Supplementary Material for

Mechanism-Informed Machine Learning for Rational Catalyst Design: Application to Regioselectivity of Allyl Acetate Hydroformylation

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1 Details of the correlation between experimental l/b ratios and ΔΔG

1.1 Experimental results

All ligands were purchased from Shanghai Bide Pharmatech Co., Ltd. and used without further purification. During the hydroformylation of allyl acetate, the molar ratio of ligand to metal center is 10. An excess of ligand facilitates effective coordination with the catalyst center, leading to the formation of a homogeneous and stable active species. The overall aldehyde selectivity presented in Table S1 refers to the proportion of 4-acetoxybutyraldehyde and 2-methyl-3-acetoxypropionaldehyde among all reaction products.

Table S1 Experimental results of allyl acetate hydroformylation

Entry	Ligand	Conversion	Total Aldehyde Selectivity	l/b
1	P1	99.99%	98.24%	0.584
2	P2	99.91%	77.12%	0.744
3	P3	99.96%	94.37%	0.796
4	P4	94.29%	95.30%	0.656
5	P5	99.86%	98.30%	0.611
6	P6	99.97%	97.72%	0.661
7	P7	99.96%	97.51%	0.675
8	P8	99.97%	87.12%	0.704
9	P9	99.84%	97.54%	0.632
10	P10	81.28%	94.42%	0.648
11	P11	44.27%	96.92%	0.612
12	2P1	99.45%	92.24%	8.926
13	2P2	99.85%	89.58%	2.567
14	2P3	99.73%	37.84%	3.013
15	2P4	99.83%	47.44%	1.318
16	2P5	99.79%	71.57%	0.754
17	2P6	99.97%	71.54%	0.804
18	2P7	78.95%	81.13%	1.410

1.2 Olefin coordination configurations

To compare the coordination stability of allyl acetate across different ligand systems, DFT calculations were performed on 18 representative mono- and bidentate phosphine catalysts, focusing on the relative position and orientation of the acetoxy functional group with respect to the catalyst structure. Computational details are as follows: geometry optimizations were carried out using the M06-2X functional with a mixed basis set, SDD for Rh and 6-31G* for all other atoms. Single-point energy calculations were performed at the M06-2X/def2-TZVP level, including solvent effects of toluene. The final energies were corrected for vibrational frequencies at 353.15 K and 20 bar.

For each catalyst, both equatorial-equatorial and equatorial-axial coordination modes of the two phosphorus atoms in the ligand were considered. For the olefin substrate, different spatial orientations of the acetoxy group relative to the catalyst center were examined. Certain ligand conformations could not be optimized to stable minima and were thus omitted from the figure. The energies shown are relative to the lowest-energy configuration of each catalyst.

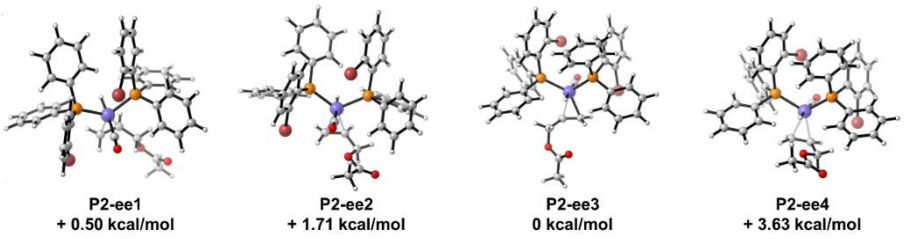


Figure S1. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P2.

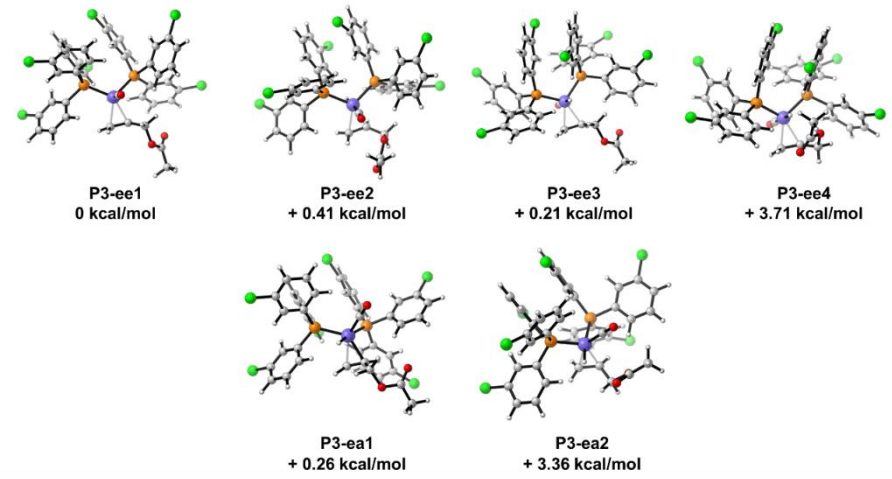


Figure S2. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P3.

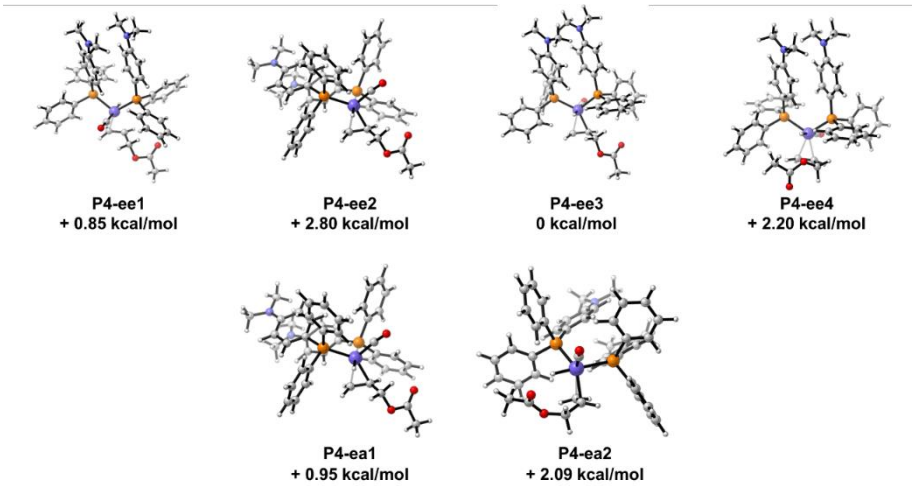


Figure S3. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P4.

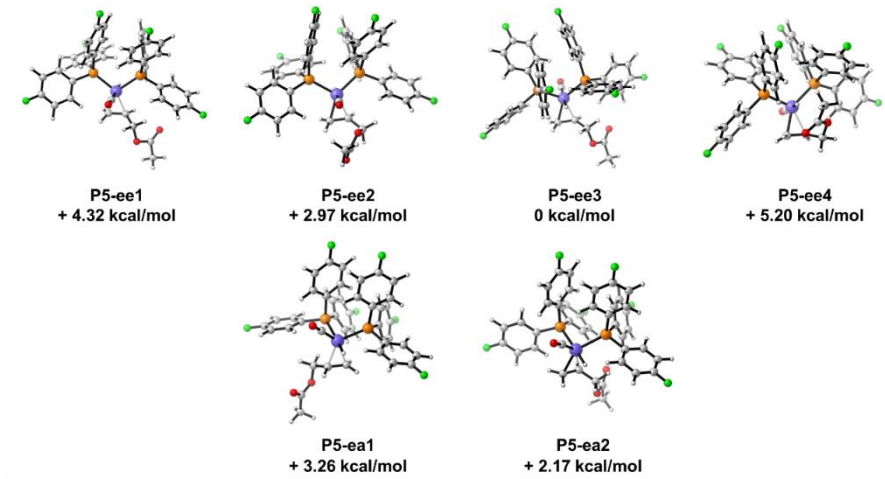


Figure S4. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P5.

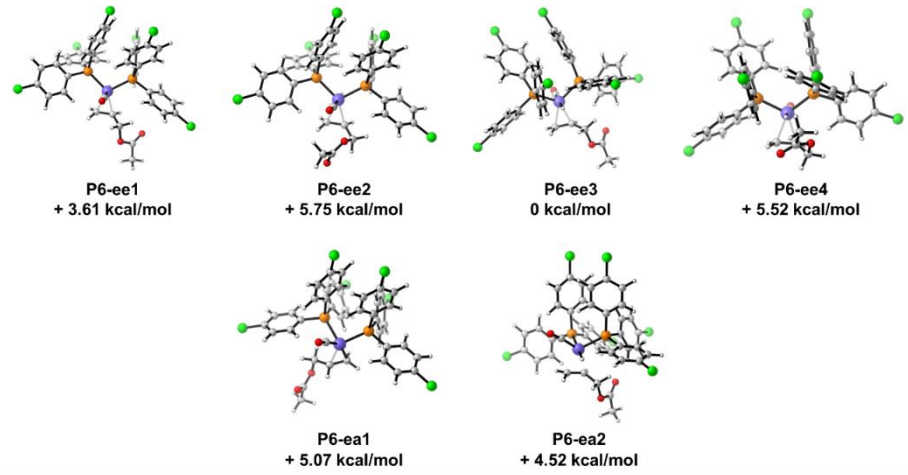


Figure S5. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P6.

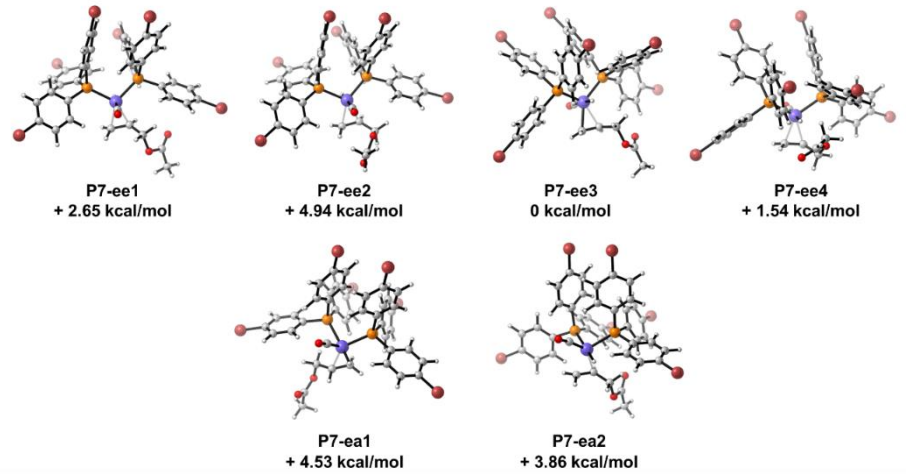


Figure S6. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P7.

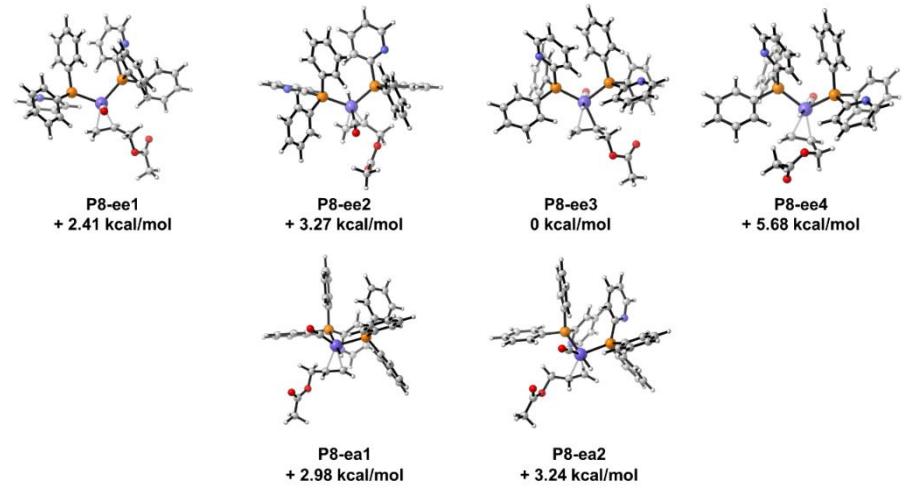


Figure S7. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P8.

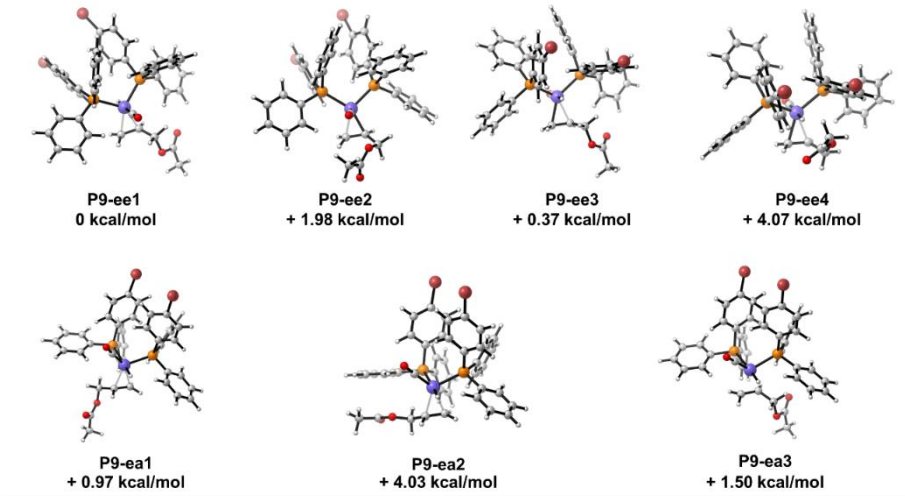


Figure S8. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P9.

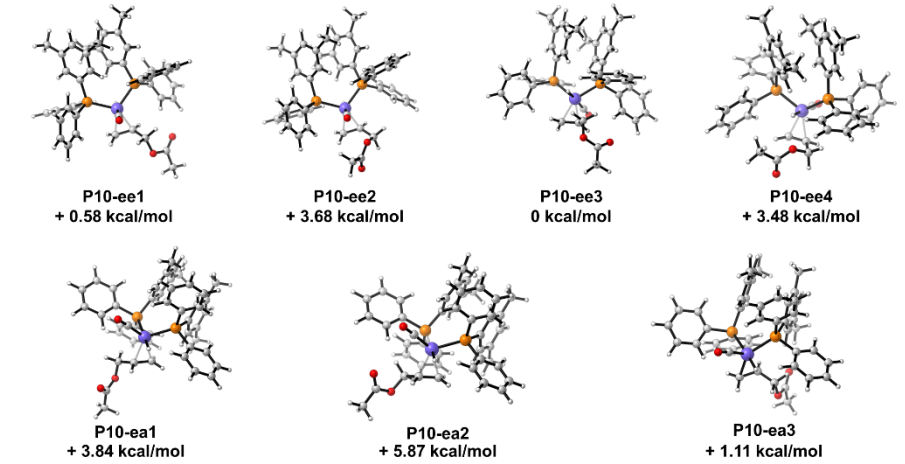


Figure S9. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P10.

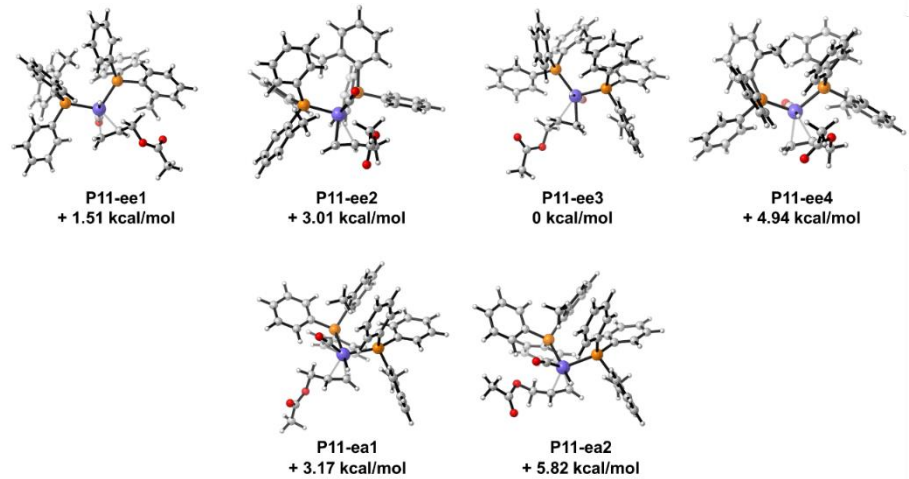


Figure S10. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand P11.

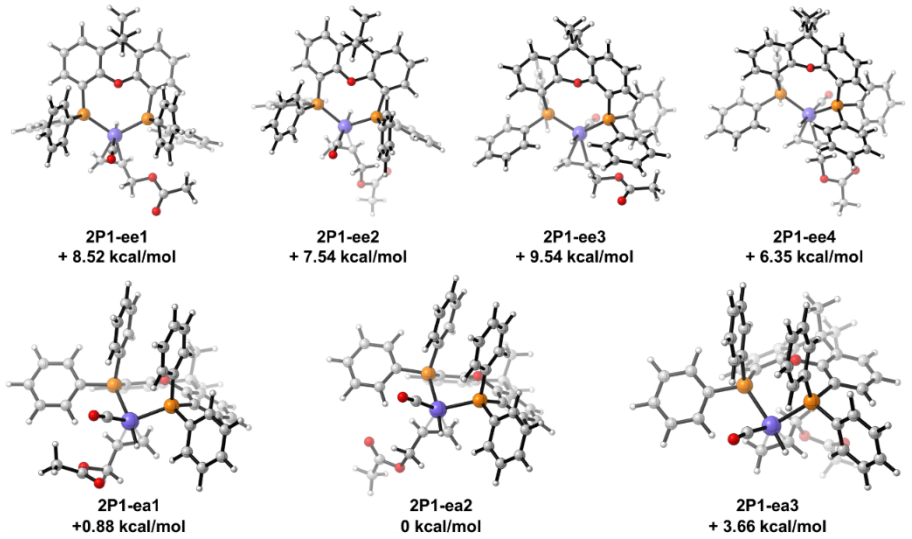


Figure S11. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P1.

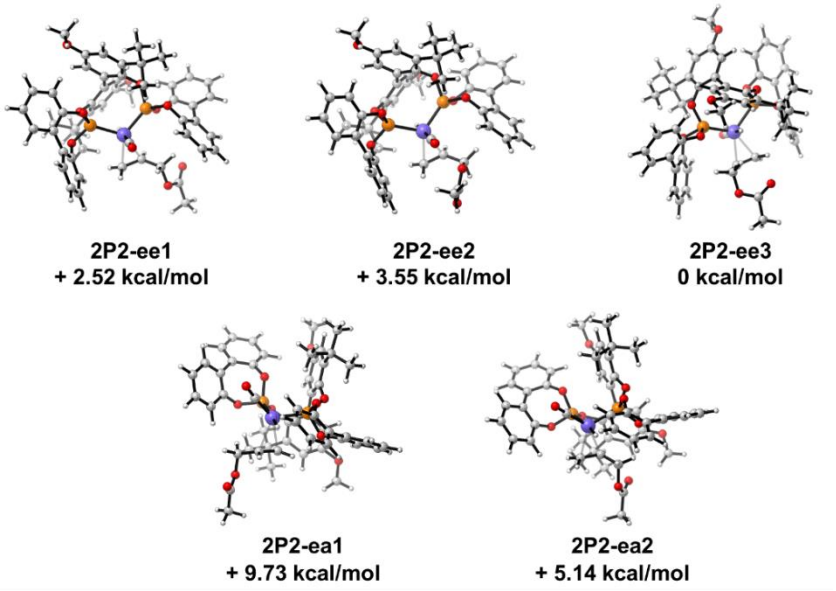


Figure S12. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P2.

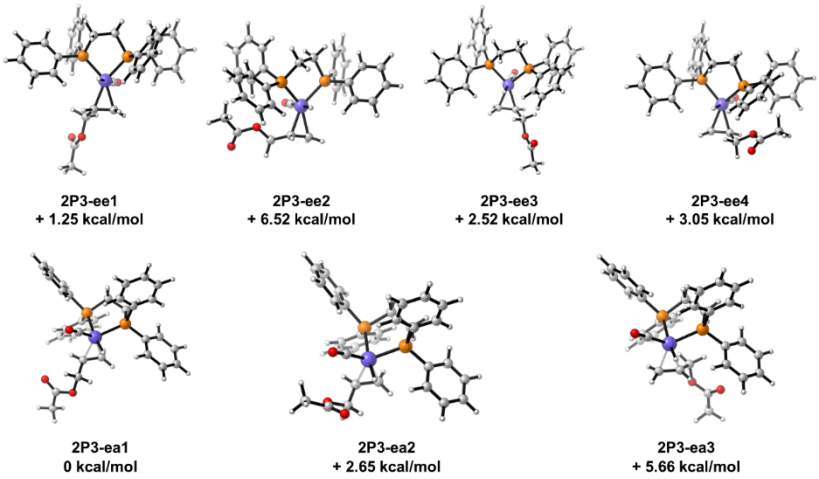


Figure S13. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P3.

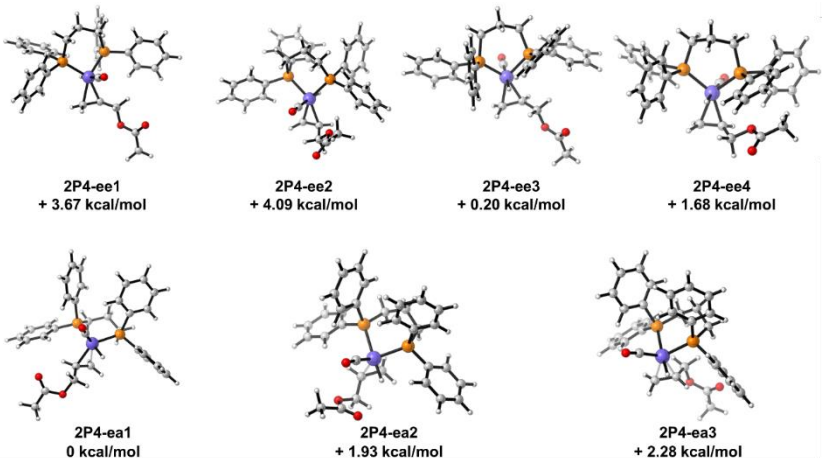


Figure S14. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P4.

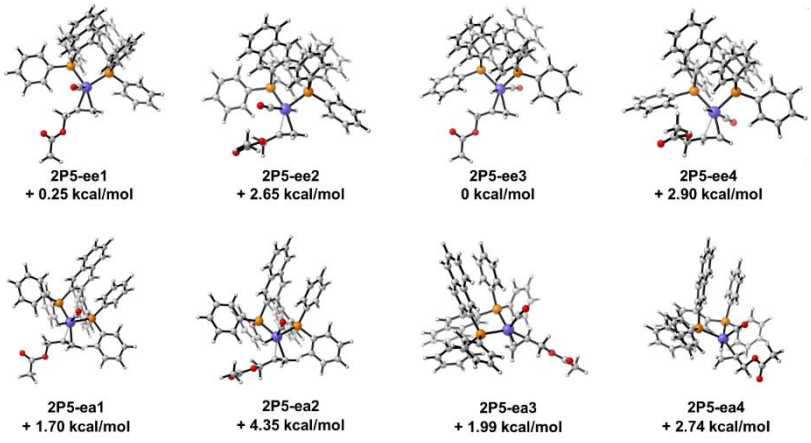


Figure S15. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P5.

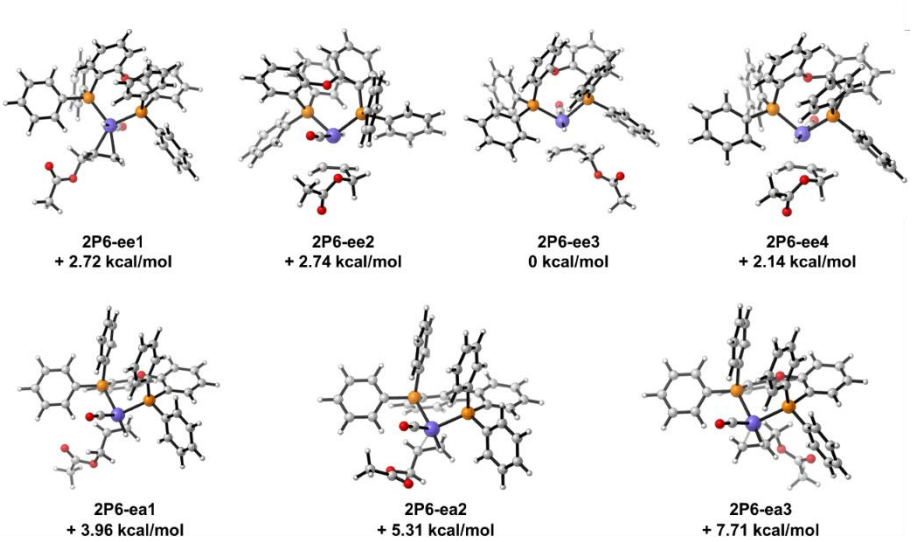


Figure S16. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P6.

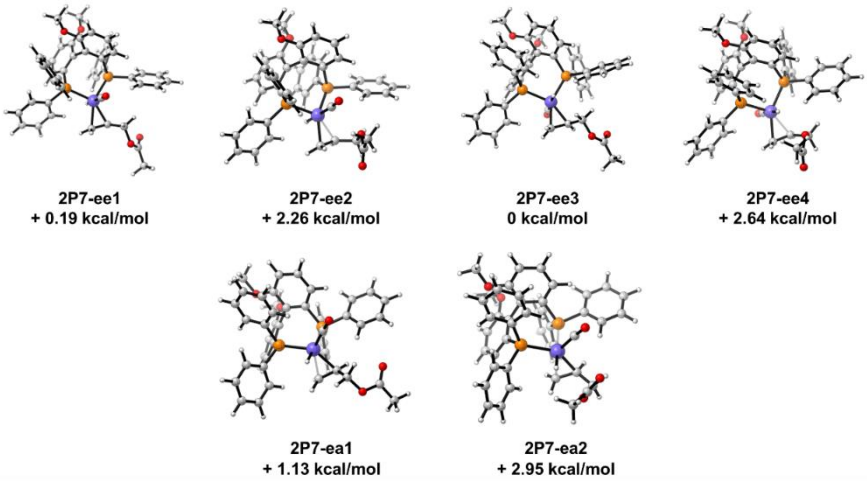


Figure S17. Olefin coordination configurations and relative energies of the Rh catalyst modified with ligand 2P7.

2 Stable structure search and parameters extraction

2.1 Stable structure search

The initial conformer sampling was performed using unconstrained molecular dynamics (MD). A 100ps NVT simulation at an elevated temperature of 400 K was performed to efficiently explore the conformational space. The semi-empirical method GFN0-xTB[1,2] was employed for the dynamics, using a time step of 1fs and constraining the X-H bonds via the SHAKE algorithm. The self-consistent charge (SCC) accuracy was set to 2.0. The trajectory was sampled every 50fs, yielding a total of 2000 snapshot conformers for subsequent analysis.

These structures were then subjected to a two-step clustering and filtering process using the Molclus/isostat toolkit[3]. Both clustering stages applied a strict energy difference threshold of 0.5kcal/mol and a geometric distance threshold of 0.2 Å (with the temperature parameter set to 350K) to ensure the selected conformers were truly low-energy and geometrically distinct. In the first clustering step, up to 50 unique conformers were identified. A second, more stringent clustering stage was subsequently applied to select a final set of 10 representative conformers, which were then further optimized at the GFN2-xTB[4] level.

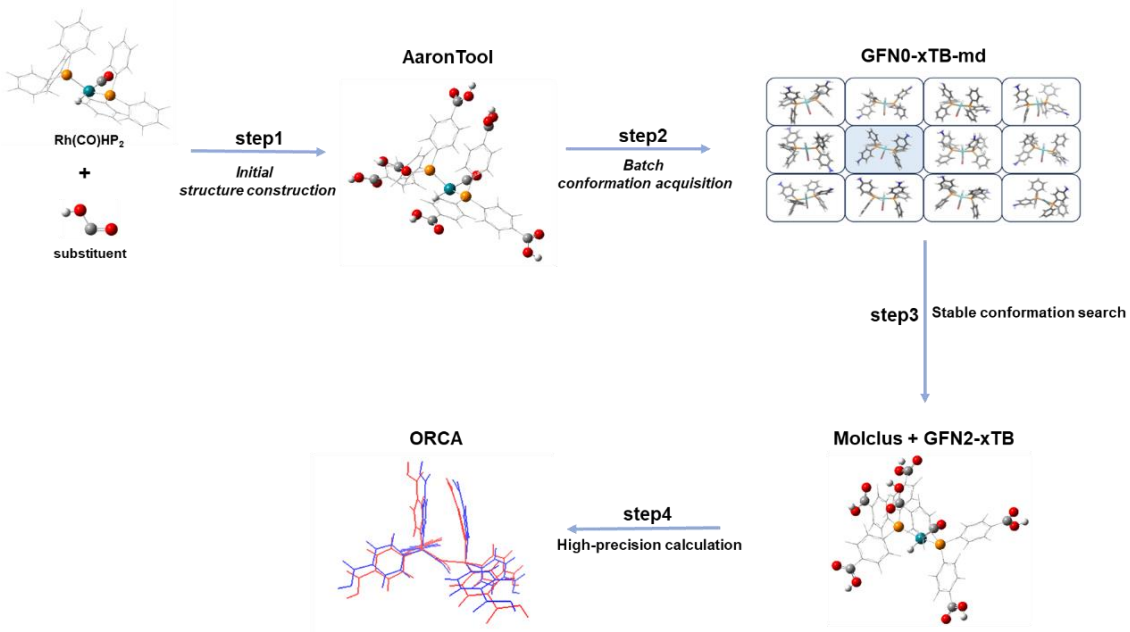


Figure S18. Workflow for stable conformer search.

```
\$md
   temp=400        # in K, thermostat temperature
   time=100        # in ps, total run time of simulation
   dump=50         # in fs, interval for trajectory printout
   step=1        # in fs, time step for propagation
   velo=false      # also write out velocities
   nvt=true        # perform simulation in NVT ensemble
   hmass=1         # do not change mass of hydrogens (default:4 times)
   shake=1         # use SHAKE algorithm to constrain bonds 0 = off, 1 = X-H only, 2 = all bonds
   sccacc=2.0      # accuracy of xTB calculation in dynamics
   restart=false   # read velocities from "mdrestart"
\$end
```

Figure S19. GFN0-xTB parameter settings.

The descriptor set can be categorized into four groups:

(I) **Steric parameters of ligands**: reflecting the intrinsic spatial properties of ligands;

(II) **Coordination parameters of substrate-catalyst complexes**: describing the interaction patterns between the substrate and the metal center;

(III) **Electronic parameters**: characterizing charge distribution and electronic effects within the system;

(IV) **Atomic parameters**: capturing the coupled influence of geometric and electronic factors.

2.2 Steric parameters of ligands

2.2.1 Buried volume and octant analysis

The buried volume refers to the percentage of spatial volume occupied by a ligand within a defined distance from the metal center, which is commonly used to quantify its steric size or steric hindrance.

This study employed morfeus to extract the buried volume of ligand structures, where H atoms, metal atoms, CO groups, and substrates were excluded by default. The buried volume fraction (V_bur) of the ligand was calculated with a default radius of 3.5 Å, and additional values were obtained at radii of 1.0, 2.0, 3.0, 4.0, and 5.0 Å.

To further quantify the spatial distribution of buried volume, octant buried volume analysis was performed. Specifically, the Rh atom was set as the origin, the CO bond direction was defined as the z-axis, and the plane containing the P atoms

was used to define the xz-plane. The buried volume fraction in each of the eight octants (buried_volume_n, n = 0-7) was computed at a radius of 3.5 Å, along with the maximum and minimum buried volume values (buried_volume_max, buried_volume_min).

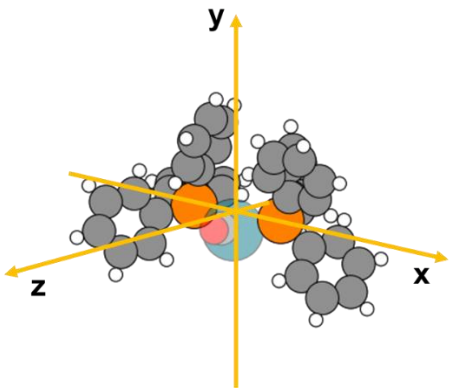


Figure S20. Schematic illustration of the octant division (Rh and CO were shown only for clarity in defining the coordinate system, but were not included in the actual calculation).

2.2.2 Sterimol parameters

Sterimol parameters are a set of steric descriptors used to quantify the three-dimensional size and shape of a substituent or ligand. They consist of three values: L, B1, and B5. L represents the length of the substituent along the bond axis connecting it to the parent atom or metal center. B1 and B5 denote the minimum and maximum radii of the substituent perpendicular to the bond axis, respectively, capturing the steric bulk in the narrowest and widest directions. Sterimol parameters are widely used in organometallic chemistry and catalysis to relate ligand sterics to reactivity and selectivity.

2.2.3 Cone angle, pyramidalization, solid angle

With the metal atom as the vertex and the metal-ligand bond as the cone axis, a hypothetical cone is formed by the space covered by the outermost atoms of the ligand, and the apex angle of this cone is defined as the cone angle. The magnitude of the cone angle reflects the steric hindrance of the ligand around the metal center.

In the context of ligand characterization, pyramidalization is commonly used to describe the extent to which the substituents around the phosphorus atom in a phosphine ligand deviate from an ideal planar geometry. This parameter quantitatively reflects the geometric distortion and electronic distribution of the ligand, providing valuable insights into its steric and electronic effects.

The ligand solid angle represents the solid angle of the complete shadow cast by a ligand on a sphere as viewed from the metal center, reflecting the spatial occupancy of the ligand around the metal. From solid angle, a solid “cone” angle can be derived, which is analogous to Tolman’s cone angle and quantifies the directional spatial shielding provided by the ligand. The G parameter measures the overall extent to which the ligand shields the metal coordination sphere, representing the steric protection effect of the ligand. These parameters provide a quantitative description of ligand steric effects and can guide catalyst design and prediction of reaction selectivity.

Table S2 Ligand space parameter names and definitions table

Feature	Definition	Access
V_bur	Fraction of buried volume of the ligand at a radius of 3.5 Å in the olefin-coordinated stable structure.	Morfeus
V_bur_1	Fraction of buried volume of the ligand at a radius of 1 Å in the olefin-coordinated stable structure.	Morfeus
V_bur_2	Fraction of buried volume of the ligand at a radius of 2 Å in the olefin-coordinated stable structure.	Morfeus
V_bur_3	Fraction of buried volume of the ligand at a radius of 3 Å in the olefin-coordinated stable structure.	Morfeus
V_bur_4	Fraction of buried volume of the ligand at a radius of 4 Å in the olefin-coordinated stable structure.	Morfeus
V_bur_5	Fraction of buried volume of the ligand at a radius of 5 Å in the olefin-coordinated stable structure.	Morfeus
percent_buried_volume_0	Percentage of the volume blocked by the ligand in the 0th octant (+X, +Y, +Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_1	Percentage of the volume blocked by the ligand in the 1st octant (–X, +Y, +Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_2	Percentage of the volume blocked by the ligand in the 2nd octant (–X, –Y, +Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_3	Percentage of the volume blocked by the ligand in the 3rd octant (+X, –Y, +Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_4	Percentage of the volume blocked by the ligand in the 4th octant (+X, +Y, –Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_5	Percentage of the volume blocked by the ligand in the 5th octant (–X, +Y, –Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_6	Percentage of the volume blocked by the ligand in the 6th octant (–X, –Y, –Z) of the sphere relative to the total volume of that octant.	Morfeus
percent_buried_volume_7	Percentage of the volume blocked by the ligand in the 7th octant (+X, –Y, –Z) of the sphere relative to the total volume of that octant.	Morfeus
buried_volume_0	Volume blocked by the ligand in the 0th octant (+X, +Y, +Z) of the sphere.	Morfeus
buried_volume_1	Volume blocked by the ligand in the 1st octant (–X, +Y, +Z) of the sphere.	Morfeus
buried_volume_2	Volume blocked by the ligand in the 2nd octant (–X, –Y, +Z) of the sphere.	Morfeus

Feature	Definition	Access
buried_volume_3	Volume blocked by the ligand in the 3rd octant (+X, –Y, +Z) of the sphere.	Morfeus
buried_volume_4	Volume blocked by the ligand in the 4th octant (+X, +Y, –Z) of the sphere.	Morfeus
buried_volume_5	Volume blocked by the ligand in the 5th octant (–X, +Y, –Z) of the sphere.	Morfeus
buried_volume_6	Volume blocked by the ligand in the 6th octant (–X, –Y, –Z) of the sphere.	Morfeus
buried_volume_7	Volume blocked by the ligand in the 7th octant (+X, –Y, –Z) of the sphere.	Morfeus
free_volume_0	Volume unblocked by the ligand in the 0th octant (+X, +Y, +Z) of the sphere.	Morfeus
free_volume_1	Volume unblocked by the ligand in the 1st octant (–X, +Y, +Z) of the sphere.	Morfeus
free_volume_2	Volume unblocked by the ligand in the 2nd octant (–X, –Y, +Z) of the sphere.	Morfeus
free_volume_3	Volume unblocked by the ligand in the 3rd octant (+X, –Y, +Z) of the sphere.	Morfeus
free_volume_4	Volume unblocked by the ligand in the 4th octant (+X, +Y, –Z) of the sphere	Morfeus
free_volume_5	Volume unblocked by the ligand in the 5th octant (–X, +Y, –Z) of the sphere.	Morfeus
free_volume_6	Volume unblocked by the ligand in the 6th octant (–X, –Y, –Z) of the sphere.	Morfeus
free_volume_7	Volume unblocked by the ligand in the 7th octant (+X, –Y, –Z) of the sphere.	Morfeus
percent_buried_volume_max	Maximum percentage of the ligand-blocked volume among the eight octants.	Morfeus
percent_buried_volume_min	Minimum percentage of the ligand-blocked volume among the eight octants.	Morfeus
free_volume_max	Maximum volume unblocked by the ligand among the eight octants.	Morfeus
free_volume_min	Minimum volume unblocked by the ligand among the eight octants.	Morfeus
buried_volume_max	Maximum volume blocked by the ligand among the eight octants.	Morfeus
buried_volume_min	Minimum volume blocked by the ligand among the eight octants.	Morfeus
Sterimol_L	Maximum length of the ligand measured along the anchoring bond direction.	Morfeus
Sterimol_B1	Minimum lateral width of the substituent in the plane perpendicular to L.	Morfeus

Feature	Definition	Access
Sterimol_B5	Maximum lateral width of the substituent in the plane perpendicular to L.	Morfeus
Buried_Sterimol_L	Maximum length of the ligand measured along the anchoring bond direction, considering the spatial overlap between the metal center and the ligand.	Morfeus
Buried_Sterimol_B1	B1 value considering the spatial overlap with the metal center, representing the minimum lateral width of the ligand in the practically accessible space.	Morfeus
Buried_Sterimol_B5	B5 value considering the spatial overlap with the metal center, representing the maximum lateral width of the ligand in the practically accessible space.	Morfeus
Cone Angle	The apex angle of a hypothetical cone formed by the ligand around the metal center, representing steric hindrance.	Morfeus
Pyramidalization_P	Degree of pyramidalization at the ligand's P atom.	Morfeus
Pyramidalization_P_angle	Pyramidalization angle at the ligand's P atom.	Morfeus
Solid Angle	Solid angle of the ligand as seen from the metal center.	Morfeus
Solid Angle (cone)	Cone angle derived from the solid angle.	Morfeus
Solid Angle (G)	Overall extent to which the ligand shields the metal coordination sphere	Morfeus

2.3 Coordination structure parameters between substrate and catalyst

2.3.1 Structural parameters

Based on the optimized geometric coordinates, structure parameters including bond lengths, bond angles, and dihedral angles were extracted using script. The numbering of the P atoms is assigned according to their distance from the Rh center: the phosphorus atom closer to Rh is denoted as P1, and the farther one as P2. For clarity, H atoms attached to phenyl rings are omitted in the Figure S4.

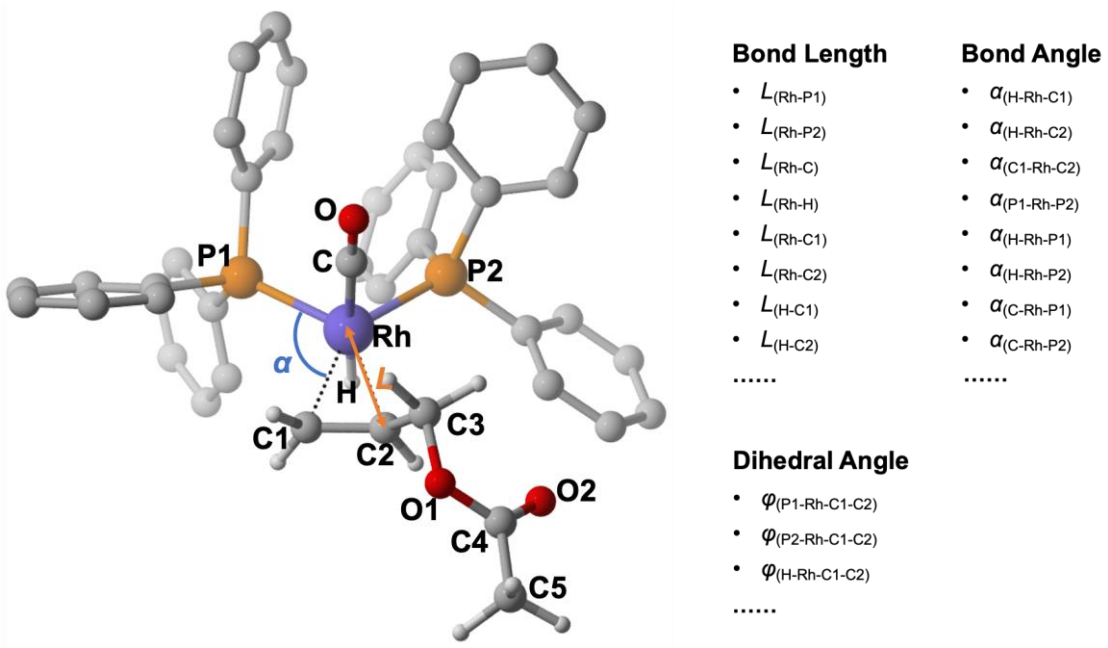


Figure S21. Schematic overview of structural parameter extraction.

