Supplementary Materials: Searching Anti-Zika Virus Activity in 1*H*-1,2,3-triazole based compounds

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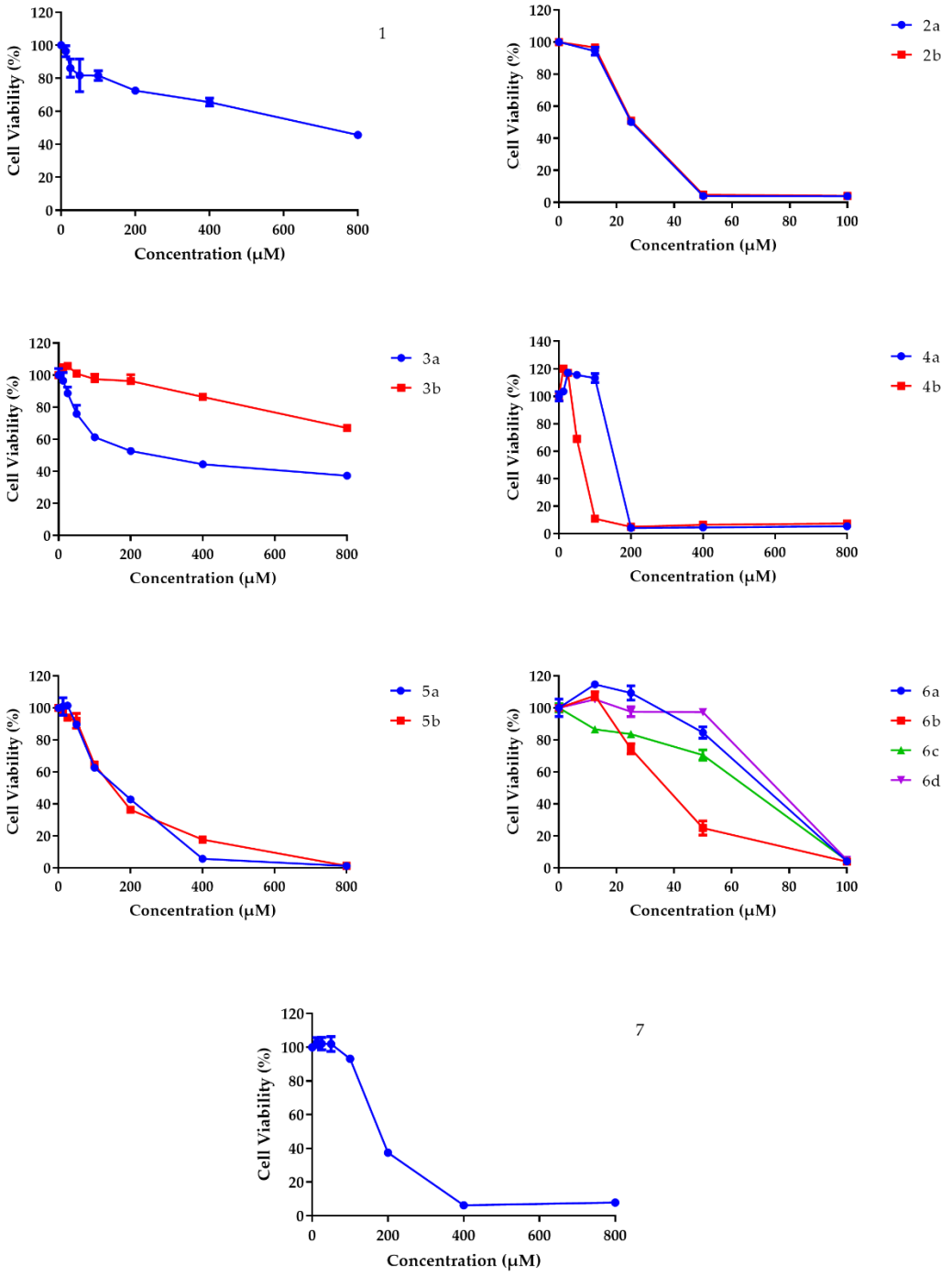

