Supplementary Materials

of the manuscript entitled:

Vibrational Properties of Benzoxaboroles and Their Interactions with *Candida albicans*' LeuRS

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The best structures obtained in the docking studies to *Candida albicans* leucyl t-RNA synthetase (Figures S31-S98). Coordinates of the best structures obtained in the docking studies to *Candida albicans* leucyl t-RNA synthetase (Tables S31-S98). Experimental IR and Raman spectra of investigated benzoxaboroles.

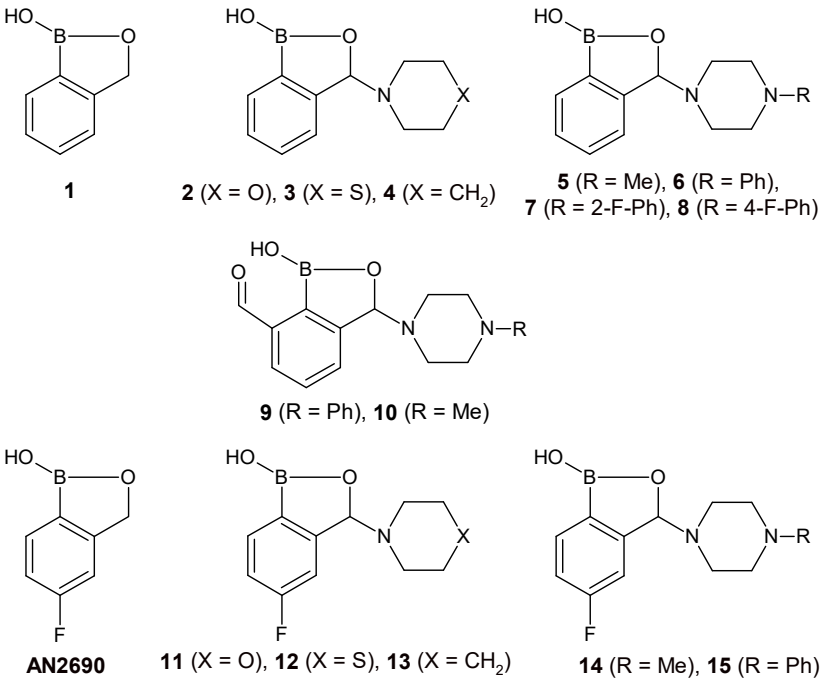


Figure S1. Structures of investigated compounds.

Table S1.Chosen results of docking studies of **(1-15)-AMP** spiroboronates with *Candida albicans* LeuRS.

Cmpd	Structure of the spiroboronate	The lowest binding energy [kcal/mol]	Numer of structures	Mean binding energy [kcal/mol]	Inhibition constant [nM]	Number of hydrogen bonds: aminoacids involved
AN2690	AN2690-AMP	-11.89	17	-10.80	1.93	5: Leu404, Lys407, Leu317, Lys483, Lys 483 [1]
1	1-1-AMP	-11.28	11	-10.63	5.41	5: Leu404, Lys407, Leu317, Lys483, Lys 483
	1-2-AMP	-11.51	17	-10.60	3.63	5: Leu404, Lys407, Leu317, Lys483, Lys483
2	2-*R*-1-AMP	-11.40	5	-11.02	4.39	4: Lys407, Gly410, Lys483, Lys483
	2-*R*-2-AMP	-11.36	19	-10.82	4.68	3: Lys407, Lys483, Lys483
	2-*S*-1-AMP	-9.92	1	-9.92	53.52	3: Leu317, Leu404, Lys407
	2-*S*-2-AMP	-12.02	3	-10.49	1.53	3: Lys483, Lys483, Tyr487
3	3-*R*-1-AMP	-13.04	2	-12.48	0.28	3: Leu317, Lys483, Lys483
	3-*R*-2-AMP	-11.81	23	-10.88	2.21	4: Lys407, Leu317, Lys483, Lys483
	3-*S*-1-AMP	-9.65	1	-9.65	85.11	3: Lys407, Lys483, Lys483
	3-*S*-2-AMP	-9.88	12	-9.44	57.36	1: Lys483
4	4-*R*-1-AMP	-12.86	4	-12.29	0.38	4: Leu404, Lys407, Lys483, Lys483
	4-*R*-2-AMP	-11.36	14	-10.45	4.69	4: Leu317, Lys407, Lys483, Lys483
	4-*S*-1-AMP	-9.18	1	-9.18	186.36	2: Lys407, Lys483
	4-*S*-2-AMP	-9.94	9	-9.35	51.79	2: Thr402, Thr402
5	5-*R*-1-AMP	-9.21	44	-8.59	176.64	3: Lys407, Lys483, Lys483
	5-*R*-2-AMP	-12.21	13	-11.16	1.12	4: Leu317, Lys407, Lys483, Lys483
	5-*S*-1-AMP	-9.23	128	-8.85	170.43	1: Lys393
	5-*S*-2-AMP	-9.86	15	-9.27	59.56	1: Lys407
6	6-*R*-1-AMP	-12.73	20	-11.93	0.47	2: Lys407, Lys483,
	6-*R*-2-AMP	-10.95	28	-10.24	9.40	2: Lys407, Lys483,
	6-*S*-1-AMP	-11.36	1	-11.36	4.70	4: Lys407, Lys483, Lys483, Lys483,
	6-*S*-2-AMP	-11.61	3	-10.74	3.11	3: Lys407, Lys483, Lys483
	6-*S*-1-c-AMP	-9.72	83	-9.27	74.74	1: not analyzed
	6-*S*-2-c-AMP	-10.35	5	-9.94	26.07	3: not analyzed
7	7-*R*-1-AMP	-10.89	21	-10.13	10.41	2: Lys407, Lys483
	7-*R*-2-AMP	-12.24	27	-11.65	1.07	3: Lys407, Lys483, Lys483
	7-*S*-1-AMP	-10.75	2	-10.54	13.27	3: Lys407, Lys483, Lys483
	7-*S*-2-AMP	-11.06	1	-11.06	7.85	3: Lys407, Lys483, Lys483
	7-*R*-1-c-AMP	-10.86	22	-10.06	10.95	2: not analyzed
	7-*R*-2-c-AMP	-12.11	18	-11.48	1.33	4: not analyzed
8	8-*R*-1-AMP	-12.11	24	-11.33	1.32	2: Lys407, Lys483
	8-*R*-2-AMP	-10.20	11	-9.53	33.64	1: Lys407
	8-*S*-1-AMP	-10.31	30	-9.33	27.57	3: Lys407, Lys483, Lys483

	8-*S*-2-AMP	-11.14	1	-11.14	6.82	4: Lys407, Lys483, Lys483, Lys483
	8-*R*-1-c-AMP	-12.20	29	-11.37	1.15	3: not analyzed
	8-*R*-2-c-AMP	-10.09	15	-9.76	39.85	3: not analyzed
9	9-*R*-1-AMP	-12.87	26	-12.00	0.37	3: Lys403, Lys483, Lys483
	9-*R*-2-AMP	-10.53	5	-9.49	19.18	5: Leu404, Lys407, Lys483, Lys483, Lys483
	9-*S*-1-AMP	-12.06	1	-12.06	1.45	3: Lys407, Lys483, Lys483
	9-*S*-2-AMP	-10.50	3	-10.30	20.14	2: Lys407, Lys483
	9-*R*-1-c-AMP	-12.66	22	-12.04	0.53	3: not analyzed
	9-*R*-2-c-AMP	-10.35	18	-9.77	26.10	3: not analyzed
10	10-*R*-1-AMP	-12.17	1	-12.17	1.21	4: Leu404, Lys407, Thr413, Lys483
	10-*R*-2-AMP	-11.94	14	-11.08	1.76	2: Lys407, Lys483
	10-*S*-1-AMP	-9.97	1	-9.97	49.18	2: Lys407, Lys483
	10-*S*-2-AMP	-9.29	4	-8.95	154.66	3: Lys407, Lys483, Lys483
11	11-*R*-1-AMP	-11.20	11	-10.67	6.15	2: Lys407, Lys483
	11-*R*-2-AMP	-10.78	1	-10.78	12.53	5: Leu317, Lys407, Gly410, Lys483, Lys483
	11-*S*-1-AMP	-11.10	5	10.45	7.33	1: Lys407
	11-*S*-2-AMP	-9.91	3	-9.59	54.15	4: Thr321, Lys407, Lys483, Lys483
12	12-*R*-1-AMP	-11.68	19	-11.08	2.76	4: Thr321, Lys407, Lys483, Lys483
	12-*R*-2-AMP	-9.94	36	-9.41	61.49	3: Arg427, Arg427, Asn431
	12-*S*-1-AMP	-11.64	2	-10.80	2.94	3: Tyr487, Lys483, Lys483
	12-*S*-2-AMP	-10.47	2	-10.09	21.10	3: Lys407, Lys483, Lys483
13	13-*R*-1-AMP	-11.85	24	-11.25	2.05	2: Lys407, Lys483
	13-*R*-2-AMP	-10.49	1	-10.49	20.40	1: Lys407
	13-*S*-1-AMP	-10.36	1	-10.36	25.64	2: Lys407, Lys483
	13-*S*-2-AMP	-8.98	7	-8.59	263.12	1: Lys407
14	14-*R*-1-AMP	-11.26	12	-10.52	5.57	2: Lys407, Lys483
	14-*R*-2-AMP	-9.36	17	-8.85	138.23	3: Lys407, Lys483, Lys483
	14-*S*-1-AMP	-8.82	24	-8.15	345.46	3: Lys407, Lys483, Lys510
	14-*S*-2-AMP	8.73	1	-8.73	396.82	3: Lys407, Lys483, Lys483
15	15-*R*-1-AMP	-10.68	25	-9.97	14.87	2: Lys407, Lys483
	15-*R*-2-AMP	-12.92	18	-11.71	0.34	3: Lys407, Lys483, Lys483
	15-*S*-1-AMP	-9.59	4	-9.26	93.19	1: Asn461
	15-*S*-2-AMP	-11.08	1	-11.08	7.60	2: Lys407, Lys483

[1] Adamczyk-Woźniak, A.; Gozdalik, J.T.; Wieczorek, D.; Madura, I.D.; Kaczorowska, E.; Brzezińska, E.; Sporzyński, A.; Lipok, J. Synthesis, Properties and Antimicrobial Activity of 5-Trifluoromethyl-2-formylphenylboronic Acid. *Molecules* **2020**, *25*, a799, doi:10.3390/molecules25040799.

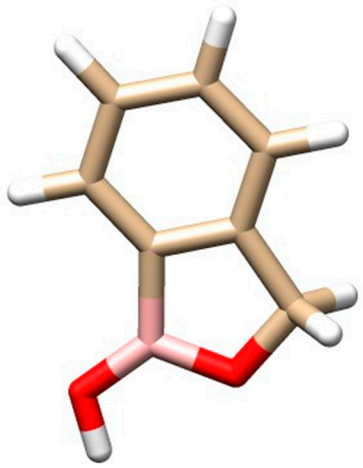


Figure S2 Structure 1

Table S2. Coordinates of structure 1

Coordinates of the input structure	Coordinates of the optimized structure
C -3.46272 0.78487 0.09690	C -0.08264 -0.49102 0.00055
C -4.55267 -0.08335 0.05845	C 0.87178 -1.50734 0.00035
C -4.29373 -1.45980 -0.04772	C 2.22128 -1.17590 -0.00008
C -2.96549 -1.92698 -0.11198	C 2.61959 0.16254 -0.00033
C -1.89314 -1.01842 -0.07016	C 1.67821 1.18702 -0.00019
C -2.17699 0.34612 0.03574	C 0.33215 0.84551 0.00026
B -3.34477 2.29080 0.20363	B -1.63444 -0.42338 0.00022
O -1.93253 2.70652 0.20309	O -2.02183 0.89938 -0.00017
C -1.20204 1.48651 0.09691	C -0.86914 1.75771 0.00017
O -4.46650 3.22043 0.30069	O -2.52873 -1.44297 -0.00037
H -4.68072 3.45247 -0.63803	H -3.43953 -1.12789 -0.00106
H -0.54798 1.36455 0.98654	H -0.91196 2.39832 0.88572
H -0.58943 1.49759 -0.82975	H -0.91166 2.39889 -0.88496
H -5.56737 0.29003 0.10862	H 0.56527 -2.54737 0.00059
H -5.11590 -2.16276 -0.08026	H 2.97288 -1.95667 -0.00027
H -2.77014 -2.98827 -0.19375	H 3.67599 0.40563 -0.00073
H -0.87039 -1.36896 -0.11891	H 1.99835 2.22359 -0.00047

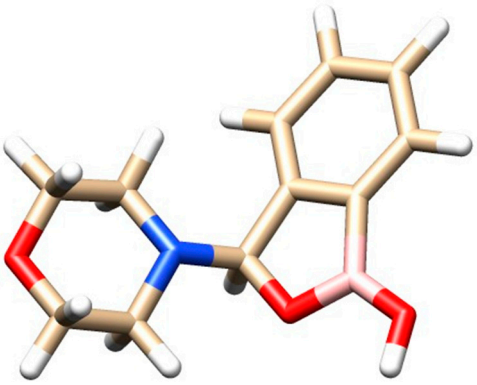


Figure S3. Structure 2-*R*

Table S3. Coordinates of structure 2-*R*

Coordinates of the input structure	Coordinates of the optimized structure
C 3.33300 -0.11500 -0.63500	C 3.32989 -0.11227 -0.63006
C 3.60400 -1.46400 -0.43700	C 3.59938 -1.46288 -0.44131
C 2.67800 -2.27700 0.21600	C 2.67095 -2.27992 0.20293
C 1.46200 -1.76300 0.65700	C 1.45388 -1.76768 0.64554
C 1.18000 -0.42200 0.42200	C 1.17469 -0.42501 0.41994
O 0.31200 1.76000 0.56200	O 0.30539 1.75597 0.57071
C -0.04200 0.38700 0.83300	C -0.04795 0.38309 0.83116
N -1.26600 0.10800 0.09500	N -1.26564 0.10619 0.08096
C -2.37100 0.94100 0.59200	C -2.37351 0.94555 0.55691
C -1.66700 -1.29900 0.05000	C -1.68206 -1.29594 0.05763
C -2.90300 -1.45900 -0.82800	C -2.92948 -1.44257 -0.80519
C -3.60100 0.77300 -0.28600	C -3.59702 0.73827 -0.31992
O -3.99000 -0.63700 -0.30300	O -3.99346 -0.62598 -0.34256
O 2.03900 3.00700 -0.53500	O 2.03741 3.00978 -0.51206
H 1.46800 3.75700 -0.33700	H 1.46734 3.76059 -0.31179
H -0.20700 0.32200 1.92200	H -0.22271 0.30903 1.91838
H 4.06600 0.52500 -1.11200	H 4.06491 0.53089 -1.10065
H 4.54600 -1.88500 -0.77000	H 4.54098 -1.88238 -0.77583
H 2.91100 -3.32100 0.39000	H 2.90215 -3.32567 0.36960
H 0.76600 -2.40500 1.18300	H 0.75694 -2.41252 1.16722
H -0.85700 -1.88700 -0.37900	H -0.88943 -1.90477 -0.37534
H -1.89300 -1.69500 1.05600	H -1.90141 -1.67909 1.07102
H -3.21400 -2.50700 -0.82100	H -3.29136 -2.47133 -0.77405
H -2.62800 -1.19000 -1.86200	H -2.68243 -1.18489 -1.84485
H -2.04600 1.98000 0.58500	H -2.06299 1.98885 0.51983
H -2.63100 0.66700 1.63000	H -2.63253 0.70056 1.60274
H -4.42200 1.36400 0.12600	H -4.44594 1.30145 0.07014
H -3.36900 1.16200 -1.29200	H -3.38150 1.08317 -1.34099
B 1.51300 1.83500 -0.10500	B 1.51005 1.83524 -0.09101
C 2.12000 0.41000 -0.19700	C 2.11665 0.41075 -0.19027

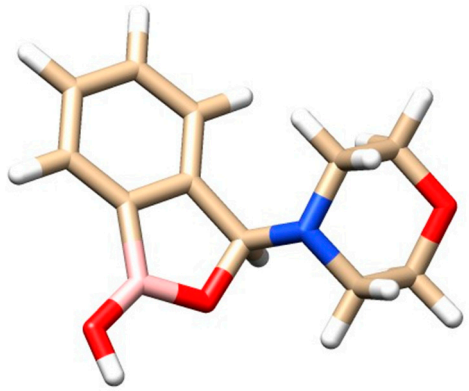


Figure S4. Structure 2-*S*

Table S4. Coordinates of structure 2-*S*

Coordinates of the input structure	Coordinates of the optimized structure
C 2.14000 0.29300 0.04600	C 2.13334 0.30001 0.05111
C 3.35200 0.36900 0.22900	C 3.34731 -0.35545 0.24108
C 3.40600 1.75000 0.07800	C 3.40978 -1.73584 0.08991
C 2.25900 2.46300 -0.27100	C 2.26943 -2.45452 -0.26789
C 1.04200 1.81200 -0.45200	C 1.04978 -1.80988 -0.45699
C 0.98700 0.43500 -0.26900	C 0.98649 -0.43366 -0.27159
B 1.70300 1.78200 -0.00600	B 1.68866 1.78709 -0.00442
O 0.37900 1.84100 -0.36600	O 0.36593 1.83841 -0.37265
C -0.19300 0.50800 -0.45300	C -0.19663 0.50290 -0.46090
N -1.23300 0.43600 0.55300	N -1.23781 0.42627 0.54636
C -2.38800 1.29200 0.24400	C -2.39887 1.27275 0.23504
C -3.41200 0.60400 -0.66200	C -3.41540 0.56025 -0.65391
O -3.84200 0.64700 -0.03200	O -3.83194 -0.67143 -0.07203
C -2.71000 1.55400 0.17500	C -2.72695 -1.53870 0.15601
C -1.67700 0.85900 1.06700	C -1.68398 -0.87183 1.05250
H -2.02600 2.21600 -0.20500	H -2.04986 2.19596 -0.22769
H -2.87600 1.54700 1.18900	H -2.88322 1.53853 1.18018
H -4.28300 1.25300 -0.78900	H -4.31787 1.16232 -0.77530
H -2.97200 0.44300 -1.66200	H -2.99399 0.37234 -1.65316
H -3.07000 2.46100 0.66900	H -3.13383 -2.43359 0.63145
H -2.23600 1.85900 -0.77600	H -2.28384 -1.83305 -0.80843
H -0.81700 1.50100 1.24400	H -0.82965 -1.52591 1.21521
H -2.14800 0.67000 2.03800	H -2.14466 -0.69194 2.03012
H 0.16600 2.38000 -0.74200	H 0.18003 -2.38316 -0.75564
H 2.31600 3.53600 -0.40900	H 2.33369 -3.52745 -0.40755
H 4.34300 2.27700 0.21400	H 4.34905 -2.25758 0.23151
H 4.24900 0.18900 0.47000	H 4.23998 0.20771 0.48880
O 2.45900 2.88700 0.20800	O 2.43674 2.89632 0.21291
H 1.95200 3.70000 0.10300	H 1.92709 3.70701 0.10422
H -0.58000 0.43600 -1.48100	H -0.58317 0.42690 -1.48820

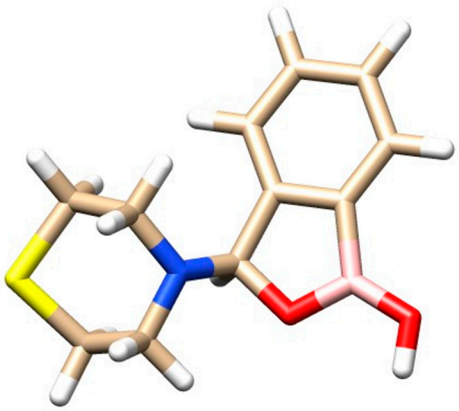


Figure S5. Structure 3-*R*

Table S5. Coordinates of structure 3-*R*

Coordinates of the input structure	Coordinates of the optimized structure
C -1.20220 1.12779 -0.13645	C -2.42269 0.235148 0.03692
C -2.28529 0.75492 -0.93045	C -3.60691 -0.477729 0.20742
C -2.68744 -0.58778 -0.90760	C -3.60182 -1.858887 0.05214
C -1.99605 -1.51599 -0.10832	C -2.42314 -2.521332 -0.28938
C -0.90846 -1.10166 0.67949	C -1.23298 -1.819001 -0.45891
C -0.53055 0.25141 0.66482	C -1.23729 -0.441578 -0.27119
B -0.49798 2.44697 0.05244	B -2.05071 1.741761 -0.00531
O 0.67940 2.28438 0.91276	O -0.72633 1.858911 -0.35234
C 0.60134 0.94669 1.41369	C -0.09782 0.553131 -0.44408
N 0.39859 1.00470 2.89343	N 0.94260 0.516936 0.56479
C 1.41369 1.83876 3.57939	C 2.03048 1.465555 0.31447
C 2.81729 1.21854 3.54848	C 3.09138 0.981991 -0.67851
S 2.87237 -0.36706 4.44674	S 3.91369 -0.560501 -0.12078
C 0.23497 -0.28513 3.59719	C 1.40576 -0.752925 1.10961
C 1.49561 -1.15423 3.54609	C 2.39682 -1.529078 0.23383
O -0.81765 3.68051 -0.66003	O -2.85472 2.812047 0.20598
H -1.43456 4.16502 -0.05531	H -2.38485 3.647717 0.10785
H -0.37643 -1.83164 1.27210	H -0.33292 -2.350978 -0.74273
H -2.29997 -2.55470 -0.10398	H -2.43357 -3.595818 -0.43128
H -3.52263 -0.91226 -1.51449	H -4.51722 -2.425042 0.17843
H -2.79721 1.47739 -1.55306	H -4.52859 0.041970 0.44354
H -0.02280 -0.09574 4.66291	H 1.89463 -0.532793 2.06383
H -0.63891 -0.83064 3.20415	H 0.54239 -1.379637 1.33172
H 1.27152 -2.10785 4.06849	H 2.73651 -2.427974 0.75138
H 1.79925 -1.40960 2.51073	H 1.94511 -1.836997 -0.71202
H 1.11127 1.99733 4.63821	H 2.51357 1.679104 1.27234
H 1.45393 2.85061 3.12382	H 1.58738 2.395907 -0.04326
H 3.50706 1.91428 4.07076	H 3.88768 1.721752 -0.77527
H 3.20556 1.09039 2.51812	H 2.66675 0.820895 -1.67208
H 1.54250 0.42426 1.14645	H 0.29723 0.503112 -1.46993

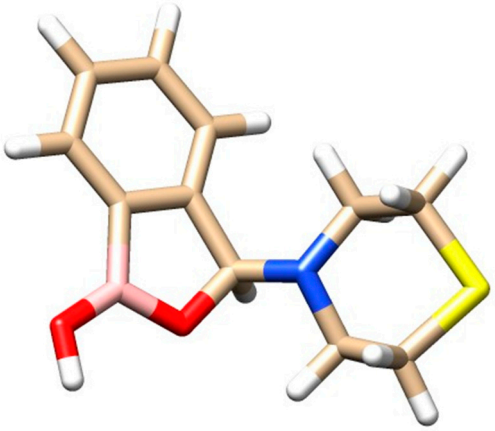


Figure S6. Structure 3-*S*

Table S6. Coordinates of structure 3-*S*

Coordinates of the input structure				Coordinates of the optimized structure			
C	-1.21900	1.38819	-0.30393	C	-2.39680	0.37202	-0.23309
C	-2.46083	0.92378	-0.73403	C	-3.58098	-0.19395	-0.69860
C	-2.80464	-0.40365	-0.44304	C	-3.83244	-1.54072	-0.46412
C	-1.91233	-1.22065	0.27424	C	-2.91633	-2.31076	0.25179
C	-0.66864	-0.71618	0.69107	C	-1.72834	-1.75545	0.72019
C	-0.32549	0.60853	0.37034	C	-1.46386	-0.41813	0.44744
B	-0.55724	2.73827	-0.40869	B	-1.82936	1.81425	-0.15932
O	0.70904	2.74983	0.33245	O	-0.65604	1.78888	0.55926
C	0.94370	1.38888	0.70816	C	-0.27820	0.43279	0.88143
N	2.17949	0.91486	0.01289	N	0.98735	0.17430	0.20260
C	3.32199	1.76037	0.44461	C	2.04354	1.02655	0.76707
C	4.59735	1.46557	-0.34177	C	3.26702	1.10287	-0.13345
S	5.20961	-0.20074	0.02831	S	4.06369	-0.52720	-0.36927
C	2.46663	-0.52199	0.22630	C	1.39367	-1.22813	0.12059
C	3.69061	-0.99428	-0.56126	C	2.54606	-1.42280	-0.85875
O	-1.16736	3.93072	-0.99013	O	-2.36618	2.95844	-0.64638
H	-1.68004	4.33777	-0.24675	H	-1.82500	3.73117	-0.44929
H	1.07222	1.34763	1.81356	H	-0.15964	0.40205	1.97737
H	-0.00166	-1.34998	1.25885	H	-1.04128	-2.36351	1.29669
H	-2.18705	-2.24041	0.51071	H	-3.13464	-3.35287	0.45444
H	-3.76254	-0.79567	-0.75924	H	-4.75148	-1.99301	-0.81798
H	-3.14488	1.56993	-1.26908	H	-4.30858	0.41431	-1.22387
H	2.58951	-0.74762	1.30920	H	1.68293	-1.63605	1.10505
H	1.64649	-1.12899	-0.19380	H	0.55084	-1.80831	-0.25127
H	3.80863	-2.08824	-0.41025	H	2.82125	-2.47713	-0.90581
H	3.56500	-0.81929	-1.65128	H	2.24498	-1.09806	-1.85633
H	3.51566	1.63897	1.53460	H	2.34497	0.67098	1.76716
H	3.09486	2.83144	0.25426	H	1.63060	2.02924	0.87656
H	5.38325	2.18179	-0.02156	H	4.02446	1.74667	0.31513
H	4.44667	1.59796	-1.43445	H	2.99469	1.51394	-1.10713

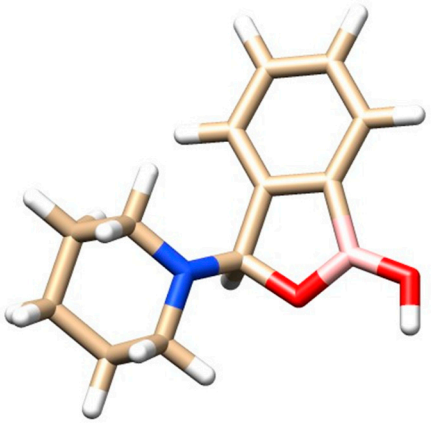


Figure S7. Structure 4-*R*

Table S7. Coordinates of structure 4-*R*

Coordinates of the input structure	Coordinates of the optimized structure
C -2.40602 -0.65044 -0.06085	C -2.14280 0.29511 0.04197
C -3.65717 -1.25681 0.03600	C -3.35712 -0.36343 0.21915
C -3.73158 -2.64536 -0.14024	C -3.41327 -1.74455 0.07366
C -2.56659 -3.38272 -0.41846	C -2.26541 -2.46070 -0.26474
C -1.32212 -2.73541 -0.50788	C -1.04562 -1.81290 -0.44118
C -1.25817 -1.34665 -0.30438	C -0.98893 -0.43531 -0.26308
B -1.97495 0.79078 0.03526	B -1.70241 1.78314 -0.01008
O -2.87304 1.92757 0.21808	O -2.45744 2.89085 0.19556
O -0.54610 0.92219 -0.27064	O -0.37577 1.83901 -0.35923
C -0.04997 -0.41706 -0.35048	C 0.19419 0.50494 -0.44205
N 0.91841 -0.62840 0.76840	N 1.22976 0.42885 0.56917
C 2.00110 0.39020 0.77822	C 2.37666 1.30039 0.27617
C 3.00618 0.17571 -0.37036	C 3.40162 0.67027 -0.67854
C 1.51757 -1.97945 0.88567	C 1.66835 -0.87486 1.06610
C 2.48735 -2.28034 -0.26991	C 2.67248 -1.59721 0.15253
C 3.60355 -1.23079 -0.27984	C 3.87146 -0.69081 -0.15264
H -3.15565 2.17390 -0.69877	H -1.94717 3.70182 0.09201
H -4.54754 -0.67362 0.23294	H -4.25460 0.19806 0.45315
H -2.63004 -4.45244 -0.56963	H -2.32367 -3.53481 -0.39839
H -4.68781 -3.14796 -0.07495	H -4.35254 -2.26895 0.20555
H -0.44084 -3.31409 -0.74387	H -0.16959 -2.38509 -0.72232
H 0.74445 -2.75701 0.98539	H 0.79872 -1.49601 1.26965
H 2.08240 -2.03971 1.84284	H 2.15152 -0.69282 2.03397
H 2.93222 -3.28952 -0.13652	H 3.00267 -2.52409 0.63221
H 1.94440 -2.27285 -1.23799	H 2.18441 -1.88508 -0.78587
H 4.18729 -1.31474 0.66361	H 4.44918 -0.54093 0.76782
H 4.29520 -1.41050 -1.13033	H 4.54542 -1.16981 -0.86824
H 2.50282 0.30715 -1.35026	H 2.95425 0.54541 -1.67105
H 3.81865 0.93084 -0.30737	H 4.25017 1.34970 -0.80432
H 1.58729 1.41914 0.72827	H 1.99744 2.24343 -0.11551
H 2.54556 0.33001 1.74692	H 2.86656 1.52609 1.23057
H 0.42702 -0.54803 -1.34299	H 0.58694 0.43084 -1.46773

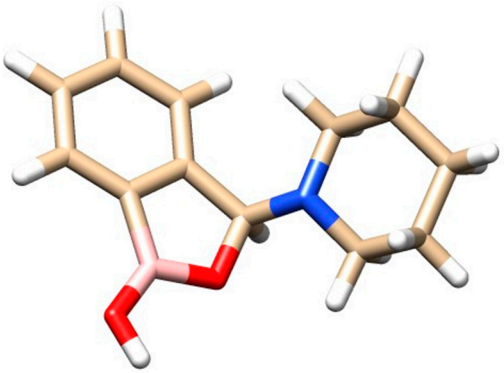


Figure S8. Structure 4-*S*

Table S8. Coordinates of structure 4-*S*

Coordinates of the input structure	Coordinates of the optimized structure
C -1.89995 -0.49197 -0.19879	C -2.11926 0.41245 -0.202680
C -3.00172 -1.20692 -0.66464	C -3.33291 -0.10798 -0.644807
C -2.99406 -2.60015 -0.51468	C -3.61390 -1.45375 -0.439910
C -1.90179 -3.23504 0.10312	C -2.69628 -2.26820 0.223012
C -0.80805 -2.47980 0.56045	C -1.47892 -1.75853 0.667233
C -0.81626 -1.08582 0.38066	C -1.18692 -0.42126 0.424908
C 0.22995 -0.04812 0.78271	C 0.03710 0.38428 0.840165
B -1.60093 0.98440 -0.16694	B -1.50734 1.83524 -0.111188
O -2.51102 2.03675 -0.60998	O -2.02610 3.00788 -0.550278
O -0.35018 1.24033 0.55472	O -0.31257 1.75838 0.565470
N 1.50713 -0.13820 0.01406	N 1.26599 0.10255 0.111796
C 2.39816 0.98576 0.40675	C 2.36819 0.93010 0.623824
C 3.68944 0.99100 -0.41794	C 3.59722 0.82989 -0.275488
C 2.21491 -1.42860 0.19675	C 1.65460 -1.30690 0.049024
C 3.51527 -1.47344 -0.61815	C 2.86601 -1.49270 -0.866916
C 4.43247 -0.32472 -0.21581	C 4.04636 -0.62438 -0.427731
H -3.07414 2.23049 0.18153	H -1.45318 3.75698 -0.351707
H 0.41620 -0.15633 1.87504	H 0.19293 0.32116 1.931207
H 0.01094 -2.98356 1.05299	H -0.78981 -2.40128 1.201769
H -1.90655 -4.30957 0.23180	H -2.93622 -3.30988 0.402591
H -3.83502 -3.18571 -0.86260	H -4.55601 -1.87106 -0.775885
H -3.84329 -0.70223 -1.12157	H -4.05977 0.53431 -1.129161
H 1.61263 -2.26067 -0.20291	H 0.82191 -1.88517 -0.344932
H 2.43364 -1.60389 1.27416	H 1.89369 -1.70717 1.054051
H 4.03189 -2.44352 -0.45473	H 3.14528 -2.55025 -0.878015
H 3.27098 -1.38651 -1.69978	H 2.57168 -1.22374 -1.886148
H 4.72302 -0.43199 0.85242	H 4.42891 -0.98854 0.533457
H 5.35580 -0.33993 -0.83359	H 4.86937 -0.70419 -1.143162
H 4.33577 1.83863 -0.10505	H 4.40062 1.44322 0.142529
H 3.43873 1.12033 -1.49380	H 3.34844 1.24491 -1.257169
H 1.90287 1.96305 0.22343	H 2.02073 1.95990 0.676869
H 2.64873 0.92216 1.49018	H 2.63772 0.61855 1.651735

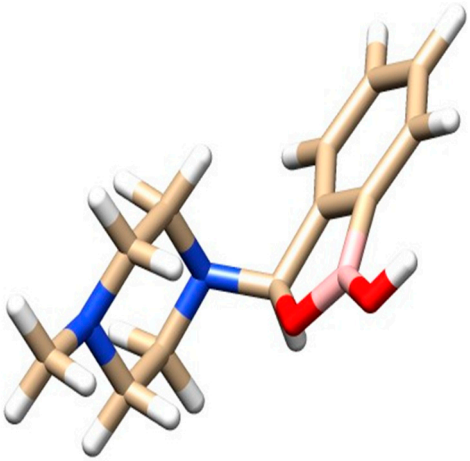


Figure S9. Structure 5-*R*

Table S9. Coordinates of structure 5-*R*

Coordinates of the input structure	Coordinates of the optimized structure
O -0.24616 -2.15253 1.53053	O 0.00670 1.14341 -0.89514
B -1.35927 -2.96032 2.05877	B -1.08670 1.78752 -0.38354
C -2.38484 -1.92640 2.62923	C -2.17628 0.72675 -0.02088
C -1.84830 -0.66938 2.37387	C -1.60768 -0.49997 -0.37159
C -0.50631 -0.75279 1.65303	C -0.23849 -0.31268 -0.99546
C -3.59151 -2.14537 3.28139	C -3.45596 0.75182 0.53231
C -4.29079 -1.00664 3.69301	C -4.14266 -0.44143 0.72738
C -3.77447 0.27352 3.45411	C -3.55657 -1.65820 0.37469
C -2.55122 0.45698 2.79862	C -2.28105 -1.69814 -0.18037
N -0.58137 -0.07387 0.36760	N 0.78365 -1.13618 -0.46149
C -0.09291 -0.82831 -0.77148	C 1.06871 -1.05957 0.97411
C 1.43883 -0.93621 -0.78516	C 2.13707 -0.02111 1.32715
C 0.04060 1.23884 0.37065	C 2.01599 -1.25634 -1.24150
C 1.57622 1.16825 0.33920	C 3.06463 -0.20202 -0.88360
N 2.03562 0.38778 -0.79617	N 3.35308 -0.25964 0.54960
C 3.48310 0.33869 -0.88100	C 4.41610 0.65800 0.92267
O -1.37488 -4.41214 2.24848	O -1.07647 3.14198 -0.26167
H -3.97146 -3.16383 3.46391	H -3.92417 1.68981 0.81509
H -5.25518 -1.11963 4.21629	H -5.13754 -0.43150 1.15724
H -2.15392 1.46987 2.62742	H -1.81908 -2.64104 -0.44913
H -0.42918 -0.31224 -1.70196	H 1.42590 -2.04395 1.29489
H -0.57673 -1.83211 -0.80996	H 0.14493 -0.84944 1.51365
H 1.74942 -1.48570 -1.70514	H 2.38393 -0.11240 2.38941
H 1.80375 -1.51886 0.09342	H 1.74317 0.99456 1.15831
H -0.30498 1.82526 1.25325	H 1.76922 -1.20012 -2.30373
H -0.31998 1.79870 -0.52466	H 2.44229 -2.24641 -1.04616
H 1.97467 0.73879 1.28833	H 2.70781 0.79595 -1.18854
H 1.97739 2.20584 0.25328	H 3.98853 -0.41194 -1.43114
H -2.10406 -4.82207 2.68171	H -1.89133 3.48892 0.11062
H 3.92762 -0.16827 0.00672	H 4.16137 1.71591 0.73220
H 3.79422 -0.20507 -1.80189	H 4.63992 0.55015 1.98656
H 3.89760 1.36983 -0.95480	H 5.32233 0.42115 0.36052
H -4.34094 1.15663 3.79480	H -4.10187 -2.58093 0.53634
H 0.26321 -0.32134 2.29383	H -0.28377 -0.51124 -2.07013

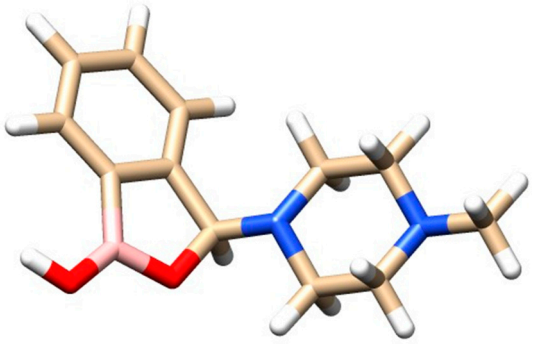


Figure S10. Structure 5-*S*

Table S10. Coordinates of structure 5-*S*

Coordinates of the input structure	Coordinates of the optimized structure
O -1.49201 -2.81163 0.50724	O -0.78766 1.78148 0.589175
B -2.22737 -3.27218 1.80187	B -1.94736 1.79237 -0.142471
C -2.64431 -1.95353 2.53591	C -2.47483 0.32967 -0.252455
C -2.21311 -0.90018 1.77676	C -1.52703 -0.44374 0.427478
C -1.49201 -1.35281 0.50724	C -0.37535 0.43869 0.889506
C -3.32818 -1.79339 3.73989	C -3.63017 -0.26953 -0.748381
C -3.56948 -0.47699 4.16472	C -3.84020 -1.62910 -0.547749
C -3.13024 0.61666 3.39142	C -2.90902 -2.38166 0.165930
C -2.44306 0.41550 2.18161	C -1.74905 -1.79460 0.665713
N -0.11092 -0.84932 0.50724	N 0.89446 0.21556 0.209852
C 0.57158 -1.29083 -0.71758	C 1.91831 1.14236 0.710493
C 2.01845 -0.76335 -0.71758	C 3.20111 1.00567 -0.093671
C -0.12494 0.61976 0.55797	C 1.39314 -1.15705 0.268425
C 1.32189 1.14722 0.55797	C 2.68364 -1.28251 -0.532665
N 2.00438 0.70573 -0.66681	N 3.69998 -0.36400 -0.036724
C 3.38544 1.20928 -0.66680	C 4.95905 -0.51539 -0.744660
O -2.49036 -4.72784 2.26487	O -2.44398 2.97581 -0.582692
H -2.01484 -0.97947 -0.37331	H -0.25666 0.38664 1.986067
H -3.65743 -2.64308 4.31956	H -4.37738 0.31495 -1.276472
H -4.09576 -0.30102 5.09126	H -4.73724 -2.10418 -0.927220
H -2.10472 1.25042 1.58594	H -1.05053 -2.39013 1.240906
H 0.04318 -0.90221 -1.58814	H 2.13876 0.94403 1.774494
H 0.58198 -2.38013 -0.75523	H 1.53540 2.15728 0.626085
H 2.52454 -1.09068 -1.62579	H 3.95928 1.67307 0.324874
H 2.54686 -1.15194 0.15298	H 3.01180 1.32431 -1.135192
H -0.63102 0.94714 1.46616	H 0.65391 -1.82687 -0.167468
H -0.65333 1.00835 -0.31261	H 1.58638 -1.48103 1.307432
H 1.85030 0.75866 1.42855	H 2.45824 -1.09927 -1.599689
H 1.31148 2.23653 0.59557	H 3.06034 -2.30527 -0.443973
H -2.96447 -4.71743 3.09957	H -3.26438 2.87954 -1.072942
H 3.91384 0.82073 0.20378	H 4.87663 -0.29392 -1.824327
H 3.89153 0.88191 -1.57499	H 5.70593 0.15727 -0.317515
H 3.37500 2.29858 -0.62921	H 5.32399 -1.53921 -0.636158
H -3.32424 1.62270 3.73297	H -3.09326 -3.43515 0.341913

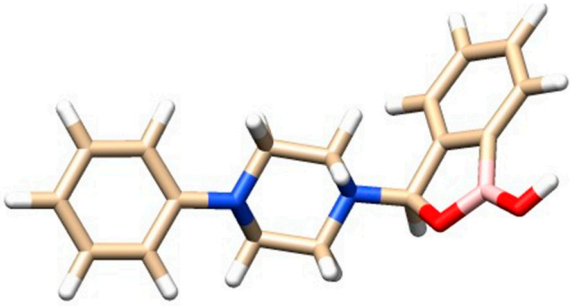


Figure S11. Structure 6-*R*

Table S11. Coordinates of structure 6-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
O	0.64918	-1.78753	1.84247	O	-2.27987	-1.84970	0.05628
B	-0.23111	-2.87706	2.30694	B	-3.41366	-1.58496	-0.66558
C	-1.44696	-2.16801	2.99442	C	-3.86927	-0.11900	-0.36826
C	-1.19176	-0.80375	2.92359	C	-2.92451	0.36750	0.53844
C	0.12875	-0.51473	2.22575	C	-1.91306	-0.70389	0.89122
C	-2.58950	-2.71306	3.56579	C	-4.90616	0.71502	-0.78460
C	-3.51148	-1.80511	4.09694	C	-4.98123	2.01374	-0.29338
C	-3.27633	-0.42481	4.04026	C	-4.02521	2.48348	0.60862
C	-2.11605	0.09358	3.45355	C	-2.98562	1.66171	1.03460
N	-0.04174	0.37667	1.09065	N	-0.54683	-0.31097	0.76025
C	-0.86289	-0.19315	0.02948	C	-0.12861	0.09878	-0.58155
C	-1.15721	0.84947	-1.05876	C	1.26187	0.72325	-0.53368
C	1.23981	0.82858	0.56618	C	0.40465	-1.27403	1.31676
C	1.04858	1.91676	-0.50102	C	1.79447	-0.65652	1.37511
N	0.11238	1.40638	-1.48357	N	2.22065	-0.20813	0.04652
C	0.36858	1.55891	-2.80014	C	3.59414	0.06002	-0.12909
C	-0.13072	2.67035	-3.48256	C	4.06282	1.25457	-0.69334
C	0.13298	2.81968	-4.84565	C	5.42427	1.46214	-0.89471
C	0.89181	1.86031	-5.51964	C	6.35334	0.49937	-0.52963
C	1.39063	0.75138	-4.83257	C	5.89884	-0.69008	0.03504
C	1.12868	0.59772	-3.46971	C	4.54541	-0.91105	0.22775
O	-0.15446	-4.28373	1.90713	O	-3.93611	-2.54559	-1.47161
H	-0.73320	3.42677	-2.95204	H	3.37045	2.03821	-0.96704
H	-2.75621	-3.80225	3.59499	H	-5.65614	0.36604	-1.48790
H	-4.43747	-2.18253	4.56230	H	-5.78378	2.66895	-0.61148
H	-4.02311	0.26899	4.46190	H	-4.09419	3.49944	0.97998
H	-1.93655	1.17995	3.40198	H	-2.23748	2.02474	1.72973
H	-1.83839	-0.53993	0.44336	H	-0.83614	0.83509	-0.96528
H	-0.35508	-1.07810	-0.42341	H	-0.11571	-0.75629	-1.27184
H	-1.79036	1.67421	-0.65468	H	1.21414	1.66814	0.03331
H	-1.69997	0.37695	-1.91213	H	1.57182	0.95641	-1.55307
H	1.80678	-0.03309	0.13840	H	0.43723	-2.19706	0.72025
H	1.85224	1.25825	1.39369	H	0.08524	-1.53527	2.32877
H	2.02813	2.17924	-0.96736	H	2.49781	-1.39399	1.75568
H	0.61840	2.84113	-0.04852	H	1.78249	0.19088	2.08022
H	-0.26138	3.69395	-5.39066	H	5.75497	2.39700	-1.33313
H	1.09618	1.97757	-6.59732	H	7.41203	0.66618	-0.68518
H	1.98861	-0.00549	-5.36765	H	6.60609	-1.46257	0.31496
H	1.51896	-0.28043	-2.92793	H	4.21511	-1.86072	0.62903
H	-0.83530	-4.88305	2.16126	H	-4.72751	-2.25708	-1.93352
H	0.80174	-0.06355	2.95794	H	-2.05375	-1.03737	1.92390

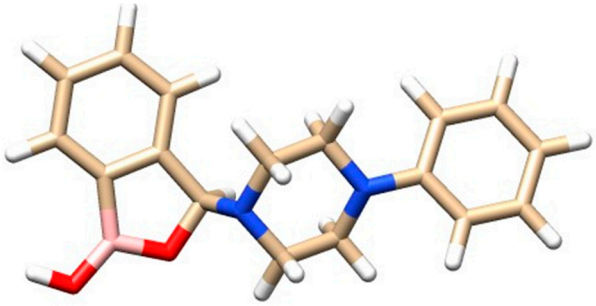


Figure S12. Structure 6-*S*

Table S12. Coordinates of structure 6-*S*

Coordinates of the input structure				Coordinates of the optimized structure		
O	-0.87730	-2.76346	0.81051	O	-2.34405	-1.77323	-0.55259
B	-1.61266	-3.22400	2.10514	B	-3.67117	-1.51358	-0.33220
C	-2.02960	-1.90535	2.83918	C	-3.84774	0.02436	-0.13701
C	-1.59839	-0.85200	2.08003	C	-2.55404	0.54942	-0.23385
C	-0.87730	-1.30464	0.81051	C	-1.54814	-0.57970	-0.39701
C	-2.71346	-1.74522	4.04316	C	-4.93458	0.88566	-0.00641
C	-2.95477	-0.42882	4.46800	C	-4.72594	2.26009	0.00878
C	-2.51553	0.66484	3.69470	C	-3.43690	2.77285	-0.12680
C	-1.82835	0.46367	2.48489	C	-2.34149	1.92250	-0.25499
N	0.50379	-0.80114	0.81051	N	-0.67886	-0.80903	0.74688
C	1.18695	-1.24307	-0.41548	C	0.29269	-1.88536	0.52092
C	0.39048	-0.78427	-1.65102	C	1.54763	-1.42384	-0.22225
C	0.48980	0.66922	0.86451	C	-0.01322	0.32044	1.38547
C	-0.34260	1.22642	-0.30526	C	1.24546	0.81378	0.65985
N	0.16027	0.66324	-1.56314	N	2.17825	-0.29059	0.46792
C	0.40197	1.44507	-2.59886	C	3.50386	0.02262	0.10155
C	0.17858	2.82377	-2.50239	C	3.90970	1.32527	-0.22111
C	0.43492	3.65298	-3.60089	C	5.23745	1.60276	-0.53292
C	0.91465	3.10350	-4.79585	C	6.19184	0.59667	-0.54511
C	1.13803	1.72481	-4.89232	C	5.79974	-0.70156	-0.22765
C	0.88169	0.89560	-3.79382	C	4.48341	-0.98555	0.09507
O	-1.87565	-4.67967	2.56815	O	-4.56462	-2.53450	-0.36026
H	-0.19150	3.24765	-1.58057	H	3.19089	2.13221	-0.24394
H	-1.40012	-0.93130	-0.07004	H	-0.99999	-0.47058	-1.34465
H	-3.04272	-2.59491	4.62284	H	-5.94583	0.49762	0.06768
H	-3.48105	-0.25284	5.39453	H	-5.56571	2.93796	0.10658
H	-2.70953	1.67087	4.03624	H	-3.28546	3.84593	-0.14020
H	-1.49001	1.29859	1.88921	H	-1.34980	2.33994	-0.38284
H	1.26217	-2.33048	-0.41492	H	-0.19642	-2.69075	-0.02484
H	2.18724	-0.81121	-0.44708	H	0.58726	-2.27594	1.49998
H	-0.56751	-1.30329	-1.68223	H	1.29670	-1.14449	-1.25949
H	0.95653	-1.00790	-2.55528	H	2.24971	-2.25302	-0.28054
H	1.51121	1.04321	0.79417	H	0.28743	-0.01273	2.38432
H	0.05073	0.99137	1.80873	H	-0.71437	1.14130	1.52090
H	-0.25424	2.31249	-0.33243	H	1.72493	1.57652	1.27620
H	-1.38846	0.94833	-0.17511	H	0.97334	1.28858	-0.30009
H	0.26259	4.71654	-3.52648	H	5.51853	2.62051	-0.77937
H	1.11240	3.74318	-5.64327	H	7.22330	0.81631	-0.79141
H	1.50811	1.30093	-5.81415	H	6.53112	-1.50173	-0.21691
H	1.05402	-0.16797	-3.86824	H	4.21408	-1.99524	0.37729
H	-2.34976	-4.66925	3.40284	H	-5.46858	-2.24782	-0.20762

