Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Loading of chromenones on superparamagnetic iron oxide–modified dextran core–shell nanoparticles. Openness to bind to β–cyclodextrin and DNA†

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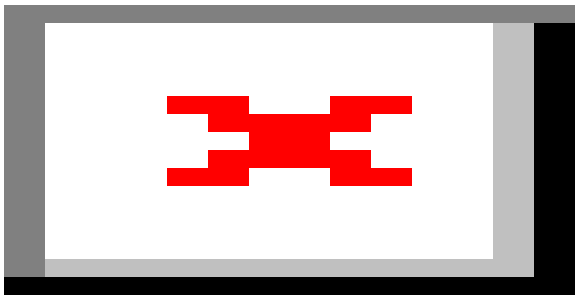
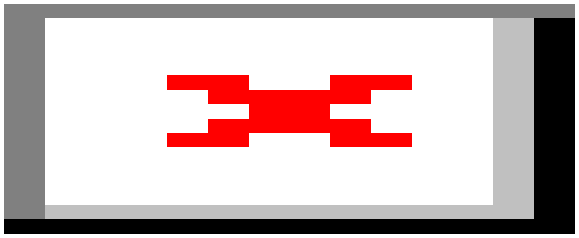


SI 1 Molecular structure of chromenones (a) PC, (b) DC, (c) DHC, (d) BTC, and (e) BIC

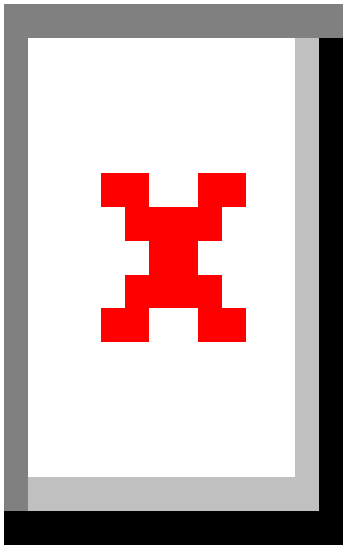
SI 2A IR spectral data for dextran–coated and aminoethylamino–dextran–coated SPIONs

Dextran–coated SPIONs		Aminoethylamino–dextran–coated SPIONs	
3433.64 (broad)	–O–H str	3415.31 (broad)	–O–H str
–	–	3792.33	–N–H str
2764.46 2426.01 2362.37	Aliphatic –C–H str	2358.52 –	Aliphatic –C–H str

1384.64	O–H in plane bending in coupling with –C–H wagging, In plane bending bands	1383.68	O–H in plane bending in coupling with –C–H wagging, In plane bending bands
1117.55 to 1068.37	–C–O str	–	–C–O str
1597.73	–C=C str coupled with C–C str	1597.73	–C=C str coupled with C–C str
838.88 600.72	–C–H out of plane bending	–	–C–H out of plane bending
535.1	Fe–O bonding	550.5	Fe–O bonding
498.50 476.33 434.86	Due to dextran	491.75 – 433.90	Due to dextran



SI 2B IR spectra for (a) dextran–coated SPIONs and (b) aminoethylamino–dextran–coated SPIONs



SI 3 X–ray photoelectron spectra for the expanded spectra of aminoethylamino–modified dextran–coated SPIONs corresponding to (a) Fe 2p, (b) N 1s, (c) O 1s, (d) P 2p, and (e) C 1s

