Electronic Supplementary Information (ESI)

for

Scrutinising the role of intramolecular hydrogen bonding in water exchange dynamics of Gd(III) complexes

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ESI Summary

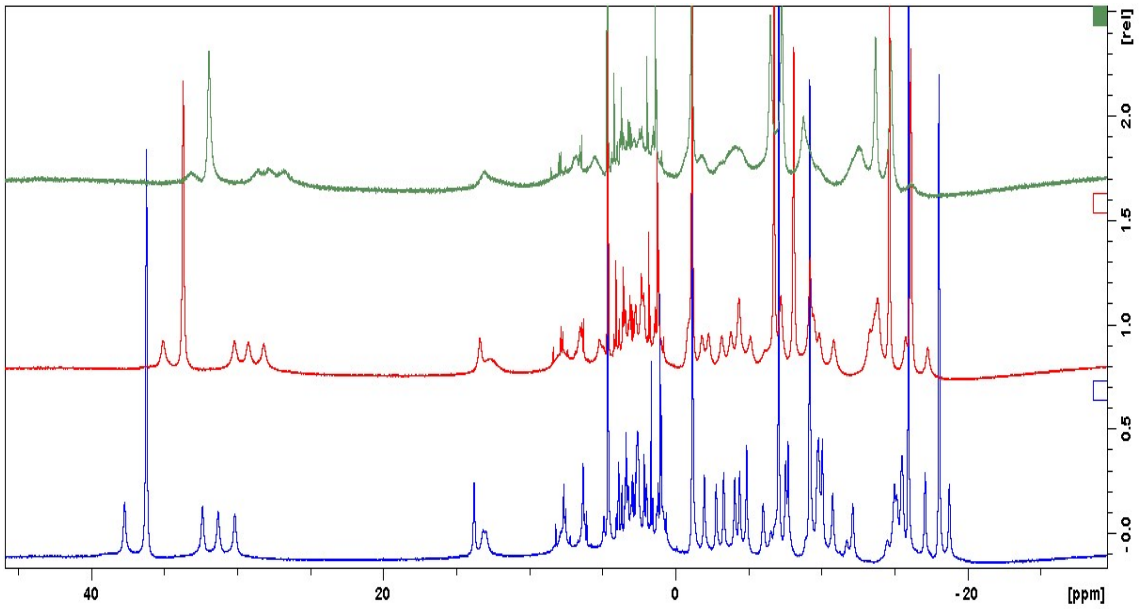


Figure S1. ^{1}H NMR spectra at 310 K (top), 298K (middle) and 278 K (bottom) for EuDO3A-DiHAP (D_2O, pH 7).

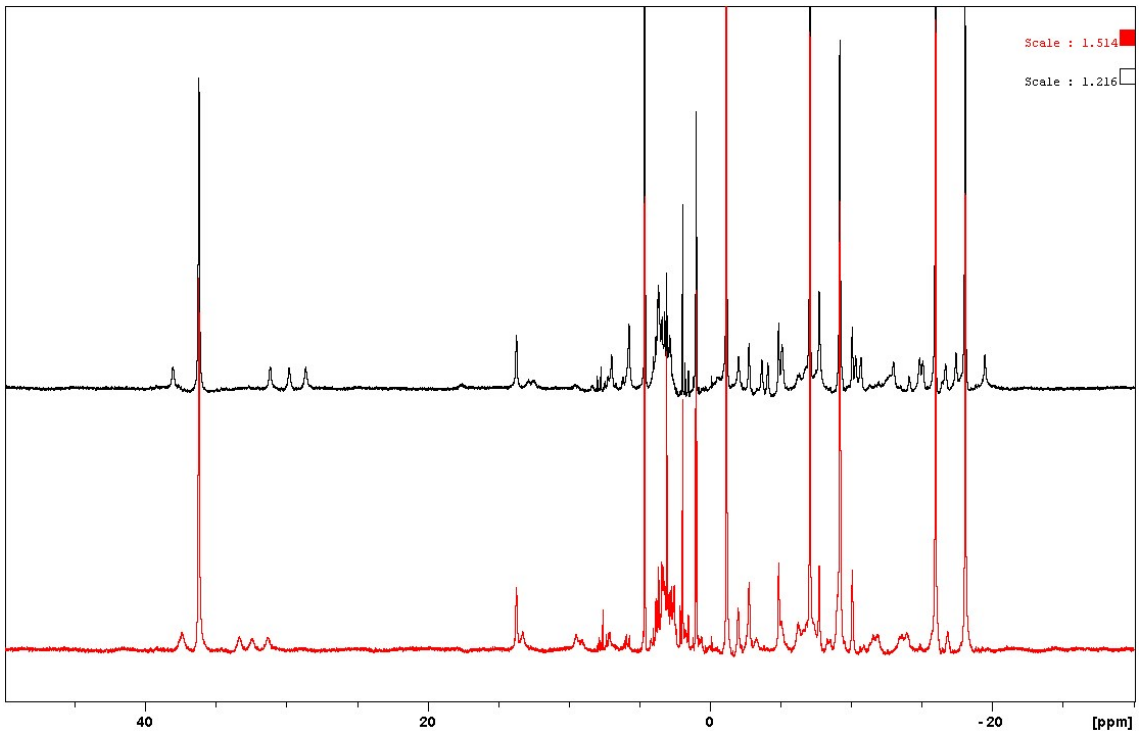


Figure S2. ^{1}H NMR spectra at 283 K for EuDO3A-DiHAP (D_2O) at pH 4 (top) and pH 9 (bottom).

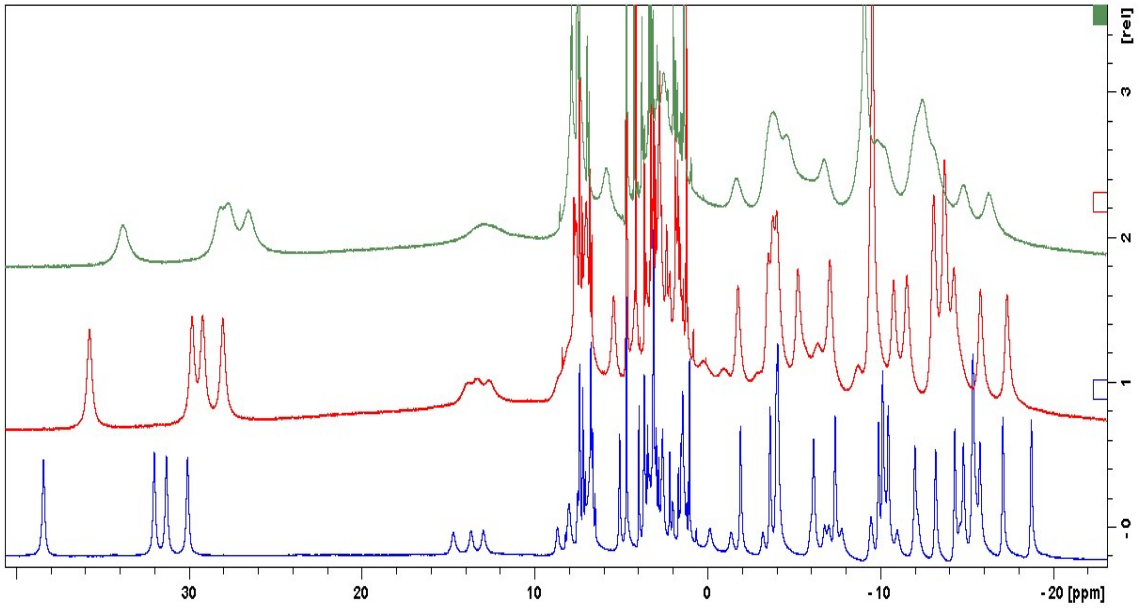


Figure S3. ^{1}H NMR spectra at 310 K (top), 298K (middle) and 278 K (bottom) for EuDO3A-AnAP (D_2O, pH 7).

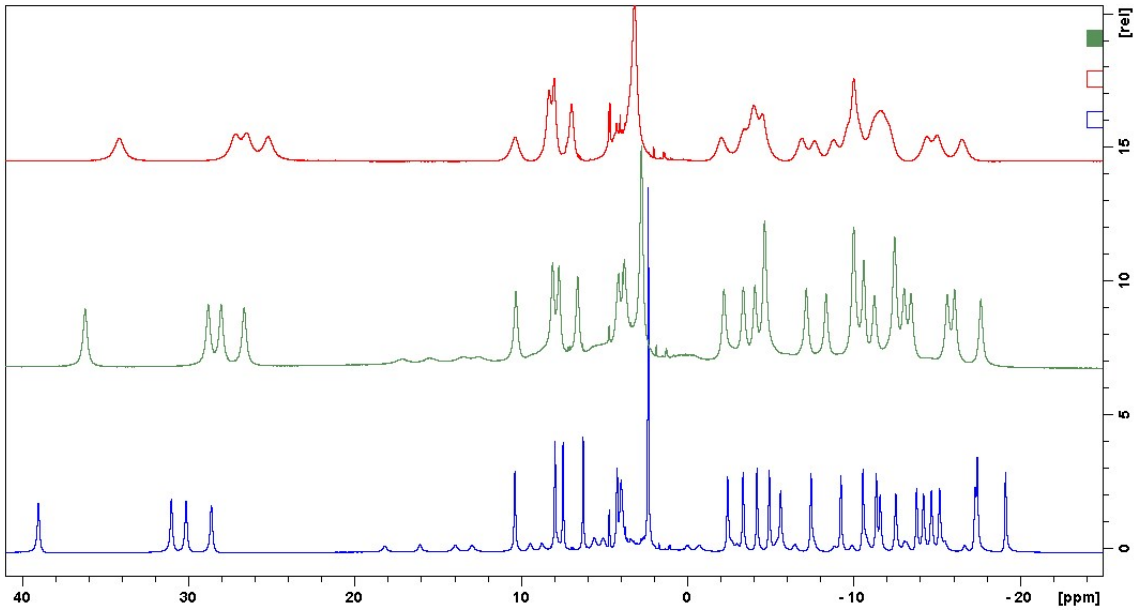


Figure S4. ^{1}H NMR spectra at 310 K (top), 298K (middle) and 278 K (bottom) for EuDO3A-*o*MAP (D_2O, pH 7).

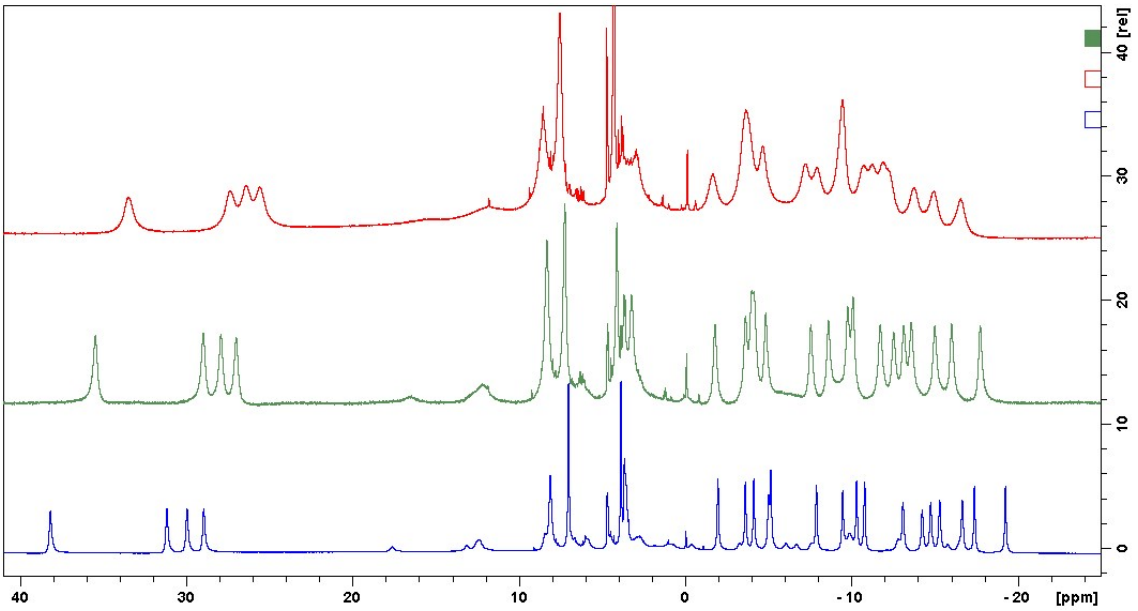


Figure S5. ^{1}H NMR spectra at 310 K (top), 298K (middle) and 278 K (bottom) for EuDO3A-*p*MAP (D_2O, pH 7).

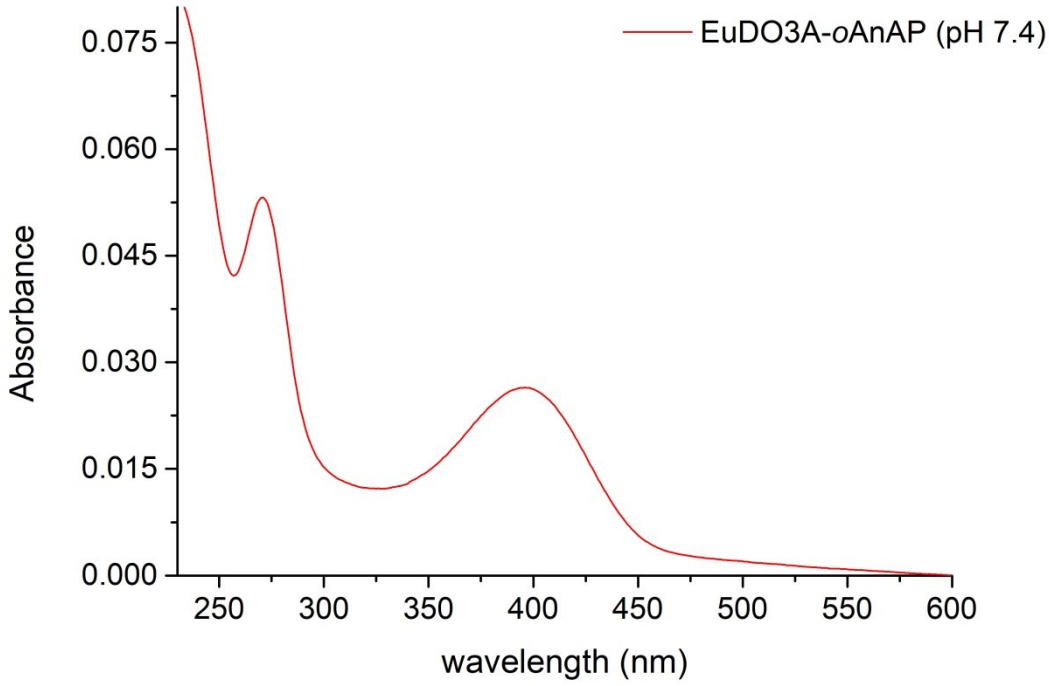


Figure S6. Absorption spectrum of the EuDO3A-oAnAP complex recorded in aqueous solution (10^{-4} M, d = 0.1 cm).

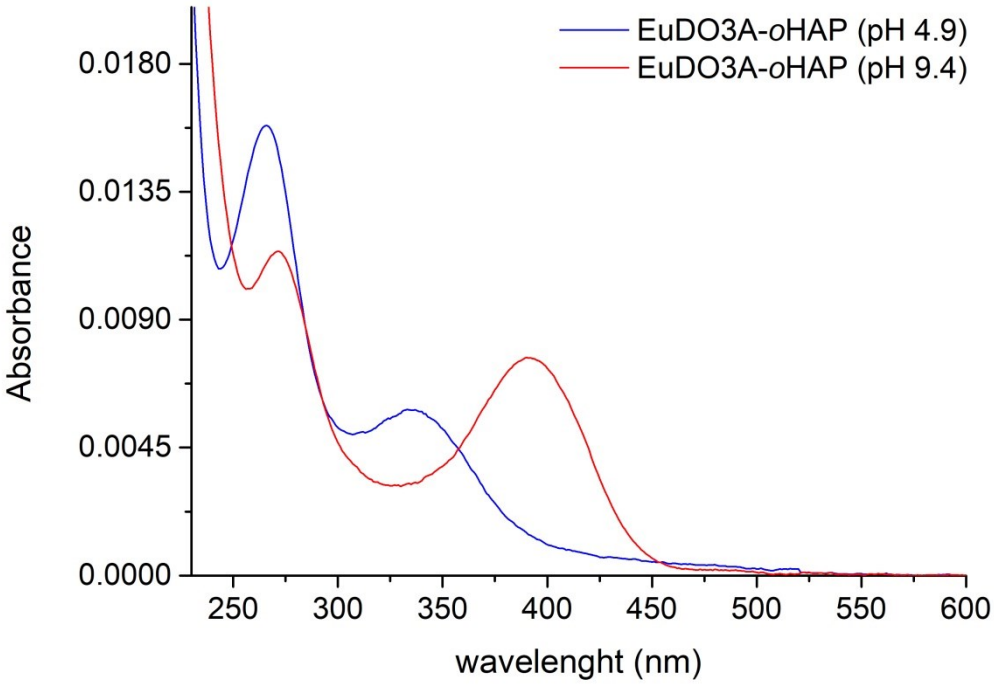


Figure S7. Absorption spectra of the EuDO3A-oHAP complex recorded in aqueous solution at different pH values (10^{-4} M, d = 0.1 cm).

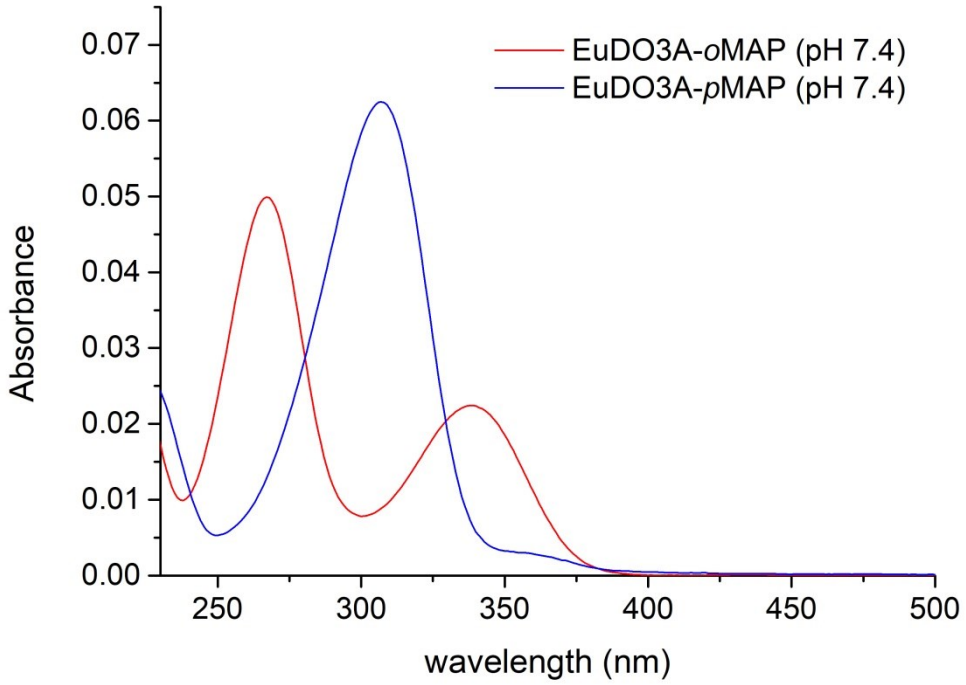


Figure S8. Absorption spectra of the EuDO3A-*o*MAP and EuDO3A-*p*MAP complexes recorded in aqueous solution at different pH values (10^{-4} M, $d = 0.1$ cm).

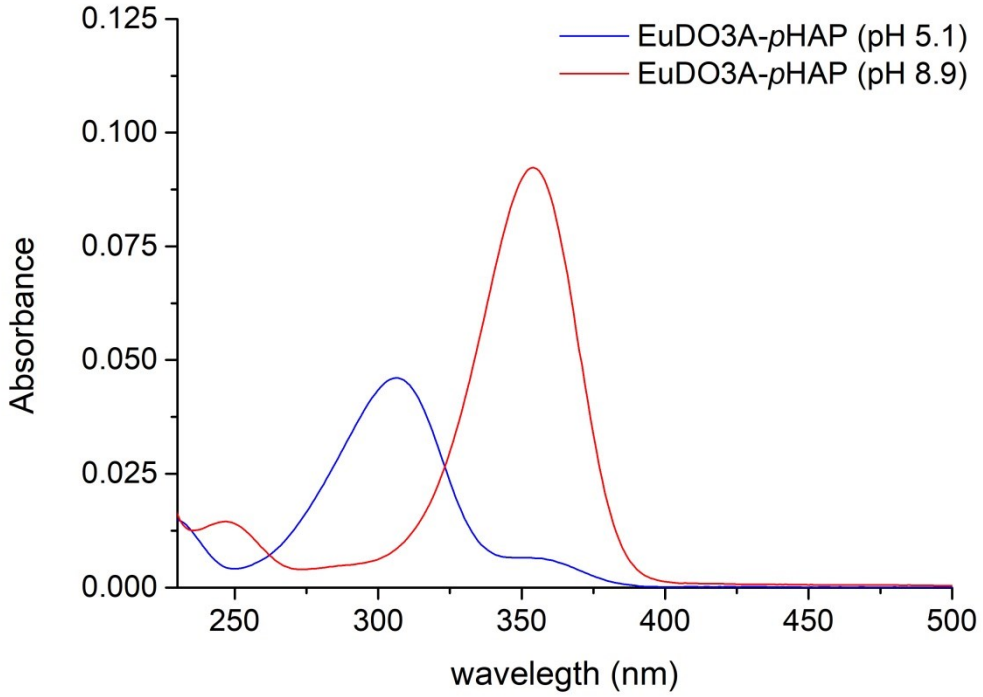


Figure S9. Absorption spectra of the EuDO3A-*p*HAP complex recorded in aqueous solution at different pH values (10^{-4} M, d = 0.1 cm).

