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

Supporting Information: On the Applicability of Functional-Group Symmetry-Adapted Perturbation Theory and Other Partitioning Models for a Chiral Recognition – the Case of Popular Drug Molecules Interacting with Chiral Phases

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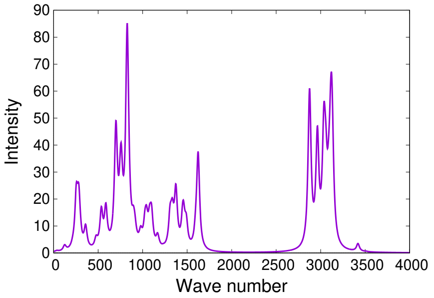
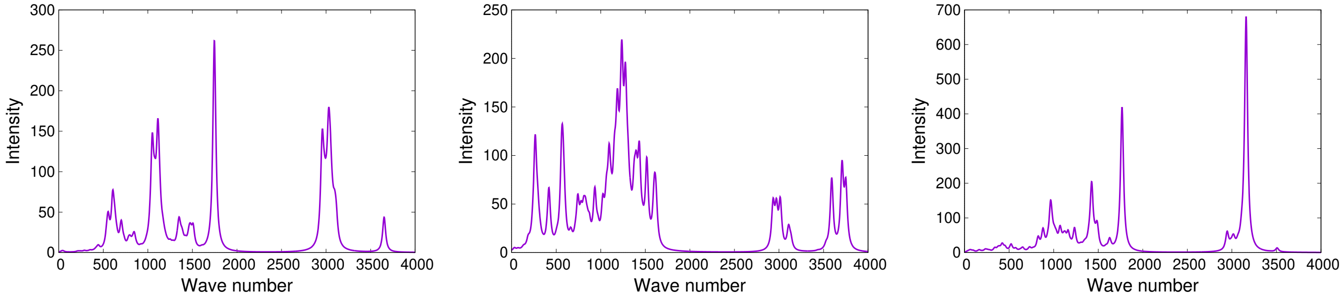
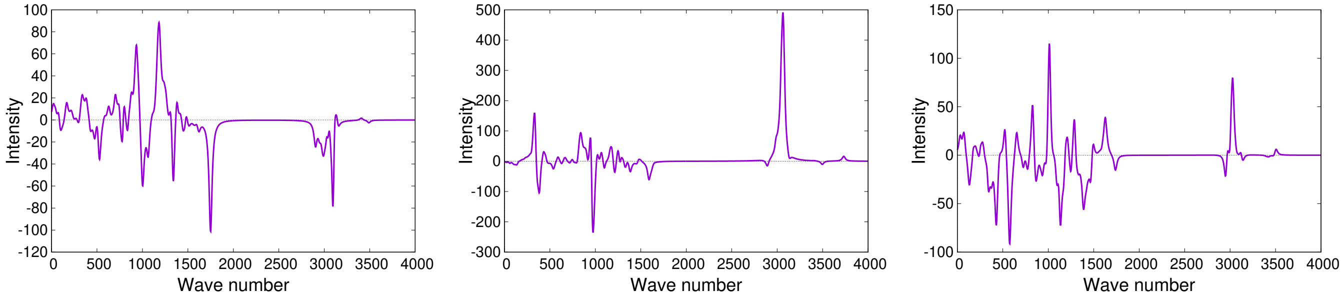


(a) phenethylamine (**Phe**) (b) proline (**Pro**)

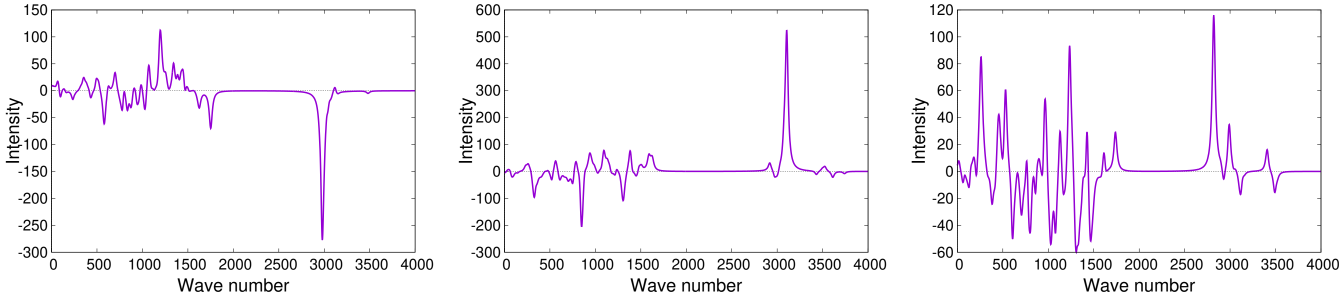


(c) ibuprofen (**Ibu**) (d) norepinephrine (**Nor**) (e) baclofen (**Bac**)

Figure FS1: Simulated B97-D3/aug-cc-pVTZ IR spectra for the monomers under study.

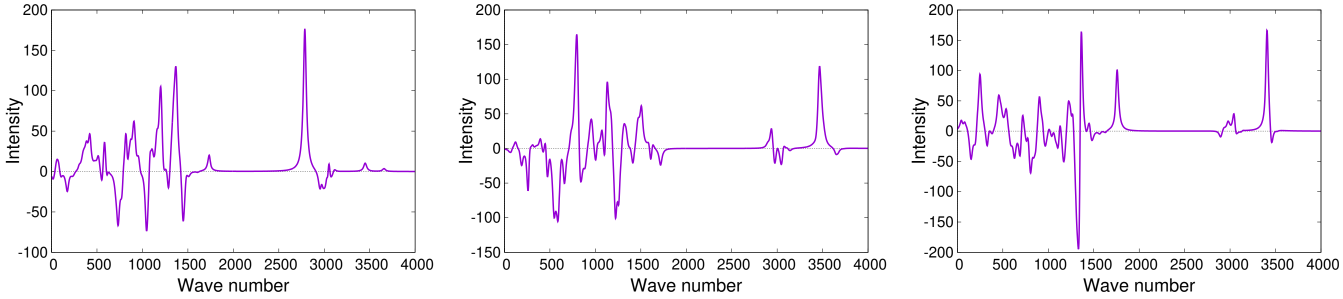


(a) (R)**Ibu** – (R)**Phe** (b) (R)**Nor** – (R)**Phe** (c) (R)**Bac** – (R)**Phe**

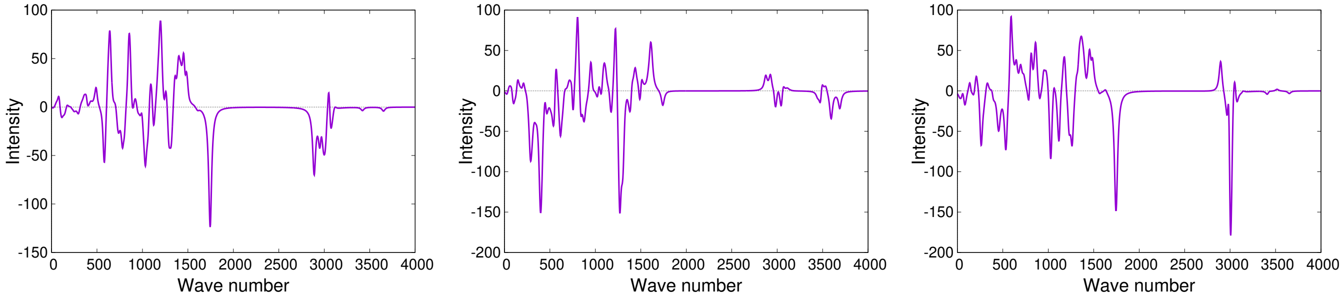


(d) (S)**Ibu** – (R)**Phe** (e) (S)**Nor** – (R)**Phe** (f) (S)**Bac** – (R)**Phe**

Figure FS2: Simulated B97-D3/aug-cc-pVTZ VCD spectra for complexes with phenethylamine.

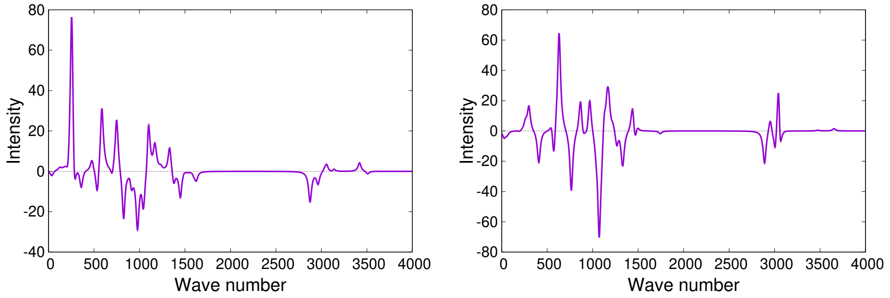


(a) (R)**Ibu** – (R)**Pro** (b) (R)**Nor** – (R)**Pro** (c) (R)**Bac** – (R)**Pro**

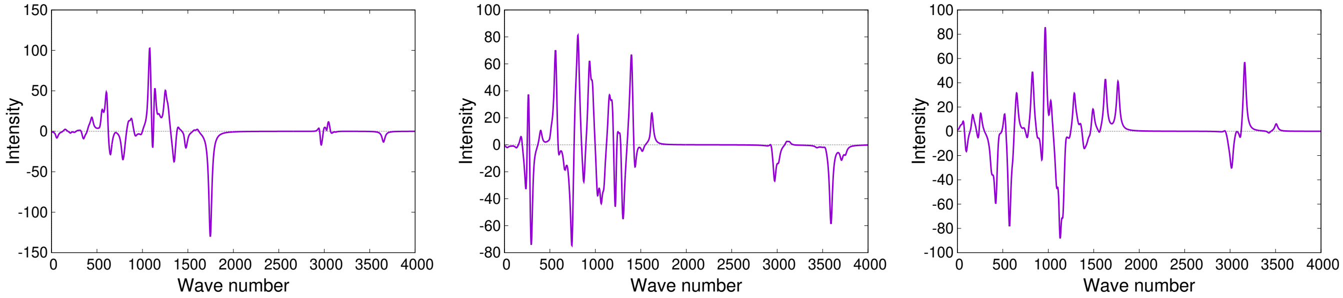


(d) (S)**Ibu** – (R)**Pro** (e) (S)**Nor** – (R)**Pro** (f) (S)**Bac** – (R)**Pro**

Figure FS3: Simulated B97-D3/aug-cc-pVTZ VCD spectra for complexes with proline.



(a) phenethylamine ((R)-**Phe**) (b) proline ((S)-**Pro**)



(c) ibuprofen ((R)-**Ibu**) (d) norepinephrine ((S)-**Nor**) (e) baclofen ((S)-**Bac**)

Figure FS4: Simulated B97-D3/aug-cc-pVTZ VCD spectra for the monomers under study.

Table TS1: B97-D3/aug-cc-pVTZ optimized geometry of the (S)**Bac** – (S)**Phe** complex.

At.	X	Y	Z	At.	X	Y	Z
C	5.071 623 1	−3.405 941 3	0.083 628 7	C	0.709 173 3	−0.014 141 9	−0.493 074 2
C	6.204 299 6	−3.284 759 0	1.089 627 5	C	2.230 795 4	−0.270 978 1	−0.543 494 5
C	6.513 254 3	−2.025 120 0	1.622 887 7	C	2.792 258 4	−0.419 143 5	0.863 184 6
C	7.566 567 2	−1.850 286 3	2.520 983 0	C	3.568 715 1	0.598 682 1	1.431 760 6
C	8.332 176 8	−2.955 374 3	2.893 911 1	C	4.061 679 6	0.485 958 5	2.736 010 2
C	8.048 505 5	−4.224 253 7	2.388 294 8	C	3.789 904 9	−0.658 095 4	3.488 917 7
Cl	9.660 488 0	−2.751 012 1	4.025 790 2	C	3.018 077 0	−1.681 250 2	2.930 074 6
C	6.985 399 8	−4.377 833 3	1.495 084 7	C	2.517 049 7	−1.560 515 1	1.632 369 1
C	5.594 002 9	−3.499 481 0	−1.368 929 1	N	2.603 952 2	−1.434 759 2	−1.380 818 3
N	5.962 150 8	−4.887 567 9	−1.746 810 8	H	2.284 877 9	−1.268 786 2	−2.332 732 9
H	6.320 274 7	−4.906 904 2	−2.697 824 0	H	2.099 142 4	−2.261 948 9	−1.066 016 1
H	6.709 354 6	−5.230 698 5	−1.148 890 9	H	0.315 124 2	0.133 237 9	−1.505 756 9
C	4.092 110 5	−4.544 184 4	0.477 282 9	H	0.475 309 9	0.873 751 5	0.106 432 3
C	2.948 186 4	−4.752 497 4	−0.512 840 0	H	0.198 808 8	−0.874 828 1	−0.046 038 9
O	1.808 622 7	−4.379 536 3	−0.305 075 3	H	2.711 374 9	0.604 104 0	−1.000 128 1
O	3.274 903 5	−5.392 721 7	−1.652 071 3	H	3.790 994 9	1.489 988 8	0.847 732 4
H	4.273 854 2	−5.481 777 1	−1.703 366 6	H	4.663 087 3	1.287 486 9	3.158 400 4
H	4.502 443 3	−2.472 991 9	0.112 598 2	H	4.181 352 6	−0.755 940 1	4.498 038 5
H	5.904 994 9	−1.167 002 0	1.349 933 5	H	2.805 791 8	−2.578 219 3	3.507 046 4
H	7.786 623 6	−0.871 499 9	2.935 058 4	H	1.929 450 1	−2.372 646 3	1.211 435 1
H	8.644 404 4	−5.077 101 7	2.697 192 5				
H	6.761 132 2	−5.379 531 4	1.136 564 2				
H	4.791 046 4	−3.178 015 8	−2.039 849 4				
H	6.427 757 1	−2.793 292 2	−1.485 266 6				
H	4.632 628 4	−5.491 125 3	0.576 911 3				
H	3.655 276 3	−4.298 444 9	1.446 835 8				

Table TS2: B97-D3/aug-cc-pVTZ optimized geometry of the (S)**Bac** – (S)**Pro** complex.