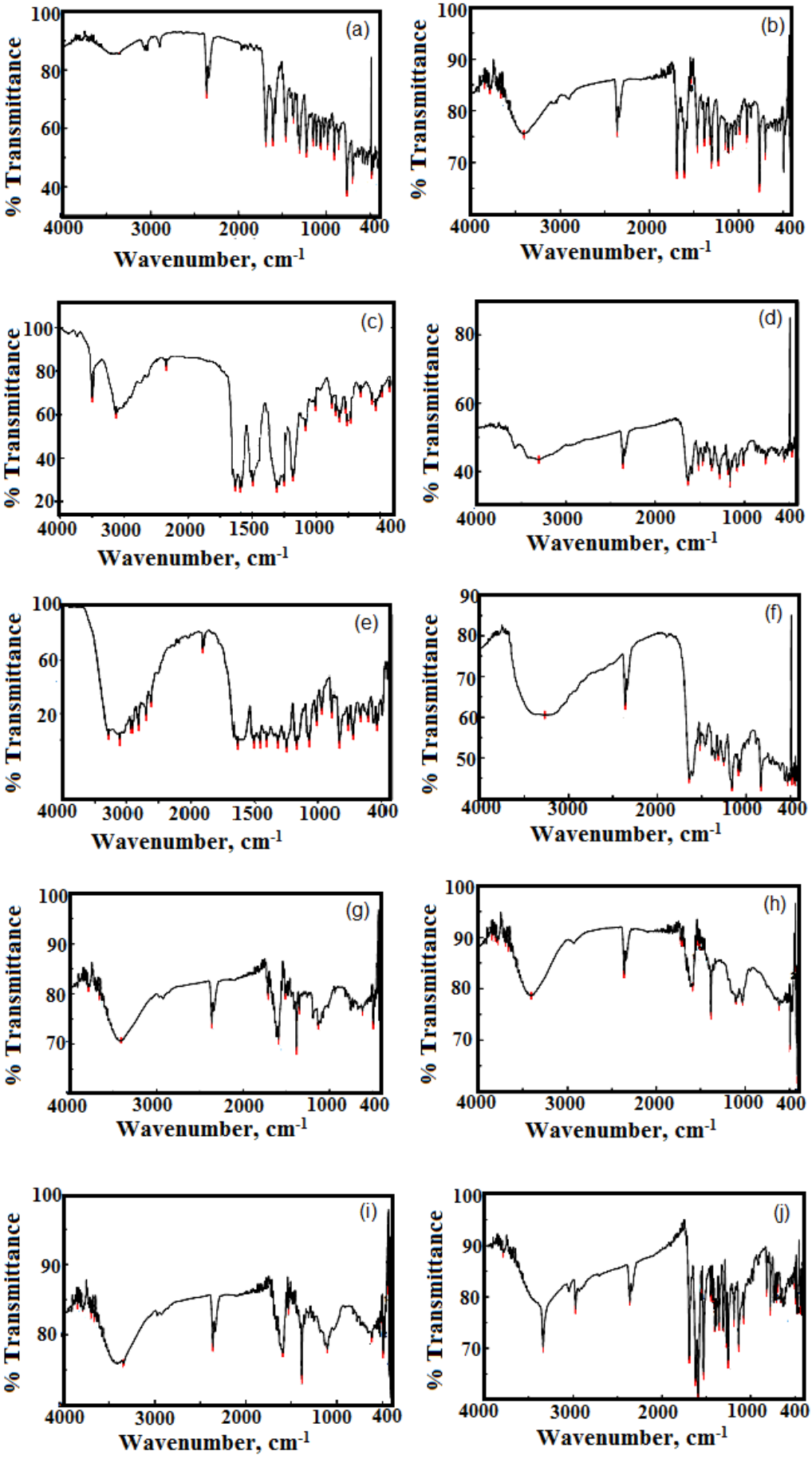
SI 4 FTIR spectral data of free chromenones, and CHR–SPIONs

CHRs	Types of Bonds	CHRs	CHR–SPIONs
PC	O–H str	–	3357.46
	C=O	1690.3	1688.37
	Aromatic C=C str	1605.45,1530.24	1605.45
	C–O str coupled with C–H wagging	1383.68,1321.96, 1303.64,1148.4	1373.07,1302.68 1148.4
	Aliphatic C–H str	3039.26,2896.56	3039.26,2896.56
	Aliphatic C–H bend	1461.78	1460.81
	–C–OH str	–	1079.94,921.80

