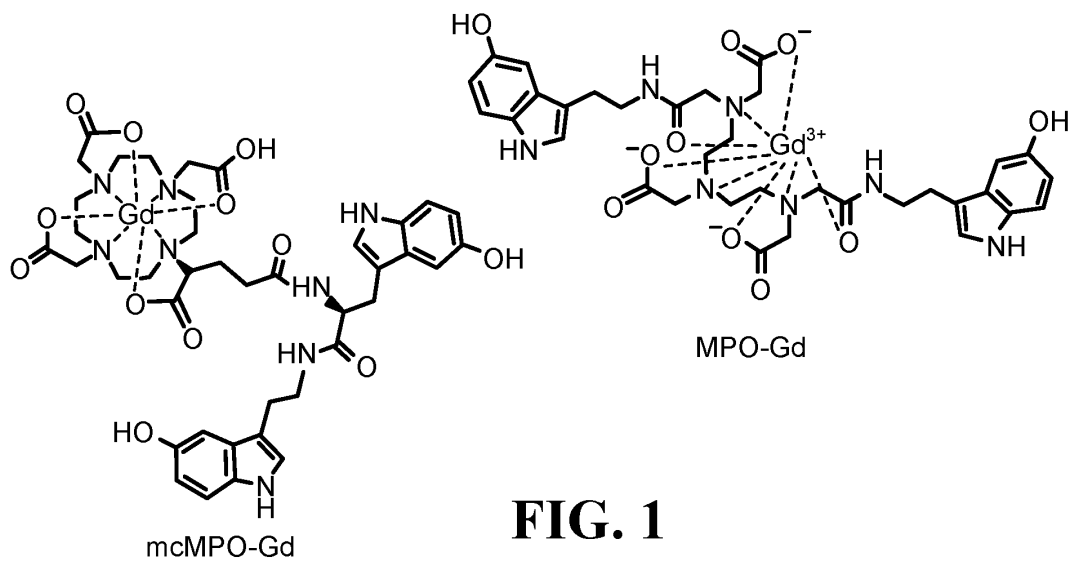
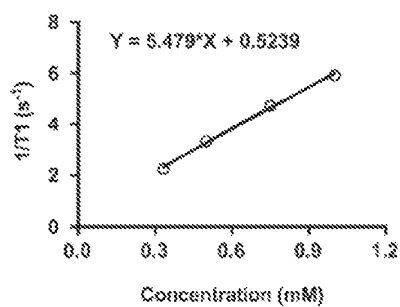