Figure S1. Graphical results for cytotoxicity assay of triazole derivates in Vero cells. Cell viability was determined by the MTT method and statistical analysis was performed in GraphPad Prism program. In brief, $1x10^4$ Vero cells were plated in 96-well microplates for 24h. The compounds were distributed in concentrations between 800-12,5 μM and incubated for 5 days. After reading the ODs by MTT method on spectrophotometer at 570nm, the graphical formation and determination of CC20 and CC50 was made on GraphPad Pris

Table S1: Missing residues in RdRp (*5U04*) protein.

Sequence	Range
YHGSYEAPTQGSASS	306-320
GIAMTDTTPYGQQRVFKEKVDTR	341-363
ALGAIFEE	409-416
MMGKREKKQGEFGKAK	455-470
DDTAGWDT	534-541
KVVKVLRPAEGGKTVMDIISRQDQRGSGQ	577-605
RKDTQ	690-694

Table S2: Model generated after filling loops for RdRp protein (5U04).

Entry	Code	ERRAT	PROSA	VERIFY-3D	PROCHECK			
					Favoured	Additional Favoured	Generously Favoured	Disallowed
1	Model-1	64.2361	-7.42	77.42%	87.8% (462)	8.9% (47)	1.9% (10)	1.3% (7)
2	Model-2	65.2324	-7.43	81.61%	89.5% (471)	8.7% (46)	0.8% (4)	1.0% (5)
3	Model-3	64.9573	-7.18	82.94%	88.8% (467)	9.1% (48)	1.5% (8)	0.6% (3)
4	Model-4	70.7612	-7.82	79.77%	90.9% (478)	7.0% (37)	1.0% (5)	1.1% (6)
5	Model-5	68.4119	-7.03	-79.26%	88.2% (464)	10.1% (53)	1.3% (7)	0.4% (2)
6	Model-6	60.7639	-5.77	-72.91%	87.1% (458)	8.7% (46)	2.3% (12)	1.9% (10)
7	Model-7	62.9948	-6.98	80.43%	88.0% (463)	8.9% (47)	1.7% (9)	1.3% (7)
8	Model-8	69.4017	-7.26	84.62%	88.2% (464)	9.7% (51)	1.3% (7)	0.8% (4)
9	**Model-9**	**70.5882**	**-7.69**	**84.95%**	**89.5% (471)**	**7.8% (41)**	**1.5% (8)**	**1.1% (6)**
10	Model-10	60.0349	-5.51	82.94%	89.4% (470)	8.6% (45)	1.3% (7)	0.8% (4)
11	Model-11	63.6522	-7.62	78.93%	87.3% (459)	9.5% (50)	1.5% (8)	1.7% (9)
12	Model-12	63.1488	-6.46	76.09%	87.8% (462)	9.7% (51)	1.3% (7)	1.1% (6)
13	Model-13	64.2123	-6.39	87.12%	89.2% (469)	8.9% (47)	1.5% (8)	0.4% (2)
14	Model-14	69.5502	-6.28	80.60%	89.2% (469)	8.7% (46)	1.0% (5)	1.1% (6)
15	Model-15	68.3566	-6.01	83.44%	88.8% (467)	8.4% (44)	1.9% (10)	1.0% (5)

