

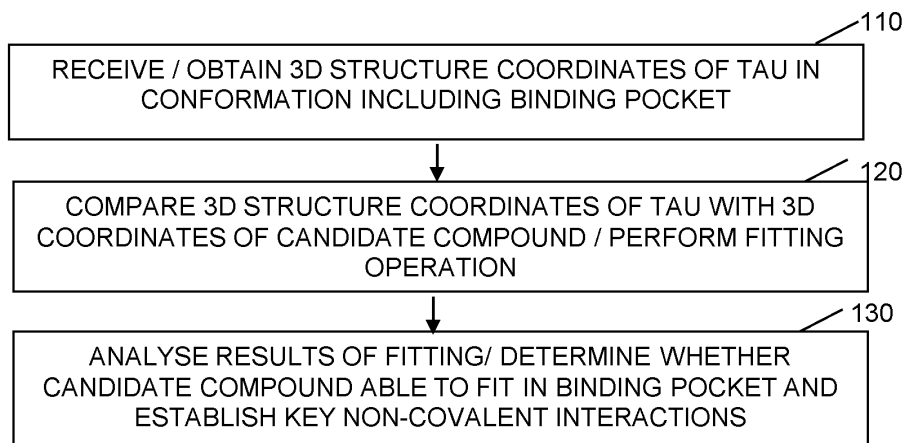


Figure 1

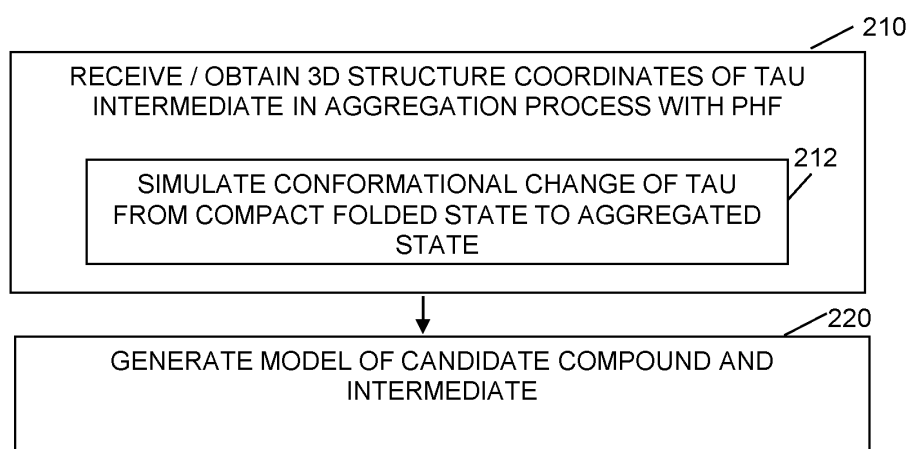


Figure 2

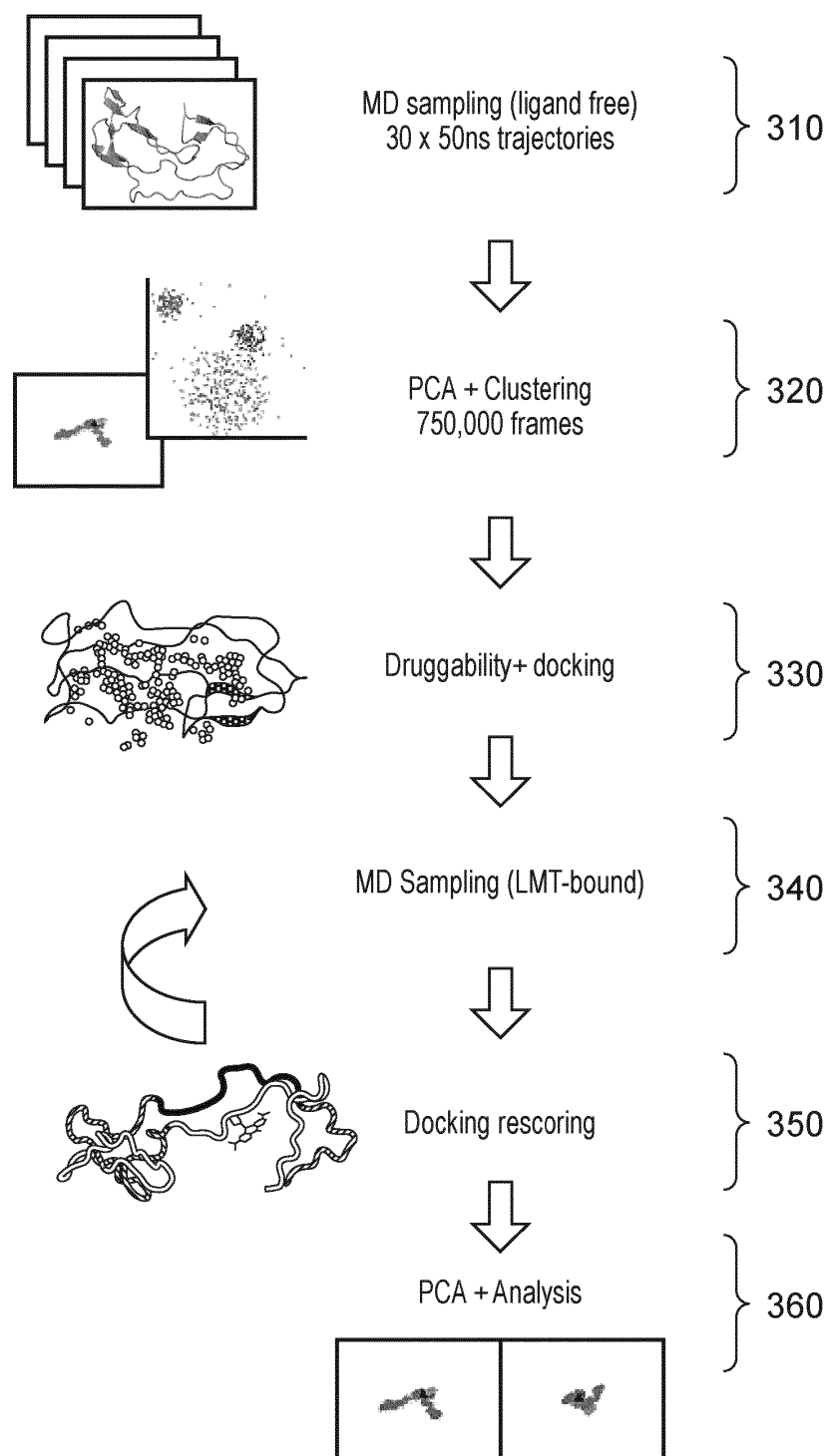


FIG. 3

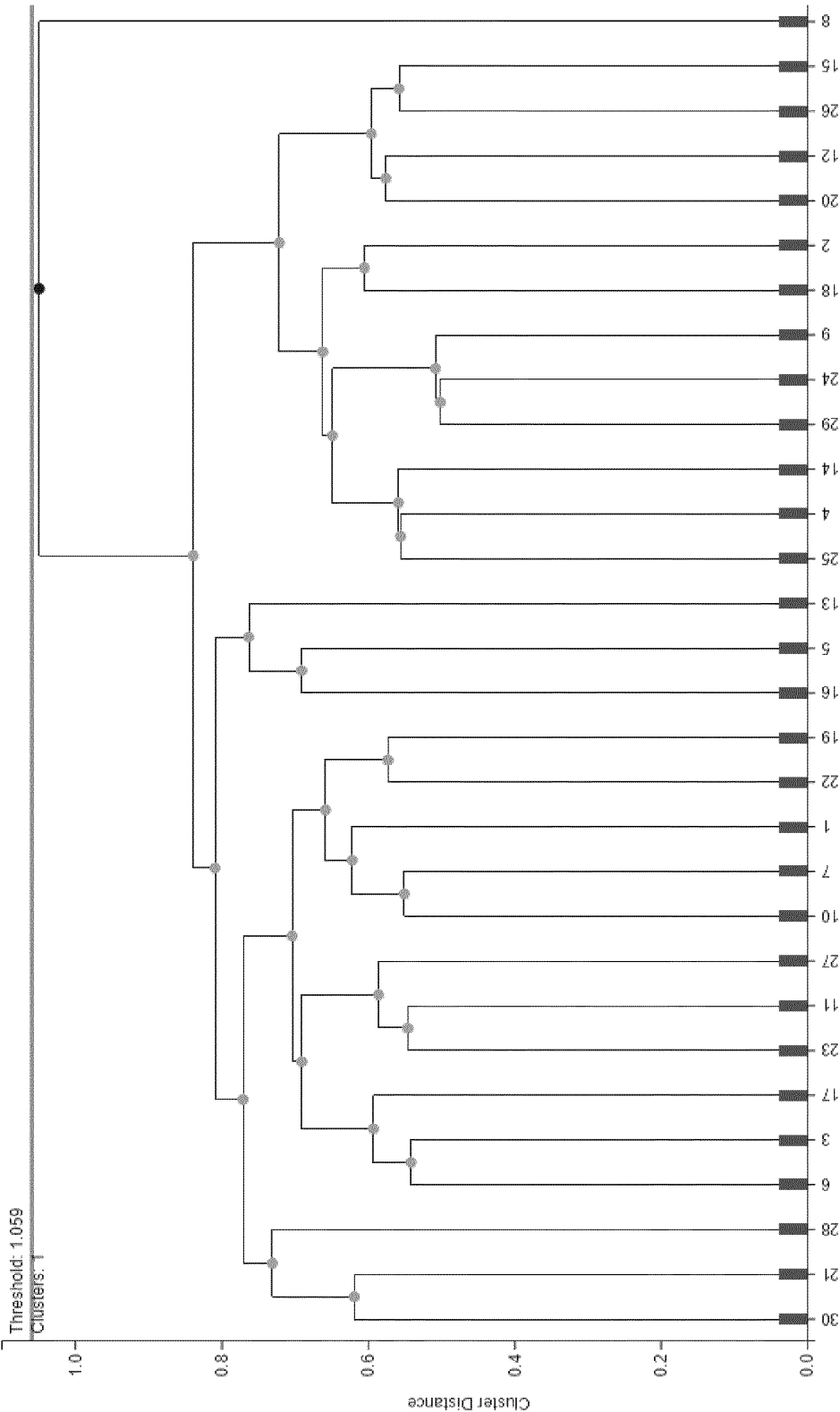


FIG. 4A

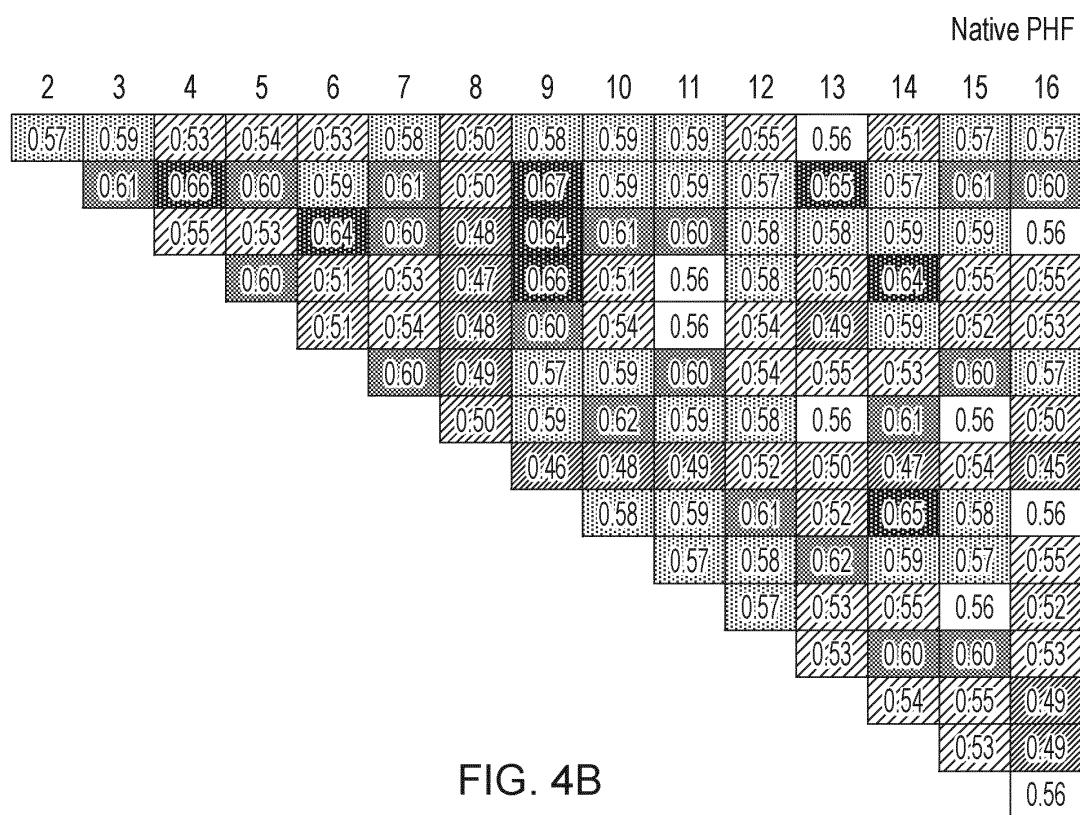


FIG. 4B

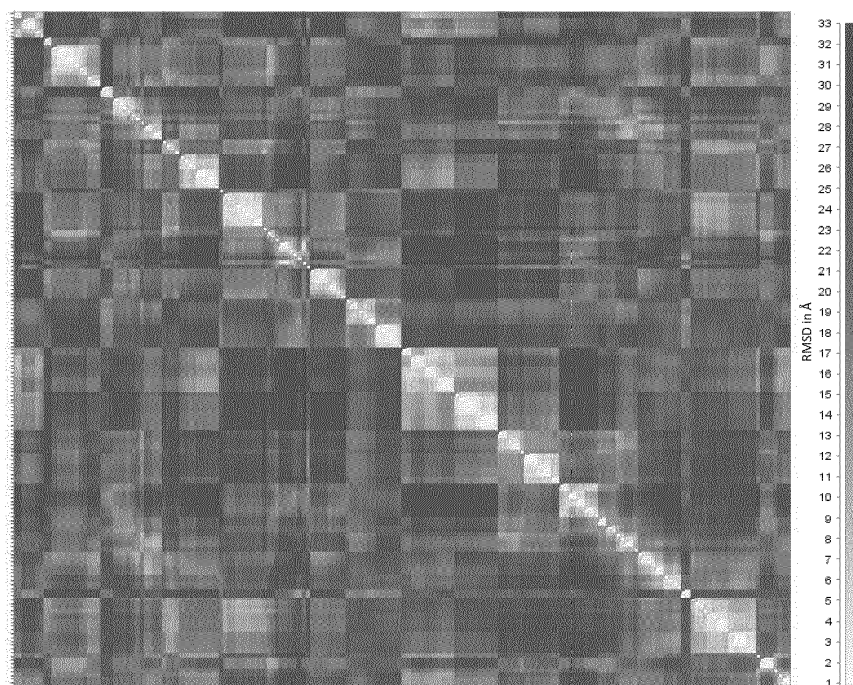


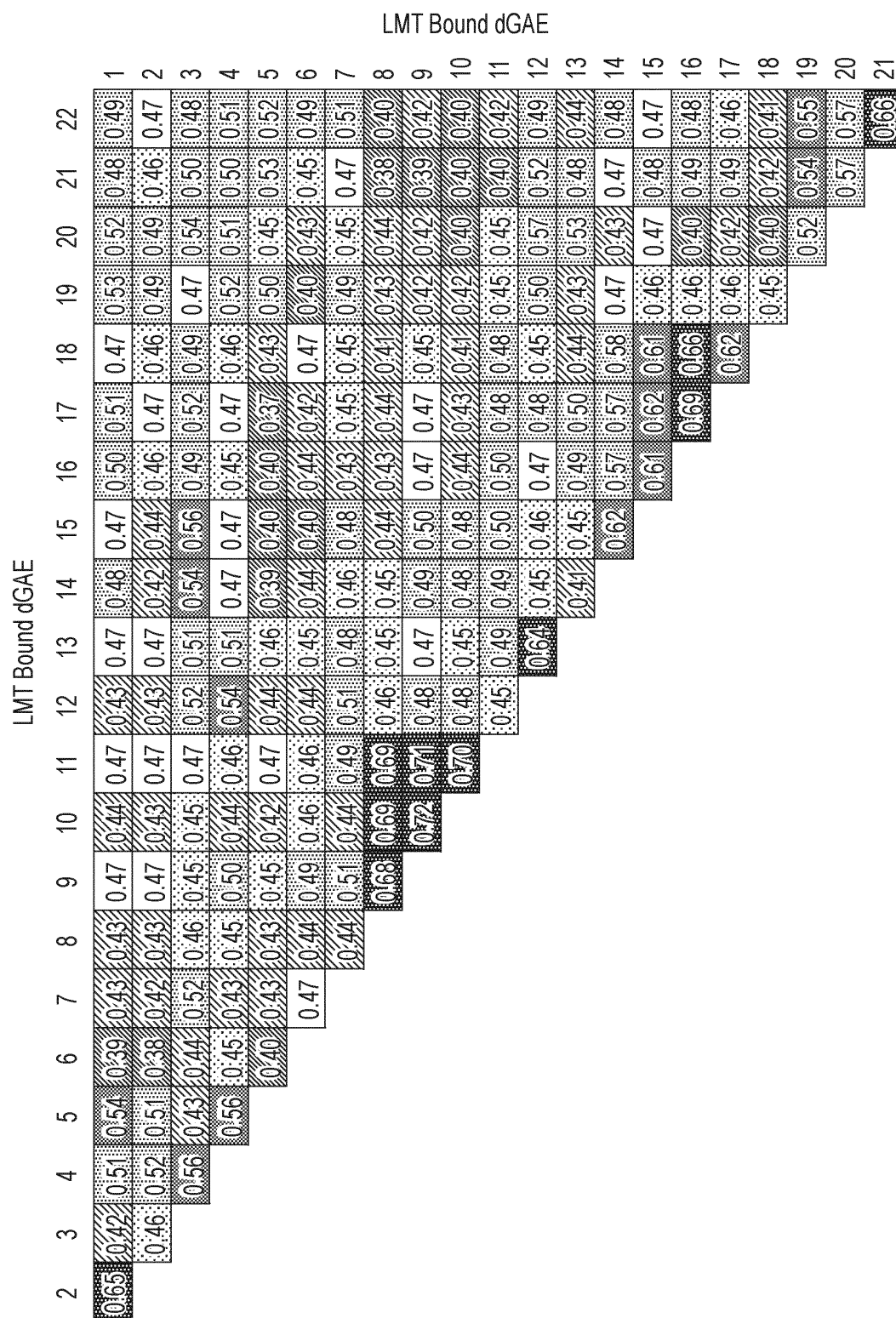
FIG. 5

single strand

17	18	19	20	21	22	23	24	25	26	27	28	29	30	
0.54	0.58	0.56	0.57	0.55	0.56	0.54	0.60	0.62	0.60	0.56	0.55	0.59	0.54	1
0.54	0.65	0.60	0.57	0.62	0.54	0.60	0.60	0.64	0.60	0.61	0.60	0.57	0.62	2
0.60	0.54	0.59	0.56	0.62	0.60	0.57	0.60	0.58	0.63	0.61	0.56	0.65	0.58	3
0.58	0.57	0.57	0.56	0.47	0.56	0.63	0.61	0.63	0.56	0.59	0.47	0.60	0.59	4
0.53	0.57	0.56	0.55	0.53	0.53	0.54	0.56	0.56	0.51	0.51	0.47	0.55	0.50	5
0.63	0.50	0.54	0.56	0.62	0.56	0.56	0.57	0.54	0.60	0.55	0.60	0.63	0.57	6
0.59	0.56	0.59	0.57	0.58	0.57	0.55	0.62	0.57	0.58	0.55	0.52	0.58	0.52	7
0.48	0.47	0.41	0.45	0.45	0.45	0.51	0.49	0.48	0.51	0.49	0.49	0.47	0.43	8
0.63	0.63	0.63	0.61	0.52	0.60	0.61	0.67	0.65	0.63	0.58	0.55	0.67	0.60	9
0.58	0.54	0.57	0.57	0.61	0.57	0.54	0.64	0.57	0.60	0.59	0.53	0.60	0.54	10
0.58	0.50	0.58	0.56	0.54	0.55	0.63	0.59	0.60	0.55	0.62	0.55	0.55	0.52	11
0.60	0.58	0.55	0.61	0.52	0.55	0.62	0.64	0.60	0.60	0.59	0.54	0.58	0.55	12
0.51	0.48	0.50	0.55	0.56	0.51	0.49	0.59	0.49	0.52	0.54	0.49	0.54	0.46	13
0.55	0.63	0.61	0.61	0.55	0.56	0.59	0.61	0.63	0.59	0.58	0.50	0.61	0.55	14
0.55	0.56	0.51	0.61	0.53	0.53	0.56	0.61	0.55	0.63	0.53	0.59	0.58	0.54	15
0.56	0.52	0.53	0.51	0.53	0.52	0.53	0.54	0.54	0.49	0.52	0.51	0.54	0.50	16
	0.54	0.55	0.57	0.56	0.61	0.56	0.64	0.58	0.61	0.56	0.56	0.62	0.54	17
		0.57	0.61	0.50	0.54	0.53	0.61	0.63	0.58	0.52	0.51	0.59	0.57	18
			0.55	0.60	0.61	0.57	0.60	0.60	0.58	0.55	0.50	0.58	0.59	19
				0.52	0.58	0.55	0.68	0.58	0.61	0.50	0.53	0.61	0.54	20
					0.54	0.54	0.55	0.51	0.57	0.51	0.51	0.54	0.60	21
						0.55	0.58	0.57	0.57	0.54	0.51	0.57	0.57	22
							0.60	0.64	0.55	0.60	0.53	0.54	0.53	23
								0.60	0.63	0.59	0.56	0.67	0.59	24
									0.58	0.59	0.55	0.63	0.57	25
