}$$

The false positive rate (FNR) and true negative rate (TNR) of the classifier are estimated to be 0.075 and 0.78 respectively (means obtained through K=5 cross validation). P(T = Gel) is the proportion of gelling candidates in the population of candidates suggested by BO for GOx at iteration four, which can be estimated to be the ~ 20/24 = 0.83 observed to gel at this iteration without the use of the classifier. Using the aforementioned values in Bayes' rule gives a sizable probability of 0.32 to gel given it is predicted to not gel. As partial validation to the values used in this estimation, (0.32) (24) = 7.68 ~ 8 copolymers would be expected to gel in a set of 24 copolymers predicted not to gel using the classifier, which is quite close to the seven that were observed to gel. Thus, keeping the BO agnostic to the gelling and using the classifier as a screening tool is a viable but suboptimal way to avoid gelling candidates.

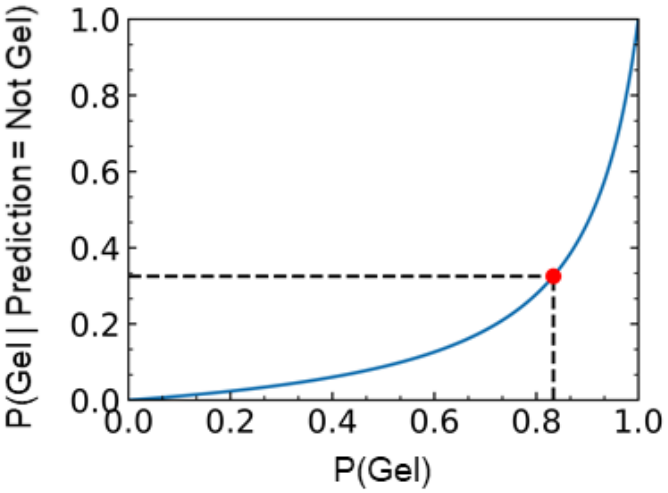

Fig. S12| Impact of the prior on probability of gelling given a prediction of "not-gelling". Using the false negative rate (FNR) and true positive rate (TPR) of the classifier, estimated as means from K=5 cross validation, and a prior informed by the proportion of candidates observed to gel without use of the classifier, we estimate the probability of gelling to be 0.32.

To simultaneously address both shortcomings, the classifier was retrained with gelation data up to iteration four and directly incorporated into the optimization objective itself for iteration five (full exploit of the GOx campaign). Here, the probability of not gelling predicted by the RFC was used as a multiplicative factor for values predicted by the GPR model. In this way, the exploit round for GOx was reframed from selecting the candidates that had the highest predicted REA to instead candidates that had the highest "expected REA", valuing the REA of gelled polymers at 0% since we do not consider them as viable materials for PPHs:

$$E[REA] = \sum \mu_i(x)\ p_i(x) = \mu_i(x) * \big(1 - p_i(x)\big) + 0 * p(x) = \mu_i(x) * (1 - p_i(x))$$

Optimization with this objective function accounts for gelation behavior and allows for risks in selecting candidates with high probability of gelling if there is a suitably high predicted REA. Accordingly, candidates produced from this round of active learning had only 3/24 polymers gel and had the highest mean REA of any iteration of the GOx campaign. This objective resembles that used by Gardner et al. in performing BO with black-box constraints, which in this case are gelling regions of the chemical space.[1]

Polymer Seed Library

#	DP	DEAEMA	2-HPMA	SPMA	BMA	DMAPMA	MMA	PEGMA	TEAMA	HRP REA	GOx REA	Lip REA
1	200	0.1	0.2	0	0	0	0.5	0.2	0	1.8%	21.0%	-4.8%
2	200	0.1	0.2	0	0	0	0.55	0.15	0	1.2%	22.4%	-4.9%
3	200	0.1	0.2	0	0	0	0.6	0.1	0	1.5%	26.2%	1.1%
4	200	0.1	0.2	0	0	0	0.65	0.05	0	0.7%	26.5%	26.8%
5	200	0.1	0.2	0	0	0	0.7	0	0	0.7%	26.1%	11.5%
6	200	0.1	0	0	0	0	0.5	0.4	0	0.8%	13.3%	-3.5%
7	200	0.1	0	0	0	0	0.55	0.35	0	0.6%	11.5%	-4.0%
8	200	0.1	0	0	0	0	0.6	0.3	0	0.8%	9.5%	-3.7%
9	200	0.1	0	0	0	0	0.65	0.25	0	1.3%	25.2%	-2.9%
10	200	0.1	0	0	0	0	0.7	0.2	0	2.0%	30.4%	-4.7%
11	200	0	0.3	0	0	0	0.5	0.2	0	1.0%	4.8%	3.3%
12	200	0.05	0.25	0	0	0	0.5	0.2	0	0.7%	6.4%	-5.0%
13	200	0.1	0.2	0	0	0	0.5	0.2	0	0.6%	32.1%	-3.9%
14	200	0.15	0.15	0	0	0	0.5	0.2	0	0.8%	24.9%	-4.4%
15	200	0.2	0.1	0	0	0	0.5	0.2	0	1.1%	15.4%	-3.1%
16	200	0.25	0.05	0	0	0	0.5	0.2	0	1.1%	12.6%	-4.3%
17	200	0.3	0	0	0	0	0.5	0.2	0	1.3%	22.4%	-3.0%
18	200	0.1	0.2	0	0	0	0	0.7	0	0.8%	7.8%	-4.4%
19	200	0.1	0.2	0	0	0	0.05	0.65	0	0.6%	8.1%	-3.2%
20	200	0.1	0.2	0	0	0	0.1	0.6	0	0.4%	10.3%	-3.3%
21	200	0.1	0.2	0	0	0	0.15	0.55	0	0.5%	11.7%	-3.4%
22	200	0.1	0.2	0	0	0	0.2	0.5	0	0.6%	9.0%	-5.1%
23	200	0.1	0.2	0	0	0	0.25	0.45	0	0.6%	8.3%	-5.5%
24	200	0.1	0.2	0	0	0	0.3	0.4	0	0.9%	8.0%	-5.4%
25	200	0.1	0.2	0	0	0	0.35	0.35	0	1.4%	13.1%	-5.2%
26	200	0.1	0.2	0	0	0	0.4	0.3	0	0.7%	17.0%	-5.5%
27	200	0.1	0.2	0	0	0	0.45	0.35	0	1.0%	10.4%	-5.2%
28	200	0.1	0.2	0	0.5	0	0	0.2	0	0.7%	10.7%	62.5%
29	200	0.1	0.2	0	0.55	0	0	0.15	0	0.7%	9.5%	64.3%
30	200	0.1	0.2	0	0.6	0	0	0.1	0	1.9%	7.5%	12.6%
31	200	0.1	0.2	0	0.65	0	0	0.05	0	2.2%	5.9%	19.4%
32	200	0.1	0.2	0	0.7	0	0	0	0	0.6%	4.7%	20.7%
33	200	0.1	0	0	0.5	0	0	0.4	0	1.2%	5.2%	-5.1%
34	200	0.1	0	0	0.55	0	0	0.35	0	0.6%	6.3%	-5.4%
35	200	0.1	0	0	0.6	0	0	0.3	0	0.8%	6.8%	-5.1%
36	200	0.1	0	0	0.65	0	0	0.25	0	0.9%	6.7%	-3.7%
37	200	0.1	0	0	0.7	0	0	0.2	0	1.3%	5.3%	1.2%
38	200	0	0.3	0	0.5	0	0	0.2	0	0.5%	5.2%	-3.2%
39	200	0.05	0.25	0	0.5	0	0	0.2	0	0.6%	5.8%	7.3%
40	200	0.1	0.2	0	0.5	0	0	0.2	0	0.8%	3.7%	14.0%
41	200	0.15	0.15	0	0.5	0	0	0.2	0	0.7%	5.1%	-2.8%

42	200	0.2	0.1	0	0.5	0	0	0.2	0	0.8%	6.2%	1.5%
43	200	0.25	0.05	0	0.5	0	0	0.2	0	0.9%	6.1%	-0.8%
44	200	0.3	0	0	0.5	0	0	0.2	0	1.1%	6.3%	-0.2%
45	200	0.1	0.2	0	0	0	0	0.7	0	0.8%	5.0%	-2.9%
46	200	0.1	0.2	0	0.05	0	0	0.65	0	0.7%	5.7%	-3.9%
47	200	0.1	0.2	0	0.1	0	0	0.6	0	0.8%	5.3%	-4.2%
48	200	0.1	0.2	0	0.15	0	0	0.55	0	0.6%	2.2%	-3.6%
49	200	0.1	0.2	0	0.2	0	0	0.5	0	1.0%	2.8%	-1.7%
50	200	0.1	0.2	0	0.25	0	0	0.45	0	1.1%	3.6%	-5.6%
51	200	0.1	0.2	0	0.3	0	0	0.4	0	0.7%	4.7%	-5.9%
52	200	0.1	0.2	0	0.35	0	0	0.35	0	1.1%	5.5%	-5.0%
53	200	0.1	0.2	0	0.4	0	0	0.3	0	0.9%	7.9%	-4.7%
54	200	0.1	0.2	0	0.45	0	0	0.25	0	1.0%	8.4%	-4.9%
55	200	0	0.2	0.1	0	0	0.5	0.2	0	1.1%	1.3%	1.0%
56	200	0	0.2	0.1	0	0	0.55	0.15	0	1.7%	1.2%	0.5%
57	200	0	0.2	0.1	0	0	0.6	0.1	0	6.8%	1.3%	1.1%
58	200	0	0.2	0.1	0	0	0.65	0.05	0	12.8%	1.5%	1.3%
59	200	0	0.2	0.1	0	0	0.7	0	0	12.7%	1.3%	1.4%
60	200	0	0	0.1	0	0	0.5	0.4	0	1.0%	0.9%	0.5%
61	200	0	0	0.1	0	0	0.55	0.35	0	1.0%	0.7%	3.1%
62	200	0	0	0.1	0	0	0.6	0.3	0	1.2%	0.8%	0.7%
63	200	0	0	0.1	0	0	0.65	0.25	0	0.8%	2.0%	0.2%
64	200	0	0	0.1	0	0	0.7	0.2	0	1.9%	3.4%	-0.8%
65	200	0	0.3	0	0	0	0.5	0.2	0	3.3%	3.3%	2.9%
66	200	0	0.25	0.05	0	0	0.5	0.2	0	2.2%	2.2%	0.9%
67	200	0	0.2	0.1	0	0	0.5	0.2	0	2.8%	3.3%	-1.6%
68	200	0	0.15	0.15	0	0	0.5	0.2	0	1.9%	0.0%	-1.6%
69	200	0	0.1	0.2	0	0	0.5	0.2	0	2.4%	2.0%	0.9%
70	200	0	0.05	0.25	0	0	0.5	0.2	0	2.0%	1.0%	0.4%
71	200	0	0	0.3	0	0	0.5	0.2	0	1.2%	1.6%	11.4%
72	200	0	0.2	0.1	0	0	0	0.7	0	1.9%	3.4%	8.0%
73	200	0	0.2	0.1	0	0	0.05	0.65	0	1.1%	3.6%	4.0%
74	200	0	0.2	0.1	0	0	0.1	0.6	0	1.2%	5.3%	3.6%
75	200	0	0.2	0.1	0	0	0.15	0.55	0	1.6%	3.6%	4.6%
76	200	0	0.2	0.1	0	0	0.2	0.5	0	1.4%	3.0%	5.7%
77	200	0	0.2	0.1	0	0	0.25	0.45	0	1.7%	2.6%	5.6%
78	200	0	0.2	0.1	0	0	0.3	0.4	0	2.0%	1.2%	3.0%
79	200	0	0.2	0.1	0	0	0.35	0.35	0	0.9%	2.0%	0.8%
80	200	0	0.2	0.1	0	0	0.4	0.3	0	2.5%	3.8%	0.8%
81	200	0	0.2	0.1	0	0	0.45	0.35	0	1.7%	4.1%	0.9%
82	200	0	0.2	0.1	0.5	0	0	0.2	0	3.0%	4.9%	-0.1%
83	200	0	0.2	0.1	0.55	0	0	0.15	0	3.2%	3.8%	0.2%
84	200	0	0.2	0.1	0.6	0	0	0.1	0	2.4%	3.6%	0.5%
85	200	0	0.2	0.1	0.65	0	0	0.05	0	6.8%	3.4%	1.0%