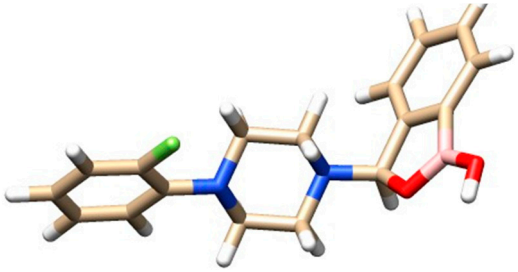


Figure S13. Structure 7-*R*

Table S13. Coordinates of structure 7-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
F	11.30504	2.93257	-0.24839	F	-3.23149	0.96845	-2.02891
O	10.16827	0.57543	6.25395	O	4.13828	2.84730	-0.40828
H	11.05971	0.47105	5.97455	H	3.66732	3.61934	-0.07484
O	10.03124	3.07695	5.46119	O	2.46451	1.64441	0.81933
N	8.88931	4.45241	3.82998	N	0.74159	-0.06096	0.90870
N	9.47962	4.67774	1.05052	N	-2.04941	0.11851	0.32932
C	7.90770	2.19970	6.35519	C	4.02527	0.23139	-0.30862
C	6.86043	1.44797	6.89752	C	5.04290	-0.35687	-1.05768
H	7.02489	0.49125	7.29651	H	5.76421	0.25818	-1.58391
C	5.57807	2.02773	6.88951	C	5.12380	-1.74330	-1.12596
H	4.76400	1.49656	7.28973	H	5.91049	-2.21293	-1.70504
C	5.37548	3.31479	6.35024	C	4.19459	-2.54080	-0.45489
H	4.41021	3.73149	6.35335	H	4.26911	-3.62015	-0.52200
C	6.44602	4.04922	5.80398	C	3.17434	-1.96562	0.29724
H	6.28769	5.00497	5.39811	H	2.44682	-2.58161	0.81305
C	7.72478	3.47211	5.80578	C	3.10687	-0.58108	0.36054
C	9.02025	4.06028	5.26087	C	2.11301	0.25303	1.14311
H	9.26594	4.93938	5.86224	H	2.28785	0.15466	2.21846
C	10.07297	5.23498	3.38157	C	-0.18580	0.58159	1.83940
H	10.97102	4.61249	3.40153	H	-0.24599	1.66554	1.66462
H	10.22526	6.08898	4.04566	H	0.17443	0.42257	2.85883
C	9.85313	5.77002	1.94479	C	-1.57697	-0.02560	1.70098
H	9.05969	6.52069	1.95474	H	-1.53593	-1.08268	2.01261
H	10.77697	6.23738	1.59689	H	-2.26244	0.49951	2.36816
C	8.40785	3.78243	1.47687	C	-1.11631	-0.49754	-0.62499
H	8.35633	2.91564	0.81444	H	-1.47013	-0.32026	-1.63685
H	7.45425	4.31376	1.43542	H	-1.06761	-1.58560	-0.46053
C	8.66400	3.29176	2.92315	C	0.27609	0.09759	-0.47136
H	7.79030	2.72357	3.24842	H	0.96299	-0.42373	-1.13921
H	9.53270	2.62883	2.92748	H	0.24963	1.15643	-0.76398
C	9.70861	4.82787	-0.34227	C	-3.42105	-0.08347	0.09424
C	9.04247	5.82470	-1.07962	C	-4.29102	-0.66772	1.02487
H	8.36373	6.47042	-0.60273	H	-3.89452	-1.03434	1.96157
C	9.27632	5.95934	-2.45838	C	-5.65323	-0.79693	0.77142
H	8.77646	6.70449	-3.00558	H	-6.29019	-1.25282	1.51984
C	10.17679	5.09753	-3.10610	C	-6.19134	-0.36183	-0.43038
H	10.35172	5.19810	-4.13750	H	-7.24959	-0.46473	-0.63409
C	10.84252	4.10055	-2.37397	C	-5.35327	0.22069	-1.37714
H	11.51611	3.45585	-2.85896	H	-5.72732	0.59225	-2.32286
C	10.60870	3.96514	-0.99503	C	-4.00990	0.35768	-1.10160
B	9.51941	1.88588	6.17234	B	3.57575	1.68612	0.01137

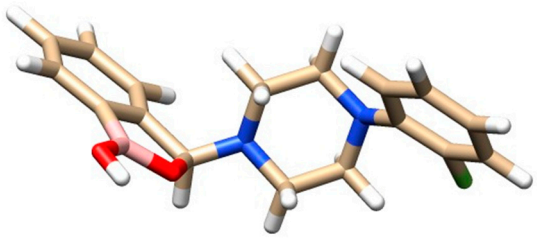


Figure S14. Structure 7-*S*

Table S14. Coordinates of structure 7-*S*

Coordinates of the input structure				Coordinates of the optimized structure		
N	1.28241	0.02166	3.55275	N	-0.64834	-0.78848	0.562995
C	0.75810	-0.26823	4.86826	C	-0.23767	-0.23466	-0.732141
C	1.52607	1.42576	3.30950	C	0.46321	-0.78449	1.520060
C	0.42906	2.38940	3.81490	C	1.63814	-1.59319	0.969229
C	-0.33592	0.70431	5.36424	C	0.95393	-1.03213	-1.268855
N	-0.06088	2.11508	5.15752	N	2.07374	-1.08897	-0.336707
C	0.58625	2.81710	6.20614	C	3.11190	-0.15535	-0.422744
C	0.47750	4.24545	6.27223	C	4.34690	-0.39177	0.207255
C	1.03401	4.96000	7.35150	C	5.42086	0.46722	0.120476
C	1.69336	4.28629	8.37554	C	5.31860	1.62390	-0.646218
C	1.81061	2.89604	8.32689	C	4.12645	1.88594	-1.305573
C	1.27523	2.17625	7.26109	C	3.04425	1.02110	-1.187441
F	-0.15947	4.94399	5.30223	F	4.51298	-1.53608	0.920318
H	0.33558	-1.31099	4.88297	H	-1.07267	-0.31363	-1.430365
H	1.63348	-0.23506	5.57864	H	0.02744	0.82805	-0.640300
H	1.67689	1.61641	2.21145	H	0.11745	-1.23839	2.452726
H	2.49233	1.67366	3.83802	H	0.79428	0.23992	1.748129
H	-0.46663	2.32523	3.13373	H	1.32464	-2.63519	0.844232
H	0.83121	3.43824	3.76011	H	2.46616	-1.57619	1.670562
H	-0.53511	0.50319	6.45130	H	1.28980	-0.63011	-2.223898
H	-1.28700	0.49369	4.79146	H	0.62447	-2.06224	-1.444761
H	0.93135	6.05493	7.37205	H	6.33416	0.20093	0.637772
H	2.11933	4.85030	9.21762	H	6.16035	2.29951	-0.727195
H	2.33539	2.36095	9.13220	H	4.02257	2.78028	-1.908236
H	1.40092	1.08220	7.24993	H	2.12114	1.27160	-1.691069
C	-0.87475	-2.52176	2.44993	C	-3.78896	0.71139	0.040002
C	-0.70152	-1.11687	2.41824	C	-3.09313	-0.48561	0.226123
C	-2.13546	-3.08565	2.40953	C	-4.97105	0.70984	-0.698532
C	-3.24598	-2.23115	2.33103	C	-5.43525	-0.48445	-1.238472
C	-3.07792	-0.84977	2.29085	C	-4.72516	-1.67139	-1.046766
C	-1.79785	-0.27672	2.33396	C	-3.54432	-1.68347	-0.309898
B	0.56339	-3.08365	2.49104	B	-2.93983	1.78383	0.780922
O	1.49121	-2.05330	2.45935	O	-1.83911	1.17785	1.338155
C	0.78327	-0.75974	2.44493	C	-1.86834	-0.27299	1.092724
O	1.01889	-4.33621	2.51636	O	-3.18430	3.11374	0.893139
H	-2.26995	-4.17678	2.43439	H	-5.52437	1.62942	-0.852546
H	-4.25826	-2.66077	2.29755	H	-6.35321	-0.49882	-1.814581
H	-3.95834	-0.19281	2.22434	H	-5.09872	-2.59338	-1.477396
H	-1.68245	0.81612	2.30060	H	-2.98812	-2.60223	-0.163816
H	1.98254	-4.27885	2.52337	H	-2.50498	3.56522	1.406754
H	1.09074	-0.28190	1.46904	H	-2.01068	-0.72903	2.076761

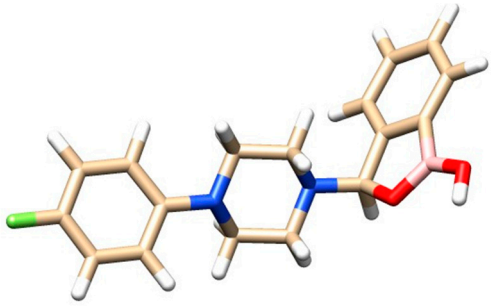


Figure S15. Structure 8-*R*

Table S15. Coordinates of structure 8-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
F	11.87800	2.01136	7.81950	F	7.28917	0.55309	-0.53359
O	2.65676	7.08018	13.05108	O	-4.40810	-2.41227	-1.55436
H	3.41057	7.49396	13.43075	H	-3.95390	-3.26233	-1.56586
O	3.57041	7.27797	10.59512	O	-2.70191	-1.83545	0.03073
N	4.32084	5.87782	8.76940	N	-0.94290	-0.33884	0.77107
N	6.85304	4.58961	8.51286	N	1.83381	-0.29136	0.09605
C	1.42277	6.07886	10.76318	C	-4.24036	-0.06201	-0.40912
C	0.23588	5.45027	11.15326	C	-5.25171	0.79435	-0.84120
H	-0.11649	5.51345	12.13987	H	-5.98902	0.45588	-1.56042
C	-0.46830	4.73257	10.16853	C	-5.30629	2.09055	-0.34103
H	-1.36626	4.24739	10.42011	H	-6.08799	2.76605	-0.66872
C	0.01927	4.65907	8.84746	C	-4.35769	2.53360	0.58285
H	-0.52088	4.11840	8.12545	H	-4.41246	3.54818	0.96053
C	1.22105	5.29584	8.48124	C	-3.34375	1.68784	1.02338
H	1.58227	5.23233	7.49701	H	-2.60249	2.03086	1.73591
C	1.92816	6.00788	9.46170	C	-3.30162	0.39594	0.51838
C	3.24639	6.75643	9.30974	C	-2.31892	-0.69846	0.88233
H	3.07755	7.59335	8.62718	H	-2.48210	-1.03847	1.90914
C	5.52554	6.67187	8.40550	C	-0.01987	-1.32276	1.33685
H	5.97180	7.11748	9.29809	H	0.00464	-2.24407	0.73655
H	5.24617	7.47347	7.71776	H	-0.35985	-1.58233	2.34253
C	6.57445	5.77367	7.70395	C	1.38174	-0.73487	1.41848
H	6.19285	5.46149	6.72904	H	1.37842	0.10878	2.12817
H	7.48823	6.35236	7.55340	H	2.06544	-1.48921	1.80341
C	5.71390	3.82556	9.01519	C	0.90514	0.67076	-0.48423
H	6.05227	3.08827	9.74652	H	1.23597	0.91222	-1.49549
H	5.22883	3.30487	8.18649	H	0.86821	1.60786	0.09646
C	4.69300	4.77109	9.69489	C	-0.49743	0.07744	-0.55948
H	3.80952	4.18520	9.95605	H	-1.18448	0.83206	-0.94411
H	5.13059	5.17070	10.61298	H	-0.49147	-0.76932	-1.26033
C	8.09986	3.93313	8.33084	C	3.21682	-0.03593	-0.04482
C	9.25282	4.46017	8.94169	C	4.14149	-1.04563	0.26890
H	9.18640	5.32912	9.52993	H	3.78439	-2.00883	0.61011
C	10.49624	3.82803	8.77444	C	5.50393	-0.84997	0.11536
H	11.35298	4.22616	9.23488	H	6.21390	-1.63237	0.35163
C	10.59395	2.66476	7.99306	C	5.95945	0.36377	-0.37341
C	9.44644	2.13583	7.37912	C	5.08438	1.37707	-0.70444
H	9.51734	1.26693	6.79211	H	5.46933	2.31578	-1.08229
C	8.20306	2.76808	7.54736	C	3.71703	1.17836	-0.53137
H	7.35156	2.36789	7.07866	H	3.04511	1.98987	-0.77176
B	2.52018	6.99112	11.59562	B	-3.81890	-1.52910	-0.70971

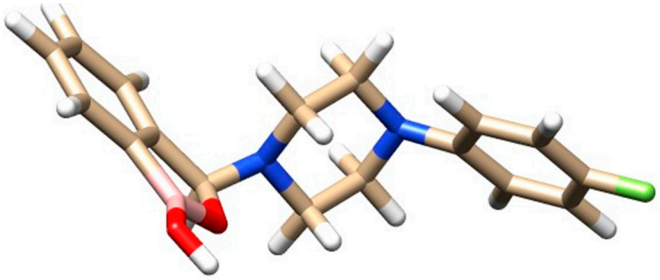


Figure S16. Structure 8-*S*

Table S16. Coordinates of structure 8-*S*

Coordinates of the input structure				Coordinates of the optimized structure			
N	1.28058	0.03663	3.53989	N	-0.85378	-0.88547	0.65723
C	0.77521	-0.26708	4.85995	C	-0.34883	-0.42848	-0.64300
C	1.49478	1.44546	3.29804	C	0.21827	-0.94155	1.65591
C	0.39170	2.39109	3.82640	C	1.33597	-1.87301	1.17941
C	-0.33639	0.68074	5.36341	C	0.77373	-1.36358	-1.09870
N	-0.08132	2.09699	5.17087	N	1.85403	-1.46982	-0.12697
C	0.57496	2.79884	6.21606	C	2.98953	-0.64860	-0.21397
C	0.50466	4.21697	6.22649	C	4.11575	-0.92133	0.58455
C	1.05438	4.95568	7.26591	C	5.27294	-0.16481	0.49113
C	1.69308	4.29753	8.33674	C	5.33183	0.87338	-0.42223
C	1.77526	2.89167	8.34370	C	4.25559	1.16801	-1.23371
C	1.23021	2.15894	7.29463	C	3.08944	0.41808	-1.12176
H	-0.00510	4.74941	5.40818	H	4.10012	-1.76058	1.26720
H	0.37809	-1.31960	4.87678	H	-1.16489	-0.45474	-1.36687
H	1.65484	-0.21199	5.56378	H	0.02007	0.60533	-0.58416
H	1.62361	1.64259	2.19833	H	-0.20050	-1.32378	2.59088
H	2.46538	1.70822	3.81150	H	0.63416	0.05695	1.85710
H	-0.50898	2.32543	3.15212	H	0.94039	-2.89141	1.09834
H	0.78701	3.44270	3.77774	H	2.13670	-1.88439	1.91491
H	-0.53506	0.46666	6.44798	H	1.17106	-1.05288	-2.06349
H	-1.28302	0.45952	4.78729	H	0.35003	-2.36571	-1.22994
H	0.99086	6.05346	7.26497	H	6.13593	-0.38683	1.10613
F	2.22615	5.01492	9.35309	F	6.46467	1.60804	-0.52105
H	2.27746	2.38118	9.17813	H	4.32290	1.98921	-1.93614
H	1.32486	1.06227	7.32077	H	2.24901	0.68936	-1.74457
C	-0.87206	-2.51552	2.44794	C	-3.80746	0.89184	-0.04347
C	-0.70044	-1.11033	2.40760	C	-3.24218	-0.36035	0.20934
C	-2.13239	-3.08160	2.40944	C	-4.95075	0.98089	-0.83567
C	-3.24417	-2.22898	2.32373	C	-5.50642	-0.17983	-1.36230
C	-3.07776	-0.84707	2.27425	C	-4.92592	-1.42322	-1.10383
C	-1.79829	-0.27211	2.31546	C	-3.78562	-1.52583	-0.31234
B	0.56677	-3.07528	2.49403	B	-2.88791	1.90120	0.70230
O	1.49325	-2.04341	2.45730	O	-1.87650	1.20956	1.32568
C	0.78391	-0.75138	2.43523	C	-2.03815	-0.23823	1.12123
O	1.02388	-4.32679	2.52716	O	-3.00387	3.25142	0.76347
H	-2.26538	-4.17270	2.44129	H	-5.40304	1.94443	-1.04182
H	-4.25589	-2.65997	2.29187	H	-6.39523	-0.12393	-1.98006
H	-3.95904	-0.19202	2.20170	H	-5.36941	-2.31811	-1.52517
H	-1.68409	0.82035	2.27390	H	-3.32936	-2.48898	-0.11472
H	1.98752	-4.26848	2.53497	H	-2.30363	3.65268	1.29052
H	1.09261	-0.27690	1.45812	H	-2.26188	-0.64597	2.11129

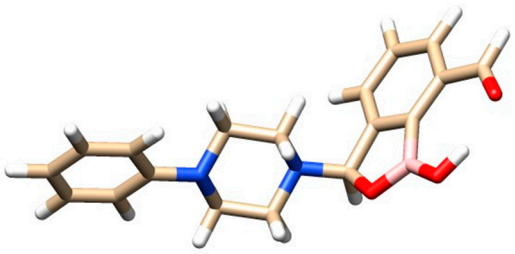


Figure S17. Structure 9-*R*

Table S17. Coordinates of structure 9-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
O	1.13994	-2.06992	2.25346	O	-1.77737	-1.51252	1.04716
B	0.12638	-3.08764	2.59610	B	-2.95398	-1.53142	0.33464
C	-0.94769	-2.33257	3.46625	C	-3.36799	-0.03769	0.05190
C	-0.50472	-1.01314	3.53903	C	-2.36925	0.72954	0.63930
C	0.79035	-0.79396	2.77593	C	-1.34928	-0.15132	1.33480
C	-2.12630	-2.74917	4.08535	C	-4.42347	0.61007	-0.61152
C	-2.84979	-1.79166	4.81081	C	-4.44023	2.00708	-0.66547
C	-2.40121	-0.46829	4.89688	C	-3.42575	2.75613	-0.07454
C	-1.22571	-0.06361	4.25880	C	-2.37898	2.11989	0.58502
N	0.65104	0.21283	1.73616	N	0.00978	0.11938	0.98257
C	-0.31159	-0.15385	0.70410	C	0.34515	-0.07268	-0.43124
C	-0.53867	1.00496	-0.27822	C	1.74520	0.45844	-0.70580
C	1.94044	0.55248	1.14844	C	0.98497	-0.56907	1.83153
C	1.81756	1.73973	0.18180	C	2.38970	-0.03977	1.56621
N	0.76218	1.42496	-0.76060	N	2.73121	-0.19532	0.15894
C	1.02143	1.42229	-2.08550	C	4.08754	-0.07638	-0.21118
O	0.40368	-4.52662	2.55968	O	-3.55966	-2.67755	-0.01354
C	-2.59535	-4.01865	4.00927	C	-5.52057	-0.12635	-1.26125
H	-3.79063	-2.05402	5.32452	H	-5.25321	2.51185	-1.17657
H	-0.87368	0.97929	4.31851	H	-1.58006	2.69324	1.04087
H	-1.29366	-0.40403	1.16869	H	-0.37071	0.47561	-1.04589
H	0.03870	-1.05611	0.14799	H	0.29612	-1.13397	-0.71105
H	-1.02046	1.86960	0.23605	H	1.75703	1.54903	-0.54420
H	-1.20386	0.68588	-1.11594	H	1.99609	0.27671	-1.74858
H	2.36583	-0.33156	0.61541	H	0.96737	-1.65449	1.66044
H	2.65606	0.83604	1.95589	H	0.72639	-0.38731	2.87758
H	2.78850	1.92634	-0.33629	H	3.09637	-0.61387	2.16659
H	1.53419	2.66842	0.73070	H	2.44468	1.01419	1.88738
H	-0.19034	-5.14159	2.94587	H	-4.37181	-2.47027	-0.51085
H	-2.98714	0.27017	5.46990	H	-3.45282	3.83761	-0.13030
O	-2.10584	-4.94541	3.41177	O	-5.64351	-1.33493	-1.30422
H	-3.54602	-4.22025	4.55439	H	-6.28502	0.51367	-1.74498
C	1.48819	0.25753	-2.69860	C	4.48740	-0.42546	-1.51225
C	1.75496	0.25799	-4.06916	C	5.81611	-0.35180	-1.89521
C	1.55520	1.41872	-4.81962	C	6.79533	0.05984	-0.99418
C	1.08833	2.58117	-4.20215	C	6.41511	0.39769	0.29602
C	0.82011	2.58518	-2.83184	C	5.08035	0.33968	0.68633
H	1.64637	-0.65985	-2.10666	H	3.75146	-0.78967	-2.21778
H	2.12360	-0.65897	-4.55909	H	6.09220	-0.63483	-2.90462
H	1.76626	1.41731	-5.90236	H	7.83464	0.10918	-1.29450
H	0.93119	3.49661	-4.79714	H	7.15973	0.72326	1.01365
H	0.45118	3.50352	-2.34456	H	4.81901	0.63506	1.69283
H	1.55378	-0.48591	3.49369	H	-1.42828	-0.03347	2.42026

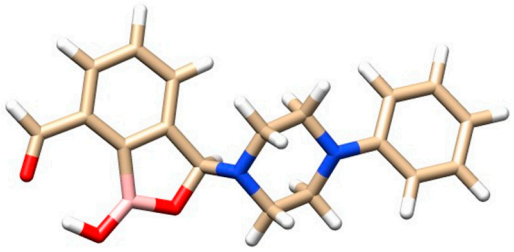


Figure S18. Structure 9-*S*

Table S18. Coordinates of structure 9-*S*

Coordinates of the input structure				Coordinates of the optimized structure			
O	-0.22895	-2.97917	1.39954	O	-1.78627	-1.73435	-0.58172
B	-0.96431	-3.43971	2.69417	B	-3.12362	-1.49406	-0.36456
C	-1.38125	-2.12107	3.42821	C	-3.29614	0.05594	-0.16014
C	-0.95005	-1.06771	2.66906	C	-2.00846	0.58010	-0.24355
C	-0.22895	-1.52035	1.39954	C	-0.99850	-0.54767	-0.40499
C	-2.06512	-1.96093	4.63220	C	-4.38847	0.92781	-0.02702
C	-2.30643	-0.64453	5.05703	C	-4.16408	2.30736	-0.00060
C	-1.86719	0.44913	4.28373	C	-2.87700	2.81745	-0.12996
C	-1.18001	0.24796	3.07392	C	-1.79110	1.95629	-0.25900
N	1.15213	-1.01685	1.39954	N	-0.14725	-0.77699	0.75463
C	1.83529	-1.45878	0.17355	C	0.81618	-1.86613	0.54653
C	1.03882	-0.99998	-1.06199	C	2.07735	-1.42638	-0.19918
C	1.13814	0.45351	1.45355	C	0.53114	0.35251	1.38087
C	0.30574	1.01071	0.28377	C	1.79453	0.82634	0.65073
N	0.80906	0.44633	-0.97491	N	2.71685	-0.28857	0.47546
C	1.05080	1.22759	-2.01105	C	4.04593	0.00834	0.10569
O	-1.22730	-4.89538	3.15718	O	-4.03527	-2.47664	-0.39464
H	-0.75178	-1.14701	0.51899	H	-0.43487	-0.42112	-1.34179
C	-2.51023	-3.10958	5.41583	C	-5.77878	0.45016	0.06783
H	-2.83271	-0.46856	5.98356	H	-5.00514	2.98487	0.10124
H	-0.84166	1.08288	2.47824	H	-0.79596	2.36616	-0.38429
H	1.91015	-2.54621	0.17434	H	0.32098	-2.67431	0.01097
H	2.83573	-1.02726	0.14174	H	1.10272	-2.24411	1.53261
H	0.08075	-1.51885	-1.09301	H	1.83307	-1.16132	-1.24167
H	1.60490	-1.22415	-1.96610	H	2.77186	-2.26276	-0.24214
H	2.15966	0.82717	1.38297	H	0.82864	0.02556	2.38244
H	0.69932	0.77600	2.39776	H	-0.16082	1.18243	1.51205
H	0.39429	2.09675	0.25607	H	2.27981	1.59296	1.25773
H	-0.74017	0.73285	0.41399	H	1.52848	1.29179	-0.31597
H	-1.70141	-4.88496	3.99187	H	-4.91954	-2.09506	-0.24435
H	-2.06119	1.45516	4.62528	H	-2.71901	3.88900	-0.13765
O	-2.28565	-4.24168	5.02045	O	-6.14374	-0.70827	0.02436
H	-3.03829	-2.95709	6.34550	H	-6.53409	1.25184	0.18914
C	1.53052	0.67745	-3.20571	C	5.01710	-1.00754	0.11829
C	1.78693	1.50606	-4.30465	C	6.33610	-0.73940	-0.20710
C	1.56361	2.88481	-4.20893	C	6.73866	0.55012	-0.54626
C	1.08389	3.43496	-3.01427	C	5.79237	1.56377	-0.55310
C	0.82749	2.60635	-1.91533	C	4.46197	1.30192	-0.23876
H	1.70280	-0.38617	-3.27955	H	4.73932	-2.01006	0.41735
H	2.15699	1.08166	-5.22624	H	7.06121	-1.54484	-0.18137
H	1.76140	3.52403	-5.05668	H	7.77217	0.75737	-0.79457
H	0.91161	4.49857	-2.94042	H	6.08190	2.57485	-0.81652
H	0.45742	3.03074	-0.99373	H	3.74968	2.11410	-0.27656

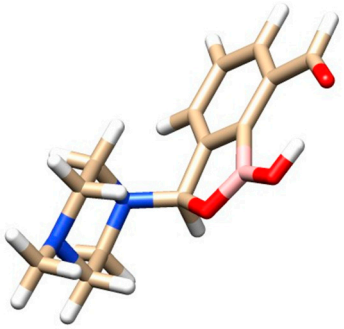


Figure S19. Structure 10-*R*

Table S19. Coordinates of structure 10-*R*

Coordinates of the input structure	Coordinates of the optimized structure
O -0.23349 1.21475 -0.79069	O 0.30325 0.82966 -1.04534
B -1.64664 1.61669 -0.63176	B -0.91619 1.33372 -0.66020
C -2.39633 0.27976 -0.28119	C -1.82307 0.12264 -0.22133
C -1.40615 -0.71177 -0.26056	C -1.03026 -1.00401 -0.40102
C -0.01103 -0.15623 -0.51069	C 0.32250 -0.63823 -0.98502
C -3.75300 -0.00454 -0.05325	C -3.12984 -0.03483 0.27097
C -4.10077 -1.35392 0.15960	C -3.59680 -1.31869 0.56887
C -3.12030 -2.36435 0.15906	C -2.78290 -2.43388 0.38651
C -1.76481 -2.05143 -0.04647	C -1.48890 -2.28318 -0.10131
N 0.85345 -0.37139 0.68734	N 1.43325 -1.21130 -0.31315
C 1.65793 0.80260 1.12247	C 1.63494 -0.88685 1.10264
C 2.86739 1.05754 0.18634	C 2.51229 0.34839 1.32567
C 1.72671 -1.57399 0.58414	C 2.70495 -1.23836 -1.03804
C 2.96354 -1.33410 -0.32346	C 3.55744 0.01099 -0.81278
N 3.73190 -0.15073 0.14453	N 3.78504 0.20029 0.61968
C 4.92633 0.07862 -0.70630	C 4.67426 1.32023 0.88039
O -2.21256 2.76540 -1.35041	O -1.18654 2.64953 -0.68095
H -5.10464 -1.61676 0.33176	H -4.60500 -1.44503 0.94910
H -1.04327 -2.81301 -0.04707	H -0.84334 -3.14290 -0.23899
H 2.03409 0.61121 2.13151	H 2.12228 -1.74687 1.57391
H 1.03470 1.69707 1.17286	H 0.66512 -0.75089 1.58271
H 3.43853 1.90078 0.58184	H 2.72097 0.44620 2.39541
H 2.51454 1.31399 -0.81494	H 1.97302 1.25353 1.00264
H 1.16213 -2.42301 0.19728	H 2.50242 -1.37312 -2.10257
H 2.07579 -1.83692 1.58651	H 3.27086 -2.10931 -0.69017
H 2.64174 -1.19530 -1.35779	H 3.06337 0.88605 -1.26752
H 3.60066 -2.22070 -0.27634	H 4.52696 -0.12054 -1.30267
H -3.13243 2.82728 -1.52487	H -2.09844 2.79137 -0.36710
H 4.63507 0.28909 -1.73714	H 4.26568 2.28613 0.53427
H 5.49934 0.92301 -0.31877	H 4.86446 1.39797 1.95332
H 5.56656 -0.80533 -0.69051	H 5.63033 1.15665 0.37801
H -3.40398 -3.36371 0.32049	H -3.15957 -3.42066 0.62709
H 0.41053 -0.62136 -1.40283	H 0.37468 -0.96836 -2.02703
C -4.79659 1.02878 -0.00258	C -4.03598 1.10406 0.49144
O -4.54628 2.14430 0.45393	O -3.77876 2.27435 0.28512
H -5.80602 0.74042 -0.07167	H -5.03620 0.83030 0.88226

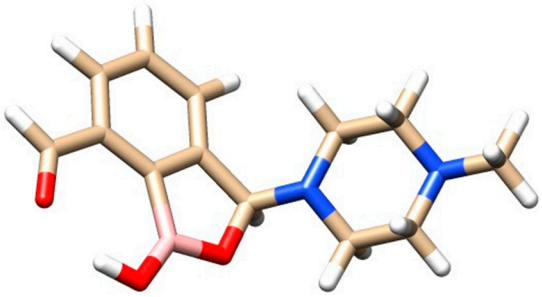


Figure S20. Structure 10-*S*

Table S20. Coordinates of structure 10-*S*

Coordinates of the input structure	Coordinates of the optimized structure
O -1.44269 -2.75662 0.44869	O -0.35563 -1.57476 -0.94325
B -2.17805 -3.21717 1.74332	B -1.57018 -1.57164 -0.29448
C -2.59499 -1.89852 2.47736	C -1.99509 -0.07122 -0.09995
C -2.16379 -0.84517 1.71821	C -0.94907 0.67482 -0.63723
C -1.44269 -1.29780 0.44869	C 0.17351 -0.25425 -1.08500
C -3.27886 -1.73838 3.68134	C -3.14382 0.58559 0.36850
C -3.52016 -0.42198 4.10618	C -3.22478 1.97756 0.26758
C -3.08093 0.67167 3.33288	C -2.19283 2.70514 -0.31466
C -2.39375 0.47051 2.12307	C -1.05111 2.05728 -0.77834
N -0.06161 -0.79431 0.44869	N 1.38699 -0.17866 -0.28055
C 0.62090 -1.23582 -0.77612	C 2.38024 -1.15553 -0.75007
C 2.06777 -0.70834 -0.77612	C 3.58763 -1.17217 0.17261
C -0.07562 0.67477 0.49942	C 1.99319 1.14900 -0.20235
C 1.37121 1.20223 0.49942	C 3.20904 1.12069 0.71636
N 2.05370 0.76074 -0.72535	N 4.19363 0.15295 0.25223
C 3.43476 1.26429 -0.72535	C 5.38821 0.15603 1.07869
O -2.44104 -4.67283 2.20633	O -2.20605 -2.70910 0.02022
H -1.96552 -0.92446 -0.43186	H 0.39363 -0.11185 -2.15810
C -3.72396 -2.88704 4.46497	C -4.28785 -0.13566 0.95143
H -4.04644 -0.24601 5.03271	H -4.11013 2.49022 0.62833
H -2.05540 1.30543 1.52739	H -0.26597 2.63232 -1.25417
H 0.09250 -0.84720 -1.64668	H 2.71310 -0.91203 -1.77452
H 0.63130 -2.32512 -0.81377	H 1.91458 -2.13843 -0.76811
H 2.57385 -1.03567 -1.68433	H 4.32849 -1.87353 -0.22015
H 2.59618 -1.09693 0.09444	H 3.27693 -1.53551 1.16913
H -0.58170 1.00215 1.40762	H 1.27186 1.85107 0.21340
H -0.60401 1.06336 -0.37115	H 2.30533 1.51890 -1.19622
H 1.89962 0.81367 1.37000	H 2.87129 0.89445 1.74476
H 1.36080 2.29154 0.53703	H 3.66887 2.11275 0.72880
H -2.91515 -4.66242 3.04102	H -3.05394 -2.49132 0.44901
H 3.96316 0.87574 0.14524	H 5.18718 -0.12514 2.12830
H 3.94085 0.93692 -1.63354	H 6.11855 -0.54781 0.67395
H 3.42432 2.35359 -0.68775	H 5.83877 1.15102 1.07455
H -3.27493 1.67771 3.67442	H -2.28014 3.78013 -0.41504
O -3.49939 -4.01913 4.06960	O -4.38833 -1.34062 1.07599
H -4.25203 -2.73454 5.39465	H -5.11521 0.51516 1.29763

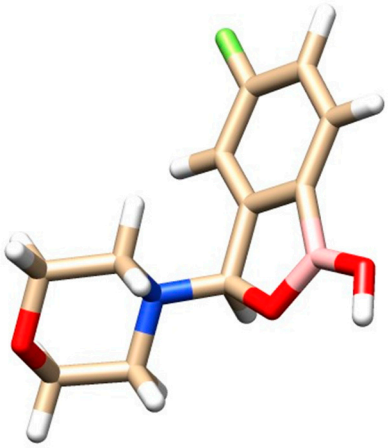


Figure S21. Structure 11-*R*

Table S21. Coordinates of structure 11-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
C	0.15591	-1.84956	0.77240	C	-1.81115	0.96173	0.09019
C	-0.93792	-2.69137	0.91969	C	-3.09413	0.63863	0.53119
C	-2.15945	-2.07266	1.20223	C	-3.55135	-0.66845	0.42172
C	-2.24351	-0.68294	1.36356	C	-2.71191	-1.63143	-0.12691
C	-1.10723	0.12471	1.23086	C	-1.43230	-1.35148	-0.57742
C	0.10250	-0.46377	0.86637	C	-1.00399	-0.03757	-0.45832
B	1.75750	-2.21592	0.58379	B	-0.93813	2.24658	0.04473
O	2.42557	-0.90301	0.68678	O	0.28298	1.93936	-0.50813
C	1.47904	0.16993	0.69555	C	0.32909	0.52601	-0.90846
F	-3.40247	-0.13152	1.68539	F	-3.16644	-2.89747	-0.22215
N	1.65401	0.96435	-0.50877	N	1.47408	-0.17205	-0.42471
C	0.97546	2.24150	-0.57906	C	2.73295	0.24398	-1.05146
C	1.63791	0.27332	-1.78081	C	1.61609	-0.23205	1.03460
C	0.24212	0.22698	-2.40453	C	2.76381	-1.16741	1.38900
C	-0.36000	2.20815	-1.33587	C	3.84600	-0.70630	-0.63286
O	-0.22613	1.54478	-2.57078	O	3.97958	-0.75407	0.78008
O	2.38061	-3.51411	0.85315	O	-1.26396	3.49361	0.46715
H	-0.83560	-3.78655	0.85114	H	-3.73705	1.39843	0.96016
H	-3.06049	-2.69269	1.34280	H	-4.53975	-0.96090	0.75241
H	-1.16556	1.20700	1.42733	H	-0.81052	-2.13548	-0.99061
H	1.72691	0.78004	1.59456	H	0.39193	0.53499	-2.00055
H	1.65827	2.93381	-1.12570	H	3.00363	1.27107	-0.76649
H	0.84653	2.67900	0.43828	H	2.61287	0.21339	-2.13794
H	2.06823	-0.75033	-1.69858	H	0.68903	-0.60805	1.47104
H	2.31506	0.82999	-2.47084	H	1.81652	0.76286	1.45675
H	-0.49360	-0.35239	-1.79965	H	2.51686	-2.19141	1.07436
H	0.27921	-0.22012	-3.42495	H	2.94105	-1.16307	2.46523
H	-0.70013	3.24243	-1.57513	H	4.80657	-0.36820	-1.02394
H	-1.18389	1.71514	-0.77606	H	3.63777	-1.71274	-1.02384
H	3.31786	-3.58053	0.91881	H	-0.54641	4.12275	0.33178

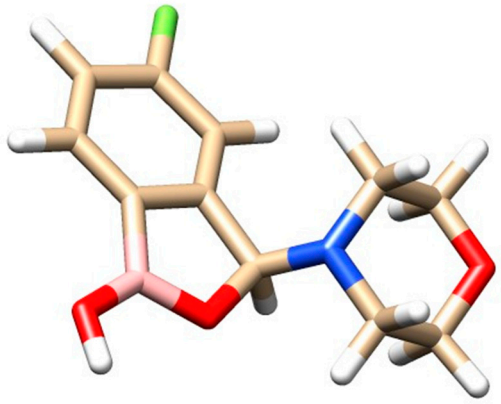


Figure S22. Structure 11-*S*

Table S22. Coordinates of structure 11-*S*

Coordinates of the input structure				Coordinates of the optimized structure			
C	0.11154	-1.90731	1.37743	C	1.83234	0.92675	0.07680
C	-0.55000	-2.38741	2.49948	C	3.15111	0.53354	0.29528
C	-1.81304	-1.84402	2.75178	C	3.49904	-0.80732	0.19491
C	-2.37286	-0.89312	1.88791	C	2.51472	-1.72683	-0.14121
C	-1.67684	-0.45468	0.75439	C	1.19262	-1.37537	-0.36377
C	-0.38990	-0.93804	0.51661	C	0.86092	-0.03317	-0.22728
B	1.53718	-2.39779	0.70108	B	1.10009	2.28958	-0.03651
O	1.57809	-1.65392	-0.57169	O	-0.20113	2.06023	-0.41715
C	0.56087	-0.64835	-0.64842	C	-0.48452	0.63954	-0.45593
F	-3.58760	-0.42694	2.12911	F	2.86041	-3.02454	-0.26458
N	1.22659	0.64694	-0.55222	N	-1.49443	0.39020	0.55638
C	0.35410	1.80159	-0.45447	C	-1.69437	-0.96518	1.07343
C	2.15158	0.87747	-1.65147	C	-2.79478	0.99451	0.22420
C	1.43541	1.20944	-2.96746	C	-3.64734	0.09218	-0.66498
C	-0.37245	2.09195	-1.77123	C	-2.57437	-1.82808	0.17026
O	0.57335	2.31108	-2.79313	O	-3.82305	-1.19324	-0.07735
O	2.21376	-3.67118	0.96137	O	1.60768	3.53272	0.14382
H	-0.11123	-3.17406	3.13457	H	3.91104	1.26993	0.52930
H	-2.38957	-2.19484	3.62393	H	4.51243	-1.15339	0.35269
H	-2.14963	0.25424	0.05599	H	0.48289	-2.14338	-0.64298
H	0.97619	2.68759	-0.18420	H	-2.19841	-0.86471	2.04070
H	-0.35328	1.69690	0.39657	H	-0.73512	-1.44331	1.26254
H	2.83063	0.00420	-1.78775	H	-2.62504	1.96278	-0.24648
H	2.81828	1.72849	-1.37517	H	-3.32933	1.17043	1.16302
H	0.84359	0.35633	-3.37293	H	-3.19269	-0.01607	-1.66135
H	2.16996	1.51287	-3.74910	H	-4.64790	0.50864	-0.79539
H	-0.96950	3.03007	-1.69457	H	-2.80519	-2.78208	0.64844
H	-1.05878	1.27179	-2.08575	H	-2.06911	-2.03649	-0.78609
H	2.89162	-3.97019	0.37972	H	0.94959	4.22193	0.00007
H	0.01749	-0.76186	-1.58553	H	-0.83655	0.44617	-1.48015

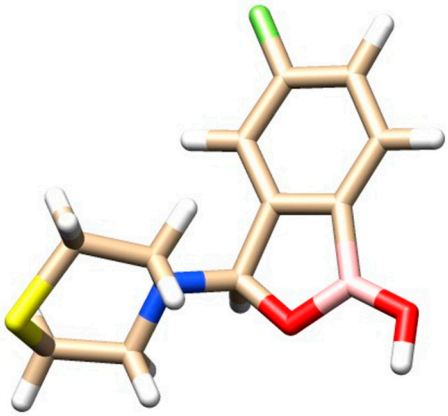


Figure S23. Structure 12-*R*

Table S23. Coordinates of structure 12-*R*

Coordinates of the input structure				Coordinates of the optimized structure		
C	0.15591	-1.84953	0.77234	C	2.15253	0.87691	-0.13202
C	-0.93792	-2.69135	0.91968	C	3.39379	0.43362	-0.58786
C	-2.15945	-2.07265	1.20226	C	3.74086	-0.90422	-0.44891
C	-2.24351	-0.68292	1.36353	C	2.83487	-1.77657	0.14378
C	-1.10724	0.12471	1.23077	C	1.59335	-1.37623	0.60993
C	0.10254	-0.46372	0.86628	C	1.27510	-0.03463	0.46008
B	1.75749	-2.21592	0.58372	B	1.39347	2.23290	-0.10612
O	2.42562	-0.90305	0.68684	O	0.16279	2.04606	0.47914
C	1.47916	0.16995	0.69559	C	0.00687	0.65414	0.92464
F	-3.40246	-0.13150	1.68542	F	3.18246	-3.07344	0.26764
N	1.65448	0.96442	-0.50860	N	1.21044	0.04563	0.49643
C	0.97551	2.24126	-0.57918	C	2.39812	0.56354	1.18385
C	1.63782	0.27358	-1.78071	C	1.38192	-0.04161	-0.95856
C	0.24174	0.22829	-2.40392	C	2.44337	-1.06627	-1.33692
C	-0.35960	2.20689	-1.33665	C	3.58032	-0.38865	1.05939
S	-0.22580	1.54424	-2.56963	S	4.09686	-0.63684	-0.67897
O	2.38061	-3.51412	0.85312	O	1.81489	3.43508	-0.57100
H	-0.83557	-3.78653	0.85115	H	4.08944	1.12379	-1.05088
H	-3.06046	-2.69270	1.34294	H	4.69346	-1.28897	-0.79000
H	-1.16561	1.20700	1.42722	H	0.91701	-2.09279	1.05831
H	1.72695	0.77999	1.59466	H	0.01983	0.69966	2.01686
H	1.65832	2.93375	-1.12562	H	2.68140	1.55601	0.80616
H	0.84602	2.67884	0.43805	H	2.14682	0.67140	2.24322
H	2.06767	-0.75028	-1.69874	H	0.42871	-0.35027	-1.39275
H	2.31508	0.83008	-2.47080	H	1.64540	0.93465	-1.38747
H	-0.49381	-0.35176	-1.79945	H	2.16169	-2.05822	-0.97889
H	0.27874	-0.21861	-3.42445	H	2.55660	-1.10871	-2.42077
H	-0.69966	3.24113	-1.57619	H	4.45055	0.01916	1.57493
H	-1.18373	1.71464	-0.77648	H	3.33611	-1.35615	1.50244
H	3.31786	-3.58047	0.91881	H	1.15727	4.12755	-0.44029

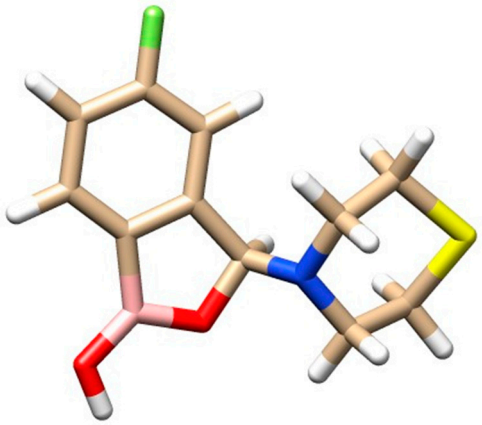


Figure S24. Structure 12-*S*

Table S24. Coordinates of structure 12-*S*

Coordinates of the input structure	Coordinates of the optimized structure
C 0.11148 -1.90746 1.37746	C 2.16565 0.83075 0.05598
C -0.55003 -2.38769 2.49945	C 3.45416 0.33861 0.25357
C -1.81301 -1.84421 2.75187	C 3.69578 -1.02569 0.16040
C -2.37279 -0.89322 1.88810	C 2.63646 -1.86841 -0.14733
C -1.67681 -0.45470 0.75459	C 1.34169 -1.41741 -0.34955
C -0.38989 -0.93807 0.51675	C 1.11617 -0.05239 -0.22094
B 1.53714 -2.39795 0.70119	B 1.54088 2.24544 -0.04866
O 1.57818 -1.65397 -0.57151	O 0.21650 2.11696 -0.39706
C 0.56098 -0.64834 -0.64819	C -0.17808 0.72410 -0.42866
F -3.58748 -0.42697 2.12941	F 2.87711 -3.19023 -0.26248
N 1.22675 0.64693 -0.55187	N -1.18867 0.54946 0.59954
C 0.35426 1.80162 -0.45482	C -1.47320 -0.78647 1.11360
C 2.15130 0.87761 -1.65146	C -2.40566 1.33173 0.35471
C 1.43415 1.21057 -2.96672	C -3.37871 0.72142 -0.65752
C -0.37089 2.09165 -1.77245	C -2.32573 -1.67964 0.20428
S 0.57386 2.31065 -2.79223	S -3.96647 -0.94005 -0.14645
O 2.21372 -3.67128 0.96180	O 2.14707 3.44594 0.11276
H -0.11120 -3.17444 3.13438	H 4.27240 1.01654 0.46658
H -2.38952 -2.19498 3.62407	H 4.68218 -1.44789 0.30297
H -2.14966 0.25430 0.05633	H 0.57063 -2.13250 -0.60494
H 0.97608 2.68765 -0.18394	H -2.00412 -0.65642 2.06140
H -0.35397 1.69701 0.39552	H -0.53307 -1.28627 1.34557
H 2.82989 0.00412 -1.78863	H -2.10284 2.32416 0.01933
H 2.81849 1.72824 -1.37516	H -2.91944 1.45039 1.31279
H 0.84250 0.35747 -3.37250	H -2.93374 0.65268 -1.65258
H 2.16855 1.51381 -3.74858	H -4.27507 1.33817 -0.73916
H -0.96836 3.02953 -1.69607	H -2.53083 -2.63312 0.69407
H -1.05740 1.27161 -2.08693	H -1.82243 -1.89131 -0.74226
H 2.89162 -3.97046 0.38033	H 1.54265 4.18450 -0.02111
H 0.01764 -0.76180 -1.58532	H -0.56041 0.55775 -1.44729