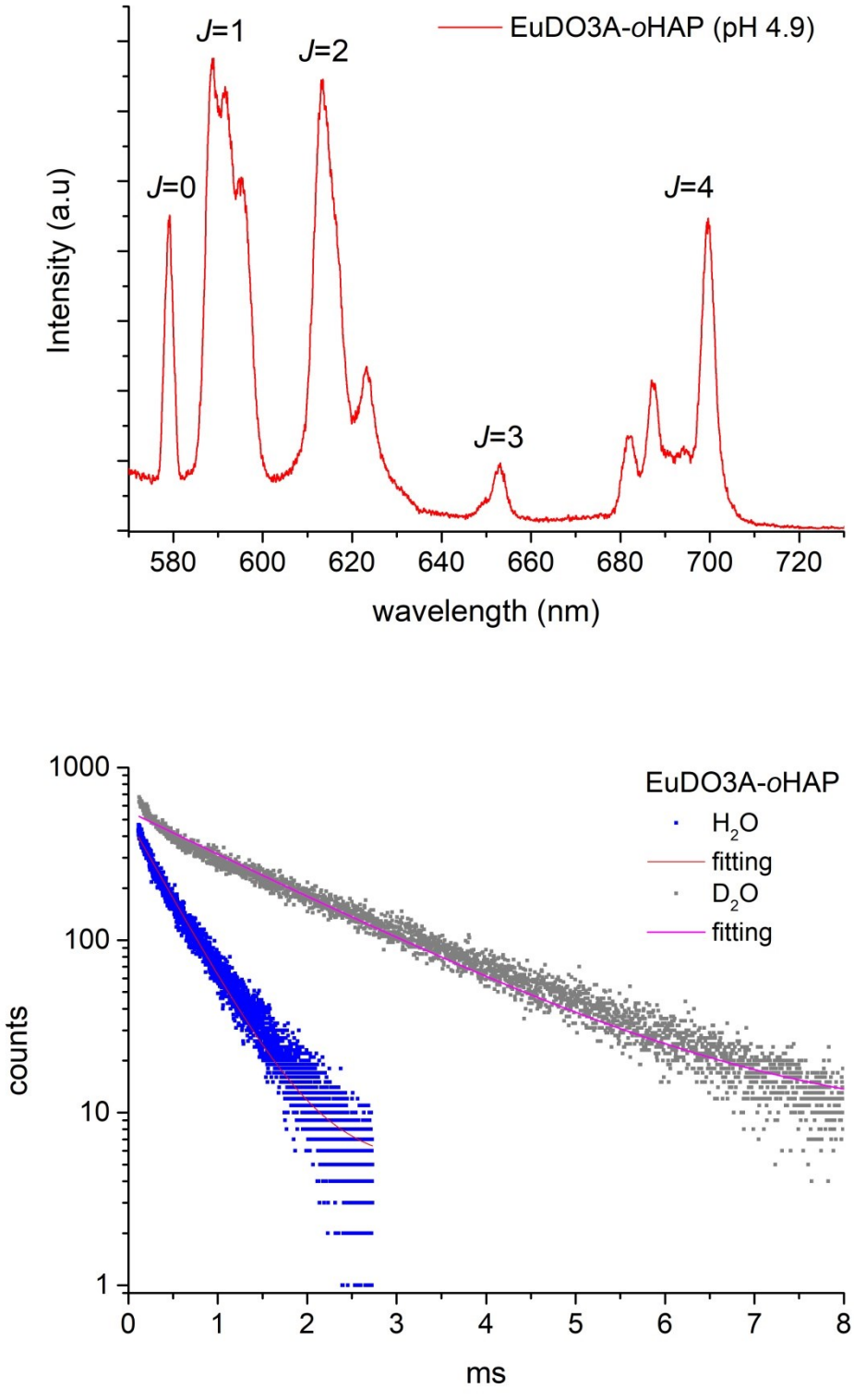


Figure S10. Emission spectrum (top) and decay curves (bottom) of the EuDO3A-*o*HAP complex (10^{-4} M, pH 4.9, λ_{exc} = 350 nm, bandpass = 2 nm, λ_{em} = 613 nm). The distortion of the baseline in the emission spectrum is due to residual ligand emission.

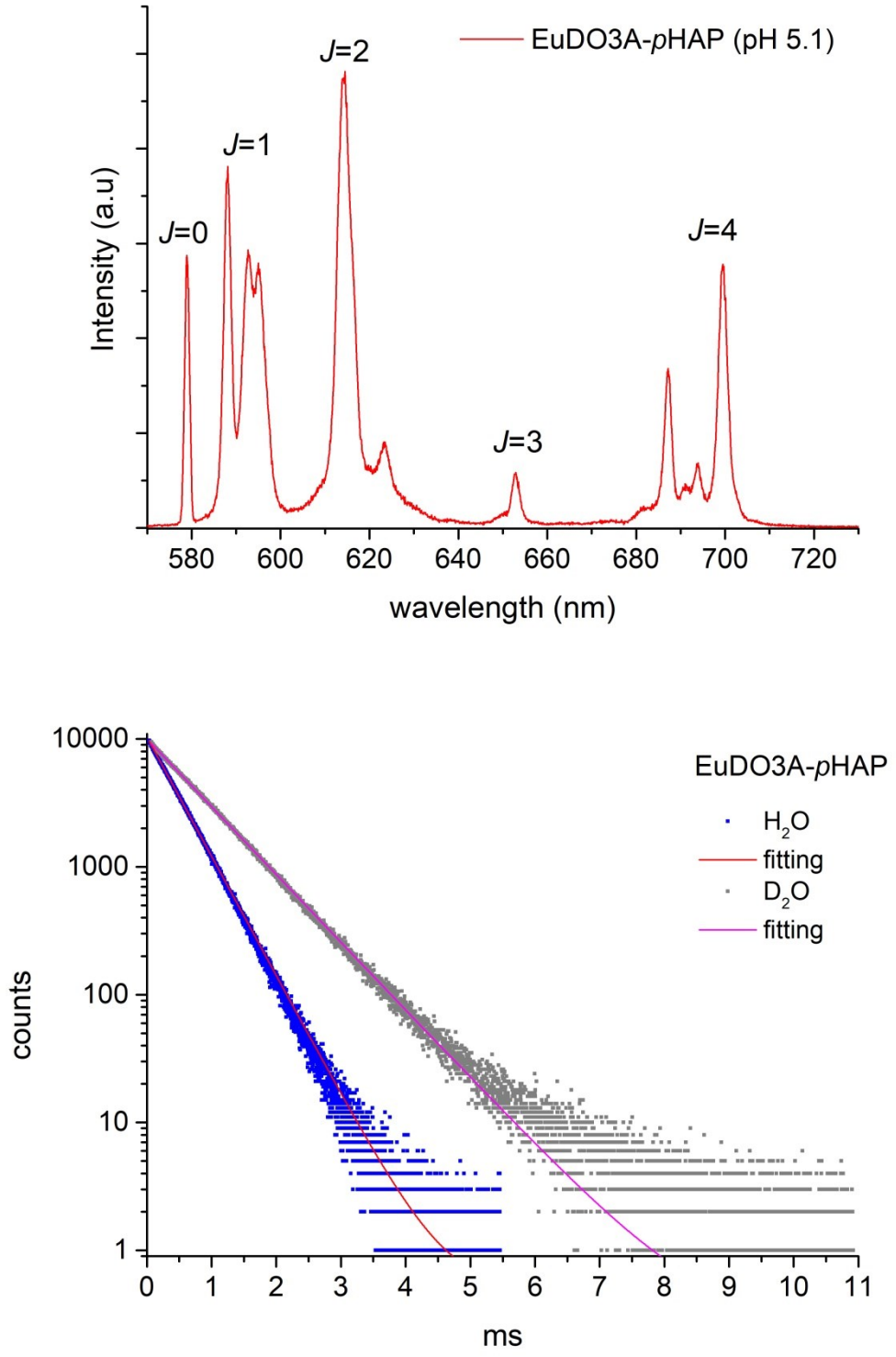


Figure S11. Emission spectrum (top) and decay curves (bottom) of the EuDO3A-*o*HAP complex (10^{-4} M, pH 5.1, λ_{exc} = 314 nm, bandpass = 1 nm, λ_{em} = 613 nm).

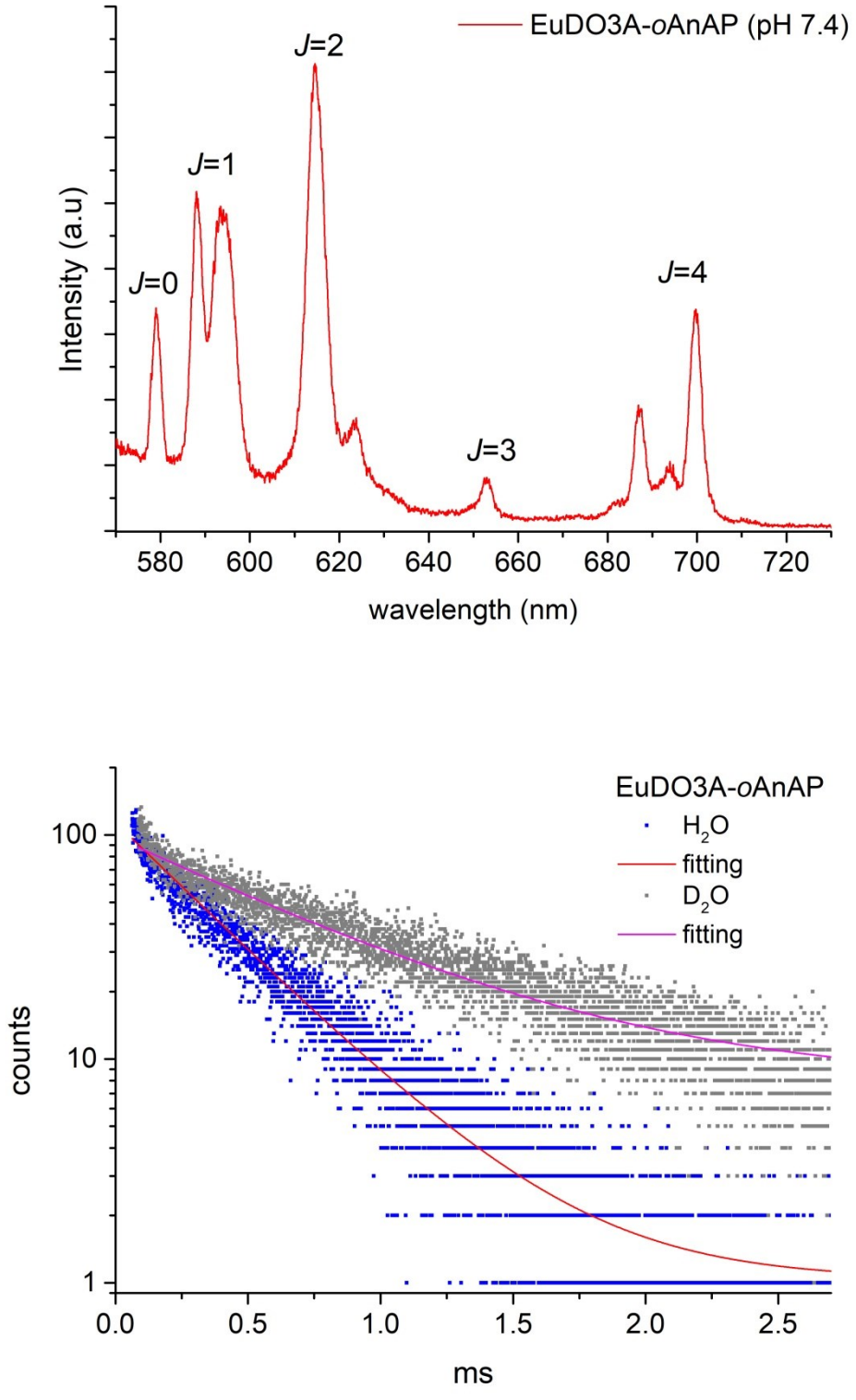


Figure S12. Emission spectrum (top) and decay curves (bottom) of the EuDO3A-*o*AnAP complex (10^{-4} M, pH 7.4, λ_{exc} = 400 nm, bandpass = 2 nm, λ_{em} = 613 nm). The distortion of the baseline in the emission spectrum is due to residual ligand emission.

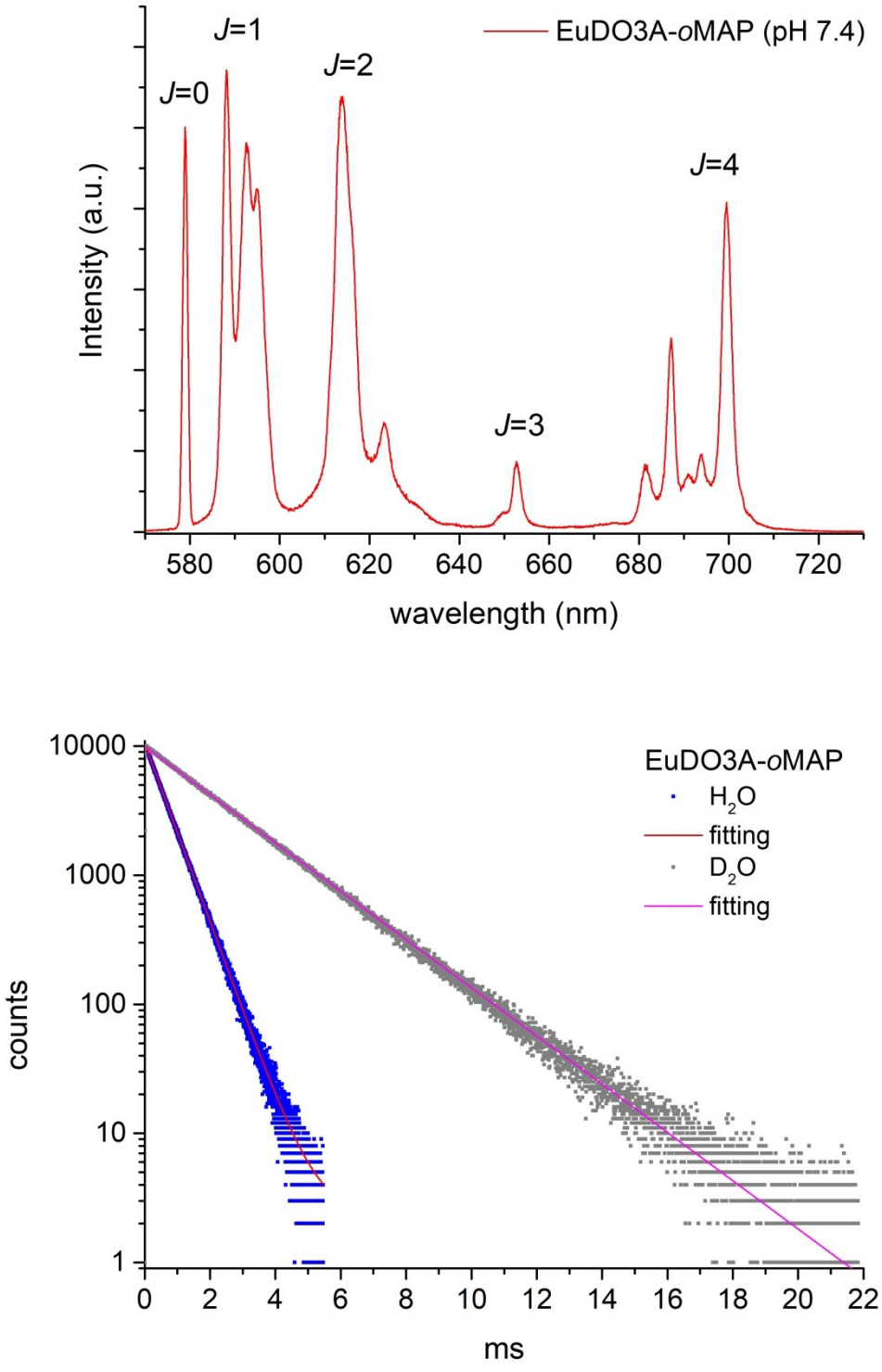


Figure S13. Emission spectrum (top) and decay curves (bottom) of the EuDO3A-*o*MAP complex (10^{-4} M, pH 7.4, λ_{exc} = 350 nm, bandpass = 1 nm, λ_{em} = 613 nm).

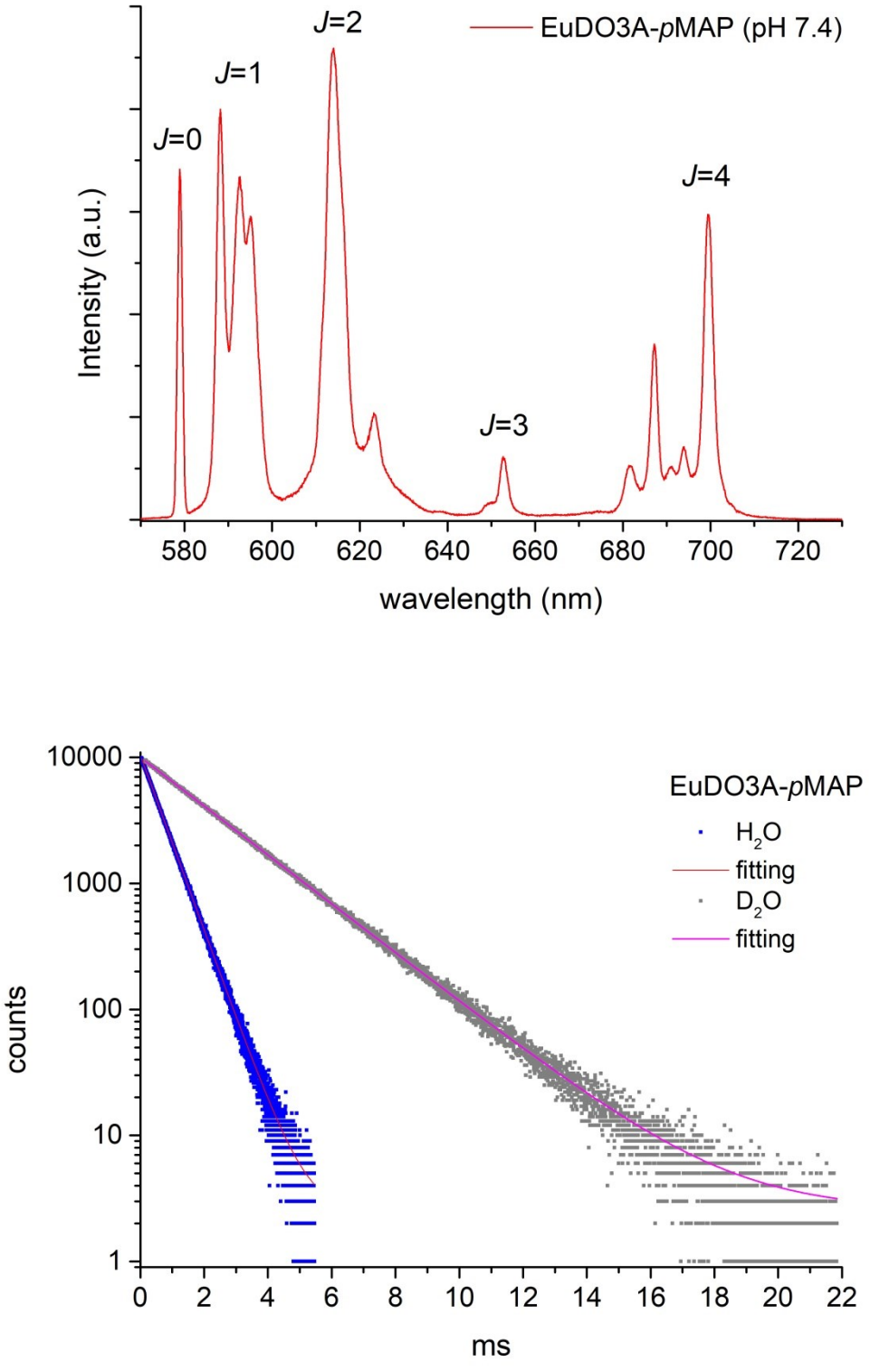


Figure S14. Emission spectrum (top) and decay curves (bottom) of the EuDO3A-*p*MAP complex (10^{-4} M, pH 7.4, λ_{exc} = 312 nm, bandpass = 1 nm, λ_{em} = 613 nm).

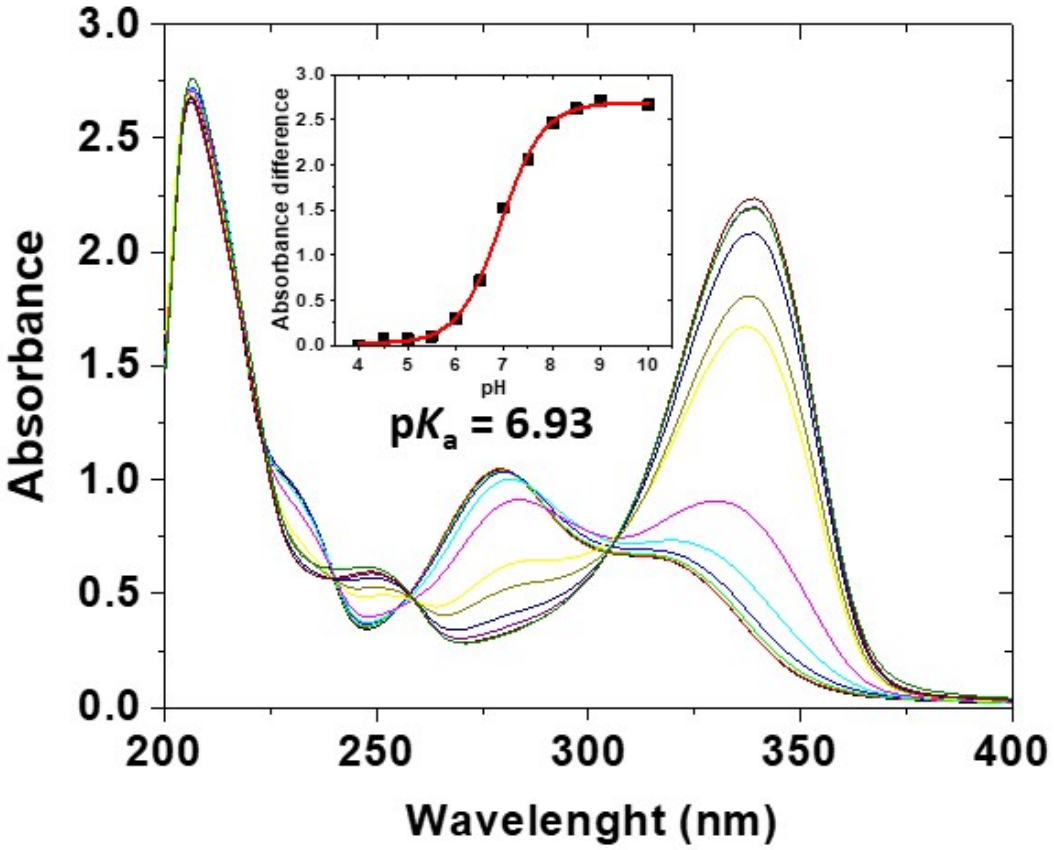


Figure S15. UV spectra (λ = 200−400 nm) of DO3A-DiHAP (4×10^{-4} M) in different aqueous solutions ranging from pH 4.1 to 10.2 (0.1 M NaCl, 298 K). The absorbances are normalized to zero for λ = 600 nm. Insert: plot of the total absorbance difference vs pH to determine the pK_a. The total absorbance difference is the sum of the absolute absorbance difference values at the chosen wavelengths (i.e. 280 and 340 nm).

