Supplementary Information

Mesoporous polymeric nanoparticles for effective treatment of inflammatory diseases: an *in vivo* study

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Supporting Figures:

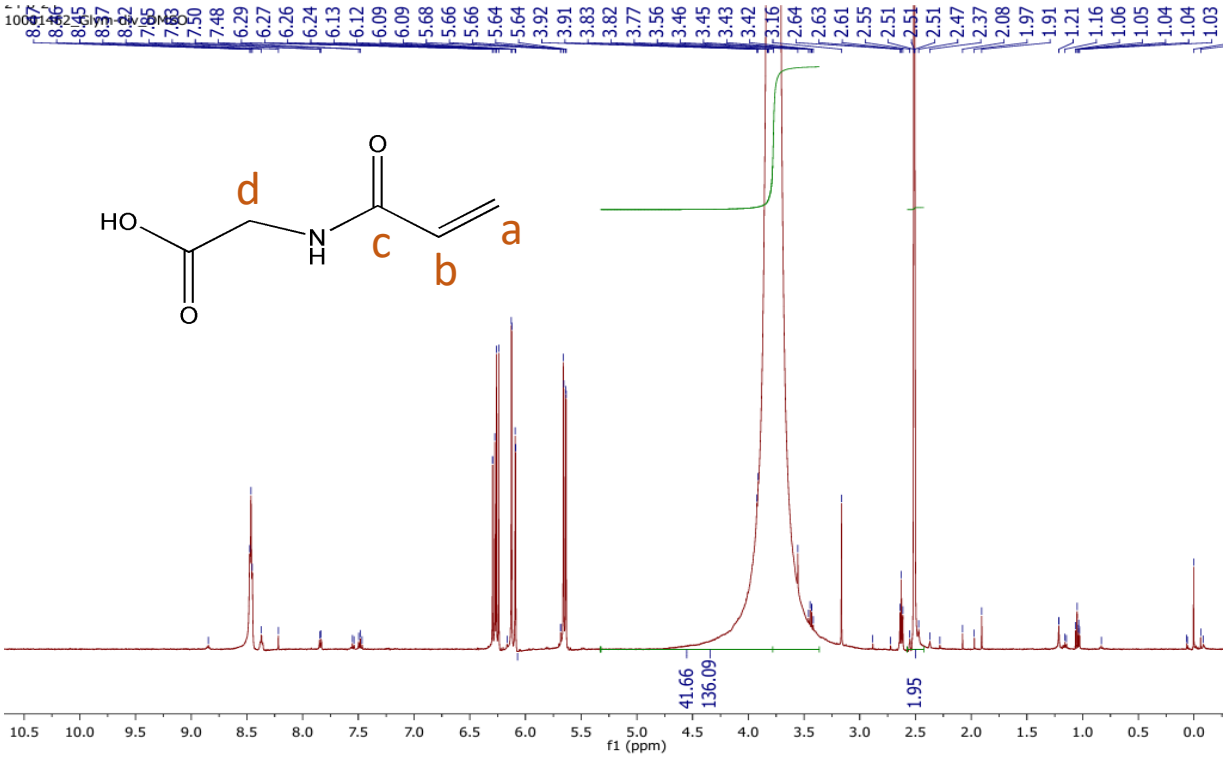

Figure S1: ^{1}H NMR spectroscopy results for monomer synthesized from glycine and N-acryloyl chloride