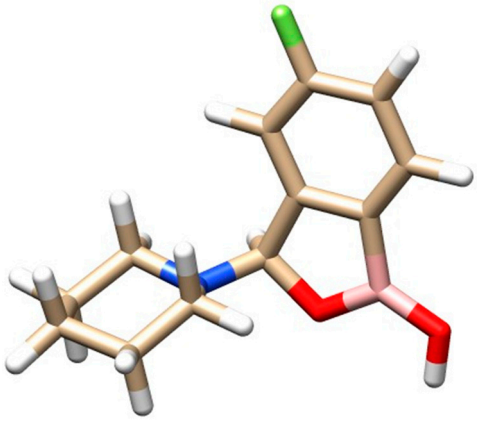


Figure S25. Structure 13-*R*

Table S25. Coordinates of structure 13-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
C	-0.13836	-2.08184	0.98390	C	-1.87739	0.86458	0.05713
C	-1.21428	-2.95480	1.06733	C	-3.09662	0.41919	0.56554
C	-2.47958	-2.36741	1.15952	C	-3.38924	-0.93868	0.56284
C	-2.62813	-0.97398	1.18337	C	-2.45278	-1.82376	0.04313
C	-1.51238	-0.13034	1.11126	C	-1.23322	-1.41960	-0.47574
C	-0.24438	-0.69556	0.98245	C	-0.96004	-0.05818	-0.45384
B	1.48277	-2.39919	0.92429	B	-1.19098	2.24262	-0.13576
O	2.10515	-1.06242	0.96072	O	0.04645	2.04903	-0.70478
C	1.12566	-0.02098	0.90237	C	0.29495	0.64712	-0.96707
F	-3.83721	-0.44825	1.29662	F	-2.74731	-3.14033	0.04015
N	1.34817	0.75793	-0.30679	N	1.56935	0.27346	-0.41654
C	0.78368	2.09504	-0.26874	C	2.28563	-0.78870	-1.11441
C	1.03142	0.04974	-1.53526	C	1.63860	0.15496	1.03857
C	1.50188	0.82729	-2.77296	C	3.09554	0.20069	1.50090
C	1.25371	2.93833	-1.46282	C	3.76449	-0.77427	-0.72446
C	0.90592	2.23932	-2.78191	C	3.93023	-0.87306	0.79563
O	2.13615	-3.66704	1.25666	O	-1.66652	3.47317	0.17783
H	-1.07082	-4.04751	1.07352	H	-3.81996	1.12397	0.95919
H	-3.37141	-3.01179	1.23356	H	-4.32339	-1.32722	0.94770
H	-1.64111	0.96142	1.16747	H	-0.55048	-2.15876	-0.87465
H	1.30414	0.59407	1.81443	H	0.37248	0.53055	-2.05221
H	1.09653	2.60862	0.67081	H	2.17723	-0.63027	-2.19046
H	-0.32886	2.04498	-0.27884	H	1.87067	-1.78821	-0.88857
H	-0.06829	-0.12512	-1.60588	H	1.17052	-0.78013	1.39145
H	1.53499	-0.94512	-1.53688	H	1.08069	0.98307	1.47736
H	1.21078	0.28344	-3.70387	H	3.13713	0.06871	2.58580
H	2.61627	0.89471	-2.76562	H	3.50321	1.19089	1.27549
H	2.35837	3.08725	-1.39972	H	4.21017	0.15826	-1.08387
H	0.78214	3.95014	-1.43057	H	4.28125	-1.59942	-1.22312
H	3.07193	-3.70032	1.35851	H	-1.04200	4.17189	-0.04783
H	1.29977	2.82328	-3.64832	H	4.98427	-0.78248	1.07152
H	-0.20279	2.17950	-2.89605	H	3.60315	-1.86458	1.13172

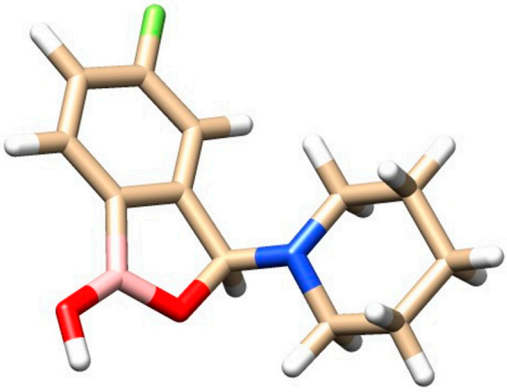


Figure S26. Structure 13-*S*

Table S26. Coordinates of structure 13-*S*

Coordinates of the input structure	Coordinates of the optimized structure
C -0.52641 -2.28344 -0.33108	C -1.78034 0.98391 -0.22444
C -1.65728 -3.08857 -0.33069	C -3.06216 0.70162 -0.69156
C -2.87369 -2.44575 -0.57843	C -3.58626 -0.57593 -0.54348
C -2.91976 -1.07054 -0.84416	C -2.81610 -1.54047 0.09179
C -1.74895 -0.30208 -0.85710	C -1.53766 -1.29852 0.56914
C -0.53222 -0.91024 -0.54650	C -1.01849 -0.02412 0.37740
B 1.06821 -2.70225 -0.21617	B -0.92888 2.27007 -0.07705
O 1.76888 -1.43694 -0.50591	O 0.22609 1.95762 0.60245
C 0.87869 -0.31584 -0.52546	C 0.32452 0.53673 0.82980
F -4.08017 -0.49711 -1.11919	F -3.33941 -2.77216 0.26212
N 1.16094 0.50602 0.64950	N 1.49181 0.06336 0.09960
C 0.22370 1.59911 0.84977	C 1.63184 -1.39186 0.01846
C 2.53792 0.98501 0.63208	C 2.71507 0.68038 0.63563
C 2.91012 1.75947 1.90394	C 3.92004 0.37738 -0.25045
C 0.52319 2.41171 2.11884	C 2.80604 -1.77460 -0.88454
C 1.95886 2.94296 2.10105	C 4.11238 -1.13077 -0.41766
O 1.61665 -4.04334 -0.43507	O -1.22741 3.53016 -0.47532
H -1.58921 -4.17751 -0.17486	H -3.65928 1.47731 -1.15671
H -3.80431 -3.03697 -0.60104	H -4.57888 -0.83584 -0.88812
H -1.79123 0.76712 -1.12035	H -1.00477 -2.09201 1.07642
H -0.80219 1.18919 0.98330	H 0.71868 -1.81142 -0.39752
H 0.22453 2.27050 -0.04193	H 1.78063 -1.84103 1.02013
H 2.70245 1.63654 -0.25943	H 2.91119 0.31570 1.66245
H 3.23875 0.12169 0.54887	H 2.55191 1.75421 0.69786
H 3.96359 2.12468 1.83990	H 4.81149 0.83707 0.18573
H 2.85007 1.07789 2.78619	H 3.76137 0.84112 -1.22903
H 0.38055 1.76365 3.01699	H 2.57829 -1.44656 -1.90350
H -0.19530 3.26188 2.21033	H 2.89622 -2.86436 -0.90717
H 2.54143 -4.15525 -0.57447	H -0.53440 4.15996 -0.24767
H 1.06502 0.24099 -1.47378	H 0.45071 0.40775 1.91895
H 2.19102 3.47797 3.05326	H 4.91980 -1.34374 -1.12340
H 2.08255 3.67371 1.26649	H 4.41075 -1.56729 0.54304

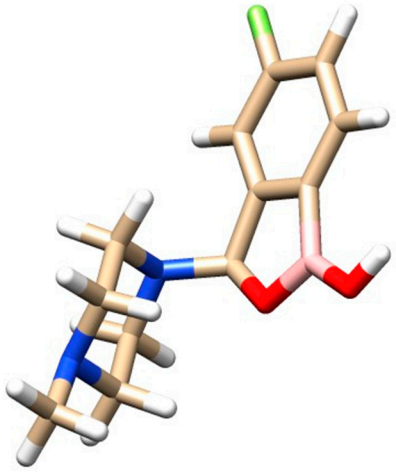


Figure S27. Structure 14-*R*

Table S27. Coordinates of structure 14-*R*

Coordinates of the input structure	Coordinates of the optimized structure
O -0.26952 -2.13898 1.54677	O 0.43745 1.32882 -0.84100
B -1.38530 -2.94390 2.07396	B -0.58357 2.07409 -0.31452
C -2.40707 -1.90697 2.64569	C -1.80095 1.13687 -0.03254
C -1.86712 -0.65158 2.39178	C -1.37436 -0.12933 -0.44032
C -0.52564 -0.73853 1.67049	C 0.02281 -0.07723 -1.02830
C -3.61434 -2.12013 3.29796	C -3.08341 1.28300 0.49699
C -4.30727 -0.97789 3.71038	C -3.91592 0.17714 0.61418
C -3.79271 0.30411 3.47382	C -3.44610 -1.06332 0.19869
C -2.56774 0.47589 2.81699	C -2.18135 -1.25185 -0.33314
N -0.59905 -0.05810 0.38577	N 0.91991 -1.04944 -0.52312
C -0.11494 -0.81338 -0.75459	C 1.18590 -1.07735 0.91802
C 1.41635 -0.92728 -0.77018	C 2.38028 -0.21312 1.33130
C 0.02823 1.25208 0.38968	C 2.13756 -1.30053 -1.29532
C 1.56352 1.17519 0.35662	C 3.31294 -0.41741 -0.87470
N 2.01851 0.39429 -0.78021	N 3.56546 -0.58136 0.55686
C 3.46569 0.33942 -0.86676	C 4.73751 0.16337 0.98538
O -1.40369 -4.39525 2.26744	O -0.41108 3.40816 -0.11803
H -3.99918 -3.13679 3.48040	H -3.44747 2.25171 0.82403
H -5.27149 -1.08946 4.23379	H -4.91628 0.25102 1.02106
F -4.46929 1.36584 3.88119	F -4.26108 -2.13002 0.32330
H -2.16608 1.48637 2.64331	H -1.85132 -2.23754 -0.63566
H -0.45020 -0.29502 -1.68417	H 1.39636 -2.11499 1.19774
H -0.60278 -1.81522 -0.79348	H 0.29024 -0.76395 1.45518
H 1.72369 -1.47683 -1.69124	H 2.59341 -0.38525 2.39073
H 1.78000 -1.51249 0.10723	H 2.13191 0.85346 1.20571
H -0.31408 1.83881 1.27336	H 1.91909 -1.16176 -2.35613
H -0.33104 1.81445 -0.50458	H 2.42149 -2.34744 -1.14339
H 1.96117 0.74291 1.30483	H 3.10121 0.63361 -1.13454
H 1.96887 2.21124 0.27162	H 4.20903 -0.72550 -1.42189
H -2.13381 -4.80136 2.70270	H -1.18509 3.83601 0.25702
H 3.90912 -0.17077 0.01964	H 4.63279 1.25369 0.84223
H 3.77353 -0.20414 -1.78886	H 4.92550 -0.02258 2.04530
H 3.88435 1.36898 -0.93940	H 5.61257 -0.16978 0.42279
H 0.24531 -0.30986 2.31146	H -0.02385 -0.21255 -2.11265

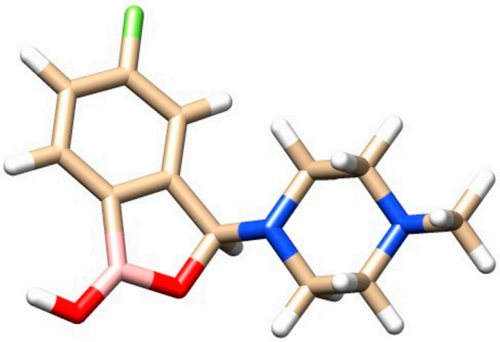


Figure S28 Structure 14-*S*

Table S28. Coordinates of structure 14-*S*

Coordinates of the input structure				Coordinates of the optimized structure			
O	-1.50275	-2.80051	0.51818	O	-0.33502	2.04603	0.623072
B	-2.23811	-3.26106	1.81281	B	-1.47640	2.23349	-0.115049
C	-2.65505	-1.94241	2.54685	C	-2.19107	0.85879	-0.273379
C	-2.22384	-0.88906	1.78770	C	-1.35941	-0.05391	0.386361
C	-1.50275	-1.34169	0.51818	C	-0.10573	0.65354	0.884026
C	-3.33892	-1.78227	3.75083	C	-3.41198	0.43018	-0.790284
C	-3.58022	-0.46587	4.17566	C	-3.80734	-0.89266	-0.636966
C	-3.14098	0.62778	3.40236	C	-2.97133	-1.75835	0.054074
C	-2.45380	0.42661	2.19256	C	-1.74956	-1.37193	0.582786
N	-0.12166	-0.83820	0.51818	N	1.12965	0.28363	0.207029
C	0.56084	-1.27971	-0.70664	C	2.26063	1.05438	0.742293
C	2.00771	-0.75223	-0.70664	C	3.52259	0.77487	-0.057397
C	-0.13568	0.63088	0.56891	C	1.44496	-1.14392	0.227453
C	1.31115	1.15834	0.56891	C	2.71691	-1.41286	-0.568160
N	1.99370	0.71684	-0.65591	N	3.83851	-0.64912	-0.038360
C	3.37478	1.22034	-0.65591	C	5.07482	-0.94209	-0.742243
O	-2.50110	-4.71672	2.27582	O	-1.80515	3.48533	-0.520666
H	-2.02557	-0.96835	-0.36237	H	-0.01035	0.55149	1.979333
H	-3.66817	-2.63196	4.33050	H	-4.07354	1.12087	-1.303109
H	-4.10650	-0.28990	5.10220	H	-4.74993	-1.26136	-1.020392
F	-3.37989	1.86670	3.82297	F	-3.36957	-3.03457	0.228372
H	-2.11546	1.26154	1.59688	H	-1.16008	-2.09370	1.132786
H	0.03245	-0.89112	-1.57721	H	2.44144	0.79851	1.801333
H	0.57124	-2.36901	-0.74425	H	2.01394	2.11249	0.685403
H	2.51381	-1.07961	-1.61482	H	4.35685	1.32561	0.385193
H	2.53608	-1.14082	0.16395	H	3.38601	1.14545	-1.089891
H	-0.64176	0.95826	1.47710	H	0.63129	-1.69970	-0.235195
H	-0.66407	1.01947	-0.30167	H	1.58292	-1.52061	1.257279
H	1.83953	0.76975	1.43950	H	2.52853	-1.17234	-1.631021
H	1.30076	2.24764	0.60654	H	2.95609	-2.47805	-0.506615
H	-2.97521	-4.70631	3.11051	H	-2.62530	3.51869	-1.019378
H	3.90317	0.83176	0.21467	H	5.03373	-0.67770	-1.814488
H	3.88085	0.89296	-1.56410	H	5.89840	-0.38685	-0.288177
H	3.36438	2.30964	-0.61830	H	5.30144	-2.00772	-0.664482

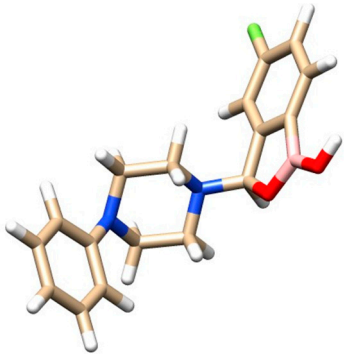


Figure S29. Structure 15-*R*

Table S29. Coordinates of structure 15-*R*

Coordinates of the input structure				Coordinates of the optimized structure			
O	0.33719	-1.93804	1.36751	O	1.22411	1.87576	0.75673
B	-0.44755	-2.98004	2.06026	B	2.24868	2.29991	-0.04918
C	-1.41164	-2.20831	3.02388	C	3.21345	1.09869	-0.30839
C	-1.12878	-0.85910	2.85315	C	2.64638	0.03241	0.39427
C	-0.00750	-0.63794	1.85007	C	1.40549	0.47698	1.14208
C	-2.37163	-2.69051	3.90401	C	4.39076	0.88792	-1.02643
C	-3.07170	-1.73180	4.64428	C	4.98103	-0.36962	-1.03773
C	-2.81058	-0.36216	4.49361	C	4.37720	-1.40085	-0.32786
C	-1.83134	0.08636	3.59795	C	3.20978	-1.23444	0.39901
N	-0.41568	0.28869	0.80416	N	0.25005	-0.33504	0.93460
C	-0.96507	-0.36900	-0.37597	C	-0.22234	-0.42037	-0.45287
C	-1.49527	0.64460	-1.40353	C	-1.31230	-1.49050	-0.56991
C	0.64436	1.22792	0.46813	C	-0.85360	-0.02970	1.85406
C	0.15883	2.29733	-0.52171	C	-1.93427	-1.10270	1.71557
N	-0.43324	1.60572	-1.65364	N	-2.41878	-1.23528	0.34901
C	0.25391	1.56887	-2.81863	C	-3.56993	-0.56429	-0.08590
C	-0.13666	2.39065	-3.87891	C	-4.13511	-0.87006	-1.33842
C	0.58737	2.37235	-5.07453	C	-5.29870	-0.25468	-1.77051
C	1.70270	1.54218	-5.20962	C	-5.95538	0.67689	-0.97188
C	2.08818	0.71710	-4.15179	C	-5.41532	0.98086	0.26991
C	1.36290	0.72881	-2.95928	C	-4.23989	0.38188	0.70772
O	-0.47191	-4.41197	1.75469	O	2.27659	3.58904	-0.47470
H	-1.00711	3.06146	-3.77317	H	-3.67710	-1.62372	-1.96565
H	-2.56024	-3.77082	4.01569	H	4.85932	1.69317	-1.58301
H	-3.83978	-2.06117	5.36394	H	5.89371	-0.57121	-1.58364
F	-3.48719	0.51653	5.21547	F	4.95596	-2.61794	-0.35128
H	-1.61045	1.16069	3.48800	H	2.76911	-2.06748	0.93181
H	-1.80552	-1.03424	-0.06700	H	0.61855	-0.68699	-1.09575
H	-0.18659	-1.00225	-0.86476	H	-0.62247	0.54352	-0.79833
H	-2.37748	1.19062	-0.99121	H	-0.87998	-2.46981	-0.33642
H	-1.81891	0.13724	-2.34351	H	-1.67391	-1.52255	-1.59433
H	1.52349	0.67742	0.05742	H	-1.27530	0.96566	1.65535
H	0.98229	1.75343	1.39231	H	-0.46239	-0.03191	2.87512
H	0.99610	2.96454	-0.83744	H	-2.76617	-0.90941	2.39006
H	-0.62485	2.93718	-0.05006	H	-1.49704	-2.06525	2.00580
H	0.28707	3.02617	-5.91144	H	-5.70567	-0.52111	-2.73954
H	2.28288	1.54126	-6.14741	H	-6.86742	1.15182	-1.31094
H	2.97312	0.06481	-4.25338	H	-5.90176	1.70855	0.90977
H	1.68735	0.07699	-2.13272	H	-3.83664	0.67604	1.66653
H	-1.06372	-4.98115	2.21798	H	3.03089	3.78514	-1.03622
H	0.85063	-0.24620	2.40238	H	1.59933	0.49095	2.21901

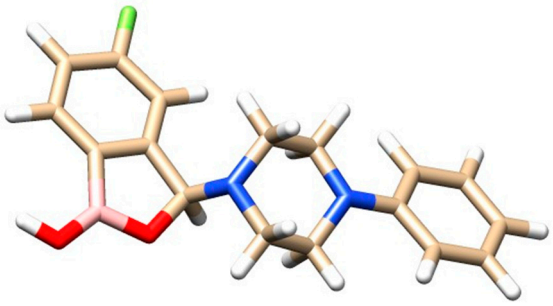


Figure S30. Structure 15-*S*

Table S30. Coordinates of structure 15-*S*

Coordinates of the input structure	Coordinates of the optimized structure
O -1.49341 -2.56223 0.84771	O -2.02243 -2.08905 -0.56496
B -1.75579 -3.12259 2.18617	B -3.36946 -1.93765 -0.35801
C -1.90867 -1.87206 3.11551	C -3.66699 -0.42303 -0.14284
C -1.64412 -0.75952 2.32423	C -2.41669 0.20236 -0.21587
C -1.25299 -1.15482 0.90178	C -1.32337 -0.84305 -0.38279
C -2.31530 -1.80994 4.44207	C -4.81789 0.35191 -0.01365
C -2.47331 -0.53217 4.98645	C -4.72503 1.73730 0.02702
C -2.25789 0.61298 4.20843	C -3.47082 2.32088 -0.08274
C -1.86809 0.50556 2.86779	C -2.30232 1.58622 -0.21158
N 0.15406 -0.92196 0.59866	N -0.45560 -1.01795 0.77261
C 0.56133 -1.47188 -0.69023	C 0.57946 -2.03762 0.55958
C -0.04357 -0.71388 -1.88325	C 1.80472 -1.51388 -0.19179
C 0.59487 0.46296 0.67536	C 0.14636 0.15537 1.39798
C -0.02910 1.34787 -0.41355	C 1.36907 0.71490 0.66027
N 0.21953 0.70375 -1.69351	N 2.36635 -0.33273 0.47816
C 0.51956 1.46713 -2.76627	C 3.66842 0.05744 0.09995
C -0.50553 2.03520 -3.52562	C 3.99106 1.37972 -0.23645
C -0.18818 2.82377 -4.63337	C 5.29747 1.73577 -0.55824
C 1.14796 3.04095 -4.97698	C 6.31187 0.79018 -0.56768
C 2.16970 2.47072 -4.21447	C 6.00228 -0.52700 -0.23754
C 1.85698 1.68157 -3.10582	C 4.70776 -0.88872 0.09563
O -2.28978 -4.45970 2.45855	O -4.17706 -3.02596 -0.41370
H -1.56111 1.86416 -3.25465	H 3.22375 2.14056 -0.26228
H -1.94401 -0.67697 0.17144	H -0.77441 -0.67400 -1.32116
H -2.52958 -2.72266 5.02174	H -5.79776 -0.11099 0.04283
H -2.80564 -0.42596 6.03257	H -5.59687 2.37141 0.12285
F -2.45680 1.80937 4.73760	F -3.38299 3.66593 -0.07176
H -1.75505 1.41202 2.25215	H -1.36070 2.10932 -0.31663
H 0.30394 -2.55471 -0.74992	H 0.13991 -2.87862 0.02597
H 1.67477 -1.43540 -0.75536	H 0.89614 -2.39438 1.54433
H -1.14318 -0.87418 -1.96742	H 1.53961 -1.26940 -1.23427
H 0.42081 -1.07849 -2.83049	H 2.55459 -2.30119 -0.23480
H 1.70578 0.48653 0.57224	H 0.47111 -0.15213 2.39724
H 0.40851 0.87518 1.69106	H -0.60101 0.93432 1.53352
H 0.43373 2.36302 -0.38277	H 1.80306 1.51320 1.26496
H -1.12740 1.47288 -0.27283	H 1.06458 1.16122 -0.30380
H -0.99340 3.27538 -5.23707	H 5.51394 2.76677 -0.81445
H 1.39673 3.66432 -5.85240	H 7.32650 1.07084 -0.82174
H 3.22425 2.64382 -4.48781	H 6.78157 -1.28052 -0.22511
H 2.66383 1.23119 -2.50312	H 4.50263 -1.91059 0.38757
H -2.60685 -4.67218 3.31978	H -5.10387 -2.81861 -0.27052

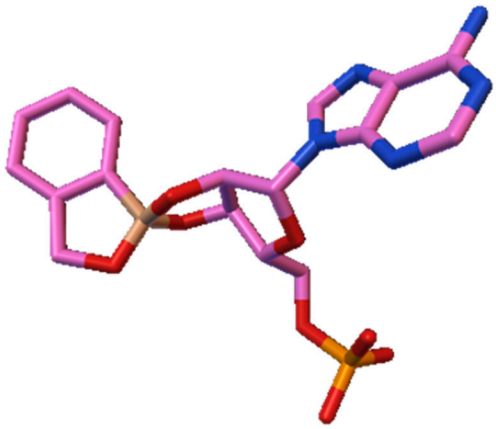


Figure S31. The best structure obtained in the docking studies of 1-AMP-1.

Table S31. Coordinates of the best 1-AMP-1 spiroester.

C	*25.619*	*59.456*	*11.385*
C	*26.700*	*58.588*	*11.532*
C	*27.282*	*58.026*	*10.402*
C	*26.787*	*58.324*	*9.130*
C	*25.708*	*59.187*	*8.971*
C	*25.135*	*59.746*	*10.106*
O	*23.784*	*60.965*	*11.599*
C	*23.970*	*60.699*	*10.198*
C	*23.793*	*60.520*	*15.364*
O	*24.690*	*61.382*	*16.075*
C	*24.635*	*59.552*	*14.546*
O	*24.130*	*59.324*	*13.237*
C	*25.900*	*60.340*	*14.350*
O	*25.681*	*60.979*	*13.109*
C	*25.991*	*61.310*	*15.526*
B	*24.720*	*60.269*	*12.348*
N	*26.930*	*60.791*	*16.551*
C	*27.394*	*59.526*	*16.632*
N	*28.232*	*59.403*	*17.684*
C	*28.294*	*60.616*	*18.284*
C	*28.995*	*61.163*	*19.451*
C	*27.429*	*61.515*	*17.550*
N	*29.814*	*60.363*	*20.179*
N	*28.800*	*62.461*	*19.759*
C	*27.985*	*63.244*	*19.026*
N	*27.306*	*62.803*	*17.955*
C	*22.894*	*59.871*	*16.405*
O	*21.647*	*60.589*	*16.384*
P	*21.302*	*61.692*	*17.520*
O	*20.201*	*62.485*	*16.852*
O	*22.563*	*62.473*	*17.768*
O	*20.824*	*60.783*	*18.641*

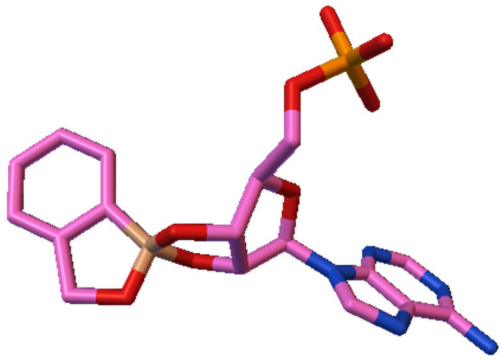


Figure S32. The best structure obtained in the docking studies of 1-AMP-2.

Table S32. Coordinates of the best 1-AMP-2 spiroester.

C	*24.736*	*60.551*	*11.023*
C	*23.784*	*61.568*	*10.986*
C	*23.323*	*62.026*	*9.757*
C	*23.809*	*61.474*	*8.569*
C	*24.759*	*60.459*	*8.593*
C	*25.213*	*60.008*	*9.825*
O	*26.334*	*58.859*	*11.549*
C	*26.228*	*58.932*	*10.117*
C	*24.164*	*60.507*	*14.905*
O	*25.048*	*61.342*	*15.662*
C	*24.986*	*59.356*	*14.341*
O	*24.659*	*59.029*	*12.997*
C	*26.358*	*59.966*	*14.277*
O	*26.416*	*60.469*	*12.958*
C	*26.397*	*61.056*	*15.346*
B	*25.497*	*59.785*	*12.125*
N	*27.093*	*60.564*	*16.560*
C	*27.189*	*59.275*	*16.951*
N	*27.895*	*59.187*	*18.099*
C	*28.248*	*60.449*	*18.443*
C	*28.998*	*61.052*	*19.551*
C	*27.708*	*61.346*	*17.445*
N	*29.521*	*60.257*	*20.520*
N	*29.145*	*62.392*	*19.565*
C	*28.622*	*63.167*	*18.596*
N	*27.915*	*62.681*	*17.562*
C	*23.041*	*60.096*	*15.844*
O	*22.127*	*61.205*	*15.911*
P	*21.890*	*62.007*	*17.299*
O	*21.045*	*63.173*	*16.839*
O	*23.249*	*62.394*	*17.817*
O	*21.127*	*60.957*	*18.090*

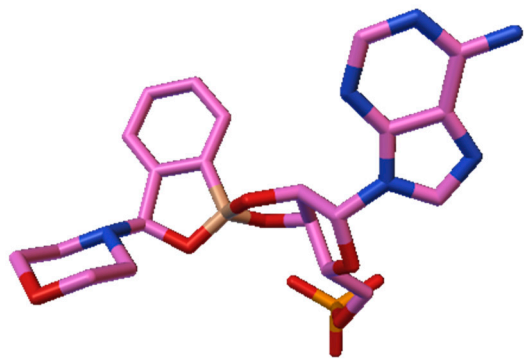


Figure S33. The best structure obtained in the docking studies of 2-R-1-AMP.

Table S33. Coordinates of the best 2-R-1-AMP spiroester.

C	*27.815*	*63.150*	*15.090*
C	*28.829*	*64.100*	*15.152*
C	*29.636*	*64.192*	*16.285*
C	*29.462*	*63.323*	*17.359*
C	*28.473*	*62.349*	*17.275*
O	*26.826*	*60.753*	*17.802*
C	*28.054*	*61.317*	*18.312*
C	*27.632*	*62.277*	*16.159*
C	*23.767*	*60.010*	*15.612*
O	*23.973*	*59.000*	*14.616*
C	*24.634*	*61.205*	*15.241*
O	*25.283*	*61.804*	*16.355*
C	*25.731*	*60.552*	*14.448*
O	*26.723*	*60.313*	*15.425*
C	*25.136*	*59.275*	*13.859*
B	*26.559*	*61.192*	*16.524*
N	*28.979*	*60.211*	*18.517*
C	*28.312*	*58.925*	*18.261*
C	*29.317*	*57.786*	*18.310*
O	*29.969*	*57.774*	*19.619*
C	*30.658*	*59.040*	*19.856*
C	*29.656*	*60.188*	*19.814*
C	*22.272*	*60.285*	*15.652*
O	*21.939*	*60.575*	*17.022*
P	*21.468*	*62.060*	*17.467*
O	*20.519*	*61.752*	*18.603*
O	*20.812*	*62.688*	*16.268*
O	*22.800*	*62.644*	*17.908*
N	*24.762*	*59.487*	*12.440*
C	*23.524*	*59.356*	*11.918*
N	*23.543*	*59.627*	*10.595*
C	*24.824*	*59.930*	*10.273*
C	*25.524*	*60.303*	*9.039*
C	*25.619*	*59.820*	*11.477*
N	*24.828*	*60.414*	*7.878*
N	*26.851*	*60.529*	*9.103*
C	*27.528*	*60.417*	*10.262*
N	*26.951*	*60.068*	*11.424*

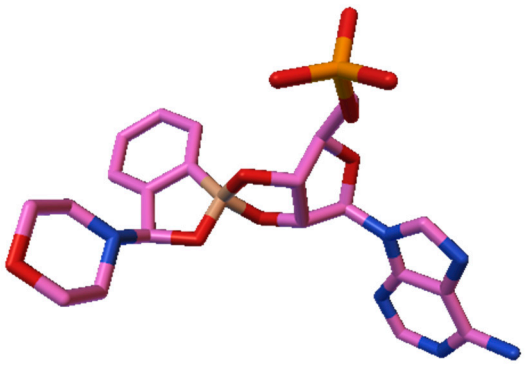


Figure S34. The best structure obtained in the docking studies of 2-R-2-AMP.

Table S34. Coordinates of the best 2-R-2-AMP spiroester.

C	*27.847*	*59.883*	*18.682*
C	*28.745*	*59.677*	*19.724*
C	*29.781*	*60.584*	*19.947*
C	*29.921*	*61.719*	*19.152*
C	*28.997*	*61.939*	*18.137*
O	*27.946*	*62.656*	*16.157*
C	*28.948*	*63.065*	*17.113*
C	*27.977*	*61.014*	*17.881*
C	*24.699*	*59.754*	*16.126*
O	*24.941*	*58.828*	*15.060*
C	*25.201*	*61.118*	*15.674*
O	*25.889*	*61.836*	*16.690*
C	*26.257*	*60.738*	*14.674*
O	*27.434*	*60.718*	*15.454*
C	*25.863*	*59.366*	*14.131*
B	*27.278*	*61.525*	*16.608*
N	*28.544*	*64.369*	*17.621*
C	*29.084*	*65.444*	*16.775*
C	*28.526*	*66.791*	*17.205*
O	*28.866*	*67.025*	*18.609*
C	*28.301*	*65.974*	*19.452*
C	*28.859*	*64.620*	*19.028*
C	*23.211*	*59.685*	*16.434*
O	*22.668*	*60.989*	*16.160*
P	*21.655*	*61.704*	*17.204*
O	*20.576*	*62.219*	*16.279*
O	*22.437*	*62.783*	*17.902*
O	*21.239*	*60.504*	*18.040*
N	*25.206*	*59.503*	*12.809*
C	*23.894*	*59.736*	*12.596*
N	*23.641*	*59.807*	*11.271*
C	*24.820*	*59.608*	*10.633*
C	*25.245*	*59.553*	*9.230*
C	*25.836*	*59.393*	*11.641*
N	*24.332*	*59.741*	*8.243*
N	*26.546*	*59.318*	*8.967*
C	*27.441*	*59.136*	*9.957*
N	*27.116*	*59.162*	*11.260*

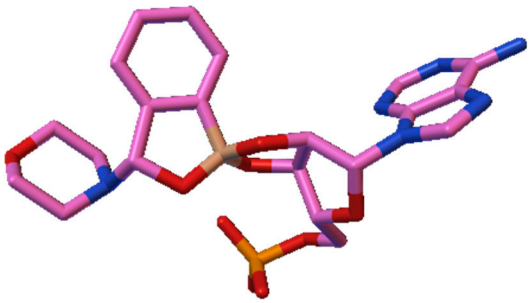


Figure S35. The best structure obtained in the docking studies of 2-S-1-AMP.

Table S35. Coordinates of the best 2-S-1-AMP spiroester.

C	*27.573*	*62.295*	*14.836*
C	*27.597*	*63.331*	*13.905*
C	*28.518*	*64.362*	*14.051*
C	*29.422*	*64.349*	*15.114*
C	*29.404*	*63.321*	*16.053*
C	*28.460*	*62.309*	*15.919*
O	*27.309*	*60.254*	*16.033*
C	*28.266*	*61.063*	*16.770*
C	*24.303*	*59.395*	*13.805*
O	*24.652*	*58.724*	*12.588*
C	*24.854*	*60.812*	*13.725*
O	*25.435*	*61.266*	*14.940*
C	*26.006*	*60.637*	*12.776*
O	*27.096*	*60.412*	*13.646*
C	*25.667*	*59.431*	*11.902*
B	*26.824*	*60.945*	*14.930*
N	*27.706*	*61.270*	*18.090*
C	*28.449*	*60.563*	*19.144*
C	*29.636*	*61.370*	*19.676*
O	*29.155*	*62.669*	*20.155*
C	*28.513*	*63.427*	*19.078*
C	*27.336*	*62.613*	*18.534*
C	*22.791*	*59.299*	*13.939*
O	*22.423*	*60.083*	*15.088*
P	*23.072*	*59.783*	*16.542*
O	*21.844*	*59.748*	*17.424*
O	*24.016*	*60.916*	*16.841*
O	*23.694*	*58.420*	*16.284*
N	*25.151*	*59.878*	*10.585*
C	*25.374*	*59.272*	*9.400*
N	*24.752*	*59.945*	*8.407*
C	*24.128*	*61.003*	*8.978*
C	*23.301*	*62.110*	*8.486*
C	*24.405*	*60.965*	*10.398*
N	*23.014*	*62.199*	*7.162*
N	*22.845*	*63.011*	*9.380*
C	*23.135*	*62.909*	*10.691*
N	*23.896*	*61.928*	*11.205*

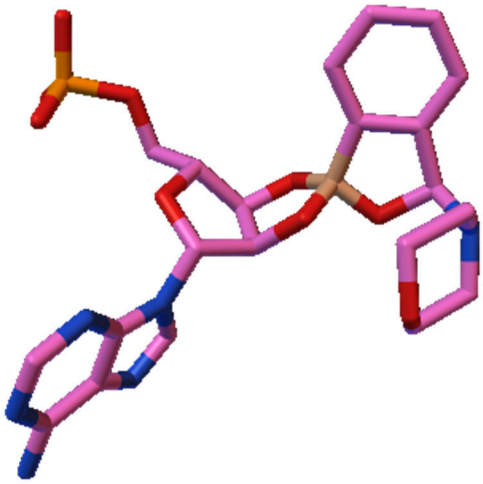


Figure S36. The best structure obtained in the docking studies of 2-S-2-AMP.

Table S36. Coordinates of the best 2-S-2-AMP spiroester.

C	*23.865*	*61.410*	*11.165*
C	*23.234*	*62.617*	*11.459*
C	*22.769*	*63.416*	*10.420*
C	*22.917*	*63.003*	*9.096*
C	*23.551*	*61.801*	*8.791*
C	*24.041*	*61.020*	*9.832*
O	*24.794*	*59.219*	*11.152*
C	*24.719*	*59.659*	*9.770*
C	*23.639*	*60.885*	*15.014*
O	*24.812*	*61.317*	*15.714*
C	*24.009*	*59.639*	*14.221*
O	*23.453*	*59.611*	*12.913*
C	*25.485*	*59.834*	*14.019*
O	*25.547*	*60.480*	*12.764*
C	*25.968*	*60.705*	*15.177*
B	*24.378*	*60.211*	*12.010*
N	*26.072*	*59.641*	*9.254*
C	*26.759*	*60.933*	*9.407*
C	*27.432*	*61.088*	*10.772*
O	*28.361*	*59.973*	*10.977*
C	*27.662*	*58.686*	*10.939*
C	*26.973*	*58.538*	*9.579*
C	*22.555*	*60.685*	*16.061*
O	*21.879*	*61.947*	*16.207*
P	*21.627*	*62.590*	*17.673*
O	*23.042*	*62.782*	*18.170*
O	*20.827*	*61.588*	*18.459*
O	*20.923*	*63.880*	*17.283*
N	*26.612*	*59.868*	*16.218*
C	*26.408*	*58.548*	*16.413*
N	*27.159*	*58.106*	*17.445*
C	*27.848*	*59.173*	*17.916*
C	*28.815*	*59.389*	*18.999*
C	*27.476*	*60.325*	*17.123*
N	*29.195*	*58.345*	*19.778*
N	*29.300*	*60.633*	*19.180*
C	*28.915*	*61.659*	*18.397*
N	*28.027*	*61.532*	*17.398*

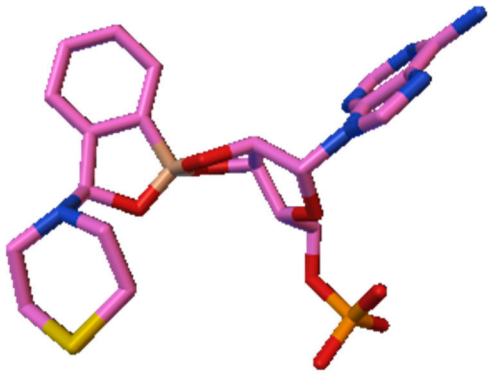


Figure S37. The best structure obtained in the docking studies of 3-R-1-AMP.

Table S37. Coordinates of the best 3-R-1-AMP spiroester.

C	*25.616*	*59.444*	*11.468*
C	*26.670*	*58.560*	*11.689*
C	*27.304*	*57.967*	*10.605*
C	*26.876*	*58.241*	*9.307*
C	*25.826*	*59.125*	*9.072*
C	*25.217*	*59.741*	*10.159*
O	*23.680*	*60.825*	*11.582*
C	*24.030*	*60.694*	*10.179*
C	*23.723*	*60.636*	*15.390*
O	*24.559*	*61.623*	*16.007*
C	*24.627*	*59.677*	*14.629*
O	*24.117*	*59.304*	*13.355*
C	*25.817*	*60.547*	*14.338*
O	*25.522*	*61.064*	*13.057*
C	*25.851*	*61.613*	*15.432*
B	*24.609*	*60.219*	*12.379*
N	*24.276*	*62.035*	*9.683*
C	*24.555*	*63.006*	*10.743*
C	*23.314*	*63.580*	*11.433*
S	*22.204*	*64.450*	*10.258*
C	*22.092*	*63.119*	*9.000*
C	*23.473*	*62.584*	*8.598*
C	*22.902*	*60.002*	*16.502*
O	*21.659*	*60.724*	*16.566*
P	*21.481*	*61.990*	*17.561*
O	*20.680*	*62.943*	*16.702*
O	*22.863*	*62.477*	*17.901*
O	*20.685*	*61.342*	*18.682*
N	*26.849*	*61.256*	*16.469*
C	*27.822*	*62.062*	*16.943*
N	*28.548*	*61.417*	*17.882*
C	*28.025*	*60.173*	*17.998*
C	*28.332*	*58.989*	*18.809*
C	*26.927*	*60.066*	*17.062*
N	*29.356*	*59.031*	*19.699*
N	*27.572*	*57.888*	*18.642*
C	*26.557*	*57.862*	*17.756*
N	*26.232*	*58.906*	*16.975*

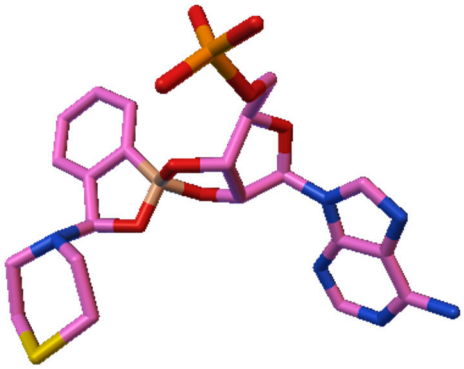


Figure S38. The best structure obtained in the docking studies of 3-R-2-AMP.

Table S38. Coordinates of the best 3-R-2-AMP spiroester.

C	*27.103*	*59.994*	*17.351*
C	*26.685*	*58.784*	*17.898*
C	*27.418*	*58.211*	*18.931*
C	*28.571*	*58.837*	*19.401*
C	*28.997*	*60.049*	*18.864*
C	*28.243*	*60.633*	*17.854*
O	*27.538*	*61.903*	*15.995*
C	*28.513*	*61.911*	*17.072*
C	*23.909*	*59.624*	*15.140*
O	*24.121*	*58.882*	*13.932*
C	*24.643*	*60.950*	*15.001*
O	*25.324*	*61.350*	*16.183*
C	*25.727*	*60.597*	*14.022*
O	*26.807*	*60.247*	*14.863*
C	*25.197*	*59.428*	*13.194*
B	*26.655*	*60.843*	*16.139*
N	*28.330*	*63.155*	*17.794*
C	*27.453*	*64.105*	*17.106*
C	*28.133*	*64.935*	*16.014*
S	*29.520*	*65.944*	*16.670*
C	*30.395*	*64.601*	*17.561*
C	*29.453*	*63.796*	*18.466*
C	*22.404*	*59.736*	*15.324*
O	*22.135*	*61.088*	*15.738*
P	*21.400*	*61.396*	*17.148*
O	*19.966*	*61.592*	*16.710*
O	*22.046*	*62.630*	*17.717*
O	*21.656*	*60.087*	*17.877*
N	*24.700*	*59.908*	*11.882*
C	*23.405*	*60.059*	*11.531*
N	*23.315*	*60.519*	*10.264*
C	*24.581*	*60.656*	*9.803*
C	*25.185*	*61.093*	*8.539*
C	*25.482*	*60.240*	*10.857*
N	*24.387*	*61.488*	*7.514*
N	*26.529*	*61.090*	*8.440*
C	*27.308*	*60.697*	*9.466*
N	*26.821*	*60.275*	*10.644*

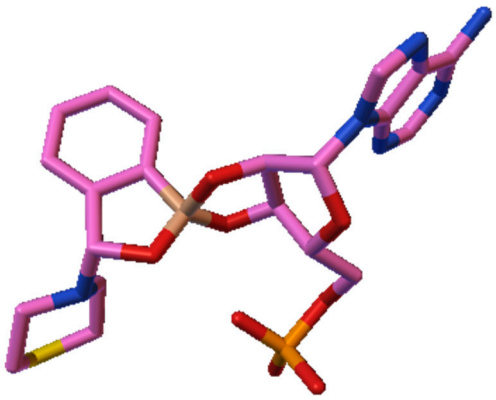


Figure S39. The best structure obtained in the docking studies of 3-S-1-AMP.

Table S39. Coordinates of the best 3-S-1-AMP spiroester.

C	*29.889*	*65.462*	*16.132*
C	*29.323*	*65.019*	*17.324*
C	*28.351*	*64.028*	*17.274*
O	*26.943*	*62.221*	*17.813*
C	*27.620*	*63.342*	*18.422*
C	*25.016*	*60.089*	*15.329*
O	*25.730*	*58.906*	*14.950*
C	*25.772*	*61.284*	*14.767*
O	*25.853*	*62.381*	*15.668*
C	*27.172*	*60.743*	*14.676*
O	*27.741*	*61.139*	*15.907*
C	*27.040*	*59.229*	*14.525*
B	*27.044*	*62.251*	*16.441*
N	*26.602*	*64.132*	*19.104*
C	*27.161*	*64.720*	*20.331*
C	*26.080*	*65.213*	*21.280*
S	*25.064*	*66.546*	*20.549*
C	*24.670*	*65.668*	*18.992*
C	*25.905*	*65.123*	*18.285*
C	*23.595*	*59.924*	*14.812*
O	*22.863*	*61.092*	*15.225*
P	*22.664*	*61.436*	*16.796*
O	*22.240*	*60.095*	*17.352*
O	*21.606*	*62.502*	*16.880*
O	*24.082*	*61.843*	*17.164*
N	*27.208*	*58.835*	*13.105*
C	*28.164*	*58.017*	*12.617*
N	*28.019*	*57.873*	*11.282*
C	*26.951*	*58.622*	*10.918*
C	*26.268*	*58.911*	*9.652*
C	*26.435*	*59.262*	*12.109*
N	*26.713*	*58.343*	*8.503*
N	*25.204*	*59.739*	*9.677*
C	*24.772*	*60.294*	*10.826*
N	*25.358*	*60.081*	*12.015*

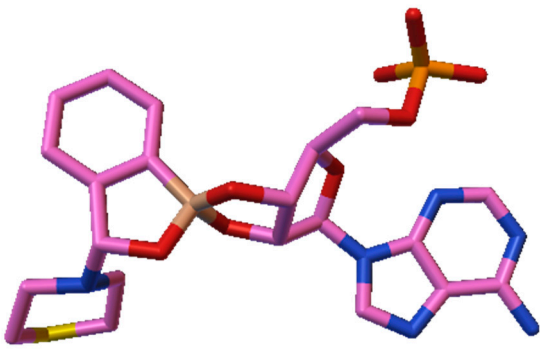


Figure S40. The best structure obtained in the docking studies of 3-S-2-AMP.

Table S40. Coordinates of the best 3-S-2-AMP spiroester.

C	*26.950*	*67.455*	*17.627*
C	*25.592*	*67.405*	*17.324*
C	*24.857*	*68.586*	*17.286*
C	*25.483*	*69.809*	*17.525*
C	*26.840*	*69.869*	*17.831*
C	*27.560*	*68.683*	*17.908*
O	*29.290*	*67.088*	*17.866*
C	*29.045*	*68.478*	*18.173*
C	*26.873*	*63.630*	*16.602*
O	*26.686*	*62.742*	*17.711*
C	*28.262*	*64.239*	*16.727*
O	*28.305*	*65.627*	*16.420*
C	*28.498*	*64.156*	*18.209*
O	*28.056*	*65.416*	*18.668*
C	*27.650*	*62.991*	*18.717*
B	*28.094*	*66.368*	*17.620*
N	*29.495*	*68.693*	*19.544*
C	*29.538*	*70.132*	*19.840*
C	*30.358*	*70.442*	*21.082*
S	*29.657*	*69.681*	*22.591*
C	*29.515*	*67.988*	*21.913*
C	*28.783*	*67.938*	*20.575*
C	*26.641*	*62.809*	*15.343*
O	*26.278*	*61.484*	*15.770*
P	*24.738*	*60.984*	*15.713*
O	*24.159*	*61.633*	*16.949*
O	*24.764*	*59.480*	*15.759*
O	*24.295*	*61.624*	*14.407*
N	*28.490*	*61.784*	*18.904*
C	*29.749*	*61.762*	*19.391*
N	*30.213*	*60.494*	*19.429*
C	*29.227*	*59.698*	*18.949*
C	*29.075*	*58.257*	*18.718*
C	*28.110*	*60.546*	*18.592*
N	*30.094*	*57.415*	*19.029*
N	*27.911*	*57.814*	*18.202*
C	*26.908*	*58.661*	*17.900*
N	*26.987*	*59.990*	*18.075*

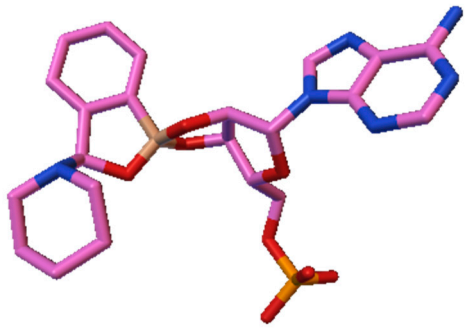


Figure S41. The best structure obtained in the docking studies of 4-R-1-AMP.

Table S41. Coordinates of the best 4-R-1-AMP spiroester.