										0.55	0.57	0.65	0.57	26
											0.53	0.56	0.48	27
												0.60	0.54	28
													0.58	29
														30

Native PHF single strand

FIG. 4B (Continued)



Limit bound											
name	1	2	3	4	5	6	7	8	9	10	11
1	0.47	0.44	0.47	0.41	0.47	0.41	0.49	0.47	0.46	0.44	0.47
2	0.48	0.49	0.46	0.48	0.46	0.40	0.51	0.49	0.53	0.47	0.51
3	0.50	0.45	0.52	0.53	0.46	0.42	0.48	0.49	0.51	0.45	0.53
4	0.46	0.44	0.41	0.41	0.43	0.40	0.47	0.41	0.52	0.45	0.47
5	0.47	0.49	0.43	0.44	0.45	0.38	0.45	0.43	0.44	0.43	0.47
6	0.45	0.44	0.54	0.49	0.50	0.42	0.49	0.44	0.45	0.44	0.49
7	0.43	0.41	0.51	0.44	0.43	0.38	0.43	0.41	0.46	0.44	0.47
8	0.38	0.41	0.37	0.35	0.43	0.37	0.40	0.38	0.41	0.40	0.42
9	0.48	0.47	0.46	0.48	0.51	0.38	0.47	0.46	0.51	0.47	0.50
10	0.46	0.45	0.53	0.45	0.47	0.41	0.47	0.44	0.46	0.41	0.45
11	0.41	0.39	0.42	0.47	0.49	0.39	0.41	0.40	0.42	0.40	0.43
12	0.43	0.46	0.45	0.45	0.45	0.38	0.50	0.45	0.47	0.46	0.47
13	0.45	0.47	0.48	0.46	0.42	0.38	0.40	0.37	0.41	0.41	0.35
14	0.45	0.45	0.42	0.40	0.41	0.34	0.44	0.41	0.46	0.43	0.45
15	0.45	0.46	0.43	0.43	0.44	0.37	0.45	0.43	0.43	0.42	0.48
16	0.47	0.43	0.53	0.48	0.50	0.46	0.61	0.53	0.53	0.54	0.55
17	0.49	0.42	0.50	0.47	0.46	0.43	0.52	0.46	0.50	0.42	0.49
18	0.47	0.45	0.40	0.38	0.43	0.35	0.47	0.45	0.48	0.44	0.52
19	0.50	0.43	0.49	0.45	0.44	0.39	0.45	0.49	0.51	0.47	0.52
20	0.45	0.48	0.44	0.39	0.46	0.34	0.43	0.42	0.43	0.41	0.43
21	0.50	0.43	0.49	0.47	0.41	0.44	0.42	0.45	0.48	0.45	0.51
22	0.46	0.44	0.47	0.43	0.46	0.40	0.48	0.50	0.48	0.44	0.50
23	0.44	0.44	0.45	0.47	0.47	0.40	0.47	0.46	0.48	0.45	0.47
24	0.47	0.46	0.49	0.45	0.47	0.34	0.44	0.44	0.46	0.43	0.46
25	0.41	0.43	0.47	0.44	0.49	0.38	0.47	0.46	0.46	0.42	0.48
26	0.46	0.45	0.48	0.43	0.42	0.35	0.44	0.44	0.48	0.42	0.51
27	0.46	0.43	0.44	0.44	0.49	0.41	0.47	0.42	0.47	0.43	0.47
28	0.43	0.39	0.47	0.46	0.40	0.44	0.44	0.46	0.42	0.40	0.46
29	0.48	0.47	0.53	0.47	0.47	0.40	0.47	0.48	0.49	0.47	0.49
30	0.51	0.46	0.41	0.41	0.42	0.41	0.43	0.51	0.51	0.46	0.51
AVERAGE	0.46	0.44	0.46	0.44	0.45	0.39	0.46	0.45	0.47	0.44	0.48

