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Supplementary Materials: Adsorption of Selected Molecules on $(TiO_2)_{20}$ Nano-Clusters: A Density-Functional-Theory Study

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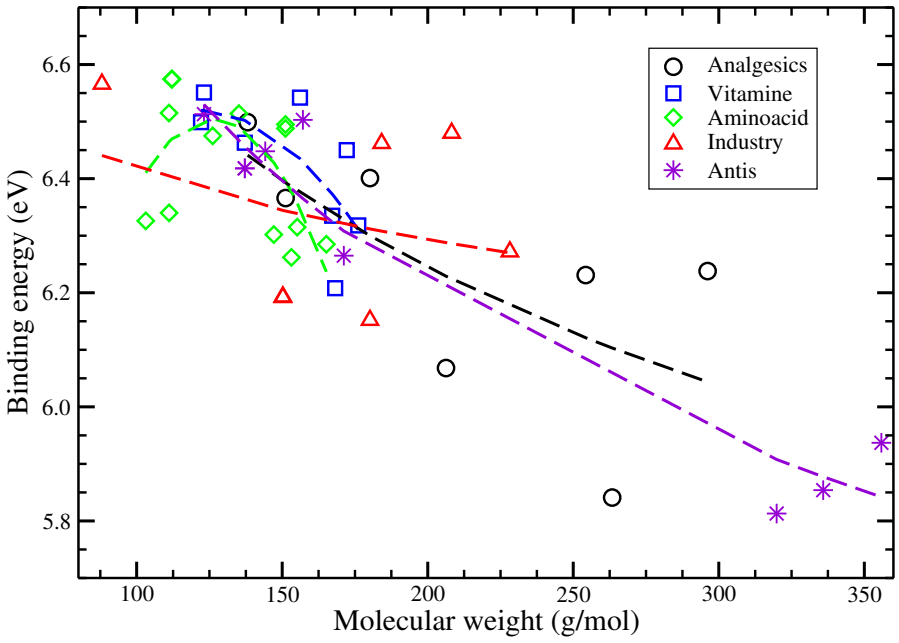

Figure S1. Illustration of the Binding energies of the different molecules here considered as a function of the molecular weight. Calculated with the SIESTA code within the PBE approximation. The lines are a visual aid to illustrate the dependency.

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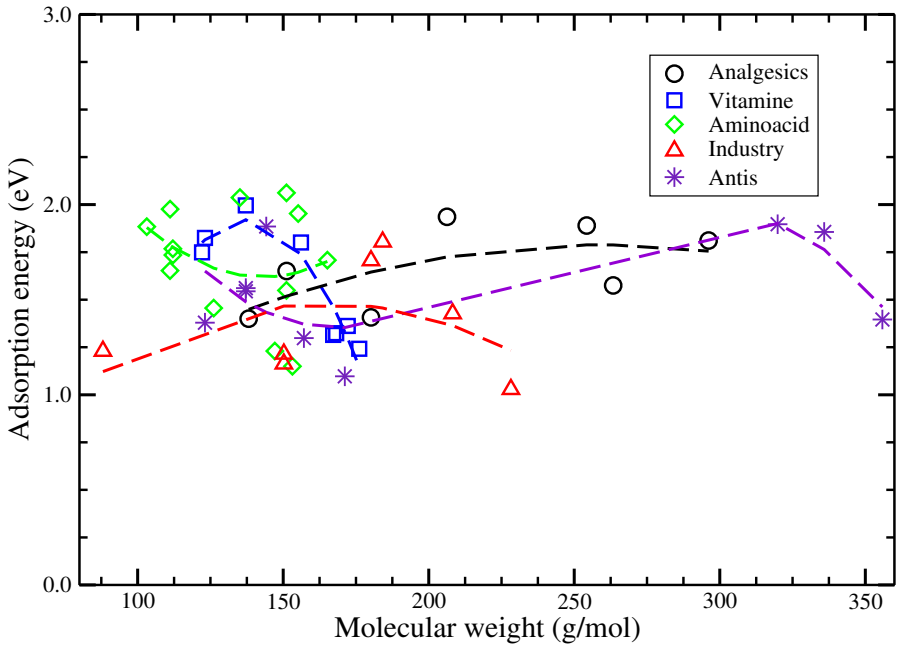

Figure S2. Illustration of the Adsorption energies of the different molecules here considered as a function of the molecular weight. Calculated with the SIESTA code within the PBE approximation. The lines are a visual aid to illustrate the dependency.

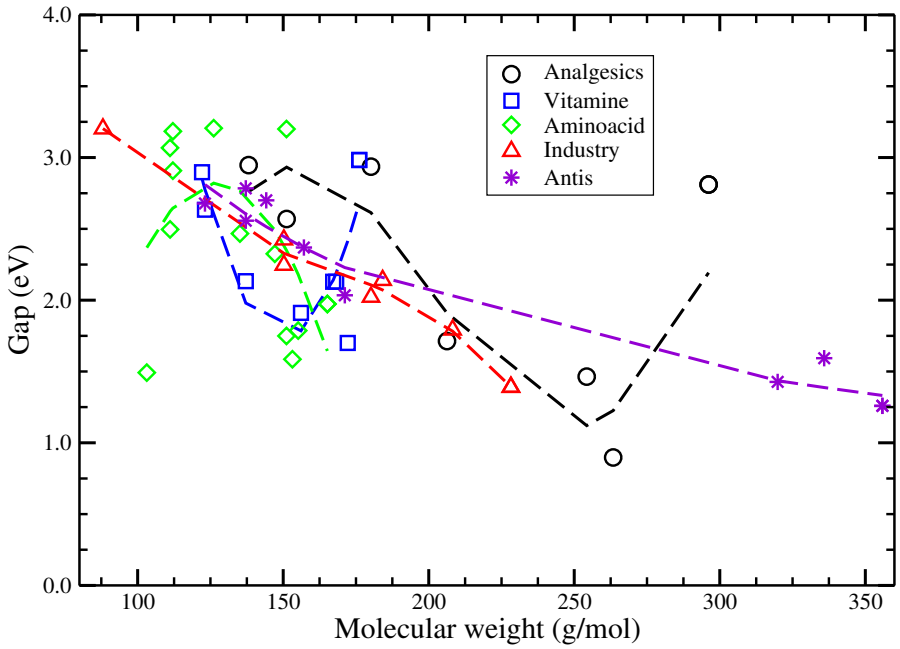

Figure S3. Illustration of the Homo-Lumo gap of the different molecules here considered as a function of the molecular weight. Calculated with the SIESTA code within the PBE approximation. The lines are a visual aid to illustrate the dependency.

1. supplementary information

		PBE (SIESTA)		
Type	Molecule	Ebind (eV/atom) Molecule	Ebind (eV/atom) Complex	Eads (eV) Molecule
Vitaminic-like	B3(1)	4.862	6.499	1.749
	B3(2)	5.014	6.551	1.825
	B10	4.875	6.463	1.996
	B13	5.071	6.542	1.801
	B6(1)	4.718	6.335	1.315
	B6(2)	4.474	6.208	1.324
	K3	5.160	6.450	1.362
	C	4.573	6.318	1.242
Aminoacid/hormones	DMG	4.132	6.326	1.884
	Cytosine	4.708	6.515	1.653
	Histamine	4.318	6.340	1.976
	Uracil-Bind O	4.905	6.574	1.735
	Uracil-Bind N		6.575	1.768
	Thymine	4.765	6.475	1.456
	Adenine	4.917	6.514	2.037
	Glutamic	4.415	6.302	1.230
	Guanine-Bind O	4.924	6.488	1.549
	Guanine-Bind N		6.495	2.062
	Dopanime	4.528	6.262	1.150
	Histidine	4.525	6.315	1.953
	Fenilalanine	4.663	6.285	1.708

		PBE (SIESTA)		
Type	Molecule	Ebind (eV/atom) Molecule	Ebind (eV/atom) Complex	Eads (eV) Molecule
Analgesics	Salicylic	4.988	6.499	1.400
	Paracetamol	4.744	6.366	1.651
	Aspirin	4.966	6.401	1.407
	Ibuprofen	4.536	6.068	1.936
	Tramadol	4.391	5.841	1.575
Anti-inflamatory	Enantyum	4.995	6.231	1.890
	Diclofenac	4.897	6.238	1.811
Antibiotics	Pyrazinamide	4.845	6.513	1.379
	Isoniazid-Bind O	4.698	6.418	1.544
	Isoniazid-Bind N		6.418	1.561
Anti-virals	Favipiravir	4.913	6.503	1.298
	Chloroquine	4.440	5.813	1.897
	Hydroxychloroquine	4.534	5.854	1.856
Anti-parasites	Aminoquinoline	4.986	6.448	1.885
	Metronidazole	4.458	6.265	1.097
	Amodiaquinine	4.705	5.937	1.396
Industry	Biotinidase	4.568	6.566	1.230
	Thymol	4.497	6.193	1.215
	Carva	4.498	6.192	1.163
	Glucose	4.263	6.152	1.706
	Galic-acid	4.970	6.462	1.804
	Anthraquinone	5.424	6.480	1.427
	Resveratrol	4.980	6.272	1.029

		B3LYP (G09)		
Type	Molecule	Ebind (eV/atom) Molecule	Ebind (eV/atom) Complex	Eads (eV) Molecule
Vitaminic-like	B3(1)	4.867	5.854	1.515
	B3(2)	5.010	5.893	1.449
	B10	4.896	5.838	1.730
	B13	4.983	5.874	1.278
	B6(1)	4.711	5.736	1.173
	B6(2)	4.481	5.634	1.141
	K3	5.196	5.863	1.230
	C	4.509	5.699	1.206
Aminoacid/hormones	DMG	4.175	5.696	1.563
	Cytosine	4.680	5.852	1.823
	Histamine	4.348	5.718	1.847
	Uracil-Bind O	4.863	5.893	1.436
	Uracil-Bind N		6.167	1.389
	Thymine	6.065	6.092	1.369
	Adenine	4.847	5.851	1.628
	Glutamic	4.401	5.688	1.169
	Guanine-Bind O	4.836	5.834	1.504
	Guanine-Bind N		5.834	1.491
	Dopanime	4.567	5.681	0.852
	Histidine	4.504	5.702	1.552
	Fenilalanine	4.699	5.711	1.385