2.3.2 **Dispersion descriptor**

The SASA is defined as the area traced by the center of a probe sphere (typically with a radius of 1.4 Å) as it rolls over the molecular surface, while the solvent-accessible volume corresponds to the volume accessible to the probe center. In this study, the total SASA value as well as atom-specific SASA values for Rh, P, H, and C atoms were calculated using morfeus.

P_int is a quantitative descriptor derived from electron density isosurfaces, used to evaluate the strength of dispersion interactions between atoms or ligands and their surrounding environment. In this study, the dispersion interaction strengths of Rh, P, H, and C atoms were collected using the morfeus package.

Table S3. Correspondence table of names and definitions of substrate and catalyst coordination structure parameters.

Feature	Definition	Access
L(Rh-P1)	The distance between the Rh atom and the closer P atom in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(Rh-P2)	The distance between the Rh atom and the farther P atom in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(Rh-P)	The average distance between the Rh atom and the P atoms in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(Rh-H)	The distance between the Rh atom and the adjacent H atom in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(Rh-C)	The distance between the Rh atom and the C atom of the coordinated carbonyl group in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(Rh-C1)	The distance between the Rh atom and the β-C atom of the coordinated olefin in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(Rh-C2)	The distance between the Rh atom and the α-C atom of the coordinated olefin in the olefin-coordinated stable structure.	DFT calculation based on M06-2X/6-31G*/SDD
L((Rh-C1)-(Rh-C2))	The difference in distance between the Rh atom and the β-C vs.α-C atoms of the coordinated olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(H-C1)	The distance between the H atom involved in hydrogen transfer and the β-C atom of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
L(H-C2)	The distance between the H atom involved in hydrogen transfer and the α-C atom of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
α(H-Rh-C1)	The bond angle among the H atom (involved in hydrogen transfer), the Rh atom, and the β-C atom of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
α(H-Rh-C2)	The bond angle among the H atom (involved in hydrogen transfer), the Rh atom, and the α-C atom of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
α(C1-Rh-C2)	The bond angle among the β-C atom, the Rh atom, and the α-C atom of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
α(H-Rh-P1)	The bond angle among the H atom (involved in hydrogen transfer), the Rh atom, and the closer P atom in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
α(H-Rh-P2)	The bond angle among the H atom (involved in hydrogen transfer), the Rh atom, and the farther P atom in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
α(C-Rh-P1)	The bond angle among the C atom of the carbonyl group, the Rh atom, and the closer P atom in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD

Feature	Definition	Access
α(C-Rh-P2)	The bond angle among the C atom of the carbonyl group, the Rh atom, and the farther P atom in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
φ(P1-Rh-C1-C2)	The dihedral angle formed by the closer P atom, the Rh atom, and the β-C and α-C atoms of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
φ(P2-Rh-C1-C2)	The dihedral angle formed by the farther P atom, the Rh atom, and the β-C and α-C atoms of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
φ(H-Rh-C1-C2)	The dihedral angle formed by the H atom (involved in hydrogen transfer), the Rh atom, and the β-C and α-C atoms of the olefin in the stable olefin coordination structure.	DFT calculation based on M06-2X/6-31G*/SDD
SASA Area	Solvent-accessible surface area of the molecule.	Morfeus
SASA Volume	Solvent-accessible volume of the molecule.	Morfeus
SASA_Rh	Solvent-accessible surface area of the Rh atom in the olefin-coordinated structure.	Morfeus
SASA_P1	Solvent-accessible surface area of the P1 atom in the olefin-coordinated structure.	Morfeus
SASA_P2	Solvent-accessible surface area of the P2 atom in the olefin-coordinated structure.	Morfeus
SASA_H	Solvent-accessible surface area of the H atom bonded to Rh in the olefin-coordinated structure.	Morfeus
SASA_C	Solvent-accessible surface area of the carbon atom of the CO group bonded to Rh in the olefin-coordinated structure.	Morfeus
P_int_Rh	Sum of dispersion interaction energies between Rh atom and its neighboring atoms.	Morfeus
P_int_P1	Sum of dispersion interactions between the P atom near Rh and its surrounding atoms.	Morfeus
P_int_P2	Sum of dispersion interactions between the P atom far from Rh and its surrounding atoms.	Morfeus
P_int_C	Sum of dispersion interactions between the CO carbon atom bonded to Rh and its neighboring atoms.	Morfeus
P_int_H	Sum of dispersion interactions between the H atom bonded to Rh and its neighboring atoms.	Morfeus

2.4 Electronic parameters

The NPA charges of Rh, H, C, P1, P2, and the C atoms bonded to them in the catalyst structure were calculated using NBO 3.1, along with the NPA charges of the olefin backbone atoms.

Table S4 Correspondence table between names and definitions of electronic parameters

Feature	Definition	Access
HOMO	Highest Occupied Molecular Orbital	DFT calculation based on M06-2X/6-31G*/SDD
LUMO	Lowest Unoccupied Molecular Orbital	DFT calculation based on M06-2X/6-31G*/SDD
μ	Chemical potential	$\mu = (E_{HOMO}+E_{LUMO})/2$
η	Chemical hardness	$\eta = (E_{HOMO}-E_{LUMO})/2$
ω	Electronegativity index	$\omega = \mu^2/2\eta$
NBO_Rh	NPA charge of the Rh atom in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_H	NPA charge of the H atom bonded to Rh in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_C	NPA charge of the carbonyl C atom bonded to Rh in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P1	NPA charge of the P atom closer to Rh in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P2	NPA charge of the P atom farther from Rh in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P1C1	NPA charge of the C atom closest to P1 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P1C2	NPA charge of the second-closest C atom to P1 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P1C3	NPA charge of the farthest C atom bonded to P1 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P2C1	NPA charge of the C atom closest to P2 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P2C2	NPA charge of the second-closest C atom to P2 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_P2C3	NPA charge of the farthest C atom bonded to P2 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_C1	NPA charge of the β-C atom of the olefin in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_C2	NPA charge of the α-C atom of the olefin in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_C3	NPA charge of the C atom bonded to α-C, excluding β-C, in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_O1	NPA charge of the O atom bonded to C3 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_C4	NPA charge of the C atom bonded to O1 in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures
NBO_O2	NPA charge of the O atom bonded to C4, excluding O1, in the olefin-coordinated structure.	from NBO 3.1 on M06-2X/6-31G*/SDD optimized structures

2.5 Atomic parameters

The chemical shielding tensors of each atom in the $RhH(CO)(AA)P_2$ structure were calculated using the GIAO method, and isotropic and anisotropic components were extracted for nine atoms (Rh, P1, P2, H, C, C1, C2, C3, and O1), along with tensor components in different coordinate directions (XX, YY, ZZ, XY, XZ, YX, YZ, ZX, ZY).

Table S5 Atomic parameter name and definition correspondence table

Feature	Definition	Access
Rh_Isotropic	Isotropic component of the tensor of the Rh atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_Anisotropy	Anisotropy of the tensor of the Rh atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_XX	Diagonal tensor element in the X direction, representing the response strength of the Rh atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_YY	Diagonal tensor element in the Y direction, representing the response strength of the Rh atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the Rh atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_XY	Tensor component X-Y, representing the coupling of the Rh atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_YX	Tensor component Y-X, representing the coupling of the Rh atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_XZ	Tensor component X-Z, representing the coupling of the Rh atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_ZX	Tensor component Z-X, representing the coupling of the Rh atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_YZ	Tensor component Y-Z, representing the coupling of the Rh atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
Rh_ZY	Tensor component Z-Y, representing the coupling of the Rh atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_Isotropic	Isotropic component of the tensor of the P1 atom (the P atom proximal to the Rh atom).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_Anisotropy	Anisotropy of the tensor of the P1 atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_XX	Diagonal tensor element in the X direction, representing the response strength of the P1 atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_YY	Diagonal tensor element in the Y direction, representing the response strength of the P1 atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures

Feature	Definition	Access
P1_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the P1 atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_XY	Tensor component X-Y, representing the coupling of the P1 atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_YX	Tensor component Y-X, representing the coupling of the P1 atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_XZ	Tensor component X-Z, representing the coupling of the P1 atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_ZX	Tensor component Z-X, representing the coupling of the P1 atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_YZ	Tensor component Y-Z, representing the coupling of the P1 atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P1_ZY	Tensor component Z-Y, representing the coupling of the P1 atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_Isotropic	Isotropic component of the tensor of the P2 atom (the P atom distal to the Rh atom).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_Anisotropy	Anisotropy of the tensor of the P2 atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_XX	Diagonal tensor element in the X direction, representing the response strength of the P2 atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_YY	Diagonal tensor element in the Y direction, representing the response strength of the P2 atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the P2 atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_XY	Tensor component X-Y, representing the coupling of the P2 atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_YX	Tensor component Y-X, representing the coupling of the P2 atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_XZ	Tensor component X-Z, representing the coupling of the P2 atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_ZX	Tensor component Z-X, representing the coupling of the P2 atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_YZ	Tensor component Y-Z, representing the coupling of the P2 atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
P2_ZY	Tensor component Z-Y, representing the coupling of the P2 atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_Isotropic	Isotropic component of the tensor of the carbon atom (the carbonyl C atom bound to Rh).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_Anisotropy	Anisotropy of the tensor of the C atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_XX	Diagonal tensor element in the X direction, representing the response strength of the C atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures

Feature	Definition	Access
C_YY	Diagonal tensor element in the Y direction, representing the response strength of the C atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the C atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_XY	Tensor component X-Y, representing the coupling of the C atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_YX	Tensor component Y-X, representing the coupling of the C atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_XZ	Tensor component X-Z, representing the coupling of the C atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_ZX	Tensor component Z-X, representing the coupling of the C atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_YZ	Tensor component Y-Z, representing the coupling of the C atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C_ZY	Tensor component Z-Y, representing the coupling of the C atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_Isotropic	Isotropic component of the tensor of the hydrogen atom (the H atom bound to Rh).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_Anisotropy	Anisotropy of the tensor of the H atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_XX	Diagonal tensor element in the X direction, representing the response strength of the H atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_YY	Diagonal tensor element in the Y direction, representing the response strength of the H atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the H atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_XY	Tensor component X-Y, representing the coupling of the H atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_YX	Tensor component Y-X, representing the coupling of the H atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_XZ	Tensor component X-Z, representing the coupling of the H atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_ZX	Tensor component Z-X, representing the coupling of the H atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_YZ	Tensor component Y-Z, representing the coupling of the H atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
H_ZY	Tensor component Z-Y, representing the coupling of the H atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_Isotropic	Isotropic component of the tensor of the olefin β-C atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_Anisotropy	Anisotropy of the tensor of the olefin β-C atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures

Feature	Definition	Access
C1_XX	Diagonal tensor element in the X direction, representing the response strength of the olefin β-C atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_YY	Diagonal tensor element in the Y direction, representing the response strength of the olefin α-C atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the olefin β-C atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_XY	Tensor component X-Y, representing the coupling of the olefin β-C atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_YX	Tensor component Y-X, representing the coupling of the olefin β-C atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_XZ	Tensor component X-Z, representing the coupling of the olefin β-C atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_ZX	Tensor component Z-X, representing the coupling of the olefin β-C atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_YZ	Tensor component Y-Z, representing the coupling of the olefin β-C atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C1_ZY	Tensor component Z-Y, representing the coupling of the olefin β-C atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_Isotropic	Isotropic component of the tensor of the olefin α-C atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_Anisotropy	Anisotropy of the tensor of the olefin α-C atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_XX	Diagonal tensor element in the X direction, representing the response strength of the olefin α-C atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_YY	Diagonal tensor element in the Y direction, representing the response strength of the olefin α-C atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the olefin α-C atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_XY	Tensor component X-Y, representing the coupling of the olefin α-C atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_YX	Tensor component Y-X, representing the coupling of the olefin α-C atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_XZ	Tensor component X-Z, representing the coupling of the olefin α-C atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_ZX	Tensor component Z-X, representing the coupling of the olefin α-C atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_YZ	Tensor component Y-Z, representing the coupling of the olefin α-C atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C2_ZY	Tensor component Z-Y, representing the coupling of the olefin α-C atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_Isotropic	Isotropic tensor component of the olefin C3 atom (the non-βC atom connected to the α-C atom).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures

Feature	Definition	Access
C3_Anisotropy	Anisotropy of the tensor of the olefin C3 atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_XX	Diagonal tensor element in the X direction, representing the response strength of the olefin C3 atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_YY	Diagonal tensor element in the Y direction, representing the response strength of the olefin C3 atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the olefin C3 atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_XY	Tensor component X-Y, representing the coupling of the olefin C3 atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_YX	Tensor component Y-X, representing the coupling of the olefin C3 atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_XZ	Tensor component X-Z, representing the coupling of the olefin C3 atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_ZX	Tensor component Z-X, representing the coupling of the olefin C3 atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_YZ	Tensor component Y-Z, representing the coupling of the olefin C3 atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C3_ZY	Tensor component Z-Y, representing the coupling of the olefin C3 atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_Isotropic	Isotropic tensor component of the olefin O1 atom (the oxygen atom near to the C=C bond)	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_Anisotropy	Anisotropy of the tensor of the olefin O1 atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_XX	Diagonal tensor element in the X direction, representing the response strength of the olefin O1 atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_YY	Diagonal tensor element in the Y direction, representing the response strength of the olefin O1 atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the olefin O1 atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_XY	Tensor component X-Y, representing the coupling of the olefin O1 atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_YX	Tensor component Y-X, representing the coupling of the olefin O1 atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_XZ	Tensor component X-Z, representing the coupling of the olefin O1 atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_ZX	Tensor component Z-X, representing the coupling of the olefin O1 atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_YZ	Tensor component Y-Z, representing the coupling of the olefin O1 atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O1_ZY	Tensor component Z-Y, representing the coupling of the olefin O1 atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures

Feature	Definition	Access
C4_Isotropic	Isotropic tensor component of the olefin C4 atom (the non-C3 C atom connected to O1).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_Anisotropy	Anisotropy of the tensor of the olefin C4 atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_XX	Diagonal tensor element in the X direction, representing the response strength of the olefin C4 atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_YY	Diagonal tensor element in the Y direction, representing the response strength of the olefin C4 atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the olefin C4 atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_XY	Tensor component X-Y, representing the coupling of the olefin C4 atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_YX	Tensor component Y-X, representing the coupling of the olefin C4 atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_XZ	Tensor component X-Z, representing the coupling of the olefin C4 atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_ZX	Tensor component Z-X, representing the coupling of the olefin C4 atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_YZ	Tensor component Y-Z, representing the coupling of the olefin C4 atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
C4_ZY	Tensor component Z-Y, representing the coupling of the olefin C4 atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_Isotropic	Isotropic tensor component of the olefin O2 atom (the O atom connected to C4).	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_Anisotropy	Anisotropy of the tensor of the olefin O2 atom.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_XX	Diagonal tensor element in the X direction, representing the response strength of the olefin O2 atom to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_YY	Diagonal tensor element in the Y direction, representing the response strength of the olefin O2 atom to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_ZZ	Diagonal tensor element in the Z direction, representing the response strength of the olefin O2 atom to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_XY	Tensor component X-Y, representing the coupling of the olefin O2 atom's response in the Y direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_YX	Tensor component Y-X, representing the coupling of the olefin O2 atom's response in the X direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_XZ	Tensor component X-Z, representing the coupling of the olefin O2 atom's response in the Z direction to an external field applied along X.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_ZX	Tensor component Z-X, representing the coupling of the olefin O2 atom's response in the X direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_YZ	Tensor component Y-Z, representing the coupling of the olefin O2 atom's response in the Z direction to an external field applied along Y.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures
O2_ZY	Tensor component Z-Y, representing the coupling of the olefin O2 atom's response in the Y direction to an external field applied along Z.	from GIAO calculations on M06-2X/6-31G/SDD optimized structures

3 Local descriptor extraction method

Atom-Centered Symmetry Functions (ACSF)

The ACSF descriptor transforms Cartesian coordinates into a set of symmetry functions that describe the chemical environment of each atom. It utilizes internal coordinates such as interatomic distances to represent molecular structures, ensuring that the energy remains invariant under translational and rotational operations. The local environment around each atom is characterized through radial and angular functions, which convert geometric information into numerical features based on predefined symmetry functions.

In this study, the xyz files of key atoms involved in the reaction region (Rh, P1, P2, H, C, O, C1, C2, C3, and O1) were extracted from computational output files. The ACSF descriptors were then generated using Dscribe. Key parameters include species types, cutoff radius, radial function parameters, angular function parameters, and extended angular function parameters, with detailed settings provided in Table S6. The resulting ACSF feature dimension for each atom is 330.

Smooth Overlap of Atomic Positions (SOAP)

The SOAP descriptor converts the local atomic environment into a continuous three-dimensional atomic density distribution via a spherical harmonic expansion of the atomic density. This is followed by the computation of overlap integrals between atomic environments. In this work, the SOAP descriptors were generated using Dscribe, based on the same reaction region files as those used for ACSF. We employed spherical Gaussian-type orbitals as the radial basis functions, with a cutoff radius of 6.0 Å for the local region. The number of radial basis functions was set to 8, and the maximum degree of spherical harmonics was set to 6. The resulting SOAP feature dimension for each atom is 5740.

Local Many-Body Tensor Representation (LMBTR)

The LMBTR encodes multi-body interactions by representing interatomic distances and angular distributions in the form of histograms, thereby capturing bonding interactions. The LMBTR descriptors were generated using the Dscribe

package based on the full computational files, considering all elements present in the dataset. In this study, both pairwise (k = 2) and three-body (k = 3) LMBTR descriptors were computed, yielding feature dimensions of 1900 and 20,000, respectively.

Table S6 Parameter settings for local descriptor extraction

Descriptor	Parameter setting	Dimension
ACSF	species: Rh, C, O, P, H r_cut: 6.0 g2_params: [[5,4],[2.5,3],[1,2],[0.4,1.5],[0.2,1],[0.1,0.5]] g3_params: [0.5,1,1.5,2,2.5] g4_params: [[5,1,-1], [5,1,1], [2.5,1,-1], [2.5,1,1], [1,1,-1], [1,1,1], [5,2,-1], [5,2,1], [2.5,2,-1], [2.5,2,1], [1,2,-1], [1,2,1], [5,3,-1], [5,3,1], [2.5,3,-1], [2.5,3,1], [1,3,-1], [1,3,1]]	3300
SOAP	species: Rh, C, O, P, H r_cut: 6.0 n_max: 8 l_max: 6 periodic: False	57400
LMBTR-k2	species: Rh, C, O, P, H, Br, F, Cl, S, N geometry: {function: inverse_distance} grid: {min: 0, max: 5, n: 100, sigma: 0.1} weighting: {function: exp, scale: 0.5, threshold: 1e-3} periodic: False normalization: l2	1900
LMBTR-k3	species: Rh, C, O, P, H, Br, F, Cl, S, N geometry: {function: cosine} grid: {min: 0, max: 5, n: 200, sigma: 0.01} weighting: {function: exp, scale: 0.5, threshold: 1e-3} periodic: False normalization: l2	20000

4 Details of interpretable machine learning model construction

4.1 Overview of ligand structures in the training set

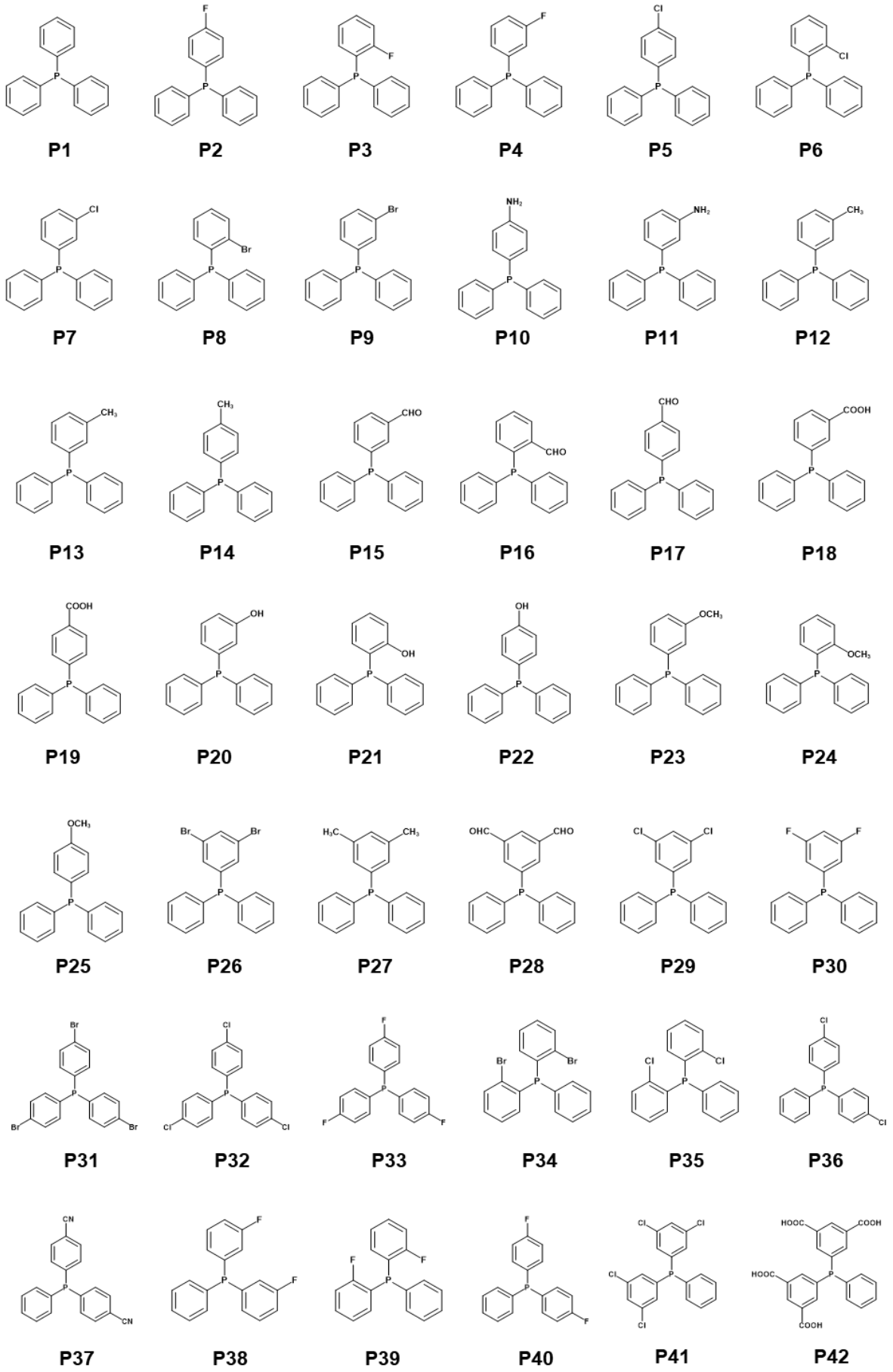


Figure S22. Ligand structures of the training set

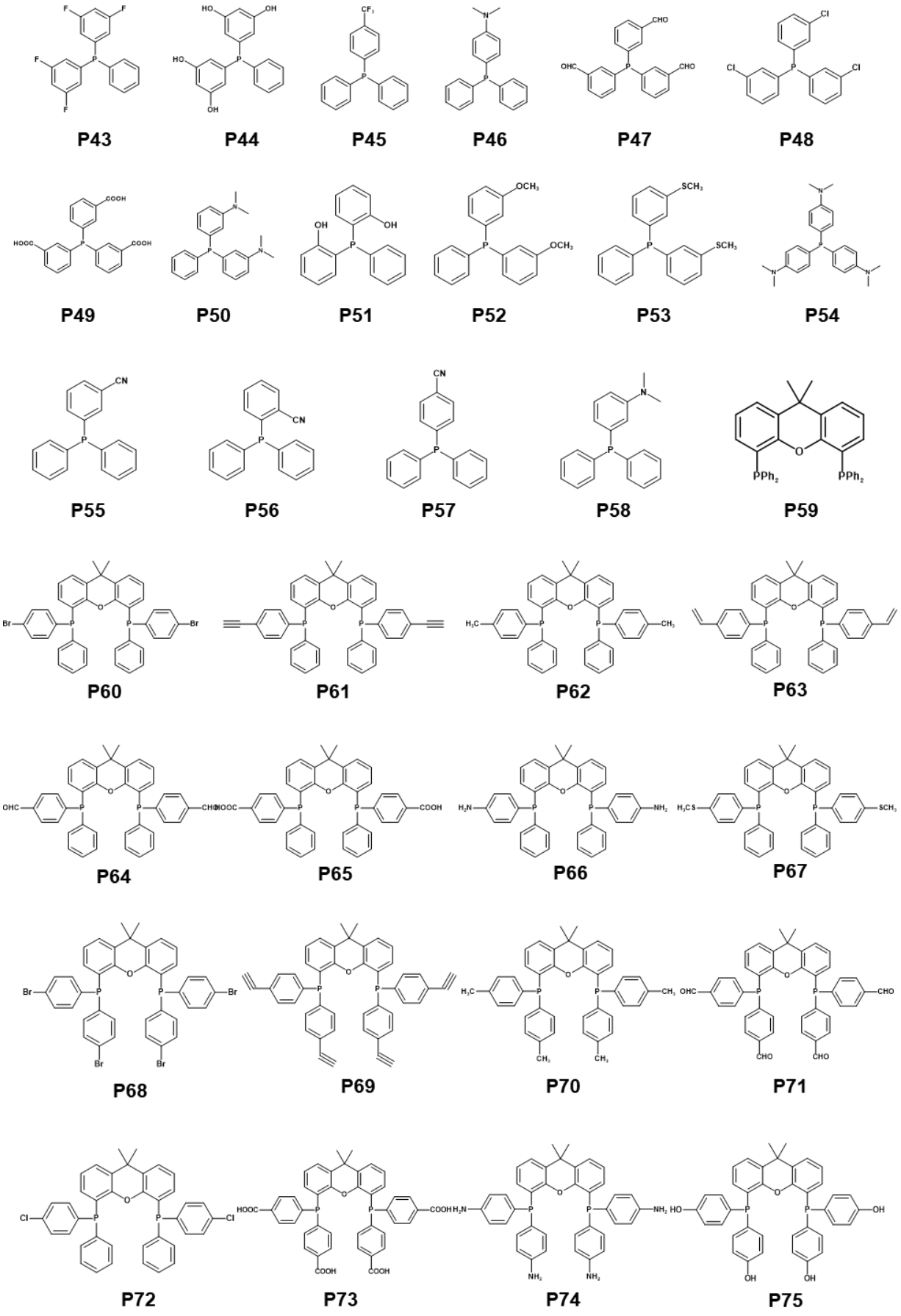


Figure S22. Ligand structures of the training set (continued)

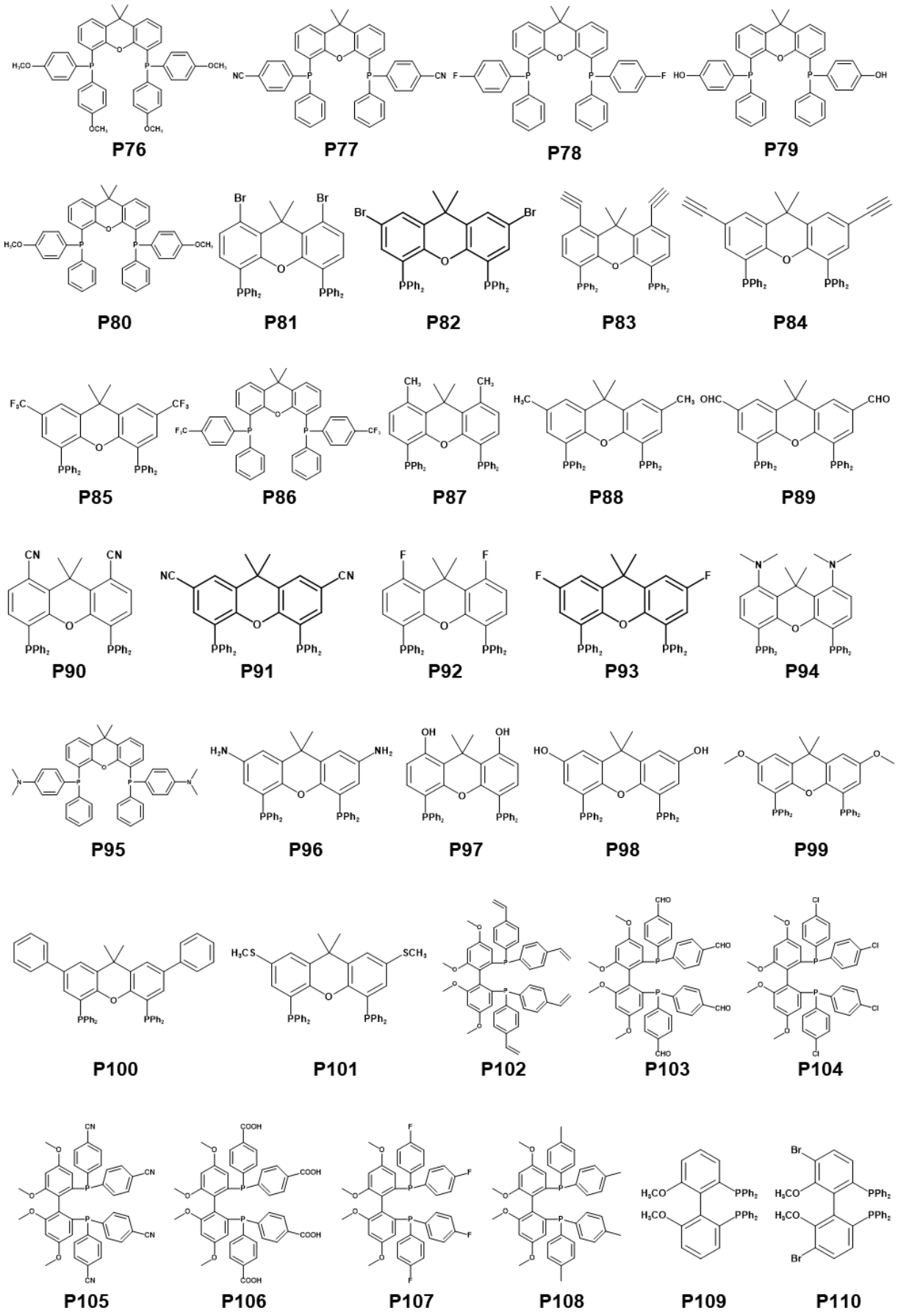


Figure S22. Ligand structures of the training set (continued)

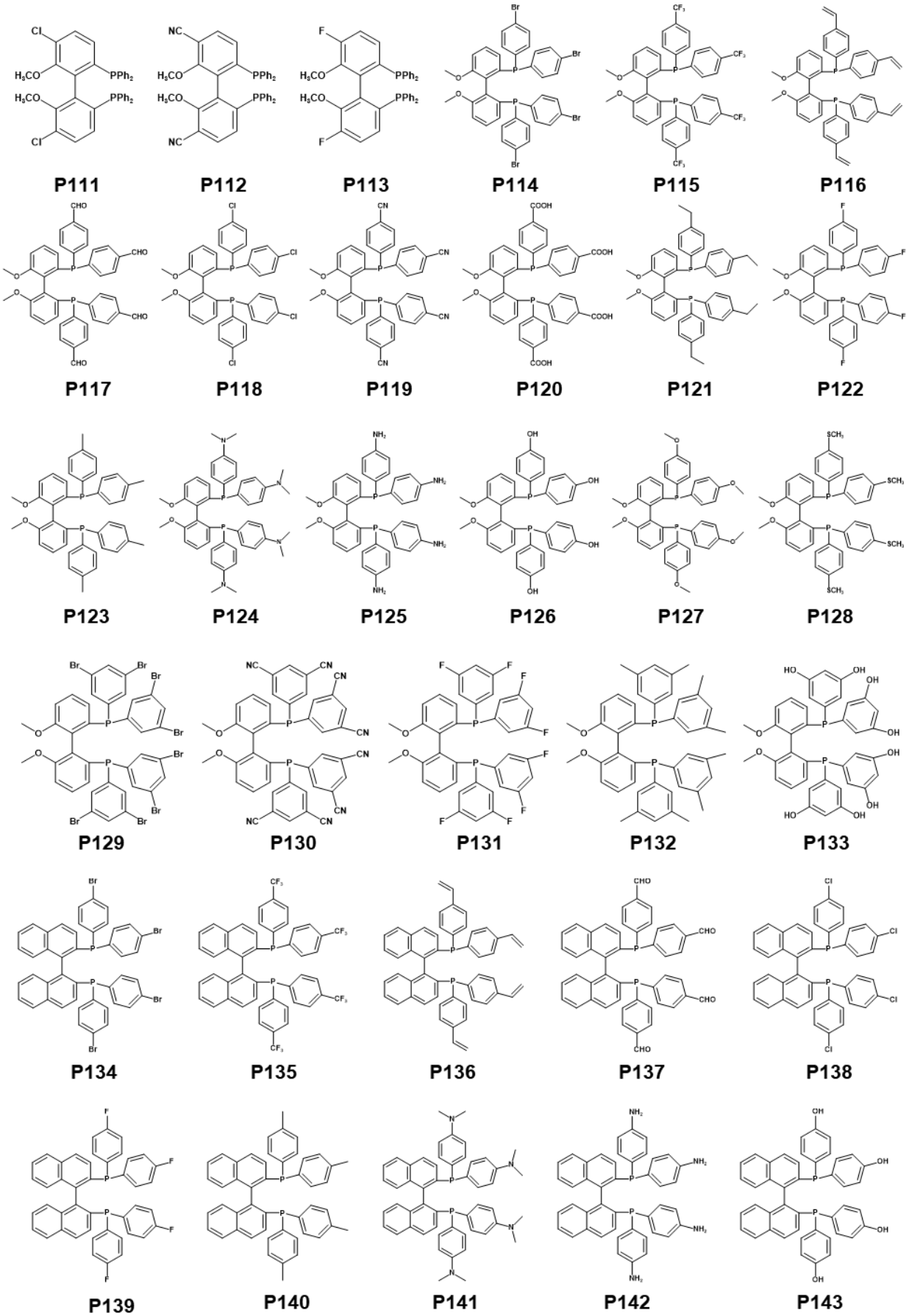


Figure S22. Ligand structures of the training set (continued)

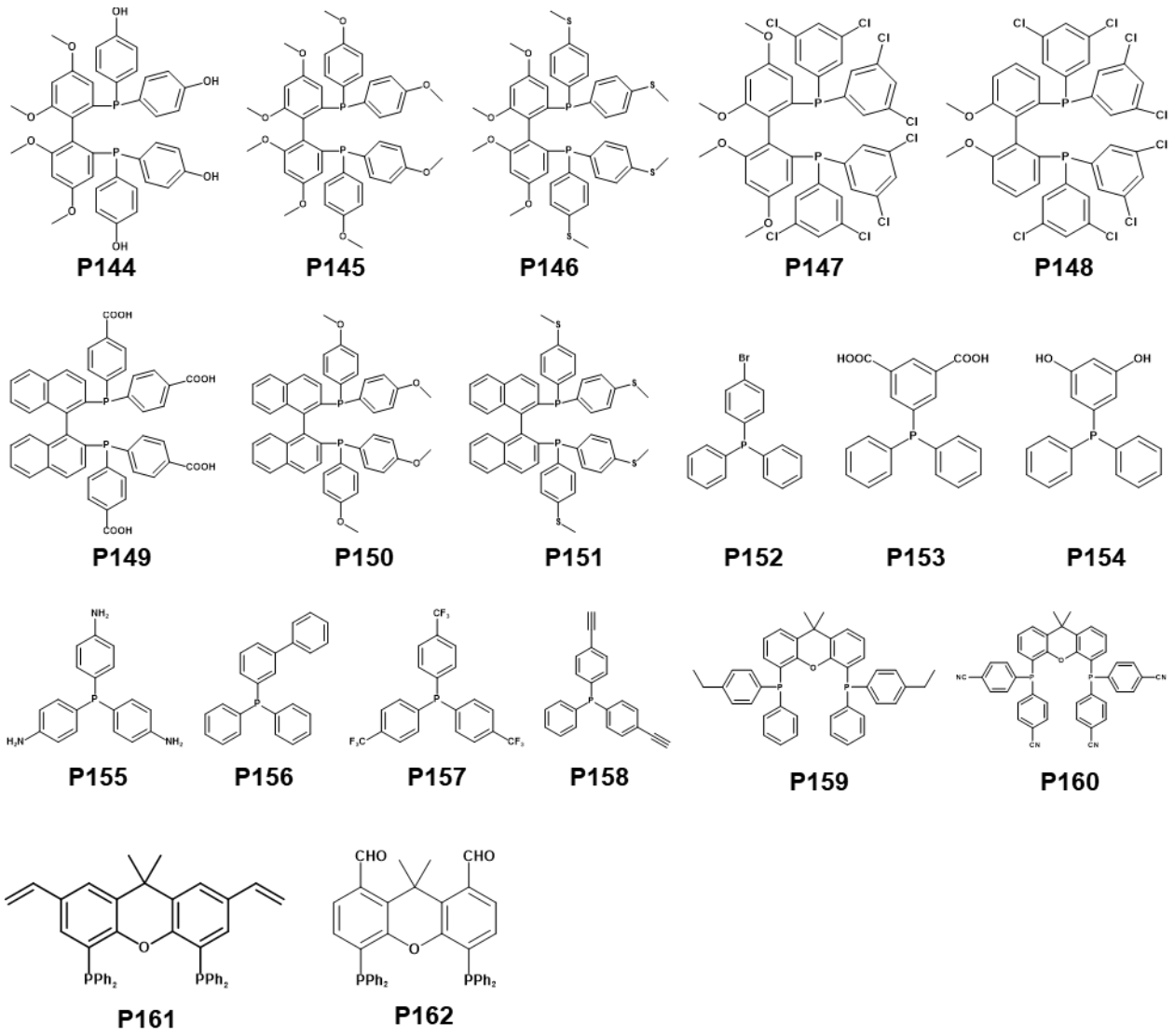


Figure S22. Ligand structures of the training set (continued)

4.2 Machine Learning Model Feature Screening Process

4.2.1 Evaluation metrics

(1) Coefficient of Determination, R^2

The R^2 measures the proportion of variance in the observed data that can be explained by the predictive model. Its value can be negative (indicating the model performs worse than simply using the mean) and ranges up to 1.0 for perfect prediction. A higher R^2 indicates stronger explanatory power of the model.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

(2) Root Mean Squared Error, RMSE

RMSE is the square root of MSE, which retains the same unit as the target variable, making it more interpretable in practice. RMSE is widely used in regression problems to evaluate the magnitude of prediction errors. A lower RMSE indicates better model performance.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

(3) Mean Absolute Error, MAE

MAE represents the average of the absolute differences between observed and predicted values. Unlike RMSE, MAE penalizes all deviations linearly, making it more robust to outliers. It provides a straightforward measure of the average predictive deviation of the model.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

4.2.2 Pearson correlation analysis

Pearson correlation analysis was employed to evaluate the linear dependence between descriptors and to mitigate redundancy. The Pearson correlation coefficient quantifies the strength and direction of a linear relationship between two variables, ranging from –1 (perfect negative correlation) to +1 (perfect positive correlation). Features with very high correlations often convey overlapping information, which can lead to multicollinearity and reduce the robustness of machine learning models.

In this study, a coefficient of 0.90 was used as a reference threshold. When the absolute correlation coefficient between two features exceeded 0.90, they were carefully examined for redundancy. In most cases, one of the correlated features was removed; however, some features with $|r| > 0.90$ were retained due to their distinct chemical relevance. Based on this procedure, 167 features were selected for subsequent modeling.

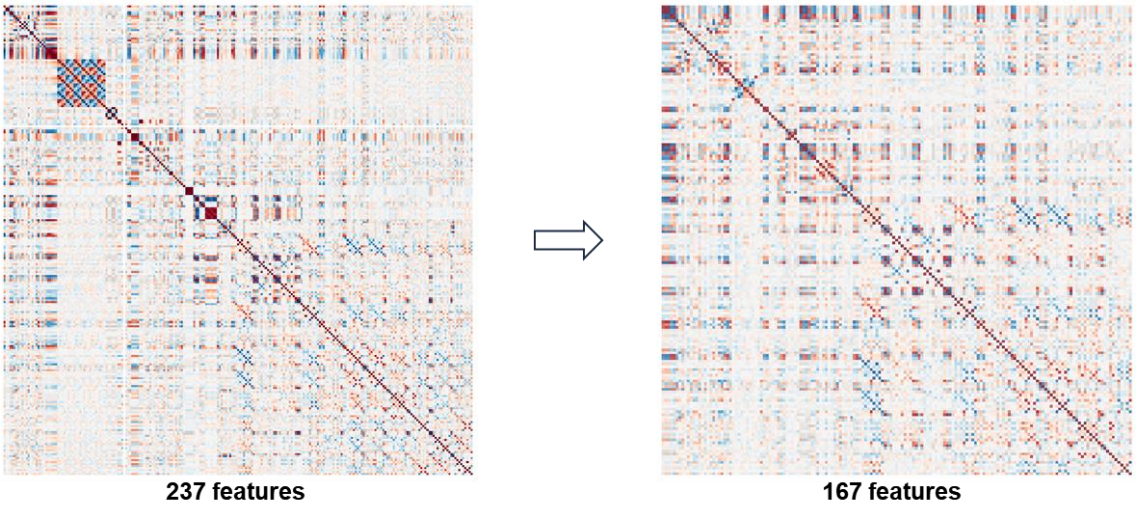


Figure S23. Comparison of features before and after screening using Pearson correlation analysis.

