Supplementary material

Surface induced dissociation yields quaternary substructure of refractory noncovalent Phosphorylase B and Glutamate Dehydrogenase complexes

Xin Ma; Mowei Zhou; Vicki H. Wysocki*

Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio 43210, United States

Permanent address: 876 Biological Sciences Building, 484 W 12th Ave, Columbus, OH 43210, USA.

*Corresponding author. Address reprint requests to Prof. Vicki H. Wysocki, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210. Email: wysocki.11@osu.edu. Phone: (614) 292-8687

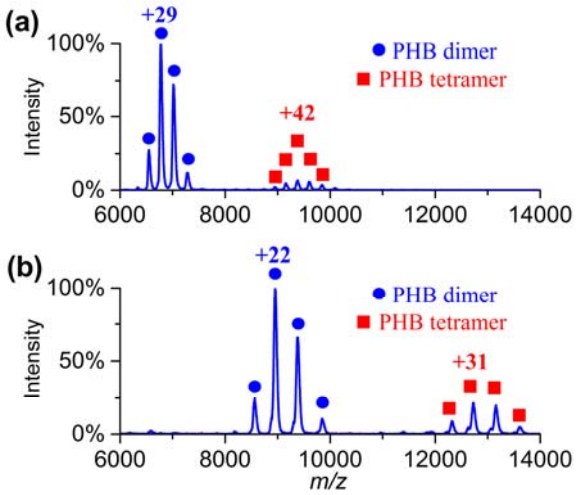

Figure S-1. Mass spectra of PHB in ammonium acetate before and after adding TEAA. (a) Mass spectrum of PHB in ammonium acetate. PHB dimer is the major species and a small amount of PHB tetramer is observed. The +29 peak is the highest of the PHB dimer peaks. (b) Mass spectrum of PHB in ammonium acetate after adding 10% (v/v) TEAA. PHB dimer is the major species and PHB tetramer is observed. The +22 peak is the highest of the PHB dimer peaks.

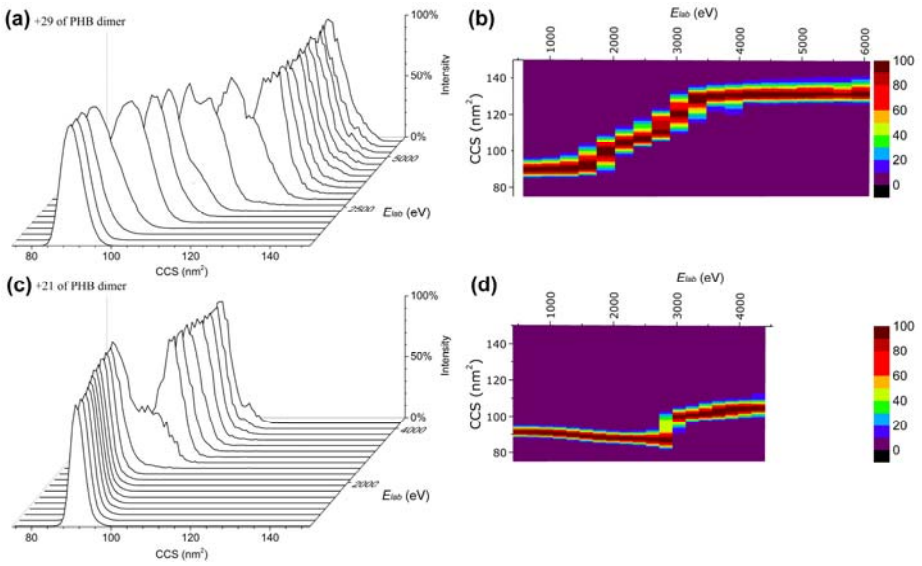

Figure S-2. The CCS change of PHB dimer at different CID E_{lab}. Each drift time plot is normalized to the highest intensity in that plot. (a) CCS of PHB dimer at +29 at CID E_{lab} from 580 to 5800 eV. The precursor begins to unfold at 1500 eV and the CCS reaches ~100 nm^2 at 2000 eV. It is stable until E_{lab} 2300 eV and then increases to ~130 nm^2. The CCS does not change when the E_{lab} is higher than 3200 eV. (b) An alternative representation of the data in (a). (c) CCS of PHB dimer at +21 at CID E_{lab} from 420 to 4200 eV. The CCS decreases slightly and reaches ~85 nm^2 at 2500 eV. It increases abruptly to ~100 nm^2 when the E_{lab} is higher than 3000 eV. (d) An alternative representation of the data in (c).