C	*25.733*	*59.481*	*11.621*
C	*26.743*	*58.534*	*11.770*
C	*27.283*	*57.926*	*10.641*
C	*26.800*	*58.250*	*9.374*
C	*25.793*	*59.197*	*9.213*
C	*25.279*	*59.826*	*10.342*
O	*23.891*	*60.968*	*11.866*
C	*24.156*	*60.847*	*10.443*
C	*23.943*	*60.386*	*15.650*
O	*24.819*	*61.264*	*16.367*
C	*24.806*	*59.477*	*14.786*
O	*24.283*	*59.265*	*13.482*
C	*26.033*	*60.322*	*14.587*
O	*25.762*	*60.986*	*13.371*
C	*26.110*	*61.261*	*15.790*
B	*24.815*	*60.259*	*12.609*
N	*24.457*	*62.178*	*9.957*
C	*24.589*	*63.163*	*11.041*
C	*23.249*	*63.747*	*11.512*
C	*22.468*	*64.336*	*10.332*
C	*22.333*	*63.307*	*9.203*
C	*23.707*	*62.730*	*8.828*
C	*23.094*	*59.671*	*16.690*
O	*21.745*	*60.140*	*16.521*
P	*21.142*	*61.301*	*17.477*
O	*19.880*	*61.683*	*16.736*
O	*22.174*	*62.393*	*17.544*
O	*20.901*	*60.504*	*18.749*
N	*27.091*	*60.753*	*16.779*
C	*27.664*	*59.530*	*16.772*
N	*28.510*	*59.405*	*17.817*
C	*28.467*	*60.572*	*18.502*
C	*29.119*	*61.092*	*19.710*
C	*27.526*	*61.443*	*17.831*
N	*30.005*	*60.316*	*20.383*
N	*28.812*	*62.343*	*20.110*
C	*27.932*	*63.103*	*19.431*
N	*27.293*	*62.683*	*18.327*

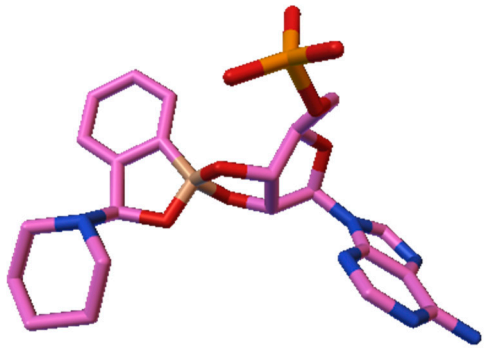


Figure S42. The best structure obtained in the docking studies of 4-R-2-AMP.

Table S42. Coordinates of the best 4-R-2-AMP spiroester.

C	*27.270*	*60.442*	*17.200*
C	*26.894*	*59.261*	*17.836*
C	*27.659*	*58.781*	*18.893*
C	*28.803*	*59.467*	*19.299*
C	*29.186*	*60.649*	*18.672*
C	*28.399*	*61.143*	*17.637*
O	*27.630*	*62.263*	*15.711*
C	*28.622*	*62.371*	*16.767*
C	*24.071*	*59.817*	*15.066*
O	*24.304*	*58.972*	*13.932*
C	*24.765*	*61.145*	*14.801*
O	*25.435*	*61.675*	*15.938*
C	*25.858*	*60.734*	*13.855*
O	*26.949*	*60.497*	*14.721*
C	*25.362*	*59.478*	*13.142*
B	*26.781*	*61.205*	*15.936*
N	*28.413*	*63.654*	*17.408*
C	*27.891*	*64.673*	*16.486*
C	*28.981*	*65.375*	*15.662*
C	*30.058*	*65.968*	*16.577*
C	*30.598*	*64.902*	*17.539*
C	*29.445*	*64.209*	*18.282*
C	*22.564*	*59.901*	*15.245*
O	*22.270*	*61.242*	*15.678*
P	*21.666*	*61.526*	*17.154*
O	*20.307*	*62.100*	*16.823*
O	*22.598*	*62.494*	*17.829*
O	*21.627*	*60.110*	*17.706*
N	*24.850*	*59.818*	*11.792*
C	*24.837*	*58.999*	*10.720*
N	*24.297*	*59.632*	*9.655*
C	*23.968*	*60.881*	*10.064*
C	*23.365*	*62.057*	*9.427*
C	*24.347*	*61.004*	*11.456*
N	*22.997*	*62.000*	*8.122*
N	*23.192*	*63.167*	*10.173*
C	*23.560*	*63.208*	*11.468*
N	*24.128*	*62.172*	*12.107*

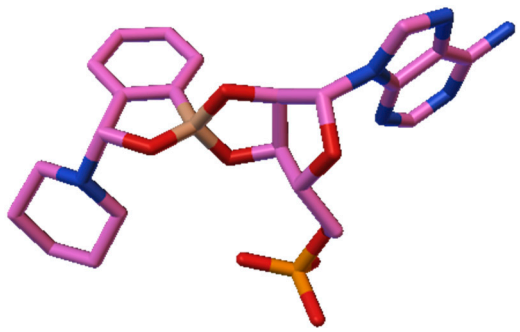


Figure S43. The best structure obtained in the docking studies of 4-S-1-AMP.

Table S43. Coordinates of the best 4-S-1-AMP spiroester.

C	*28.015*	*63.576*	*16.680*
C	*28.139*	*64.157*	*15.420*
C	*28.849*	*65.345*	*15.284*
C	*29.450*	*65.933*	*16.397*
C	*29.330*	*65.361*	*17.660*
C	*28.586*	*64.195*	*17.797*
C	*28.340*	*63.354*	*19.042*
O	*27.739*	*62.135*	*18.553*
C	*25.469*	*59.856*	*16.478*
O	*26.187*	*58.805*	*15.819*
C	*25.903*	*61.174*	*15.852*
O	*26.097*	*62.217*	*16.799*
C	*27.279*	*60.834*	*15.352*
O	*28.109*	*61.231*	*16.424*
C	*27.287*	*59.327*	*15.101*
B	*27.458*	*62.204*	*17.221*
N	*27.425*	*63.916*	*20.025*
C	*27.866*	*65.257*	*20.433*
C	*27.065*	*65.762*	*21.629*
C	*25.566*	*65.764*	*21.322*
C	*25.136*	*64.389*	*20.805*
C	*26.011*	*63.924*	*19.639*
C	*23.990*	*59.531*	*16.334*
O	*23.340*	*60.735*	*15.891*
P	*22.415*	*61.601*	*16.900*
O	*21.649*	*62.480*	*15.936*
O	*23.346*	*62.351*	*17.813*
O	*21.585*	*60.491*	*17.525*
N	*27.112*	*59.044*	*13.656*
C	*27.905*	*58.256*	*12.900*
N	*27.452*	*58.219*	*11.628*
C	*26.350*	*59.005*	*11.579*
C	*25.401*	*59.399*	*10.532*
C	*26.141*	*59.555*	*12.901*
N	*25.553*	*58.918*	*9.271*
N	*24.396*	*60.234*	*10.864*
C	*24.256*	*60.701*	*12.119*
N	*25.096*	*60.390*	*13.121*

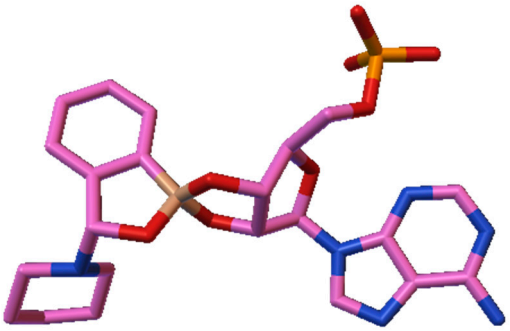


Figure S44. The best structure obtained in the docking studies of 4-S-2-AMP.

Table S44. Coordinates of the best 4-S-2-AMP spiroester.

C	*26.794*	*67.212*	*17.692*
C	*25.419*	*67.126*	*17.495*
C	*24.666*	*68.292*	*17.414*
C	*25.289*	*69.535*	*17.508*
C	*26.663*	*69.633*	*17.707*
C	*27.406*	*68.462*	*17.825*
C	*28.908*	*68.293*	*18.001*
O	*29.149*	*66.884*	*17.793*
C	*26.774*	*63.387*	*16.756*
O	*26.621*	*62.528*	*17.892*
C	*28.156*	*64.020*	*16.839*
O	*28.173*	*65.398*	*16.493*
C	*28.420*	*63.980*	*18.318*
O	*27.968*	*65.247*	*18.750*
C	*27.598*	*62.818*	*18.872*
B	*27.973*	*66.169*	*17.676*
N	*29.444*	*68.629*	*19.312*
C	*29.497*	*70.087*	*19.489*
C	*30.274*	*70.462*	*20.749*
C	*29.666*	*69.795*	*21.983*
C	*29.524*	*68.290*	*21.750*
C	*28.780*	*67.987*	*20.449*
C	*26.531*	*62.529*	*15.524*
O	*25.829*	*61.354*	*15.966*
P	*24.288*	*61.094*	*15.537*
O	*24.278*	*59.597*	*15.324*
O	*24.040*	*61.897*	*14.290*
O	*23.577*	*61.548*	*16.801*
N	*28.460*	*61.628*	*19.077*
C	*29.622*	*61.600*	*19.762*
N	*30.140*	*60.352*	*19.752*
C	*29.288*	*59.577*	*19.039*
C	*29.252*	*58.164*	*18.645*
C	*28.201*	*60.418*	*18.586*
N	*30.249*	*57.331*	*19.037*
N	*28.211*	*57.737*	*17.901*
C	*27.228*	*58.575*	*17.522*
N	*27.207*	*59.880*	*17.837*

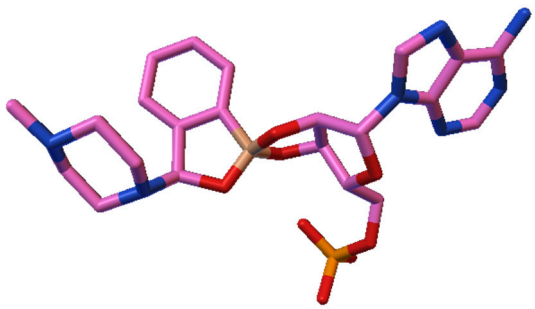


Figure S45. The best structure obtained in the docking studies of 5-R-1-AMP.

Table S45. Coordinates of the best 5-R-1-AMP spiroester.

O	*24.002*	*66.555*	*17.597*
C	*23.290*	*67.992*	*19.367*
C	*24.679*	*68.086*	*19.264*
C	*25.217*	*67.151*	*18.198*
C	*22.624*	*68.754*	*20.327*
C	*23.352*	*69.594*	*21.162*
C	*24.740*	*69.679*	*21.042*
C	*25.417*	*68.923*	*20.089*
C	*20.473*	*65.207*	*17.186*
O	*19.652*	*65.986*	*16.307*
C	*20.758*	*66.052*	*18.420*
O	*22.100*	*65.955*	*18.878*
C	*20.627*	*67.445*	*17.871*
O	*21.956*	*67.767*	*17.516*
C	*19.683*	*67.351*	*16.675*
B	*22.872*	*66.977*	*18.252*
N	*26.118*	*67.742*	*17.278*
C	*27.556*	*67.620*	*17.526*
C	*28.128*	*68.768*	*18.364*
N	*27.797*	*70.055*	*17.752*
C	*26.345*	*70.208*	*17.634*
C	*28.397*	*71.163*	*18.476*
C	*25.776*	*69.075*	*16.777*
C	*19.721*	*63.912*	*17.452*
O	*20.444*	*62.866*	*16.779*
P	*21.706*	*62.137*	*17.486*
O	*22.543*	*61.744*	*16.290*
O	*21.159*	*60.974*	*18.267*
O	*22.272*	*63.298*	*18.288*
N	*18.319*	*67.789*	*17.059*
C	*17.886*	*69.066*	*17.129*
N	*16.590*	*69.100*	*17.507*
C	*16.197*	*67.816*	*17.686*
C	*14.949*	*67.158*	*18.090*
C	*17.334*	*66.964*	*17.408*
N	*13.853*	*67.909*	*18.369*
N	*14.935*	*65.812*	*18.167*
C	*16.030*	*65.080*	*17.886*
N	*17.205*	*65.619*	*17.522*

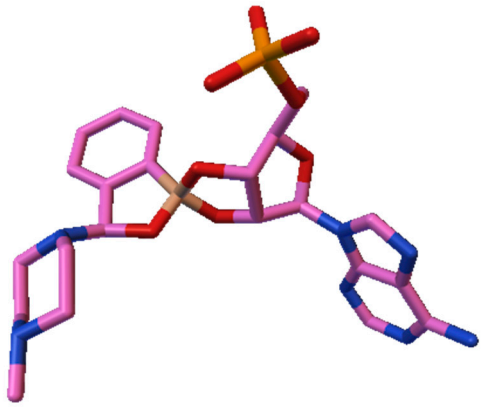


Figure S46. The best structure obtained in the docking studies of 5-R-2-AMP.

Table S46. Coordinates of the best 5-R-2-AMP spiroester.

O	*27.458*	*62.306*	*16.115*
C	*27.451*	*60.315*	*17.434*
C	*28.435*	*61.167*	*17.940*
C	*28.543*	*62.434*	*17.114*
C	*27.239*	*59.081*	*18.047*
C	*28.005*	*58.720*	*19.150*
C	*28.979*	*59.589*	*19.646*
C	*29.205*	*60.823*	*19.043*
C	*24.266*	*59.465*	*15.363*
O	*24.528*	*58.766*	*14.140*
C	*24.776*	*60.890*	*15.199*
O	*25.446*	*61.391*	*16.348*
C	*25.849*	*60.711*	*14.162*
O	*27.013*	*60.534*	*14.944*
C	*25.466*	*59.474*	*13.352*
B	*26.836*	*61.098*	*16.231*
N	*28.541*	*63.641*	*17.856*
C	*27.602*	*64.699*	*17.473*
C	*28.180*	*65.682*	*16.451*
N	*29.444*	*66.235*	*16.937*
C	*30.409*	*65.164*	*17.190*
C	*29.977*	*67.235*	*16.028*
C	*29.843*	*64.194*	*18.229*
C	*22.773*	*59.341*	*15.625*
O	*22.249*	*60.680*	*15.692*
P	*21.574*	*61.242*	*17.053*
O	*20.198*	*61.642*	*16.570*
O	*22.424*	*62.393*	*17.519*
O	*21.594*	*59.983*	*17.904*
N	*24.833*	*59.872*	*12.071*
C	*23.576*	*60.340*	*11.920*
N	*23.331*	*60.606*	*10.619*
C	*24.456*	*60.294*	*9.933*
C	*24.858*	*60.336*	*8.522*
C	*25.429*	*59.799*	*10.883*
N	*23.983*	*60.786*	*7.587*
N	*26.102*	*59.925*	*8.202*
C	*26.960*	*59.483*	*9.141*
N	*26.651*	*59.408*	*10.446*

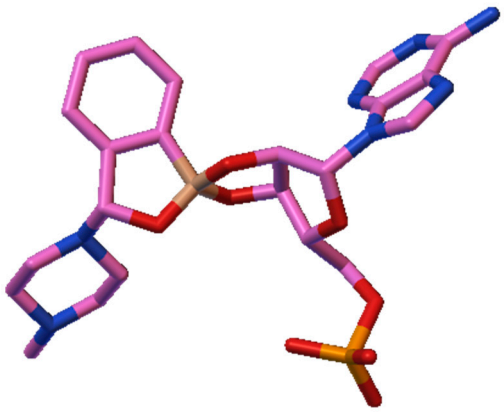


Figure S47. The best structure obtained in the docking studies of 5-S-1-AMP.

Table S47. Coordinates of the best 5-S-1-AMP spiroester.

O	*39.300*	*51.240*	*-0.771*
C	*37.530*	*51.777*	*0.726*
C	*38.730*	*52.237*	*1.281*
C	*39.900*	*51.817*	*0.401*
C	*36.321*	*52.065*	*1.356*
C	*36.316*	*52.823*	*2.522*
C	*37.514*	*53.309*	*3.042*
C	*38.730*	*53.027*	*2.423*
C	*36.891*	*49.412*	*-3.122*
O	*36.134*	*50.251*	*-4.004*
C	*36.412*	*49.684*	*-1.703*
O	*37.465*	*49.752*	*-0.750*
C	*35.895*	*51.091*	*-1.820*
O	*37.013*	*51.867*	*-1.442*
C	*35.488*	*51.280*	*-3.280*
B	*37.900*	*51.105*	*-0.644*
N	*40.783*	*50.809*	*0.973*
C	*40.778*	*49.591*	*0.153*
C	*41.587*	*48.492*	*0.823*
N	*42.959*	*48.932*	*1.053*
C	*42.963*	*50.140*	*1.866*
C	*43.776*	*47.883*	*1.636*
C	*42.157*	*51.251*	*1.203*
C	*36.697*	*47.983*	*-3.605*
O	*36.879*	*47.997*	*-5.032*
P	*38.357*	*48.136*	*-5.681*
O	*38.141*	*49.228*	*-6.704*
O	*38.702*	*46.796*	*-6.272*
O	*39.148*	*48.573*	*-4.459*
N	*34.019*	*51.138*	*-3.428*
C	*33.263*	*51.692*	*-4.399*
N	*31.966*	*51.353*	*-4.232*
C	*31.901*	*50.573*	*-3.127*
C	*30.826*	*49.889*	*-2.399*
C	*33.242*	*50.449*	*-2.595*
N	*29.548*	*49.977*	*-2.850*
N	*31.150*	*49.185*	*-1.296*
C	*32.423*	*49.105*	*-0.863*
N	*33.451*	*49.716*	*-1.474*

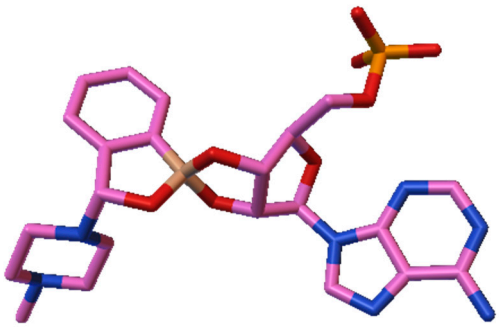


Figure S48. The best structure obtained in the docking studies of 5-S-2-AMP.

Table S48. Coordinates of the best 5-S-2-AMP spiroester.

O	*28.986*	*66.760*	*17.566*
C	*26.630*	*67.094*	*17.601*
C	*27.252*	*68.347*	*17.539*
C	*28.763*	*68.178*	*17.622*
C	*25.243*	*67.006*	*17.522*
C	*24.488*	*68.162*	*17.364*
C	*25.119*	*69.400*	*17.263*
C	*26.506*	*69.503*	*17.342*
C	*26.535*	*63.224*	*16.867*
O	*26.465*	*62.405*	*18.040*
C	*27.911*	*63.874*	*16.839*
O	*27.888*	*65.239*	*16.444*
C	*28.269*	*63.890*	*18.299*
O	*27.830*	*65.167*	*18.714*
C	*27.499*	*62.740*	*18.945*
B	*27.755*	*66.050*	*17.610*
N	*29.380*	*68.663*	*18.851*
C	*29.412*	*70.132*	*18.867*
C	*30.179*	*70.634*	*20.079*
N	*29.577*	*70.136*	*21.312*
C	*29.544*	*68.680*	*21.293*
C	*30.249*	*70.649*	*22.493*
C	*28.775*	*68.163*	*20.084*
C	*26.225*	*62.320*	*15.684*
O	*25.531*	*61.173*	*16.207*
P	*23.984*	*60.888*	*15.821*
O	*23.262*	*61.414*	*17.041*
O	*23.850*	*59.404*	*15.616*
O	*23.848*	*61.768*	*14.588*
N	*28.387*	*61.568*	*19.136*
C	*29.542*	*61.553*	*19.834*
N	*30.090*	*60.319*	*19.804*
C	*29.265*	*59.539*	*19.066*
C	*29.267*	*58.133*	*18.644*
C	*28.163*	*60.362*	*18.617*
N	*30.280*	*57.317*	*19.030*
N	*28.246*	*57.697*	*17.879*
C	*27.247*	*58.518*	*17.505*
N	*27.190*	*59.816*	*17.847*

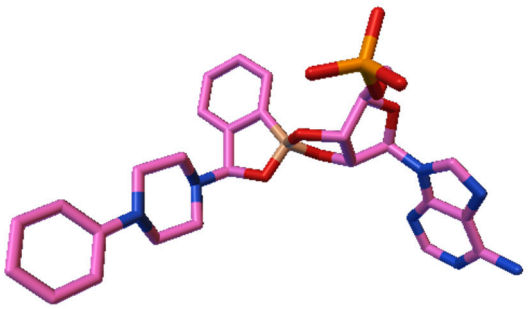


Figure S49. The best structure obtained in the docking studies of 6-R-1-AMP.

Table S49. Coordinates of the best 6-R-1-AMP spiroester.

O	*28.074*	*62.503*	*16.091*
C	*27.947*	*60.813*	*17.773*
C	*29.021*	*61.651*	*18.077*
C	*29.191*	*62.720*	*17.014*
C	*27.657*	*59.744*	*18.619*
C	*28.440*	*59.531*	*19.749*
C	*29.507*	*60.382*	*20.037*
C	*29.810*	*61.452*	*19.201*
C	*24.605*	*59.816*	*16.028*
O	*24.745*	*58.853*	*14.976*
C	*25.219*	*61.122*	*15.542*
O	*25.986*	*61.793*	*16.532*
C	*26.218*	*60.632*	*14.532*
O	*27.403*	*60.521*	*15.293*
C	*25.694*	*59.290*	*14.023*
B	*27.340*	*61.359*	*16.434*
N	*29.276*	*64.055*	*17.510*
C	*28.289*	*64.420*	*18.528*
C	*28.642*	*65.771*	*19.145*
N	*28.729*	*66.797*	*18.114*
C	*29.685*	*66.425*	*17.067*
C	*29.326*	*65.076*	*16.462*
C	*28.717*	*68.147*	*18.521*
C	*28.729*	*69.210*	*17.607*
C	*28.766*	*70.529*	*18.048*
C	*28.775*	*70.827*	*19.402*
C	*28.759*	*69.780*	*20.320*
C	*28.736*	*68.462*	*19.891*
C	*23.123*	*59.885*	*16.361*
O	*22.722*	*61.257*	*16.196*
P	*21.733*	*61.970*	*17.264*
O	*20.689*	*62.578*	*16.355*
O	*22.558*	*62.976*	*18.019*
O	*21.253*	*60.754*	*18.039*
N	*25.029*	*59.462*	*12.708*
C	*23.699*	*59.568*	*12.501*
N	*23.442*	*59.718*	*11.183*
C	*24.637*	*59.701*	*10.544*
C	*25.068*	*59.806*	*9.146*
C	*25.669*	*59.517*	*11.542*
N	*24.142*	*59.974*	*8.167*
N	*26.388*	*59.737*	*8.879*
C	*27.295*	*59.573*	*9.860*
N	*26.967*	*59.458*	*11.158*

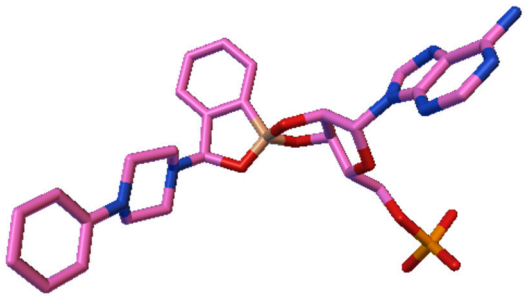


Figure S50. The best structure obtained in the docking studies of 6-R-2-AMP.

Table S50. Coordinates of the best 6-R-2-AMP spiroester.

O	*25.844*	*61.752*	*16.963*
C	*27.790*	*61.462*	*18.316*
C	*27.497*	*60.240*	*17.707*
C	*26.236*	*60.344*	*16.872*
C	*28.899*	*61.555*	*19.157*
C	*29.691*	*60.432*	*19.373*
C	*29.383*	*59.221*	*18.751*
C	*28.279*	*59.114*	*17.912*
C	*25.261*	*65.259*	*18.312*
O	*25.941*	*66.296*	*17.595*
C	*26.316*	*64.410*	*19.007*
O	*26.055*	*63.014*	*18.944*
C	*27.513*	*64.629*	*18.125*
O	*27.438*	*63.546*	*17.222*
C	*27.316*	*65.990*	*17.460*
B	*26.688*	*62.483*	*17.782*
N	*26.359*	*59.867*	*15.533*
C	*27.392*	*60.512*	*14.720*
C	*27.586*	*59.752*	*13.412*
N	*26.329*	*59.663*	*12.680*
C	*25.275*	*59.055*	*13.496*
C	*25.092*	*59.818*	*14.800*
C	*26.379*	*59.295*	*11.320*
C	*25.241*	*59.280*	*10.500*
C	*25.322*	*58.865*	*9.174*
C	*26.533*	*58.469*	*8.625*
C	*27.670*	*58.484*	*9.428*
C	*27.597*	*58.883*	*10.753*
C	*24.272*	*65.946*	*19.240*
O	*23.526*	*64.907*	*19.899*
P	*22.720*	*63.791*	*19.043*
O	*22.030*	*63.007*	*20.136*
O	*23.746*	*63.006*	*18.273*
O	*21.793*	*64.688*	*18.238*
N	*28.121*	*67.024*	*18.155*
C	*28.823*	*68.013*	*17.562*
N	*29.435*	*68.775*	*18.494*
C	*29.116*	*68.253*	*19.702*
C	*29.441*	*68.583*	*21.095*
C	*28.272*	*67.100*	*19.475*
N	*30.234*	*69.650*	*21.365*
N	*28.929*	*67.804*	*22.069*
C	*28.142*	*66.749*	*21.786*
N	*27.816*	*66.386*	*20.534*

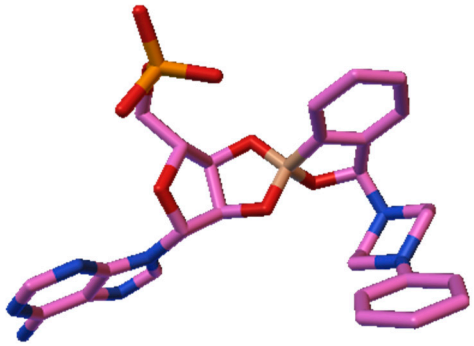


Figure S51. The best structure obtained in the docking studies of 6-S-1-AMP.

Table S51. Coordinates of the best 6-S-1-AMP spiroester.

O	*27.592*	*61.271*	*15.657*
C	*25.230*	*61.031*	*15.822*
C	*25.732*	*59.942*	*15.100*
C	*27.228*	*60.110*	*14.882*
C	*23.879*	*61.074*	*16.157*
C	*23.044*	*60.025*	*15.786*
C	*23.563*	*58.929*	*15.101*
C	*24.911*	*58.875*	*14.757*
C	*25.557*	*64.034*	*18.338*
O	*25.553*	*65.342*	*17.752*
C	*26.864*	*63.358*	*17.949*
O	*26.714*	*61.990*	*17.593*
C	*27.202*	*64.065*	*16.666*
O	*26.636*	*63.221*	*15.685*
C	*26.539*	*65.439*	*16.743*
B	*26.489*	*61.905*	*16.188*
N	*27.630*	*60.385*	*13.512*
C	*26.785*	*59.709*	*12.520*
C	*25.499*	*60.471*	*12.198*
N	*25.797*	*61.846*	*11.776*
C	*26.594*	*62.557*	*12.768*
C	*27.866*	*61.761*	*13.090*
C	*24.760*	*62.555*	*11.132*
C	*23.971*	*61.988*	*10.123*
C	*22.927*	*62.705*	*9.545*
C	*22.648*	*64.004*	*9.943*
C	*23.427*	*64.578*	*10.945*
C	*24.460*	*63.868*	*11.534*
C	*25.350*	*64.225*	*19.832*
O	*24.127*	*63.548*	*20.174*
P	*22.764*	*63.825*	*19.343*
O	*21.707*	*63.493*	*20.372*
O	*22.780*	*62.902*	*18.155*
O	*22.916*	*65.311*	*19.063*
N	*27.534*	*66.471*	*17.123*
C	*28.875*	*66.314*	*17.132*
N	*29.476*	*67.458*	*17.528*
C	*28.492*	*68.354*	*17.779*
C	*28.450*	*69.748*	*18.236*
C	*27.225*	*67.700*	*17.530*
N	*29.608*	*70.408*	*18.491*
N	*27.244*	*70.332*	*18.385*
C	*26.102*	*69.665*	*18.126*
N	*26.071*	*68.386*	*17.717*

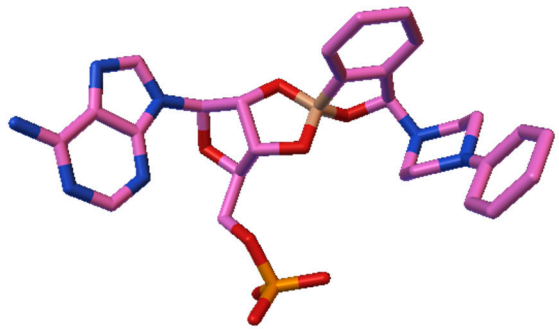


Figure S52. The best structure obtained in the docking studies of 6-S-2-AMP.

Table S52. Coordinates of the best 6-S-2-AMP spiroester.

O	*27.552*	*61.938*	*18.344*
C	*28.292*	*63.359*	*16.584*
C	*28.761*	*63.882*	*17.795*
C	*28.223*	*63.059*	*18.956*
C	*28.682*	*63.945*	*15.382*
C	*29.547*	*65.032*	*15.395*
C	*30.038*	*65.520*	*16.604*
C	*29.654*	*64.946*	*17.813*
C	*25.210*	*60.033*	*16.091*
O	*25.809*	*58.933*	*15.395*
C	*25.812*	*61.315*	*15.533*
O	*26.111*	*62.284*	*16.529*
C	*27.147*	*60.834*	*15.037*
O	*27.997*	*61.079*	*16.138*
C	*26.978*	*59.349*	*14.717*
B	*27.452*	*62.088*	*16.970*
N	*27.235*	*63.730*	*19.788*
C	*27.764*	*64.926*	*20.452*
C	*27.732*	*66.175*	*19.570*
N	*26.376*	*66.421*	*19.059*
C	*25.847*	*65.261*	*18.349*
C	*25.912*	*64.019*	*19.246*
C	*26.118*	*67.698*	*18.519*
C	*27.050*	*68.743*	*18.577*
C	*26.776*	*69.976*	*17.991*
C	*25.571*	*70.208*	*17.347*
C	*24.636*	*69.176*	*17.286*
C	*24.903*	*67.943*	*17.855*
C	*23.706*	*59.896*	*15.912*
O	*23.155*	*61.223*	*15.982*
P	*21.929*	*61.564*	*16.985*
O	*20.874*	*62.057*	*16.021*
O	*22.427*	*62.610*	*17.945*
O	*21.656*	*60.181*	*17.555*
N	*26.798*	*59.154*	*13.258*
C	*27.775*	*58.877*	*12.369*
N	*27.257*	*58.759*	*11.127*
C	*25.924*	*58.972*	*11.234*
C	*24.797*	*58.998*	*10.294*
C	*25.631*	*59.246*	*12.625*
N	*25.015*	*58.754*	*8.977*
N	*23.567*	*59.261*	*10.781*
C	*23.366*	*59.499*	*12.091*
N	*24.354*	*59.503*	*13.001*

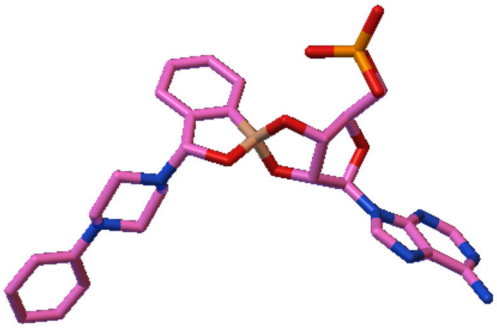


Figure S53. The best structure obtained in the docking studies of 6-S-c-1-AMP.

Table S73. Coordinates of the best 6-S-c-1-AMP spiroester.

O	*35.678*	*48.187*	*-0.683*
C	*37.049*	*49.642*	*0.561*
C	*36.663*	*48.189*	*0.400*
C	*36.330*	*50.455*	*-0.308*
C	*38.017*	*50.146*	*1.415*
C	*36.588*	*51.826*	*-0.300*
C	*37.564*	*52.336*	*0.535*
C	*38.276*	*51.506*	*1.380*
C	*34.204*	*51.287*	*-3.447*
O	*32.830*	*51.565*	*-3.149*
C	*34.439*	*49.804*	*-3.198*
O	*35.673*	*49.524*	*-2.550*
C	*33.379*	*49.495*	*-2.178*
O	*34.062*	*49.666*	*-0.954*
C	*32.260*	*50.512*	*-2.398*
B	*35.459*	*49.517*	*-1.141*
N	*36.162*	*47.604*	*1.615*
C	*35.443*	*48.538*	*2.482*
C	*34.753*	*47.772*	*3.596*
N	*35.762*	*47.070*	*4.405*
C	*36.530*	*46.149*	*3.536*
C	*37.175*	*46.890*	*2.389*
C	*35.269*	*46.399*	*5.575*
C	*34.034*	*46.655*	*6.150*
C	*33.629*	*45.960*	*7.288*
C	*34.443*	*45.009*	*7.856*
C	*35.675*	*44.752*	*7.295*
C	*36.086*	*45.435*	*6.164*
C	*34.442*	*51.745*	*-4.877*
O	*35.866*	*51.734*	*-5.087*
P	*36.595*	*50.460*	*-5.774*
O	*37.423*	*49.927*	*-4.627*
O	*37.404*	*50.989*	*-6.927*
O	*35.383*	*49.609*	*-6.117*
N	*31.151*	*49.900*	*-3.170*
C	*31.114*	*48.634*	*-3.636*
N	*29.954*	*48.411*	*-4.292*
C	*29.246*	*49.564*	*-4.243*
C	*27.940*	*50.003*	*-4.748*
C	*30.038*	*50.539*	*-3.524*
N	*27.157*	*49.132*	*-5.435*
N	*27.557*	*51.273*	*-4.505*
C	*28.343*	*52.125*	*-3.820*
N	*29.553*	*51.791*	*-3.341*

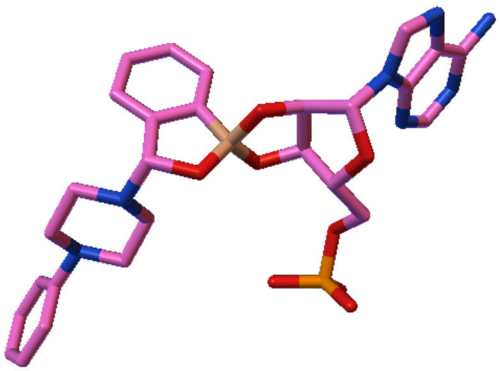


Figure S54. The best structure obtained in the docking studies of 6-S-c-2-AMP.

Table S54. Coordinates of the best 6-S-c-2-AMP spiroester.

O	*27.502*	*62.220*	*18.260*
C	*28.739*	*64.077*	*17.509*
C	*28.282*	*63.354*	*18.757*
C	*28.241*	*63.470*	*16.362*
C	*29.577*	*65.180*	*17.459*
C	*28.592*	*64.006*	*15.122*
C	*29.443*	*65.092*	*15.061*
C	*29.935*	*65.671*	*16.215*
C	*25.236*	*60.165*	*15.929*
O	*25.872*	*59.002*	*15.384*
C	*25.928*	*61.387*	*15.340*
O	*26.151*	*62.425*	*16.284*
C	*27.292*	*60.841*	*15.023*
O	*28.032*	*61.155*	*16.184*
C	*27.116*	*59.340*	*14.802*
B	*27.435*	*62.237*	*16.876*
N	*27.537*	*64.198*	*19.652*
C	*26.265*	*64.680*	*19.110*
C	*25.459*	*65.342*	*20.213*
N	*26.206*	*66.496*	*20.741*
C	*27.515*	*66.034*	*21.256*
C	*28.305*	*65.321*	*20.184*
C	*25.514*	*67.299*	*21.709*
C	*25.201*	*68.636*	*21.521*
C	*24.527*	*69.346*	*22.513*
C	*24.160*	*68.737*	*23.688*
C	*24.473*	*67.408*	*23.886*
C	*25.141*	*66.694*	*22.907*
C	*23.755*	*60.045*	*15.605*
O	*23.175*	*61.344*	*15.819*
P	*22.033*	*61.571*	*16.945*
O	*21.898*	*60.182*	*17.528*
O	*20.804*	*62.062*	*16.230*
O	*22.743*	*62.562*	*17.853*
N	*27.079*	*59.033*	*13.351*
C	*28.051*	*58.416*	*12.647*
N	*27.686*	*58.296*	*11.352*
C	*26.458*	*58.855*	*11.236*
C	*25.511*	*59.062*	*10.133*
C	*26.073*	*59.350*	*12.540*
N	*25.823*	*58.624*	*8.887*
N	*24.347*	*59.686*	*10.403*
C	*24.049*	*60.114*	*11.645*
N	*24.875*	*59.967*	*12.694*

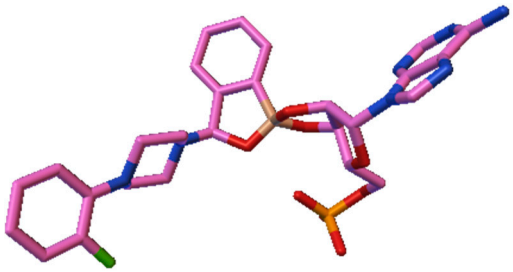


Figure S55. The best structure obtained in the docking studies of 7-R-1-AMP.

Table S55. Coordinates of the best 7-R-1-AMP spiroester.

O	*26.032*	*61.816*	*17.276*
C	*27.996*	*61.559*	*18.609*
C	*29.107*	*61.675*	*19.444*
C	*29.932*	*60.574*	*19.635*
C	*29.656*	*59.362*	*18.999*
C	*28.550*	*59.233*	*18.163*
C	*27.731*	*60.339*	*17.983*
C	*26.464*	*60.416*	*17.157*
C	*25.300*	*65.297*	*18.466*
O	*25.954*	*66.296*	*17.673*
C	*26.377*	*64.528*	*19.220*
O	*26.152*	*63.125*	*19.260*
C	*27.568*	*64.712*	*18.321*
O	*27.520*	*63.564*	*17.500*
C	*27.336*	*66.016*	*17.559*
B	*26.798*	*62.526*	*18.139*
N	*26.592*	*59.967*	*15.808*
C	*25.332*	*59.537*	*15.201*
C	*25.603*	*58.815*	*13.885*
N	*26.333*	*59.692*	*12.977*
C	*27.590*	*60.157*	*13.582*
C	*27.318*	*60.860*	*14.903*
C	*26.381*	*59.321*	*11.622*
C	*27.523*	*58.802*	*10.997*
C	*27.508*	*58.396*	*9.667*
C	*26.354*	*58.512*	*8.907*
C	*25.203*	*59.026*	*9.496*
C	*25.230*	*59.406*	*10.821*
F	*24.080*	*59.864*	*11.374*
C	*24.295*	*66.025*	*19.343*
O	*23.458*	*65.020*	*19.941*
P	*22.695*	*63.920*	*19.028*
O	*21.942*	*63.125*	*20.070*
O	*23.758*	*63.139*	*18.304*
O	*21.818*	*64.833*	*18.185*
N	*28.115*	*67.118*	*18.174*
C	*28.603*	*68.199*	*17.530*
N	*29.258*	*69.002*	*18.396*
C	*29.187*	*68.412*	*19.613*
C	*29.679*	*68.738*	*20.956*
C	*28.454*	*67.173*	*19.460*
N	*30.379*	*69.885*	*21.155*
N	*29.412*	*67.878*	*21.959*
C	*28.715*	*66.745*	*21.746*
N	*28.247*	*66.381*	*20.541*

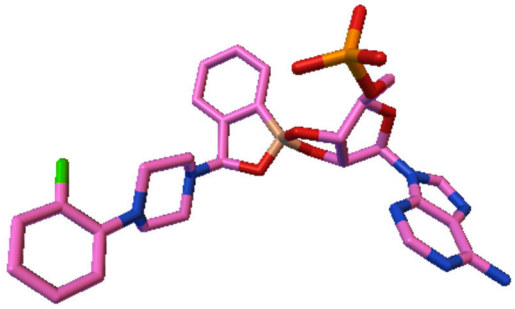


Figure S56. The best structure obtained in the docking studies of 7-R-2-AMP.

Table S56. Coordinates of the best 7-R-2-AMP spiroester.

O	*27.745*	*62.322*	*15.703*
C	*27.436*	*60.469*	*17.178*
C	*27.047*	*59.323*	*17.869*
C	*27.713*	*58.975*	*19.039*
C	*28.759*	*59.765*	*19.520*
C	*29.157*	*60.913*	*18.838*
C	*28.488*	*61.246*	*17.669*
C	*28.774*	*62.416*	*16.751*
C	*24.209*	*59.880*	*15.072*
O	*24.397*	*59.068*	*13.907*
C	*24.919*	*61.205*	*14.831*
O	*25.627*	*61.687*	*15.965*
C	*25.980*	*60.806*	*13.843*
O	*27.088*	*60.523*	*14.672*
C	*25.443*	*59.581*	*13.105*
B	*26.964*	*61.195*	*15.913*
N	*28.824*	*63.690*	*17.391*
C	*29.415*	*64.748*	*16.573*
C	*29.690*	*65.982*	*17.423*
N	*28.453*	*66.447*	*18.039*
C	*27.827*	*65.389*	*18.846*
C	*27.573*	*64.151*	*17.998*
C	*28.450*	*67.743*	*18.584*
C	*28.343*	*68.909*	*17.814*
C	*28.288*	*70.170*	*18.400*
C	*28.355*	*70.311*	*19.777*
C	*28.465*	*69.172*	*20.571*
C	*28.500*	*67.930*	*19.975*
F	*28.565*	*66.841*	*20.779*
C	*22.708*	*59.985*	*15.293*
O	*22.439*	*61.340*	*15.695*
P	*21.785*	*61.665*	*17.141*
O	*20.520*	*62.394*	*16.748*
O	*22.779*	*62.511*	*17.890*
O	*21.556*	*60.254*	*17.657*
N	*24.903*	*59.972*	*11.781*
C	*24.845*	*59.188*	*10.684*
N	*24.290*	*59.863*	*9.655*
C	*23.996*	*61.104*	*10.110*
C	*23.398*	*62.310*	*9.526*
C	*24.413*	*61.177*	*11.494*
N	*22.995*	*62.301*	*8.230*
N	*23.266*	*63.399*	*10.310*
C	*23.669*	*63.394*	*11.595*
N	*24.234*	*62.328*	*12.187*

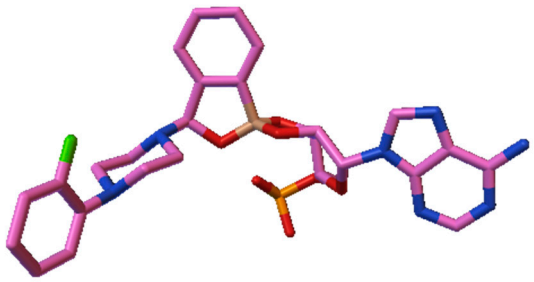


Figure S57. The best structure obtained in the docking studies of 7-R-c-1-AMP

Table S57. Coordinates of the best 7-R-c-1-AMP spiroester.

O	*25.726*	*61.633*	*17.117*
C	*27.836*	*61.486*	*18.234*
C	*29.014*	*61.631*	*18.969*
C	*29.821*	*60.525*	*19.198*
C	*29.478*	*59.280*	*18.680*
C	*28.327*	*59.119*	*17.923*
C	*27.521*	*60.232*	*17.716*
C	*26.206*	*60.257*	*16.972*
C	*25.127*	*65.238*	*18.358*
O	*25.683*	*66.260*	*17.521*
C	*26.286*	*64.476*	*18.986*
O	*26.087*	*63.069*	*19.025*
C	*27.376*	*64.693*	*17.975*
O	*27.263*	*63.557*	*17.144*
C	*27.050*	*66.004*	*17.262*
B	*26.625*	*62.498*	*17.835*
N	*26.341*	*59.857*	*15.594*
C	*25.199*	*59.102*	*15.073*
C	*25.545*	*58.533*	*13.706*
N	*25.840*	*59.645*	*12.783*
C	*26.978*	*60.434*	*13.312*
C	*26.662*	*60.963*	*14.694*
C	*26.040*	*59.277*	*11.417*
C	*25.144*	*59.534*	*10.384*
C	*25.434*	*59.162*	*9.072*
C	*26.620*	*58.520*	*8.770*
C	*27.537*	*58.257*	*9.779*
C	*27.228*	*58.641*	*11.064*
F	*28.128*	*58.388*	*12.047*
C	*24.205*	*65.937*	*19.345*
O	*23.383*	*64.917*	*19.940*
P	*22.524*	*63.897*	*19.019*
O	*21.692*	*63.175*	*20.056*
O	*23.512*	*63.020*	*18.300*
O	*21.743*	*64.890*	*18.174*
N	*27.870*	*67.110*	*17.814*
C	*29.070*	*66.981*	*18.419*
N	*29.536*	*68.192*	*18.795*
C	*28.606*	*69.104*	*18.425*
C	*28.481*	*70.562*	*18.535*
C	*27.512*	*68.392*	*17.800*
N	*29.474*	*71.281*	*19.118*
N	*27.369*	*71.145*	*18.042*
C	*26.393*	*70.419*	*17.464*
N	*26.439*	*69.083*	*17.343*

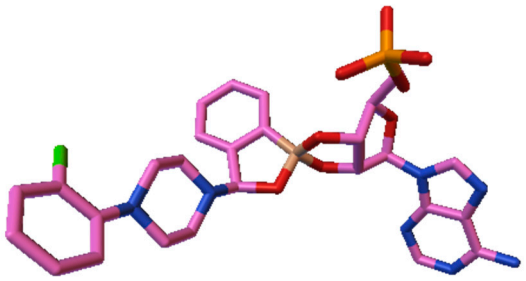


Figure S58. The best structure obtained in the docking studies of 7R-c-2-AMP.

Table S58. Coordinates of the best 7-R-c-2-AMP spiroester.

O	*27.583*	*62.781*	*15.927*
C	*27.699*	*60.940*	*17.450*
C	*27.611*	*59.751*	*18.176*
C	*28.497*	*59.518*	*19.219*
C	*29.456*	*60.466*	*19.559*
C	*29.542*	*61.666*	*18.868*
C	*28.660*	*61.879*	*17.816*
C	*28.626*	*63.087*	*16.909*
C	*24.531*	*59.572*	*15.535*
O	*24.847*	*58.767*	*14.393*
C	*24.921*	*61.008*	*15.210*
O	*25.549*	*61.685*	*16.291*
C	*26.004*	*60.804*	*14.188*
O	*27.179*	*60.810*	*14.971*
C	*25.722*	*59.458*	*13.522*
B	*26.959*	*61.495*	*16.191*
N	*28.375*	*64.311*	*17.623*
C	*28.378*	*64.171*	*19.081*
C	*27.870*	*65.455*	*19.719*
N	*28.769*	*66.564*	*19.349*
C	*28.796*	*66.701*	*17.873*
C	*29.253*	*65.412*	*17.225*
C	*28.509*	*67.812*	*19.993*
C	*28.204*	*68.999*	*19.335*
C	*27.938*	*70.167*	*20.049*
C	*27.979*	*70.171*	*21.430*
C	*28.274*	*69.000*	*22.114*
C	*28.527*	*67.860*	*21.385*
F	*28.809*	*66.714*	*22.056*
C	*23.054*	*59.356*	*15.825*
O	*22.430*	*60.653*	*15.799*
P	*21.740*	*61.271*	*17.129*
O	*20.508*	*61.932*	*16.554*
O	*22.731*	*62.228*	*17.731*
O	*21.458*	*59.994*	*17.904*
N	*25.056*	*59.660*	*12.212*
C	*23.734*	*59.542*	*11.969*
N	*23.474*	*59.798*	*10.668*
C	*24.660*	*60.079*	*10.077*
C	*25.084*	*60.428*	*8.716*
C	*25.692*	*59.971*	*11.085*
N	*24.158*	*60.537*	*7.730*
N	*26.398*	*60.636*	*8.493*
C	*27.305*	*60.527*	*9.483*
N	*26.985*	*60.199*	*10.745*

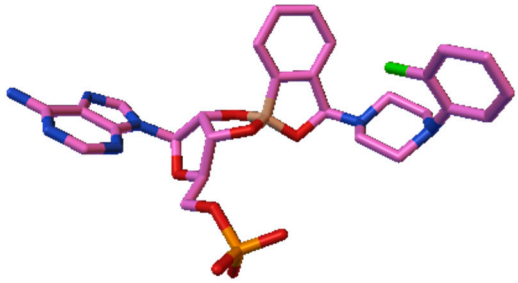


Figure S59. The best structure obtained in the docking studies of 7-S-1-AMP.