86	200	0	0.2	0.1	0.7	0	0	0	0	1.3%	1.4%	39.9%
87	200	0	0	0.1	0.5	0	0	0.4	0	0.6%	2.5%	0.3%
88	200	0	0	0.1	0.55	0	0	0.35	0	1.1%	4.1%	-0.1%
89	200	0	0	0.1	0.6	0	0	0.3	0	2.0%	4.2%	-0.1%
90	200	0	0	0.1	0.65	0	0	0.25	0	1.6%	4.7%	0.1%
91	200	0	0	0.1	0.7	0	0	0.2	0	0.7%	4.6%	0.1%
92	200	0	0.3	0	0.5	0	0	0.2	0	3.9%	5.8%	-0.2%
93	200	0	0.25	0.05	0.5	0	0	0.2	0	3.9%	3.5%	-1.4%
94	200	0	0.2	0.1	0.5	0	0	0.2	0	4.8%	2.1%	0.3%
95	200	0	0.15	0.15	0.5	0	0	0.2	0	1.4%	2.1%	0.1%
96	200	0	0.1	0.2	0.5	0	0	0.2	0	2.9%	3.3%	0.2%
97	200	0	0.05	0.25	0.5	0	0	0.2	0	2.4%	3.4%	0.3%
98	200	0	0	0.3	0.5	0	0	0.2	0	1.8%	4.5%	0.5%
99	200	0	0.2	0.1	0	0	0	0.7	0	1.3%	4.1%	0.1%
100	200	0	0.2	0.1	0.05	0	0	0.65	0	4.3%	3.7%	0.0%
101	200	0	0.2	0.1	0.1	0	0	0.6	0	0.9%	2.9%	1.0%
102	200	0	0.2	0.1	0.15	0	0	0.55	0	1.3%	1.5%	1.2%
103	200	0	0.2	0.1	0.2	0	0	0.5	0	3.5%	1.9%	-0.3%
104	200	0	0.2	0.1	0.25	0	0	0.45	0	2.3%	3.5%	-0.6%
105	200	0	0.2	0.1	0.3	0	0	0.4	0	1.0%	4.7%	-0.7%
106	200	0	0.2	0.1	0.35	0	0	0.35	0	1.4%	5.0%	-0.4%
107	200	0	0.2	0.1	0.4	0	0	0.3	0	1.4%	4.9%	-0.4%
108	200	0	0.2	0.1	0.45	0	0	0.25	0	1.5%	4.5%	-0.4%
109	200	0.05	0	0	0	0	0.65	0.3	0	0.4%	15.0%	0.2%
110	200	0.1	0	0	0	0	0.6	0.3	0	0.6%	13.6%	-1.1%
111	200	0.15	0	0	0	0	0.55	0.3	0	0.6%	10.3%	-1.8%
112	200	0.2	0	0	0	0	0.5	0.3	0	0.8%	7.6%	-1.6%
113	200	0.25	0	0	0	0	0.45	0.3	0	0.9%	5.2%	-1.9%
114	200	0.3	0	0	0	0	0.4	0.3	0	0.9%	4.8%	-1.5%
115	200	0.35	0	0	0	0	0.35	0.3	0	0.9%	4.1%	-0.4%
116	200	0.4	0	0	0	0	0.3	0.3	0	0.8%	5.2%	-0.9%
117	200	0.45	0	0	0	0	0.25	0.3	0	0.6%	12.1%	-3.4%
118	200	0.5	0	0	0	0	0.2	0.3	0	0.7%	14.2%	-1.1%
119	200	0.05	0	0	0.65	0	0	0.3	0	0.4%	21.7%	-1.6%
120	200	0.1	0	0	0.6	0	0	0.3	0	0.5%	21.3%	-0.7%
121	200	0.15	0	0	0.55	0	0	0.3	0	0.6%	18.3%	-1.5%
122	200	0.2	0	0	0.5	0	0	0.3	0	0.8%	16.1%	-1.2%
123	200	0.25	0	0	0.45	0	0	0.3	0	0.6%	16.4%	-1.4%
124	200	0.3	0	0	0.4	0	0	0.3	0	0.8%	9.8%	-1.6%
125	200	0.35	0	0	0.35	0	0	0.3	0	0.5%	26.4%	-1.2%
126	200	0.4	0	0	0.3	0	0	0.3	0	0.6%	25.3%	-0.7%
127	200	0.45	0	0	0.25	0	0	0.3	0	0.9%	28.4%	-0.9%
128	200	0.5	0	0	0.2	0	0	0.3	0	0.9%	27.9%	-0.6%
129	200	0	0	0	0	0.05	0.65	0.3	0	0.4%	28.9%	-0.5%

130	200	0	0	0	0	0.1	0.6	0.3	0	0.4%	30.3%	-1.0%
131	200	0	0	0	0	0.15	0.55	0.3	0	0.6%	26.3%	-1.3%
132	200	0	0	0	0	0.2	0.5	0.3	0	0.7%	20.4%	-1.1%
133	200	0	0	0	0	0.25	0.45	0.3	0	0.7%	23.2%	-1.5%
134	200	0	0	0	0	0.3	0.4	0.3	0	1.0%	28.5%	-1.1%
135	200	0	0	0	0	0.35	0.35	0.3	0	0.9%	30.0%	2.7%
136	200	0	0	0	0	0.4	0.3	0.3	0	1.0%	31.1%	4.8%
137	200	0	0	0	0	0.45	0.25	0.3	0	1.0%	28.9%	-0.6%
138	200	0	0	0	0	0.5	0.2	0.3	0	1.2%	25.5%	1.3%
139	200	0	0	0	0.65	0.05	0	0.3	0	0.4%	9.3%	-1.6%
140	200	0	0	0	0.6	0.1	0	0.3	0	0.5%	8.3%	-1.4%
141	200	0	0	0	0.55	0.15	0	0.3	0	0.7%	12.5%	0.2%
142	200	0	0	0	0.5	0.2	0	0.3	0	0.5%	22.8%	6.0%
143	200	0	0	0	0.45	0.25	0	0.3	0	0.6%	31.7%	15.7%
144	200	0	0	0	0.4	0.3	0	0.3	0	0.7%	26.2%	20.5%
145	200	0	0	0	0.35	0.35	0	0.3	0	0.8%	25.2%	16.6%
146	200	0	0	0	0.3	0.4	0	0.3	0	0.6%	23.2%	10.7%
147	200	0	0	0	0.25	0.45	0	0.3	0	1.1%	27.5%	8.0%
148	200	0	0	0	0.2	0.5	0	0.3	0	0.7%	26.0%	0.0%
149	200	0	0	0	0	0	0.65	0.3	0.05	0.3%	5.1%	-1.8%
150	200	0	0	0	0	0	0.6	0.3	0.1	0.2%	11.8%	-1.5%
151	200	0	0	0	0	0	0.55	0.3	0.15	0.3%	6.9%	-0.7%
152	200	0	0	0	0	0	0.5	0.3	0.2	0.5%	5.0%	-0.1%
153	200	0	0	0	0	0	0.45	0.3	0.25	0.5%	4.5%	-0.7%
154	200	0	0	0	0	0	0.4	0.3	0.3	10.7%	3.4%	-1.1%
155	200	0	0	0	0	0	0.35	0.3	0.35	1.7%	3.4%	-0.5%
156	200	0	0	0	0	0	0.3	0.3	0.4	30.9%	2.1%	0.9%
157	200	0	0	0	0	0	0.25	0.3	0.45	43.7%	2.7%	-0.6%
158	200	0	0	0	0	0	0.2	0.3	0.5	44.5%	4.1%	1.5%
159	200	0	0	0	0.65	0	0	0.3	0.05	0.8%	26.2%	41.7%
160	200	0	0	0	0.6	0	0	0.3	0.1	1.0%	10.1%	44.7%
161	200	0	0	0	0.55	0	0	0.3	0.15	1.6%	4.1%	31.1%
162	200	0	0	0	0.5	0	0	0.3	0.2	38.1%	6.1%	15.0%
163	200	0	0	0	0.45	0	0	0.3	0.25	30.1%	4.2%	5.6%
164	200	0	0	0	0.4	0	0	0.3	0.3	31.4%	2.1%	0.4%
165	200	0	0	0	0.35	0	0	0.3	0.35	44.1%	2.5%	-1.0%
166	200	0	0	0	0.3	0	0	0.3	0.4	36.0%	3.6%	-0.1%
167	200	0	0	0	0.25	0	0	0.3	0.45	31.4%	3.8%	-1.0%
168	200	0	0	0	0.2	0	0	0.3	0.5	34.0%	3.5%	-1.0%
169	100	0.1	0.2	0	0	0	0.5	0.2	0	3.0%	28.9%	1.5%
170	100	0.1	0.2	0	0	0	0.55	0.15	0	4.9%	33.4%	-0.1%
171	100	0.1	0.2	0	0	0	0.6	0.1	0	4.7%	30.8%	4.3%
172	100	0.1	0.2	0	0	0	0.65	0.05	0	5.7%	27.4%	14.9%
173	100	0.1	0.2	0	0	0	0.7	0	0	6.1%	32.5%	3.1%

