Electronic Supplementary Material (ESI) for RSC Advances.

The effect of heterocyclic π bridges on second order nonlinear optical properties of compounds formed between ferrocenyl and corannulenyl

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Table S1 The energies (*E*, a.u.) of the endo-n and exo-n (n = 1-5) compounds obtained by the B2PLYP functional.

Compound	**endo-1**	**endo-2**	**endo-3**	**endo-4**	**endo-5**
E	-2415.017401	-2645.612370	-2639.645234	-2659.501495	-2982.396382
Compound	**exo-1**	**exo-2**	**exo-3**	**exo-4**	**exo-5**
E	-2415.017109	-2645.612471	-2639.646737	-2659.501079	-2982.394052

Table S2 The relative energies (E_{rel}, kcal/mol) between endo and exo conformers obtained by the MP2 functional.

Compound	E_{rel}	Compound	E_{rel}
endo-1	0	**exo-1**	-0.05
endo-2	0	**exo-2**	-0.15
endo-3	0	**exo-3**	-1.02
endo-4	0	**exo-4**	0.11
endo-5	0	**exo-5**	4.69

Table S3 The bowl depth (Å) for endo-n and exo-n (n = 3-5) compounds.

Compound	**endo-3**	**exo-3**	**endo-4**	**exo-4**	**endo-5**	**exo-5**
Depth	0.881	0.866	0.866	0.860	0.871	0.870

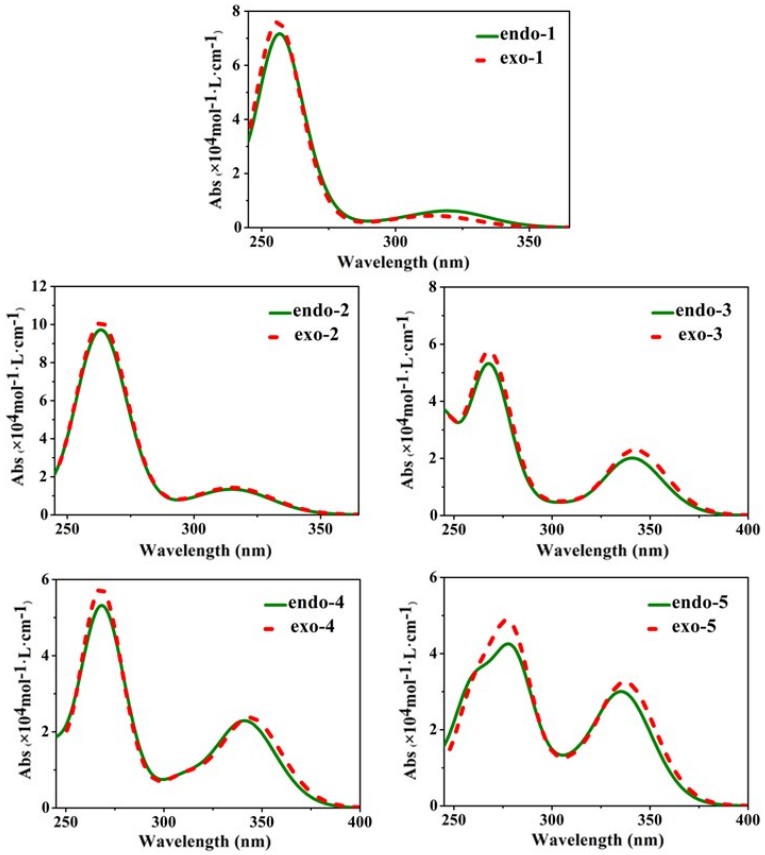

Fig. S1 UV-vis spectra of endo-n and exo-n (n = 1-5) compounds.

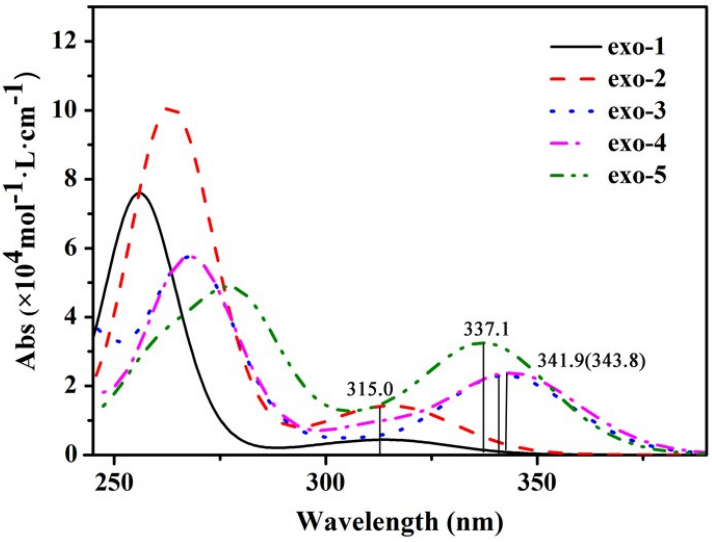

Fig. S2 UV-vis spectra of exo-n (n = 1-5) compounds.

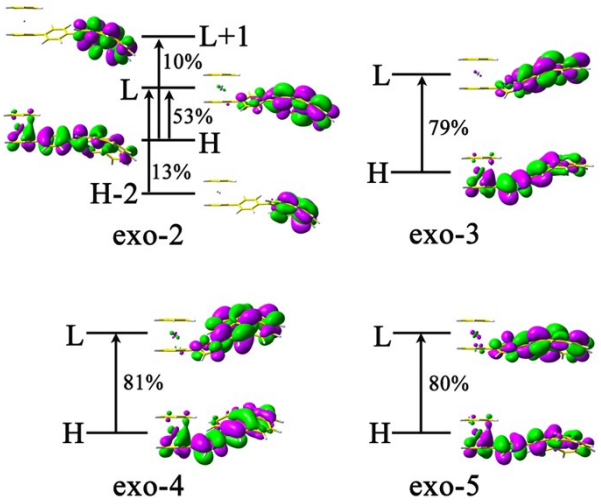

Fig. S3 Molecular orbitals corresponding to the dominant electron transitions of exo-n (n = 2-5) compounds (H = HOMO, L = LUMO, H-2 = HOMO-2, L+1 = LUMO+1, etc.).