FIG. 7

confirmation											AVERAGE
12	13	14	15	16	17	18	19	20	21	22	
0.43	0.50	0.43	0.41	0.48	0.48	0.44	0.44	0.48	0.49	0.43	0.45
0.45	0.55	0.45	0.40	0.45	0.46	0.44	0.45	0.48	0.49	0.49	0.47
0.46	0.52	0.49	0.44	0.44	0.49	0.42	0.45	0.51	0.51	0.49	0.48
0.39	0.43	0.44	0.41	0.37	0.42	0.41	0.37	0.39	0.46	0.43	0.43
0.40	0.41	0.44	0.40	0.49	0.50	0.46	0.39	0.39	0.45	0.42	0.44
0.56	0.54	0.57	0.47	0.42	0.51	0.41	0.48	0.54	0.56	0.51	0.49
0.48	0.49	0.47	0.41	0.44	0.45	0.45	0.43	0.44	0.47	0.49	0.45
0.41	0.44	0.39	0.36	0.41	0.44	0.35	0.40	0.41	0.48	0.42	0.40
0.45	0.55	0.46	0.45	0.44	0.45	0.43	0.42	0.49	0.53	0.49	0.47
0.47	0.46	0.46	0.44	0.45	0.49	0.42	0.46	0.48	0.50	0.49	0.46
0.42	0.45	0.40	0.34	0.44	0.48	0.42	0.42	0.43	0.49	0.45	0.42
0.43	0.48	0.45	0.39	0.54	0.50	0.48	0.44	0.42	0.49	0.48	0.46
0.46	0.46	0.44	0.42	0.48	0.53	0.43	0.45	0.45	0.47	0.42	0.44
0.40	0.43	0.43	0.38	0.42	0.45	0.42	0.36	0.41	0.45	0.44	0.42
0.43	0.52	0.43	0.43	0.46	0.47	0.44	0.43	0.47	0.50	0.46	0.45
0.48	0.49	0.49	0.48	0.45	0.46	0.45	0.45	0.49	0.48	0.43	0.49
0.54	0.55	0.48	0.41	0.43	0.46	0.40	0.44	0.52	0.50	0.49	0.47
0.44	0.47	0.40	0.37	0.46	0.48	0.47	0.43	0.42	0.48	0.45	0.44
0.47	0.47	0.50	0.43	0.48	0.46	0.46	0.41	0.44	0.47	0.48	0.46
0.43	0.54	0.44	0.39	0.45	0.48	0.39	0.43	0.42	0.46	0.45	0.43
0.50	0.46	0.57	0.48	0.50	0.55	0.47	0.47	0.48	0.47	0.49	0.48
0.42	0.48	0.49	0.41	0.40	0.45	0.41	0.41	0.48	0.50	0.49	0.45
0.41	0.42	0.47	0.42	0.42	0.48	0.47	0.42	0.42	0.45	0.46	0.45
0.47	0.53	0.44	0.41	0.44	0.46	0.39	0.46	0.48	0.46	0.49	0.45
0.42	0.47	0.41	0.40	0.42	0.46	0.41	0.42	0.48	0.47	0.49	0.44
0.46	0.50	0.47	0.40	0.40	0.42	0.37	0.42	0.46	0.53	0.48	0.44
0.41	0.46	0.39	0.39	0.43	0.49	0.39	0.43	0.44	0.46	0.46	0.44
0.44	0.50	0.45	0.39	0.44	0.45	0.38	0.45	0.53	0.49	0.50	0.44
0.51	0.55	0.47	0.42	0.43	0.41	0.37	0.48	0.49	0.56	0.51	0.47
0.44	0.44	0.56	0.43	0.40	0.44	0.46	0.41	0.44	0.48	0.47	0.46
0.45	0.49	0.46	0.41	0.44	0.47	0.42	0.43	0.46	0.49	0.47	

FIG. 7 (Continued)