At.	X	Y	Z	At.	X	Y	Z
C	1.015 016 7	0.919 810 7	0.787 043 5	C	−1.766 290 3	−2.612 491 5	2.547 015 5
C	−0.355 147 4	1.114 520 9	0.962 372 7	C	−0.286 240 1	−2.187 111 0	2.766 726 2
C	−1.250 561 6	0.303 938 3	0.262 327 6	C	−0.386 115 6	−1.199 000 4	3.947 085 5
C	−0.795 385 2	−0.685 515 1	−0.606 712 2	N	−1.711 468 1	−0.545 590 6	3.835 135 3
C	0.581 369 1	−0.856 920 5	−0.774 478 8	C	−2.598 034 8	−1.682 365 2	3.484 655 5
C	1.508 176 7	−0.060 499 9	−0.087 667 6	H	−1.678 157 6	0.050 210 2	3.006 354 0
C	3.000 256 4	−0.263 911 2	−0.270 908 5	C	0.726 748 1	−0.175 361 7	4.114 411 8
C	3.653 868 5	−0.814 755 0	1.014 539 5	O	1.900 186 3	−0.365 211 7	3.858 489 6
C	3.280 816 9	−2.275 906 1	1.254 619 1	O	0.323 983 3	1.003 492 8	4.635 820 1
O	3.366 978 4	−3.120 695 0	0.389 492 9	H	−0.644 769 9	0.931 049 2	4.779 791 0
O	2.875 500 5	−2.609 156 3	2.503 675 5	H	−1.928 997 9	−3.667 065 2	2.788 756 0
C	3.691 300 9	1.035 854 7	−0.740 523 9	H	−2.054 756 1	−2.463 469 2	1.502 857 2
N	5.098 002 8	0.779 391 5	−1.078 704 0	H	0.107 791 0	−1.667 284 2	1.890 869 5
Cl	−2.980 393 0	0.518 093 9	0.511 638 7	H	0.381 025 6	−3.023 790 0	2.975 192 1
H	2.655 037 2	−1.807 339 4	3.028 007 9	H	−0.393 436 0	−1.768 004 7	4.891 303 3
H	5.161 708 8	0.188 004 0	−1.903 079 7	H	−2.865 255 4	−2.202 921 5	4.411 747 7
H	5.579 575 8	1.646 108 7	−1.296 555 5	H	−3.514 704 9	−1.309 259 4	3.022 481 1
H	1.703 915 9	1.536 780 8	1.356 545 1				
H	−0.724 185 7	1.885 437 4	1.631 867 3				
H	−1.504 052 6	−1.314 588 3	−1.135 461 6				
H	0.940 294 2	−1.637 081 2	−1.440 944 0				
H	3.149 246 1	−1.019 841 0	−1.052 014 7				
H	3.403 423 1	−0.182 474 5	1.870 848 4				
H	4.741 548 3	−0.784 933 0	0.879 953 6				
H	3.099 838 2	1.456 027 5	−1.572 158 5				
H	3.672 343 4	1.775 822 0	0.069 585 9				

Table TS3: B97-D3/aug-cc-pVTZ optimized geometry of the (R)**Ibu** – (R)**Phe** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−1.499 135 9	0.332 860 5	−1.369 405 5	C	2.332 595 6	−0.516 009 0	−6.280 534 9
C	−0.240 749 4	0.250 432 4	−2.252 415 3	C	2.466 547 2	−1.169 009 0	−7.515 464 5
C	0.034 386 7	−1.187 572 1	−2.683 109 8	C	2.915 554 3	−2.488 233 0	−7.584 648 2
C	−0.651 925 3	−1.726 098 0	−3.779 059 9	C	3.248 853 0	−3.174 739 4	−6.412 641 5
C	−0.430 650 8	−3.039 447 3	−4.194 141 1	C	3.125 373 5	−2.530 968 5	−5.181 053 6
C	0.480 708 7	−3.863 214 3	−3.523 131 9	C	2.666 226 1	−1.212 383 7	−5.112 976 4
C	1.141 448 0	−3.332 827 7	−2.406 610 6	C	1.787 909 5	0.904 777 0	−6.264 727 4
C	0.925 363 2	−2.018 980 2	−1.990 133 1	C	0.256 420 9	0.918 962 1	−6.384 386 1
C	0.745 705 5	−5.281 041 9	−3.968 414 2	N	2.176 505 5	1.625 692 7	−5.027 046 1
C	0.081 952 2	−6.357 446 8	−3.074 548 3	H	3.191 624 3	1.643 146 3	−4.945 320 2
C	−1.448 116 6	−6.246 767 8	−3.103 932 4	H	1.877 170 6	2.595 471 1	−5.098 085 9
C	0.540 204 5	−7.758 481 5	−3.502 295 3	H	2.217 061 3	−0.636 314 8	−8.431 807 5
C	0.976 943 1	0.840 703 6	−1.518 778 9	H	3.012 583 1	−2.976 788 2	−8.551 101 6
O	1.064 899 9	0.879 177 5	−0.311 015 3	H	3.601 747 6	−4.201 704 9	−6.461 578 4
O	1.989 025 8	1.284 173 0	−2.294 042 6	H	3.367 595 2	−3.055 765 8	−4.262 059 5
H	1.811 047 9	1.244 319 8	−3.276 584 3	H	2.554 386 9	−0.742 863 7	−4.142 179 8
H	−2.355 582 0	−0.093 212 9	−1.901 816 8	H	2.197 893 4	1.418 611 1	−7.150 128 7
H	−1.722 268 1	1.371 801 9	−1.105 309 9	H	−0.186 417 8	0.395 318 3	−5.533 862 2
H	−1.340 993 2	−0.227 177 3	−0.444 509 3	H	−0.054 893 9	0.413 325 2	−7.303 055 5
H	−0.405 794 7	0.844 349 6	−3.162 012 1	H	−0.124 630 2	1.947 635 0	−6.409 032 1
H	−1.369 181 3	−1.109 526 3	−4.316 694 7				
H	−0.961 352 7	−3.426 217 4	−5.061 663 6				
H	1.851 933 3	−3.953 859 4	−1.863 663 3				
H	1.460 152 0	−1.634 550 1	−1.125 347 0				
H	0.396 133 5	−5.418 686 5	−5.000 742 8				
H	1.830 049 4	−5.457 476 3	−3.978 185 9				
H	0.419 533 6	−6.180 791 8	−2.042 867 6				
H	−1.822 574 3	−6.413 251 7	−4.122 927 9				
H	−1.784 115 0	−5.256 830 2	−2.779 076 3				
H	−1.907 056 9	−6.997 654 9	−2.450 661 2				
H	0.234 177 5	−7.962 708 3	−4.536 763 3				
H	0.096 538 9	−8.531 051 0	−2.863 673 8				
H	1.631 186 1	−7.856 104 8	−3.448 776 1				

Table TS4: B97-D3/aug-cc-pVTZ optimized geometry of the (R)**Ibu** – (R)**Pro** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−1.522 857 8	0.503 710 9	−1.099 841 2	C	3.720 964 3	−0.479 471 4	−6.219 425 9
C	−0.337 278 4	0.373 083 2	−2.070 805 8	C	4.728 567 7	−0.336 358 5	−5.069 008 3
C	−0.145 548 2	−1.059 679 1	−2.528 434 4	C	4.037 201 5	−1.112 181 8	−3.915 115 3
C	−0.591 635 0	−1.482 277 3	−3.784 940 6	N	2.589 166 6	−0.916 951 5	−4.133 227 8
C	−0.373 423 5	−2.791 579 5	−4.223 691 0	C	2.377 596 1	−0.335 038 5	−5.491 013 7
C	0.299 801 4	−3.720 217 8	−3.419 631 9	H	2.107 426 5	−1.808 788 9	−4.055 549 9
C	0.719 545 9	−3.300 357 7	−2.146 738 0	C	4.420 562 1	−2.589 365 5	−3.940 009 6
C	0.495 739 1	−1.997 808 9	−1.705 753 3	O	3.709 000 8	−3.501 206 8	−4.302 229 1
C	0.555 356 3	−5.134 826 2	−3.878 420 3	O	5.697 162 1	−2.769 149 1	−3.499 051 4
C	−0.379 605 1	−6.179 632 0	−3.220 908 0	H	5.882 294 6	−3.722 057 8	−3.551 692 9
C	−1.847 347 5	−5.937 692 9	−3.597 510 0	H	3.863 236 0	0.268 975 1	−7.004 435 5
C	0.059 050 2	−7.599 576 5	−3.604 037 2	H	3.801 602 0	−1.474 989 1	−6.671 025 6
C	0.944 210 3	1.001 093 6	−1.463 721 1	H	4.827 348 4	0.713 831 0	−4.774 076 3
O	0.920 080 8	1.680 873 2	−0.459 717 7	H	5.725 031 7	−0.723 633 3	−5.292 069 2
O	2.092 993 7	0.806 920 0	−2.135 413 7	H	4.340 204 7	−0.711 045 0	−2.941 077 4
H	2.062 533 3	0.130 370 9	−2.894 582 5	H	1.549 696 3	−0.844 034 1	−5.991 440 6
H	−2.438 498 7	0.141 307 3	−1.578 830 9	H	2.111 122 8	0.724 756 3	−5.384 242 2
H	−1.655 432 0	1.544 129 4	−0.793 489 7				
H	−1.341 282 4	−0.092 309 6	−0.200 242 1				
H	−0.548 624 7	0.982 633 9	−2.962 252 6				
H	−1.093 534 0	−0.772 478 7	−4.440 232 4				
H	−0.716 729 8	−3.093 719 7	−5.211 025 9				
H	1.246 556 3	−4.002 859 0	−1.504 088 0				
H	0.856 027 4	−1.690 300 0	−0.726 286 1				
H	0.440 665 5	−5.200 052 0	−4.968 904 3				
H	1.596 685 3	−5.397 809 2	−3.655 763 8				
H	−0.281 662 6	−6.068 326 5	−2.131 063 4				
H	−1.983 626 7	−6.039 631 7	−4.682 547 6				
H	−2.174 949 3	−4.933 264 6	−3.310 248 0				
H	−2.503 088 8	−6.665 981 7	−3.106 845 7				
H	−0.009 554 5	−7.741 717 2	−4.690 478 6				
H	−0.579 945 5	−8.351 783 8	−3.127 155 9				
H	1.096 194 3	−7.791 531 8	−3.304 707 1				

Table TS5: B97-D3/aug-cc-pVTZ optimized geometry of the (S)**Nor** – (S)**Phe** complex.

At.	X	Y	Z	At.	X	Y	Z
C	6.330 080 2	−3.497 409 1	1.620 417 0	C	0.958 676 0	−0.046 215 1	−0.195 358 5
C	5.859 725 8	−2.621 728 9	0.638 534 2	C	2.479 387 5	−0.110 262 3	0.020 603 8
C	6.248 607 5	−1.277 016 2	0.607 752 6	C	2.868 980 9	−0.574 870 2	1.415 146 1
C	7.165 579 3	−0.827 087 6	1.587 058 4	C	3.780 951 8	0.165 206 0	2.175 629 0
C	7.639 116 9	−1.710 633 5	2.556 637 0	C	4.195 238 0	−0.285 039 5	3.430 667 3
C	7.223 648 4	−3.049 840 0	2.598 413 5	C	3.700 673 2	−1.485 284 1	3.944 271 1
C	7.669 150 5	−3.944 579 3	3.734 778 0	C	2.787 535 9	−2.231 824 7	3.194 328 7
O	7.828 563 2	−5.320 916 3	3.337 366 6	C	2.375 223 1	−1.777 861 2	1.939 741 9
H	8.278 173 3	−5.326 415 3	2.482 855 2	N	3.173 129 1	−0.976 194 0	−0.981 282 3
C	6.651 430 2	−3.956 271 1	4.904 918 4	H	2.882 301 7	−0.719 919 7	−1.922 809 0
N	5.320 058 8	−4.473 582 4	4.591 023 6	H	2.892 600 2	−1.944 465 0	−0.840 937 1
H	4.907 842 2	−3.916 051 7	3.846 447 7	H	0.731 311 7	0.338 135 9	−1.196 920 0
H	5.418 325 1	−5.415 162 2	4.219 765 7	H	0.490 555 4	0.613 824 6	0.542 941 6
O	7.535 916 5	0.498 023 2	1.541 689 6	H	0.504 619 9	−1.038 729 9	−0.100 978 6
H	8.181 069 9	0.659 672 0	2.241 830 9	H	2.892 180 7	0.894 967 9	−0.125 293 6
O	5.791 520 8	−0.389 461 5	−0.309 967 9	H	4.203 519 0	1.078 172 0	1.764 638 1
H	4.909 327 4	−0.701 839 8	−0.661 906 9	H	4.918 992 0	0.294 870 2	3.996 977 5
H	6.004 682 0	−4.533 114 1	1.626 544 6	H	4.029 509 8	−1.849 971 6	4.913 386 9
H	5.169 889 4	−2.975 321 9	−0.122 804 0	H	2.403 349 7	−3.169 423 1	3.588 007 0
H	8.336 630 3	−1.340 571 5	3.309 621 7	H	1.665 312 2	−2.372 847 5	1.368 639 8
H	8.625 052 0	−3.562 331 6	4.135 339 9				
H	6.556 976 0	−2.928 838 5	5.277 611 4				
H	7.078 586 2	−4.564 791 3	5.711 673 4				

Table TS6: B97-D3/aug-cc-pVTZ optimized geometry of the (R)**Nor** – (R)**Pro** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−0.286 697 8	−2.765 713 0	−2.207 864 1	C	1.418 384 5	−6.187 890 1	−0.450 588 7
C	0.170 882 9	−3.449 656 4	−3.338 782 6	C	2.484 134 8	−5.350 392 3	−1.203 085 7
C	−0.324 234 2	−4.717 888 1	−3.634 810 8	C	3.015 651 9	−6.344 291 0	−2.293 916 0
C	−1.304 569 0	−5.297 390 5	−2.804 584 6	N	1.915 574 9	−7.254 181 7	−2.603 875 2
C	−1.756 756 6	−4.611 525 4	−1.679 532 6	C	1.237 420 3	−7.478 234 2	−1.310 989 5
C	−1.246 830 5	−3.343 985 4	−1.368 969 9	H	1.275 769 6	−6.795 707 4	−3.246 179 3
C	−1.660 584 2	−2.647 858 1	−0.090 714 0	C	3.520 221 9	−5.593 333 2	−3.503 687 6
C	−0.833 952 4	−3.159 548 5	1.111 488 8	O	2.866 075 3	−5.268 186 3	−4.480 656 4
N	0.582 491 2	−2.801 873 7	0.961 682 3	O	4.823 546 6	−5.246 419 2	−3.370 210 2
O	−3.060 526 1	−2.896 830 2	0.132 834 3	H	5.059 782 9	−4.717 375 4	−4.151 893 0
O	−1.796 112 3	−6.547 645 1	−3.077 079 5	H	1.744 724 2	−6.433 512 0	0.565 366 3
O	0.083 575 8	−5.470 949 7	−4.717 217 7	H	0.480 384 9	−5.633 179 5	−0.377 517 7
H	0.976 167 9	−3.292 904 1	0.163 393 7	H	2.016 986 4	−4.492 678 1	−1.695 310 8
H	1.108 293 9	−3.099 653 0	1.777 880 9	H	3.289 988 6	−4.985 681 0	−0.559 769 9
H	−3.306 169 8	−2.475 708 8	0.966 073 2	H	3.850 607 2	−6.918 117 4	−1.872 688 3
H	−1.374 385 0	−6.852 778 9	−3.895 705 4	H	1.711 598 0	−8.332 428 5	−0.811 475 0
H	1.041 522 1	−5.327 041 6	−4.856 202 6	H	0.187 865 1	−7.727 755 5	−1.485 308 4
H	0.108 307 4	−1.780 422 0	−1.976 416 2				
H	0.918 503 3	−3.009 988 3	−3.993 696 4				
H	−2.507 338 7	−5.072 145 1	−1.045 445 1				
H	−1.471 204 9	−1.568 465 3	−0.197 063 8				
H	−1.028 785 5	−4.241 745 4	1.208 060 8				
H	−1.211 314 3	−2.671 921 5	2.021 456 9				

Table TS7: B97-D3/aug-cc-pVTZ optimized geometry of the (S)**Bac** – (R)**Phe** complex.