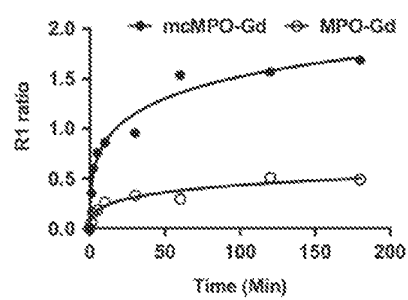
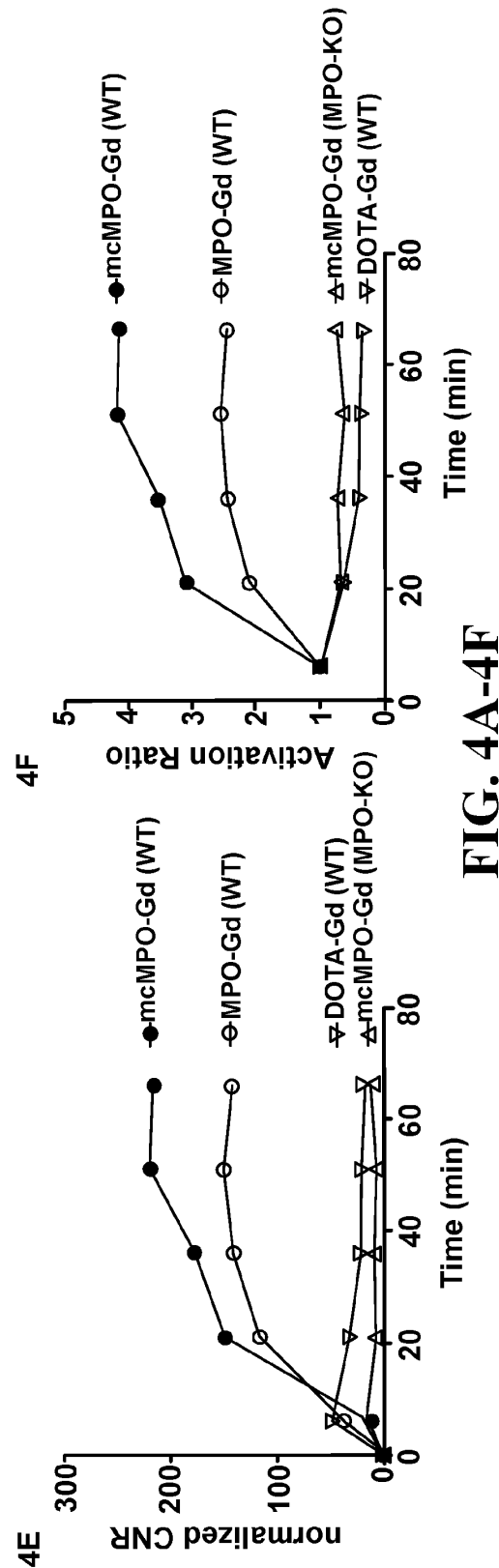
