Electronic Supplementary Information

Highly efficient extraction of actinides with pillar[5]arene-derived diglycolamides in ionic liquid via a unique mechanism involving competitive host-guest interactions

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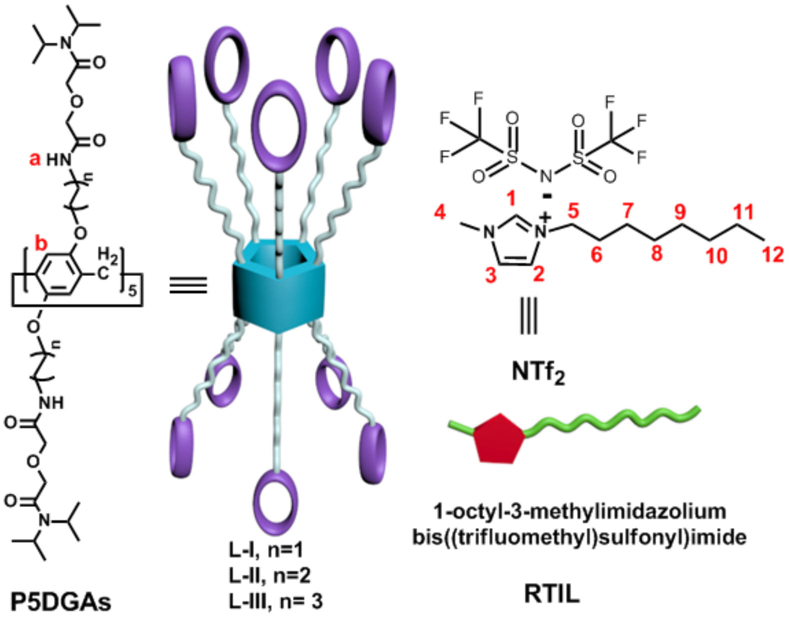
1. Partial 2D NOESY spectrum of L-I and $C_8minNTf_2$



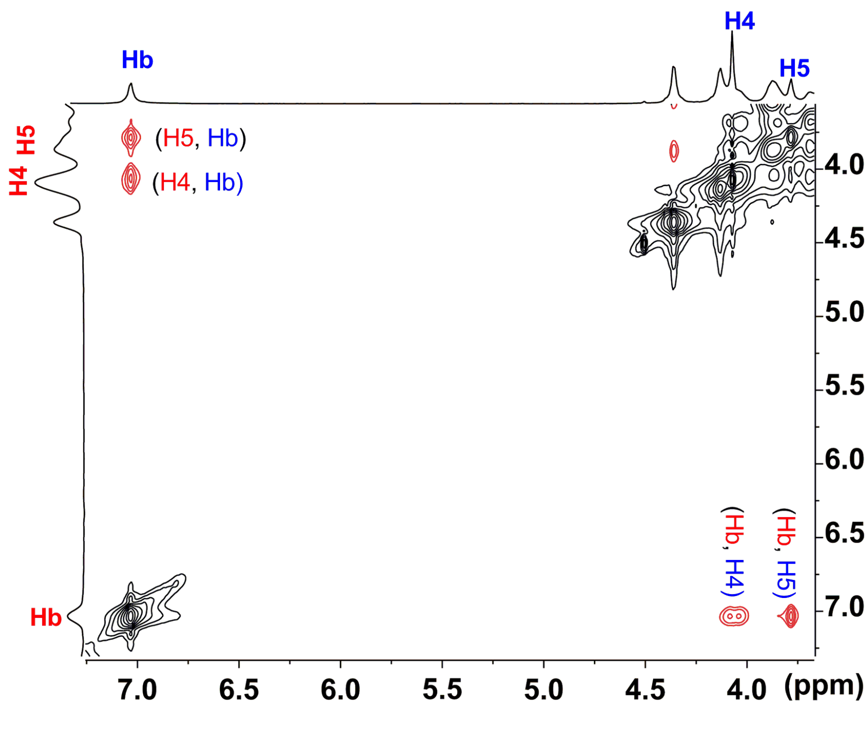


Fig. S1 Partial 2D NOESY spectrum (400 MHz, acetone-d_6, 298 K, mixing time = 0.3 s) of **L-I** (10.0 mM) and $C_8minNTf_2$ (10.0 mM).

2. [1]H NMR titration of P5DGAs and $C_8minNTf_2$

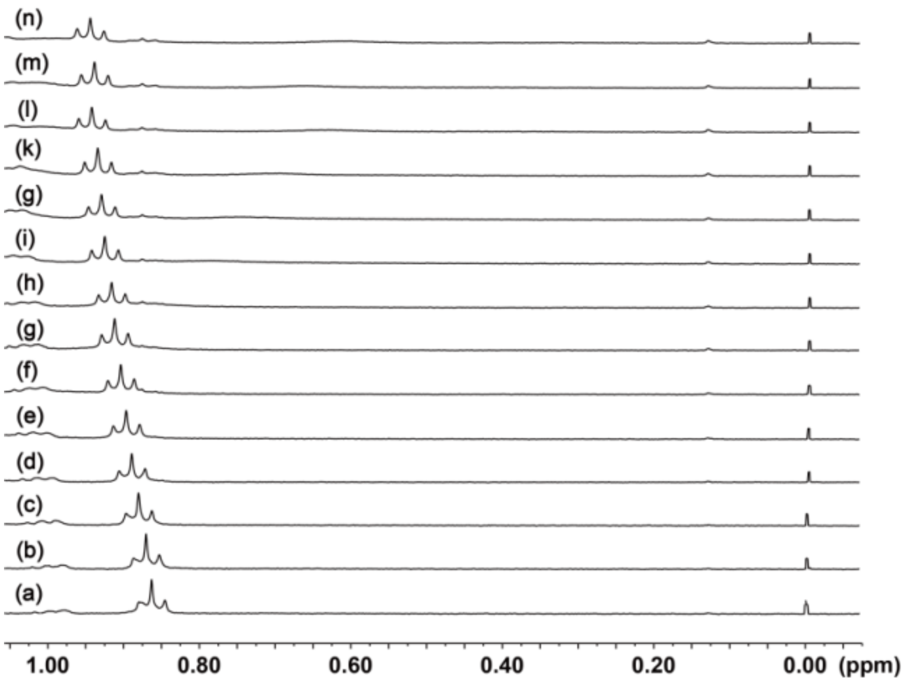


Fig. S2 Stacked plots of ^{1}H NMR (400 MHz, 298 K) spectra of compound **L-I** (2.0 mM) with $C_8minNTf_2$ (0-2.5 equiv.) at different concentration in acetone-d_6.

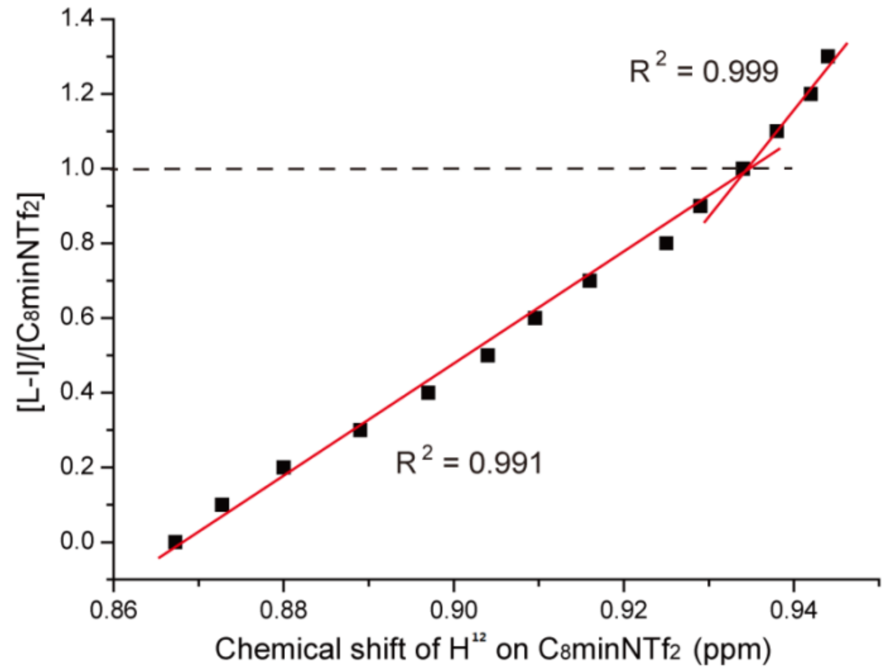


Fig. S3 Mole ratio plot for the complexation between **L-I** and $C_8minNTf_2$, indicating a 1:1 stoichiometry.

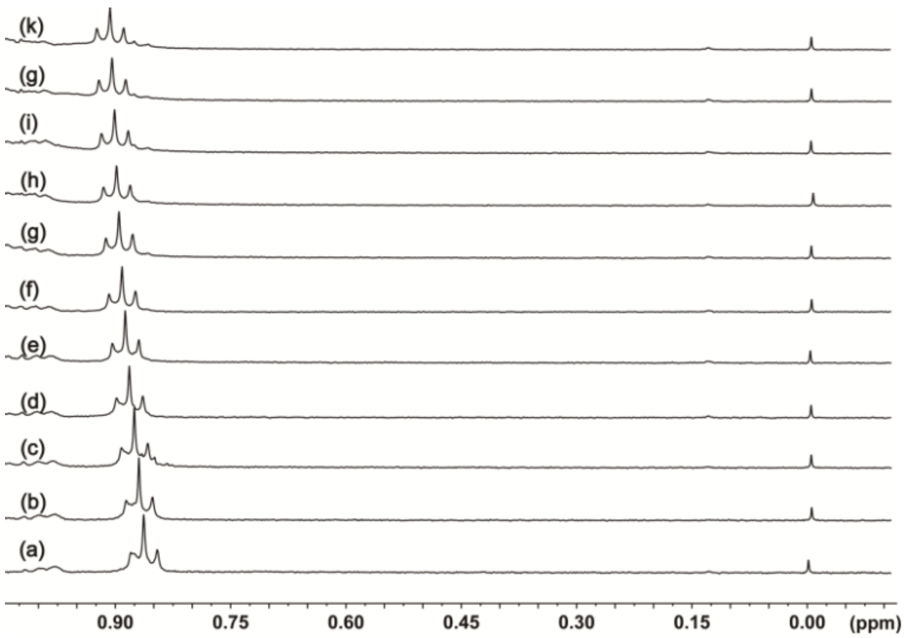


Fig. S4 Stacked plots of ^{1}H NMR (400 MHz, 298 K) spectra of compound **L-II** (2.0 mM) with $C_8minNTf_2$ (0-2.0 equiv.) at different concentration in acetone-d_6.

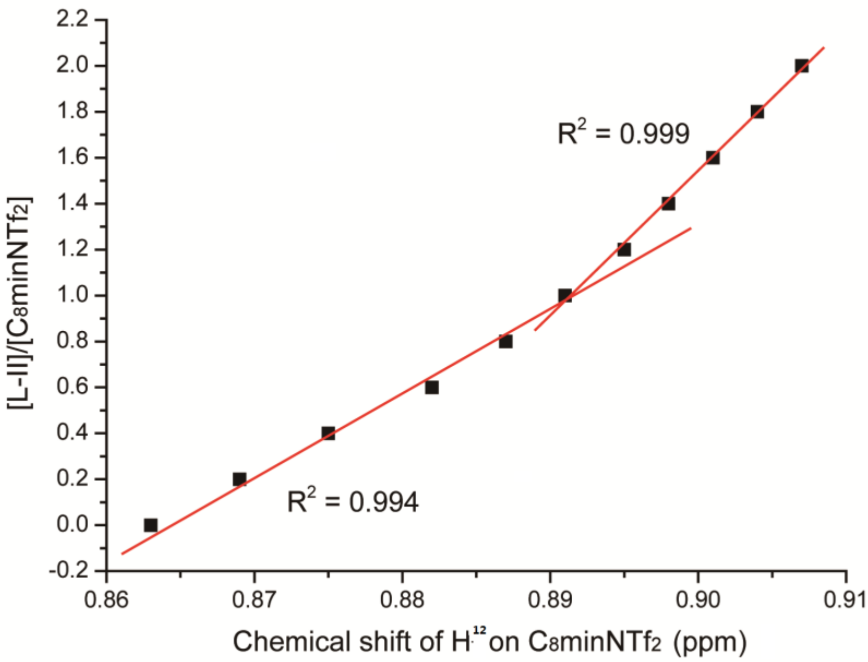


Fig. S5 Mole ratio plot for the complexation between **L-II** and $C_8minNTf_2$, indicating a 1:1 stoichiometry.

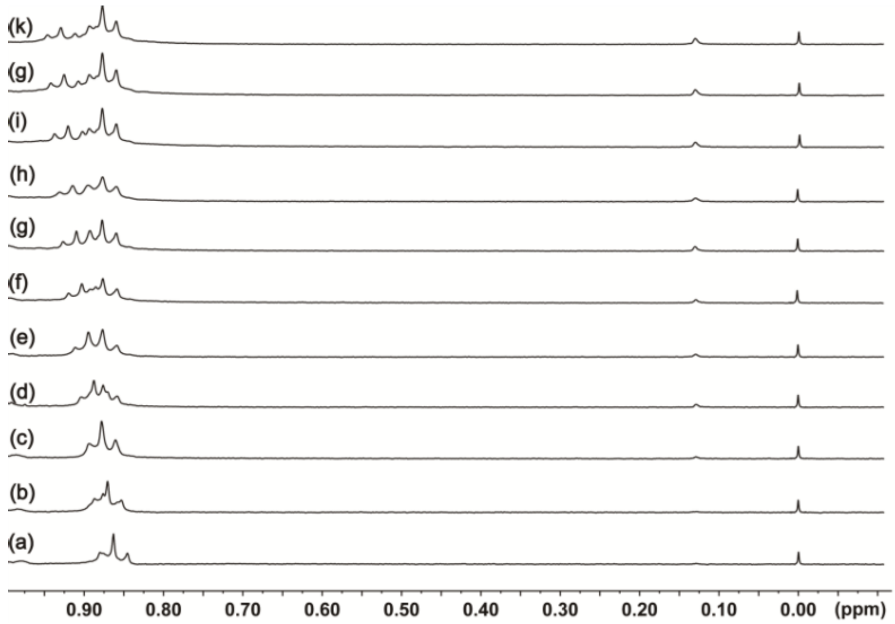


Fig. S6 Stacked plots of [1]H NMR (400 MHz, 298 K) spectra of compound **L-III** (2.0 mM) with $C_8minNTf_2$ (0- 2.0 equiv.) at different concentration in acetone-d_6.

