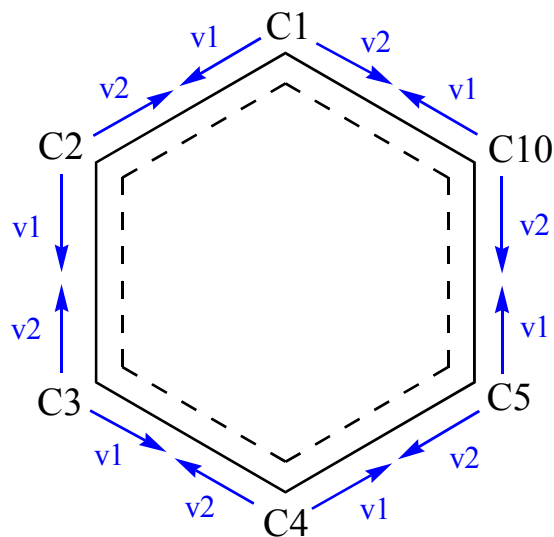


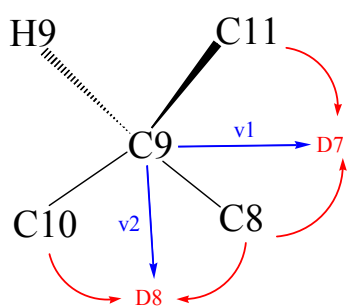
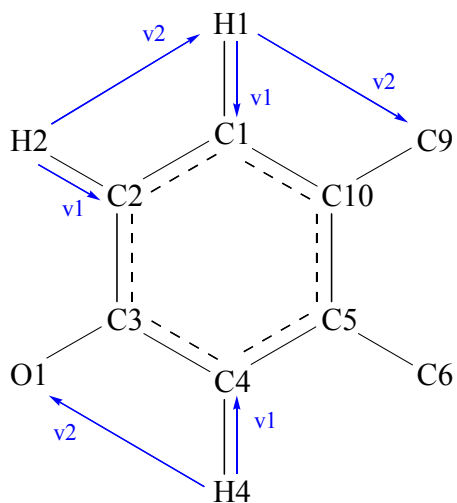
Supplemental Material

Diagrams corresponding to vector definitions in Tables 1 and 2.

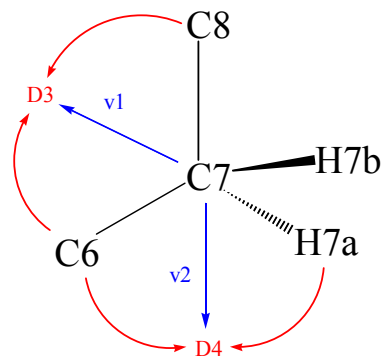
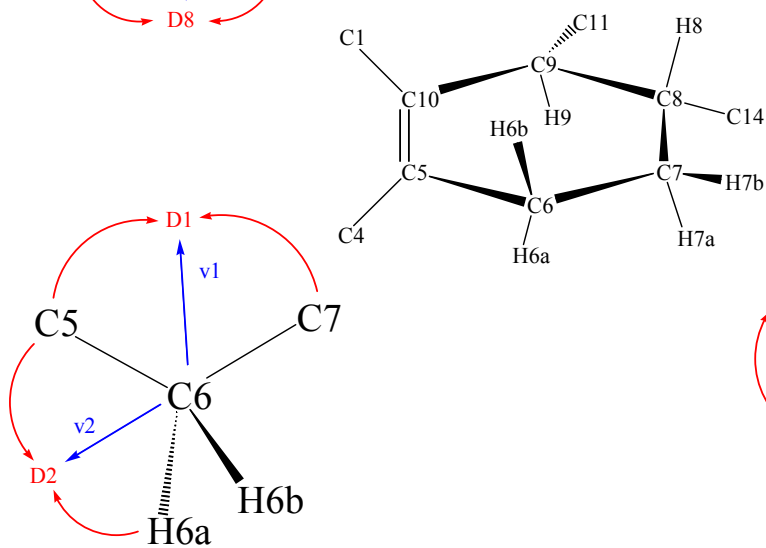
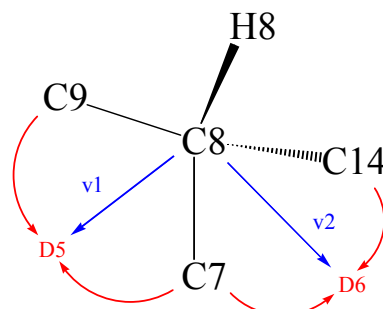
A Ring