4.2.3 Univariate analysis

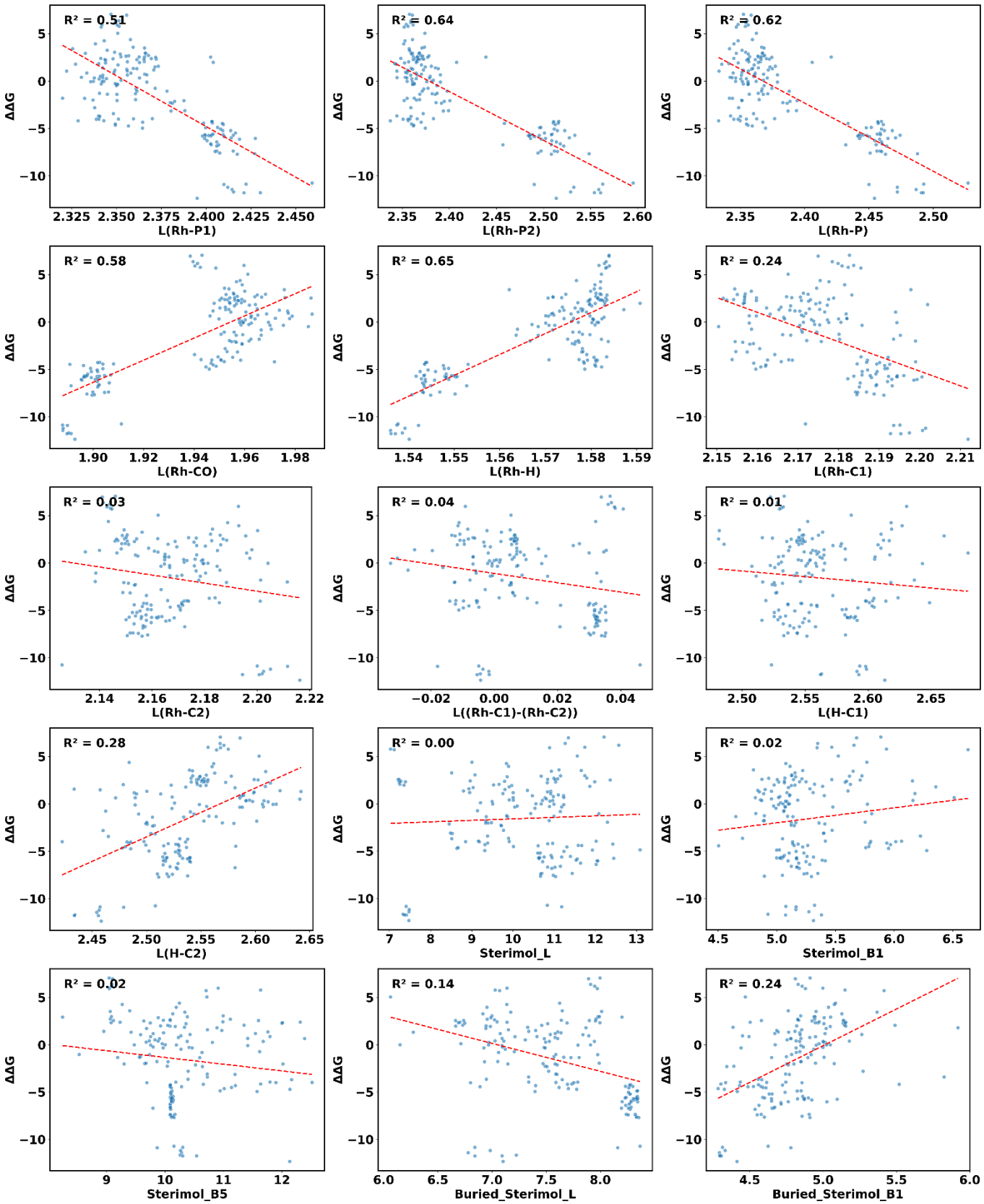


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG.

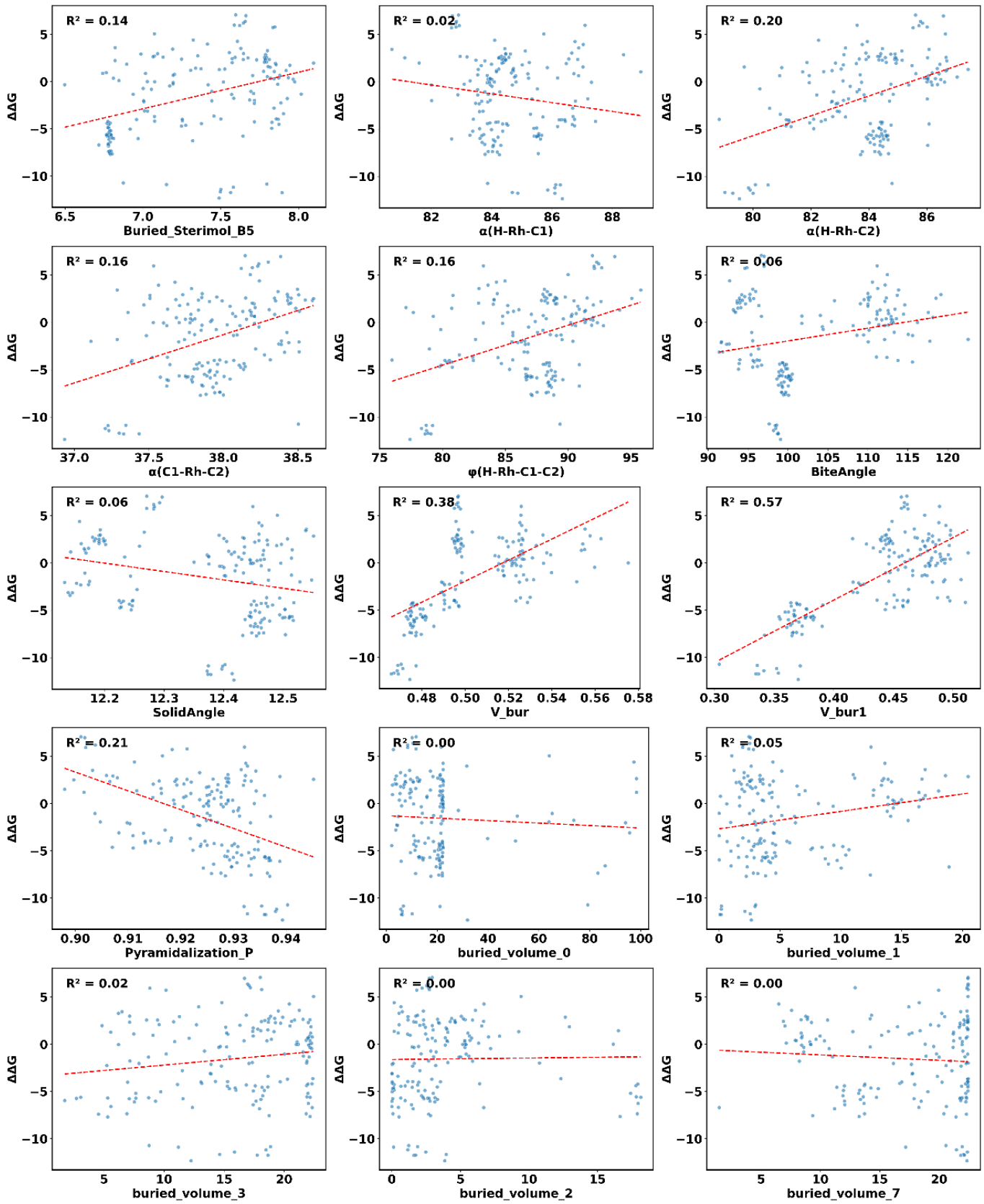


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

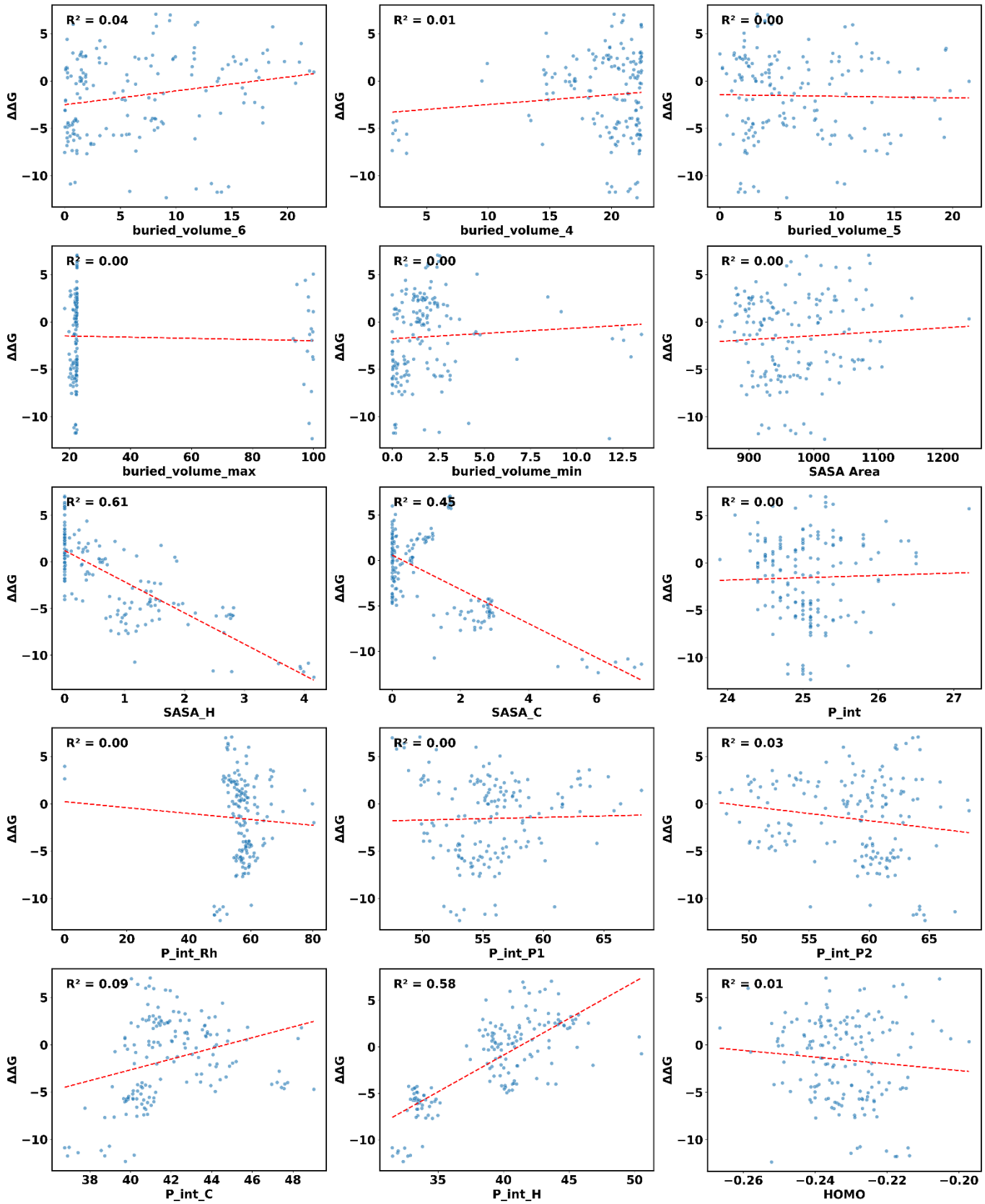


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

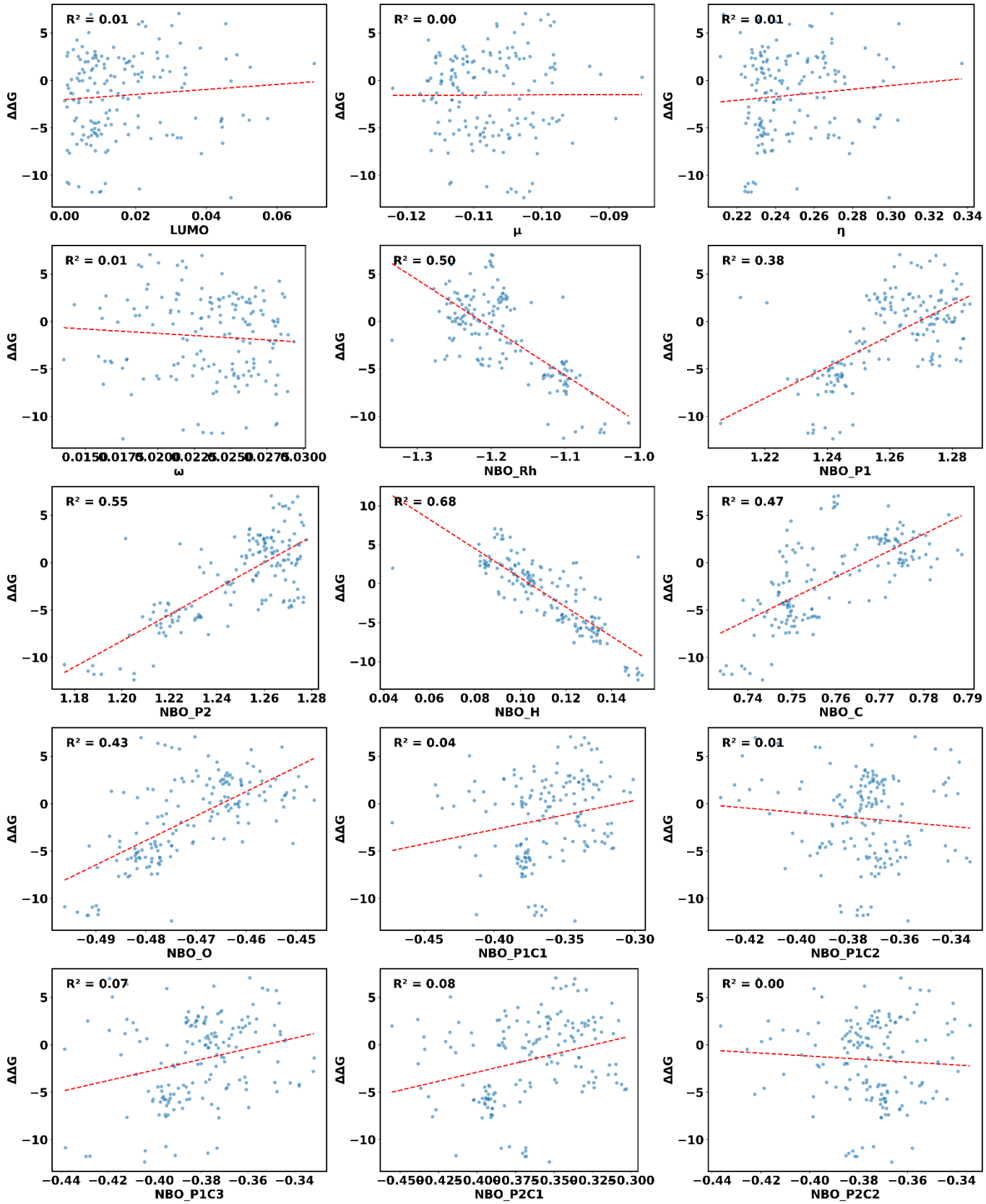


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

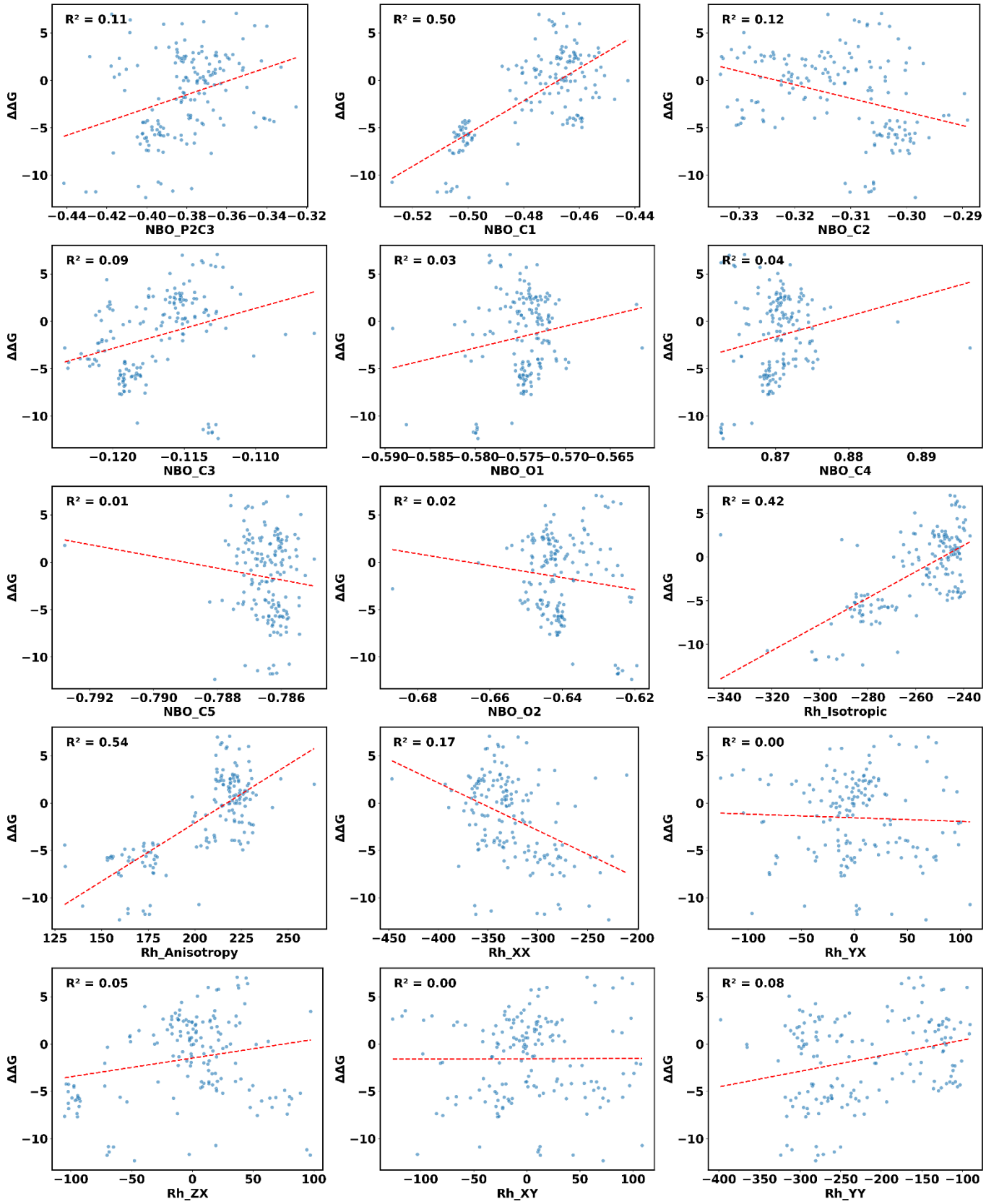


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

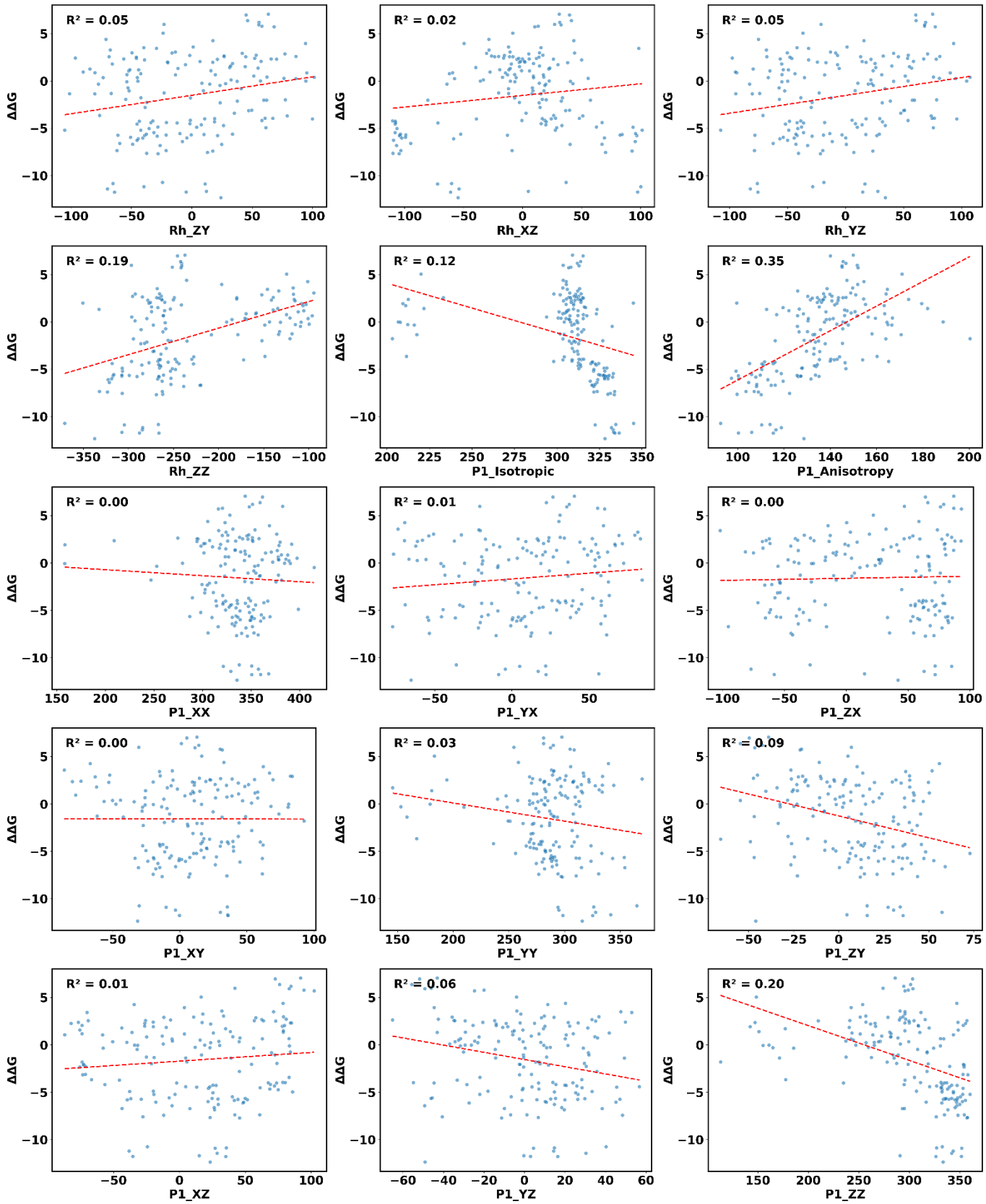


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

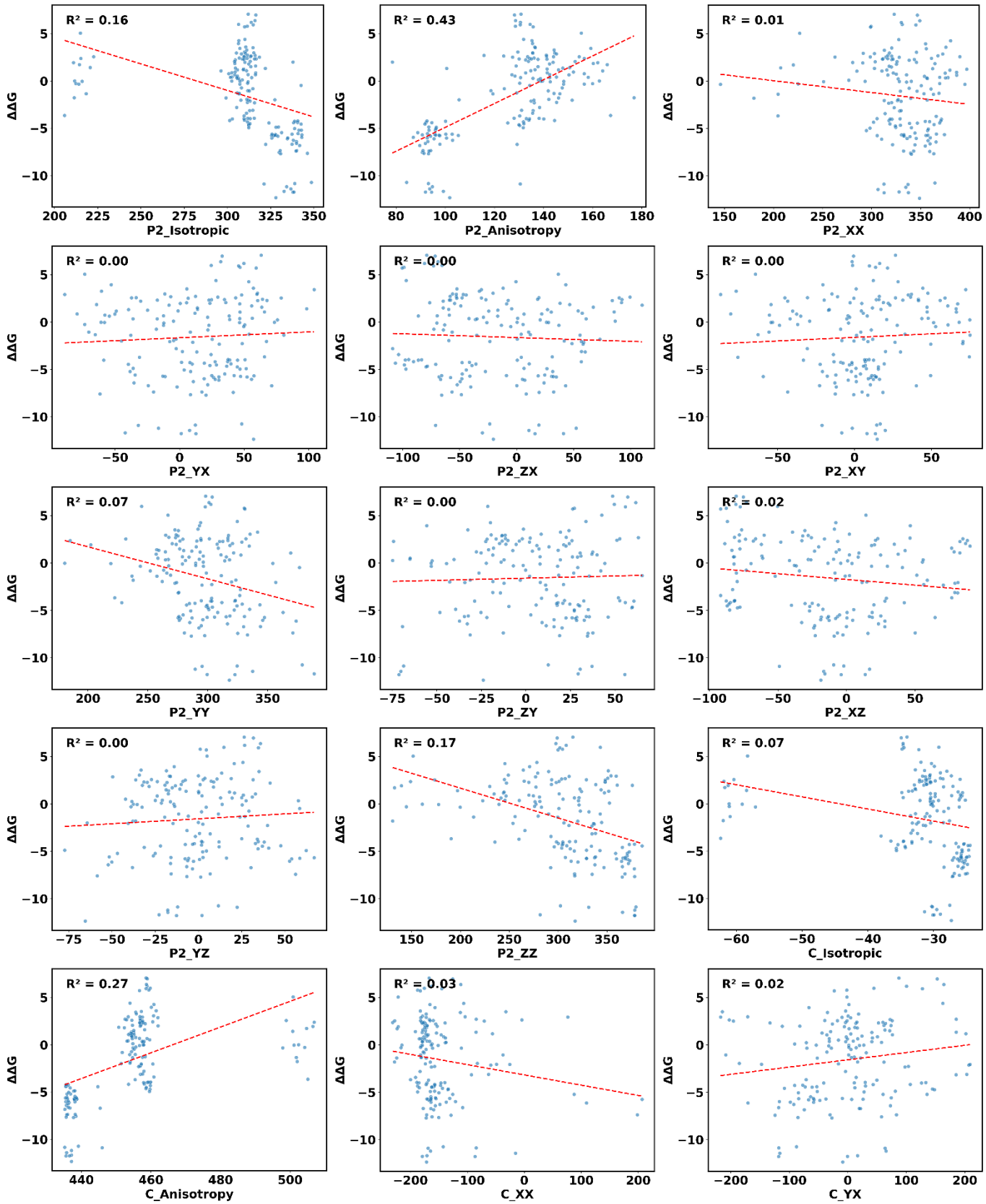


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

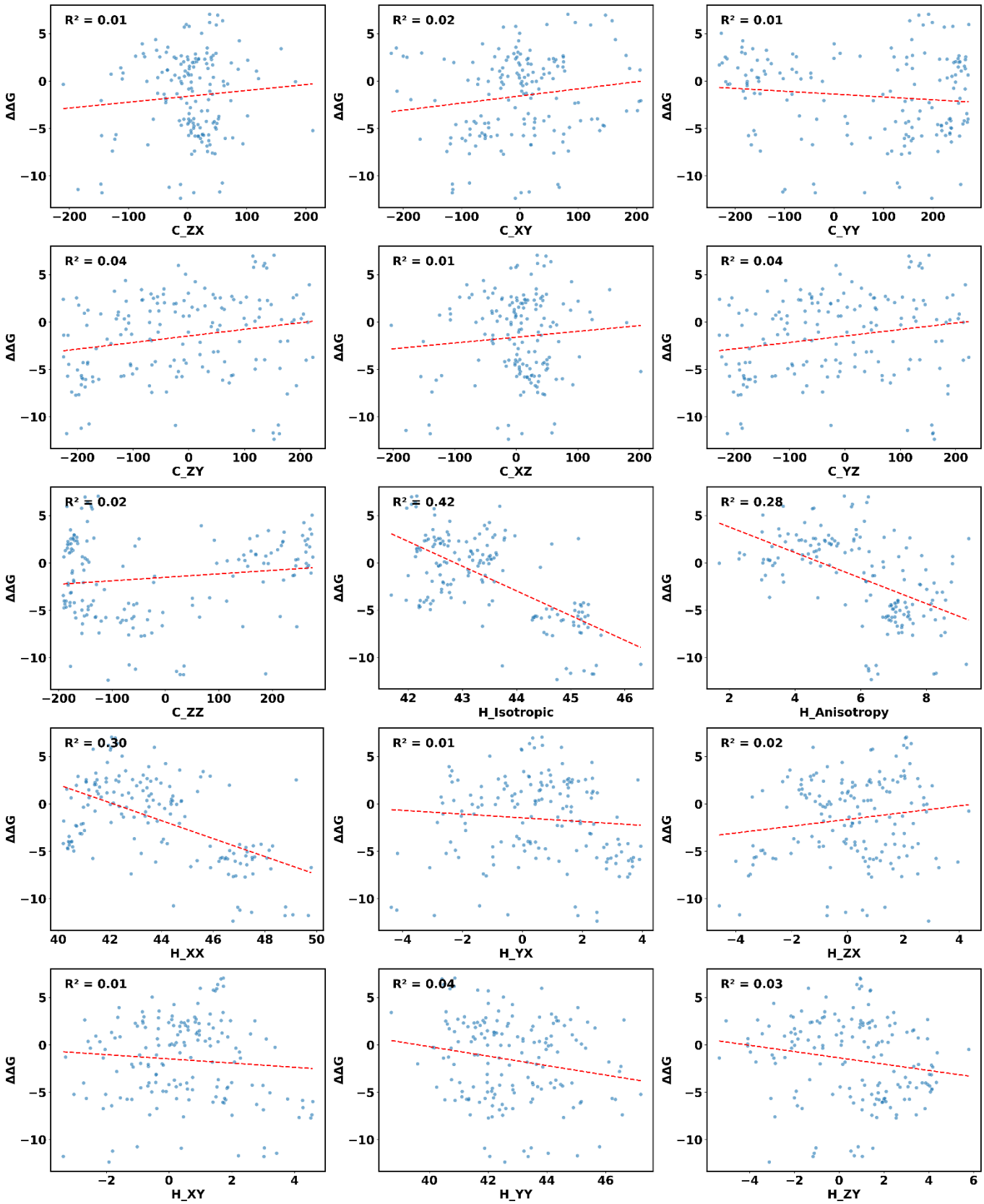


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

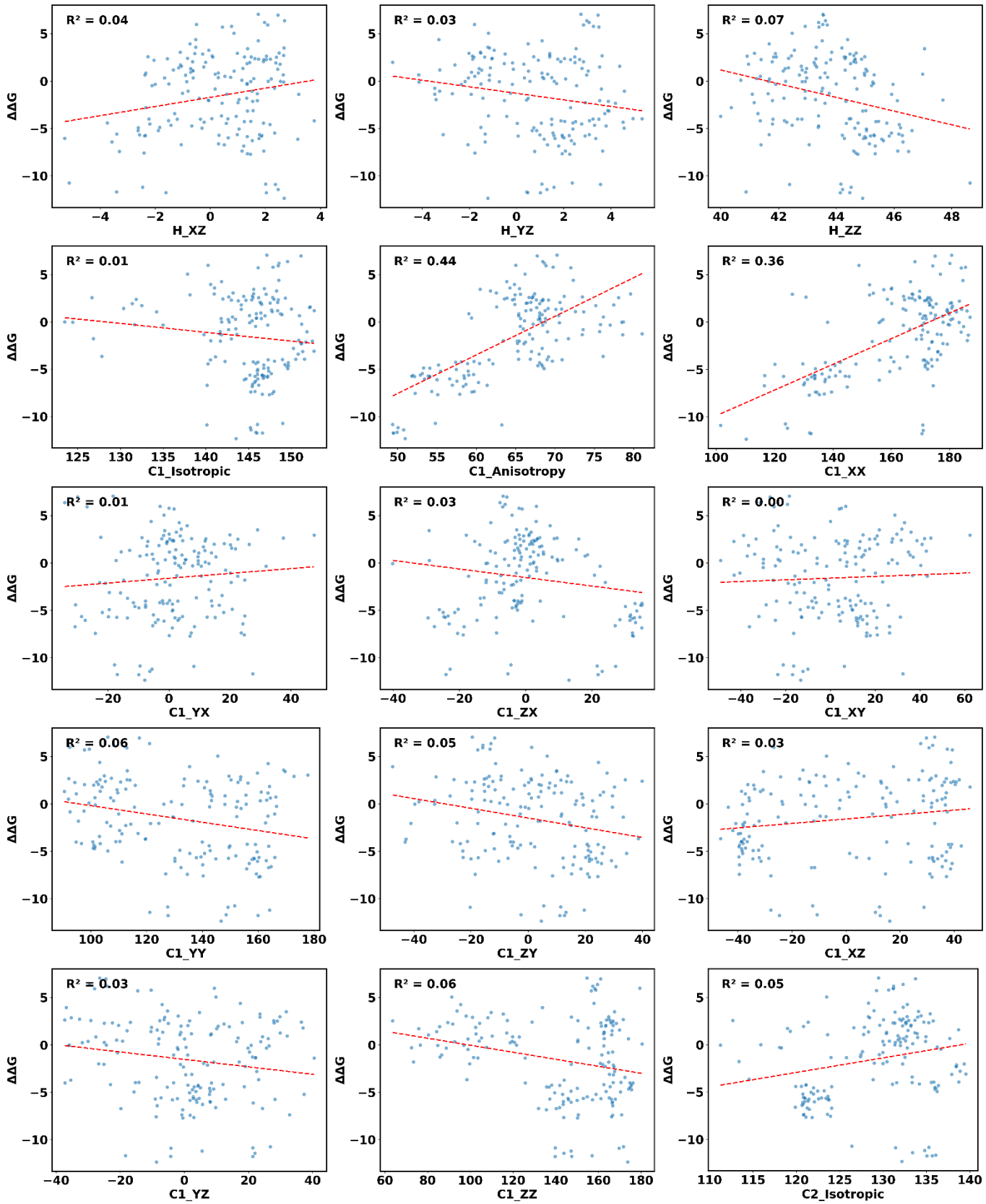


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

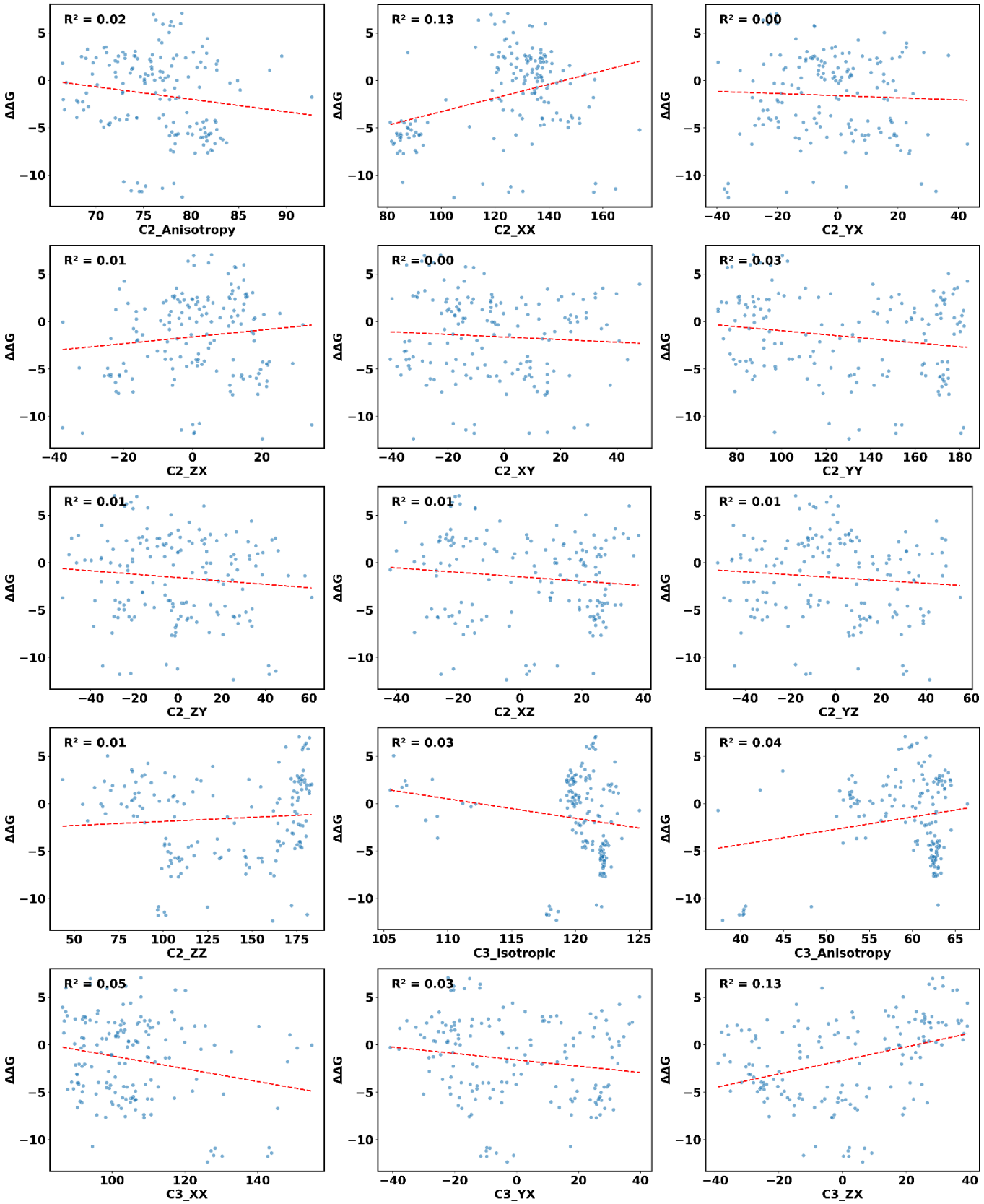


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

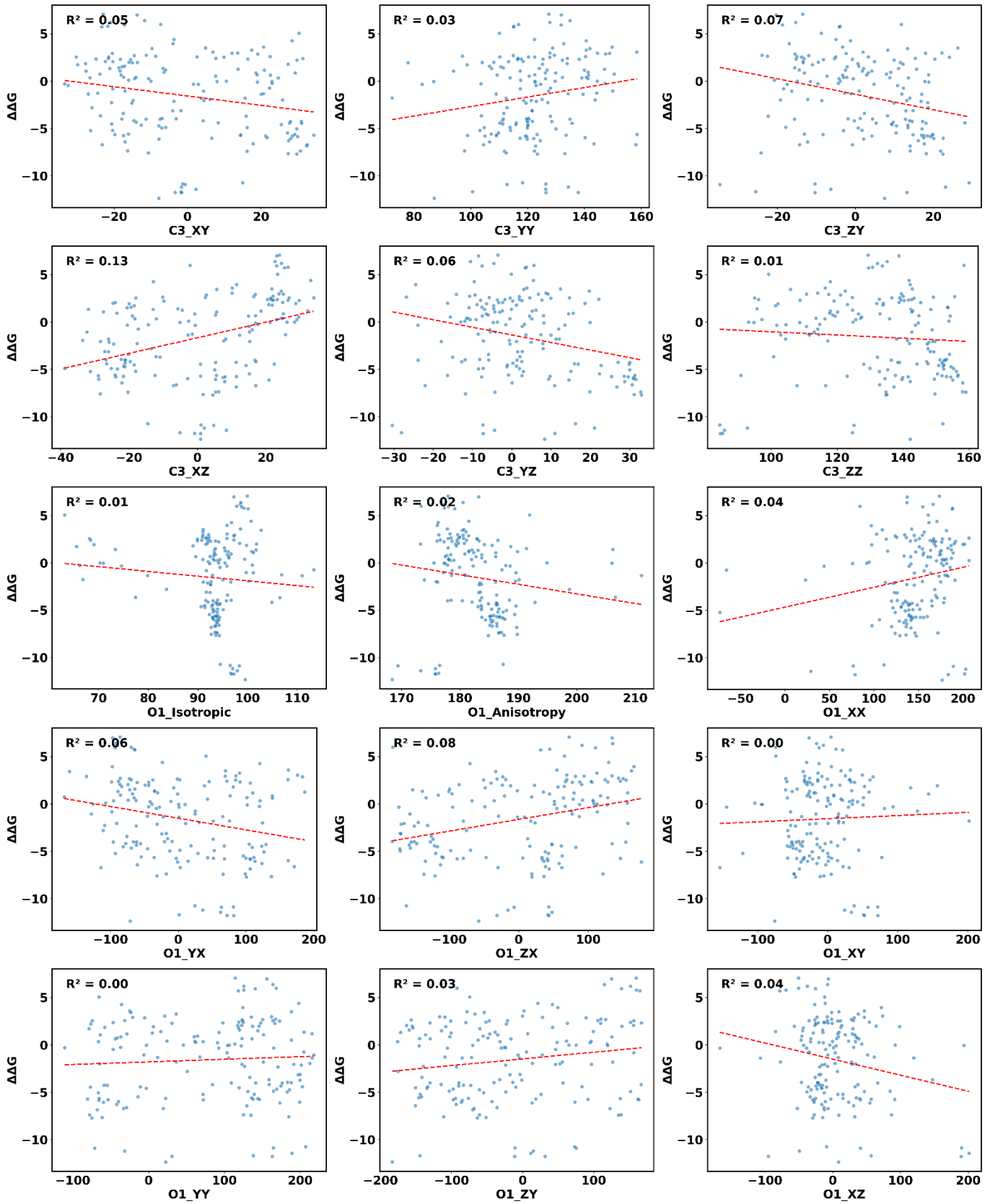


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

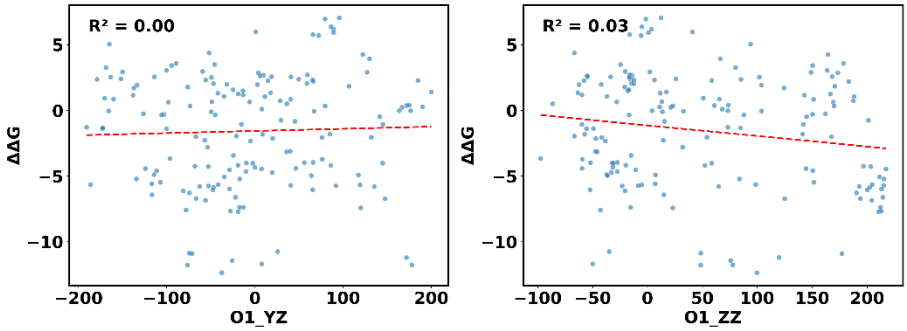


Figure S24. Scatter plot and fitted curve of descriptors and ΔΔG (continued).

