

Fig S1.IR spectrum of the ligand



Fig S2.IR spectrum of the gadolinium(III) complex.



Fig. S3.1H NMR of the ligand



Fig. S4 13C NMR of the ligand

Table SI. X-Ray diffraction data of the ligand

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *Position*, °2*θ* | *Height*, cts | *FWHM Left*, °2*θ* | *d-spacing*, Å | *Relative Intensity*, % |
| 6.5918 | 31.74 | 0.2007 | 13.40930 | 4.21 |
| 12.5018 | 193.97 | 0.3011 | 7.08047 | 25.71 |
| 13.8603 | 146.73 | 0.1004 | 6.38936 | 19.45 |
| 14.6777 | 84.35 | 0.2007 | 6.03533 | 11.18 |
| 16.1904 | 78.56 | 0.8029 | 5.47469 | 10.41 |
| 17.6736 | 336.73 | 0.1673 | 5.01846 | 44.64 |
| 20.6472 | 81.18 | 0.1004 | 4.30192 | 10.76 |
| 22.0253 | 110.87 | 0.3346 | 4.03577 | 14.70 |
| 23.1856 | 60.92 | 0.2007 | 3.83638 | 8.08 |
| 25.1860 | 754.40 | 0.0836 | 3.53602 | 100.00 |
| 25.5258 | 431.35 | 0.1338 | 3.48971 | 57.18 |
| 26.4798 | 219.37 | 0.1338 | 3.36611 | 29.08 |
| 27.0251 | 204.74 | 0.2007 | 3.29942 | 27.14 |
| 28.0630 | 241.07 | 0.1338 | 3.17971 | 31.96 |
| 28.4829 | 304.67 | 0.1004 | 3.13379 | 40.39 |
| 30.3330 | 77.39 | 0.5353 | 2.94673 | 10.26 |
| 32.1389 | 72.14 | 0.3346 | 2.78515 | 9.56 |
| 36.7059 | 47.66 | 0.6691 | 2.44843 | 6.32 |
| 43.6109 | 63.34 | 0.2007 | 2.07545 | 8.40 |
| 54.5215 | 34.69 | 0.5353 | 1.68312 | 4.60 |