

Supporting Information

Taylor dispersion analysis for measurement of diffusivity and size of gadolinium-based contrast agents

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Table S1. Structure of ligands tested as Gd^{3+} , Eu^{3+} or Y^{3+} complexes.

Class of Ligand	Structure of Ligand	Ionicity of Ln-Complex	Name and Chemical Formula of Ligand					
Open-chain		Non-Ionic	DTPA-BMA $R_1 = R_2 =$		$C_{16}H_{29}N_5O_8$ Mw = 419.44 g/mol			
		Ionic	BOPTA $R_1 =$; $R_2 =$		$C_{21}H_{29}N_3O_{11}$ Mw = 499.47 g/mol			
Macrocyclic		Ionic	DOTA $R =$				$C_{16}H_{28}N_4O_8$ Mw = 404.42 g/mol	
		Non ionic	HP-D03A $R =$		BT-DO3A $R =$		$C_{17}H_{32}N_4O_7$ Mw = 404.46 g/mol	$C_{18}H_{34}N_4O_9$ Mw = 450.49 g/mol
	Pyclen based Structure 	Non ionic	PCTA $R = H$ $C_{17}H_{24}N_4O_6$ Mw = 380.40 g/mol	PCTA D1 $R =$	PCTA D2 $R =$	PCTA D3 $R =$		$C_{110}H_{165}Br_9N_{16}O_{60}$ Mw = 3390.72 g/mol

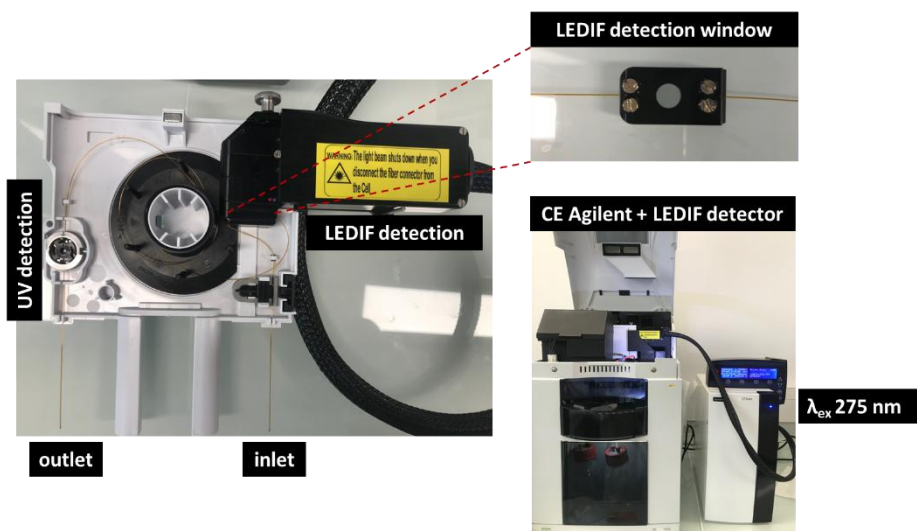


Fig. S1. Pictures of the TDA setup with UV and LEDIF detectors.

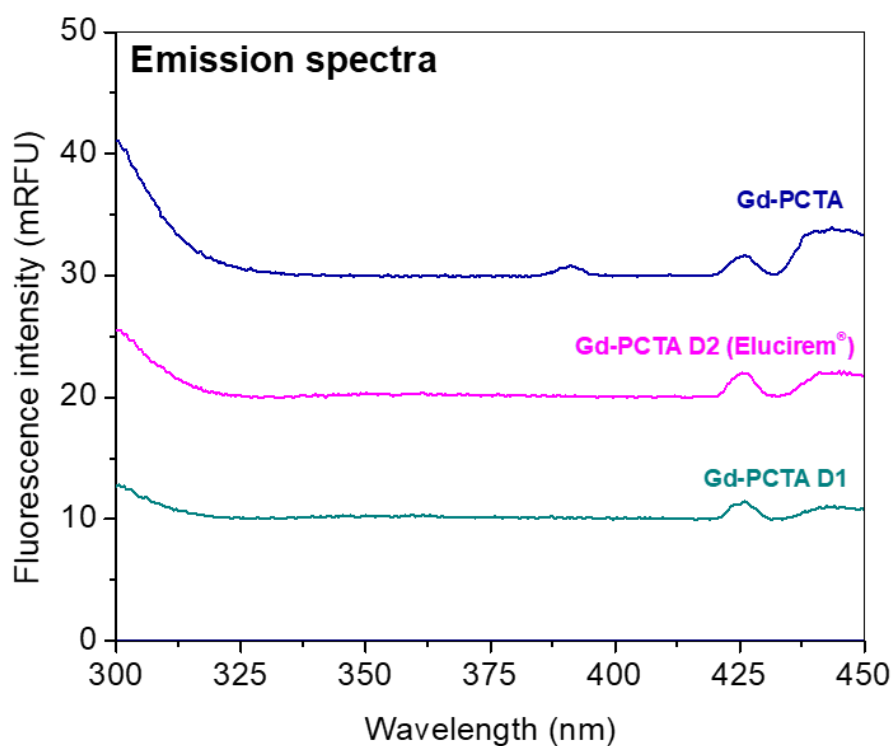


Fig. S2. Emission spectra (excitation wavelength 275 nm) of Gd-PCTA, Gd-PCTA D1 and Gd-PCTA D2 at a concentration of 5.0 mM. GBCA were diluted in 10 mM Tris-HCl buffer pH 7.4. Sensitivity of spectrofluorometer was set at medium level.

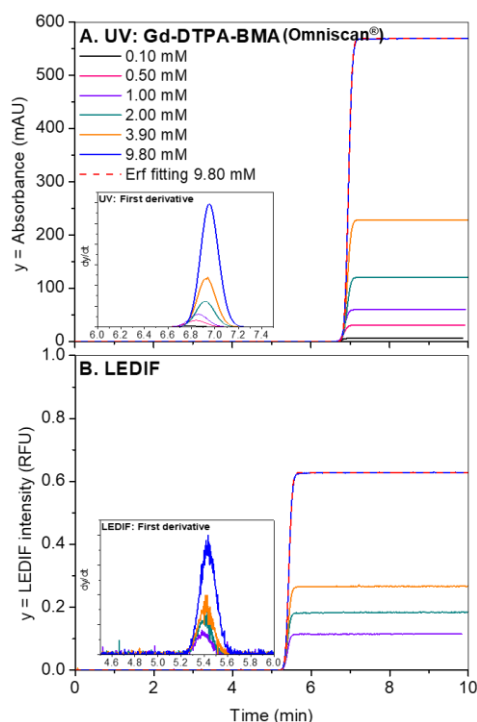


Fig. S3. Frontal Taylorgrams of Gd-DTPA-BMA at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal Taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: ultrapure water, mobilization pressure 100 mbar.

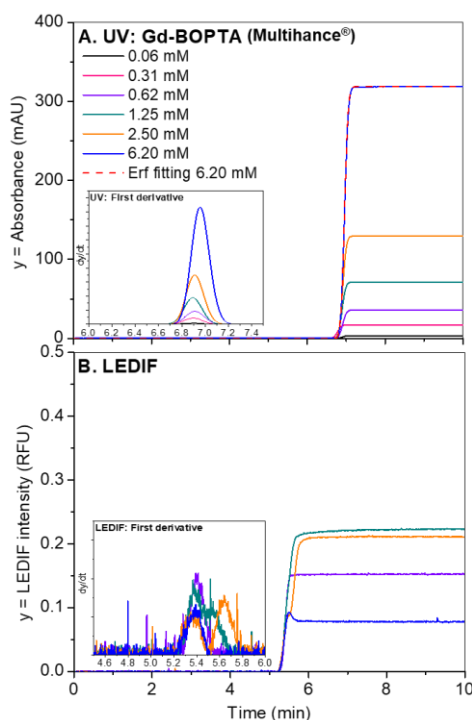


Fig. S4. Frontal Taylorgrams of Gd-BOPTA at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal Taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: ultrapure water, mobilization pressure 100 mbar.