4.2.4 PLSR feature engineering workflow

PLSR is a multivariate statistical method that projects high-dimensional predictor variables into a small number of latent variables while maximizing the covariance with the response variable. Compared with conventional regression techniques, PLSR is particularly advantageous in handling datasets with strong multicollinearity, high dimensionality, and limited sample sizes, as it effectively reduces the risk of overfitting and improves model robustness. In this study, the spatial and electronic descriptors of phosphine ligands are numerous and highly correlated, making direct modeling with the raw feature space unreliable. By incorporating PLSR as a preprocessing step for dimensionality reduction and information extraction, the essential structure–property correlations can be preserved while redundant and noisy features are eliminated. This strategy provides a compact and physically meaningful feature set for subsequent nonlinear learning with algorithms such as XGBoost.

Data preprocessing was first performed by reading a feature matrix containing 167 descriptors and the target variable data. The sample indices were shuffled using a random seed of 42 to eliminate potential sequential bias while maintaining the correspondence between features and the target variable. All features were subjected to standardization, a process rigorously implemented within each iteration of the cross-validation loop. For every training-validation split, the StandardScaler was exclusively fitted on the current training subset to compute feature-wise means and standard deviations. These derived parameters were subsequently applied to transform both the training and validation sets. This methodology strictly prevents the validation

data from contributing to the estimation of scaling parameters, thereby accurately simulating the scenario of model prediction on unseen data. This approach effectively eliminates the influence of variable scales and ensures the reliability and validity of the model evaluation.

Subsequently, a PLS model was constructed to evaluate the impact of 1 to 19 principal components. The stability of the model was assessed using 100 repetitions of 5-fold cross-validation, each time employing a different random seed (from 1 to 100) to evaluate model performance across various data splits.

Feature selection was then conducted by ranking feature importance based on the absolute values of the PLS coefficients. An iterative approach was adopted to progressively remove the least important features: initially, two features were eliminated per iteration, followed by the removal of one feature per iteration in later stages. After each elimination step, the model was retrained and re-evaluated based on the current feature importance ranking.

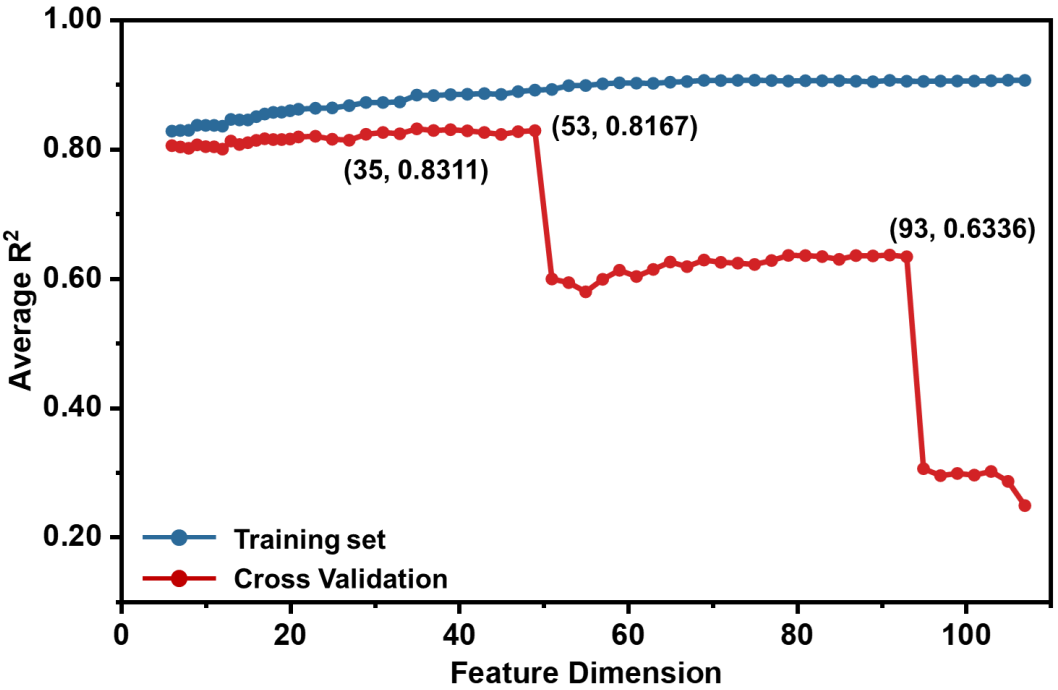


Figure S25. Variation of training set and cross-validation R^2 with feature dimension during PLS-based feature selection (k=4, note that cross-validation R^2 values become negative when the number of features exceeds 107, which is not shown in the plot).

SASA_H	P_int_H	Buried_Sterimol_B1	α(H-Rh-C2)	L(Rh-C2)	L(Rh-H)
Rh_Anisotropy	Φ(H-Rh-C1-C2)	P_int_Rh	C3_Anisotropy	L(H-C2)	α(C1-Rh-C2)
NBO_C3	H_Anisotropy	L(Rh-P2)	NBO_O	O1_Anisotropy	H_ZY
V_bur	NBO_P2	C2_Anisotropy	L(Rh-P)	L((Rh-C1)-(Rh-C2))	L(Rh-CO)
O1_ZX	Sterimol_L	Sterimol_B5	Rh_XX	C3_ZX	C3_XZ
C1_XZ	Pyramidalization_P	P1_XY	V_bur1	C2_XY	SASA_C
P1_YZ	P_int	P2_YX	H_YZ	C2_XZ	buried_volume_6
P1_YY	L(Rh-P1)	C1_XX	H_YY	P1_Anisotropy	C1_XY
NBO_C1	NBO_H	Rh_ZX	C3_ZY	buried_volume_min	α(H-Rh-C1)
C1_Anisotropy	C_Anisotropy	NBO_P2C3	NBO_P1C2	H_Isotropic	C_XZ
Rh_Isotropic	L(Rh-C1)	P_int_P2	Buried_Sterimol_L	HOMO	O1_XZ
C_ZX	P1_XX	C3_XX	P2_XY	P2_YZ	Rh_XZ
C2_YZ	μ	Rh_ZZ	O1_YZ	C2_YY	C2_ZZ
Rh_YY	P_int_P1	buried_volume_1	buried_volume_4	P1_ZZ	L(H-C1)
P2_YY	Sterimol_B1	C3_YY	P1_XZ	P_int_C	buried_volume_5
H_ZX	H_XX	P2_Anisotropy			

Figure S26. High-importance features identified from different subsets during PLS-based feature reduction (35 features, shown in green; 53 features, shown in green & blue; and 93 features, representing all features).

4.2.5 Nonlinear machine Learning methods for comparative study

In this study, we employed a diverse set of machine learning algorithms to evaluate and enhance the predictive performance of catalyst design models. These algorithms span different methodological families, including ensemble learning, kernel-based approaches, and neural networks, each with distinct strengths in handling small-sample, high-dimensional datasets. Ensemble learning methods, such as boosting and random forests, are particularly effective at reducing variance and improving generalization. Kernel-based models, including support vector regression and Gaussian processes, are powerful for capturing nonlinear relationships with limited data. Neural networks, represented here by multilayer perceptrons, provide flexible function approximation capabilities, enabling the modeling of complex descriptors.

eXtreme Gradient Boosting (XGBoost)[5]

XGBoost is an advanced implementation of gradient boosting designed for high efficiency and scalability. It introduces regularization techniques (both L1 and L2) to prevent overfitting, which is particularly important in small-sample conditions. The algorithm builds additive models sequentially, each new tree correcting the residuals of previous ones. Its sparsity-aware algorithms and parallelization make it highly

efficient for high-dimensional datasets. XGBoost has become one of the most widely adopted methods for regression and classification in scientific applications.

Categorical Boosting (CatBoost)[6]

CatBoost is a gradient boosting algorithm developed with a focus on categorical variables. Unlike many other boosting methods, it natively handles categorical features, reducing the need for extensive preprocessing such as one-hot encoding. It employs an ordered boosting scheme, which helps to mitigate prediction shift and overfitting. The algorithm also incorporates efficient symmetric tree structures to balance accuracy and computational speed. CatBoost is particularly advantageous in datasets containing mixed numerical and categorical descriptors.

Adaptive Boosting (AdaBoost)[7]

AdaBoost is one of the earliest and most influential boosting algorithms. It works by sequentially combining multiple weak learners, typically shallow decision trees, to create a strong predictor. Each subsequent learner is trained to emphasize samples that were previously misclassified or mispredicted. This adaptiveness makes it powerful for improving accuracy on challenging datasets. Although sensitive to noisy data, AdaBoost remains a robust baseline for regression and classification tasks.

Gradient Boosting Regression (GBR)[8]

Gradient Boosting Regression is a variant of boosting specialized for regression tasks. It builds models sequentially, and each one fitted to the residuals of the previous ensemble. By minimizing a differentiable loss function, GBR effectively handles nonlinear dependencies. The method can achieve strong predictive accuracy, though it may require careful tuning to prevent overfitting. It serves as a foundation for more advanced boosting frameworks like XGBoost and LightGBM.

Light Gradient Boosting Machine (LightGBM)[9]

LightGBM is a highly efficient gradient boosting framework developed for large-scale and high-dimensional data. It employs histogram-based algorithms that significantly reduce computation and memory usage. Its leaf-wise tree growth strategy allows deeper trees with fewer iterations, enhancing accuracy. LightGBM supports parallel and distributed training, making it suitable for big data applications. It is often preferred when model speed and scalability are critical.

Random Forest (RF)[10]

Random Forest is an ensemble method based on bagging, constructing multiple decision trees on bootstrapped subsets of the data. Predictions are obtained by averaging the results of individual trees, reducing variance and improving generalization. The method is robust to overfitting and relatively insensitive to parameter settings. It also provides feature importance measures, making it valuable for feature selection. RF remains one of the most widely used algorithms for both regression and classification.

Support Vector Regression (SVR)[11]

SVR extends support vector machines to regression problems by introducing an epsilon-insensitive loss function. It uses kernel functions, such as radial basis functions (RBF), to map data into higher-dimensional spaces where linear separation is feasible. SVR is especially powerful for small-sample, high-dimensional datasets. Its performance depends heavily on kernel choice and hyperparameter tuning. Despite higher computational cost, SVR remains a strong candidate for nonlinear regression tasks.

Gaussian Processes (GP)[12]

GP provide a non-parametric Bayesian framework for regression. They model data as distributions over functions, allowing not only predictions but also uncertainty quantification. GPs are especially useful for small datasets, where uncertainty estimates can guide model interpretation and further data collection. Their kernel

functions allow flexible modeling of complex, nonlinear relationships. However, computational cost scales cubically with the number of samples, limiting their use on very large datasets.

Multi-Layer Perceptron (MLP)[13]

MLPs are feedforward artificial neural networks consisting of input, hidden, and output layers. They use nonlinear activation functions to capture complex mappings between inputs and outputs. With sufficient hidden units and layers, MLPs can approximate arbitrary continuous functions. They are flexible and widely applied to regression, classification, and feature learning.

4.2.6 Machine learning model optimization process (XGBoost example)

A feature subset initially screened by PLS was loaded, and sample indices were shuffled using a random seed of 42 while strictly maintaining the correspondence between features and the target variable.

The process then proceeded to the iterative feature selection and model training phase. Bayesian Optimization was employed to automatically tune the hyperparameters of XGBoost, including the number of trees, maximum depth, learning rate, and others. Each optimization run executed 20 initial points and 50 iterations to identify the optimal parameter combination. During each training-validation split of the cross-validation, all features underwent rigorous standardization: the StandardScaler computed the mean and variance solely based on the current training set, and the same parameters were applied to transform the validation set. This approach ensured that the validation data did not participate in the calculation of any scaling parameters, effectively eliminating the influence of varying scales and preventing data leakage.

Based on the optimized model, SHAP values were computed for each feature. Features were ranked according to their mean absolute SHAP importance, and the least important feature was eliminated in each iteration. This procedure was repeated until only one feature remained, thereby achieving progressive refinement of the

feature space. During each iteration, model performance was evaluated using 10 repeats of 5-fold cross-validation, with comprehensive metrics including R^2, RMSE, and MAE recorded for both training and validation sets.

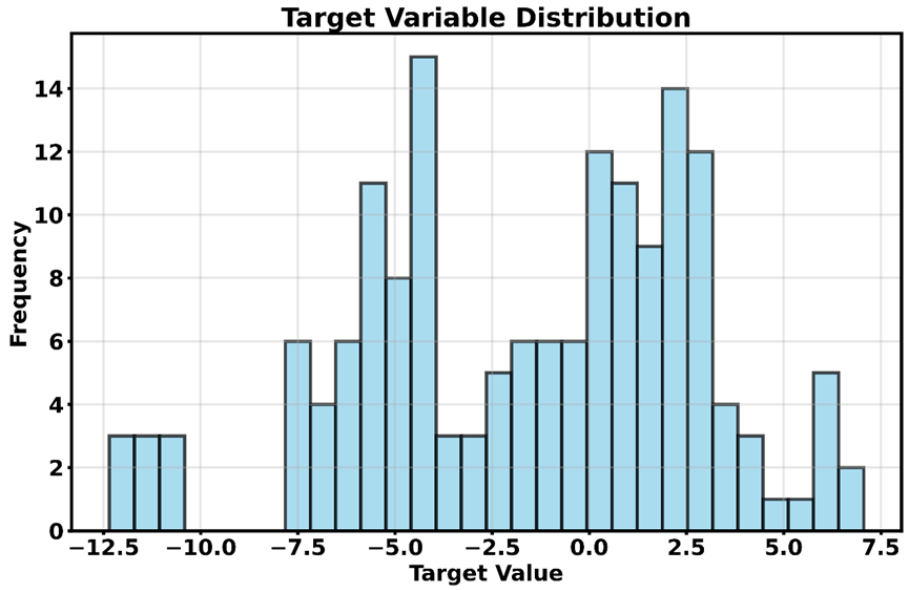


Figure S27. Distribution of target values in the training set.

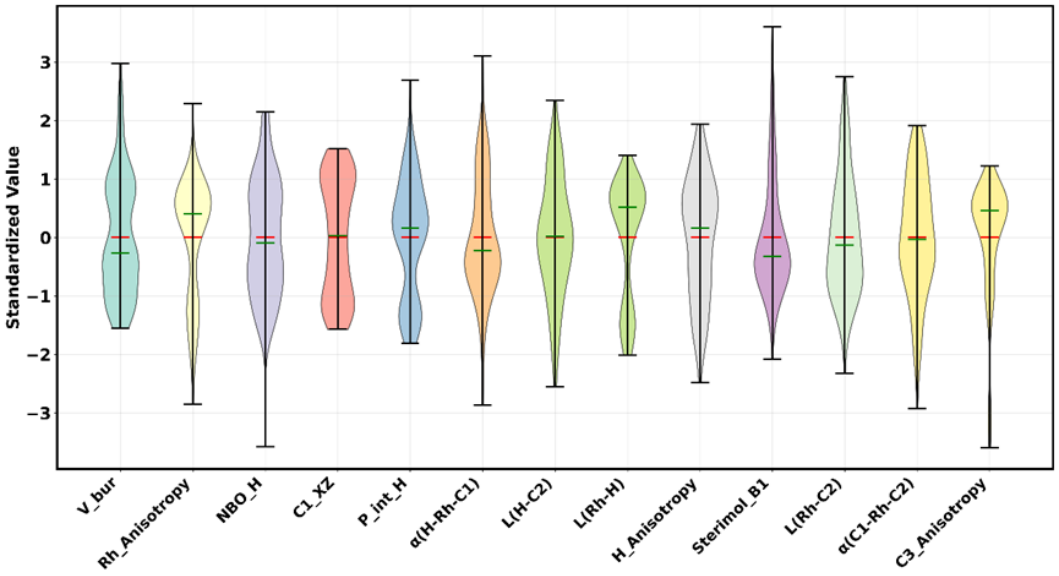


Figure S28. Violin plot of xgboost optimized feature set.

4.2.7 Details of model performance

During the feature selection process, machine learning models were subsequently constructed based on the first R^2 inflection point (93 features), the second R^2 inflection point (53 features), and the feature set size corresponding to optimal performance (35 features) identified through PLSR cross-validation. Experimental results indicate that for most models, the optimal feature subset selected from the initial set of 93 features achieved the best performance. Moreover, certain features within this optimal subset were not included in the smaller initial feature sets. The Venn diagram in the figure below illustrates the optimal feature subsets selected from the three initial feature sets for four representative models—XGBoost, GBR, LightGBM, and RF. Features unique to the 93-feature set are color-coded according to their source set.

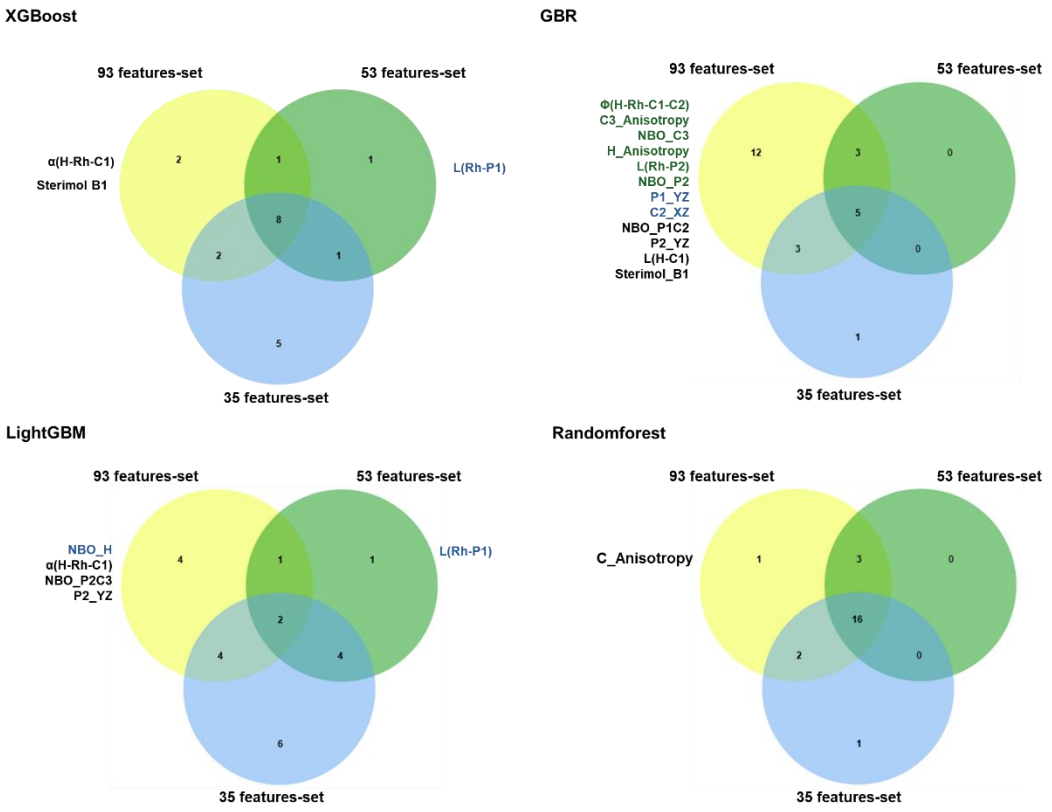


Figure S29. Venn diagram illustrating the optimal feature subsets selected by multiple machine learning models from different initial feature sets (yellow: 93 features-set; green: 53 features-set; blue: 35 features-set).

Among all models, the final optimal descriptor subset derived from the 93-feature set exhibited markedly superior performance in most cases compared to those obtained from the 53- or 35-feature sets. Notably, several key descriptors in the 93-feature set were absent from the smaller sets, indicating that a larger initial feature space is essential to retain descriptors with critical contributions to model performance (see SI for details). Accordingly, subsequent analyses in this study were conducted based on the 93-feature set.

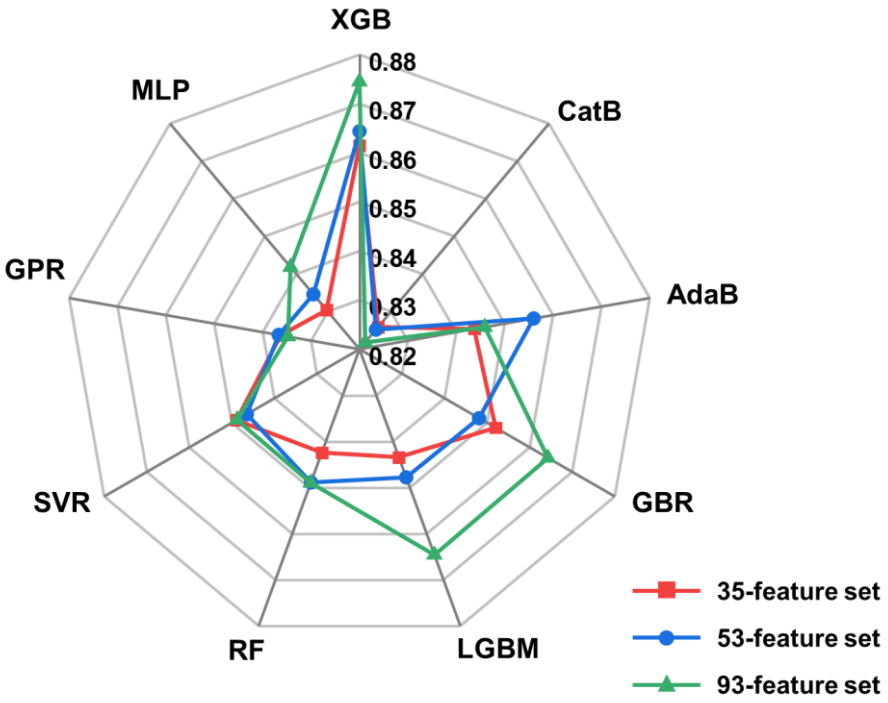


Figure S30. Comparison of the optimal performance of various machine learning models across different feature sets.

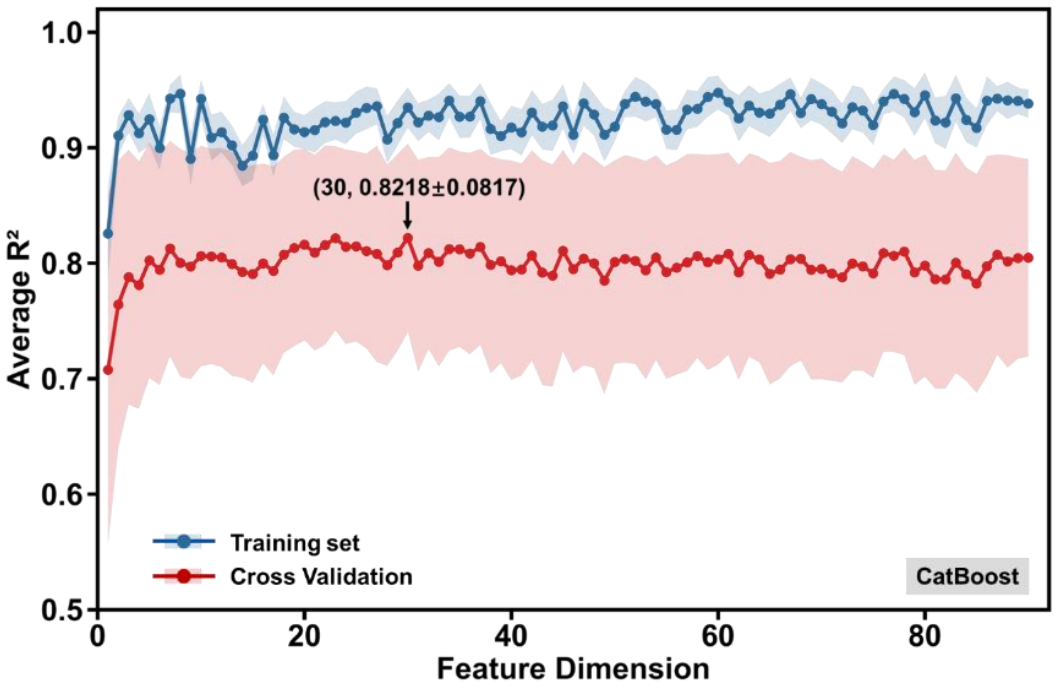


Figure S31. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the CatBoost model.

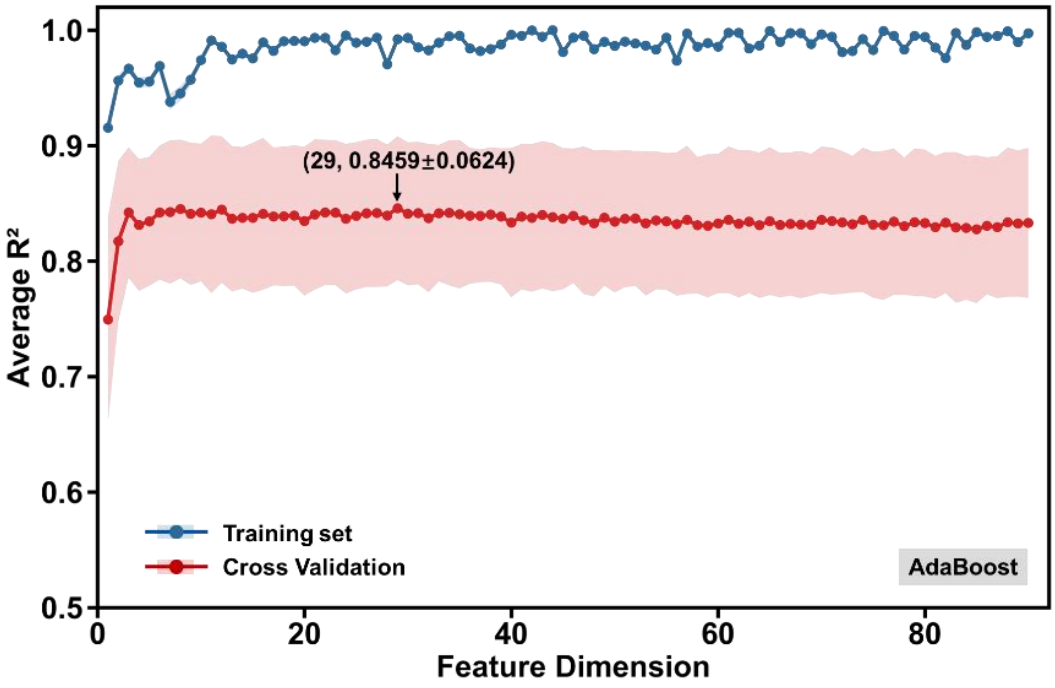


Figure S32. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the AdaBoost model.

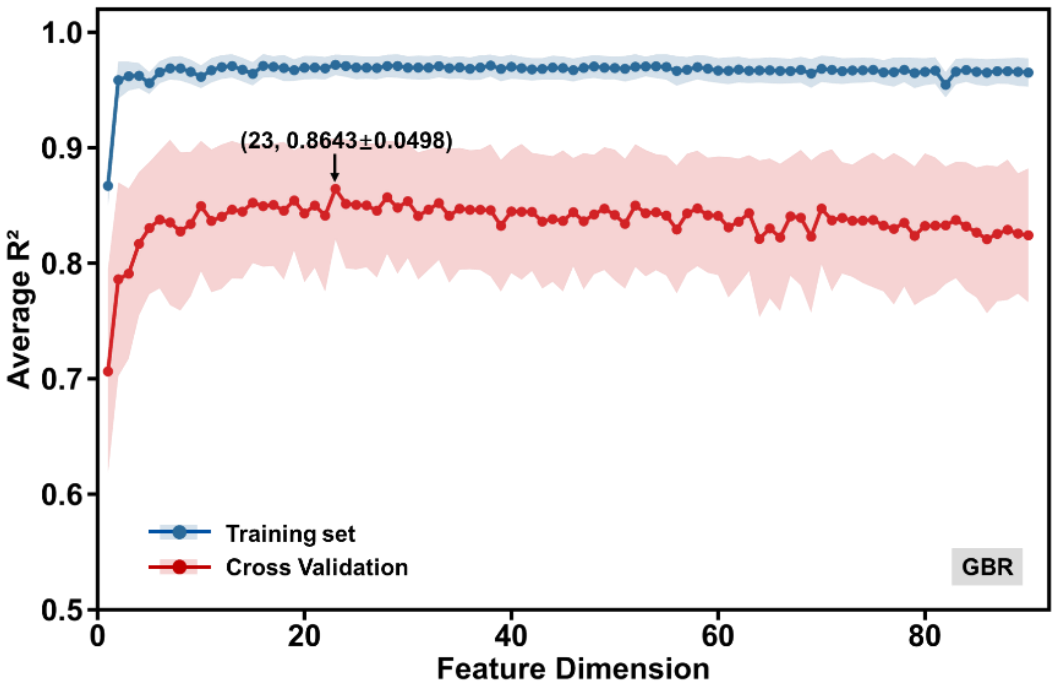


Figure S33. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the GBR model.

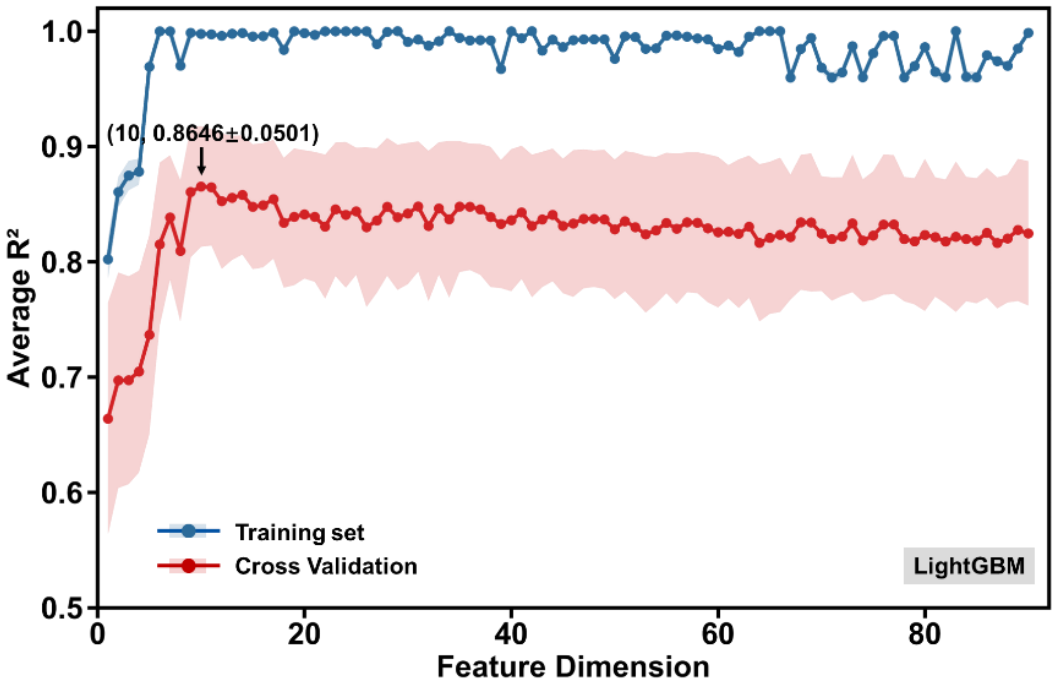


Figure S34. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the LightGBM model.

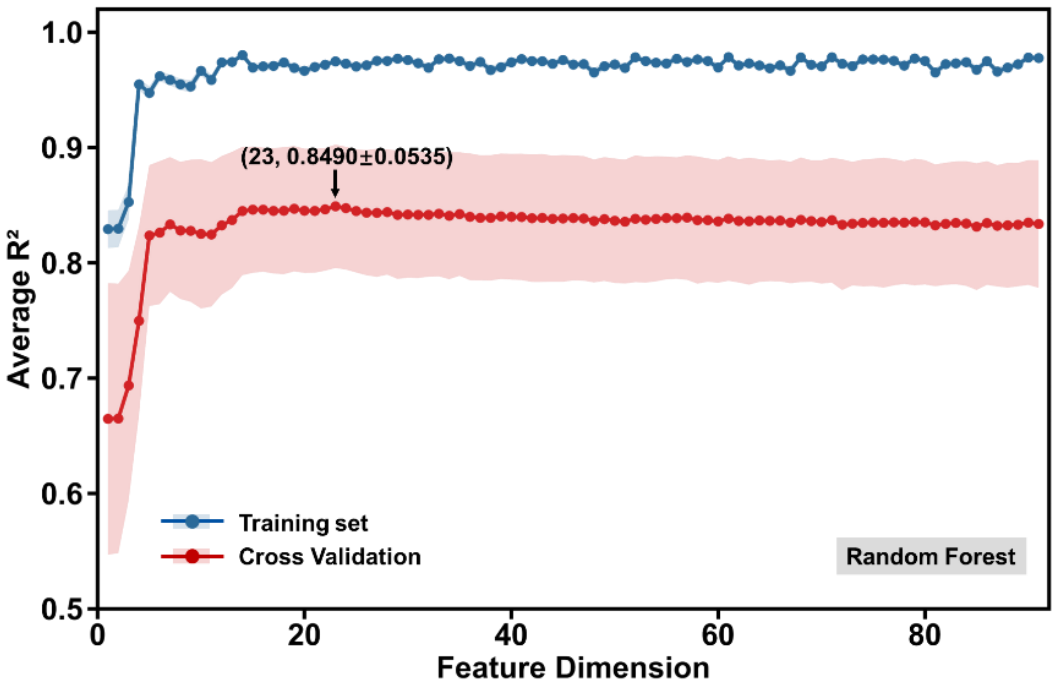


Figure S35. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the Random Forest model.

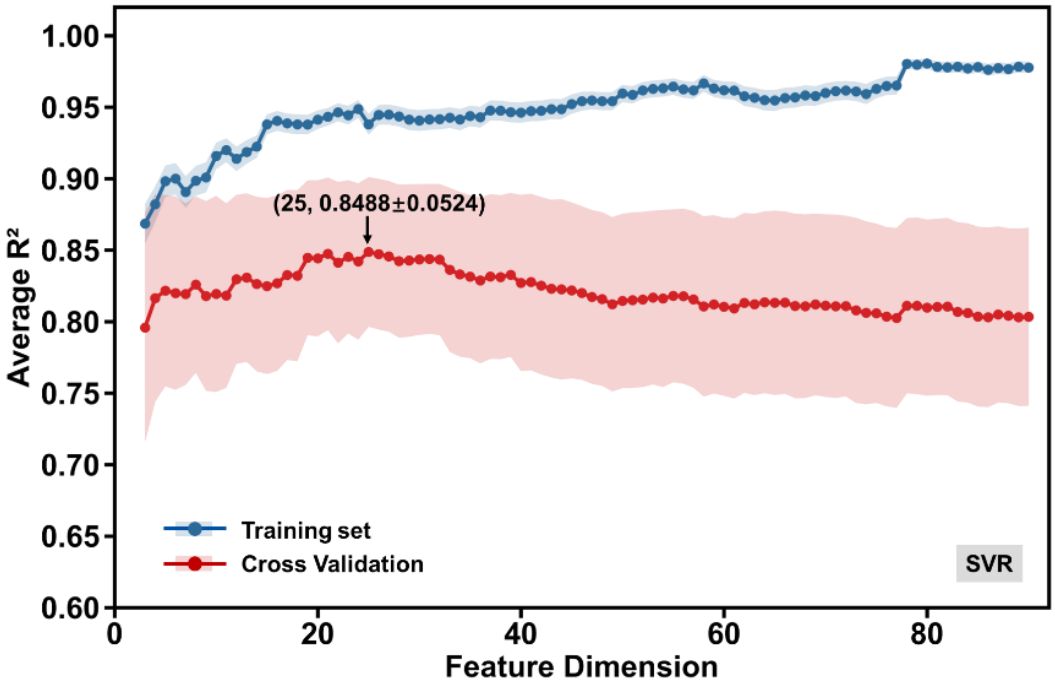


Figure S36. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the SVR model.

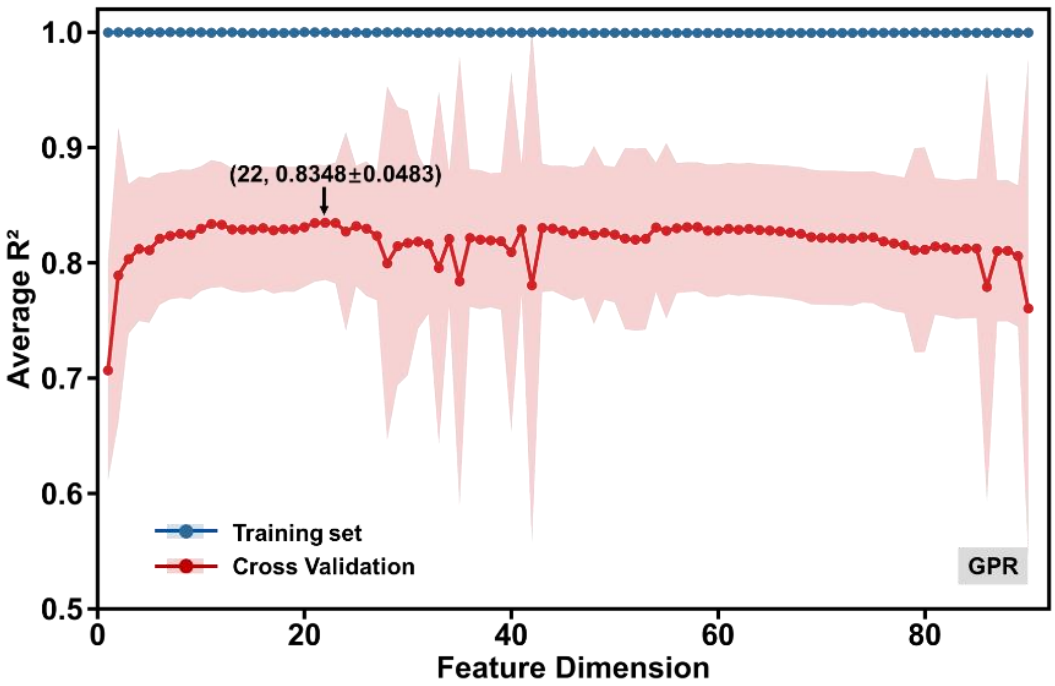


Figure S37. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the GPR model.

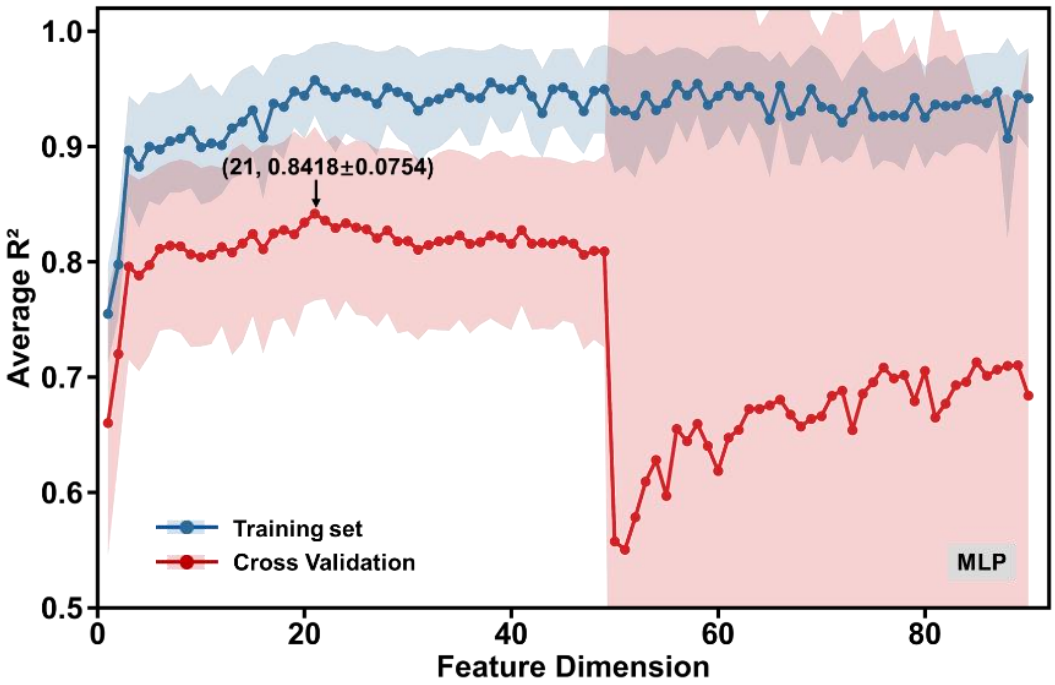


Figure S38. Variation of training and cross-validation R^2 values with feature dimensionality during the feature selection process for the MLP model.

Table S7 Optimal parameters and selected features of various machine learning models constructed on the 93-feature set.