²⁹⁷IKHVPGGGSVQIVY KPVDSLKVTS KCGSLGNIHH KPGGGQVEVK SEKLDFKDRV QSKIGSLDNI THVPGGGNKK IETHKLTFR E NAKAKTDHGAE³⁹¹

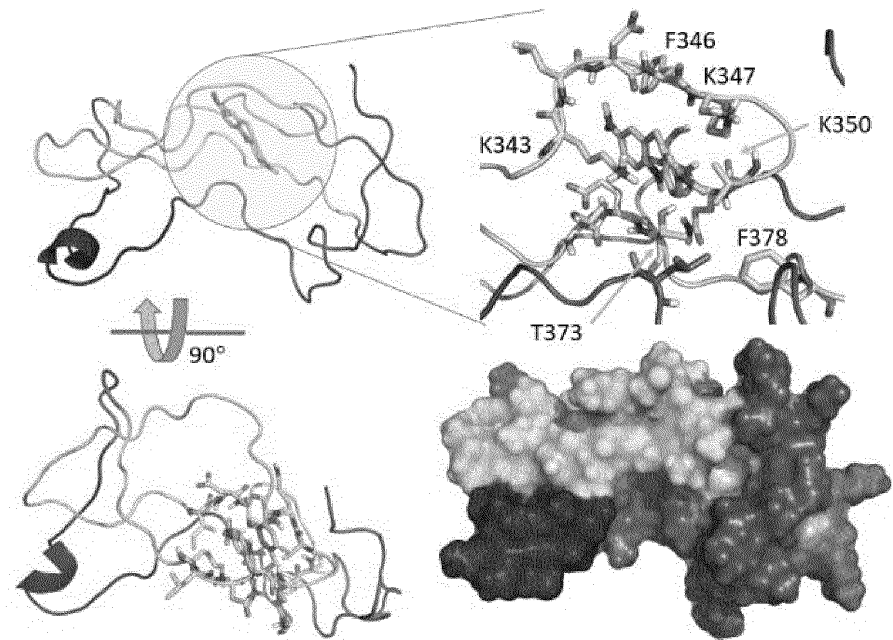


Figure 8A

First vs Previous LMT pocket stability

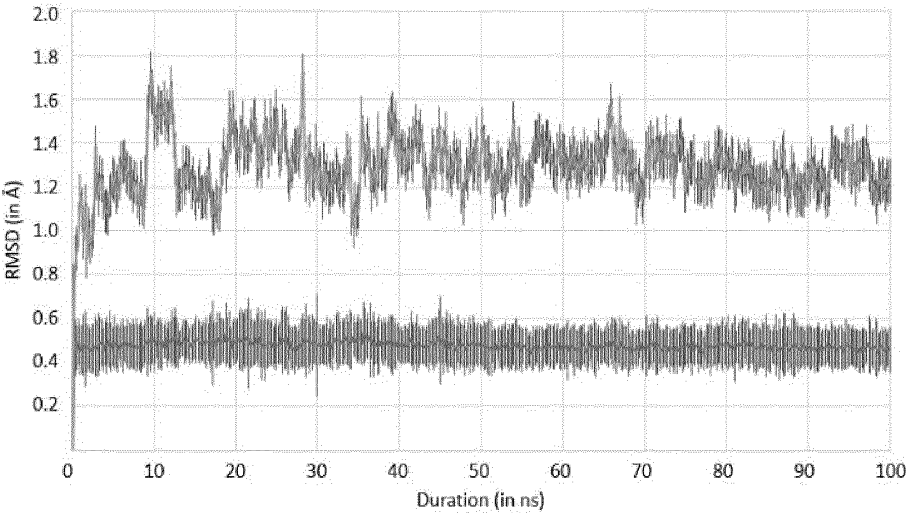


Figure 8B

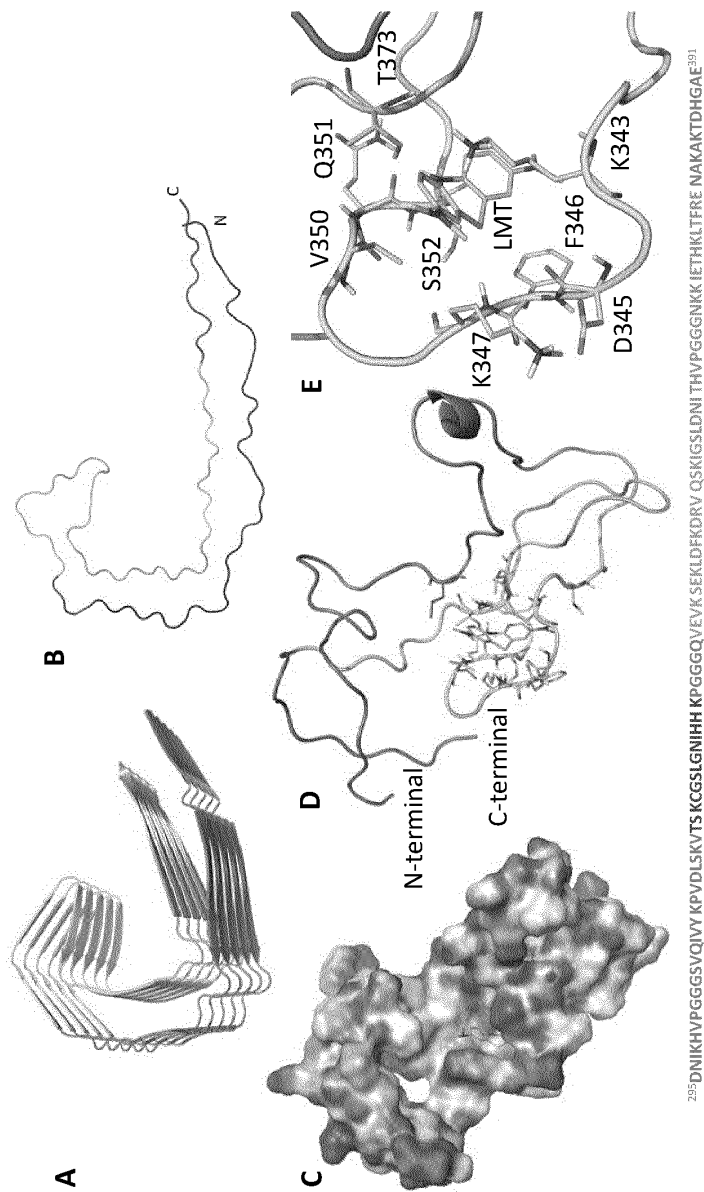


Figure 9

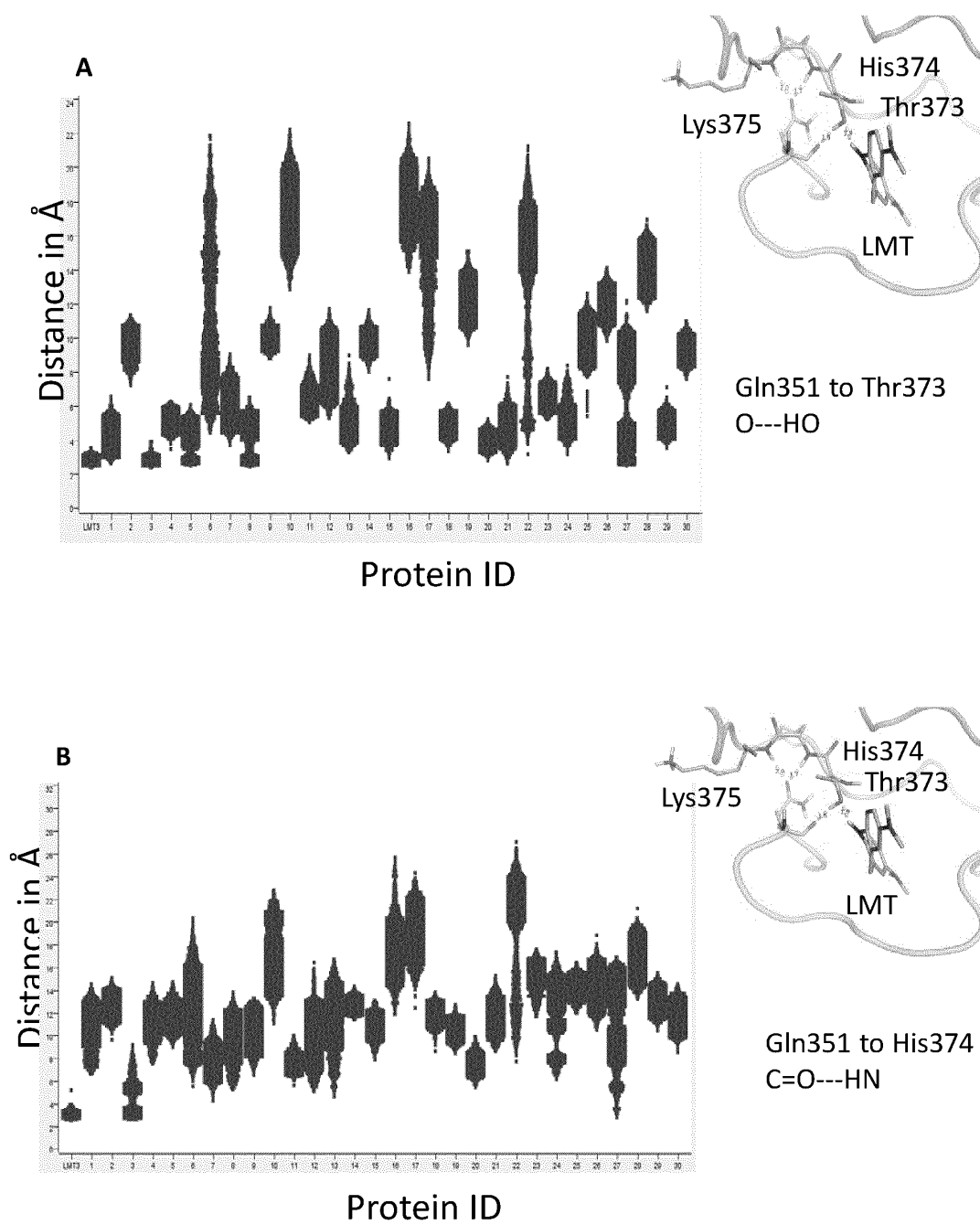


Figure 10

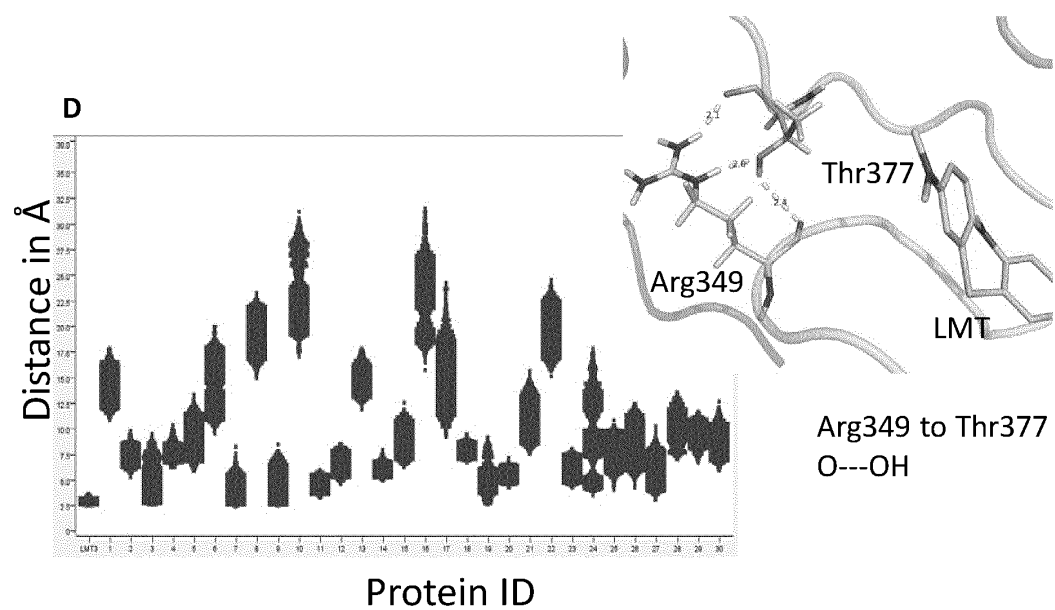
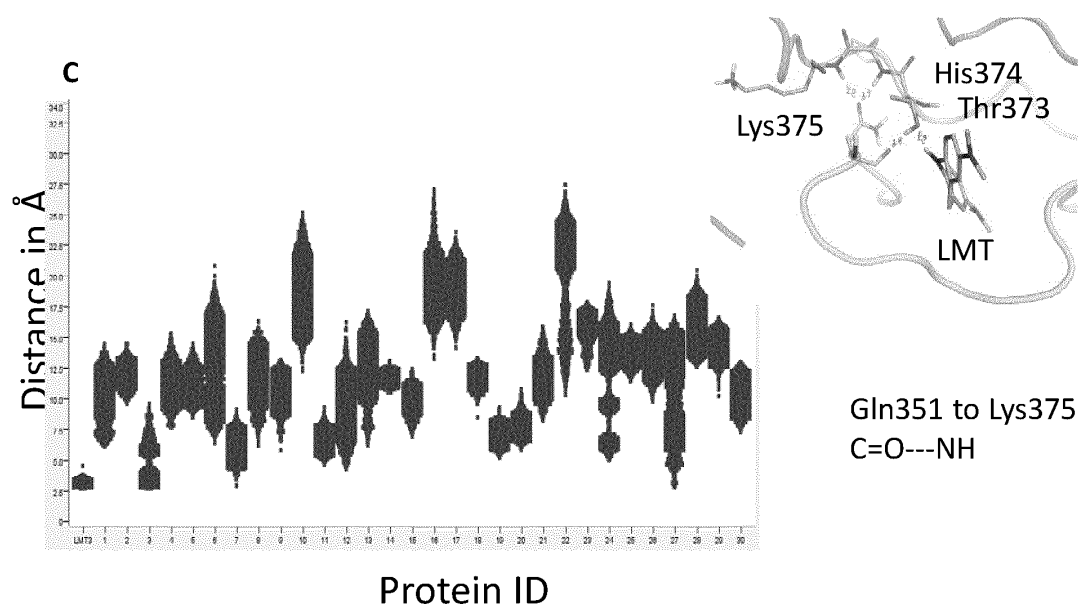


Figure 10 (continued)

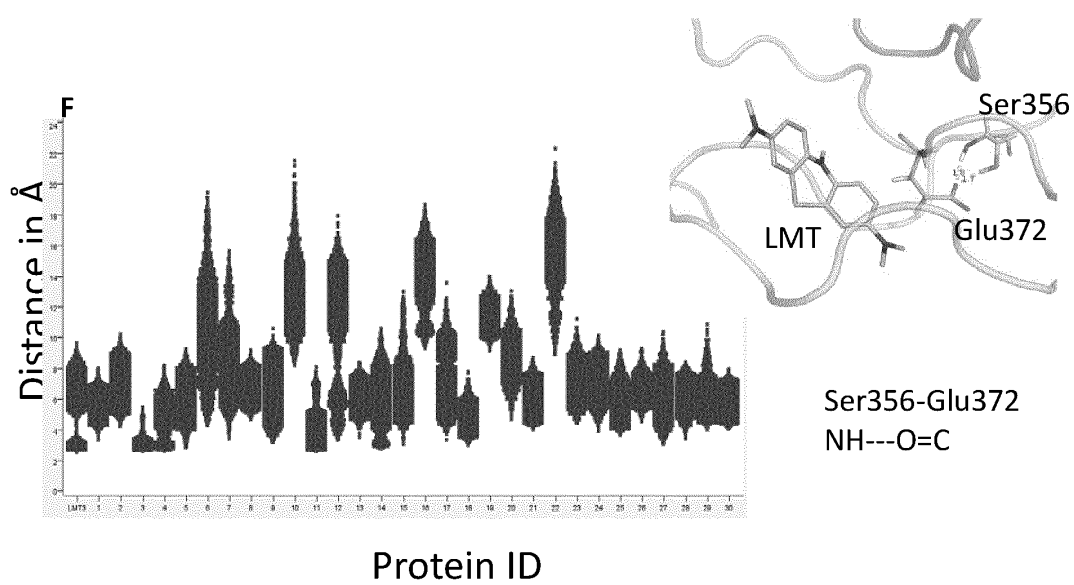
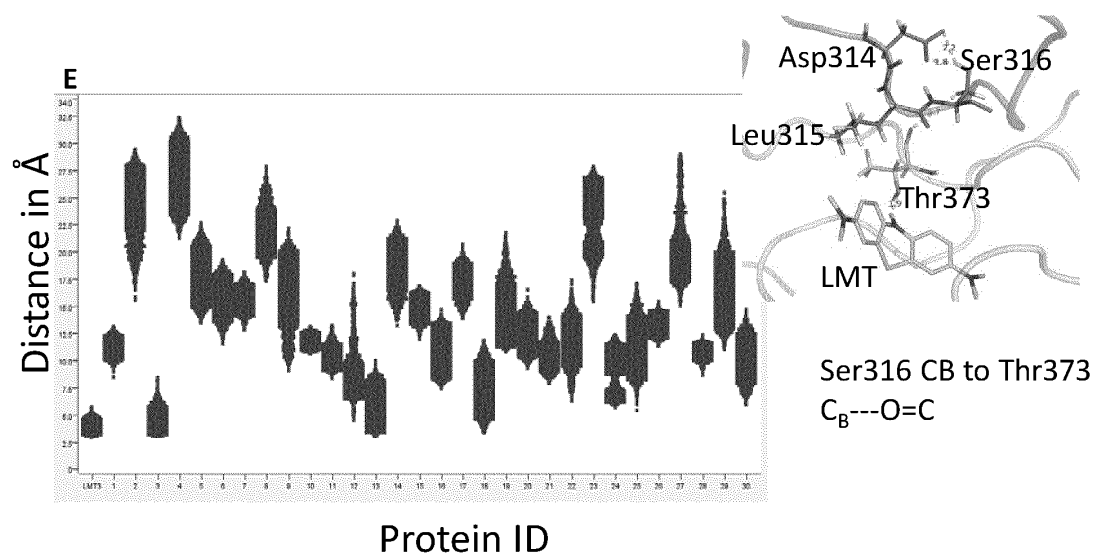


Figure 10 (continued)

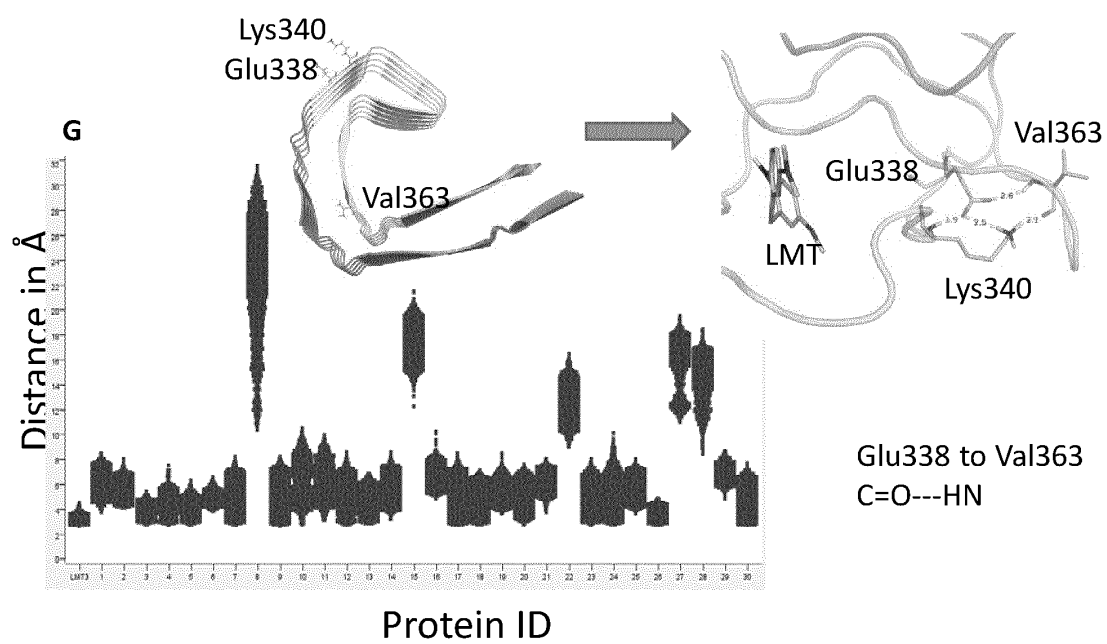


Figure 10 (continued)