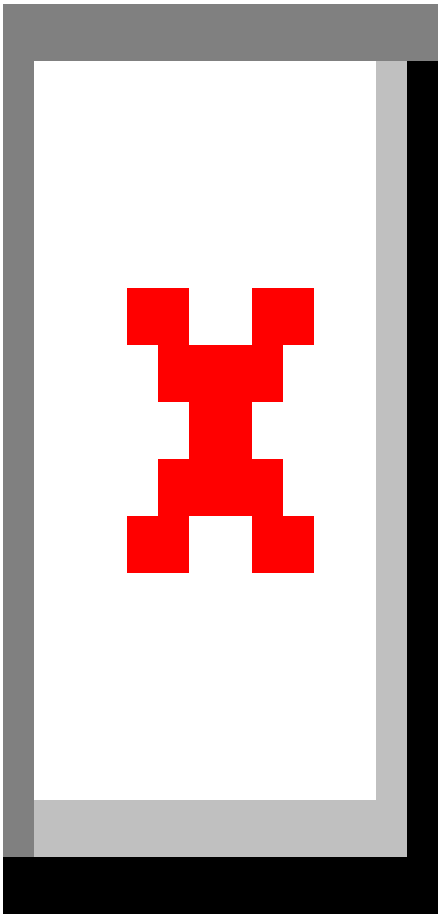
	Chelate compounds O–H str	–	2360.44,2340.19
	Deformation vibrations–C–H outside plane, related to substitution of aromatic rings of multi–ring compounds, N–H def out of plane	800–500	800–500
	Fe–O bond stretching	–	~548.6
	N–H str	–	3790.4
DC	O–H str	3496.94	3302.5(broad)
	C=O	1631.78	1630.52
	Aromatic C=C str	1587.42,1498.69	1587.13,1512.88
	C–O str and O–H in plane coupled with C–H wagging	1400.32,1309.67, 1290.38,1180.44	1401.03,1365.35, 1277.61,1186.97
	Aliphatic C–H str	3041.74,2964.59	2973.7
	Aliphatic C–H bend	1498.69	1465.63
	Chelate compounds O–H str	2357.01,2328.08	2360.44,2340.19
	–C–OH str	1082, 1020,873,819	1435.74,1074.16, 1010.16,971.97
	Deformation vibrations–C–H outside plane, related to substitution of aromatic rings of multi–ring compounds, N–H def out of plane	800–500	800–500
	Fe–O bond stretching	–	~557.3
	N–H str	–	3789.44

DHC	O–H str	3285.76 (broad)	3263.93 (broad)
	C=O	1641.54	1640.16
	Aromatic C=C str	1497.30, a band merged with	1517.7
	C–O str and O–H in plane coupled with C–H wagging	C=O 1390.41,1311.86,	1349.93,1312.32, 1250.61
	Aliphatic C–H str	1253.2,1180.28	2916.81
	Aliphatic C–H bend	3115.29, 2919.55	1467.56
	Chelate compounds O–H str	1464.16	2360.44
	–C–OH str	2703.98,2622.35	1084.76
	Deformation vibrations–C–H outside plane, related to substitution of aromatic rings of multi–ring compounds, N–H def out of plane	1081.33,1013.21, 968.06 800–500	800–500
	Fe–O bond stretching	–	~559.2
	N–H str	–	Merged with O–H
BTC	C=O	1710.55	1712.48
	Aromatic C=C str	1589.06,1511.92	1589.06,1509.03
	C–O str coupled with C–H wagging	1383.68,1348,	1383.68,1348
	Aliphatic C–H str	1312.32,1259.29,	
	Aliphatic C–H bend	2924.52	3039.26, 2935
	Chelate compounds O–H str	1466.6	1414.53
	–C–N str	2360.44,2340.19	2357,2335
	–C–OH str	1132.01	1130.87
	Deformation vibrations–C–H outside plane, related to substitution of aromatic rings of multi–ring compounds, N–H def out of plane	1076.08,1013.41 938.19,818.63 800–500	1076.08,939.163, 818.63 800–500
	Fe–O bond stretching		
	N–H str	–	~548.6
		–	3454.85 (broad), Merged with O–H
BIC	C=O	1709.59	1725.98