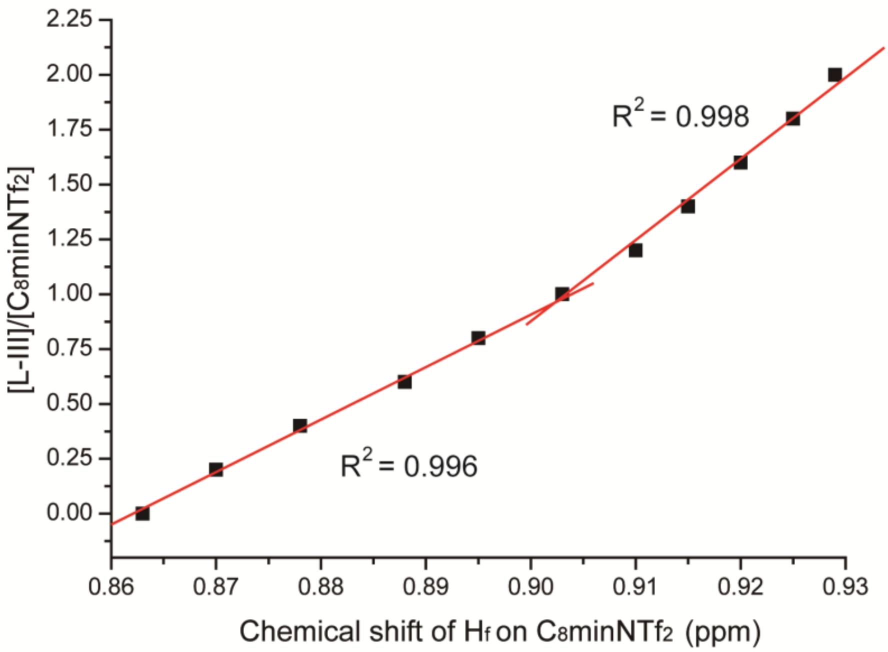


Fig. S7 Mole ratio plot for the complexation between **L-III** and $C_8minNTf_2$, indicating a 1:1 stoichiometry.

3. Job's plot for the complexation between L-I and C_8minNTf$_2$

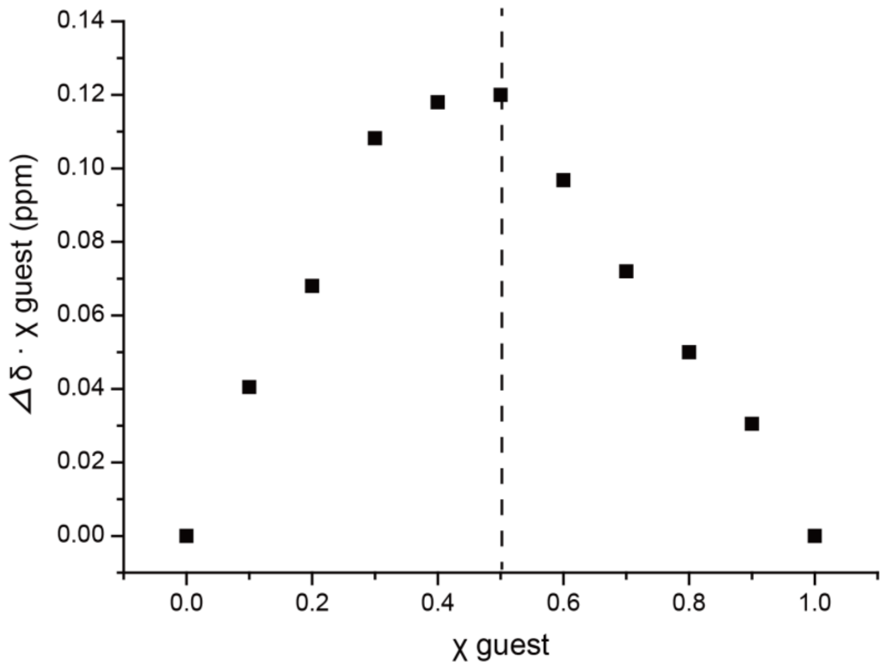


Fig. S8 Job's plot for the complexation between **L-I** and C_8minNTf$_2$; [**L-I**] + [C_8minNTf$_2$] = 10.0 mM, indicating a 1:1 stoichiometry.

4. ESI HR-MS for P5DGAs-Eu^{3+} complexes

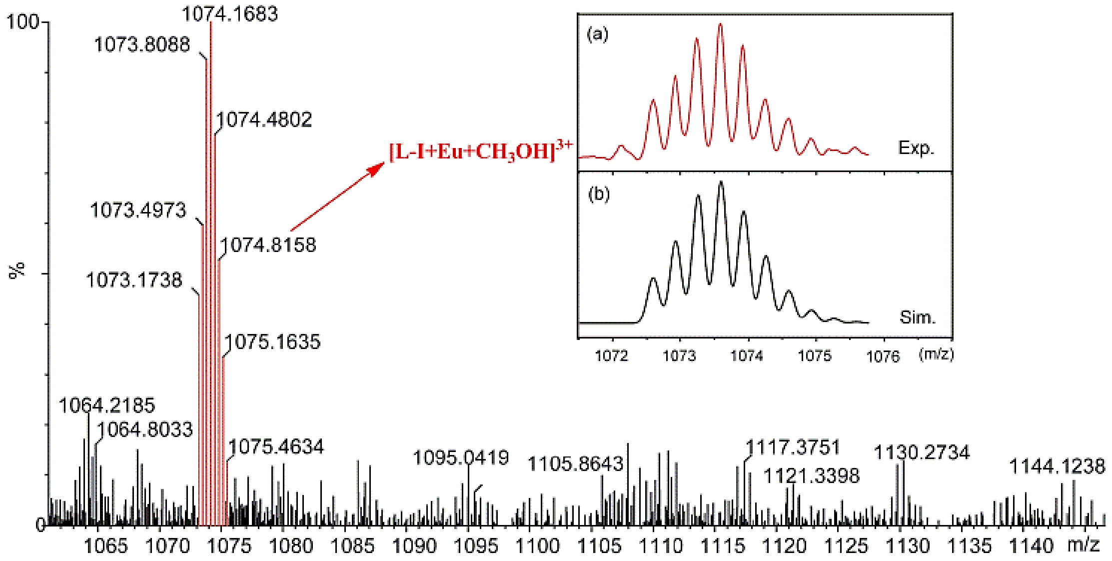


Fig. S9 HRESI-MS spectrum of the 1:1 (M:L) complex formed between **L-I** and Eu^{3+}. Inset: (a) experimental isotope distribution; (b) computer simulation.

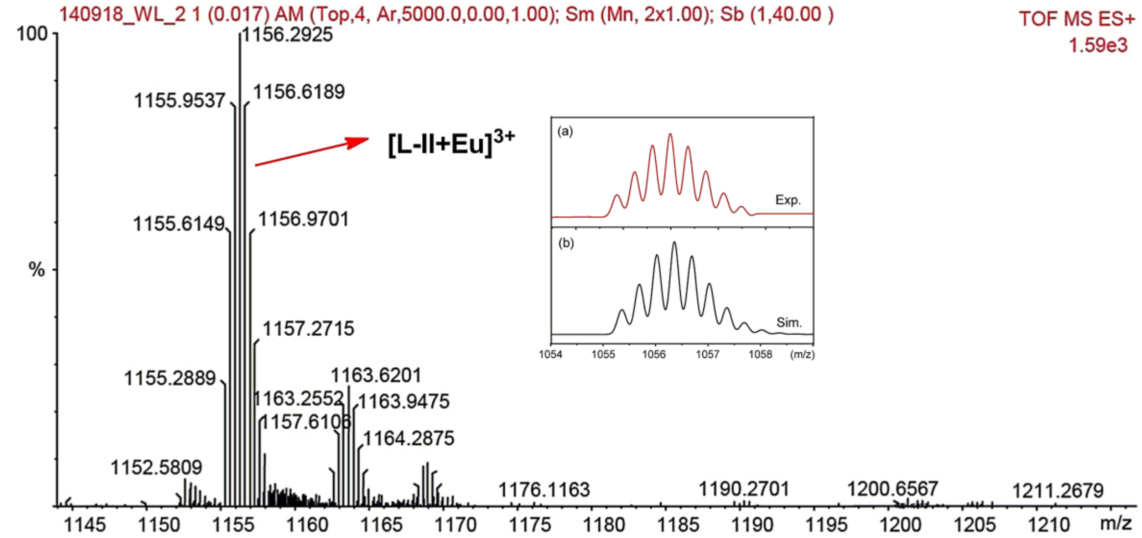


Fig. S10 HRESI-MS spectrum of the 1:1 (M:L) complex formed between **L-II** and Eu^{3+} (inset: experimental isotope distribution (red) and computer simulation (black)).

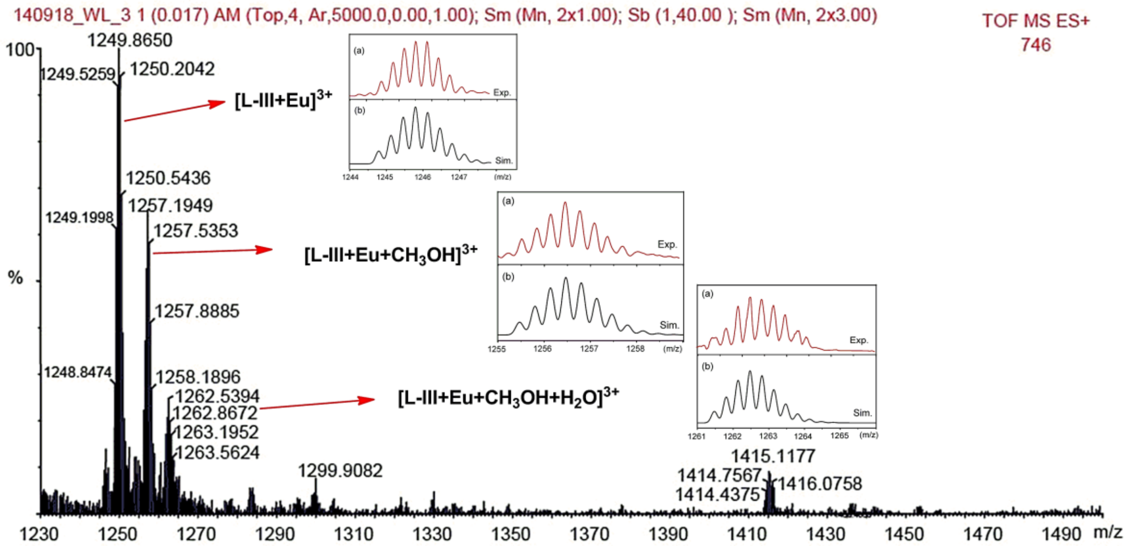


Fig. S11 HRESI-MS spectrum of the 1:1 (M:L) complex formed between **L-III** and Eu^{3+} (inset: experimental isotope distribution (red) and computer simulation (black)).

5. ESI HR-MS for P5DGAs-C_8mim^+ complexes

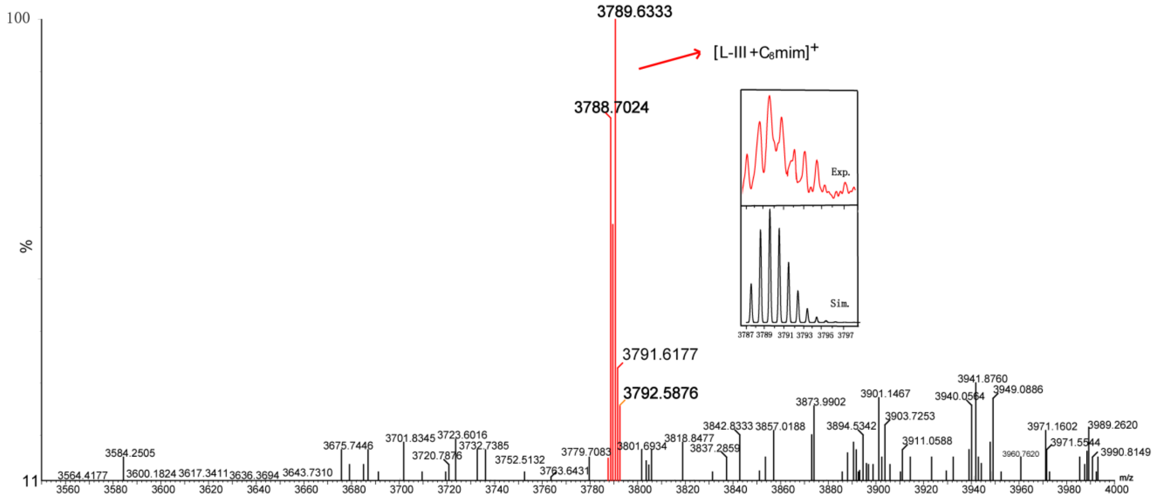


Fig. S12 HRESI-MS spectrum of the 1:1 (M : L) complex formed between **L-III** and C_8mim^+ (inset: experimental isotope distribution (red) and computer simulation (black)).

6. Density functional theory (DFT) calculations of L-I

The structure **L-I** was optimized by the density functional theory (DFT) method at the M062X/6-31G (d, p) level by employing the Gaussian 09 program. [S1]

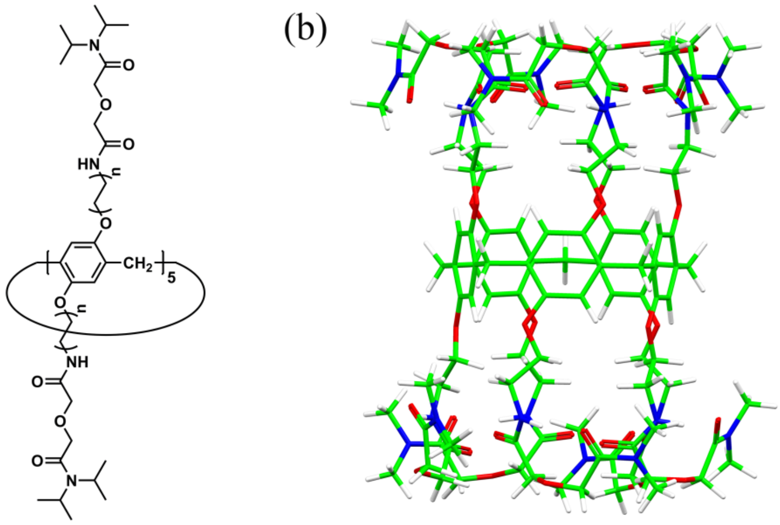


Fig. S13 (a) Chemical structure of **L-I** and (b) Geometry optimized molecular model of DGA-pillar[5]arene at the M062X/6-31G (d, p) level.