174	100	0.1	0	0	0	0	0.5	0.4	0	2.9%	26.9%	0.0%
175	100	0.1	0	0	0	0	0.55	0.35	0	3.8%	22.4%	-0.5%
176	100	0.1	0	0	0	0	0.6	0.3	0	3.1%	22.5%	0.0%
177	100	0.1	0	0	0	0	0.65	0.25	0	2.5%	39.8%	1.9%
178	100	0.1	0	0	0	0	0.7	0.2	0	3.3%	56.2%	0.2%
179	100	0	0.3	0	0	0	0.5	0.2	0	53.9%	12.0%	1.2%
180	100	0.05	0.25	0	0	0	0.5	0.2	0	2.5%	12.7%	-0.8%
181	100	0.1	0.2	0	0	0	0.5	0.2	0	46.1%	62.3%	-0.5%
182	100	0.15	0.15	0	0	0	0.5	0.2	0	6.1%	57.7%	0.0%
183	100	0.2	0.1	0	0	0	0.5	0.2	0	6.5%	40.3%	0.5%
184	100	0.25	0.05	0	0	0	0.5	0.2	0	3.5%	35.9%	0.0%
185	100	0.3	0	0	0	0	0.5	0.2	0	14.5%	33.5%	1.4%
186	100	0.1	0.2	0	0	0	0	0.7	0	2.4%	9.4%	-0.9%
187	100	0.1	0.2	0	0	0	0.05	0.65	0	4.9%	11.5%	-0.1%
188	100	0.1	0.2	0	0	0	0.1	0.6	0	3.7%	11.8%	-0.1%
189	100	0.1	0.2	0	0	0	0.15	0.55	0	5.0%	12.3%	-0.1%
190	100	0.1	0.2	0	0	0	0.2	0.5	0	3.7%	13.9%	-0.4%
191	100	0.1	0.2	0	0	0	0.25	0.45	0	3.3%	11.8%	0.1%
192	100	0.1	0.2	0	0	0	0.3	0.4	0	3.5%	9.9%	-0.6%
193	100	0.1	0.2	0	0	0	0.35	0.35	0	2.2%	8.5%	0.3%
194	100	0.1	0.2	0	0	0	0.4	0.3	0	3.3%	12.4%	-0.7%
195	100	0.1	0.2	0	0	0	0.45	0.35	0	3.3%	11.9%	-0.7%
196	100	0.1	0.2	0	0.5	0	0	0.2	0	3.2%	14.4%	0.4%
197	100	0.1	0.2	0	0.55	0	0	0.15	0	8.2%	9.7%	5.7%
198	100	0.1	0.2	0	0.6	0	0	0.1	0	1.9%	10.0%	0.4%
199	100	0.1	0.2	0	0.65	0	0	0.05	0	1.3%	7.3%	0.8%
200	100	0.1	0.2	0	0.7	0	0	0	0	1.4%	6.0%	0.9%
201	100	0.1	0	0	0.5	0	0	0.4	0	2.8%	7.7%	-0.2%
202	100	0.1	0	0	0.55	0	0	0.35	0	4.6%	11.2%	-0.7%
203	100	0.1	0	0	0.6	0	0	0.3	0	4.0%	11.0%	-0.1%
204	100	0.1	0	0	0.65	0	0	0.25	0	4.6%	11.3%	1.2%
205	100	0.1	0	0	0.7	0	0	0.2	0	9.7%	9.8%	4.6%
206	100	0	0.3	0	0.5	0	0	0.2	0	14.3%	11.4%	1.0%
207	100	0.05	0.25	0	0.5	0	0	0.2	0	3.5%	9.0%	3.5%
208	100	0.1	0.2	0	0.5	0	0	0.2	0	2.8%	12.7%	0.7%
209	100	0.15	0.15	0	0.5	0	0	0.2	0	2.3%	8.6%	9.3%
210	100	0.2	0.1	0	0.5	0	0	0.2	0	3.1%	10.4%	6.7%
211	100	0.25	0.05	0	0.5	0	0	0.2	0	3.2%	10.9%	3.0%
212	100	0.3	0	0	0.5	0	0	0.2	0	4.0%	9.8%	3.7%
213	100	0.1	0.2	0	0	0	0	0.7	0	2.8%	10.8%	0.6%
214	100	0.1	0.2	0	0.05	0	0	0.65	0	4.1%	11.2%	-0.6%
215	100	0.1	0.2	0	0.1	0	0	0.6	0	2.3%	10.4%	0.0%
216	100	0.1	0.2	0	0.15	0	0	0.55	0	3.3%	9.6%	1.3%
217	100	0.1	0.2	0	0.2	0	0	0.5	0	1.3%	8.0%	3.7%

218	100	0.1	0.2	0	0.25	0	0	0.45	0	2.5%	10.0%	-0.4%
219	100	0.1	0.2	0	0.3	0	0	0.4	0	2.7%	13.1%	-0.8%
220	100	0.1	0.2	0	0.35	0	0	0.35	0	4.8%	11.8%	-0.3%
221	100	0.1	0.2	0	0.4	0	0	0.3	0	4.0%	13.7%	-0.1%
222	100	0.1	0.2	0	0.45	0	0	0.35	0	4.1%	13.5%	-0.3%
223	100	0	0.2	0.1	0	0	0.5	0.2	0	27.0%	1.2%	-2.2%
224	100	0	0.2	0.1	0	0	0.55	0.15	0	20.2%	1.5%	-1.6%
225	100	0	0.2	0.1	0	0	0.6	0.1	0	49.4%	2.0%	-1.1%
226	100	0	0.2	0.1	0	0	0.65	0.05	0	24.2%	2.3%	-0.6%
227	100	0	0.2	0.1	0	0	0.7	0	0	32.3%	2.5%	-0.2%
228	100	0	0	0.1	0	0	0.5	0.4	0	46.5%	2.6%	-2.9%
229	100	0	0	0.1	0	0	0.55	0.35	0	47.6%	2.2%	-2.7%
230	100	0	0	0.1	0	0	0.6	0.3	0	47.7%	1.9%	-2.4%
231	100	0	0	0.1	0	0	0.65	0.25	0	32.1%	2.2%	-2.9%
232	100	0	0	0.1	0	0	0.7	0.2	0	35.1%	5.7%	-2.6%
233	100	0	0.3	0	0	0	0.5	0.2	0	62.9%	7.2%	7.3%
234	100	0	0.25	0.05	0	0	0.5	0.2	0	55.0%	7.8%	10.5%
235	100	0	0.2	0.1	0	0	0.5	0.2	0	32.6%	8.2%	1.7%
236	100	0	0.15	0.15	0	0	0.5	0.2	0	28.5%	8.3%	-0.4%
237	100	0	0.1	0.2	0	0	0.5	0.2	0	28.0%	4.7%	2.7%
238	100	0	0.05	0.25	0	0	0.5	0.2	0	18.8%	1.5%	4.8%
239	100	0	0	0.3	0	0	0.5	0.2	0	14.8%	1.6%	19.4%
240	100	0	0.2	0.1	0	0	0	0.7	0	43.3%	5.8%	9.0%
241	100	0	0.2	0.1	0	0	0.05	0.65	0	45.4%	8.0%	18.8%
242	100	0	0.2	0.1	0	0	0.1	0.6	0	35.4%	10.2%	20.6%
243	100	0	0.2	0.1	0	0	0.15	0.55	0	50.4%	11.0%	17.9%
244	100	0	0.2	0.1	0	0	0.2	0.5	0	51.0%	11.8%	7.9%
245	100	0	0.2	0.1	0	0	0.25	0.45	0	35.6%	8.8%	10.7%
246	100	0	0.2	0.1	0	0	0.3	0.4	0	10.2%	1.9%	9.0%
247	100	0	0.2	0.1	0	0	0.35	0.35	0	37.6%	2.0%	10.8%
248	100	0	0.2	0.1	0	0	0.4	0.3	0	55.1%	7.4%	1.9%
249	100	0	0.2	0.1	0	0	0.45	0.35	0	48.4%	10.8%	1.0%
250	100	0	0.2	0.1	0.5	0	0	0.2	0	22.1%	14.0%	0.7%
251	100	0	0.2	0.1	0.55	0	0	0.15	0	10.4%	14.7%	1.7%
252	100	0	0.2	0.1	0.6	0	0	0.1	0	3.1%	14.3%	3.6%
253	100	0	0.2	0.1	0.65	0	0	0.05	0	5.1%	9.3%	3.7%
254	100	0	0.2	0.1	0.7	0	0	0	0	0.0%	2.6%	1.0%
255	100	0	0	0.1	0.5	0	0	0.4	0	0.0%	2.8%	-2.5%
256	100	0	0	0.1	0.55	0	0	0.35	0	0.0%	8.2%	-2.0%
257	100	0	0	0.1	0.6	0	0	0.3	0	0.0%	11.6%	-1.4%
258	100	0	0	0.1	0.65	0	0	0.25	0	0.0%	12.7%	2.9%
259	100	0	0	0.1	0.7	0	0	0.2	0	0.0%	14.5%	27.3%
260	100	0	0.3	0	0.5	0	0	0.2	0	0.0%	16.6%	0.2%
261	100	0	0.25	0.05	0.5	0	0	0.2	0	0.0%	12.5%	-0.3%

262	100	0	0.2	0.1	0.5	0	0	0.2	0	0.0%	3.1%	-1.3%
263	100	0	0.15	0.15	0.5	0	0	0.2	0	20.4%	6.5%	1.3%
264	100	0	0.1	0.2	0.5	0	0	0.2	0	3.0%	7.1%	1.9%
265	100	0	0.05	0.25	0.5	0	0	0.2	0	0.7%	7.4%	2.2%
266	100	0	0	0.3	0.5	0	0	0.2	0	1.9%	7.1%	1.0%
267	100	0	0.2	0.1	0	0	0	0.7	0	3.5%	5.9%	8.3%
268	100	0	0.2	0.1	0.05	0	0	0.65	0	30.7%	5.6%	-0.1%
269	100	0	0.2	0.1	0.1	0	0	0.6	0	1.4%	4.6%	0.4%
270	100	0	0.2	0.1	0.15	0	0	0.55	0	0.6%	3.4%	3.2%
271	100	0	0.2	0.1	0.2	0	0	0.5	0	6.4%	7.2%	4.4%
272	100	0	0.2	0.1	0.25	0	0	0.45	0	6.4%	8.8%	0.3%
273	100	0	0.2	0.1	0.3	0	0	0.4	0	13.8%	10.7%	-0.4%
274	100	0	0.2	0.1	0.35	0	0	0.35	0	7.2%	11.0%	-0.4%
275	100	0	0.2	0.1	0.4	0	0	0.3	0	4.6%	10.9%	-0.6%
276	100	0	0.2	0.1	0.45	0	0	0.25	0	3.6%	10.9%	-0.5%
277	100	0.05	0	0	0	0	0.65	0.3	0	-1.6%	7.9%	0.2%
278	100	0.1	0	0	0	0	0.6	0.3	0	22.0%	21.5%	0.2%
279	100	0.15	0	0	0	0	0.55	0.3	0	28.2%	26.6%	-0.6%
280	100	0.2	0	0	0	0	0.5	0.3	0	41.2%	30.6%	0.0%
281	100	0.25	0	0	0	0	0.45	0.3	0	29.8%	35.0%	0.2%
282	100	0.3	0	0	0	0	0.4	0.3	0	39.4%	31.8%	0.1%
283	100	0.35	0	0	0	0	0.35	0.3	0	41.7%	28.8%	0.3%
284	100	0.4	0	0	0	0	0.3	0.3	0	36.6%	27.2%	0.5%
285	100	0.45	0	0	0	0	0.25	0.3	0	73.4%	27.2%	0.0%
286	100	0.5	0	0	0	0	0.2	0.3	0	74.7%	18.9%	0.4%
287	100	0.05	0	0	0.65	0	0	0.3	0	-1.3%	11.7%	1.8%
288	100	0.1	0	0	0.6	0	0	0.3	0	0.2%	35.1%	1.1%
289	100	0.15	0	0	0.55	0	0	0.3	0	0.3%	44.0%	0.7%
290	100	0.2	0	0	0.5	0	0	0.3	0	2.9%	45.0%	0.9%
291	100	0.25	0	0	0.45	0	0	0.3	0	2.4%	42.7%	1.1%
292	100	0.3	0	0	0.4	0	0	0.3	0	3.3%	39.2%	0.6%
293	100	0.35	0	0	0.35	0	0	0.3	0	3.0%	36.9%	0.2%
294	100	0.4	0	0	0.3	0	0	0.3	0	78.4%	27.4%	0.1%
295	100	0.45	0	0	0.25	0	0	0.3	0	110.0%	31.9%	-0.3%
296	100	0.5	0	0	0.2	0	0	0.3	0	93.1%	28.3%	1.9%
297	100	0	0	0	0	0.05	0.65	0.3	0	20.4%	14.2%	3.5%
298	100	0	0	0	0	0.1	0.6	0.3	0	22.2%	15.1%	8.0%
299	100	0	0	0	0	0.15	0.55	0.3	0	14.8%	18.0%	0.7%
300	100	0	0	0	0	0.2	0.5	0.3	0	0.0%	20.6%	2.0%
301	100	0	0	0	0	0.25	0.45	0.3	0	0.4%	18.3%	1.8%
302	100	0	0	0	0	0.3	0.4	0.3	0	16.3%	16.4%	0.8%
303	100	0	0	0	0	0.35	0.35	0.3	0	4.4%	27.0%	4.5%
304	100	0	0	0	0	0.4	0.3	0.3	0	10.3%	33.4%	1.3%
305	100	0	0	0	0	0.45	0.25	0.3	0	-0.3%	39.5%	3.5%