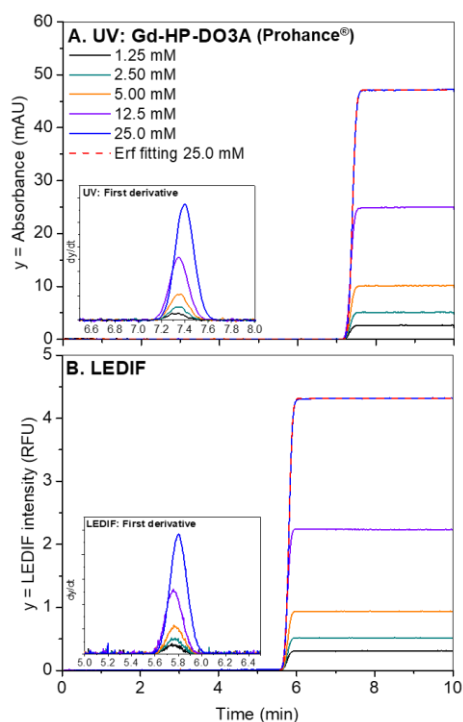


Fig. S5. Frontal Taylorgrams of Gd-HP-DO3A at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal Taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: 10 mM Tris-HCl buffer (pH 7.4), mobilization pressure 100 mbar.

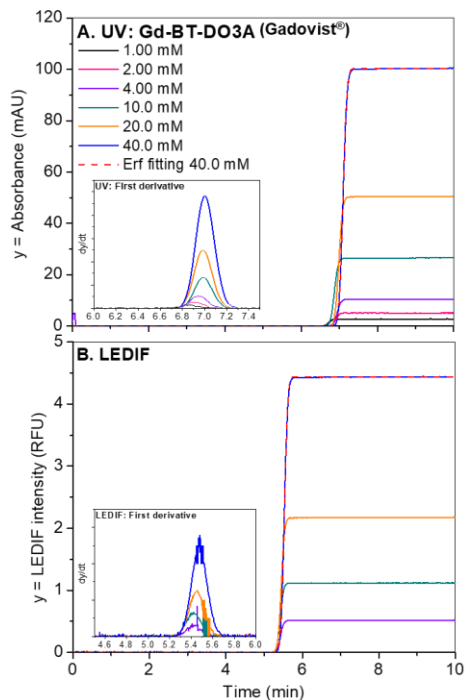


Fig. S6. Frontal Taylorgrams of Gd-BT-DO3A at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal Taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: 10 mM Tris-HCl buffer (pH 7.4), mobilization pressure 100 mbar.

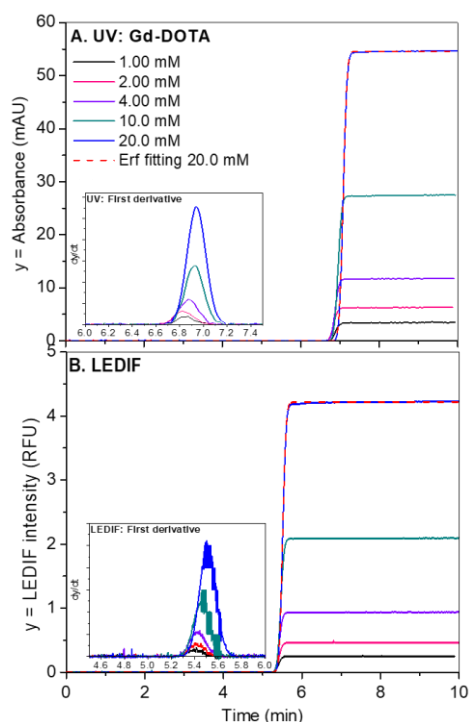


Fig. S7. Frontal taylorgrams of Gd-DOTA at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: 10 mM Tris-HCl buffer (pH 7.4), mobilization pressure 100 mbar.

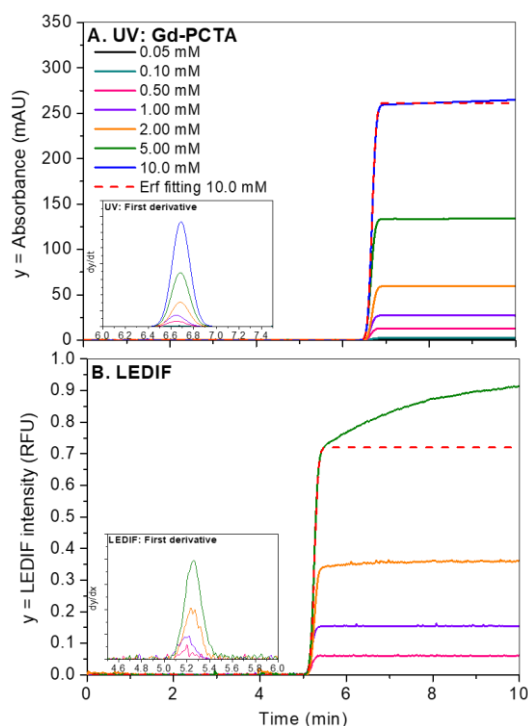


Fig. S8. Frontal taylorgrams of Gd-PCTA at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: 10 mM Tris-HCl buffer (pH 7.4), mobilization pressure 100 mbar.

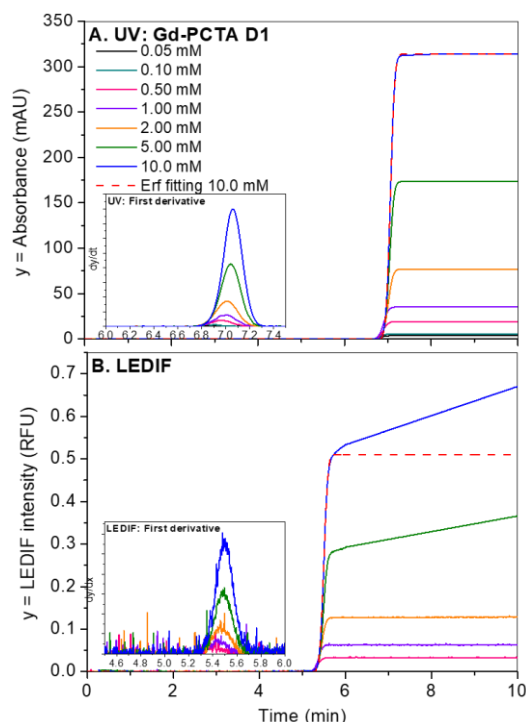


Fig. S9. Frontal taylorgrams of Gd-PCTA D1 at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: 10 mM Tris-HCl buffer (pH 7.4), mobilization pressure 100 mbar.

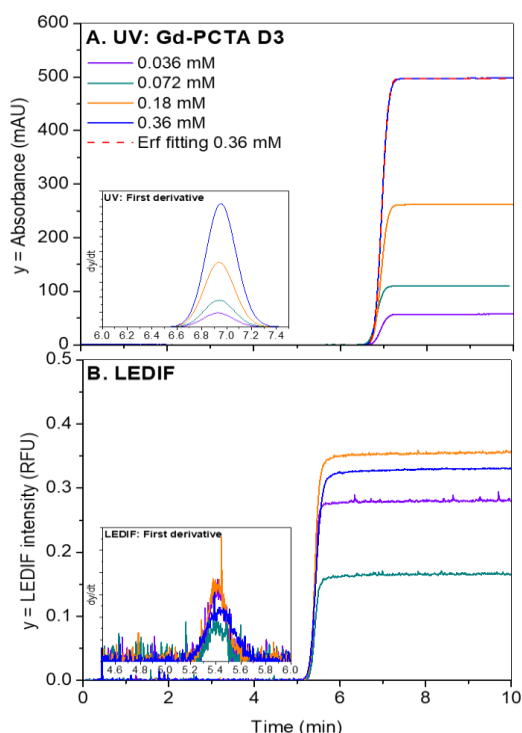


Fig. S10. Frontal taylorgrams of Gd-PCTA D3 at different concentrations using (A) UV 200 nm and (B) LEDIF detector (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm). Erf fitting to calculate D_h and D is plotted in a red dotted line. The inset photo is the first derivative of the frontal taylorgram. Experimental conditions: fused silica capillary of 65 cm total length (44 cm to LEDIF detector, 56.5 cm to UV detector) x 50 μm i.d., eluent: 10 mM Tris-HCl buffer (pH 7.4), mobilization pressure 100 mbar.