Table S1 Atomic coordinates for the optimized structure of **L-I**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.081520	1.251575	3.891965
2	6	0	-1.165066	-0.119124	4.123771
3	6	0	-0.010155	-0.887059	4.258498
4	6	0	1.234231	-0.259100	4.150219
5	6	0	1.317720	1.110799	3.912564

6	6	0	0.163556	1.880039	3.786579
7	8	0	-2.172765	2.070098	3.762269
8	6	0	-3.465421	1.510833	3.843955
9	6	0	-4.413437	2.703295	3.834595
10	7	0	-5.780390	2.292966	4.063551
11	6	0	-6.690288	2.290245	3.076618
12	6	0	-8.014130	1.616409	3.412445
13	8	0	-8.195389	1.417624	4.799932
14	6	0	-8.405506	0.096923	5.221692
15	6	0	-7.116591	-0.526773	5.778417
16	7	0	-7.171983	-1.836121	6.125514
17	8	0	2.327180	-1.074266	4.297781
18	6	0	3.608032	-0.492543	4.225789
19	6	0	4.593239	-1.576807	4.639337
20	7	0	5.936255	-1.036408	4.681127
21	6	0	6.763446	-1.179228	3.627957
22	6	0	7.974406	-0.258076	3.622955
23	8	0	8.254695	0.271684	4.904497
24	6	0	8.423907	1.664639	4.951665
25	6	0	7.086539	2.375904	5.208751
26	7	0	7.105259	3.730489	5.252352
27	6	0	0.244821	3.362402	3.495509
28	6	0	-0.078156	-2.385707	4.452454
29	6	0	-6.000448	-2.477971	6.693968
30	6	0	-8.316605	-2.709411	5.942753
31	8	0	-6.115779	0.160331	5.953637
32	8	0	-6.529529	2.780245	1.959000
33	8	0	6.591286	-1.966462	2.699544
34	8	0	6.071701	1.724622	5.438819
35	6	0	8.241683	4.560821	4.909351
36	6	0	5.903674	4.461068	5.611978
37	6	0	-1.048737	4.036512	-0.023900
38	6	0	-1.014001	3.796518	1.345617
39	6	0	0.203925	3.645649	2.009231
40	6	0	1.391894	3.724888	1.272189
41	6	0	1.353819	3.992413	-0.095502
42	6	0	0.137900	4.159884	-0.754441
43	8	0	-2.199759	4.175587	-0.752007
44	6	0	-3.457856	4.086702	-0.119558
45	6	0	-4.448592	4.418160	-1.229877
46	7	0	-5.798765	4.563459	-0.740230
47	6	0	-6.759067	3.675180	-1.033253
48	6	0	-8.084574	3.883934	-0.311733
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51	6	0	-7.022092	5.482987	2.426244
52	7	0	-7.026650	5.383433	3.777988
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54	6	0	3.788727	3.832041	1.354394
55	6	0	4.810111	3.893453	2.486188
56	7	0	6.068676	4.439309	2.021890
57	6	0	7.180377	3.700270	1.911745
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67	8	0	-6.652360	2.745202	-1.833061
68	8	0	7.339659	2.573482	2.380389
69	8	0	5.636096	6.392677	0.016387
70	6	0	7.032292	6.306519	-3.296464
71	6	0	4.776113	6.948729	-2.437091
72	6	0	-1.245119	-3.352650	2.438084
73	6	0	-1.233241	-3.985756	1.198386
74	6	0	-0.027928	-4.361032	0.606350
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76	6	0	1.155086	-3.468669	2.524348
77	6	0	-0.049501	-3.102199	3.120273
78	8	0	-2.382861	-2.933412	3.073867
79	6	0	-3.648593	-3.239567	2.529680
80	6	0	-4.631975	-2.858083	3.629532
81	7	0	-5.988983	-3.230522	3.303096
82	6	0	-6.908060	-2.314946	2.964561
83	6	0	-8.244809	-2.867243	2.488825
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87	7	0	-7.235339	-6.513478	0.083542
88	8	0	2.312879	-4.470482	0.628450
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90	6	0	4.582812	-4.821888	0.277383
91	7	0	5.937471	-4.611381	0.725275
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93	6	0	8.125348	-3.572993	0.730832

94	8	0	8.425569	-4.558026	1.696170
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99	6	0	-6.039986	-7.236212	-0.310743
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137	8	0	-6.762974	-0.913107	-3.077774

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139	8	0	6.384205	1.799263	-5.560410
140	6	0	8.513886	-1.006201	-6.367518
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145	6	0	1.224659	-2.382968	-3.277989
146	6	0	1.228686	-3.389823	-2.314999
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163	6	0	8.186116	-2.257805	-3.216701
164	8	0	8.198605	-3.524181	-3.844058
165	6	0	8.113193	-4.646629	-3.005862
166	6	0	6.702045	-5.247094	-2.988266
167	7	0	6.455416	-6.239173	-2.095829
168	6	0	-6.020275	-1.846303	-6.892403
169	6	0	-8.324872	-1.161327	-6.440325
170	8	0	-6.208372	-3.565766	-4.762741
171	8	0	-6.693733	-3.342559	-0.000613
172	8	0	6.870754	-0.281057	-3.094431
173	8	0	5.860863	-4.896612	-3.809802
174	6	0	7.451163	-6.797906	-1.198078
175	6	0	5.210010	-6.977223	-2.253996
176	1	0	-2.123884	-0.623252	4.180267
177	1	0	2.274841	1.607367	3.793697
178	1	0	-3.666556	0.837360	2.998882
179	1	0	-3.595972	0.942674	4.776334
180	1	0	-4.085487	3.394595	4.617694
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182	1	0	-5.992792	1.722350	4.885535
183	1	0	-8.819497	2.259129	3.033452
184	1	0	-8.019082	0.669314	2.863445
185	1	0	-9.152320	0.121102	6.025503
186	1	0	-8.793551	-0.516781	4.403646
187	1	0	3.826914	-0.139448	3.207610
188	1	0	3.695644	0.362463	4.910507
189	1	0	4.304383	-1.956784	5.624272
190	1	0	4.583436	-2.409336	3.930163
191	1	0	6.101803	-0.202763	5.248338
192	1	0	8.835581	-0.838807	3.265332
193	1	0	7.766846	0.535024	2.894479
194	1	0	9.098374	1.880919	5.788524
195	1	0	8.868746	2.035567	4.024395
196	1	0	-0.592546	3.871519	3.979393
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210	1	0	-5.976996	5.203836	0.037246
211	1	0	-8.884181	3.796125	-1.058677
212	1	0	-8.170601	3.063017	0.406272
213	1	0	-8.721426	4.187692	2.060155
214	1	0	-9.072109	5.926572	1.959494
215	1	0	4.070452	3.073318	0.611219
216	1	0	3.743995	4.808269	0.850831
217	1	0	4.386681	4.531889	3.268224
218	1	0	5.001660	2.906359	2.917255
219	1	0	6.042280	5.311298	1.488609
220	1	0	9.194300	4.367811	1.908153
221	1	0	8.606477	3.698162	0.365870
222	1	0	8.511523	6.758801	-0.900523
223	1	0	8.239220	5.025500	-1.171948
224	1	0	0.946708	4.970220	-2.563331
225	1	0	-0.823829	4.971206	-2.486900

226	1	0	-5.924730	6.649915	5.048710
227	1	0	-8.293383	5.621517	5.417739
228	1	0	7.806551	5.562164	-3.106611
229	1	0	4.550949	6.861179	-3.500853
230	1	0	-2.153011	-4.170800	0.653235
231	1	0	2.075815	-3.233498	3.046884
232	1	0	-3.844321	-2.672467	1.608772
233	1	0	-3.736784	-4.312007	2.302346
234	1	0	-4.310605	-3.364457	4.545575
235	1	0	-4.611480	-1.779314	3.809082
236	1	0	-6.188137	-4.202384	3.053156
237	1	0	-9.032336	-2.334184	3.036997
238	1	0	-8.314815	-2.616759	1.426222
239	1	0	-9.300488	-5.824528	1.819774
240	1	0	-8.883895	-4.483436	0.729590
241	1	0	3.728368	-3.066988	1.231458
242	1	0	3.660062	-4.554357	2.212120
243	1	0	4.359333	-5.893806	0.243044
244	1	0	4.497980	-4.419727	-0.736183
245	1	0	6.221441	-4.934752	1.653316
246	1	0	8.880590	-3.614550	-0.065530
247	1	0	8.117799	-2.565732	1.158020
248	1	0	9.508086	-4.687168	3.403260
249	1	0	8.936546	-3.051815	3.011081
250	1	0	-0.868604	-5.625477	-0.902155
251	1	0	0.902744	-5.613689	-0.856943
252	1	0	-6.187626	-8.316760	-0.198899
253	1	0	-8.098610	-6.043492	-1.780841
254	1	0	9.511440	-3.124722	5.057394
255	1	0	6.701759	-4.679686	6.917763
256	1	0	-2.084922	2.902332	-2.955574
257	1	0	2.169237	0.698360	-4.197123
258	1	0	-3.735568	1.129513	-2.812216
259	1	0	-3.641804	2.043597	-4.339435
260	1	0	-4.241375	-0.057586	-5.578433
261	1	0	-4.578848	-0.867980	-4.037805
262	1	0	-6.060294	1.589162	-4.871642
263	1	0	-8.978801	0.208035	-3.798557
264	1	0	-8.207492	1.352549	-2.662517
265	1	0	-8.747138	3.284231	-3.212328
266	1	0	-9.088203	3.740796	-4.896812
267	1	0	3.769394	1.688847	-2.569515
268	1	0	3.769545	2.229369	-4.269557
269	1	0	4.398250	4.524302	-3.523061

270	1	0	4.565133	3.950876	-1.853078
271	1	0	6.245439	2.900565	-4.090829
272	1	0	8.982645	2.916009	-2.044978
273	1	0	8.187416	1.340854	-2.325640
274	1	0	8.921631	0.571528	-4.138071
275	1	0	9.429139	1.627900	-5.479058
276	1	0	-0.861023	-0.919282	-5.484055
277	1	0	0.911815	-0.936323	-5.486795
278	1	0	-5.585333	6.472570	-2.922014
279	1	0	-7.903095	6.002611	-2.078395
280	1	0	9.388954	-0.622986	-5.844792
281	1	0	6.008431	-1.528014	-6.874323
282	1	0	-2.110178	-2.045087	-3.724610
283	1	0	2.157933	-3.754560	-1.888337
284	1	0	-3.713018	-2.466216	-1.924962
285	1	0	-3.704918	-3.575083	-3.321164
286	1	0	-4.284355	-5.460636	-1.762456
287	1	0	-4.547970	-4.293381	-0.454186
288	1	0	-6.128056	-4.198853	-2.988601
289	1	0	-8.971005	-3.581931	-1.205589
290	1	0	-8.186993	-2.160071	-1.950026
291	1	0	-9.246477	-3.485481	-4.889315
292	1	0	-8.851554	-2.044762	-3.922189
293	1	0	3.832658	-2.095250	-2.330091
294	1	0	3.698733	-3.366299	-3.572001
295	1	0	4.273573	-1.633103	-5.315825
296	1	0	4.660831	-0.480577	-4.024290
297	1	0	6.068658	-3.096745	-4.279588
298	1	0	9.034275	-1.676721	-3.599302
299	1	0	8.271010	-2.336032	-2.129903
300	1	0	8.790906	-5.412846	-3.405614
301	1	0	8.439644	-4.400027	-1.994382
302	1	0	-6.172424	-2.283109	-7.886292
303	1	0	-8.530201	-1.271040	-7.510900
304	1	0	8.178335	-6.045146	-0.892836
305	1	0	4.981313	-7.488665	-1.317717
306	1	0	5.388670	0.145184	-6.778676
307	1	0	6.430993	-0.345208	-8.140149
308	1	0	8.241061	-1.978647	-5.937707
309	1	0	8.790008	-1.157750	-7.417396
310	1	0	4.026417	6.405295	-1.859580
311	1	0	4.734995	8.003731	-2.145141
312	1	0	6.494435	5.970745	-4.185934
313	1	0	7.503644	7.274254	-3.511611

314	1	0	7.985738	5.196837	4.052550
315	1	0	8.505735	5.207893	5.753841
316	1	0	5.064526	3.768762	5.645998
317	1	0	5.715784	5.237320	4.863598
318	1	0	8.332764	-1.999405	5.773682
319	1	0	8.898973	-3.421857	6.681476
320	1	0	5.582341	-4.472248	5.543891
321	1	0	6.122748	-3.050333	6.481966
322	1	0	6.952966	-7.133083	-0.285707
323	1	0	7.981404	-7.647014	-1.648473
324	1	0	4.405276	-6.284760	-2.500372
325	1	0	5.287025	-7.720058	-3.056687
326	1	0	-4.981633	5.753583	3.829589
327	1	0	-5.640802	4.903068	5.256447
328	1	0	-9.070487	4.899653	4.011288
329	1	0	-7.949243	3.927599	4.994362
330	1	0	-5.138098	-1.827457	6.559328
331	1	0	-5.831908	-3.430835	6.183096
332	1	0	-9.207751	-2.152971	5.657079
333	1	0	-8.534411	-3.225194	6.884555
334	1	0	-5.209498	-6.917450	0.316531
335	1	0	-5.820183	-7.016678	-1.359980
336	1	0	-9.258886	-6.195738	-0.440017
337	1	0	-8.514768	-7.641542	-1.118063
338	1	0	-5.182555	-2.340258	-6.403576
339	1	0	-5.810451	-0.778033	-7.004307
340	1	0	-9.231486	-1.430273	-5.900462
341	1	0	-8.090022	-0.108210	-6.238014
342	1	0	-4.961143	5.370813	-4.183445
343	1	0	-5.874506	6.832185	-4.643000
344	1	0	-9.046214	5.374160	-3.290149
345	1	0	-8.239710	6.915658	-3.567586

The total electronic energy is calculated to be -8585.55887489 a.u.