Table S59. Coordinates of the best 7-S-1-AMP spiroester.

C	*28.199*	*63.423*	*16.199*
C	*28.647*	*64.045*	*17.367*
C	*28.651*	*63.883*	*14.962*
C	*29.537*	*64.953*	*14.915*
C	*29.972*	*65.565*	*16.093*
C	*29.530*	*65.114*	*17.334*
O	*27.173*	*62.335*	*18.060*
C	*28.077*	*63.365*	*18.596*
C	*25.083*	*60.218*	*15.616*
O	*25.725*	*59.031*	*15.135*
C	*25.838*	*61.412*	*15.049*
O	*26.024*	*62.465*	*15.986*
C	*27.206*	*60.831*	*14.830*
O	*27.879*	*61.154*	*16.030*
C	*27.010*	*59.330*	*14.626*
B	*27.264*	*62.262*	*16.661*
N	*27.456*	*64.234*	*19.542*
C	*28.270*	*65.373*	*19.982*
C	*27.566*	*66.079*	*21.144*
N	*26.204*	*66.492*	*20.825*
C	*25.418*	*65.356*	*20.334*
C	*26.106*	*64.662*	*19.159*
C	*25.951*	*67.783*	*20.350*
C	*26.297*	*68.148*	*19.036*
C	*26.032*	*69.388*	*18.497*
F	*26.903*	*67.231*	*18.237*
C	*25.363*	*70.341*	*19.257*
C	*24.980*	*70.018*	*20.550*
C	*25.277*	*68.770*	*21.088*
C	*23.623*	*60.123*	*15.202*
O	*22.980*	*61.326*	*15.661*
P	*21.877*	*61.279*	*16.847*
O	*22.291*	*62.459*	*17.696*
O	*22.023*	*59.946*	*17.528*
O	*20.607*	*61.505*	*16.042*
N	*27.059*	*58.995*	*13.182*
C	*28.105*	*58.444*	*12.531*
N	*27.804*	*58.272*	*11.226*
C	*26.541*	*58.729*	*11.048*
C	*25.628*	*58.840*	*9.905*
C	*26.064*	*59.216*	*12.325*
N	*26.025*	*58.405*	*8.682*
N	*24.408*	*59.374*	*10.114*
C	*24.026*	*59.800*	*11.334*
N	*24.817*	*59.738*	*12.418*

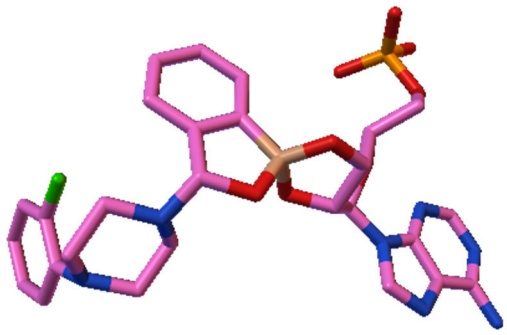


Figure S60. The best structure obtained in the docking studies of 7-S-2-AMP.

Table S60. Coordinates of the best 7-S-2-AMP spiroester.

C	*25.750*	*63.685*	*18.405*
O	*25.695*	*64.933*	*17.704*
C	*27.067*	*63.011*	*18.047*
O	*26.948*	*61.613*	*17.820*
C	*27.355*	*63.607*	*16.697*
O	*26.792*	*62.661*	*15.811*
C	*26.655*	*64.964*	*16.665*
B	*26.694*	*61.393*	*16.435*
C	*25.351*	*60.698*	*16.040*
C	*25.693*	*59.733*	*15.090*
C	*24.016*	*60.849*	*16.414*
C	*23.050*	*60.036*	*15.832*
C	*23.408*	*59.079*	*14.880*
C	*24.738*	*58.917*	*14.500*
O	*27.712*	*60.796*	*15.697*
C	*27.191*	*59.701*	*14.864*
N	*27.604*	*59.773*	*13.501*
C	*27.131*	*58.685*	*12.638*
C	*27.827*	*58.778*	*11.277*
N	*27.659*	*60.076*	*10.634*
C	*28.086*	*61.157*	*11.527*
C	*27.376*	*61.082*	*12.879*
C	*26.620*	*60.283*	*9.721*
C	*25.327*	*59.793*	*9.979*
C	*24.253*	*60.005*	*9.142*
F	*25.104*	*59.096*	*11.123*
C	*24.418*	*60.762*	*7.987*
C	*25.671*	*61.286*	*7.704*
C	*26.750*	*61.042*	*8.547*
C	*25.572*	*64.006*	*19.881*
O	*24.487*	*64.946*	*19.974*
P	*22.953*	*64.471*	*19.755*
O	*22.884*	*63.243*	*20.635*
O	*22.788*	*64.189*	*18.287*
O	*22.215*	*65.678*	*20.310*
N	*27.628*	*66.052*	*16.925*
C	*28.937*	*66.041*	*16.598*
N	*29.524*	*67.196*	*16.980*
C	*28.565*	*67.950*	*17.566*
C	*28.526*	*69.278*	*18.191*
C	*27.332*	*67.193*	*17.543*
N	*29.655*	*70.030*	*18.244*
N	*27.351*	*69.712*	*18.690*
C	*26.238*	*68.956*	*18.627*
N	*26.209*	*67.730*	*18.081*

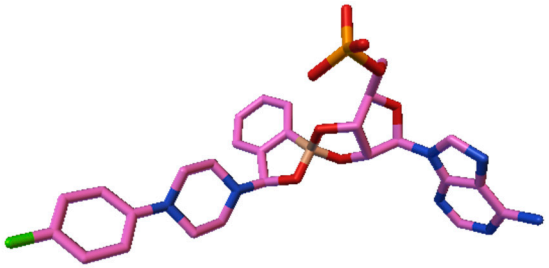


Figure S61. The best structure obtained in the docking studies of 8-R-1-AMP.

Table S61. Coordinates of the best 8-R-1-AMP spiroester.

O	*27.566*	*62.643*	*15.954*
C	*27.631*	*60.751*	*17.410*
C	*27.472*	*59.547*	*18.095*
C	*28.226*	*59.310*	*19.240*
C	*29.134*	*60.266*	*19.700*
C	*29.304*	*61.470*	*19.023*
C	*28.546*	*61.694*	*17.883*
C	*28.593*	*62.907*	*16.975*
C	*24.433*	*59.595*	*15.467*
O	*24.705*	*58.843*	*14.278*
C	*24.856*	*61.035*	*15.209*
O	*25.524*	*61.638*	*16.309*
C	*25.912*	*60.857*	*14.154*
O	*27.102*	*60.791*	*14.912*
C	*25.581*	*59.555*	*13.426*
B	*26.925*	*61.417*	*16.170*
N	*28.436*	*64.163*	*17.632*
C	*28.071*	*64.059*	*19.044*
C	*27.664*	*65.424*	*19.578*
N	*28.742*	*66.398*	*19.386*
C	*29.127*	*66.488*	*17.983*
C	*29.530*	*65.118*	*17.453*
C	*28.643*	*67.603*	*20.118*
C	*28.633*	*67.559*	*21.522*
C	*28.569*	*68.717*	*22.280*
C	*28.529*	*69.942*	*21.636*
F	*28.478*	*71.075*	*22.374*
C	*28.549*	*70.029*	*20.259*
C	*28.597*	*68.861*	*19.504*
C	*22.957*	*59.403*	*15.777*
O	*22.343*	*60.703*	*15.706*
P	*21.781*	*61.431*	*17.040*
O	*21.341*	*60.249*	*17.872*
O	*20.658*	*62.333*	*16.605*
O	*23.051*	*62.104*	*17.535*
N	*24.894*	*59.843*	*12.143*
C	*23.573*	*60.066*	*11.984*
N	*23.292*	*60.298*	*10.683*
C	*24.462*	*60.213*	*10.006*
C	*24.860*	*60.348*	*8.600*
C	*25.503*	*59.899*	*10.960*
N	*23.924*	*60.636*	*7.660*
N	*26.162*	*60.184*	*8.288*
C	*27.080*	*59.901*	*9.231*
N	*26.781*	*59.752*	*10.532*

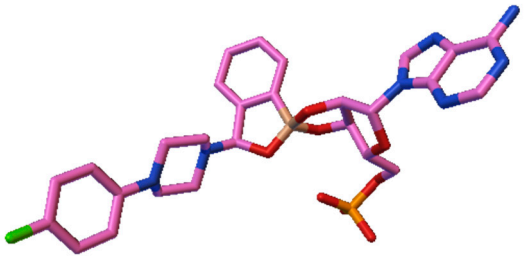


Figure S62. The best structure obtained in the docking studies of 8-R-2-AMP.

Table S62. Coordinates of the best 8-R-2-AMP spiroester.

O	*25.908*	*62.141*	*17.191*
C	*27.853*	*61.985*	*18.568*
C	*28.946*	*62.164*	*19.413*
C	*29.781*	*61.083*	*19.684*
C	*29.529*	*59.834*	*19.115*
C	*28.438*	*59.643*	*18.271*
C	*27.612*	*60.728*	*18.011*
C	*26.359*	*60.741*	*17.160*
C	*25.232*	*65.551*	*18.846*
O	*25.874*	*66.678*	*18.235*
C	*26.318*	*64.673*	*19.451*
O	*26.104*	*63.282*	*19.249*
C	*27.502*	*65.019*	*18.592*
O	*27.459*	*64.030*	*17.585*
C	*27.257*	*66.433*	*18.068*
B	*26.748*	*62.892*	*18.038*
N	*26.515*	*60.220*	*15.841*
C	*25.260*	*59.824*	*15.201*
C	*25.549*	*59.040*	*13.929*
N	*26.380*	*59.826*	*13.013*
C	*27.622*	*60.244*	*13.653*
C	*27.324*	*61.027*	*14.927*
C	*26.451*	*59.370*	*11.677*
C	*25.281*	*59.319*	*10.902*
C	*25.310*	*58.910*	*9.579*
C	*26.524*	*58.560*	*9.008*
F	*26.555*	*58.170*	*7.713*
C	*27.696*	*58.608*	*9.732*
C	*27.656*	*59.004*	*11.065*
C	*24.225*	*66.109*	*19.841*
O	*23.538*	*64.983*	*20.414*
P	*22.601*	*64.027*	*19.500*
O	*22.012*	*63.096*	*20.536*
O	*23.504*	*63.352*	*18.504*
O	*21.621*	*65.053*	*18.955*
N	*28.031*	*67.419*	*18.861*
C	*28.703*	*67.165*	*20.004*
N	*29.298*	*68.290*	*20.456*
C	*28.989*	*69.278*	*19.582*
C	*29.297*	*70.709*	*19.482*
C	*28.147*	*68.708*	*18.552*
N	*30.076*	*71.297*	*20.425*
N	*28.790*	*71.398*	*18.440*
C	*28.019*	*70.800*	*17.510*
N	*27.690*	*69.499*	*17.550*



Figure S62. The best structure obtained in the docking studies of 8-R-c-1-AMP.

Table S62. Coordinates of the best 8-R-c-1-AMP spiroester.

O	*27.546*	*62.619*	*15.898*
C	*27.594*	*60.715*	*17.319*
C	*27.424*	*59.518*	*18.002*
C	*28.195*	*59.262*	*19.117*
C	*29.125*	*60.179*	*19.565*
C	*29.316*	*61.374*	*18.894*
C	*28.543*	*61.626*	*17.774*
C	*28.586*	*62.846*	*16.898*
C	*24.409*	*59.607*	*15.405*
O	*24.642*	*58.827*	*14.225*
C	*24.865*	*61.030*	*15.114*
O	*25.567*	*61.634*	*16.193*
C	*25.899*	*60.806*	*14.047*
O	*27.100*	*60.721*	*14.787*
C	*25.522*	*59.501*	*13.347*
B	*26.960*	*61.373*	*16.036*
N	*28.445*	*64.083*	*17.593*
C	*28.104*	*63.929*	*18.998*
C	*27.678*	*65.260*	*19.566*
N	*28.732*	*66.269*	*19.404*
C	*29.155*	*66.368*	*18.011*
C	*29.567*	*65.010*	*17.478*
C	*28.482*	*67.493*	*20.070*
C	*28.300*	*67.502*	*21.445*
C	*28.054*	*68.670*	*22.137*
C	*28.006*	*69.843*	*21.455*
F	*27.757*	*70.995*	*22.145*
C	*28.195*	*69.888*	*20.117*
C	*28.429*	*68.719*	*19.413*
C	*22.933*	*59.459*	*15.741*
O	*22.376*	*60.785*	*15.759*
P	*21.677*	*61.377*	*17.096*
O	*20.392*	*61.949*	*16.543*
O	*22.618*	*62.405*	*17.663*
O	*21.497*	*60.096*	*17.895*
N	*24.823*	*59.784*	*12.070*
C	*23.486*	*59.800*	*11.885*
N	*23.196*	*60.097*	*10.599*
C	*24.377*	*60.267*	*9.958*
C	*24.775*	*60.591*	*8.583*
C	*25.437*	*60.046*	*10.918*
N	*23.822*	*60.803*	*7.640*
N	*26.091*	*60.672*	*8.303*
C	*27.026*	*60.462*	*9.251*
N	*26.730*	*60.150*	*10.523*

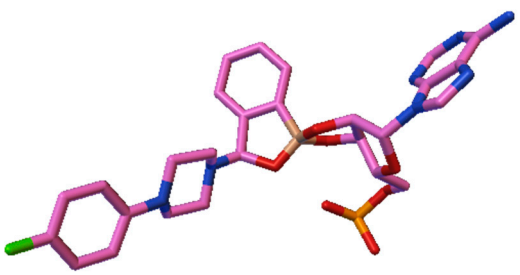


Figure S63. The best structure obtained in the docking studies of 8-R-c-2-AMP.

Table S63. Coordinates of the best 8-R-c-2-AMP spiroester.

O	*25.782*	*62.113*	*16.989*
C	*27.729*	*61.800*	*18.315*
C	*28.846*	*61.873*	*19.137*
C	*29.619*	*60.746*	*19.325*
C	*29.303*	*59.554*	*18.704*
C	*28.190*	*59.458*	*17.887*
C	*27.415*	*60.589*	*17.704*
C	*26.171*	*60.710*	*16.870*
C	*25.150*	*65.497*	*18.579*
O	*25.787*	*66.582*	*17.892*
C	*26.243*	*64.636*	*19.195*
O	*26.006*	*63.240*	*19.071*
C	*27.405*	*64.921*	*18.285*
O	*27.319*	*63.883*	*17.332*
C	*27.161*	*66.310*	*17.697*
B	*26.608*	*62.779*	*17.864*
N	*26.313*	*60.272*	*15.520*
C	*25.054*	*60.188*	*14.798*
C	*25.259*	*59.437*	*13.506*
N	*26.284*	*60.081*	*12.674*
C	*27.528*	*60.261*	*13.418*
C	*27.276*	*61.013*	*14.709*
C	*26.407*	*59.540*	*11.371*
C	*27.661*	*59.217*	*10.876*
C	*27.830*	*58.687*	*9.614*
C	*26.735*	*58.463*	*8.841*
F	*26.910*	*57.944*	*7.590*
C	*25.491*	*58.744*	*9.286*
C	*25.315*	*59.288*	*10.547*
C	*24.182*	*66.118*	*19.573*
O	*23.511*	*65.032*	*20.236*
P	*22.574*	*64.002*	*19.407*
O	*21.959*	*63.184*	*20.520*
O	*23.482*	*63.222*	*18.496*
O	*21.615*	*64.981*	*18.750*
N	*27.971*	*67.324*	*18.415*
C	*28.490*	*68.449*	*17.879*
N	*29.168*	*69.144*	*18.817*
C	*29.081*	*68.438*	*19.970*
C	*29.583*	*68.617*	*21.337*
C	*28.313*	*67.242*	*19.699*
N	*30.315*	*69.718*	*21.647*
N	*29.292*	*67.670*	*22.252*
C	*28.563*	*66.584*	*21.931*
N	*28.084*	*66.354*	*20.697*

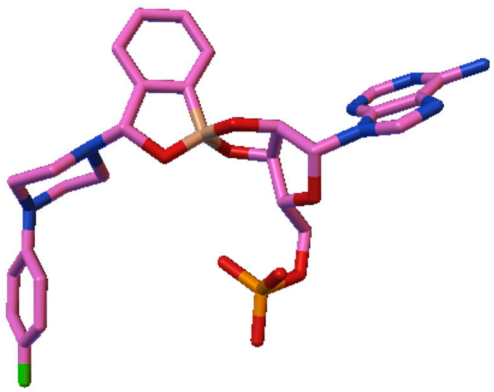


Figure S64. The best structure obtained in the docking studies of 8-S-1-AMP.

Table S64. Coordinates of the best 8-S-1-AMP spiroester.

C	*24.907*	*68.127*	*18.463*
C	*26.213*	*67.916*	*18.016*
C	*24.568*	*69.348*	*19.042*
C	*25.540*	*70.336*	*19.166*
C	*26.842*	*70.108*	*18.717*
C	*27.192*	*68.893*	*18.136*
O	*25.039*	*65.918*	*17.564*
C	*26.356*	*66.549*	*17.378*
C	*21.383*	*65.242*	*18.528*
O	*20.452*	*65.577*	*17.492*
C	*22.006*	*66.539*	*19.026*
O	*23.404*	*66.445*	*19.264*
C	*21.870*	*67.425*	*17.819*
O	*23.106*	*67.248*	*17.160*
C	*20.676*	*66.894*	*17.027*
B	*24.097*	*66.809*	*18.073*
N	*27.442*	*65.760*	*17.863*
C	*27.160*	*64.967*	*19.064*
C	*28.464*	*64.355*	*19.584*
N	*29.169*	*63.567*	*18.581*
C	*29.397*	*64.356*	*17.366*
C	*28.094*	*64.948*	*16.830*
C	*28.968*	*62.186*	*18.499*
C	*29.579*	*61.313*	*19.418*
C	*29.381*	*59.949*	*19.417*
C	*28.516*	*59.378*	*18.488*
C	*27.873*	*60.204*	*17.577*
F	*28.320*	*58.200*	*18.510*
C	*28.103*	*61.575*	*17.577*
C	*20.607*	*64.457*	*19.574*
O	*20.501*	*63.107*	*19.088*
P	*21.499*	*62.556*	*17.936*
O	*20.973*	*63.267*	*16.710*
O	*21.341*	*61.061*	*17.899*
O	*22.824*	*63.096*	*18.448*
N	*19.473*	*67.721*	*17.291*
C	*18.478*	*67.975*	*16.415*
N	*17.540*	*68.760*	*16.988*
C	*17.956*	*69.011*	*18.253*
C	*17.427*	*69.779*	*19.386*
C	*19.226*	*68.345*	*18.441*
N	*16.242*	*70.430*	*19.263*
N	*18.147*	*69.809*	*20.526*
C	*19.320*	*69.157*	*20.634*
N	*19.865*	*68.446*	*19.632*

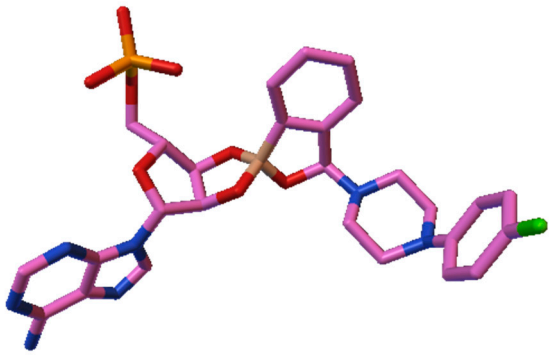


Figure S65. The best structure obtained in the docking studies of 8-S-2-AMP.

Table S65. Coordinates of the best 8-S-2-AMP spiroester.

C	*25.131*	*61.071*	*16.148*
C	*25.653*	*59.996*	*15.424*
C	*23.762*	*61.126*	*16.403*
C	*22.939*	*60.110*	*15.930*
C	*23.476*	*59.045*	*15.204*
C	*24.842*	*58.977*	*14.943*
O	*27.489*	*61.388*	*15.938*
C	*27.159*	*60.104*	*15.299*
C	*25.653*	*64.058*	*18.701*
O	*25.571*	*65.384*	*18.164*
C	*26.917*	*63.414*	*18.148*
O	*26.743*	*62.056*	*17.765*
C	*27.103*	*64.167*	*16.860*
O	*26.441*	*63.347*	*15.920*
C	*26.438*	*65.528*	*17.056*
B	*26.364*	*62.013*	*16.391*
N	*27.674*	*59.973*	*13.976*
C	*27.182*	*58.817*	*13.218*
C	*27.978*	*58.689*	*11.917*
N	*27.957*	*59.902*	*11.108*
C	*28.399*	*61.059*	*11.893*
C	*27.590*	*61.205*	*13.183*
C	*27.005*	*60.059*	*10.096*
C	*26.008*	*59.089*	*9.888*
C	*25.016*	*59.209*	*8.939*
C	*24.954*	*60.352*	*8.147*
C	*25.903*	*61.347*	*8.334*
F	*23.998*	*60.477*	*7.293*
C	*26.911*	*61.199*	*9.279*
C	*25.611*	*64.198*	*20.215*
O	*24.378*	*63.600*	*20.654*
P	*22.998*	*63.849*	*19.843*
O	*21.978*	*63.242*	*20.781*
O	*23.129*	*63.133*	*18.526*
O	*22.980*	*65.368*	*19.801*
N	*27.457*	*66.562*	*17.359*
C	*28.781*	*66.348*	*17.512*
N	*29.414*	*67.511*	*17.777*
C	*28.468*	*68.480*	*17.797*
C	*28.470*	*69.930*	*18.025*
C	*27.189*	*67.853*	*17.540*
N	*29.641*	*70.569*	*18.277*
N	*27.293*	*70.584*	*17.972*
C	*26.139*	*69.937*	*17.718*
N	*26.066*	*68.612*	*17.513*

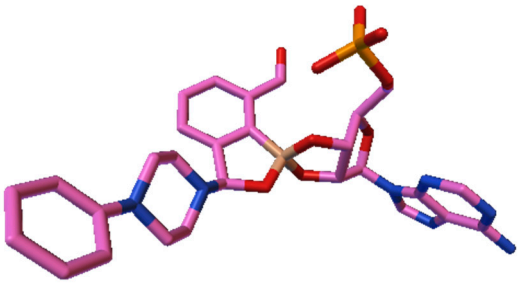


Figure S66. The best structure obtained in the docking studies of 9-R-1-AMP.

Table S66. Coordinates of the best 9-R-1-AMP spiroester.

O	*28.074*	*62.777*	*15.357*
C	*27.795*	*61.138*	*17.069*
C	*28.690*	*62.099*	*17.526*
C	*28.950*	*63.146*	*16.460*
C	*27.459*	*60.065*	*17.911*
C	*28.033*	*59.991*	*19.184*
C	*28.923*	*60.967*	*19.623*
C	*29.260*	*62.032*	*18.793*
C	*24.986*	*59.711*	*14.731*
O	*25.438*	*58.782*	*13.738*
C	*25.499*	*61.090*	*14.340*
O	*25.982*	*61.850*	*15.440*
C	*26.719*	*60.743*	*13.534*
O	*27.752*	*60.785*	*14.496*
C	*26.476*	*59.348*	*12.961*
B	*27.377*	*61.599*	*15.593*
N	*28.793*	*64.496*	*16.902*
C	*29.786*	*65.445*	*16.391*
C	*29.377*	*66.866*	*16.754*
N	*29.214*	*67.009*	*18.203*
C	*28.255*	*66.048*	*18.727*
C	*28.669*	*64.629*	*18.356*
C	*29.185*	*68.323*	*18.718*
C	*29.129*	*69.414*	*17.836*
C	*29.134*	*70.717*	*18.309*
C	*29.210*	*70.977*	*19.675*
C	*29.277*	*69.908*	*20.556*
C	*29.259*	*68.596*	*20.090*
C	*26.519*	*59.005*	*17.508*
O	*26.056*	*58.146*	*18.234*
C	*23.472*	*59.580*	*14.794*
O	*22.960*	*60.860*	*15.206*
P	*22.775*	*61.216*	*16.776*
O	*24.166*	*61.677*	*17.151*
O	*22.337*	*59.952*	*17.462*
O	*21.753*	*62.337*	*16.679*
N	*26.040*	*59.439*	*11.547*
C	*26.562*	*58.751*	*10.510*
N	*25.924*	*59.076*	*9.365*
C	*24.981*	*59.994*	*9.685*
C	*23.970*	*60.749*	*8.936*
C	*25.071*	*60.241*	*11.108*
N	*23.845*	*60.561*	*7.598*
N	*23.186*	*61.610*	*9.616*
C	*23.319*	*61.784*	*10.945*
N	*24.232*	*61.135*	*11.686*



Figure S67. The best structure obtained in the docking studies of 9-R-2-AMP.

Table S67. Coordinates of the best 9-R-2-AMP spiroester.

O	*25.506*	*61.669*	*16.873*
C	*27.559*	*61.426*	*18.067*
C	*27.226*	*60.193*	*17.516*
C	*25.900*	*60.270*	*16.784*
C	*28.744*	*61.539*	*18.814*
C	*29.554*	*60.414*	*18.983*
C	*29.204*	*59.191*	*18.418*
C	*28.031*	*59.071*	*17.678*
C	*24.976*	*65.153*	*18.266*
O	*25.583*	*66.191*	*17.487*
C	*26.095*	*64.319*	*18.875*
O	*25.843*	*62.920*	*18.844*
C	*27.209*	*64.542*	*17.891*
O	*27.068*	*63.451*	*17.005*
C	*26.943*	*65.896*	*17.237*
B	*26.379*	*62.386*	*17.636*
N	*25.926*	*59.757*	*15.450*
C	*27.226*	*59.817*	*14.775*
C	*27.165*	*59.044*	*13.465*
N	*26.102*	*59.564*	*12.601*
C	*24.811*	*59.541*	*13.272*
C	*24.882*	*60.312*	*14.586*
C	*26.148*	*59.199*	*11.239*
C	*25.012*	*59.381*	*10.431*
C	*25.015*	*59.001*	*9.099*
C	*26.143*	*58.416*	*8.528*
C	*27.266*	*58.223*	*9.316*
C	*27.277*	*58.614*	*10.653*
C	*29.172*	*62.806*	*19.430*
O	*28.498*	*63.513*	*20.156*
C	*24.064*	*65.839*	*19.271*
O	*22.718*	*65.442*	*18.952*
P	*22.181*	*63.956*	*19.313*
O	*20.764*	*64.243*	*19.756*
O	*23.072*	*63.421*	*20.400*
O	*22.286*	*63.294*	*17.949*
N	*27.795*	*66.943*	*17.853*
C	*28.973*	*66.739*	*18.479*
N	*29.479*	*67.913*	*18.916*
C	*28.597*	*68.878*	*18.563*
C	*28.530*	*70.335*	*18.730*
C	*27.491*	*68.239*	*17.884*
N	*29.537*	*70.986*	*19.365*
N	*27.456*	*70.983*	*18.236*
C	*26.465*	*70.324*	*17.606*
N	*26.459*	*68.992*	*17.431*

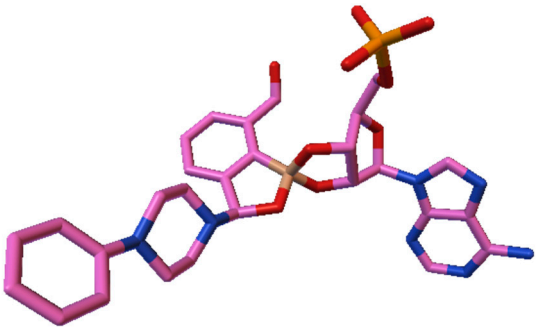


Figure S68. The best structure obtained in the docking studies of 9-R-c-1-AMP.

Table S68. Coordinates of the best 9-R-c-1-AMP spiroester.

O	*27.566*	*62.706*	*15.725*
C	*28.634*	*63.020*	*16.664*
C	*27.726*	*60.896*	*17.261*
C	*28.653*	*61.856*	*17.615*
C	*27.627*	*59.731*	*18.050*
C	*29.492*	*61.707*	*18.719*
C	*28.458*	*59.596*	*19.151*
C	*29.377*	*60.566*	*19.480*
C	*24.586*	*59.567*	*15.378*
O	*24.864*	*58.805*	*14.197*
C	*24.947*	*61.017*	*15.088*
O	*25.611*	*61.664*	*16.165*
C	*25.990*	*60.862*	*14.016*
O	*27.196*	*60.855*	*14.752*
C	*25.696*	*59.536*	*13.316*
B	*27.018*	*61.495*	*16.003*
N	*28.467*	*64.286*	*17.309*
C	*29.595*	*65.194*	*17.139*
C	*29.241*	*66.569*	*17.636*
N	*28.799*	*66.542*	*19.025*
C	*27.759*	*65.544*	*19.268*
C	*28.155*	*64.195*	*18.730*
C	*28.684*	*67.776*	*19.685*
C	*28.600*	*67.874*	*21.061*
C	*28.574*	*69.107*	*21.688*
C	*28.602*	*70.270*	*20.991*
C	*28.651*	*70.186*	*19.633*
C	*28.692*	*68.970*	*18.986*
C	*26.691*	*58.662*	*17.725*
O	*25.993*	*58.068*	*18.511*
C	*23.124*	*59.323*	*15.720*
O	*22.480*	*60.609*	*15.738*
P	*21.477*	*61.021*	*16.942*
O	*21.657*	*59.864*	*17.899*
O	*20.099*	*61.122*	*16.347*
O	*22.124*	*62.317*	*17.402*
N	*24.975*	*59.775*	*12.042*
C	*23.636*	*59.758*	*11.874*
N	*23.324*	*60.019*	*10.586*
C	*24.493*	*60.198*	*9.925*
C	*24.866*	*60.498*	*8.538*
C	*25.569*	*60.021*	*10.876*
N	*23.897*	*60.667*	*7.602*
N	*26.177*	*60.599*	*8.239*
C	*27.127*	*60.430*	*9.179*
N	*26.854*	*60.143*	*10.462*

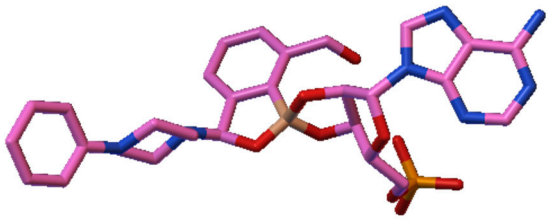


Figure S69. The best structure obtained in the docking studies of 9-R-c-2-AMP.

Table S69. Coordinates of the best 9-R-c-2-AMP spiroester.

O	*34.159*	*72.961*	*-0.403*
C	*33.278*	*71.846*	*-0.092*
C	*35.035*	*71.872*	*1.522*
C	*33.908*	*71.191*	*1.106*
C	*35.736*	*71.389*	*2.647*
C	*33.443*	*70.052*	*1.762*
C	*35.273*	*70.250*	*3.287*
C	*34.144*	*69.592*	*2.855*
C	*36.622*	*75.856*	*0.250*
O	*37.915*	*75.689*	*-0.344*
C	*36.473*	*74.798*	*1.335*
O	*35.187*	*74.192*	*1.366*
C	*37.403*	*73.725*	*0.844*
O	*36.546*	*72.883*	*0.101*
C	*38.458*	*74.426*	*-0.011*
B	*35.205*	*73.038*	*0.530*
N	*33.079*	*70.955*	*-1.195*
C	*33.914*	*71.248*	*-2.354*
C	*33.821*	*70.135*	*-3.361*
N	*32.441*	*69.886*	*-3.762*
C	*31.542*	*69.722*	*-2.622*
C	*31.694*	*70.848*	*-1.635*
C	*32.237*	*69.057*	*-4.876*
C	*31.420*	*69.422*	*-5.931*
C	*31.305*	*68.622*	*-7.052*
C	*31.958*	*67.440*	*-7.166*
C	*32.740*	*67.054*	*-6.119*
C	*32.883*	*67.839*	*-4.996*
C	*36.919*	*72.068*	*3.163*
O	*36.946*	*73.171*	*3.653*
C	*36.547*	*77.294*	*0.737*
O	*35.376*	*77.393*	*1.567*
P	*35.506*	*77.609*	*3.168*
O	*34.092*	*77.991*	*3.541*
O	*36.518*	*78.702*	*3.381*
O	*35.907*	*76.207*	*3.597*
N	*39.707*	*74.617*	*0.766*
C	*40.439*	*73.640*	*1.342*
N	*41.515*	*74.168*	*1.965*
C	*41.457*	*75.509*	*1.783*
C	*42.287*	*76.649*	*2.190*
C	*40.267*	*75.799*	*1.013*
N	*43.412*	*76.436*	*2.919*
N	*41.898*	*77.885*	*1.817*
C	*40.780*	*78.081*	*1.092*
N	*39.971*	*77.084*	*0.697*

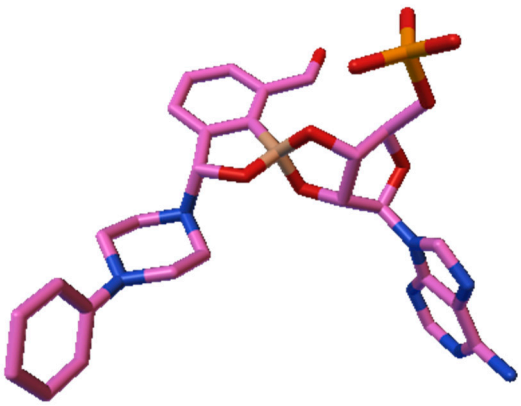


Figure S70. The best structure obtained in the docking studies of 9-S-1-AMP.

Table S70. Coordinates of the best 9-S-1-AMP spiroester.

O	*27.069*	*62.603*	*16.539*
C	*27.366*	*60.552*	*17.709*
C	*28.305*	*61.466*	*18.182*
C	*28.220*	*62.758*	*17.381*
C	*27.258*	*59.293*	*18.322*
C	*28.083*	*58.989*	*19.408*
C	*28.985*	*59.927*	*19.896*
C	*29.097*	*61.174*	*19.290*
C	*24.280*	*59.474*	*15.423*
O	*24.710*	*58.877*	*14.193*
C	*24.643*	*60.951*	*15.371*
O	*25.164*	*61.453*	*16.594*
C	*25.807*	*60.945*	*14.419*
O	*26.918*	*60.846*	*15.285*
C	*25.623*	*59.723*	*13.521*
B	*26.583*	*61.313*	*16.579*
N	*29.355*	*63.008*	*16.502*
C	*28.975*	*63.709*	*15.269*
C	*28.868*	*65.226*	*15.441*
N	*30.111*	*65.781*	*15.991*
C	*30.486*	*65.135*	*17.243*
C	*30.564*	*63.615*	*17.048*
C	*30.286*	*67.177*	*15.892*
C	*29.745*	*68.020*	*16.876*
C	*29.873*	*69.396*	*16.787*
C	*30.534*	*69.984*	*15.712*
C	*31.066*	*69.163*	*14.728*
C	*30.953*	*67.778*	*14.814*
C	*26.290*	*58.275*	*17.879*
O	*26.155*	*57.161*	*18.347*
C	*22.793*	*59.180*	*15.554*
O	*22.125*	*60.450*	*15.654*
P	*21.589*	*60.998*	*17.082*
O	*20.182*	*61.428*	*16.736*
O	*22.498*	*62.126*	*17.487*
O	*21.666*	*59.723*	*17.906*
N	*25.052*	*60.125*	*12.213*
C	*23.935*	*60.860*	*12.028*
N	*23.708*	*61.041*	*10.709*
C	*24.702*	*60.401*	*10.046*
C	*25.047*	*60.200*	*8.634*
C	*25.567*	*59.790*	*11.032*
N	*24.266*	*60.746*	*7.667*
N	*26.145*	*59.474*	*8.344*
C	*26.912*	*58.941*	*9.315*
N	*26.646*	*59.076*	*10.624*

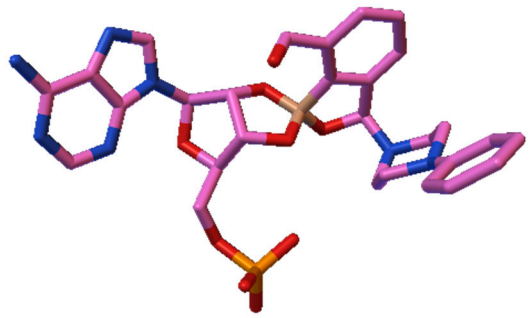


Figure S71. The best structure obtained in the docking studies of 9-S-2-AMP.

Table S71. Coordinates of the best 9-S-2-AMP spiroester.

O	*27.321*	*61.965*	*18.250*
C	*28.340*	*63.499*	*16.744*
C	*28.734*	*63.829*	*18.039*
C	*28.016*	*62.937*	*19.042*
C	*28.898*	*64.190*	*15.657*
C	*29.854*	*65.182*	*15.893*
C	*30.269*	*65.470*	*17.188*
C	*29.716*	*64.790*	*18.270*
C	*25.138*	*60.545*	*15.420*
O	*25.744*	*59.486*	*14.669*
C	*25.915*	*61.821*	*15.128*
O	*26.140*	*62.627*	*16.277*
C	*27.266*	*61.277*	*14.756*
O	*27.962*	*61.301*	*15.985*
C	*27.030*	*59.867*	*14.218*
B	*27.383*	*62.248*	*16.865*
N	*27.013*	*63.614*	*19.854*
C	*27.500*	*64.878*	*20.422*
C	*27.404*	*66.056*	*19.452*
N	*26.034*	*66.210*	*18.945*
C	*25.542*	*64.982*	*18.332*
C	*25.671*	*63.813*	*19.317*
C	*25.718*	*67.432*	*18.317*
C	*26.423*	*68.598*	*18.663*
C	*26.111*	*69.818*	*18.087*
C	*25.084*	*69.926*	*17.155*
C	*24.374*	*68.785*	*16.810*
C	*24.686*	*67.552*	*17.375*
C	*28.532*	*63.899*	*14.259*
O	*27.505*	*64.232*	*13.703*
C	*23.671*	*60.579*	*15.022*
O	*22.910*	*60.321*	*16.216*
P	*22.167*	*61.526*	*17.005*
O	*21.282*	*60.762*	*17.965*
O	*21.416*	*62.326*	*15.976*
O	*23.364*	*62.197*	*17.660*
N	*27.051*	*59.870*	*12.735*
C	*28.104*	*60.198*	*11.958*
N	*27.774*	*60.089*	*10.653*
C	*26.481*	*59.689*	*10.605*
C	*25.524*	*59.392*	*9.533*
C	*26.007*	*59.563*	*11.967*
N	*25.913*	*59.500*	*8.236*
N	*24.277*	*59.015*	*9.878*
C	*23.906*	*58.911*	*11.169*
N	*24.728*	*59.179*	*12.197*

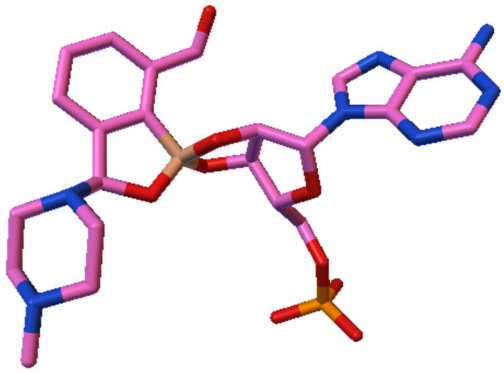


Figure S72. The best structure obtained in the docking studies of 10-R-1-AMP.

Table S72. Coordinates of the best 10-R-1-AMP spiroester.

O	*24.026*	*61.211*	*11.825*
C	*25.722*	*59.596*	*11.363*
C	*25.265*	*60.104*	*10.153*
C	*24.135*	*61.096*	*10.364*
C	*26.739*	*58.626*	*11.354*
C	*27.267*	*58.202*	*10.131*
C	*26.799*	*58.729*	*8.930*
C	*25.790*	*59.688*	*8.934*
C	*24.036*	*60.501*	*15.563*
O	*24.992*	*61.270*	*16.302*
C	*24.807*	*59.532*	*14.678*
O	*24.268*	*59.405*	*13.368*
C	*26.112*	*60.256*	*14.500*
O	*25.911*	*60.973*	*13.299*
C	*26.278*	*61.154*	*15.724*
B	*24.898*	*60.362*	*12.520*
N	*24.282*	*62.320*	*9.662*
C	*24.228*	*63.573*	*10.423*
C	*22.816*	*64.152*	*10.543*
N	*22.214*	*64.300*	*9.219*
C	*22.160*	*63.008*	*8.533*
C	*20.904*	*64.926*	*9.292*
C	*23.572*	*62.442*	*8.388*
C	*27.281*	*58.036*	*12.588*
O	*28.424*	*57.659*	*12.760*
C	*23.118*	*59.848*	*16.585*
O	*22.455*	*60.913*	*17.289*
P	*20.909*	*60.768*	*17.754*
O	*20.740*	*61.982*	*18.639*
O	*20.792*	*59.455*	*18.479*
O	*20.212*	*60.875*	*16.408*
N	*27.202*	*60.527*	*16.701*
C	*27.651*	*59.255*	*16.665*
N	*28.478*	*59.021*	*17.706*
C	*28.549*	*60.170*	*18.419*
C	*29.246*	*60.595*	*19.639*
C	*27.701*	*61.146*	*17.769*
N	*30.050*	*59.718*	*20.294*
N	*29.064*	*61.859*	*20.069*
C	*28.265*	*62.719*	*19.408*
N	*27.590*	*62.391*	*18.294*

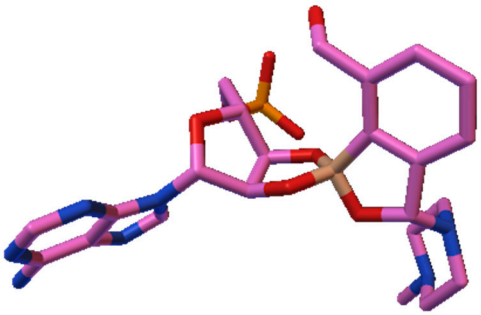


Figure S73. The best structure obtained in the docking studies of 10-R-2-AMP.

Table S73. Coordinates of the best 10-R-2-AMP spiroester.

O	*27.617*	*62.659*	*16.616*
C	*27.850*	*60.521*	*17.652*
C	*28.779*	*61.384*	*18.221*
C	*28.732*	*62.753*	*17.567*
C	*27.784*	*59.193*	*18.106*
C	*28.651*	*58.775*	*19.121*
C	*29.570*	*59.658*	*19.683*
C	*29.640*	*60.974*	*19.235*
C	*24.635*	*59.679*	*15.563*
O	*24.915*	*59.170*	*14.253*
C	*25.033*	*61.149*	*15.581*
O	*25.695*	*61.544*	*16.775*
C	*26.087*	*61.192*	*14.511*
O	*27.282*	*61.005*	*15.241*
C	*25.774*	*60.046*	*13.550*
B	*27.100*	*61.378*	*16.595*
N	*28.678*	*63.842*	*18.475*
C	*27.421*	*64.092*	*19.189*
C	*26.479*	*65.044*	*18.447*
N	*27.171*	*66.291*	*18.121*
C	*28.348*	*66.022*	*17.295*
C	*26.279*	*67.249*	*17.489*
C	*29.302*	*65.094*	*18.046*
C	*26.831*	*58.214*	*17.558*
O	*25.859*	*57.763*	*18.130*
C	*23.164*	*59.406*	*15.833*
O	*22.482*	*60.670*	*15.742*
P	*21.685*	*61.279*	*17.014*
O	*20.374*	*61.691*	*16.384*
O	*22.507*	*62.425*	*17.537*
O	*21.593*	*60.041*	*17.892*
N	*25.078*	*60.559*	*12.345*
C	*24.137*	*61.527*	*12.325*
N	*23.720*	*61.746*	*11.059*
C	*24.408*	*60.893*	*10.264*
C	*24.436*	*60.610*	*8.824*
C	*25.281*	*60.108*	*11.109*
N	*23.633*	*61.312*	*7.985*
N	*25.274*	*59.651*	*8.380*
C	*26.067*	*58.964*	*9.225*
N	*26.081*	*59.165*	*10.553*

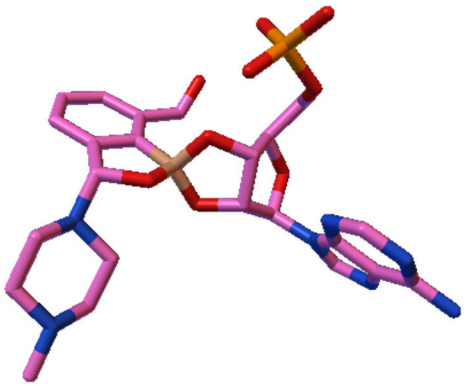


Figure S74. The best structure obtained in the docking studies of 10-S-1-AMP.

Table S74. Coordinates of the best 10-S-1-AMP spiroester.

O	*26.729*	*63.710*	*16.609*
C	*27.609*	*61.756*	*17.643*
C	*27.923*	*62.855*	*18.439*
C	*27.474*	*64.139*	*17.752*
C	*27.926*	*60.464*	*18.091*
C	*28.532*	*60.302*	*19.340*
C	*28.796*	*61.405*	*20.145*
C	*28.485*	*62.689*	*19.703*
C	*25.505*	*59.884*	*14.940*
O	*26.194*	*59.580*	*13.721*
C	*25.294*	*61.391*	*14.987*
O	*25.522*	*61.957*	*16.271*
C	*26.428*	*61.884*	*14.132*
O	*27.446*	*62.137*	*15.078*
C	*26.763*	*60.750*	*13.165*
B	*26.889*	*62.351*	*16.362*
N	*28.558*	*64.988*	*17.275*
C	*28.687*	*64.890*	*15.814*
C	*29.903*	*65.666*	*15.334*
N	*29.810*	*67.067*	*15.731*
C	*29.682*	*67.163*	*17.179*
C	*30.929*	*67.849*	*15.233*
C	*28.464*	*66.391*	*17.673*
C	*27.628*	*59.256*	*17.303*
O	*26.804*	*58.406*	*17.578*
C	*24.229*	*59.056*	*14.938*
O	*23.134*	*59.976*	*15.094*
P	*22.640*	*60.439*	*16.566*
O	*21.137*	*60.363*	*16.421*
O	*23.170*	*61.829*	*16.788*
O	*23.241*	*59.329*	*17.413*
N	*26.158*	*61.009*	*11.836*
C	*26.595*	*60.520*	*10.657*
N	*25.807*	*60.955*	*9.650*
C	*24.854*	*61.741*	*10.206*
C	*23.716*	*62.513*	*9.694*
C	*25.097*	*61.787*	*11.632*
N	*23.446*	*62.511*	*8.364*
N	*22.967*	*63.204*	*10.577*
C	*23.246*	*63.195*	*11.895*
N	*24.278*	*62.520*	*12.426*

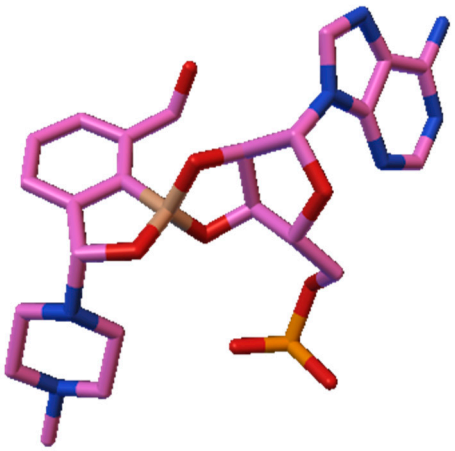


Figure S75. The best structure obtained in the docking studies of 10-S-2-AMP.

Table S75. Coordinates of the best 10-S-2-AMP spiroester.