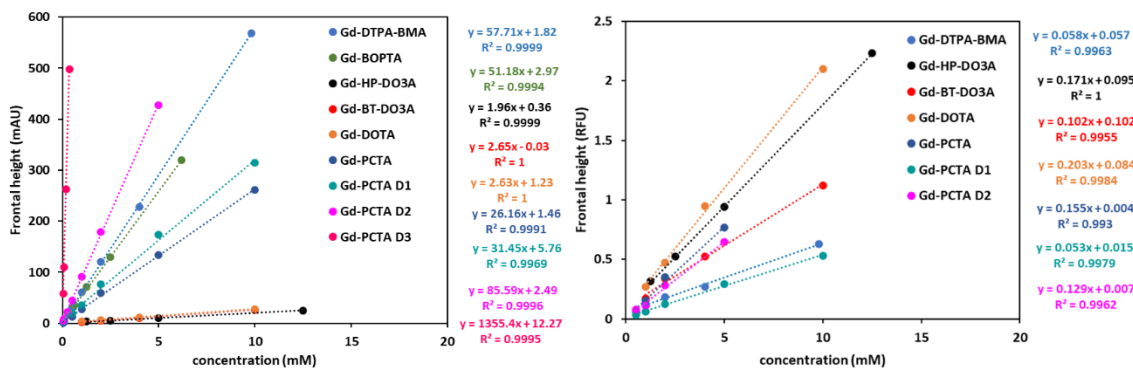


Fig. S11. Linear calibrations of GBCA using UV at 200 nm and LEDIF detection (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm).

Table S2. Cartesian coordinates (Å) obtained after geometry optimization of Gd-DTPA-BMA using DFT (Charge = 0 Multiplicity = 8).

Gd	0.04314	0.13259	-0.10157
O	1.99164	0.35743	-1.66373
O	1.37875	1.33921	1.42862
O	3.36754	2.24135	1.8054
O	-1.56767	1.11042	1.353
O	-2.47979	1.3492	3.36488
O	0.18389	-2.00454	-1.06736
O	-0.46367	-4.02574	-1.72409
O	-1.82517	0.59165	-1.71695
O	0.06419	2.53953	-0.89617
N	2.4456	-1.0636	0.61189
N	-0.1828	-1.1925	2.17024
N	-2.31503	-1.45492	-0.00716
C	2.04537	-2.15486	1.50204
H	1.53997	-2.90511	0.89673
C	1.13966	-1.67304	2.62179
C	-1.0842	-2.34158	1.96771
H	-1.27374	-2.82956	2.93076
H	-0.57294	-3.06893	1.33957
C	-2.42537	-1.98023	1.35453
H	-3.05623	-2.87564	1.37922
H	-2.9257	-1.23944	1.97485
C	3.03313	-1.54197	-0.62856
H	4.07621	-1.85123	-0.50789
H	2.4573	-2.39388	-0.98563
C	2.90824	-0.47457	-1.69889
C	3.30708	-0.06349	1.25034
H	4.17863	0.13454	0.62762
H	3.69751	-0.43177	2.20286
C	2.63645	1.28341	1.51798
C	-0.74057	-0.24485	3.14539
H	0.08112	0.32598	3.57508
H	-1.24169	-0.7688	3.96343
C	-1.69344	0.81664	2.59041
C	-2.14325	-2.51552	-0.99819
H	-2.70944	-3.4117	-0.7303
H	-2.53095	-2.17224	-1.9589
C	-0.69163	-2.9047	-1.27717
C	-3.41968	-0.57959	-0.35644
H	-3.64598	0.06778	0.49026
H	-4.33335	-1.12692	-0.61287
C	-3.01444	0.33955	-1.4935
O	1.92439	4.16273	0.39028
H	0.71867	3.0982	-0.4327
H	-0.80533	2.93873	-0.72297
H	2.43128	3.56235	0.97137
H	2.56951	4.55448	-0.19832
H	2.91983	-2.63371	1.95804
H	1.01607	-2.48401	3.34627
H	1.62923	-0.85646	3.14697
N	3.79681	-0.49627	-2.68032
N	-3.99062	0.89191	-2.20004
H	4.53938	-1.17181	-2.64153
H	-4.93837	0.61637	-2.01163
C	3.73532	0.41405	-3.80659
H	3.85213	1.44467	-3.47392
H	4.5382	0.16786	-4.49423

H	2.78039	0.31973	-4.32145
C	-3.73685	1.84518	-3.26258
H	-4.67768	2.30563	-3.54775
H	-3.04916	2.61509	-2.91734
H	-3.29991	1.35361	-4.13152
O	-2.40085	3.37047	0.12438
H	-2.27261	2.56819	0.66966
H	-3.25197	3.26968	-0.30112

Table S3. Cartesian coordinates (Å) obtained after geometry optimization of Gd-BOPTA using DFT (Charge = -2 Multiplicity = 8).

Gd	-1.44603	0.24559	0.04036
O	-3.54886	0.44311	-1.2371
O	-4.9068	-0.3513	-2.81271
O	-2.95887	-0.39525	1.7996
O	-5.12843	-0.78655	2.09124
O	-0.20863	0.77469	1.99857
O	0.90647	0.16838	3.82467
O	-0.77486	-0.76024	-2.00566
O	0.58248	-1.40628	-3.64132
O	-0.41262	2.21026	-0.91467
O	0.98277	3.83925	-0.36388
O	-2.55824	2.37359	0.92635
N	-2.88043	-2.06899	-0.41884
N	-0.23189	-1.87121	1.06232
N	1.35216	0.24883	-0.53771
C	-1.88927	-3.14117	-0.34599
H	-1.23874	-3.04564	-1.2132
C	-1.07581	-3.07553	0.93632
C	1.03765	-2.07055	0.34231
H	1.61476	-2.85977	0.84103
H	0.8046	-2.43469	-0.65669
C	1.92911	-0.83982	0.25075
H	2.88734	-1.1632	-0.16732
H	2.15066	-0.4671	1.24852
C	-3.43823	-1.89207	-1.7543
H	-4.20655	-2.63764	-1.98121
H	-2.63524	-1.98805	-2.48184
C	-4.03174	-0.49461	-1.96044
C	-3.95247	-2.18393	0.57313
H	-4.92036	-2.26128	0.0782
H	-3.84099	-3.09831	1.16157
C	-4.02757	-1.02469	1.56974
C	0.00532	-1.55761	2.47543
H	-0.8996	-1.79613	3.03303
H	0.81874	-2.16358	2.88524
C	0.27763	-0.0833	2.79399
C	1.4765	0.02052	-1.96912
H	2.43528	-0.43907	-2.2286
H	1.42869	0.9775	-2.4901
C	0.34898	-0.80138	-2.59245
C	1.77348	1.59129	-0.13211
H	1.78996	1.59949	0.95796
C	0.70263	2.63705	-0.51281
O	-5.25037	1.70326	0.54926
H	-3.52774	2.32915	0.90004