Model	Optimal Parameters	Optimal Feature Set
XGBoost	alpha: 0.395, colsample_bytree: 0.84, gamma: 0.37, learning_rate: 0.02, max_depth: 6, min_child_weight: 7.7, n_estimators: 426, reg_lambda: 0.84, subsample: 0.75	V_bur, Rh_Anisotropy, NBO_H, C1_XZ, P_int_H, α(H-Rh-C1), L(H-C2), L(Rh-H), H_Anisotropy, Sterimol_B1, L(Rh-C2), α(C1-Rh-C2), C3_Anisotropy
Catboost	bagging_temperature: 0.37, colsample_bylevel: 0.92, depth: 3, iterations: 287, l2_leaf_reg: 8.65, learning_rate: 0.115, random_strength: 1.37	P_int_H, Rh_Anisotropy, SASA_H, L(H-C2), H_Anisotropy, NBO_H, L(Rh-P1), α(C1-Rh-C2), NBO_O, C3_XZ, NBO_C3, α(H-Rh-C1), C2_YZ, H_Isotropic, Buried_Sterimol_B1, C2_XZ, φ(H-Rh-C1-C2), P2_YY, C2_XY, buried_volume_1, C2_Anisotropy, NBO_P2, NBO_P1C2, Sterimol_B1, Pyramidalization_P, O1_Anisotropy, C1_XZ, Sterimol_L, α(H-Rh-C2), P1_XZ
Adaboost	learning_rate: 0.023, max_depth: 7, min_samples_leaf: 4, min_samples_split: 5, n_estimators: 175	V_bur, Rh_Anisotropy, NBO_H, φ(H-Rh-C1-C2), P1_YZ, C1_XZ, SASA_C, L(Rh-H), L(Rh-P2), L(H-C2), C3_Anisotropy, P_int_P1, P2_YZ, P_int_H, C1_Anisotropy, C1_XX, Buried_Sterimol_B1, NBO_C3, NBO_P2, C2_XY, C1_XY, O1_Anisotropy, P1_XX, L((Rh-C1)-(Rh-C2)), H_Anisotropy, L(Rh-P1), C2_YZ, NBO_C1
GBR	learning_rate: 0.19, max_depth: 3, max_features: 0.49, min_samples_split: 4, n_estimators: 200	P_int_H, L(Rh-H), L(Rh-C2), Rh_Anisotropy, φ(H-Rh-C1-C2), C3_Anisotropy, L(H-C2), α(C1-Rh-C2), NBO_C3, H_Anisotropy, L(Rh-P2), V_bur, NBO_P2, L((Rh-C1)-(Rh-C2)), L(Rh-CO), C1_XZ, SASA_C, P1_YZ, C2_XZ, P1_Anisotropy, NBO_C1, NBO_H, α(H-Rh-C1), Rh_Isotropic, P2_YZ, P_int_P1, H_XX
lightGBM	colsample_bytree: 0.9, learning_rate: 0.2, max_depth: 3, min_child_samples: 10, min_split_gain: 0.0, n_estimators: 309, num_leaves: 134,	Buried_Sterimol_B1, Rh_Anisotropy, C3_Anisotropy, NBO_C3, O1_Anisotropy, NBO_P2, C2_XZ, NBO_H, α(H-Rh-C1), NBO_P2C3, P2_YZ

	reg_alpha: 0.0, reg_lambda: 50.0, subsample: 0.9, boosting_type: gbdt	
Randomforest	max_depth: 10, max_features: 0.3, max_samples: 1.0, min_samples_leaf: 2, min_samples_split: 2, n_estimators: 212	SASA_H, P_int_H, H-Rh-C2, L(Rh-H), L(Rh-C2), Rh_Anisotropy, φ(H-Rh-C1-C2), C3_Anisotropy, L(H-C2), NBO_C3, H_Anisotropy, L(Rh-P2), V_bur, L(Rh-P), L((Rh-C1)-(Rh-C2)), L(Rh-CO), C1_XZ, V_bur_1, SASA_C, NBO_C1, NBO_H, C_Anisotropy
SVR	C: 49.6, gamma: 0.006, epsilon: 0.01, kernel: 'rbf'	P_int_H, α(H-Rh-C2), L(Rh-H), L(Rh-C2), Rh_Anisotropy, α(C1-Rh-C2), NBO_C3, H_Anisotropy, L(Rh-P2), H_ZY, O1_Anisotropy, V_bur, NBO_P2, L(Rh-P), L((Rh-C1)-(Rh-C2)), L(Rh-CO), Sterimol_L, O1_ZX, Pyramidalization_P, V_bur_1, H_YZ, L(Rh-P1), C_Anisotropy, C2_YZ, P_int_P1
GPR	alpha: 0.006, kernel_type: 0.52, length_scale: 5.36	Rh_Anisotropy, L(Rh-H), P_int_H, NBO_C3, L(Rh-C2), C1_XZ, SASA_H, L(Rh-P2), L(Rh-P), α(H-Rh-C2), V_bur, H_Anisotropy, C3_Anisotropy, Buried_Sterimol_B1, L(H-C2), α(C1-Rh-C2), L(Rh-P1), buried_volume_5, NBO_P2, L(Rh-CO), P1_XX, O1_Anisotropy
MLP	alpha: 0.006, arch_idx: 1.42, batch_size: 9, learning_rate_init: 0.01, hidden_layer_sizes: (64, 32)	P_int_H, H-Rh-C2, L(Rh-H), L(Rh-C2), Rh_Anisotropy, φ(H-Rh-C1-C2), P_int_Rh, C3_Anisotropy, H_Anisotropy, V_bur, NBO_P2, L((Rh-C1)-(Rh-C2)), L(Rh-CO), Sterimol_L, O1_ZX, C1_XX, C1_XY, Buried_Sterimol_L, C2_YZ, P2_YY, P1_XZ

4.3.5 Supplementary SHAP and PDP analyses

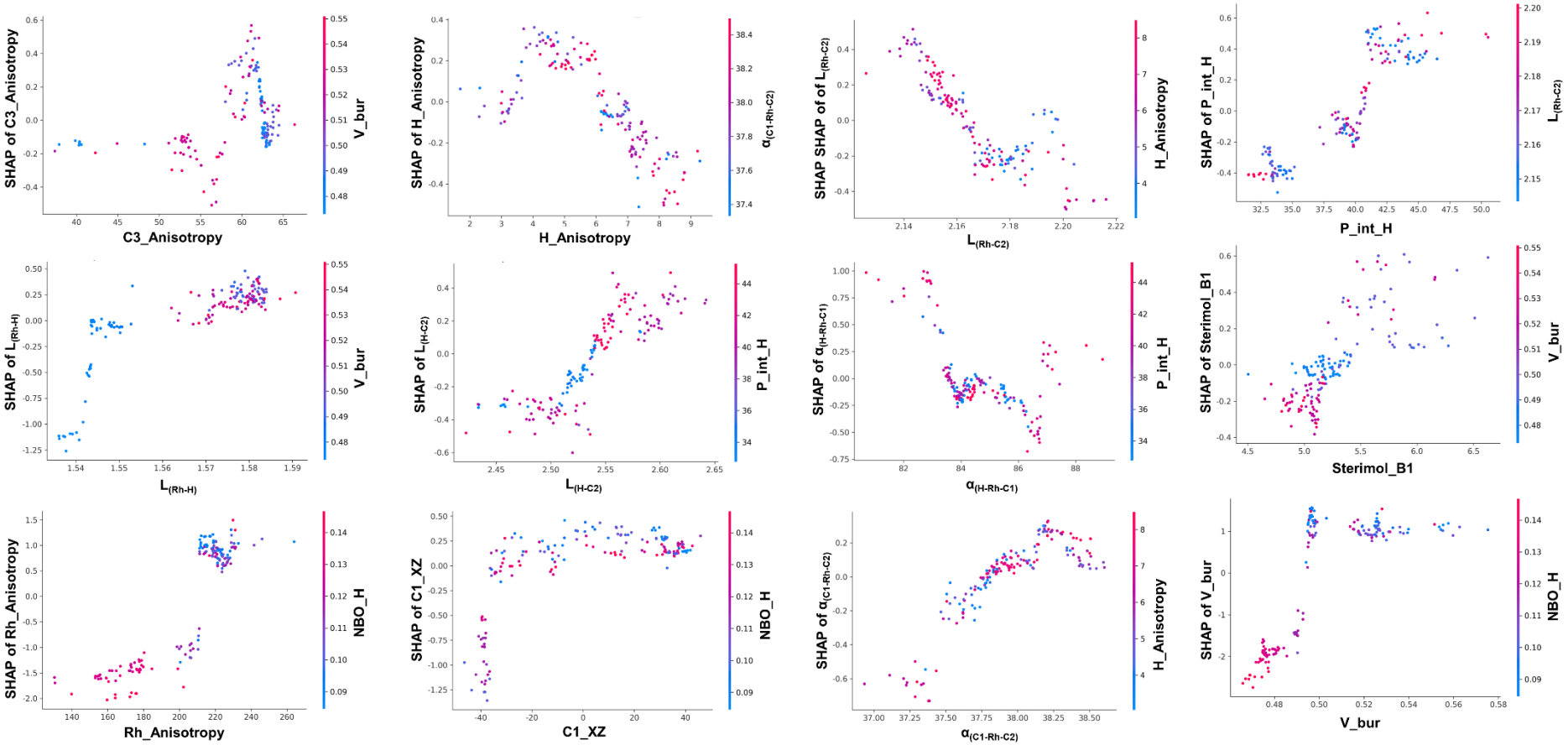


Figure S39. SHAP dependence plots revealing key feature interactions

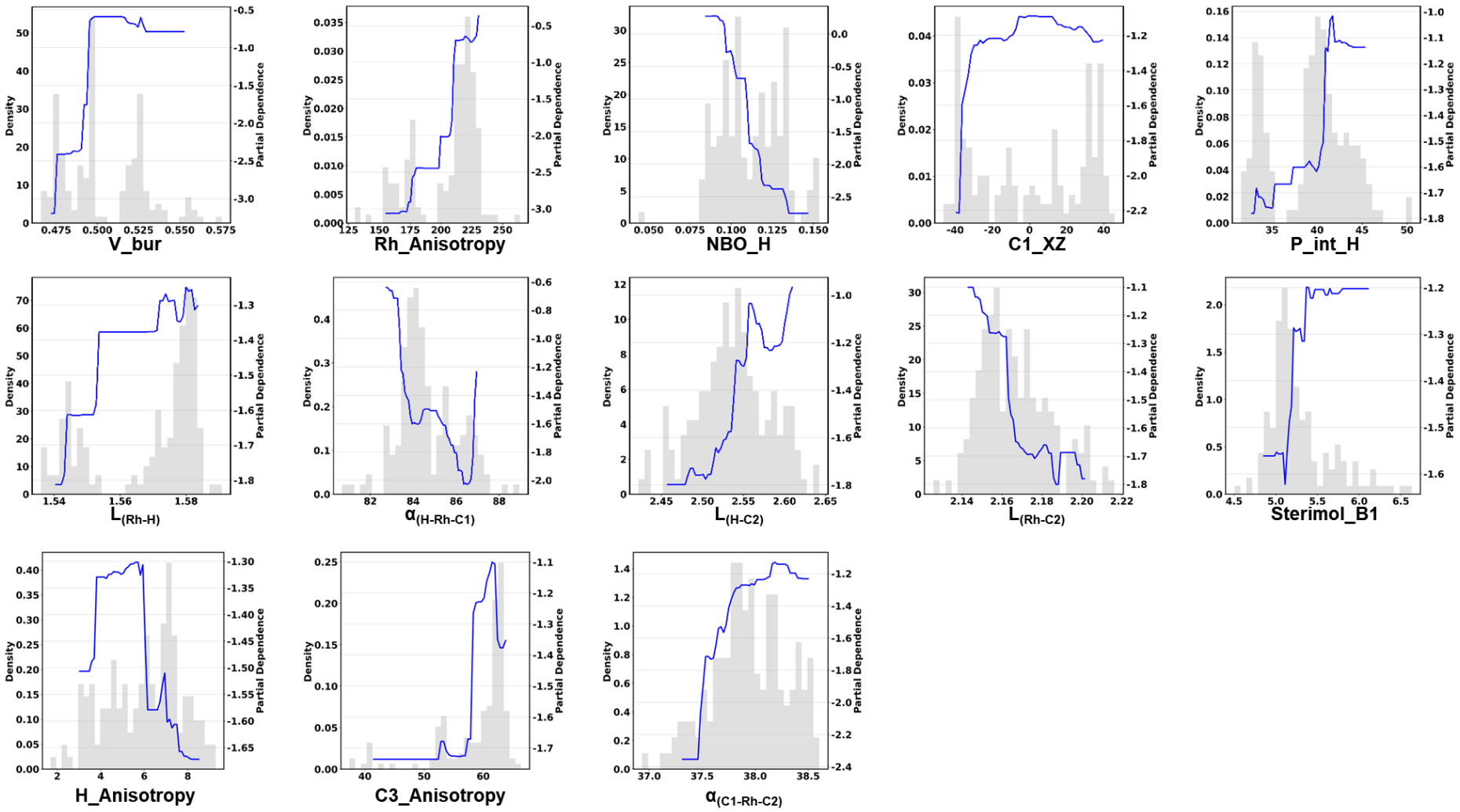


Figure S40. Partial dependence plots for key features

5 Performance of local descriptor models

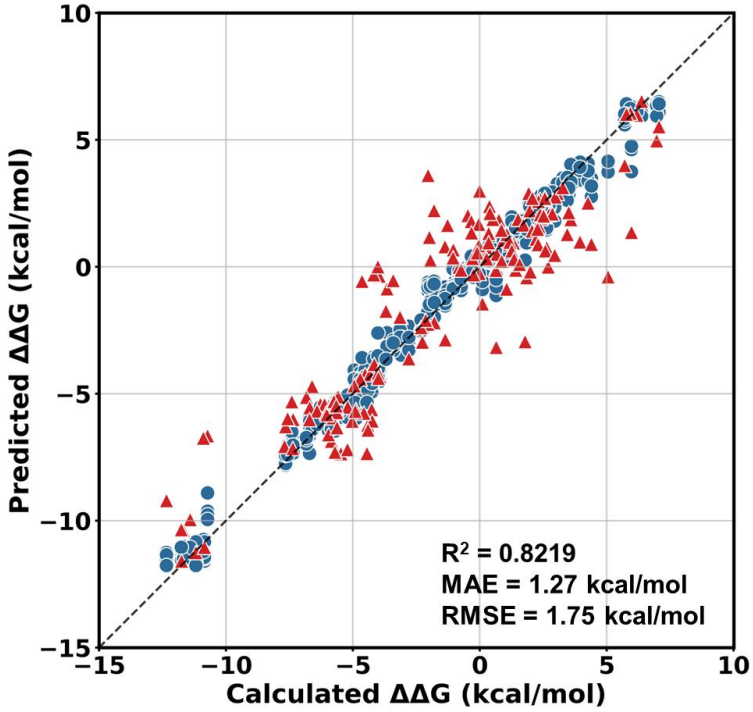


Figure S41. Cross-validation performance comparison of XGBoost model based on SOAP descriptors.

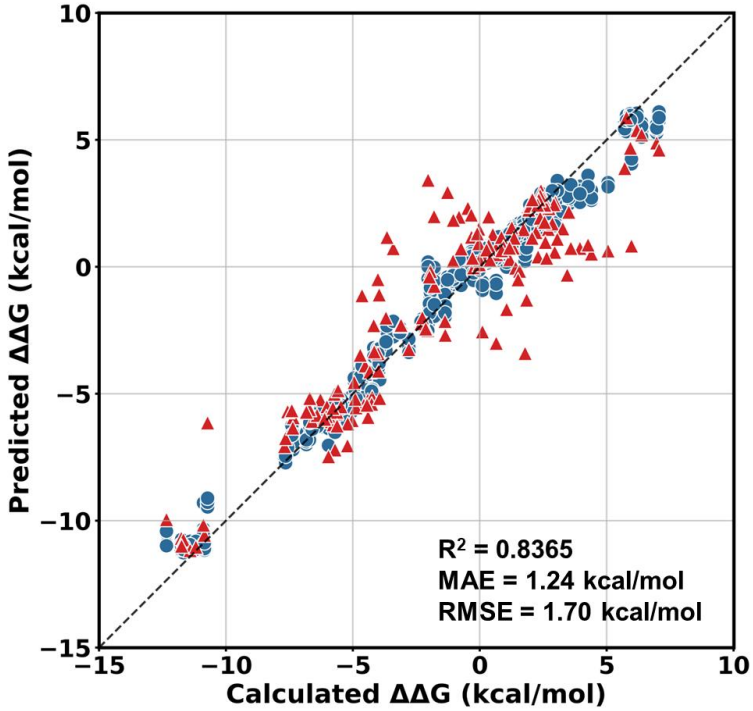


Figure S42. Cross-validation performance comparison of XGBoost model based on ACSF descriptors.

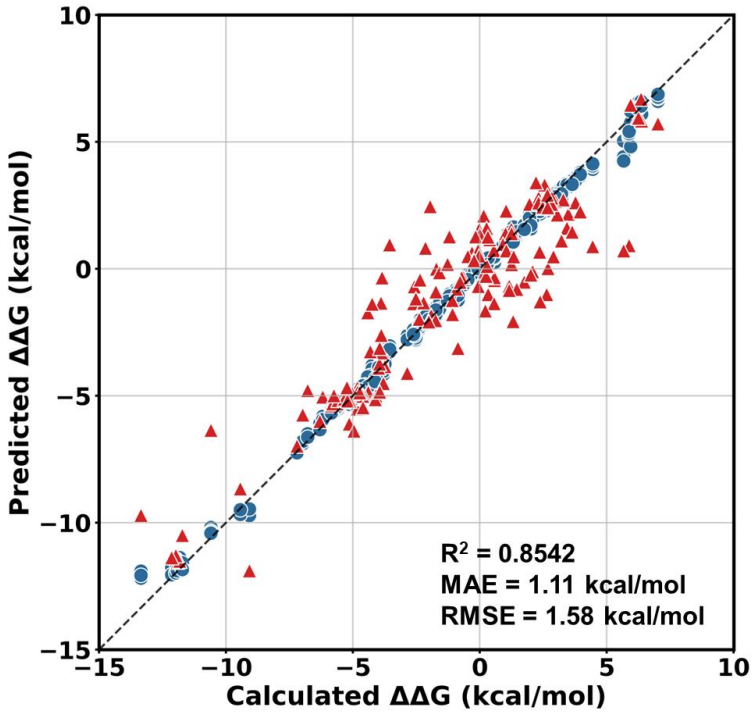


Figure S43. Cross-validation performance comparison of XGBoost models based on LMBTR-k3 descriptors.

6 Model prediction details

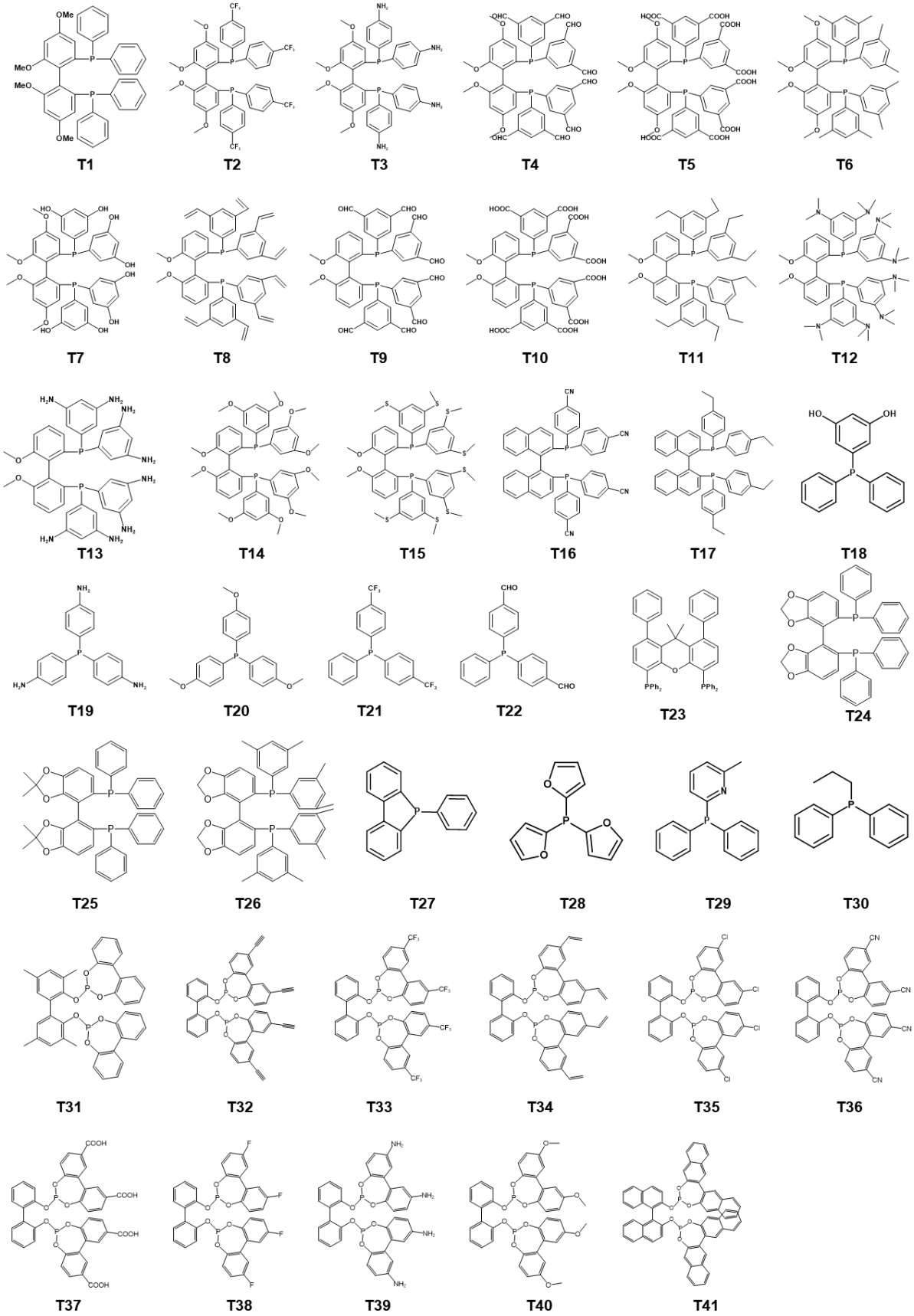


Figure S44. Structures of ligands included in the test set.

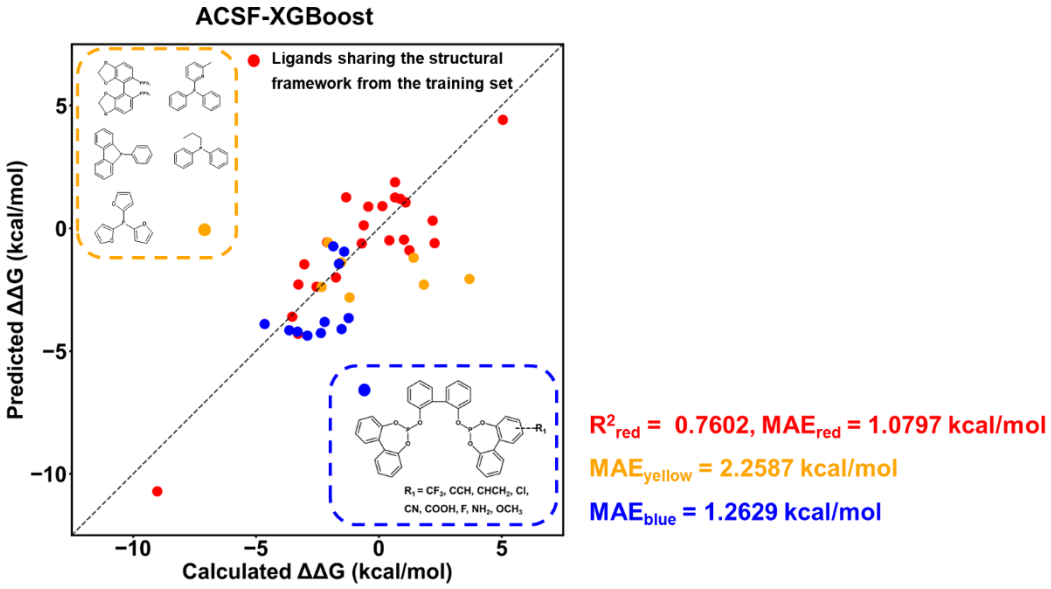


Figure S45. Performance of the trained ACSF-XGBoost model on the external test set (red: ligands sharing the same backbone structure as those in the training set; yellow: other alkylphosphine or arylphosphine ligands; blue: bisphosphite ligands).

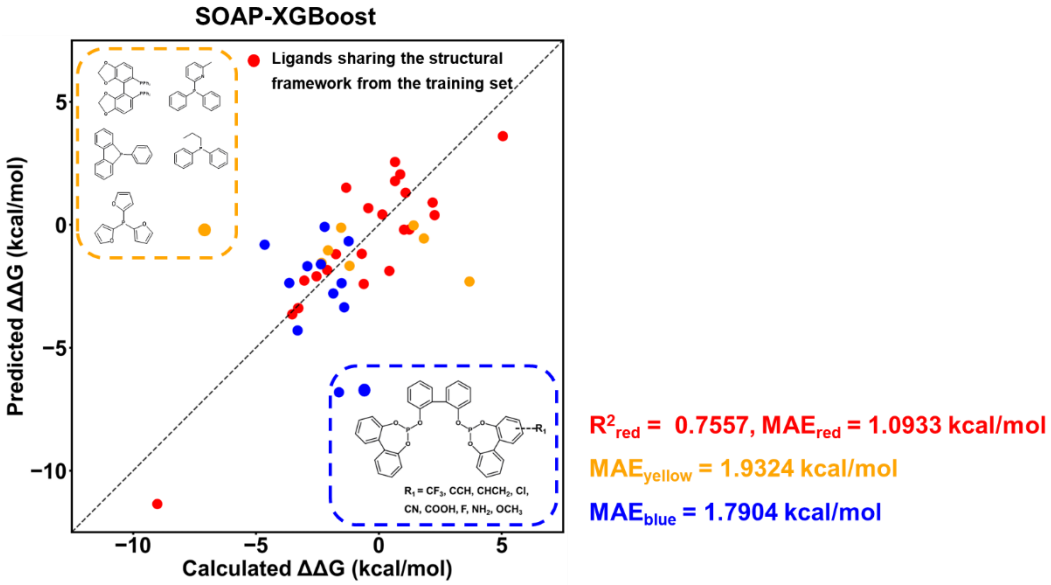


Figure S46. Performance of the trained SOAP-XGBoost model on the external test set (red: ligands sharing the same backbone structure as those in the training set; yellow: other alkylphosphine or arylphosphine ligands; blue: bisphosphite ligands).

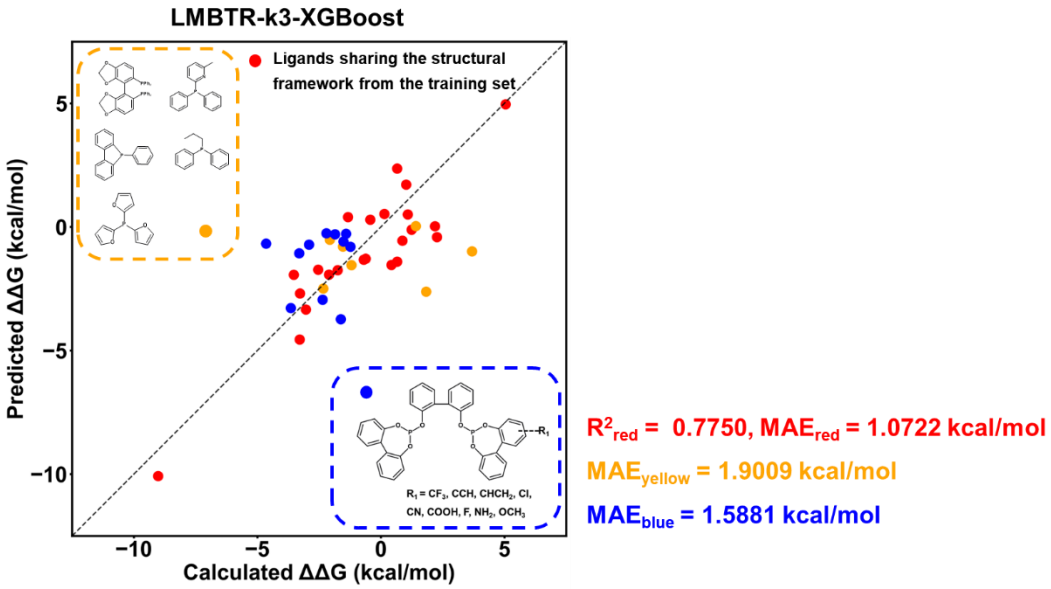


Figure S47. Performance of the trained LMBTR-k3-XGBoost model on the external test set (red: ligands sharing the same backbone structure as those in the training set; yellow: other alkylphosphine or arylphosphine ligands; blue: bisphosphite ligands).

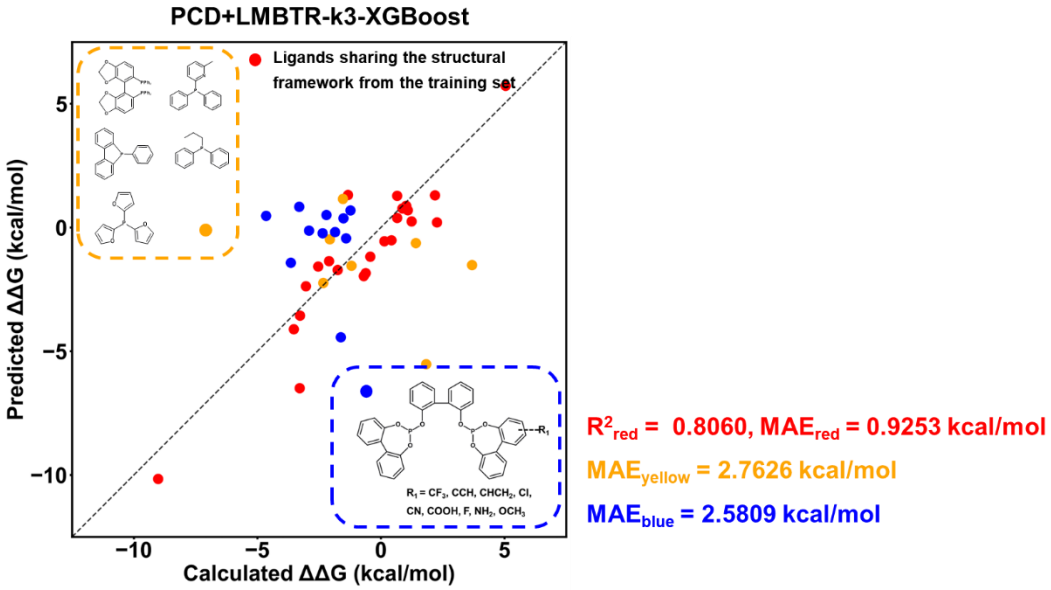


Figure S48. Performance of the trained PCD+LMBTR-k3-XGBoost model on the external test set (red: ligands sharing the same backbone structure as those in the training set; yellow: other alkylphosphine or arylphosphine ligands; blue: bisphosphite ligands).

Table S8 Comparison between predicted and actual values obtained from the optimized XGBoost model

Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}
P1	2.970	2.272	**P22**	2.369	2.403	**P43**	-1.807	-0.731
P2	2.578	1.995	**P23**	2.214	1.640	**P44**	-1.379	-1.754
P3	0.848	1.120	**P24**	1.323	1.160	**P45**	-2.046	-0.317
P4	-1.366	-0.982	**P25**	1.254	1.692	**P46**	-0.247	0.004
P5	0.242	0.226	**P26**	2.288	2.489	**P47**	-4.184	-3.636
P6	3.584	3.364	**P27**	0.267	0.182	**P48**	2.407	2.205
P7	1.164	1.328	**P28**	-4.018	-3.239	**P49**	-0.049	0.356
P8	-0.013	0.109	**P29**	0.401	0.185	**P50**	0.513	0.238
P9	1.926	1.921	**P30**	-0.019	0.075	**P51**	1.980	1.905
P10	2.689	0.928	**P31**	0.666	0.162	**P52**	2.946	1.132
P11	1.714	1.552	**P32**	1.840	1.748	**P53**	1.057	0.754
P12	-0.290	0.228	**P33**	-0.822	-0.396	**P54**	0.346	0.646
P13	1.047	0.215	**P34**	-0.103	0.061	**P55**	0.342	0.356
P14	3.052	2.937	**P35**	2.546	2.630	**P56**	2.860	1.718
P15	0.628	0.493	**P36**	-0.334	-0.244	**P57**	0.931	0.360
P16	1.406	0.438	**P37**	5.971	5.122	**P58**	-1.274	-1.171
P17	-3.656	-2.024	**P38**	4.255	3.563	**P59**	-5.494	-6.468
P18	-0.345	0.078	**P39**	-0.473	-0.107	**P60**	-7.363	-6.719
P19	0.862	1.083	**P40**	-0.041	-0.009	**P61**	-7.412	-5.216
P20	0.747	0.424	**P41**	0.377	0.558	**P62**	-5.794	-5.656
P21	-1.993	-2.024	**P42**	3.434	2.145	**P63**	-5.663	-5.595

Table S8 Comparison between predicted and actual values obtained from the optimized XGBoost model (continued)

Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}
P64	-5.729	-5.571	**P85**	-10.009	-10.721	**P106**	1.344	0.292
P65	-6.121	-5.929	**P86**	-5.630	-5.422	**P107**	-2.132	-2.573
P66	-5.206	-5.146	**P87**	-11.192	-11.243	**P108**	-4.645	-3.812
P67	-5.749	-5.230	**P88**	-5.038	-5.067	**P109**	2.914	3.049
P68	-4.406	-4.717	**P89**	-6.049	-6.141	**P110**	1.963	2.208
P69	-6.417	-6.606	**P90**	-7.701	-7.419	**P111**	-2.270	-1.870
P70	-5.853	-5.786	**P91**	-5.779	-6.046	**P112**	2.556	2.607
P71	-4.908	-5.186	**P92**	-7.656	-7.075	**P113**	3.266	3.121
P72	-5.582	-5.305	**P93**	-5.633	-5.693	**P114**	2.555	2.164
P73	-6.030	-5.844	**P94**	-5.969	-6.320	**P115**	-4.947	-4.720
P74	-4.577	-4.708	**P95**	-11.678	-10.556	**P116**	-3.999	-4.075
P75	-5.469	-5.177	**P96**	-10.852	-10.665	**P117**	-4.333	-4.531
P76	-7.573	-5.135	**P97**	-11.763	-11.242	**P118**	2.063	2.221
P77	-4.423	-4.458	**P98**	-6.704	-5.064	**P119**	2.268	2.355
P78	-4.241	-4.399	**P99**	-9.945	-4.820	**P120**	5.775	5.836
P79	-6.840	-4.710	**P100**	-4.879	-5.021	**P121**	2.378	2.695
P80	-4.451	-5.092	**P101**	-10.894	-10.426	**P122**	-2.323	-2.388
P81	-5.217	-5.874	**P102**	-4.719	-4.634	**P123**	-4.519	-4.640
P82	-6.278	-5.919	**P103**	-4.167	-4.511	**P124**	0.646	-0.328
P83	-5.705	-6.176	**P104**	-3.144	-2.876	**P125**	1.500	1.440
P84	-4.268	-4.772	**P105**	-4.014	-3.490	**P126**	1.569	0.977

Table S8 Comparison between predicted and actual values obtained from the optimized XGBoost model (continued)

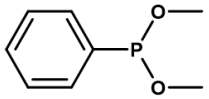
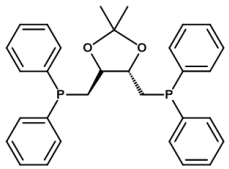
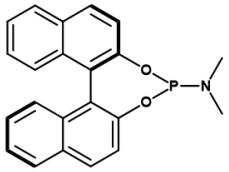
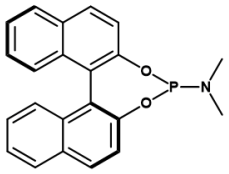
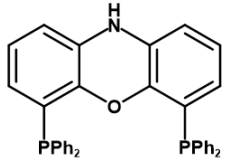
Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}
P127	2.321	2.518	**P139**	5.928	6.161	**P151**	-1.947	-1.630
P128	-3.945	-3.531	**P140**	3.502	3.204	**P152**	2.632	2.438
P129	5.707	5.990	**P141**	2.509	3.028	**P153**	3.943	3.650
P130	1.783	1.290	**P142**	6.966	6.283	**P154**	-1.328	1.680
P131	2.052	2.266	**P143**	6.372	6.407	**P155**	5.047	4.556
P132	-3.414	-2.142	**P144**	-3.108	-2.753	**P156**	-1.792	-1.709
P133	-2.800	-2.986	**P145**	1.176	1.524	**P157**	-0.744	-1.240
P134	2.316	2.936	**P146**	-2.050	-2.292	**P158**	-3.703	-3.792
P135	7.056	6.542	**P147**	4.389	3.801	**P159**	-10.734	-7.053
P136	6.184	6.466	**P148**	1.067	0.895	**P160**	-12.351	-11.571
P137	2.716	2.545	**P149**	-3.968	-3.374	**P161**	-7.369	-7.282
P138	2.967	2.751	**P150**	-1.059	-0.671	**P162**	-6.615	-6.314

* The dataset was split into 80% training and 20% test sets, using a random seed of 42.

Table S9 Comparison between actual and predicted values of the training set using the XGBoost model.

Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}	Sample	Actual_Value / kcal·mol^{-1}	Predicted_Value / kcal·mol^{-1}
T1	-2.536	-3.278	**T24**	-1.189	-1.761
T2	-3.528	-1.576	**T25**	1.414	0.491
T3	-3.035	-2.711	**T26**	-2.332	-1.701
T4	0.659	-0.315	**T27**	1.832	-1.149
T5	2.269	1.717	**T28**	-1.539	0.428
T6	-3.277	-2.458	**T29**	3.687	1.135
T7	-1.750	-2.948	**T30**	-2.068	-0.242
T8	-0.693	0.460	**T31**	-1.231	-0.048
T9	0.868	0.469	**T32**	-2.206	-2.169
T10	1.241	1.481	**T33**	-3.308	-2.126
T11	1.088	0.592	**T34**	-1.413	-2.289
T12	-0.613	-1.197	**T35**	-3.645	-3.555
T13	-3.287	-3.064	**T36**	-1.519	-0.886
T14	-2.103	-0.958	**T37**	-1.857	-3.604
T15	0.427	1.159	**T38**	-4.645	-0.609
T16	1.020	0.649	**T39**	-2.913	-4.005
T17	0.143	-0.101	**T40**	2.358	-2.909
T18	-1.328	1.632	**T41**	-1.626	-3.101
T19	5.047	4.568			
T20	2.188	2.789			
T21	0.660	0.069			
T22	-0.427	-0.847			
T23	-9.015	-11.163			

Table S10 Experimental results of allyl acetate hydroformylation

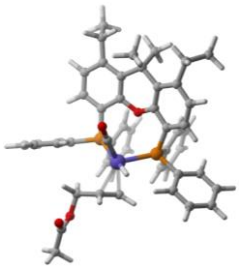
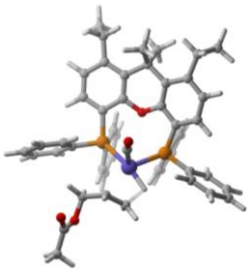
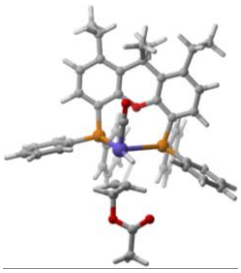
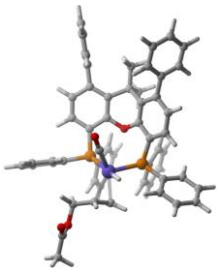
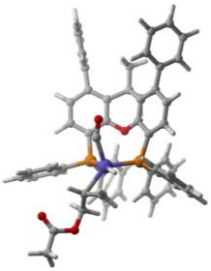
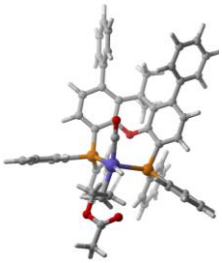
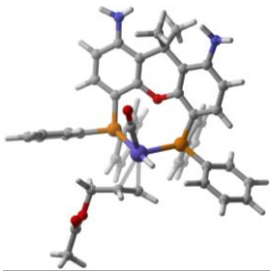
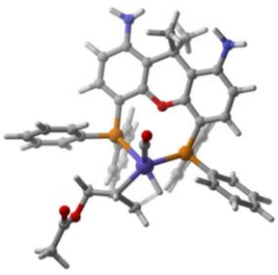
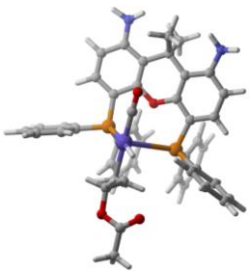
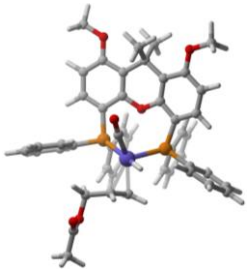
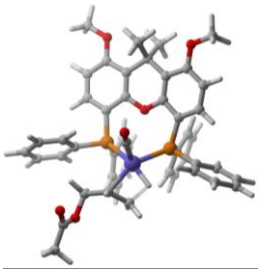
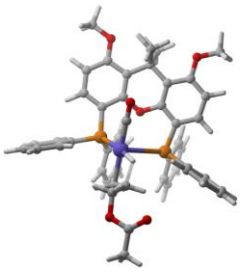
Ligand	Conversion	T/K	P/bar	Selectivity[a]					l/b[b]
				l*	b*	p*	n*	i*	
	13.20%	353	20	43.93%	9.11%	46.44%	0.26%	0.26%	5
	99.64%	353	20	63.64%	32.50%	0.26%	3.06%	0.55%	2
	84.69%	353	20	71.68%	0.09%	---	8.34%	19.89%	816
	74.76%	333	20	76.11%	5.07%	---	4.42%	14.40%	15
	78.25%	353	20	69.48%	0.22%	---	9.35%	20.96%	320
	64.38%	333	20	73.00%	9.69%	---	2.33%	14.97%	8
	99.37%	353	20	81.65%	1.66%	2.06%	8.43%	6.20%	49

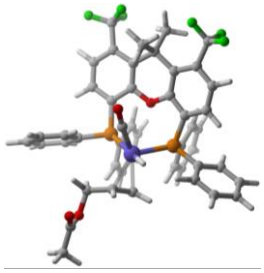
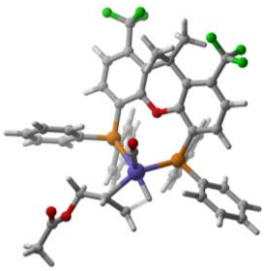
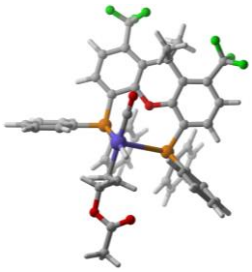
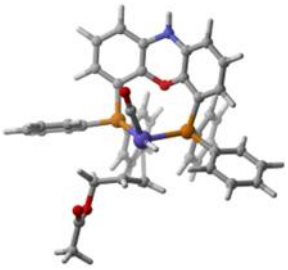
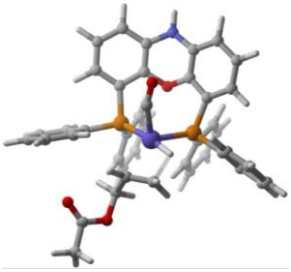
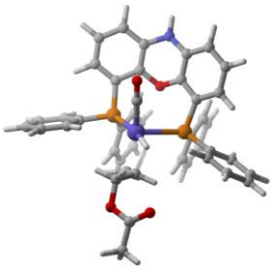
[a] l*, b*, p*, n*, i* represent the selectivity of 4-acetoxybutyraldehyde, 2-methyl-3-acetoxypropionaldehyde, propyl acetate, n-butyraldehyde and isobutyraldehyde,

respectively.

