Mapping the Azolog Space Enables the Optical Control of New Biological Targets

Johannes Morstein[†,§], Mahendra Awale[‡,§], Jean-Louis Reymond[‡*], Dirk Trauner[†*]

[†]Department of Chemistry, New York University, 100 Washington Square East, New York, NY 10003-6699, USA.

[‡]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland.

[§]These authors contributed equally

Supporting Information

Table of Contents

Analysis of linker-protein contacts

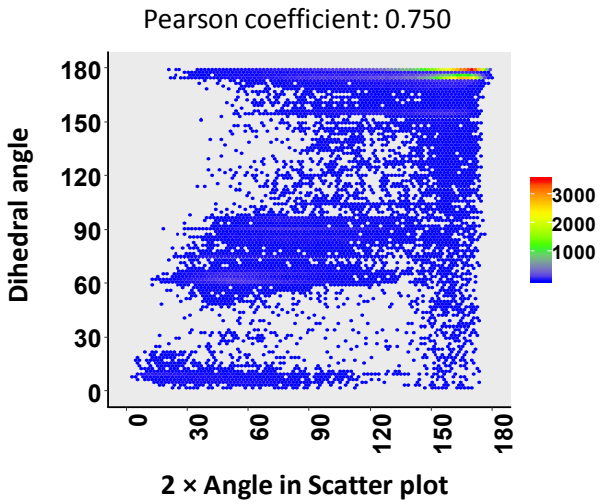
For each of the four linker types (-CO-NH-, -CH_2-NH-, -SO_2NH- and -CH_2-O-), 30 PDB entries were randomly selected and protein-ligand contacts were analyzed. For each selected PDB entry, the search was carried out on the "https://www.rcsb.org/" website and the "2D Diagram & Interactions" section was manually inspected to determined the protein-ligand interactions. Where the linker group has formed a H-bonding interaction with the protein, the corresponding PDB entry is marked as 1 in Table SI 1.

Table SI 1. Analysis of linker-protein contacts.

PDB ID	-CO-NH-	PDB ID	-CH_2-NH-	PDB ID	-SO_2NH-	PDB ID	-CH_2-O-
3pyy	1	4jhi	0	2d41	0	5j89	0
4n9b	1	5bwv	0	2o4p	0	4luz	0
4krs	1	4i13	0	4cax	0	4uga	0
3aea	1	2r3l	1	2g0g	0	3hr1	1
2vtn	1	3bmc	0	4xv9	0	4mse	0
3vs0	0	4yqq	1	4yfn	0	4kiu	0
3dzu	1	4p8m	0	3hkc	0	4jsh	0
5t3q	1	4qjo	0	4nqm	0	2r4b	0
4qo9	1	4x5f	0	2ynd	0	1u1f	0
4bhn	1	4kjj	0	4wgi	0	4y2t	0
3pyh	1	4cmf	0	3tye	1	3ad5	0
4g9r	1	4qrd	1	4nqn	1	4n4s	0
4o91	1	4gg5	0	2hoc	0	4nem	0
1xm4	0	4jev	0	3qk0	0	5adb	0
5mvd	0	4qre	1	1fvv	1	3u16	0
4jts	1	3h7w	1	4jxh	1	3h0a	0
1dne	1	3tyu	0	4tu4	1	3gnw	0
4agw	1	5bwu	0	2obf	1	5g6p	0
1wm0	0	3tr9	0	5fg6	0	3kzz	0
4k0y	0	1g2m	1	4wmx	0	5ufj	0
3v6s	0	5sy3	0	2ea2	0	3chp	0
3ps6	0	3et7	1	3cdb	0	4jsm	0
2uym	0	5h24	1	4tpt	1	4v26	0
3cd7	1	4yq6	1	4xv2	1	5i8b	0
4rx5	1	4pss	0	5ar8	1	4iae	1
5t2p	1	2dhf	0	2xyx	0	3ic2	0
3r9h	0	4ypw	1	1uvt	0	3ewj	0
4kiq	1	5sy2	1	2fhy	1	4zyc	0
2vtt	0	1kms	0	4yad	0	4dgg	0
4gii	0	4ky4	0	4asp	1	3fxv	0
Total H-Bonds	**19**		**11**		**11**		**2**