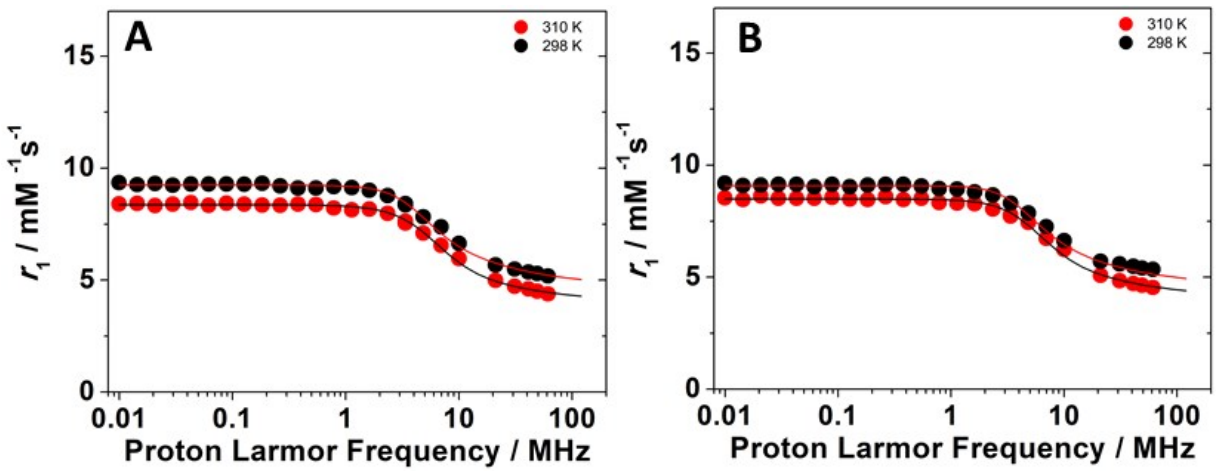


Figure S16. ^{1}H NMRD profiles recorded at 298 (black) and 310 K (red) for (A) GdDO3A-oMAP at pH 7.4 and (B) GdDO3A-pMAP at pH 7.4.

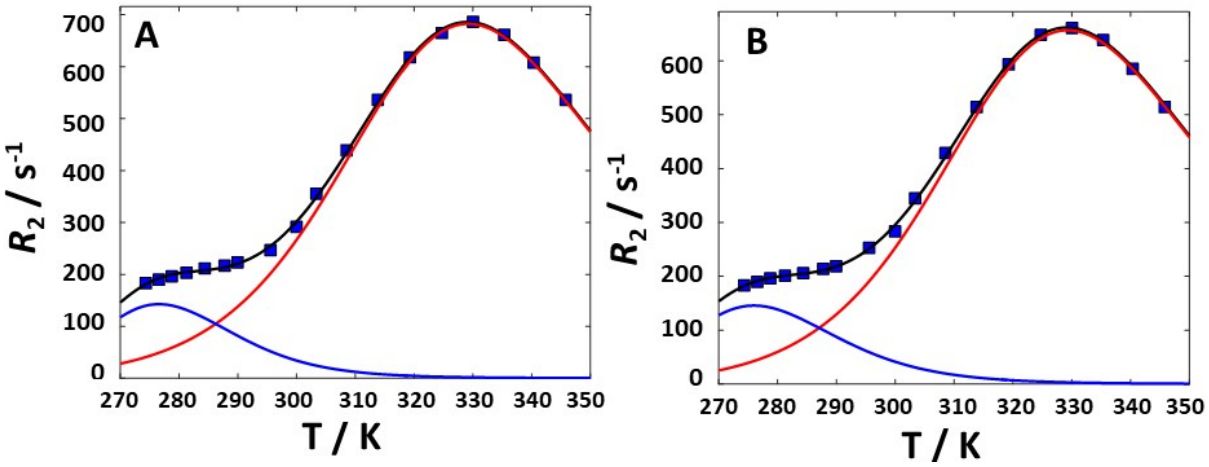
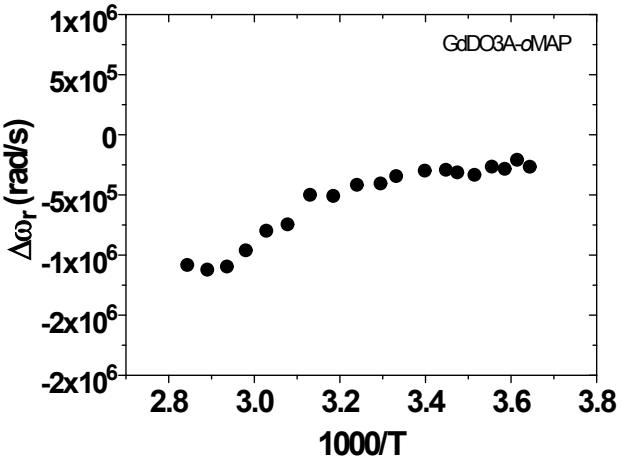


Figure S17. Transverse ^{17}O NMR relaxation rates measured at 11.74 T and pH 7.4 for: (A) GdDO3A-*o*MAP (18.4 mM) and (B) GdDO3A-*p*MAP (19.2 mM). The red and blue lines represent the calculated contributions of the isomeric species SAP and TSAP, respectively.

A



B

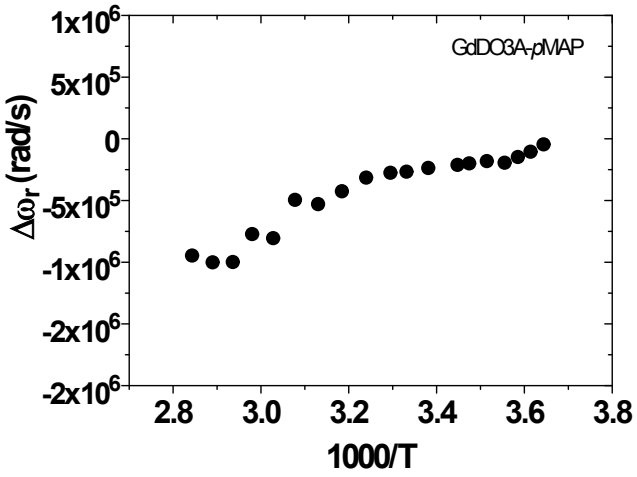
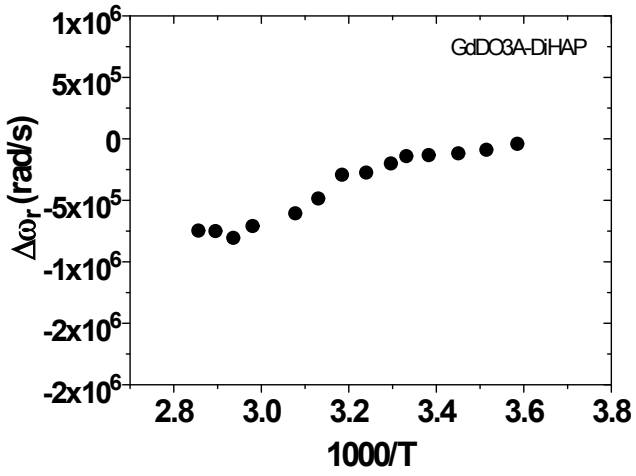


Figure S18. Reduced transverse ^{17}O chemical shifts measured at 11.74 T (pH 7) for GdDO3A-*o*MAP (A) and GdDO3A-*p*MAP (B).

A



B

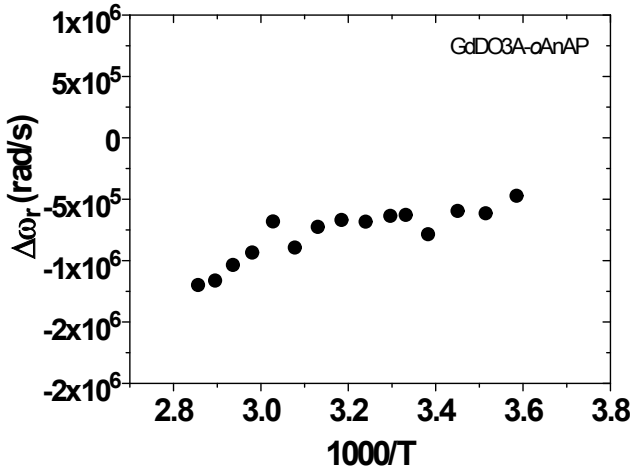


Figure S19. Reduced transverse ^{17}O chemical shifts measured at 11.74 T (pH 7) for GdDO3A-DiHAP (A) and GdDO3A-oAnAP (B).