At.	X	Y	Z	At.	X	Y	Z
C	0.894 243 2	1.644 457 5	0.015 252 5	C	−0.795 532 2	−1.400 017 5	3.543 334 7
C	−0.458 335 1	1.863 362 7	0.285 513 0	C	−2.179 359 2	−1.291 870 1	3.360 289 5
C	−1.316 363 2	0.767 058 8	0.391 811 3	C	−2.896 625 4	−2.290 195 9	2.695 029 5
C	−0.838 023 2	−0.533 500 8	0.234 774 2	C	−2.231 657 0	−3.412 625 6	2.197 704 0
C	0.516 041 4	−0.728 091 3	−0.046 478 5	C	−0.848 540 4	−3.529 090 1	2.373 597 8
C	1.406 297 4	0.348 889 4	−0.162 325 4	C	−0.136 237 5	−2.533 913 9	3.043 796 2
C	2.887 016 9	0.102 210 5	−0.386 796 0	C	−0.040 428 0	−0.298 287 9	4.270 746 8
C	3.637 714 9	0.024 785 4	0.970 311 1	C	0.692 315 7	−0.807 611 9	5.518 833 5
C	3.528 791 8	−1.363 831 5	1.603 241 7	N	0.958 374 6	0.340 278 6	3.356 342 6
O	4.001 211 9	−2.341 404 1	1.058 670 7	H	0.505 208 0	0.616 570 6	2.487 273 1
O	2.917 284 2	−1.458 741 4	2.798 200 1	H	1.306 527 6	1.193 720 0	3.788 169 3
C	3.531 020 5	1.140 125 1	−1.329 193 3	H	−2.702 463 0	−0.411 183 5	3.726 198 2
N	4.912 354 1	0.756 536 0	−1.645 607 4	H	−3.969 037 6	−2.182 651 0	2.555 716 5
Cl	−3.017 835 5	1.038 264 3	0.736 093 1	H	−2.784 455 7	−4.190 138 8	1.676 278 8
H	2.287 692 7	−0.685 176 2	2.987 430 8	H	−0.320 456 5	−4.397 175 8	1.987 003 7
H	4.932 515 5	−0.131 913 7	−2.139 100 7	H	0.937 760 8	−2.633 528 0	3.157 772 6
H	5.349 327 3	1.446 250 4	−2.248 446 9	H	−0.782 428 8	0.450 421 3	4.587 386 1
H	1.551 673 0	2.506 331 5	−0.052 927 2	H	1.436 186 6	−1.562 318 1	5.247 939 3
H	−0.845 322 5	2.869 582 7	0.412 294 8	H	−0.020 303 5	−1.252 785 4	6.219 831 4
H	−1.505 939 1	−1.378 590 0	0.356 709 8	H	1.207 276 6	0.017 118 1	6.026 677 9
H	0.888 744 1	−1.743 820 3	−0.152 523 4				
H	3.003 436 8	−0.879 231 8	−0.864 911 4				
H	3.281 677 0	0.814 148 3	1.640 884 9				
H	4.703 264 9	0.183 560 3	0.772 438 0				
H	2.878 907 9	1.248 114 5	−2.213 162 4				
H	3.570 477 5	2.120 909 0	−0.838 075 1				

Table TS8: B97-D3/aug-cc-pVTZ optimized geometry of the (R)**Bac** – (S)**Pro** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−0.473 994 8	0.769 112 9	0.411 223 2	C	1.002 142 1	−0.345 922 2	3.869 770 7
C	0.917 064 0	0.661 856 5	0.346 075 4	C	1.609 599 1	−1.569 326 7	3.134 695 4
C	1.484 892 4	−0.387 274 8	−0.375 972 7	C	0.372 486 9	−2.298 010 5	2.536 935 3
C	0.682 193 8	−1.315 855 6	−1.039 339 2	N	−0.757 689 1	−1.992 171 9	3.438 716 0
C	−0.706 050 0	−1.186 837 1	−0.968 907 9	C	−0.535 118 7	−0.589 456 4	3.860 136 4
C	−1.310 708 2	−0.149 043 3	−0.241 186 7	H	−0.683 455 3	−2.616 940 3	4.241 561 0
C	−2.824 173 6	−0.093 630 2	−0.124 710 5	C	0.587 170 2	−3.795 610 2	2.448 888 0
C	−3.304 985 9	−0.954 769 6	1.067 691 8	O	0.359 823 9	−4.572 993 1	3.350 515 9
C	−3.143 964 8	−2.450 129 9	0.792 769 4	O	1.121 535 7	−4.157 634 8	1.255 025 9
O	−3.552 528 5	−2.959 099 5	−0.231 425 2	H	1.256 522 6	−5.120 398 7	1.287 724 3
O	−2.549 425 7	−3.189 918 4	1.746 962 9	H	1.248 228 3	0.588 546 1	3.357 211 1
C	−3.381 138 7	1.340 046 2	−0.033 894 4	H	1.387 663 1	−0.274 071 0	4.890 942 0
N	−4.847 281 9	1.324 591 9	−0.130 874 3	H	2.323 889 1	−1.293 119 6	2.356 351 4
Cl	3.233 942 8	−0.551 115 6	−0.429 708 2	H	2.114 070 9	−2.233 108 9	3.844 617 7
H	−2.094 938 0	−2.628 125 7	2.444 673 9	H	0.147 135 1	−1.899 557 4	1.545 235 8
H	−5.137 650 2	0.999 278 9	−1.049 041 8	H	−1.013 691 8	−0.411 299 3	4.827 017 4
H	−5.225 844 7	2.259 081 0	−0.012 693 7	H	−1.007 807 9	0.067 249 1	3.122 797 2
H	−0.900 497 3	1.587 729 9	0.983 628 3				
H	1.555 276 3	1.379 047 5	0.852 166 4				
H	1.137 097 9	−2.133 469 7	−1.588 124 6				
H	−1.334 659 0	−1.920 350 3	−1.466 422 8				
H	−3.246 683 1	−0.554 738 3	−1.026 676 1				
H	−4.376 844 5	−0.771 340 2	1.207 611 2				
H	−2.788 463 7	−0.651 175 5	1.983 309 9				
H	−3.124 411 1	1.781 943 9	0.937 872 7				
H	−2.886 728 2	1.953 010 3	−0.807 148 8				

Table TS9: B97-D3/aug-cc-pVTZ optimized geometry of the (R)**Ibu** – (S)**Phe** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−0.883 623 3	0.098 625 8	−0.538 108 5	C	2.218 184 8	−0.700 473 4	−5.743 563 5
C	0.017 207 0	0.294 184 5	−1.770 012 7	C	3.368 023 6	−0.524 002 4	−4.965 558 1
C	0.128 893 0	−0.996 014 1	−2.572 583 1	C	4.327 055 1	−1.538 142 8	−4.870 265 1
C	−0.862 849 0	−1.326 706 9	−3.504 631 3	C	4.153 016 8	−2.742 040 7	−5.553 197 9
C	−0.815 272 7	−2.530 789 3	−4.210 095 4	C	3.006 409 8	−2.929 429 3	−6.330 783 8
C	0.225 944 4	−3.444 921 2	−4.006 628 4	C	2.049 363 6	−1.920 422 4	−6.417 166 0
C	1.214 218 2	−3.112 728 7	−3.070 599 5	C	1.138 786 2	0.362 888 8	−5.893 169 7
C	1.168 766 8	−1.912 067 0	−2.363 933 8	C	1.015 956 9	0.839 696 6	−7.355 064 6
C	0.282 685 7	−4.762 855 5	−4.739 077 2	N	1.342 403 7	1.502 953 6	−4.964 370 1
C	−0.184 763 4	−5.970 526 9	−3.888 940 5	H	0.547 122 8	2.132 540 5	−5.042 760 7
C	−1.663 796 7	−5.848 510 6	−3.499 535 3	H	2.150 036 9	2.045 760 8	−5.269 423 9
C	0.079 595 7	−7.283 262 2	−4.638 966 6	H	3.519 388 8	0.386 883 4	−4.397 111 5
C	1.404 568 6	0.823 576 2	−1.354 800 6	H	5.206 777 1	−1.383 777 7	−4.250 711 5
O	1.815 799 2	0.786 560 4	−0.215 328 8	H	4.898 605 3	−3.529 378 0	−5.476 951 5
O	2.160 481 7	1.326 518 3	−2.349 452 9	H	2.850 822 9	−3.866 551 1	−6.858 991 8
H	1.721 074 8	1.271 998 0	−3.252 424 4	H	1.147 457 3	−2.090 956 8	−7.000 094 9
H	−1.872 956 1	−0.250 120 4	−0.851 675 8	H	0.191 231 8	−0.100 797 0	−5.592 854 0
H	−0.989 502 7	1.035 133 4	0.018 023 2	H	1.951 152 8	1.314 980 4	−7.674 880 4
H	−0.442 419 0	−0.644 095 6	0.131 533 2	H	0.201 407 7	1.567 695 2	−7.452 615 0
H	−0.434 850 5	1.054 551 9	−2.423 240 1	H	0.812 960 0	0.005 646 4	−8.033 504 0
H	−1.684 041 9	−0.632 853 4	−3.679 488 3				
H	−1.595 926 6	−2.763 444 7	−4.932 094 6				
H	2.043 996 2	−3.796 898 9	−2.907 477 1				
H	1.955 514 9	−1.679 911 7	−1.650 474 9				
H	−0.334 981 4	−4.715 760 5	−5.647 125 3				
H	1.314 576 2	−4.944 250 1	−5.066 008 4				
H	0.414 428 5	−5.970 795 3	−2.966 757 7				
H	−2.295 367 4	−5.840 831 9	−4.398 223 5				
H	−1.856 621 4	−4.925 079 7	−2.944 190 3				
H	−1.975 577 7	−6.695 294 7	−2.877 494 4				
H	−0.489 609 8	−7.311 526 9	−5.577 566 7				
H	−0.224 009 5	−8.148 493 2	−4.038 296 1				
H	1.142 085 2	−7.395 220 7	−4.886 205 1				

Table TS10: B97-D3/aug-cc-pVTZ optimized geometry of the (R)**Ibu** – (S)**Pro** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−1.328 913 4	0.354 191 7	−1.150 160 7	C	1.252 049 5	−0.377 370 1	−6.725 109 4
C	−0.095 247 2	0.338 737 1	−2.068 758 9	C	2.571 036 1	−1.124 033 9	−6.464 677 0
C	0.146 363 0	−1.053 396 5	−2.633 893 3	C	2.825 909 9	−0.824 017 3	−4.965 851 7
C	−0.525 214 5	−1.468 309 1	−3.790 251 1	N	2.373 664 9	0.568 320 3	−4.761 691 4
C	−0.336 943 2	−2.749 021 7	−4.314 243 7	C	1.292 178 3	0.835 379 5	−5.756 321 5
C	0.532 475 1	−3.659 772 8	−3.700 206 3	H	3.172 641 7	1.171 528 1	−4.950 979 2
C	1.189 896 3	−3.248 235 3	−2.531 188 1	C	4.290 674 7	−0.968 893 1	−4.608 111 0
C	0.999 221 9	−1.970 898 4	−2.003 097 7	O	5.105 870 5	−0.072 764 4	−4.643 521 3
C	0.736 590 5	−5.052 984 2	−4.245 178 8	O	4.600 722 8	−2.254 975 7	−4.291 435 7
C	−0.012 773 9	−6.150 389 8	−3.447 926 6	H	5.557 724 2	−2.276 586 8	−4.118 703 0
C	−1.532 423 6	−5.943 976 5	−3.495 781 9	H	1.148 412 7	−0.068 636 2	−7.769 295 0
C	0.369 687 3	−7.541 183 4	−3.971 918 3	H	0.406 853 5	−1.024 888 8	−6.476 585 1
C	1.149 009 9	0.877 902 8	−1.329 564 7	H	3.385 375 1	−0.697 720 4	−7.063 112 9
O	1.172 037 8	1.063 323 1	−0.131 319 3	H	2.510 852 1	−2.196 309 9	−6.667 644 6
O	2.226 645 8	1.125 920 1	−2.092 365 9	H	2.231 486 8	−1.501 300 3	−4.348 880 5
H	2.110 829 5	0.893 290 3	−3.069 090 5	H	0.336 735 2	0.948 553 4	−5.234 620 4
H	−2.208 217 7	0.000 366 4	−1.698 675 2	H	1.500 668 5	1.775 110 3	−6.277 461 2
H	−1.518 320 2	1.364 085 1	−0.775 105 0				
H	−1.161 864 7	−0.298 720 4	−0.289 419 4				
H	−0.275 927 7	1.015 426 1	−2.916 116 7				
H	−1.200 100 9	−0.776 942 6	−4.291 199 3				
H	−0.867 080 0	−3.044 231 2	−5.217 748 7				
H	1.873 908 9	−3.934 663 0	−2.036 122 8				
H	1.533 995 5	−1.677 025 4	−1.103 031 0				
H	0.406 220 0	−5.097 512 3	−5.292 290 5				
H	1.808 840 4	−5.291 041 9	−4.239 571 3				
H	0.311 825 5	−6.071 974 8	−2.400 129 6				
H	−1.893 881 0	−6.005 735 5	−4.531 053 1				
H	−1.817 529 3	−4.965 151 7	−3.096 971 6				
H	−2.049 061 7	−6.715 293 2	−2.913 515 3				
H	0.070 773 2	−7.651 155 5	−5.022 703 0				
H	−0.131 202 9	−8.329 245 3	−3.398 037 4				
H	1.451 525 1	−7.708 777 0	−3.910 363 9				

Table TS11: B97-D3/aug-cc-pVTZ optimized geometry of the (S)**Nor** – (R)**Phe** complex.