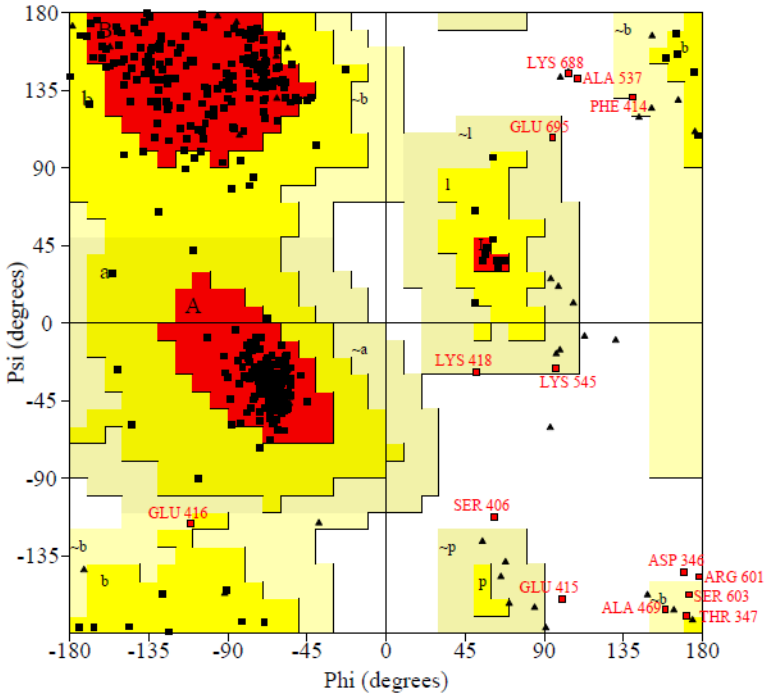

Figure S2. Ramachandran map of top scored modeled RdRp (5U04) protein.

