

Comparing the PyBEST-PPP results with experimental values in 'Targeting Excited States in All-Trans Polyenes

C10H12-S3	t	U	k	single-Excitation (ev) H->L (5,6)	Exp
	-4.5	4.3	3.0	3.21731735	3.57
	-4.5	5.0	3.0	3.37591925	3.57
	-4.5	5.5	3.0	3.49242706	3.57
	-4.5	5.7	3.0	3.53964189	3.57
	-4.5	5.8	3.0	3.56336642	3.57
	-4.5	6.0	3.0	3.61103693eV	3.57
C12H14-S3				single-Excitation (ev) H->L (6,7)	
	-4.5	4.3	3.0	2.72448501	3.31
	-4.5	5.0	3.0	2.85892489	3.31
	-4.5	5.5	3.0	2.956793	3.31
	-4.5	5.7	3.0	2.9962171	3.31
	-4.5	5.8	3.0	3.0159727	3.31
	-4.5	6.0	3.0	3.0555545	3.31
	-4.5	7.0	3.0	3.2541014	3.31
	-4.5	7.3	3.0	3.3136476	3.31
	-4.5	8.0	3.0	3.4521811	3.31
C14H16-S3				single-Excitation (ev) H->L (7,8)	
	-4.5	4.3	3.0	2.36533575	3.12
	-4.5	5.0	3.0	2.4818704	3.12
	-4.5	5.5	3.0	2.5657621	3.12
	-4.5	5.7	3.0	2.5993048	3.12
	-4.5	5.8	3.0	2.6160565	3.12
	-4.5	6.0	3.0	2.6495002	3.12
	-4.5	7.0	3.0	2.814665	3.12
	-4.5	7.3	3.0	2.8632844	3.12
	-4.5	8.0	3.0	2.9746199	3.12
	-4.5	9.0	3.0	3.1289953	3.12