At.	X	Y	Z	At.	X	Y	Z
C	−7.633 501 9	−1.578 255 8	2.526 283 4	C	−1.130 873 9	0.309 342 6	−0.300 381 0
C	−7.126 315 7	−0.615 438 0	1.647 225 1	C	−2.579 581 8	−0.200 584 2	−0.153 912 2
C	−6.312 637 1	−0.981 518 6	0.577 177 3	C	−2.858 766 8	−0.631 623 0	1.280 094 6
C	−5.988 627 5	−2.340 858 2	0.371 803 7	C	−2.958 584 4	0.359 516 9	2.269 170 2
C	−6.515 941 9	−3.288 003 7	1.252 111 5	C	−3.195 430 5	0.026 429 3	3.601 994 4
C	−7.329 390 0	−2.926 390 2	2.333 594 1	C	−3.336 484 8	−1.315 189 9	3.972 026 4
C	−7.782 186 9	−4.000 348 1	3.320 330 5	C	−3.247 019 8	−2.308 366 1	2.996 783 7
O	−8.797 913 6	−3.551 310 0	4.216 132 3	C	−3.008 311 2	−1.968 926 9	1.660 930 4
H	−8.316 055 9	−3.130 260 2	4.948 301 5	N	−2.903 529 1	−1.265 644 6	−1.130 984 7
C	−6.575 196 8	−4.521 633 9	4.135 159 5	H	−2.873 516 0	−0.877 244 1	−2.069 766 7
N	−6.109 072 5	−3.438 251 2	5.016 423 1	H	−2.191 031 1	−1.992 621 9	−1.103 127 3
H	−5.427 279 7	−3.777 503 5	5.685 981 4	H	−0.952 829 5	0.672 049 1	−1.319 760 0
H	−5.665 736 5	−2.708 604 8	4.464 237 4	H	−0.424 331 7	−0.502 346 3	−0.088 277 7
O	−5.198 149 5	−2.759 655 3	−0.653 166 8	H	−0.924 965 1	1.125 737 6	0.399 678 3
H	−4.498 682 6	−2.081 733 4	−0.870 602 6	H	−3.268 371 7	0.621 439 2	−0.379 062 8
O	−5.793 894 4	−0.062 288 0	−0.319 238 5	H	−2.859 601 3	1.406 553 7	1.987 727 5
H	−6.128 437 0	0.810 876 4	−0.080 206 8	H	−3.277 659 6	0.810 497 6	4.350 461 7
H	−8.275 107 7	−1.282 441 8	3.349 188 7	H	−3.522 174 7	−1.577 982 9	5.010 380 4
H	−7.369 513 3	0.437 010 6	1.793 130 7	H	−3.380 674 3	−3.352 559 6	3.267 199 3
H	−6.253 916 0	−4.329 653 7	1.077 445 1	H	−2.987 736 9	−2.757 613 3	0.916 365 6
H	−8.207 940 0	−4.843 411 2	2.759 527 2				
H	−5.806 112 0	−4.901 425 7	3.443 539 3				
H	−6.915 917 5	−5.352 764 9	4.763 082 9				

Table TS12: B97-D3/aug-cc-pVTZ optimized geometry of the (S)**Nor** – (R)**Pro** complex.

At.	X	Y	Z	At.	X	Y	Z
C	0.948 238 7	−2.454 625 6	3.633 227 7	C	1.163 855 1	−0.854 196 0	−0.298 075 8
C	1.412 243 6	−1.136 759 9	3.607 535 9	C	1.438 953 8	0.588 898 1	0.149 568 0
C	0.514 936 0	−0.068 463 4	3.637 660 0	C	0.064 867 0	1.274 716 8	−0.114 934 4
C	−0.872 394 2	−0.328 272 9	3.668 291 8	N	−0.944 463 6	0.221 024 2	−0.019 962 3
C	−1.318 403 3	−1.648 314 1	3.710 969 7	C	−0.274 876 4	−1.086 507 6	0.183 467 9
C	−0.421 553 0	−2.724 937 9	3.693 001 6	C	−0.169 419 4	2.446 213 8	0.829 776 1
C	−0.963 561 9	−4.151 221 2	3.661 913 7	O	−0.996 039 2	2.482 706 9	1.719 570 9
O	−0.003 849 0	−5.124 790 7	4.063 912 9	O	0.623 339 8	3.528 377 0	0.631 498 5
H	0.451 195 0	−5.380 842 9	3.242 617 3	H	−1.619 354 5	0.424 049 9	0.708 453 1
C	−1.490 220 2	−4.501 416 0	2.248 726 6	H	1.237 855 0	3.361 531 5	−0.099 472 3
N	−0.336 581 0	−4.652 505 0	1.345 990 6	H	1.221 430 3	−0.932 053 0	−1.390 298 2
H	−0.607 438 5	−5.083 578 4	0.469 361 4	H	1.868 183 8	−1.567 580 9	0.139 018 1
H	0.067 391 8	−3.744 866 7	1.135 568 8	H	1.666 681 4	0.617 701 5	1.218 698 8
O	−1.790 721 7	0.700 336 5	3.715 586 0	H	2.259 002 8	1.066 262 3	−0.396 916 3
H	−1.610 196 1	1.336 096 9	2.994 554 0	H	0.068 233 5	1.700 777 5	−1.135 016 7
O	1.020 868 8	1.209 309 0	3.627 003 4	H	−0.273 019 8	−1.382 724 9	1.239 640 4
H	0.296 495 9	1.838 379 4	3.759 076 4	H	−0.785 479 4	−1.866 240 5	−0.394 708 0
H	1.654 856 3	−3.278 131 2	3.637 765 4				
H	2.476 481 0	−0.917 288 2	3.588 437 4				
H	−2.392 627 9	−1.817 525 5	3.748 524 5				
H	−1.804 259 0	−4.220 585 1	4.365 412 4				
H	−2.006 656 3	−5.466 380 7	2.301 878 0				
H	−2.214 994 8	−3.735 570 9	1.930 675 9				

Table TS13: B97-D3/aug-cc-pVTZ optimized geometry of the baclofen.

At.	X	Y	Z
C	5.034 417 7	−3.402 037 8	0.108 244 5
C	6.179 237 8	−3.284 525 8	1.105 606 9
C	6.537 773 9	−2.022 331 3	1.602 042 5
C	7.611 514 6	−1.855 488 4	2.477 638 5
C	8.350 934 2	−2.973 428 2	2.865 726 6
C	8.020 802 4	−4.243 990 9	2.393 964 5
Cl	9.703 364 9	−2.781 087 3	3.966 327 7
C	6.938 699 2	−4.388 751 4	1.522 877 3
C	5.568 456 0	−3.471 743 2	−1.345 717 2
N	6.021 770 4	−4.836 356 3	−1.700 224 4
H	6.377 798 9	−4.850 515 8	−2.651 939 1
H	6.789 919 8	−5.120 504 0	−1.098 051 9
C	4.065 890 2	−4.557 808 4	0.474 962 5
C	2.943 437 6	−4.776 541 6	−0.543 723 9
O	1.804 563 1	−4.407 182 9	−0.370 489 6
O	3.310 868 6	−5.435 508 2	−1.670 723 0
H	4.302 757 9	−5.524 334 7	−1.687 846 1
H	4.458 520 6	−2.470 161 8	0.162 253 3
H	5.963 159 2	−1.147 833 5	1.304 242 4
H	7.871 681 5	−0.873 473 7	2.859 289 8
H	8.597 820 0	−5.106 720 5	2.710 912 9
H	6.683 844 8	−5.390 731 7	1.188 342 6
H	4.755 217 8	−3.216 849 8	−2.033 559 9
H	6.356 617 0	−2.714 162 9	−1.463 184 9
H	4.621 552 1	−5.494 873 0	0.577 588 2
H	3.601 461 0	−4.332 010 7	1.437 100 0

Table TS14: B97-D3/aug-cc-pVTZ optimized geometry of the ibuprofen.

At.	X	Y	Z
C	−0.667 998 4	−0.568 767 6	−1.090 282 7
C	0.714 766 0	−0.444 247 8	−0.966 621 3
C	1.329 561 4	−0.528 692 9	0.291 565 0
C	0.522 803 2	−0.738 914 2	1.414 358 2
C	−0.862 634 9	−0.866 118 6	1.284 844 0
C	−1.482 740 7	−0.782 924 8	0.032 315 9
H	−1.126 046 3	−0.497 953 8	−2.075 060 5
H	1.325 508 4	−0.271 768 9	−1.849 556 5
H	0.979 478 6	−0.804 370 9	2.400 063 4
H	−1.471 673 5	−1.028 727 3	2.171 629 0
C	−2.983 364 1	−0.871 859 7	−0.114 953 5
H	−3.229 533 2	−1.554 713 2	−0.939 327 8
H	−3.422 565 6	−1.301 564 7	0.795 546 8
C	−3.665 379 1	0.491 425 5	−0.391 702 9
C	−3.433 439 9	1.482 619 5	0.756 287 6
H	−3.868 712 7	1.097 062 1	1.687 903 3
H	−2.365 972 2	1.652 806 4	0.929 136 2
H	−3.905 018 3	2.447 968 5	0.539 542 5
C	2.845 840 7	−0.423 386 6	0.429 582 4
C	3.300 672 2	0.905 021 0	−0.168 350 8
O	3.205 413 0	1.920 728 6	0.741 328 5
H	3.461 436 4	2.733 776 2	0.273 297 5
O	3.673 440 3	1.079 026 8	−1.307 798 7
C	−5.164 781 0	0.289 316 5	−0.649 728 4
H	−5.652 631 9	−0.134 251 1	0.237 976 0
H	−5.657 445 5	1.241 085 3	−0.879 676 8
H	−5.337 858 4	−0.396 361 6	−1.487 754 7
H	−3.208 957 7	0.907 438 3	−1.301 638 4
C	3.573 719 0	−1.599 969 8	−0.242 110 2
H	4.656 806 2	−1.520 267 0	−0.101 181 4
H	3.226 449 4	−2.542 330 4	0.192 194 5
H	3.370 530 0	−1.610 637 8	−1.315 814 0
H	3.086 648 6	−0.398 625 9	1.497 658 0

Table TS15: B97-D3/aug-cc-pVTZ optimized geometry of the norepinephrine.

At.	X	Y	Z
C	−0.549 399 5	−0.206 398 7	−0.514 674 5
C	0.247 569 1	0.906 345 3	−0.228 350 9
C	1.602 319 5	0.755 452 4	0.064 347 4
C	2.191 381 0	−0.520 849 0	0.080 053 2
C	1.399 294 5	−1.632 907 5	−0.209 658 0
C	0.043 900 6	−1.476 008 5	−0.504 755 6
O	2.447 733 9	1.813 321 3	0.350 545 5
H	1.960 018 8	2.642 600 4	0.276 030 0
O	3.521 587 1	−0.695 755 3	0.364 876 6
H	3.913 988 9	0.174 159 5	0.526 565 1
C	−2.040 623 0	−0.048 001 7	−0.815 079 8
O	−2.440 239 2	1.316 145 4	−0.940 020 6
C	−2.901 774 8	−0.732 460 7	0.269 961 5
N	−2.765 267 7	0.034 782 8	1.519 820 6
H	−1.848 161 2	−0.121 636 6	1.929 036 7
H	−3.460 918 2	−0.244 867 5	2.202 326 6
H	−2.658 847 7	1.591 914 1	−0.032 411 0
H	−0.195 738 8	1.899 217 2	−0.257 361 8
H	1.864 884 2	−2.614 328 4	−0.204 480 6
H	−0.552 248 9	−2.355 472 8	−0.736 976 3
H	−2.615 229 9	−1.791 550 0	0.356 490 9
H	−2.256 783 8	−0.528 066 9	−1.779 095 1
H	−3.949 966 9	−0.684 750 7	−0.045 630 6

Table TS16: B97-D3/aug-cc-pVTZ optimized geometry of the phenethylamine

At.	X	Y	Z
C	2.316 478 1	−0.514 000 0	−6.337 050 1
C	2.613 026 0	−1.135 893 5	−7.556 851 7
C	3.073 238 3	−2.455 007 9	−7.596 442 4
C	3.247 187 8	−3.170 483 9	−6.408 945 8
C	2.955 443 4	−2.557 871 6	−5.186 294 9
C	2.491 804 6	−1.240 841 9	−5.150 767 2
C	1.764 893 8	0.904 098 6	−6.313 555 1
C	0.230 644 8	0.889 545 8	−6.200 564 4
N	2.316 194 7	1.653 699 1	−5.166 405 3
H	3.328 515 5	1.712 969 5	−5.239 016 2
H	1.958 018 0	2.604 738 9	−5.169 239 5
H	2.484 739 7	−0.580 950 6	−8.484 828 5
H	3.301 729 8	−2.920 296 2	−8.552 349 3
H	3.610 670 6	−4.194 701 6	−6.435 529 2
H	3.090 857 7	−3.107 285 7	−4.257 504 5
H	2.268 745 6	−0.759 750 4	−4.202 761 0
H	2.024 036 0	1.372 013 6	−7.280 317 3
H	−0.068 911 7	0.406 317 6	−5.264 826 2
H	−0.209 420 9	0.339 817 3	−7.038 574 4
H	−0.167 785 9	1.912 041 6	−6.209 866 9

Table TS17: B97-D3/aug-cc-pVTZ optimized geometry of the proline.

At.	X	Y	Z
C	1.236 608 3	−0.363 083 0	−6.724 062 8
C	2.419 588 0	−1.286 917 6	−6.386 309 1
C	2.733 952 5	−0.941 562 6	−4.893 955 7
N	2.000 642 0	0.298 100 5	−4.607 178 4
C	1.545 148 7	0.879 041 8	−5.884 413 5
H	2.584 028 6	0.945 169 6	−4.086 849 2
C	4.236 571 9	−0.816 867 2	−4.671 360 8
O	4.841 391 1	0.212 865 4	−4.462 519 2
O	4.847 903 3	−2.036 874 5	−4.736 887 4
H	5.797 529 3	−1.879 928 5	−4.599 539 5
H	1.163 701 4	−0.147 270 4	−7.794 111 5
H	0.292 802 8	−0.811 125 6	−6.393 194 4
H	3.278 459 3	−1.036 944 6	−7.019 115 1
H	2.206 008 6	−2.349 626 2	−6.520 478 4
H	2.385 990 4	−1.753 883 1	−4.240 717 6
H	0.669 006 8	1.516 197 4	−5.720 471 1
H	2.323 523 5	1.484 103 4	−6.382 837 2

Table TS18: Components[1] of the stabilization energy[2] as well as thermodynamic parameters for the complexes[3,4,5] under study.