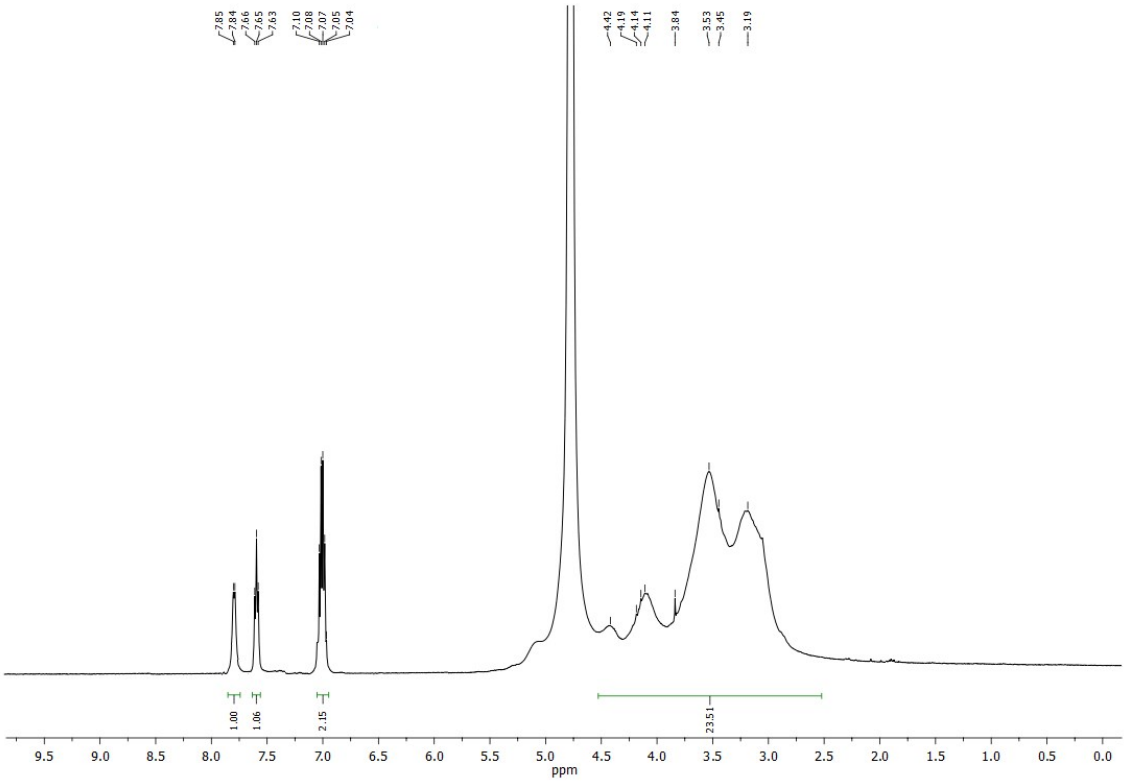


Figure S20a. ^{1}H NMR spectrum of **DO3A-oAnAP**

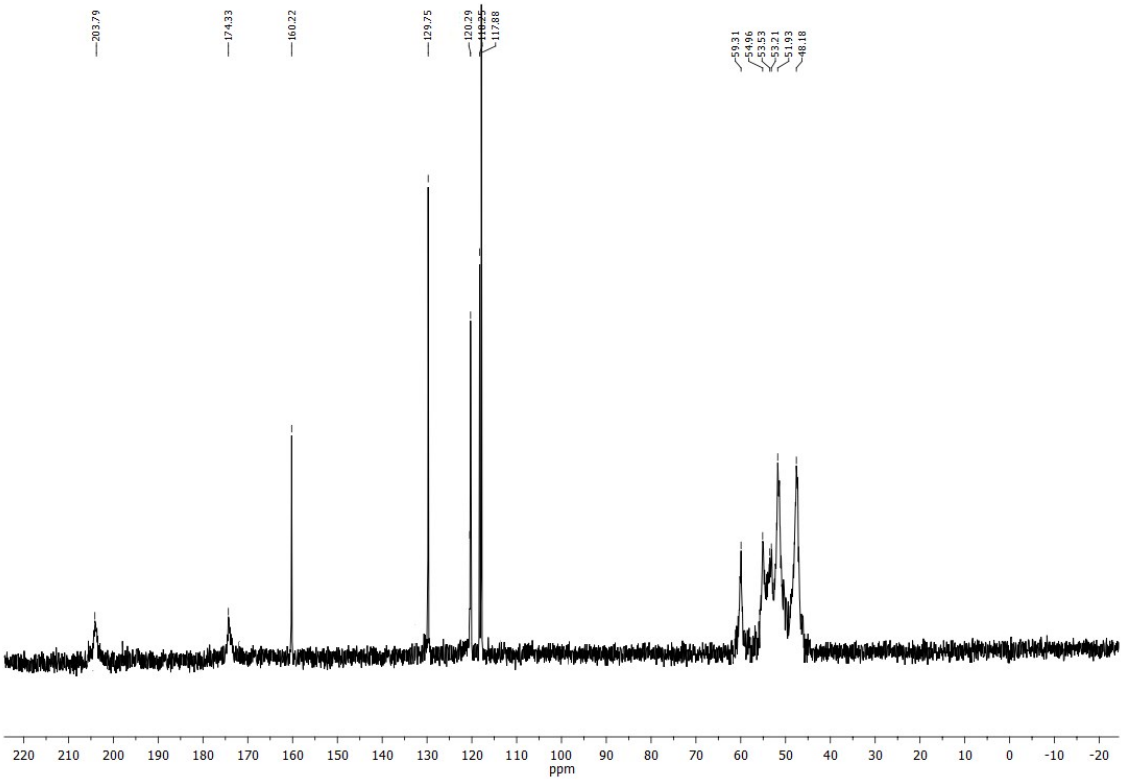


Figure S20b. ^{13}C NMR spectrum of **DO3A-oAnAP**

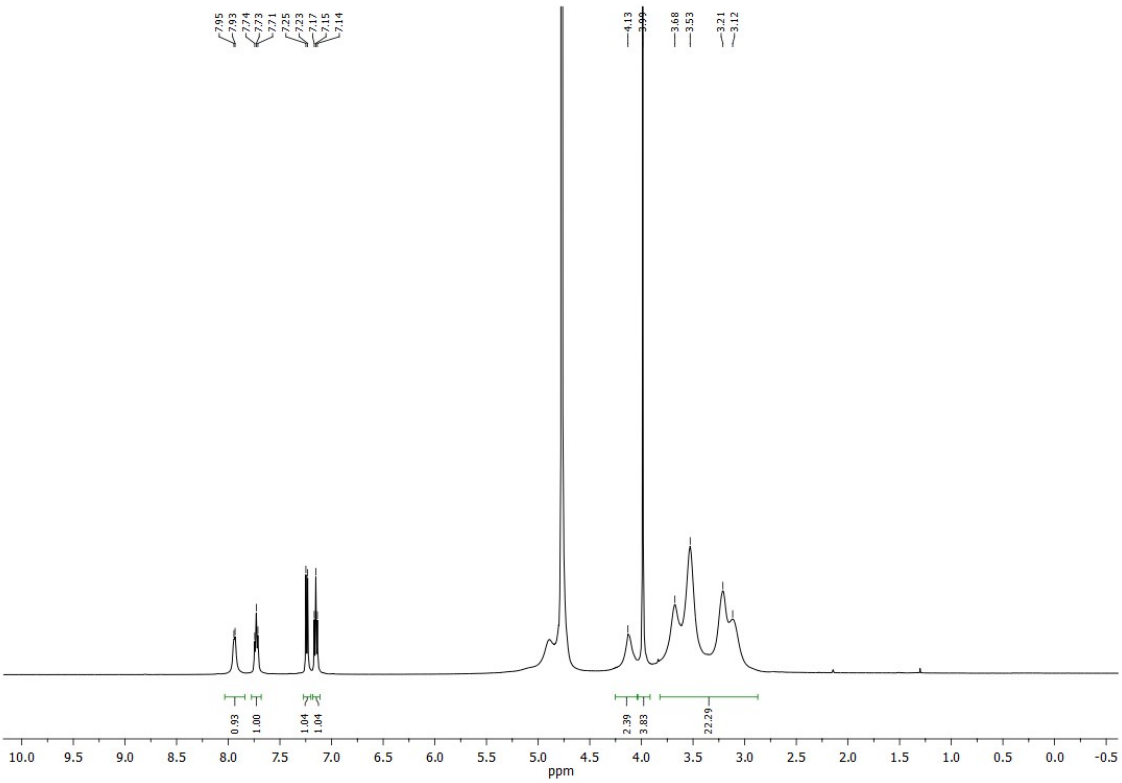


Figure S21a. ^{1}H NMR spectrum of **DO3A-oMAP**

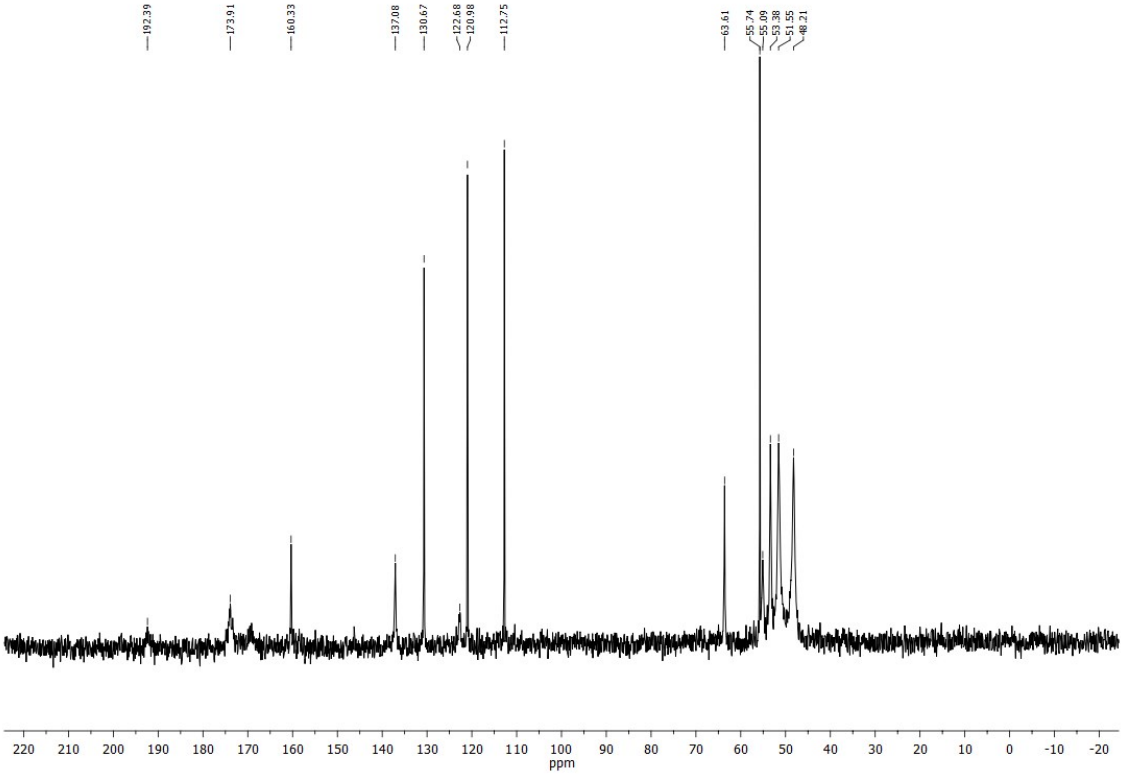


Figure S21b. ^{13}C NMR spectrum of **DO3A-oMAP**

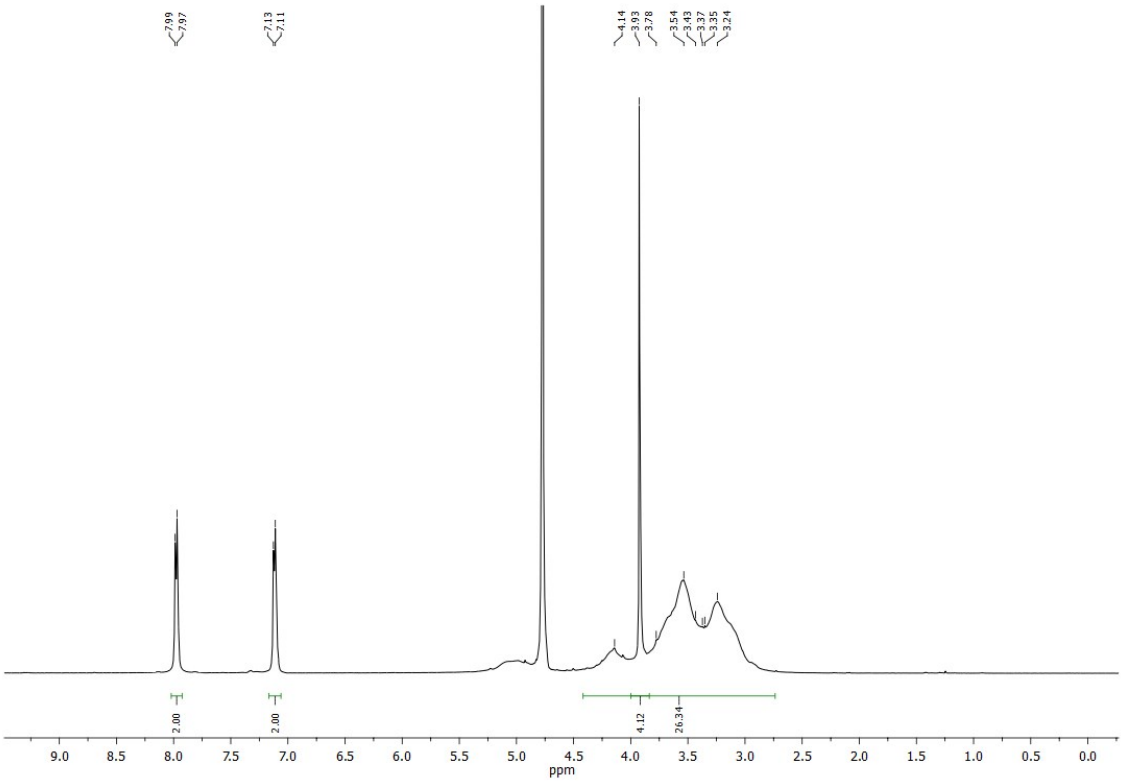


Figure S22a. ^{1}H NMR spectrum of **DO3A-pMAP**

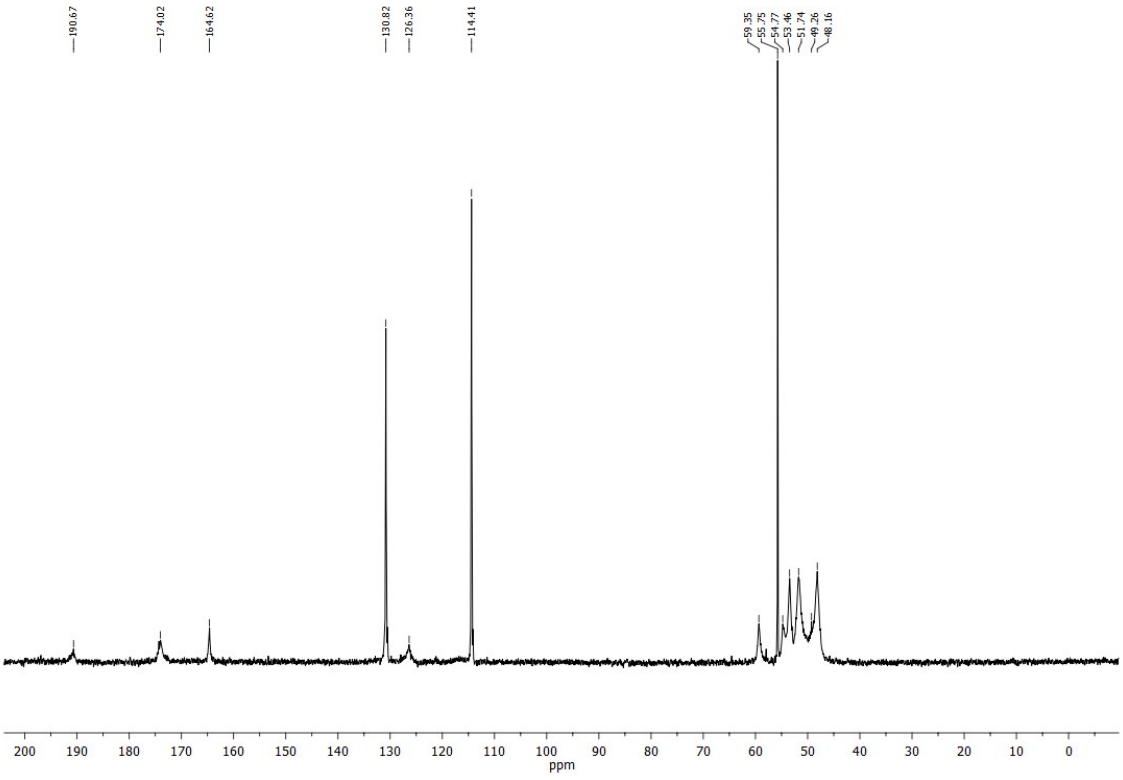


Figure S22b. ^{13}C NMR spectrum of **DO3A-pMAP**

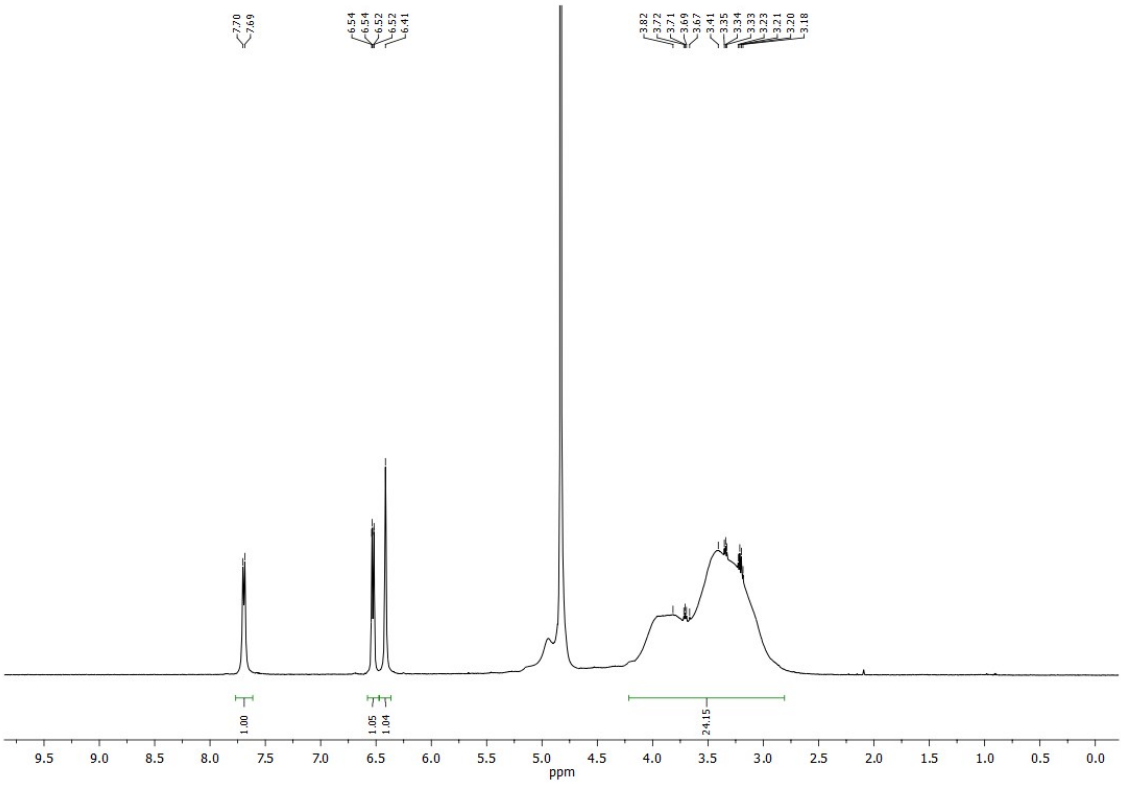


Figure S23a. ^{1}H NMR spectrum of **DO3A-DiHAP**

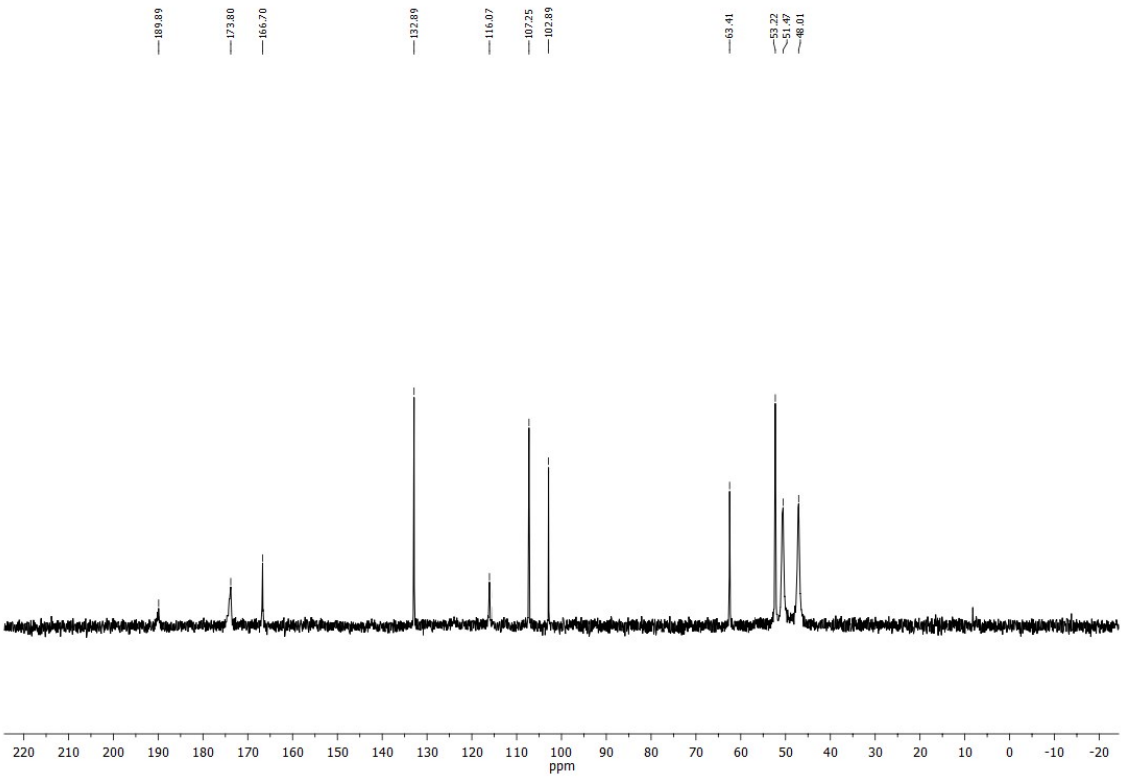


Figure S23b. ^{13}C NMR spectrum of **DO3A-DiHAP**

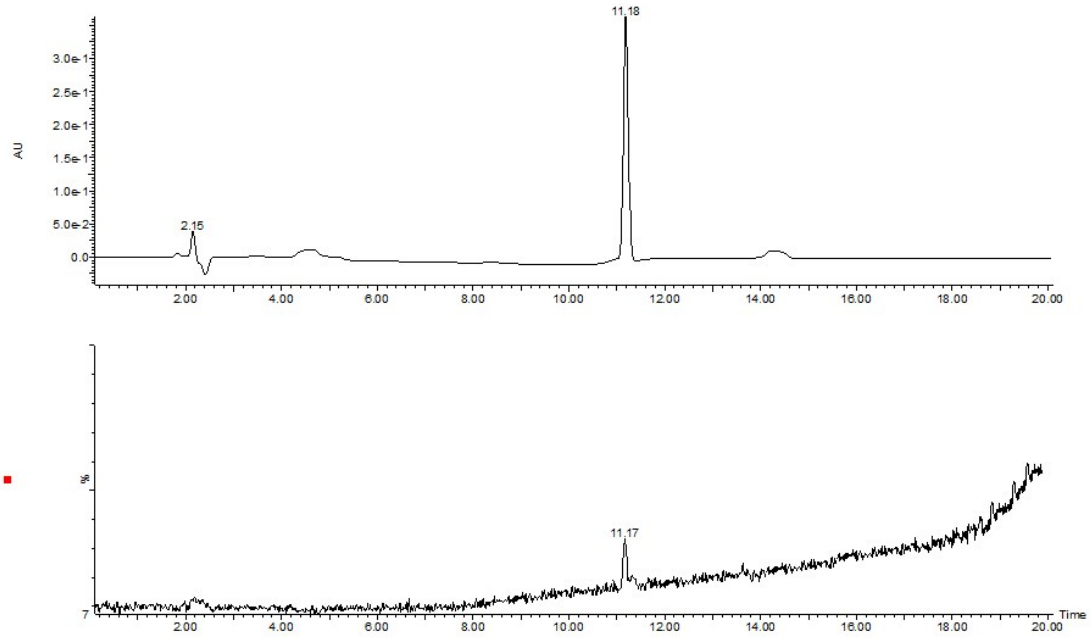


Figure S24a. HPLC-MS chromatogram of **DO3A-oAnAP**

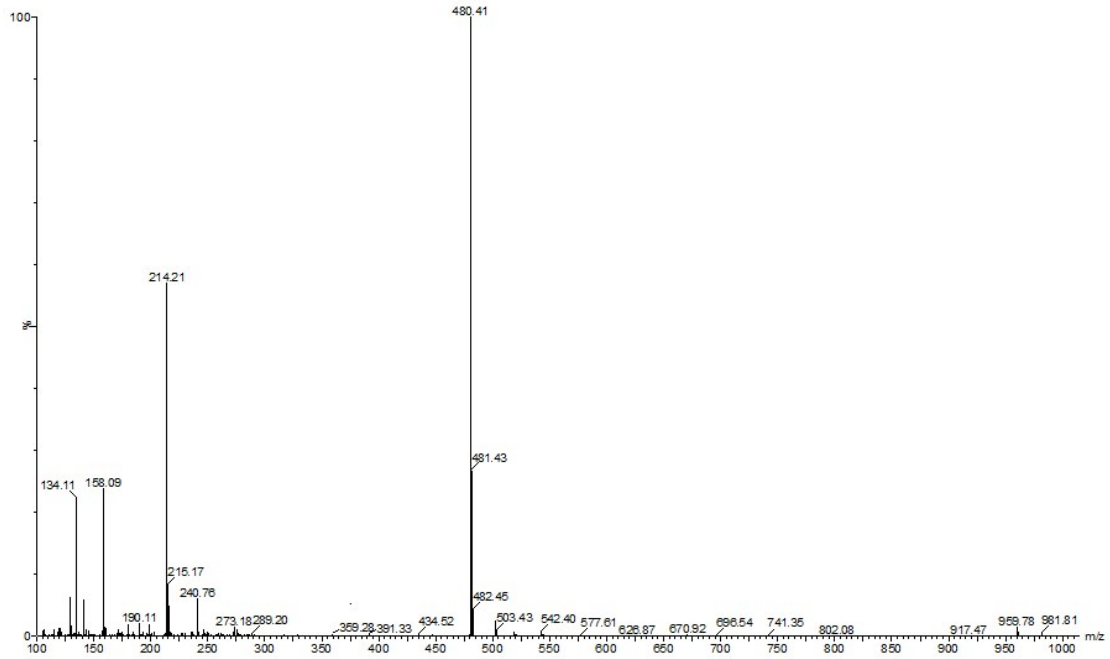


Figure S24b. MS spectrum of **DO3A-oAnAP**

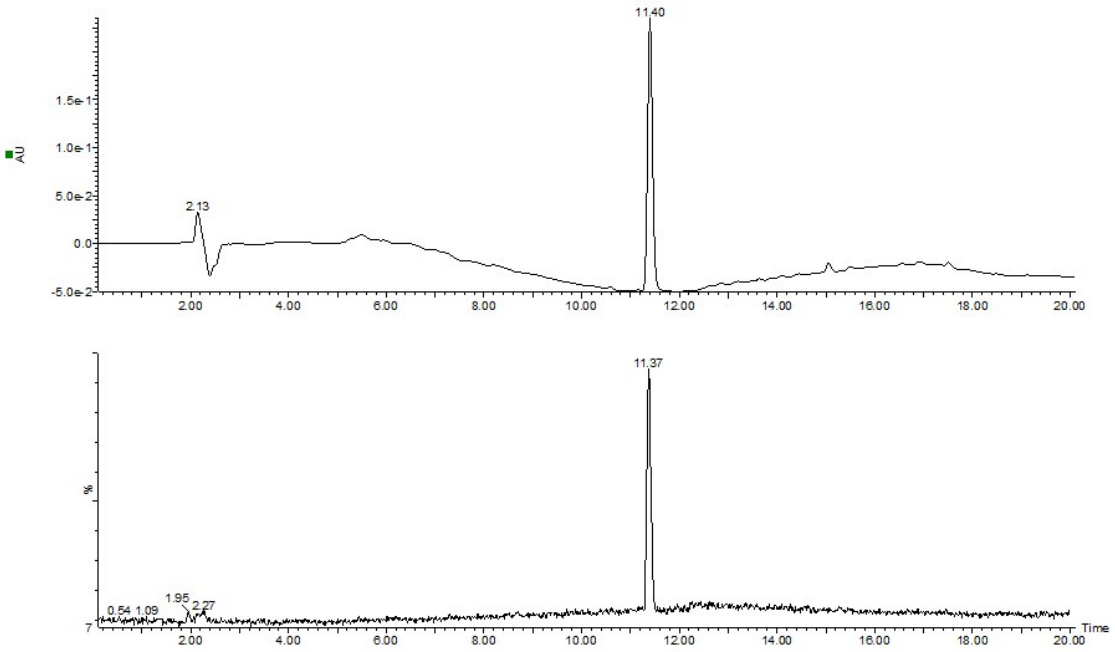


Figure S25a. HPLC-MS chromatogram of **DO3A-oMAP**

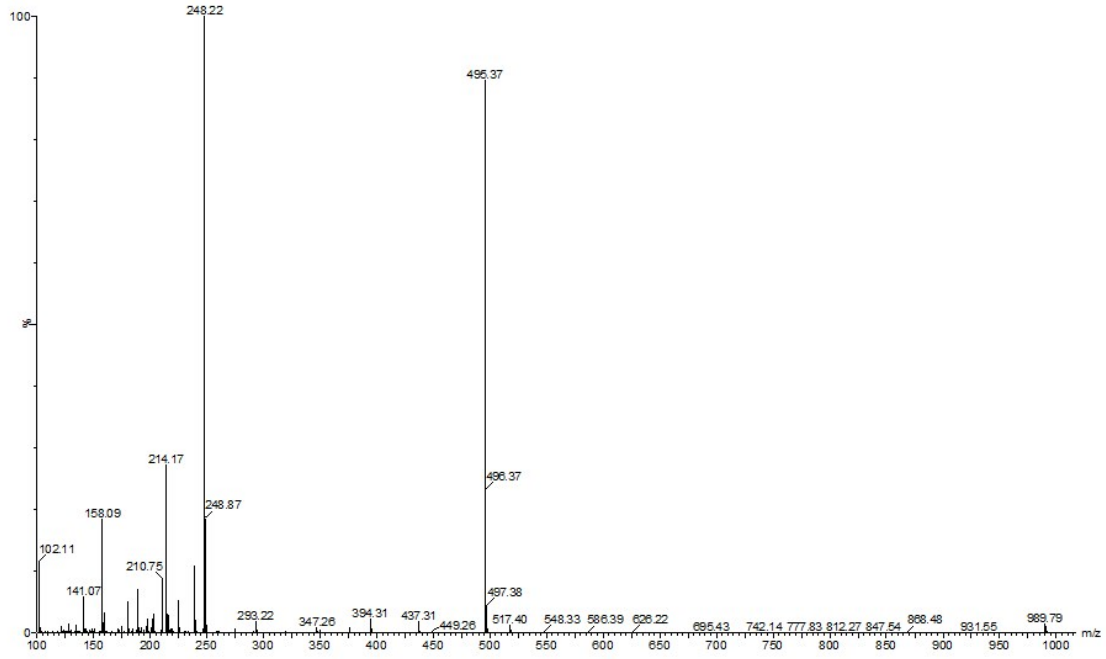


Figure S25b. MS spectrum of **DO3A-oMAP**

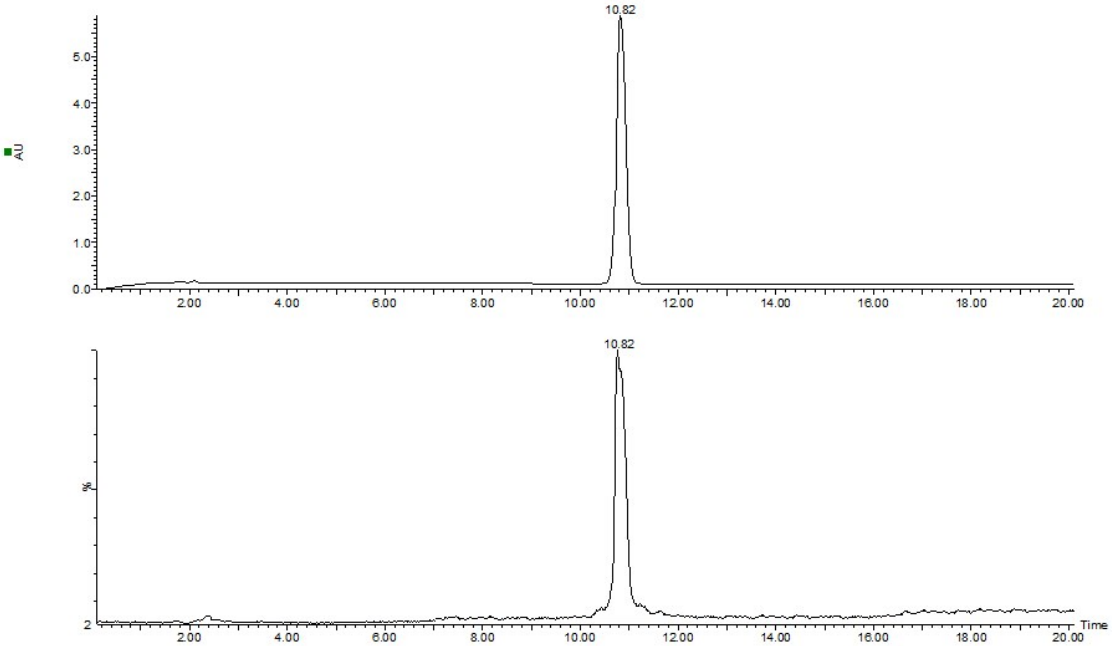


Figure S26a. HPLC-MS chromatogram of **DO3A-pMAP**

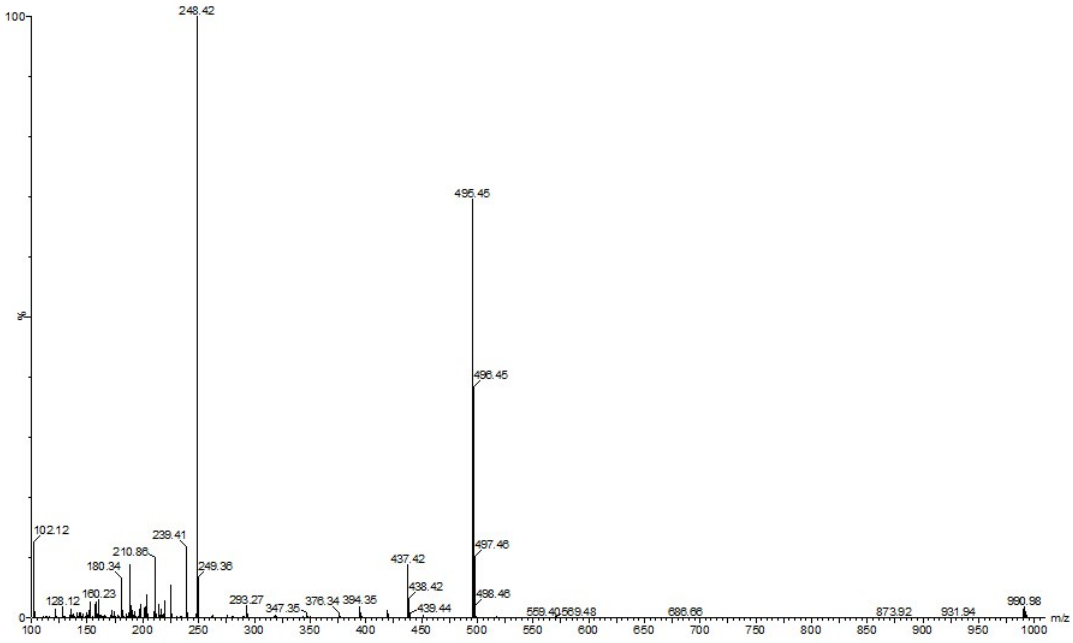


Figure S26b. MS spectrum of **DO3A-pMAP**

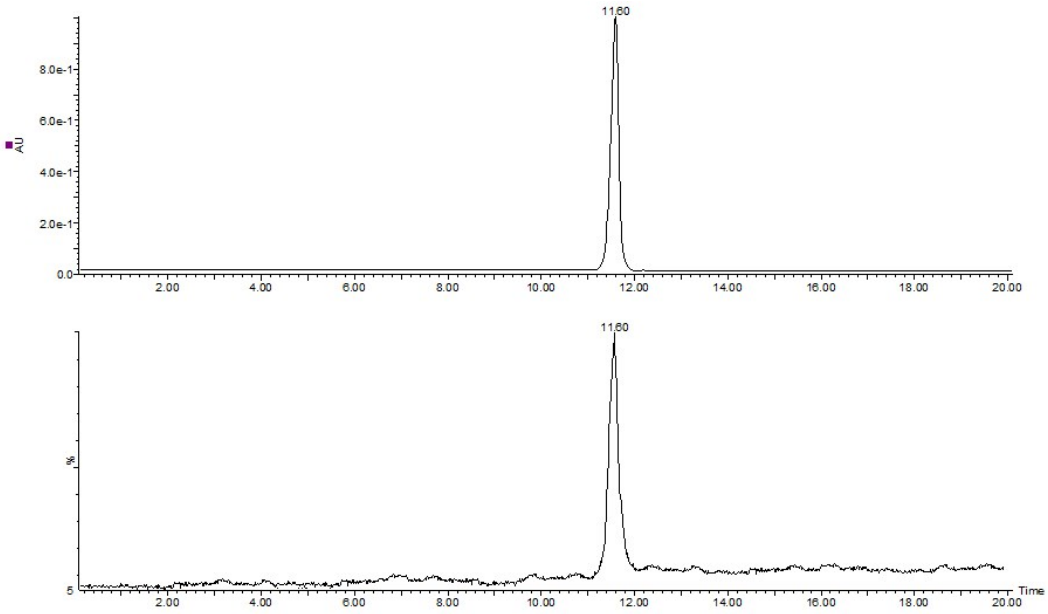


Figure S27a. HPLC-MS chromatogram of **DO3A-DiHAP**