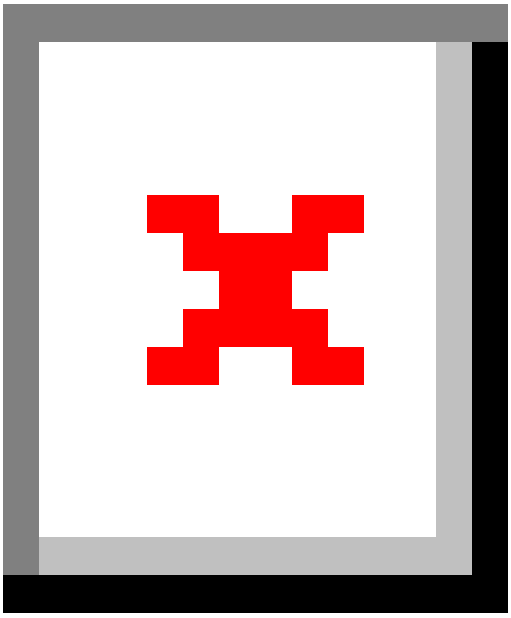
	Aromatic C=C str	1592.91, 1530.24	1591.95,1530.24
	C–O str coupled with C–H wagging	1383.68,1354.75	1383.68,1311.36
		1252.54	1253.5
	Aliphatic C–H str	2970.8,2907.16	3045.05,2930.31
	Aliphatic C–H bend	1467.56	1468.53
	Chelate compounds O–H str	2359.48,2339.23	2360.44,2340.19
	–C–N str	1137.12	1134.96
	–C–OH str	818.63	1012.45, 973.87,
			915.05,819.59
		800–500	800–500
	Deformation vibrations–C–H outside plane, related to substitution of aromatic rings of multi–ring compounds, N–H def out of plane		
	Fe–O bond stretching	–	~547.6
	N–H str	3343	3338.18, 3789.4



SI 5 FTIR spectra of Chromenones and Chromenones conjugated onto SPIONs of (a-b) PC, (c-d) DC, (e-f) DHC, (g-h) BTC, and (i-j) BIC



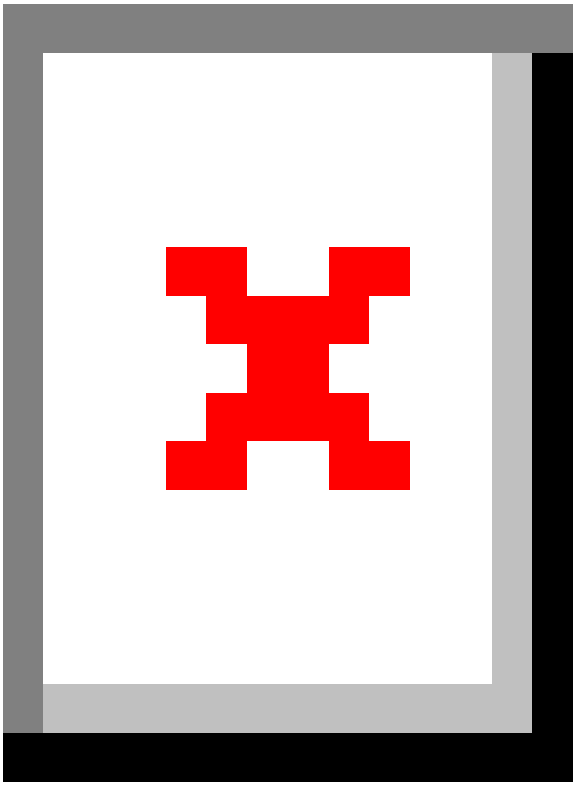
SI 6 Molecular docking poses of complex of oligomeric part of dextran (Blue) and CHR (Dark brown) (a) PC, (b) DC, (c) DHC, (d) BTC, and (e) BIC (Hydrogen binding– – –and Atom–atom interaction – – –)



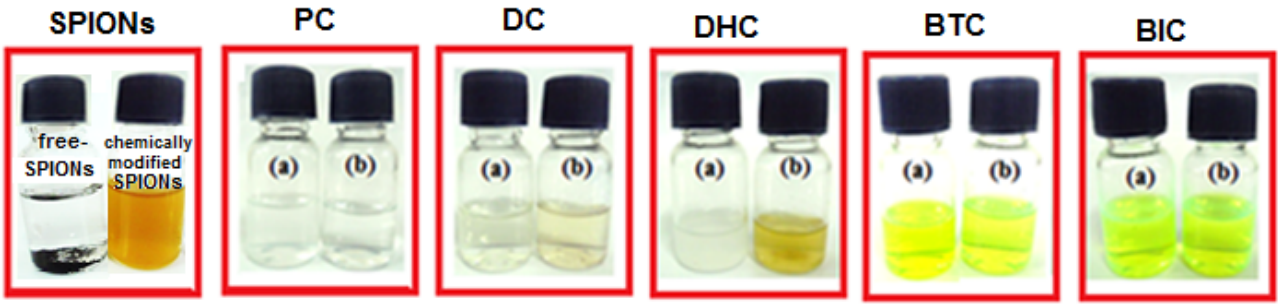
SI 7 Molecular docking poses of complex of oligomeric part of aminoethylamino-dextran (Blue) and CHR (Dark brown) (a) DC, (b) DHC, (c) BTC, and (d) BIC (Hydrogen binding– – –and Atom–atom interaction – – –)