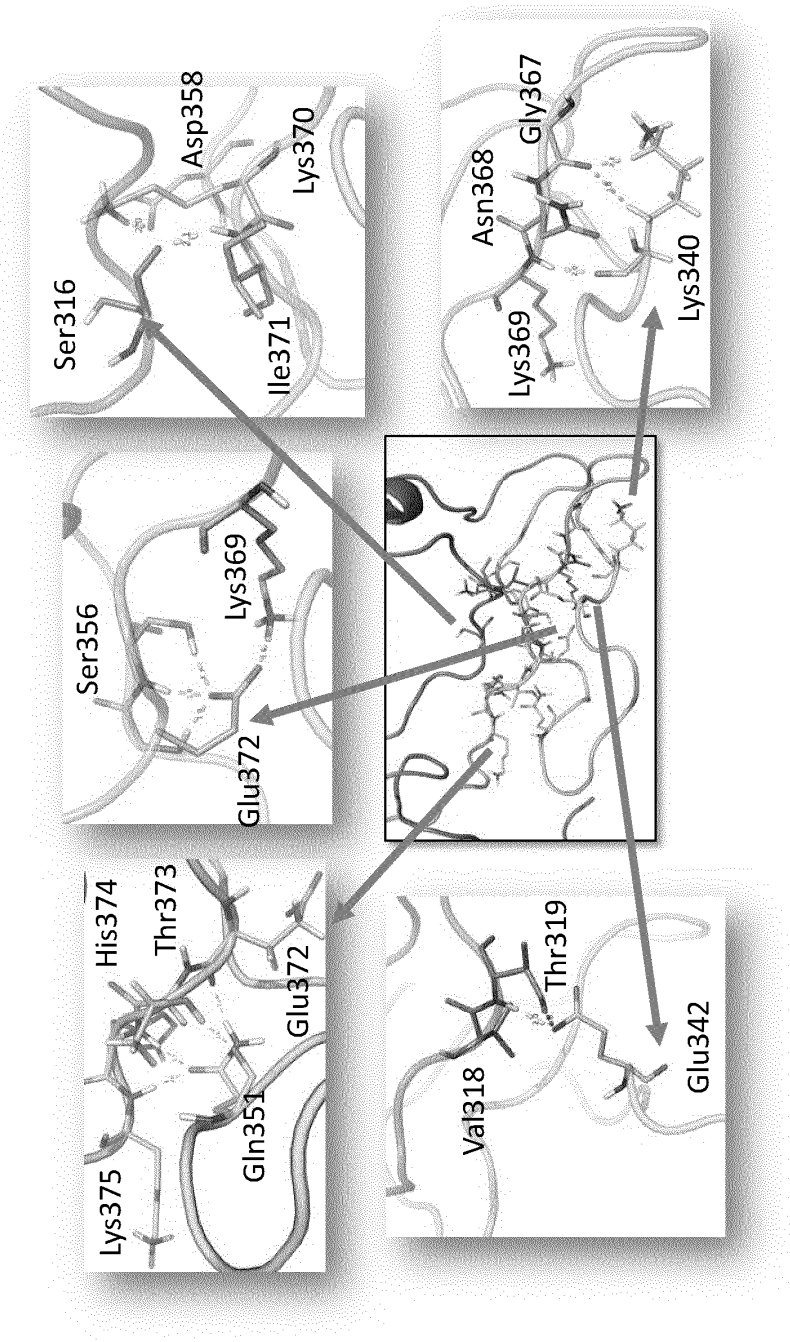


Figure 11

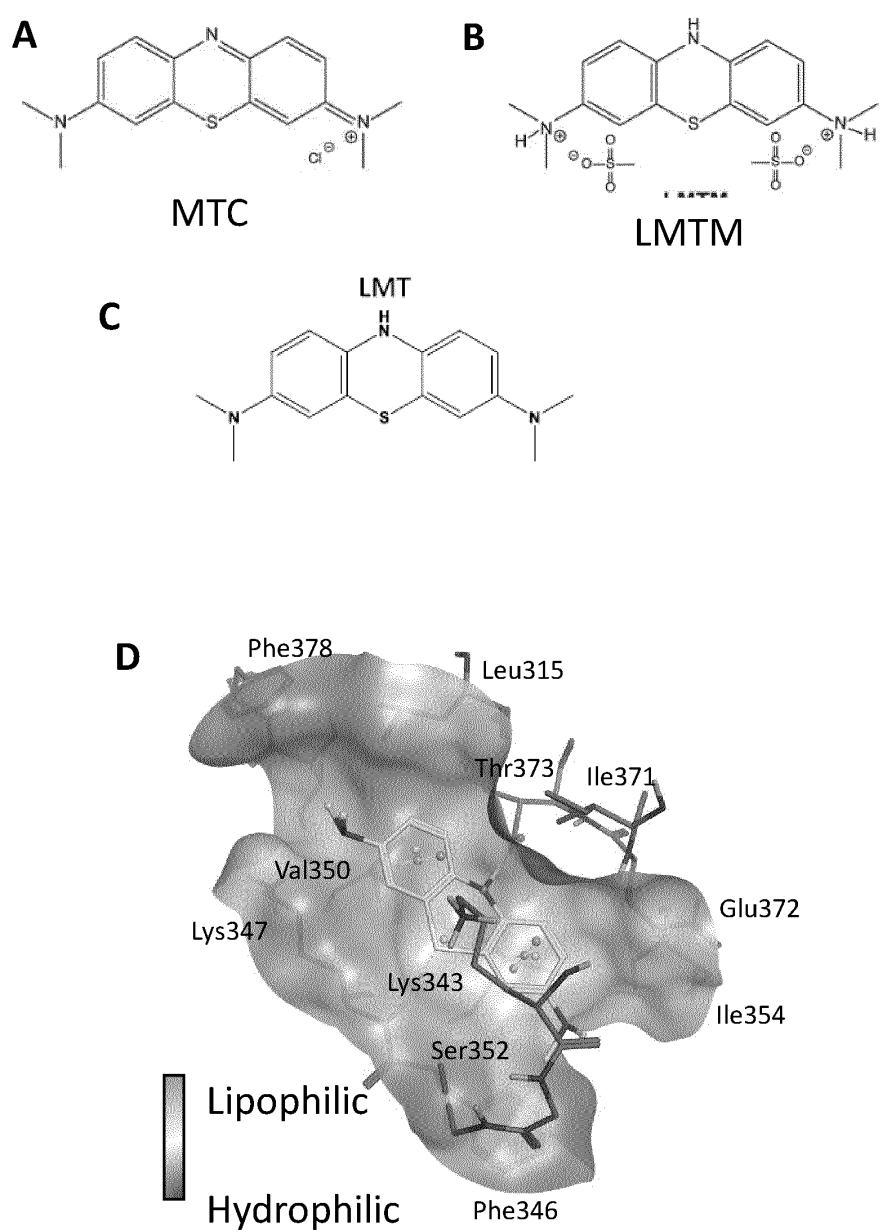


Figure 12

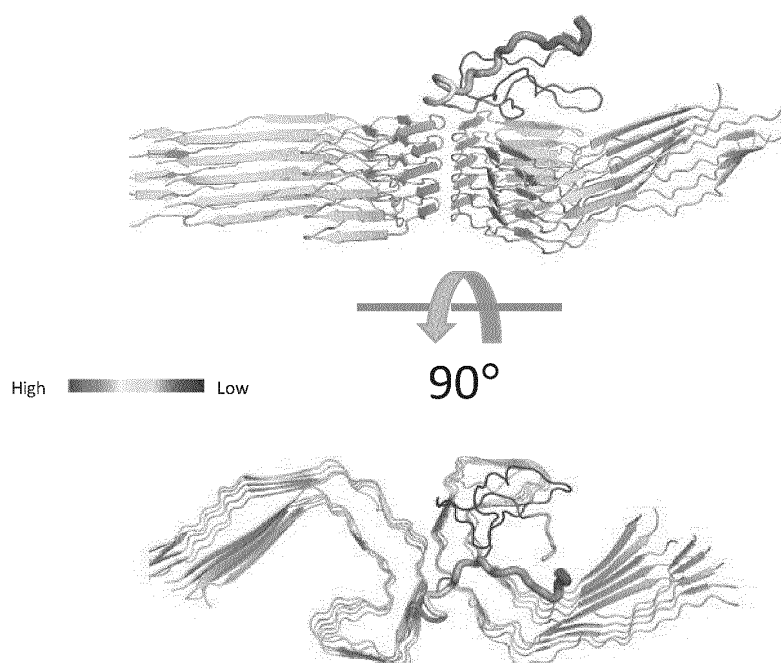


FIG. 13

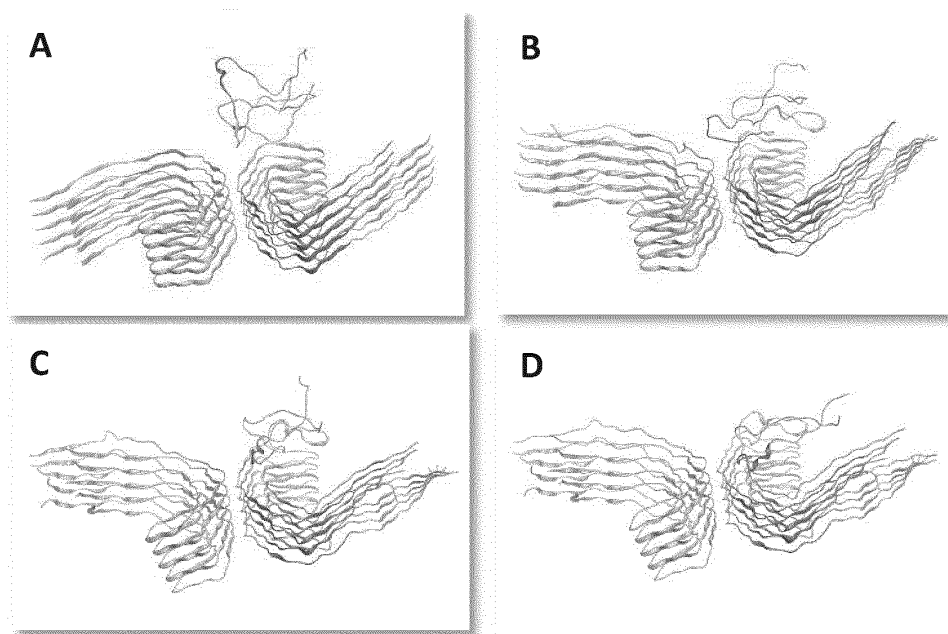


FIG. 14

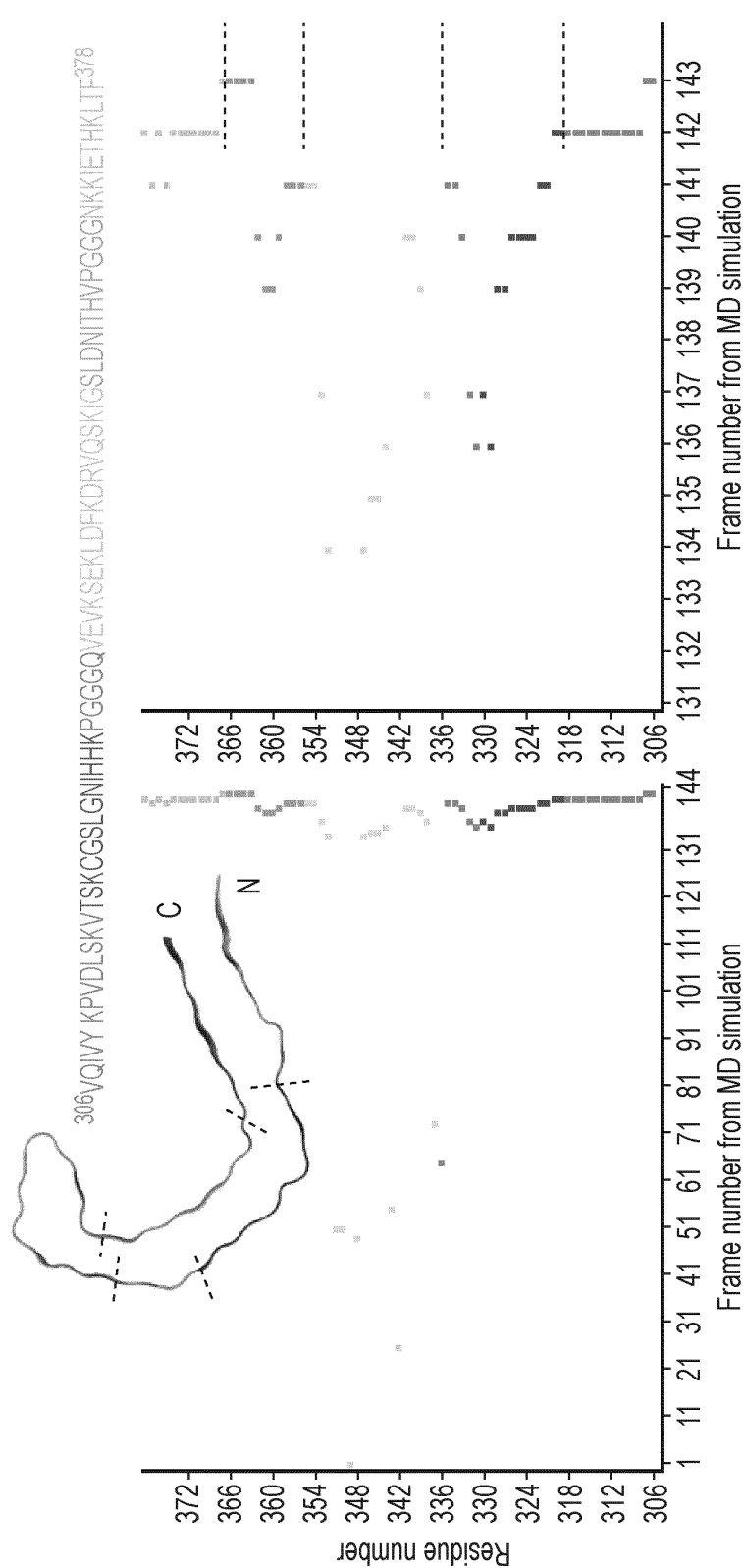
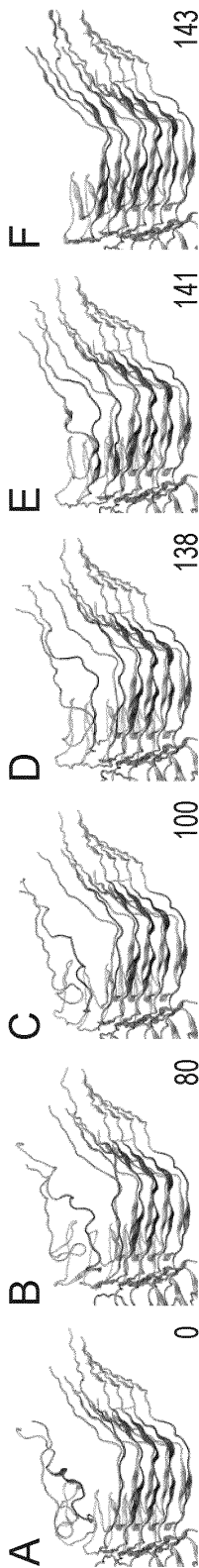