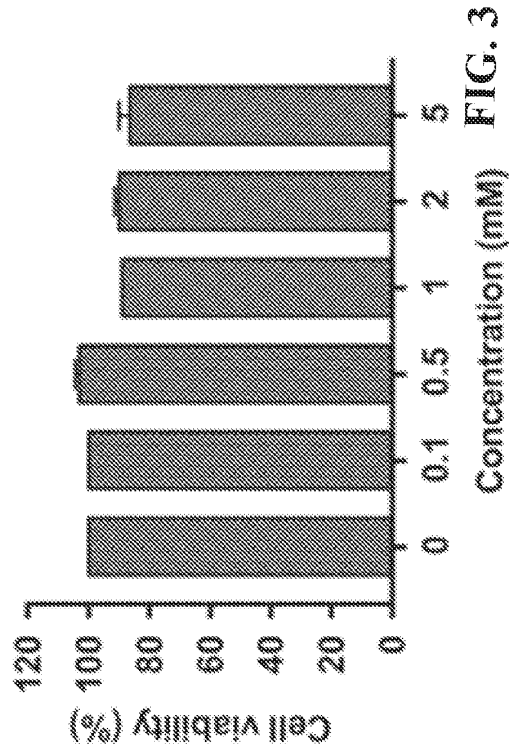
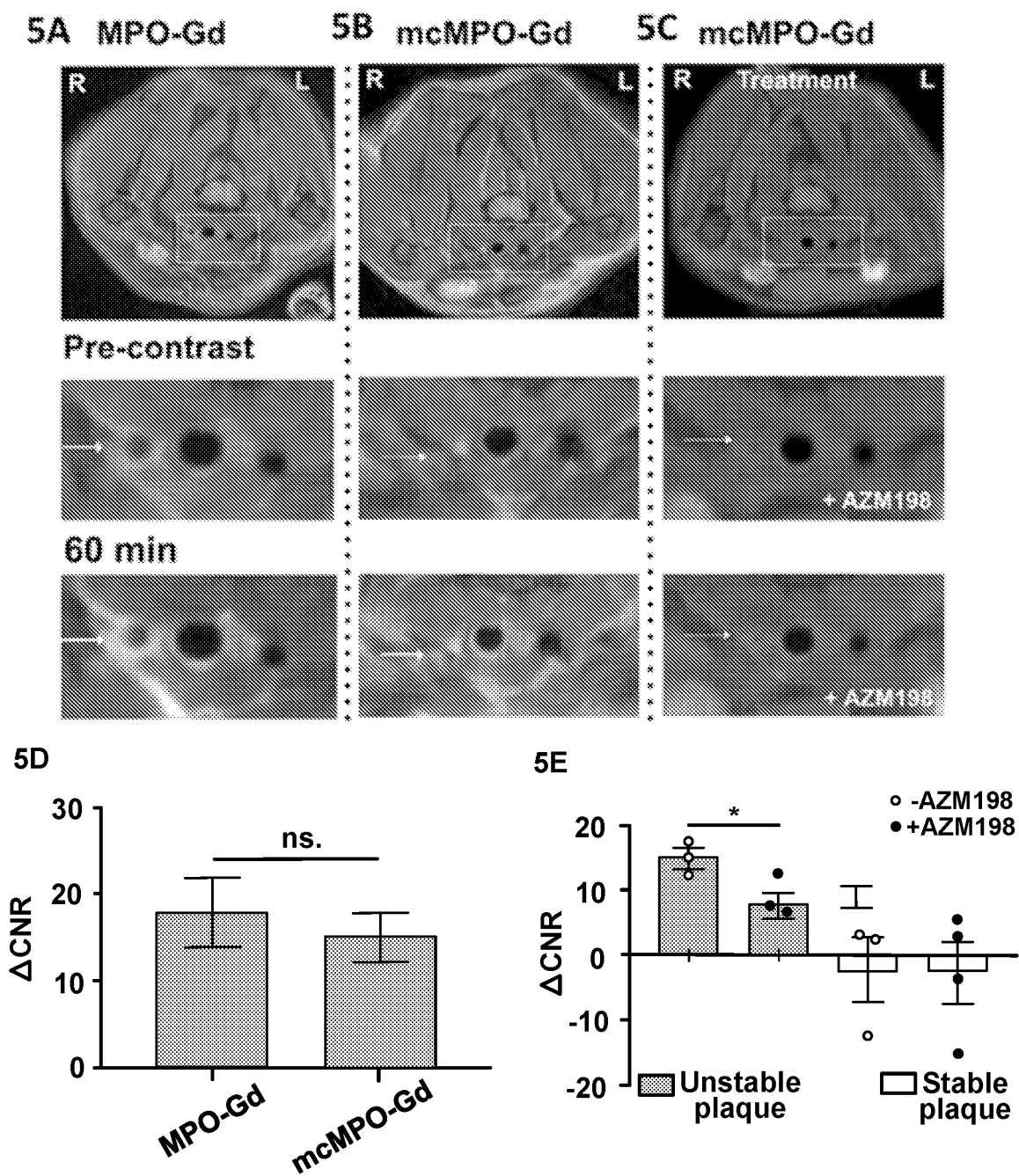