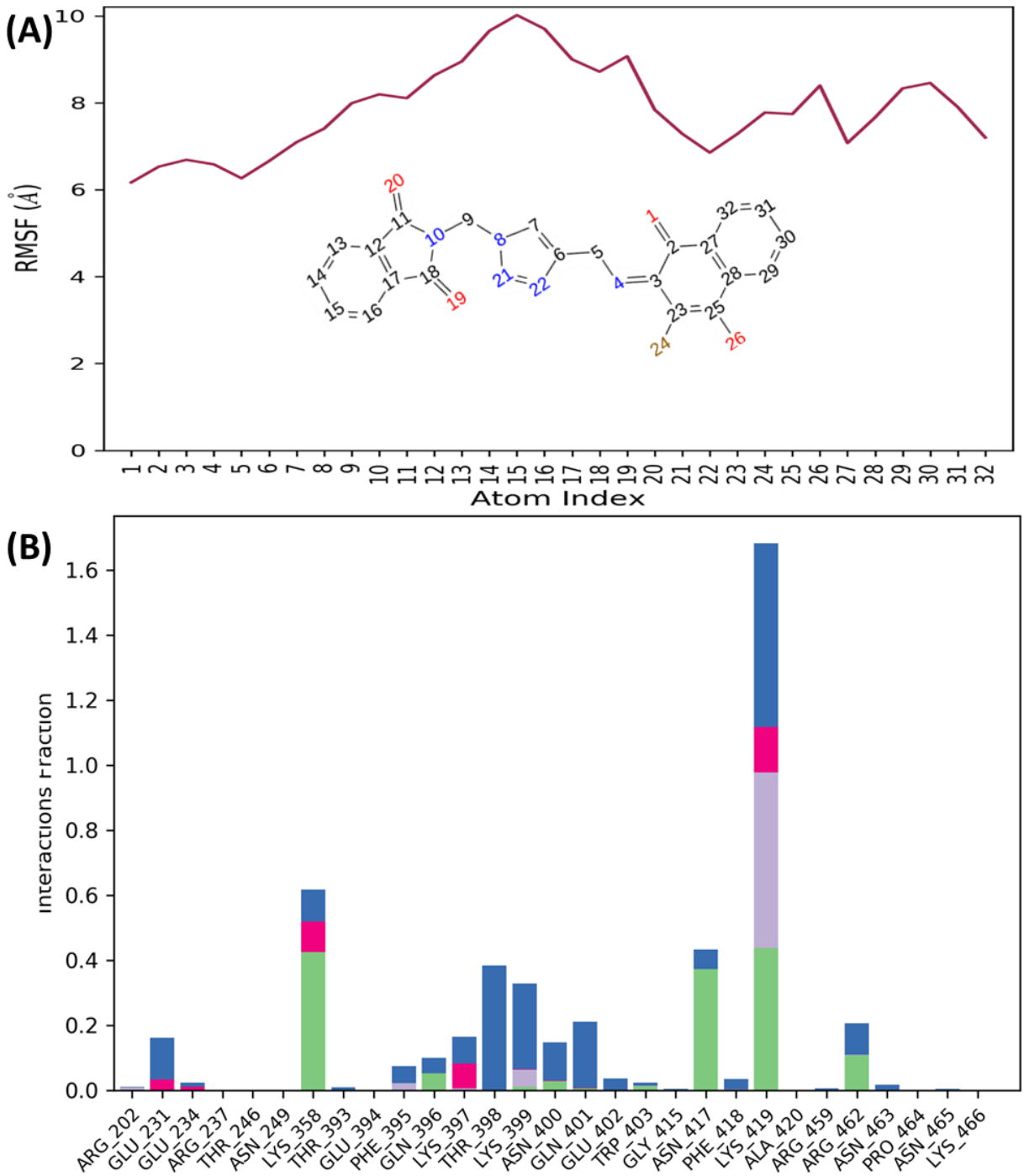

Figure S3. MD simulation of **4b**-helicase (6MH3) complex. A) Ligand RMSF-fluctuations of each atom of compound **4b** with respect to protein; B) Histogram plot showed interacting residues with compound **4b** during MD simulation (H-bond: green, hydrophobic: grey, salt bridge interaction: pink, and water bridge interaction: blue).

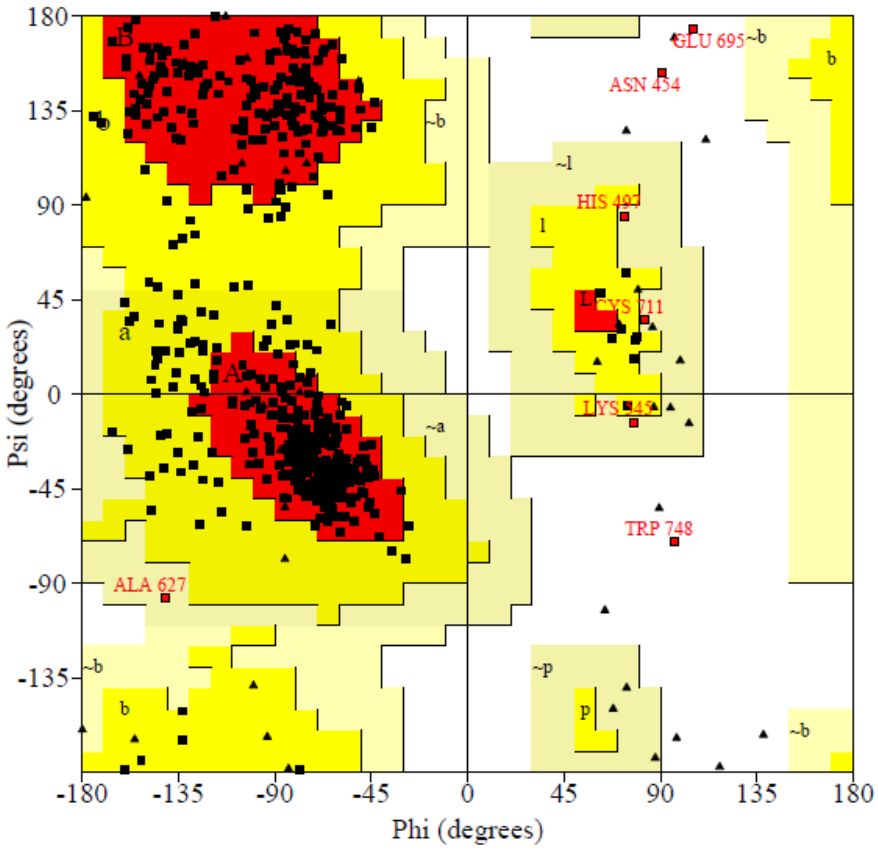

Figure S4. Ramachandran map after MD Simulation for **4b**-RdRp (5U04) complex.