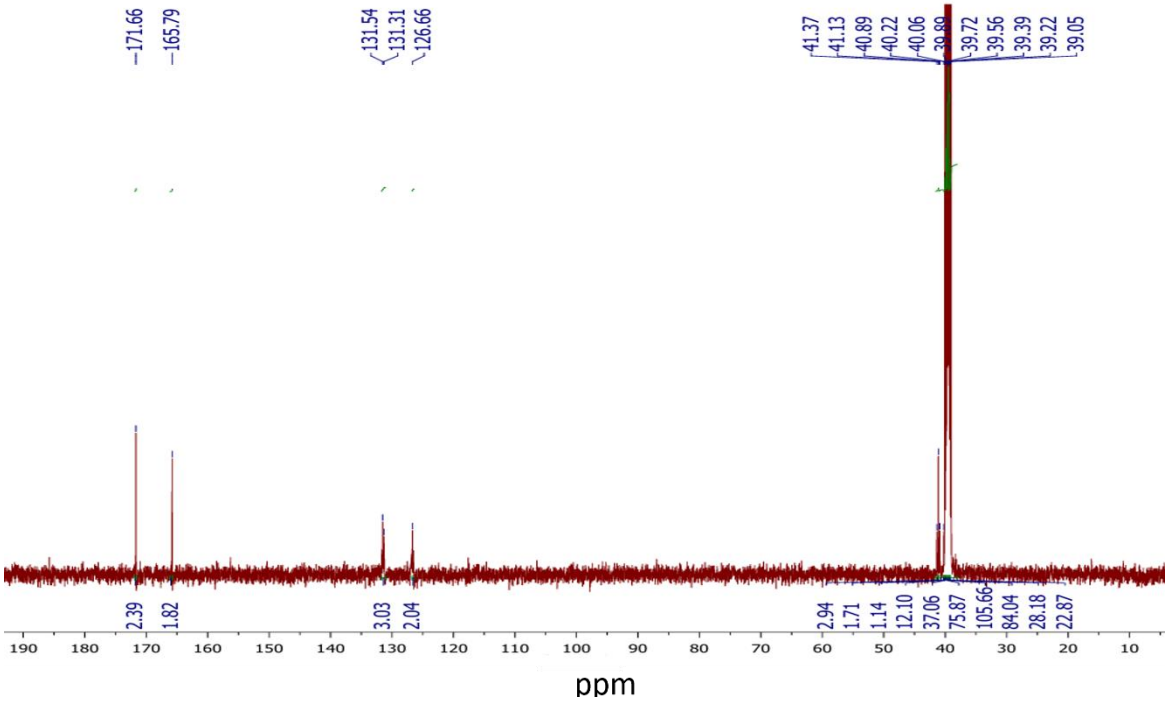

Figure: S2 ^{13}C NMR spectroscopy results for monomer synthesized from glycine and N-acryloyl chloride

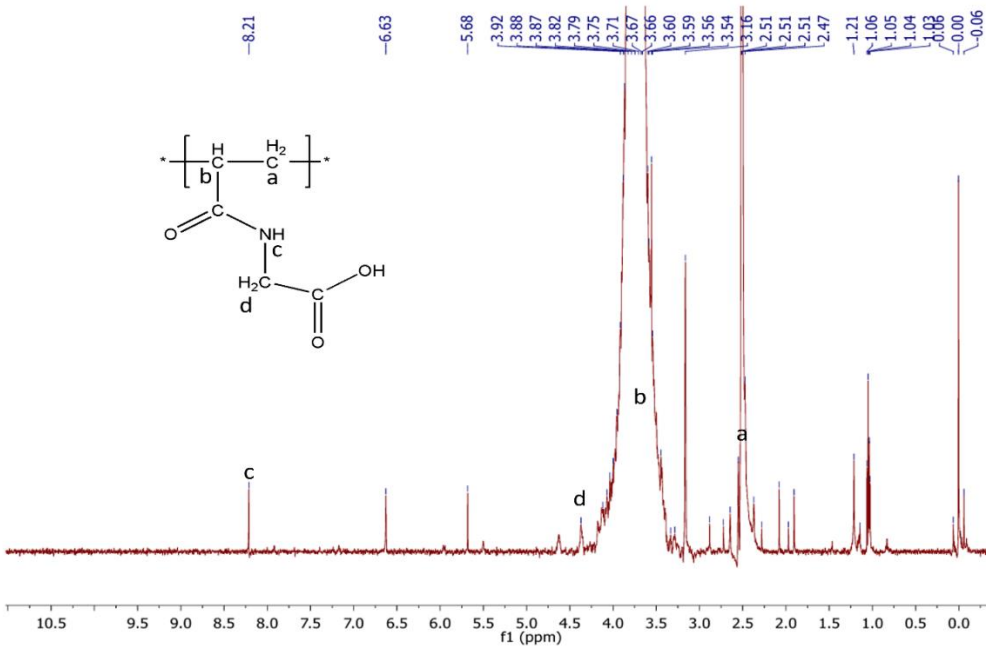

Figure S3: [1]H NMR spectroscopy results for polymer synthesized (GlyNPs)