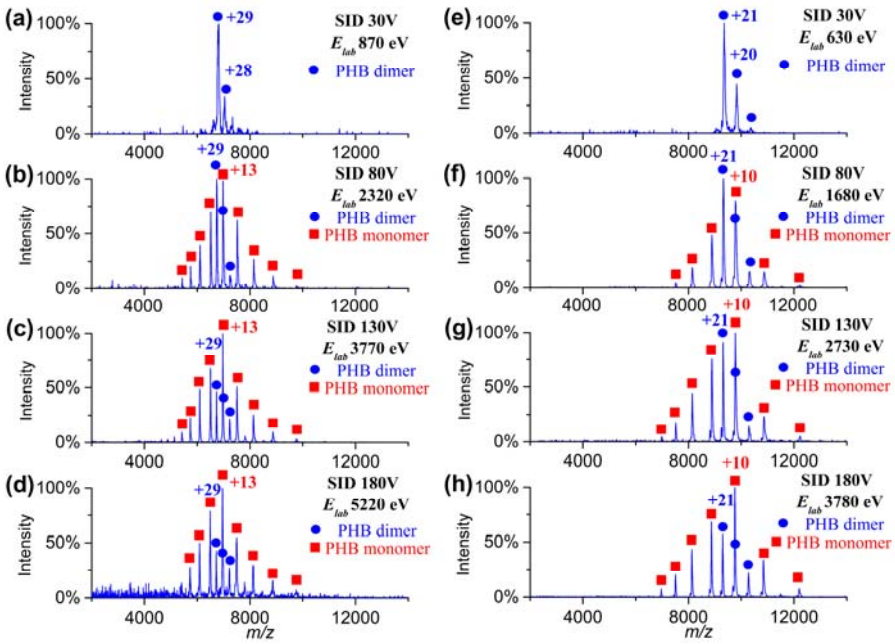

Figure S-3. (a) Selected SID spectra of +29 PHB dimer at SID acceleration voltages 30-180 V (E_{lab} 870-5220 eV). (b) Selected SID spectra of +21 PHB dimer at SID acceleration voltages 30-180 V (E_{lab} 630-3780 eV). Only 4 spectra are plotted for simplicity.

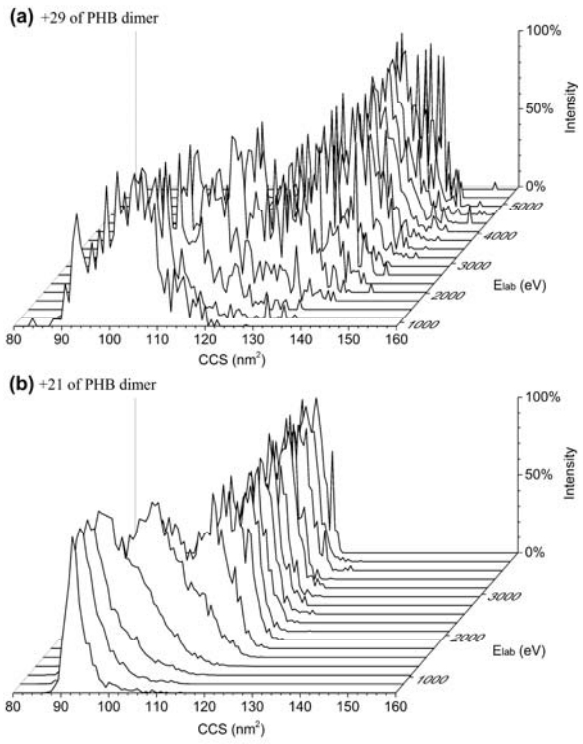

Figure S-4. The CCS change of PHB dimer precursor at different SID E_{lab}. Each drift time plot is normalized to the highest intensity in that plot. (a) PHB dimer at +29 precursor CCSs at SID E_{lab} from 870 to 5510 eV. The precursor begins to unfold at 870 eV and the CCS reaches ~140 nm^2 when the E_{lab} is higher than 2500 eV. (b) PHB dimer at +21 precursor CCSs at SID E_{lab} from 630 to 3990 eV. The CCS of the precursor begins to increase at 1300 eV and reaches ~120 nm^2 and is stable when the E_{lab} is higher than 1800 eV. Signal to noise is poorer for these drift time plots than for those of CID, because precursor fragments by SID.