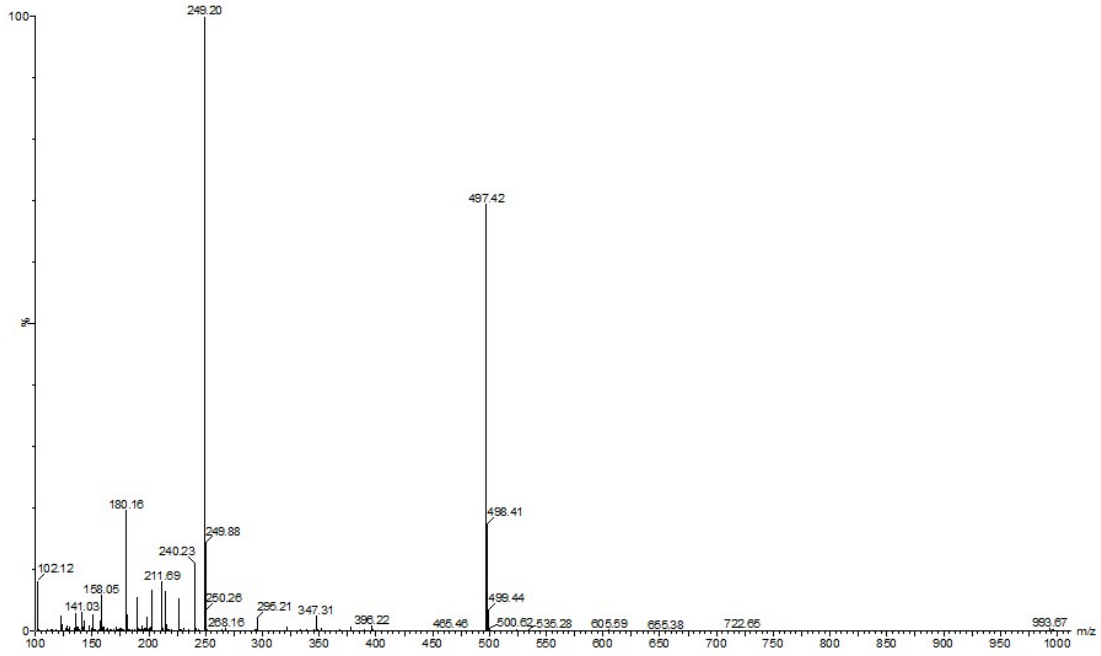


Figure S27b. MS spectrum of **DO3A-DiHAP**

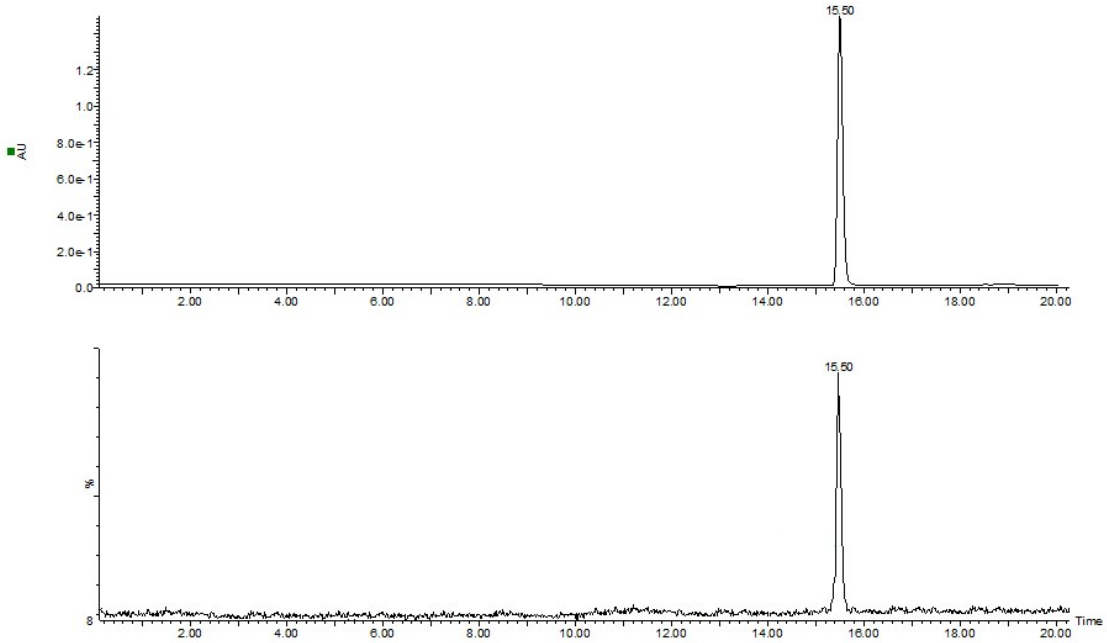


Figure S28a. HPLC-MS chromatogram of **GdDO3A-oAnAP**

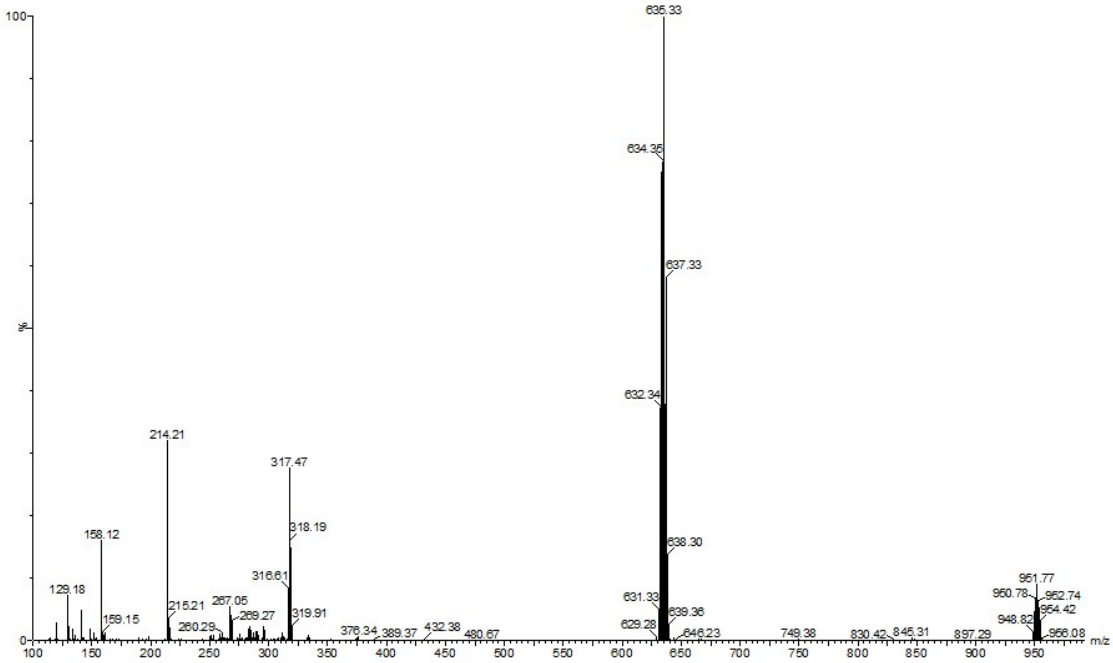


Figure S28b. MS spectrum of **GdDO3A-oAnAP**

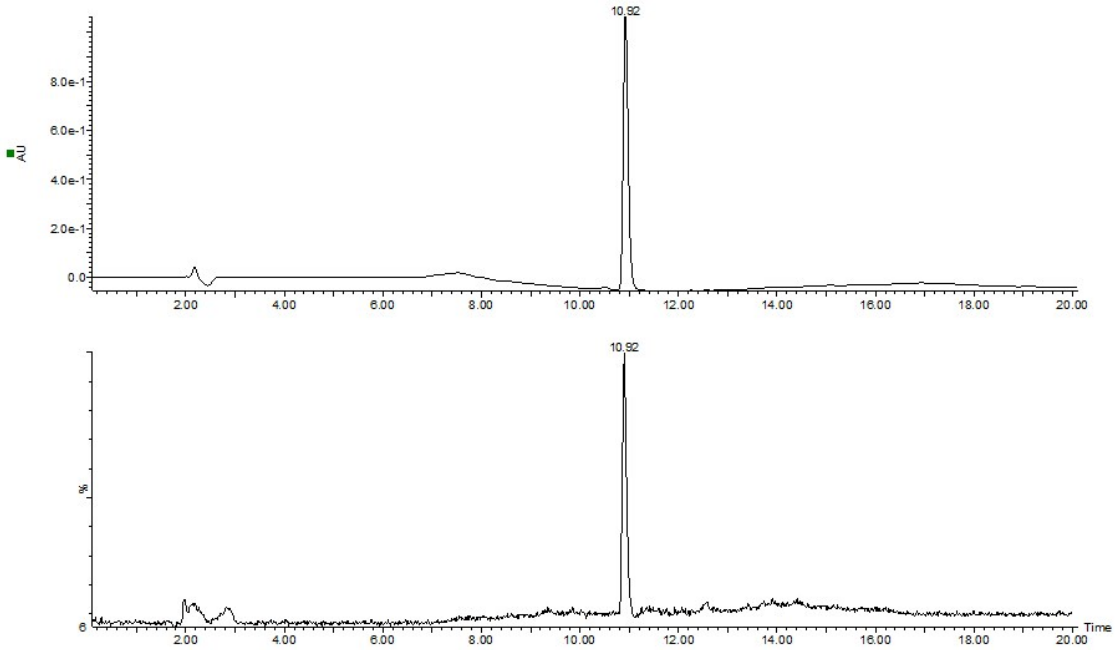


Figure S29a. HPLC-MS chromatogram of **GdDO3A-oMAP**

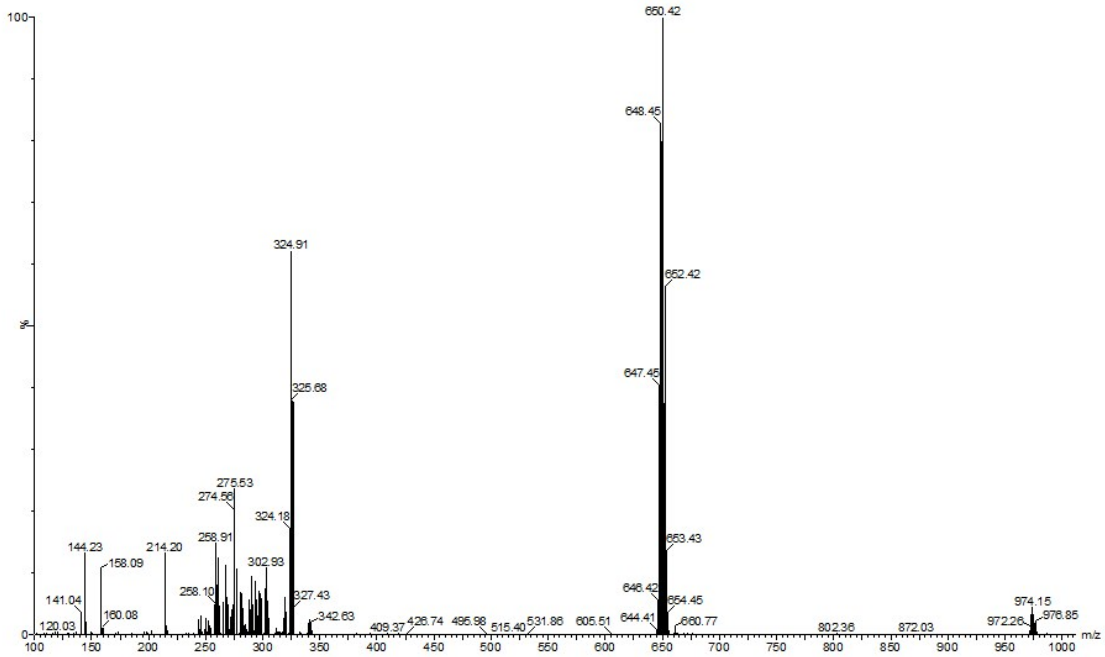


Figure S29b. MS spectrum of **GdDO3A-oMAP**

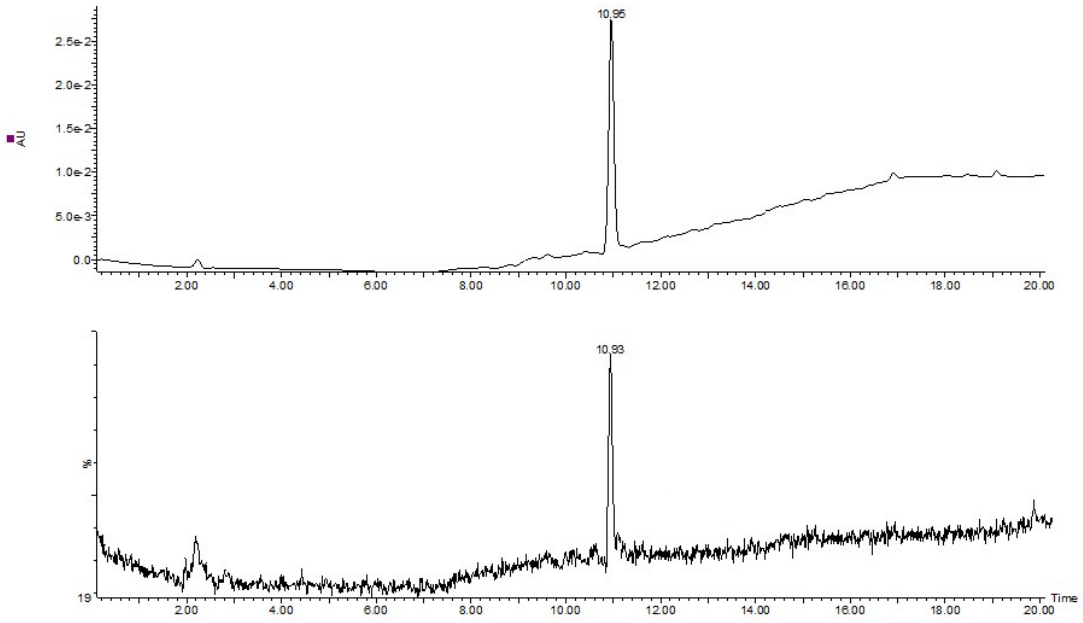


Figure S30a. HPLC-MS chromatogram of **GdDO3A-pMAP**

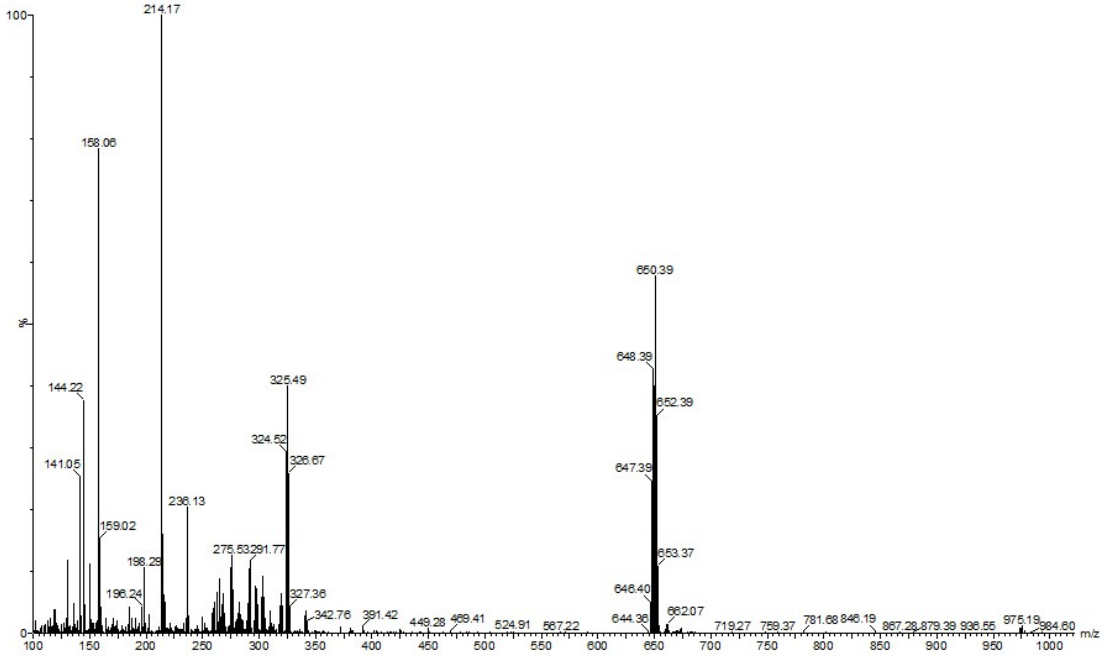


Figure S30b. MS spectrum of **GdDO3A-pMAP**

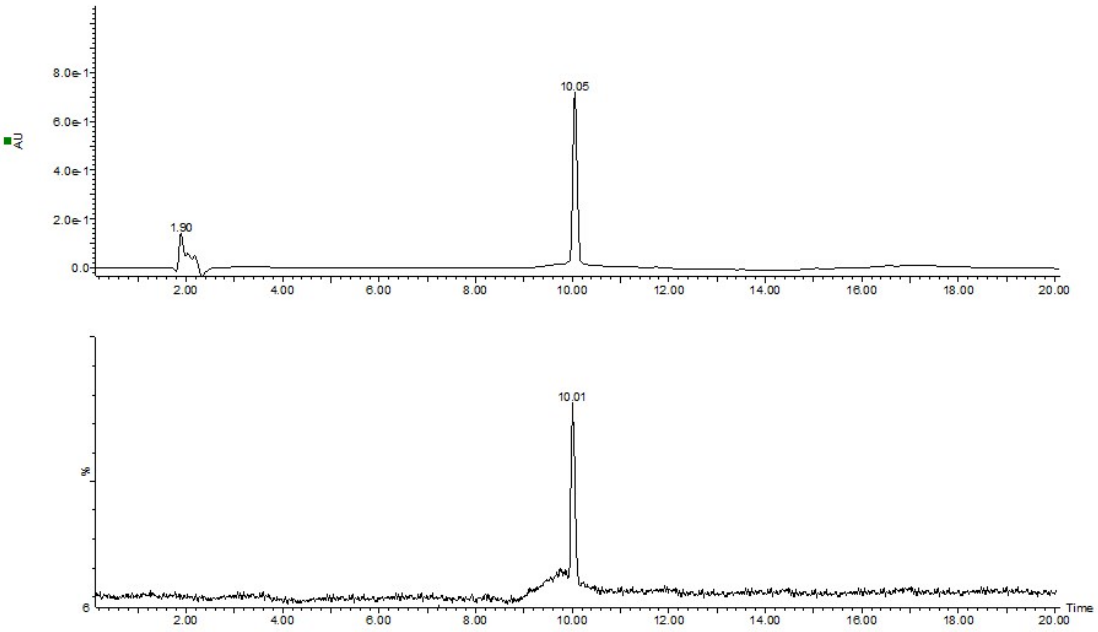


Figure S31a. HPLC-MS chromatogram of **GdDO3A-DiHAP**

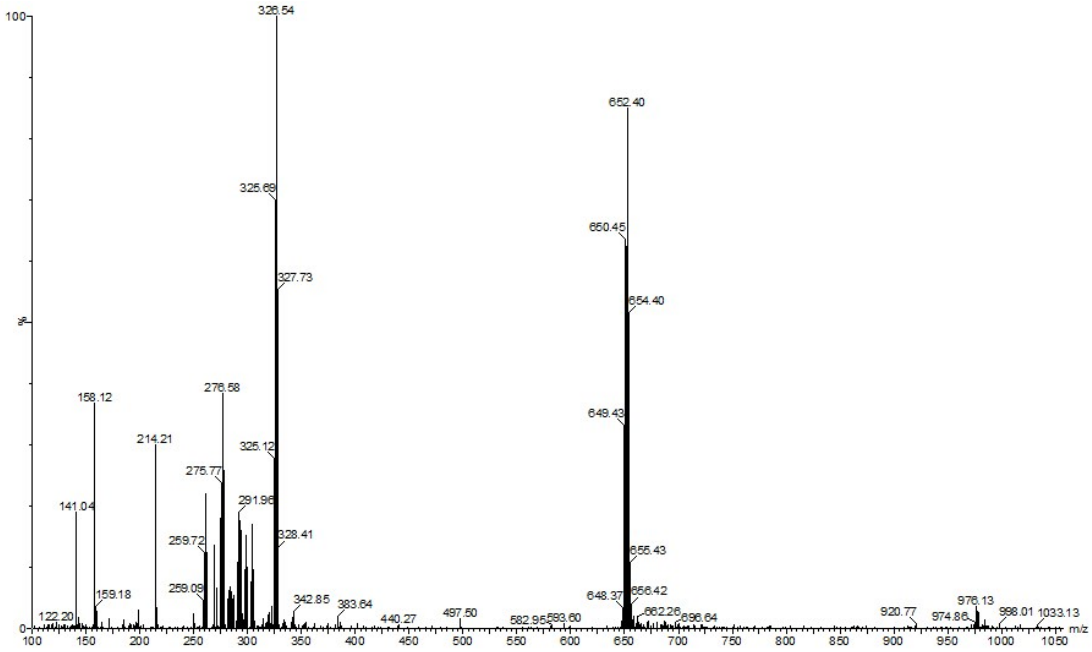


Figure S31b. MS spectrum of **GdDO3A-DiHAP**

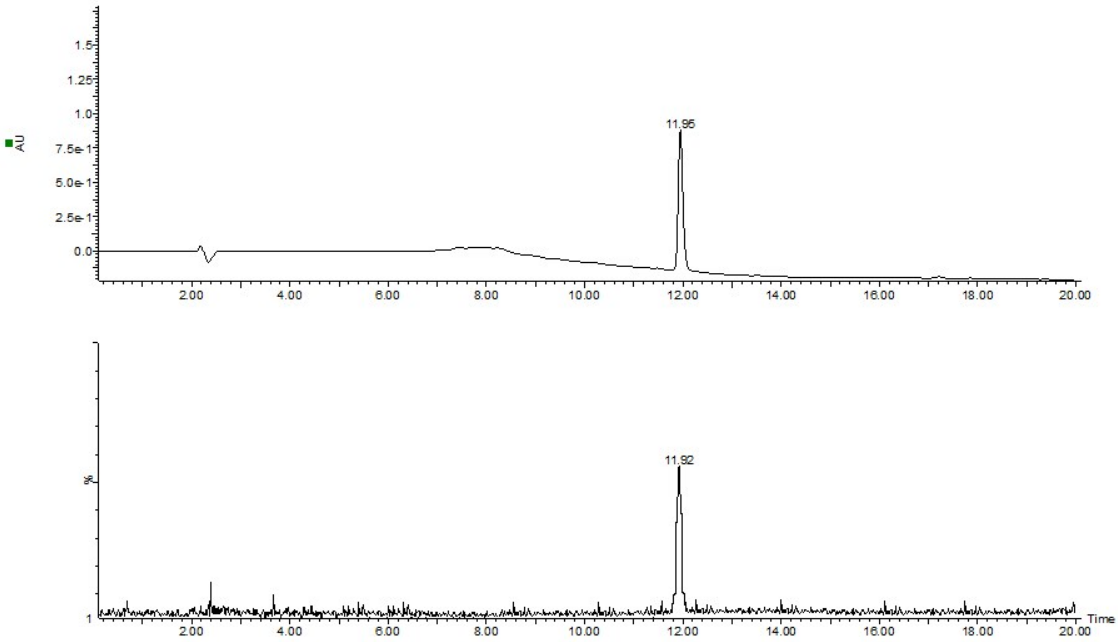


Figure S32a. HPLC-MS chromatogram of **EuDO3A-oAnAP**

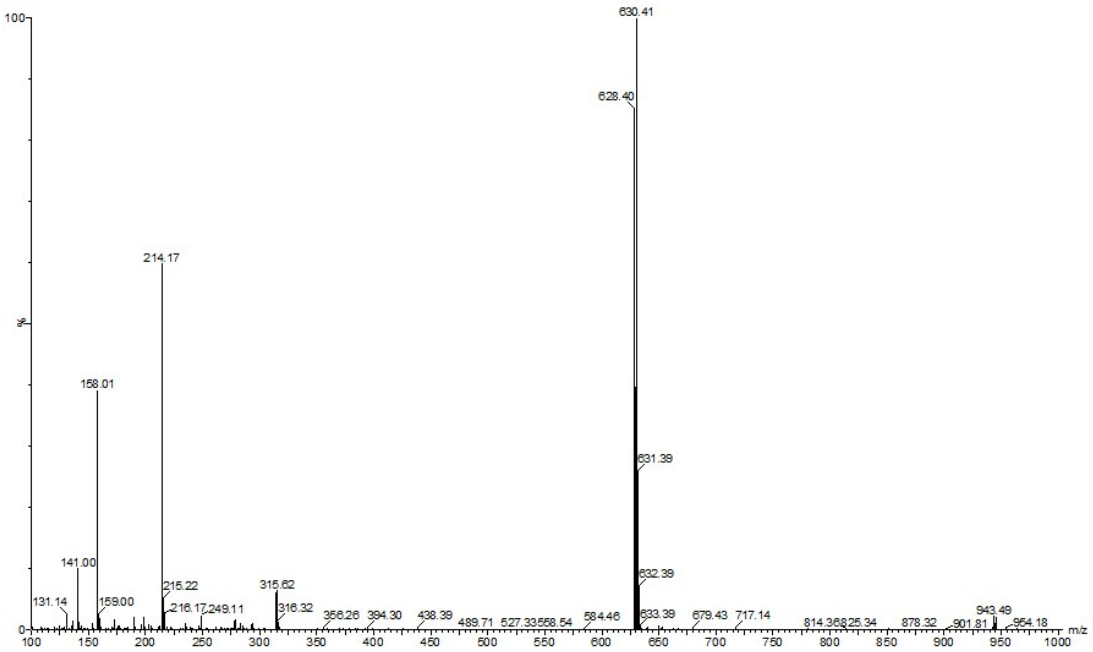


Figure S32b. MS spectrum of **EuDO3A-oAnAP**

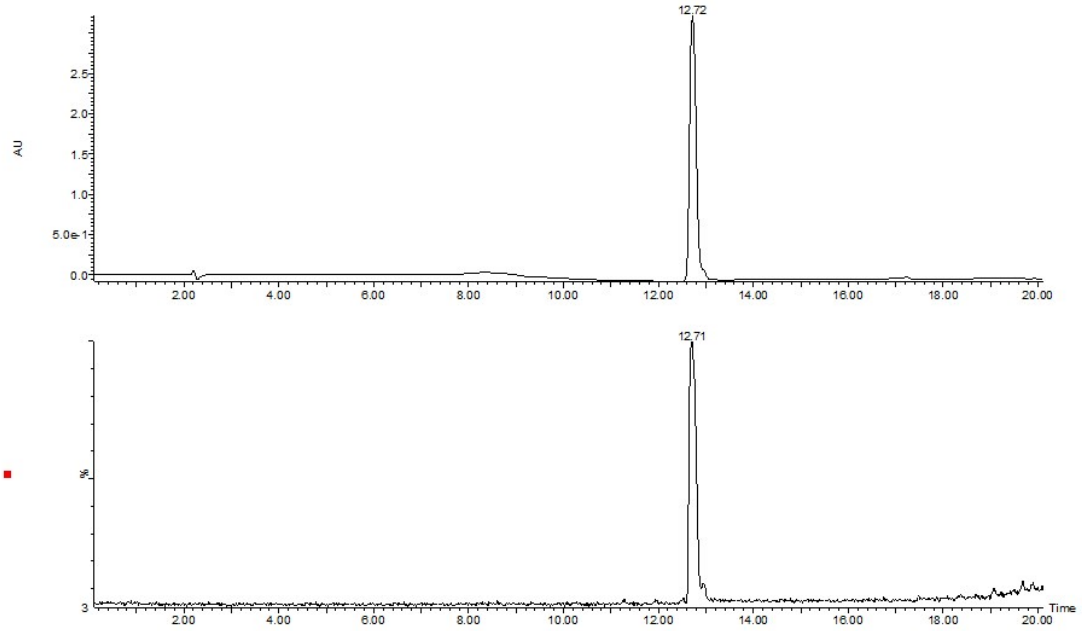


Figure S33a. HPLC-MS chromatogram of **EuDO3A-oMAP**

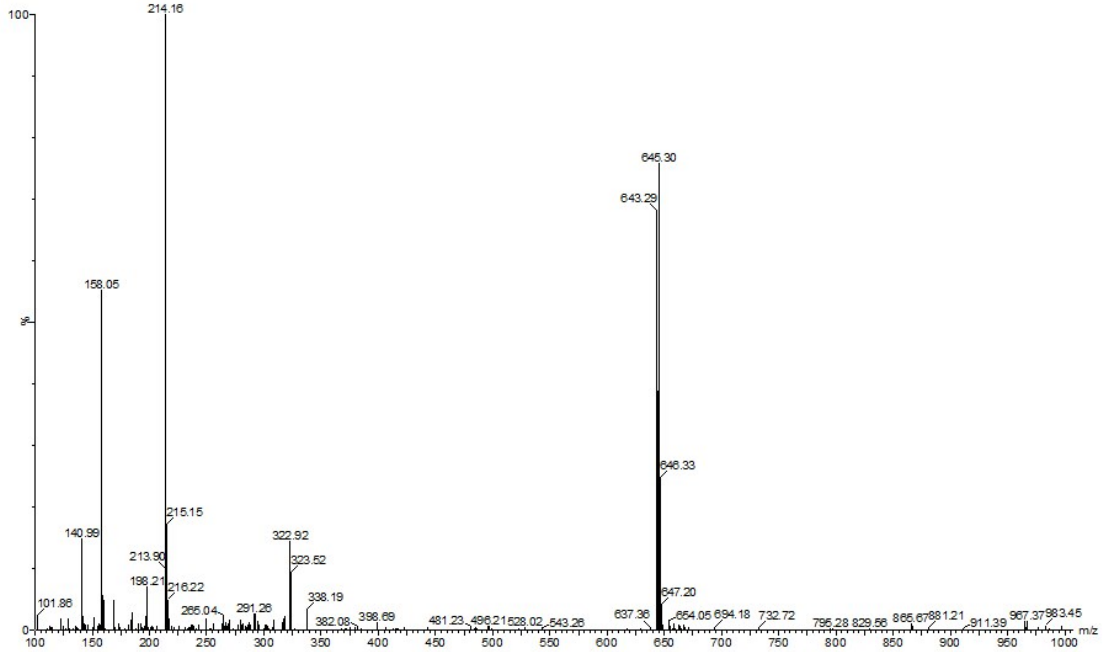


Figure S33b. MS spectrum of **EuDO3A-oMAP**

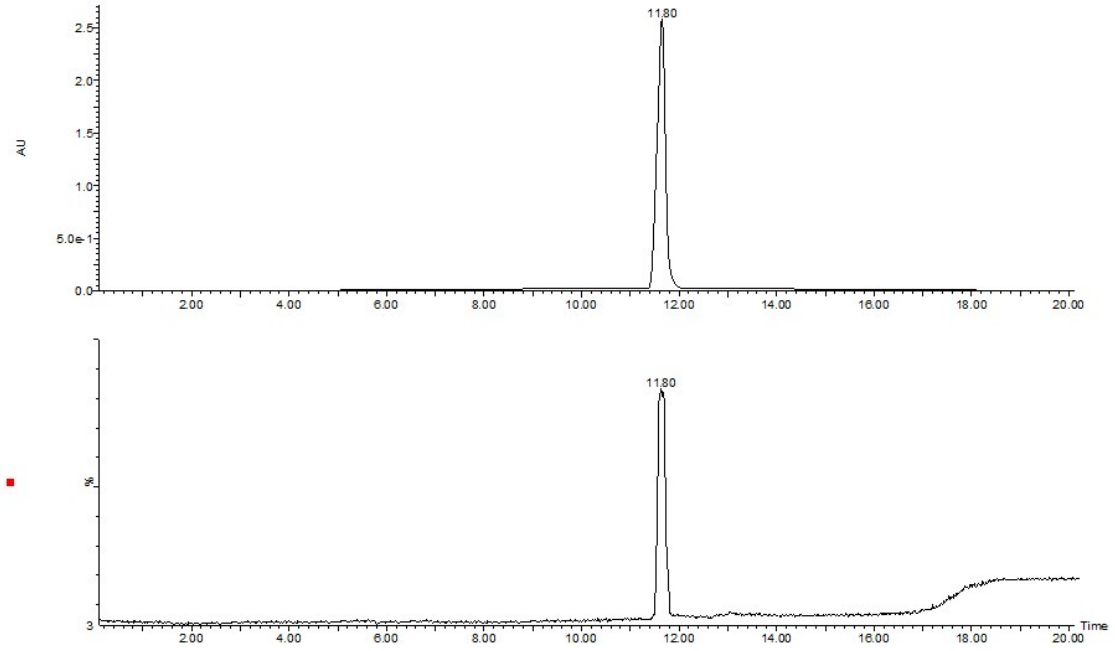


Figure S34a. HPLC-MS chromatogram of **EuDO3A-pMAP**

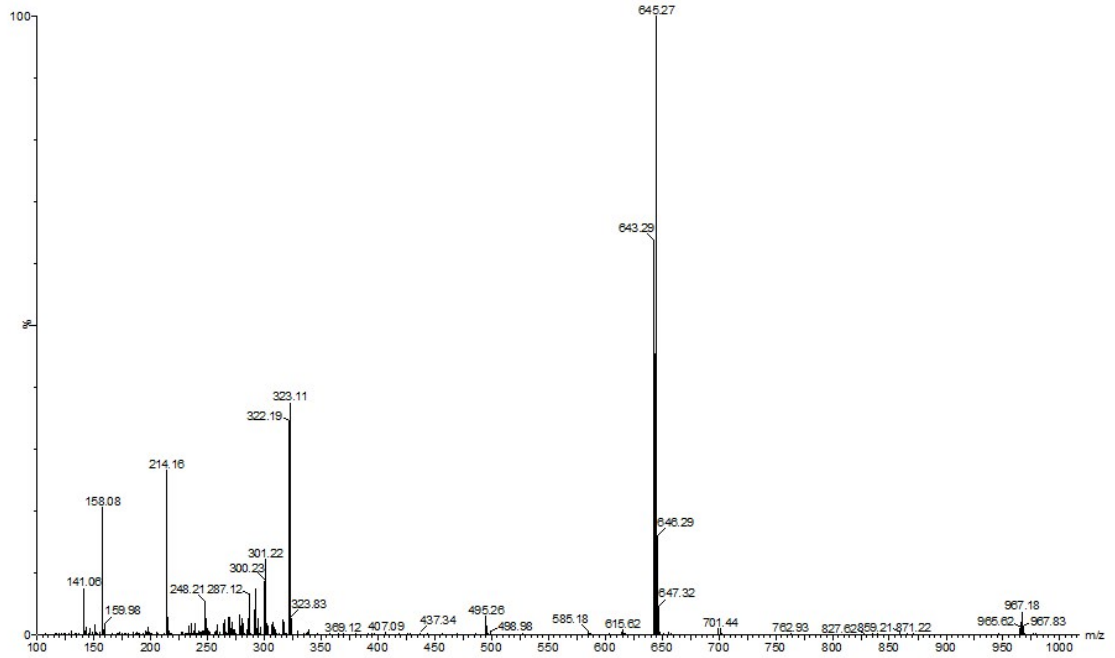


Figure S34b. MS spectrum of **EuDO3A-pMAP**