O	*27.641*	*61.961*	*18.384*
C	*28.204*	*63.456*	*16.622*
C	*28.742*	*63.952*	*17.808*
C	*28.305*	*63.079*	*18.978*
C	*28.489*	*64.105*	*15.410*
C	*29.325*	*65.225*	*15.413*
C	*29.893*	*65.680*	*16.598*
C	*29.610*	*65.041*	*17.802*
C	*25.221*	*60.044*	*16.049*
O	*25.846*	*58.988*	*15.310*
C	*25.786*	*61.362*	*15.539*
O	*26.063*	*62.300*	*16.570*
C	*27.131*	*60.936*	*15.020*
O	*27.979*	*61.162*	*16.127*
C	*27.001*	*59.461*	*14.644*
B	*27.411*	*62.124*	*16.999*
N	*27.363*	*63.713*	*19.894*
C	*27.803*	*65.076*	*20.225*
C	*26.899*	*65.685*	*21.285*
N	*25.514*	*65.707*	*20.828*
C	*25.078*	*64.357*	*20.499*
C	*24.633*	*66.340*	*21.795*
C	*25.976*	*63.736*	*19.435*
C	*27.955*	*63.641*	*14.118*
O	*28.560*	*63.001*	*13.280*
C	*23.720*	*59.873*	*15.870*
O	*23.160*	*61.194*	*15.764*
P	*22.381*	*61.870*	*17.014*
O	*21.499*	*62.880*	*16.314*
O	*23.428*	*62.477*	*17.906*
O	*21.635*	*60.660*	*17.552*
N	*26.820*	*59.316*	*13.179*
C	*27.806*	*59.196*	*12.267*
N	*27.284*	*59.080*	*11.026*
C	*25.937*	*59.133*	*11.159*
C	*24.799*	*59.073*	*10.234*
C	*25.639*	*59.304*	*12.565*
N	*25.021*	*58.920*	*8.904*
N	*23.556*	*59.170*	*10.747*
C	*23.351*	*59.320*	*12.070*
N	*24.347*	*59.394*	*12.9*

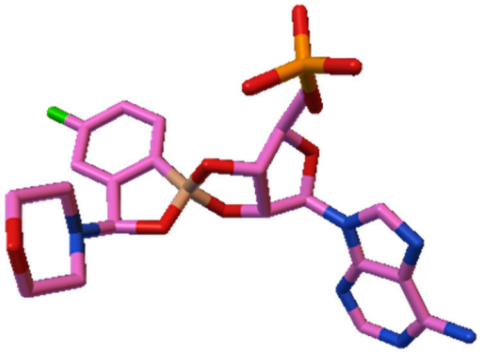


Figure S76. The best structure obtained in the docking studies of 11-R-1-AMP.

Table S76. Coordinates of the best 11-R-1-AMP spiroester.

C	*27.917*	*60.690*	*17.614*
C	*27.818*	*59.512*	*18.352*
C	*28.668*	*59.301*	*19.431*
C	*29.603*	*60.278*	*19.752*
C	*29.734*	*61.461*	*19.043*
C	*28.875*	*61.643*	*17.971*
O	*27.728*	*62.537*	*16.113*
C	*28.844*	*62.825*	*17.023*
F	*30.419*	*60.063*	*20.804*
C	*24.587*	*59.517*	*15.885*
O	*24.779*	*58.720*	*14.710*
C	*25.027*	*60.937*	*15.555*
O	*25.766*	*61.561*	*16.598*
C	*26.022*	*60.699*	*14.454*
O	*27.249*	*60.630*	*15.150*
C	*25.624*	*59.382*	*13.790*
B	*27.153*	*61.302*	*16.393*
N	*28.758*	*64.101*	*17.653*
C	*28.658*	*65.223*	*16.713*
C	*28.796*	*66.534*	*17.473*
O	*27.817*	*66.646*	*18.494*
C	*27.919*	*65.566*	*19.412*
C	*27.752*	*64.222*	*18.714*
C	*23.126*	*59.370*	*16.279*
O	*22.484*	*60.620*	*15.970*
P	*21.497*	*61.335*	*17.039*
O	*21.283*	*60.228*	*18.046*
O	*20.257*	*61.736*	*16.288*
O	*22.398*	*62.457*	*17.528*
N	*24.876*	*59.643*	*12.535*
C	*23.545*	*59.839*	*12.431*
N	*23.203*	*60.051*	*11.142*
C	*24.344*	*59.982*	*10.415*
C	*24.678*	*60.110*	*8.992*
C	*25.432*	*59.698*	*11.326*
N	*23.695*	*60.370*	*8.091*
N	*25.967*	*59.968*	*8.625*
C	*26.931*	*59.712*	*9.530*
N	*26.692*	*59.572*	*10.844*

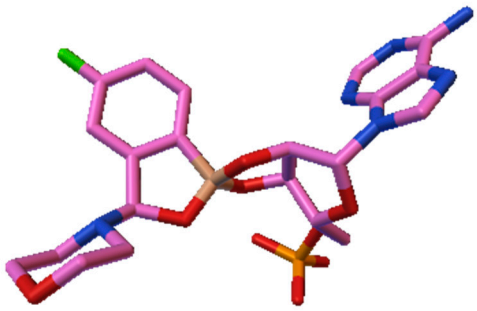


Figure S80. The best structure obtained in the docking studies of 11-R-2-AMP.

Table S80. Coordinates of the best 11-R-2-AMP spiroester.

C	*27.412*	*62.337*	*16.159*
C	*27.633*	*63.368*	*15.246*
C	*28.637*	*64.297*	*15.487*
C	*29.404*	*64.177*	*16.640*
C	*29.216*	*63.169*	*17.571*
C	*28.206*	*62.257*	*17.306*
O	*26.712*	*60.434*	*17.418*
C	*27.780*	*61.095*	*18.181*
F	*30.378*	*65.083*	*16.858*
C	*23.715*	*59.814*	*15.188*
O	*23.995*	*58.993*	*14.048*
C	*24.453*	*61.132*	*15.000*
O	*25.065*	*61.616*	*16.188*
C	*25.591*	*60.718*	*14.109*
O	*26.622*	*60.433*	*15.031*
C	*25.110*	*59.492*	*13.336*
B	*26.398*	*61.114*	*16.253*
N	*28.833*	*60.218*	*18.574*
C	*29.135*	*60.258*	*20.008*
C	*30.406*	*59.465*	*20.281*
O	*30.283*	*58.124*	*19.832*
C	*29.999*	*58.082*	*18.439*
C	*28.717*	*58.831*	*18.108*
C	*22.201*	*59.931*	*15.281*
O	*21.916*	*61.239*	*15.807*
P	*21.296*	*61.422*	*17.293*
O	*21.482*	*60.038*	*17.874*
O	*19.859*	*61.831*	*17.121*
O	*22.247*	*62.466*	*17.855*
N	*24.686*	*59.879*	*11.968*
C	*24.709*	*59.085*	*10.877*
N	*24.251*	*59.759*	*9.799*
C	*23.938*	*61.008*	*10.218*
C	*23.409*	*62.217*	*9.576*
C	*24.240*	*61.088*	*11.631*
N	*23.115*	*62.201*	*8.251*
N	*23.228*	*63.315*	*10.338*
C	*23.523*	*63.315*	*11.652*
N	*24.021*	*62.248*	*12.297*

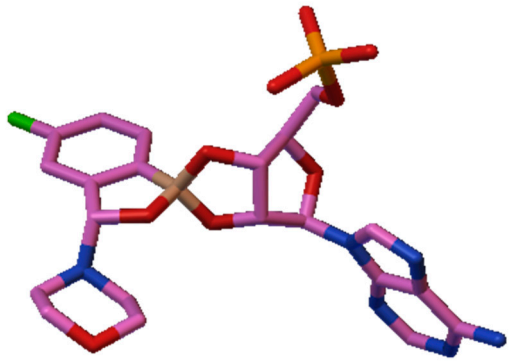


Figure S81. The best structure obtained in the docking studies of 11-S-1-AMP.

Table S81. Coordinates of the best 11-S-1-AMP.

C	*28.020*	*60.616*	*17.720*
C	*27.985*	*59.306*	*18.194*
C	*28.808*	*58.929*	*19.248*
C	*29.639*	*59.885*	*19.817*
C	*29.703*	*61.196*	*19.373*
C	*28.894*	*61.543*	*18.298*
O	*27.590*	*62.746*	*16.750*
C	*28.724*	*62.904*	*17.638*
F	*30.418*	*59.525*	*20.859*
C	*24.899*	*59.462*	*15.748*
O	*25.209*	*58.977*	*14.435*
C	*25.123*	*60.968*	*15.748*
O	*25.759*	*61.448*	*16.925*
C	*26.144*	*61.124*	*14.656*
O	*27.367*	*61.082*	*15.362*
C	*25.947*	*59.941*	*13.709*
B	*27.170*	*61.444*	*16.717*
N	*29.834*	*63.350*	*16.818*
C	*30.588*	*64.547*	*17.196*
C	*29.913*	*65.846*	*16.759*
O	*29.652*	*65.836*	*15.360*
C	*28.840*	*64.725*	*14.991*
C	*29.497*	*63.404*	*15.386*
C	*23.475*	*59.023*	*16.050*
O	*22.616*	*60.120*	*15.693*
P	*21.724*	*60.877*	*16.814*
O	*21.645*	*59.829*	*17.901*
O	*20.402*	*61.204*	*16.174*
O	*22.638*	*62.047*	*17.141*
N	*25.172*	*60.359*	*12.516*
C	*24.038*	*61.090*	*12.523*
N	*23.602*	*61.289*	*11.261*
C	*24.478*	*60.664*	*10.438*
C	*24.592*	*60.485*	*8.986*
C	*25.492*	*60.043*	*11.263*
N	*23.664*	*61.040*	*8.165*
N	*25.631*	*59.768*	*8.513*
C	*26.545*	*59.225*	*9.339*
N	*26.493*	*59.341*	*10.676*

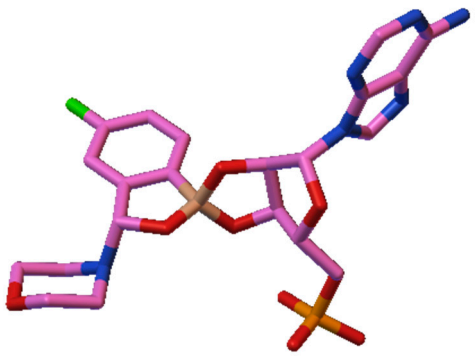


Figure S82. The best structure obtained in the docking studies of 11-S-2-AMP.

Table S82. Coordinates of the best 11-S-2-AMP spiroester.

C	*27.390*	*62.691*	*15.943*
C	*27.239*	*63.942*	*15.349*
C	*28.134*	*64.962*	*15.648*
C	*29.176*	*64.698*	*16.527*
C	*29.358*	*63.467*	*17.138*
C	*28.432*	*62.472*	*16.850*
O	*27.386*	*60.386*	*16.534*
C	*28.410*	*61.028*	*17.333*
F	*30.060*	*65.681*	*16.795*
C	*24.167*	*59.806*	*14.621*
O	*24.402*	*59.432*	*13.257*
C	*24.612*	*61.253*	*14.785*
O	*25.312*	*61.499*	*15.997*
C	*25.644*	*61.379*	*13.699*
O	*26.847*	*61.079*	*14.376*
C	*25.274*	*60.352*	*12.631*
B	*26.706*	*61.312*	*15.766*
N	*28.037*	*60.835*	*18.721*
C	*28.619*	*61.683*	*19.762*
C	*30.006*	*61.220*	*20.207*
O	*29.977*	*59.859*	*20.623*
C	*29.497*	*59.009*	*19.587*
C	*28.098*	*59.423*	*19.135*
C	*22.694*	*59.549*	*14.896*
O	*22.155*	*60.764*	*15.448*
P	*21.811*	*60.879*	*17.027*
O	*20.299*	*60.905*	*17.010*
O	*22.445*	*62.151*	*17.522*
O	*22.406*	*59.573*	*17.529*
N	*24.569*	*61.011*	*11.504*
C	*23.550*	*61.889*	*11.612*
N	*23.149*	*62.292*	*10.387*
C	*23.930*	*61.650*	*9.486*
C	*24.022*	*61.627*	*8.021*
C	*24.845*	*60.801*	*10.219*
N	*23.184*	*62.399*	*7.283*
N	*24.951*	*60.832*	*7.454*
C	*25.777*	*60.073*	*8.199*
N	*25.738*	*60.039*	*9.542*

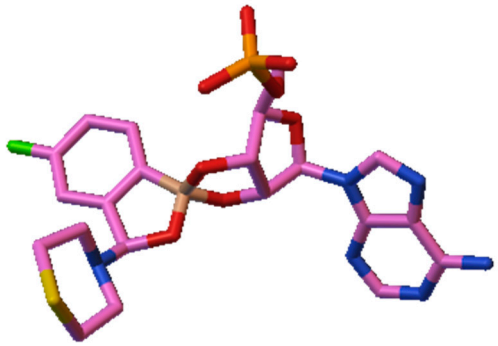


Figure S83. The best structure obtained in the docking studies of 12-R-1-AMP.

Table S83. Coordinates of the best 12-R-1-AMP spiroester.

C	*27.797*	*60.771*	*17.560*
C	*27.569*	*59.651*	*18.357*
C	*28.354*	*59.434*	*19.482*
C	*29.357*	*60.348*	*19.790*
C	*29.616*	*61.473*	*19.024*
C	*28.817*	*61.662*	*17.905*
O	*27.827*	*62.534*	*15.950*
C	*28.930*	*62.781*	*16.890*
F	*30.107*	*60.129*	*20.887*
C	*24.494*	*59.777*	*15.718*
O	*24.693*	*58.883*	*14.616*
C	*25.074*	*61.129*	*15.325*
O	*25.794*	*61.765*	*16.373*
C	*26.114*	*60.732*	*14.315*
O	*27.283*	*60.616*	*15.099*
C	*25.649*	*59.406*	*13.715*
B	*27.164*	*61.382*	*16.284*
N	*28.936*	*64.100*	*17.434*
C	*29.018*	*65.155*	*16.417*
C	*29.482*	*66.477*	*17.013*
S	*28.325*	*67.116*	*18.279*
C	*28.238*	*65.588*	*19.283*
C	*27.906*	*64.360*	*18.447*
C	*23.003*	*59.777*	*16.017*
O	*22.567*	*61.147*	*15.958*
P	*21.704*	*61.797*	*17.166*
O	*20.588*	*62.482*	*16.410*
O	*22.620*	*62.738*	*17.901*
O	*21.278*	*60.537*	*17.901*
N	*25.010*	*59.633*	*12.396*
C	*23.683*	*59.640*	*12.149*
N	*23.453*	*59.881*	*10.840*
C	*24.662*	*60.024*	*10.247*
C	*25.123*	*60.289*	*8.879*
C	*25.676*	*59.845*	*11.263*
N	*24.215*	*60.459*	*7.884*
N	*26.451*	*60.359*	*8.657*
C	*27.340*	*60.190*	*9.654*
N	*26.986*	*59.934*	*10.924*

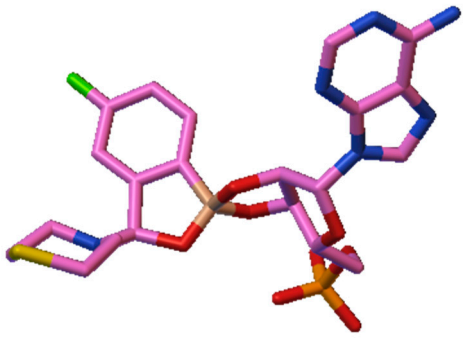


Figure S84. The best structure obtained in the docking studies of 12-R-2-AMP.

Table S84. Coordinates of the best 12-R-2-AMP spiroester.

C	*34.938*	*71.593*	*1.917*
C	*35.533*	*70.931*	*2.991*
C	*34.845*	*69.911*	*3.636*
C	*33.572*	*69.568*	*3.190*
C	*32.948*	*70.202*	*2.127*
C	*33.657*	*71.218*	*1.504*
O	*34.324*	*72.959*	*0.057*
C	*33.179*	*72.087*	*0.357*
F	*32.919*	*68.574*	*3.820*
C	*37.420*	*75.072*	*0.399*
O	*38.552*	*74.573*	*-0.324*
C	*37.128*	*74.096*	*1.530*
O	*35.742*	*73.843*	*1.720*
C	*37.691*	*72.816*	*0.979*
O	*36.568*	*72.220*	*0.363*
C	*38.787*	*73.215*	*-0.007*
B	*35.369*	*72.718*	*0.927*
N	*32.684*	*71.379*	*-0.778*
C	*33.737*	*70.951*	*-1.706*
C	*33.173*	*70.628*	*-3.084*
S	*31.973*	*69.247*	*-3.043*
C	*30.917*	*69.918*	*-1.707*
C	*31.718*	*70.315*	*-0.475*
C	*37.772*	*76.484*	*0.841*
O	*37.205*	*76.664*	*2.151*
P	*35.783*	*77.417*	*2.347*
O	*34.890*	*76.630*	*1.415*
O	*35.989*	*78.851*	*1.941*
O	*35.537*	*77.148*	*3.822*
N	*40.122*	*73.081*	*0.624*
C	*40.840*	*74.079*	*1.181*
N	*42.008*	*73.602*	*1.663*
C	*42.030*	*72.273*	*1.399*
C	*42.982*	*71.182*	*1.641*
C	*40.805*	*71.940*	*0.705*
N	*44.150*	*71.439*	*2.282*
N	*42.654*	*69.946*	*1.214*
C	*41.490*	*69.706*	*0.581*
N	*40.582*	*70.660*	*0.319*

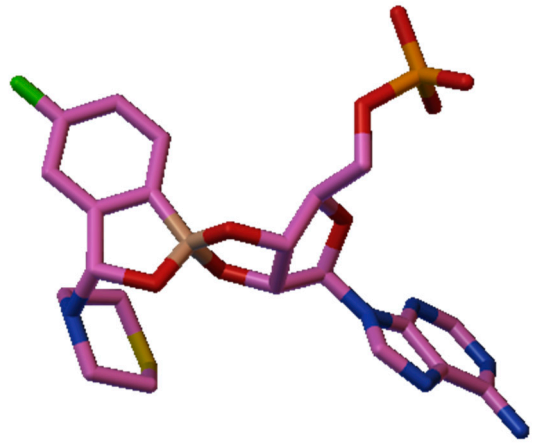


Figure S85. The best structure obtained in the docking studies of 12-S-1-AMP.

Table S85. Coordinates of the best 12-S-1-AMP spiroester.

C	*23.571*	*61.775*	*11.456*
C	*23.105*	*63.031*	*11.834*
C	*22.632*	*63.914*	*10.871*
C	*22.625*	*63.505*	*9.544*
C	*23.080*	*62.263*	*9.130*
C	*23.576*	*61.409*	*10.106*
O	*24.254*	*59.501*	*11.308*
C	*24.096*	*59.985*	*9.952*
F	*22.144*	*64.353*	*8.611*
C	*23.528*	*61.117*	*15.270*
O	*24.758*	*61.432*	*15.934*
C	*23.770*	*59.883*	*14.411*
O	*23.159*	*59.953*	*13.130*
C	*25.247*	*59.979*	*14.151*
O	*25.303*	*60.673*	*12.922*
C	*25.842*	*60.762*	*15.320*
B	*24.087*	*60.523*	*12.211*
N	*25.390*	*59.854*	*9.304*
C	*26.251*	*58.724*	*9.636*
C	*26.995*	*58.827*	*10.974*
S	*28.084*	*60.301*	*11.045*
C	*26.847*	*61.542*	*10.501*
C	*26.125*	*61.121*	*9.218*
C	*22.476*	*60.949*	*16.356*
O	*21.820*	*62.222*	*16.500*
P	*21.659*	*62.915*	*17.956*
O	*23.093*	*63.250*	*18.296*
O	*21.032*	*61.890*	*18.861*
O	*20.808*	*64.120*	*17.587*
N	*26.465*	*59.836*	*16.296*
C	*26.208*	*58.516*	*16.412*
N	*26.955*	*57.980*	*17.402*
C	*27.696*	*58.985*	*17.926*
C	*28.687*	*59.093*	*19.003*
C	*27.361*	*60.199*	*17.212*
N	*29.035*	*57.988*	*19.710*
N	*29.227*	*60.303*	*19.253*
C	*28.874*	*61.391*	*18.541*
N	*27.966*	*61.363*	*17.552*

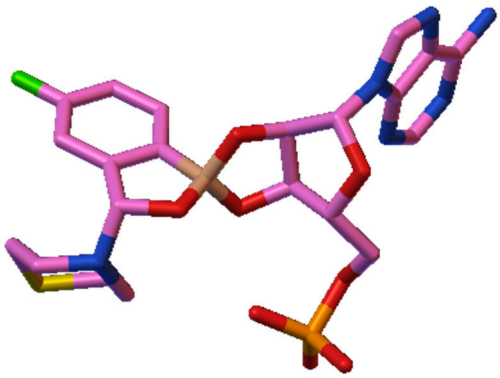


Figure S86. The best structure obtained in the docking studies of 12-S-2-AMP.

Table S86. Coordinates of the best 12-S-2-AMP spiroester.

C	*27.966*	*63.348*	*16.353*
C	*28.329*	*63.964*	*15.158*
C	*29.225*	*65.027*	*15.170*
C	*29.748*	*65.438*	*16.388*
C	*29.411*	*64.852*	*17.597*
C	*28.491*	*63.812*	*17.566*
O	*27.233*	*61.891*	*18.084*
C	*27.974*	*62.961*	*18.718*
F	*30.636*	*66.454*	*16.395*
C	*25.042*	*59.932*	*15.741*
O	*25.724*	*58.830*	*15.128*
C	*25.653*	*61.214*	*15.194*
O	*25.846*	*62.219*	*16.181*
C	*27.036*	*60.757*	*14.820*
O	*27.788*	*61.058*	*15.977*
C	*26.933*	*59.261*	*14.533*
B	*27.153*	*62.074*	*16.733*
N	*27.058*	*63.626*	*19.629*
C	*25.732*	*64.015*	*19.162*
C	*25.681*	*65.273*	*18.285*
S	*26.338*	*66.747*	*19.153*
C	*27.915*	*66.006*	*19.731*
C	*27.701*	*64.665*	*20.442*
C	*23.562*	*59.747*	*15.447*
O	*22.961*	*61.053*	*15.495*
P	*22.348*	*61.638*	*16.876*
O	*21.809*	*60.384*	*17.526*
O	*21.293*	*62.640*	*16.496*
O	*23.612*	*62.181*	*17.523*
N	*26.875*	*59.019*	*13.071*
C	*27.716*	*58.236*	*12.363*
N	*27.371*	*58.241*	*11.057*
C	*26.291*	*59.050*	*10.937*
C	*25.442*	*59.490*	*9.825*
C	*25.981*	*59.569*	*12.252*
N	*25.691*	*59.039*	*8.569*
N	*24.427*	*60.335*	*10.094*
C	*24.190*	*60.773*	*11.346*
N	*24.936*	*60.419*	*12.405*

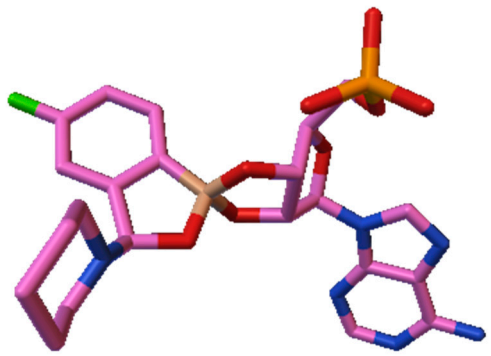


Figure S87. The best structure obtained in the docking studies of 13-R-1-AMP.

Table S87. Coordinates of the best 13-R-1-AMP spiroester.

C	*27.791*	*60.782*	*17.602*
C	*27.675*	*59.598*	*18.330*
C	*28.546*	*59.350*	*19.384*
C	*29.522*	*60.292*	*19.683*
C	*29.672*	*61.477*	*18.980*
C	*28.784*	*61.707*	*17.937*
O	*27.634*	*62.634*	*16.111*
C	*28.738*	*62.918*	*17.005*
F	*30.366*	*60.040*	*20.704*
C	*24.609*	*59.490*	*15.811*
O	*24.880*	*58.718*	*14.634*
C	*24.979*	*60.936*	*15.509*
O	*25.651*	*61.587*	*16.579*
C	*26.018*	*60.767*	*14.436*
O	*27.226*	*60.757*	*15.168*
C	*25.713*	*59.438*	*13.746*
B	*27.055*	*61.408*	*16.414*
N	*28.567*	*64.224*	*17.581*
C	*29.625*	*65.191*	*17.308*
C	*29.125*	*66.610*	*17.574*
C	*28.582*	*66.742*	*19.000*
C	*27.536*	*65.658*	*19.281*
C	*28.088*	*64.269*	*18.961*
C	*23.147*	*59.258*	*16.158*
O	*22.446*	*60.473*	*15.841*
P	*21.942*	*61.474*	*17.011*
O	*20.976*	*62.362*	*16.260*
O	*23.160*	*62.187*	*17.531*
O	*21.276*	*60.479*	*17.948*
N	*24.991*	*59.671*	*12.472*
C	*23.651*	*59.730*	*12.320*
N	*23.337*	*59.960*	*11.027*
C	*24.505*	*60.043*	*10.346*
C	*24.877*	*60.267*	*8.944*
C	*25.582*	*59.837*	*11.291*
N	*23.907*	*60.459*	*8.014*
N	*26.187*	*60.277*	*8.627*
C	*27.138*	*60.086*	*9.561*
N	*26.866*	*59.864*	*10.858*

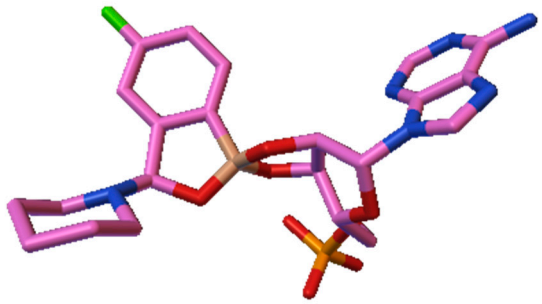


Figure S88. The best structure obtained in the docking studies of 13-R-2-AMP.

Table S88. Coordinates of the best 13-R-2-AMP spiroester.

C	*27.195*	*62.401*	*16.080*
C	*27.340*	*63.447*	*15.169*
C	*28.259*	*64.458*	*15.422*
C	*29.011*	*64.402*	*16.589*
C	*28.893*	*63.383*	*17.520*
C	*27.974*	*62.380*	*17.240*
O	*26.622*	*60.461*	*17.341*
C	*27.643*	*61.157*	*18.096*
F	*29.897*	*65.391*	*16.828*
C	*23.623*	*59.766*	*15.140*
O	*23.917*	*58.946*	*14.002*
C	*24.332*	*61.099*	*14.943*
O	*24.938*	*61.601*	*16.126*
C	*25.475*	*60.706*	*14.049*
O	*26.516*	*60.448*	*14.968*
C	*25.018*	*59.467*	*13.283*
B	*26.282*	*61.129*	*16.188*
N	*28.701*	*60.244*	*18.431*
C	*28.494*	*58.850*	*18.053*
C	*29.824*	*58.099*	*18.045*
C	*30.533*	*58.227*	*19.398*
C	*30.658*	*59.698*	*19.805*
C	*29.299*	*60.398*	*19.756*
C	*22.108*	*59.850*	*15.237*
O	*21.796*	*61.157*	*15.752*
P	*21.228*	*61.343*	*17.258*
O	*21.634*	*60.037*	*17.903*
O	*19.741*	*61.539*	*17.144*
O	*22.047*	*62.541*	*17.709*
N	*24.581*	*59.838*	*11.915*
C	*24.583*	*59.028*	*10.835*
N	*24.118*	*59.691*	*9.754*
C	*23.822*	*60.949*	*10.159*
C	*23.296*	*62.154*	*9.507*
C	*24.142*	*61.046*	*11.567*
N	*22.985*	*62.122*	*8.186*
N	*23.135*	*63.264*	*10.255*
C	*23.447*	*63.281*	*11.565*
N	*23.942*	*62.218*	*12.219*

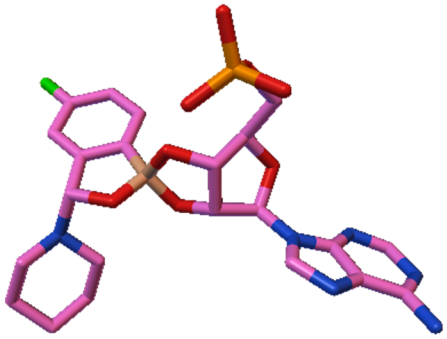


Figure S89. The best structure obtained in the docking studies of 13-S-1-AMP.

Table S89. Coordinates of the best 13-S-1-AMP spiroester.

C	*27.776*	*61.328*	*17.570*
C	*28.143*	*59.994*	*17.743*
C	*28.934*	*59.632*	*18.825*
C	*29.325*	*60.615*	*19.722*
C	*28.984*	*61.950*	*19.582*
C	*28.222*	*62.298*	*18.473*
O	*26.745*	*63.397*	*17.011*
C	*27.665*	*63.665*	*18.089*
F	*30.070*	*60.254*	*20.788*
C	*25.346*	*59.799*	*14.998*
O	*25.844*	*59.751*	*13.655*
C	*25.089*	*61.259*	*15.343*
O	*25.496*	*61.613*	*16.659*
C	*26.054*	*61.962*	*14.429*
O	*27.199*	*62.116*	*15.242*
C	*26.274*	*61.032*	*13.237*
B	*26.844*	*62.073*	*16.612*
N	*28.634*	*64.632*	*17.598*
C	*28.414*	*66.015*	*18.030*
C	*29.564*	*66.915*	*17.575*
C	*29.771*	*66.848*	*16.061*
C	*29.907*	*65.390*	*15.618*
C	*28.742*	*64.550*	*16.133*
C	*24.118*	*58.902*	*15.040*
O	*23.600*	*58.967*	*16.380*
P	*22.391*	*59.979*	*16.757*
O	*21.733*	*59.254*	*17.909*
O	*21.528*	*60.104*	*15.532*
O	*23.187*	*61.208*	*17.166*
N	*25.456*	*61.473*	*12.081*
C	*24.567*	*62.489*	*12.081*
N	*24.004*	*62.616*	*10.859*
C	*24.546*	*61.655*	*10.073*
C	*24.379*	*61.241*	*8.675*
C	*25.481*	*60.900*	*10.880*
N	*23.510*	*61.910*	*7.875*
N	*25.108*	*60.198*	*8.229*
C	*25.968*	*59.545*	*9.034*
N	*26.159*	*59.866*	*10.325*

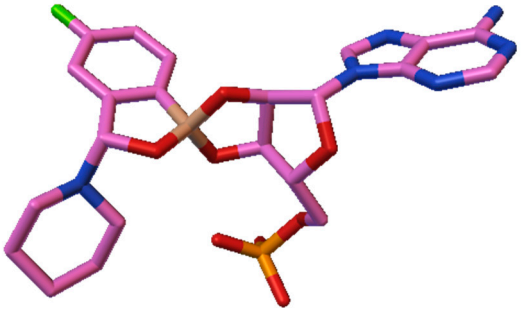


Figure S90. The best structure obtained in the docking studies of 13-S-2-AMP.

Table S90. Coordinates of the best 13-S-2-AMP spiroester.

C	*28.001*	*61.235*	*18.519*
C	*28.579*	*61.124*	*19.782*
C	*29.203*	*59.940*	*20.154*
C	*29.252*	*58.898*	*19.239*
C	*28.689*	*58.969*	*17.975*
C	*28.035*	*60.149*	*17.636*
O	*27.097*	*61.938*	*16.435*
C	*27.370*	*60.527*	*16.318*
F	*29.886*	*57.761*	*19.593*
C	*26.004*	*65.235*	*17.946*
O	*27.013*	*66.252*	*17.898*
C	*26.483*	*64.156*	*18.907*
O	*26.227*	*62.834*	*18.452*
C	*27.975*	*64.320*	*18.829*
O	*28.339*	*63.393*	*17.827*
C	*28.230*	*65.773*	*18.435*
B	*27.355*	*62.382*	*17.705*
N	*26.106*	*59.864*	*16.031*
C	*26.014*	*59.230*	*14.714*
C	*24.706*	*58.449*	*14.577*
C	*23.488*	*59.338*	*14.836*
C	*23.644*	*60.063*	*16.173*
C	*24.984*	*60.791*	*16.247*
C	*24.708*	*65.924*	*18.345*
O	*24.125*	*65.136*	*19.398*
P	*23.025*	*63.993*	*19.069*
O	*22.621*	*63.549*	*20.457*
O	*23.723*	*62.934*	*18.261*
O	*21.976*	*64.827*	*18.352*
N	*28.592*	*66.575*	*19.629*
C	*28.755*	*66.102*	*20.882*
N	*29.086*	*67.107*	*21.722*
C	*29.127*	*68.241*	*20.983*
C	*29.409*	*69.654*	*21.263*
C	*28.787*	*67.892*	*19.620*
N	*29.726*	*70.039*	*22.525*
N	*29.345*	*70.531*	*20.241*
C	*29.031*	*70.134*	*18.993*
N	*28.750*	*68.860*	*18.671*

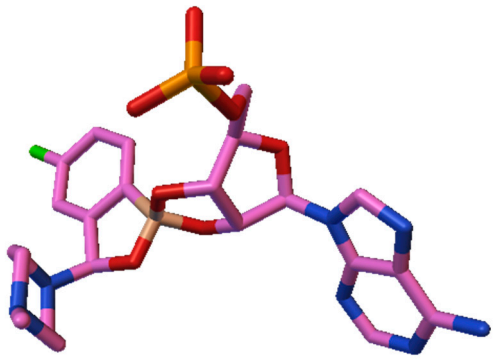


Figure S91. The best structure obtained in the docking studies of 14-R-1-AMP.

Table S91. Coordinates of the best 14-R-1-AMP spiroester.

O	*27.908*	*62.544*	*16.151*
C	*27.912*	*60.674*	*17.635*
C	*28.930*	*61.546*	*18.028*
C	*29.033*	*62.732*	*17.090*
C	*27.700*	*59.504*	*18.364*
C	*28.498*	*59.219*	*19.465*
C	*29.497*	*60.117*	*19.821*
C	*29.741*	*61.290*	*19.124*
F	*30.261*	*59.832*	*20.895*
C	*24.617*	*59.690*	*15.826*
O	*24.794*	*58.889*	*14.652*
C	*25.122*	*61.091*	*15.509*
O	*25.869*	*61.680*	*16.566*
C	*26.123*	*60.816*	*14.423*
O	*27.335*	*60.693*	*15.138*
C	*25.680*	*59.519*	*13.747*
B	*27.247*	*61.364*	*16.382*
N	*29.090*	*63.995*	*17.728*
C	*28.155*	*64.269*	*18.823*
C	*26.846*	*64.912*	*18.357*
N	*27.122*	*66.113*	*17.570*
C	*27.949*	*65.786*	*16.407*
C	*25.898*	*66.794*	*17.183*
C	*29.269*	*65.170*	*16.873*
C	*23.145*	*59.604*	*16.196*
O	*22.594*	*60.922*	*16.024*
P	*21.633*	*61.576*	*17.153*
O	*21.267*	*60.365*	*17.982*
O	*20.473*	*62.204*	*16.430*
O	*22.615*	*62.520*	*17.829*
N	*24.965*	*59.815*	*12.482*
C	*23.627*	*59.815*	*12.309*
N	*23.320*	*60.131*	*11.032*
C	*24.492*	*60.328*	*10.383*
C	*24.872*	*60.682*	*9.010*
C	*25.564*	*60.105*	*11.329*
N	*23.908*	*60.897*	*8.080*
N	*26.185*	*60.786*	*8.720*
C	*27.131*	*60.572*	*9.654*
N	*26.852*	*60.234*	*10.924*

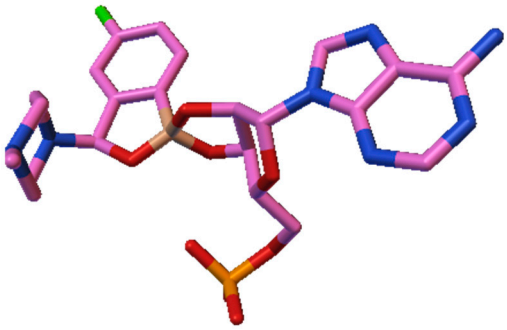


Figure S92. The best structure obtained in the docking studies of 14-R-2-AMP.

Table S92. Coordinates of the best 14-R-2-AMP spiroester.

O	*25.881*	*61.548*	*17.155*
C	*27.917*	*61.465*	*18.397*
C	*27.654*	*60.185*	*17.904*
C	*26.337*	*60.143*	*17.154*
C	*29.073*	*61.678*	*19.149*
C	*29.943*	*60.625*	*19.399*
C	*29.641*	*59.370*	*18.885*
C	*28.505*	*59.114*	*18.134*
F	*30.496*	*58.356*	*19.128*
C	*25.187*	*65.086*	*18.278*
O	*25.747*	*66.088*	*17.419*
C	*26.342*	*64.362*	*18.955*
O	*26.162*	*62.955*	*19.037*
C	*27.452*	*64.562*	*17.961*
O	*27.373*	*63.398*	*17.166*
C	*27.123*	*65.844*	*17.199*
B	*26.734*	*62.353*	*17.878*
N	*26.393*	*59.520*	*15.883*
C	*27.550*	*59.783*	*15.023*
C	*27.351*	*60.975*	*14.084*
N	*26.126*	*60.806*	*13.303*
C	*24.967*	*60.679*	*14.187*
C	*25.952*	*61.881*	*12.340*
C	*25.153*	*59.472*	*15.107*
C	*24.234*	*65.803*	*19.221*
O	*23.442*	*64.788*	*19.864*
P	*22.459*	*63.830*	*19.003*
O	*23.450*	*62.947*	*18.279*
O	*21.656*	*64.726*	*18.100*
O	*21.709*	*63.135*	*20.127*
N	*27.916*	*66.979*	*17.731*
C	*29.130*	*66.893*	*18.314*
N	*29.561*	*68.121*	*18.677*
C	*28.595*	*69.000*	*18.321*
C	*28.422*	*70.453*	*18.428*
C	*27.514*	*68.248*	*17.719*
N	*29.401*	*71.207*	*18.990*
N	*27.283*	*70.996*	*17.954*
C	*26.321*	*70.236*	*17.397*
N	*26.410*	*68.901*	*17.279*

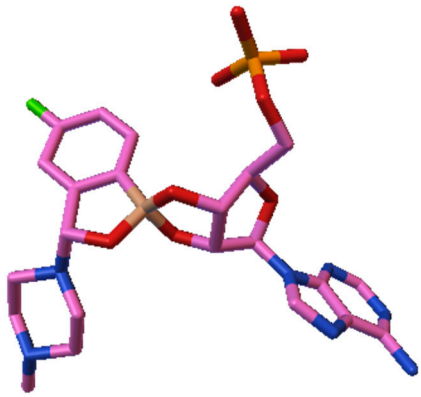


Figure S93. The best structure obtained in the docking studies of 14-S-1-AMP.

Table S93. Coordinates of the best 14-S-1-AMP spiroester.

O	*15.464*	*64.177*	*18.162*
C	*17.412*	*65.331*	*17.431*
C	*16.420*	*66.277*	*17.720*
C	*15.124*	*65.569*	*18.091*
C	*18.693*	*65.758*	*17.090*
C	*18.989*	*67.116*	*17.053*
C	*17.988*	*68.020*	*17.381*
C	*16.702*	*67.636*	*17.725*
F	*18.283*	*69.336*	*17.374*
C	*19.059*	*61.782*	*17.127*
O	*18.884*	*61.216*	*15.823*
C	*17.696*	*61.808*	*17.805*
O	*17.444*	*63.004*	*18.531*
C	*16.769*	*61.860*	*16.623*
O	*16.555*	*63.246*	*16.454*
C	*17.518*	*61.213*	*15.459*
B	*16.803*	*63.938*	*17.665*
N	*14.042*	*65.702*	*17.124*
C	*13.188*	*64.506*	*17.141*
C	*12.146*	*64.580*	*16.036*
N	*11.326*	*65.778*	*16.183*
C	*12.173*	*66.963*	*16.167*
C	*10.279*	*65.847*	*15.177*
C	*13.221*	*66.903*	*17.274*
C	*20.113*	*60.942*	*17.831*
O	*20.779*	*61.807*	*18.767*
P	*21.930*	*62.837*	*18.276*
O	*22.499*	*63.311*	*19.594*
O	*21.244*	*63.911*	*17.477*
O	*22.836*	*61.884*	*17.514*
N	*17.062*	*59.814*	*15.267*
C	*16.325*	*59.094*	*16.139*
N	*16.088*	*57.860*	*15.642*
C	*16.694*	*57.799*	*14.432*
C	*16.832*	*56.775*	*13.390*
C	*17.343*	*59.072*	*14.198*
N	*16.249*	*55.561*	*13.559*
N	*17.539*	*57.083*	*12.284*
C	*18.110*	*58.293*	*12.129*
N	*18.033*	*59.269*	*13.048*

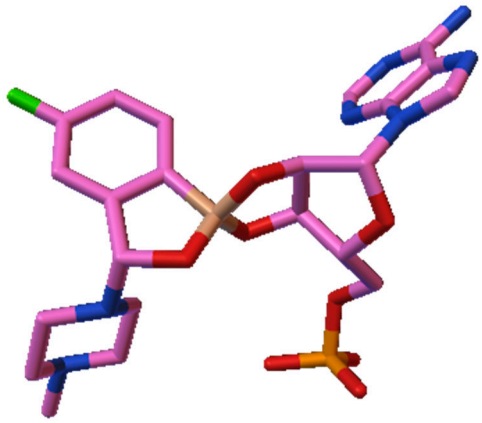


Figure S94. The best structure obtained in the docking studies of 14-S-2-AMP.

Table S94. Coordinates of the best 14-S-2-AMP spiroester.

O	*27.553*	*62.005*	*18.047*
C	*28.283*	*63.410*	*16.271*
C	*28.650*	*64.004*	*17.485*
C	*28.107*	*63.184*	*18.648*
C	*28.698*	*63.981*	*15.070*
C	*29.484*	*65.126*	*15.079*
C	*29.857*	*65.665*	*16.303*
C	*29.466*	*65.127*	*17.519*
F	*30.645*	*66.759*	*16.310*
C	*25.233*	*60.041*	*15.681*
O	*25.857*	*58.922*	*15.039*
C	*25.890*	*61.306*	*15.146*
O	*26.141*	*62.284*	*16.146*
C	*27.246*	*60.796*	*14.743*
O	*28.028*	*61.044*	*15.893*
C	*27.074*	*59.310*	*14.432*
B	*27.448*	*62.073*	*16.675*
N	*27.043*	*63.819*	*19.415*
C	*27.598*	*64.837*	*20.318*
C	*26.511*	*65.399*	*21.220*
N	*25.432*	*65.975*	*20.425*
C	*24.882*	*64.966*	*19.530*
C	*24.404*	*66.578*	*21.258*
C	*25.962*	*64.396*	*18.618*
C	*23.741*	*59.925*	*15.407*
O	*23.162*	*61.208*	*15.706*
P	*21.979*	*61.351*	*16.805*
O	*22.068*	*60.023*	*17.524*
O	*20.698*	*61.557*	*16.044*
O	*22.500*	*62.531*	*17.609*
N	*26.984*	*59.097*	*12.967*
C	*27.310*	*57.964*	*12.310*
N	*27.103*	*58.117*	*10.984*
C	*26.641*	*59.377*	*10.800*
C	*26.233*	*60.174*	*9.637*
C	*26.581*	*60.019*	*12.096*
N	*26.275*	*59.624*	*8.397*
N	*25.821*	*61.441*	*9.847*
C	*25.782*	*61.972*	*11.084*
N	*26.152*	*61.302*	*12.187*

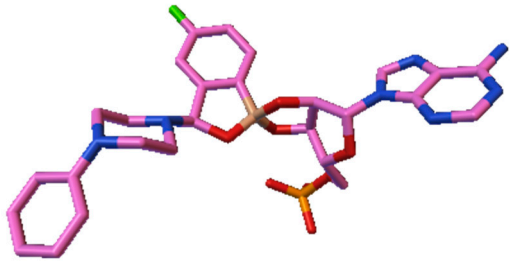


Figure S95. The best structure obtained in the docking studies of 15-R-1-AMP.

Table S95. Coordinates of the best 15-R-1-AMP spiroester.

O	*26.484*	*62.192*	*16.060*
C	*27.683*	*61.324*	*17.931*
C	*27.612*	*60.325*	*16.955*
C	*26.810*	*60.798*	*15.759*
C	*28.350*	*61.054*	*19.128*
C	*28.933*	*59.810*	*19.333*
C	*28.840*	*58.852*	*18.331*
C	*28.185*	*59.076*	*17.131*
F	*29.413*	*57.650*	*18.539*
C	*25.593*	*65.322*	*18.017*
O	*26.567*	*66.370*	*17.931*
C	*26.223*	*64.169*	*18.786*
O	*25.926*	*62.891*	*18.238*
C	*27.685*	*64.386*	*18.516*
O	*27.918*	*63.574*	*17.384*
C	*27.857*	*65.878*	*18.240*
B	*26.943*	*62.550*	*17.298*
N	*27.443*	*60.611*	*14.494*
C	*27.217*	*61.678*	*13.510*
C	*28.126*	*61.469*	*12.294*
N	*27.931*	*60.150*	*11.696*
C	*28.109*	*59.102*	*12.692*
C	*27.201*	*59.286*	*13.907*
C	*27.074*	*59.980*	*10.601*
C	*26.681*	*58.688*	*10.206*
C	*25.799*	*58.495*	*9.156*
C	*25.260*	*59.578*	*8.466*
C	*25.630*	*60.858*	*8.852*
C	*26.527*	*61.063*	*9.893*
C	*24.356*	*65.928*	*18.662*
O	*23.791*	*64.914*	*19.512*
P	*22.579*	*63.973*	*18.993*
O	*21.947*	*63.541*	*20.297*
O	*23.201*	*62.852*	*18.207*
O	*21.763*	*64.991*	*18.213*
N	*28.372*	*66.570*	*19.447*
C	*28.557*	*66.012*	*20.662*
N	*29.042*	*66.928*	*21.527*
C	*29.161*	*68.092*	*20.845*
C	*29.609*	*69.450*	*21.176*
C	*28.706*	*67.858*	*19.491*
N	*30.040*	*69.727*	*22.433*
N	*29.579*	*70.385*	*20.205*
C	*29.151*	*70.094*	*18.962*
N	*28.717*	*68.876*	*18.596*

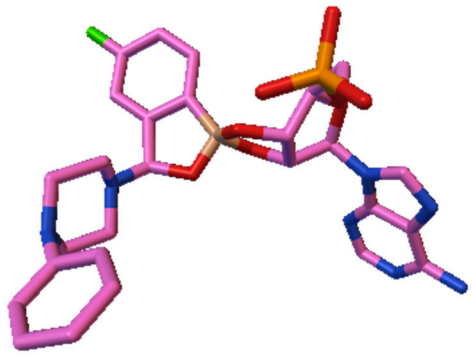


Figure S96. The best structure obtained in the docking studies of 15-R-2-AMP.

Table S96. Coordinates of the best 15-R-2-AMP spiroester.

O	*27.652*	*62.666*	*16.055*
C	*27.791*	*60.855*	*17.601*
C	*28.782*	*61.785*	*17.925*
C	*28.783*	*62.937*	*16.941*
C	*27.667*	*59.701*	*18.376*
C	*28.519*	*59.491*	*19.453*
C	*29.486*	*60.447*	*19.739*
C	*29.645*	*61.605*	*18.995*
F	*30.304*	*60.236*	*20.789*
C	*24.492*	*59.680*	*15.779*
O	*24.740*	*58.852*	*14.636*
C	*24.955*	*61.089*	*15.436*
O	*25.643*	*61.736*	*16.499*
C	*26.003*	*60.820*	*14.393*
O	*27.193*	*60.764*	*15.152*
C	*25.633*	*59.488*	*13.743*
B	*27.037*	*61.468*	*16.371*
N	*28.760*	*64.237*	*17.530*
C	*27.621*	*64.506*	*18.419*
C	*27.836*	*65.833*	*19.155*
N	*28.051*	*66.938*	*18.223*
C	*29.149*	*66.639*	*17.314*
C	*28.946*	*65.324*	*16.561*
C	*26.988*	*67.766*	*17.837*
C	*25.771*	*67.202*	*17.411*
C	*24.691*	*67.999*	*17.071*
C	*24.771*	*69.387*	*17.153*
C	*25.961*	*69.957*	*17.582*
C	*27.057*	*69.168*	*17.911*
C	*23.012*	*59.548*	*16.101*
O	*22.432*	*60.855*	*15.937*
P	*21.625*	*61.565*	*17.150*
O	*20.446*	*62.167*	*16.420*
O	*22.555*	*62.576*	*17.762*
O	*21.280*	*60.348*	*17.993*
N	*24.952*	*59.719*	*12.446*
C	*23.617*	*59.741*	*12.244*
N	*23.345*	*59.981*	*10.943*
C	*24.535*	*60.108*	*10.308*
C	*24.952*	*60.362*	*8.924*
C	*25.582*	*59.919*	*11.290*
N	*24.013*	*60.540*	*7.961*
N	*26.273*	*60.415*	*8.657*
C	*27.193*	*60.238*	*9.623*
N	*26.880*	*59.990*	*10.906*

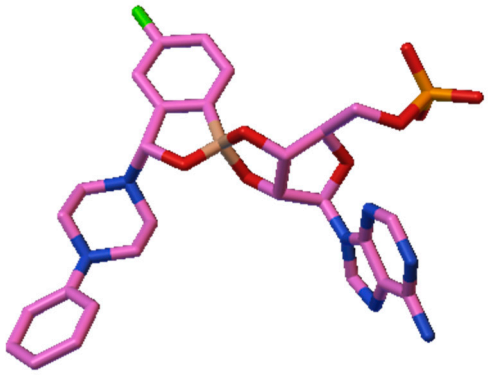


Figure S97. The best structure obtained in the docking studies of 15-S-1-AMP.