FIG. 15

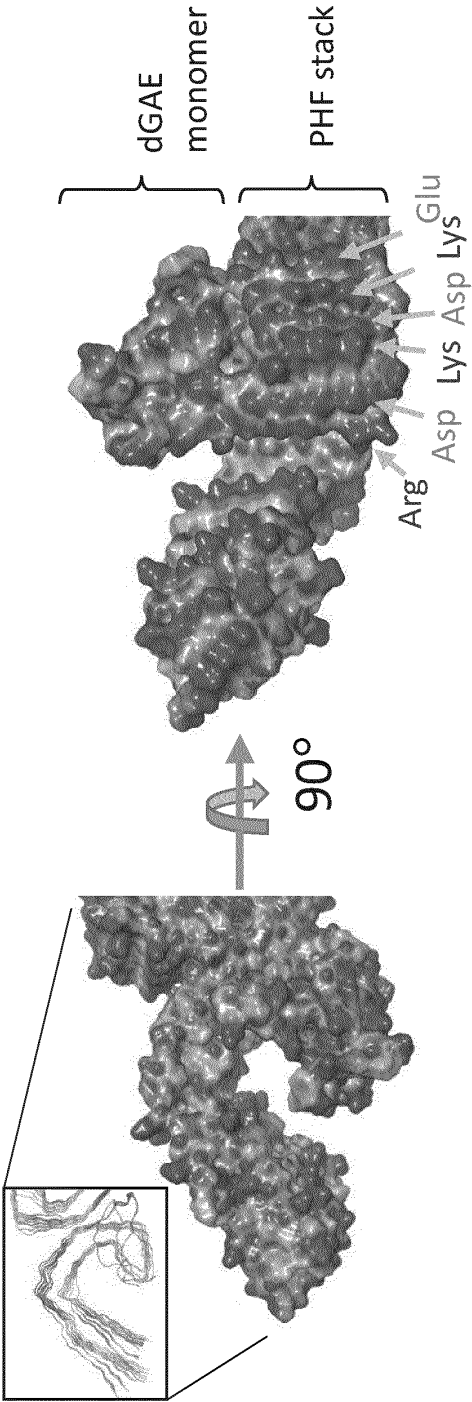


FIG. 16B

FIG. 16A

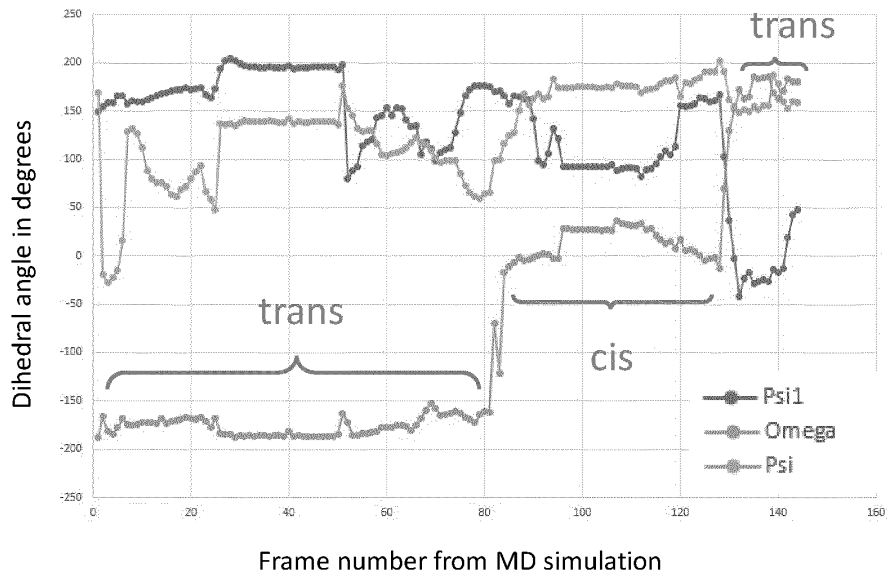


Figure 17A

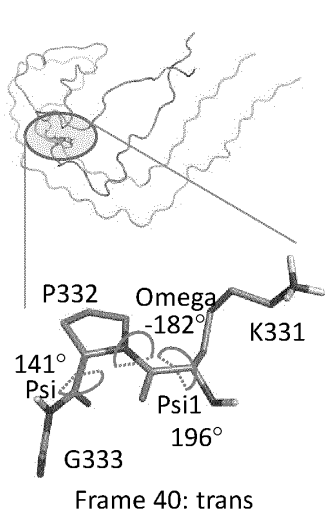


Figure 17B

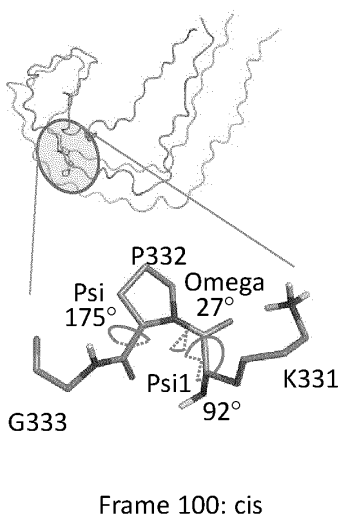


Figure 17C

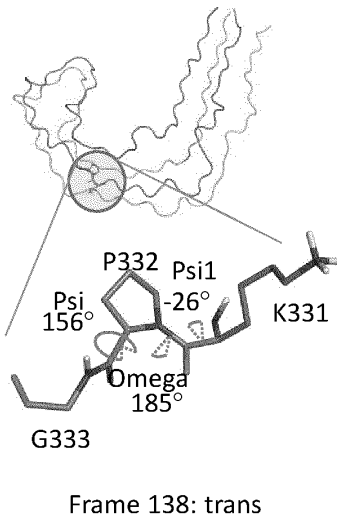


Figure 17D

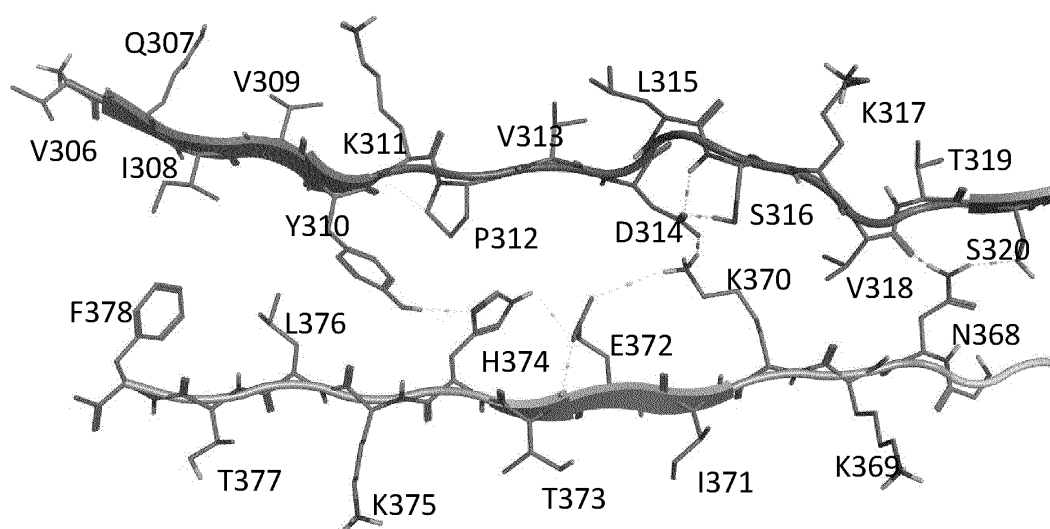