H	-2.27579	3.23109	0.56207
H	-5.34163	0.98262	1.18969
H	-4.79426	1.28288	-0.20234
H	-2.36326	-4.12986	-0.39454
H	-0.45934	-3.97804	1.0097
H	-1.75514	-3.0916	1.78573
O	-1.546	4.86092	0.08964
H	-1.44232	5.43175	0.85085
H	-0.64092	4.55507	-0.13246
C	3.14769	2.03231	-0.62243
H	3.17608	2.09411	-1.71756
H	3.35881	3.03163	-0.23238
O	4.1054	1.1038	-0.17194
C	5.39988	1.3567	-0.67341
H	5.78106	2.30802	-0.28468
H	5.35819	1.43777	-1.76737
C	6.3001	0.22317	-0.27298
C	6.06929	-1.05358	-0.77943
C	7.35427	0.41738	0.60953
C	6.87603	-2.11604	-0.40731
H	5.24917	-1.21143	-1.46924
C	8.17025	-0.64437	0.98034
H	7.53947	1.40571	1.012
C	7.93106	-1.91248	0.47448
H	6.68679	-3.10358	-0.80718
H	8.98937	-0.47952	1.66789
H	8.56378	-2.74117	0.76376

Table S4. Cartesian coordinates (Å) obtained after geometry optimization of Gd-HP-DO3A using DFT (Charge = 0 Multiplicity = 8).

N	-0.74784	1.05888	-2.17619
C	0.46132	1.46371	-2.91411
C	1.57264	0.43245	-2.88239
N	2.06383	0.115	-1.53276
C	2.71647	-1.20528	-1.53259
C	1.72666	-2.35694	-1.51868
N	0.87919	-2.40992	-0.31719
C	-0.25352	-3.32562	-0.53246
C	-1.37648	-2.74573	-1.3828
N	-1.9336	-1.46787	-0.90756
C	-2.51159	-0.71288	-2.03746
C	-1.47817	0.00082	-2.89159
C	-1.59597	2.22946	-1.90064
C	-2.1888	2.30051	-0.49287
O	-2.01074	1.31083	0.27444
O	-2.79188	3.33315	-0.17754
C	2.94912	1.16018	-1.00634
C	2.28107	2.23245	-0.13963
O	3.01484	3.09507	0.34746
O	1.0305	2.14201	0.0623
C	1.65464	-2.8192	0.85979
C	2.41367	-1.69552	1.56953
O	3.40887	-1.98332	2.22354
O	1.90898	-0.52501	1.46764
C	-2.96824	-1.63085	0.12911
C	-2.46858	-2.11581	1.48634

O	-1.24262	-1.44586	1.80655
H	-1.00626	3.13506	-2.02147
H	-2.42052	2.29693	-2.61662
H	3.49133	1.66566	-1.81106
H	3.69628	0.7005	-0.36285
H	2.35414	-3.62357	0.61682
H	0.96158	-3.2018	1.60936
H	-3.4141	-0.6496	0.27808
H	-3.75252	-2.31464	-0.2168
H	0.8208	2.38821	-2.47031
H	0.22083	1.67541	-3.96189
H	2.39475	0.80324	-3.50422
H	1.23566	-0.48985	-3.34867
H	3.3603	-1.31897	-2.41112
H	3.36635	-1.26791	-0.66397
H	2.28714	-3.29303	-1.62276
H	1.07519	-2.28992	-2.38782
H	0.08388	-4.24988	-1.0151
H	-0.6315	-3.60929	0.44272
H	-1.01341	-2.59397	-2.39707
H	-2.16738	-3.50065	-1.45507
H	-3.20875	0.01565	-1.63196
H	-3.09219	-1.38014	-2.6829
H	-0.75636	-0.71838	-3.27221
H	-1.98793	0.4196	-3.76664
O	2.37369	1.70869	2.97974
H	2.4436	0.86451	2.4958
H	2.58262	2.37569	2.31419
Gd	-0.02283	0.06235	0.18534
H	-0.90524	1.8391	2.50166
O	-0.31622	1.05806	2.52872
H	0.5561	1.38327	2.81871
H	-2.24121	-3.1805	1.45035
C	-3.5124	-1.88021	2.55666
H	-4.43716	-2.39598	2.30102
H	-3.16576	-2.25999	3.51714
H	-3.72885	-0.8143	2.65141
H	-1.34009	-0.87635	2.57611
O	-1.96735	3.30072	2.51878
H	-2.33913	3.33805	1.6168
H	-1.48733	4.12112	2.63243

Table S5. Cartesian coordinates (Å) obtained after geometry optimization of Gd-BT-DO3A using DFT (Charge = 0 Multiplicity = 8).

N	0.42317	1.43955	-2.11572
C	1.77135	1.35893	-2.70423
C	2.3592	-0.03846	-2.68274
N	2.50448	-0.60663	-1.33342
C	2.58054	-2.07699	-1.41272
C	1.22571	-2.7329	-1.60958
N	0.28059	-2.49949	-0.5059
C	-1.08528	-2.86041	-0.92173
C	-1.75897	-1.83032	-1.81653
N	-1.86023	-0.47242	-1.25049
C	-1.91376	0.53148	-2.337
C	-0.57711	0.82322	-2.99884
C	0.08805	2.83344	-1.78375

C	-0.64125	3.03548	-0.45521
O	-0.95978	2.00393	0.20388
O	-0.85327	4.19678	-0.0876
C	3.66192	-0.04691	-0.61962
C	3.37675	1.13965	0.3075
O	4.3256	1.58437	0.95465
O	2.17998	1.56053	0.387
C	0.66883	-3.25594	0.69129
C	1.71015	-2.58262	1.58817
O	2.40342	-3.28774	2.3106
O	1.73947	-1.30409	1.55434
C	-3.01602	-0.25868	-0.33522
C	-2.85553	-0.97369	1.02071
O	-1.5043	-0.89191	1.46113
H	1.00635	3.41102	-1.70796
H	-0.50944	3.2961	-2.57488
H	4.45139	0.25115	-1.31558
H	4.08385	-0.81464	0.0252
H	1.01738	-4.25942	0.43298
H	-0.21102	-3.36732	1.32523
H	-3.00398	0.8097	-0.12316
H	2.41648	2.02698	-2.13983
H	1.76255	1.71225	-3.74106
H	3.33218	-0.00551	-3.18418
H	1.73988	-0.71128	-3.27033
H	3.23366	-2.38544	-2.23539
H	3.03811	-2.44698	-0.4994
H	1.38085	-3.80858	-1.74907
H	0.77052	-2.3662	-2.52753
H	-1.08375	-3.81565	-1.45868
H	-1.67126	-3.0151	-0.02291
H	-1.20487	-1.75471	-2.74943
H	-2.74146	-2.22243	-2.09309
H	-2.3237	1.44967	-1.92411
H	-2.59356	0.21083	-3.13151
H	-0.15917	-0.09901	-3.39622
H	-0.76687	1.47158	-3.86175
O	2.78419	0.46036	3.3628
H	2.59867	-0.30863	2.79171
H	3.32537	1.0342	2.80742
Gd	0.39747	0.08455	0.14962
H	-0.09922	1.89673	2.5807
O	0.1473	0.94917	2.57007
H	1.02331	0.88411	2.99397
H	-3.10193	-2.03181	0.91764
C	-3.74342	-0.41163	2.12718
H	-3.38226	-0.81776	3.07533
H	-3.65527	0.67937	2.15655
H	-1.39992	-0.35172	2.25491
O	-0.55459	3.63655	2.66471
H	-0.73193	3.88815	1.73833
H	0.14791	4.21619	2.95931
C	-4.37726	-0.57637	-0.99051
H	-4.64885	-1.62368	-0.82112
H	-4.30173	-0.43563	-2.06701
O	-5.08508	-0.81086	1.9144
H	-5.60827	-0.55837	2.67571
O	-5.40476	0.2812	-0.55154
H	-5.59312	0.03393	0.36368

Table S6. Cartesian coordinates (Å) obtained after geometry optimization of Gd-DOTA using DFT (Charge = -1 Multiplicity = 8).