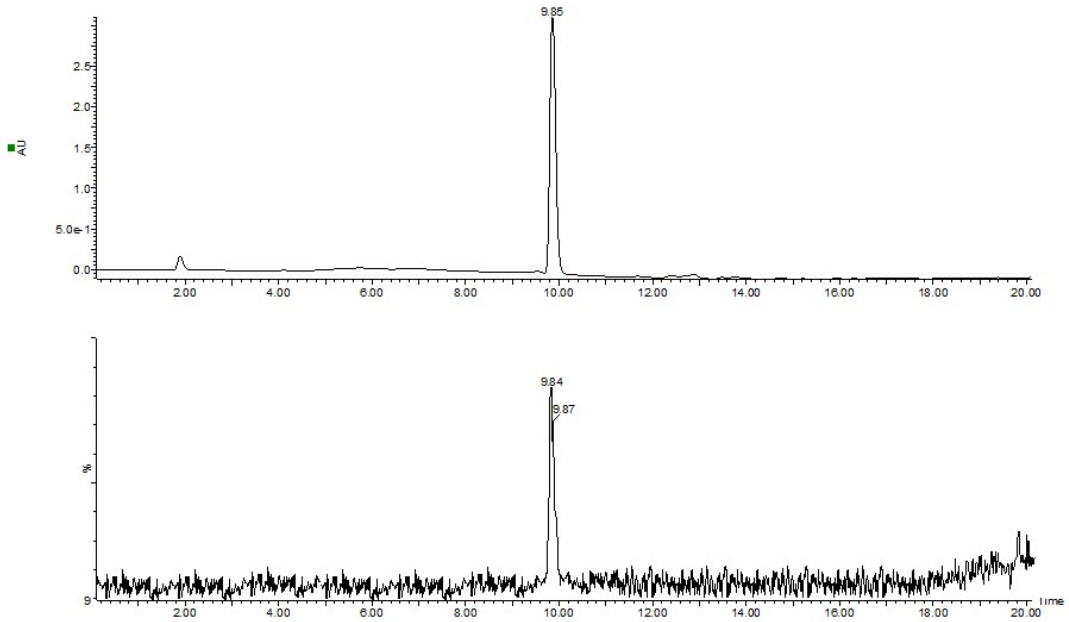


Figure S35a. HPLC-MS chromatogram of **EuDO3A-DiHAP**

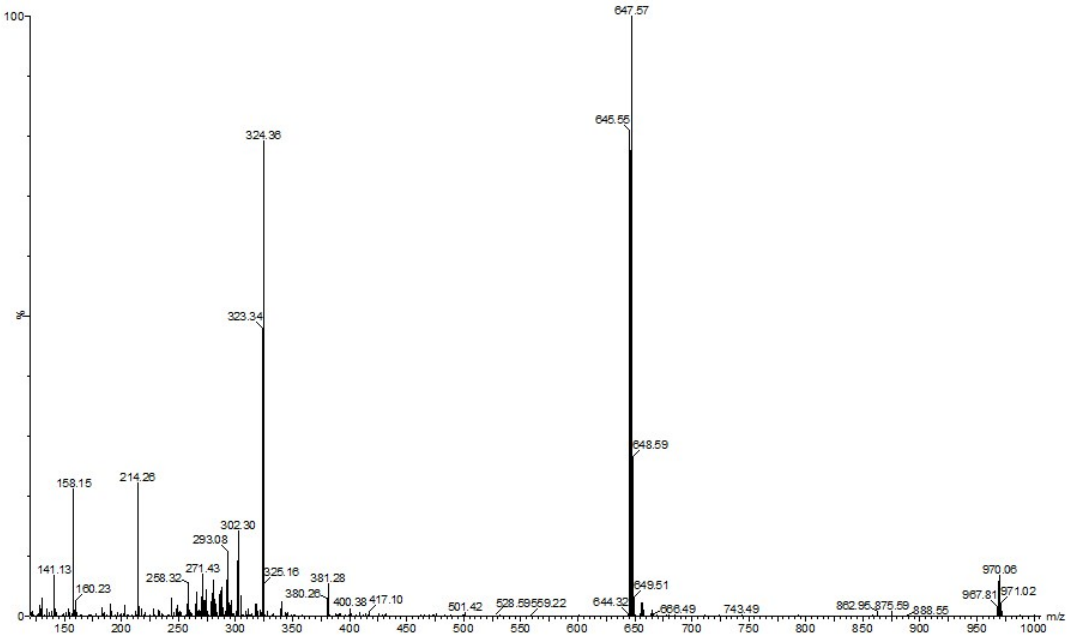


Figure S35b. MS spectrum of **EuDO3A-DiHAP**

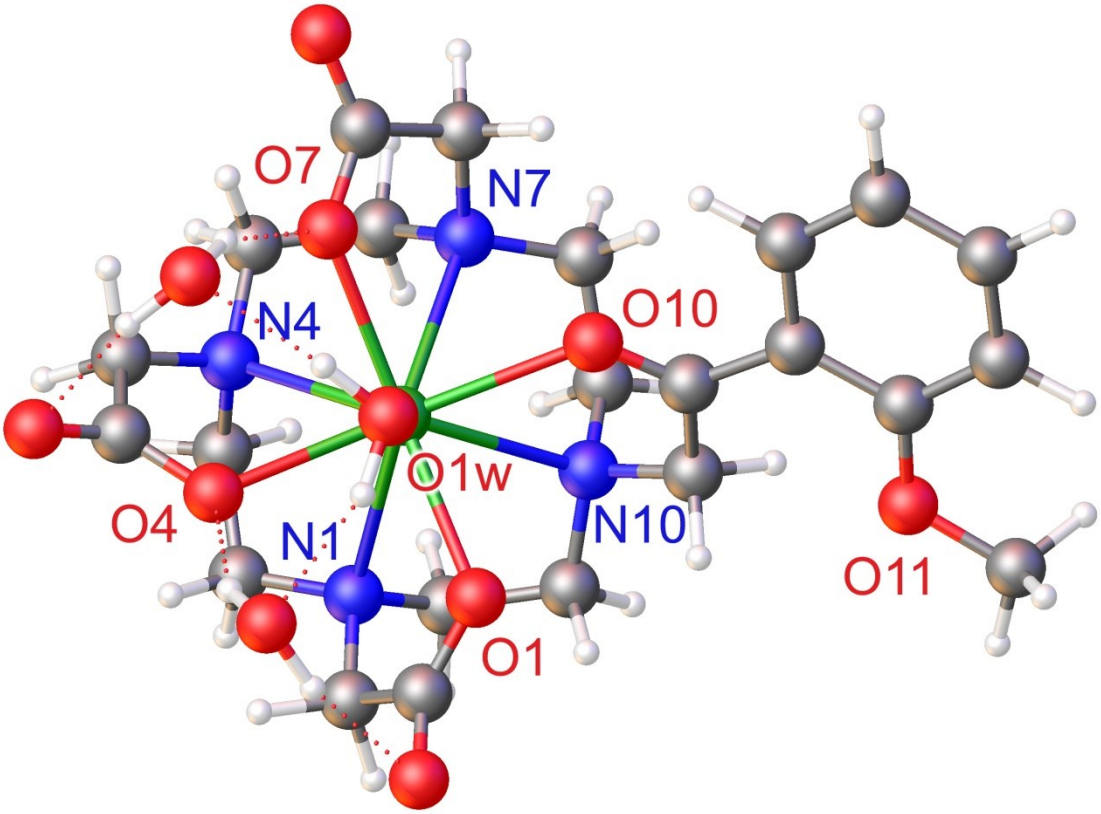


Figure S36. Structure of the GdDO3A-*o*MAP·3H_2O complex obtained with DFT calculations.

Table S1. Energies of the $^7F_1$ level (cm^{-1}) observed in the emission spectra of EuDO3A-*p*HAP, EuDO3A-*o*HAP, EuDO3A-*o*AnAP, EuDO3A-*p*MAP and EuDO3A-oMAP.

DO3A-*o*HAP	**DO3A-*p*HAP**	**DO3A-*o*MAP**	**DO3A-*p*MAP**	**DO3A-*o*AnAP**
296	270	273	273	264
371	402	405	402	*a*
473	467	467	470	*a*

[a] Unresolved components due to poor resolution associated to weak emission.

Table S2. Bond distances (Å) of the metal coordination environments obtained with DFT calculations.[a]

	DO3A-*o*HAP	**DO3A-*p*HAP**	**DO3A-*o*MAP**	**DO3A-*p*MAP**	**DO3A-*o*AnAP**	**DO3A-DiHAP**	**DO3A-AP**
Gd1-N1	2.665	2.674	2.677	2.692	2.680	2.670	2.673
Gd1-N4	2.654	2.690	2.684	2.695	2.678	2.666	2.667
Gd1-N7	2.711	2.704	2.704	2.696	2.688	2.707	2.690
Gd1-N10	2.701	2.718	2.701	2.714	2.705	2.701	2.714
Gd1-O1	2.358	2.363	2.365	2.364	2.368	2.360	2.366
Gd1-O4	2.377	2.387	2.387	2.363	2.392	2.379	2.385
Gd1-O7	2.399	2.383	2.382	2.382	2.385	2.398	2.381
Gd1-O10	2.456	2.461	2.465	2.492	2.429	2.443	2.481
Gd1-O1w	2.516	2.518	2.520	2.493	2.523	2.518	2.516

[a] See Figure 5 and S43 for labelling.