SI8 Docking and E_{model} score of oligomeric part of dextran and aminoethylamino-dextran

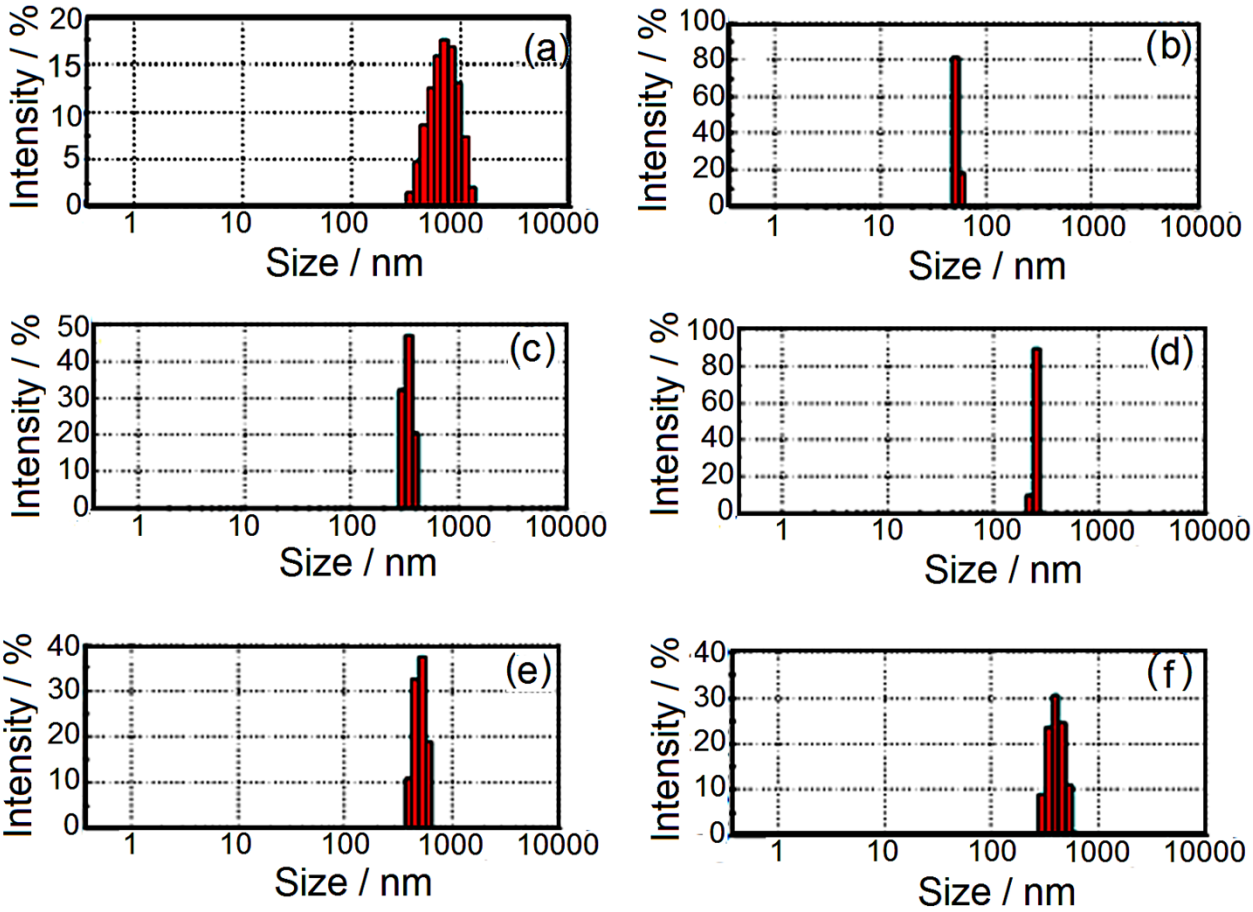
CHRs	Dextran (Kcal mol^{-1})		Aminoethylamino attached dextran(Kcal mol^{-1})	
	Docking score	E_{model} score	Docking score	E_{model} score
PC	0.640	–24.021	–	–
DC	–1.357	–32.471	–2.55291	–31.8915
DHC	–0.710	–28.494	–1.09581	–32.3933
BTC	–0.500	–40.389	–0.46448	–38.0988
BIC	–0.886	–29.441	–0.65794	–41.3116