Table S97. Coordinates of the best 15-S-1-AMP spiroester.

O	*41.091*	*72.182*	*0.512*
C	*41.639*	*74.198*	*1.649*
C	*42.830*	*73.539*	*1.325*
C	*42.520*	*72.191*	*0.687*
C	*41.689*	*75.465*	*2.225*
C	*42.914*	*76.076*	*2.461*
C	*44.071*	*75.405*	*2.093*
C	*44.064*	*74.143*	*1.520*
F	*45.258*	*76.010*	*2.297*
C	*37.783*	*74.889*	*1.266*
O	*36.994*	*74.401*	*2.358*
C	*38.301*	*73.683*	*0.496*
O	*39.656*	*73.810*	*0.084*
C	*38.309*	*72.622*	*1.560*
O	*39.627*	*72.692*	*2.062*
C	*37.247*	*73.027*	*2.581*
B	*40.495*	*73.264*	*1.099*
N	*42.848*	*71.032*	*1.503*
C	*41.685*	*70.176*	*1.771*
C	*41.373*	*69.199*	*0.635*
N	*42.552*	*68.389*	*0.302*
C	*43.711*	*69.216*	*-0.015*
C	*43.986*	*70.197*	*1.132*
C	*42.334*	*67.236*	*-0.483*
C	*43.221*	*66.149*	*-0.489*
C	*42.947*	*65.010*	*-1.240*
C	*41.798*	*64.923*	*-2.012*
C	*40.911*	*65.997*	*-2.014*
C	*41.168*	*67.131*	*-1.260*
C	*36.892*	*75.829*	*0.470*
O	*35.694*	*76.023*	*1.243*
P	*35.533*	*77.306*	*2.220*
O	*35.897*	*76.716*	*3.563*
O	*34.104*	*77.762*	*2.111*
O	*36.594*	*78.224*	*1.635*
N	*36.000*	*72.254*	*2.362*
C	*35.528*	*71.269*	*3.154*
N	*34.368*	*70.786*	*2.660*
C	*34.104*	*71.478*	*1.526*
C	*33.036*	*71.457*	*0.520*
C	*35.181*	*72.425*	*1.326*
N	*32.004*	*70.585*	*0.654*
N	*33.116*	*72.319*	*-0.513*
C	*34.144*	*73.180*	*-0.631*
N	*35.160*	*73.243*	*0.246*

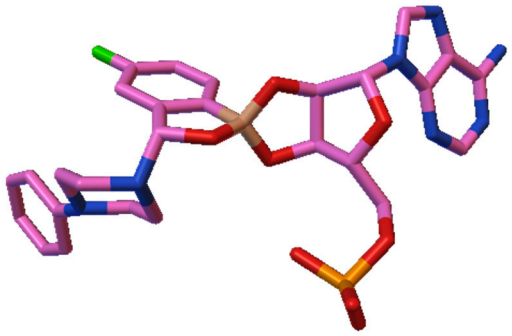


Figure S98. The best structure obtained in the docking studies of 15-S-2-AMP.

Table S98. Coordinates of the best 15-S-2-AMP spiroester.

O	*26.915*	*62.035*	*17.934*
C	*28.051*	*63.288*	*16.260*
C	*28.381*	*63.824*	*17.511*
C	*27.595*	*63.115*	*18.603*
C	*28.677*	*63.775*	*15.115*
C	*29.634*	*64.777*	*15.215*
C	*29.960*	*65.258*	*16.476*
C	*29.360*	*64.800*	*17.639*
F	*30.909*	*66.210*	*16.577*
C	*24.957*	*60.150*	*15.218*
O	*25.612*	*58.961*	*14.760*
C	*25.795*	*61.340*	*14.771*
O	*25.915*	*62.354*	*15.760*
C	*27.163*	*60.726*	*14.667*
O	*27.722*	*60.988*	*15.937*
C	*26.948*	*59.239*	*14.391*
B	*27.076*	*62.092*	*16.545*
N	*26.565*	*63.921*	*19.243*
C	*27.100*	*64.810*	*20.282*
C	*27.677*	*66.115*	*19.729*
N	*26.688*	*66.816*	*18.901*
C	*26.174*	*65.969*	*17.832*
C	*25.621*	*64.663*	*18.415*
C	*26.952*	*68.169*	*18.599*
C	*28.244*	*68.715*	*18.651*
C	*28.472*	*70.042*	*18.300*
C	*27.427*	*70.864*	*17.903*
C	*26.141*	*70.334*	*17.850*
C	*25.905*	*69.011*	*18.186*
C	*23.543*	*60.112*	*14.660*
O	*22.685*	*59.670*	*15.726*
P	*22.027*	*60.731*	*16.760*
O	*21.622*	*59.831*	*17.905*
O	*20.872*	*61.379*	*16.045*
O	*23.234*	*61.607*	*17.051*
N	*27.130*	*58.950*	*12.947*
C	*28.276*	*58.548*	*12.357*
N	*28.083*	*58.375*	*11.032*
C	*26.788*	*58.681*	*10.778*
C	*25.944*	*58.712*	*9.578*
C	*26.174*	*59.073*	*12.029*
N	*26.470*	*58.361*	*8.377*
N	*24.657*	*59.089*	*9.715*
C	*24.148*	*59.432*	*10.914*
N	*24.869*	*59.438*	*12.047*