		B3LYP (G09)		
Type	Molecule	Ebind (eV/atom) Molecule	Ebind (eV/atom) Complex	Eads (eV) Molecule
Analgesics	Salicylic	4.993	5.866	1.432
	Paracetamol	4.772	5.769	1.584
	Aspirin	4.969	5.805	1.294
	Ibuprofen	4.614	5.572	1.366
	Tramadol	4.451	5.398	1.020
Anti-inflamatory	Enantyum	5.039	5.722	1.343
	Diclofenac	4.890	5.694	1.273
Antibiotics	Pyrazinamide	4.802	5.854	1.410
	Isoniazid-Bind O	4.670	5.784	1.426
	Isoniazid-Bind N		5.781	1.231
Anti-virals	Favipiravir	4.829	5.844	1.359
	Chloroquine	4.495	5.385	1.354
	Hydroxychloroquine	4.483	5.371	1.299
Anti-parasites	Aminoquinoline	5.025	5.844	1.650
	Metronidazole	4.358	5.642	0.988
	Amodiaquinine	4.838	5.492	0.617
Industry	Biotinidase	4.561	5.877	1.222
	Thymol	4.590	5.650	0.958
	Carva	4.591	5.651	1.003
	Glucose	4.225	5.563	1.373
	Galic-acid	4.923	5.828	1.423
	Anthraquinone	5.454	5.912	1.181
	Resveratrol	5.014	5.736	0.587

		M06-L (G09)		
Type	Molecule	Ebind (eV/atom) Molecule	Ebind (eV/atom) Complex	Eads (eV) Molecule
Vitaminic-like	B3(1)	4.898	6.299	1.648
	B3(2)	5.056	6.346	1.505
	B10	4.938	6.274	1.801
	B13	5.035	6.324	1.455
	B6(1)	4.748	6.153	1.319
	B6(2)	4.496	6.030	1.272
	K3	5.266	6.287	1.357
	C	4.541	6.118	1.322
Aminoacid/hormones	DMG	4.168	6.126	1.576
	Cytosine	4.692	6.303	1.828
	Histamine	4.339	6.144	1.989
	Uracil-Bind O	4.894	6.355	1.521
	Uracil-Bind N		6.638	1.593
	Thymine	6.097	6.542	1.431
	Adenine	4.858	6.293	1.788
	Glutamic	4.418	6.108	1.270
	Guanine-Bind O	4.854	6.271	1.569
	Guanine-Bind N		6.273	1.757
	Dopanime	4.589	6.088	0.968
	Histidine	4.514	6.115	1.604
	Fenilalanine	4.729	6.115	1.449

		M06-L (G09)		
Type	Molecule	Ebind (eV/atom) Molecule	Ebind (eV/atom) Complex	Eads (eV) Molecule
Analgesics	Salicylic	5.049	6.311	1.534
	Paracetamol	4.808	6.189	1.669
	Aspirin	5.025	6.226	1.431
	Ibuprofen	4.646	5.937	1.500
	Tramadol	4.474	5.726	1.351
Anti-inflamatory	Enantyum	5.099	6.098	1.535
	Diclofenac	4.966	6.086	1.435
Antibiotics	Pyrazinamide	4.823	6.301	1.460
	Isoniazid-Bind O	4.687	6.215	1.541
	Isoniazid-Bind N		6.213	1.390
Anti-virals	Favipiravir	4.861	6.289	1.422
	Chloroquine	4.518	5.703	1.743
	Hydroxychloroquine	4.506	5.686	1.707
Anti-parasites	Aminoquinoline	5.067	6.272	1.900
	Metronidazole	4.375	6.054	1.151
	Amodiaquinine	4.880	5.821	1.080
Industry	Biotinidase	4.584	6.348	1.207
	Thymol	4.617	6.045	1.079
	Carva	4.617	6.045	1.110
	Glucose	4.230	5.957	1.542
	Galic-acid	4.981	6.263	1.504
	Anthraquinone	5.539	6.329	1.416
	Resveratrol	5.071	6.125	0.750

1.1. coordinates

Vitaminic-like
B3(1)
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C 0.642832 5.287764 1.019334
H 0.876245 6.376607 1.070211
N 0.142904 4.740412 2.149805

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C -0.160048 3.428532 2.104297
C 0.579371 3.198767 -0.214136
H -0.574822 2.970417 3.031018
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B10

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Aminoacid/hormones

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Cytosine

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Histamine

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Uracil-Bind O
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Thymine

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Adenine

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Glutamic
Guanine-Bind O
76
N -0.051024 2.229307 0.900361
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C -0.119274 3.607048 0.869522
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H -0.043096 2.793157 -4.568177
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Ti -3.177511 -6.154772 2.252664
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Guanine-Bind N
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Dopamine

82
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Phenylalanine

83
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O -2.253670 -10.283397 0.253872
O 0.632915 -10.790109 0.385429

O -3.158703 -8.058021 1.223174
O 1.643856 -9.276840 -5.039501
O 1.258724 -2.108423 0.546144
O -0.361013 -3.787864 -0.528594
O -1.714420 -9.612142 -4.951629
O -2.641850 -4.496158 -1.910974
O -1.774777 -6.582895 3.095541
O -0.768870 -10.651002 2.864335
O -3.744324 -9.844455 2.949756
O 3.278732 -6.988050 -0.461815
O -1.801502 -2.040987 0.669960
O -0.199870 -5.770895 -2.255054
O -3.621823 -9.588909 -2.399268

Analgesics

Salicylic

76
C 0.073108 2.520150 1.210034
C 0.026300 3.307102 2.402753
C 0.027966 3.189259 -0.046562
H 0.059291 2.562735 -0.963903
C -0.056060 4.715866 2.338716
C -0.052892 4.594044 -0.116990
H -0.085065 5.099342 -1.104449
H -0.091627 5.299118 3.285434
C -0.093877 5.357857 1.080408
H -0.158172 6.466442 1.037598
C 0.165651 1.036132 1.228518
O 0.250089 0.375514 2.394377
H 0.210201 1.056264 3.130581
O 0.170776 0.377933 0.143852
O 0.057174 2.639807 3.626489
H 0.037403 3.313928 4.346084
O -0.769912 -4.037211 -4.035107
O -4.862617 -6.705129 2.757631
O 2.962451 -4.957092 1.742741
O 2.036094 -8.778710 1.154495
Ti -1.503002 -3.795757 1.369057
Ti -3.179177 -5.997877 2.209530
Ti -4.815848 -8.405818 2.008382
O 3.992867 -7.859136 2.550034
O 1.107107 -8.514594 -1.378043
Ti -0.781383 -3.605884 -2.199200
Ti 1.588429 -4.102415 0.781825
O -0.367215 -1.794558 -1.878135
O -1.748707 -7.904070 -1.216459
Ti -3.765625 -8.550279 -0.710726
Ti -2.206581 -9.611197 1.906065
Ti 3.495223 -9.579444 2.048378
Ti -0.211056 -6.543499 2.068482
Ti -0.197675 -8.338406 -5.414407
Ti 2.992532 -8.921356 -0.698036
Ti 0.007907 -1.730092 -0.047542
Ti 2.702925 -6.781814 1.674579
Ti -0.608274 -9.500076 -0.784044

Ti 0.620834 -10.133841 1.902276
Ti 1.809631 -8.471101 -3.298305
Ti -2.398199 -6.001720 -1.373642
Ti 1.694897 -6.150934 -1.361789
Ti -2.096403 -8.689913 -3.213933
Ti -0.721339 -5.878879 -4.007435
O -2.991787 -4.155824 2.431222
O 4.160831 -9.970494 0.377377
O 0.973409 -6.219751 0.496648
O -4.044532 -6.667057 -1.051860
O -1.047340 -10.122345 -2.413141
O 0.014615 -4.472409 2.230853
O -0.557040 -8.521560 1.481041
O 2.257987 -6.713292 -3.106422
O 2.197577 -10.688712 2.812894
O 1.281824 -6.922614 2.990893
O -1.943888 -5.638104 0.616378
O 3.273470 -9.313294 -2.482665
O -2.368672 -6.534599 -3.386423
O -5.323124 -8.919646 0.282660
O -0.368957 -6.543916 -5.763879
O -0.160137 -7.862226 -3.579506
O 2.267223 -4.488722 -0.998725
O -2.418906 -10.067050 0.109155
O 0.431928 -10.770033 0.197993
O -3.183006 -7.863577 1.232124
O 1.507722 -9.017585 -5.098452
O 1.631543 -2.243325 0.777294
O -0.197545 -3.710915 -0.237172
O -1.854280 -9.118788 -5.035178
O -2.466795 -4.128450 -1.721027
O -1.758905 -6.598687 3.188225
O -0.969665 -10.760644 2.667337
O -3.859623 -9.740393 2.842678
O 3.284970 -7.106223 -0.386706
O -1.414031 -1.924645 1.115907
O -0.142799 -5.576966 -2.092336
O -3.746708 -9.127571 -2.479854

Paracetamol

80
C -0.046083 3.713988 0.421781
C -0.043337 4.192613 1.761236
C -0.062654 4.644401 -0.653369
H -0.047248 4.265249 -1.697706
C -0.061089 5.578200 2.016864
C -0.074562 6.029022 -0.401182
H -0.079290 6.754065 -1.244300
H -0.047006 5.953918 3.061186
C -0.069202 6.504516 0.937779
O -0.057670 7.851617 1.242454
H -0.064432 8.332865 0.379878
N 0.054412 2.346998 0.056177
C -0.055170 1.194305 0.745668
C -0.610881 1.099426 2.143604

