FW: follow-up

Michael R Shirts

Mon 3/25/2019 11:15 AM

To: Benjamin Joseph Coscia <Benjamin.Coscia@Colorado.EDU>;

Cc: Theodore L Fobe <Theodore.Fobe@Colorado.EDU>; Garrett Andrew Meek <Garrett.Meek@Colorado.EDU>;

4 attachments (131 KB)

Terphenyl_pent_trans_mm2.pdb; Terphenyl_pent_trans_mmf94.pdb; Terphenyl_oct_trans_mmf94.pdb; Terphenyl_16mer_trans_mm2.pdb;

FYI, all. PDBs for systems from Gellman's group on their new monomers. Ben can rapidly put together atomistic systems, so I've talked to him a bit about generating these to run, and starting some exploratory runs just to get information. I think that would be the fastest route to helping Sam. I think then Lenny and Garrett can analyze the results. I will engage Adam a bit more.

See below from Sam:

- We are eager to pursue a collaboration on atomistic simulations of the terphenyl oligomers. I have cc'd Adam Kleman on this message -- he is leading the experimental work. I will let Adam provide the information you request. He'll lead this exchange going forward, but I'll stay in the loop.

Best,
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Michael Shirts
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Department of Chemical and Biological Engineering
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From: Adam F Kleman <kleman2@wisc.edu>
Date: Monday, March 25, 2019 at 10:40 AM
To: Michael R Shirts <Michael.Shirts@Colorado.EDU>
Cc: SAMUEL H GELLMAN <gellman@chem.wisc.edu>
Subject: Re: follow-up

Hi Michael,

I was very excited when I heard you may be willing to perform some simulations for our terphenyl oligomers. I'd be grateful for any simulations or structures you could provide. I've been trying to grow x-ray quality crystals with no luck.
I believe having some computational support would enable me to more thoughtfully choose variations on the structure to synthesize. I understand if time does not permit, but if you'd like to try any sort of simulation that provides us with some structural information, I'd appreciate the attempt.
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To this end, I've attached several pdb-format files of the quick simulations we've performed. Another group member did the computational work here, and from what I understand the calculations are not particularly advanced (only took him a few minutes to draw, a few hours to compute). If these would be more useful to you in a different format, I may be able to provide that (I can put you in contact with this other group member as well if needed). If you'd like any more information, please let me know. I am interested in some variations on these structures with other amino acids interspersed, but I think this is enough for now.

Thanks for your time,

-Adam Kleman

> On Mar 25, 2019, at 10:44 AM, SAMUEL H GELLMAN <gellman@chem.wisc.edu> wrote:
>
> Michael,
>
> We are eager to pursue a collaboration on atomistic simulations of the terphenyl oligomers. I have cc'd Adam Kleman on this message -- he is leading the experimental work. I will let Adam provide the information you request. He'll lead this exchange going forward, but I'll stay in the loop.
>
> Sam
>
> Sam Gellman
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>
> ---
>
> **From:** Michael R Shirts <Michael.Shirts@Colorado.EDU>
> **Sent:** Saturday, March 23, 2019 6:51 AM
> **To:** SAMUEL H GELLMAN
> **Subject:** Re: follow-up
>
> - Those subunits I sent to you are not necessarily flat. The u umost stable conformation of biphenyl has a twist about the bond between the rings.
>
> Yes, I saw the structures – was writing too fast. The effective number of degrees is low given the number of atoms, which would be more amenable to addressing hypotheses with CG modeling.

- We are flying blind on this project -- no computational component (and no collaborator). If you are interested, I'd be happy to talk about this possibility.

We'd be interested in trying a few off-the-shelf things (might take a couple of weekas as we're doing a big push to get our CG modeling workflow complete). If you had a short oligamer in machine readable format (like what you used to visualize it on slide 1), that would simplify the attempt.

Best,
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From: SAMUEL H GELLMAN <gellman@chem.wisc.edu>
Date: Friday, March 22, 2019 at 9:51 AM
To: Michael R Shirts <Michael.Shirts@Colorado.EDU>
Subject: Re: follow-up

Thanks, Michael. I enjoyed the conversation as well.

Those subunits I sent to you are not necessarily flat. The most stable conformation of biphenyl has a twist about the bond between the rings.

We are flying blind on this project -- no computational component (and no collaborator). If you are interested, I'd be happy to talk about this possibility.

Sam

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From: Michael R Shirts <Michael.Shirts@Colorado.EDU>
Sent: Thursday, March 21, 2019 6:25 PM
To: SAMUEL H GELLMAN
Subject: Re: follow-up

Hi, Sam-

Excellent to talk with you! The stereo terochemical patterning hypothesis and the importance of repeated torsional units is interesting – we will have to think about how to access features like that.

Those new monomers are very interesting, and potentially the sort of things that could be examined a bit more easily with CG models since they have relatively little chemical detail (mostly flat and bulky). We make sure we are thinking about it as we examine our model space.

It's possible we could do some atomistic modeling of these new moonomers as well just to get some more detail on how they might fold up, if you needed it; but I'm guessing you already have collaborators on that (assuming that you actually want or need those sorts of simulations at this point in time!)

Best,
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From: SAMUEL H GELLMAN <gellman@chem.wisc.edu>
Date: Monday, March 18, 2019 at 6:10 PM
To: Michael R Shirts <Michael.Shirts@Colorado.EDU>
Subject: follow-up

Michael,

Very nice to talk with you and your students today. I hope that at least a little of what I said made sense.

Attached is the paper from the Hungarians on the "stereochemical patterning hypothesis." Possibly interesting on your end.

Also attached are a few ppt slides about new types of subunits we are exploring. These have a very different profile of rigidity/flexibility/hydrophobicity relative to other building blocks that have been examined empirically. Or that's my hunch, anyway. If you can't make sense of these slides, we can discuss.

Good luck! I look forward to staying in touch.
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Sam

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