SI 9 Energy dispersive X–ray spectra of (a) naked Iron oxide, (b) dextran–coated SPIONs, (c) aminoethylamino–dextran–coated SPIONs,[1] and of CHR–SPIONs of (d) PC, (e) DC, (f) DHC, (g) BTC, (h) BIC



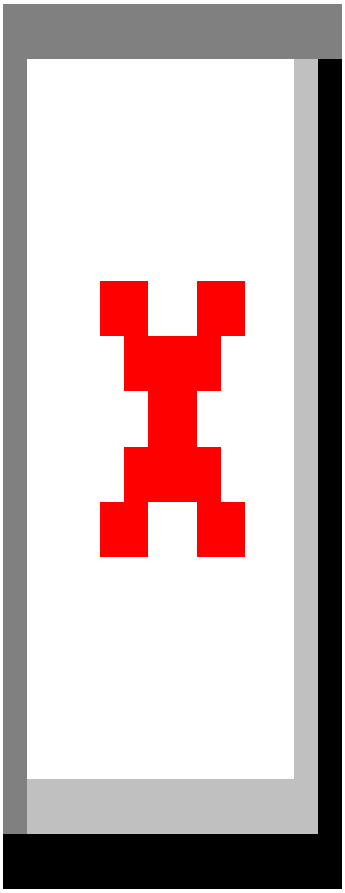
SI 10 Photographic images for the dispersion of free-SPIONs, chemically modified SPIONs, chromenones and the corresponding chromenones conjugated onto chemically modified SPIONs of PC, DC, DHC, BTC, BIC in aqueous medium



SI 11 Size distributions of (a) aminoethylamino–dextran–coated SPIONs, and CHR–SPIONs of (b) PC, (c) DC, (d) DHC, (e) BTC, and (f) BIC

SI 12 Particle size and magnetic properties of aminoethylamino–modified dextran–coated SPIONs and CHR–SPIONs

Sample		Particle diameter nm	Coercivity, H_c (G)	M_S (emu/g)	M_R (emu/g)
Aminoethylamino–modified dextran–coated SPIONs		723.7	0.65	0	0
CHR– SPIONs	PC	52.2	3.34	4.94	0
	DC	338.0	0.72	0	0
	DHC	251.5	0.74	1.75	0
	BTC	508.6	0.61	62.31	0
	BIC	564.4	2.04	4.44	0