H 0.372028 2.187031 -0.911754
H -0.009516 3.485192 2.606892
O 0.330797 0.141887 0.117704
H -1.388403 1.864558 2.343973
H 0.205952 1.236234 2.889698
H -1.029983 0.076776 2.268817
O -0.840985 -4.110122 -3.926823
O -4.866311 -6.885262 2.791106
O 2.968113 -5.124260 1.825706
O 2.045493 -8.914893 1.155201
Ti -1.494440 -3.936492 1.504219
Ti -3.176618 -6.167461 2.283896
Ti -4.806682 -8.583651 2.031173
O 4.012957 -8.032781 2.558162
O 1.130934 -8.647222 -1.391481
Ti -0.798183 -3.722129 -2.079056
Ti 1.585088 -4.271261 0.886687
O -0.385482 -1.925648 -1.733404
O -1.732036 -8.027287 -1.182517
Ti -3.721857 -8.699295 -0.677879
Ti -2.196065 -9.775828 1.920710
Ti 3.505325 -9.742213 2.024601
Ti -0.206928 -6.719535 2.139058
Ti -0.206156 -8.359297 -5.398037
Ti 3.005660 -9.026938 -0.722069
Ti 0.031729 -1.875542 0.097447
Ti 2.706515 -6.947987 1.721663
Ti -0.599413 -9.622320 -0.792227
Ti 0.637399 -10.281724 1.887566
Ti 1.832132 -8.508126 -3.312797
Ti -2.397835 -6.119970 -1.269596
Ti 1.694000 -6.252545 -1.307282
Ti -2.096904 -8.773946 -3.201846
Ti -0.790389 -5.948629 -3.932942
O -3.000038 -4.322060 2.532050
O 4.156375 -10.110260 0.342353
O 0.973348 -6.367485 0.563501
O -4.033396 -6.805304 -0.962827
O -1.042520 -10.218316 -2.427273
O 0.017302 -4.644333 2.341353
O -0.549261 -8.668826 1.507047
O 2.249769 -6.750964 -3.070065
O 2.216889 -10.861881 2.775949
O 1.294820 -7.105184 3.048943
O -1.939366 -5.775674 0.711289
O 3.329373 -9.318178 -2.521422
O -2.409804 -6.638568 -3.301210
O -5.284986 -9.087794 0.300269
O -0.449947 -6.570059 -5.707223
O -0.160580 -7.925182 -3.557082
O 2.252303 -4.596836 -0.910570
O -2.393241 -10.214471 0.111377
O 0.444195 -10.896796 0.178062
O -3.162347 -8.026461 1.286002

O 1.527878 -8.994818 -5.127237
O 1.645986 -2.417045 0.905091
O -0.225948 -3.857553 -0.108184
O -1.849562 -9.176081 -5.027070
O -2.486839 -4.251477 -1.606723
O -1.755767 -6.778675 3.260629
O -0.947981 -10.922362 2.659875
O -3.850812 -9.926802 2.851551
O 3.282366 -7.214646 -0.364087
O -1.352373 -2.043658 1.318886
O -0.157515 -5.681422 -2.021837
O -3.734142 -9.241445 -2.457722

Aspirin

81
C 0.151811 2.500786 1.192155
C 0.179867 3.320401 2.365381
C 0.048282 3.132459 -0.078560
H 0.026576 2.483132 -0.979384
C 0.110891 4.727713 2.272547
C -0.025088 4.536832 -0.179650
H -0.104116 5.016590 -1.177541
H 0.128475 5.344301 3.190997
C 0.007546 5.329614 0.996352
H -0.043133 6.436889 0.928945
C 0.223312 1.010992 1.235300
O 0.353646 0.378555 2.410471
H 0.381484 1.100634 3.115423
O 0.159835 0.333925 0.164677
O 0.359985 2.655317 3.599947
C -0.427846 3.053539 4.752308
O -1.158695 4.025126 4.747495
C -0.164451 2.067829 5.866345
H 0.745315 1.462704 5.665155
H -1.037638 1.376749 5.954451
H -0.067953 2.608778 6.831969
O -0.846846 -4.124328 -3.967742
O -4.856054 -6.808542 2.832797
O 2.956342 -4.996626 1.800463
O 2.042187 -8.822177 1.208624
Ti -1.505840 -3.876576 1.410501
Ti -3.181957 -6.090164 2.265400
Ti -4.816258 -8.508957 2.079878
O 4.015997 -7.893952 2.570780
O 1.117940 -8.599811 -1.331193
Ti -0.803963 -3.688750 -2.132512
Ti 1.582366 -4.154457 0.833742
O -0.425742 -1.866773 -1.814117
O -1.747687 -7.997703 -1.161830
Ti -3.762091 -8.653685 -0.640584
Ti -2.198927 -9.691960 1.967443
Ti 3.504783 -9.624199 2.094546
Ti -0.210897 -6.619181 2.123865
Ti -0.208004 -8.406961 -5.354794
Ti 2.997250 -8.977716 -0.663002

Ti -0.004169 -1.788418 0.007795
Ti 2.703234 -6.825992 1.725550
Ti -0.602867 -9.578843 -0.726187
Ti 0.640180 -10.186548 1.963467
Ti 1.815529 -8.507926 -3.258662
Ti -2.400382 -6.097261 -1.281907
Ti 1.695776 -6.201982 -1.311400
Ti -2.100535 -8.788835 -3.152730
Ti -0.789346 -5.965445 -3.934296
O -3.031905 -4.240402 2.427377
O 4.152801 -10.038059 0.423509
O 0.981940 -6.282830 0.555236
O -4.045207 -6.766941 -0.955576
O -1.046622 -10.212654 -2.348673
O 0.008519 -4.536300 2.279203
O -0.553709 -8.585664 1.527530
O 2.241741 -6.746464 -3.066172
O 2.221847 -10.741755 2.866889
O 1.290485 -6.966566 3.053014
O -1.912127 -5.752142 0.683326
O 3.300623 -9.326371 -2.451624
O -2.413954 -6.634742 -3.300762
O -5.317850 -9.024905 0.356008
O -0.443828 -6.621012 -5.695208
O -0.170180 -7.939518 -3.517437
O 2.254062 -4.534700 -0.955086
O -2.405323 -10.160013 0.170915
O 0.443359 -10.836236 0.267494
O -3.180748 -7.959879 1.306047
O 1.519153 -9.044108 -5.059199
O 1.632654 -2.291425 0.802079
O -0.204198 -3.782809 -0.176363
O -1.848815 -9.219421 -4.970013
O -2.478652 -4.221600 -1.621226
O -1.753218 -6.648465 3.257760
O -0.945447 -10.801804 2.754097
O -3.854601 -9.847866 2.895824
O 3.279307 -7.154128 -0.356554
O -1.395554 -1.998984 1.201026
O -0.163235 -5.658411 -2.032090
O -3.749322 -9.226156 -2.413875

Ibuprofen

93
C 1.661718 2.989502 -0.921272
C 0.950959 3.408198 0.233997
C 1.875234 3.927527 -1.963927
H 2.425710 3.603119 -2.872141
C 0.484908 4.739235 0.341323
C 1.409074 5.256384 -1.851154
H 1.608142 5.980613 -2.667962
H -0.052705 5.069465 1.254031
C 0.707824 5.685593 -0.693052
C 0.268571 7.131047 -0.539714
H -0.409315 7.217299 0.344872

H -0.318244 7.453177 -1.436217
C 1.456444 8.109662 -0.346075
C 2.232503 7.772884 0.939643
H 1.568337 7.896768 1.828597
H 3.110969 8.443773 1.072019
H 2.587709 6.717365 0.926733
C 0.949282 9.561966 -0.328498
H 1.789868 10.285222 -0.220906
H 0.254771 9.714130 0.532025
H 0.392215 9.807768 -1.263111
C 2.245673 1.580013 -1.042173
H 2.845143 1.553056 -1.983648
H 3.566162 0.187378 0.055298
H 3.930868 1.943381 0.301645
H 2.498670 1.188143 1.097712
C 3.115863 1.198710 0.173921
H 0.780457 2.691605 1.062230
C 1.137587 0.540978 -1.247024
O 0.548121 0.066532 -0.152333
O 0.835032 0.140387 -2.416183
H 0.033981 -0.994594 -2.201886
H 2.142744 7.976009 -1.224184
O -0.835853 -4.112373 -3.942861
O -4.882446 -6.913769 2.800607
O 2.928803 -5.098354 1.834510
O 2.034492 -8.904988 1.146719
Ti -1.520085 -3.933567 1.492219
Ti -3.197497 -6.193192 2.275137
Ti -4.872925 -8.597045 2.005441
O 3.989056 -8.013383 2.552436
O 1.111051 -8.622151 -1.374956
Ti -0.820622 -3.743577 -2.110566
Ti 1.536156 -4.252251 0.908586
O -0.450048 -1.874000 -1.765298
O -1.752342 -8.031148 -1.205382
Ti -3.782163 -8.702357 -0.700353
Ti -2.233251 -9.767757 1.893812
Ti 3.497194 -9.731974 2.018559
Ti -0.233104 -6.735533 2.103040
Ti -0.207003 -8.387420 -5.403302
Ti 2.994973 -9.003135 -0.711656
Ti 0.009545 -1.794145 0.219044
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Ti -0.605810 -9.624686 -0.790119
Ti 0.616890 -10.266208 1.892855
Ti 1.814886 -8.490097 -3.295983
Ti -2.406244 -6.144066 -1.284106
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Ti -2.100937 -8.796504 -3.205122
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O -3.041197 -4.344537 2.484709
O 4.160073 -10.076824 0.339086
O 0.953186 -6.328963 0.544688
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O -0.026970 -4.655274 2.330079
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O 3.299701 -9.318704 -2.505231
O -2.410517 -6.634883 -3.337432
O -5.347054 -9.091299 0.264556
O -0.456553 -6.597873 -5.730810
O -0.171488 -7.918708 -3.560295
O 2.219630 -4.536544 -0.898999
O -2.432415 -10.208715 0.090001
O 0.424269 -10.894496 0.187393
O -3.221969 -8.030325 1.252862
O 1.520496 -9.015739 -5.099286
O 1.565067 -2.393615 1.049055
O -0.255517 -3.766432 -0.127247
O -1.840750 -9.208257 -5.026917
O -2.490026 -4.257963 -1.643830
O -1.771459 -6.809650 3.236232
O -0.972829 -10.881523 2.666993
O -3.903724 -9.945375 2.795186
O 3.266773 -7.179609 -0.358235
O -1.347884 -2.029590 1.408308
O -0.174380 -5.666118 -2.029532
O -3.750766 -9.240467 -2.480849

Tramadol

104
C 2.048589 2.276338 -3.579635
O 3.126529 1.557734 -4.068828
C 3.871059 2.199807 -5.119370
H 4.312000 3.169504 -4.779106
H 4.687589 1.503833 -5.400184
H 3.236873 2.407022 -6.014672
H -1.022174 4.093592 -1.919521
C -0.165304 3.575614 -2.386124
C 1.362357 1.669769 -2.495002
H 1.752984 0.721155 -2.086542
C 0.259386 2.311654 -1.890954
C 1.632170 3.542481 -4.068935
C 0.521398 4.179367 -3.462464
H 2.165247 4.025586 -4.907639
H 0.187145 5.167076 -3.840260
C 1.608177 2.740171 0.669415
H 1.774316 3.469802 -0.156053
H 1.827726 3.281458 1.634006
N 2.552448 1.639528 0.455934
C 2.786070 0.866852 1.680251
C 3.818306 2.157797 -0.069211
H 1.885154 0.288515 1.966866
H 3.632716 2.671088 -1.038238
H 3.608998 0.140475 1.509073

