Electronic Supplementary Information (ESI)

Effect of Hydroxy Groups on X-ray-induced Decomposition of Azobenzene Derivatives

Koki Ogawara^a, Naoya leda^a, Hideo Takakura^a, Kohei Nakajima^a, Akari Mukaimine^b, Mei Harad^a, Kazuaki Hashimoto^a, Osamu Inanami^c, and Mikako Ogawa^{a,b}

- a. Laboratory of Bioanalysis and Molecular Imaging, Graduate School of Pharmaceutical Sciences, Hokkaido University, N12, W6, Kita-ku, Sapporo, Hokkaido, Japan.
- b. WPI-ICReDD, Hokkaido University, N21, W10, Kita-ku Sapporo, Hokkaido, Japan.
- c. Graduate School of Veterinary Medicine, Hokkaido University, N18, W9, Kita-ku Sapporo, Hokkaido, Japan.

Table of contents

Fig. S1 MS spectrums of 3-ABA released from AZO1-4	3
Fig. S2 MS spectrums of byproducts generated from AZO1 and AZO2	4
Fig. S3 ¹ H spectrum of AZO1 in CD ₃ OD (containing CDCl ₃ as a cosolvent)	5
Fig. S4 ¹³ C spectrum of AZO1 in DMSO- <i>d</i> ₆	6
Fig. S5 ¹ H spectrum of AZO2 in CD ₃ OD	7
Fig. S6 ¹³ C spectrum of AZO2 in DMSO- <i>d</i> ₆	8
Fig. S7 ¹ H spectrum of AZO3 in CD ₃ OD	9
Fig. S8 ¹³ C spectrum of AZO3 in DMSO- d_6	10
Fig. S9 ¹ H spectrum of AZO4 in CD ₃ OD	11
Fig. S10 ¹³ C spectrum of AZO4 in DMSO- d_6	12



Fig. S1 MS spectrums of 3-ABA released from AZO1–4 after X-ray irradiation for (a) AZO1, (b) AZO2, (c) AZO3, and (d) AZO4. (positive scan mode)





(b) Byproduct detected from AZO2 after X-ray irradiation



Fig. S2 MS spectrums of byproducts generated from (a) AZO1 (positive scan mode) and (b) AZO2 (negative scan mode) after X-ray irradiation.



Fig. S3 ¹H spectrum of AZO1 in CD₃OD (containing CDCl₃ as a cosolvent)



Fig. S4 ¹³C spectrum of AZO1 in DMSO- d_6



Fig. S5 ¹H spectrum of AZO2 in CD_3OD



Fig. S6 ¹³C spectrum of AZO2 in DMSO- d_6



Fig. S7 ¹H spectrum of AZO3 in CD_3OD



Fig. S8¹³C spectrum of AZO3 in DMSO- d_6



Fig. S9¹H spectrum of AZO4 in CD_3OD



Fig. S10 ¹³C spectrum of AZO4 in DMSO- d_6