306	100	0	0	0	0	0.5	0.2	0.3	0	-0.3%	40.3%	6.3%
307	100	0	0	0	0.65	0.05	0	0.3	0	18.7%	15.1%	0.0%
308	100	0	0	0	0.6	0.1	0	0.3	0	30.7%	23.8%	1.2%
309	100	0	0	0	0.55	0.15	0	0.3	0	-0.6%	23.0%	3.7%
310	100	0	0	0	0.5	0.2	0	0.3	0	19.4%	18.1%	5.9%
311	100	0	0	0	0.45	0.25	0	0.3	0	5.1%	33.7%	6.7%
312	100	0	0	0	0.4	0.3	0	0.3	0	8.3%	34.7%	5.9%
313	100	0	0	0	0.35	0.35	0	0.3	0	22.0%	38.1%	7.4%
314	100	0	0	0	0.3	0.4	0	0.3	0	19.4%	37.5%	5.4%
315	100	0	0	0	0.25	0.45	0	0.3	0	0.7%	43.3%	4.0%
316	100	0	0	0	0.2	0.5	0	0.3	0	34.2%	34.4%	1.2%
317	100	0	0	0	0	0	0.65	0.3	0.05	19.7%	8.9%	0.1%
318	100	0	0	0	0	0	0.6	0.3	0.1	28.5%	13.6%	0.1%
319	100	0	0	0	0	0	0.55	0.3	0.15	31.3%	10.8%	0.1%
320	100	0	0	0	0	0	0.5	0.3	0.2	34.2%	11.3%	1.0%
321	100	0	0	0	0	0	0.45	0.3	0.25	26.7%	8.4%	7.2%
322	100	0	0	0	0	0	0.4	0.3	0.3	34.2%	8.3%	1.3%
323	100	0	0	0	0	0	0.35	0.3	0.35	79.6%	8.0%	1.5%
324	100	0	0	0	0	0	0.3	0.3	0.4	48.2%	8.4%	2.7%
325	100	0	0	0	0	0	0.25	0.3	0.45	36.1%	6.8%	3.0%
326	100	0	0	0	0	0	0.2	0.3	0.5	42.0%	4.7%	3.9%
327	100	0	0	0	0.65	0	0	0.3	0.05	-1.3%	16.8%	13.4%
328	100	0	0	0	0.6	0	0	0.3	0.1	0.8%	10.6%	23.7%
329	100	0	0	0	0.55	0	0	0.3	0.15	6.4%	8.6%	18.0%
330	100	0	0	0	0.5	0	0	0.3	0.2	10.3%	11.1%	7.7%
331	100	0	0	0	0.45	0	0	0.3	0.25	5.0%	9.9%	1.9%
332	100	0	0	0	0.4	0	0	0.3	0.3	21.2%	7.8%	0.5%
333	100	0	0	0	0.35	0	0	0.3	0.35	31.6%	5.8%	2.0%
334	100	0	0	0	0.3	0	0	0.3	0.4	2.3%	5.5%	2.0%
335	100	0	0	0	0.25	0	0	0.3	0.45	5.9%	5.8%	3.1%
336	100	0	0	0	0.2	0	0	0.3	0.5	17.4%	7.8%	1.8%
337	50	0.1	0.2	0	0	0	0.5	0.2	0	55.7%	16.2%	-0.1%
338	50	0.1	0.2	0	0	0	0.55	0.15	0	38.7%	14.2%	-0.5%
339	50	0.1	0.2	0	0	0	0.6	0.1	0	50.7%	20.6%	1.6%
340	50	0.1	0.2	0	0	0	0.65	0.05	0	48.2%	15.5%	9.5%
341	50	0.1	0.2	0	0	0	0.7	0	0	35.4%	19.9%	4.8%
342	50	0.1	0	0	0	0	0.5	0.4	0	72.6%	8.4%	0.0%
343	50	0.1	0	0	0	0	0.55	0.35	0	56.5%	10.0%	-0.8%
344	50	0.1	0	0	0	0	0.6	0.3	0	52.3%	12.2%	-0.4%
345	50	0.1	0	0	0	0	0.65	0.25	0	61.2%	20.6%	-0.6%
346	50	0.1	0	0	0	0	0.7	0.2	0	30.1%	29.5%	-0.6%
347	50	0	0.3	0	0	0	0.5	0.2	0	33.4%	5.8%	-0.4%
348	50	0.05	0.25	0	0	0	0.5	0.2	0	39.1%	8.2%	-2.0%
349	50	0.1	0.2	0	0	0	0.5	0.2	0	45.3%	32.2%	-2.0%

350	50	0.15	0.15	0	0	0	0.5	0.2	0	38.1%	27.7%	-0.6%
351	50	0.2	0.1	0	0	0	0.5	0.2	0	45.8%	18.6%	0.2%
352	50	0.25	0.05	0	0	0	0.5	0.2	0	62.4%	13.4%	-1.4%
353	50	0.3	0	0	0	0	0.5	0.2	0	49.8%	13.6%	1.5%
354	50	0.1	0.2	0	0	0	0	0.7	0	47.6%	7.3%	-1.8%
355	50	0.1	0.2	0	0	0	0.05	0.65	0	49.3%	8.2%	-1.4%
356	50	0.1	0.2	0	0	0	0.1	0.6	0	25.6%	9.3%	-1.8%
357	50	0.1	0.2	0	0	0	0.15	0.55	0	33.5%	15.2%	-1.8%
358	50	0.1	0.2	0	0	0	0.2	0.5	0	29.1%	24.4%	-1.6%
359	50	0.1	0.2	0	0	0	0.25	0.45	0	37.8%	28.2%	-1.2%
360	50	0.1	0.2	0	0	0	0.3	0.4	0	5.5%	21.0%	-1.4%
361	50	0.1	0.2	0	0	0	0.35	0.35	0	41.4%	13.5%	-1.0%
362	50	0.1	0.2	0	0	0	0.4	0.3	0	24.3%	28.6%	-1.3%
363	50	0.1	0.2	0	0	0	0.45	0.35	0	21.6%	25.1%	-1.4%
364	50	0.1	0.2	0	0.5	0	0	0.2	0	1.3%	18.4%	10.5%
365	50	0.1	0.2	0	0.55	0	0	0.15	0	0.7%	7.1%	-0.3%
366	50	0.1	0.2	0	0.6	0	0	0.1	0	1.0%	6.4%	-0.6%
367	50	0.1	0.2	0	0.65	0	0	0.05	0	-0.1%	4.3%	-0.3%
368	50	0.1	0.2	0	0.7	0	0	0	0	-0.5%	2.7%	1.4%
369	50	0.1	0	0	0.5	0	0	0.4	0	1.0%	2.8%	-1.2%
370	50	0.1	0	0	0.55	0	0	0.35	0	0.1%	10.1%	-0.8%
371	50	0.1	0	0	0.6	0	0	0.3	0	-0.2%	10.8%	-0.4%
372	50	0.1	0	0	0.65	0	0	0.25	0	-0.7%	15.0%	-0.1%
373	50	0.1	0	0	0.7	0	0	0.2	0	-0.8%	22.6%	-0.5%
374	50	0	0.3	0	0.5	0	0	0.2	0	5.2%	7.6%	-1.1%
375	50	0.05	0.25	0	0.5	0	0	0.2	0	-0.2%	8.0%	0.1%
376	50	0.1	0.2	0	0.5	0	0	0.2	0	-0.8%	9.2%	-0.1%
377	50	0.15	0.15	0	0.5	0	0	0.2	0	-0.2%	3.5%	0.1%
378	50	0.2	0.1	0	0.5	0	0	0.2	0	-0.7%	7.9%	2.1%
379	50	0.25	0.05	0	0.5	0	0	0.2	0	-0.6%	8.0%	1.1%
380	50	0.3	0	0	0.5	0	0	0.2	0	-0.3%	8.7%	1.0%
381	50	0.1	0.2	0	0	0	0	0.7	0	25.7%	7.5%	0.7%
382	50	0.1	0.2	0	0.05	0	0	0.65	0	29.5%	6.9%	1.3%
383	50	0.1	0.2	0	0.1	0	0	0.6	0	13.9%	4.4%	0.4%
384	50	0.1	0.2	0	0.15	0	0	0.55	0	-0.2%	2.1%	0.3%
385	50	0.1	0.2	0	0.2	0	0	0.5	0	-0.8%	6.2%	0.6%
386	50	0.1	0.2	0	0.25	0	0	0.45	0	-0.8%	11.9%	0.4%
387	50	0.1	0.2	0	0.3	0	0	0.4	0	0.0%	9.1%	0.4%
388	50	0.1	0.2	0	0.35	0	0	0.35	0	-0.4%	9.3%	0.6%
389	50	0.1	0.2	0	0.4	0	0	0.3	0	0.4%	10.1%	0.3%
390	50	0.1	0.2	0	0.45	0	0	0.25	0	0.9%	8.3%	0.2%
391	50	0	0.2	0.1	0	0	0.5	0.2	0	70.7%	2.6%	1.6%
392	50	0	0.2	0.1	0	0	0.55	0.15	0	93.0%	3.3%	0.9%
393	50	0	0.2	0.1	0	0	0.6	0.1	0	72.2%	4.7%	-0.8%