H 4.517005 1.312176 -0.245989
H 3.061117 1.524467 2.550769
H 4.327545 2.887367 0.621540
H -0.409231 3.384277 0.624616
O -0.042064 0.247436 -0.629455
H -0.219529 -0.092871 -1.554335
C -0.403247 1.701652 -0.645493
C -1.951152 1.769974 -0.687342
H -2.307094 1.250912 -1.609506
H -2.239304 2.842175 -0.787160
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H -2.433767 0.052891 0.567561
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C -0.475202 1.672971 1.898682
H -0.142294 0.609227 1.936427
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H -0.065100 2.158108 2.815410
H -2.320866 2.817546 1.973455
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O -4.860192 -6.798267 2.849681
O 2.950197 -5.028031 1.864227
O 2.044491 -8.847745 1.249766
Ti -1.495677 -3.869020 1.492376
Ti -3.173844 -6.098324 2.308721
Ti -4.815530 -8.510971 2.118355
O 4.004474 -7.943813 2.639124
O 1.133409 -8.641796 -1.290524
Ti -0.802189 -3.722566 -2.099415
Ti 1.577541 -4.184485 0.914393
O -0.359548 -1.932701 -1.818326
O -1.734767 -8.023557 -1.107117
Ti -3.729262 -8.684458 -0.590563
Ti -2.199790 -9.697028 2.030551
Ti 3.506615 -9.667387 2.125592
Ti -0.219701 -6.634749 2.191790
Ti -0.198067 -8.437728 -5.302194
Ti 3.008661 -8.983011 -0.617011
Ti 0.006791 -1.795752 0.078897
Ti 2.702657 -6.867568 1.794078
Ti -0.597634 -9.603798 -0.672932
Ti 0.636561 -10.197293 2.017260
Ti 1.841120 -8.509343 -3.205964
Ti -2.389910 -6.112190 -1.219764
Ti 1.698020 -6.202266 -1.241183
Ti -2.086311 -8.811363 -3.099971
Ti -0.775611 -5.997134 -3.890966
O -3.033034 -4.244381 2.471114
O 4.158289 -10.056948 0.449055
O 0.972953 -6.273075 0.618437
O -4.026345 -6.784035 -0.879899
O -1.044479 -10.241204 -2.291752
O 0.007010 -4.549787 2.356913

O -0.552263 -8.591598 1.574644
O 2.245504 -6.743592 -2.993005
O 2.222743 -10.765711 2.905505
O 1.283354 -7.022910 3.104283
O -1.885253 -5.750548 0.749077
O 3.343431 -9.299325 -2.406037
O -2.395418 -6.663291 -3.247308
O -5.290085 -9.053239 0.398433
O -0.441306 -6.655611 -5.651847
O -0.156153 -7.959378 -3.466090
O 2.250920 -4.533435 -0.871367
O -2.400832 -10.174671 0.234048
O 0.433065 -10.860888 0.332673
O -3.166462 -7.965743 1.361635
O 1.537555 -9.056934 -5.002275
O 1.580623 -2.291944 0.930441
O -0.222963 -3.760286 -0.114929
O -1.838325 -9.248151 -4.916306
O -2.482024 -4.246915 -1.572051
O -1.757287 -6.660228 3.321015
O -0.945827 -10.796558 2.826027
O -3.858255 -9.842958 2.952699
O 3.273527 -7.158049 -0.280515
O -1.346872 -1.973288 1.300248
O -0.153528 -5.669881 -1.973012
O -3.736112 -9.247672 -2.360711

Anti-inflamatory

Enantyum

93
C 0.889467 3.351636 -1.188606
C 0.121248 3.668947 -0.034534
C 1.046635 4.333873 -2.192402
C -0.241633 5.946537 -0.867467
H -0.674583 6.959028 -0.737416
H 1.605730 4.105438 -3.120202
C -0.455565 4.950290 0.114728
C 0.516861 5.642709 -2.028944
C 0.766971 6.639126 -3.138619
O 0.800178 6.255020 -4.327999
C 1.019992 8.087037 -2.801697
C 1.474796 8.513630 -1.522877
H 1.607880 7.768867 -0.712756
C 0.889143 9.043533 -3.847108
H 0.566335 8.680313 -4.846657
C 1.632120 10.823149 -2.333935
H 1.874385 11.892561 -2.149889
C 1.781732 9.874683 -1.291886
H 2.148863 10.191554 -0.292431
C 1.183562 10.403685 -3.613827
H 1.070482 11.143332 -4.435466
H -1.063851 5.182303 1.013986
C 1.582128 1.985750 -1.287139
H 2.165332 1.842078 -0.344118
C 2.512342 1.835554 -2.505708

H 3.011344 0.841871 -2.501554
H 3.301306 2.617437 -2.498334
H 1.939003 1.926641 -3.452998
H -0.014355 2.902214 0.758733
C 0.556724 0.842237 -1.309555
O 0.382216 0.183214 -0.163917
O -0.036670 0.523369 -2.384229
H -0.450231 -0.812786 -2.159345
O -0.900813 -4.029308 -3.946457
O -4.890474 -6.896803 2.706860
O 2.901016 -5.051476 1.839849
O 2.044968 -8.864645 1.164354
Ti -1.525707 -3.897135 1.424881
Ti -3.213665 -6.162509 2.170816
Ti -4.828295 -8.609012 1.989965
O 3.976974 -7.952519 2.579685
O 1.122835 -8.573880 -1.381508
Ti -0.892444 -3.669904 -2.120495
Ti 1.530609 -4.204329 0.891220
O -0.563907 -1.802248 -1.742469
O -1.732030 -8.001621 -1.210711
Ti -3.736139 -8.706679 -0.711338
Ti -2.191601 -9.768275 1.876755
Ti 3.518866 -9.679804 2.043228
Ti -0.266038 -6.702294 2.054931
Ti -0.176845 -8.293486 -5.407294
Ti 3.000197 -8.961536 -0.698376
Ti 0.006025 -1.720731 0.215363
Ti 2.673814 -6.884363 1.728199
Ti -0.576608 -9.591629 -0.797440
Ti 0.663901 -10.250531 1.868577
Ti 1.837706 -8.453615 -3.297275
Ti -2.419035 -6.122656 -1.311373
Ti 1.713810 -6.165040 -1.314864
Ti -2.060703 -8.752756 -3.216218
Ti -0.779641 -5.884344 -3.953492
O -3.082741 -4.313211 2.361490
O 4.172976 -10.024392 0.362230
O 0.957410 -6.290314 0.521562
O -4.047535 -6.805237 -0.985635
O -0.994579 -10.174538 -2.452113
O -0.046282 -4.616124 2.280624
O -0.556444 -8.650256 1.424160
O 2.259932 -6.691977 -3.071495
O 2.239125 -10.824836 2.768492
O 1.225211 -7.066448 2.998356
O -1.908009 -5.783279 0.635543
O 3.314465 -9.282219 -2.489359
O -2.391817 -6.592681 -3.334608
O -5.297984 -9.115568 0.257971
O -0.396338 -6.493640 -5.713917
O -0.149843 -7.849097 -3.561083
O 2.245506 -4.504227 -0.898501
O -2.378505 -10.215277 0.066956

O 0.474128 -10.866311 0.160181
O -3.181070 -8.040466 1.227944
O 1.530211 -8.971865 -5.099722
O 1.567591 -2.338615 1.009407
O -0.252364 -3.696900 -0.166148
O -1.818393 -9.106849 -5.051204
O -2.539919 -4.227668 -1.626958
O -1.806233 -6.737158 3.184144
O -0.918729 -10.861576 2.659235
O -3.842726 -9.935558 2.802838
O 3.277595 -7.140750 -0.357798
O -1.328889 -1.995553 1.417640
O -0.161461 -5.573067 -2.048825
O -3.710982 -9.221567 -2.495488
Diclofenac
90
C -1.757447 0.876826 3.656891
C -1.936099 1.348510 4.980288
H -2.318794 0.661641 5.763643
C -1.267991 1.736032 2.643530
C -1.138145 3.565191 4.295648
H -0.890858 4.621296 4.526269
C -1.169642 1.234487 1.210401
H -1.806585 1.867727 0.539415
H -1.575251 0.198320 1.158639
C 0.227885 1.196093 0.584646
O 0.606388 0.165958 -0.054345
O 1.036236 2.229561 0.659895
H 0.518738 3.004345 1.187647
C -1.627766 2.694006 5.297626
C -0.959659 3.081624 2.981955
N -0.458948 3.916681 1.892003
H -1.228820 4.039268 1.205180
C 0.035862 5.222787 2.198335
C 1.270396 5.409935 2.888768
Cl 2.191976 4.003058 3.403049
C -0.657155 6.388728 1.756877
Cl -2.173141 6.196006 0.862977
C 1.051028 7.843488 2.715613
H 1.446247 8.859711 2.919524
C 1.766669 6.708208 3.162133
H 2.725762 6.811995 3.711220
C -0.158934 7.690991 2.000053
H -0.728447 8.568802 1.630907
H -1.767392 3.074679 6.330590
H -1.996848 -0.172174 3.383426
O -0.856323 -4.180996 -4.035211
O -4.853897 -6.786539 2.788861
O 2.964888 -5.066459 1.783776
O 2.031457 -8.886060 1.214889
Ti -1.485766 -3.877198 1.322957
Ti -3.178098 -6.078672 2.219836
Ti -4.806487 -8.501793 2.065408
O 3.985594 -7.961640 2.608847