7. Density functional theory (DFT) calculations of a model complex

The complex structure P5DGA ⊃ C_2mim^+ was optimized by the density functional theory (DFT) method at the M062X/6-31G (d, p) level by employing the Gaussian 09 program.[S1]

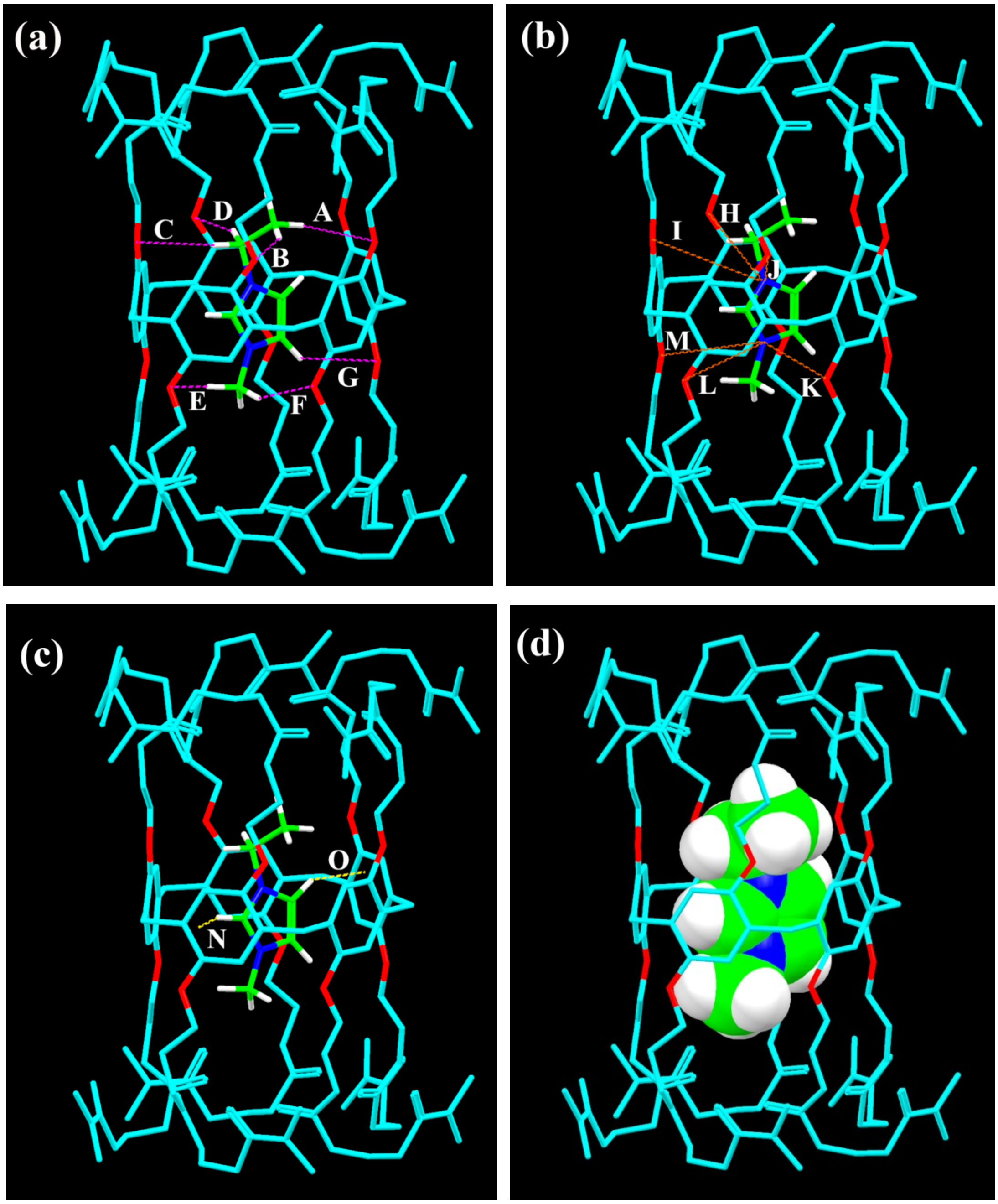

Fig. S14 Four side views (a), (b), (c) and (d) of optimized geometry of **L-I** ⊃ C_2min^+ at the M062X /6-31G (d, p) level. C_2min^+ is accommodated in the cavity of **L-I** (green = C, white = H, red = O and blue = N). All terminal isopropyl groups of each chain in the host molecule are replaced by methyl groups for simplicity and hydrogens except the ones involved in hydrogen bonding between host and guest are omitted for clarity. The dashed pink lines in (a) indicate intermolecular H-bonds A-G with A = 2.814 Å (124.19°), B = 2.556 Å (151.11°), C = 2.791 Å (163.52°), D = 2.485 Å (157.63°), E = 2.463 Å (142.57°), F = 2.447 Å (148.55°), G = 2.687 Å (133.38°). The dashed orange lines in (b) indicate the $N^+\cdots O$ interaction H-M with H = 4.075 Å, I = 4.520 Å, J = 4.374 Å, K = 3.660 Å, L = 4.152 Å, M = 4.105 Å). The dashed yellow lines in (c) indicate the C-H···π interaction N and O with N = 2.378 Å, O = 2.347 Å.

Table S2 Atomic coordinates for the optimized structure of the **L-I**-C_2mim^+.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.211753	-1.609741	3.563698
2	6	0	1.190775	-0.249141	3.866076
3	6	0	-0.019269	0.439281	3.943755
4	6	0	-1.206462	-0.254426	3.687584
5	6	0	-1.191627	-1.627083	3.461478
6	6	0	0.015494	-2.321911	3.412790
7	8	0	2.356060	-2.338358	3.399863
8	6	0	3.612460	-1.771673	3.725877
9	6	0	4.592309	-2.935593	3.652231
10	7	0	5.940780	-2.514240	3.945259
11	6	0	6.846371	-2.352058	2.965026
12	6	0	8.155168	-1.698967	3.385980
13	8	0	8.281675	-1.560726	4.785013
14	6	0	8.389111	-0.253270	5.279131
15	6	0	7.046658	0.268371	5.812181
16	7	0	7.013005	1.563264	6.207006
17	8	0	-2.349231	0.502694	3.688067
18	6	0	-3.607659	-0.128975	3.852647
19	6	0	-4.530187	0.967548	4.369201
20	7	0	-5.886881	0.498999	4.504540
21	6	0	-6.800120	0.771525	3.556580
22	6	0	-8.115266	0.016950	3.683517
23	8	0	-8.246561	-0.654053	4.918300
24	6	0	-8.385985	-2.048255	4.866178
25	6	0	-7.057553	-2.766715	5.145531
26	7	0	-7.054766	-4.112905	5.003660
27	6	0	0.054593	-3.811174	3.147584
28	6	0	-0.082291	1.907521	4.299380
29	6	0	5.790239	2.110263	6.766456
30	6	0	8.125471	2.495956	6.144265
31	8	0	6.080312	-0.480820	5.918537
32	8	0	6.696639	-2.704089	1.795767
33	8	0	-6.642878	1.571170	2.634278
34	8	0	-6.075314	-2.139969	5.531472
35	6	0	-8.184475	-4.920525	4.576105
36	6	0	-5.845229	-4.861165	5.296152
37	6	0	1.304997	-4.401849	-0.408899
38	6	0	1.296245	-4.229646	0.975958
39	6	0	0.089780	-4.088907	1.662821
40	6	0	-1.110602	-4.131847	0.942994
41	6	0	-1.104113	-4.327660	-0.434276
42	6	0	0.100555	-4.456955	-1.122842

43	8	0	2.437911	-4.498766	-1.164231
44	6	0	3.706014	-4.351259	-0.555344
45	6	0	4.703517	-4.572780	-1.684957
46	7	0	6.060918	-4.596064	-1.198854
47	6	0	6.888906	-3.552027	-1.366684
48	6	0	8.214291	-3.652184	-0.623875
49	8	0	8.452281	-4.938733	-0.093406
50	6	0	8.608361	-5.027733	1.297378
51	6	0	7.311120	-5.470518	1.989851
52	7	0	7.316325	-5.476880	3.343746
53	8	0	-2.248138	-3.918353	1.671320
54	6	0	-3.526992	-4.145501	1.103490
55	6	0	-4.469530	-4.149188	2.301837
56	7	0	-5.841336	-4.363214	1.915471
57	6	0	-6.737749	-3.363370	1.932468
58	6	0	-8.089142	-3.694546	1.314722
59	8	0	-8.251153	-5.067384	1.036160
60	6	0	-8.421955	-5.426309	-0.308055
61	6	0	-7.128823	-5.981728	-0.921588
62	7	0	-7.162165	-6.241682	-2.249835
63	6	0	0.123083	-4.481933	-2.632666
64	6	0	6.134347	-5.914109	4.064750
65	6	0	8.425688	-5.063592	4.185786
66	8	0	6.347729	-5.849184	1.330185
67	8	0	6.657558	-2.566429	-2.067244
68	8	0	-6.551727	-2.245296	2.413052
69	8	0	-6.151445	-6.222447	-0.219423
70	6	0	-8.282803	-5.953486	-3.130502
71	6	0	-5.986817	-6.784968	-2.906945
72	6	0	1.098309	3.137015	2.453422
73	6	0	1.109968	3.971351	1.339917
74	6	0	-0.087637	4.439047	0.791823
75	6	0	-1.296564	4.055674	1.383759
76	6	0	-1.303776	3.256275	2.527780
77	6	0	-0.110064	2.789808	3.073567
78	8	0	2.219645	2.604357	3.017200
79	6	0	3.501040	3.049544	2.607320
80	6	0	4.444583	2.519340	3.677899
81	7	0	5.801853	2.945260	3.450362
82	6	0	6.751220	2.076765	3.066878
83	6	0	8.083952	2.703790	2.683098
84	8	0	8.178899	4.061744	3.053644
85	6	0	8.359997	4.991057	2.020382
86	6	0	7.055963	5.726965	1.680237

87	7	0	7.103675	6.572493	0.623082
88	8	0	-2.432969	4.460697	0.735846
89	6	0	-3.692869	4.340287	1.374593
90	6	0	-4.663162	5.061138	0.447990
91	7	0	-6.030884	4.887878	0.873751
92	6	0	-6.815885	3.958076	0.295718
93	6	0	-8.128547	3.680271	1.013575
94	8	0	-8.370663	4.564323	2.087218
95	6	0	-8.487098	3.979604	3.356302
96	6	0	-7.163358	4.027029	4.133598
97	7	0	-7.145933	3.406578	5.335885
98	6	0	-0.094610	5.195800	-0.519311
99	6	0	5.927230	7.342549	0.261626
100	6	0	8.244246	6.749678	-0.260478
101	8	0	6.055302	5.589598	2.377573
102	8	0	6.619202	0.854197	3.020324
103	8	0	-6.553858	3.356950	-0.744813
104	8	0	-6.196675	4.640930	3.690355
105	6	0	-8.258794	2.685816	5.930984
106	6	0	-5.940396	3.442717	6.144392
107	6	0	1.233558	-0.994853	-3.703209
108	6	0	1.275309	-2.320899	-3.277632
109	6	0	0.098311	-3.053022	-3.130907
110	6	0	-1.127747	-2.415588	-3.354813
111	6	0	-1.168303	-1.093537	-3.791767
112	6	0	0.011243	-0.381197	-4.001529
113	8	0	2.348141	-0.214523	-3.862828
114	6	0	3.632171	-0.816942	-3.863154
115	6	0	4.551157	0.210678	-4.510166
116	7	0	5.921099	-0.242217	-4.531923
117	6	0	6.819446	0.246685	-3.659760
118	6	0	8.159994	-0.471348	-3.632026
119	8	0	8.342767	-1.336450	-4.730809
120	6	0	8.550353	-2.691626	-4.438231
121	6	0	7.271384	-3.517207	-4.635165
122	7	0	7.340480	-4.824426	-4.287645
123	8	0	-2.238395	-3.180310	-3.135372
124	6	0	-3.520183	-2.612057	-3.307634
125	6	0	-4.493910	-3.762998	-3.093860
126	7	0	-5.855864	-3.352561	-3.332682
127	6	0	-6.676308	-3.034454	-2.317313
128	6	0	-7.995592	-2.397154	-2.732104
129	8	0	-8.260053	-2.544771	-4.111446
130	6	0	-8.467267	-1.365231	-4.840306

131	6	0	-7.192485	-0.918594	-5.570929
132	7	0	-7.261058	0.249907	-6.250766
133	6	0	-0.013002	1.013576	-4.585324
134	6	0	6.190793	-5.686402	-4.494893
135	6	0	8.483414	-5.469228	-3.663061
136	8	0	6.271842	-3.015918	-5.140652
137	8	0	6.631047	1.206411	-2.912685
138	8	0	-6.433320	-3.219168	-1.124666
139	8	0	-6.189074	-1.625548	-5.568358
140	6	0	-8.416679	1.128835	-6.306386
141	6	0	-6.112077	0.707322	-7.011275
142	6	0	1.130925	3.643635	-2.080512
143	6	0	1.153218	2.625193	-3.030630
144	6	0	-0.033523	2.102421	-3.539380
145	6	0	-1.255139	2.606891	-3.070284
146	6	0	-1.276917	3.646617	-2.140876
147	6	0	-0.086178	4.177696	-1.639434
148	8	0	2.254808	4.160377	-1.499581
149	6	0	3.536485	3.779938	-1.968948
150	6	0	4.503218	4.696767	-1.231303
151	7	0	5.864951	4.491066	-1.658014
152	6	0	6.728376	3.776988	-0.915448
153	6	0	8.063944	3.478587	-1.582653
154	8	0	8.257987	4.205126	-2.777719
155	6	0	8.428941	3.452809	-3.948906
156	6	0	7.123224	3.333448	-4.748181
157	7	0	7.150504	2.530395	-5.837594
158	8	0	-2.374485	2.020546	-3.584391
159	6	0	-3.649102	2.554805	-3.276196
160	6	0	-4.610059	1.866669	-4.235574
161	7	0	-5.973860	2.280374	-4.005694
162	6	0	-6.831739	1.481598	-3.347815
163	6	0	-8.168481	2.112458	-2.987522
164	8	0	-8.390447	3.344978	-3.637281
165	6	0	-8.578897	4.463296	-2.814168
166	6	0	-7.294994	5.293785	-2.676899
167	7	0	-7.343182	6.335191	-1.812102
168	6	0	5.964236	2.397060	-6.663673
169	6	0	8.293824	1.753984	-6.287017
170	8	0	6.131692	3.983359	-4.428624
171	8	0	6.518361	3.381420	0.230915
172	8	0	-6.613877	0.310236	-3.040446
173	8	0	-6.310832	5.045494	-3.365814
174	6	0	-8.472008	6.664024	-0.957642