N	1.53703	0.10788	2.00597
C	0.88168	1.02874	2.94841
C	-0.61967	0.83201	3.04363
N	-1.34613	1.08249	1.79184
C	-2.67993	0.46609	1.84779
C	-2.6511	-1.03684	1.64813
N	-2.1007	-1.46312	0.35413
C	-1.71716	-2.8829	0.4167
C	-0.41438	-3.11873	1.16424
N	0.75003	-2.44613	0.57122
C	1.8451	-2.33497	1.54889
C	1.62651	-1.24102	2.57849
C	2.84998	0.62053	1.60024
C	3.21897	0.42177	0.12984
O	2.40347	-0.19063	-0.61613
O	4.29427	0.90829	-0.24885
C	-1.44617	2.51467	1.49522
C	-0.34527	3.09334	0.6032
O	-0.44117	4.29469	0.31702
O	0.54578	2.30847	0.17296
C	-3.05114	-1.22293	-0.73523
C	-3.08017	0.21045	-1.27659
O	-4.12171	0.6259	-1.77458
O	-1.98186	0.86062	-1.21452
C	1.20587	-3.14112	-0.63556
C	0.41872	-2.81826	-1.91054
O	0.39426	-3.66695	-2.80148
O	-0.11501	-1.66592	-1.97272
H	2.87648	1.69603	1.75999
H	3.65253	0.1923	2.20984
H	-1.49499	3.11216	2.41165
H	-2.37263	2.69724	0.95358
H	-4.06686	-1.51373	-0.4518
H	-2.75226	-1.83604	-1.58594
H	2.22619	-2.82063	-0.84587
H	1.21793	-4.22526	-0.49042
H	1.08907	2.04379	2.62196
H	1.30365	0.91942	3.95445
H	-0.99739	1.49031	3.83556
H	-0.83659	-0.18337	3.36627
H	-3.16762	0.67356	2.8076
H	-3.29828	0.9243	1.08048
H	-3.67202	-1.41918	1.7668
H	-2.05911	-1.49659	2.43615
H	-2.50074	-3.47413	0.90446
H	-1.63315	-3.25596	-0.60028
H	-0.51787	-2.77797	2.19176
H	-0.24072	-4.20006	1.21537
H	2.7614	-2.13578	0.99934
H	1.98829	-3.28386	2.07858
H	0.71039	-1.43962	3.13004
H	2.44137	-1.29092	3.31062
O	-1.25156	3.25888	-2.36402
H	-1.7075	2.49316	-1.9666
H	-0.96347	3.7863	-1.60725
Gd	0.06963	0.0073	-0.30916
H	1.61014	1.44679	-2.51578

O	0.66963	1.18772	-2.49116
H	0.15431	2.00994	-2.54982
O	3.36859	1.95707	-2.65645
H	3.75868	1.52944	-3.41884
H	3.78418	1.53324	-1.87994

Table S7. Cartesian coordinates (Å) obtained after geometry optimization of Gd-PCTA using DFT (Charge = 0 Multiplicity = 8).

O	0.4142	2.23404	-1.06202
O	0.61418	0.99178	2.23314
O	1.79168	-1.50782	1.08376
N	-1.95014	-0.3922	-1.13665
N	-1.68842	1.90549	0.51897
N	-1.53279	-0.77603	1.8683
N	-0.27009	-2.49933	-0.28317
C	-2.90788	0.53628	-1.18007
C	-4.15994	0.27336	-1.71017
H	-4.91473	1.04631	-1.72344
C	-4.42495	-0.99461	-2.19425
H	-5.39551	-1.23121	-2.60798
C	-3.44376	-1.9653	-2.10971
H	-3.62849	-2.97697	-2.44094
C	-2.21476	-1.62809	-1.56742
C	-2.5752	1.90525	-0.64921
H	-2.07129	2.44288	-1.45234
H	-3.50113	2.4472	-0.43203
C	-2.38672	1.59465	1.77195
H	-3.33029	2.14796	1.84034
H	-1.76284	1.93804	2.59283
C	-2.70331	0.11742	1.93968
H	-3.2168	-0.01072	2.89878
H	-3.40715	-0.19022	1.17115
C	-1.97419	-2.14369	1.542
H	-2.80611	-2.07323	0.84673
H	-2.36124	-2.64506	2.4355
C	-0.88385	-3.01735	0.95154
H	-0.08525	-3.14249	1.6792
H	-1.30697	-4.01224	0.77147
C	-1.11672	-2.65467	-1.46699
H	-0.48139	-2.5238	-2.34232
H	-1.55161	-3.65786	-1.51792
C	-0.98969	3.18772	0.60239
C	-0.76754	-0.75384	3.11868
C	1.03132	-3.14005	-0.47743
O	1.10855	-0.57927	-2.22151
C	2.12667	-2.47336	0.35214
C	0.14912	0.46167	3.29745
C	0.10341	3.30853	-0.45381
O	3.29273	-2.89373	0.21238
O	0.41067	0.82574	4.43892
O	0.64872	4.39948	-0.63083
H	1.10672	0.1852	-2.83026
O	1.16274	1.78141	-3.60482
O	3.60076	-1.80425	-2.35548
H	3.67295	-2.31919	-1.53554
H	3.66785	-2.43873	-3.06956

H	0.93753	2.16214	-2.73367
H	0.41558	1.97236	-4.17215
H	2.00614	-0.95703	-2.28564
O	2.65041	0.91673	-0.07131
H	3.43104	0.4491	0.27362
H	2.91895	1.78249	-0.42643
O	3.24958	3.45877	-1.05882
H	3.81455	3.97332	-0.48221
H	2.3674	3.87135	-0.9948
O	4.79871	-0.62787	0.82908
H	4.32428	-1.47559	0.72551
H	4.89348	-0.50877	1.77442
H	-0.49215	3.2528	1.5694
H	-0.10285	-1.61772	3.13852
H	1.32552	-3.05773	-1.52132
H	1.00681	-4.20817	-0.23884
H	-1.42915	-0.8249	3.98621
H	-1.66906	4.04157	0.51878
Gd	0.29062	0.11328	0.10738

Table S8. Cartesian coordinates (Å) obtained after geometry optimization of Gd-PCTA D1 using DFT (Charge = -3 Multiplicity = 8).

O	-1.78054	-2.28089	-0.34195
O	-1.09686	0.9367	-1.60161
O	1.78653	0.19776	-1.6048
N	-0.08345	-0.85106	2.33195
N	-2.43074	-0.07222	0.9239
N	-0.08532	1.84442	0.82883
N	2.29146	-0.09885	0.96742
C	-1.24486	-0.82957	2.98963
C	-1.30125	-0.83199	4.3735
H	-2.25779	-0.80618	4.87518
C	-0.1181	-0.84214	5.08905
H	-0.13156	-0.83698	6.17026
C	1.08224	-0.82267	4.40334
H	2.02557	-0.78908	4.92908
C	1.06128	-0.82189	3.01824
C	-2.51515	-0.82304	2.17953
H	-2.74309	-1.86161	1.93929
H	-3.33204	-0.45486	2.80715
C	-2.55191	1.37764	1.11802
H	-3.35756	1.61625	1.8208
H	-2.83302	1.81977	0.16511
C	-1.29128	2.03735	1.65414
H	-1.50543	3.10031	1.78996
H	-1.07896	1.64723	2.64565
C	1.1196	2.02622	1.65761
H	0.90336	1.64267	2.65073
H	1.34817	3.08725	1.79074
C	2.37327	1.36377	1.11718
H	2.61405	1.77961	0.14204
H	3.19308	1.63499	1.78984
C	2.35424	-0.81299	2.24355
H	2.59745	-1.85283	2.02598
H	3.14631	-0.41858	2.88756
C	-3.42162	-0.56884	-0.05344
C	-0.06097	2.71901	-0.37207