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Ti -0.792123 -3.732620 -2.202420
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O -1.733934 -8.021326 -1.167239
Ti -3.729493 -8.672847 -0.638119
Ti -2.204169 -9.726036 1.961825
Ti 3.488295 -9.683830 2.121479
Ti -0.217852 -6.637212 2.112831
Ti -0.205751 -8.480160 -5.370852
Ti 2.990734 -9.040428 -0.637465
Ti 0.093266 -1.835069 -0.094763
Ti 2.697230 -6.888938 1.723972
Ti -0.601545 -9.614792 -0.739748
Ti 0.619556 -10.241698 1.958973
Ti 1.811032 -8.591419 -3.254429
Ti -2.390900 -6.118952 -1.312474
Ti 1.690573 -6.287088 -1.331181
Ti -2.098809 -8.808969 -3.161471
Ti -0.786447 -6.017240 -3.985949
O -3.029014 -4.216060 2.317685
O 4.157553 -10.078815 0.453648
O 0.975794 -6.335421 0.544875
O -4.027994 -6.783291 -0.963036
O -1.038610 -10.243782 -2.361269
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O -0.560422 -8.623234 1.572415
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O 2.185305 -10.789721 2.886692
O 1.275903 -7.005571 3.040208
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O 3.267165 -9.432689 -2.424362
O -2.409711 -6.686479 -3.325878
O -5.295899 -9.033846 0.349983
O -0.441582 -6.698354 -5.739285
O -0.163649 -7.977057 -3.541415
O 2.277868 -4.630502 -0.974237
O -2.406905 -10.176850 0.158661
O 0.442071 -10.872639 0.251969
O -3.161281 -7.967626 1.301865
O 1.510137 -9.135928 -5.053702
O 1.675267 -2.375978 0.774932
O -0.170086 -3.824401 -0.249770
O -1.853249 -9.269673 -4.971632
O -2.468230 -4.243442 -1.661429
O -1.765518 -6.615707 3.238138
O -0.973476 -10.881127 2.713647
O -3.857193 -9.843635 2.898626
O 3.285056 -7.226632 -0.347115
O -1.328180 -1.976278 1.084654
O -0.145959 -5.690995 -2.092208
O -3.739442 -9.246928 -2.407675

Antibiotics

Pyrazinamide

74
N -1.805176 0.995498 1.811714
N -1.727584 3.803288 2.452190
C -0.979932 1.873749 1.188451
C -0.951174 3.258426 1.501728
H -0.250855 3.940411 0.968156
C -2.595910 1.546803 2.747096
C -2.551807 2.932989 3.071711
H -3.297099 0.860541 3.274097
H -3.212973 3.345733 3.867334
N 0.465855 2.141160 -0.781800
H 0.136094 3.103224 -0.878508
H 1.138512 1.764116 -1.457596
C -0.000584 1.322362 0.180135
O 0.439739 0.138218 0.257693
O -0.787213 -4.120104 -3.920306
O -4.849614 -6.832613 2.850291
O 2.986792 -5.094399 1.826681
O 2.030971 -8.894775 1.180686
Ti -1.489969 -3.937321 1.493789
Ti -3.150412 -6.152042 2.310690
Ti -4.843336 -8.519586 2.065148
O 4.023020 -8.017181 2.554844
O 1.105595 -8.649170 -1.359903
Ti -0.771901 -3.698471 -2.081217
Ti 1.596202 -4.233638 0.902269
O -0.386798 -1.888548 -1.719597
O -1.745841 -8.010198 -1.167548
Ti -3.768707 -8.654219 -0.651413
Ti -2.231838 -9.722371 1.946438
Ti 3.486847 -9.727818 2.048362
Ti -0.188606 -6.692524 2.142778
Ti -0.233840 -8.399521 -5.360994
Ti 2.978167 -9.022475 -0.690464
Ti 0.014231 -1.864273 0.124288
Ti 2.729293 -6.919744 1.721729
Ti -0.620575 -9.599589 -0.736135
Ti 0.607712 -10.233371 1.949409
Ti 1.815920 -8.505250 -3.279663
Ti -2.379663 -6.100451 -1.268220
Ti 1.702133 -6.214344 -1.294150
Ti -2.115965 -8.786522 -3.157145
Ti -0.767456 -5.965654 -3.915549
O -2.984447 -4.311490 2.538722
O 4.120001 -10.124221 0.364758
O 0.993603 -6.332328 0.567969
O -4.027488 -6.762698 -0.959804
O -1.085130 -10.225582 -2.357911
O 0.033367 -4.629520 2.338346
O -0.570088 -8.628932 1.498526
O 2.232585 -6.741884 -3.061264
O 2.188208 -10.805364 2.845674
O 1.313170 -7.082341 3.049475
O -1.917454 -5.774363 0.716881

O 3.299155 -9.330324 -2.484275
O -2.399010 -6.622392 -3.294680
O -5.336810 -9.013871 0.333176
O -0.459681 -6.610524 -5.687664
O -0.177247 -7.946188 -3.521131
O 2.260032 -4.555343 -0.908490
O -2.441877 -10.175981 0.151502
O 0.390925 -10.883656 0.257200
O -3.193347 -7.980205 1.302496
O 1.501003 -9.030890 -5.079761
O 1.625680 -2.380517 0.960289
O -0.189899 -3.824372 -0.113986
O -1.870408 -9.214578 -4.975541
O -2.457419 -4.225316 -1.603495
O -1.726512 -6.755556 3.279618
O -0.983014 -10.829680 2.745161
O -3.895381 -9.872020 2.869198
O 3.282108 -7.207716 -0.356405
O -1.395197 -2.068342 1.296001
O -0.157647 -5.679277 -1.995246
O -3.769834 -9.214695 -2.427269
Isoniazid-Bind O
77
C -1.573449 1.074236 2.121863
H -1.511084 -0.029635 1.982603
C -1.813085 3.802294 2.522594
H -1.919714 4.893188 2.716485
C -0.805435 1.956175 1.320872
C -0.924582 3.354531 1.521160
H -0.330257 4.081894 0.928452
C -2.435804 1.652156 3.080578
N -2.557640 2.977810 3.287604
H -3.063854 0.989781 3.718307
N 0.578387 2.133701 -0.691743
H 0.476259 3.149874 -0.651239
N 1.508050 1.623688 -1.608841
H 1.029907 1.540323 -2.524895
H 1.656212 0.641808 -1.310468
C 0.077813 1.366766 0.286035
O 0.382246 0.124358 0.298362
O -0.799189 -4.123870 -3.950920
O -4.840089 -6.808855 2.860086
O 2.987997 -5.065984 1.815567
O 2.041263 -8.870297 1.193362
Ti -1.483051 -3.909445 1.446572
Ti -3.152859 -6.115177 2.304128
Ti -4.827104 -8.506477 2.094609
O 4.025144 -7.977272 2.564305
O 1.108621 -8.617808 -1.348216
Ti -0.775319 -3.698813 -2.116912
Ti 1.603021 -4.219596 0.877241
O -0.350729 -1.884827 -1.784639
O -1.737275 -7.995929 -1.153244
Ti -3.754151 -8.644958 -0.624315

Ti -2.206066 -9.692528 1.975054
Ti 3.507251 -9.694479 2.062092
Ti -0.192644 -6.652896 2.137775
Ti -0.233552 -8.408819 -5.356973
Ti 2.982127 -9.003680 -0.682834
Ti 0.042631 -1.849635 0.056585
Ti 2.725100 -6.893581 1.723765
Ti -0.614963 -9.589387 -0.724134
Ti 0.631830 -10.210349 1.962793
Ti 1.815831 -8.506167 -3.274418
Ti -2.378929 -6.094694 -1.269406
Ti 1.703783 -6.213612 -1.304970
Ti -2.112790 -8.782356 -3.144615
Ti -0.774612 -5.970188 -3.925942
O -2.988520 -4.262796 2.476996
O 4.138019 -10.081304 0.376603
O 0.994960 -6.311157 0.563538
O -4.022611 -6.750968 -0.934112
O -1.074261 -10.215186 -2.346525
O 0.035884 -4.578337 2.314709
O -0.554924 -8.600819 1.516987
O 2.238051 -6.743049 -3.067399
O 2.215296 -10.787798 2.848591
O 1.310777 -7.035880 3.048697
O -1.899426 -5.765439 0.710170
O 3.295451 -9.330870 -2.474171
O -2.404222 -6.624976 -3.291120
O -5.316204 -9.011995 0.364032
O -0.461254 -6.620797 -5.692612
O -0.175774 -7.942310 -3.519186
O 2.262705 -4.552092 -0.930482
O -2.421797 -10.158755 0.177545
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O -3.181437 -7.960413 1.322144
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O -2.455872 -4.217191 -1.612701
O -1.728008 -6.703434 3.280605
O -0.957583 -10.802441 2.763360
O -3.868779 -9.849343 2.898993
O 3.284687 -7.187058 -0.358582
O -1.388837 -2.029675 1.226152
O -0.156262 -5.669971 -2.015655
O -3.758634 -9.213113 -2.396112

Isoniazid-Bind N

77
C 0.267545 1.997840 -1.830386
H 0.004447 2.439834 -2.814026
C 0.938457 0.813126 0.583978
H 1.207217 0.284661 1.523522
C 1.332551 2.554213 -1.080661
C 1.643239 1.959061 0.171606

H 2.458251 2.338713 0.817262
C -0.386562 0.852157 -1.337795
N -0.047910 0.257946 -0.162629
H -1.175820 0.338186 -1.927781
N 3.088566 4.225043 -0.878403
H 3.391937 3.661457 -0.082077
N 4.104255 5.046818 -1.408751
H 3.872622 6.025282 -1.156743
H 3.936728 5.023071 -2.435920
C 2.118782 3.697342 -1.694091
O 1.908504 4.110998 -2.857027
O -1.204377 -4.257748 -3.917087
O -4.992976 -7.221946 2.885816
O 2.679752 -4.944352 1.815049
O 2.033977 -8.803714 1.198650
Ti -1.838184 -4.092547 1.499473
Ti -3.360117 -6.411942 2.334463
Ti -4.848381 -8.921305 2.143945
O 3.941220 -7.762356 2.565238
O 1.064114 -8.617454 -1.324481
Ti -1.214784 -3.843141 -2.079002
Ti 1.245262 -4.193496 0.874877
O -1.004361 -2.002837 -1.733928
O -1.825797 -8.205079 -1.105092
Ti -3.790965 -8.996803 -0.575216
Ti -2.147386 -9.932308 2.017345
Ti 3.561196 -9.515103 2.066600
Ti -0.369086 -6.753561 2.153387
Ti -0.332087 -8.499511 -5.334768
Ti 2.969433 -8.884220 -0.680749
Ti -0.513854 -1.921805 0.091056
Ti 2.555841 -6.790300 1.725265
Ti -0.578514 -9.718189 -0.692853
Ti 0.728553 -10.239150 1.976078
Ti 1.732544 -8.487433 -3.264762
Ti -2.608957 -6.362586 -1.238108
Ti 1.486968 -6.196665 -1.299477
Ti -2.147651 -9.003267 -3.099992
Ti -1.011226 -6.092416 -3.903551
O -3.302376 -4.556096 2.544116
O 4.214709 -9.858722 0.380359
O 0.782728 -6.324706 0.571676
O -4.200843 -7.130712 -0.891269
O -0.993084 -10.359995 -2.321035
O -0.279303 -4.666886 2.339470
O -0.578539 -8.725093 1.538872
O 2.047014 -6.701813 -3.062539
O 2.350892 -10.694362 2.858791
O 1.164907 -7.032079 3.055852
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O -2.583740 -6.882871 -3.256302
O -5.324505 -9.455496 0.422384
O -0.664890 -6.725036 -5.669744