394	50	0	0.2	0.1	0	0	0.65	0.05	0	80.4%	5.5%	0.9%
395	50	0	0.2	0.1	0	0	0.7	0	0	48.8%	6.3%	-1.2%
396	50	0	0	0.1	0	0	0.5	0.4	0	81.7%	4.3%	0.5%
397	50	0	0	0.1	0	0	0.55	0.35	0	167.7%	3.9%	0.5%
398	50	0	0	0.1	0	0	0.6	0.3	0	42.2%	2.7%	-1.4%
399	50	0	0	0.1	0	0	0.65	0.25	0	42.4%	4.3%	-0.8%
400	50	0	0	0.1	0	0	0.7	0.2	0	53.7%	9.8%	-0.9%
401	50	0	0.3	0	0	0	0.5	0.2	0	61.8%	10.8%	1.3%
402	50	0	0.25	0.05	0	0	0.5	0.2	0	74.0%	13.6%	-0.9%
403	50	0	0.2	0.1	0	0	0.5	0.2	0	40.8%	13.4%	-1.3%
404	50	0	0.15	0.15	0	0	0.5	0.2	0	54.4%	12.2%	0.8%
405	50	0	0.1	0.2	0	0	0.5	0.2	0	56.3%	10.3%	-0.6%
406	50	0	0.05	0.25	0	0	0.5	0.2	0	69.2%	4.6%	0.5%
407	50	0	0	0.3	0	0	0.5	0.2	0	39.7%	3.9%	1.8%
408	50	0	0.2	0.1	0	0	0	0.7	0	40.5%	10.1%	-0.6%
409	50	0	0.2	0.1	0	0	0.05	0.65	0	45.6%	14.1%	-0.6%
410	50	0	0.2	0.1	0	0	0.1	0.6	0	66.7%	15.0%	-0.6%
411	50	0	0.2	0.1	0	0	0.15	0.55	0	83.8%	15.9%	2.1%
412	50	0	0.2	0.1	0	0	0.2	0.5	0	58.7%	16.1%	-0.8%
413	50	0	0.2	0.1	0	0	0.25	0.45	0	59.8%	14.5%	-1.0%
414	50	0	0.2	0.1	0	0	0.3	0.4	0	56.6%	5.1%	-1.1%
415	50	0	0.2	0.1	0	0	0.35	0.35	0	112.6%	4.2%	0.6%
416	50	0	0.2	0.1	0	0	0.4	0.3	0	29.8%	11.2%	-0.4%
417	50	0	0.2	0.1	0	0	0.45	0.35	0	37.3%	12.9%	-0.7%
418	50	0	0.2	0.1	0.5	0	0	0.2	0	14.8%	19.9%	-1.2%
419	50	0	0.2	0.1	0.55	0	0	0.15	0	13.0%	21.8%	-0.7%
420	50	0	0.2	0.1	0.6	0	0	0.1	0	32.5%	21.5%	-0.5%
421	50	0	0.2	0.1	0.65	0	0	0.05	0	17.1%	17.0%	-0.2%
422	50	0	0.2	0.1	0.7	0	0	0	0	14.9%	6.6%	12.2%
423	50	0	0	0.1	0.5	0	0	0.4	0	30.1%	3.4%	-0.8%
424	50	0	0	0.1	0.55	0	0	0.35	0	25.6%	10.7%	-0.6%
425	50	0	0	0.1	0.6	0	0	0.3	0	18.0%	13.5%	-1.3%
426	50	0	0	0.1	0.65	0	0	0.25	0	11.0%	18.9%	-0.6%
427	50	0	0	0.1	0.7	0	0	0.2	0	21.3%	20.2%	0.0%
428	50	0	0.3	0	0.5	0	0	0.2	0	37.9%	17.0%	3.1%
429	50	0	0.25	0.05	0.5	0	0	0.2	0	34.4%	17.0%	-3.4%
430	50	0	0.2	0.1	0.5	0	0	0.2	0	52.3%	6.3%	-1.0%
431	50	0	0.15	0.15	0.5	0	0	0.2	0	35.5%	5.6%	-0.7%
432	50	0	0.1	0.2	0.5	0	0	0.2	0	13.8%	16.7%	-0.7%
433	50	0	0.05	0.25	0.5	0	0	0.2	0	17.4%	21.9%	-3.4%
434	50	0	0	0.3	0.5	0	0	0.2	0	17.7%	22.7%	-0.6%
435	50	0	0.2	0.1	0	0	0	0.7	0	67.0%	16.9%	-0.3%
436	50	0	0.2	0.1	0.05	0	0	0.65	0	78.4%	18.4%	1.0%
437	50	0	0.2	0.1	0.1	0	0	0.6	0	83.4%	13.1%	-1.0%

438	50	0	0.2	0.1	0.15	0	0	0.55	0	58.9%	5.1%	-0.9%
439	50	0	0.2	0.1	0.2	0	0	0.5	0	102.0%	4.5%	-0.3%
440	50	0	0.2	0.1	0.25	0	0	0.45	0	23.6%	13.5%	-1.4%
441	50	0	0.2	0.1	0.3	0	0	0.4	0	31.2%	17.4%	-1.5%
442	50	0	0.2	0.1	0.35	0	0	0.35	0	40.5%	19.1%	-1.5%
443	50	0	0.2	0.1	0.4	0	0	0.3	0	69.0%	22.5%	-1.4%
444	50	0	0.2	0.1	0.45	0	0	0.35	0	90.6%	20.1%	1.8%
445	50	0.05	0	0	0	0	0.65	0.3	0	0.4%	1.3%	-1.6%
446	50	0.1	0	0	0	0	0.6	0.3	0	0.6%	17.2%	-1.4%
447	50	0.15	0	0	0	0	0.55	0.3	0	0.8%	15.0%	-0.3%
448	50	0.2	0	0	0	0	0.5	0.3	0	0.6%	14.2%	0.3%
449	50	0.25	0	0	0	0	0.45	0.3	0	0.6%	12.6%	-0.1%
450	50	0.3	0	0	0	0	0.4	0.3	0	0.5%	11.6%	0.3%
451	50	0.35	0	0	0	0	0.35	0.3	0	0.4%	11.0%	-0.1%
452	50	0.4	0	0	0	0	0.3	0.3	0	0.5%	9.6%	-0.5%
453	50	0.45	0	0	0	0	0.25	0.3	0	0.5%	14.2%	-0.7%
454	50	0.5	0	0	0	0	0.2	0.3	0	0.9%	22.6%	0.8%
455	50	0.05	0	0	0.65	0	0	0.3	0	0.1%	16.5%	-1.5%
456	50	0.1	0	0	0.6	0	0	0.3	0	0.5%	12.9%	-1.3%
457	50	0.15	0	0	0.55	0	0	0.3	0	0.5%	23.9%	-0.9%
458	50	0.2	0	0	0.5	0	0	0.3	0	0.5%	30.4%	-0.6%
459	50	0.25	0	0	0.45	0	0	0.3	0	0.5%	26.3%	-0.8%
460	50	0.3	0	0	0.4	0	0	0.3	0	0.6%	16.0%	-1.0%
461	50	0.35	0	0	0.35	0	0	0.3	0	0.3%	19.2%	-0.7%
462	50	0.4	0	0	0.3	0	0	0.3	0	0.5%	26.1%	-0.1%
463	50	0.45	0	0	0.25	0	0	0.3	0	0.6%	31.6%	0.1%
464	50	0.5	0	0	0.2	0	0	0.3	0	1.4%	36.0%	0.8%
465	50	0	0	0	0	0.05	0.65	0.3	0	0.6%	7.6%	-0.7%
466	50	0	0	0	0	0.1	0.6	0.3	0	0.7%	7.9%	-0.7%
467	50	0	0	0	0	0.15	0.55	0.3	0	0.5%	6.6%	-0.2%
468	50	0	0	0	0	0.2	0.5	0.3	0	0.3%	2.5%	-0.8%
469	50	0	0	0	0	0.25	0.45	0.3	0	0.6%	4.5%	0.1%
470	50	0	0	0	0	0.3	0.4	0.3	0	5.9%	15.6%	4.3%
471	50	0	0	0	0	0.35	0.35	0.3	0	7.3%	24.1%	8.9%
472	50	0	0	0	0	0.4	0.3	0.3	0	5.6%	34.7%	12.2%
473	50	0	0	0	0	0.45	0.25	0.3	0	4.3%	23.7%	15.4%
474	50	0	0	0	0	0.5	0.2	0.3	0	6.7%	24.9%	16.8%
475	50	0	0	0	0.65	0.05	0	0.3	0	0.4%	6.9%	0.8%
476	50	0	0	0	0.6	0.1	0	0.3	0	0.5%	2.1%	2.2%
477	50	0	0	0	0.55	0.15	0	0.3	0	0.5%	2.3%	1.8%
478	50	0	0	0	0.5	0.2	0	0.3	0	1.0%	8.1%	6.9%
479	50	0	0	0	0.45	0.25	0	0.3	0	0.8%	10.3%	12.2%
480	50	0	0	0	0.4	0.3	0	0.3	0	1.2%	13.6%	11.3%
481	50	0	0	0	0.35	0.35	0	0.3	0	14.1%	16.0%	10.8%

482	50	0	0	0	0.3	0.4	0	0.3	0	22.9%	24.4%	8.4%
483	50	0	0	0	0.25	0.45	0	0.3	0	8.5%	22.9%	2.3%
484	50	0	0	0	0.2	0.5	0	0.3	0	1.7%	13.3%	-1.3%
485	50	0	0	0	0	0	0.65	0.3	0.05	3.8%	1.7%	-1.8%
486	50	0	0	0	0	0	0.6	0.3	0.1	17.1%	6.2%	-0.5%
487	50	0	0	0	0	0	0.55	0.3	0.15	29.1%	18.3%	1.6%
488	50	0	0	0	0	0	0.5	0.3	0.2	33.9%	10.7%	1.7%
489	50	0	0	0	0	0	0.45	0.3	0.25	35.2%	10.0%	2.9%
490	50	0	0	0	0	0	0.4	0.3	0.3	31.6%	9.6%	2.7%
491	50	0	0	0	0	0	0.35	0.3	0.35	28.6%	4.4%	3.2%
492	50	0	0	0	0	0	0.3	0.3	0.4	29.1%	1.4%	3.5%
493	50	0	0	0	0	0	0.25	0.3	0.45	33.2%	1.7%	7.7%
494	50	0	0	0	0	0	0.2	0.3	0.5	25.6%	4.3%	15.0%
495	50	0	0	0	0.65	0	0	0.3	0.05	32.2%	8.0%	43.7%
496	50	0	0	0	0.6	0	0	0.3	0.1	22.0%	16.0%	45.5%
497	50	0	0	0	0.55	0	0	0.3	0.15	33.1%	11.7%	32.4%
498	50	0	0	0	0.5	0	0	0.3	0.2	26.0%	8.4%	16.9%
499	50	0	0	0	0.45	0	0	0.3	0.25	25.1%	5.6%	8.8%
500	50	0	0	0	0.4	0	0	0.3	0.3	27.7%	1.8%	2.5%
501	50	0	0	0	0.35	0	0	0.3	0.35	44.6%	1.6%	1.9%
502	50	0	0	0	0.3	0	0	0.3	0.4	21.7%	5.1%	0.2%
503	50	0	0	0	0.25	0	0	0.3	0.45	39.6%	6.9%	0.2%
504	50	0	0	0	0.2	0	0	0.3	0.5	35.1%	7.2%	-1.5%