Figure 18A

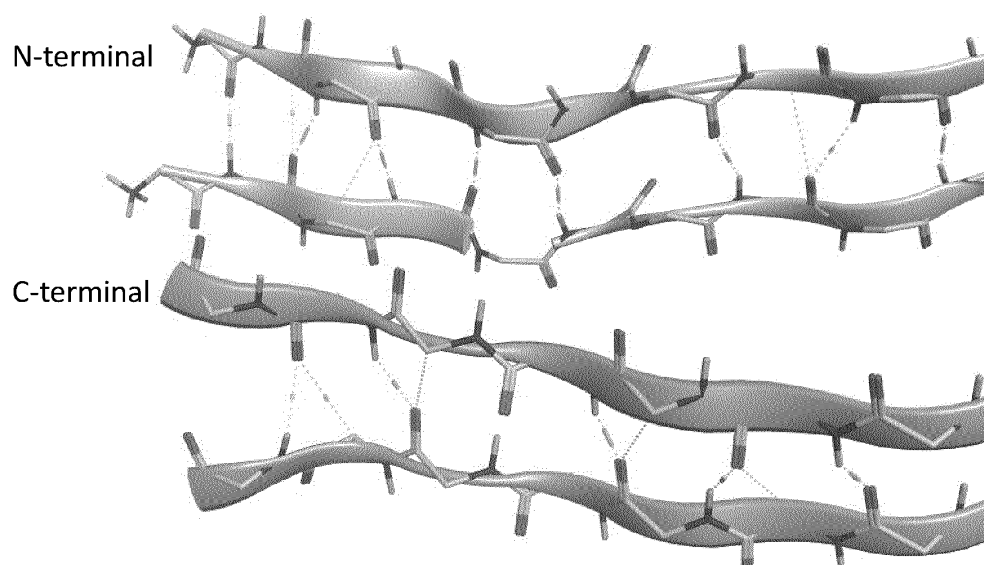


Figure 18B

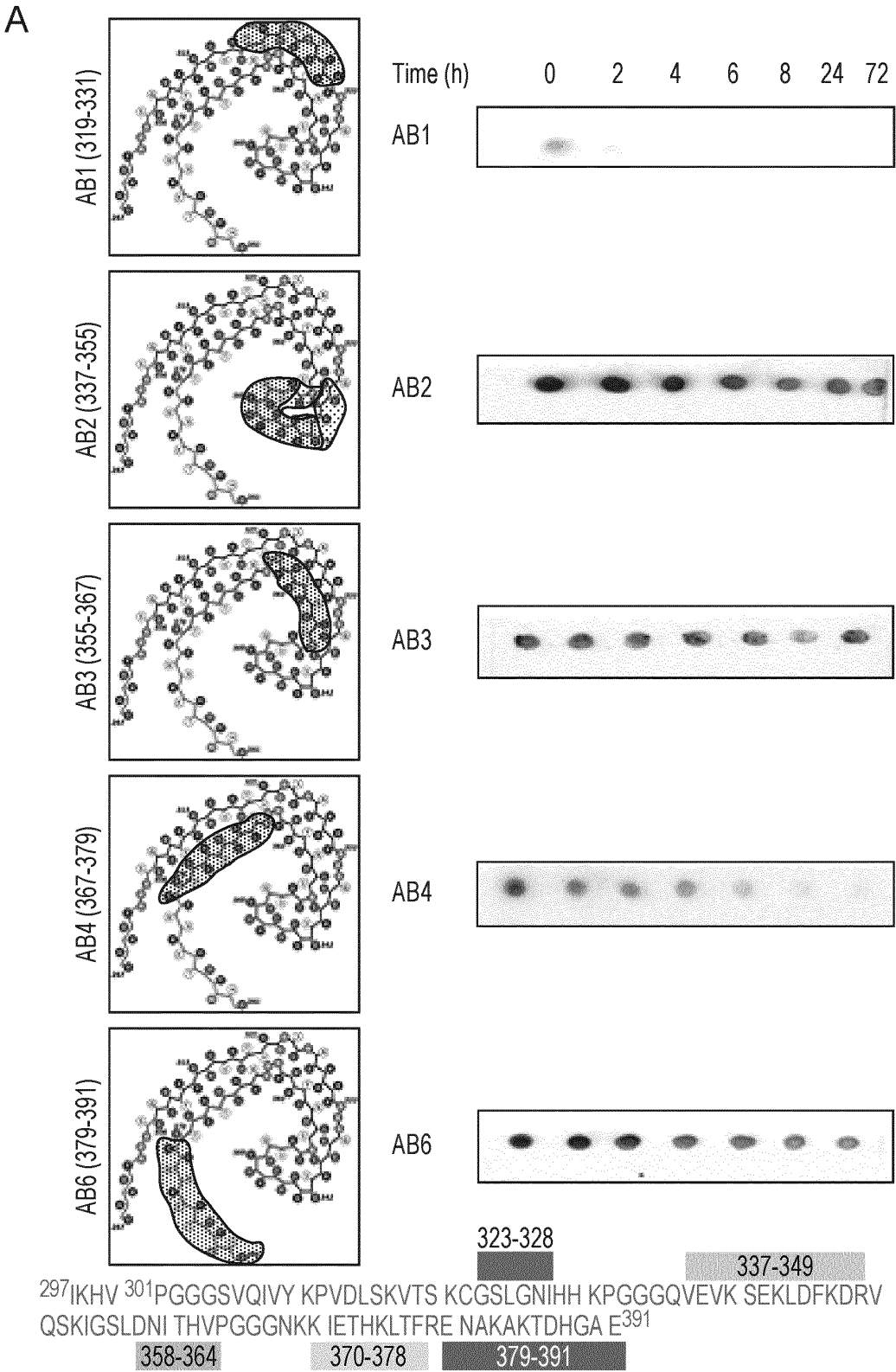


FIG. 19

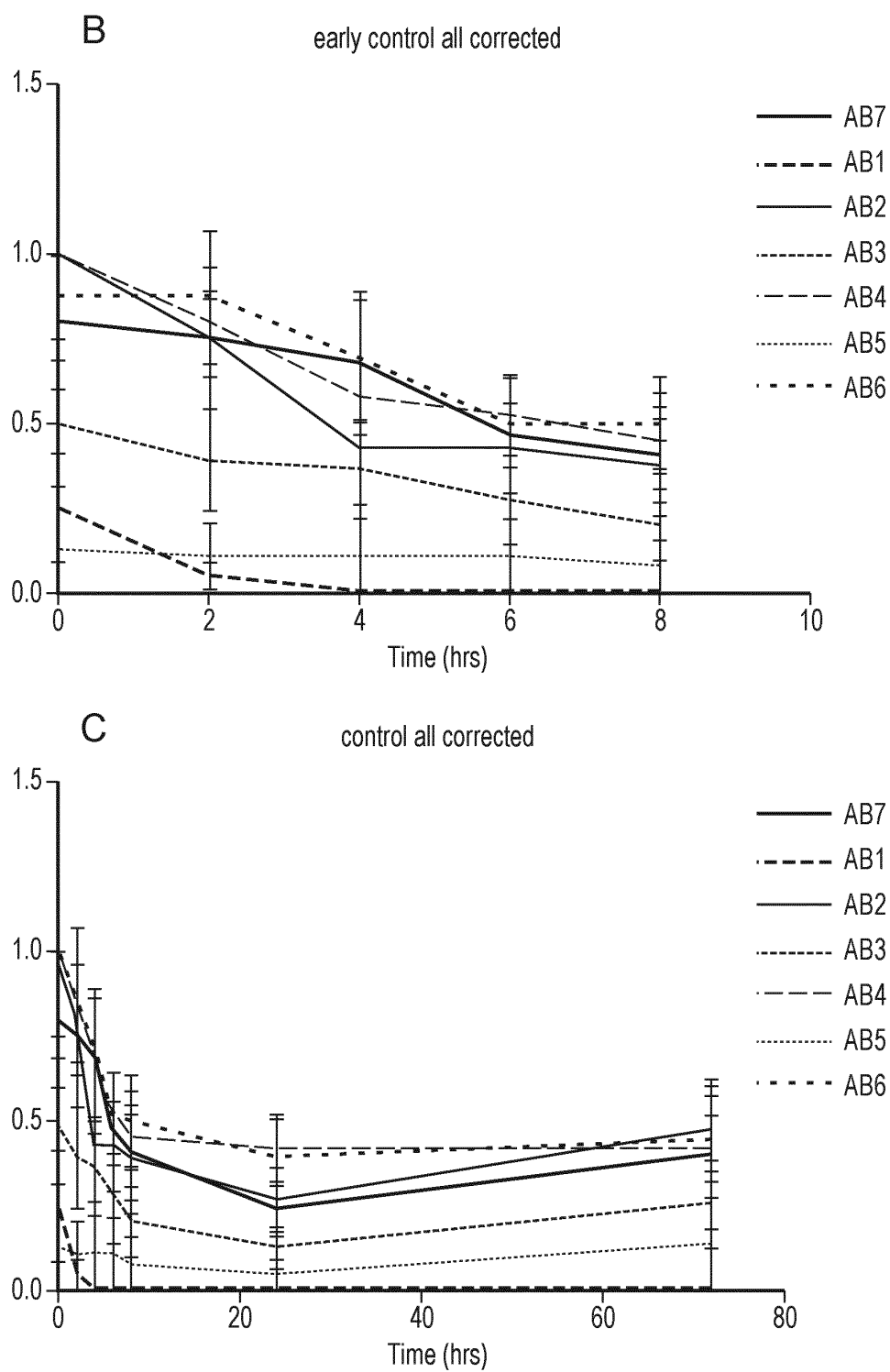


FIG. 19 (Continued)

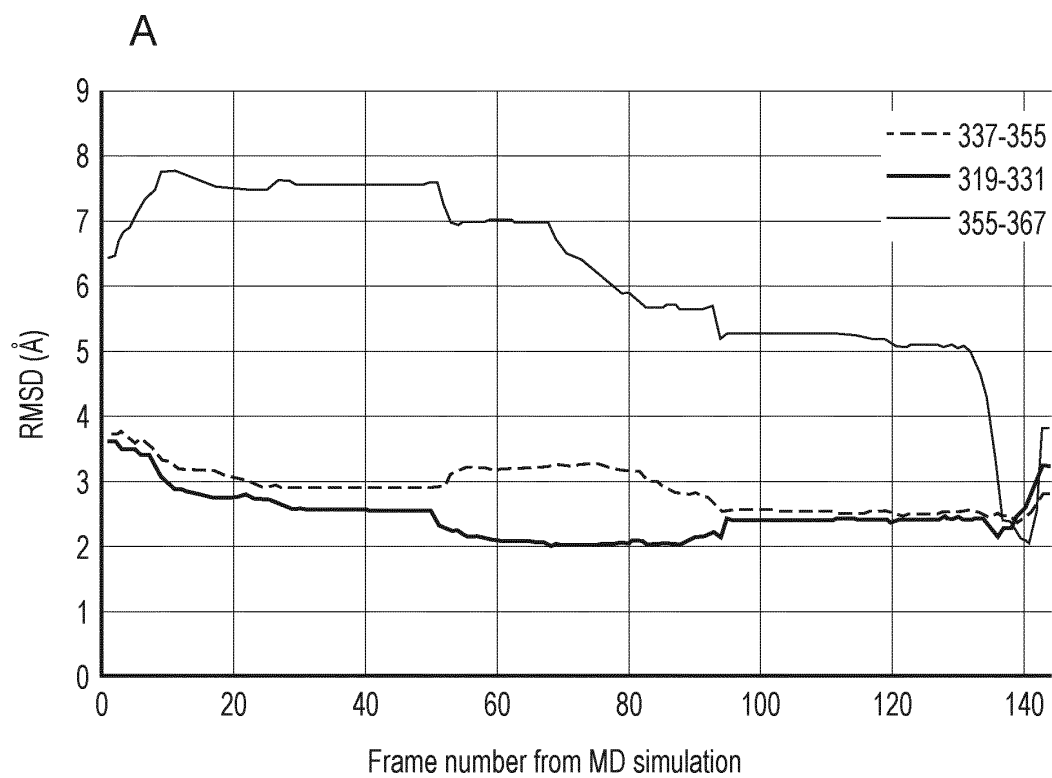


FIG. 20

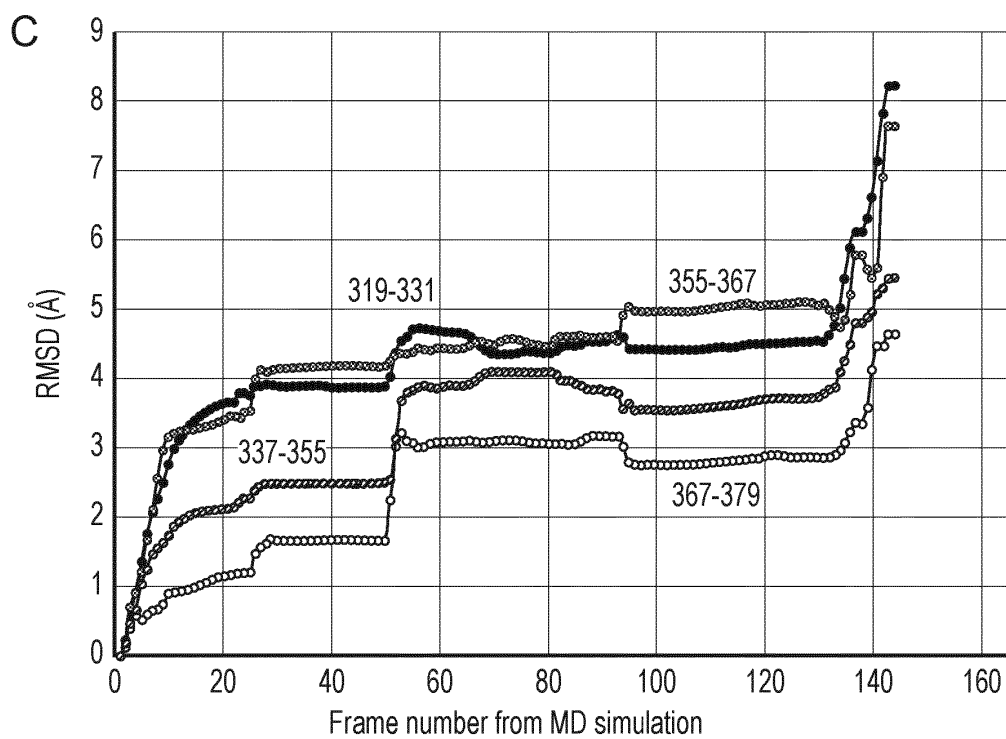
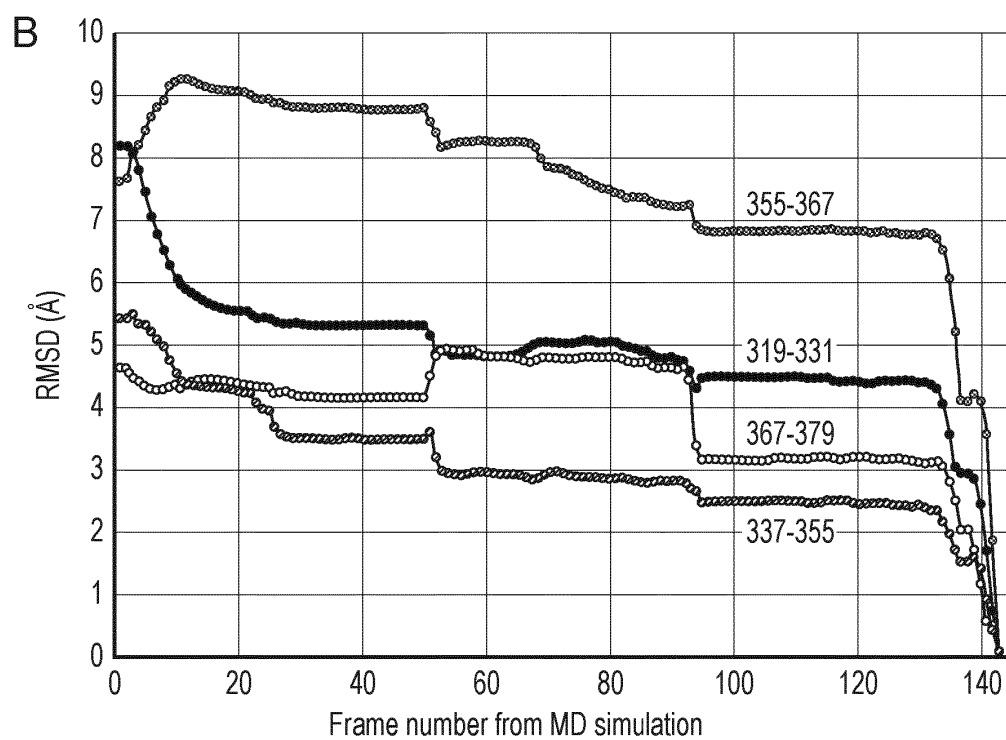


FIG. 20 (Continued)