[b] l/b represents the linear-to-branched ratio, which is the ratio of 4-acetoxybutyraldehyde to 2-methyl-3-acetoxypropionaldehyde.

Table S11 Theoretically calculated structures and energies of the selected ligands.

No	Coordination structure	TS-l	TS-b
L1		 ΔG = -3294.768309 Hatree	 ΔG = -3294.768309 Hatree
L2		 ΔG = -2989.955236 Hatree	 ΔG = -2989.973864 Hatree
L3		 ΔG = -2943.526959 Hatree	 ΔG = -2943.544252 Hatree
L4		 ΔG = -3061.834489 Hatree	 ΔG = -3061.853217 Hatree

No	Coordination structure	TS-l	TS-b
L5		 ΔG = -3506.99677 Hatree	 ΔG = -3507.014967 Hatree
E5		 ΔG = -2769.477058 Hatree	 ΔG = -2769.489103 Hatree

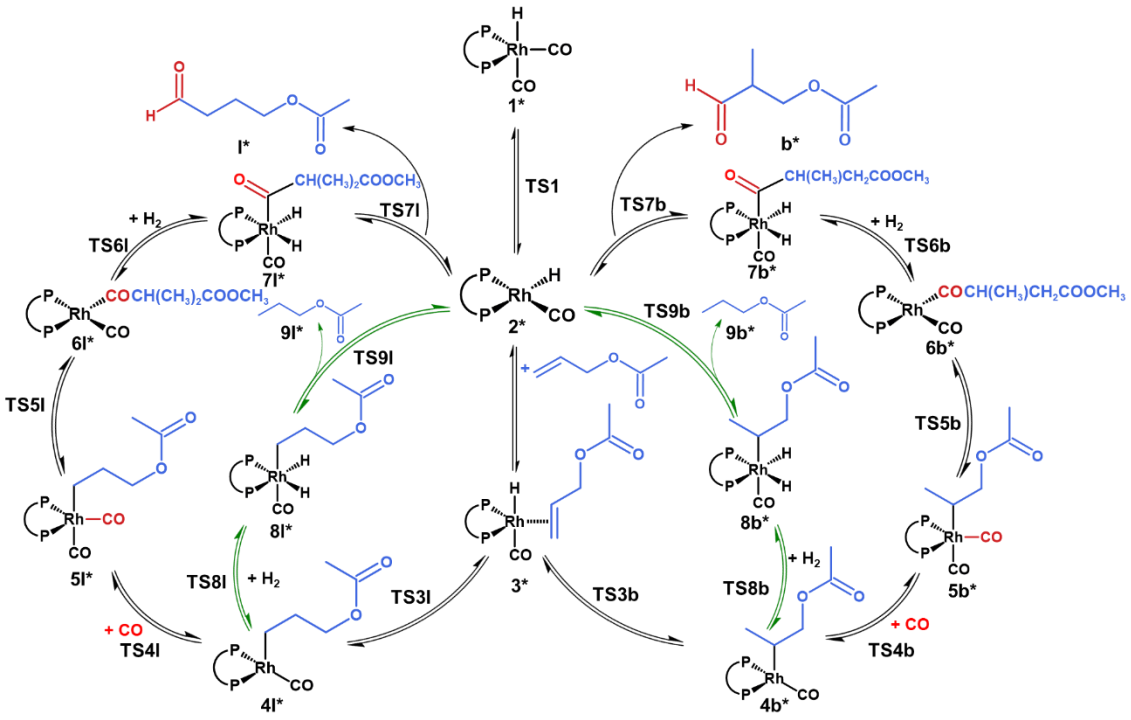


Figure S49. Network diagram of the hydroformylation reaction of allyl acetate[14].

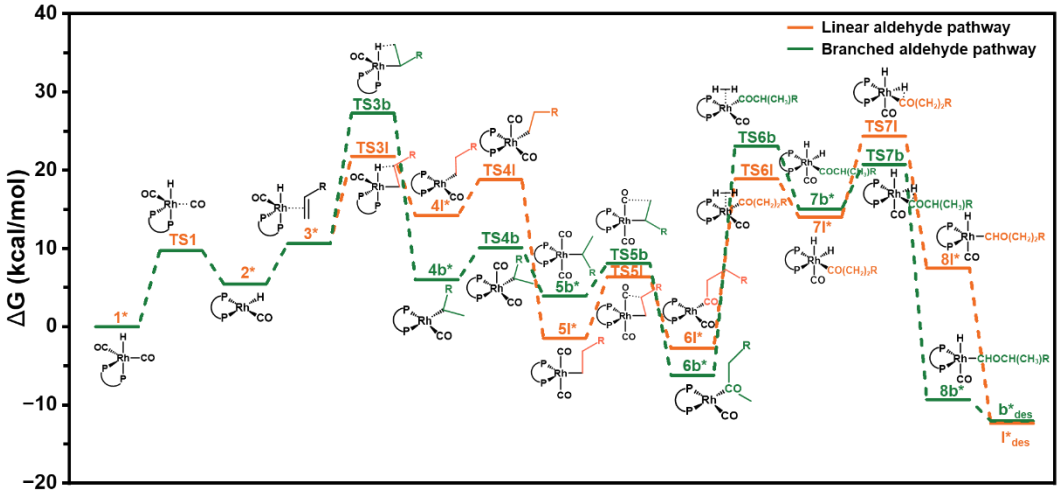


Figure S50. Free energy profiles for the hydroformylation of allyl acetate catalyzed by $RhH(CO)_2$(Xantphos)[14].

7 Structural coordinates

1*

H	7.186383	10.29417	3.715676
H	7.138759	7.841296	3.98924
H	8.831917	3.746354	4.513735
H	10.98558	3.079163	3.478975
H	12.7546	6.767237	4.793339
H	10.6133	7.427058	5.835337
H	3.003665	3.615634	5.521166
H	0.718639	2.910067	4.894615
H	-0.57135	7.006156	5.001834
H	1.702772	7.70942	5.648593
H	4.023343	9.953401	3.071978
H	3.982308	7.567188	3.711426
C	7.548835	9.849596	4.636998
C	7.52239	8.467552	4.791222
C	9.583039	5.622535	5.250685
C	9.697468	4.399868	4.582342
C	10.90774	4.029017	3.99838
C	12.00807	4.878038	4.074232
C	11.89974	6.100719	4.736429
C	10.69379	6.472229	5.322552
C	2.51581	5.710531	5.616499
C	2.220287	4.359346	5.406428
C	0.932281	3.962121	5.055068
C	-0.07408	4.912819	4.903106
C	0.209725	6.260586	5.114105
C	1.495056	6.65787	5.474529
C	4.267501	7.951746	5.816473
C	4.352157	10.65223	5.085632
C	4.151993	9.672453	4.112949
C	4.127496	8.33058	4.473895
H	8.80125	8.254678	7.935639
H	8.817086	10.70816	7.668622
H	4.59267	8.661193	7.827183
H	4.698423	11.03713	7.174206
C	7.980782	7.8802	5.974873
C	8.444114	8.697076	7.009908
C	8.457367	10.08221	6.857822
C	8.015018	10.65926	5.670841
C	4.476399	8.935988	6.783136
C	4.527629	10.28042	6.41463
H	10.38047	4.938119	7.666475
H	8.686342	4.897777	11.62562
H	10.57216	4.447476	10.08673
H	3.820381	5.388569	11.85884
H	1.826005	5.640684	8.055591
H	1.753405	5.274285	10.49457
C	9.556772	5.163622	8.335765
C	8.378458	5.725962	7.830771
C	7.358296	6.013906	8.724632
C	7.428035	5.712722	10.08552
C	8.60221	5.142192	10.57086
C	9.659733	4.886006	9.696899
C	5.061841	6.211767	8.821597
C	5.059884	5.937544	10.19165
C	3.852229	5.598992	10.79375
C	2.694365	5.528186	10.01794
C	2.731383	5.744219	8.643619
C	3.941236	6.075	8.01499
O	6.234609	6.648726	8.241089
H	4.95881	3.895709	4.619406
C	6.401104	5.198405	3.410263
O	6.59615	5.358064	2.287509
P	7.993385	6.048267	6.065328
P	4.209139	6.154572	6.18799
Rh	6.070728	4.809024	5.235262
H	4.382302	11.70063	4.804657
H	8.02566	11.73857	5.553139
H	-1.07628	4.605218	4.621404
H	12.94878	4.591695	3.61434
C	6.396725	3.301784	6.376072
O	6.573345	2.3535	6.999228
N	6.294813	6.008238	10.86114
H	6.299266	5.624422	11.79838

2*

H	7.087265	9.958007	3.482829
H	7.051032	7.538138	3.996497
H	8.658796	3.973889	4.179121
H	10.76428	3.415482	3.001381
H	12.78933	6.537513	5.149388
H	10.6853	7.099914	6.318733
H	3.159872	3.893233	4.68912
H	0.916947	3.395334	3.75268
H	-0.61715	6.995845	5.525528
H	1.624011	7.505222	6.43096
H	3.766952	9.867571	3.156728
H	3.712466	7.500341	3.842925
C	7.460435	9.604251	4.438761
C	7.441042	8.244299	4.727343
C	9.5369	5.550652	5.348987
C	9.567621	4.524296	4.403013
C	10.75293	4.215054	3.73518
C	11.91286	4.931957	4.008181
C	11.88816	5.968897	4.942435
C	10.70588	6.281231	5.603031
C	2.538207	5.717603	5.635313
C	2.329567	4.5678	4.872444
C	1.065978	4.290388	4.348302
C	0.005137	5.157342	4.585675
C	0.206517	6.313024	5.34237
C	1.466311	6.59577	5.855987
C	4.282684	7.898849	5.887386
C	4.347045	10.58688	5.104447
C	4.012284	9.599139	4.179833
C	3.987432	8.26391	4.567119
H	8.74092	8.339112	7.868695
H	8.746595	10.75717	7.363761
H	4.875486	8.633553	7.829604

H	4.940594	10.99119	7.133216	C	-1.2519	-0.48836	5.031577
C	7.915239	7.775138	5.957042	C	-0.07906	-1.00434	4.488108
C	8.378406	8.689324	6.90582	C	0.00473	-1.27929	3.124705
C	8.384818	10.05367	6.620012	C	1.072604	1.91556	1.836023
C	7.935018	10.51122	5.385007	C	-0.05272	2.300918	2.573829
C	4.633182	8.891901	6.804289	C	0.015559	2.419549	3.957536
C	4.665603	10.22883	6.410745	C	1.206258	2.137999	4.625034
H	10.377	4.977951	7.867878	C	2.323854	1.733589	3.901489
H	8.680738	5.168734	11.81911	C	2.259549	1.624645	2.513054
H	10.57182	4.64201	10.30892	C	1.052034	3.696139	-0.3516
H	3.821862	5.524877	11.99812	C	1.306625	6.434606	-0.89562
H	1.841301	5.528936	8.180909	C	2.088556	5.843123	0.09694
H	1.771603	5.257548	10.6316	C	1.959145	4.485892	0.369434
C	9.553876	5.250727	8.519397	H	-2.80537	-3.01697	2.269831
C	8.377512	5.782828	7.977536	H	-4.60657	-4.61831	1.744006
C	7.354596	6.112897	8.856215	H	-0.4377	3.701385	-1.90393
C	7.421613	5.884613	10.23048	H	-0.21553	6.115205	-2.38346
C	8.598565	5.353785	10.7521	C	-2.45539	-2.47569	0.210629
C	9.657785	5.054451	9.894929	C	-3.09707	-3.17552	1.236296
C	5.048432	6.266348	8.933882	C	-4.11089	-4.08541	0.938617
C	5.047876	6.052153	10.314	C	-4.48109	-4.3157	-0.38366
C	3.850957	5.69189	10.92531	C	0.273127	4.298923	-1.34211
C	2.702121	5.53754	10.14926	C	0.399661	5.661795	-1.61264
C	2.736226	5.702529	8.767477	H	-0.82644	-4.34055	0.034445
C	3.931715	6.066336	8.132817	H	1.093997	-5.74524	-0.59634
O	6.217006	6.702418	8.342458	H	3.387713	3.022466	-1.48238
H	4.789533	3.511253	5.945818	H	5.416641	1.839423	-2.26684
P	7.956851	5.954025	6.19422	C	0.160741	-3.89837	-0.03439
P	4.203964	6.105438	6.307623	C	0.338742	-2.52961	0.22267
Rh	6.015695	4.514933	5.91086	C	1.63106	-2.03067	0.14139
H	4.367318	11.63035	4.804863	C	2.723514	-2.79428	-0.2835
H	7.94167	11.57409	5.162843	C	2.519918	-4.14329	-0.55163
H	-0.97763	4.940025	4.178858	C	1.244899	-4.68913	-0.39973
H	12.83586	4.691107	3.490039	C	2.777245	-0.06614	-0.26574
C	6.920363	2.930096	5.791559	C	3.892401	-0.76447	-0.72539
O	7.415546	1.890805	5.73745	C	4.849289	-0.06128	-1.45395
N	6.276245	6.197016	10.98476	C	4.663242	1.299276	-1.70314
H	6.284498	5.850036	11.9364	C	3.5245	1.969362	-1.25992
				C	2.548751	1.274596	-0.53561
3*				O	1.853298	-0.7262	0.518918
				P	-1.04441	-1.32482	0.483256
H	-4.11648	-3.80778	-2.44686	P	0.903243	1.891249	0.000289
H	-2.33847	-2.17359	-1.92015	H	1.404132	7.49539	-1.10461
H	-3.11809	-0.29432	2.203474	H	-5.27038	-5.02483	-0.61231
H	-3.25943	0.180584	4.618115	H	1.258114	2.224398	5.706233
H	0.779166	-1.19405	5.125275	H	-1.31389	-0.2808	6.095487
H	0.923083	-1.68777	2.714639	Rh	-0.90023	0.682588	-1.06497
H	-0.98484	2.515436	2.058027	H	-0.76802	1.768128	-2.14945
H	-0.86619	2.718365	4.515987	C	-0.16256	-0.42595	-2.39706
H	3.253675	1.506956	4.414502	O	0.354497	-1.05042	-3.21394
H	3.144595	1.323965	1.959644	C	-2.44059	1.965684	-0.14717
H	2.796636	6.441193	0.662028	C	-3.01528	1.300891	-1.24344
H	2.565865	4.033606	1.149787	C	-4.06938	0.256258	-1.03166
C	-3.83452	-3.63351	-1.41332	O	-5.37211	0.872204	-0.86547
C	-2.83114	-2.71683	-1.11669	C	-5.98875	1.258758	-1.99044
C	-1.0894	-1.03581	2.291681	C	-7.31808	1.90054	-1.68569
C	-2.25735	-0.48843	2.840378	O	-5.52815	1.108895	-3.0983
C	-2.34225	-0.22661	4.203867	H	-2.69622	1.640565	0.860708

H	-2.13553	3.005858	-0.22707
H	-3.10983	1.827564	-2.18899
H	-3.91561	-0.29025	-0.09925
H	-4.13219	-0.45148	-1.86
H	-7.15645	2.810377	-1.10155
H	-7.92964	1.224393	-1.08378
H	-7.82714	2.143077	-2.61715
H	5.730706	-0.57572	-1.8251
H	3.352017	-4.76039	-0.87755
N	3.957307	-2.1338	-0.4164
H	4.674103	-2.65516	-0.90647
TS3l			
651.56i			
H	-4.9066	-3.92972	-1.502
H	-3.03814	-2.28446	-1.36636
H	-3.02051	-0.74647	2.413244
H	-3.02423	-0.10764	4.795084
H	1.143037	-1.11304	5.069367
H	1.149213	-1.77124	2.699054
H	-1.07768	2.354454	2.378862
H	-0.75528	2.669499	4.805665
H	3.435236	1.838523	4.354546
H	3.123093	1.561474	1.921944
H	1.45281	6.724051	0.556996
H	1.552614	4.403476	1.399846
C	-4.26935	-3.90289	-0.6236
C	-3.2257	-2.98103	-0.5514
C	-0.93408	-1.301	2.384976
C	-2.1027	-0.82079	2.991349
C	-2.10787	-0.46623	4.336128
C	-0.94036	-0.5745	5.089728
C	0.227242	-1.03723	4.491423
C	0.232174	-1.40381	3.146746
C	1.002259	1.949165	1.978227
C	-0.0835	2.253828	2.80875
C	0.096975	2.433035	4.175823
C	1.364259	2.28468	4.736931
C	2.445929	1.958945	3.923277
C	2.268472	1.796792	2.549936
C	0.633598	3.549077	-0.35433
C	0.529323	6.180739	-1.31083
C	1.070426	5.912617	-0.05484
C	1.125767	4.604546	0.421252
H	-1.99801	-3.79266	2.51498
H	-3.85047	-5.42752	2.384161
H	-0.29811	3.014253	-2.22293
H	-0.38695	5.33675	-3.06976
C	-2.4005	-2.93609	0.575539
C	-2.63349	-3.82377	1.633454
C	-3.67548	-4.74288	1.560168
C	-4.49493	-4.78235	0.431572
C	0.088266	3.829057	-1.61405
C	0.041237	5.135961	-2.09275
H	-0.55455	-4.71967	0.137929
H	1.468562	-5.92549	-0.61112
H	2.962836	3.070552	-1.38203
H	5.035264	2.06642	-2.2884
C	0.385412	-4.18847	0.034751
C	0.447299	-2.81591	0.310869
C	1.674525	-2.18015	0.168408
C	2.811497	-2.82819	-0.31997
C	2.728105	-4.1896	-0.59723
C	1.522942	-4.86308	-0.39845
C	2.606854	-0.09523	-0.26507
C	3.761151	-0.6874	-0.78101
C	4.635769	0.104158	-1.52004
C	4.343716	1.453908	-1.7194
C	3.179453	2.021402	-1.20923
C	2.278299	1.237706	-0.47626
O	1.768663	-0.85252	0.529012
P	-1.01435	-1.73295	0.599642
P	0.6482	1.787453	0.180051
H	0.485175	7.201551	-1.6775
H	-5.30971	-5.49775	0.378483
H	1.505536	2.414918	5.805656
H	-0.94003	-0.29171	6.13815
Rh	-1.18322	0.010371	-0.95802
H	-1.61344	1.120461	-2.06968
C	-0.10142	-0.82937	-2.20947
O	0.561873	-1.37964	-2.97563
C	-2.95973	0.839099	0.050186
C	-2.93571	1.458569	-1.21864
C	-3.93826	1.04285	-2.2727
O	-5.18455	1.733158	-2.07267
C	-5.21941	3.008381	-2.49839
C	-6.56645	3.62852	-2.24007
O	-4.27972	3.564058	-3.01594
H	-3.66304	0.023307	0.210896
H	-2.68855	1.409295	0.933097
H	-2.65728	2.51099	-1.26313
H	-4.17711	-0.01698	-2.17091
H	-3.57902	1.248077	-3.283
H	-6.76303	3.637517	-1.16487
H	-7.34776	3.030577	-2.71512
H	-6.57896	4.644956	-2.63002
H	5.539622	-0.33424	-1.93287
H	3.601274	-4.71593	-0.97171
N	3.965862	-2.05141	-0.50799
H	4.696472	-2.49369	-1.05228
4l*			
H	3.392187	-4.28312	1.191412
H	1.408753	-2.92942	0.672498
H	-2.62544	-1.47313	0.312451
H	-4.34845	-3.12753	-0.3804
H	-2.75527	-5.95061	2.439988
H	-1.05283	-4.29477	3.141437
H	0.627803	3.242366	-0.41018
H	1.324692	5.139805	-1.7996
H	5.277558	4.933211	-0.1038
H	4.566905	3.031987	1.314854
H	5.663884	-1.01481	-0.17628
H	3.82722	0.623836	-0.31965
C	2.814757	-3.84792	2.001104

C	1.695777	-3.07577	1.709564	C	-1.26689	1.608504	1.887973
C	-1.74075	-2.77035	1.77911	C	-2.01003	2.038703	0.617065
C	-2.66928	-2.45301	0.784492	C	-2.30285	3.531974	0.61595
C	-3.63189	-3.38278	0.393959	O	-3.04645	3.937688	-0.54753
C	-3.66371	-4.6401	0.990684	C	-2.34353	4.182327	-1.66043
C	-2.73444	-4.9682	1.978513	C	-3.24945	4.558379	-2.80305
C	-1.77695	-4.03833	2.371881	O	-1.13723	4.10792	-1.72825
C	2.544505	3.018761	0.559732	H	-0.80728	2.475049	2.38053
C	1.644968	3.617738	-0.32578	H	-1.95627	1.155444	2.606685
C	2.042086	4.693427	-1.11848	H	-2.95037	1.488775	0.500554
C	3.348527	5.166859	-1.03725	H	-1.37283	4.106998	0.665766
C	4.257067	4.567229	-0.16257	H	-2.9388	3.800254	1.462218
C	3.858496	3.498468	0.63448	H	-3.90401	3.715391	-3.03964
C	3.370846	0.55683	1.790328	H	-2.64889	4.817245	-3.67344
C	5.450982	-1.31338	1.948215	H	-3.88351	5.399808	-2.51434
C	5.119024	-0.73998	0.72165				
C	4.083749	0.18573	0.642482	TS4l			
H	0.748575	-2.28674	4.875157	43.14i			
H	2.736535	-3.63995	5.387615	H	3.827153	-4.1349	1.67282
H	3.161464	0.238459	3.915649	H	1.761164	-3.08544	0.86431
H	4.990716	-1.40023	4.049186	H	-2.55715	-2.26686	0.220091
C	0.937901	-2.49561	2.734637	H	-4.07234	-4.17861	-0.24074
C	1.324727	-2.71288	4.059942	H	-2.20273	-6.41128	2.918767
C	2.449437	-3.48419	4.351979	H	-0.70684	-4.49694	3.391512
C	3.197793	-4.0512	3.325797	H	0.801236	2.376206	-1.45774
C	3.709844	-0.02154	3.016186	H	1.719913	4.013964	-3.0863
C	4.744994	-0.95156	3.091618	H	5.048332	4.740269	-0.46765
H	-2.94381	-2.18536	3.998054	H	4.128633	3.112859	1.155859
H	-2.44324	0.556329	7.275946	H	5.709167	-1.21513	0.134369
H	-3.72812	-1.23552	6.140601	H	3.763892	0.190503	-0.41848
H	0.6908	4.189187	6.591569	C	3.127282	-3.71206	2.386978
H	2.556081	4.373894	2.724333	C	1.961553	-3.10695	1.93033
H	1.967756	5.438862	4.867551	C	-1.54324	-3.25207	1.840755
C	-2.36098	-1.41675	4.49424	C	-2.49129	-3.17378	0.817027
C	-1.16919	-0.96378	3.914579	C	-3.33933	-4.24915	0.55672
C	-0.45297	0.01786	4.591325	C	-3.23625	-5.41351	1.312851
C	-0.89416	0.586522	5.787541	C	-2.28712	-5.50215	2.331473
C	-2.08479	0.127669	6.344594	C	-1.44473	-4.42661	2.596293
C	-2.80383	-0.8776	5.699424	C	2.392716	2.65499	-0.0405
C	1.03767	1.769191	4.245646	C	1.724944	2.908049	-1.24041
C	0.643466	2.376176	5.442411	C	2.244693	3.824014	-2.15532
C	0.985117	3.705787	5.664468	C	3.436503	4.485026	-1.8762
C	1.697118	4.403407	4.689805	C	4.114797	4.229943	-0.68305
C	2.038927	3.799408	3.484517	C	3.597401	3.317599	0.229322
C	1.703024	2.459809	3.236249	C	3.181692	0.503608	1.637866
O	0.759889	0.427741	4.077571	C	5.397269	-1.09443	2.264702
P	-0.52927	-1.4755	2.265855	C	5.091188	-0.81692	0.933328
P	1.902528	1.644335	1.590051	C	3.991332	-0.02513	0.623278
H	-4.4075	-5.3687	0.68338	H	0.630858	-2.18616	4.916018
H	3.666157	5.998827	-1.65845	H	2.698892	-3.24289	5.719995
H	6.253729	-2.04183	2.010212	H	2.889331	0.62023	3.774331
H	4.076389	-4.64685	3.554481	H	4.82688	-0.78785	4.316751
N	-0.09205	1.59364	6.350006	C	1.046382	-2.54266	2.827388
H	-0.5212	2.110265	7.108179	C	1.327149	-2.60378	4.195703
H	-1.40915	1.822807	-0.2919	C	2.497731	-3.20753	4.653523
C	1.050424	-0.64556	-0.38946	C	3.400711	-3.76148	3.752346
O	1.533255	-1.14543	-1.30687	C	3.498754	0.226227	2.969134
Rh	0.090226	0.321823	0.940974	C	4.600451	-0.57081	3.277315

H	-2.9228	-2.45704	3.86634	H	-2.60045	2.607361	3.039751
H	-2.80799	0.712616	6.773394	H	1.359729	1.741419	4.463445
H	-3.8772	-1.32335	5.843667	H	2.060889	1.155986	2.175059
H	-0.16713	4.541479	5.584697	H	1.451322	6.074841	-0.44114
H	1.742515	4.383399	1.743563	H	1.250929	3.856884	0.636155
H	0.910631	5.677482	3.654677	C	-3.64913	-4.64919	-2.2328
C	-2.43101	-1.58202	4.277702	C	-2.72833	-3.67243	-1.85253
C	-1.25824	-1.0985	3.683215	C	-1.68792	-1.77219	1.580561
C	-0.65326	0.014391	4.257038	C	-3.05337	-1.4827	1.714485
C	-1.19896	0.690967	5.349682	C	-3.56116	-1.00202	2.917801
C	-2.36928	0.200501	5.92194	C	-2.71243	-0.80676	4.004593
C	-2.9692	-0.94038	5.38986	C	-1.35591	-1.09309	3.879768
C	0.644347	1.851552	3.691457	C	-0.84271	-1.56848	2.675632
C	0.123465	2.576766	4.765225	C	0.127609	1.547529	1.298696
C	0.23693	3.963891	4.758053	C	-1.1847	1.96135	1.56137
C	0.845329	4.595279	3.676203	C	-1.57828	2.292453	2.853412
C	1.32959	3.860729	2.597848	C	-0.66364	2.215675	3.902116
C	1.238183	2.462573	2.588001	C	0.641361	1.80217	3.651378
O	0.540913	0.472142	3.735242	C	1.036533	1.467135	2.357179
P	-0.49394	-1.77418	2.152413	C	0.673497	2.845743	-1.18
P	1.67314	1.428836	1.1229	C	0.903434	5.353123	-2.39598
H	-3.89043	-6.25504	1.106946	C	1.162185	5.211866	-1.03283
H	3.8436	5.195625	-2.58885	C	1.048302	3.964346	-0.42634
H	6.250834	-1.71936	2.509662	H	-2.51635	-4.39359	1.463038
H	4.315397	-4.22503	4.109455	H	-4.14392	-6.12743	0.785851
N	-0.52039	1.843955	5.782949	H	0.095384	2.130056	-3.12304
H	-1.03244	2.410436	6.448767	H	0.316518	4.352583	-4.21063
H	-0.56057	3.006503	0.458822	C	-2.30813	-3.57668	-0.52422
C	1.21406	-1.14514	-0.55579	C	-2.82955	-4.46753	0.424595
O	1.804001	-1.68886	-1.38017	C	-3.74629	-5.44149	0.044469
Rh	0.045825	-0.09981	0.545683	C	-4.15711	-5.53306	-1.28638
C	-1.4477	1.18384	1.29873	C	0.409328	2.996564	-2.54455
C	-1.54397	2.5412	0.591048	C	0.527761	4.245426	-3.15137
C	-2.40457	3.518343	1.38053	H	-0.39287	-5.28913	-0.03363
O	-2.75163	4.685942	0.6111	H	1.78291	-6.43606	0.155114
C	-1.81251	5.632775	0.484529	H	3.256549	2.443145	-1.20509
C	-2.32135	6.796102	-0.32882	H	5.543011	1.501198	-1.12207
O	-0.7146	5.571179	0.986464	C	0.505118	-4.71266	0.157985
H	-1.35899	1.362774	2.374423	C	0.428118	-3.31796	0.286065
H	-2.40328	0.648436	1.168868	C	1.611675	-2.63153	0.529523
H	-1.9789	2.431359	-0.41152	C	2.861988	-3.25355	0.57508
H	-1.88059	3.829629	2.291703	C	2.915189	-4.6374	0.442474
H	-3.36559	3.070846	1.645991	C	1.734794	-5.35673	0.253365
H	-2.92877	6.446185	-1.16471	C	2.602199	-0.55587	0.20081
H	-1.47673	7.384531	-0.68472	C	3.876781	-1.12304	0.225636
H	-2.95267	7.42453	0.30663	C	4.940939	-0.36723	-0.25902
C	-1.21874	0.329832	-1.84866	C	4.706697	0.916723	-0.75335
O	-2.05411	-0.41318	-1.65031	C	3.421608	1.451323	-0.7975
				C	2.336708	0.701257	-0.3252
5l*				O	1.54773	-1.26773	0.735136
				P	-1.06985	-2.29879	-0.06906
H	-3.97138	-4.71185	-3.26738	P	0.55867	1.163901	-0.44817
H	-2.3353	-2.9709	-2.58404	H	0.98919	6.327852	-2.86609
H	-3.72701	-1.64767	0.877626	H	-4.87661	-6.29089	-1.58046
H	-4.62139	-0.78527	3.004263	H	-0.97	2.472893	4.911554
H	-0.68665	-0.93868	4.720443	H	-3.10635	-0.43099	4.944055
H	0.218664	-1.77674	2.597358	Rh	-0.71395	-0.57434	-1.83343
H	-1.89827	2.042866	0.746302	H	-3.0349	1.653605	-2.841

C	0.957482	-1.3908	-2.39688	H	1.51708	1.361739	-3.51854
O	1.926863	-1.89292	-2.73702	H	1.788719	3.223781	-5.1168
C	-2.59766	0.227297	-1.25194	C	-2.21395	-3.78856	-0.84364
C	-2.93422	1.632462	-1.74877	C	-2.9434	-4.51429	0.107479
C	-4.22608	2.136177	-1.13032	C	-3.76086	-5.56639	-0.29157
O	-4.472	3.463943	-1.62001	C	-3.85988	-5.90042	-1.64297
C	-5.53958	4.089976	-1.10679	C	1.217469	2.367856	-3.23312
C	-5.69344	5.470121	-1.69118	C	1.368431	3.41591	-4.13464
O	-6.27074	3.593307	-0.28257	H	-0.3743	-5.32428	0.24723
H	-3.39733	-0.46366	-1.55568	H	1.767893	-6.30824	0.994404
H	-2.59391	0.231231	-0.15609	H	3.2113	2.433686	-1.27538
H	-2.13229	2.340728	-1.50233	H	5.465478	1.639188	-0.63051
H	-4.16446	2.168035	-0.03572	C	0.459852	-4.67966	0.502139
H	-5.07619	1.496658	-1.39305	C	0.327087	-3.28839	0.395194
H	-5.82057	5.398656	-2.77432	C	1.420809	-2.50219	0.733462
H	-4.78926	6.053953	-1.50207	C	2.656989	-3.03983	1.100551
H	-6.55743	5.95985	-1.24495	C	2.772061	-4.42358	1.194352
H	5.944399	-0.78244	-0.25118	C	1.669396	-5.23104	0.912694
H	3.874243	-5.14567	0.48012	C	2.382724	-0.42961	0.310735
N	3.987549	-2.4271	0.737164	C	3.646683	-0.91356	0.656738
H	4.879235	-2.87944	0.575971	C	4.761215	-0.1568	0.307261
C	-1.45378	-0.42013	-3.5299	C	4.591692	1.05054	-0.37167
O	-1.97563	-0.34677	-4.55564	C	3.325239	1.501384	-0.73197
				C	2.191219	0.746535	-0.40152
TS5l				O	1.266716	-1.13231	0.718936
305.79i				P	-1.09924	-2.41572	-0.36525
H	-3.22082	-5.43517	-3.6455	P	0.450581	1.136013	-0.86103
H	-1.76301	-3.55098	-2.93206	H	1.070232	5.51976	-4.49009
H	-3.81111	-1.4604	-0.15521	H	-4.5019	-6.71919	-1.9525
H	-5.056	-0.21402	1.568074	H	-1.64686	3.716992	3.794808
H	-1.6916	-0.52758	4.222241	H	-4.01236	0.231298	3.779249
H	-0.41408	-1.71005	2.479623	Rh	-0.47534	-0.91568	-2.29171
H	-2.21695	1.351029	0.260144	H	-2.80951	1.997663	-3.5627
H	-3.15458	2.524045	2.209921	C	1.105932	-1.84012	-2.62857
H	0.803125	3.729626	3.392828	O	2.093468	-2.388	-2.84707
H	1.739593	2.598864	1.404846	C	-2.57526	-0.0301	-2.81393
H	0.099713	5.934945	-2.24406	C	-2.79776	1.463746	-2.60631
H	-0.14261	4.084914	-0.63129	C	-4.08318	1.719777	-1.83273
C	-3.14117	-5.18122	-2.59328	O	-4.07794	3.085689	-1.38686
C	-2.32087	-4.12567	-2.19581	C	-4.51211	3.327385	-0.14224
C	-2.01285	-1.65255	1.031312	C	-4.26357	4.759078	0.248987
C	-3.33092	-1.23467	0.794538	O	-5.00238	2.487808	0.579265
C	-4.04644	-0.55381	1.774727	H	-3.16341	-0.43034	-3.64163
C	-3.4571	-0.30068	3.012879	H	-2.88399	-0.5844	-1.92158
C	-2.15484	-0.72425	3.260382	H	-1.98109	1.899743	-2.02149
C	-1.43096	-1.39203	2.274047	H	-4.14534	1.068961	-0.95542
C	-0.17529	1.916264	0.683196	H	-4.97684	1.559097	-2.44456
C	-1.55215	1.897726	0.926973	H	-4.49484	5.432947	-0.57745
C	-2.08268	2.551413	2.039211	H	-3.2004	4.865811	0.489112
C	-1.2363	3.213399	2.924894	H	-4.85708	5.00548	1.128491
C	0.14003	3.220281	2.700256	H	5.754603	-0.51032	0.567578
C	0.667752	2.57932	1.583412	H	3.721855	-4.86485	1.481754
C	0.680904	2.59527	-1.95769	N	3.704494	-2.13822	1.342698
C	0.964664	4.703474	-3.78248	H	4.625371	-2.55379	1.41158
C	0.419721	4.935796	-2.52326	C	-0.90694	-0.17631	-3.89994
C	0.282276	3.889567	-1.6115	O	-0.94841	0.273904	-4.97639
H	-2.87078	-4.25073	1.159734				
H	-4.32347	-6.1245	0.450164	6l*			

H	-1.09303	-6.66165	-3.40658
H	-0.22163	-4.4887	-2.61591
H	-3.59183	-1.93914	-0.92123
H	-5.29531	-0.7593	0.432135
H	-2.63374	-0.79651	3.805586
H	-0.92907	-1.96806	2.459193
H	-2.17036	0.792894	0.183166
H	-3.1943	2.030406	2.061546
H	0.534259	4.055825	2.758881
H	1.547243	2.84926	0.854447
H	0.697363	5.623847	-2.79502
H	0.138436	3.933366	-1.09138
C	-1.54671	-6.18031	-2.5462
C	-1.05868	-4.95514	-2.1017
C	-2.14213	-2.03024	0.677234
C	-3.38132	-1.68523	0.116086
C	-4.34057	-1.02337	0.876845
C	-4.07274	-0.70156	2.208169
C	-2.84775	-1.04834	2.771604
C	-1.88402	-1.70964	2.011147
C	-0.25494	1.765355	0.366893
C	-1.58133	1.526402	0.73209
C	-2.15655	2.213558	1.801199
C	-1.39945	3.130538	2.524607
C	-0.06325	3.352848	2.186924
C	0.506705	2.672271	1.116232
C	0.790288	2.262703	-2.29488
C	1.429172	4.186643	-4.22125
C	0.882265	4.574341	-3.00154
C	0.568709	3.61753	-2.03713
H	-3.1541	-4.45589	0.52976
H	-4.0354	-6.61936	-0.27579
H	1.445487	0.820705	-3.75663
H	2.053706	2.524584	-5.44338
C	-1.63445	-4.32023	-0.99519
C	-2.7059	-4.93208	-0.33749
C	-3.19999	-6.1542	-0.78962
C	-2.62232	-6.77878	-1.8928
C	1.315733	1.877796	-3.53463
C	1.647085	2.835335	-4.48644
H	-0.11743	-5.46857	0.732615
H	1.900213	-6.15666	1.984863
H	3.209539	2.109956	-1.56755
H	5.395704	1.567939	-0.55492
C	0.62121	-4.72844	1.021318
C	0.435351	-3.38204	0.674155
C	1.396882	-2.47011	1.08095
C	2.586663	-2.85104	1.707259
C	2.759473	-4.19148	2.03677
C	1.763111	-5.11493	1.714806
C	2.292249	-0.44611	0.437846
C	3.52262	-0.77824	1.0125
C	4.646098	-0.04514	0.643968
C	4.517849	0.994415	-0.27689
C	3.287127	1.300555	-0.85003
C	2.145749	0.564945	-0.49978
O	1.167697	-1.12867	0.854812
P	-0.87848	-2.74271	-0.44383
P	0.435356	0.907674	-1.10759
H	1.674575	4.933849	-4.96948
H	-3.01053	-7.7298	-2.24351
H	-1.84582	3.664924	3.358093
H	-4.81811	-0.18036	2.800969
Rh	-0.86207	-0.93251	-2.20755
H	-2.87901	3.050091	-3.11682
C	-1.11606	-2.05352	-3.65189
O	-1.17115	-2.70679	-4.59754
C	-3.03538	0.930358	-2.68525
C	-2.89522	2.389999	-2.24446
C	-3.9855	2.793071	-1.27071
O	-3.60071	4.050764	-0.69926
C	-4.18365	4.384389	0.460553
C	-3.60938	5.667029	1.000778
O	-5.04404	3.721698	0.992132
H	-3.84142	0.815967	-3.42075
H	-3.27888	0.298768	-1.82214
H	-1.93838	2.528528	-1.73078
H	-4.08754	2.057752	-0.46513
H	-4.96338	2.901224	-1.75278
H	-3.70217	6.461399	0.256414
H	-2.54456	5.520673	1.204071
H	-4.13083	5.943983	1.91579
H	5.61236	-0.28614	1.077527
H	3.670261	-4.51102	2.534613
N	3.534879	-1.84106	1.931698
H	4.454496	-2.16293	2.207976
C	-1.72024	0.449348	-3.34359
O	-1.39024	0.931274	-4.40459

TS6l
962.40i

H	-2.87175	-5.52463	-3.16972
H	-1.24107	-3.76592	-2.58229
H	-3.25644	-0.54492	-0.23293
H	-4.42435	0.817261	1.461778
H	-1.31826	-0.10943	4.294649
H	-0.16015	-1.47394	2.594876
H	-1.3857	2.224581	-0.22018
H	-2.20635	3.295379	1.844676
H	1.57171	2.535581	3.743456
H	2.393451	1.467114	1.689795
H	2.71784	5.714007	-1.70251
H	2.175264	3.734101	-0.32268
C	-2.96507	-4.99798	-2.22527
C	-2.04919	-4.00228	-1.89585
C	-1.63866	-1.10786	1.066227
C	-2.83416	-0.44605	0.763417
C	-3.50054	0.30724	1.722434
C	-2.95514	0.418952	3.00152
C	-1.75212	-0.21222	3.304692
C	-1.09297	-0.97821	2.343506
C	0.557361	1.765407	0.587778
C	-0.73998	2.288367	0.648856
C	-1.1949	2.901534	1.811974
C	-0.36832	2.995237	2.929086