Active Learning Polymer Iterations – Horseradish Peroxidase (HRP)											
Polymer	**DP**	**DEAEMA**	**2-HPMA**	**SPMA**	**BMA**	**DMAPMA**	**MMA**	**PEGMA**	**TEAMA**	**REA**	**Std Dev.**
I1-1	125	0.48	0	0	0.2	0	0	0.32	0	-2%	1%
I1-2	50	0	0.16	0.27	0.07	0	0	0.5	0	14%	2%
I1-3	50	0	0	0.1	0	0	0.44	0.41	0.05	11%	1%
I1-4	100	0.45	0	0	0.15	0	0.1	0.3	0	-2%	0%
I1-5	75	0	0	0.13	0	0	0.55	0.27	0.05	15%	1%
I1-6	50	0.14	0.05	0	0	0	0.72	0.09	0	61%	9%
I1-7	50	0	0	0.21	0	0	0.65	0.14	0	12%	0%
I1-8	50	0.28	0	0	0	0	0.65	0	0.07	65%	5%
I1-9	125	0.46	0	0	0.16	0	0	0.25	0.13	-1%	0%
I1-10	50	0.31	0	0	0.08	0	0.61	0	0	-1%	1%
I1-11	50	0	0	0	0	0	0.39	0.52	0.09	16%	2%
I1-12	50	0.24	0	0.13	0.07	0	0.56	0	0	48%	8%
I1-13	125	0.43	0	0	0.1	0.13	0	0.34	0	49%	4%
I1-14	75	0	0	0.15	0	0	0.69	0	0.16	41%	1%
I1-15	50	0.17	0	0.15	0	0.05	0.63	0	0	52%	16%
I1-16	125	0.39	0	0	0.09	0	0.07	0.45	0	-1%	0%
I1-17	50	0.25	0	0	0	0.15	0.6	0	0	-1%	1%
I1-18	125	0.35	0	0	0.08	0	0	0.38	0.19	-2%	0%
I1-19	125	0.37	0	0.15	0	0	0	0.35	0.13	-2%	0%
I1-20	125	0.38	0	0.24	0.09	0	0	0.29	0	56%	5%
I1-21	75	0	0	0.11	0.26	0	0.63	0	0	13%	5%
I1-22	50	0.2	0	0	0	0	0.54	0	0.26	59%	7%
I1-23	50	0.11	0	0.09	0.24	0	0.56	0	0	30%	7%
I1-24	50	0	0	0.38	0.14	0	0	0.48	0	30%	21%
I2-1	50	0.27	0	0.06	0	0	0.59	0	0.08	46%	3%
I2-2	75	0	0.14	0.13	0	0	0.15	0.58	0	18%	3%
I2-3	50	0.32	0.08	0	0	0	0.6	0	0	40%	7%
I2-4	75	0	0.33	0.09	0	0	0.39	0.19	0	36%	5%
I2-5	50	0	0.11	0.2	0.32	0	0	0.37	0	54%	8%
I2-6	50	0.28	0	0	0.07	0	0.59	0.06	0	46%	3%
I2-7	50	0.25	0	0.12	0.13	0	0.5	0	0	39%	1%
I2-8	100	0.33	0	0.33	0.12	0	0	0.22	0	32%	10%
I2-9	75	0	0	0	0	0	0.59	0.12	0.29	55%	8%
I2-10	50	0	0.32	0.08	0	0	0.22	0.38	0	17%	2%
I2-11	50	0.16	0	0.11	0	0	0.57	0	0.16	49%	7%
I2-12	75	0.54	0	0	0.29	0	0	0.17	0	45%	8%
I2-13	50	0	0	0.24	0.31	0	0	0.45	0	29%	6%
I2-14	125	0.39	0	0.38	0.09	0	0	0.14	0	40%	10%
I2-15	50	0.34	0.06	0	0	0.07	0.53	0	0	46%	11%
I2-16	125	0.32	0	0.44	0	0	0	0.24	0	43%	8%
I2-17	100	0.58	0	0	0	0	0.31	0.11	0	48%	18%

I2-18	75	0	0.19	0	0	0	0.48	0.07	0.26	54%	10%
I2-19	50	0	0.21	0	0	0	0.53	0	0.26	41%	9%
I2-20	50	0.43	0.1	0	0	0	0.47	0	0	48%	4%
I2-21	100	0.55	0	0.13	0.26	0	0	0.06	0	37%	10%
I2-22	100	0.64	0	0	0.3	0.06	0	0	0	-2%	1%
I2-23	100	0.6	0.08	0	0.32	0	0	0	0	-2%	0%
I2-24	100	0.42	0	0.36	0.22	0	0	0	0	36%	15%
I3-1	75	0	0.15	0.07	0	0	0.63	0	0.15	64%	7%
I3-2	100	0.48	0	0	0.29	0	0	0.23	0	-2%	0%
I3-3	50	0.19	0	0.1	0	0	0.59	0.12	0	52%	2%
I3-4	50	0	0.31	0.09	0	0	0	0.6	0	36%	7%
I3-5	100	0	0	0.07	0	0	0.62	0.15	0.16	56%	1%
I3-6	50	0.36	0	0	0	0	0.53	0.11	0	40%	11%
I3-7	50	0	0	0.17	0	0	0.52	0.31	0	27%	3%
I3-8	50	0.05	0	0	0	0	0.63	0.13	0.19	-2%	0%
I3-9	125	0.29	0	0.35	0.1	0	0	0.26	0	-1%	1%
I3-10	75	0	0.07	0	0	0	0.44	0.16	0.33	52%	7%
I3-11	50	0.28	0.18	0	0	0	0.44	0.1	0	42%	6%
I3-12	75	0	0.34	0.09	0	0	0.57	0	0	55%	5%
I3-13	50	0	0	0.16	0.17	0	0	0.67	0	44%	4%
I3-14	50	0	0.11	0	0.11	0	0.59	0	0.19	52%	6%
I3-15	50	0	0	0	0.11	0.06	0.65	0	0.18	32%	3%
I3-16	125	0.53	0	0	0	0	0.3	0.17	0	-1%	1%
I3-17	75	0.11	0	0	0	0	0.4	0.1	0.39	-2%	0%
I3-18	50	0.23	0.16	0	0	0	0.42	0	0.19	33%	7%
I3-19	75	0.1	0	0	0.11	0	0.39	0	0.4	-1%	1%
I3-20	50	0	0	0.07	0.19	0	0.46	0	0.28	59%	9%
I3-21	150	0	0.19	0	0	0	0.14	0.25	0.42	39%	7%
I3-22	75	0	0	0.16	0	0	0.38	0	0.46	60%	8%
I3-23	100	0.63	0	0	0	0	0.32	0.05	0	41%	6%
I3-24	75	0	0	0	0.24	0	0.33	0.08	0.35	38%	11%
I4-1	50	0	0.25	0.16	0	0	0.59	0	0	43%	6%
I4-2	100	0.47	0	0	0	0	0.32	0.21	0	54%	13%
I4-3	50	0	0.14	0.18	0.35	0	0	0.33	0	34%	5%
I4-4	50	0.29	0.08	0	0	0	0.52	0	0.11	52%	15%
I4-5	50	0	0.27	0.06	0	0	0.11	0.56	0	32%	4%
I4-6	75	0	0.25	0.09	0	0	0.55	0.11	0	48%	19%
I4-7	75	0	0.18	0	0	0	0.42	0.22	0.18	53%	14%
I4-8	75	0	0.18	0	0.15	0	0.51	0	0.16	48%	14%
I4-9	75	0	0.27	0	0	0	0.57	0	0.16	60%	2%
I4-10	125	0.48	0	0.35	0	0	0	0.17	0	19%	2%
I4-11	75	0	0.08	0	0	0	0.26	0.35	0.31	38%	5%
I4-12	50	0	0.18	0.18	0	0	0.48	0	0.16	41%	7%
I4-13	100	0	0	0.16	0	0	0.56	0	0.28	48%	11%

I4-14	100	0	0.1	0.12	0	0	0.57	0	0.21	47%	20%
I4-15	150	0	0	0	0	0	0.22	0.33	0.45	37%	1%
I4-16	100	0.51	0	0.32	0	0	0	0.17	0	38%	6%
I4-17	75	0	0	0.2	0.16	0	0.43	0	0.21	48%	8%
I4-18	50	0	0.28	0	0.2	0	0.52	0	0	21%	19%
I4-19	75	0	0.12	0.24	0	0	0.42	0	0.22	47%	2%
I4-20	75	0	0	0.34	0	0	0.4	0	0.26	37%	4%
I4-21	50	0	0.16	0.28	0	0	0.36	0	0.2	41%	3%
I4-22	50	0	0	0.33	0	0.06	0.38	0	0.23	44%	6%
I4-23	125	0	0	0.25	0	0	0.15	0.08	0.52	69%	10%
I4-24	100	0.49	0	0.3	0	0	0.21	0	0	41%	27%
I5-1	75	0	0.13	0.12	0	0	0.53	0	0.22	56%	3%
I5-2	75	0	0.18	0.09	0	0	0.55	0	0.18	50%	7%
I5-3	50	0	0.21	0.11	0	0	0.58	0.1	0	22%	4%
I5-4	50	0.29	0.09	0	0	0	0.54	0.08	0	47%	4%
I5-5	75	0	0.19	0.09	0	0	0.6	0	0.12	55%	3%
I5-6	50	0.23	0.12	0	0	0	0.56	0.09	0	34%	5%
I5-7	75	0	0.12	0.15	0	0	0.58	0	0.15	49%	21%
I5-8	50	0	0.22	0.11	0	0	0.52	0.15	0	17%	5%
I5-9	75	0	0.24	0.1	0	0	0.52	0	0.14	59%	9%
I5-10	50	0	0.17	0.12	0.08	0	0	0.63	0	16%	4%
I5-11	75	0	0.09	0.19	0	0	0.48	0	0.24	54%	13%
I5-12	50	0	0.15	0.15	0	0	0.56	0.14	0	52%	9%
I5-13	50	0	0.27	0.09	0	0	0.54	0.1	0	42%	12%
I5-14	75	0	0.19	0.1	0	0	0.49	0	0.22	57%	11%
I5-15	75	0	0.1	0.1	0	0	0.6	0	0.2	59%	16%
I5-16	50	0	0.2	0.09	0	0	0.08	0.63	0	10%	1%
I5-17	50	0.16	0.14	0.11	0	0	0.59	0	0	0%	0%
I5-18	75	0	0.14	0.13	0	0	0.47	0	0.26	71%	17%
I5-19	50	0.23	0.08	0.09	0	0	0.6	0	0	30%	3%
I5-20	50	0	0.17	0.13	0	0	0.5	0.2	0	54%	11%
I5-21	75	0	0.04	0.17	0	0	0.55	0	0.24	81%	7%
I5-22	50	0.09	0.16	0.12	0	0	0.63	0	0	-1%	0%
I5-23	50	0.27	0	0.05	0	0	0.59	0.09	0	30%	4%
I5-24	50	0.22	0	0.1	0	0	0.61	0.07	0	63%	6%