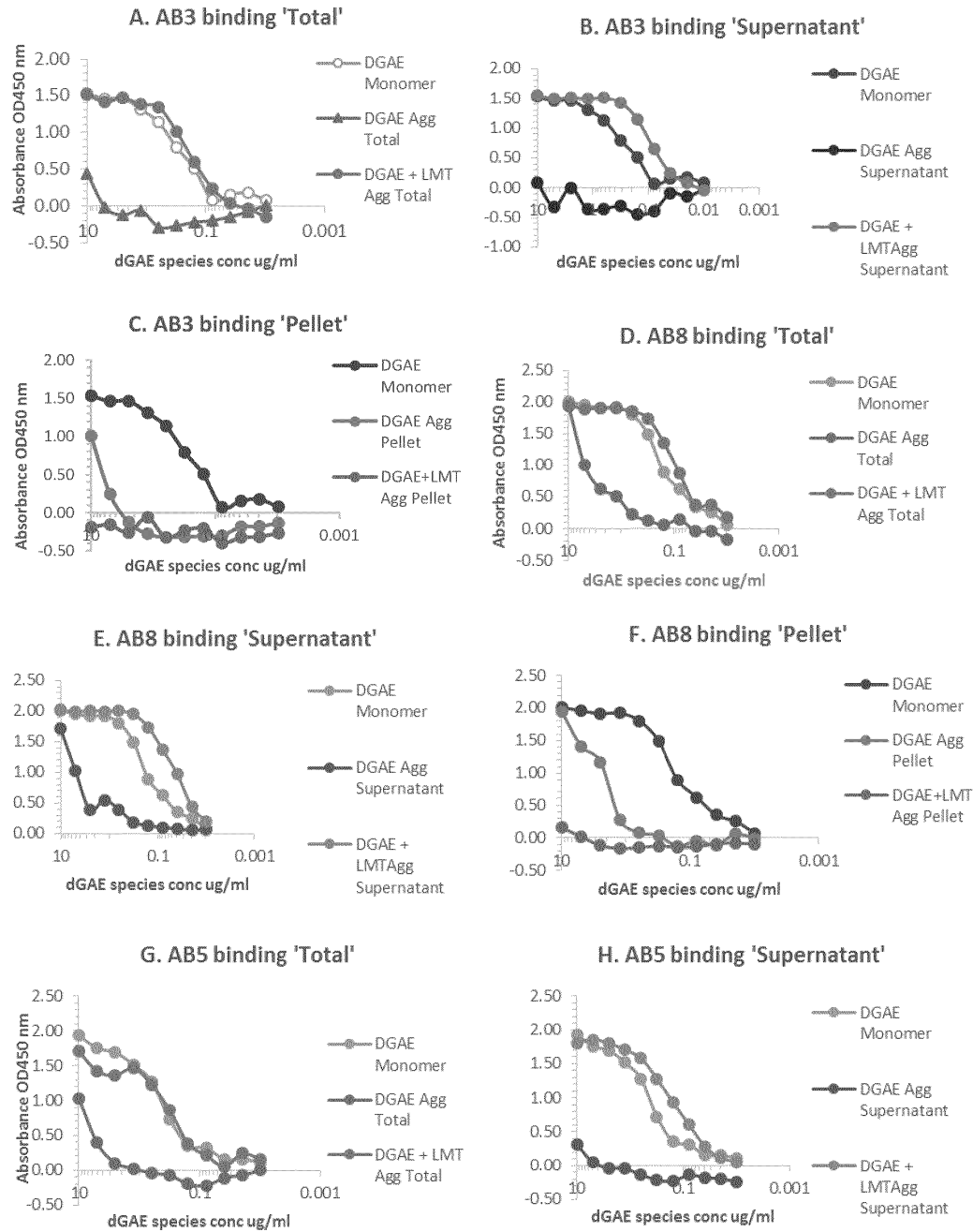


Figure 21

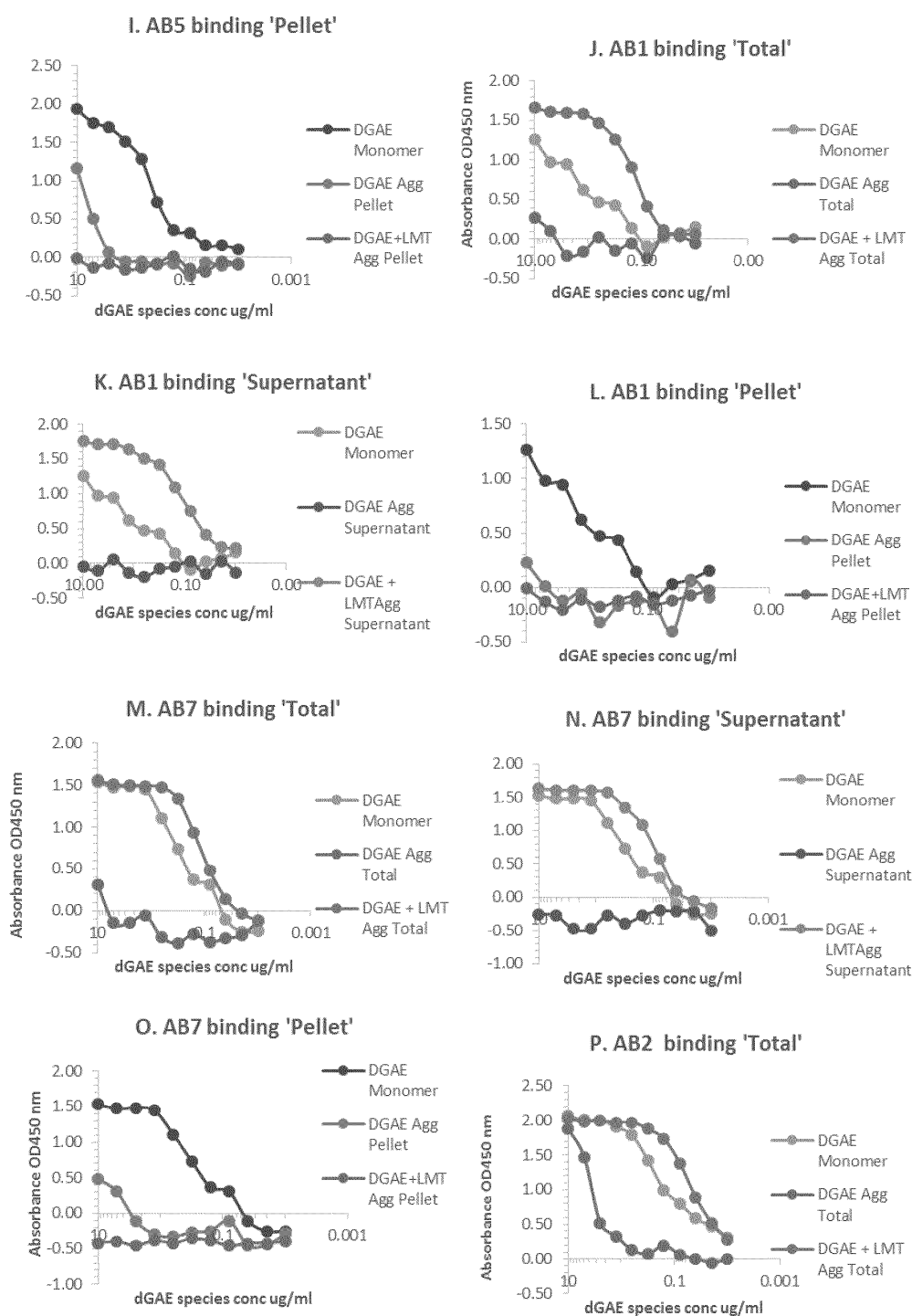


Figure 21 (continued)

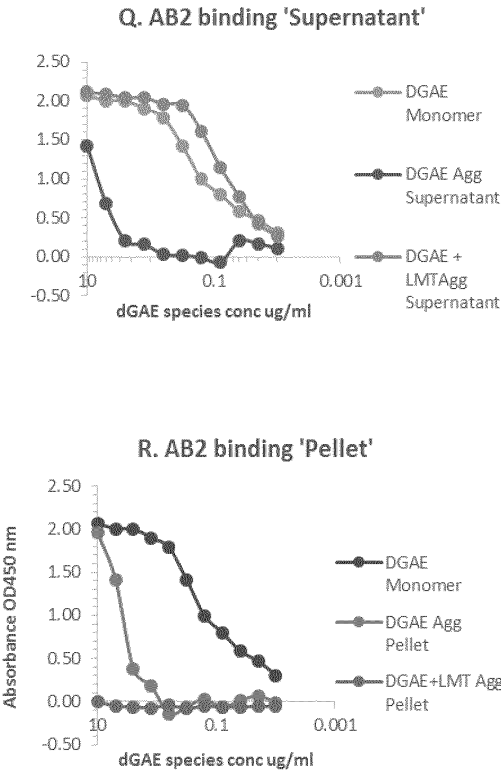


Figure 21 (continued)

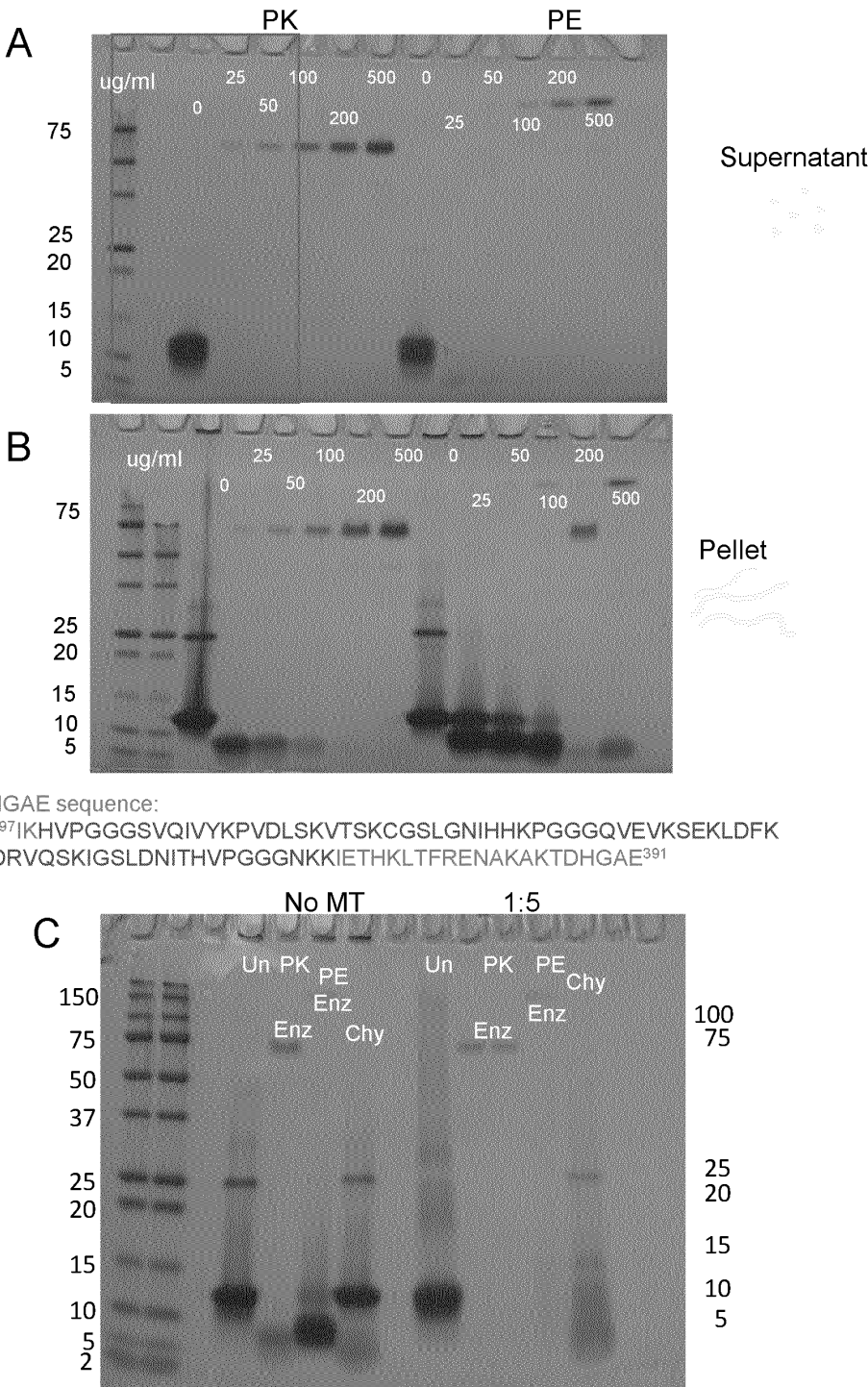


Figure 22

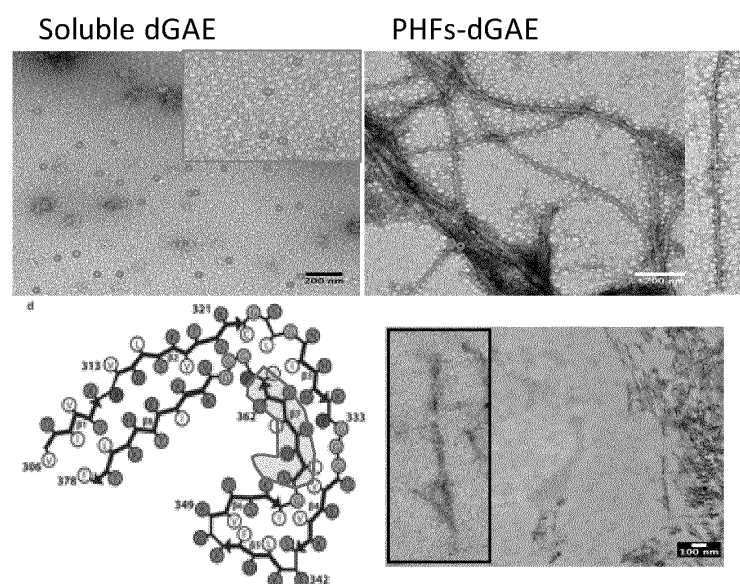


Figure 23A

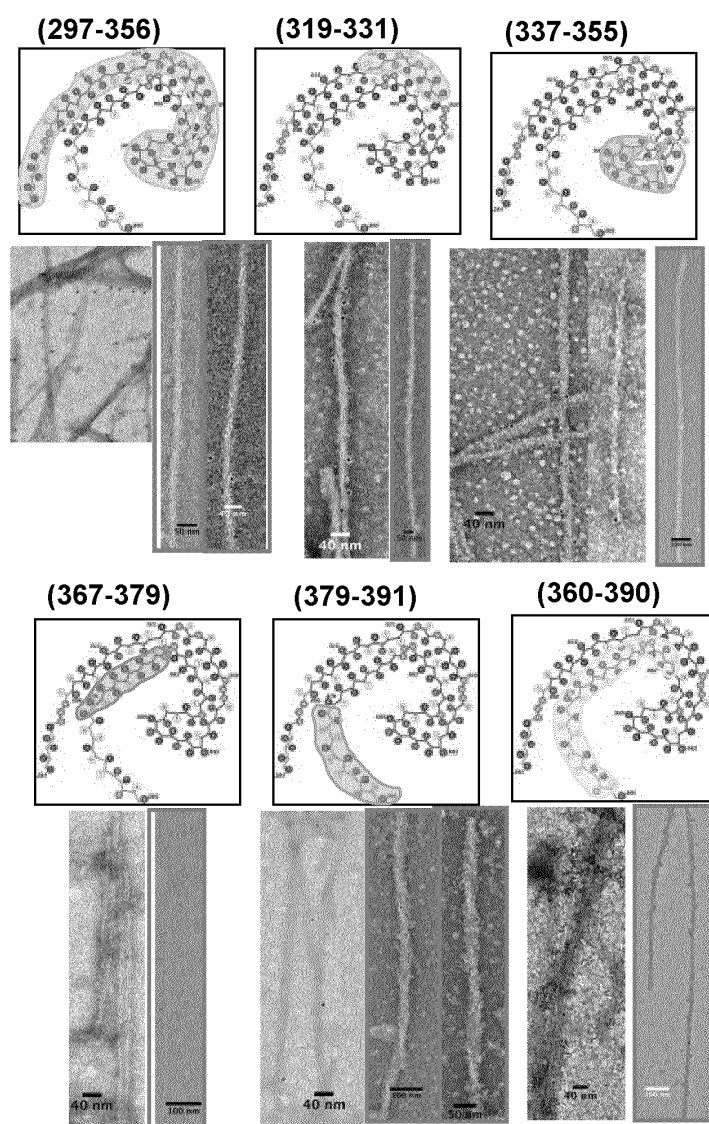


Figure 23B