C	0.918743	2.469034	2.878501	H	6.196873	-1.27752	0.365672
C	1.381281	1.858125	1.714636	H	3.508424	-5.16952	1.686741
C	1.495626	2.552696	-1.99584	N	3.941732	-2.48009	1.37016
C	2.097975	4.79392	-3.55011	H	4.784989	-3.03515	1.451278
C	2.316099	4.822126	-2.17313	C	-1.65541	0.477881	-2.50346
C	2.012309	3.707484	-1.39731	O	-1.62371	1.67873	-2.28557
H	-3.27576	-3.12118	1.149356	H	1.419703	-1.65555	-2.0873
H	-4.91048	-4.87154	0.555428	H	1.474409	-0.76369	-2.93782
H	0.846151	1.64173	-3.8277				
H	1.392744	3.630133	-5.21851	7l*			
C	-2.15176	-3.31191	-0.68262				
C	-3.18712	-3.64	0.199742	H	-2.37717	-5.86885	-2.92549
C	-4.10848	-4.62986	-0.13497	H	-0.77801	-4.1587	-2.1595
C	-4.00071	-5.30875	-1.34688	H	-3.16886	-0.35928	-0.22227
C	1.271543	2.532861	-3.37394	H	-4.37476	0.917256	1.513251
C	1.574654	3.650815	-4.14854	H	-1.4384	-0.32059	4.410137
H	-0.62676	-5.00807	0.505718	H	-0.27109	-1.63954	2.677803
H	1.329407	-6.2868	1.311346	H	-1.37413	2.036593	-0.07732
H	4.058649	1.884451	-1.63044	H	-2.099	3.093313	2.031659
H	6.187038	0.779369	-1.01155	H	1.872133	2.661267	3.612723
C	0.305363	-4.4959	0.719368	H	2.600134	1.619986	1.511142
C	0.405056	-3.11165	0.524319	H	1.518982	5.910319	-1.97131
C	1.612766	-2.50301	0.833973	H	0.980892	3.961878	-0.56204
C	2.753433	-3.21443	1.210769	C	-2.66951	-5.17146	-2.14695
C	2.640544	-4.5912	1.383752	C	-1.77301	-4.19772	-1.72191
C	1.412135	-5.21548	1.161793	C	-1.65687	-1.10238	1.114233
C	2.876473	-0.66054	0.246202	C	-2.80127	-0.35954	0.80031
C	4.058462	-1.32041	0.583405	C	-3.48207	0.355766	1.778362
C	5.259131	-0.78846	0.118634	C	-2.99103	0.360651	3.084691
C	5.245975	0.369306	-0.66051	C	-1.83016	-0.34083	3.397896
C	4.050415	0.995807	-1.00793	C	-1.16535	-1.08	2.419393
C	2.834722	0.468153	-0.55901	C	0.655981	1.739375	0.571521
O	1.685643	-1.12965	0.760435	C	-0.66747	2.162884	0.734631
P	-0.86472	-2.05668	-0.29362	C	-1.06832	2.770682	1.921484
P	1.147311	1.05057	-1.00615	C	-0.16109	2.949396	2.962306
H	2.330337	5.665848	-4.15379	C	1.155732	2.524581	2.808582
H	-4.72144	-6.07806	-1.60546	C	1.56541	1.928675	1.618598
H	-0.7279	3.472024	3.836065	C	1.542863	2.512388	-2.05709
H	-3.46105	1.013522	3.756308	C	2.17188	4.728917	-3.64739
Rh	0.033433	-0.75468	-2.25579	C	1.67268	4.909132	-2.36142
H	-4.98273	0.472766	-3.61171	C	1.366335	3.807094	-1.56438
C	-0.48822	-1.6123	-3.82044	H	-3.68236	-2.70925	0.665416
O	-0.74378	-2.14929	-4.80305	H	-5.27718	-4.41563	-0.10886
C	-2.99083	-0.11027	-3.00623	H	2.19269	1.334981	-3.74537
C	-4.15294	0.882262	-3.02593	H	2.754864	3.288761	-5.1417
C	-4.65908	1.225393	-1.63864	C	-2.12717	-3.2878	-0.71509
O	-5.70004	2.201982	-1.7935	C	-3.39296	-3.38492	-0.13223
C	-6.2805	2.626653	-0.66539	C	-4.29522	-4.35602	-0.56751
C	-7.3346	3.663534	-0.94981	C	-3.93954	-5.24616	-1.57549
O	-5.98231	2.219962	0.434355	C	2.044361	2.337723	-3.35299
H	-2.79955	-0.4644	-4.02776	C	2.363728	3.438971	-4.14038
H	-3.22367	-1.01749	-2.42935	H	-0.68388	-4.96205	0.657863
H	-3.82357	1.805426	-3.51195	H	1.256565	-6.2475	1.485597
H	-3.86607	1.64401	-1.01079	H	4.106757	1.833669	-1.69895
H	-5.0775	0.348971	-1.12854	H	6.225283	0.723689	-1.05972
H	-8.07669	3.257234	-1.6412	C	0.264521	-4.4636	0.825246
H	-6.87368	4.530426	-1.43005	C	0.395195	-3.09303	0.559016
H	-7.81164	3.962575	-0.01797	C	1.618718	-2.49972	0.825244

C	2.750837	-3.21858	1.218064	C	-3.6499	-3.64785	-2.62237
C	2.609067	-4.58273	1.452304	C	-2.54948	-2.92948	-2.16141
C	1.36179	-5.18725	1.281665	C	-1.67662	-0.42055	1.051338
C	2.904284	-0.69239	0.188625	C	-2.85125	0.322606	0.880445
C	4.079115	-1.35607	0.537784	C	-3.35822	1.100314	1.915935
C	5.284454	-0.83523	0.071584	C	-2.67904	1.169074	3.130252
C	5.280393	0.31771	-0.71438	C	-1.49708	0.452882	3.300483
C	4.089432	0.946405	-1.07514	C	-0.99828	-0.34278	2.271482
C	2.870497	0.420148	-0.63646	C	1.051368	2.069332	0.530926
O	1.708792	-1.1331	0.713821	C	-0.21712	2.659806	0.543373
P	-0.86828	-2.02651	-0.25076	C	-0.64539	3.365655	1.664005
P	1.180783	1.025151	-1.04236	C	0.176378	3.471327	2.784059
H	2.409811	5.588872	-4.26558	C	1.431923	2.86897	2.782583
H	-4.6446	-5.99964	-1.91178	C	1.871642	2.172463	1.658686
H	-0.47841	3.418085	3.888955	C	2.321858	2.61277	-1.98699
H	-3.50746	0.925875	3.854674	C	3.547452	4.605611	-3.52184
Rh	-0.07608	-0.69377	-2.20114	C	3.309524	4.815263	-2.16545
H	-5.08003	0.581982	-3.5595	C	2.704173	3.822311	-1.3982
C	-0.62594	-1.8802	-3.52358	H	-3.68704	-2.12493	0.937734
O	-0.88525	-2.56189	-4.40514	H	-5.64136	-3.37227	0.114298
C	-3.08245	0.006003	-2.9529	H	2.255548	1.473287	-3.81106
C	-4.25549	0.985355	-2.96207	H	3.355558	3.231989	-5.17038
C	-4.76218	1.281668	-1.56434	C	-2.54988	-2.35792	-0.88309
O	-5.84791	2.213484	-1.68284	C	-3.6683	-2.54559	-0.0622
C	-6.40428	2.614437	-0.53448	C	-4.77481	-3.25243	-0.52804
C	-7.51317	3.603033	-0.77933	C	-4.77127	-3.79895	-1.80969
O	-6.04782	2.223511	0.553908	C	2.558978	2.41071	-3.35148
H	-2.85091	-0.30662	-3.98096	C	3.174711	3.400278	-4.11332
H	-3.3255	-0.92555	-2.41891	H	-1.39844	-4.38402	0.264921
H	-3.93423	1.924641	-3.4218	H	0.252388	-6.04354	1.063751
H	-3.97898	1.723969	-0.94071	H	4.633939	1.54984	-1.39562
H	-5.13282	0.377051	-1.06544	H	6.482918	0.070324	-0.6691
H	-8.26194	3.162728	-1.4421	C	-0.39271	-4.06939	0.523014
H	-7.10963	4.488401	-1.27714	C	-0.02705	-2.72259	0.394316
H	-7.96773	3.882557	0.169629	C	1.265457	-2.36825	0.752861
H	6.218843	-1.32566	0.328302	C	2.231502	-3.2949	1.151909
H	3.467739	-5.16729	1.769168	C	1.85371	-4.63003	1.260381
N	3.952758	-2.50235	1.341416	C	0.540815	-5.00234	0.96521
H	4.788814	-3.06629	1.432995	C	2.887812	-0.77887	0.314594
C	-1.7633	0.576373	-2.3856	C	3.903511	-1.6564	0.690775
O	-1.73474	1.778542	-2.15909	C	5.210429	-1.33875	0.326559
H	1.315142	-1.54765	-2.17556	C	5.460768	-0.17412	-0.39989
H	0.469777	0.087952	-3.41755	C	4.423316	0.664284	-0.80478
				C	3.104206	0.348109	-0.46325
TS7l				O	1.600701	-1.03179	0.735847
742.11i				P	-1.05922	-1.4043	-0.37165
H	-3.63264	-4.07936	-3.61825	P	1.588289	1.236105	-1.01452
H	-1.68022	-2.80853	-2.80194	H	4.019098	5.381096	-4.11732
H	-3.40976	0.256533	-0.04663	H	-5.6374	-4.34373	-2.17197
H	-4.28951	1.637498	1.765448	H	-0.16477	4.014419	3.660481
H	-0.95719	0.507727	4.240865	H	-3.06766	1.779168	3.940199
H	-0.08319	-0.90257	2.43003	Rh	0.138894	-0.22939	-2.30352
H	-0.86817	2.558545	-0.32137	H	-4.57327	0.443338	-4.55235
H	-1.63297	3.816274	1.667014	C	0.158147	-1.30066	-3.81564
H	2.074688	2.943124	3.654533	O	0.235623	-1.96318	-4.75286
H	2.858605	1.718557	1.66064	C	-2.57036	0.355594	-3.7702
H	3.594805	5.753965	-1.70089	C	-4.00201	0.886951	-3.73008
H	2.526348	3.991685	-0.34029	C	-4.65754	0.530533	-2.4101

O	-6.06362	0.799855	-2.49481
C	-6.71904	0.738832	-1.32624
C	-8.18421	1.03595	-1.50556
O	-6.18156	0.476945	-0.27479
H	-2.09608	0.567198	-4.73858
H	-2.56832	-0.73548	-3.66635
H	-4.01206	1.973494	-3.86076
H	-4.23646	1.131324	-1.60496
H	-4.51681	-0.53209	-2.16564
H	-8.62334	0.317276	-2.20196
H	-8.30818	2.032625	-1.93627
H	-8.68738	0.978908	-0.54177
H	6.024534	-1.99929	0.610176
H	2.582192	-5.37253	1.573293
N	3.524047	-2.80419	1.408478
H	4.242556	-3.51093	1.506468
C	-1.64212	0.943347	-2.70355
O	-2.00313	1.887356	-2.03361
H	1.33416	-1.25069	-1.9789
H	-0.13886	1.04047	-3.2388
l*			
H	-2.54458	-5.56967	-3.95353
H	-1.27461	-3.60935	-3.10782
H	-3.90479	-2.37849	-0.19279
H	-5.40845	-1.08779	1.259092
H	-2.01814	0.672323	3.217237
H	-0.50606	-0.61728	1.777356
H	-1.1019	2.729111	-1.50948
H	-2.46698	3.99448	0.118309
H	0.110418	2.665673	3.290603
H	1.449399	1.377106	1.676063
H	2.66329	5.488916	-2.59796
H	1.919279	3.772861	-0.98199
C	-2.58603	-5.3132	-2.89962
C	-1.87349	-4.2098	-2.42802
C	-2.08773	-1.61838	0.699133
C	-3.47887	-1.72469	0.562155
C	-4.33355	-0.99119	1.381708
C	-3.81752	-0.12586	2.343588
C	-2.43644	-0.00647	2.480844
C	-1.57808	-0.74294	1.666943
C	0.247253	1.934969	-0.02898
C	-0.85337	2.69298	-0.45005
C	-1.61152	3.41864	0.463464
C	-1.27519	3.40105	1.817007
C	-0.16859	2.670235	2.240956
C	0.58872	1.939082	1.325788
C	1.625017	2.248636	-2.48217
C	2.463287	4.19377	-4.30952
C	2.393641	4.497857	-2.94951
C	1.975058	3.531874	-2.04061
H	-2.72972	-4.38208	0.855781
H	-3.98527	-6.33592	0.021119
H	1.40876	0.963368	-4.18859
H	2.158449	2.684159	-5.81384
C	-1.91253	-3.86306	-1.0755
C	-2.68337	-4.64247	-0.19885
C	-3.39343	-5.74176	-0.6681
C	-3.34576	-6.07867	-2.02194
C	1.693571	1.954273	-3.84568
C	2.113653	2.92325	-4.75606
H	-0.43082	-5.22771	0.550913
H	1.453734	-6.19379	1.791851
H	4.003919	1.912626	-1.45069
H	6.036344	1.08334	-0.31492
C	0.378837	-4.58337	0.869669
C	0.352473	-3.21525	0.558675
C	1.434285	-2.44792	0.978441
C	2.543786	-2.9943	1.632842
C	2.544597	-4.35208	1.931464
C	1.453037	-5.13402	1.559905
C	2.650605	-0.54466	0.427611
C	3.789749	-1.04562	1.060236
C	5.017172	-0.45056	0.784265
C	5.077266	0.620729	-0.10716
C	3.933418	1.092755	-0.74434
C	2.690506	0.500063	-0.48543
O	1.422941	-1.08368	0.759274
P	-0.93208	-2.40955	-0.51157
P	1.104261	0.926403	-1.3155
H	2.785451	4.950261	-5.01843
H	-3.90225	-6.93609	-2.3874
H	-1.86832	3.960245	2.533874
H	-4.48653	0.470805	2.95445
Rh	0.178754	-1.14921	-2.36508
H	-4.61288	1.87775	-2.56786
C	0.698869	-1.76615	-4.0172
O	1.065249	-2.17437	-5.03509
C	-3.0249	0.579631	-1.8691
C	-3.86594	1.846151	-1.768
C	-4.53563	1.910147	-0.41047
O	-5.14547	3.201134	-0.27844
C	-5.73309	3.435277	0.906339
C	-6.31394	4.823224	0.961616
O	-5.77228	2.620921	1.798084
H	-3.64124	-0.32767	-1.91564
H	-2.40014	0.455505	-0.96804
H	-3.22981	2.726562	-1.89836
H	-3.80551	1.777348	0.395249
H	-5.3011	1.136217	-0.29012
H	-7.01755	4.964088	0.137756
H	-5.51506	5.560125	0.84374
H	-6.81717	4.968939	1.915952
H	5.916943	-0.82449	1.263884
H	3.396461	-4.79111	2.442596
N	3.606272	-2.12621	1.937457
H	4.457591	-2.58281	2.241537
C	-2.07482	0.561859	-3.03123
O	-1.80012	1.508732	-3.72496
H	1.438863	-1.88712	-1.96012
H	-1.62137	-0.44761	-3.2588
TS3b			
705.53i			

H	-4.67035	-3.04663	-2.44165	P	0.901683	1.819099	0.094929
H	-2.72264	-1.60568	-1.93343	H	1.312948	7.349987	-1.37848
H	-3.10745	-0.48573	2.219568	H	-5.53053	-4.62223	-0.72512
H	-3.23216	-0.22324	4.663653	H	0.93456	2.227704	5.796036
H	0.877875	-1.42454	4.998124	H	-1.23797	-0.69718	6.07325
H	1.000064	-1.71754	2.562316	Rh	-0.7973	0.690482	-1.00517
H	-1.1627	2.109444	2.046101	H	-0.81366	2.046377	-1.86246
H	-1.18739	2.368814	4.513783	C	0.166815	-0.29176	-2.43535
H	3.074263	1.835217	4.601795	O	1.092955	-0.69683	-2.98659
H	3.103104	1.635343	2.138725	C	-2.33431	2.286086	-1.67303
H	1.303459	6.724572	1.023236	C	-2.98428	1.071188	-1.36956
H	1.15186	4.359243	1.693267	C	-3.79785	0.957756	-0.1157
C	-4.19252	-3.11141	-1.46998	O	-5.10422	1.57077	-0.27082
C	-3.10522	-2.29	-1.18195	C	-5.98935	0.868022	-0.99324
C	-1.04536	-1.1242	2.210848	C	-7.30195	1.602484	-1.10309
C	-2.22737	-0.68711	2.824322	O	-5.7542	-0.20841	-1.48799
C	-2.30138	-0.54395	4.205219	H	-2.34368	3.094026	-0.94353
C	-1.18515	-0.81333	4.994903	H	-2.31671	2.623514	-2.70756
C	-0.00068	-1.22412	4.392627	H	-3.3448	0.470961	-2.19949
C	0.069963	-1.38612	3.009956	H	-3.33627	1.510229	0.70655
C	0.97098	1.873969	1.92984	H	-3.95699	-0.08507	0.169324
C	-0.23357	2.073736	2.612095	H	-7.1468	2.550542	-1.62473
C	-0.24595	2.216218	3.995344	H	-7.68467	1.833122	-0.10606
C	0.944856	2.130706	4.714464	H	-8.01537	0.987892	-1.6499
C	2.144866	1.908183	4.045082	H	5.823993	-0.55	-1.61851
C	2.160546	1.787879	2.656809	H	3.270654	-4.72227	-1.2197
C	1.043033	3.612013	-0.32689	N	3.955463	-2.1858	-0.42808
C	1.240608	6.30708	-1.08604	H	4.669614	-2.67686	-0.95127
C	1.234112	5.956076	0.259439				
C	1.14438	4.616735	0.638898	4b*			
H	-2.51768	-3.2752	2.01748				
H	-4.44028	-4.73352	1.502796	H	-3.90518	-3.6811	-2.64311
H	0.981796	3.204623	-2.44473	H	-2.06131	-2.17587	-1.98537
H	1.165321	5.573788	-3.11176	H	-2.99133	0.048763	2.299847
C	-2.50141	-2.32706	0.077667	H	-3.11558	0.277792	4.748346
C	-2.98719	-3.22188	1.039635	H	0.675776	-1.70641	5.125964
C	-4.0694	-4.04671	0.748146	H	0.772443	-2.00341	2.682868
C	-4.6775	-3.98795	-0.50485	H	-0.84935	2.377345	2.210969
C	1.048882	3.97689	-1.68127	H	-0.7684	2.424178	4.682189
C	1.154644	5.311162	-2.05836	H	3.389544	1.351059	4.567371
H	-0.92689	-4.22419	-0.42921	H	3.319992	1.326371	2.0997
H	0.964832	-5.62786	-1.1558	H	3.285062	6.353776	0.728715
H	3.507851	3.044362	-1.11661	H	3.077052	3.912901	1.048756
H	5.566485	1.900322	-1.86754	C	-3.77101	-3.41937	-1.59827
C	0.080807	-3.8252	-0.40155	C	-2.74222	-2.56151	-1.22945
C	0.304228	-2.51073	0.033332	C	-1.11088	-1.01743	2.316928
C	1.615862	-2.06352	0.054886	C	-2.1902	-0.35262	2.916381
C	2.695471	-2.81446	-0.41566	C	-2.2615	-0.21952	4.298689
C	2.450884	-4.11169	-0.85171	C	-1.23272	-0.71252	5.09994
C	1.148912	-4.61254	-0.82069	C	-0.13757	-1.33558	4.50992
C	2.818961	-0.10842	-0.14059	C	-0.07911	-1.49687	3.126357
C	3.937792	-0.79109	-0.61471	C	1.233297	1.863392	1.989684
C	4.934776	-0.0514	-1.24338	C	0.085318	2.165512	2.728941
C	4.778014	1.328061	-1.3898	C	0.129875	2.193098	4.11859
C	3.622046	1.97672	-0.96145	C	1.319309	1.900991	4.783552
C	2.600232	1.244058	-0.34398	C	2.461774	1.584591	4.054066
O	1.869905	-0.81145	0.568738	C	2.421637	1.568754	2.661114
P	-1.02467	-1.26544	0.373324	C	1.258576	3.745992	-0.1027

C	1.480119	6.515997	-0.43927	H	4.581817	-2.76864	-0.89889
C	2.446842	5.821724	0.289927				
C	2.331825	4.447702	0.464168	TS4b			
H	-3.2602	-2.51265	2.130572	40.01i			
H	-5.11102	-3.99222	1.46679	H	2.722033	-2.75531	-0.27479
H	-0.5605	3.919747	-1.23961	H	1.023578	-0.99944	0.165743
H	-0.36013	6.368481	-1.5453	H	-3.59862	0.305735	2.363904
C	-2.54781	-2.21568	0.114835	H	-5.70703	-0.74111	1.621671
C	-3.40621	-2.74414	1.080657	H	-3.53028	-4.21753	0.34511
C	-4.44868	-3.59117	0.705837	H	-1.41906	-3.17275	1.083428
C	-4.63239	-3.93109	-0.62982	H	1.037077	4.51179	1.265438
C	0.289121	4.451065	-0.81987	H	2.028602	6.643932	0.495957
C	0.400435	5.831927	-0.98698	H	5.945377	4.888514	0.686062
H	-1.0138	-4.15701	-0.06124	H	4.960727	2.768907	1.484663
H	0.829811	-5.65606	-0.69089	H	4.97195	-0.60929	-0.96596
H	3.618524	2.988224	-1.33325	H	3.352192	1.150414	-0.35961
H	5.577241	1.714127	-2.14772	C	2.149815	-2.77855	0.64742
C	-0.00468	-3.76715	-0.11685	C	1.199707	-1.78984	0.893223
C	0.241998	-2.41172	0.159056	C	-2.35907	-1.3588	1.767704
C	1.563293	-1.99176	0.119268	C	-3.57926	-0.68496	1.912686
C	2.617301	-2.80889	-0.30626	C	-4.76997	-1.27527	1.500558
C	2.343473	-4.13746	-0.60755	C	-4.75482	-2.5465	0.92835
C	1.037755	-4.61257	-0.47944	C	-3.54742	-3.22362	0.782841
C	2.835413	-0.09285	-0.19399	C	-2.35497	-2.6347	1.201695
C	3.910144	-0.84054	-0.67241	C	2.93032	3.495021	1.423855
C	4.906763	-0.17171	-1.3793	C	2.11479	4.597723	1.145997
C	4.796212	1.20319	-1.59468	C	2.672654	5.797172	0.71093
C	3.697793	1.925237	-1.13255	C	4.051101	5.903221	0.540981
C	2.688928	1.266788	-0.41909	C	4.870517	4.810104	0.815897
O	1.864374	-0.72217	0.555672	C	4.31461	3.613031	1.261177
P	-1.0879	-1.15662	0.483729	C	3.377295	0.683325	1.750358
P	1.083752	1.93414	0.159636	C	5.192789	-1.32963	1.054944
H	1.567995	7.589858	-0.57144	C	4.672139	-0.48939	0.070713
H	-5.44354	-4.59263	-0.91729	C	3.759167	0.501419	0.413482
H	1.35168	1.912323	5.868772	H	0.121816	-2.83346	3.946636
H	-1.28034	-0.59992	6.178747	H	1.832115	-4.56383	3.519937
Rh	-0.86034	0.949615	-0.91707	H	3.609283	-0.0429	3.769025
H	-2.99518	2.757196	-2.55051	H	5.191168	-1.82674	3.148788
C	-0.35046	1.64616	-2.51993	C	0.46031	-1.8042	2.080976
O	0.062756	1.947899	-3.55541	C	0.69336	-2.81079	3.022771
C	-3.2086	1.714071	-2.81948	C	1.654204	-3.7894	2.780235
C	-2.82939	0.75212	-1.68937	C	2.380772	-3.7763	1.59157
C	-3.64709	1.054523	-0.44086	C	3.897648	-0.1637	2.729567
O	-5.03008	1.40283	-0.71324	C	4.797071	-1.17035	2.379116
C	-5.85651	0.382459	-0.978	H	-3.01597	-1.50521	4.262912
C	-7.22696	0.885659	-1.35911	H	-1.36537	-0.23458	8.024368
O	-5.53731	-0.78132	-0.91948	H	-3.16937	-1.32358	6.715854
H	-4.27864	1.656207	-3.06104	H	2.286663	2.992634	7.750367
H	-2.65563	1.487794	-3.7357	H	3.49767	4.146009	3.78782
H	-3.06238	-0.26512	-2.0127	H	3.493116	4.530558	6.224256
H	-3.27229	1.941308	0.086028	C	-2.20619	-1.04724	4.818604
H	-3.65676	0.197735	0.238546	C	-1.07748	-0.55957	4.144514
H	-7.16095	1.433436	-2.30345	C	-0.0531	-0.03111	4.913395
H	-7.59822	1.578155	-0.60029	C	-0.13854	0.126061	6.298323
H	-7.90747	0.042541	-1.46853	C	-1.27754	-0.33969	6.947058
H	5.759119	-0.72376	-1.76424	C	-2.29203	-0.94266	6.20388
H	3.145163	-4.79403	-0.93276	C	1.701487	1.468573	4.78707
N	3.889882	-2.21867	-0.40464	C	1.65492	1.68646	6.16767

C	2.307703	2.801983	6.681319	C	2.307057	4.566042	0.955173
C	2.980923	3.665685	5.816282	C	2.966268	5.699601	0.481647
C	2.989551	3.447331	4.442694	C	4.356461	5.758955	0.502826
C	2.330906	2.331665	3.903845	C	5.09023	4.683407	1.002707
O	1.112507	0.334091	4.27315	C	4.434511	3.55218	1.478151
P	-0.82249	-0.51204	2.314619	C	3.334223	0.684507	1.838851
P	2.130193	1.984164	2.101976	C	5.209897	-1.29804	1.231376
H	-5.68129	-3.00678	0.60007	C	4.723704	-0.46671	0.223037
H	4.486312	6.834622	0.192617	C	3.782998	0.511926	0.522467
H	5.899899	-2.10886	0.78731	H	0.480653	-2.61457	4.138007
H	3.130522	-4.53898	1.403888	H	2.309866	-4.22616	3.724388
N	0.93949	0.757954	6.939345	H	3.463471	-0.04954	3.863716
H	0.775312	1.027802	7.901527	H	5.105066	-1.80678	3.31988
H	-1.75932	3.43857	-1.11555	C	0.546735	-1.77986	2.150362
C	0.614837	2.377918	-0.5176	C	0.965271	-2.6446	3.165306
O	1.022607	2.812648	-1.50705	C	1.991131	-3.55774	2.930176
Rh	-0.02617	1.538623	0.955755	C	2.60046	-3.61792	1.679203
C	-2.3712	2.883946	-0.39393	C	3.809221	-0.1625	2.840879
C	-1.81982	1.477092	-0.13638	C	4.742622	-1.15168	2.533664
C	-1.79108	0.721846	-1.44924	H	-3.09239	-1.57557	4.177559
O	-1.32681	-0.62494	-1.22846	H	-1.66198	-0.07702	7.949667
C	-1.27356	-1.39995	-2.31877	H	-3.38523	-1.2566	6.612693
C	-0.87844	-2.81457	-1.98183	H	2.036553	3.100585	7.77967
O	-1.53819	-1.00775	-3.43205	H	3.493874	4.150171	3.873442
H	-3.39654	2.849516	-0.79336	H	3.37444	4.574954	6.301785
H	-2.39623	3.47135	0.5301	C	-2.32619	-1.06885	4.75457
H	-2.5389	0.962866	0.506604	C	-1.17335	-0.59384	4.11371
H	-1.13524	1.198413	-2.18709	C	-0.21039	0.03007	4.895696
H	-2.79162	0.654336	-1.90111	C	-0.36382	0.23703	6.268166
H	-0.0549	-2.83	-1.26435	C	-1.52273	-0.22795	6.883252
H	-0.60581	-3.34067	-2.89605	C	-2.48949	-0.88727	6.124519
H	-1.73403	-3.31372	-1.51665	C	1.552561	1.547403	4.812176
C	-0.93474	3.116077	3.838804	C	1.444532	1.792197	6.18498
O	-0.55964	4.128005	3.496786	C	2.107899	2.893774	6.715821
				C	2.856275	3.72098	5.878875
5b*				C	2.930433	3.4792	4.511613
				C	2.261329	2.379032	3.95545
H	2.690981	-2.77152	-0.29969	O	0.965514	0.419408	4.282252
H	0.88533	-1.12253	0.129915	P	-0.86935	-0.61902	2.297999
H	-3.47599	-0.06311	1.132306	P	2.134375	2.037067	2.150544
H	-5.32056	-1.46739	0.297171	H	-5.16074	-3.94347	0.433
H	-3.15016	-4.9928	1.445793	H	4.869674	6.639268	0.128702
H	-1.29767	-3.58972	2.26582	H	5.943922	-2.06363	0.999088
H	1.22191	4.513209	0.926791	H	3.399735	-4.33016	1.497104
H	2.389766	6.531879	0.090536	N	0.672519	0.900868	6.943428
H	6.174726	4.724857	1.02151	H	0.453452	1.207236	7.883406
H	5.011879	2.718873	1.869374	H	-1.6624	4.055327	-0.62863
H	5.077312	-0.57925	-0.79728	C	0.567554	2.020917	-0.50114
H	3.416154	1.164495	-0.26709	O	0.97524	2.224807	-1.55901
C	2.199526	-2.74718	0.668059	Rh	-0.11607	1.907909	1.24409
C	1.186283	-1.82401	0.906973	C	-2.39323	3.598859	0.049417
C	-2.25167	-1.72157	1.756135	C	-2.03046	2.140943	0.351833
C	-3.40217	-1.14254	1.209619	C	-2.26985	1.36221	-0.93397
C	-4.44524	-1.93547	0.736341	O	-1.66959	0.054568	-0.90668
C	-4.35478	-3.32339	0.812616	C	-2.13649	-0.82338	-1.81002
C	-3.22508	-3.91193	1.377282	C	-1.43441	-2.15079	-1.70501
C	-2.18068	-3.1175	1.845524	O	-3.00637	-0.56242	-2.60825
C	3.035222	3.482708	1.456532	H	-3.38133	3.67868	-0.42955

H	-2.42122	4.206116	0.958291
H	-2.72973	1.775162	1.112937
H	-1.85089	1.899289	-1.79507
H	-3.34303	1.235548	-1.12335
H	-0.36856	-2.02122	-1.91389
H	-1.86994	-2.84404	-2.42337
H	-1.53036	-2.54643	-0.68994
C	-0.77562	3.031654	2.67599
O	-1.11488	3.808755	3.448079

TS5b
279.37i

H	3.181852	-2.75166	-0.36439
H	1.564574	-0.92657	0.058
H	-3.06116	0.63348	1.750913
H	-5.11435	-0.09963	0.587398
H	-3.13472	-3.71662	-0.62208
H	-1.09281	-3.00475	0.569618
H	1.449301	4.570724	0.801926
H	2.630096	6.61564	0.02003
H	6.333493	5.042013	1.526685
H	5.155058	3.014707	2.31279
H	5.298297	-0.37813	-0.69393
H	3.670374	1.393513	-0.15187
C	2.535943	-2.79655	0.506657
C	1.624434	-1.77086	0.741713
C	-1.93898	-1.14119	1.249393
C	-3.07994	-0.3268	1.237642
C	-4.23601	-0.73843	0.582938
C	-4.25906	-1.96176	-0.08725
C	-3.1259	-2.7704	-0.09086
C	-1.97184	-2.36726	0.579107
C	3.219657	3.671515	1.618107
C	2.517165	4.689126	0.969244
C	3.183359	5.83202	0.527859
C	4.554211	5.960936	0.729174
C	5.263289	4.946107	1.372921
C	4.600334	3.806074	1.814605
C	3.538274	0.866068	1.93986
C	5.367158	-1.15608	1.31631
C	4.930172	-0.28006	0.322788
C	4.01461	0.719799	0.629418
H	0.242801	-2.92776	3.626992
H	1.891684	-4.7268	3.227564
H	3.62511	0.08606	3.950891
H	5.218757	-1.70539	3.391788
C	0.787706	-1.81423	1.861794
C	0.889632	-2.88542	2.754846
C	1.814965	-3.90089	2.527103
C	2.634831	-3.86	1.401135
C	3.980152	-0.01203	2.930579
C	4.886932	-1.02354	2.615067
H	-2.80293	-1.60746	3.682036
H	-1.7098	-0.33603	7.647488
H	-3.28088	-1.47498	6.105292
H	1.800932	3.054047	7.880778
H	3.39796	4.359353	4.106877
H	3.094893	4.683505	6.534544
C	-2.09041	-1.13699	4.351367
C	-0.90213	-0.59855	3.838061
C	-0.00942	-0.03593	4.739292
C	-0.28223	0.10042	6.101764
C	-1.47572	-0.4229	6.590552
C	-2.35966	-1.05548	5.714817
C	1.661896	1.558841	4.849004
C	1.434709	1.748531	6.214925
C	1.960964	2.88574	6.81993
C	2.684049	3.801295	6.055301
C	2.863297	3.616268	4.687736
C	2.336411	2.479617	4.057821
O	1.21212	0.394247	4.264542
P	-0.43662	-0.46691	2.061868
P	2.31335	2.200281	2.23731
H	-5.15548	-2.27823	-0.61225
H	5.074005	6.847878	0.380523
H	6.076403	-1.94222	1.075704
H	3.353973	-4.65388	1.223866
N	0.676756	0.770675	6.880052
H	0.378886	1.017361	7.81611
H	-0.42868	3.542056	-2.031
C	0.842553	1.838746	-0.44095
O	1.439926	1.851562	-1.45074
Rh	0.258093	1.85443	1.294207
C	-1.24106	3.418618	-1.30549
C	-1.14777	2.070299	-0.60793
C	-1.35928	0.897977	-1.53908
O	-2.7391	0.91439	-1.96195
C	-3.15153	-0.16731	-2.63686
C	-4.61162	-0.06047	-2.99577
O	-2.42994	-1.09192	-2.92707
H	-2.19077	3.505662	-1.84782
H	-1.18157	4.2391	-0.58486
H	-1.91504	2.002338	0.169482
H	-1.16349	-0.06174	-1.05205
H	-0.72517	0.968834	-2.42972
H	-5.19559	0.205949	-2.11203
H	-4.95367	-1.00951	-3.4069
H	-4.74654	0.731692	-3.7378
C	-0.68518	2.907195	2.683264
O	-1.167	3.607722	3.451575

6b*

H	2.644214	-3.17319	-0.57164
H	0.88055	-1.48492	-0.21794
H	-3.02348	0.32305	0.721977
H	-5.15274	-0.74282	0.012627
H	-3.64345	-4.56732	1.264658
H	-1.53022	-3.49806	1.989921
H	0.95869	4.615378	1.162939
H	1.832342	6.831657	0.458915
H	5.847885	5.416568	1.036518
H	4.975019	3.216866	1.750972
H	5.457836	0.014219	-0.89383
H	3.833607	1.755938	-0.27132
C	2.211548	-3.04826	0.416013

C	1.212074	-2.10007	0.612424	C	0.190068	3.107986	-1.85851
C	-2.1475	-1.51368	1.41418	C	-0.41213	1.840511	-1.24769
C	-3.16924	-0.74755	0.848366	C	-0.78149	0.869034	-2.35461
C	-4.36308	-1.34676	0.448495	O	-1.20809	-0.36092	-1.75409
C	-4.53622	-2.72075	0.602811	C	-1.36288	-1.39029	-2.60738
C	-3.51305	-3.49563	1.151088	C	-1.72194	-2.65803	-1.88494
C	-2.32401	-2.89514	1.555445	O	-1.22558	-1.27741	-3.80219
C	2.905249	3.770768	1.497901	H	-0.50343	3.574339	-2.56649
C	2.031022	4.798767	1.133901	H	0.432493	3.8388	-1.08249
C	2.521933	6.042029	0.740249	H	-1.31148	2.095272	-0.66774
C	3.895864	6.26425	0.701373	H	0.095734	0.670829	-2.97646
C	4.776324	5.245386	1.064237	H	-1.58361	1.258705	-2.9904
C	4.28523	4.005805	1.46438	H	-0.96079	-2.88931	-1.1342
C	3.457016	0.949331	1.69434	H	-1.80233	-3.47097	-2.60537
C	5.289801	-1.04353	0.975346	H	-2.67021	-2.52479	-1.35675
C	4.988204	-0.01705	0.084341	C	-0.88576	2.489337	2.944409
C	4.072588	0.969419	0.437562	O	-1.48955	3.146374	3.661896
H	0.687679	-2.56277	3.943281				
H	2.467343	-4.23125	3.589353	TS6b			
H	3.286346	-0.13933	3.555523	251.13i			
H	4.895476	-1.87744	2.922213	H	2.840779	-2.46234	-0.62134
C	0.65224	-1.91551	1.882923	H	1.099228	-0.79738	-0.097
C	1.11277	-2.68985	2.951938	H	-2.97916	0.473507	0.541467
C	2.116883	-3.63561	2.751721	H	-5.0004	-0.64866	-0.37444
C	2.667076	-3.81657	1.485535	H	-3.65656	-4.38269	1.275295
C	3.762461	-0.08783	2.583121	H	-1.6346	-3.26752	2.157206
C	4.673905	-1.07656	2.223678	H	1.122213	4.441037	0.715541
H	-2.95544	-1.61954	3.820996	H	2.200966	6.492916	-0.18086
H	-1.65017	-0.30318	7.700936	H	6.005689	5.103164	1.251458
H	-3.32943	-1.40868	6.248421	H	4.930683	3.056821	2.126797
H	1.948575	2.947039	7.772783	H	5.37915	-0.10482	-0.8115
H	3.372837	4.262128	3.937746	H	3.674087	1.572769	-0.23388
H	3.213758	4.562646	6.376993	C	2.301297	-2.52924	0.318313
C	-2.19879	-1.15347	4.442164	C	1.31747	-1.58902	0.612947
C	-1.01898	-0.66727	3.861269	C	-2.18147	-1.31674	1.412213
C	-0.07807	-0.09214	4.709208	C	-3.13414	-0.5912	0.696396
C	-0.28612	0.065236	6.081439	C	-4.26861	-1.22221	0.185809
C	-1.46977	-0.41335	6.63565	C	-4.46007	-2.58505	0.396869
C	-2.41077	-1.03023	5.812703	C	-3.51244	-3.31908	1.112769
C	1.626282	1.483567	4.734008	C	-2.37607	-2.68993	1.610615
C	1.474578	1.670608	6.111535	C	2.947776	3.623901	1.490882
C	2.051961	2.789121	6.703214	C	2.191541	4.596393	0.835317
C	2.756064	3.695691	5.912391	C	2.79946	5.746947	0.33275
C	2.854266	3.521477	4.535839	C	4.169783	5.93227	0.483757
C	2.269803	2.407015	3.915257	C	4.935363	4.96419	1.135258
O	1.130148	0.317748	4.183996	C	4.32962	3.814752	1.630681
P	-0.65993	-0.64091	2.047678	C	3.363103	0.833181	1.767009
P	2.165194	2.192906	2.079323	C	5.301046	-1.0881	1.104273
H	-5.46373	-3.18999	0.289709	C	4.923165	-0.12266	0.173873
H	4.282187	7.228875	0.387436	C	3.961452	0.828631	0.499341
H	5.999252	-1.8169	0.696394	H	0.425087	-2.70598	3.700928
H	3.453737	-4.54959	1.333686	H	2.184804	-4.35459	3.180026
N	0.730026	0.705345	6.81007	H	3.307531	-0.16936	3.683524
H	0.484812	0.958194	7.759638	H	4.988043	-1.84467	3.0958
H	1.114106	2.858136	-2.3897	C	0.619241	-1.65472	1.824667
C	0.66491	1.139396	-0.34601	C	0.946309	-2.65237	2.748662
O	1.58825	0.591182	-0.91093	C	1.939023	-3.58469	2.454843
Rh	0.056266	1.546515	1.471849	C	2.611339	-3.52965	1.23667

C	3.747175	-0.14142	2.694175	H	-4.92955	-0.7572	-0.43372
C	4.707745	-1.09456	2.36239	H	-3.54214	-4.44247	1.28778
H	-3.01481	-1.47781	3.879817	H	-1.56993	-3.27344	2.204099
H	-1.54755	-0.42355	7.784393	H	1.257115	4.349919	0.48419
H	-3.30335	-1.39501	6.329946	H	2.455305	6.297829	-0.46428
H	2.096335	2.790227	7.862215	H	6.092928	4.956205	1.386543
H	3.402639	4.211655	4.019199	H	4.899591	3.003341	2.315136
H	3.309355	4.446299	6.47245	H	5.27968	-0.18994	-0.81792
C	-2.22025	-1.08251	4.503107	H	3.555313	1.472869	-0.23266
C	-1.03815	-0.61187	3.915953	C	2.305178	-2.48022	0.29899
C	-0.05045	-0.12711	4.7656	C	1.325149	-1.54694	0.626367
C	-0.21287	-0.02227	6.147754	C	-2.14284	-1.34089	1.428271
C	-1.39748	-0.48945	6.710827	C	-3.09241	-0.64505	0.679454
C	-2.38397	-1.02851	5.885564	C	-4.20007	-1.3087	0.150991
C	1.686113	1.413147	4.799663	C	-4.36742	-2.67246	0.373384
C	1.572581	1.554463	6.184114	C	-3.41966	-3.37746	1.117565
C	2.168313	2.658017	6.786662	C	-2.31072	-2.71713	1.635299
C	2.843345	3.589304	5.997556	C	2.986576	3.561071	1.484303
C	2.905332	3.453289	4.613443	C	2.312476	4.490529	0.691726
C	2.309051	2.351242	3.984351	C	2.9909	5.585806	0.15575
O	1.143556	0.285479	4.211805	C	4.347086	5.759674	0.40867
P	-0.72399	-0.43124	2.103386	C	5.032266	4.830576	1.19292
P	2.104581	2.132509	2.157264	C	4.358613	3.734907	1.719641
H	-5.34337	-3.07782	0.002508	C	3.341175	0.793038	1.801554
H	4.645146	6.825752	0.090984	C	5.287009	-1.11069	1.130555
H	6.05149	-1.83054	0.849173	C	4.858329	-0.18356	0.182892
H	3.387329	-4.25471	1.010071	C	3.888532	0.757854	0.511358
N	0.836428	0.571738	6.870939	H	0.498328	-2.70929	3.717916
H	0.618539	0.797406	7.834056	H	2.256699	-4.34469	3.138836
H	0.318918	3.240687	-2.50659	H	3.361293	-0.14675	3.748813
C	0.224502	1.649969	-0.3057	H	5.053073	-1.81647	3.151064
O	1.361224	1.477704	-0.71642	C	0.652733	-1.63721	1.850518
Rh	-0.28174	1.926153	1.612561	C	1.001801	-2.64249	2.756857
C	-0.68313	3.166318	-2.07319	C	1.991563	-3.5664	2.429775
C	-0.86333	1.799556	-1.40782	C	2.6359	-3.49228	1.197447
C	-0.70214	0.690106	-2.42668	C	3.767907	-0.14648	2.744192
O	-0.96131	-0.54339	-1.74176	C	4.733781	-1.09307	2.406855
C	-0.87154	-1.65696	-2.48916	H	-2.99059	-1.53657	3.917308
C	-1.21152	-2.87973	-1.68433	H	-1.55557	-0.42113	7.817797
O	-0.56988	-1.64008	-3.65904	H	-3.28733	-1.43947	6.368988
H	-1.42292	3.31932	-2.86499	H	2.043447	2.854501	7.872909
H	-0.79725	3.973506	-1.34191	H	3.364408	4.238651	4.021901
H	-1.8616	1.728033	-0.96738	H	3.24674	4.505825	6.470288
H	0.314726	0.676389	-2.82798	C	-2.20582	-1.12332	4.541441
H	-1.40838	0.792632	-3.25722	C	-1.03032	-0.63514	3.957504
H	-0.54463	-2.95375	-0.82006	C	-0.05365	-0.1231	4.802853
H	-1.11908	-3.76484	-2.31237	C	-0.22245	-0.00789	6.18317
H	-2.23279	-2.78792	-1.30213	C	-1.40046	-0.49384	6.745397
C	-0.84644	2.519421	3.455764	C	-2.37395	-1.06023	5.923193
O	-1.20593	2.948531	4.448938	C	1.663426	1.437298	4.825537
H	-1.71977	2.752188	1.012877	C	1.540301	1.59334	6.207543
H	-1.09066	3.364858	0.987712	C	2.123076	2.709717	6.799538
				C	2.794224	3.637354	6.003423
7b*				C	2.87024	3.483018	4.621746
				C	2.291191	2.365918	4.003594
H	2.82451	-2.40075	-0.65082	O	1.13376	0.30047	4.242911
H	1.08712	-0.74267	-0.06569	P	-0.70838	-0.44838	2.151992
H	-2.95986	0.418695	0.510695	P	2.10155	2.108631	2.181381