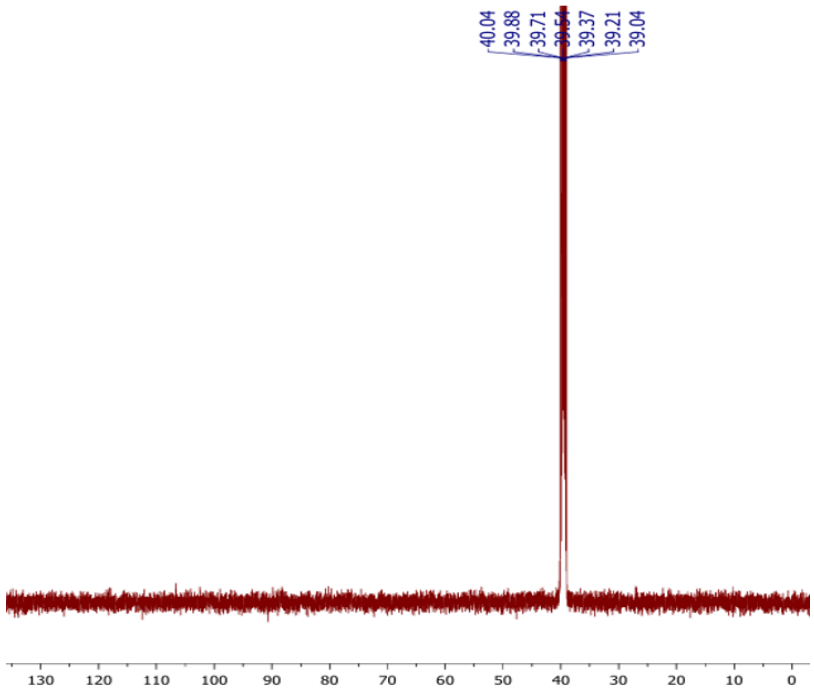

Figure: S4 [13] C-NMR spectroscopy results for polymer synthesized (GlyNPs)

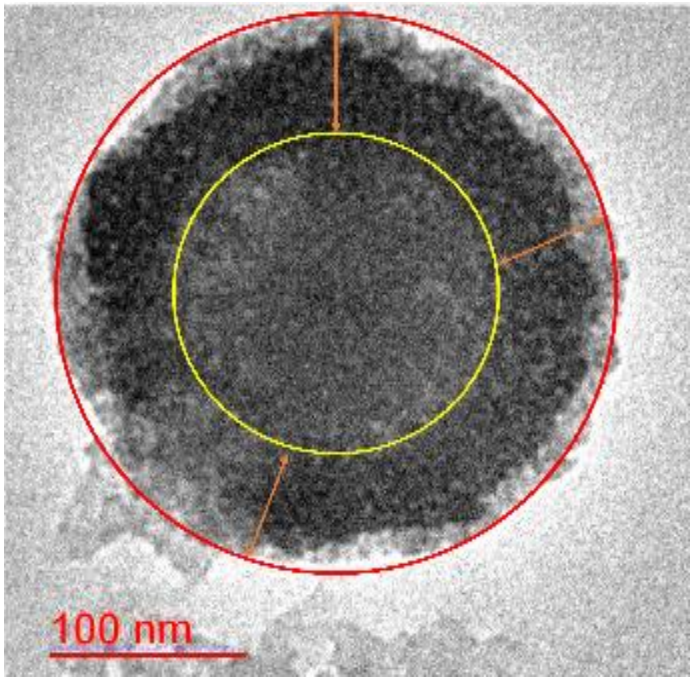

Figure S5: HR-TEM image of porous GlyNPs shows the hollow core and solid shell.