Table S3. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-AP·3H_2O system (0 Imaginary Frequencies).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	-1.762231	-1.970112	-1.133201
2	6	-3.096806	-1.484252	-1.549319
3	6	-3.064453	-0.082514	-2.135214
4	7	-2.550410	0.948320	-1.206558
5	6	-2.126097	2.138628	-1.977434
6	6	-0.778483	1.955440	-2.656698
7	7	0.340951	1.683856	-1.726974
8	6	1.482066	1.130390	-2.486527
9	6	1.303881	-0.342558	-2.820951
10	7	1.134201	-1.214411	-1.638033
11	6	0.516994	-2.500113	-2.042156
12	6	-0.975170	-2.383868	-2.311388
13	6	-1.898363	-3.076630	-0.168359
14	6	-0.831722	-3.131944	0.931796
15	8	0.031729	-2.195001	0.956775
16	8	-0.930561	-4.039084	1.759771
17	6	-3.561614	1.324802	-0.200466
18	6	-3.524776	0.530856	1.109440
19	8	-4.328278	0.837677	1.985914
20	8	-2.608190	-0.355909	1.222432
21	6	0.739230	2.915282	-1.022893
22	6	-0.158341	3.278654	0.165685

23	8	-0.277709	4.449825	0.490179
24	8	-0.691898	2.276382	0.773246
25	6	2.426463	-1.465107	-0.988645
26	6	2.823445	-0.369081	-0.021570
27	8	1.948638	0.333005	0.476264
28	1	-2.840056	-2.955529	0.368142
29	1	-1.939879	-4.049855	-0.671653
30	1	-4.577228	1.278385	-0.610691
31	1	-3.384558	2.358751	0.097923
32	1	0.798904	3.769342	-1.706305
33	1	1.732782	2.758123	-0.595040
34	1	2.342295	-2.362507	-0.366782
35	1	3.212422	-1.646987	-1.728547
36	1	-3.740380	-1.493546	-0.671884
37	1	-3.543720	-2.161251	-2.289194
38	1	-4.078045	0.180452	-2.465063
39	1	-2.440803	-0.073390	-3.029324
40	1	-2.868494	2.385364	-2.747331
41	1	-2.086484	2.989295	-1.299500
42	1	-0.562352	2.855017	-3.248082
43	1	-0.837834	1.129371	-3.365005
44	1	1.628398	1.681690	-3.424222
45	1	2.389771	1.280748	-1.902700
46	1	0.426728	-0.465980	-3.454507
47	1	2.162860	-0.674062	-3.418852
48	1	0.686799	-3.217759	-1.241506
49	1	1.005480	-2.894401	-2.942353
50	1	-1.152178	-1.664147	-3.110862
51	1	-1.333099	-3.352358	-2.685579
52	8	-1.888540	2.241610	3.209386
53	1	-1.579520	2.500127	2.318990
54	1	-0.663602	0.895611	3.009839
55	64	-0.489017	-0.021068	0.180736
56	8	-0.132644	0.149417	2.665364
57	1	-0.547930	-0.637867	3.071134
58	6	4.235365	-0.165767	0.347392
59	6	5.248067	-1.041925	-0.056962
60	6	4.554639	0.947971	1.133536
61	6	6.560645	-0.805333	0.324532
62	6	5.867872	1.187074	1.500019
63	6	6.870882	0.309242	1.096365
64	1	7.342306	-1.488586	0.016346
65	1	6.113156	2.054774	2.100123
66	1	-2.760510	1.854716	3.060479
67	8	-1.888962	-1.817668	3.487494
68	1	-1.610273	-2.675857	3.139798
69	1	-2.372768	-1.399021	2.752164
70	1	3.762562	1.619007	1.441526
71	1	7.898869	0.495475	1.384824
72	1	5.024874	-1.915863	-0.655739

E(RwB97XD) = -1866.9753619 Hartree
Zero-point correction = 0.597500
Thermal correction to Energy = 0.634516
Thermal correction to Enthalpy = 0.635461
Thermal correction to Gibbs Free Energy = 0.531105
Sum of electronic and zero-point Energies = -1866.377861
Sum of electronic and thermal Energies = -1866.340845
Sum of electronic and thermal Enthalpies = -1866.339901

Sum of electronic and thermal Free Energies= -1866.444257

Table S4. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-AP·3H_2O system (1 Imaginary Frequency).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	-1.613553	-1.999083	-1.209733
2	6	-3.017783	-1.634174	-1.509040
3	6	-3.161338	-0.211867	-2.023835
4	7	-2.695572	0.815598	-1.067958
5	6	-2.441563	2.087982	-1.782606
6	6	-1.129537	2.087854	-2.553118
7	7	0.068758	1.863780	-1.710665
8	6	1.211086	1.467717	-2.565497
9	6	1.146048	0.009620	-2.994234
10	7	1.147980	-0.946151	-1.862763
11	6	0.625908	-2.263183	-2.303307
12	6	-0.883990	-2.280027	-2.462850
13	6	-1.566538	-3.155469	-0.292196
14	6	-0.439824	-3.139427	0.749585
15	8	0.319131	-2.112234	0.778130
16	8	-0.388661	-4.088811	1.529471
17	6	-3.664447	1.019271	0.024546
18	6	-3.449679	0.160548	1.274433
19	8	-4.245359	0.287067	2.198700
20	8	-2.406075	-0.586705	1.294872
21	6	0.397401	3.078021	-0.940205
22	6	-0.443105	3.267370	0.328379
23	8	-0.651215	4.393376	0.747851
24	8	-0.833860	2.174192	0.891969
25	6	2.502262	-1.114671	-1.318938
26	6	2.846661	-0.128871	-0.225712
27	8	1.950685	0.525599	0.301367
28	1	-2.484593	-3.169532	0.296056
29	1	-1.525706	-4.102490	-0.841914
30	1	-4.696261	0.886477	-0.319788
31	1	-3.576440	2.047134	0.379194
32	1	0.328026	3.978214	-1.559687
33	1	1.428836	2.990606	-0.589292
34	1	2.574024	-2.095450	-0.839080
35	1	3.256132	-1.090133	-2.113266
36	1	-3.592517	-1.746725	-0.591544
37	1	-3.447498	-2.320861	-2.249245
38	1	-4.213749	-0.037088	-2.282102
39	1	-2.595861	-0.094498	-2.948358
40	1	-3.254095	2.304294	-2.487636
41	1	-2.439917	2.895028	-1.051818
42	1	-1.038797	3.044858	-3.082962
43	1	-1.154444	1.313348	-3.319838
44	1	1.257016	2.093218	-3.465507
45	1	2.131510	1.654663	-2.012786
46	1	0.239627	-0.160340	-3.573989
47	1	1.986359	-0.197179	-3.668770
48	1	0.917329	-3.002557	-1.558778

49	1	1.084830	-2.560063	-3.254377
50	1	-1.188506	-1.545738	-3.208442
51	1	-1.177518	-3.260567	-2.859842
52	8	-2.018025	2.017562	3.376624
53	1	-1.681153	2.226479	2.483964
54	1	-0.665236	0.744191	3.580966
55	64	-0.453279	-0.011399	0.086974
56	8	0.024712	0.061352	3.524315
57	1	-0.470171	-0.773065	3.581206
58	6	4.236924	0.003769	0.239914
59	6	5.269600	-0.797351	-0.259919
60	6	4.511850	0.949771	1.234656
61	6	6.557473	-0.653615	0.234099
62	6	5.800736	1.095137	1.718062
63	6	6.823110	0.291988	1.218899
64	1	7.354070	-1.279111	-0.149196
65	1	6.011395	1.829904	2.485421
66	1	-2.828526	1.517709	3.222773
67	8	-1.692812	-2.189387	3.446579
68	1	-1.249141	-2.930061	3.013446
69	1	-2.105496	-1.691581	2.716832
70	1	3.704575	1.561957	1.616540
71	1	7.831350	0.403060	1.600652
72	1	5.081438	-1.542018	-1.023040

E(RwB97XD) = -1866.9641052 Hartree
Zero-point correction = 0.597574
Thermal correction to Energy = 0.634273
Thermal correction to Enthalpy = 0.635217
Thermal correction to Gibbs Free Energy = 0.530565
Sum of electronic and zero-point Energies = -1866.366531
Sum of electronic and thermal Energies = -1866.329833
Sum of electronic and thermal Enthalpies = -1866.328889
Sum of electronic and thermal Free Energies = -1866.433541

Table S5. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*o*HAP·4H_2O system (0 Imaginary Frequencies).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	2.505121	-1.966729	0.738511
2	6	3.763804	-1.342587	1.204296
3	6	3.534396	-0.095310	2.040724
4	7	2.822970	0.983215	1.322596
5	6	2.248980	1.940008	2.295615
6	6	1.000474	1.412306	2.981199
7	7	-0.125055	1.132609	2.061691
8	6	-1.109448	0.263450	2.741839
9	6	-0.677806	-1.192426	2.788077
10	7	-0.438189	-1.788157	1.455515
11	6	0.388925	-3.011418	1.591713
12	6	1.858174	-2.707352	1.838758
13	6	2.767080	-2.846299	-0.415623
14	6	1.674700	-2.868063	-1.490606
15	8	0.667303	-2.106771	-1.314848

16	8	1.880712	-3.566018	-2.484471
17	6	3.712630	1.686570	0.377881
18	6	3.692829	1.173197	-1.065949
19	8	4.356968	1.784348	-1.898619
20	8	2.931104	0.174303	-1.315686
21	6	-0.769247	2.382780	1.624111
22	6	-0.206090	3.008622	0.346382
23	8	-0.645460	4.105430	0.005145
24	8	0.656230	2.324976	-0.304817
25	6	-1.711871	-2.126323	0.802841
26	6	-2.344888	-0.941442	0.103889
27	8	-1.572341	-0.053543	-0.317635
28	1	3.656828	-2.486006	-0.932783
29	1	2.975760	-3.875272	-0.100183
30	1	4.750571	1.692962	0.730815
31	1	3.395890	2.727616	0.309374
32	1	-0.751583	3.143251	2.413690
33	1	-1.822635	2.193770	1.408362
34	1	-1.510711	-2.838778	-0.003337
35	1	-2.397105	-2.604820	1.507469
36	1	4.348527	-1.082685	0.323700
37	1	4.356696	-2.055142	1.792423
38	1	4.506451	0.267951	2.399428
39	1	2.957922	-0.350543	2.929519
40	1	2.986205	2.195244	3.067847
41	1	2.012611	2.859766	1.763723
42	1	0.688279	2.140124	3.741640
43	1	1.237107	0.493590	3.517054
44	1	-1.286613	0.604428	3.769954
45	1	-2.063445	0.355837	2.223499
46	1	0.240949	-1.282966	3.365592
47	1	-1.439496	-1.767253	3.330657
48	1	0.285597	-3.588998	0.674883
49	1	0.016904	-3.635692	2.413949
50	1	1.967046	-2.128275	2.755718
51	1	2.380052	-3.657528	2.014069
52	8	1.663910	2.916452	-2.774626
53	1	1.372878	2.971075	-1.845142
54	1	0.683843	1.375583	-2.767255
55	64	0.865835	-0.059013	-0.157829
56	8	0.295820	0.505171	-2.544804
57	1	0.793830	-0.118138	-3.110982
58	6	-3.757249	-0.843105	-0.130989
59	6	-4.670431	-1.817762	0.330160
60	6	-4.283867	0.273459	-0.845639
61	6	-6.017601	-1.706870	0.114904
62	1	-4.308188	-2.684232	0.866655
63	6	-5.649176	0.393150	-1.054482
64	6	-6.511978	-0.585489	-0.579939
65	1	-6.698692	-2.467747	0.476662
66	1	-6.036637	1.247360	-1.594055
67	1	2.593861	2.660195	-2.721665
68	8	2.285408	-0.942697	-3.800567
69	1	2.181895	-1.884568	-3.605974
70	1	2.749853	-0.582649	-3.023416
71	1	-2.573112	0.998779	-1.147234
72	8	-3.469356	3.751191	0.297630
73	1	-2.549177	4.036154	0.190184
74	1	-3.577603	3.061466	-0.365013
75	8	-3.502898	1.241089	-1.340025

76	8	-7.817299	-0.413296	-0.814315
77	1	-8.326773	-1.143257	-0.450814

E(RwB97XD) = -2093.8873186 Hartree
Zero-point correction = 0.633825
Thermal correction to Energy = 0.675124
Thermal correction to Enthalpy = 0.676068
Thermal correction to Gibbs Free Energy = 0.563376
Sum of electronic and zero-point Energies = -2093.253493
Sum of electronic and thermal Energies = -2093.212195
Sum of electronic and thermal Enthalpies = -2093.211250
Sum of electronic and thermal Free Energies = -2093.323942

Table S6. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*o*HAP·4H_2O system (1 Imaginary Frequency).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	2.478485	-1.844499	0.620647
2	6	3.809175	-1.232716	0.846491
3	6	3.728941	0.109529	1.559155
4	7	2.937124	1.119379	0.824085
5	6	2.533646	2.217984	1.730490
6	6	1.391047	1.833645	2.655100
7	7	0.146010	1.460926	1.947321
8	6	-0.733411	0.699941	2.863567
9	6	-0.313387	-0.752491	3.013665
10	7	-0.309085	-1.513424	1.743943
11	6	0.501670	-2.744482	1.899158
12	6	1.998856	-2.476116	1.870681
13	6	2.547946	-2.832788	-0.470663
14	6	1.209531	-3.112270	-1.158060
15	8	0.362173	-2.136745	-1.133570
16	8	1.034858	-4.179355	-1.722292
17	6	3.706097	1.656099	-0.314461
18	6	3.656461	0.791093	-1.579935
19	8	4.614454	0.786771	-2.337187
20	8	2.542550	0.171458	-1.775476
21	6	-0.558390	2.654465	1.441848
22	6	-0.196472	3.098681	0.022472
23	8	-0.687348	4.148111	-0.388489
24	8	0.554271	2.318533	-0.658364
25	6	-1.679346	-1.864292	1.339665
26	6	-2.339642	-0.778788	0.511296
27	8	-1.617484	0.089422	0.017699
28	1	3.185398	-2.422466	-1.257770
29	1	2.989388	-3.776471	-0.133372
30	1	4.748233	1.847159	-0.038690
31	1	3.251271	2.605203	-0.608297
32	1	-0.432987	3.510144	2.114926
33	1	-1.629616	2.447485	1.393752
34	1	-1.645367	-2.737350	0.681225
35	1	-2.287323	-2.135277	2.207967
36	1	4.293115	-1.106857	-0.121550
37	1	4.448942	-1.903855	1.432737

38	1	4.749677	0.477995	1.723452
39	1	3.287914	-0.021758	2.547284
40	1	3.383810	2.545848	2.341965
41	1	2.235344	3.064202	1.113368
42	1	1.198173	2.671583	3.337312
43	1	1.689616	0.992549	3.280815
44	1	-0.746791	1.160006	3.859520
45	1	-1.753188	0.757612	2.486079
46	1	0.690314	-0.800383	3.433240
47	1	-0.975252	-1.235931	3.743762
48	1	0.233978	-3.430256	1.096964
49	1	0.259977	-3.249665	2.842726
50	1	2.274504	-1.829687	2.703686
51	1	2.521637	-3.427166	2.033839
52	8	0.881955	1.995055	-3.382124
53	1	0.783610	2.376495	-2.490808
54	1	-0.687537	1.026454	-3.114491
55	64	0.793264	-0.000557	-0.202895
56	8	-1.391716	0.524389	-2.669781
57	1	-1.385217	-0.389586	-3.014605
58	6	-3.771997	-0.765585	0.263035
59	6	-4.628478	-1.664882	0.931168
60	6	-4.343344	0.195242	-0.610661
61	6	-5.995081	-1.603784	0.784648
62	1	-4.208520	-2.418760	1.583756
63	6	-5.735820	0.259950	-0.728348
64	6	-6.546379	-0.620587	-0.042393
65	1	-6.633114	-2.302299	1.310082
66	1	-6.153325	1.009921	-1.388711
67	1	-7.621875	-0.552537	-0.158387
68	1	1.553825	1.316057	-3.236877
69	8	-1.427209	-2.150271	-3.157974
70	1	-0.807880	-2.296581	-2.412144
71	1	-0.973424	-2.500864	-3.926533
72	8	-3.661637	1.085890	-1.343227
73	1	-2.729440	0.838619	-1.542318
74	8	-3.453574	3.614680	0.142700
75	1	-2.576964	3.972883	-0.058575
76	1	-3.527607	2.845886	-0.434841

E(RwB97XD) = -2018.645529 Hartree
Zero-point correction = 0.626596
Thermal correction to Energy = 0.667048
Thermal correction to Enthalpy = 0.667993
Thermal correction to Gibbs Free Energy = 0.556006
Sum of electronic and zero-point Energies = -2018.018933
Sum of electronic and thermal Energies = -2017.978481
Sum of electronic and thermal Enthalpies = -2017.977536
Sum of electronic and thermal Free Energies = -2018.089523

Table S7. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-DiHAP·4H_2O system (0 Imaginary Frequencies).

Center Number	Coordinates (Angstroms) X	Y	Z

1	7	2.505121	-1.966729	0.738511
2	6	3.763804	-1.342587	1.204296
3	6	3.534396	-0.095310	2.040724
4	7	2.822970	0.983215	1.322596
5	6	2.248980	1.940008	2.295615
6	6	1.000474	1.412306	2.981199
7	7	-0.125055	1.132609	2.061691
8	6	-1.109448	0.263450	2.741839
9	6	-0.677806	-1.192426	2.788077
10	7	-0.438189	-1.788157	1.455515
11	6	0.388925	-3.011418	1.591713
12	6	1.858174	-2.707352	1.838758
13	6	2.767080	-2.846299	-0.415623
14	6	1.674700	-2.868063	-1.490606
15	8	0.667303	-2.106771	-1.314848
16	8	1.880712	-3.566018	-2.484471
17	6	3.712630	1.686570	0.377881
18	6	3.692829	1.173197	-1.065949
19	8	4.356968	1.784348	-1.898619
20	8	2.931104	0.174303	-1.315686
21	6	-0.769247	2.382780	1.624111
22	6	-0.206090	3.008622	0.346382
23	8	-0.645460	4.105430	0.005145
24	8	0.656230	2.324976	-0.304817
25	6	-1.711871	-2.126323	0.802841
26	6	-2.344888	-0.941442	0.103889
27	8	-1.572341	-0.053543	-0.317635
28	1	3.656828	-2.486006	-0.932783
29	1	2.975760	-3.875272	-0.100183
30	1	4.750571	1.692962	0.730815
31	1	3.395890	2.727616	0.309374
32	1	-0.751583	3.143251	2.413690
33	1	-1.822635	2.193770	1.408362
34	1	-1.510711	-2.838778	-0.003337
35	1	-2.397105	-2.604820	1.507469
36	1	4.348527	-1.082685	0.323700
37	1	4.356696	-2.055142	1.792423
38	1	4.506451	0.267951	2.399428
39	1	2.957922	-0.350543	2.929519
40	1	2.986205	2.195244	3.067847
41	1	2.012611	2.859766	1.763723
42	1	0.688279	2.140124	3.741640
43	1	1.237107	0.493590	3.517054
44	1	-1.286613	0.604428	3.769954
45	1	-2.063445	0.355837	2.223499
46	1	0.240949	-1.282966	3.365592
47	1	-1.439496	-1.767253	3.330657
48	1	0.285597	-3.588998	0.674883
49	1	0.016904	-3.635692	2.413949
50	1	1.967046	-2.128275	2.755718
51	1	2.380052	-3.657528	2.014069
52	8	1.663910	2.916452	-2.774626
53	1	1.372878	2.971075	-1.845142
54	1	0.683843	1.375583	-2.767255
55	64	0.865835	-0.059013	-0.157829
56	8	0.295820	0.505171	-2.544804
57	1	0.793830	-0.118138	-3.110982
58	6	-3.757249	-0.843105	-0.130989
59	6	-4.670431	-1.817762	0.330160
60	6	-4.283867	0.273459	-0.845639

61	6	-6.017601	-1.706870	0.114904
62	1	-4.308188	-2.684232	0.866655
63	6	-5.649176	0.393150	-1.054482
64	6	-6.511978	-0.585489	-0.579939
65	1	-6.698692	-2.467747	0.476662
66	1	-6.036637	1.247360	-1.594055
67	1	2.593861	2.660195	-2.721665
68	8	2.285408	-0.942697	-3.800567
69	1	2.181895	-1.884568	-3.605974
70	1	2.749853	-0.582649	-3.023416
71	1	-2.573112	0.998779	-1.147234
72	8	-3.469356	3.751191	0.297630
73	1	-2.549177	4.036154	0.190184
74	1	-3.577603	3.061466	-0.365013
75	8	-3.502898	1.241089	-1.340025
76	8	-7.817299	-0.413296	-0.814315
77	1	-8.326773	-1.143257	-0.450814

E(RwB97XD) = -2093.8873186 Hartree
Zero-point correction = 0.633825
Thermal correction to Energy = 0.675124
Thermal correction to Enthalpy = 0.676068
Thermal correction to Gibbs Free Energy = 0.563376
Sum of electronic and zero-point Energies = -2093.253493
Sum of electronic and thermal Energies = -2093.212195
Sum of electronic and thermal Enthalpies = -2093.211250
Sum of electronic and thermal Free Energies = -2093.323942

Table S8. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-DiHAP·4H_2O system (1 Imaginary Frequency).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	-2.660356	-1.877630	-0.568384
2	6	-3.953065	-1.257135	-0.938009
3	6	-3.779862	0.009921	-1.761854
4	7	-3.011268	1.063440	-1.065250
5	6	-2.510696	2.064382	-2.033479
6	6	-1.311352	1.574028	-2.826917
7	7	-0.132176	1.230270	-1.999328
8	6	0.780456	0.368820	-2.784625
9	6	0.322398	-1.079124	-2.846472
10	7	0.202495	-1.727800	-1.522893
11	6	-0.638893	-2.941004	-1.627308
12	6	-2.122356	-2.624622	-1.725426
13	6	-2.831146	-2.765032	0.595936
14	6	-1.551471	-3.010798	1.400224
15	8	-0.683804	-2.054843	1.355582
16	8	-1.442314	-4.030743	2.059753
17	6	-3.844611	1.719926	-0.041406
18	6	-3.922145	0.962144	1.288603
19	8	-4.932849	1.049472	1.968262
20	8	-2.848600	0.327424	1.618209
21	6	0.578942	2.442430	-1.552231
22	6	0.106555	3.045197	-0.226265
23	8	0.604961	4.114148	0.122628

24	8	-0.742662	2.370018	0.448237
25	6	1.525336	-2.085958	-0.996259
26	6	2.194803	-0.921419	-0.298762
27	8	1.448889	-0.059793	0.197515
28	1	-3.510221	-2.273225	1.296910
29	1	-3.273258	-3.725625	0.310974
30	1	-4.855502	1.918388	-0.412291
31	1	-3.379236	2.676654	0.208126
32	1	0.554962	3.227938	-2.316466
33	1	1.631344	2.202305	-1.386705
34	1	1.397609	-2.833924	-0.207524
35	1	2.152483	-2.529033	-1.774211
36	1	-4.497581	-1.031574	-0.021792
37	1	-4.573023	-1.962617	-1.505327
38	1	-4.773139	0.387504	-2.037000
39	1	-3.271040	-0.224827	-2.696492
40	1	-3.301836	2.347883	-2.739373
41	1	-2.241334	2.959540	-1.475815
42	1	-1.040945	2.344690	-3.560233
43	1	-1.590224	0.690534	-3.400878
44	1	0.879730	0.743899	-3.810969
45	1	1.774236	0.429554	-2.342533
46	1	-0.649133	-1.132828	-3.336031
47	1	1.019499	-1.639399	-3.483377
48	1	-0.449865	-3.561678	-0.752628
49	1	-0.353832	-3.535608	-2.504655
50	1	-2.315251	-2.042439	-2.626249
51	1	-2.668603	-3.568981	-1.847479
52	8	-1.457369	2.463171	3.114093
53	1	-1.240462	2.691336	2.191731
54	1	0.177607	1.505674	3.050801
55	64	-0.974225	0.005353	0.236338
56	8	0.923824	1.017535	2.669237
57	1	0.947851	0.141240	3.095339
58	6	3.619372	-0.813942	-0.149744
59	6	4.506509	-1.708805	-0.787371
60	6	4.181029	0.244941	0.622033
61	6	5.866337	-1.573952	-0.698725
62	1	4.112778	-2.527993	-1.373676
63	6	5.560216	0.387150	0.701485
64	6	6.397510	-0.505843	0.047935
65	1	6.525080	-2.271739	-1.201912
66	1	5.979300	1.195914	1.285799
67	1	-2.061172	1.718134	3.002802
68	8	1.030685	-1.639125	3.406956
69	1	0.432210	-1.934581	2.689559
70	1	0.600960	-1.916062	4.218077
71	8	3.458689	1.143035	1.300619
72	1	2.502060	0.933731	1.288146
73	8	3.388405	3.645206	-0.290342
74	1	2.486436	3.972967	-0.154479
75	1	3.472207	2.934129	0.353932
76	8	7.716135	-0.305677	0.165861
77	1	8.203756	-0.976857	-0.319784