Table S3: Site score of predicted binding site by Site Map for helicase protein (6MH3).

Binding Sites	Site Score	Residues
Site 3	**1.097**	**196, 197, 198, 199, 200, 201, 202, 228, 231, 286, 288, 316, 317, 415, 417, 455, 459, 462**
Site 1	1.055	224, 225, 226, 244, 245, 246, 262, 263, 264, 265, 267, 268, 271, 287, 288, 289, 290, 291, 292, 293, 298, 318, 320, 321, 322, 363, 364, 365, 366, 367, 368, 369, 370, 385, 386, 387, 388, 389, 390, 391, 392, 393, 394, 407, 408, 409, 410, 411, 413, 414, 429, 430, 431, 432, 442, 445, 448, 449, 451, 452, 456, 479, 480, 481, 484, 486, 487, 489, 493, 508, 514, 533, 536, 537, 540, 541, 542, 543, 597, 598, 599, 601, 602, 603, 604, 605, 608, 609, 617

Site 2	0.948	269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 300, 304, 309, 495, 496, 497, 498, 499, 500, 501, 502, 503, 504, 523, 524, 525, 526, 529, 530, 533, 534, 537, 538
Site 4	0.928	227, 230, 231, 358, 392, 395, 396, 398, 399, 401, 403, 417, 418, 419, 420, 421, 460, 461, 462, 463, 466, 469
Site 5	0.698	233, 236, 237, 238, 239, 240, 241, 243, 250, 251, 252, 253, 256

Table S4: Site score of predicted binding site by Site Map for RdRp protein ((5U04)).

Binding Sites	**Site Score**	**Residues**
Site 1	**1.008**	338, 339, 340, 341, 342, 343, 344, 345, 346, 416, 417, 418, 420, 486, 490, 513, 533, 534, 535, 536, 539, 540, 541, 542, 543, 544, 545, 547, 548, 551, 570, 573, 574, 575, 576, 604, 605, 607, 608, 609, 611, 612, 620, 623, 663, 664, 665, 666, 667, 676, 691, 702, 709, 710, 711, 712, 713, 714, 731, 732, 734, 735, 738, 739, 742, 743, 744, 745, 746, 747, 748, 749, 752, 753, 756, 760, 763, 768, 792, 793, 794, 795, 796, 797, 798, 799, 800, 801, 803, 805, 806, 848
Site 3	1.002	358, 359, 360, 361, 362, 363, 365, 368, 633, 636, 637, 681, 684, 685, 689, 692, 693, 695, 696
Site 2	0.980	758, 762, 765, 769, 772, 775, 776, 779, 782, 785, 786, 787, 788, 808, 809, 810, 811, 812, 834, 835, 836, 840, 858, 883, 884, 885, 886, 887, 888
Site 4	0.907	400, 403, 404, 412, 413, 415, 416, 417, 419, 422, 454, 455, 459, 465, 470, 471, 472, 473, 476, 479, 483, 487, 491, 494, 495, 602, 603, 604, 605, 606, 607
Site 5	0.764	354, 355, 356, 358, 626, 627, 629, 631, 632, 633, 675, 678, 679, 680, 681, 696, 698