175	6	0	-6.182088	7.192088	-1.652741
176	1	0	2.112119	0.298492	4.037190
177	1	0	-2.113031	-2.176031	3.300713
178	1	0	3.899181	-0.985966	3.013135
179	1	0	3.603600	-1.337712	4.735068
180	1	0	4.266840	-3.704126	4.360787
181	1	0	4.587415	-3.370350	2.648055
182	1	0	6.120971	-2.014215	4.819448
183	1	0	8.974046	-2.330477	3.018309
184	1	0	8.188439	-0.732970	2.872973
185	1	0	9.106495	-0.272446	6.108808
186	1	0	8.772118	0.422124	4.508085
187	1	0	-3.982846	-0.536174	2.901474
188	1	0	-3.547713	-0.950743	4.577546
189	1	0	-4.145967	1.315126	5.333163
190	1	0	-4.536785	1.817318	3.678606
191	1	0	-6.070557	-0.312964	5.100576
192	1	0	-8.930835	0.744543	3.581481
193	1	0	-8.143676	-0.676744	2.837014
194	1	0	-9.104425	-2.336377	5.643476
195	1	0	-8.785852	-2.361484	3.897371
196	1	0	0.940067	-4.241160	3.619830
197	1	0	-0.832496	-4.276853	3.583151
198	1	0	0.789592	2.165865	4.905032
199	1	0	-0.982167	2.092451	4.890959
200	1	0	5.888657	2.246198	7.849635
201	1	0	7.927859	3.284468	5.407285
202	1	0	-9.105246	-4.340844	4.538644
203	1	0	-5.939552	-5.390333	6.251276
204	1	0	2.221355	-4.169302	1.540566
205	1	0	-2.028030	-4.330489	-1.003616
206	1	0	3.825372	-3.349921	-0.115981
207	1	0	3.859985	-5.097186	0.236181
208	1	0	4.455014	-5.524219	-2.165913
209	1	0	4.625213	-3.779158	-2.434214
210	1	0	6.306611	-5.259091	-0.458910
211	1	0	9.013432	-3.407412	-1.335525
212	1	0	8.180838	-2.885794	0.156826
213	1	0	8.946636	-4.073364	1.712101
214	1	0	9.379873	-5.782434	1.492821
215	1	0	-3.808486	-3.354918	0.390911
216	1	0	-3.564844	-5.108873	0.577487
217	1	0	-4.134642	-4.933783	2.987926
218	1	0	-4.416558	-3.191171	2.828419

219	1	0	-6.071924	-5.182050	1.346214
220	1	0	-8.866893	-3.383254	2.023425
221	1	0	-8.161156	-3.079521	0.412686
222	1	0	-9.187064	-6.211861	-0.346838
223	1	0	-8.777900	-4.575276	-0.896213
224	1	0	-0.748707	-5.019407	-3.010228
225	1	0	1.025220	-4.983175	-2.986467
226	1	0	6.299621	-6.899438	4.515127
227	1	0	8.616669	-5.837888	4.936151
228	1	0	-8.096083	-5.047989	-3.722059
229	1	0	-5.772965	-6.195756	-3.803901
230	1	0	2.041787	4.245157	0.857650
231	1	0	-2.237572	2.966932	3.000666
232	1	0	3.765728	2.655207	1.614873
233	1	0	3.545599	4.146453	2.568146
234	1	0	4.082624	2.878458	4.646977
235	1	0	4.434035	1.424960	3.695456
236	1	0	5.992312	3.939734	3.300803
237	1	0	8.878338	2.139947	3.187812
238	1	0	8.178912	2.566669	1.601685
239	1	0	9.092838	5.732049	2.363527
240	1	0	8.758886	4.504531	1.125669
241	1	0	-3.996697	3.289623	1.486060
242	1	0	-3.675280	4.796163	2.372924
243	1	0	-4.399909	6.122403	0.416024
244	1	0	-4.574235	4.655156	-0.564826
245	1	0	-6.274172	5.132362	1.835691
246	1	0	-8.938381	3.784139	0.279972
247	1	0	-8.075822	2.637580	1.343716
248	1	0	-9.239520	4.552233	3.911430
249	1	0	-8.831184	2.942905	3.277947
250	1	0	0.788864	5.833620	-0.585912
251	1	0	-0.987770	5.819250	-0.585998
252	1	0	6.081216	8.404114	0.485524
253	1	0	8.066000	6.264261	-1.229088
254	1	0	-9.183230	2.837976	5.376593
255	1	0	-6.057948	4.139613	6.982078
256	1	0	2.218953	-2.810480	-3.057067
257	1	0	-2.110590	-0.595969	-3.996730
258	1	0	3.968302	-1.049904	-2.841731
259	1	0	3.631197	-1.747357	-4.445628
260	1	0	4.191581	0.401334	-5.526411
261	1	0	4.520407	1.151885	-3.953230
262	1	0	6.143104	-1.142062	-4.968525

263	1	0	8.949138	0.291331	-3.637881
264	1	0	8.188146	-1.008388	-2.678726
265	1	0	8.923472	-2.816240	-3.417402
266	1	0	9.312768	-3.067122	-5.131910
267	1	0	-3.698858	-1.804240	-2.581896
268	1	0	-3.644162	-2.199373	-4.318120
269	1	0	-4.216224	-4.571930	-3.776575
270	1	0	-4.428942	-4.140751	-2.068810
271	1	0	-6.104893	-2.979043	-4.252391
272	1	0	-8.797652	-2.878773	-2.158299
273	1	0	-7.928490	-1.343884	-2.439093
274	1	0	-8.822561	-0.561404	-4.187853
275	1	0	-9.243087	-1.572723	-5.586994
276	1	0	0.873683	1.145998	-5.210611
277	1	0	-0.896173	1.113387	-5.220128
278	1	0	6.005409	-6.262384	-3.583193
279	1	0	8.280852	-5.678141	-2.604627
280	1	0	-9.294135	0.674957	-5.848948
281	1	0	-5.935076	1.763821	-6.788373
282	1	0	2.092091	2.211719	-3.385807
283	1	0	-2.215542	4.047241	-1.770968
284	1	0	3.753191	2.724793	-1.744358
285	1	0	3.621572	3.925291	-3.054266
286	1	0	4.196433	5.730135	-1.420665
287	1	0	4.457444	4.516259	-0.152659
288	1	0	6.088671	4.587632	-2.652346
289	1	0	8.858063	3.744963	-0.873140
290	1	0	8.080531	2.397368	-1.751470
291	1	0	9.168303	3.974551	-4.568764
292	1	0	8.816230	2.456267	-3.716481
293	1	0	-3.932659	2.350328	-2.233823
294	1	0	-3.672348	3.642034	-3.430196
295	1	0	-4.304503	2.104999	-5.259092
296	1	0	-4.563020	0.781512	-4.106614
297	1	0	-6.204706	3.277156	-4.036114
298	1	0	-8.958805	1.407332	-3.275405
299	1	0	-8.163133	2.218007	-1.897970
300	1	0	-9.348164	5.090792	-3.280976
301	1	0	-8.939994	4.161839	-1.825944
302	1	0	6.110602	2.894774	-7.628988
303	1	0	8.487946	1.972244	-7.342631
304	1	0	-8.266568	6.384393	0.084061
305	1	0	-5.984310	7.330488	-0.585506
306	1	0	-5.242948	0.115030	-6.731159

307	1	0	-6.294865	0.598969	-8.086484
308	1	0	-8.202556	2.076090	-5.795865
309	1	0	-8.660376	1.343682	-7.352333
310	1	0	-5.143111	-6.738270	-2.220826
311	1	0	-6.158851	-7.826213	-3.201647
312	1	0	-8.417103	-6.794565	-3.817445
313	1	0	-9.213330	-5.835255	-2.577290
314	1	0	-7.996181	-5.353441	3.585384
315	1	0	-8.336313	-5.737225	5.289628
316	1	0	-5.004665	-4.171389	5.348085
317	1	0	-5.680842	-5.594216	4.500884
318	1	0	-8.042479	1.611164	5.974296
319	1	0	-8.421268	3.050477	6.950743
320	1	0	-5.105572	3.763168	5.523623
321	1	0	-5.750415	2.440937	6.540745
322	1	0	-8.647945	7.743454	-0.998537
323	1	0	-9.386110	6.171943	-1.286440
324	1	0	-5.326270	6.721580	-2.133487
325	1	0	-6.361368	8.172353	-2.108498
326	1	0	5.296647	-5.970234	3.372012
327	1	0	5.916596	-5.193949	4.859356
328	1	0	9.341317	-4.928646	3.612207
329	1	0	8.187980	-4.126932	4.706127
330	1	0	4.969859	1.424452	6.562190
331	1	0	5.592140	3.082921	6.305790
332	1	0	9.057465	1.997232	5.883786
333	1	0	8.262613	2.962663	7.125493
334	1	0	5.073450	6.973650	0.827199
335	1	0	5.742301	7.232815	-0.811492
336	1	0	9.159939	6.352325	0.174195
337	1	0	8.400079	7.819414	-0.432119
338	1	0	5.120594	2.851160	-6.147225
339	1	0	5.770000	1.334426	-6.839957
340	1	0	9.195252	1.999572	-5.728280
341	1	0	8.094409	0.680088	-6.183532
342	1	0	5.323843	-5.072088	-4.730717
343	1	0	6.377593	-6.383957	-5.319290
344	1	0	9.384483	-4.862904	-3.739173
345	1	0	8.681649	-6.417969	-4.171972
346	6	0	-0.391629	1.079792	-0.076723
347	7	0	0.566623	0.168468	-0.218362
348	6	0	0.009752	-1.086790	-0.107420
349	6	0	-1.321649	-0.907422	0.108366
350	7	0	-1.549364	0.450749	0.117502

351	6	0	-2.830918	1.109874	0.349174
352	6	0	1.989674	0.469203	-0.426594
353	6	0	2.828414	-0.048241	0.731888
354	1	0	-0.252269	2.151560	-0.117347
355	1	0	0.594097	-1.991211	-0.188130
356	1	0	-2.109273	-1.625070	0.277847
357	1	0	-3.044417	1.108955	1.421197
358	1	0	-2.754815	2.136825	-0.015511
359	1	0	-3.613296	0.581252	-0.197427
360	1	0	2.276321	0.040388	-1.391873
361	1	0	2.061012	1.558066	-0.509042
362	1	0	2.538321	0.466546	1.653544
363	1	0	2.683400	-1.124455	0.882714
364	1	0	3.889589	0.134214	0.537845

The total electronic energy is calculated to be -8930.07888197 a.u.

8 Determination of the extracted species by Am (III) extraction

The equilibrium constant (K_1) of eqn. (1) and extraction constant for cation exchange mechanism (K_{ex}, eqn. (2)) are defined as eqn. (S1), (S2):

$$K_1 = \frac{[\mathrm{P5DGA} \bullet C_8\mathrm{mim}]^+_{IL}}{[\mathrm{P5DGA}]_{IL} \bullet [C_8\mathrm{mim}]^+_{IL}} \qquad \text{(S1)}$$

$$\mathrm{K_{ex}} = \frac{[(\mathrm{Am(NO_3)_m} \bullet \mathrm{P5DGA})]_{\mathrm{IL}}^{(3-\mathrm{m})}}{[\mathrm{Am^{3+}}]_{\mathrm{aq}} \bullet [\mathrm{NO_3^-}]_{\mathrm{aq}}^{\mathrm{m}}} \bullet \frac{[\mathrm{C_8mim}]_{\mathrm{aq}}^{(3-\mathrm{m})}}{[\mathrm{C_8mim}]_{\mathrm{IL}}^{(2-\mathrm{m})} \bullet [\mathrm{C_8mim} \bullet \mathrm{P5DGA}]_{\mathrm{IL}}^{+}} \qquad \text{(S2)}$$

Substituting $[\mathrm{C_8mim{\bullet}P5DGA}]^+_{\mathrm{IL}}$ of eqn. (S1) into eqn. (S2) and assuming that $[NO_3^-]^m_{aq}$, $[\mathrm{C_8mim}^{(3\text{-}m)}]_{\mathrm{IL}}$, K_1 and $[\mathrm{P5DGA}]_{IL}$ are constant, $D_{Am} = [(Am(NO_3)_m \bullet P5DGA)]_{IL}{}^{(3-m)} / [Am^{3+}]_{aq}$, then $\mathrm{K'_{ex}}$ is given as follows:

$$K'_{ex} = D_{Am} \bullet [C_8mim]^{(3-m)}_{aq} \qquad \text{(S3)}$$

Taking the logarithm of eqn. (S3) and fitting the experimental data in Fig. S16 gives a slope of ca. -1.

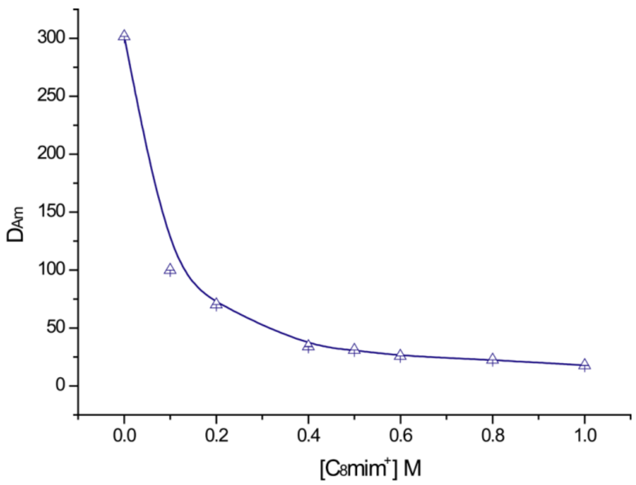

Fig. S15 Effect of C_8mim^+ concentration on Am^{3+} extraction with **L-III** in the $C_8mimNTf_2$, aq : or = 1:1, at 25 ± 1.0 °C, **[L-III]** = 10^{-4} M, $[HNO_3]$ = 0.5 M.

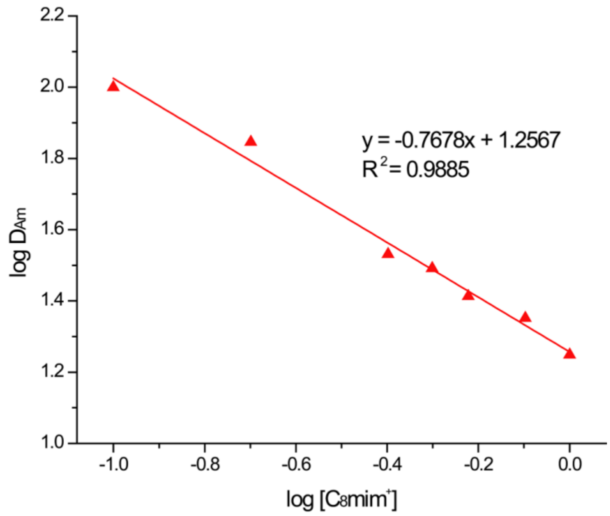

Fig. S16 Dependency of Am^{3+} distribution ratio (D_{Am}) on C_8mim^+ concentration with **L-III** in the $C_8mimNTf_2$, aq : or = 1:1, at 25 ± 1.0 °C, **[L-III]** = 10^{-4} M, $[HNO_3]$ = 0.5 M.