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O 0.560928 -10.901185 0.280214
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O 1.431351 -9.038314 -5.061069
O 1.143186 -2.322494 0.904935
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O -1.910998 -9.411674 -4.925957
O -2.843573 -4.504804 -1.584235
O -1.893796 -6.918305 3.297865
O -0.807047 -10.960974 2.772057
O -3.786538 -10.184893 2.958969
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O -0.402625 -5.755754 -2.003626
O -3.756533 -9.553342 -2.347903

Anti-virals

Favipiravir

75
N -2.130855 0.901238 1.544970
N -2.261815 3.689339 2.244296
C -1.340245 1.832130 0.948938
C -1.441622 3.221113 1.284862
O -0.662640 4.153651 0.628283
H -0.916803 5.022400 1.039599
C -2.970867 1.390930 2.439953
C -3.038444 2.763616 2.828191
F -3.838571 0.515740 3.046846
H -3.742108 3.082819 3.629862
N 0.049990 2.141871 -1.051237
H -0.185936 3.141028 -1.005153
H 0.801514 1.816122 -1.669643
C -0.315841 1.330801 -0.044470
O 0.199749 0.179460 0.063866
O -0.853007 -4.148623 -4.018738
O -4.855248 -6.802073 2.848684
O 2.969924 -5.063524 1.760145
O 2.042392 -8.882235 1.190541
Ti -1.497574 -3.908709 1.407415
Ti -3.175012 -6.095435 2.288383
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O 4.017411 -7.959314 2.559860
O 1.109777 -8.644553 -1.345252
Ti -0.800743 -3.714179 -2.181212
Ti 1.591293 -4.222187 0.804832
O -0.416050 -1.907197 -1.847332
O -1.734616 -8.011676 -1.148678
Ti -3.745394 -8.661012 -0.609352
Ti -2.203711 -9.708901 1.993081
Ti 3.507652 -9.680641 2.075845
Ti -0.205844 -6.643722 2.117851
Ti -0.231394 -8.456406 -5.375448
Ti 2.992808 -9.030492 -0.681756

Ti 0.010571 -1.861141 -0.002972
Ti 2.710762 -6.892740 1.698865
Ti -0.603530 -9.614727 -0.707717
Ti 0.633532 -10.219101 1.986169
Ti 1.802892 -8.581496 -3.280119
Ti -2.396743 -6.107075 -1.295919
Ti 1.689023 -6.264531 -1.336938
Ti -2.099567 -8.802685 -3.128174
Ti -0.797773 -5.992520 -3.982983
O -3.011970 -4.249175 2.447016
O 4.158385 -10.077318 0.400418
O 0.974956 -6.325929 0.530926
O -4.033969 -6.776685 -0.948991
O -1.049546 -10.236704 -2.334220
O 0.030041 -4.576000 2.259069
O -0.553781 -8.614700 1.544259
O 2.258045 -6.826878 -3.075807
O 2.221418 -10.782010 2.868672
O 1.301521 -7.023349 3.026647
O -1.926632 -5.766222 0.680779
O 3.274821 -9.416263 -2.467476
O -2.415970 -6.660141 -3.317852
O -5.311474 -9.020777 0.377421
O -0.456892 -6.669630 -5.736408
O -0.170199 -7.959542 -3.543266
O 2.262086 -4.601867 -0.979257
O -2.413651 -10.170213 0.194623
O 0.424744 -10.877509 0.292382
O -3.174721 -7.966371 1.333601
O 1.483411 -9.124994 -5.074373
O 1.638162 -2.354988 0.794352
O -0.206047 -3.820341 -0.209828
O -1.869820 -9.245561 -4.952388
O -2.476385 -4.238390 -1.655362
O -1.739063 -6.665531 3.262060
O -0.954547 -10.826272 2.775476
O -3.858388 -9.844596 2.927774
O 3.280580 -7.213991 -0.369038
O -1.366902 -2.046754 1.209947
O -0.151109 -5.677440 -2.082333
O -3.743756 -9.239101 -2.378292

Chloroquine

108
C -0.126903 3.121896 -0.454887
N 0.056123 0.266048 -0.065872
C -0.048086 2.554005 0.889367
C 0.049880 1.118872 1.030491
C -0.058062 2.210842 -1.544971
C 0.016690 0.829621 -1.295991
H -0.103386 2.573399 -2.583527
H 0.018663 0.114707 -2.145356
N -0.250267 4.459516 -0.635130
C -1.738282 4.922982 -2.580324
C 0.091843 9.034504 -2.435978

C -0.763772 9.934068 -4.533277
C 1.160925 12.245555 -4.115239
H 0.421528 12.400669 -4.932038
H -1.683334 9.488741 -4.066506
H -1.021909 10.985613 -4.797798
H -0.187177 8.095992 -5.590235
H 0.536769 9.601070 -6.255705
H -1.918460 3.839917 -2.751239
H -1.788992 5.445451 -3.558409
H -2.551226 5.316830 -1.929485
H -0.333658 5.038500 0.201842
C -0.366750 5.167973 -1.917932
H 0.447615 4.794435 -2.592392
C -0.018368 7.557715 -2.855539
H 0.797663 6.769297 -1.003668
H -0.981036 7.022154 -0.977959
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H -0.856385 9.310455 -1.878979
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H 1.345845 11.206426 -2.202933
H -0.323414 11.758751 -2.571717
H 2.082490 11.816958 -4.570822
H 1.401611 13.245107 -3.689901
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H -0.909696 7.420817 -3.510958
C -0.060594 3.361570 2.070332
C 0.139059 0.545849 2.339773
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C 0.025873 2.795335 3.346856
C 0.128358 1.373204 3.473504
H 0.018861 3.431962 4.255072
Cl 0.240840 0.666226 5.079486
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O -4.849750 -6.924240 2.846585
O 2.965675 -5.112162 1.765803
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Ti 1.573231 -4.290899 0.821335
O -0.366739 -2.013691 -1.831577
O -1.731584 -8.114353 -1.147060
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Ti -2.179197 -9.806567 1.995238
Ti 3.518521 -9.723755 2.090741
Ti -0.205760 -6.724202 2.127414

Ti -0.213541 -8.517896 -5.365783
Ti 2.998105 -9.093044 -0.671296
Ti -0.001514 -1.908620 0.025240
Ti 2.710614 -6.940813 1.706870
Ti -0.588936 -9.696848 -0.719410
Ti 0.658913 -10.298918 1.981560
Ti 1.818438 -8.617169 -3.273022
Ti -2.400962 -6.213572 -1.271186
Ti 1.694808 -6.315250 -1.321815
Ti -2.095592 -8.902153 -3.140539
Ti -0.796273 -6.087755 -3.939296
O -3.024555 -4.356799 2.447101
O 4.160930 -10.141389 0.417638
O 0.978868 -6.387926 0.543876
O -4.033544 -6.895406 -0.935148
O -1.036495 -10.327630 -2.342156
O 0.016592 -4.655267 2.291635
O -0.541437 -8.700195 1.556562
O 2.250562 -6.858766 -3.070687
O 2.244729 -10.842568 2.877055
O 1.308849 -7.071811 3.038697
O -1.912534 -5.861952 0.702140
O 3.299880 -9.441778 -2.460088
O -2.416480 -6.760664 -3.292194
O -5.285127 -9.160500 0.376353
O -0.455841 -6.735418 -5.707097
O -0.165190 -8.046595 -3.527924
O 2.245322 -4.642787 -0.965285
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O 0.459115 -10.944899 0.281729
O -3.163650 -8.073158 1.334263
O 1.515274 -9.155140 -5.071482
O 1.595213 -2.415047 0.851250
O -0.231181 -3.917693 -0.171726
O -1.848530 -9.333857 -4.961734
O -2.485455 -4.345322 -1.631543
O -1.735139 -6.763008 3.273571
O -0.927949 -10.930422 2.760467
O -3.835098 -9.954976 2.930675
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O -1.365210 -2.108136 1.244898
O -0.156669 -5.776837 -2.041489
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Hydroxychloroquine

109
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C -0.230137 2.549341 0.884982
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C 0.124297 2.229106 -1.527270
C 0.184042 0.847050 -1.279831
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H 0.310208 0.143844 -2.129360
N -0.251852 4.461825 -0.640893

C -1.538045 4.843566 -2.743190
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C -0.690792 9.929630 -4.610248
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O 0.273126 12.875754 -4.968856
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H -1.394381 9.089514 -4.412647
H -1.299109 10.869961 -4.569833
H 0.553235 8.810810 -6.008406
H 0.617107 10.575349 -6.271868
H -1.647046 3.752350 -2.920606
H -1.504330 5.355235 -3.727499
H -2.436657 5.201619 -2.191817
H -0.505430 5.027823 0.170375
C -0.262367 5.159375 -1.935045
H 0.639018 4.825509 -2.512282
C 0.058046 7.558403 -2.853447
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H -1.067332 6.980204 -1.082533
C -0.138000 6.663406 -1.623050
H 0.792272 9.212576 -1.645715
H -0.976153 9.264308 -1.973407
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H -0.533944 4.448771 1.967375
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Cl -0.505593 0.640923 5.063610
O -0.842022 -4.245497 -4.014242
O -4.851928 -6.824920 2.845175
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O 2.053217 -8.887340 1.203602
Ti -1.496189 -3.939450 1.402068
Ti -3.168684 -6.120918 2.290570
Ti -4.814063 -8.530665 2.103494
O 4.036544 -7.960589 2.556472
O 1.115306 -8.675613 -1.339227
Ti -0.787566 -3.801518 -2.177319
Ti 1.583432 -4.248079 0.802954
O -0.350085 -1.992209 -1.881205
O -1.740064 -8.067936 -1.143108
Ti -3.748417 -8.712361 -0.607726