C	3.33432	-0.59546	0.04176
O	1.20754	-2.84072	0.11416
C	2.89431	-0.36457	-1.41083
C	-1.03769	2.20504	-1.45732
C	-2.99318	-1.9531	-0.55883
O	3.62585	-0.80341	-2.32363
O	-1.66958	3.00418	-2.13883
O	-3.79314	-2.65923	-1.17728
H	0.58376	-3.58513	0.2119
O	-0.79231	-4.71901	0.17543
O	3.17648	-3.49605	-1.76595
H	3.52245	-2.63095	-2.04477
H	3.91586	-3.95485	-1.36611
H	-1.32887	-3.93982	-0.07402
H	-1.10602	-4.98307	1.04049
H	1.83874	-3.11812	-0.5751
O	-0.03803	-1.80684	-2.45899
H	0.56239	-1.62147	-3.20199
H	-0.69626	-2.47064	-2.72902
O	-2.04036	-3.65054	-3.10755
H	-2.46322	-3.47467	-3.94816
H	-2.70205	-3.41304	-2.42971
O	1.87145	-1.24352	-4.41151
H	2.5407	-0.99592	-3.74137
H	1.62242	-0.41894	-4.82969
H	-3.31727	0.08128	-0.92615
H	0.92139	2.55904	-0.82361
H	3.34664	-1.67814	0.16239
C	-4.88137	-0.52174	0.42194
H	-5.13186	-1.43544	0.96181
H	-4.99478	0.29503	1.13514
C	-5.8677	-0.30279	-0.71417
H	-5.78139	-1.10542	-1.44617
H	-5.61339	0.61957	-1.24616
C	-0.22871	4.21539	-0.09081
H	0.13213	4.44888	0.91073
H	-1.28498	4.47929	-0.11075
C	0.53277	5.07729	-1.08519
H	0.18679	4.87693	-2.09992
H	1.59375	4.80699	-1.06877
C	4.75593	-0.0863	0.33736
H	4.90857	0.89751	-0.10865
H	4.85503	0.04993	1.41464
C	5.8503	-1.03891	-0.11786
H	5.82467	-1.16574	-1.19896
H	5.6704	-2.03281	0.30525
Gd	-0.04402	-0.60944	-0.25633
C	-7.34572	-0.19008	-0.29928
O	-8.16702	-0.10428	-1.24313
C	0.45506	6.59693	-0.84777
O	0.98024	7.31095	-1.73517
C	7.28057	-0.63304	0.28649
O	8.20025	-1.32339	-0.21313
O	7.42279	0.32539	1.07823
O	-0.10113	7.00655	0.19586
O	-7.62048	-0.18202	0.92173

Table S9. Cartesian coordinates (Å) obtained after geometry optimization of Gd-PCTA D2 using DFT (Charge = 0 Multiplicity = 8).

O	-1.71171	-3.16143	-0.39864
O	-0.99471	-0.23904	-2.19158
O	1.88847	-0.96072	-2.0042
N	-0.05201	-1.26415	2.01592
N	-2.37498	-0.75658	0.445
N	-0.01357	1.10594	0.04591
N	2.35638	-0.77559	0.58782
C	-1.22608	-1.12036	2.63509
C	-1.31052	-0.86205	3.99288
H	-2.27681	-0.7435	4.46133
C	-0.14209	-0.73637	4.72151
H	-0.17718	-0.5277	5.78181
C	1.07153	-0.8465	4.0689
H	2.00429	-0.7149	4.59807
C	1.07854	-1.10687	2.70842
C	-2.48059	-1.27052	1.81415
H	-2.69764	-2.3375	1.76019
H	-3.3106	-0.80166	2.35066
C	-2.49051	0.70528	0.37044
H	-3.30304	1.07105	1.0076
H	-2.75706	0.96782	-0.65058
C	-1.23491	1.44901	0.79761
H	-1.44808	2.51909	0.73511
H	-1.04181	1.24757	1.84707
C	1.17627	1.43817	0.85053
H	0.93997	1.24254	1.89237
H	1.40692	2.50564	0.79367
C	2.43828	0.68943	0.46461
H	2.69615	0.91771	-0.5667
H	3.24513	1.08401	1.09049
C	2.38821	-1.24472	1.97469
H	2.62825	-2.30765	1.95575
H	3.16805	-0.74042	2.55379
C	-3.34416	-1.42046	-0.44582
C	0.03848	1.73174	-1.29573
C	3.40515	-1.43538	-0.21408
O	1.27665	-3.61813	0.23587
C	2.99678	-1.46654	-1.69609
C	-0.92474	1.0315	-2.28621
C	-2.91916	-2.8773	-0.6843
O	3.75487	-2.0473	-2.49886
O	-1.53284	1.70075	-3.11302
O	-3.72058	-3.678	-1.16904
H	0.6519	-4.32201	0.4977
O	-0.73019	-5.42119	0.69124
O	3.21076	-4.62198	-1.50434
H	3.58635	-3.83776	-1.93555
H	3.94073	-5.04422	-1.05046
H	-1.26701	-4.73011	0.25758
H	-1.06442	-5.48497	1.58618
H	1.89241	-4.03395	-0.39606
O	0.08415	-3.09201	-2.50567
H	0.69583	-3.04429	-3.26137
H	-0.57112	-3.79541	-2.6591
O	-1.90464	-5.02654	-2.83271
H	-2.30435	-5.03749	-3.70252
H	-2.58938	-4.67078	-2.23644

O	2.01884	-2.88775	-4.49919
H	2.68242	-2.50718	-3.89106
H	1.77535	-2.16971	-5.08403
H	-3.22565	-0.93822	-1.41926
H	1.0285	1.49233	-1.69119
H	3.40933	-2.47871	0.09891
C	-4.81182	-1.29288	-0.00868
H	-5.04502	-2.08798	0.70209
H	-4.93159	-0.34158	0.51301
C	-5.77279	-1.33288	-1.18993
H	-5.66216	-2.27633	-1.72386
H	-5.51842	-0.54443	-1.9013
C	-0.13592	3.25468	-1.30661
H	0.2247	3.6675	-0.36302
H	-1.19807	3.48638	-1.38807
C	0.63042	3.89552	-2.45617
H	0.28008	3.48773	-3.40503
H	1.69071	3.64434	-2.38445
C	4.82603	-0.88364	0.00438
H	4.97093	0.00661	-0.61057
H	4.9062	-0.57427	1.04855
C	5.90679	-1.91807	-0.28514
H	5.86634	-2.21735	-1.33235
H	5.72193	-2.82207	0.29804
Gd	0.0352	-1.51831	-0.56972
C	-7.25241	-1.16929	-0.9033
O	-8.05411	-1.09744	-1.82904
C	0.57344	5.40457	-2.59205
O	1.25763	5.97292	-3.43685
C	7.3443	-1.53047	0.00011
O	8.22799	-2.37971	-0.0334
N	-0.24612	6.06719	-1.75768
N	-7.62888	-1.11023	0.38592
N	7.59896	-0.23368	0.25752
H	-6.94113	-1.20885	1.11135
H	-0.81067	5.55466	-1.10385
H	6.83307	0.40896	0.33848
C	8.91364	0.25904	0.59864
H	9.65211	-0.40353	0.15203
H	9.0343	1.25391	0.16836
C	-0.40638	7.50287	-1.758
H	0.44266	7.94065	-2.27839
H	-1.31707	7.78388	-2.29463
C	-8.99996	-0.96334	0.81678
H	-9.57758	-0.56004	-0.01212
H	-9.42164	-1.93667	1.08387
C	-9.07788	-0.0345	2.01105
H	-8.69828	0.95235	1.71944
C	-0.47627	8.02414	-0.33711
H	0.4594	7.77611	0.17874
C	9.13185	0.32925	2.09948
C	10.54147	0.77398	2.43351
H	10.73458	1.7492	1.97587
H	11.26199	0.05125	2.03877
C	-0.66548	9.52661	-0.2993
H	-1.58441	9.79202	-0.8304
H	0.17959	10.01913	-0.78996
C	-10.50056	0.12163	2.50707
H	-10.90056	-0.85911	2.78138
H	-11.12432	0.54744	1.71521

O	10.62414	0.85714	3.84685
H	11.39349	1.37207	4.08638
O	-1.55807	7.3684	0.30399
H	-1.68246	7.79396	1.15519
O	-0.74923	9.89559	1.06708
H	-1.12732	10.77145	1.13268
O	-8.2511	-0.578	3.0272
H	-8.4019	-0.06135	3.82179
O	-10.45085	0.97862	3.63535
H	-11.26889	0.90049	4.12445
H	8.96977	-0.6682	2.52632
O	8.18509	1.2369	2.63506
H	8.44309	1.40329	3.54471

Table S10. Cartesian coordinates (Å) obtained after geometry optimization of Y-PCTA using DFT (Charge = 0 Multiplicity = 1).