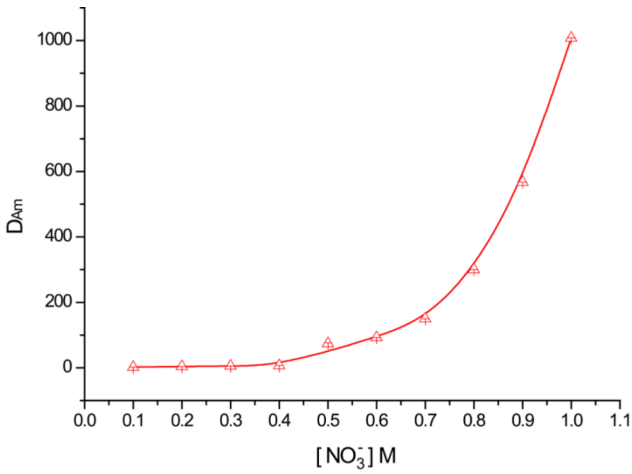

Fig. S17 Effect of sodium nitrate concentration on Am^{3+} extraction with **L-III** in $C_8mimNTf_2$, aq : or = 1:1, at 25 ± 1.0 °C, [L-III] = 10^{-4} M, $[HNO_3]$ = 0.05 M.

9 ^{1}H NMR titration of TFA and L-I-C$_8$minNTf$_2$ complex

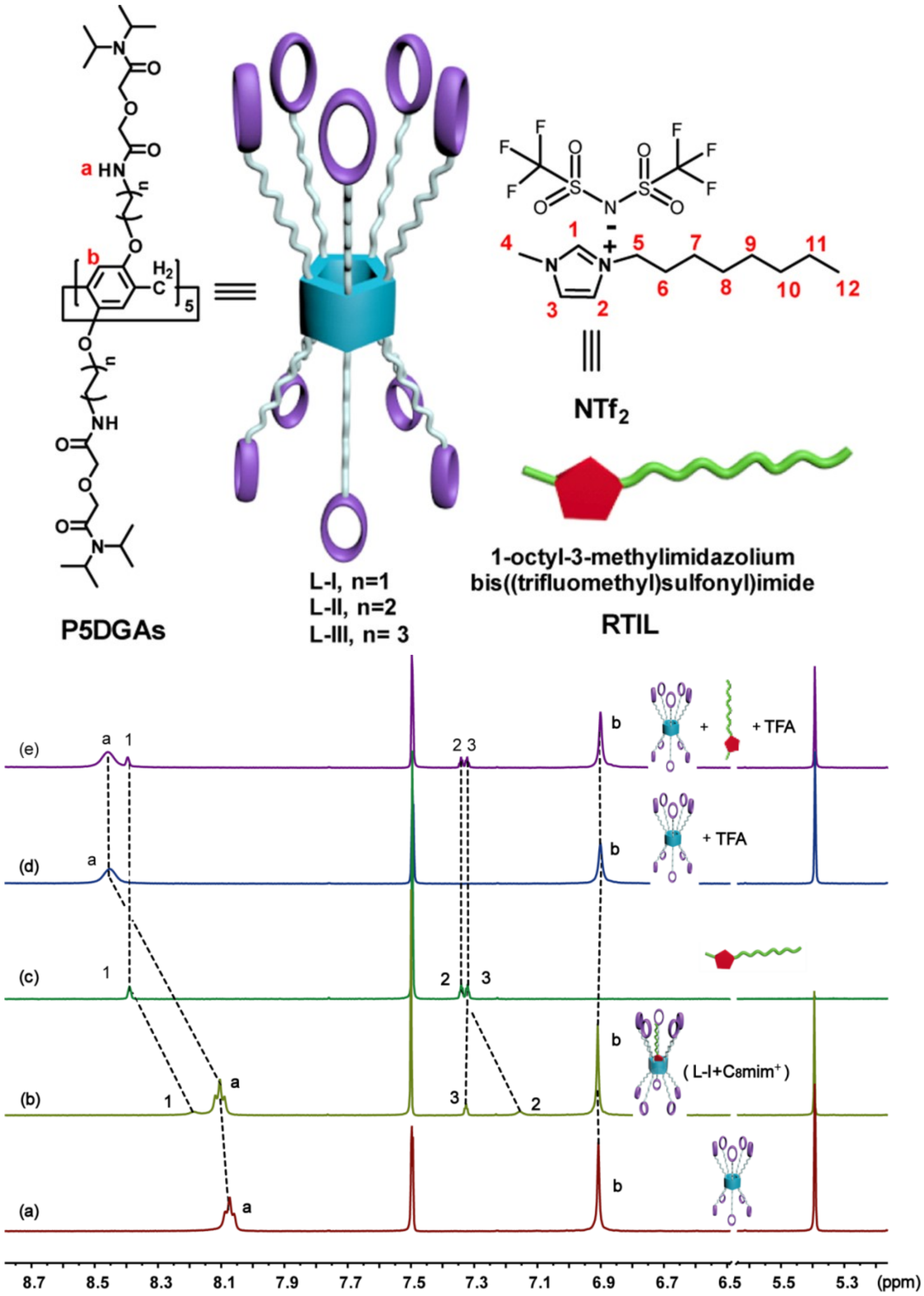

Fig. S18 Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3CN$, 1:1, v/v) of a) **L-I** (2.0 mM); b) **L-I** +C_8mim^+ (2.0 mM for each); c) C_8mim^+ (2.0 mM); d) **L-I** (2.0 mM) + TFA (80.0 mM); e) **L-I** (2.0 mM)+ C_8mim^+ (2.0 mM) + TFA (80.0 mM).

10 UV-vis spectrophotometric titration of P5DGAs with $C_8minNTf_2$

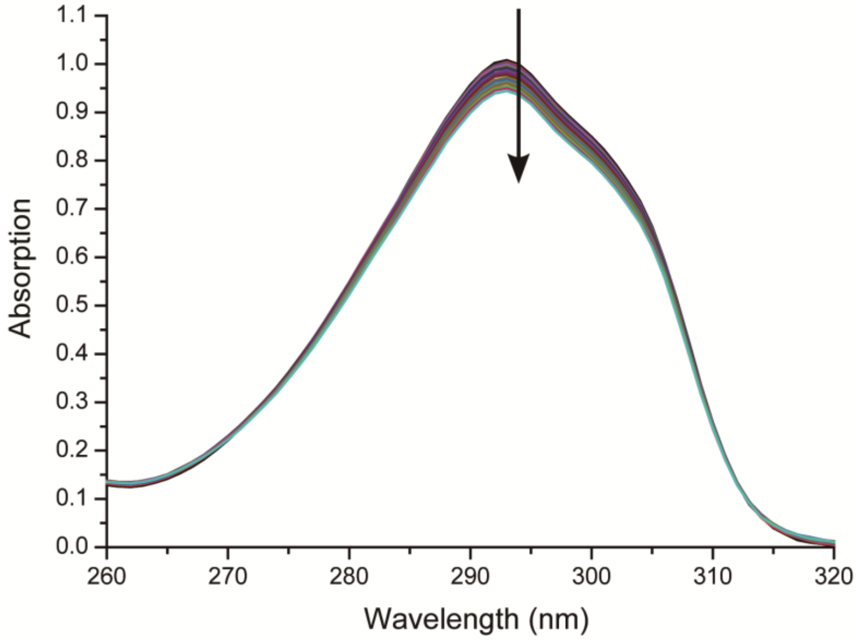

Fig. S19 UV-vis spectrophotometric titration of **L-I** (4.0×10^{-5} M) with $C_8minNTf_2$ (0-3.0 equiv.) in CH_3CN. The binding constant ($Ka = 3.8 \pm 0.3 \times 10^3\ M^{-1}$) fitted with the ReactLab EQUILIBRIA software.

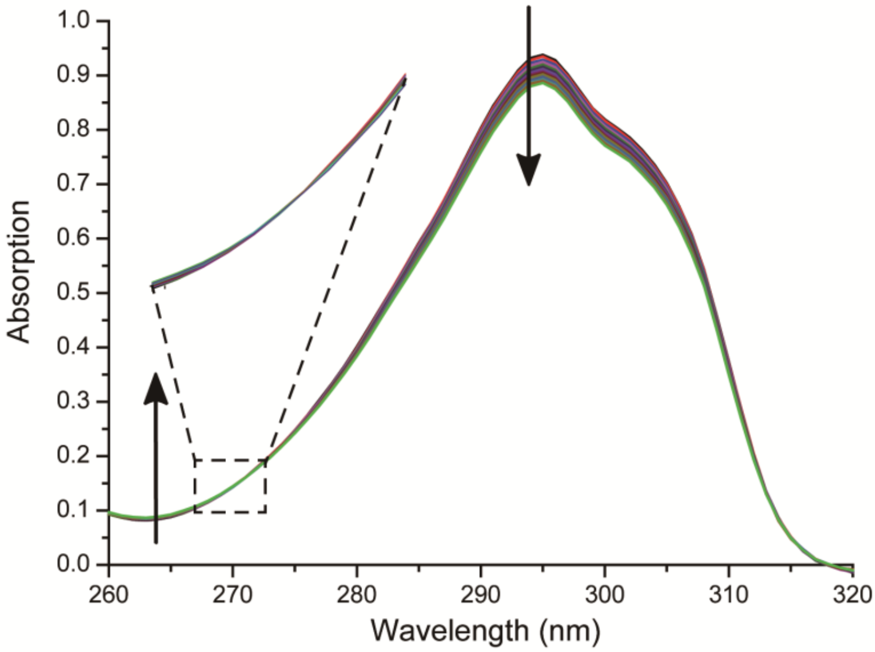

Fig. S20 UV-vis spectrophotometric titration of **L-II** (4.0×10^{-5} M) with $C_8minNTf_2$ (0-3.0 equiv.) in CH_3CN. The binding constant ($Ka = 2.0 \pm 0.4 \times 10^3\ M^{-1}$) fitted with the ReactLab EQUILIBRIA software.

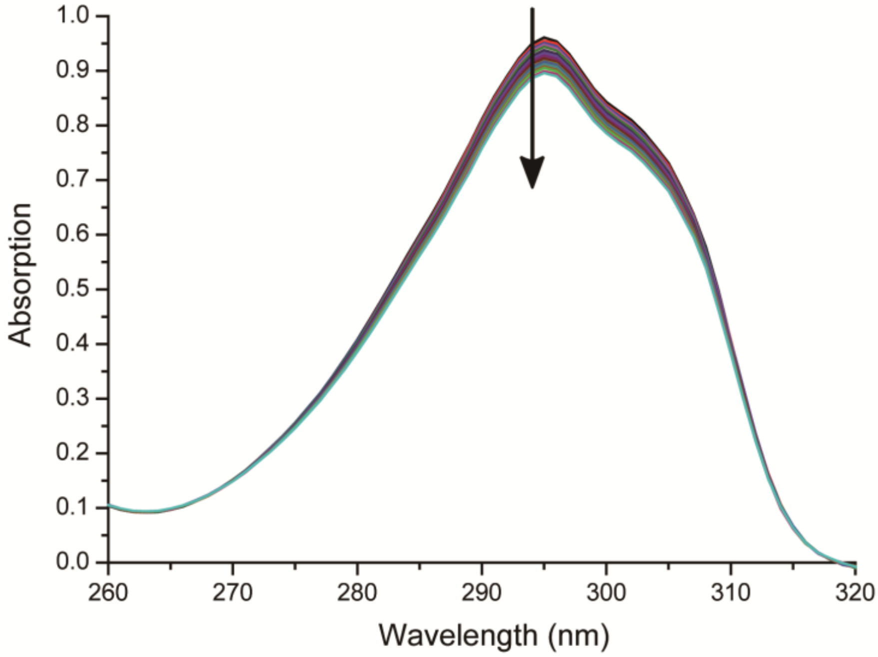

Fig. S21 UV-vis spectrophotometric titration of **L-III** (4.0×10^{-5} M) with $C_8minNTf_2$ (0-3.0 equiv.) in CH_3CN. The binding constant (Ka = $1.0 \pm 0.2 \times 10^3$ M^{-1}) fitted with the ReactLab EQUILIBRIA software.

11 UV-vis spectrophotometric titration of P5DGAs with Eu^{3+}

The binding constant Ka defined as the concentration ratio (Ka = $[M_xL_y^{n+}]^x/[M^{n+}]^x[L]^y$) was determined in methanol by UV−vis spectrophotometric titration at 25 °C. The titration experiments were carried out in a 1.0 cm quartz cell. Factor analysis and mathematical treatment of the spectrophotometric data were performed and fitted with the ReactLab EQUILIBRIA software.