Ti -2.200353 -9.727055 2.006995
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Ti -0.198743 -6.681672 2.125789
Ti -0.216949 -8.528602 -5.374116
Ti 2.994215 -9.076507 -0.671682
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Ti 0.643743 -10.215087 2.000075
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O 1.312642 -7.042922 3.034637
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O -2.414189 -6.748848 -3.316808
O -5.311870 -9.062700 0.382703
O -0.457344 -6.748236 -5.734596
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O -1.736503 -6.705506 3.262867
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O -3.737740 -9.321508 -2.369225

Anti-parasites

Aminoquinoline

79
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N 0.054115 0.271917 -0.043238
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C -0.165607 2.389184 -1.234512

C -0.114997 0.978210 -1.178753
H -0.303971 2.898761 -2.209471
H -0.230318 0.375966 -2.107796
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H -0.312718 4.989006 0.814983
H -0.474382 4.950983 -0.882712
C 0.226121 3.084489 2.464958
C 0.370014 0.253147 2.376613
H 0.437132 -0.855184 2.348190
H 0.178316 4.191969 2.505064
C 0.394085 2.356501 3.649966
C 0.471794 0.930163 3.598298
H 0.472567 2.885755 4.622468
H 0.612799 0.347575 4.532398
O -0.896994 -4.227789 -3.993162
O -4.861926 -6.941851 2.788104
O 2.939949 -5.058033 1.749388
O 2.059637 -8.889049 1.181929
Ti -1.527812 -3.991225 1.405150
Ti -3.176577 -6.223754 2.256480
Ti -4.797837 -8.650988 2.046591
O 4.031679 -7.956773 2.544472
O 1.125592 -8.684528 -1.370754
Ti -0.872418 -3.805586 -2.157131
Ti 1.541456 -4.245549 0.800402
O -0.480680 -1.981197 -1.867258
O -1.727294 -8.125200 -1.185347
Ti -3.729139 -8.798468 -0.674752
Ti -2.165481 -9.800148 1.946008
Ti 3.531601 -9.686607 2.059365
Ti -0.211452 -6.731476 2.099935
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Ti -0.066356 -1.901355 -0.035794
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Ti -0.574231 -9.695894 -0.767041
Ti 0.677128 -10.253331 1.944051
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Ti -2.402593 -6.231286 -1.301854
Ti 1.703797 -6.284575 -1.334139
Ti -2.070608 -8.902488 -3.190594
Ti -0.787990 -6.066921 -3.957225
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O -3.819694 -9.969081 2.878096
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O -1.426113 -2.111830 1.189750
O -0.169579 -5.753327 -2.062262
O -3.713050 -9.368973 -2.446276

Metronidazole

81
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O -0.371291 -2.017482 -1.863560
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Ti -3.747304 -8.759019 -0.608855
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Ti -0.005557 -1.973638 -0.020230
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Ti -2.098660 -8.902519 -3.127577
Ti -0.798149 -6.096223 -3.986077
O -3.022324 -4.344821 2.447377
O 4.150037 -10.152809 0.421691
O 0.976965 -6.400008 0.534941
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O -1.041062 -10.320829 -2.322501
O 0.007358 -4.653366 2.261777
O -0.553771 -8.690100 1.542334
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O 2.223517 -10.814588 2.903811
O 1.300926 -7.071374 3.036248
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O 3.281673 -9.489185 -2.451373
O -2.417470 -6.760829 -3.319438
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O 3.280993 -7.276106 -0.364054
O -1.420429 -2.124186 1.156879
O -0.152065 -5.773183 -2.083499
O -3.741415 -9.341539 -2.374980

Amodiaquinine

107
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N 0.236913 8.897965 1.356124
C -1.247361 6.886330 1.216245

C -0.822031 8.214463 0.797133
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C 0.873232 8.275611 2.347271
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H 1.724017 8.825909 2.810810
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H -1.569048 -1.041762 4.913286
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H -1.492826 0.887418 6.594176
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H 1.939041 -0.847640 4.895233
H 0.513344 -1.940278 4.753638
H 1.003999 0.077295 7.090231
H 1.242635 -1.713866 7.154194
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C -1.557024 8.874510 -0.246692
H -1.223404 9.882990 -0.570622
H -2.740792 5.300172 0.976720
C -3.119075 6.961451 -0.381882
C -2.675682 8.254351 -0.821432
H -4.024866 6.508980 -0.837027
Cl -3.583409 9.069032 -2.096744
C -0.323165 3.692437 0.638092
H -0.509298 4.589814 0.019036
C 0.328140 1.349271 0.818911
C 0.074913 2.483858 0.023503
H 0.215471 2.428393 -1.075333
O 0.793174 0.159349 0.167039
H 1.559408 -0.224715 0.677404
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O 1.125734 -8.683049 -1.357722
Ti -0.892042 -3.758458 -2.286795

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O -1.729926 -8.058449 -1.156756
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Ti -0.219763 -8.571722 -5.372816
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Ti -0.119499 -1.806836 -0.204056
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Ti 1.689650 -6.202564 -1.400235
Ti -2.097600 -8.895175 -3.136690
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O -3.060202 -4.222060 2.331503
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O 2.266185 -10.656205 2.908395
O 1.278336 -6.866415 2.961196
O -1.927889 -5.755157 0.618894
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O -5.278142 -9.106794 0.393142
O -0.453194 -6.792855 -5.754104
O -0.175012 -8.047664 -3.545058
O 2.220702 -4.525425 -1.074166
O -2.375684 -10.195382 0.226024
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O 1.504199 -9.206567 -5.056619
O 1.553198 -2.262406 0.651508
O -0.259120 -3.775916 -0.327868
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O -2.539789 -4.312896 -1.735640
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O -3.825117 -9.834246 2.950471
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O -1.515258 -1.962223 0.966629
O -0.179470 -5.692538 -2.132657
O -3.735255 -9.326048 -2.365351
Industry
Biotinidase
70
C 0.126789 1.575709 0.088494

O 0.058010 2.243132 -1.091675
O 0.055458 2.369421 1.188837
C -0.051138 3.682415 -0.802216
C -0.055696 3.767282 0.743333
O 0.255819 0.345628 0.166241
H 0.822086 4.192391 -1.268689
H -0.990630 4.055607 -1.268564
H 0.813296 4.327721 1.156631
H -0.998819 4.187068 1.160661
O -0.847646 -4.106502 -3.977484
O -4.861585 -6.780819 2.784371
O 2.960994 -4.966126 1.796724
O 2.050465 -8.789995 1.203636
Ti -1.505980 -3.833780 1.413779
Ti -3.179895 -6.065655 2.242288
Ti -4.805972 -8.494448 2.063961
O 4.020971 -7.859941 2.571609
O 1.119710 -8.574957 -1.329937
Ti -0.805065 -3.665222 -2.141954
Ti 1.588661 -4.127141 0.834310
O -0.436799 -1.843777 -1.824227
O -1.741815 -7.975463 -1.160646
Ti -3.732100 -8.640167 -0.643146
Ti -2.187452 -9.678638 1.970791
Ti 3.520685 -9.585568 2.085896
Ti -0.211034 -6.592522 2.121884
Ti -0.206242 -8.393132 -5.356202
Ti 3.000056 -8.940229 -0.668731
Ti 0.003120 -1.766145 0.001040
Ti 2.705032 -6.796592 1.722870
Ti -0.595821 -9.553399 -0.721349
Ti 0.662008 -10.154516 1.957040
Ti 1.814345 -8.489167 -3.258527
Ti -2.398809 -6.075443 -1.291492
Ti 1.694523 -6.174883 -1.312507
Ti -2.095997 -8.771922 -3.157651
Ti -0.785583 -5.944856 -3.945079
O -3.028719 -4.216159 2.421260
O 4.164948 -9.988284 0.410279
O 0.983612 -6.246117 0.554537
O -4.037838 -6.751140 -0.956529
O -1.036905 -10.185002 -2.347311
O 0.005630 -4.513892 2.272984
O -0.545542 -8.563201 1.522380
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O 2.243238 -10.701331 2.864417
O 1.293870 -6.939964 3.047100
O -1.907971 -5.710373 0.673688
O 3.298199 -9.309706 -2.454698
O -2.408738 -6.620047 -3.306796
O -5.292111 -9.022785 0.346236
O -0.444239 -6.608017 -5.702337
O -0.167242 -7.914774 -3.521295
O 2.253722 -4.507701 -0.957187

O -2.386799 -10.150063 0.171051
O 0.459988 -10.808409 0.265126
O -3.161998 -7.947462 1.302008
O 1.518534 -9.030073 -5.059017
O 1.634241 -2.263266 0.803340
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O -1.844310 -9.211428 -4.970871
O -2.478610 -4.201230 -1.630816
O -1.756963 -6.625577 3.244441
O -0.923646 -10.778660 2.752006
O -3.846787 -9.833594 2.889725
O 3.281198 -7.120556 -0.358792
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O -0.161478 -5.630276 -2.034992
O -3.739436 -9.216085 -2.414042

Thymol

85
C -0.676308 2.433165 2.812818
C -0.878632 2.508002 4.310773
H -1.719272 3.190872 4.564999
H 0.036277 2.904191 4.813361
H -1.090988 1.505832 4.746376
C -1.077698 3.498880 1.963790
H -1.571279 4.385244 2.413736
C -0.063525 1.305722 2.212329
H 0.236650 0.430506 2.829015
C -0.864989 3.444980 0.567149
C 0.146940 1.282555 0.817182
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C -0.233942 2.332892 -0.053310
C -0.014560 2.235750 -1.562034
H 0.851056 1.544401 -1.723508
C 0.321644 3.596471 -2.201416
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H -1.474238 0.590015 -1.864234
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H -1.091184 1.535531 -3.343902
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H 1.494045 -0.188153 0.848291
O -0.922897 -4.230407 -4.105855
O -4.861372 -6.822122 2.751195
O 2.925040 -4.973139 1.691313
O 2.047486 -8.814133 1.169339
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Ti 1.530407 -4.168845 0.727823
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Ti -3.721101 -8.737611 -0.673799
Ti -2.182853 -9.709703 1.954705
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Ti -0.220625 -6.619683 2.035699
Ti -0.210013 -8.545686 -5.403942
Ti 3.002418 -8.992902 -0.701588
Ti -0.097729 -1.840767 -0.173322
Ti 2.700410 -6.810912 1.641132
Ti -0.593048 -9.644058 -0.754651
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O 2.212969 -6.816992 -3.146527
O 2.248620 -10.697020 2.864080
O 1.284154 -6.931891 2.965499
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O -2.380358 -10.211689 0.160948
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O -3.734820 -9.326651 -2.437691