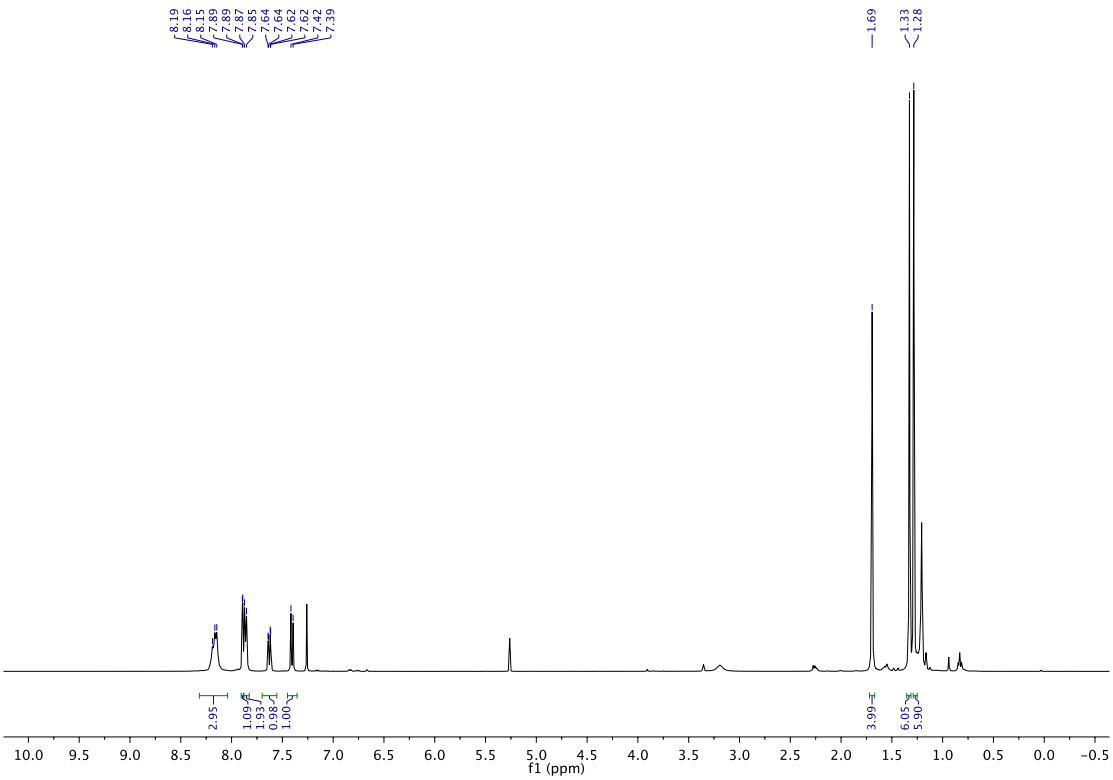
Correlation between similarity scatter plot and dihedral angle

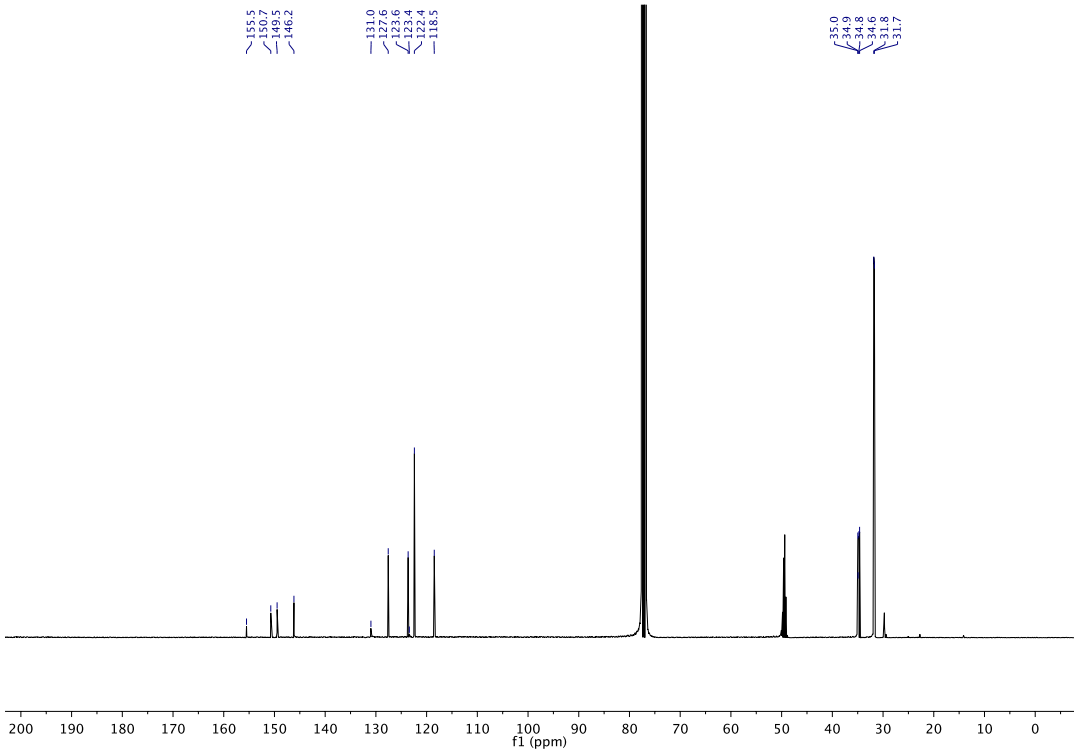
Table SI 2. Correlation between the position of each molecule in the similarity scatter plot (Figure 3/5) and the measured dihedral angle across the two-atom linker (Figure 2/4).



^{1}H and ^{13}C NMR Spectra

Azo80





LTH4 Photoswitch