System	E_{int}^{DFT}	E_{int}^{SAPT}	E_{Def}^{A}	E_{Def}^{B}	E_{Def}	ΔZPVE	$E_{Def} + \Delta$ZPVE	E_{Stab}	ΔH^0	ΔG^0
(R)**Ibu** – (R)**Phe**	−64.2	−57.2	24.4	1.9	26.3	2.3	28.6	−28.6	−27.6	22.0
(R)**Ibu** – (S)**Phe**	−72.5	−65.8	22.4	7.4	29.8	4.0	33.8	−32.0	−31.7	22.0
(R)**Ibu** – (R)**Pro**	−71.7	−64.6	22.9	1.0	23.9	2.7	26.6	−38.0	−38.1	12.6
(R)**Ibu** – (S)**Pro**	−74.7	−65.8	23.6	3.7	27.4	5.4	32.7	−33.1	−33.5	20.9
(S)**Nor** – (S)**Phe**	−71.3	−64.9	25.2	7.6	32.8	6.0	38.8	−26.1	−26.0	27.2
(S)**Nor** – (R)**Phe**	−58.4	−51.3	13.2	7.1	20.3	5.9	26.3	−25.0	−25.2	28.7
(R)**Nor** – (R)**Pro**	−56.6	−50.9	18.0	4.6	22.6	6.0	28.6	−22.3	−21.8	28.2
(S)**Nor** – (R)**Pro**	−60.8	−56.9	18.9	18.7	37.6	6.4	43.9	−13.0	−13.5	39.3
(S)**Bac** – (S)**Phe**	−52.5	−50.0	1.3	7.7	9.0	11.8	20.8	−29.2	−33.8	17.5
(S)**Bac** – (R)**Phe**	−87.5	−79.2	35.1	3.1	38.2	8.9	47.1	−32.1	−36.5	15.8
(S)**Bac** – (S)**Pro**	−74.7	−71.6	22.8	15.4	38.2	10.5	48.7	−22.9	−27.6	24.5
(R)**Bac** – (S)**Pro**	−75.7	−67.2	26.6	4.1	30.6	9.9	40.5	−26.7	−31.0	18.9

[1] The E_{Def}^{X}, $X = A, B$, is the deformation energy of the monomer X, calculated at the same level, as the DFT interaction energy, i.e. as the difference of the electronic energies of the molecule X with geometry as in the dimer and with geometry optimized for the isolated molecule X. E_{Def} is the sum of deformation energies of monomers A and B. ΔZPVE is the difference between ZPVE of the dimer and the sum of ZPVE's for monomers obtained at the same DFT level as before. Finally, E_{Stab} is the sum of E_{int}^{SAPT} and the deformation and ΔZPVE terms.

[2] Energies are in kJ/mol.

[3] E_{int}^{DFT} has been computed at the B97-D3/aug-cc-pVTZ level in the dimer basis set.

[4] E_{int}^{SAPT} has been computed in the CBS limit using aug-cc-pVTZ and aug-cc-pVQZ basis sets.

[5] Thermodynamic corrections to the ΔH^0 and ΔG^0 have been computed at the B97-D3/aug-cc-pVTZ level (298.15K, 0.1MPa).

Table TS19: IQA contributions to the “interaction” energy[1] between the fragment (Frag1) of the first molecule and the fragment (Frag2) of the second molecule, E_{int}^{IQA}, for **Bac** – **Phe** complexes[2,3,4] and their differences (see the last column).

Frag1	Frag2	(S)**Bac** – (S)**Phe**	(S)**Bac** – (R)**Phe**	Diff
Ring	Ring	−26.4	−37.6	−11.2
Ring	*CH	7.2	3.8	−3.4
Ring	NH_2	−7.6	−31.3	−23.7
Ring	CH_3	0.3	0.6	0.3
Cl	Ring	1.0	−11.0	−12.0
Cl	*CH	−6.4	−11.2	−4.8
Cl	NH_2	6.0	8.9	2.9
Cl	CH_3	−0.2	−1.6	−1.4
*CH	Ring	−15.5	0.0	15.5
*CH	*CH	6.2	4.6	−1.6
*CH	NH_2	−18.2	−5.1	13.1
*CH	CH_3	0.2	0.6	0.4
CH_2−x	Ring	−2.5	0.4	2.9
CH_2−x	*CH	19.4	12.3	−7.1
CH_2−x	NH_2	−30.7	−13.1	17.6
CH_2−x	CH_3	0.7	1.5	0.8
NH_2	Ring	1.4	−0.5	−1.9
NH_2	CH	−16.9	−11.6	5.3
NH_2	NH_2	18.1	12.3	−5.8
NH_2	CH_3	−0.6	−1.4	−0.8
CH_2−y	Ring	−10.1	0.2	10.3
CH_2−y	*CH	4.2	2.6	−1.6
CH_2−y	NH_2	−4.4	−8.8	−4.4
CH_2−y	CH_3	0.1	0.3	0.2
COOH	Ring	−16.1	−19.9	−3.8
COOH	*CH	−14.0	8.5	22.5
COOH	NH_2	−15.7	−107.8	−92.1
COOH	CH_3	−0.4	−4.4	−3.9
All	All	−121.0	−208.7	−87.7

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

[3] CH_2−x – group comprising carbon connected to the NH_2 group

[4] CH_2−y – group comprising carbon connected to the COOH group

Table TS20: IQA contributions to the “interaction” energy[1] between the fragment (Frag1) of the first molecule and the fragment (Frag2) of the second molecule, E_{int}^{IQA}, for **Bac** – **Pro** complexes[2] and their differences (see the last column).

Frag1	Frag2	(S)**Bac** – (S)**Pro**	(R)**Bac** – (S)**Pro**	Diff
Ring	*Ring	−40.1	−46.9	−6.8
Ring	COOH	−15.8	−6.8	9.0
Cl	*Ring	−27.0	−13.9	13.1
Cl	COOH	0.3	3.0	2.7
*CH	*Ring	2.4	0.8	−1.6
*CH	COOH	−3.9	−1.0	2.9
CH_2-x	*Ring	6.1	3.1	−3.0
CH_2-x	COOH	−10.0	−3.0	7.0
NH_2	*Ring	−5.6	−3.0	2.6
NH_2	COOH	9.9	3.0	−7.0
CH_2-y	*Ring	1.9	−13.0	−15.0
CH_2-y	COOH	−14.2	−0.8	13.4
COOH	*Ring	−16.8	−92.0	−75.1
COOH	COOH	−62.7	−2.1	60.6
All	All	−175.5	−172.7	2.8

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

Table TS21: IQA contributions to the “interaction” energy[1] between the fragment (Frag1) of the first molecule and the fragment (Frag2) of the second molecule, $E_{\text{int}}^{\text{IQA}}$, for **Ibu** – **Phe** complexes[2,3,4,5] and their differences (see the last column).

Frag1	Frag2	(R)**Ibu** – (R)**Phe**	(R)**Ibu** – (S)**Phe**	Diff
Ring	Ring	−37.0	−31.3	5.7
Ring	*CH	−4.9	−24.5	−19.6
Ring	NH_2	4.2	4.6	0.4
Ring	CH_3	−12.7	−1.1	11.6
CH_2	Ring	−5.2	−11.6	−6.4
CH_2	*CH	1.1	1.2	0.1
CH_2	NH_2	−1.2	−1.3	−0.1
CH_2	CH_3	0.1	0.1	0.0
CH−x	Ring	−0.4	−0.4	0.0
CH−x	*CH	1.9	2.4	0.5
CH−x	NH_2	−1.8	−2.0	−0.3
CH−x	CH_3	0.2	0.1	0.0
CH_3−x	Ring	0.0	−0.2	−0.2
CH_3−x	*CH	−0.1	−0.2	0.0
CH_3−x	NH_2	0.1	0.1	0.0
CH_3−x	CH_3	0.0	0.0	0.0
CH_3−y	Ring	0.0	−0.1	−0.1
CH_3−y	*CH	−0.1	−0.1	0.0
CH_3−y	NH_2	0.1	0.1	0.0
CH_3−y	CH_3	0.0	0.0	0.0
*CH	Ring	−0.3	−0.3	0.0
*CH	*CH	1.1	1.4	0.3
*CH	NH_2	−3.2	−5.3	−2.1
*CH	CH_3	−5.2	0.1	5.2
CH_3−z	Ring	0.1	0.0	−0.1
CH_3−z	*CH	3.7	3.9	0.3
CH_3−z	NH_2	−4.6	−4.9	−0.3
CH_3−z	CH_3	0.2	0.2	0.0
COOH	Ring	−4.6	−9.1	−4.5
COOH	*CH	8.6	10.6	2.0
COOH	NH_2	−88.9	−99.1	−10.2
COOH	CH_3	0.5	0.4	0.0
All	All	−148.3	−166.2	−17.8

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

[3] CH−x – group which is located between the CH_3−x and CH_3−y

[4] CH – group comprising asymmetric carbon

[5] CH_3−z – group connected to the asymmetric carbon

Table TS22: IQA contributions to the “interaction” energy between the fragment (Frag1) of the first molecule and the fragment (Frag2) of the second molecule,[1] E_{int}^{IQA}, for **Ibu** – **Pro** complexes[2] and their differences (see the last column).

Frag1	Frag2	(R)**Ibu** – (R)**Pro**	(R)**Ibu** – (S)**Pro**	Diff
Ring	*Ring	−48.0	−61.6	−13.5
Ring	COOH	−1.4	−1.4	−0.1
CH_2	*Ring	1.7	0.3	−1.4
CH_2	COOH	−6.1	−0.5	5.6
CH−x	*Ring	1.6	1.2	−0.4
CH−x	COOH	−2.1	−0.7	1.4
CH_3−x	*Ring	0.0	0.0	0.0
CH_3−x	COOH	−0.2	−0.1	0.2
CH_3−y	*Ring	−0.1	0.0	0.0
CH_3−y	COOH	0.0	0.0	0.0
*CH	*Ring	0.1	−6.4	−6.4
*CH	COOH	−1.0	−0.6	0.4
CH_3−z	*Ring	0.6	0.2	−0.4
CH_3−z	COOH	−1.1	−0.8	0.3
COOH	*Ring	−104.8	−93.8	11.0
COOH	COOH	0.4	1.9	1.6
All	All	−160.5	−162.2	−1.8

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

Table TS23: IQA contributions to the “interaction” energy[1] between the fragment (Frag1) of the first molecule and the fragment (Frag2) of the second molecule, $E_{\mathrm{int}}^{\mathrm{IQA}}$, for **Nor** – **Phe** complexes[2,3,4,5] and their differences (see the last column).

Frag1	Frag2	(S)**Nor** – (S)**Phe**	(S)**Nor** – (R)**Phe**	Diff
Ring	Ring	−27.2	−23.4	3.8
Ring	*CH	69.9	86.7	16.8
Ring	NH_2	−94.8	−101.7	−6.9
Ring	CH_3	4.4	4.9	0.4
OH−x	Ring	−9.8	−0.9	8.8
OH−x	*CH	−33.4	−62.1	−28.7
OH−x	NH_2	−38.3	51.7	90.0
OH−x	CH_3	−2.5	−3.6	−1.1
OH−y	Ring	−4.7	−9.4	−4.8
OH−y	*CH	−29.5	−31.5	−2.1
OH−y	NH_2	31.4	−36.5	−68.0
OH−y	CH_3	−1.9	−1.8	0.1
*CH	Ring	−0.6	−2.3	−1.7
*CH	*CH	17.8	20.9	3.1
*CH	NH_2	−17.0	−19.0	−2.1
*CH	CH_3	0.9	0.9	0.0
CH_2	Ring	−2.6	−3.4	−0.8
CH_2	*CH	13.8	12.9	−0.8
CH_2	NH_2	−12.5	−11.4	1.1
CH_2	CH_3	0.7	0.5	−0.1
NH_2	Ring	−21.0	−16.5	4.5
NH_2	*CH	−10.8	−11.8	−1.0
NH_2	NH_2	9.5	10.4	0.8
NH_2	CH_3	−0.5	−0.5	0.0
OH−z	Ring	0.2	1.7	1.5
OH−z	*CH	−18.0	−18.1	−0.1
OH−z	NH_2	16.8	16.5	−0.3
OH−z	CH_3	−0.8	−0.7	0.1
All	All	−160.1	−147.6	12.5

[1] Energies are in kJ/mol.

[2] Star ($*$) denotes the asymmetric carbon.

[3] OH−x – group connected to the ring in the *para* position

[4] OH−y – group connected to the ring in the *meta* position

[5] OH−z – group connected to the asymmetric carbon

Table TS24: IQA contributions to the “interaction” energy[1] between the fragment (Frag1) of the first molecule and the fragment (Frag2) of the second molecule, $E_{\mathrm{int}}^{\mathrm{IQA}}$, for **Nor** – **Pro** complexes[2] and their differences (see the last column).

Frag1	Frag2	(R)**Nor** – (R)**Pro**	(S)**Nor** – (R)**Pro**	Diff
Ring	*Ring	12.3	2.7	−9.6
Ring	COOH	−56.8	−60.8	−4.0
OH−x	*Ring	−44.2	−35.9	8.2
OH−x	COOH	−21.9	0.8	22.7
OH−y	*Ring	−31.1	−21.9	9.3
OH−y	COOH	13.7	−23.0	−36.7
*CH	*Ring	13.0	12.1	−0.9
*CH	COOH	−9.8	−9.3	0.5
CH_2	*Ring	4.2	5.8	1.6
CH_2	COOH	−5.9	−5.0	0.9
NH_2	*Ring	−20.2	−17.2	3.1
NH_2	COOH	5.5	4.5	−1.0
OH−z	*Ring	−12.6	−10.2	2.3
OH−z	COOH	9.5	8.2	−1.3
All	All	−144.3	−149.2	−5.0

[1] Energies are in kJ/mol.
[2] Star (∗) denotes the asymmetric carbon.

Table TS25: F-SAPT/jun-cc-pVDZ interaction energy partitioning for the **Bac** – **Phe** complexes.