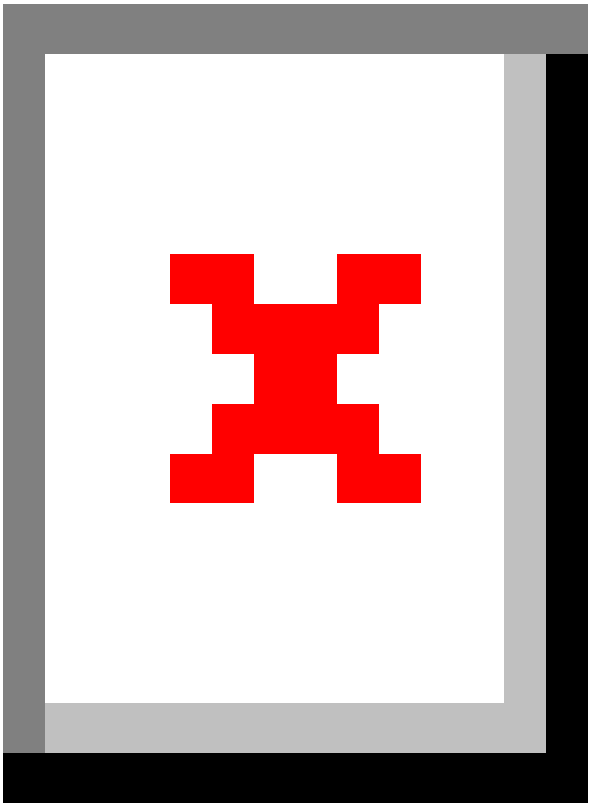
SI 13 X–ray diffraction patterns of (a) SPIONs, (b) Dextran and chromenones and their aminoethylamino–dextran–coated SPIONs conjugates (IO-DX) of (c) PC, (d) DC, (e) DHC, (f) BTC, and (g) BIC

SI14 Major peaks of CHRs, Dextran, SPIONs, and CHR–SPIONs

Compounds	2θ (deg)	
	Free CHRs	CHR–SPIONs
PC	9.4244, 16.4884 18.1424	9.3179 10.7185 25.7757 31.9277
DC	14.2889 16.7263 26.0235	24.0800 27.4000 31.1000
DHC	15.4788 20.1134 23.4927	11.0046 12.0238 17.9630 26.8000
BTC	10.2000 13.4032 15.9126	13.1084 13.8601 20.8082
BIC	7.3910 14.4279 24.0022	14.0425 23.5801 24.8892 26.0000
Free SPIONs	17.5000, 25.7000,30.4480, 35.9403,	
Aminoethylamino–modified dextran–coated SPIONs	15.8733, 23.7824,25.7000, 26.8550	
Dextran	12.6377, 21.1328, 27.2091	

SI15 Crystallite size and Strain parameter of CHRs, SPIONs, and CHRs–SPIONs

Molecule	XRD Crystallite size in nm with Strain (ε)	
	Free CHR	CHR–SPIONs
SPIONs	18 (0.0091)	
dextran–coated SPIONs	10 (0.0037)	
Aminoethylamino–dextran–coated SPIONs	45 (0.00037)	
PC	20 (0.00056)	40 (0.0004)
DC	25 (0.00041)	36 (0.00094)
DHC	23 (0.00048)	37 (0.0005)
BTC	43 (0.00045)	34 (0.00014)
BIC	40 (0.00050)	38 (0.00063)



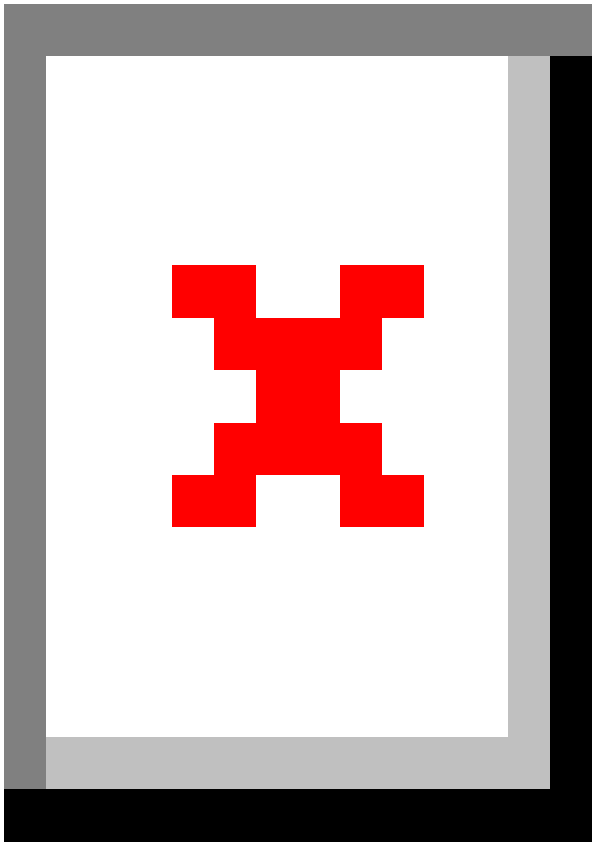
SI16 (a) Fluorescence spectra of PC loaded on CHR–SPIONs at varying concentrations of β–CD. Inset: The plot of [β–CD] *vs*. I_0/I, (b) The plot of 1/[β–CD] *vs*. $F_0/\Delta F$ for the fluorescence spectra of PC loaded on CHR–SPIONs at varying concentrations of β–CD, (b) Fluorescence spectra of DC loaded on CHR–SPIONs at varying concentrations of β–CD. Inset: The plot of 1/[β–CD] *vs*. $1/(I–I_0)$, (c) Fluorescence spectra of DHC loaded on CHR–SPIONs at varying concentrations of β–CD. Inset: The plot of $1/[\beta–CD]^2$ *vs*. $1/(I–I_0)$, (d) Fluorescence spectra of BTC loaded on CHR–SPIONs at varying concentrations of β–CD. Inset: The plot of 1/[β–CD] *vs*. $1/(I–I_0)$, and (e) Fluorescence spectra of BIC loaded on CHR–SPIONs at varying concentrations of β–CD. Inset: The plot of 1/[β–CD] *vs*. $1/(I–I_0)$.