Active Learning Polymer Iterations – Glucose Oxidase (GOx)											
Polymer	**DP**	**DEAEMA**	**2-HPMA**	**SPMA**	**BMA**	**DMAPMA**	**MMA**	**PEGMA**	**TEAMA**	**REA**	**Std Dev.**
I1-1	100	0.05	0	0	0.16	0.38	0	0.41	0	13.1%	1.2%
I1-2	100	0.2	0	0	0	0.07	0.73	0	0	10.8%	1.7%
I1-3	125	0	0	0	0.17	0.4	0.14	0.29	0	19.3%	5.5%
I1-4	100	0.21	0	0	0.35	0.17	0	0.27	0	18.2%	5.0%
I1-5	75	0.19	0	0	0	0	0.7	0.11	0	30.9%	7.4%
I1-6	75	0	0	0	0	0.45	0.33	0.22	0	15.9%	5.6%
I1-7	75	0.41	0	0.06	0.16	0	0	0.37	0	20.9%	6.0%
I1-8	75	0	0	0.06	0	0.37	0.2	0.37	0	8.7%	1.1%
I1-9	100	0	0	0	0.15	0.41	0.14	0.3	0	16.7%	0.1%
I1-10	75	0	0	0	0	0.17	0.72	0.11	0	34.1%	1.9%
I1-11	200	0.22	0	0	0	0	0.7	0.08	0	16.6%	1.0%
I1-12	125	0.18	0	0	0.37	0.19	0	0.26	0	19.6%	0.8%
I1-13	100	0.19	0	0	0	0	0.7	0.11	0	29.6%	1.6%
I1-14	150	0	0	0	0.08	0.38	0.16	0.38	0	27.7%	4.5%
I1-15	75	0.19	0	0	0	0.08	0.73	0	0	24.5%	0.5%
I1-16	75	0.21	0	0	0	0	0.72	0	0.07	21.7%	1.7%
I1-17	75	0.18	0	0	0.12	0	0.7	0	0	32.4%	1.7%
I1-18	150	0	0	0	0.16	0.4	0.15	0.29	0	15.8%	1.6%
I1-19	100	0	0	0	0	0.34	0.09	0.45	0.12	17.2%	2.5%
I1-20	150	0.21	0	0	0	0	0.69	0.1	0	32.8%	1.8%
I1-21	75	0.14	0	0	0	0.2	0.66	0	0	39.2%	3.9%
I1-22	75	0	0	0	0.08	0.33	0.11	0.48	0	23.2%	1.6%
I1-23	100	0.25	0	0	0.17	0.27	0	0.31	0	23.2%	2.1%
I1-24	175	0.31	0	0	0	0	0.69	0	0	13.3%	0.9%
I2-1	75	0.12	0	0	0	0.06	0.69	0.13	0	12.7%	1.7%
I2-2	100	0	0.06	0	0.19	0.34	0	0.41	0	13.3%	3.9%
I2-3	125	0.13	0	0	0	0.36	0.19	0.32	0	13.1%	3.8%
I2-4	100	0.19	0	0	0	0	0.71	0.1	0	22.0%	2.9%
I2-5	75	0.18	0	0	0	0.06	0.76	0	0	13.3%	3.3%
I2-6	125	0	0	0	0.18	0.37	0	0.45	0	11.4%	4.9%
I2-7	50	0.2	0	0	0	0	0.72	0.08	0	23.7%	4.7%
I2-8	125	0	0	0	0	0.49	0.27	0.24	0	1.8%	0.5%
I2-9	150	0.39	0	0	0.24	0	0	0.37	0	3.7%	0.7%
I2-10	75	0.13	0	0	0.12	0	0.75	0	0	20.1%	1.4%
I2-11	125	0.08	0	0	0	0.2	0.61	0.11	0	26.8%	1.7%
I2-12	100	0.13	0	0	0.21	0	0.66	0	0	0.3%	0.2%
I2-13	150	0	0	0	0	0.2	0.66	0.14	0	11.2%	1.0%
I2-14	125	0.21	0	0	0	0.22	0.57	0	0	21.9%	1.0%
I2-15	150	0.14	0	0	0	0.3	0.43	0.13	0	17.6%	1.9%
I2-16	100	0.19	0	0	0	0	0.63	0	0.18	7.2%	0.6%
I2-17	75	0.15	0	0	0	0	0.66	0	0.19	9.6%	1.0%

I2-18	125	0.25	0	0	0	0.42	0.17	0.16	0	12.7%	0.5%
I2-19	200	0.56	0	0	0	0	0.44	0	0	2.8%	0.3%
I2-20	100	0.29	0.32	0	0	0	0.39	0	0	23.4%	2.1%
I2-21	150	0.53	0	0	0	0	0.4	0.07	0	2.4%	0.3%
I2-22	50	0.46	0.3	0	0	0	0	0.24	0	20.7%	1.3%
I2-23	75	0.1	0	0	0.31	0	0.59	0	0	-1.8%	0.2%
I2-24	150	0.29	0.32	0	0	0	0.39	0	0	10.1%	0.6%
I3-1	125	0.16	0	0	0	0	0.66	0.18	0	24.8%	2.2%
I3-2	50	0.56	0.11	0	0	0	0	0.33	0	25.1%	4.6%
I3-3	75	0	0	0	0	0.33	0.67	0	0	43.1%	8.5%
I3-4	175	0	0	0	0.05	0.31	0.24	0.4	0	18.8%	8.7%
I3-5	200	0	0	0	0.12	0.38	0.15	0.35	0	23.4%	9.5%
I3-6	100	0	0	0	0	0.48	0.13	0.39	0	19.9%	5.4%
I3-7	75	0.23	0	0	0.47	0	0	0.3	0	41.4%	8.6%
I3-8	75	0	0	0	0.28	0.4	0.07	0.25	0	29.3%	4.2%
I3-9	75	0.46	0	0	0.22	0	0.09	0.23	0	38.0%	1.5%
I3-10	100	0	0	0	0.17	0.39	0.16	0.28	0	29.2%	8.0%
I3-11	100	0.05	0	0	0	0.27	0.68	0	0	54.3%	2.5%
I3-12	100	0	0.07	0	0.34	0.44	0	0.15	0	55.1%	3.4%
I3-13	125	0.16	0	0	0.16	0	0.55	0.13	0	52.4%	4.2%
I3-14	150	0	0	0	0.44	0.33	0	0.23	0	39.2%	4.2%
I3-15	175	0	0	0	0	0.37	0.08	0.38	0.17	12.0%	2.1%
I3-16	100	0.27	0	0	0.23	0	0.21	0.29	0	43.9%	10.0%
I3-17	75	0	0	0	0.18	0.21	0.61	0	0	42.3%	6.1%
I3-18	100	0.24	0.28	0	0	0	0.42	0.06	0	55.8%	6.9%
I3-19	150	0.38	0	0	0	0	0.47	0.15	0	29.7%	11.1%
I3-20	100	0	0	0	0.32	0.41	0	0.11	0.16	50.4%	1.5%
I3-21	50	0.48	0	0	0	0.22	0	0.3	0	50.4%	9.0%
I3-22	150	0.21	0.24	0	0	0	0.55	0	0	57.2%	18.2%
I3-23	175	0	0	0.2	0.06	0.37	0	0.37	0	8.4%	2.7%
I3-24	100	0.13	0	0	0.3	0.5	0	0.07	0	36.6%	9.0%
I4-1	125	0.25	0.17	0	0.14	0	0.44	0	0	18.2%	2.4%
I4-2	50	0.53	0	0	0.12	0.18	0	0.17	0	10.1%	1.8%
I4-3	125	0	0	0	0.45	0.43	0	0.12	0	7.6%	2.5%
I4-4	75	0.49	0	0	0.13	0.2	0	0.18	0	18.9%	8.0%
I4-5	125	0.28	0.21	0	0	0	0.46	0.05	0	47.7%	14.1%
I4-6	150	0.26	0.19	0	0.13	0	0.42	0	0	48.2%	11.6%
I4-7	100	0.19	0	0	0.21	0	0.43	0.17	0	49.2%	7.0%
I4-8	75	0.58	0	0	0	0.22	0	0.2	0	-1.2%	0.7%
I4-9	50	0.56	0	0	0	0.16	0	0.16	0.12	-1.5%	0.3%
I4-10	125	0	0	0	0.54	0.38	0	0.08	0	4.3%	0.2%
I4-11	150	0.28	0.23	0	0	0	0.4	0.09	0	50.5%	8.9%
I4-12	125	0.31	0	0	0.28	0	0.41	0	0	46.0%	2.1%
I4-13	50	0.45	0	0	0	0.28	0	0.1	0.17	35.3%	0.5%

I4-14	175	0.25	0.26	0	0	0.18	0.31	0	0	56.9%	5.9%
I4-15	50	0.61	0	0	0.14	0.19	0	0.06	0	12.5%	1.2%
I4-16	175	0.21	0.18	0	0.23	0	0.38	0	0	63.4%	1.9%
I4-17	75	0.53	0	0	0.12	0.21	0.14	0	0	3.2%	0.4%
I4-18	75	0.53	0	0.15	0.06	0.26	0	0	0	3.6%	0.1%
I4-19	75	0.57	0	0	0	0.24	0	0	0.19	6.3%	0.3%
I4-20	150	0.48	0.06	0	0.15	0	0.31	0	0	40.3%	0.5%
I4-21	75	0.64	0	0	0.13	0.23	0	0	0	26.2%	0.8%
I4-22	50	0.76	0	0	0.07	0.17	0	0	0	18.3%	0.8%
I4-23	50	0.58	0	0	0	0.17	0	0	0.25	9.0%	1.6%
I4-24	75	0.53	0	0	0	0.19	0	0	0.28	-0.5%	0.9%
I5-1	100	0	0	0	0.3	0.48	0	0.15	0.07	29.5%	7.9%
I5-2	100	0	0	0.03	0.31	0.45	0	0.21	0	39.3%	9.8%
I5-3	100	0.16	0.14	0	0	0	0.49	0.21	0	36.5%	5.4%
I5-4	50	0.45	0	0	0.06	0.2	0	0.29	0	30.9%	7.2%
I5-5	100	0	0	0	0.31	0.42	0	0.15	0.12	51.8%	7.3%
I5-6	100	0.14	0.17	0	0	0	0.54	0.15	0	44.7%	13.3%
I5-7	100	0.09	0	0	0.29	0.4	0	0.22	0	41.5%	14.5%
I5-8	100	0.06	0	0	0.24	0.49	0	0.21	0	32.5%	11.0%
I5-9	125	0.21	0.18	0	0	0	0.51	0.1	0	29.1%	5.0%
I5-10	100	0.15	0.21	0	0	0	0.49	0.15	0	56.6%	16.0%
I5-11	100	0.12	0.12	0	0	0	0.54	0.22	0	42.5%	11.0%
I5-12	100	0	0	0	0.29	0.45	0	0.1	0.16	52.0%	5.0%
I5-13	100	0	0	0	0.26	0.46	0	0.22	0.06	43.7%	4.7%
I5-14	100	0	0.1	0	0.3	0.45	0	0.15	0	55.6%	6.8%
I5-15	100	0	0.05	0	0.36	0.44	0	0.15	0	48.3%	2.7%
I5-16	100	0.18	0.18	0	0	0	0.44	0.2	0	36.1%	4.1%
I5-17	100	0.12	0.1	0	0	0	0.62	0.16	0	29.2%	6.8%
I5-18	100	0.2	0.21	0	0	0	0.5	0.09	0	50.3%	9.4%
I5-19	100	0.2	0	0	0.5	0	0	0.3	0	30.7%	4.1%
I5-20	100	0	0	0.05	0.34	0.39	0	0.22	0	67.4%	6.3%
I5-21	50	0.45	0	0	0	0.25	0	0.3	0	40.2%	2.8%
I5-22	50	0.39	0	0	0.09	0.22	0	0.3	0	51.0%	4.3%
I5-23	100	0.3	0	0	0.24	0	0.16	0.3	0	41.3%	6.7%
I5-24	100	0.24	0.12	0	0	0	0.44	0.2	0	30.0%	7.6%