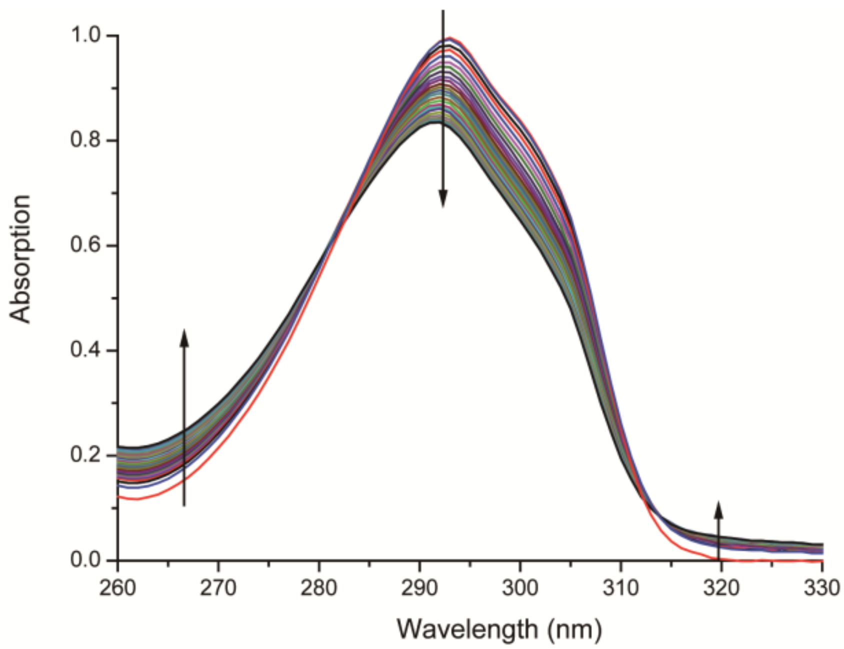

Fig. S22 UV-vis spectrophotometric titration of **L-I** (4.0×10^{-5} M) with Eu^{3+} (0-2.5 equiv.) in CH_3CN. The binding constant (Ka = $5.4 \pm 0.7 \times 10^{4}$ M^{-1}) fitted with the ReactLab EQUILIBRIA software.[S2]

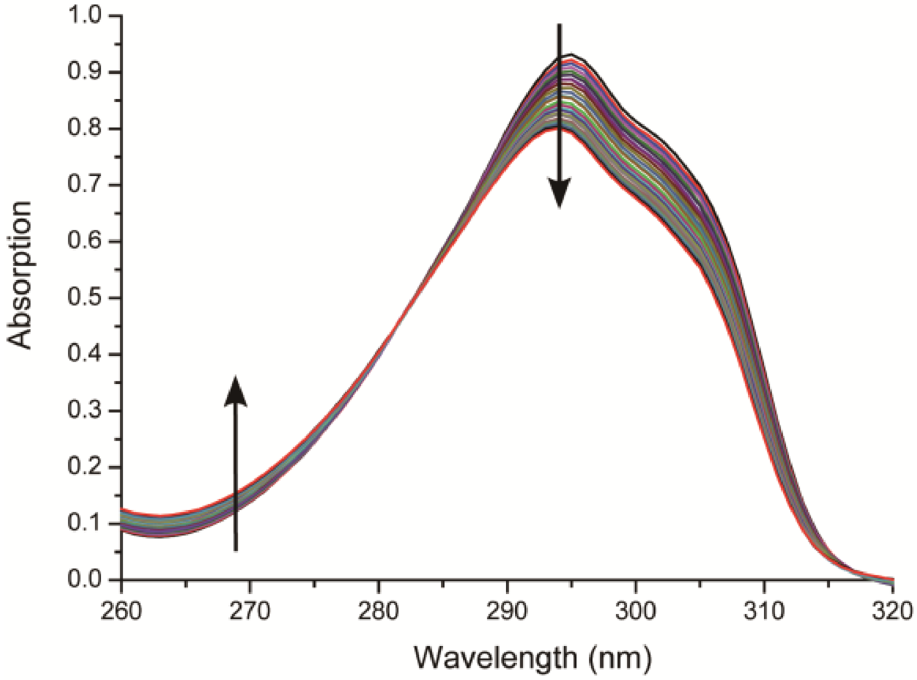

Fig. S23 UV-vis spectrophotometric titration of **L-II** (4.0×10^{-5} M) with Eu^{3+} (0-2.5 equiv.) in CH_3CN. The binding constant (Ka = $2.0 \pm 0.2 \times 10^{4}$ M^{-1}) fitted with the ReactLab EQUILIBRIA software.

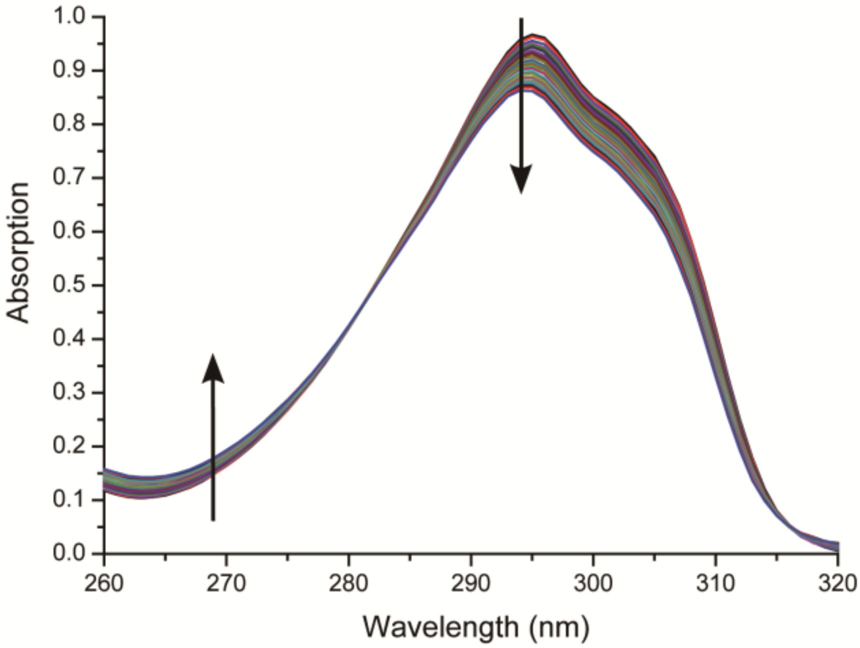

Fig. S24 UV-vis spectrophotometric titration of **L-III** (4.0×10^{-5} M) with Eu^{3+} (0-2.5 equiv.) in CH_3CN. The binding constant ($Ka = 1.2 \pm 0.3 \times 10^4\ M^{-1}$) fitted with the ReactLab EQUILIBRIA software.

12 Extraction data of actinides and fission product elements at 0.5 M HNO_3

Table S3 Comparative extraction data of actinides and fission product elements using 5.0×10^{-4} M P5DGAs in $C_8mimNTf_2$; Feed: 0.5 M HNO_3; Equilibration time: 3 h.

Metal ions	**L-I**	**L-II**	**L-III**
$D_{Am\,(III)}$	5510±25	6232±16	8411±12
$D_{Eu\,(III)}$	5877±20	6844±27	8846±32
$D_{Cs\,(I)}$	0.02±0.001	0.04±0.001	0.046±0.001
$D_{Sr\,(I)}$	0.11±0.01	0.85±0.02	0.73±0.02
$D_{Pu\,(IV)}$	125±9	176±11	321±9
$D_{Pu\,(VI)}$	1.8±0.1	3.1±0.1	5.2±0.2
$D_{U(VI)}$	1.0±0.1	2.1±0.2	4.2±0.4

13 Separation factors of Pu^{4+} over other actinides and fission products metal ions

Table S4 Comparative extraction data of actinides and fission product elements using 5.0×10^{-4} M P5DGAs in $C_8mimNTf_2$; Feed: 1.0 M HNO_3; Equilibration time: 3 h.

Metal ions	**L-I**	**L-II**	**L-III**	$SF_{\mathbf{L-I}}$[a]	$SF_{\mathbf{L-II}}$[a]	$SF_{\mathbf{L-III}}$[a]
$D_{Pu(IV)}$	93±4	52±2	41±2	--	--	--
$D_{Cs(I)}$	0.01±0.001	0.03±0.001	0.03±0.001	9.3×10^3	1.73×10^3	1.4×10^3
$D_{Sr(II)}$	0.07±0.002	0.04±0.001	0.03±0.001	1.3×10^3	1.30×10^3	1.4×10^3
$D_{Pu(VI)}$	0.31±0.01	0.22±0.01	0.19±0.01	3.0×10^2	2.4×10^2	2.2×10^2
$D_{U(VI)}$	0.16±0.01	0.38±0.01	0.50±0.02	5.8×10^2	1.4×10^2	82.0
$D_{Eu(III)}$	865±14	1731±17	7803±21	0.11	0.03	0.01

[a] SF means the separation factor values of Pu(IV) with respect to other metal ions using ligands **L-I**, **L-II** and **L-III**, i.e., $SF_{\mathbf{L-I}} = D_{Pu(IV)}/D_M$.

Table S5 Comparative extraction data of actinides and fission product elements using 5.0×10^{-4} M P5DGAs in 1-octanol; Feed: 1.0 M HNO_3; Equilibration time: 3 h.

Metal ions	**L-I**	**L-II**	**L-III**	$SF_{\mathbf{L-I}}$[a]	$SF_{\mathbf{L-II}}$[a]	$SF_{\mathbf{L-III}}$[a]
$D_{Pu(IV)}$	0.41±0.02	1.02±0.05	1.1±0.1	--	--	--
$D_{Cs(I)}$	0.008±0.002	0.020.001	0.01±0.001	5.12×10^1	5.10×10^1	1.1×10^2
$D_{Sr(II)}$	0.05±0.001	0.03±0.001	0.02±0.001	8.20	34.0	55.0
$D_{Pu(VI)}$	0.12±0.01	0.29±0.01	0.47±0.02	3.42	3.52	2.34
$D_{U(VI)}$	0.07±0.002	0.09±0.002	0.1±0.01	5.86	1.13×10^1	1.10×10^1
$D_{Eu(III)}$	12.4±0.9	63±3	52±3	0.033	0.016	0.021

[a] SF means the separation factor values of Pu(IV) with respect to other metal ions using ligands **L-I**, **L-II** and **L-III**, i.e., $SF_{\mathbf{L-I}} = D_{Pu(IV)}/D_M$.

14 Job's plot of P5DGAs and Eu^{3+}

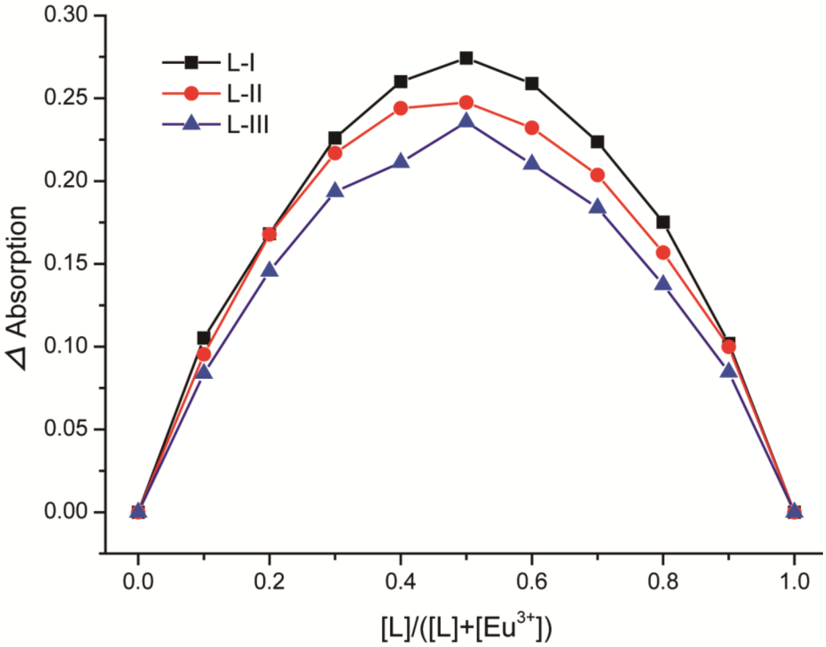

Fig. S25 Job's plot for the determination of stoichiometry in the complex formed by **L-I**, **L-II**, **L-III** and Eu^{3+} from absorbance measurements in CH_3CN, [P5DGA] + [Eu^{3+}] = 6.0×10^{-5} M.

15 FT-IR spectra of L-I and L-I-Eu^{3+} complex

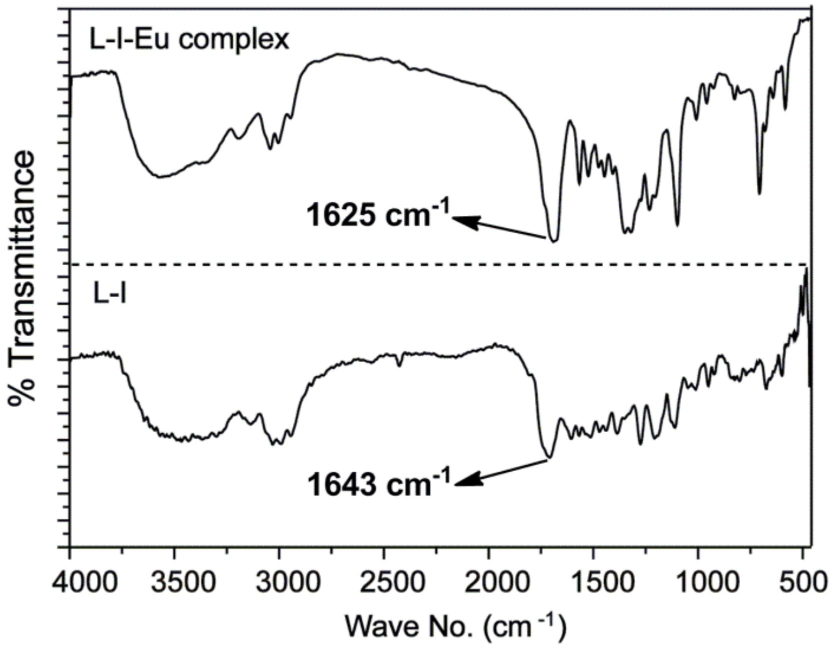

Fig. S26 FT-IR spectra of **L-I** and **L-I**-Eu complex

16 TRLFS studies of the P5DGAs-Eu^{3+} complexes

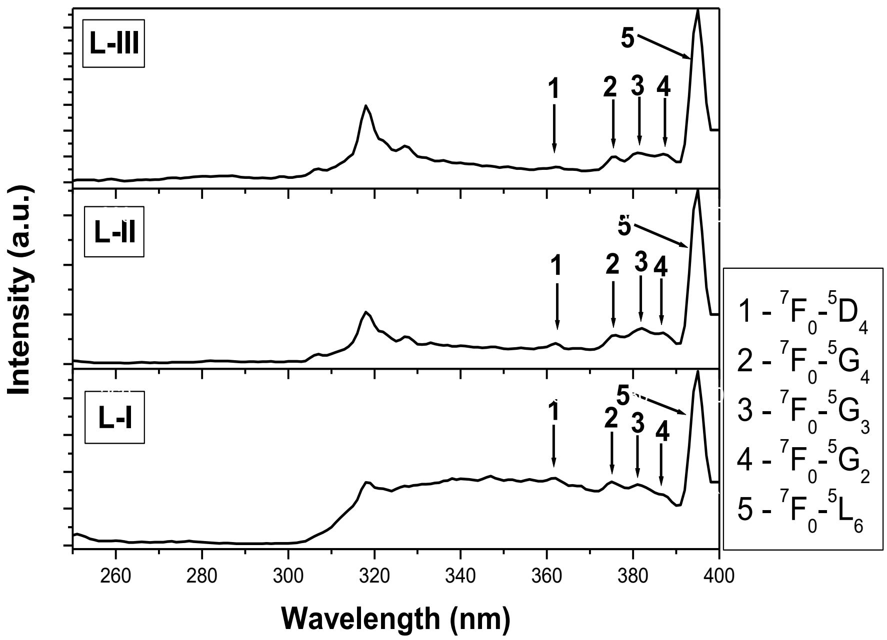

Fig. S27 Excitation spectra for different Eu^{3+}-P5DGAs complexes in $C_8mimNTf_2$.