O	-1.74952	-3.2099	-0.22784
O	-0.96329	-0.38934	-2.08521
O	1.8139	-1.22682	-1.86607
N	-0.09114	-1.30485	2.09677
N	-2.3494	-0.76782	0.4868
N	0.03749	0.96557	0.09717
N	2.30674	-0.91382	0.69324
C	-1.26317	-1.10586	2.70815
C	-1.35258	-0.8293	4.06215
H	-2.31937	-0.66819	4.51666
C	-0.18966	-0.74024	4.80359
H	-0.22797	-0.51908	5.86126
C	1.0246	-0.9019	4.16326
H	1.9571	-0.79757	4.69886
C	1.03597	-1.1776	2.80639
C	-2.51009	-1.2128	1.87594
H	-2.79527	-2.26486	1.86627
H	-3.32447	-0.66981	2.36596
C	-2.44723	0.69112	0.34739
H	-3.2888	1.08488	0.92854
H	-2.65652	0.91305	-0.69564
C	-1.18625	1.40716	0.79423
H	-1.33356	2.4844	0.65884
H	-1.04174	1.24953	1.86012
C	1.21422	1.3433	0.90103
H	0.96847	1.20221	1.9508
H	1.4428	2.40785	0.77897
C	2.45458	0.54738	0.55341
H	2.73408	0.74451	-0.4794
H	3.28224	0.90327	1.17767
C	2.34245	-1.36341	2.08513
H	2.55445	-2.43196	2.08289
H	3.14231	-0.87031	2.64689
C	-3.33459	-1.45093	-0.35071
C	0.11249	1.56264	-1.24345
C	3.35509	-1.56616	-0.09395
O	1.14368	-3.63622	0.38519
C	2.94556	-1.68235	-1.55742
C	-0.73784	0.84726	-2.2965
C	-2.94357	-2.9076	-0.56149

O	3.71865	-2.26739	-2.34045
O	-1.10947	1.48482	-3.27772
O	-3.75106	-3.69093	-1.06186
H	0.53372	-4.3335	0.69825
O	-0.81793	-5.43815	0.97066
O	3.05159	-4.7915	-1.25607
H	3.48347	-4.0555	-1.71737
H	3.74645	-5.24601	-0.77875
H	-1.36059	-4.77089	0.50879
H	-1.14536	-5.46331	1.87017
H	1.77646	-4.08606	-0.20809
O	-0.02014	-3.19957	-2.30371
H	0.62027	-3.20164	-3.0369
H	-0.65029	-3.93243	-2.42131
O	-1.94563	-5.20101	-2.56276
H	-2.31177	-5.28723	-3.4431
H	-2.64823	-4.78818	-2.02522
O	1.95232	-3.20008	-4.28419
H	2.62948	-2.79361	-3.70887
H	1.73937	-2.52964	-4.93387
H	-3.34582	-0.98378	-1.33502
H	1.13804	1.48806	-1.60602
H	3.51858	-2.57644	0.27533
H	4.31563	-1.04603	-0.02485
H	-0.15049	2.62406	-1.22011
H	-4.34861	-1.39717	0.05721
Y	-0.00738	-1.63926	-0.44668

Table S11. Cartesian coordinates (Å) obtained after geometry optimization of Y-PCTA-D1 using DFT (Charge = -3 Multiplicity = 1).

O	-1.73147	-2.23107	-0.33404
O	-1.07162	0.91086	-1.55444
O	1.72972	0.16103	-1.5674
N	-0.08501	-0.85519	2.2978
N	-2.4119	-0.0539	0.90351
N	-0.07366	1.82501	0.83011
N	2.2807	-0.1038	0.9597
C	-1.2465	-0.85009	2.96065
C	-1.30631	-0.90161	4.34327
H	-2.26491	-0.88853	4.84145
C	-0.12697	-0.94384	5.06256
H	-0.14314	-0.97771	6.14319
C	1.07332	-0.90448	4.37903
H	2.01626	-0.89285	4.90635
C	1.05659	-0.8543	2.99485
C	-2.51706	-0.80594	2.1574
H	-2.77743	-1.8378	1.92036
H	-3.32201	-0.41734	2.78817
C	-2.53934	1.39541	1.10761
H	-3.35172	1.62863	1.80459
H	-2.81199	1.84603	0.1561
C	-1.27841	2.03708	1.65612
H	-1.47556	3.10198	1.80296
H	-1.07629	1.63437	2.64543
C	1.1268	2.01867	1.66489
H	0.91233	1.6295	2.65702

H	1.34912	3.08056	1.80438
C	2.37622	1.35933	1.11964
H	2.61518	1.7807	0.14601
H	3.20255	1.62054	1.78842
C	2.35439	-0.8183	2.23435
H	2.6243	-1.8524	2.02093
H	3.13283	-0.40835	2.88544
C	-3.39995	-0.5486	-0.07725
C	-0.04683	2.71146	-0.36662
C	3.32838	-0.59249	0.03453
O	1.14974	-2.74077	0.12355
C	2.86598	-0.35682	-1.40706
C	-1.00988	2.18151	-1.45322
C	-2.95254	-1.93196	-0.56128
O	3.59362	-0.75096	-2.34139
O	-1.62337	2.96873	-2.16709
O	-3.73414	-2.66899	-1.16464
H	0.55189	-3.49262	0.30089
O	-0.79441	-4.64721	0.38786
O	3.04356	-3.45996	-1.79534
H	3.42589	-2.61735	-2.09045
H	3.77134	-3.95727	-1.42055
H	-1.33315	-3.89444	0.07436
H	-1.10214	-4.83592	1.27476
H	1.75428	-3.04264	-0.58077
O	-0.04152	-1.75713	-2.38667
H	0.54684	-1.55587	-3.13546
H	-0.66623	-2.45809	-2.64286
O	-1.93577	-3.71368	-3.01811
H	-2.34306	-3.61069	-3.87831
H	-2.62333	-3.46306	-2.37123
O	1.80665	-1.18988	-4.39884
H	2.49151	-0.93537	-3.74705
H	1.54682	-0.37081	-4.82135
H	-3.28824	0.09662	-0.95264
H	0.93898	2.55804	-0.81333
H	3.34432	-1.67637	0.14771
C	-4.86325	-0.50425	0.38385
H	-5.11189	-1.40815	0.94096
H	-4.9893	0.32664	1.07848
C	-5.8423	-0.31813	-0.76441
H	-5.74535	-1.13639	-1.47777
H	-5.59126	0.59369	-1.31561
C	-0.22263	4.20627	-0.08641
H	0.12978	4.44415	0.91714
H	-1.28025	4.46586	-0.11383
C	0.54171	5.0723	-1.07548
H	0.20861	4.86549	-2.09324
H	1.6047	4.8103	-1.04693
C	4.75055	-0.08622	0.32476
H	4.90024	0.903	-0.11002
H	4.85913	0.03616	1.40288
C	5.84104	-1.03287	-0.15246
H	5.80593	-1.14444	-1.23512
H	5.66401	-2.0329	0.25738
Y	-0.04602	-0.60761	-0.24453
C	-7.32442	-0.20837	-0.36337
O	-8.13797	-0.13353	-1.31494
C	0.45097	6.59204	-0.84478
O	0.97206	7.3072	-1.73406

C	7.27495	-0.63357	0.24499
O	8.18974	-1.32304	-0.26501
O	7.42534	0.31964	1.04161
O	-0.11006	7.00213	0.19626
O	-7.61014	-0.19279	0.85509

Table S12. Cartesian coordinates (Å) obtained after geometry optimization of Y-PCTA-D2 using DFT (Charge = 0 Multiplicity = 1).