Active Learning Polymer Iterations – Lipase (Lip)											
Polymer	**DP**	**DEAEMA**	**2-HPMA**	**SPMA**	**BMA**	**DMAPMA**	**MMA**	**PEGMA**	**TEAMA**	**REA**	**Std Dev.**
I1-1	100	0	0	0	0.7	0	0	0.15	0.15	15.1%	0.8%
I1-2	200	0	0	0	0.66	0	0	0.18	0.16	21.4%	7.1%
I1-3	75	0	0	0	0.67	0	0	0.17	0.16	39.0%	4.2%
I1-4	200	0	0.15	0	0.85	0	0	0	0	64.7%	10.1%
I1-5	200	0	0.44	0	0	0	0.56	0	0	-2.1%	0.6%
I1-6	175	0	0.4	0	0	0	0.6	0	0	-2.8%	0.4%
I1-7	200	0	0.12	0	0.82	0	0	0	0.06	6.5%	2.2%
I1-8	50	0	0	0	0.63	0	0	0.19	0.18	23.9%	2.9%
I1-9	175	0	0	0	0.67	0	0	0.17	0.16	23.0%	1.9%
I1-10	125	0	0	0.19	0	0	0.14	0.67	0	-3.2%	1.3%
I1-11	100	0	0	0.45	0	0	0.36	0.19	0	2.5%	1.5%
I1-12	125	0	0	0.45	0	0	0.37	0.18	0	26.0%	2.4%
I1-13	175	0	0.11	0	0.66	0	0	0	0.23	21.4%	5.9%
I1-14	175	0	0.06	0	0.78	0	0	0	0.16	33.8%	24.7%
I1-15	200	0	0	0	0.69	0	0	0.06	0.25	22.5%	2.9%
I1-16	150	0	0	0.43	0	0	0.31	0.26	0	-3.7%	0.5%
I1-17	200	0	0	0	0.77	0	0	0	0.23	36.7%	3.5%
I1-18	125	0	0	0.52	0	0.06	0.42	0	0	6.9%	2.4%
I1-19	125	0	0.07	0.42	0	0	0.21	0.3	0	64.5%	11.5%
I1-20	150	0	0	0.41	0	0	0.23	0.36	0	48.7%	9.0%
I1-21	150	0	0.07	0.39	0	0	0.2	0.34	0	65.9%	14.7%
I1-22	150	0	0	0	0.73	0	0	0.07	0.2	17.2%	0.5%
I1-23	150	0	0	0.36	0	0	0.21	0.35	0.08	-1.2%	0.8%
I1-24	125	0	0	0.39	0	0	0.15	0.34	0.12	21.4%	15.4%
I2-1	75	0	0	0	0.62	0	0	0.24	0.14	29.0%	3.4%
I2-2	200	0.18	0.3	0	0.52	0	0	0	0	5.2%	0.8%
I2-3	200	0.07	0.1	0	0.83	0	0	0	0	19.7%	2.9%
I2-4	200	0	0.12	0	0.77	0	0	0	0.11	18.5%	1.7%
I2-5	200	0	0.1	0.05	0.85	0	0	0	0	30.1%	0.3%
I2-6	200	0	0.39	0	0	0	0.61	0	0	-0.3%	0.2%
I2-7	150	0	0.12	0.27	0	0	0.23	0.38	0	1.9%	1.0%
I2-8	100	0	0	0	0.67	0	0	0.18	0.15	24.1%	0.2%
I2-9	150	0	0	0.46	0	0	0.13	0.41	0	29.4%	2.4%
I2-10	175	0	0.13	0	0.78	0	0	0	0.09	12.4%	7.7%
I2-11	175	0	0.15	0.05	0.8	0	0	0	0	22.5%	1.9%
I2-12	125	0	0.09	0.39	0	0	0.14	0.38	0	35.8%	2.1%
I2-13	150	0	0.12	0.39	0	0	0.12	0.37	0	33.6%	2.5%
I2-14	100	0	0.12	0.35	0	0	0.16	0.37	0	36.7%	3.0%
I2-15	125	0	0	0.39	0.09	0	0.13	0.39	0	8.0%	0.6%
I2-16	125	0	0.12	0.49	0	0	0.05	0.34	0	28.3%	2.4%
I2-17	125	0	0	0.49	0.06	0	0.06	0.39	0	23.6%	2.1%

I2-18	150	0	0.12	0.27	0	0	0.16	0.45	0	33.7%	3.6%
I2-19	150	0	0.06	0.5	0	0	0.06	0.38	0	55.2%	5.2%
I2-20	175	0	0.06	0.47	0	0.06	0	0.41	0	49.7%	4.1%
I2-21	175	0	0.12	0	0.88	0	0	0	0	40.4%	5.9%
I2-22	150	0	0.23	0.33	0	0	0	0.44	0	38.3%	1.3%
I2-23	125	0	0.24	0.35	0	0	0	0.41	0	42.2%	0.9%
I2-24	150	0	0.05	0.59	0	0	0	0.36	0	19.1%	1.0%
I3-1	200	0	0	0	0.61	0	0	0.23	0.16	13.1%	1.4%
I3-2	125	0	0.13	0.39	0	0	0.17	0.31	0	26.8%	3.9%
I3-3	200	0.21	0.26	0	0.53	0	0	0	0	1.7%	1.4%
I3-4	75	0	0	0	0.61	0	0	0.24	0.15	36.6%	3.6%
I3-5	175	0	0.12	0	0.77	0	0	0	0.11	29.4%	2.0%
I3-6	125	0	0.26	0.26	0	0	0	0.48	0	11.2%	3.0%
I3-7	150	0	0.11	0.42	0	0	0.06	0.41	0	34.8%	6.7%
I3-8	200	0	0.14	0	0.86	0	0	0	0	46.3%	7.0%
I3-9	175	0	0.12	0.41	0	0	0.06	0.41	0	56.4%	4.4%
I3-10	125	0	0.22	0.39	0	0	0.2	0.19	0	42.9%	1.1%
I3-11	175	0	0.11	0.31	0	0.09	0	0.49	0	71.1%	7.1%
I3-12	200	0	0.12	0.35	0	0	0.09	0.44	0	28.6%	0.8%
I3-13	100	0	0.23	0.2	0	0	0	0.39	0.18	15.7%	1.6%
I3-14	150	0.21	0.05	0.4	0	0	0	0.34	0	9.5%	1.1%
I3-15	200	0	0	0	0.92	0	0	0	0.08	36.1%	3.2%
I3-16	200	0	0.22	0.34	0	0	0.12	0.32	0	31.6%	2.6%
I3-17	175	0	0.47	0	0	0	0.53	0	0	0.7%	0.3%
I3-18	200	0	0.2	0.26	0	0.17	0	0.37	0	81.0%	1.5%
I3-19	150	0	0.13	0.28	0	0.27	0	0.32	0	79.8%	3.5%
I3-20	125	0.27	0.13	0.33	0	0	0	0.27	0	-1.9%	0.8%
I3-21	200	0	0.51	0.12	0	0	0.37	0	0	-2.1%	0.2%
I3-22	100	0	0.36	0.32	0	0	0.18	0.14	0	56.3%	1.6%
I3-23	125	0	0.19	0.22	0	0.28	0	0.31	0	93.9%	5.4%
I3-24	200	0	0	0.28	0.19	0.22	0	0.31	0	-0.8%	0.5%
I4-1	175	0	0.2	0.29	0	0.15	0	0.36	0	76.9%	4.2%
I4-2	100	0	0.3	0.27	0	0	0.15	0.28	0	36.2%	1.6%
I4-3	150	0	0	0.36	0	0.17	0.07	0.4	0	69.5%	6.1%
I4-4	100	0	0.22	0.29	0	0.18	0	0.31	0	56.9%	6.8%
I4-5	125	0	0.08	0.3	0	0.3	0	0.32	0	57.6%	6.9%
I4-6	150	0	0.23	0.29	0	0.17	0	0.31	0	68.9%	4.3%
I4-7	125	0	0.21	0.29	0	0.19	0	0.31	0	60.6%	3.6%
I4-8	125	0	0.19	0.38	0	0.23	0	0.2	0	66.3%	1.0%
I4-9	125	0	0.3	0.31	0	0.15	0	0.24	0	70.5%	10.5%
I4-10	175	0	0.31	0.19	0	0.19	0	0.31	0	67.7%	3.3%
I4-11	125	0	0	0.39	0	0.24	0.08	0.29	0	62.0%	3.3%
I4-12	175	0	0.07	0	0.93	0	0	0	0	52.3%	5.3%
I4-13	150	0	0.33	0.18	0	0.21	0	0.28	0	68.9%	2.7%

I4-14	175	0	0.32	0.17	0	0.29	0	0.22	0	74.8%	5.5%
I4-15	100	0	0.1	0.38	0	0.27	0	0.25	0	65.4%	2.1%
I4-16	125	0	0	0.18	0	0.28	0	0.34	0.2	76.4%	4.8%
I4-17	100	0	0.29	0.35	0	0.23	0	0.13	0	66.3%	6.7%
I4-18	100	0	0	0.36	0	0.29	0	0.27	0.08	57.4%	9.9%
I4-19	150	0	0.4	0.21	0	0.16	0	0.23	0	62.0%	2.3%
I4-20	125	0	0.34	0.34	0	0.27	0	0.06	0	59.4%	0.3%
I4-21	175	0	0.33	0.31	0	0.26	0	0.1	0	72.0%	4.1%
I4-22	125	0	0.28	0.33	0	0.29	0.1	0	0	66.4%	11.3%
I4-23	125	0	0.29	0.34	0	0.26	0	0	0.11	70.0%	7.8%
I4-24	125	0	0.3	0.33	0.12	0.25	0	0	0	36.8%	11.0%
I5-1	150	0	0.3	0.25	0	0.25	0	0.2	0	88.7%	21.8%
I5-2	150	0	0.27	0.25	0	0.22	0	0.26	0	90.5%	17.1%
I5-3	125	0	0.24	0.28	0	0.26	0	0.22	0	99.3%	13.4%
I5-4	125	0	0.19	0.28	0	0.26	0	0.27	0	67.9%	43.5%
I5-5	150	0	0.35	0.26	0	0.24	0	0.15	0	101%	18.7%
I5-6	125	0	0.27	0.32	0	0.26	0	0.15	0	88.2%	18.1%
I5-7	175	0	0.22	0.28	0	0.18	0	0.32	0	83.5%	18.6%
I5-8	175	0	0.19	0.29	0	0.14	0	0.38	0	91.1%	6.6%
I5-9	150	0	0.31	0.3	0	0.18	0	0.21	0	99.0%	7.2%
I5-10	175	0	0.14	0.31	0	0.12	0	0.43	0	74.6%	4.6%
I5-11	125	0	0.13	0.27	0	0.28	0	0.32	0	99.0%	7.4%
I5-12	150	0	0.29	0.26	0	0.32	0	0.13	0	82.8%	7.5%
I5-13	125	0	0.21	0.23	0	0.25	0	0.31	0	61.5%	6.6%
I5-14	150	0	0.15	0.32	0	0.21	0	0.32	0	59.7%	0.8%
I5-15	125	0	0	0.27	0	0.28	0	0.33	0.12	91.1%	18.7%
I5-16	175	0	0.11	0.37	0	0.12	0	0.4	0	79.0%	19.9%
I5-17	175	0	0.26	0.27	0	0.12	0	0.35	0	57.1%	10.8%
I5-18	150	0	0.12	0.27	0	0.23	0	0.38	0	87.2%	8.0%
I5-19	125	0	0.12	0.32	0	0.31	0	0.25	0	108%	9.4%
I5-20	125	0	0.23	0.33	0	0.31	0	0.13	0	93.7%	9.9%
I5-21	175	0	0.18	0.32	0	0.07	0	0.43	0	41.9%	3.5%
I5-22	150	0	0.1	0.35	0	0.19	0	0.35	0	83.4%	12.8%
I5-23	150	0	0.31	0.31	0	0.3	0	0.08	0	79.0%	2.4%
I5-24	125	0	0	0.22	0	0.28	0	0.33	0.17	105%	6.6%

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