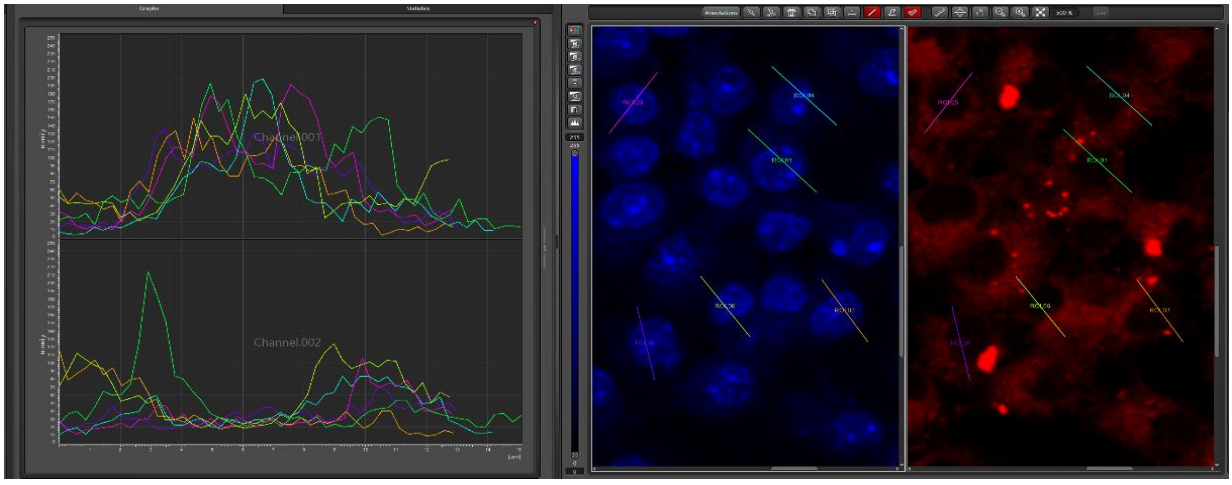

Figure S6 Represents confocal microscopy images that are showing uptake of the GlyNPs by RAW 264.7 Macrophages. (a) Intensity of the emission of lights from different position of the cells. (b) Blue colour emits from nucleus (DAPI stained). (c) Red emission observed due to the uptake of the Nile Red loaded in GlyNPs. Deep red colour exhibiting the position of the internalized GlyNPs.

Supporting Table

Table S1: Software and web tools used for network pharmacology study and *in silico* docking analysis.

S/ N	Software/Web tools/ Database name	URL
1.	Malacard	https://www.malacards.org/
2.	GeneCards database	https://www.genecards.org
3.	DisGeNet database	https://www.disgenet.org/search
4.	Venny 2.0	https://bioinfogp.cnb.csic.es/tools/venny/
5.	String tool	https://string-db.org/
6.	Cytoscape-3.9	https://cytoscape.org/download.html
7.	ShinyGo 0.77	http://bioinformatics.sdstate.edu/go/
8.	PubChem database	https://pubchem.ncbi.nlm.nih.gov/
9.	Auto Dock	https://autodock.scripps.edu/download-autodock4/

Table S2: Shows top 20 targeted genes obtained from network pharmacology study.

Rank of selected targets	Name of targeted genes	Score
1.	Ifng	1.09E+36
2.	Il6	1.09E+36
3	Cd4	1.09E+36
4.	Csf2	1.09E+36
5.	Il10	1.09E+36
6.	Itgad	1.09E+36
7.	Ptprc	1.09E+36
8.	Il1b	1.09E+36
9.	Cd80	1.09E+36
10.	Cd40	1.09E+36
11.	Ccl3	1.09E+36
12.	Cd86	1.09E+36
13.	Il18	1.09E+36
14.	Tlr2	1.09E+36
15.	Ccl4	1.09E+36
16.	Tlr1	1.09E+36
17.	Cxcl9	1.09E+36
18.	Stat1	1.09E+36
19.	Fcgr2a	1.09E+36
20.	Foxp3	1.09E+36

Table S3. Docking result of screened ligands for **COX-2** (PDB ID: **6COX**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, Ki	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-5.37	116.41 µM	HIS90
2.	Diclofenac	-5.11	178.6 µM	HIS90, ARG513
	Ligands			
3.	N-Acryloyl Glycine	-5.17	163.66 µM	ASN87, HIS90, ARG513
4.	G2	-4.09	1.0 mM	HIS90, TYR91
5.	G3	-3.39	3.25 mM	ASN87, HIS90, TYR91
6.	G4	-3.54	2.54 mM	HIS90, TYR91

Table S4. Docking result of screened ligands for NF-kβ (PDB ID: **1LE5**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, K_i	Residues involved in Hydrogen Bonding
	Reference drugs			
1..	Aspirin	-4.58	441.19 µM	ARG54, LYS241
2	Diclofenac	-4.81	298.19 µM	LYS145
	Ligands			
3.	N-Acryloyl glycine	-4.11	972.38 µM	LYS114, ASN136
4.	G2	-5.04	202.86 µM	LYS145, LYS203
5.	G3	-5.67	69.58 µM	LYS145, LYS203
6.	G4	-4.59	431.23 µM	LYS144, LYS203