O	-1.7146	-3.23734	-0.29577
O	-0.94982	-0.43635	-2.09034
O	1.82785	-1.16604	-1.88852
N	-0.08652	-1.42532	2.04232
N	-2.35799	-0.83441	0.45105
N	0.05062	0.9191	0.0995
N	2.34016	-1.00514	0.65729
C	-1.26718	-1.25091	2.65963
C	-1.36261	-1.01374	4.02672
H	-2.335	-0.87167	4.48408
C	-0.19771	-0.9393	4.77812
H	-0.24071	-0.74893	5.84488
C	1.02424	-1.07595	4.13422
H	1.95739	-0.98321	4.67798
C	1.04193	-1.31292	2.76352
C	-2.51934	-1.33845	1.82314
H	-2.79501	-2.39516	1.77158
H	-3.33503	-0.8221	2.34654
C	-2.44306	0.63462	0.37818
H	-3.26163	1.02043	1.00293
H	-2.68151	0.91158	-0.65006
C	-1.16716	1.32771	0.83544
H	-1.32674	2.41159	0.77757
H	-1.00422	1.10738	1.89104
C	1.2411	1.24581	0.91503
H	0.99385	1.05608	1.96042
H	1.49179	2.31311	0.85645
C	2.48612	0.46092	0.53923
H	2.75982	0.68266	-0.49349
H	3.30699	0.82383	1.17361
C	2.36164	-1.47165	2.04896
H	2.5904	-2.54031	2.03543
H	3.14473	-0.97224	2.63601
C	-3.32526	-1.48074	-0.46084
C	0.12859	1.5345	-1.25443
C	3.37358	-1.69868	-0.14295
O	1.16022	-3.6784	0.34758
C	2.93805	-1.70635	-1.61569
C	-0.8513	0.83436	-2.22983
C	-2.91075	-2.94663	-0.65644
O	3.65777	-2.30636	-2.4499
O	-1.4464	1.50168	-3.0775
O	-3.69339	-3.75589	-1.16995
H	0.5356	-4.32778	0.74447
O	-0.83102	-5.24433	1.25268
O	2.91987	-4.83447	-1.40606
H	3.31604	-4.08591	-1.88711
H	3.64398	-5.22422	-0.90668

H	-1.36253	-4.67744	0.65651
H	-1.07755	-4.96707	2.14072
H	1.6941	-4.16692	-0.31776
O	0.05663	-3.21787	-2.32151
H	0.62303	-3.12665	-3.11777
H	-0.57134	-3.96486	-2.4302
O	-1.78423	-5.22772	-2.57119
H	-2.13339	-5.2202	-3.46739
H	-2.50098	-4.84709	-2.02206
O	1.77186	-2.82065	-4.40724
H	2.52046	-2.6023	-3.80998
H	1.46359	-1.95922	-4.70605
H	-3.16501	-1.00981	-1.43802
H	1.11871	1.26408	-1.63989
H	3.34132	-2.74796	0.16222
C	-4.8039	-1.31944	-0.06567
H	-5.05746	-2.05824	0.7032
H	-4.93272	-0.32559	0.37782
C	-5.74414	-1.45561	-1.26244
H	-5.64119	-2.45471	-1.6939
H	-5.45336	-0.7484	-2.04708
C	-0.01571	3.06271	-1.29569
H	0.3903	3.50136	-0.37757
H	-1.08045	3.31175	-1.34663
C	0.71254	3.65958	-2.49872
H	0.28362	3.2474	-3.41716
H	1.76812	3.36658	-2.48587
C	4.81714	-1.20096	0.06958
H	4.98055	-0.28436	-0.50831
H	4.93261	-0.94421	1.12908
C	5.85738	-2.25726	-0.30141
H	5.76992	-2.50393	-1.36291
H	5.65777	-3.1856	0.24484
Y	0.02126	-1.69423	-0.49375
C	-7.22728	-1.22162	-1.02335
O	-8.00982	-1.17979	-1.97202
C	0.70555	5.17269	-2.64638
O	1.41886	5.72162	-3.48576
C	7.31786	-1.92891	-0.03502
O	8.18021	-2.7988	-0.15191
N	-0.12022	5.86437	-1.82868
N	-7.63047	-1.08001	0.2604
N	7.61081	-0.65649	0.31657
H	-6.95933	-1.10137	1.01234
H	-0.69456	5.38124	-1.15536
H	6.88135	0.03453	0.39919
C	8.95221	-0.2066	0.62118
H	9.57848	-1.08937	0.76306
H	9.35955	0.37433	-0.21613
C	-0.21988	7.30786	-1.83418
H	0.63427	7.7029	-2.38734
H	-1.13786	7.62599	-2.34479
C	-9.00008	-0.80521	0.63836
H	-9.56	-0.5826	-0.27167
H	-9.4472	-1.6875	1.1133
C	-9.05124	0.36711	1.60396
H	-8.66123	1.26322	1.09541
C	-0.22789	7.83236	-0.40824
H	0.72852	7.57067	0.07194
C	8.93953	0.65384	1.87323

C	10.31307	1.2168	2.20347
H	10.69648	1.76788	1.33467
H	11.01305	0.40352	2.43794
C	-0.40413	9.34143	-0.34567
H	-1.31989	9.62141	-0.88291
H	0.44785	9.84559	-0.8215
C	-10.46303	0.66018	2.08708
H	-10.88921	-0.2486	2.5325
H	-11.09867	0.9679	1.24585
O	10.1242	2.08007	3.31347
H	10.8531	2.70459	3.34497
O	-1.29937	7.19966	0.26899
H	-1.41261	7.69541	1.08973
O	-0.50059	9.66602	1.03208
H	-0.93644	10.51752	1.11739
O	-8.22852	0.04009	2.70987
H	-8.44341	0.69051	3.39035
O	-10.33755	1.69229	3.05246
H	-11.11871	1.68808	3.61107
H	8.5978	0.04092	2.72254
O	8.03174	1.71742	1.6465
H	8.20165	2.35384	2.35255

Appendix A. Supplementary data

Tables S1 presents the structure of the GBCA and PCTA ligands.

Fig. S1 displays TDA setup with UV and LEDIF detectors

Fig. S2. Emission spectra (excitation wavelength 275 nm) of Gd-PCTA, Gd-PCTA D1 and Gd-PCTA D2 at a concentration of 5.0 mM.

Fig. S3 to S10 present the taylorgrams obtained for Gd-DTPA-BMA, Gd-BOPTA, Gd-HP-DO3A, Gd-BT-DO3A, Gd-DOTA, Gd-PCTA, Gd-PCTA D1, Gd-PCTA D2 and Gd-PCTA D3, respectively.

Fig. S11 shows linear regression lines obtained for GBCA calibration curves in UV 200 nm and LEDIF (λ_{ex} 275 nm, $\lambda_{\text{collection}}$ 300-450 nm).

Tables S2-S12 show optimized geometries obtained with DFT.