**FIG. 1****2A****2B****FIGs. 2A-2B**

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**FIG. 5A-5E**

SUBSTITUTE SHEET (RULE 26)

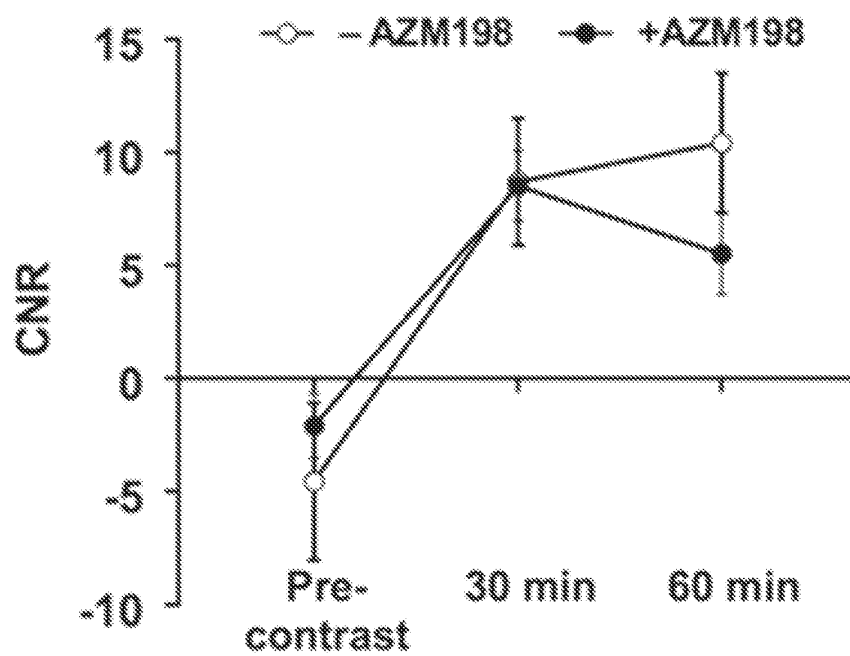


FIG. 6

SUBSTITUTE SHEET (RULE 26)

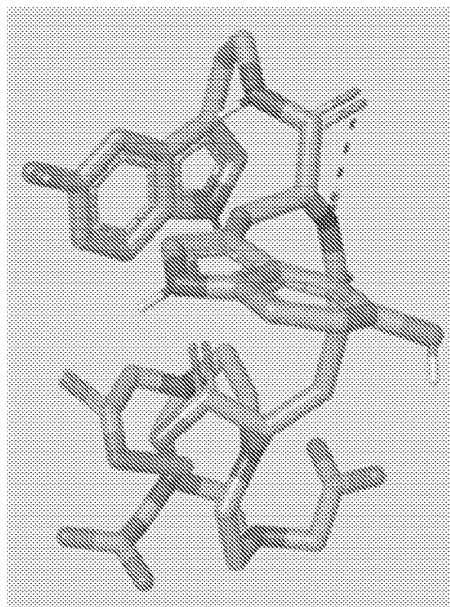
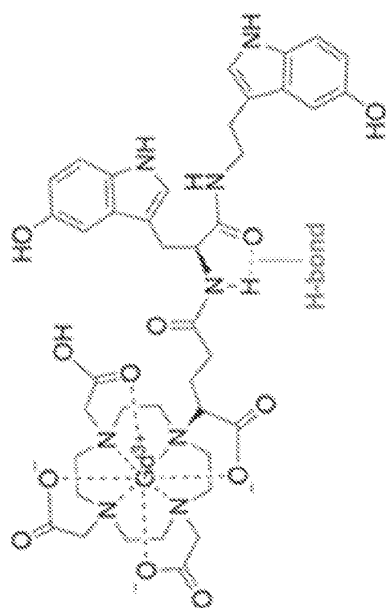


FIG. 7



SUBSTITUTE SHEET (RULE 26)

mcMPO-Gd docking

mode	affinity	dist from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-11.7	0.000	0.000
2	-11.3	1.215	3.203
3	-11.1	1.571	3.064
4	-10.7	2.015	5.157
5	-10.5	2.542	7.954
6	-10.3	2.320	8.861
7	-10.2	2.559	8.257
8	-10.1	2.165	4.971
9	-10.1	2.593	3.876
10	-10.0	2.236	6.007
11	-10.0	1.654	2.296
12	-9.9	2.127	5.143
13	-9.9	2.599	8.839
14	-9.8	2.655	8.893
15	-9.8	2.579	9.616
16	-9.6	2.334	5.601
17	-9.6	2.588	9.639
18	-9.6	2.325	3.946
19	-9.6	2.538	8.793
20	-9.5	2.688	9.549