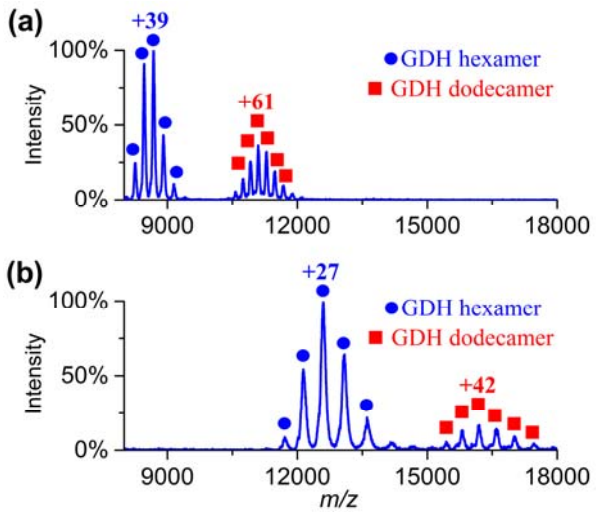

Figure S-5. Mass spectra of GDH in ammonium acetate before and after adding TEAA. (a) Mass spectrum of GDH in ammonium acetate. GDH hexamer is the major species and GDH dodecamer is observed. The +39 peak is the highest of the GDH hexamer peaks. (b) MS spectrum of GDH in ammonium acetate after adding 10% (v/v) TEAA. GDH hexamer is the major species and GDH dodecamer is observed. The +27 peak is the highest of the GDH hexamer peaks.

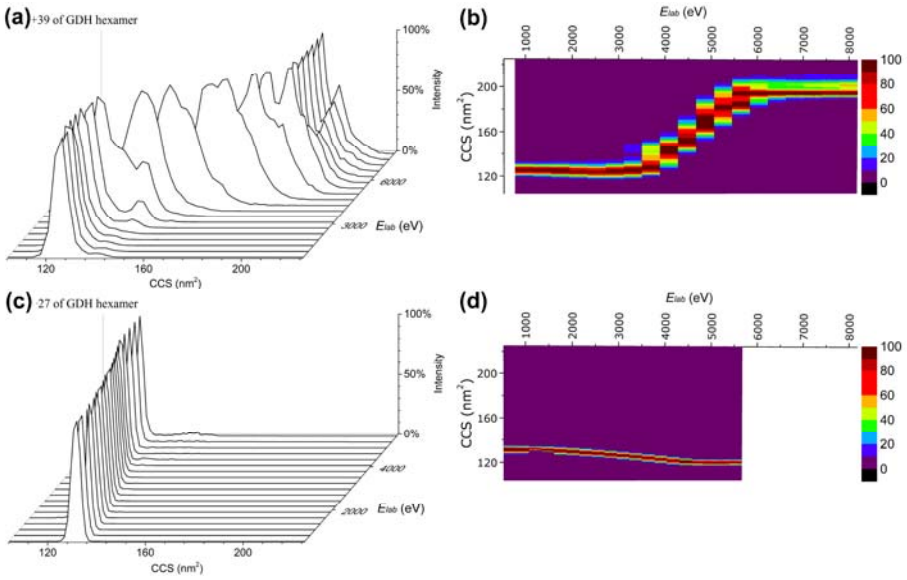

Figure S-6. The CCS change of GDH hexamer at different CID E_{lab}. Each drift time plot is normalized to the highest intensity in that plot. (a) CCS of GDH hexamer at +39 at CID E_{lab} from 780 to 7800 eV. The hexamer begins to unfold at 3000 eV and the CCS reaches ~200 nm^2 at 5000 eV. The CCS does not change when the E_{lab} is higher than 5000 eV. (b) an alternative representation of the data in (a). (c) CCS of GDH hexamer at +27 at CID E_{lab} from 540 to 5400 eV. The CCS decreases at 2000 eV and reaches ~124 nm^2 at 4000 eV. The CCS does not change when the E_{lab} is higher than 4000 eV. (d) An alternative representation of the data in (c).

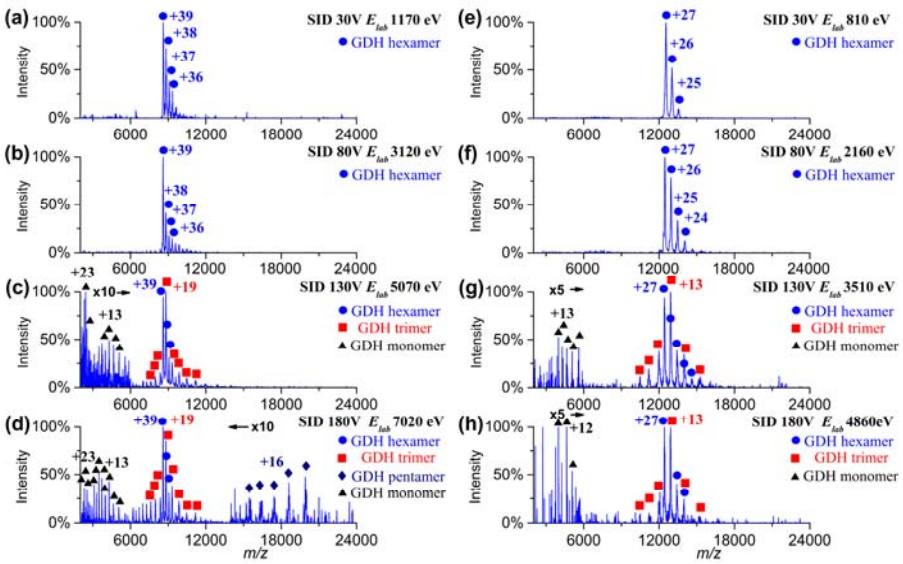

Figure S-7. (a) Selected SID spectra of +39 GDH hexamer at SID acceleration voltages 30-180 V (E_{lab} 1170-7020 eV). (b) Selected SID spectra of +27 GDH hexamer at SID acceleration voltages 30-180 V (E_{lab} 810-4860 eV). Only 4 spectra of each charge state are plotted for simplicity.