Carvacol

85
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C -0.543631 2.401347 1.348590
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H 0.427105 2.556084 1.877659

H -0.965770 1.437377 1.714137
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H -1.215387 4.366904 -0.480284
C 0.220029 1.292139 -0.827840
O 0.604349 0.148197 -0.042660
H 1.533640 0.232226 0.280173
C -0.592078 3.452358 -2.374674
C 0.381348 1.229908 -2.226347
H -0.913638 4.321484 -2.981234
C -0.027013 2.323502 -3.029955
C 0.090970 2.237846 -4.550493
H 0.790405 1.389306 -4.766282
C 0.664608 3.526420 -5.173890
H 1.656225 3.792180 -4.741207
H 0.780610 3.402031 -6.274145
H -0.026089 4.384419 -5.003329
C -1.280093 1.902861 -5.181632
H -1.710099 0.968163 -4.755009
H -2.000781 2.734399 -4.999515
H -1.178944 1.774726 -6.283137
H 0.801666 0.314688 -2.693161
O -0.861564 -4.262126 -4.050360
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O 2.914917 -4.988160 1.722063
O 2.046236 -8.828514 1.204398
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O 1.122136 -8.689162 -1.354131
Ti -0.894091 -3.792392 -2.230216
Ti 1.504681 -4.198091 0.779954
O -0.548238 -1.953480 -1.927533
O -1.739500 -8.111207 -1.190043
Ti -3.719886 -8.792451 -0.663753
Ti -2.176296 -9.775459 1.970176
Ti 3.519674 -9.607328 2.094591
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Ti -0.590065 -9.683747 -0.737103
Ti 0.672072 -10.214344 1.967395
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Ti -2.409879 -6.212784 -1.335831
Ti 1.630436 -6.252082 -1.354748
Ti -2.095914 -8.929485 -3.177165
Ti -0.803152 -6.111110 -4.002613
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O -2.424543 -6.790503 -3.369635
O -5.270203 -9.191230 0.335290
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O -0.178102 -8.065551 -3.550365
O 2.161535 -4.572612 -1.022514
O -2.366381 -10.266394 0.172658
O 0.483878 -10.891763 0.281772
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O 1.524219 -9.196846 -5.054532
O 1.525997 -2.334454 0.749209
O -0.286072 -3.836408 -0.265662
O -1.837837 -9.401711 -4.980738
O -2.557185 -4.345900 -1.725215
O -1.772638 -6.707898 3.216131
O -0.904454 -10.857930 2.759523
O -3.835145 -9.940593 2.887152
O 3.248289 -7.159550 -0.380767
O -1.486319 -2.032318 1.090856
O -0.241683 -5.763011 -2.069596
O -3.734323 -9.381313 -2.428967

Glucose

84
O -0.154907 0.266715 0.104460
C -0.379897 0.938319 1.423591
H 0.147177 0.249661 2.125309
C 0.355001 2.297330 1.453429
H -0.027770 2.856748 2.342545
C 0.076893 3.171366 0.191953
C 0.336134 2.357725 -1.098586
C -0.518720 1.073765 -1.091704
H -0.237697 0.381050 -1.930948
O 1.765458 2.117712 1.645116
H 2.105342 1.862153 0.746518
H 0.803879 4.018496 0.232637
O 1.748759 2.036317 -1.149860
H 1.859797 1.311716 -1.812266
C -1.899684 1.022256 1.782740
O -2.743500 0.164848 0.981517
H -2.375480 -0.771516 1.106918
H -2.261931 2.060571 1.625866
O -1.246444 3.725756 0.166990
H -1.793934 3.023980 -0.283737
H 0.019505 2.976668 -1.977881
O -1.886899 1.403163 -1.097643
H -2.346252 0.766599 -0.423896
H -2.015137 0.771208 2.863630
O -0.845661 -4.134183 -3.953440

O -4.852524 -6.893668 2.850455
O 2.958332 -5.067578 1.815137
O 2.047992 -8.884257 1.199393
Ti -1.505241 -3.944335 1.502157
Ti -3.179831 -6.170673 2.305662
Ti -4.812573 -8.586946 2.070690
O 4.017088 -7.965483 2.573791
O 1.109888 -8.609220 -1.328730
Ti -0.795583 -3.725589 -2.122194
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O -1.745259 -8.025085 -1.163782
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Ti 0.647527 -10.251344 1.941956
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Ti -2.402930 -6.122852 -1.274404
Ti 1.694764 -6.267726 -1.306176
Ti -2.098036 -8.800639 -3.161491
Ti -0.791537 -5.981269 -3.937824
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O -1.041557 -10.231843 -2.371346
O 0.011210 -4.622458 2.330624
O -0.547582 -8.645777 1.517485
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O -1.937581 -5.774488 0.713737
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O -2.412591 -6.647905 -3.295683
O -5.295262 -9.097459 0.342447
O -0.441825 -6.624540 -5.694882
O -0.169399 -7.948560 -3.525672
O 2.247019 -4.594859 -0.917716
O -2.395894 -10.202545 0.147066
O 0.455646 -10.879243 0.236470
O -3.175663 -8.013970 1.306032
O 1.495825 -9.098507 -5.059370
O 1.613548 -2.346727 0.855623
O -0.237891 -3.817162 -0.128013
O -1.851716 -9.219345 -4.981463
O -2.473420 -4.244744 -1.620200
O -1.746728 -6.757764 3.274251
O -0.940787 -10.878336 2.712129

O -3.848452 -9.929023 2.872565
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O -3.746678 -9.242476 -2.430771
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C -0.098294 3.064217 2.376477
C 0.155319 5.108370 1.046782
C -0.149448 2.331481 1.160004
O 0.365757 6.504603 0.976174
H -0.525004 6.935989 1.027861
C -0.326681 0.856540 1.170813
O 0.042723 0.182036 0.131133
O -0.872587 0.281898 2.220112
H -1.061100 -0.757624 1.923291
O 0.166373 5.017136 -1.376414
H -0.047634 2.358583 -1.041455
O 0.228298 5.202821 3.471417
H -0.177970 2.550701 3.356682
H 0.331082 5.967528 -1.136313
H 0.437475 6.122181 3.158228
O -0.850093 -4.211933 -4.030142
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O 2.976919 -5.061642 1.745267
O 2.055477 -8.878537 1.203960
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Ti -3.133352 -6.092860 2.284137
Ti -4.803765 -8.493760 2.119504
O 4.037987 -7.956396 2.554842
O 1.115892 -8.657073 -1.340440
Ti -0.777795 -3.778539 -2.197144
Ti 1.603285 -4.239313 0.784453
O -0.267082 -1.974544 -1.925136
O -1.732142 -8.033604 -1.141350
Ti -3.735851 -8.691380 -0.600471
Ti -2.194591 -9.703381 2.016446
Ti 3.521679 -9.686730 2.091330
Ti -0.188912 -6.668175 2.111585
Ti -0.228866 -8.507313 -5.374825
Ti 2.995109 -9.070115 -0.675255
Ti 0.107251 -1.840087 -0.112719
Ti 2.727893 -6.899281 1.698437
Ti -0.602813 -9.623514 -0.702136
Ti 0.648574 -10.209583 1.994945
Ti 1.807449 -8.611824 -3.275815
Ti -2.394236 -6.135522 -1.292148
Ti 1.695916 -6.304147 -1.343792
Ti -2.101938 -8.826992 -3.130997
Ti -0.798949 -6.049077 -3.991623
O -2.949270 -4.241572 2.448292

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O 0.060602 -4.572640 2.264040
O -0.543378 -8.614244 1.548615
O 2.259788 -6.856644 -3.085040
O 2.231054 -10.767687 2.891070
O 1.320644 -7.029576 3.026684
O -1.895078 -5.758117 0.682948
O 3.276972 -9.448886 -2.459596
O -2.417840 -6.715273 -3.318782
O -5.289731 -9.047754 0.404627
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O 2.253989 -4.634127 -0.998761
O -2.401292 -10.179756 0.220592
O 0.444290 -10.870579 0.305014
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O 1.487889 -9.165122 -5.065908
O 1.707638 -2.363943 0.665947
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O -2.463622 -4.271086 -1.676953
O -1.708680 -6.671033 3.266227
O -0.941239 -10.819056 2.788005
O -3.847427 -9.829258 2.951874
O 3.285814 -7.244943 -0.376111
O -1.255730 -1.985968 1.249248
O -0.154558 -5.721436 -2.079286
O -3.738766 -9.272071 -2.366360

Anthraquinone

84
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C 0.009553 3.621862 -1.288464
C 0.056129 2.253251 1.306329
C 0.064253 2.190700 -1.251036
C -0.067437 3.702111 3.730152
C -0.047270 3.528170 -3.737811
C -0.028876 2.281964 3.754879
C -0.008866 2.108642 -3.697333
C -0.004092 4.436448 -0.023854
C 0.136390 1.488492 0.044876
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O 0.275013 0.223719 0.084026
C -0.053170 4.399243 2.497464
C 0.037727 1.555978 2.545868
C -0.039401 4.281501 -2.538450
C 0.051343 1.434889 -2.457158
H -0.112970 4.270872 4.683359
H -0.088536 4.053395 -4.715992
H -0.048191 1.737949 4.722939
H -0.026126 1.520904 -4.640030
H -0.086931 5.508824 2.454760

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H 0.071182 0.322207 -2.405964
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Ti -3.145551 -6.095609 2.284420
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O 4.021862 -7.965818 2.565133
O 1.106555 -8.615375 -1.348499
Ti -0.781439 -3.698610 -2.119602
Ti 1.603895 -4.207184 0.871689
O -0.363573 -1.891819 -1.808297
O -1.738078 -7.995935 -1.152085
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Ti -2.206290 -9.691803 1.976364
Ti 3.505359 -9.682270 2.063051
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Ti -0.237882 -8.406495 -5.356546
Ti 2.980284 -8.998762 -0.683007
Ti 0.057695 -1.816005 0.044538
Ti 2.720305 -6.883605 1.722807
Ti -0.617173 -9.587921 -0.726299
Ti 0.632349 -10.206791 1.962681
Ti 1.813214 -8.505359 -3.275104
Ti -2.378064 -6.090231 -1.261501
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Resveratrol
89
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