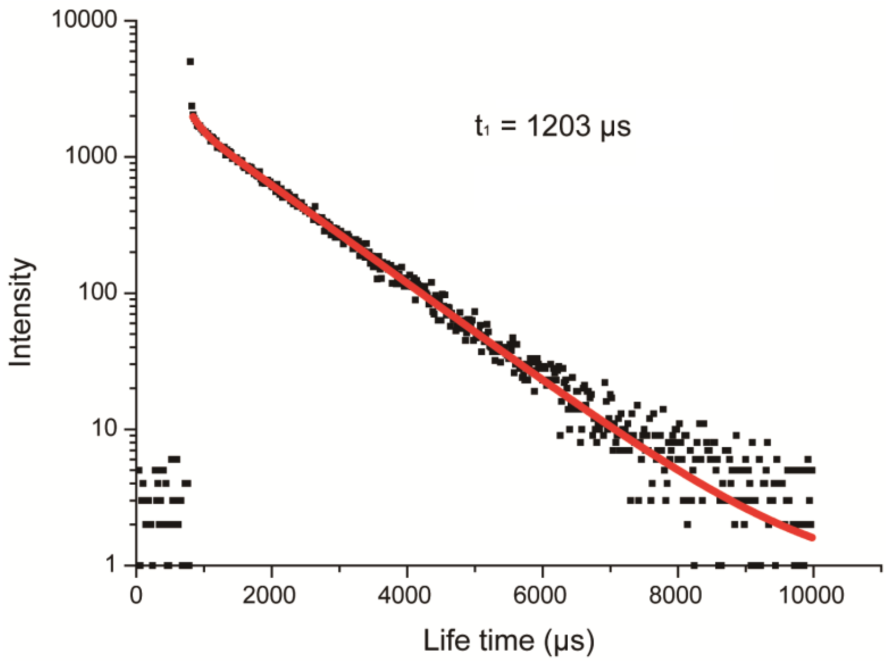

Fig. S28 Fluorescence decay profiles of Eu^{3+}-**L-I** complex.

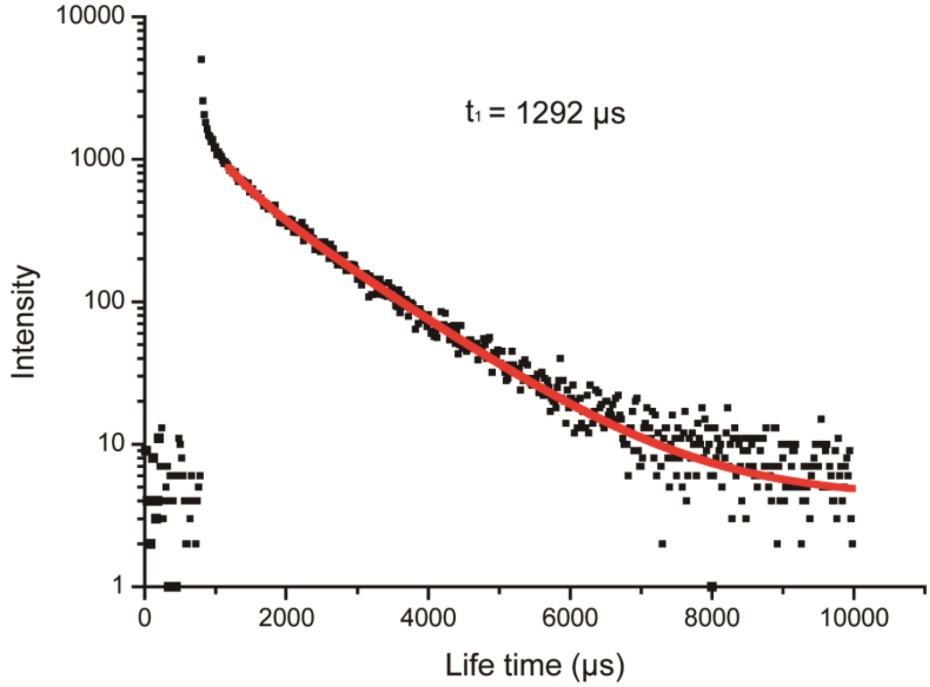

Fig. S29 Fluorescence decay profiles of Eu^{3+}-**L-II** complex.

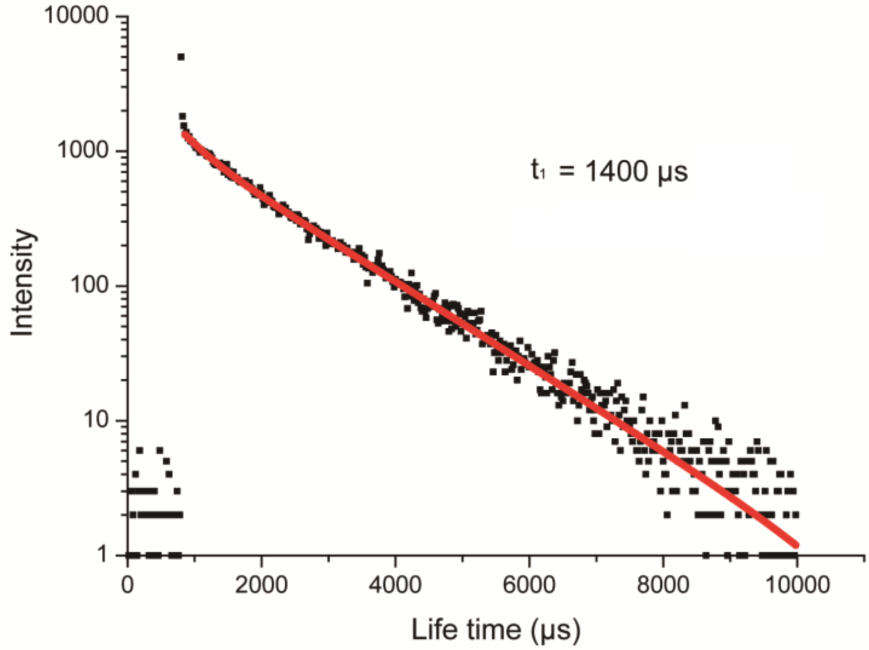

Fig. S30 Fluorescence decay profiles of Eu^{3+}-**L-III** complex.

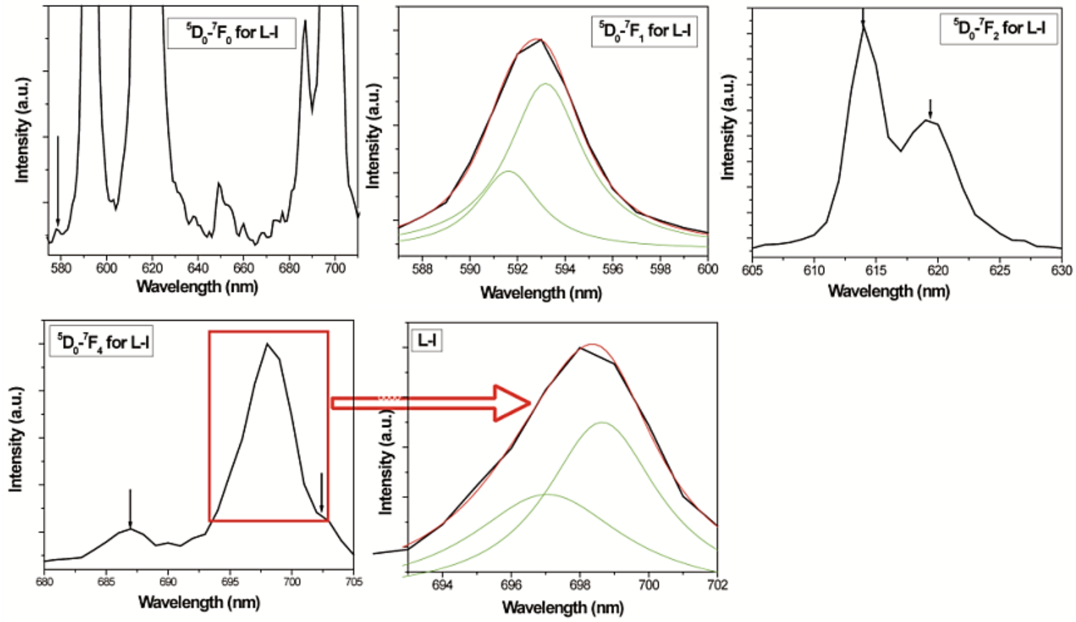

Fig. S31 Splitting pattern of different transitions for Eu^{3+}-**L-I** in C_8mimNTf_2.

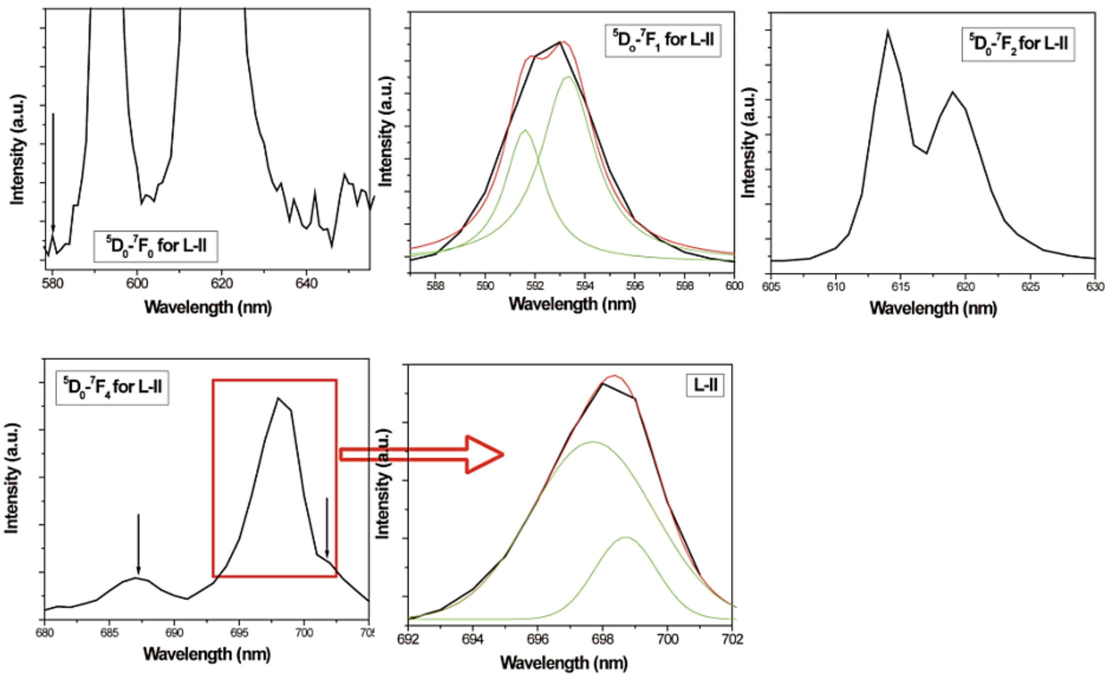

Fig. S32 Splitting pattern of different transitions for Eu^{3+}-**L-II** in C_8mimNTf_2.

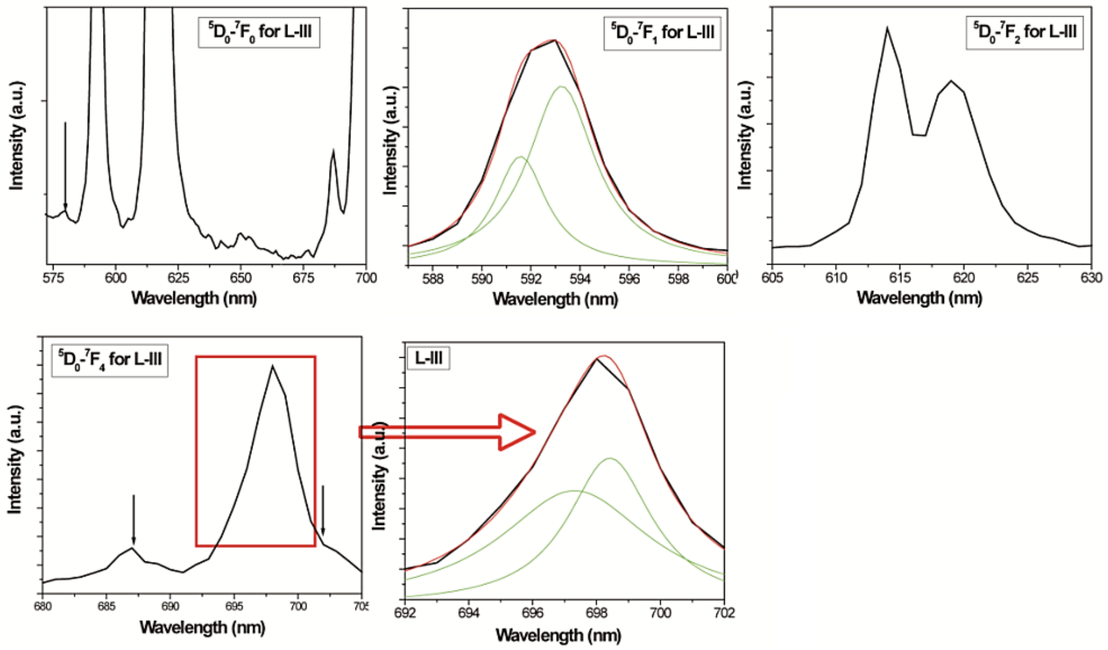

Fig. S33 Splitting pattern of different transitions for Eu^{3+}-**L-III** in $C_8mimNTf_2$.

[S1] Gaussian 09, Revision B.01, Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg,J.L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J.A., Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J.M.; Klene, M.; Knox, J.E.; Cross, J.B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Zakrzewski, V.G.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Dapprich, S.; Daniels, A.D.; Farkas, O.J.; Foresman, B.; Ortiz, J.V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.
[S1] Gaussian 09, Revision B.01, Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg,J.L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J.A., Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J.M.; Klene, M.; Knox, J.E.; Cross, J.B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Zakrzewski, V.G.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Dapprich, S.; Daniels, A.D.; Farkas, O.J.; Foresman, B.; Ortiz, J.V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.
[S2] (a) *ReactLab™ equilibria, Version 1.0,* J Plus Consulting Pty Ltd, 2010; (b) B. Y. Wang, T. Zujovic, D. A. Turner, C. M. Hadad, J. D. Badjic, *J. Org. Chem.* 2012, **77**, 2675.