Table S5. Docking result of screened ligands for **IL-6** (PDB ID: **1ALU**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, K_i	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-5.54	86.32 µM	LYS27, ARG30
2.	Diclofenac	-6.74	11.47 µM	LYS27
	Ligands			
3.	N-Acryloyl Glycine	-4.88	265.35 µM	LYS27, ARG30
4.	G2	-5.73	62.91 µM	ASP26, LYS27, ARG30
5.	G3	-4.55	461.43 µM	LYS27, ARG30
6.	G4	-4.80	303.11 µM	SER22, ASP26, ARG182

Table S6. Docking result of screened ligands for **IL-1β** (PDB ID: **5I1B**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, K_i	Residues involved in Hydrogen bonding
	Reference drugs			
1.	Aspirin	-4.62	410.65 µM	VAL3, LYS93, LYS94
2.	Diclofenac	-4.95	233.85 µM	LYS65
	Ligands			
3.	N-Acryloyl Glycine	-4.53	480.55 µM	ARG4, PHE46, LYS93
4.	G2	-4.04	1.1 mM	ARG4, GLY49, LYS93
5.	G3	-3.07	5.62 mM	VAL3, GLN48, LYS93
6.	G4	-2.1	28.9 mM	VAL3, GLN48, LYS93, LYS94

Table S7. Docking result of screened ligands for **TNF-α** (PDB ID: **2AZ5**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, K_i	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-5.59	79.74 µM	VAL74, LYS112
2.	Diclofenac	-4.89	258.8 µM	PRO70, LYS112
	Ligands			
3.	N-Acryloyl Glycine	-4.22	801.54 µM	PRO70, LYS112
4.	G2	-4.48	520.83 µM	LYS112
5.	G3	-2.69	10.76 mM	CYS69
6.	G4	-3.35	3.49 mM	PRO70, ARG103

Table S8. Docking result of screened ligands for **iNOS** (PDB ID: **4NOS**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, Ki	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-3.95	1.27 mM	HIS84
2.	Diclofenac	-4.42	574.89 µM	THR95
	Ligands			
3.	N-Acryloyl Glycine	-4.27	739.96 µM	HIS84
4.	G2	-6.00	39.95 µM	HIS84, ARG86
5.	G3	-4.57	445.37 µM	ARG83, LYS103
6.	G4	-2.50	14.64 mM	ARG86, THR95, ARG452

Table S9. Docking result of screened ligands for **TLR-4** (PDB ID: **2Z62**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, Ki	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-4.42	573.96 µM	LYS47, ILE48
2.	Diclofenac	-4.7	356.88 µM	LYS47
	Ligands			
3.	N-Acryloyl Glycine	-3.88	1.43 mM	GLN281, LYS254
4.	G2	-3.62	2.21 mM	LYS229
5.	G3	-3.26	4.09 mM	SER251, LYS282
6.	G4	-2.74	9.82 mM	LYS229, LYS 282

Table S10. Docking result of screened ligand for **MAPK-14** (PDB ID: **4F9Y**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, Ki	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-6.14	31.39 µM	LYS165
2.	Diclofenac	-6.95	7.99 µM	HIS126
	Ligands			
3.	N-Acryloyl Glycine	-4.56	457.4 µM	GLU160
4.	G2	-5.29	132.29 µM	HIS126
5.	G3	-4.44	560.18 µM	HIS126
6.	G4	-4.64	393.84 µM	HIS126

Table S11. Docking result of screened ligand for **MAPK-8** (PDB ID: **4G1W**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, Ki	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-4.66	382.33 µM	LYS220
2.	Diclofenac	-4.12	947.64 µM	LYS251
	Ligands			
3.	N-Acryloyl Glycine	-3.85	1.51 mM	LYS203, GLU204
4.	G2	-3.08	5.57 mM	TYR202, LYS203
5.	G3	-2.85	8.11 mM	TYR202, LYS203
6.	G4	-2.49	15.0 mM	TYR202, LYS203

Table S12. Docking result of screened ligands for **STAT-1** (PDB ID: **3WWT**).

S.No.	Ligands	Binding Energy (kcal/mol)	Estimated inhibition constant, Ki	Residues involved in Hydrogen Bonding
	Reference drugs			
1.	Aspirin	-3.82	1.58 mM	TYR68
2.	Diclofenac	-3.6	2.3 mM	ARG84
	Ligands			
3.	N-Acryloyl Glycine	-3.33	3.6 mM	TYR106, LYS110
4.	G2	-3.57	2.4 mM	LYS110, LYS114
5.	G3	-2.36	18.65 mM	LYS40, ARG113
6.	G4	-1.16	140.03 mM	ARG113