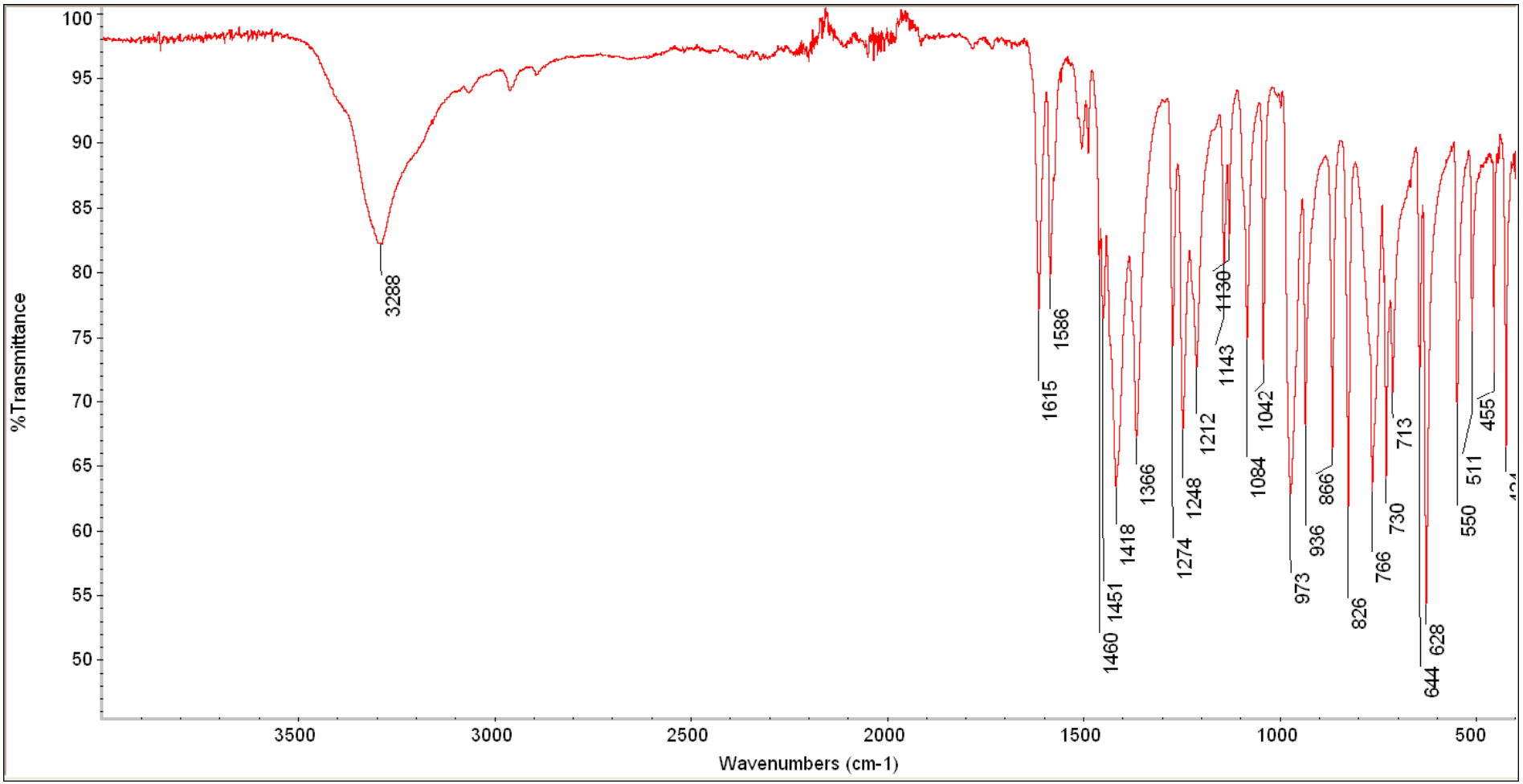


*Figure S99. IR spectrum of **AN2690** (KBr)*

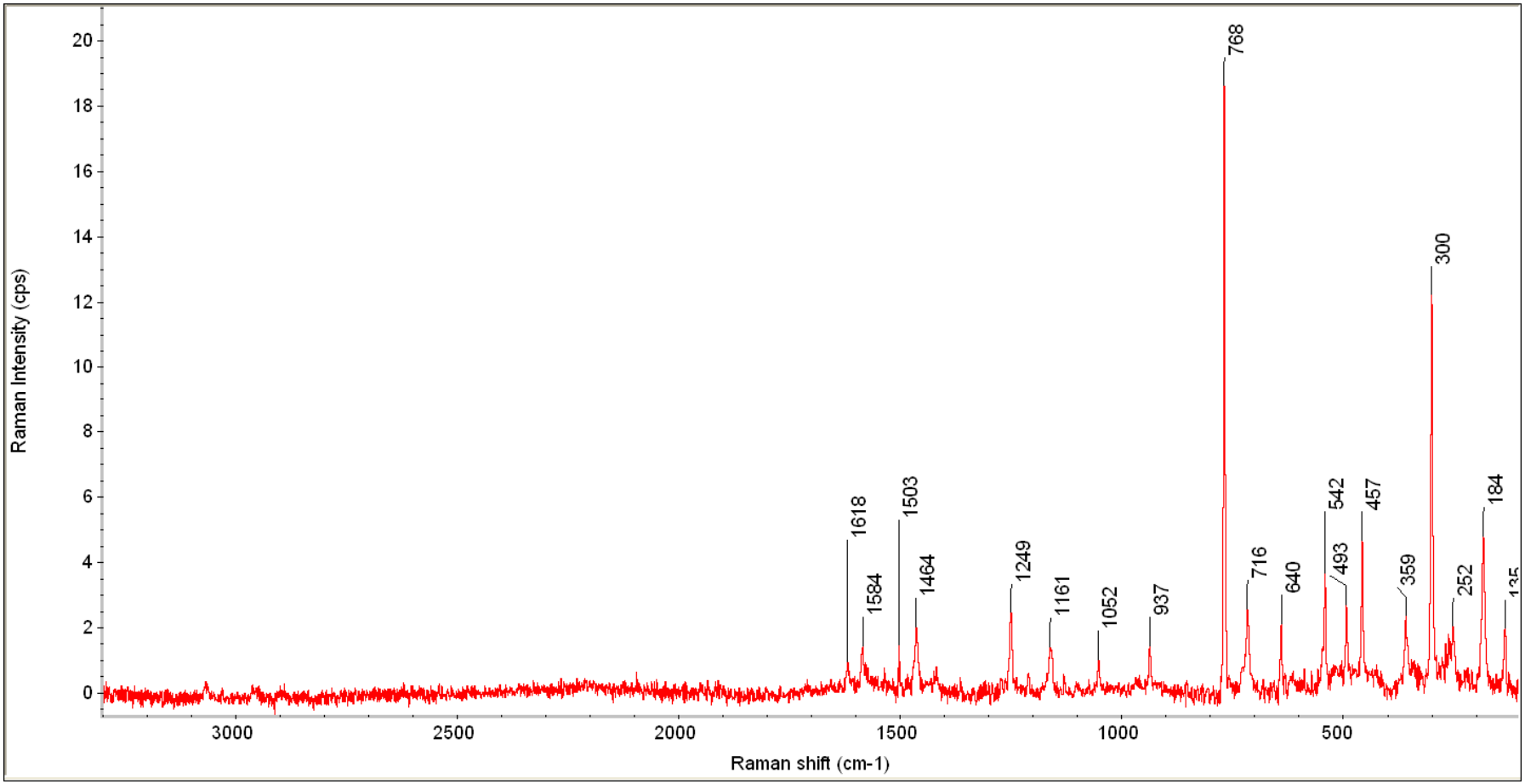


*Figure S100. Raman spectrum of **AN2690**.*

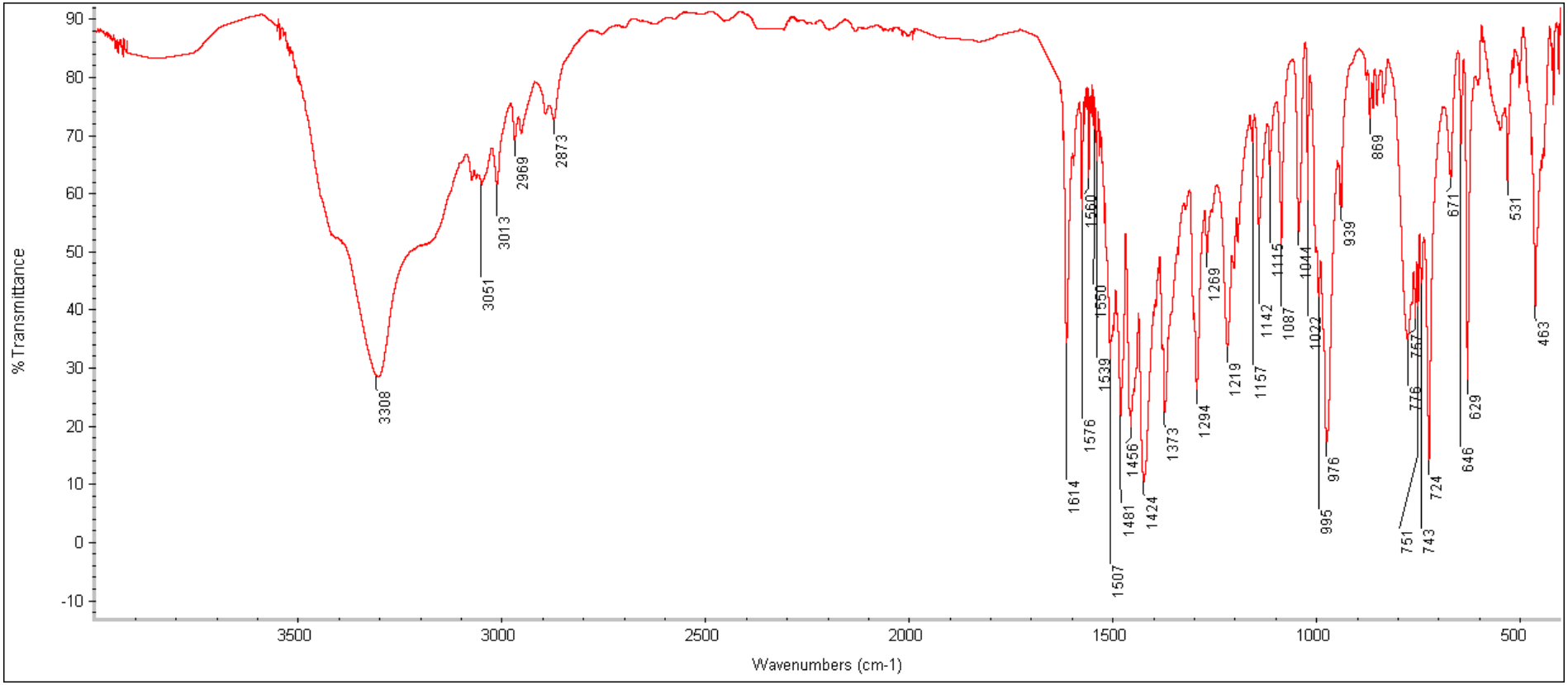


*Figure S101. IR spectrum of **1** (ATR).*

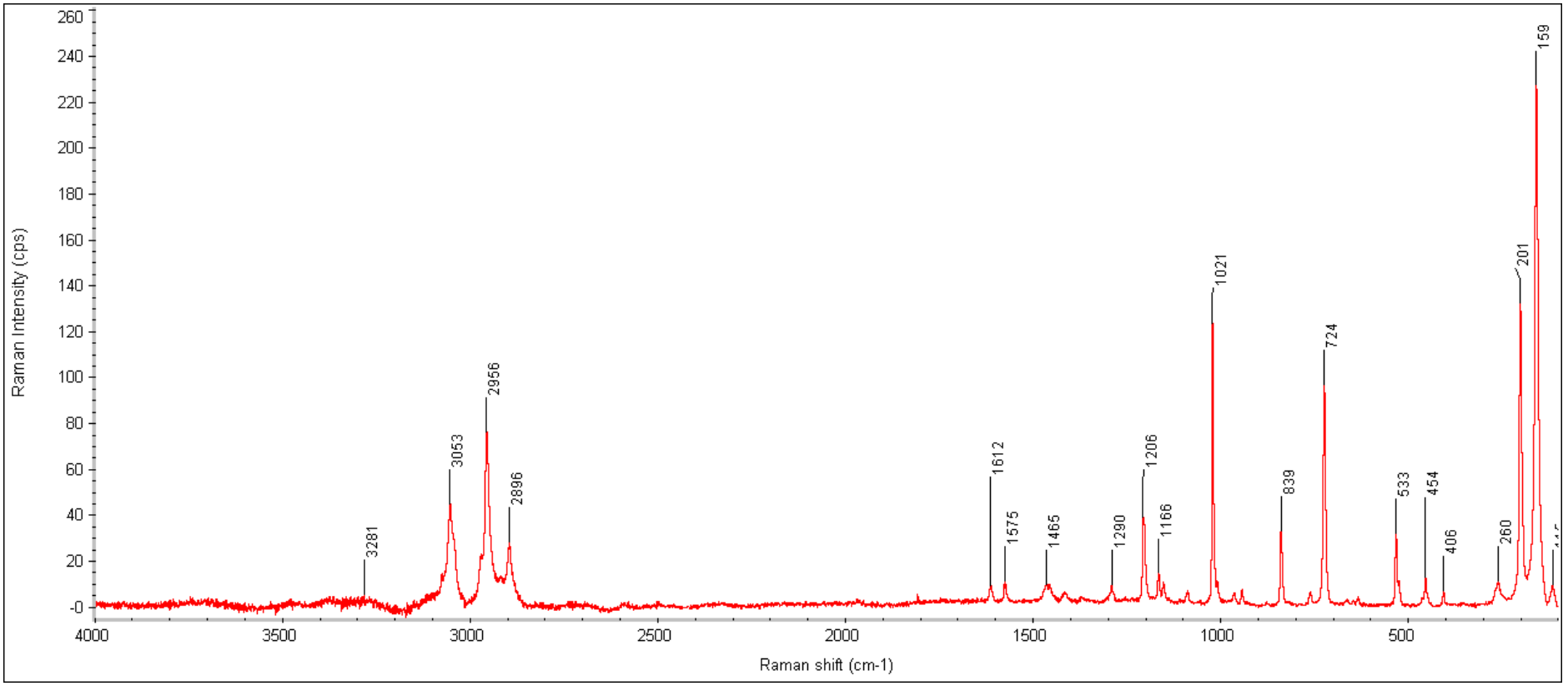


*Figure S102. Raman spectrum of **1**.*

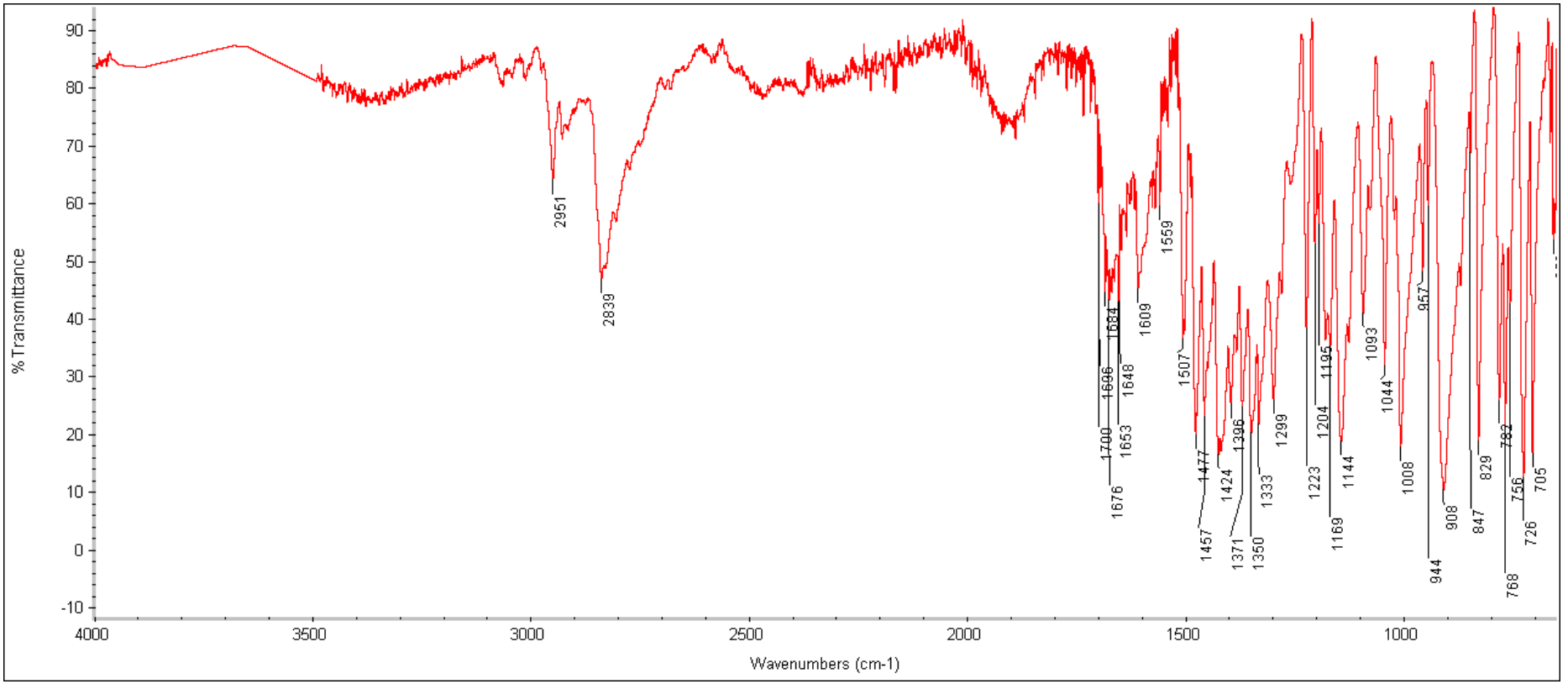


*Figure S103. IR spectrum of **5** (ATR)*

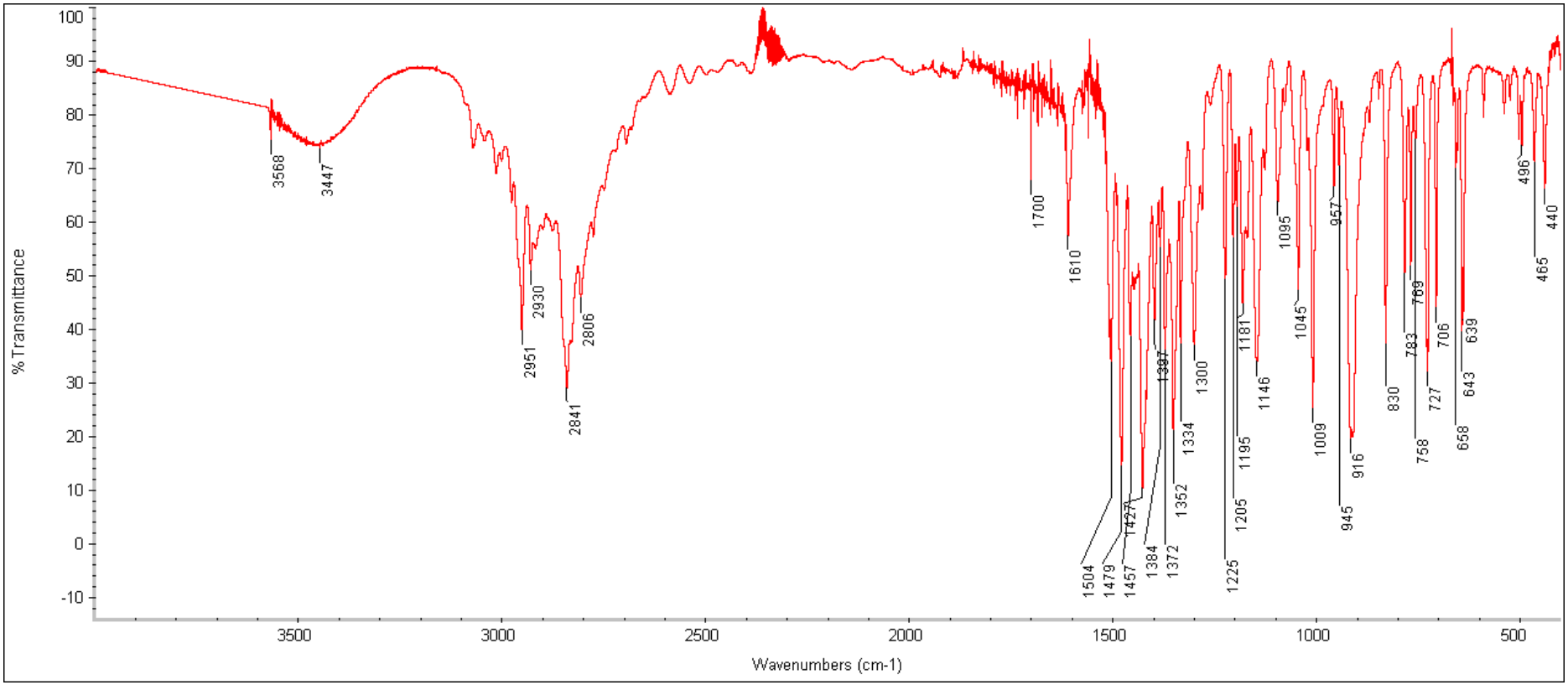


*Figure S104. IR spectrum of **5** (KBr)*

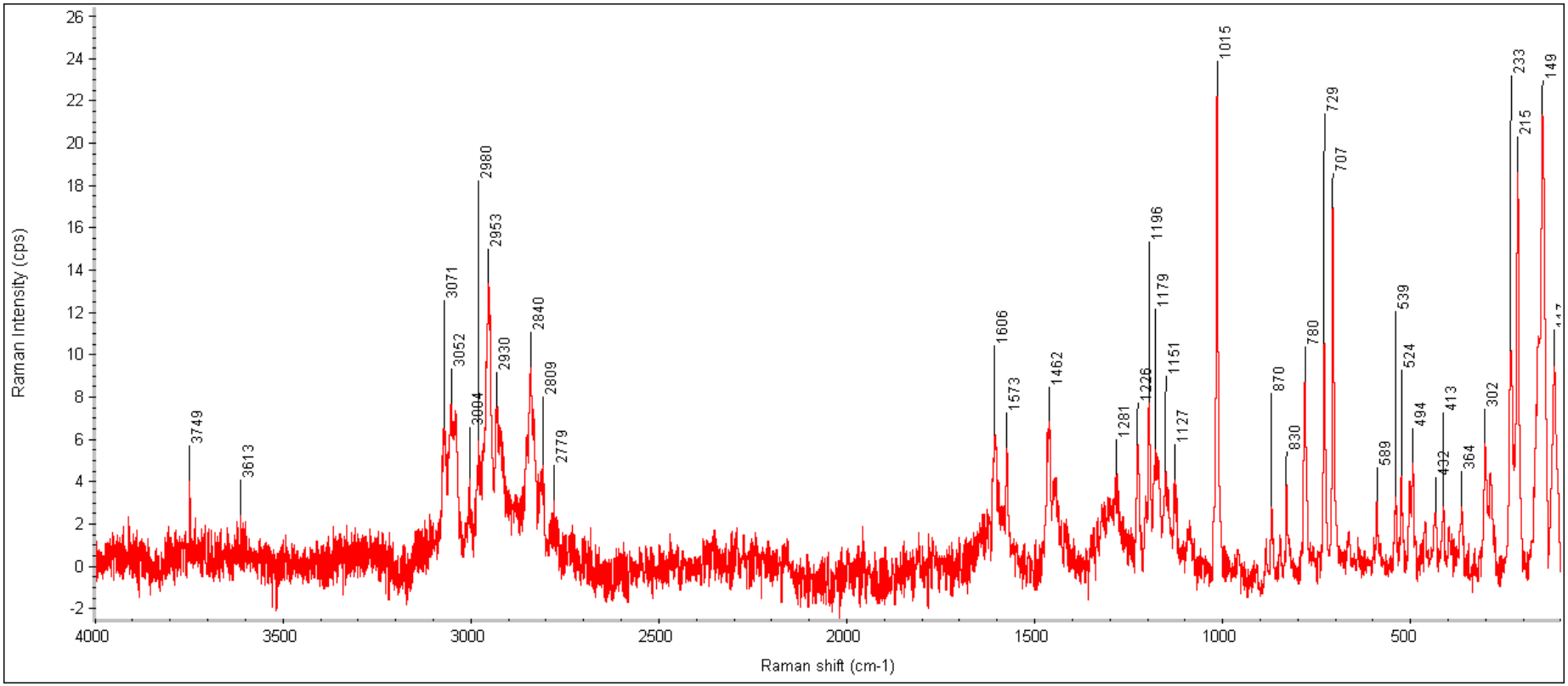


*Figure S105. Raman spectrum of **5** (KBr)*

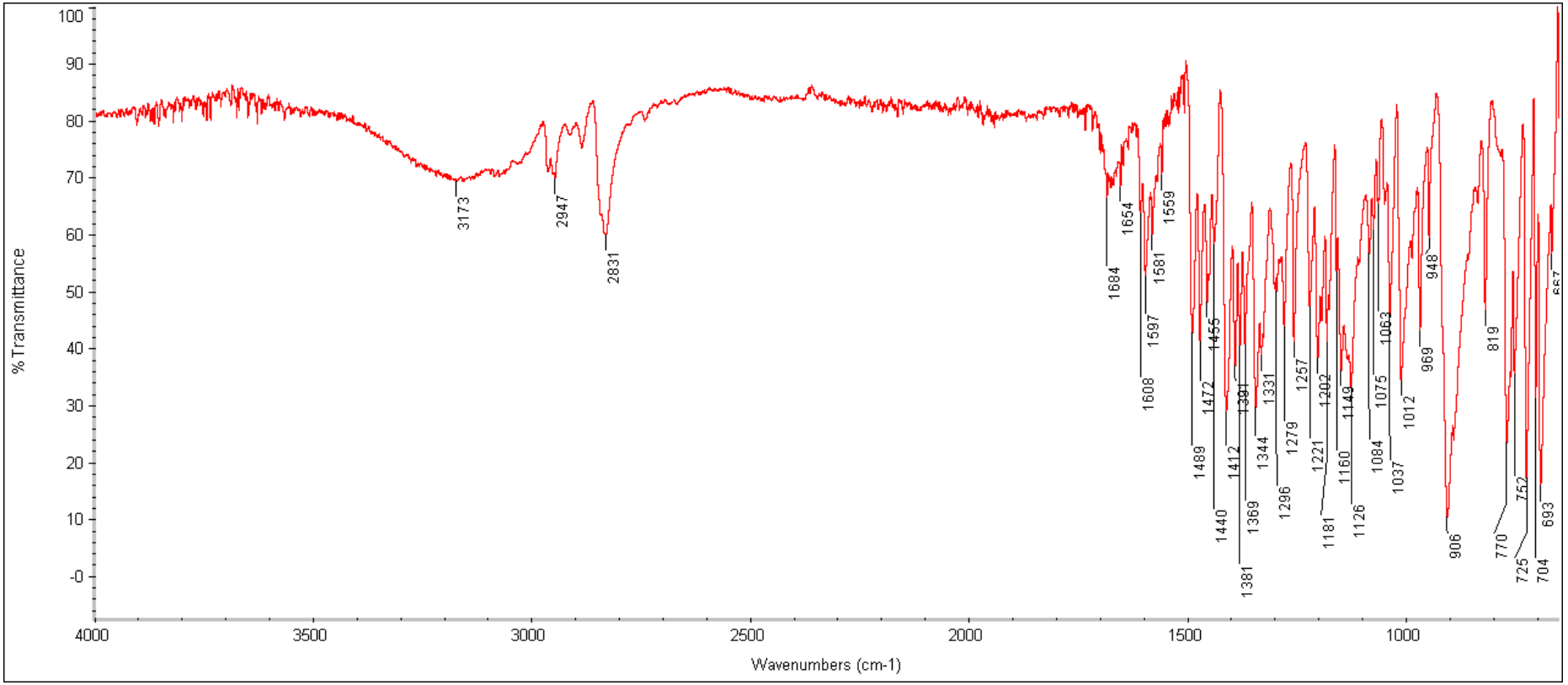


*Figure S106. IR spectrum of **6** (ATR).*

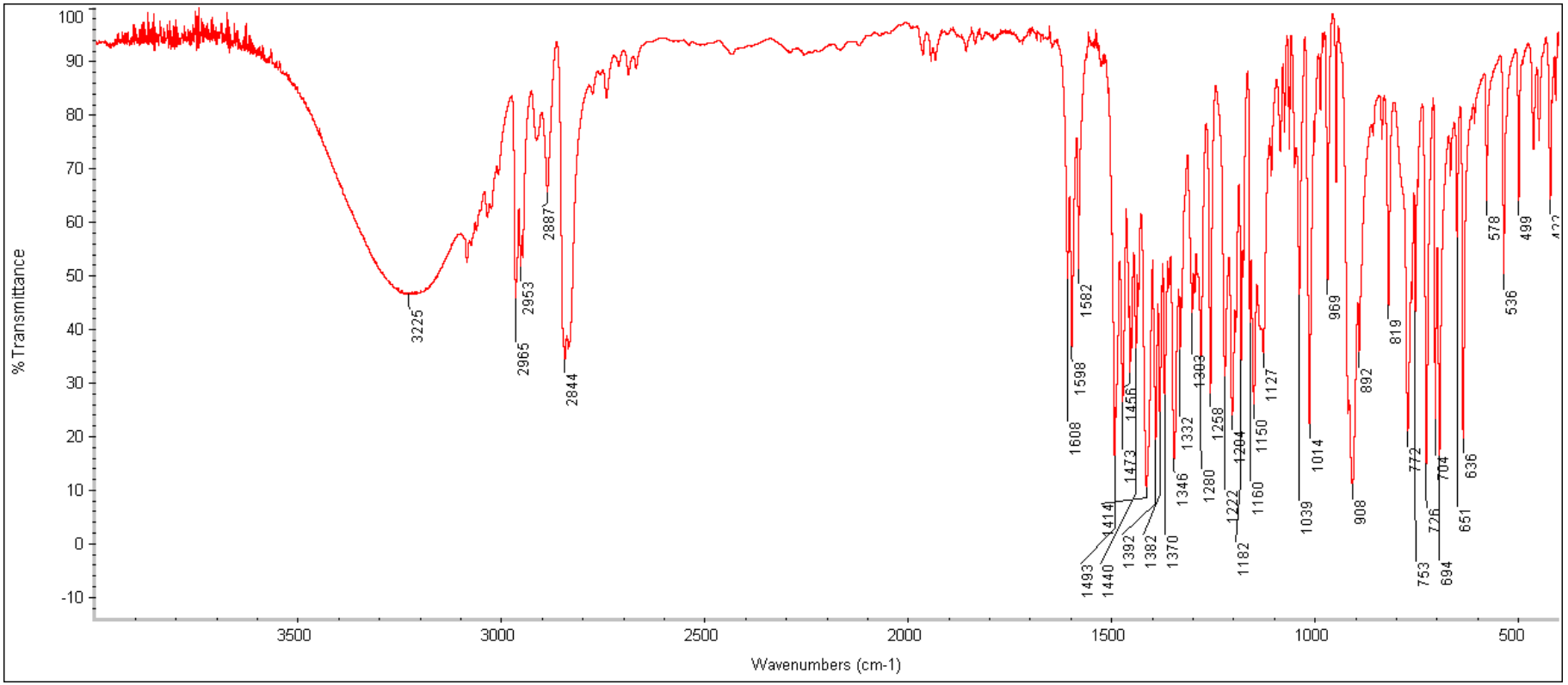


*Figure S107. IR spectrum of **6** (KBr)*

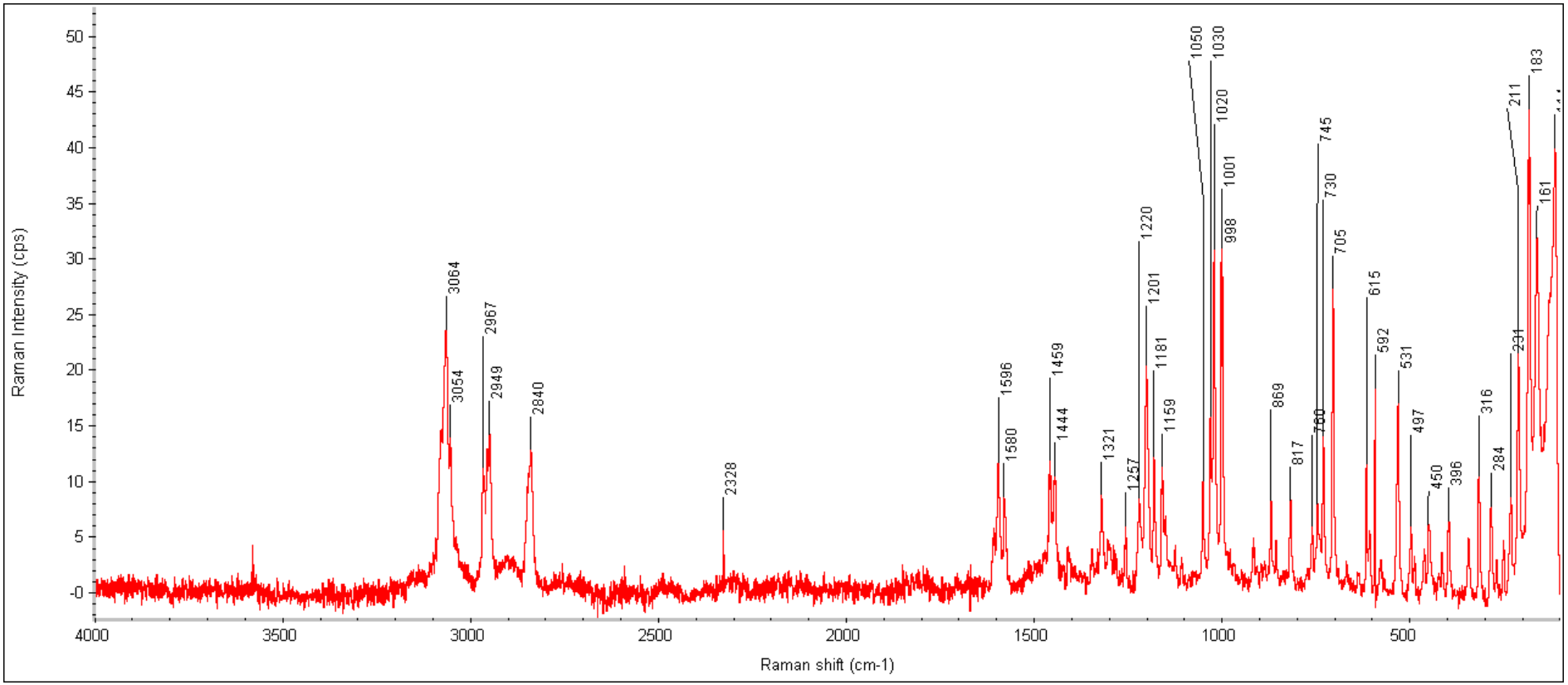


Figure S108. Raman spectrum of ***6***

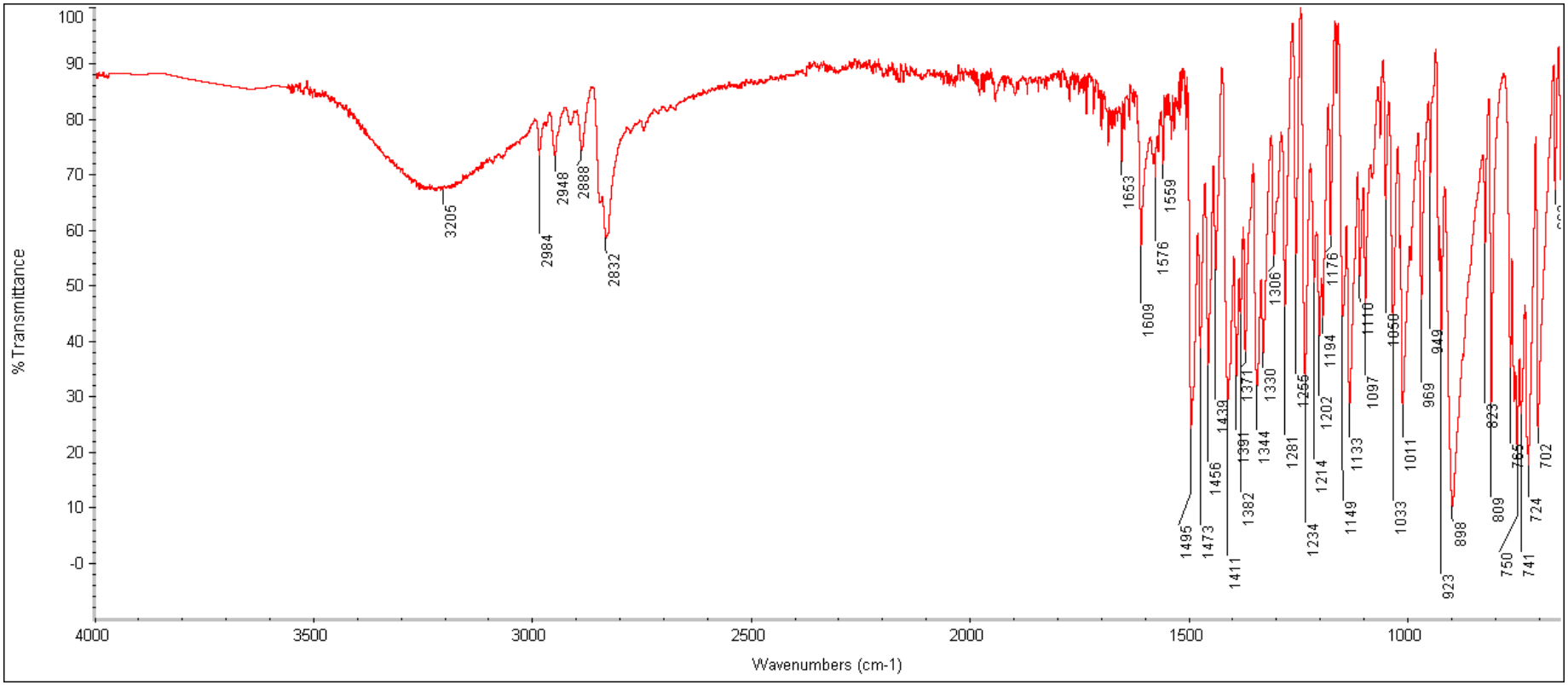


*Figure S109. IR spectrum of **7** (ATR)*

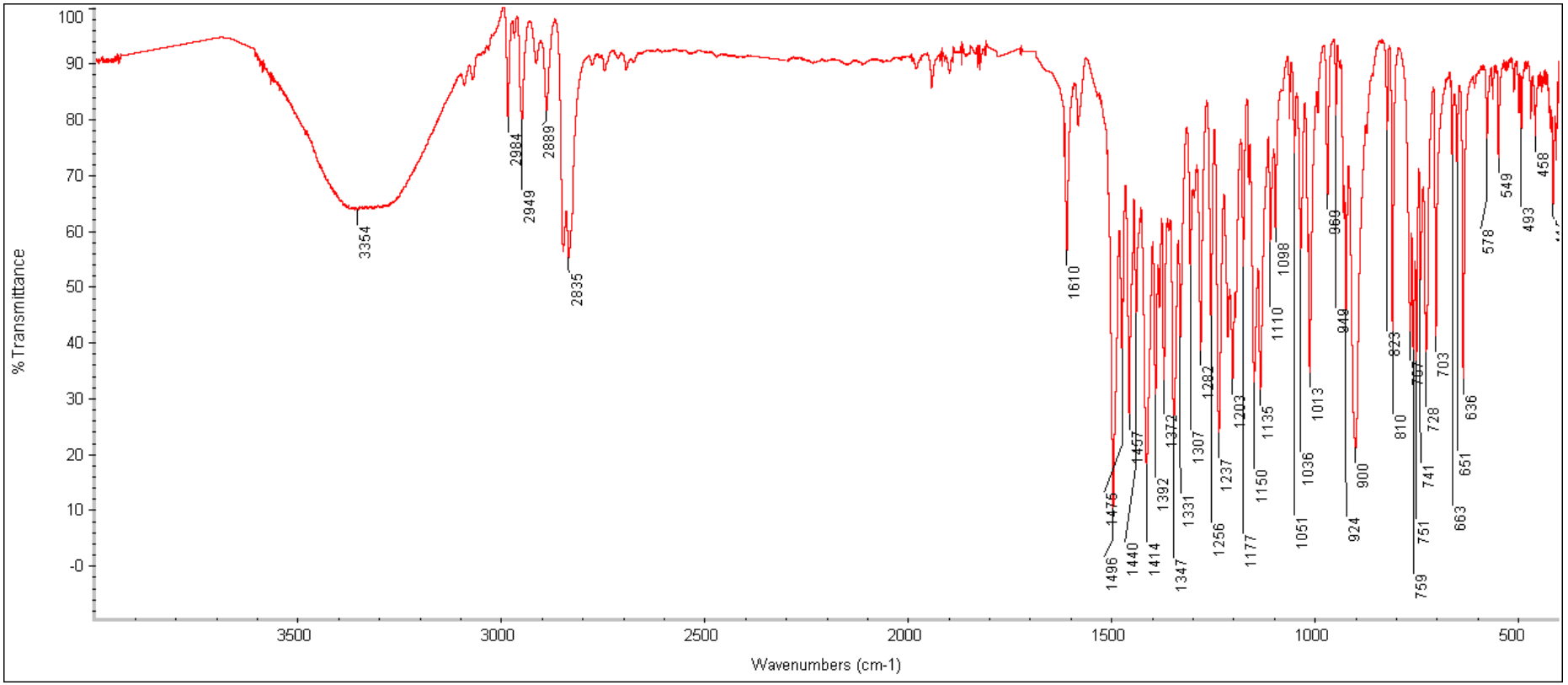


*Figure S110. IR spectrum of **7** (KBr)*

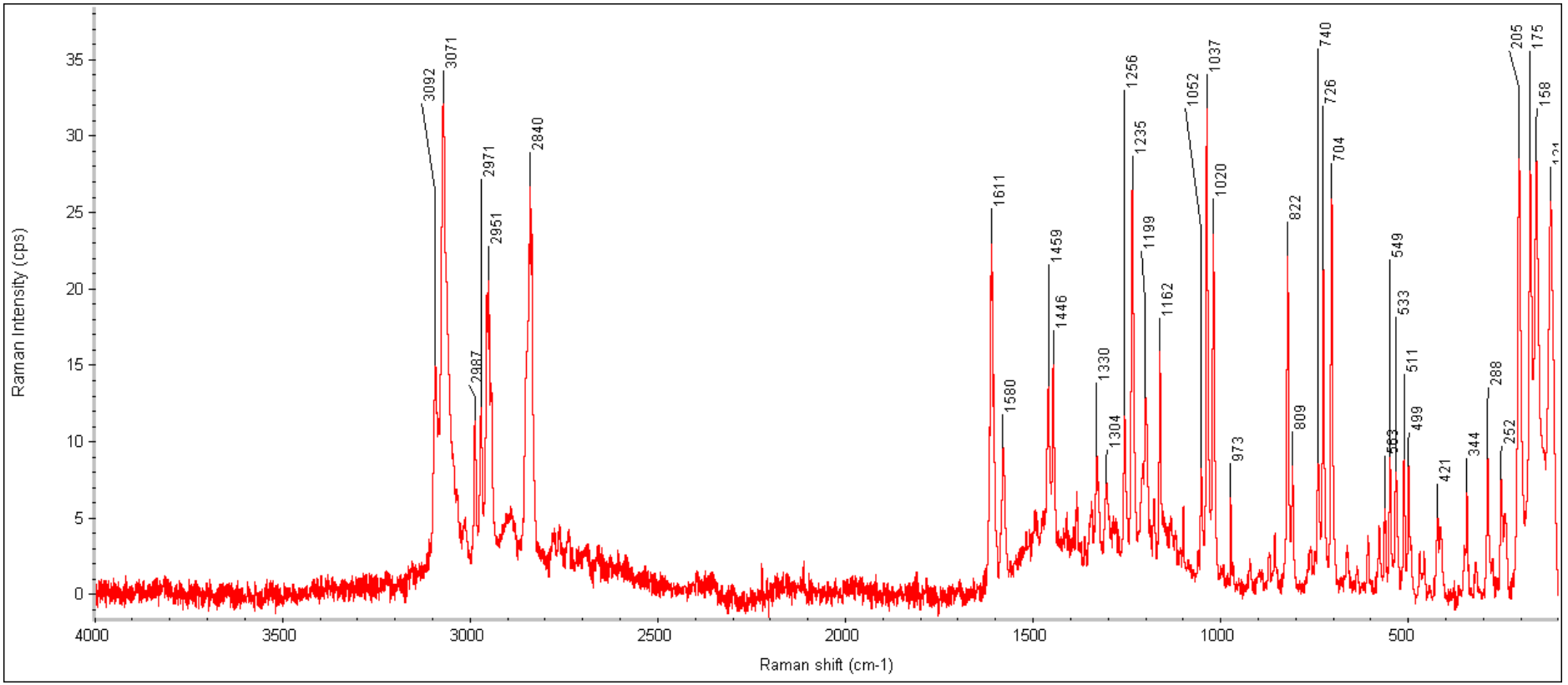


*Figure S111. Raman spectrum of **7***

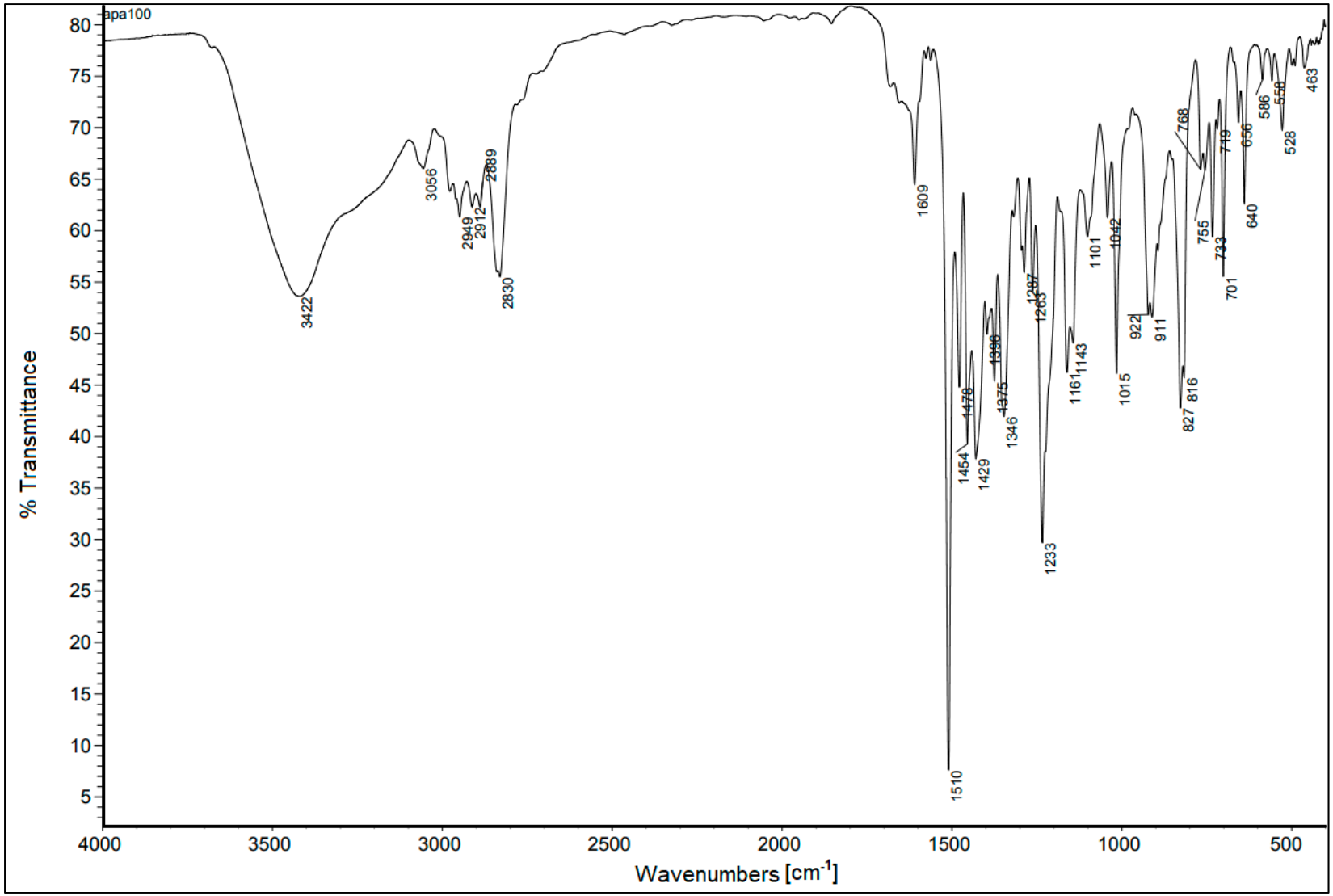


*Figure S112. IR spectrum of **8** (KBr)*

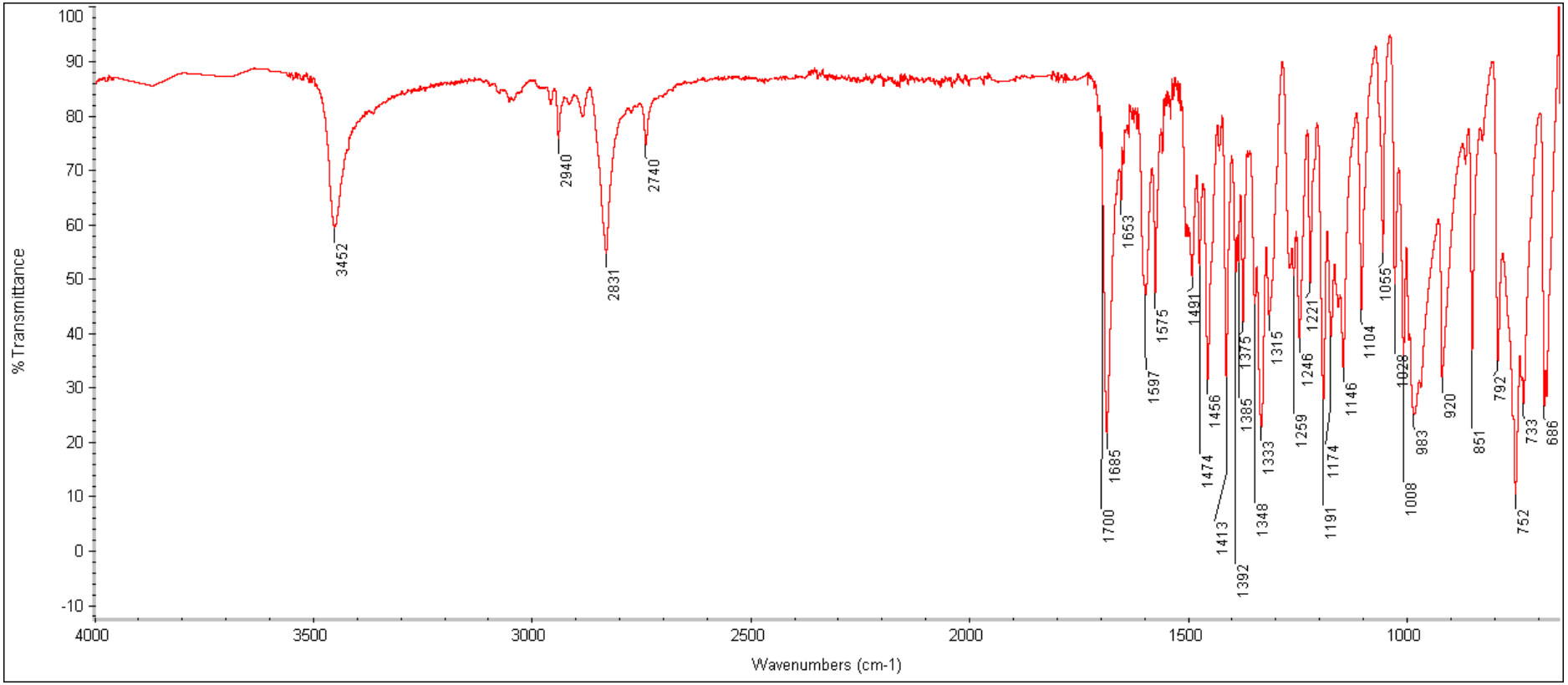


*Figure S113. IR spectrum of **9** (ATR)*

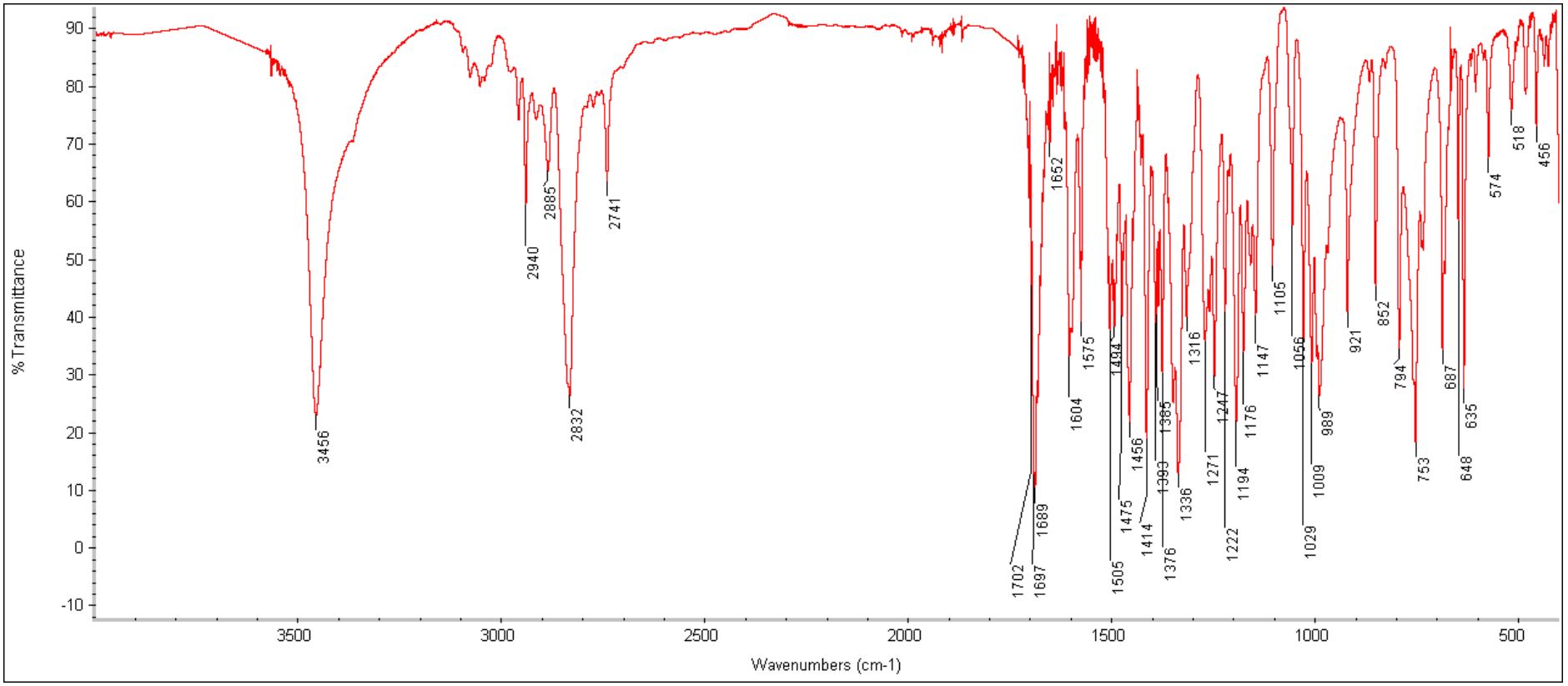


*Figure S114 IR spectrum of **9** (KBr)*

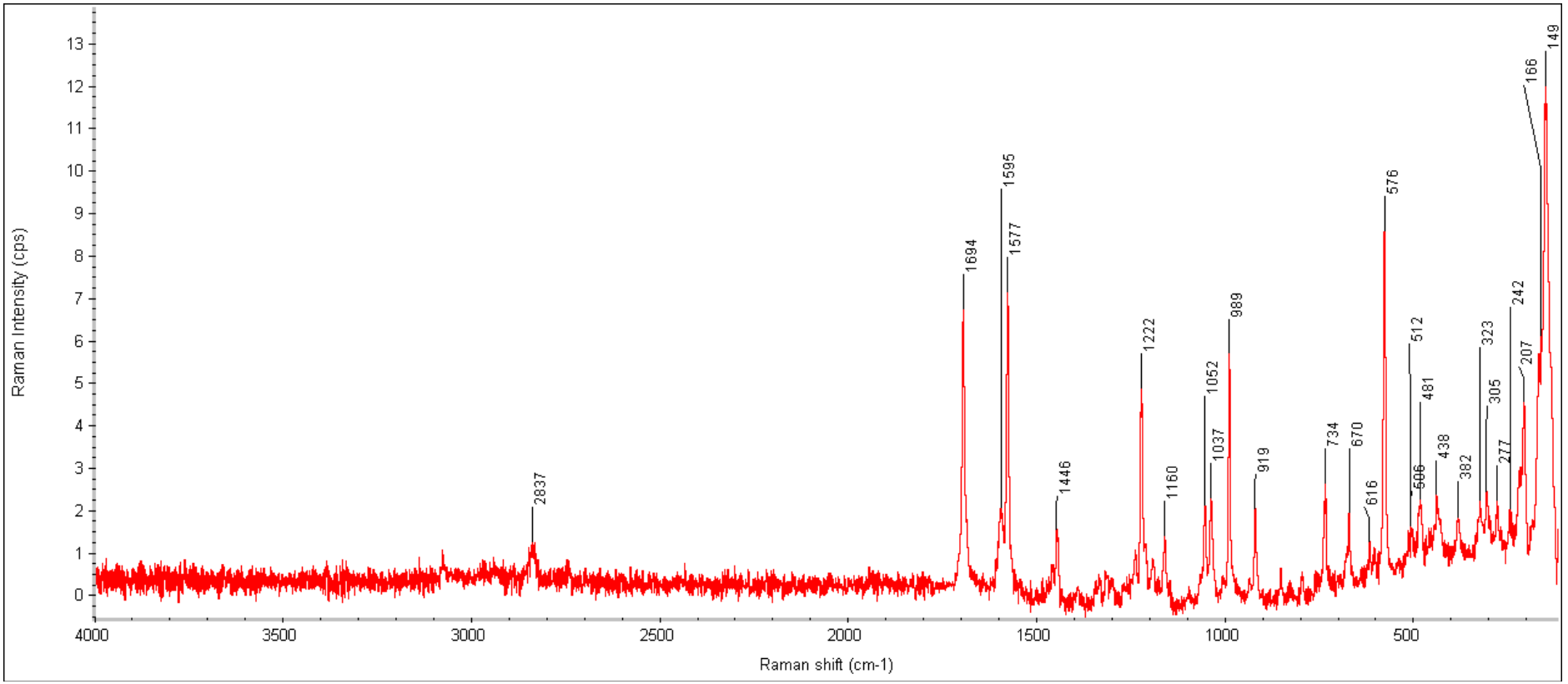


Figure S115. Raman spectrum of ***9***

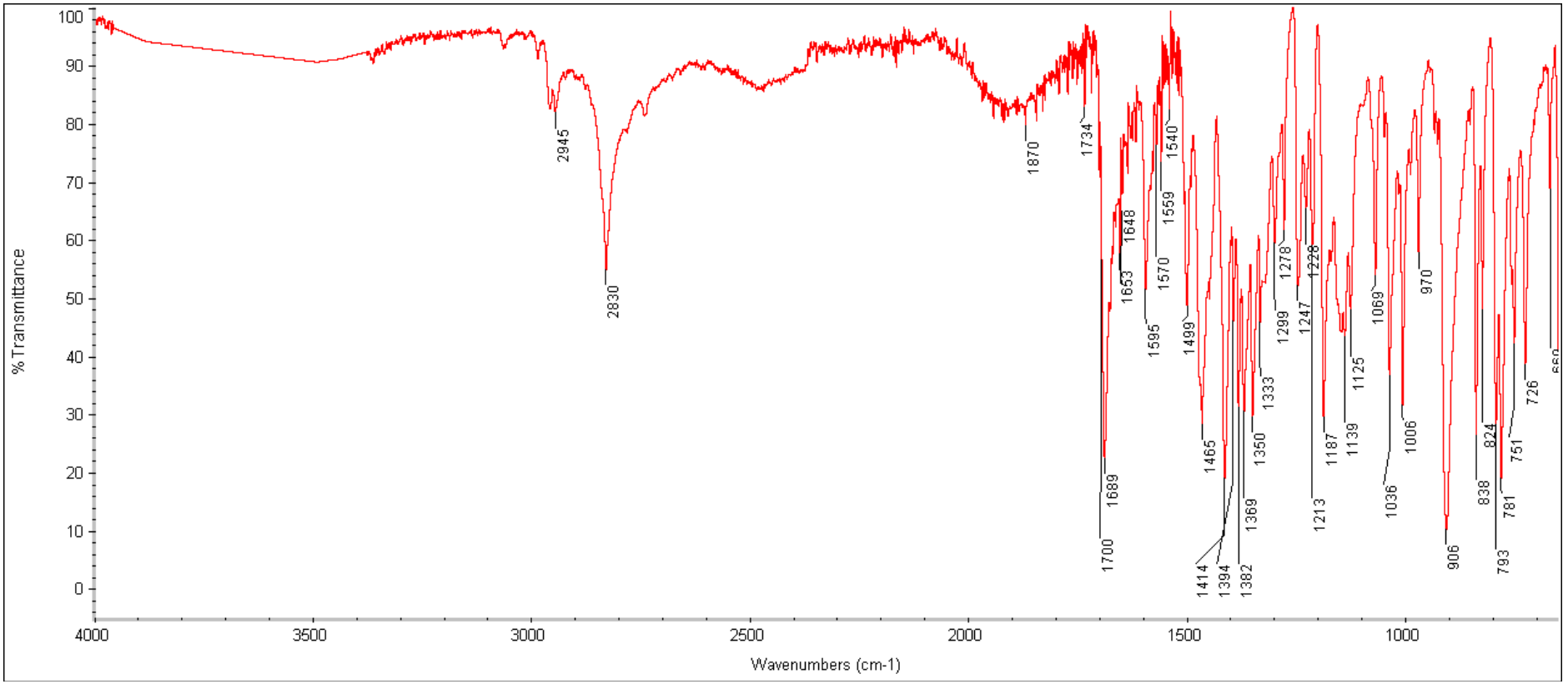


*Figure S116. IR spectrum of **10** (ATR)*

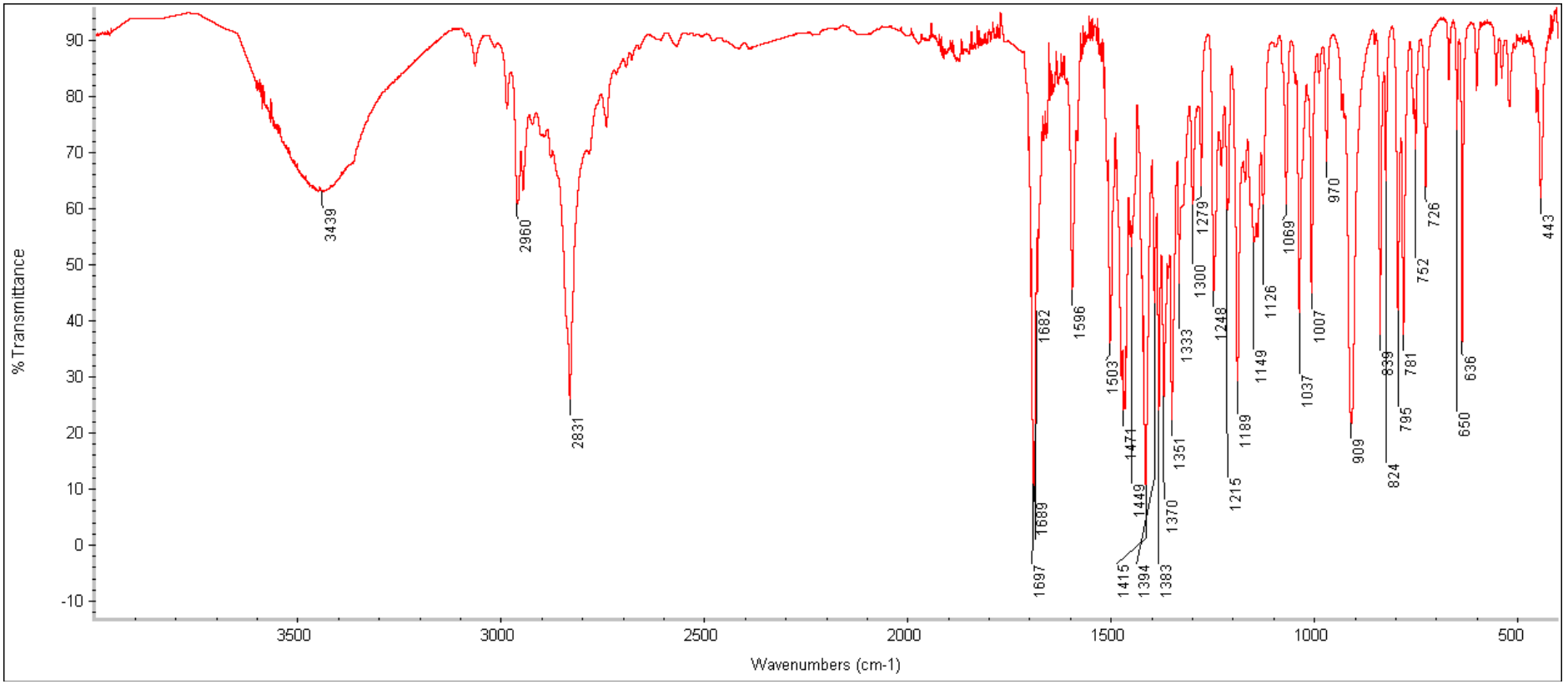


*Figure S117. IR spectrum of **10** (KBr)*

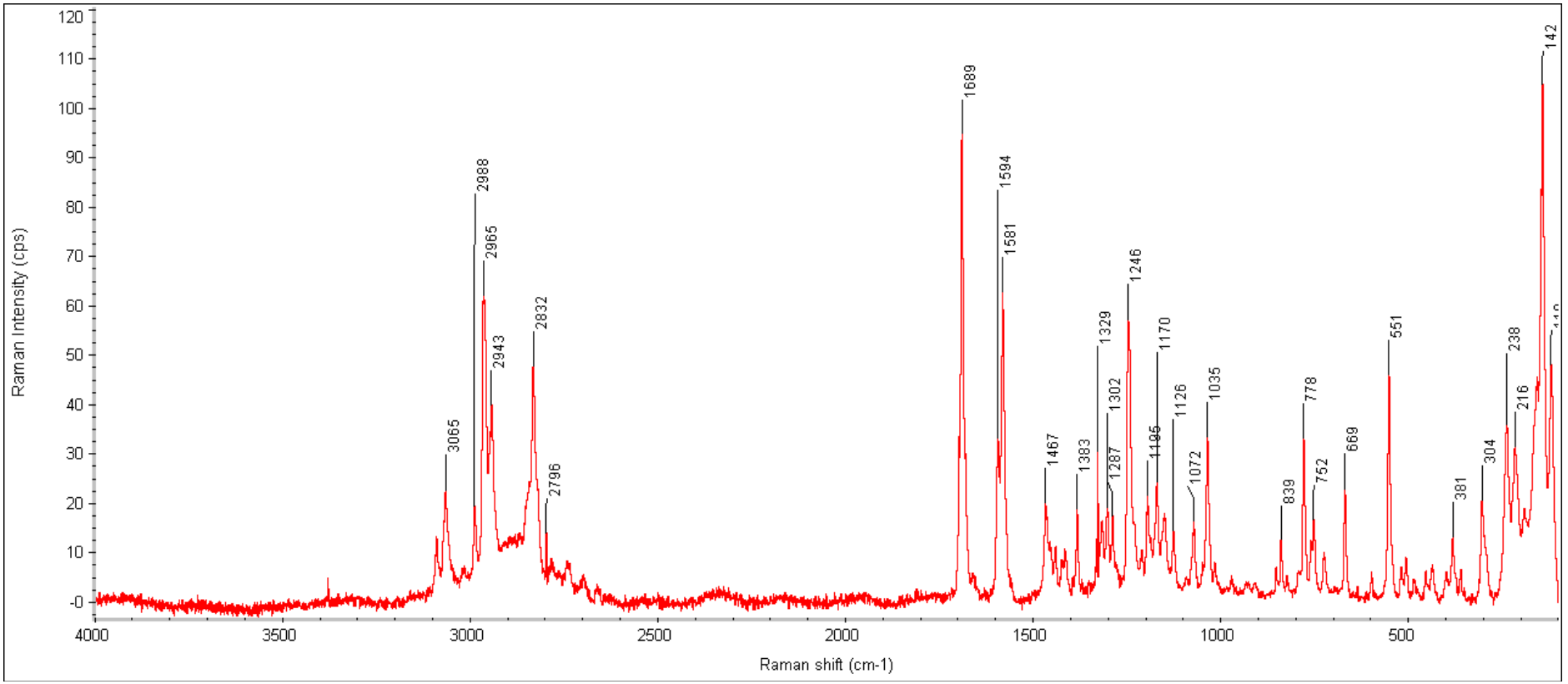


Figure S118. Raman spectrum of ***10***

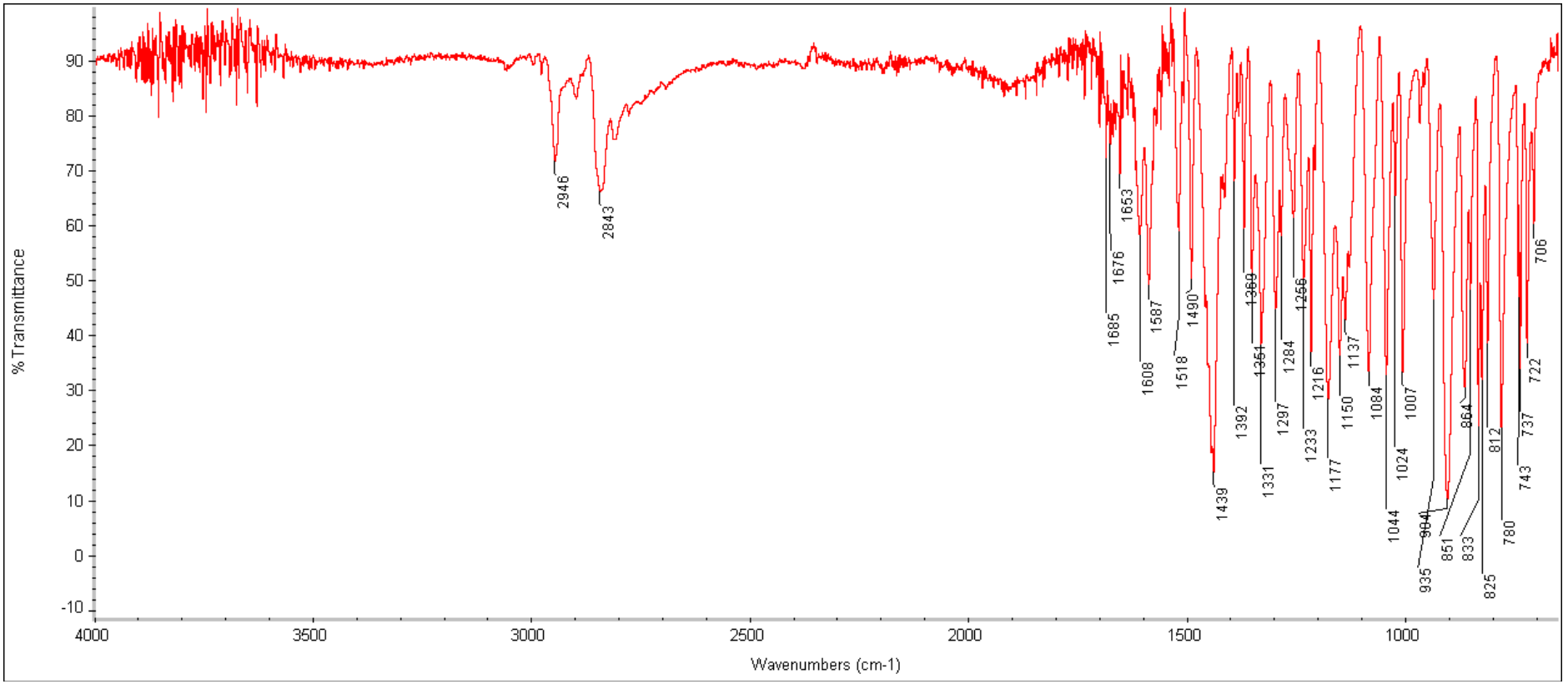


*Figure S119. IR spectrum of **14** (ATR)*

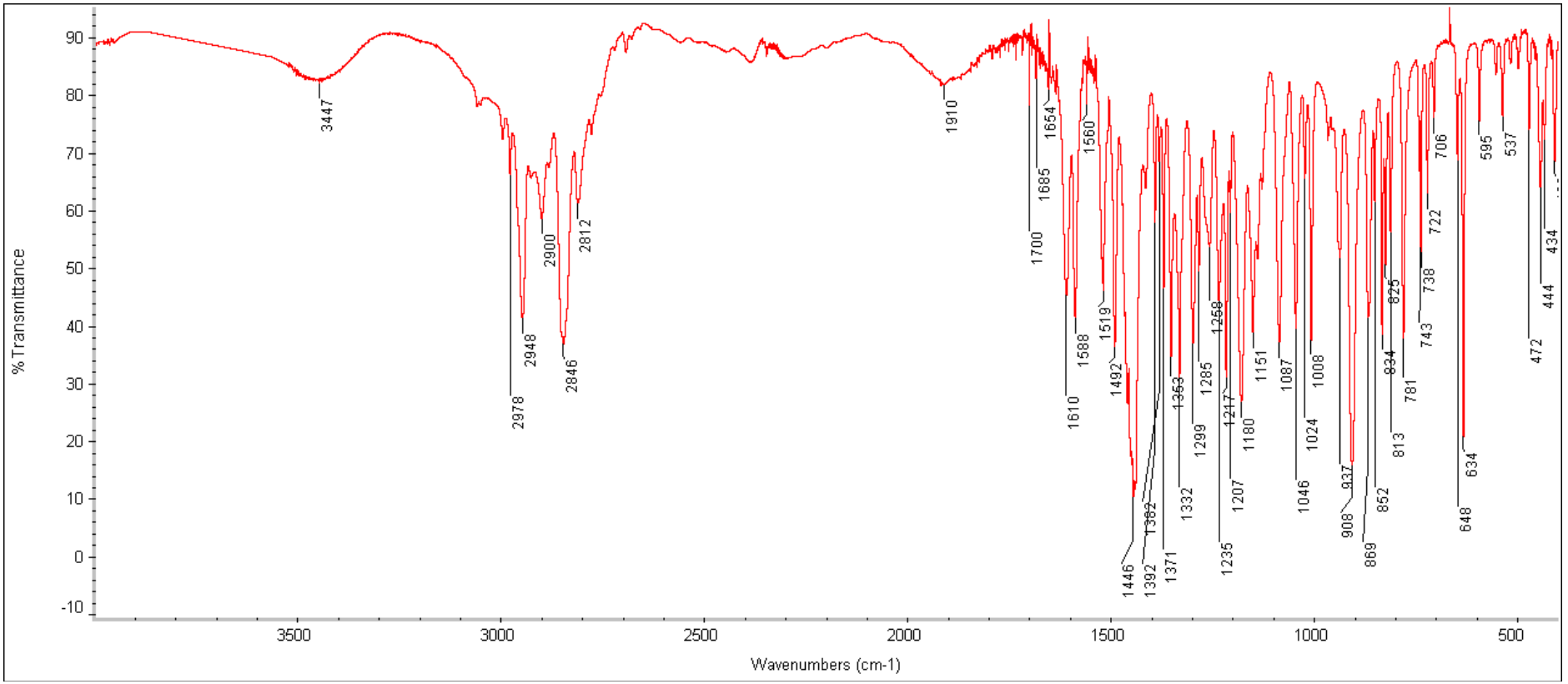


*Figure S120. IR spectrum of **14** (KBr)*

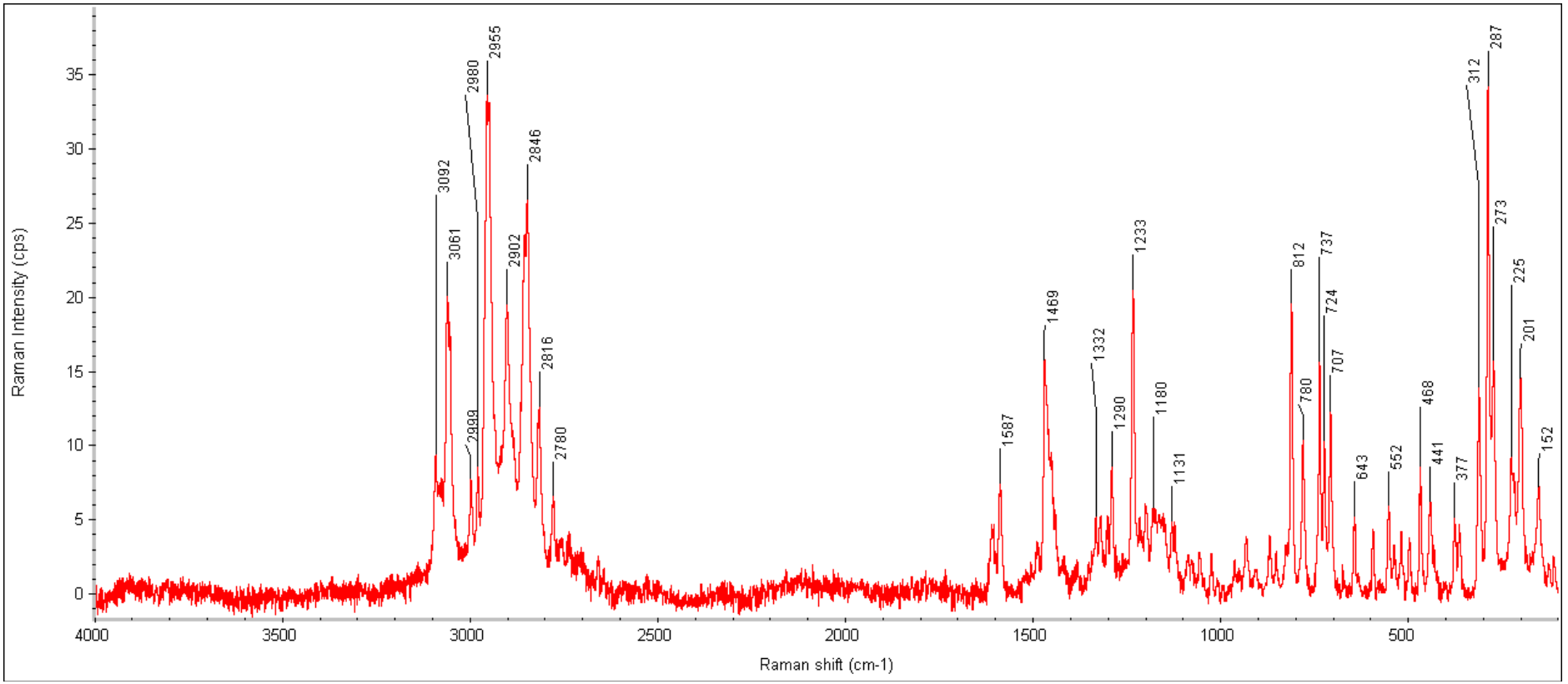


*Figure S121. Raman spectrum of **14** (KBr)*

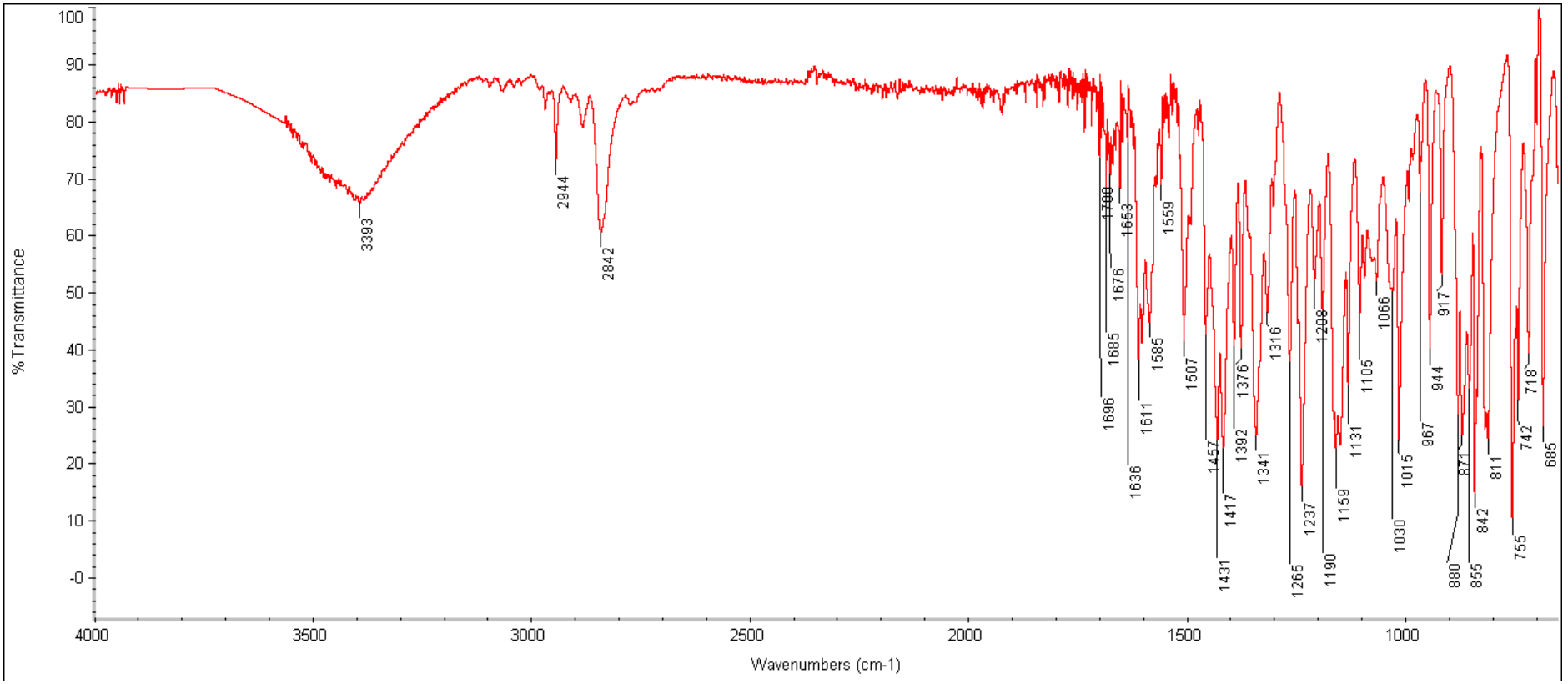


*Figure S123. IR spectrum of **15** (ATR)*

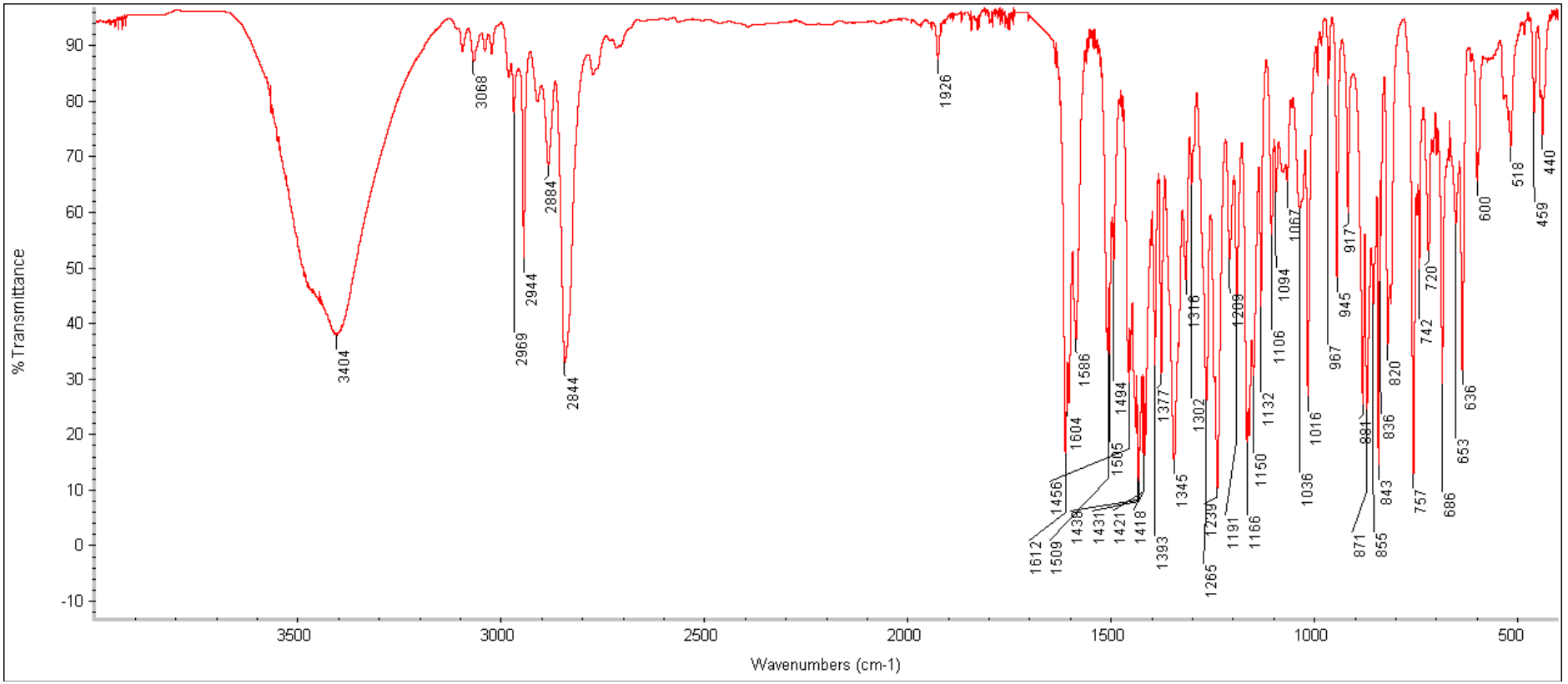


*Figure S124. IR spectrum of **15** (KBr)*

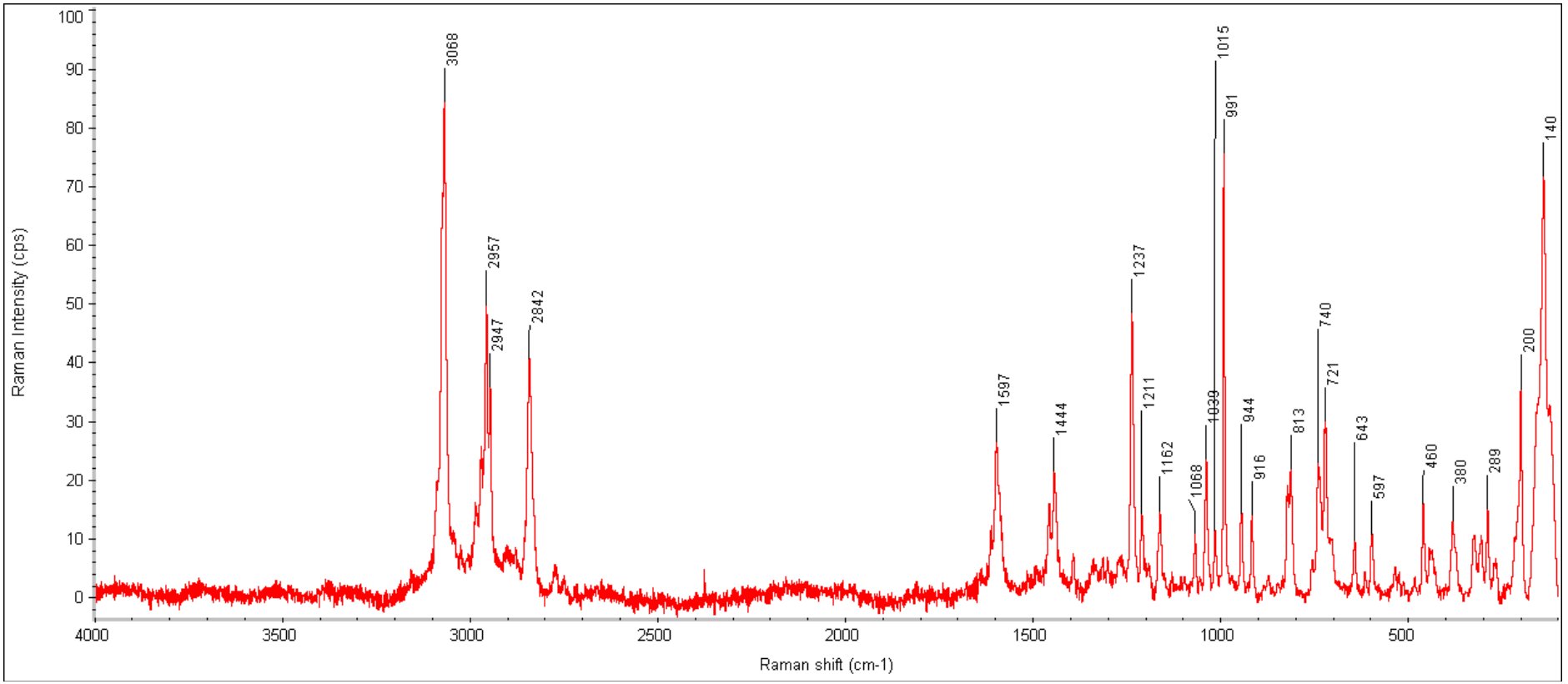


Figure S125. Raman spectrum of ***15***