		(S)**Bac** – (S)**Phe**						(S)**Bac** – (R)**Phe**						Diff
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total	Elst	Exch	IndAB	IndBA	Disp	Total	Total
Ring	Ring	−5.9	14.3	−1.3	−1.0	−16.4	−10.3	−7.7	25.7	−1.9	0.2	−23.9	−7.6	2.7
Ring	*CH	0.5	0.0	0.1	0.0	−0.4	0.1	0.7	0.4	0.7	0.5	−2.3	0.0	−0.2
Ring	NH_2	−8.6	0.1	−0.4	−0.3	−0.8	−10.0	−10.9	16.0	−2.1	−1.4	−11.5	−9.9	0.1
Ring	CH_3	2.1	0.0	0.3	0.0	−0.2	2.2	−6.1	0.2	−0.1	0.3	−0.8	−6.5	−8.7
Cl	Ring	−2.4	0.0	0.0	−0.3	−0.3	−3.1	−6.3	7.3	−0.3	−1.0	−5.7	−6.0	−2.9
Cl	*CH	0.3	0.0	0.0	0.0	0.0	0.2	1.0	0.0	0.1	−0.3	−0.3	0.5	0.2
Cl	NH_2	−1.2	0.0	0.0	−0.1	0.0	−1.3	0.9	0.0	0.0	0.4	−0.6	0.8	2.0
Cl	CH_3	0.7	0.0	0.0	0.0	0.0	0.7	1.8	0.0	0.0	−0.1	−0.1	1.6	0.9
*CH	Ring	2.9	12.9	−0.4	0.8	−7.2	9.0	0.5	0.0	0.0	−0.1	−0.4	0.1	−9.0
*CH	*CH	−1.2	0.1	−0.1	0.1	−0.6	−1.7	−0.3	0.0	0.0	−0.1	−0.1	−0.4	1.3
*CH	NH_2	9.1	7.8	−1.3	0.4	−2.9	13.0	0.0	0.1	−0.1	0.0	−0.6	−0.6	−13.7
*CH	CH_3	−3.3	0.0	0.4	0.0	−0.2	−3.1	0.4	0.0	0.0	−0.1	−0.1	0.3	3.3
CH_2−x	Ring	−4.6	0.0	0.0	−0.1	−1.2	−5.9	−0.2	0.0	0.0	0.0	−0.1	−0.3	5.5
CH_2−x	*CH	1.0	0.1	0.0	0.0	−0.3	0.9	0.9	0.0	0.0	−0.1	0.0	0.8	−0.1
CH_2−x	NH_2	5.4	4.1	−1.0	0.2	−2.1	6.6	−3.1	0.0	0.0	−0.5	−0.2	−3.8	−10.4
CH_2−x	CH_3	−0.5	0.0	0.2	0.0	−0.1	−0.4	0.1	0.0	0.0	0.0	0.0	0.1	0.5
NH_2	Ring	−1.4	0.1	0.0	−0.7	−0.4	−2.4	−0.8	0.0	0.0	−0.1	−0.1	−1.0	1.4
NH_2	*CH	−0.6	0.0	0.0	−0.1	−0.1	−0.8	−0.3	0.0	0.0	0.0	0.0	−0.3	0.5
NH_2	NH_2	−8.9	0.0	−0.2	−0.6	−0.3	−10.1	0.8	0.0	0.0	0.2	−0.1	0.9	11.0
NH_2	CH_3	2.0	0.0	0.0	−0.1	0.0	2.0	0.6	0.0	0.0	0.0	0.0	0.6	−1.3
CH_2−y	Ring	−1.2	5.7	−0.2	−0.6	−5.0	−1.3	−1.7	0.1	0.1	0.3	−0.6	−1.9	−0.6
CH_2−y	*CH	−0.2	0.0	0.0	0.0	−0.2	−0.4	−1.1	0.2	0.1	0.3	−0.3	−0.8	−0.4
CH_2−y	NH_2	−4.5	0.2	−0.3	0.0	−0.9	−5.5	7.3	3.6	−0.6	1.2	−2.2	9.3	14.8
CH_2−y	CH_3	1.1	0.0	0.1	0.0	−0.1	1.1	−0.4	0.0	0.0	0.1	−0.2	−0.4	−1.4
COOH	Ring	−16.2	7.9	−0.8	−3.2	−4.9	−17.1	−0.1	14.0	0.4	−2.5	−6.6	5.2	22.3
COOH	*CH	−1.6	0.3	−0.1	−0.4	−0.7	−2.5	8.1	0.8	1.0	−2.3	−1.7	5.9	8.4
COOH	NH_2	−24.3	14.5	−2.1	−2.7	−5.4	−19.9	−123.5	100.0	−10.2	−36.1	−15.0	−84.8	−64.9
COOH	CH_3	3.6	0.1	0.1	−0.4	−0.5	2.9	6.2	2.0	0.7	−1.2	−2.2	5.5	2.6
Ring	All	−11.8	14.4	−1.3	−1.4	−17.9	−17.9	−24.1	42.3	−3.4	−0.4	−38.5	−24.0	−6.1
Cl	All	−2.6	0.0	0.0	−0.4	−0.4	−3.4	−2.5	7.3	−0.2	−1.0	−6.7	−3.2	0.3
*CH	All	7.4	20.8	−1.3	1.3	−10.9	17.3	0.6	0.1	−0.1	−0.3	−1.1	−0.7	−18.0
CH_2−x	All	1.3	4.3	−0.8	0.1	−3.7	1.2	−2.3	0.0	0.0	−0.6	−0.4	−3.3	−4.5
NH_2	All	−9.0	0.1	−0.2	−1.5	−0.8	−11.3	0.4	0.0	0.0	0.1	−0.2	0.3	11.6
CH_2−y	All	−4.8	6.0	−0.5	−0.6	−6.3	−6.2	4.1	3.9	−0.4	2.0	−3.3	6.2	12.4
COOH	All	−38.5	22.8	−2.9	−6.6	−11.5	−36.7	−109.3	116.8	−8.2	−42.0	−25.4	−68.3	−31.6
All	Ring	−28.8	40.9	−2.7	−5.1	−35.4	−31.1	−16.3	47.1	−1.7	−3.2	−37.4	−11.5	19.5
All	*CH	−1.9	0.6	0.0	−0.4	−2.4	−4.1	9.1	1.4	1.8	−1.9	−4.8	5.5	9.6
All	NH_2	−33.0	26.7	−5.3	−3.1	−12.5	−27.1	−128.6	119.7	−13.1	−36.2	−30.1	−88.3	−61.1
All	CH_3	5.6	0.1	1.1	−0.4	−1.2	5.3	2.7	2.2	0.6	−0.9	−3.3	1.2	−4.1
All	All	−58.0	68.3	−6.9	−9.0	−51.4	−57.0	−133.2	170.4	−12.4	−42.3	−75.6	−93.0	−36.0

[1] Energies are in kJ/mol.
[2] Star (∗) denotes the asymmetric carbon.

Table TS26: F-SAPT/jun-cc-pVDZ interaction energy partitioning for the **Bac** – **Pro** complexes.

		(S)**Bac** – (S)**Pro**						(R)**Bac** – (S)**Pro**						Diff
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total	Elst	Exch	IndAB	IndBA	Disp	Total	Total
Ring	*Ring	−14.5	27.0	−1.4	0.2	−25.0	−13.9	−7.2	31.3	−0.7	−1.0	−27.1	−4.8	9.0
Ring	COOH	−12.5	8.2	−4.8	−0.5	−7.8	−17.4	−14.5	1.5	−1.2	0.3	−3.7	−17.7	−0.3
Cl	*Ring	0.0	7.9	−0.6	−0.5	−7.2	−0.5	−4.4	2.8	−0.1	−0.4	−3.4	−5.4	−4.9
Cl	COOH	−2.6	0.0	−0.5	−0.2	−0.4	−3.7	5.4	0.0	−0.1	−0.1	−0.5	4.6	8.3
*CH	*Ring	0.8	0.0	0.0	−0.2	−0.6	0.2	−2.6	0.2	−0.1	−0.5	−1.2	−4.2	−4.3
*CH	COOH	−2.9	0.2	−0.3	−0.4	−0.5	−3.9	1.7	0.0	0.0	−0.1	−0.1	1.5	5.5
CH_2−x	*Ring	0.4	0.0	0.0	0.0	−0.2	0.2	−2.1	0.0	0.0	−0.5	−0.6	−3.2	−3.4
CH_2−x	COOH	−0.4	0.0	−0.1	−0.3	−0.2	−1.0	0.4	0.0	0.0	0.0	−0.1	0.3	1.4
NH_2	*Ring	0.3	0.0	0.0	0.0	−0.1	0.3	0.6	0.0	0.0	0.3	−0.2	0.7	0.5
NH_2	COOH	1.3	0.0	0.0	0.2	−0.1	1.4	1.2	0.0	0.0	0.0	0.0	1.1	−0.2
CH_2−y	*Ring	−1.9	0.1	0.2	0.5	−0.9	−2.0	7.3	8.0	−0.8	2.5	−5.4	11.4	13.4
CH_2−y	COOH	12.8	7.4	−1.7	1.8	−3.2	17.1	−3.4	0.0	0.1	0.2	−0.3	−3.3	−20.4
COOH	*Ring	4.0	10.1	0.4	−2.2	−6.0	6.3	−101.3	83.4	−7.0	−32.4	−18.0	−75.3	−81.6
COOH	COOH	−75.8	40.4	−4.4	−15.6	−9.1	−64.5	18.3	1.6	1.2	−1.1	−2.8	17.3	81.8
Ring	All	−27.0	35.1	−6.3	−0.3	−32.8	−31.3	−21.8	32.8	−2.0	−0.8	−30.8	−22.5	8.8
Cl	All	−2.7	7.9	−1.1	−0.8	−7.6	−4.1	1.0	2.9	−0.3	−0.5	−3.9	−0.8	3.4
*CH	All	−2.1	0.2	−0.3	−0.5	−1.1	−3.8	−0.8	0.2	−0.1	−0.5	−1.3	−2.6	1.1
CH_2−x	All	0.0	0.0	−0.1	−0.3	−0.4	−0.8	−1.7	0.0	0.0	−0.5	−0.7	−2.9	−2.0
NH_2	All	1.6	0.0	0.0	0.2	−0.2	1.6	1.8	0.0	0.0	0.3	−0.2	1.9	0.2
CH_2−y	All	11.0	7.5	−1.5	2.3	−4.2	15.1	3.9	8.0	−0.7	2.7	−5.7	8.1	−7.0
COOH	All	−71.8	50.5	−4.0	−17.8	−15.1	−58.2	−83.0	85.0	−5.8	−33.5	−20.7	−58.0	0.2
All	*Ring	−10.9	45.1	−1.4	−2.2	−40.0	−9.4	−109.6	125.7	−8.8	−32.0	−55.9	−80.7	−71.3
All	COOH	−80.1	56.3	−11.9	−15.1	−21.3	−72.1	9.1	3.2	−0.1	−0.8	−7.5	3.9	76.0
All	All	−91.0	101.3	−13.3	−17.2	−61.3	−81.5	−100.5	128.9	−8.9	−32.8	−63.4	−76.8	4.7

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

Table TS27: F-SAPT/jun-cc-pVDZ interaction energy partitioning for the **Ibu** – **Phe** complexes.

		(R)**Ibu** – (R)**Phe**						(R)**Ibu** – (S)**Phe**						Diff
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total	Elst	Exch	IndAB	IndBA	Disp	Total	Total
Ring	Ring	−3.9	28.0	−1.3	−1.5	−25.5	−4.3	−14.0	21.7	−1.8	0.1	−27.1	−21.1	−16.8
Ring	*CH	−2.1	0.2	0.2	0.0	−1.1	−2.8	−4.2	14.3	0.0	0.4	−7.3	3.1	6.0
Ring	NH_2	−0.3	0.2	0.0	0.1	−1.4	−1.4	13.5	1.8	−1.2	2.1	−3.5	12.6	14.0
Ring	CH_3	−4.0	8.0	−0.3	−0.1	−5.1	−1.5	−2.9	0.1	0.5	0.1	−1.4	−3.5	−2.0
CH_2	Ring	1.3	2.0	−0.1	−0.3	−3.3	−0.4	−1.1	6.8	−0.2	−0.1	−5.4	−0.1	0.4
CH_2	*CH	0.0	0.0	0.0	−0.1	0.0	−0.1	−1.3	0.0	0.0	−0.1	−0.2	−1.5	−1.4
CH_2	NH_2	−1.3	0.0	0.0	−0.2	0.0	−1.5	−1.7	0.0	0.0	−0.3	−0.1	−2.1	−0.6
CH_2	CH_3	−0.2	0.0	0.0	−0.1	−0.1	−0.3	1.0	0.0	0.0	0.0	−0.1	0.9	1.2
CH−x	Ring	−1.8	0.0	0.0	0.1	−0.6	−2.2	−0.1	0.1	0.0	0.0	−0.9	−0.9	1.3
CH−x	*CH	0.2	0.0	0.0	0.0	0.0	0.2	−0.4	0.0	0.0	0.1	0.0	−0.3	−0.5
CH−x	NH_2	0.6	0.0	0.0	0.0	0.0	0.6	1.0	0.0	0.0	0.1	0.0	1.1	0.5
CH−x	CH_3	−0.1	0.0	0.0	0.0	0.0	−0.1	−0.1	0.0	0.0	0.0	0.0	−0.1	0.0
CH_3−x	Ring	−0.2	0.0	0.0	0.2	−0.3	−0.3	−1.6	0.1	0.0	0.1	−0.3	−1.8	−1.5
CH_3−x	*CH	0.1	0.0	0.0	0.0	0.0	0.1	0.3	0.0	0.0	0.0	0.0	0.3	0.2
CH_3−x	NH_2	−0.1	0.0	0.0	0.0	0.0	−0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.2
CH_3−x	CH_3	0.3	0.0	0.0	0.0	0.0	0.3	0.2	0.0	0.0	0.0	0.0	0.2	−0.1
CH_3−y	Ring	−0.6	0.0	0.0	0.1	−0.3	−0.8	−1.2	0.0	0.0	0.1	−0.4	−1.6	−0.8
CH_3−y	*CH	0.4	0.0	0.0	0.0	0.0	0.4	−0.6	0.0	0.0	0.0	0.0	−0.6	−1.0
CH_3−y	NH_2	−0.5	0.0	0.0	−0.1	0.0	−0.5	−0.2	0.0	0.0	−0.1	0.0	−0.3	0.3
CH_3−y	CH_3	−0.1	0.0	0.0	0.0	0.0	−0.1	0.6	0.0	0.0	0.0	0.0	0.6	0.7
*CH	Ring	−4.9	0.1	0.1	0.7	−1.1	−5.0	7.2	0.0	0.0	−0.2	−0.8	6.3	11.4
*CH	*CH	−1.8	0.1	0.0	0.3	−0.3	−1.7	12.7	0.0	0.0	−0.5	−0.5	11.7	13.4
*CH	NH_2	11.2	1.4	−0.4	1.6	−1.1	12.8	−5.2	2.2	−0.5	0.2	−1.5	−4.8	−17.6
*CH	CH_3	0.5	2.3	0.0	0.4	−1.6	1.6	−8.1	0.0	0.1	0.1	−0.1	−8.1	−9.6
CH_3−z	Ring	1.4	0.0	0.0	−0.1	−0.4	0.9	0.9	0.0	0.0	−0.1	−0.3	0.6	−0.4
CH_3−z	*CH	0.9	0.0	0.0	−0.1	−0.1	0.7	−1.3	0.0	0.0	−0.2	−0.1	−1.5	−2.3
CH_3−z	NH_2	−6.0	0.0	−0.1	−0.8	−0.2	−7.0	−6.7	0.1	−0.1	−1.0	−0.3	−8.1	−1.1
CH_3−z	CH_3	0.4	0.0	0.0	−0.2	−0.3	0.0	2.0	0.0	0.0	−0.1	0.0	1.9	1.9
COOH	Ring	8.8	2.5	0.9	−1.4	−3.3	7.6	7.5	5.7	1.0	−1.6	−4.8	7.8	0.1
COOH	*CH	10.6	1.2	0.9	−1.6	−1.2	9.9	−0.5	0.6	0.4	−1.6	−1.4	−2.5	−12.4
COOH	NH_2	−98.0	70.4	−7.2	−23.9	−11.8	−70.5	−109.3	83.5	−8.2	−29.9	−13.2	−77.1	−6.6
COOH	CH_3	1.0	0.1	0.4	−0.9	−0.8	−0.2	10.4	0.3	1.0	−0.4	−0.4	10.9	11.2
Ring	All	−10.3	36.4	−1.4	−1.5	−33.2	−10.0	−7.6	37.9	−2.5	2.6	−39.3	−8.9	1.1
CH_2	All	−0.3	2.0	−0.1	−0.6	−3.4	−2.4	−3.1	6.9	−0.2	−0.5	−5.7	−2.7	−0.3
CH−x	All	−1.1	0.0	0.0	0.2	−0.7	−1.5	0.4	0.1	0.0	0.2	−1.0	−0.3	1.2
CH_3−x	All	0.1	0.0	0.0	0.2	−0.3	0.0	−1.0	0.1	0.0	0.1	−0.4	−1.2	−1.2
CH_3−y	All	−0.8	0.0	0.0	0.0	−0.3	−1.0	−1.4	0.0	0.0	0.0	−0.5	−1.8	−0.8
*CH	All	5.1	3.8	−0.3	3.1	−4.1	7.6	6.6	2.3	−0.4	−0.4	−3.0	5.2	−2.4
CH_3−z	All	−3.2	0.1	0.0	−1.2	−1.0	−5.4	−5.0	0.1	−0.1	−1.3	−0.8	−7.2	−1.8
COOH	All	−77.7	74.2	−4.9	−27.7	−17.1	−53.2	−91.8	90.1	−5.9	−33.5	−19.8	−60.9	−7.7
All	Ring	0.2	32.6	−0.4	−2.1	−34.8	−4.4	−2.4	34.4	−1.0	−1.7	−40.1	−10.9	−6.4
All	*CH	8.3	1.4	1.1	−1.4	−2.8	6.6	4.8	15.0	0.3	−1.8	−9.6	8.7	2.1
All	NH_2	−94.4	72.0	−7.6	−23.1	−14.6	−67.7	−108.5	87.6	−10.1	−28.9	−18.6	−78.6	−10.9
All	CH_3	−2.2	10.5	0.0	−0.8	−7.9	−0.5	3.1	0.5	1.6	−0.3	−2.0	2.8	3.3
All	All	−88.2	116.5	−6.8	−27.4	−60.2	−66.0	−102.9	137.4	−9.2	−32.8	−70.4	−77.9	−11.8