MPO-Gd docking

mode	affinity	dist from best mode	
	(kcal/mol)	rmsd l.b.	rmsd u.b.
1	-9.9	0.000	0.000
2	-9.1	1.925	6.931
3	-9.0	2.324	7.314
4	-8.9	2.324	6.325
5	-8.9	2.323	7.596
6	-8.8	2.608	6.328
7	-8.7	2.120	6.526
8	-8.6	2.293	6.052
9	-8.6	2.793	6.341
10	-8.5	2.605	7.560
11	-8.4	2.485	7.223
12	-8.2	1.752	7.308
13	-8.1	2.759	7.069
14	-8.1	2.909	7.147
15	-8.0	2.538	8.363
16	-8.0	2.236	7.729
17	-8.0	2.455	7.173
18	-7.9	2.787	7.132
19	-7.9	2.324	8.133
20	-7.9	2.410	4.775

FIG. 8

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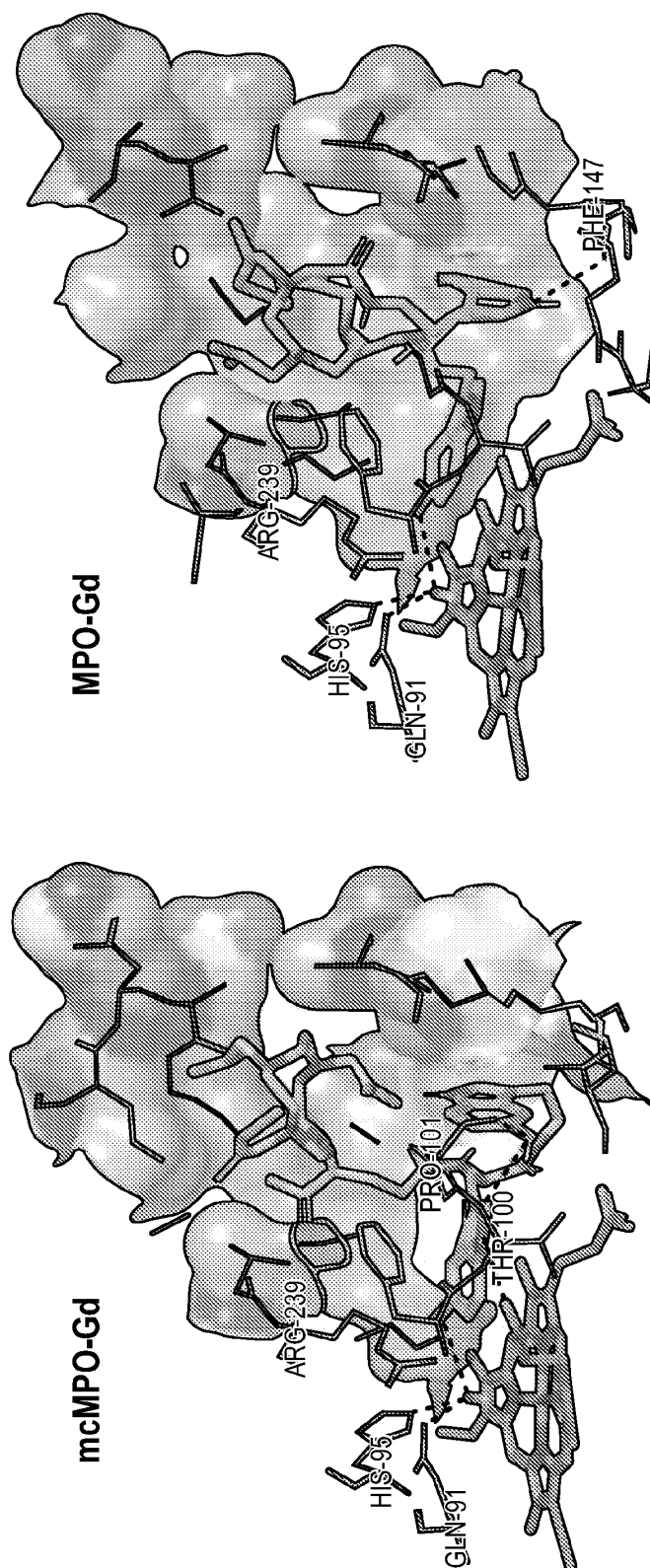


FIG. 9

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