H	-5.23041	-3.18896	-0.03526	C	3.414888	0.754719	1.740573
H	4.874652	6.611669	-0.00885	C	5.33121	-1.16782	1.047344
H	6.044467	-1.84529	0.873699	C	4.901858	-0.23592	0.104619
H	3.408099	-4.21227	0.943625	C	3.942283	0.713445	0.442551
N	0.812138	0.611859	6.90401	H	0.424895	-2.67454	3.677911
H	0.587422	0.845912	7.863508	H	2.16655	-4.33563	3.120899
H	0.126693	3.390769	-2.48933	H	3.438346	-0.18827	3.685412
C	0.059983	1.763877	-0.31268	H	5.108554	-1.87799	3.068002
O	1.215247	1.632346	-0.69235	C	0.625767	-1.59815	1.817431
Rh	-0.38391	1.95795	1.640376	C	0.944145	-2.61315	2.724699
C	-0.87104	3.269154	-2.05605	C	1.925243	-3.55064	2.410679
C	-1.0055	1.880957	-1.42588	C	2.591314	-3.48213	1.189213
C	-0.78917	0.791956	-2.45636	C	3.840005	-0.19137	2.677986
O	-0.99572	-0.45751	-1.77866	C	4.790962	-1.14806	2.329599
C	-0.86776	-1.56309	-2.53086	H	-3.09147	-1.32656	3.83066
C	-1.15764	-2.80185	-1.72957	H	-1.65023	-0.28901	7.749167
O	-0.57105	-1.53146	-3.70181	H	-3.42012	-1.19988	6.273814
H	-1.61792	3.419136	-2.84162	H	2.153264	2.759892	7.846974
H	-1.01268	4.045261	-1.29665	H	3.561536	4.065689	3.997001
H	-2.00324	1.770843	-0.99401	H	3.466208	4.330601	6.450019
H	0.228749	0.824277	-2.85363	C	-2.29112	-0.96012	4.463876
H	-1.49594	0.86738	-3.28918	C	-1.07774	-0.55105	3.895446
H	-0.47626	-2.86136	-0.87564	C	-0.08785	-0.09549	4.75623
H	-1.04528	-3.67933	-2.36504	C	-0.26974	0.034902	6.133617
H	-2.17557	-2.7465	-1.33192	C	-1.48342	-0.37474	6.679532
C	-0.96859	2.556069	3.471664	C	-2.47715	-0.881	5.842417
O	-1.39044	3.024465	4.419575	C	1.701599	1.366554	4.798901
H	-1.86631	2.096675	1.217501	C	1.580934	1.530492	6.180476
H	-0.41544	3.46064	1.219823	C	2.227177	2.610286	6.773808
				C	2.958407	3.494959	5.980136
TS7b				C	3.021415	3.342233	4.597945
431.16i				C	2.369035	2.266148	3.980138
H	2.829835	-2.38448	-0.6496	O	1.134377	0.250512	4.217988
H	1.110551	-0.69959	-0.08361	P	-0.72063	-0.38333	2.093131
H	-2.93216	0.439382	0.346972	P	2.164882	2.038874	2.157487
H	-4.90047	-0.75134	-0.57374	H	-5.25769	-3.15101	-0.04627
H	-3.62239	-4.35636	1.385093	H	4.532543	6.9589	0.437059
H	-1.6505	-3.17301	2.277586	H	6.078269	-1.9097	0.781308
H	1.068052	4.603469	1.375843	H	3.355639	-4.21383	0.945054
H	2.068585	6.749619	0.668428	N	0.791826	0.591707	6.868726
H	5.986192	5.008296	0.934994	H	0.566671	0.841299	7.824257
H	4.990399	2.866779	1.642789	H	0.102624	3.202614	-2.90456
H	5.311748	-0.24711	-0.90087	C	0.200926	1.869452	-0.53409
H	3.603083	1.429754	-0.29748	O	1.361291	1.673782	-0.87311
C	2.293173	-2.46009	0.290887	Rh	-0.29804	1.890797	1.587957
C	1.324089	-1.51167	0.607569	C	-0.86196	3.097525	-2.39825
C	-2.16351	-1.27774	1.378129	C	-0.90003	1.788036	-1.59975
C	-3.08497	-0.61081	0.571409	C	-0.66624	0.60937	-2.52124
C	-4.19394	-1.28271	0.056111	O	-0.89214	-0.58639	-1.76367
C	-4.39323	-2.62816	0.351033	C	-0.76716	-1.73616	-2.45095
C	-3.47554	-3.3056	1.155766	C	-1.11185	-2.92568	-1.60004
C	-2.3655	-2.63636	1.659234	O	-0.43819	-1.77122	-3.61313
C	2.95593	3.580272	1.540928	H	-1.6581	3.117643	-3.14803
C	2.145844	4.688466	1.271979	H	-0.99559	3.958991	-1.73627
C	2.71087	5.899781	0.877137	H	-1.87356	1.688109	-1.1122
C	4.09181	6.017184	0.748965	H	0.358955	0.612872	-2.90177
C	4.907975	4.921771	1.026172	H	-1.35404	0.625168	-3.37287
C	4.345258	3.711948	1.422736	H	-0.47701	-2.9473	-0.70986

H	-0.97955	-3.83627	-2.18308
H	-2.1487	-2.83809	-1.26117
C	-0.83165	2.764217	3.233252
O	-1.22134	3.209941	4.213934
H	-1.80152	1.954227	1.22645
H	-0.02875	2.912535	0.249443
b*			
H	2.733704	-2.57134	-0.62695
H	1.021886	-0.88991	-0.05655
H	-2.6253	0.404557	0.21114
H	-4.37038	-0.79589	-1.08333
H	-3.538	-4.38256	1.132117
H	-1.74521	-3.20796	2.363003
H	1.163178	4.493854	0.79461
H	2.338914	6.481247	-0.08511
H	6.049223	4.966527	1.464039
H	4.875225	2.97377	2.332103
H	4.999878	-0.1602	-0.92356
H	3.380628	1.532121	-0.20601
C	2.246573	-2.61136	0.34265
C	1.288392	-1.6572	0.669217
C	-2.07304	-1.31701	1.372958
C	-2.82242	-0.64627	0.404265
C	-3.81114	-1.31952	-0.31433
C	-4.06968	-2.66222	-0.05374
C	-3.33909	-3.33553	0.92646
C	-2.33749	-2.67067	1.625813
C	2.931541	3.605976	1.63876
C	2.232088	4.598891	0.950212
C	2.896551	5.719864	0.4509
C	4.26749	5.855852	0.637905
C	4.977983	4.866906	1.320526
C	4.316445	3.747751	1.811713
C	3.270236	0.825317	1.837561
C	5.129751	-1.10099	1.01334
C	4.653594	-0.15788	0.105306
C	3.728145	0.796483	0.513684
H	0.546205	-2.70118	3.822433
H	2.266258	-4.37863	3.24415
H	3.394127	-0.13943	3.766415
H	5.020752	-1.82988	3.035871
C	0.657793	-1.69287	1.918136
C	1.021533	-2.67201	2.845333
C	1.989515	-3.61998	2.518325
C	2.595647	-3.59613	1.265363
C	3.738968	-0.13419	2.738209
C	4.664672	-1.09055	2.324943
H	-3.0245	-1.53426	3.911536
H	-1.63066	-0.49615	7.849244
H	-3.35193	-1.47422	6.361381
H	2.006049	2.751977	7.992951
H	3.33197	4.202702	4.168296
H	3.223238	4.419545	6.622186
C	-2.24338	-1.14166	4.553433
C	-1.05469	-0.65662	3.995435
C	-0.08813	-0.16202	4.859783
C	-0.27243	-0.06741	6.239178
C	-1.46139	-0.55253	6.777972
C	-2.42905	-1.09741	5.933404
C	1.626229	1.388465	4.920911
C	1.498857	1.522665	6.305095
C	2.086554	2.625407	6.91737
C	2.76492	3.563201	6.138956
C	2.836965	3.436733	4.754378
C	2.250463	2.334016	4.117928
O	1.113996	0.253271	4.325517
P	-0.67678	-0.46554	2.207521
P	2.049928	2.129368	2.293746
H	-4.83637	-3.18616	-0.61563
H	4.786263	6.726677	0.249695
H	5.853047	-1.84673	0.697343
H	3.34984	-4.3351	1.011753
N	0.76157	0.53253	6.979631
H	0.5286	0.753921	7.940274
H	-0.813	3.448686	-2.89349
C	1.010404	1.787883	-1.52296
O	1.715769	1.053399	-2.17404
Rh	-0.37345	1.926465	1.922805
C	-1.02591	3.177628	-1.85426
C	-0.49706	1.778156	-1.5236
C	-1.07397	0.714476	-2.43183
O	-0.70784	-0.56005	-1.89808
C	-1.34794	-1.61847	-2.42813
C	-0.8974	-2.90145	-1.78966
O	-2.17091	-1.51485	-3.30641
H	-2.10697	3.220943	-1.69679
H	-0.56481	3.925407	-1.20085
H	-0.78123	1.558228	-0.47934
H	-0.68643	0.801708	-3.45266
H	-2.16574	0.787322	-2.4711
H	0.172593	-3.04387	-1.96569
H	-1.4632	-3.73222	-2.20915
H	-1.04802	-2.8468	-0.70765
C	-0.80271	3.699041	2.088183
O	-1.17121	4.781103	2.237271
H	-1.95525	1.82585	1.845272
H	1.458128	2.553949	-0.85173
TS8l			
711.93i			
H	3.836139	-4.21805	1.840283
H	1.874356	-3.0285	0.963245
H	-2.31499	-2.0963	0.075383
H	-3.84904	-3.97203	-0.47611
H	-2.23656	-6.23961	2.797462
H	-0.72515	-4.36444	3.356056
H	0.56537	3.296832	-0.36315
H	1.319302	5.182242	-1.73221
H	5.41031	4.212537	-0.81159
H	4.647063	2.345856	0.611225
H	5.67219	-1.52185	0.179903
H	3.771297	-0.03604	-0.31811
C	3.131027	-3.76708	2.531659
C	2.024139	-3.08588	2.037192

C	-1.42912	-3.10232	1.753607	C	-2.03896	2.289487	0.387663
C	-2.31139	-3.00357	0.674892	C	-2.4735	3.519584	1.168852
C	-3.16844	-4.05889	0.365083	O	-3.1096	4.50015	0.326044
C	-3.14296	-5.2231	1.127533	C	-2.30424	5.251387	-0.4353
C	-2.26145	-5.33148	2.203196	C	-3.10052	6.203774	-1.28917
C	-1.40967	-4.27681	2.516238	O	-1.09664	5.170201	-0.42988
C	2.553204	2.668533	0.196952	H	-0.97222	1.72681	2.169866
C	1.630416	3.478595	-0.47417	H	-2.2604	0.623534	1.733593
C	2.058634	4.552762	-1.24795	H	-2.89967	1.883913	-0.16028
C	3.421622	4.811699	-1.38065	H	-1.60809	3.980216	1.658275
C	4.34799	4.008474	-0.7185	H	-3.22444	3.27117	1.922631
C	3.917853	2.94873	0.078599	H	-3.74487	5.635835	-1.96525
C	3.314159	0.366601	1.754847	H	-2.42141	6.832395	-1.86282
C	5.470898	-1.33215	2.318171	H	-3.74459	6.820158	-0.65756
C	5.114598	-1.07267	0.996049	H	-1.14925	-0.09862	-0.84318
C	4.038138	-0.23704	0.717199	H	-0.58462	0.60456	-1.06124
H	0.618421	-2.13798	4.981096				
H	2.59103	-3.32195	5.852457	8l*			
H	3.126089	0.546216	3.897708				
H	5.009097	-0.95873	4.386748	H	-5.44169	-3.13376	-1.24813
C	1.102787	-2.49075	2.907072	H	-3.45655	-1.65071	-1.22116
C	1.321741	-2.58377	4.284496	H	-3.1206	-0.34626	2.37611
C	2.436233	-3.25955	4.779516	H	-3.11256	0.323266	4.747836
C	3.3409	-3.855	3.906324	H	0.995233	-0.8891	5.075453
C	3.676473	0.098222	3.076941	H	0.996753	-1.55874	2.70924
C	4.746555	-0.7505	3.354061	H	-0.98932	2.784868	2.040411
H	-2.95073	-2.29616	3.712337	H	-0.75401	3.149522	4.466337
H	-2.87963	0.828164	6.6739	H	3.260815	1.629783	4.308793
H	-3.97818	-1.13901	5.642702	H	3.025929	1.245291	1.887729
H	0.194064	4.51279	5.814233	H	2.372257	6.509276	0.299527
H	2.345505	4.286831	2.098843	H	2.156955	4.179158	1.084534
H	1.56	5.583804	4.041049	C	-4.71748	-3.21917	-0.44368
C	-2.44955	-1.44797	4.166734	C	-3.59548	-2.38768	-0.43512
C	-1.22201	-1.00641	3.657449	C	-1.06122	-0.99758	2.372347
C	-0.61476	0.074078	4.279469	C	-2.21271	-0.4582	2.962744
C	-1.1874	0.760146	5.351352	C	-2.21085	-0.08607	4.302835
C	-2.41193	0.312858	5.840015	C	-1.05822	-0.2445	5.06909
C	-3.02718	-0.79306	5.251563	C	0.090607	-0.77135	4.486834
C	0.827417	1.832412	3.848381	C	0.092865	-1.1465	3.144937
C	0.309237	2.563107	4.921782	C	0.997031	1.976725	1.793632
C	0.580637	3.925081	4.98675	C	-0.06117	2.514511	2.536787
C	1.341651	4.522884	3.9811	C	0.07621	2.734674	3.903221
C	1.795365	3.789636	2.88976	C	1.272184	2.419751	4.54547
C	1.524882	2.415094	2.798786	C	2.325625	1.877597	3.815775
O	0.625919	0.468746	3.82498	C	2.189827	1.654507	2.446603
P	-0.36743	-1.65634	2.165997	C	0.88601	3.566537	-0.54971
P	1.84943	1.379107	1.30238	C	1.134377	6.210675	-1.43875
H	-3.80492	-6.04816	0.883338	C	1.776572	5.802762	-0.26997
H	3.762201	5.641911	-1.99181	C	1.654096	4.489449	0.172696
H	6.304504	-1.99202	2.538892	H	-2.14118	-3.49434	2.431182
H	4.208895	-4.3803	4.293175	H	-4.12791	-4.96297	2.410745
N	-0.47654	1.863231	5.855709	H	-0.35547	3.274939	-2.28083
H	-0.99196	2.447004	6.50338	H	-0.13422	5.611794	-3.07196
H	-1.32042	2.619194	-0.3679	C	-2.65379	-2.48896	0.591007
C	1.196916	-1.14805	-0.61403	C	-2.86179	-3.41897	1.620449
O	1.830851	-1.78311	-1.32825	C	-3.97971	-4.24488	1.610431
Rh	0.006383	-0.03413	0.412472	C	-4.90974	-4.14698	0.574404
C	-1.44157	1.223373	1.316034	C	0.246113	3.984083	-1.72021

C	0.371242	5.300161	-2.16331	H	-0.93164	2.702064	2.069444
H	-0.98996	-4.46417	0.1344	H	-0.69235	3.042991	4.502628
H	0.911412	-5.87384	-0.56226	H	3.376651	1.681235	4.293456
H	3.204384	2.869825	-1.56776	H	3.142392	1.339199	1.861065
H	5.211	1.66913	-2.38247	H	2.586428	6.502455	0.260838
C	-0.00028	-4.02994	0.048502	H	2.359818	4.166207	1.029521
C	0.19351	-2.66794	0.318793	C	-4.49617	-3.28727	-0.69459
C	1.483095	-2.16615	0.190022	C	-3.37873	-2.45881	-0.5902
C	2.559888	-2.93008	-0.26641	C	-1.03152	-0.97698	2.449823
C	2.344212	-4.27883	-0.5333	C	-2.17191	-0.42953	3.053694
C	1.071407	-4.82094	-0.35573	C	-2.15599	-0.0697	4.397373
C	2.613368	-0.19745	-0.28559	C	-0.99725	-0.24212	5.151395
C	3.715948	-0.90533	-0.7642	C	0.143732	-0.76916	4.5535
C	4.655776	-0.21693	-1.52756	C	0.130317	-1.13555	3.209469
C	4.469647	1.140194	-1.79296	C	1.089656	1.99906	1.79567
C	3.344133	1.819876	-1.33229	C	0.013953	2.473618	2.556462
C	2.382929	1.140735	-0.57432	C	0.150704	2.676136	3.925319
O	1.70901	-0.84726	0.529988	C	1.362744	2.395455	4.554049
P	-1.14983	-1.43201	0.588902	C	2.431193	1.905709	3.808809
P	0.758084	1.807815	-0.0226	C	2.296939	1.707455	2.435254
H	1.227705	7.2369	-1.78018	C	0.979165	3.607502	-0.53231
H	-5.7836	-4.79101	0.566616	C	1.238552	6.25727	-1.40243
H	1.379238	2.592623	5.61208	C	1.939931	5.818021	-0.27963
H	-1.05415	0.046628	6.11519	C	1.811696	4.502066	0.153231
Rh	-1.07709	0.400065	-1.06635	H	-2.43139	-3.23965	2.580767
H	-2.62273	3.315058	-0.84451	H	-4.4175	-4.69672	2.394886
C	0.155141	-0.48468	-2.29232	H	-0.37293	3.369615	-2.1863
O	0.782343	-1.00027	-3.09633	H	-0.14157	5.712273	-2.96221
C	-2.66066	1.305674	-0.01244	C	-2.62702	-2.43285	0.588771
C	-3.3511	2.521067	-0.62987	C	-3.01041	-3.24893	1.661313
C	-4.07878	2.213768	-1.93046	C	-4.12845	-4.07064	1.556634
O	-4.90736	1.041073	-1.80759	C	-4.87438	-4.08968	0.378292
C	-6.0549	1.182855	-1.13285	C	0.278745	4.05723	-1.65508
C	-6.74189	-0.14627	-0.95277	C	0.409645	5.375846	-2.08964
O	-6.46871	2.239135	-0.71425	H	-0.98973	-4.42094	0.279593
H	-3.43048	0.543033	0.176963	H	0.888497	-5.86294	-0.42527
H	-2.27756	1.585713	0.976256	H	3.243442	2.859282	-1.62586
H	-4.08397	2.941479	0.072634	H	5.216346	1.626579	-2.47013
H	-3.37317	1.954517	-2.72056	C	0.001125	-3.99759	0.156352
H	-4.70636	3.052373	-2.24463	C	0.211567	-2.63027	0.382843
H	-6.16994	-0.74486	-0.23625	C	1.499891	-2.13927	0.217396
H	-6.766	-0.69309	-1.89816	C	2.560489	-2.9219	-0.24611
H	-7.7513	0.011367	-0.57552	C	2.329287	-4.27508	-0.47433
H	5.525101	-0.74119	-1.91319	C	1.058192	-4.80567	-0.25139
H	3.165053	-4.89656	-0.8854	C	2.634833	-0.18875	-0.30867
N	3.789303	-2.27082	-0.44027	C	3.720991	-0.91363	-0.79997
H	4.492772	-2.79718	-0.94419	C	4.655069	-0.24484	-1.58712
H	-2.25167	-0.19084	-1.87147	C	4.480097	1.111825	-1.86186
H	-1.30219	1.496349	-2.13975	C	3.372621	1.809272	-1.38487
				C	2.416627	1.150579	-0.60175
TS9l				O	1.742434	-0.81979	0.534825
959.25i				P	-1.11788	-1.38611	0.662271
H	-5.07188	-3.2983	-1.61514	P	0.816639	1.846617	-0.01677
H	-3.08641	-1.82768	-1.42518	H	1.337294	7.285351	-1.73681
H	-3.08531	-0.30797	2.477073	H	-5.74727	-4.73009	0.298447
H	-3.05079	0.341689	4.854368	H	1.469326	2.549977	5.623569
H	1.054095	-0.89348	5.131727	H	-0.9818	0.040254	6.19975
H	1.027316	-1.54875	2.760076	Rh	-1.09213	0.440699	-0.96499

H	-2.82085	3.285754	-0.79842
C	-0.17783	-0.54464	-2.28855
O	0.324987	-1.14233	-3.13184
C	-2.93111	1.290657	0.030123
C	-3.57839	2.515627	-0.60784
C	-4.25811	2.206764	-1.93602
O	-5.03263	0.995203	-1.86328
C	-6.18317	1.056251	-1.1761
C	-6.81793	-0.30553	-1.06876
O	-6.62913	2.075051	-0.70307
H	-3.71142	0.581362	0.337481
H	-2.41873	1.576251	0.952715
H	-4.32062	2.945233	0.075423
H	-3.51686	1.997019	-2.70901
H	-4.90936	3.025549	-2.25277
H	-6.18568	-0.94682	-0.44614
H	-6.88572	-0.76817	-2.05613
H	-7.80668	-0.21396	-0.62186
H	5.511177	-0.78358	-1.98235
H	3.137968	-4.90683	-0.82987
N	3.789825	-2.27619	-0.46029
H	4.475087	-2.81519	-0.9758
H	-2.64972	0.33562	-1.16298
H	-1.25707	1.516036	-2.08173

9l*

H	-5.51306	-2.70735	-0.91471
H	-3.47226	-1.30416	-0.89774
H	-2.95775	-0.62817	2.572579
H	-2.9044	-0.09658	4.97605
H	1.300653	-0.9678	5.073769
H	1.260579	-1.48436	2.673441
H	-1.07593	2.321545	1.967254
H	-0.91684	2.709043	4.4017
H	3.313902	1.97892	4.242034
H	3.161476	1.604214	1.805251
H	2.364684	6.495478	0.05021
H	2.389986	4.126742	0.749212
C	-4.70652	-2.93896	-0.22648
C	-3.54739	-2.15969	-0.23076
C	-0.85151	-1.09038	2.445578
C	-2.01657	-0.68859	3.113124
C	-1.99008	-0.39711	4.473145
C	-0.79783	-0.50224	5.186004
C	0.365176	-0.8914	4.527966
C	0.342771	-1.18257	3.16556
C	1.034367	1.952221	1.718888
C	-0.11004	2.257222	2.463992
C	-0.02087	2.479561	3.83333
C	1.212769	2.384547	4.475724
C	2.352151	2.061496	3.744893
C	2.265375	1.846878	2.370057
C	0.827906	3.531941	-0.61768
C	0.783956	6.221191	-1.38942
C	1.682294	5.789701	-0.41289
C	1.699505	4.454962	-0.02377
H	-1.83772	-3.75096	2.239715
H	-3.88843	-5.13147	2.235525
H	-0.7437	3.258857	-2.05724
H	-0.79551	5.644634	-2.73361
C	-2.49621	-2.46358	0.637798
C	-2.63833	-3.53084	1.537218
C	-3.79258	-4.30412	1.539507
C	-4.82752	-4.01164	0.649715
C	-0.06897	3.972295	-1.59403
C	-0.09151	5.313369	-1.97672
H	-0.8012	-4.46119	0.070173
H	1.104695	-5.83825	-0.66332
H	3.229108	2.888371	-1.6801
H	5.27098	1.734656	-2.47641
C	0.184284	-4.01609	-0.00333
C	0.368601	-2.66037	0.301996
C	1.652596	-2.14564	0.168042
C	2.733963	-2.89214	-0.30513
C	2.529014	-4.23681	-0.59868
C	1.259804	-4.78992	-0.43123
C	2.74615	-0.16548	-0.32128
C	3.858859	-0.85254	-0.80497
C	4.774124	-0.15191	-1.58695
C	4.549499	1.195694	-1.87152
C	3.406178	1.850437	-1.41814
C	2.473036	1.157482	-0.6392
O	1.87731	-0.82936	0.520028
P	-0.97428	-1.43491	0.637203
P	0.828234	1.770424	-0.09822
H	0.766215	7.265008	-1.68697
H	-5.72879	-4.61671	0.647814
H	1.281671	2.550439	5.546608
H	-0.77482	-0.27788	6.248164
Rh	-0.71569	0.216818	-1.13626
H	-3.25459	3.557052	0.174486
C	-1.49122	-0.78439	-2.46523
O	-1.96542	-1.39659	-3.27784
C	-3.72566	1.625893	1.035844
C	-3.97068	2.739401	0.020984
C	-3.79488	2.251599	-1.40926
O	-4.97574	1.582772	-1.88807
C	-5.98947	2.365606	-2.28725
C	-7.18172	1.538402	-2.69111
O	-5.94304	3.573655	-2.29652
H	-4.47718	0.834587	0.937671
H	-3.75812	2.000007	2.064346
H	-4.97409	3.159103	0.144507
H	-3.02203	1.478709	-1.45945
H	-3.55419	3.074028	-2.08803
H	-7.64343	1.127271	-1.78771
H	-6.86955	0.702989	-3.32204
H	-7.90363	2.165581	-3.2121
H	5.652665	-0.65923	-1.97446
H	3.353074	-4.84146	-0.96577
N	3.957043	-2.21547	-0.47181
H	4.663135	-2.73126	-0.98331
H	-2.74379	1.164776	0.866352
H	-0.41032	1.160754	-2.37706

TS8b			
854.90i			
H	3.475921	-3.77992	1.032194
H	1.722336	-2.12581	0.530601
H	-2.51282	-0.54176	0.063909
H	-4.37579	-1.94557	-0.78029
H	-3.10395	-5.17252	1.753078
H	-1.25903	-3.77224	2.615066
H	1.191696	3.9714	0.288639
H	2.229184	5.90312	-0.85486
H	6.109903	4.563334	0.413287
H	5.072527	2.637585	1.565039
H	5.501079	-1.21881	-0.20576
H	3.766452	0.535009	-0.18818
C	2.775527	-3.48978	1.808965
C	1.784605	-2.55516	1.525918
C	-1.76838	-2.06308	1.399026
C	-2.64925	-1.55372	0.439074
C	-3.69399	-2.34561	-0.03618
C	-3.8599	-3.64558	0.433662
C	-2.98099	-4.158	1.387103
C	-1.94103	-3.36963	1.8708
C	3.059912	3.171499	1.00229
C	2.27086	4.101644	0.318061
C	2.854429	5.191415	-0.32524
C	4.236403	5.356962	-0.29462
C	5.032164	4.43579	0.385826
C	4.44838	3.350544	1.033303
C	3.521373	0.516354	1.956404
C	5.476934	-1.4924	1.933053
C	5.063399	-0.90543	0.737295
C	4.086197	0.083346	0.748596
H	0.296882	-2.4154	4.579663
H	2.069096	-4.04996	5.082027
H	3.513644	0.23523	4.096311
H	5.213681	-1.54224	4.068166
C	0.87835	-2.15922	2.515731
C	0.991528	-2.70743	3.797489
C	1.991231	-3.63536	4.081725
C	2.882641	-4.03035	3.088202
C	3.937976	-0.0795	3.148277
C	4.906528	-1.08293	3.133545
H	-3.08994	-1.43012	3.525356
H	-2.37305	0.70401	7.193416
H	-3.85107	-0.66312	5.749887
H	1.334658	3.861535	7.146039
H	3.290821	4.294067	3.337226
H	2.817485	5.127546	5.615898
C	-2.42828	-0.84228	4.15256
C	-1.14339	-0.51582	3.699776
C	-0.32757	0.225672	4.542183
C	-0.74236	0.684508	5.795068
C	-2.0254	0.357613	6.224539
C	-2.85423	-0.40952	5.405381
C	1.414388	1.74631	4.510137
C	1.064277	2.233689	5.769908
C	1.584313	3.461821	6.167556
C	2.409911	4.174173	5.296387
C	2.687871	3.701301	4.016952
C	2.169825	2.468389	3.597666
O	0.960355	0.496936	4.131615
P	-0.44842	-0.96864	2.058524
P	2.203469	1.800853	1.878581
H	-4.67031	-4.26159	0.056281
H	4.694477	6.200537	-0.80142
H	6.234794	-2.26997	1.925625
H	3.66252	-4.75209	3.311201
N	0.174832	1.454518	6.531918
H	-0.21045	1.917838	7.346134
H	-0.48224	3.701077	1.9851
C	-0.08683	1.915658	-0.96119
O	-0.22868	2.544763	-1.91177
Rh	0.100722	0.819203	0.521162
C	-1.16846	2.95749	2.412079
C	-1.59955	1.920522	1.375008
C	-2.50215	2.63422	0.385034
O	-2.91798	1.7253	-0.6506
C	-3.49136	2.270229	-1.73137
C	-3.78974	1.218894	-2.76921
O	-3.72098	3.451057	-1.84624
H	-2.02978	3.507059	2.825313
H	-0.65229	2.491032	3.253807
H	-2.22999	1.181857	1.888851
H	-2.00098	3.489411	-0.08429
H	-3.41185	3.020806	0.867469
H	-2.85606	0.741237	-3.07951
H	-4.27755	1.679082	-3.6271
H	-4.43322	0.445675	-2.34177
H	1.330493	-0.06577	-0.14761
H	0.28312	-0.37029	-0.51809
8b*			
H	3.608108	-3.78869	1.082826
H	1.889635	-2.11684	0.478555
H	-2.30044	-0.50416	-0.23315
H	-4.1421	-1.85089	-1.20999
H	-2.99574	-5.18529	1.246947
H	-1.1852	-3.83021	2.246439
H	1.776303	3.538102	-0.38392
H	3.067455	5.344798	-1.50279
H	6.511742	4.327193	0.855895
H	5.218302	2.543787	1.979597
H	5.890566	-1.48416	0.332278
H	4.195696	0.280141	-0.00196
C	2.852642	-3.50648	1.80934
C	1.885392	-2.56697	1.468723
C	-1.63285	-2.07223	1.077539
C	-2.46811	-1.52641	0.098594
C	-3.49677	-2.28713	-0.45426
C	-3.68777	-3.60311	-0.0418
C	-2.85173	-4.15789	0.927038
C	-1.83098	-3.39585	1.487815
C	3.405612	2.933755	0.875427
C	2.8108	3.727746	-0.10753
C	3.539144	4.736808	-0.73715

C	4.869605	4.953738	-0.39163	H	-2.89936	1.290426	1.85076
C	5.473229	4.162019	0.586196	H	-2.59093	2.321846	0.438959
C	4.745823	3.158021	1.217224	H	-6.02031	3.850968	3.02042
C	3.63502	0.374326	2.080623	H	-6.97472	3.529011	1.542113
C	5.545585	-1.63778	2.454862	H	-5.75278	4.833454	1.579096
C	5.321674	-1.11688	1.181145	H	1.150465	0.07602	-0.37026
C	4.365621	-0.12472	0.993695	H	-0.60122	2.086722	2.073944
H	0.180172	-2.45883	4.408967				
H	1.919128	-4.10183	5.020463	TS9b			
H	3.29456	0.206108	4.205331	942.39i			
H	4.964981	-1.57515	4.526211	H	3.526181	-3.7684	0.98001
C	0.908377	-2.18772	2.39628	H	1.681745	-2.1933	0.535747
C	0.930903	-2.74537	3.677432	H	-2.13275	-1.2364	-0.26596
C	1.909668	-3.67615	4.021629	H	-3.74979	-2.91391	-1.12384
C	2.86697	-4.06192	3.08754	H	-2.97368	-5.39791	2.294671
C	3.855876	-0.15994	3.3516	H	-1.36856	-3.72642	3.147161
C	4.805	-1.1647	3.533848	H	0.84516	3.82288	0.324334
H	-3.1089	-1.48693	3.122388	H	1.741848	5.804467	-0.85438
H	-2.81363	0.999732	6.624594	H	5.734962	4.612193	0.19414
H	-4.10557	-0.5467	5.181026	H	4.837852	2.640021	1.3837
H	0.775112	4.268692	6.579874	H	5.344084	-1.20123	-0.35472
H	3.187432	4.319375	3.019668	H	3.496964	0.43704	-0.27259
H	2.403025	5.402806	5.091779	C	2.860766	-3.48107	1.788018
C	-2.52024	-0.83876	3.763564	C	1.820228	-2.59286	1.536157
C	-1.19851	-0.52616	3.41436	C	-1.66704	-2.35441	1.506203
C	-0.48282	0.295675	4.27532	C	-2.33607	-2.14046	0.300269
C	-1.03904	0.873914	5.417943	C	-3.23802	-3.08937	-0.18284
C	-2.35732	0.5634	5.740847	C	-3.47339	-4.25718	0.534564
C	-3.0813	-0.30257	4.919807	C	-2.80011	-4.48356	1.736071
C	1.220884	1.862637	4.240755	C	-1.89886	-3.54086	2.216063
C	0.716676	2.481538	5.388505	C	2.778652	3.096436	0.932007
C	1.150348	3.767962	5.692129	C	1.918071	3.998883	0.29866
C	2.060605	4.403069	4.846115	C	2.422452	5.115616	-0.36425
C	2.512063	3.789099	3.681952	C	3.796619	5.336052	-0.40525
C	2.080002	2.49521	3.349671	C	4.663118	4.442613	0.223471
O	0.839031	0.56174	3.981111	C	4.158312	3.330437	0.891794
P	-0.3602	-0.98417	1.837014	C	3.403101	0.476961	1.883642
P	2.377106	1.665113	1.723319	C	5.477121	-1.39978	1.788165
H	-4.48415	-4.19912	-0.4767	C	4.949412	-0.88272	0.605363
H	5.439893	5.734494	-0.88534	C	3.910417	0.040066	0.652231
H	6.288054	-2.41618	2.602759	H	0.502628	-2.42355	4.665469
H	3.629411	-4.78669	3.356794	H	2.362104	-3.96971	5.109581
N	-0.22093	1.756105	6.145809	H	3.541796	0.266516	4.0264
H	-0.69493	2.288405	6.86538	H	5.353236	-1.40228	3.936824
H	-0.78963	4.166575	0.598303	C	0.956457	-2.20257	2.564496
C	-0.29923	1.622612	-1.05965	C	1.16213	-2.70893	3.851258
O	-0.67315	2.004344	-2.08593	C	2.212598	-3.58898	4.103876
Rh	0.344501	0.965952	0.551433	C	3.061817	-3.97944	3.073196
C	-0.95006	4.194438	1.681487	C	3.927975	-0.05317	3.063325
C	-1.40831	2.834134	2.193058	C	4.957296	-0.99235	3.012747
C	-2.66947	2.312722	1.531828	H	-3.09968	-1.66144	3.65638
O	-3.74033	3.181129	1.929698	H	-2.39443	0.552559	7.278895
C	-4.95421	2.854201	1.456605	H	-3.85479	-0.87026	5.87295
C	-6.00171	3.828142	1.928067	H	1.175408	3.840819	7.083918
O	-5.15316	1.898245	0.746773	H	3.018069	4.257943	3.218252
H	-1.70303	4.957245	1.898919	H	2.556689	5.133435	5.481397
H	-0.0095	4.487596	2.159091	C	-2.44102	-1.05419	4.267793
H	-1.57028	2.8642	3.278535	C	-1.16469	-0.71703	3.800141

C	-0.35916	0.057914	4.623879
C	-0.77299	0.5372	5.868134
C	-2.04541	0.191861	6.315798
C	-2.8648	-0.60589	5.516806
C	1.307231	1.651994	4.509335
C	0.961982	2.15935	5.763255
C	1.423974	3.424438	6.112065
C	2.191521	4.151222	5.200401
C	2.463304	3.654681	3.928886
C	1.999905	2.384718	3.556585
O	0.912654	0.368181	4.187405
P	-0.46895	-1.1115	2.142231
P	2.027107	1.690262	1.847435
H	-4.17374	-4.99615	0.157885
H	4.193418	6.200268	-0.92862
H	6.28415	-2.12541	1.753099
H	3.880777	-4.6645	3.2707
N	0.130739	1.357223	6.567973
H	-0.25507	1.823739	7.380152
H	-0.48228	3.462978	2.374218
C	0.066922	1.507591	-0.98531
O	0.176143	1.894629	-2.06041
Rh	-0.09594	0.748208	0.709897
C	-1.34648	2.848762	2.653952
C	-1.88012	2.046891	1.465388
C	-2.33125	2.979956	0.361707
O	-3.40243	3.80961	0.86514
C	-3.83438	4.774314	0.043182
C	-4.94778	5.570836	0.674491
O	-3.37943	4.966665	-1.06015
H	-2.12823	3.51985	3.036936
H	-1.0409	2.198645	3.475691
H	-2.76671	1.502201	1.820297
H	-2.70349	2.448292	-0.52117
H	-1.5177	3.638767	0.03496
H	-5.7895	4.911282	0.900498
H	-5.26353	6.358526	-0.00772
H	-4.60409	6.003859	1.61714
H	0.888054	-0.30663	0.026764
H	-1.65031	0.748392	0.55414

9b*

H	3.608108	-3.78869	1.082826
H	1.889635	-2.11684	0.478555
H	-2.30044	-0.50416	-0.23315
H	-4.1421	-1.85089	-1.20999
H	-2.99574	-5.18529	1.246947
H	-1.1852	-3.83021	2.246439
H	1.776303	3.538102	-0.38392
H	3.067455	5.344798	-1.50279
H	6.511742	4.327193	0.855895
H	5.218302	2.543787	1.979597
H	5.890566	-1.48416	0.332278
H	4.195696	0.280141	-0.00196
C	2.852642	-3.50648	1.80934
C	1.885392	-2.56697	1.468723
C	-1.63285	-2.07223	1.077539
C	-2.46811	-1.52641	0.098594
C	-3.49677	-2.28713	-0.45426
C	-3.68777	-3.60311	-0.0418
C	-2.85173	-4.15789	0.927038
C	-1.83098	-3.39585	1.487815
C	3.405612	2.933755	0.875427
C	2.8108	3.727746	-0.10753
C	3.539144	4.736808	-0.73715
C	4.869605	4.953738	-0.39163
C	5.473229	4.162019	0.586196
C	4.745823	3.158021	1.217224
C	3.63502	0.374326	2.080623
C	5.545585	-1.63778	2.454862
C	5.321674	-1.11688	1.181145
C	4.365621	-0.12472	0.993695
H	0.180172	-2.45883	4.408967
H	1.919128	-4.10183	5.020463
H	3.29456	0.206108	4.205331
H	4.964981	-1.57515	4.526211
C	0.908377	-2.18772	2.39628
C	0.930903	-2.74537	3.677432
C	1.909668	-3.67615	4.021629
C	2.86697	-4.06192	3.08754
C	3.855876	-0.15994	3.3516
C	4.805	-1.1647	3.533848
H	-3.1089	-1.48693	3.122388
H	-2.81363	0.999732	6.624594
H	-4.10557	-0.5467	5.181026
H	0.775112	4.268692	6.579874
H	3.187432	4.319375	3.019668
H	2.403025	5.402806	5.091779
C	-2.52024	-0.83876	3.763564
C	-1.19851	-0.52616	3.41436
C	-0.48282	0.295675	4.27532
C	-1.03904	0.873914	5.417943
C	-2.35732	0.5634	5.740847
C	-3.0813	-0.30257	4.919807
C	1.220884	1.862637	4.240755
C	0.716676	2.481538	5.388505
C	1.150348	3.767962	5.692129
C	2.060605	4.403069	4.846115
C	2.512063	3.789099	3.681952
C	2.080002	2.49521	3.349671
O	0.839031	0.56174	3.981111
P	-0.3602	-0.98417	1.837014
P	2.377106	1.665113	1.723319
H	-4.48415	-4.19912	-0.4767
H	5.439893	5.734494	-0.88534
H	6.288054	-2.41618	2.602759
H	3.629411	-4.78669	3.356794
N	-0.22093	1.756105	6.145809
H	-0.69493	2.288405	6.86538
H	-0.78963	4.166575	0.598303
C	-0.29923	1.622612	-1.05965
O	-0.67315	2.004344	-2.08593
Rh	0.344501	0.965952	0.551433
C	-0.95006	4.194438	1.681487
C	-1.40831	2.834134	2.193058

C	-2.66947	2.312722	1.531828
O	-3.74033	3.181129	1.929698
C	-4.95421	2.854201	1.456605
C	-6.00171	3.828142	1.928067
O	-5.15316	1.898245	0.746773
H	-1.70303	4.957245	1.898919
H	-0.0095	4.487596	2.159091
H	-1.57028	2.8642	3.278535
H	-2.89936	1.290426	1.85076
H	-2.59093	2.321846	0.438959
H	-6.02031	3.850968	3.02042
H	-6.97472	3.529011	1.542113
H	-5.75278	4.833454	1.579096
H	1.150465	0.07602	-0.37026
H	-0.60122	2.086722	2.073944

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