E(RwB97XD) = -2093.8763053 Hartree
Zero-point correction = 0.631998
Thermal correction to Energy = 0.673458
Thermal correction to Enthalpy = 0.674402

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Thermal correction to Gibbs Free Energy = 0.560258
Sum of electronic and zero-point Energies = -2093.244308
Sum of electronic and thermal Energies = -2093.202847
Sum of electronic and thermal Enthalpies = -2093.201903
Sum of electronic and thermal Free Energies = -2093.316047
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Table S9. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*o*AnAP·3H_2O system (0 Imaginary Frequencies).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	1.912629	-2.101685	0.843283
2	6	3.270700	-1.654536	1.223581
3	6	3.275309	-0.333792	1.973955
4	7	2.702412	0.797606	1.213283
5	6	2.326569	1.878161	2.152113
6	6	1.022755	1.599881	2.883060
7	7	-0.147636	1.444889	1.992906
8	6	-1.250932	0.800760	2.737032
9	6	-1.058612	-0.699544	2.891966
10	7	-0.947513	-1.427801	1.609269
11	6	-0.302497	-2.743820	1.829558
12	6	1.202722	-2.643766	2.017459
13	6	1.987077	-3.093936	-0.244003
14	6	0.867550	-3.018860	-1.288420
15	8	0.001572	-2.094457	-1.153634
16	8	0.925965	-3.816403	-2.226393
17	6	3.644427	1.303248	0.197685
18	6	3.523190	0.675249	-1.194828
19	8	4.265618	1.098638	-2.077424
20	8	2.606424	-0.202996	-1.356805
21	6	-0.579726	2.751688	1.468251
22	6	0.237913	3.255391	0.273499
23	8	0.345543	4.457517	0.085351
24	8	0.718406	2.334078	-0.486671
25	6	-2.274022	-1.625968	1.005497
26	6	-2.734511	-0.437225	0.177738
27	8	-1.852809	0.331353	-0.245948
28	1	2.903794	-2.922498	-0.809237
29	1	2.039822	-4.117568	0.145549
30	1	4.685145	1.216278	0.531800
31	1	3.447574	2.364416	0.040339
32	1	-0.588162	3.518328	2.250941
33	1	-1.600686	2.645973	1.092390
34	1	-2.211642	-2.453218	0.292611
35	1	-3.007536	-1.900853	1.768479
36	1	3.852576	-1.551647	0.309815
37	1	3.768920	-2.409859	1.845851
38	1	4.308199	-0.104258	2.267523
39	1	2.711023	-0.436221	2.900690
40	1	3.115015	2.032806	2.900027
41	1	2.244221	2.807773	1.591494
42	1	0.843986	2.415487	3.596593
43	1	1.121449	0.690435	3.475579
44	1	-1.353830	1.241475	3.737175
45	1	-2.183305	1.007173	2.212638

46	1	-0.153842	-0.893013	3.467023
47	1	-1.890491	-1.099934	3.486188
48	1	-0.518471	-3.370521	0.965894
49	1	-0.733504	-3.241121	2.707927
50	1	1.427492	-2.010218	2.875416
51	1	1.586027	-3.643017	2.265095
52	8	1.759925	2.597617	-2.978537
53	1	1.508570	2.743251	-2.045255
54	1	0.552781	1.226415	-2.860128
55	64	0.548426	-0.020583	-0.150881
56	8	0.038719	0.443233	-2.577718
57	1	0.430878	-0.288150	-3.095118
58	6	-4.122126	-0.242817	-0.155126
59	6	-5.111862	-1.142226	0.316371
60	6	-4.526306	0.847208	-0.989430
61	6	-6.436157	-0.996056	0.001859
62	1	-4.818005	-1.977001	0.938592
63	6	-5.905019	0.978046	-1.291610
64	6	-6.825456	0.084199	-0.811421
65	1	-7.171646	-1.697841	0.372598
66	1	-6.219619	1.803855	-1.919884
67	1	-7.871168	0.214943	-1.066551
68	1	2.638889	2.200174	-2.932564
69	8	1.759996	-1.393897	-3.728978
70	1	1.508783	-2.289909	-3.465730
71	1	2.280306	-1.053797	-2.977809
72	1	-2.674798	1.636117	-1.349300
73	7	-3.665265	1.753595	-1.489543
74	1	-4.001179	2.461665	-2.119297

E(RwB97XD) = -1922.3458807 Hartree

Zero-point correction = 0.614893
Thermal correction to Energy = 0.653162
Thermal correction to Enthalpy = 0.654107
Thermal correction to Gibbs Free Energy = 0.547365
Sum of electronic and zero-point Energies = -1921.730988
Sum of electronic and thermal Energies = -1921.692718
Sum of electronic and thermal Enthalpies = -1921.691774
Sum of electronic and thermal Free Energies = -1921.798515

Table S10. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*o*AnAP·3H_2O system (1 Imaginary Frequency).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	2.113645	2.066555	-0.536253
2	6	3.495500	1.642631	-0.848668
3	6	3.536873	0.364842	-1.669002
4	7	2.901448	-0.784296	-0.993598
5	6	2.596256	-1.844223	-1.978351
6	6	1.356568	-1.544245	-2.806248
7	7	0.117262	-1.374840	-2.015263
8	6	-0.890738	-0.666702	-2.833844
9	6	-0.643762	0.832447	-2.903355
10	7	-0.667756	1.509956	-1.588888

11	6	0.004525	2.823960	-1.687143
12	6	1.519067	2.712833	-1.725973
13	6	2.113478	2.987510	0.613572
14	6	0.784210	3.068876	1.368707
15	8	0.053217	2.006973	1.312056
16	8	0.519425	4.074619	2.007304
17	6	3.776923	-1.308522	0.069102
18	6	3.690976	-0.543708	1.395020
19	8	4.679813	-0.473560	2.109156
20	8	2.522596	-0.082146	1.686966
21	6	-0.406640	-2.678829	-1.572221
22	6	0.299109	-3.261870	-0.341834
23	8	0.301570	-4.472023	-0.175679
24	8	0.801222	-2.392244	0.461997
25	6	-2.050157	1.696638	-1.125696
26	6	-2.582592	0.481326	-0.386690
27	8	-1.740341	-0.289159	0.099674
28	1	2.827375	2.607248	1.348597
29	1	2.429742	3.995632	0.324037
30	1	4.820692	-1.360094	-0.258333
31	1	3.443148	-2.320683	0.310079
32	1	-0.393317	-3.415549	-2.382956
33	1	-1.445443	-2.538346	-1.261515
34	1	-2.067106	2.501704	-0.385118
35	1	-2.697931	1.997788	-1.953682
36	1	4.029667	1.498418	0.089861
37	1	4.028436	2.430873	-1.395726
38	1	4.583226	0.132132	-1.906770
39	1	3.032726	0.522521	-2.622342
40	1	3.440824	-1.988375	-2.664682
41	1	2.466869	-2.780829	-1.439240
42	1	1.224151	-2.352324	-3.537877
43	1	1.516713	-0.633326	-3.382889
44	1	-0.903633	-1.062135	-3.857584
45	1	-1.876637	-0.868239	-2.416576
46	1	0.328272	1.018821	-3.358689
47	1	-1.388596	1.279635	-3.574760
48	1	-0.299977	3.425769	-0.832425
49	1	-0.324547	3.361658	-2.585880
50	1	1.822757	2.147354	-2.606394
51	1	1.935303	3.721336	-1.849810
52	8	1.477956	-2.384324	3.129005
53	1	1.312399	-2.637991	2.201374
54	1	-0.270924	-1.666206	3.069676
55	64	0.659416	-0.032272	0.244165
56	8	-1.071245	-1.282912	2.677227
57	1	-1.216697	-0.415630	3.097197
58	6	-3.991696	0.253051	-0.203408
59	6	-4.946661	1.104199	-0.814791
60	6	-4.452257	-0.840304	0.597664
61	6	-6.293906	0.903619	-0.678385
62	1	-4.606684	1.941487	-1.409585
63	6	-5.854438	-1.029089	0.707795
64	6	-6.740794	-0.185861	0.091772
65	1	-7.002331	1.567237	-1.156640
66	1	-6.216354	-1.859332	1.304201
67	1	-7.804485	-0.363101	0.205732
68	1	1.951504	-1.549044	3.024980
69	8	-1.518359	1.342982	3.415432
70	1	-1.003487	1.717265	2.670317

71	1	-1.082810	1.671181	4.204106
72	1	-2.649305	-1.512218	1.362383
73	7	-3.637514	-1.702358	1.237887
74	1	-4.061649	-2.351500	1.879933

E(RwB97XD) = -1922.3349016 Hartree
Zero-point correction = 0.613889
Thermal correction to Energy = 0.652051
Thermal correction to Enthalpy = 0.652995
Thermal correction to Gibbs Free Energy = 0.545024
Sum of electronic and zero-point Energies = -1921.721012
Sum of electronic and thermal Energies = -1921.682851
Sum of electronic and thermal Enthalpies = -1921.681907
Sum of electronic and thermal Free Energies = -1921.789878

Table S11. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*p*HAP·3H_2O system (0 Imaginary Frequencies).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	-1.968264	-2.003626	-1.037704
2	6	-3.359540	-1.572289	-1.303577
3	6	-3.450247	-0.168191	-1.877387
4	7	-2.890752	0.880537	-0.998634
5	6	-2.595557	2.091947	-1.795394
6	6	-1.314713	1.975217	-2.606611
7	7	-0.098025	1.750652	-1.796317
8	6	0.988459	1.253512	-2.665664
9	6	0.831464	-0.217502	-3.015706
10	7	0.820241	-1.114650	-1.840587
11	6	0.216617	-2.420202	-2.199693
12	6	-1.298812	-2.368572	-2.301814
13	6	-1.957423	-3.128617	-0.084508
14	6	-0.787566	-3.148391	0.906243
15	8	0.037315	-2.178146	0.856709
16	8	-0.769290	-4.064669	1.729670
17	6	-3.804517	1.206146	0.111711
18	6	-3.593893	0.410939	1.404364
19	8	-4.308889	0.684726	2.364835
20	8	-2.638409	-0.441187	1.412377
21	6	0.312484	2.989820	-1.116037
22	6	-0.475156	3.295719	0.162897
23	8	-0.623125	4.456541	0.512832
24	8	-0.887640	2.261779	0.810182
25	6	2.181314	-1.325857	-1.329607
26	6	2.626835	-0.270545	-0.337519
27	8	1.776644	0.430080	0.212828
28	1	-2.847772	-3.061876	0.541640
29	1	-2.001717	-4.095227	-0.599918
30	1	-4.855174	1.114337	-0.188336
31	1	-3.644887	2.246162	0.398583
32	1	0.264663	3.854279	-1.787521
33	1	1.350165	2.872838	-0.792567
34	1	2.204584	-2.262498	-0.764395
35	1	2.900710	-1.422074	-2.149768
36	1	-3.904511	-1.613778	-0.362592

37	1	-3.853971	-2.264339	-1.998070
38	1	-4.503453	0.048815	-2.099857
39	1	-2.923235	-0.127577	-2.830741
40	1	-3.420331	2.311557	-2.485940
41	1	-2.525974	2.939844	-1.116306
42	1	-1.201013	2.888973	-3.205451
43	1	-1.406995	1.153966	-3.316926
44	1	1.034804	1.829276	-3.599249
45	1	1.937049	1.417499	-2.155175
46	1	-0.099928	-0.366335	-3.560385
47	1	1.637661	-0.502916	-3.704178
48	1	0.502009	-3.140957	-1.435351
49	1	0.620760	-2.781420	-3.154100
50	1	-1.593429	-1.650308	-3.066873
51	1	-1.653146	-3.348537	-2.648800
52	8	-1.822632	2.161057	3.356432
53	1	-1.617048	2.437653	2.441800
54	1	-0.577009	0.861516	3.017653
55	64	-0.642815	-0.020754	0.172099
56	8	-0.054222	0.138883	2.615099
57	1	-0.402742	-0.666998	3.046325
58	6	4.039667	-0.126225	0.004436
59	6	5.036692	-0.961368	-0.516237
60	6	4.405792	0.876829	0.917006
61	6	6.356051	-0.805645	-0.136918
62	6	5.718517	1.046852	1.292979
63	6	6.703573	0.201801	0.767885
64	1	7.120585	-1.460818	-0.539364
65	1	6.008082	1.821000	1.992453
66	1	-2.688900	1.739290	3.291578
67	8	-1.655179	-1.901537	3.570159
68	1	-1.379531	-2.743485	3.182739
69	1	-2.221895	-1.490381	2.891670
70	1	3.636403	1.521388	1.323143
71	1	4.795329	-1.752240	-1.215224
72	8	7.966387	0.407939	1.171997
73	1	8.559699	-0.224798	0.757763

E(RwB97XD) = -1942.204832 Hartree
Zero-point correction = 0.602989
Thermal correction to Energy = 0.640869
Thermal correction to Enthalpy = 0.641813
Thermal correction to Gibbs Free Energy = 0.535906
Sum of electronic and zero-point Energies = -1941.601843
Sum of electronic and thermal Energies = -1941.563963
Sum of electronic and thermal Enthalpies = -1941.563019
Sum of electronic and thermal Free Energies = -1941.668926

Table S12. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*p*MAP·3H_2O system (0 Imaginary Frequencies).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	-2.151799	-2.074256	-0.962882
2	6	-3.552722	-1.676731	-1.230510
3	6	-3.668383	-0.304507	-1.872542

4	7	-3.111624	0.790562	-1.048674
5	6	-2.849504	1.972844	-1.900369
6	6	-1.580344	1.839386	-2.726027
7	7	-0.352795	1.664168	-1.919575
8	6	0.734931	1.140813	-2.773986
9	6	0.598177	-0.348300	-3.048949
10	7	0.610973	-1.186514	-1.829322
11	6	0.025385	-2.518270	-2.120111
12	6	-1.491196	-2.496164	-2.213511
13	6	-2.106530	-3.142820	0.054087
14	6	-0.932078	-3.075715	1.038095
15	8	-0.127813	-2.090610	0.921722
16	8	-0.884629	-3.939606	1.912431
17	6	-4.017810	1.148441	0.058988
18	6	-3.781484	0.410178	1.379246
19	8	-4.530305	0.657921	2.317612
20	8	-2.761711	-0.367595	1.432732
21	6	0.048453	2.936154	-1.290962
22	6	-0.714523	3.282195	-0.005326
23	8	-0.866555	4.453053	0.301724
24	8	-1.101532	2.268815	0.692617
25	6	1.980007	-1.354100	-1.322069
26	6	2.423636	-0.255699	-0.377087
27	8	1.568930	0.444047	0.172567
28	1	-2.996080	-3.066234	0.680156
29	1	-2.126132	-4.137562	-0.405744
30	1	-5.070056	1.035452	-0.225265
31	1	-3.864626	2.200220	0.305531
32	1	-0.027843	3.773516	-1.992724
33	1	1.094384	2.848991	-0.985311
34	1	2.022467	-2.264893	-0.717186
35	1	2.690663	-1.477377	-2.145284
36	1	-4.085613	-1.678088	-0.281288
37	1	-4.047073	-2.409656	-1.881159
38	1	-4.726058	-0.109957	-2.092420
39	1	-3.151405	-0.302352	-2.832189
40	1	-3.689706	2.152207	-2.583038
41	1	-2.779047	2.848090	-1.256588
42	1	-1.485383	2.729631	-3.361582
43	1	-1.668715	0.988785	-3.401406
44	1	0.763760	1.670483	-3.734745
45	1	1.685413	1.345239	-2.281580
46	1	-0.335784	-0.538499	-3.576086
47	1	1.402341	-0.655437	-3.729842
48	1	0.326657	-3.194685	-1.321916
49	1	0.430545	-2.919194	-3.057611
50	1	-1.805574	-1.824681	-3.012438
51	1	-1.832453	-3.498749	-2.503320
52	8	-2.147291	2.366747	3.241003
53	1	-1.841727	2.471585	2.319191
54	1	-0.818688	1.111417	3.653512
55	64	-0.849115	-0.011338	0.107621
56	8	-0.152659	0.415481	3.781977
57	1	-0.682205	-0.398178	3.808649
58	6	3.838408	-0.074637	-0.073350
59	6	4.840399	-0.881930	-0.622413
60	6	4.207758	0.937987	0.830986
61	6	6.170275	-0.699729	-0.285461
62	6	5.524403	1.134043	1.166936
63	6	6.521227	0.313469	0.613256

64	1	6.919428	-1.344134	-0.723383
65	1	5.819594	1.911710	1.860082
66	1	-2.976683	1.879718	3.171327
67	8	-1.960297	-1.774880	3.693731
68	1	-1.565724	-2.567398	3.307468
69	1	-2.382863	-1.320757	2.941572
70	1	3.436726	1.564523	1.261406
71	1	4.599157	-1.676405	-1.317139
72	8	7.772800	0.575766	1.004459
73	6	8.835504	-0.222862	0.493535
74	1	9.741687	0.166776	0.950200
75	1	8.705892	-1.271512	0.773810
76	1	8.905379	-0.132052	-0.593597

E(RwB97XD) = -1981.4902999 Hartree
Zero-point correction = 0.630152
Thermal correction to Energy = 0.670144
Thermal correction to Enthalpy = 0.671088
Thermal correction to Gibbs Free Energy = 0.559843
Sum of electronic and zero-point Energies = -1980.860148
Sum of electronic and thermal Energies = -1980.820156
Sum of electronic and thermal Enthalpies = -1980.819211
Sum of electronic and thermal Free Energies= -1980.930457

Table S13. Optimized Cartesian coordinates (Å) obtained for the GdDO3A-*o*MAP·3H_2O system (0 Imaginary Frequencies).

Center Number		Coordinates (Angstroms) X	Y	Z
1	7	-1.683417	-2.190900	-1.018841
2	6	-3.075698	-1.946709	-1.455815
3	6	-3.259869	-0.594618	-2.123078
4	7	-2.929693	0.553697	-1.253718
5	6	-2.703716	1.757160	-2.084613
6	6	-1.342382	1.767370	-2.761065
7	7	-0.198143	1.732800	-1.825443
8	6	1.022506	1.325630	-2.551794
9	6	1.075323	-0.171932	-2.811975
10	7	1.048351	-0.997320	-1.584497
11	6	0.651408	-2.386803	-1.917313
12	6	-0.838209	-2.538171	-2.178886
13	6	-1.647417	-3.252246	0.003468
14	6	-0.592849	-3.078610	1.102530
15	8	0.114335	-2.019133	1.073117
16	8	-0.554903	-3.943291	1.979861
17	6	-3.994577	0.808236	-0.264830
18	6	-3.823116	0.120761	1.093551
19	8	-4.660953	0.355437	1.960802
20	8	-2.779374	-0.603326	1.249940
21	6	-0.009462	3.044236	-1.184267
22	6	-0.951114	3.310208	-0.003568
23	8	-1.262958	4.460217	0.264961
24	8	-1.307691	2.265137	0.658795
25	6	2.372567	-1.011022	-0.946271
26	6	2.587618	0.145108	0.005026
27	8	1.604315	0.749818	0.433164

28	1	-2.600224	-3.255483	0.533996
29	1	-1.529602	-4.244606	-0.447552
30	1	-4.984010	0.552201	-0.662305
31	1	-4.010475	1.874388	-0.036685
32	1	-0.095625	3.863529	-1.906624
33	1	0.997963	3.075530	-0.761284
34	1	2.468549	-1.907364	-0.327539
35	1	3.178646	-1.058643	-1.684025
36	1	-3.714133	-2.004650	-0.576388
37	1	-3.407504	-2.728049	-2.152126
38	1	-4.298578	-0.516730	-2.470967
39	1	-2.635257	-0.536294	-3.014397
40	1	-3.474484	1.841005	-2.861846
41	1	-2.806072	2.635185	-1.449259
42	1	-1.278804	2.661907	-3.395283
43	1	-1.261082	0.911702	-3.431114
44	1	1.094793	1.847037	-3.515186
45	1	1.888321	1.637445	-1.968091
46	1	0.227967	-0.462574	-3.431536
47	1	1.975855	-0.395026	-3.398894
48	1	0.937613	-3.022475	-1.081353
49	1	1.199791	-2.741480	-2.799355
50	1	-1.132344	-1.909109	-3.018882
51	1	-1.028874	-3.573849	-2.490598
52	8	-2.486678	2.162425	3.105848
53	1	-2.221438	2.420208	2.201356
54	1	-1.063751	1.020616	2.966900
55	64	-0.731546	0.002946	0.183854
56	8	-0.419508	0.351070	2.660066
57	1	-0.712041	-0.470410	3.103139
58	6	3.930755	0.572433	0.424730
59	6	5.099342	-0.206973	0.275030
60	6	4.033256	1.841971	1.011921
61	6	6.328087	0.311332	0.691436
62	6	5.249803	2.352961	1.416429
63	6	6.394958	1.577833	1.250180
64	1	7.232373	-0.271514	0.587639
65	1	5.311726	3.340647	1.854718
66	1	-3.282439	1.629561	2.980669
67	8	-1.862388	-1.817808	3.586613
68	1	-1.451456	-2.638019	3.280504
69	1	-2.398572	-1.514065	2.831314
70	1	3.125880	2.421390	1.127330
71	1	7.359031	1.961395	1.563724
72	8	4.957537	-1.436112	-0.242195
73	6	6.105269	-2.259430	-0.419238
74	1	6.822729	-1.789360	-1.096333
75	1	6.580086	-2.476885	0.540657
76	1	5.735937	-3.181468	-0.860795

E(RwB97XD) = -1981.4964259 Hartree
Zero-point correction = 0.630709
Thermal correction to Energy = 0.670188
Thermal correction to Enthalpy = 0.671132
Thermal correction to Gibbs Free Energy = 0.561295
Sum of electronic and zero-point Energies = -1980.865717
Sum of electronic and thermal Energies = -1980.826238
Sum of electronic and thermal Enthalpies = -1980.825294
Sum of electronic and thermal Free Energies = -1980.935131