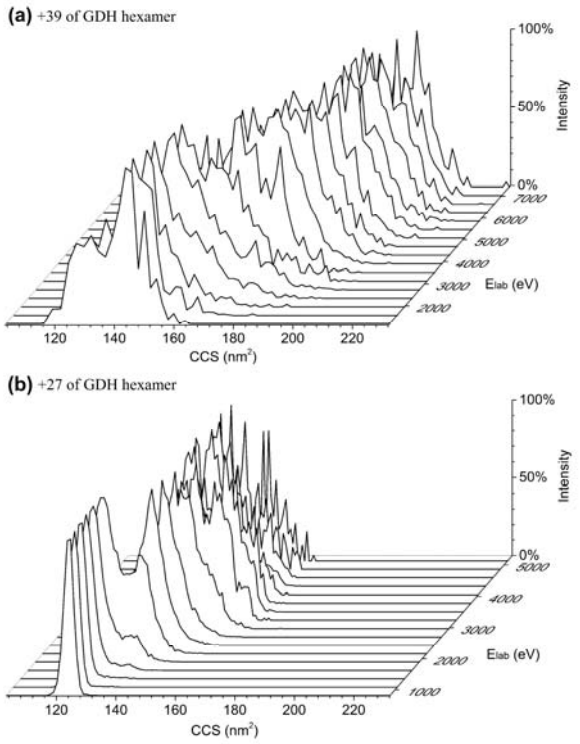

Figure S-8. The CCS change of GDH hexamer precursor at different SID E_{lab}. All the spectra are normalized to its own highest intensity. (a) GDH hexamer at +39 precursor CCSs at SID E_{lab} from 1170 to 7410 eV. The precursor begins to unfold at 1170 eV and the CCS reaches ~190 nm^2 at 3000 eV. The CCS does not change when the E_{lab} is higher than 3000 eV. (b) GDH hexamer at +27 precursor CCSs at SID E_{lab} from 810 to 5130 eV. The CCS of the precursor decreases slightly when the E_{lab} increases to 2000 eV. The CCS begins to increase at 2000 eV and reaches ~150 nm^2 at 2900 eV. The CCS does not change when the E_{lab} was higher than 2900 eV.

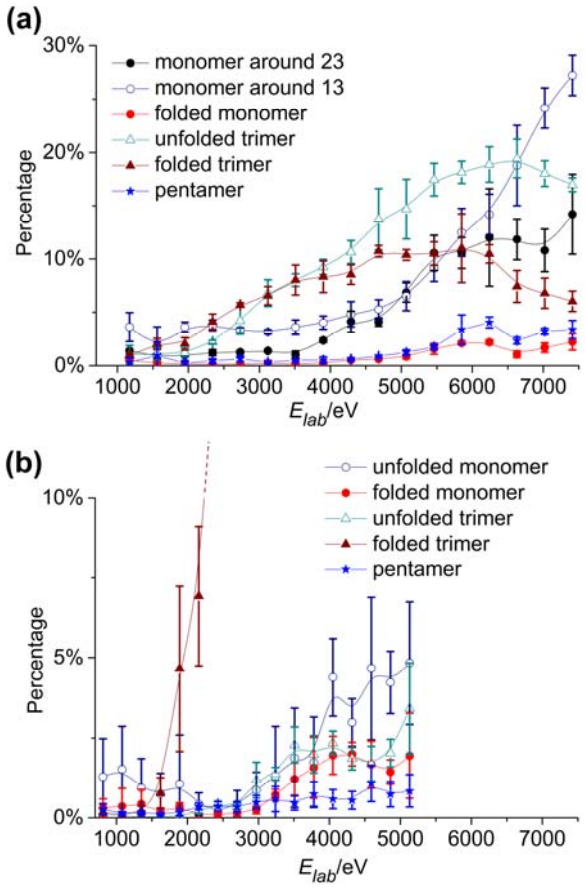

Figure S-9. Zoom-in views of the low abundance products of dissociation curves of GDH hexamer at +39 and +27. (a) Zoom-in viewsof the low abundance peaks of Figure 6b (dissociation curves of +39 GDH hexamer). (b) Zoom-in view of low abundance peaks of Figure 6d lower panel (dissociation curves of +27 GDH hexamer).