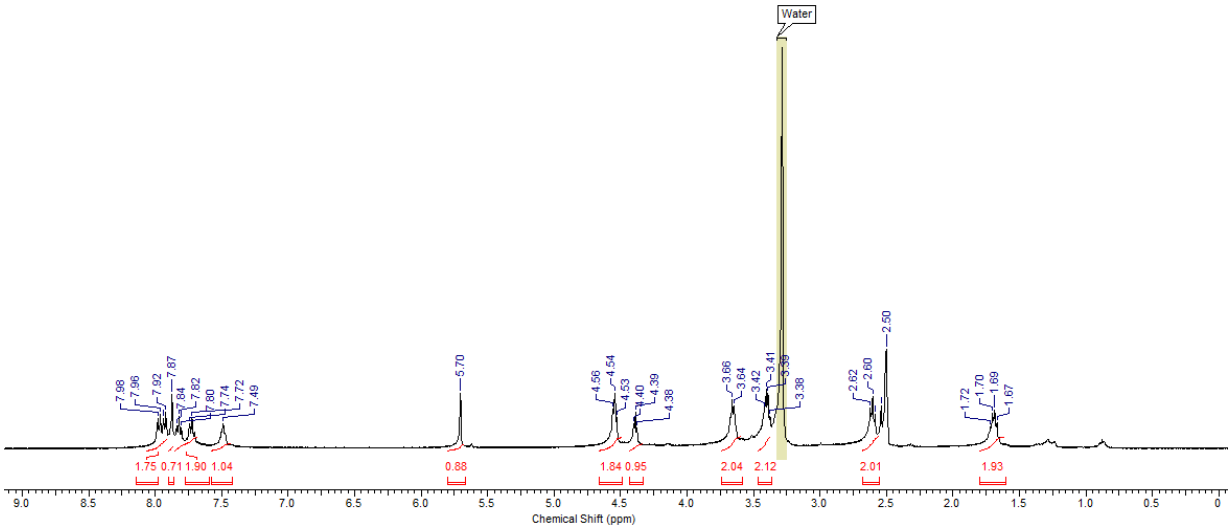

Figure S5. ^{1}H NMR of compound **5a**

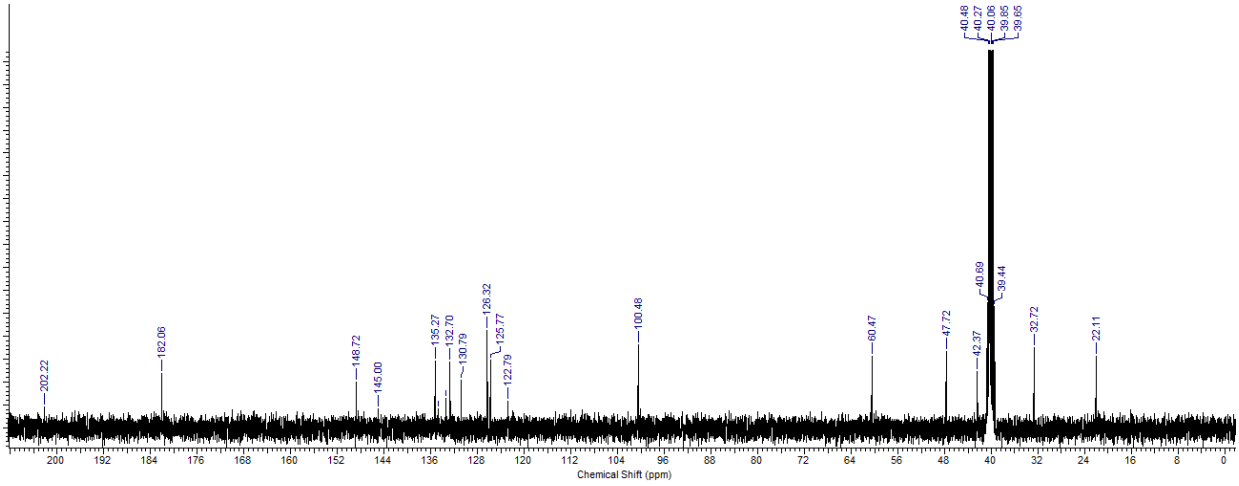

Figure S6. ^{13}C NMR of compound **5a**