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

Table TS28: F-SAPT/jun-cc-pVDZ interaction energy partitioning for the **Ibu** – **Pro** complexes.

		(R)**Ibu** – (R)**Pro**						(R)**Ibu** – (S)**Pro**						Diff
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total	Elst	Exch	IndAB	IndBA	Disp	Total	Total
Ring	*Ring	−8.9	36.2	−3.2	2.6	−23.8	2.8	−3.5	39.6	−1.8	3.4	−30.5	7.2	4.4
Ring	COOH	−7.2	2.9	0.3	0.2	−4.5	−8.4	−3.4	0.9	−0.8	0.2	−3.4	−6.5	1.8
CH_2	*Ring	−2.9	0.0	0.2	−0.6	−0.8	−4.1	−1.4	0.0	0.0	−0.6	−1.0	−3.0	1.1
CH_2	COOH	10.1	1.6	−0.7	0.0	−1.7	9.3	1.8	0.0	−0.1	0.0	−0.3	1.4	−7.9
CH−x	*Ring	1.5	0.0	0.0	0.2	−0.2	1.6	0.2	0.0	0.0	0.3	−0.3	0.3	−1.3
CH−x	COOH	−3.0	0.1	−0.1	0.0	−0.3	−3.3	0.6	0.0	0.0	0.0	−0.1	0.5	3.8
CH_3−x	*Ring	1.0	0.0	0.0	0.1	−0.1	0.9	0.0	0.0	0.0	0.1	−0.2	0.0	−0.9
CH_3−x	COOH	−2.4	0.0	0.0	0.0	−0.1	−2.5	−0.2	0.0	0.0	0.0	0.0	−0.2	2.3
CH_3−y	*Ring	0.1	0.0	0.0	−0.1	−0.1	−0.1	−0.7	0.0	0.0	0.0	−0.1	−0.8	−0.7
CH_3−y	COOH	−0.7	0.0	−0.1	0.0	−0.1	−0.9	0.8	0.0	0.0	0.0	0.0	0.7	1.7
*CH	*Ring	5.7	0.4	−0.2	1.4	−1.6	5.7	5.9	3.1	−0.4	−0.9	−3.6	4.0	−1.7
*CH	COOH	−1.9	0.0	0.1	0.0	−0.1	−1.9	−16.3	0.0	0.0	0.2	−0.2	−16.2	−14.3
CH_3−z	*Ring	−5.6	0.0	−0.1	−1.4	−0.5	−7.4	−6.3	0.1	−0.1	−1.6	−0.8	−8.7	−1.3
CH_3−z	COOH	1.8	0.0	0.0	0.0	0.0	1.7	2.6	0.0	0.0	−0.1	−0.1	2.4	0.7
COOH	*Ring	−109.1	99.7	−8.0	−40.8	−20.3	−78.5	−106.5	91.0	−7.9	−36.9	−17.8	−78.1	0.4
COOH	COOH	8.1	0.1	1.4	−0.3	−0.7	8.6	20.5	0.2	1.5	−0.6	−1.2	20.4	11.8
Ring	All	−16.1	39.1	−2.9	2.8	−28.3	−5.6	−6.9	40.5	−2.6	3.6	−34.0	0.7	6.2
CH_2	All	7.2	1.6	−0.5	−0.6	−2.5	5.3	0.4	0.0	0.0	−0.6	−1.4	−1.6	−6.8
CH−x	All	−1.4	0.1	−0.1	0.2	−0.5	−1.7	0.8	0.0	0.0	0.3	−0.3	0.8	2.5
CH_3−x	All	−1.5	0.0	0.0	0.1	−0.2	−1.6	−0.2	0.0	0.0	0.2	−0.2	−0.2	1.4
CH_3−y	All	−0.6	0.0	0.0	−0.1	−0.2	−1.0	0.1	0.0	0.0	0.0	−0.2	0.0	1.0
*CH	All	3.8	0.4	−0.1	1.4	−1.7	3.8	−10.4	3.1	−0.4	−0.7	−3.8	−12.2	−16.0
CH_3−z	All	−3.8	0.0	0.0	−1.4	−0.5	−5.7	−3.7	0.1	−0.1	−1.7	−0.9	−6.2	−0.6
COOH	All	−101.0	99.8	−6.6	−41.1	−20.9	−69.9	−85.9	91.2	−6.4	−37.5	−19.0	−57.7	12.2
All	*Ring	−118.2	136.3	−11.2	−38.5	−47.4	−79.0	−112.2	133.8	−10.2	−36.1	−54.3	−79.0	0.0
All	COOH	4.9	4.8	0.9	−0.2	−7.6	2.7	6.4	1.2	0.7	−0.4	−5.4	2.5	−0.2
All	All	−113.3	141.1	−10.3	−38.8	−55.0	−76.3	−105.8	135.0	−9.5	−36.5	−59.7	−76.5	−0.2

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

Table TS29: F-SAPT/jun-cc-pVDZ interaction energy partitioning for the **Nor** – **Phe** complexes.

		(S)**Nor** – (S)**Phe**						(S)**Nor** – (R)**Phe**						Diff
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total	Elst	Exch	IndAB	IndBA	Disp	Total	Total
Ring	Ring	13.5	22.3	−1.3	0.0	−25.0	9.6	17.4	15.8	−1.0	−0.4	−19.5	12.3	2.8
Ring	*CH	−6.7	0.2	0.1	−0.2	−1.3	−7.8	−5.7	0.1	−0.1	0.0	−1.4	−7.1	0.7
Ring	NH_2	−13.7	4.9	−2.0	−1.7	−4.5	−17.0	−16.2	0.6	−1.1	−1.6	−2.5	−20.8	−3.8
Ring	CH_3	1.1	0.0	0.7	0.0	−0.4	1.3	1.5	0.0	0.5	0.0	−0.4	1.6	0.2
OH−x	Ring	−6.2	6.4	0.9	−1.7	−5.2	−5.8	−14.2	1.5	−0.1	0.2	−3.2	−15.8	−10.0
OH−x	*CH	8.6	1.6	0.2	−1.2	−1.9	7.3	12.5	6.7	−0.1	−0.4	−2.3	16.5	9.2
OH−x	NH_2	−82.2	80.0	−7.9	−23.1	−11.7	−44.8	6.8	2.7	−0.5	1.0	−1.7	8.2	53.0
OH−x	CH_3	3.5	0.1	0.9	−0.2	−0.4	4.0	−7.9	0.2	0.1	0.1	−0.4	−7.9	−11.8
OH−y	Ring	−6.1	0.5	−0.1	−0.4	−2.1	−8.2	−3.6	6.5	1.1	−0.5	−4.6	−1.2	7.0
OH−y	*CH	2.5	0.0	0.0	−0.1	−0.1	2.3	0.7	0.5	0.2	−0.5	−1.2	−0.3	−2.6
OH−y	NH_2	−0.4	0.0	−0.1	0.0	−0.1	−0.6	−76.0	74.6	−7.4	−21.5	−10.9	−41.1	−40.5
OH−y	CH_3	−0.6	0.0	0.0	0.0	0.0	−0.6	6.5	0.2	0.9	−0.2	−0.3	7.2	7.8
*CH	Ring	−1.8	0.0	0.0	0.1	−0.7	−2.5	−1.5	0.0	0.0	−0.1	−0.6	−2.2	0.3
*CH	*CH	0.4	0.0	0.0	0.0	0.0	0.4	0.1	0.0	0.0	0.0	0.0	0.1	−0.4
*CH	NH_2	−0.5	0.0	0.0	−0.1	0.0	−0.6	−0.2	0.0	0.0	−0.1	0.0	−0.3	0.3
*CH	CH_3	0.4	0.0	0.0	0.0	0.0	0.4	0.5	0.0	0.0	0.0	0.0	0.5	0.0
CH_2	Ring	−1.3	1.0	−0.1	−0.3	−2.4	−3.0	−1.6	0.5	0.0	−0.1	−1.9	−3.1	−0.1
CH_2	*CH	0.2	0.0	0.0	0.0	0.0	0.2	−0.3	0.0	0.0	0.0	0.0	−0.3	−0.5
CH_2	NH_2	−0.4	0.0	0.0	0.0	0.0	−0.5	0.2	0.0	0.0	0.0	0.0	0.2	0.6
CH_2	CH_3	0.1	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.1	0.0
NH_2	Ring	−8.6	10.5	−0.3	−1.0	−6.5	−5.9	−4.8	9.3	−0.2	−0.6	−5.9	−2.2	3.6
NH_2	*CH	−0.1	0.0	0.0	0.0	0.0	−0.2	0.4	0.0	0.0	0.0	0.0	0.4	0.6
NH_2	NH_2	−0.9	0.0	0.0	−0.1	0.0	−1.2	−1.0	0.0	0.0	−0.1	0.0	−1.1	0.1
NH_2	CH_3	0.5	0.0	0.0	0.0	0.0	0.5	0.4	0.0	0.0	0.0	0.0	0.4	−0.1
OH−z	Ring	−1.5	0.0	0.0	0.2	−0.3	−1.6	−1.6	0.0	0.0	−0.1	−0.3	−1.9	−0.4
OH−z	*CH	−0.1	0.0	0.0	0.0	0.0	−0.1	0.5	0.0	0.0	0.0	0.0	0.5	0.6
OH−z	NH_2	−0.9	0.0	0.0	−0.2	0.0	−1.1	−0.8	0.0	0.0	−0.1	0.0	−0.9	0.2
OH−z	CH_3	0.6	0.0	0.0	0.0	0.0	0.6	0.5	0.0	0.0	0.0	0.0	0.5	−0.1
Ring	All	−5.9	27.5	−2.5	−1.9	−31.2	−14.0	−3.1	16.5	−1.7	−2.0	−23.8	−14.1	−0.1
OH−x	All	−76.2	88.2	−5.9	−26.2	−19.2	−39.3	−2.8	11.1	−0.6	0.8	−7.6	1.0	40.4
OH−y	All	−4.7	0.5	−0.1	−0.5	−2.3	−7.1	−72.4	81.8	−5.2	−22.6	−17.0	−35.4	−28.3
*CH	All	−1.4	0.0	0.0	−0.1	−0.8	−2.3	−1.2	0.0	0.0	−0.1	−0.6	−2.0	0.3
CH_2	All	−1.4	1.0	−0.1	−0.4	−2.4	−3.2	−1.6	0.5	−0.1	−0.1	−1.9	−3.2	0.1
NH_2	All	−9.1	10.5	−0.3	−1.2	−6.6	−6.7	−4.9	9.3	−0.2	−0.7	−6.0	−2.5	4.2
OH−z	All	−1.8	0.0	0.0	0.0	−0.3	−2.1	−1.3	0.0	0.0	−0.2	−0.3	−1.9	0.2
All	Ring	−11.9	40.8	−0.8	−3.1	−42.3	−17.3	−10.0	33.7	−0.3	−1.6	−35.9	−14.2	3.2
All	*CH	4.8	1.9	0.4	−1.5	−3.4	2.1	8.2	7.3	0.0	−0.9	−4.9	9.7	7.6
All	NH_2	−99.0	85.0	−10.1	−25.3	−16.4	−65.8	−87.2	77.9	−9.1	−22.4	−15.2	−55.9	9.9
All	CH_3	5.7	0.1	1.7	−0.3	−0.9	6.3	1.7	0.4	1.6	−0.1	−1.1	2.4	−4.0
All	All	−100.5	127.8	−8.9	−30.2	−62.9	−74.7	−87.4	119.3	−7.8	−24.9	−57.2	−58.0	16.7

[1] Energies are in kJ/mol.

[2] Star (∗) denotes the asymmetric carbon.

Table TS30: F-SAPT/jun-cc-pVDZ interaction energy partitioning for the **Nor** – **Pro** complexes.