SI 17 Absorption and fluorescence spectral data of CHR–SPIONs on ctDNA binding

CHRs	CHR–SPIONs			
	Absorption Maximum (nm)		Fluorescence Maximum (nm)	
	Water	DNA	Water	DNA
PC	255, 321	256, 321	280, 413	281, 414
DC	286, 381	282, 380	318	314
DHC	287	281	363	363
BTC	267, 468, 511	259, 456	511	509
BIC	264, 469	264, 471	510	511

SI18 Binding constant values of CHR–SPIONs on DNA binding

CHR loaded on modified SPIONs	K (M^{-1})
PC	7.33×10^5
DC	8.20×10^5
DHC	2.09×10^4
BTC	8.20×10^4
BIC	1.06×10^5



SI 19 Fluorescence spectra of CHR loaded on CHR–SPIONs at varying concentrations of DNA (a) PC, (b) DC, (c) DHC, (d) BTC, and (e) BIC. Inset: The plot of [DNA] versus I_0/I

SI 20. Experimental

Molecular docking

The molecular structure of the model oligomers of dextran and aminoethylamino modified dextran[2] was uploaded into Schrodinger Maestro software V 9.6 environment.[3,4] To get a proper binding affinity and molecular interaction, the receptor had to be prepared in the way of minimizing energy and potentially the molecule were fixed. The molecular receptor was prepared using the preparation work flow. All the hydrogens were added to the receptor to minimize the receptor structure with OPLS 2005 force field and the molecular mechanics engine setting was having a maximum root mean square deviation (RMSD) of 0.30 Å.[5,6] The energy minimization was performed constraining the heavy molecular atoms with the hydrogen torsion parameters turned off, to permit free rotation of the hydrogen atom. Bio–pharmacological properties of the ligands (CHR–SPIONs) were analyzed through Lipinski rule of five.[7] The compounds having less property value of Lipinski rule were restudied to obey the rule. The compounds with biologically active functional group were eliminated by applying reactive filter parameters.[8] After ensuring that the receptor and the ligand were in accurate forms of docking, the receptor grid files were generated and centered the allosteric site residues. To reduce the potential for non–polar parts of the receptor, Van der Wall's radii of the receptor atoms were scaled to 1.00 Å with a partial atomic charge of 0.27. A grid box of six maintained at 40 Å × 60 Å × 40 Å, was engaged on the primed receptor structure by selecting allosteric site receptor structure of dextran and aminoethylamino functionalized dextran groups. A three phased subsequent molecular docking was performed to know the molecular interaction. Glide high throughput virtual screening (HTVS), standard precision (SP), and extra precision (XP) methods were followed.[9,10] The XP docking method is highly accurate and offer more poses for all each ligands during docking method and reports the best pose based on the energy term, E_{model}. The best pose of each ligand was further ranked based on the energy term E_{model}. The lowest XP glide score for a ligand indicates the best binding affinity towards the receptor. The cut off XP Glide score was set up as 0 Kcal mol^{-1}.

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