		(R)**Nor** – (R)**Pro**						(S)**Nor** – (R)**Pro**						Diff
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total	Elst	Exch	IndAB	IndBA	Disp	Total	Total
Ring	*Ring	−10.9	27.8	−1.0	−0.4	−24.1	−8.7	−11.9	27.7	−0.9	−1.1	−23.7	−9.9	−1.2
Ring	COOH	−12.4	3.7	−1.7	−1.0	−4.8	−16.3	−18.6	0.9	−1.9	−1.6	−3.7	−24.8	−8.5
OH−x	*Ring	−3.4	10.0	−0.7	−0.6	−5.0	0.2	0.1	4.8	0.0	−0.8	−3.8	0.3	0.1
OH−x	COOH	−40.2	37.1	−3.9	−10.1	−7.6	−24.7	−20.0	10.5	−1.7	−3.4	−4.0	−18.5	6.2
OH−y	*Ring	1.2	2.9	−0.2	−0.7	−3.3	−0.1	5.0	0.9	0.7	0.0	−2.4	4.2	4.3
OH−y	COOH	−4.1	0.0	−0.1	−0.7	−0.2	−5.1	−33.1	40.2	−3.9	−10.8	−8.4	−16.1	−11.0
*CH	*Ring	0.5	0.0	0.0	0.1	−0.7	−0.1	3.5	0.0	0.0	0.8	−0.6	3.8	3.9
*CH	COOH	0.7	0.0	0.0	0.0	0.0	0.6	−3.9	0.0	0.0	−0.4	0.0	−4.3	−4.9
CH_2	*Ring	−0.2	1.4	−0.1	−0.2	−2.1	−1.2	−2.6	0.2	0.0	−0.6	−1.4	−4.4	−3.2
CH_2	COOH	−0.7	0.0	0.0	−0.1	−0.1	−0.8	5.1	0.0	0.0	0.4	0.0	5.5	6.3
NH_2	*Ring	−1.2	4.8	0.0	0.0	−4.5	−1.0	−0.7	4.1	0.0	−0.3	−3.6	−0.6	0.4
NH_2	COOH	1.4	0.0	0.0	0.0	−0.1	1.2	−0.4	0.0	0.0	−0.2	0.0	−0.6	−1.8
OH−z	*Ring	0.2	0.0	0.0	−0.2	−0.3	−0.2	0.6	0.0	0.0	−0.1	−0.3	0.3	0.6
OH−z	COOH	0.6	0.0	0.0	0.1	0.0	0.7	0.7	0.0	0.0	−0.1	0.0	0.6	−0.1
Ring	All	−23.4	31.5	−2.7	−1.4	−28.9	−25.0	−30.5	28.7	−2.7	−2.7	−27.4	−34.6	−9.7
OH−x	All	−43.6	47.1	−4.6	−10.6	−12.6	−24.4	−19.9	15.3	−1.6	−4.1	−7.8	−18.2	6.3
OH−y	All	−2.9	2.9	−0.2	−1.4	−3.5	−5.2	−28.1	41.1	−3.3	−10.8	−10.8	−11.9	−6.7
*CH	All	1.2	0.0	0.0	0.1	−0.8	0.6	−0.3	0.0	0.0	0.4	−0.6	−0.5	−1.1
CH_2	All	−0.9	1.4	−0.1	−0.3	−2.2	−2.1	2.5	0.2	0.0	−0.2	−1.4	1.1	3.1
NH_2	All	0.1	4.8	−0.1	−0.1	−4.6	0.2	−1.1	4.1	−0.1	−0.5	−3.6	−1.2	−1.4
OH−z	All	0.8	0.0	0.0	−0.1	−0.3	0.4	1.3	0.0	0.0	−0.2	−0.3	0.9	0.5
All	*Ring	−13.9	46.9	−2.0	−2.0	−40.1	−11.1	−6.0	37.7	−0.2	−2.0	−35.7	−6.2	4.9
All	COOH	−54.8	40.9	−5.8	−11.8	−12.8	−44.4	−70.1	51.7	−7.6	−16.0	−16.2	−58.2	−13.8
All	All	−68.7	87.8	−7.8	−13.8	−52.9	−55.5	−76.1	89.4	−7.8	−18.0	−51.9	−64.5	−9.0

[1] Energies are in kJ/mol.

[2] Star ($*$) denotes the asymmetric carbon.

1 Characteristic features of the monomers' IR spectra

Figure FS1 shows the computed IR spectra for the monomers.

In the spectrum of **Phe** two areas can be distinguished. The region up to ca. 1600 cm^{-1} is composed of peaks corresponding to the rocking movements of CH_3 and NH_2 groups (ca. 255 – 282 cm^{-1}), aromatic C-H wagging (700 cm^{-1}),C-H and N-H wagging (826 cm^{-1}), C-C-H bending (1375 cm^{-1}), and NH_2 scrissoring (1623 cm^{-1}). Next, in the region between 2875 – 3135 cm^{-1} peaks related to the C-H bonds stretching occur. N-H stretching vibrations are manifested by the small peak at ca. 3420 cm^{-1}.

The spectrum of **Pro** has a different shape. The breathing movements of the pyrrolidine ring give rise to the broad band emerging between 400 – 870 cm^{-1}. Next, the high peak at 1072 cm^{-1} is due to the coupled vibration of the ring with the O-H wagging. The sharp peak at 1743 cm^{-1} is related to the C=O stretching. The C-H bonds' stretching vibrations are found between 2980 – 3060 cm^{-1}, while the N-H and O-H stretchings can be observed at 3475 and 3653 cm^{-1}, respectively.

The spectrum for ibuprofen comprises five major peaks: (i) the broad, nonsymmetric band at ca. 600 cm^{-1} due to the wagging of OH from the carboxyl group; (ii) the double peak at ca. 1100 cm^{-1} resulting from the aliphatic C-H rocking; (iii) the high peak at 1746 cm^{-1} assigned to the C=O stretching; (iv) the double peak at ca. 3000 cm^{-1} due to the C-H stretching; (v) the 3651 cm^{-1} peak of O-H stretching. The spectrum is in line with the experimental IR ibuprofen spectra available in the literature.[1,2]

The IR spectrum of the isolated norepinephrine is similar to the experimental and simulated spectra for different conformers described in Ref.[3] Here, the whole energy range can be divided into three regions. In the broadest one, up to ca. 1600 cm^{-1}, one can distinguish three highest peaks: (i) at 264 cm^{-1} due to the out-of-plane bending of O-H bonds substituting the phenyl ring; (ii) at 562 cm^{-1} due to the wagging of the OH group connected to the chiral carbon; and (iii) 1236 cm^{-1} due to the C-C-H scissoring. Next, the C-H bonds' stretching motions give rise to the broad band at ca. 3000 cm^{-1}, while the double band between ca. 3600 – 3750 cm^{-1} is due to all the O-H stretching vibrations present in the molecule.

The spectrum computed for baclofen is also characterized by four major peaks: (i) the 966 cm^{-1} peak results from the O-H wagging; (ii) the 1426 cm^{-1} peak results from the C-O-H scissoring; (iii) the 1767 cm^{-1} peak results from the C=O stretching; and (iv) the strongest one at 3159 cm^{-1} due to the O-H stretching (note that on the left shoulder smaller peaks at ca. 3000 cm^{-1} of the C-H stretching emerge). Their positions are comparable to the experimental ones listed in.[4] The symmetric and antisymmetric stretchings of the NH_2 group give rise to the peak of very low intensity at ca. 3500 cm^{-1}.

2 Characteristic features of the VCD spectra

Table TS31: Assignment of the VCD spectrum of the (R)**Ibu** – (R)**Phe** pair.

peak position [cm^{-1}]	sign	assignment
589	-	**Ibu** ring deformation (C−H out of plane bending)
934	+	**Ibu** O−H wagging coupled to **Phe** NH_2 symmetric bend
1004	-	**Ibu** O−H wagging coupled to **Phe** *C−H wagging
1185	+	**Ibu** in plane C−H ring scissoring
1337	-	**Ibu** *C−H scissoring
1749	-	C=O stretching
3096	-	O−H stretching

Table TS32: Assignment of the VCD spectrum of the (R)**Ibu** – (S)**Phe** pair.

peak position [cm^{-1}]	sign	assignment
578	-	**Ibu** ring deformation (C−H out of plane bending)
1073	+	**Ibu** *C−CH_3 wagging
1191	+	**Phe** *C−H wagging coupled to **Ibu** in plane C−H ring scissoring
1341	+	**Ibu** *C−H wagging coupled to **Phe** in plane C−H ring scissoring
1420	+	**Ibu** O−H coupled to **Phe** in plane C−H ring scissoring
1751	-	C=O stretching
2979	-	**Ibu** O−H and CH_3 stretching coupled to **Phe** *C−H stretching
2982	+	**Ibu** O−H and CH_3 stretching coupled to **Phe** *C−H stretching

Table TS33: Assignment of the VCD spectrum of the (S)**Nor** – (S)**Phe** pair.

peak position [cm^{-1}]	sign	assignment
336	+	**Nor** O−H wagging
344	-	**Nor** O−H wagging
359	-	**Nor** O−H wagging
387	-	**Nor** N−H wagging
393	+	**Phe** N−H wagging
952	+	**Nor** in plane C−H ring scissoring coupled to C-C stretching
968	-	**Nor** O−H wagging coupled to **Phe** N−N symmetric bend
982	-	**Nor** O−H wagging coupled to **Phe** N−N and *C−C_3 symmetric bend
1589	-	**Nor** ring deformations due to C−O−H bending
3047	+	**Phe** CH_3 stretching
3063	+	**Nor** O−H stretching (the OH group forming H-bond with **Phe**) coupled to **Nor** C−H stretching in ring
3068	+	**Nor** O−H stretching (the OH group forming H-bond with **Phe**) coupled to **Nor** C−H stretching in ring

Table TS34: Assignment of the VCD spectrum of the (S)**Nor** – (R)**Phe** pair.

peak position [cm^{-1}]	sign	assignment
330	-	both NH_2 rocking
752	-	**Nor** ring C−H out of plane bending
848	-	**Nor** O−H wagging (the OH group forming H-bond with **Phe**)
1301	-	**Nor** *C−H wagging
1309	-	**Nor** *C−H wagging coupled to wagging of *C−CH_2
3104	+	**Phe** ring C−H stretching coupled to **Nor** O−H stretching (the OH group forming H-bond with **Phe**)
3106	+	**Phe** ring C−H stretching coupled to **Nor** O−H stretching (the OH group forming H-bond with **Phe**)

Table TS35: Assignment of the VCD spectrum of the (S)**Bac** – (S)**Phe** pair.

peak position [cm^{-1}]	sign	assignment
428	-	**Bac** NH_2 rocking
574	-	**Bac** skeletal movements
828	+	**Bac** ring deformation (C−H out of plane bending)
1012	+	**Bac** O−H wagging
1209	+	**Phe** C−H ring scissoring coupled to NH_2 rocking
1288	+	**Bac** CH_2 rocking
1465	-	**Bac** CH_2 scissoring coupled to C−O−H bending
1626	+	**Bac** NH_2 scissoring
3028	+	**Bac** C−H stretching coupled to O−H stretching

Table TS36: Assignment of the VCD spectrum of the (S)**Bac** – (R)**Phe** pair.

peak position [cm^{-1}]	sign	assignment
260	+	**Bac** NH_2 rocking
381	-	**Bac** ring deformation
530	+	**Bac** ring deformation (C−H out of plane bending)
606	-	**Bac** CH_2 rocking
1075	-	**Bac** O−H wagging
1236	+	**Bac** *C−H wagging
1301	-	**Bac** ring C−H rocking coupled to CH_2 rocking
1424	+	**Bac** C−O−H bending
1465	-	**Phe** *C−CH_3 rocking
2820	+	**Bac** O−H stretching (the OH group forming H-bond with **Phe**)
2991	+	**Phe** C−H stretching

Table TS37: Assignment of the VCD spectrum of the (R)**Ibu** – (R)**Pro** pair.

peak position [cm^{-1}]	sign	assignment
422	+	skeletal **Pro** movements
610	-	**Pro** O−H wagging
817	+	**Pro** N−H rocking
908	+	**Pro** ring C_2 rocking
1045	-	**Ibu** O−H wagging
1083	+	**Ibu** O−H wagging coupled to **Pro** N−H bending
1367	+	**Ibu** C−O−H bending coupled to **Pro** CH_2 rocking
1446	-	**Pro** N−H wagging
2786	+	**Ibu** O−H stretching

Table TS38: Assignment of the VCD spectrum of the (R)**Ibu** – (S)**Pro** pair.

peak position [cm^{-1}]	sign	assignment
578	-	**Ibu** ring deformation (C−H out of plane bending)
642	+	**Pro** N−H rocking coupled to ring deformations
782	-	**Ibu** ring deformation coupled to skeletal movements
792	+	**Ibu** ring deformation coupled to skeletal movements
1032	-	**Pro** asymmetric C−H bending
1089	+	**Ibu** O−H wagging coupled to **Pro** ring deformations
1291	-	**Pro** *C−H wagging
1396	+	**Ibu** C−O−H bending
1746	-	**Ibu** C=O stretching
2889	-	**Ibu** O−H stretching

Table TS39: Assignment of the VCD spectrum of the (R)**Nor** – (R)**Pro** pair.

peak position [cm^{-1}]	sign	assignment
264	-	**Nor** *C−O−H wagging
272	+	**Nor** NH_2 rocking
545	-	**Nor** ring O−H wagging
589	-	**Nor** ring O−H wagging
795	+	**Nor** ring O−H out of plane bending
1129	+	**Nor** skeletal deformations
1221	-	**Nor** *C−H wagging
1377	+	**Nor** NH_2 wagging
3464	+	**Pro** N−H stretching coupled to **Nor** O−H stretching

Table TS40: Assignment of the VCD spectrum of the (S)**Nor** – (R)**Pro** pair.

peak position [cm^{-1}]	sign	assignment
287	-	**Nor** NH_2 rocking
394	-	**Nor** ring O−H wagging
804	+	**Nor** ring C−H out of plane bending
1222	+	**Nor** *C−H wagging coupled to C−O−H bending
1267	-	**Pro** C−O−H bending coupled to ring deformations
1607	+	**Nor** ring C-C stretching

Table TS41: Assignment of the VCD spectrum of the (S)**Bac** – (S)**Pro** pair.

peak position [cm^{-1}]	sign	assignment
248	+	**Bac** NH_2 rocking
1331	-	**Pro** ring deformations
1342	-	**Bac** C−O−H bending coupled to **Pro** *C−H wagging
1354	-	**Bac** *C−H wagging
1358	+	**Bac** C−O−H bending coupled to **Pro** C−O−H bending and **Bac** *C−H wagging
1756	+	**Pro** C=O stretching
3405	+	**Bac** O−H stretching

Table TS42: Assignment of the VCD spectrum of the (R)**Bac** – (S)**Pro** pair.

peak position [cm^{-1}]	sign	assignment
262	-	**Bac** NH_2 rocking
534	-	**Bac** ring deformation (C−H out of plane bending)
589	+	**Bac** ring deformation coupled to CH_2 wagging and **Pro** O−H wagging
1027	-	**Bac** O−H wagging coupled to **Pro** ring CH_2 rocking
1120	-	**Pro** *C−H wagging coupled to O−H wagging
1263	-	**Bac** *C−H wagging coupled to CH_2 rocking
1743	-	**Bac** C=O stretching
2987	+	**Bac** O−H stretching coupled to **Pro** C−H stretching of CH_2 group in α position to N−H group
3000	-	**Bac** O−H stretching coupled **Pro** ring C−H stretching
3009	-	**Bac** O−H stretching coupled **Pro** ring C−H stretching

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