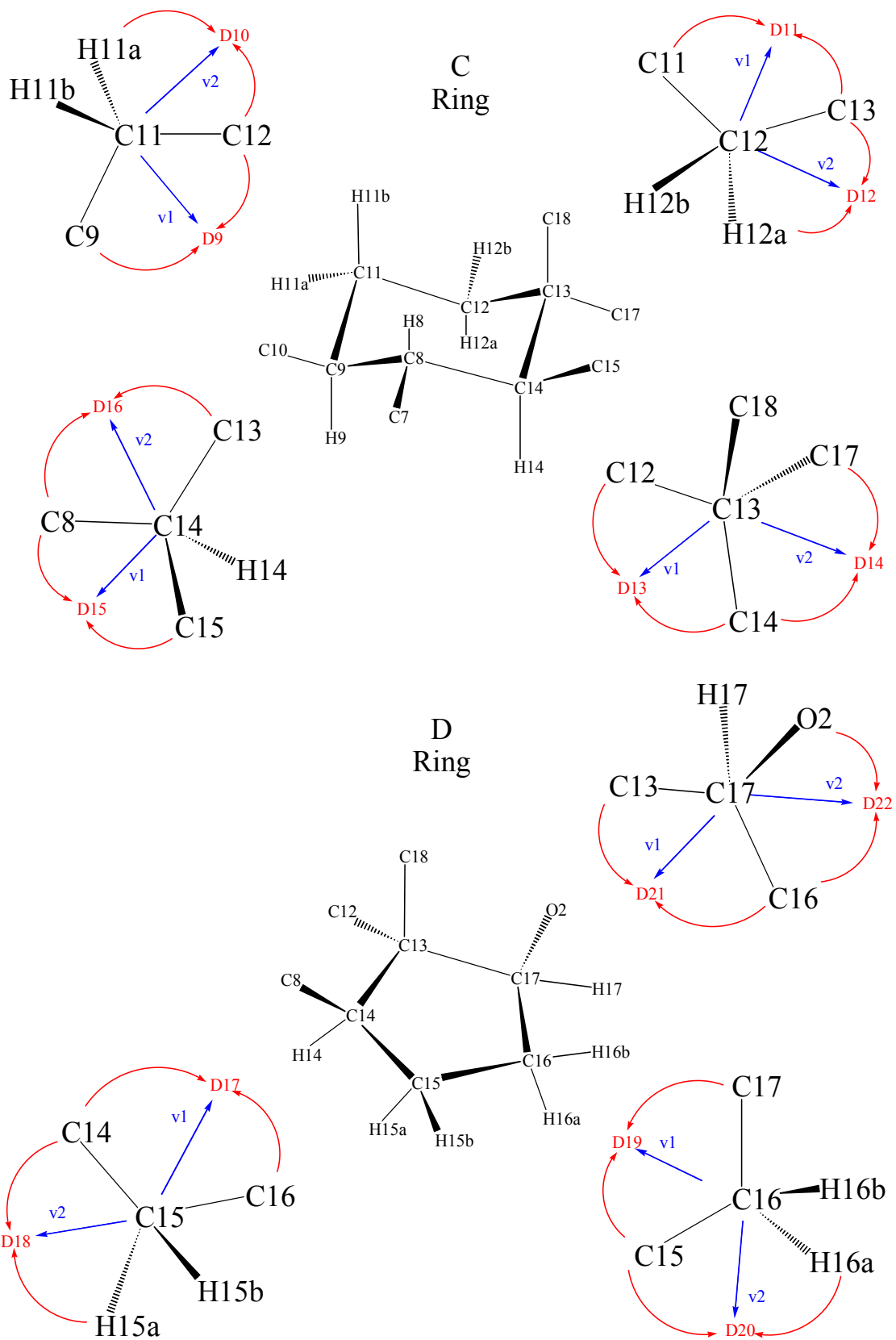


A Ring Hydrogens



B Ring

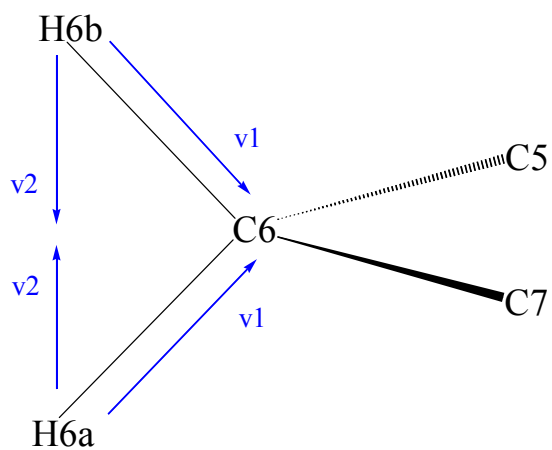




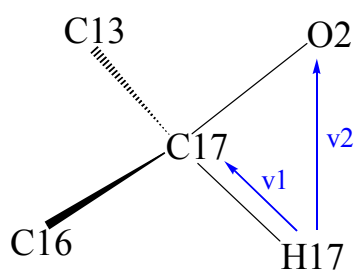
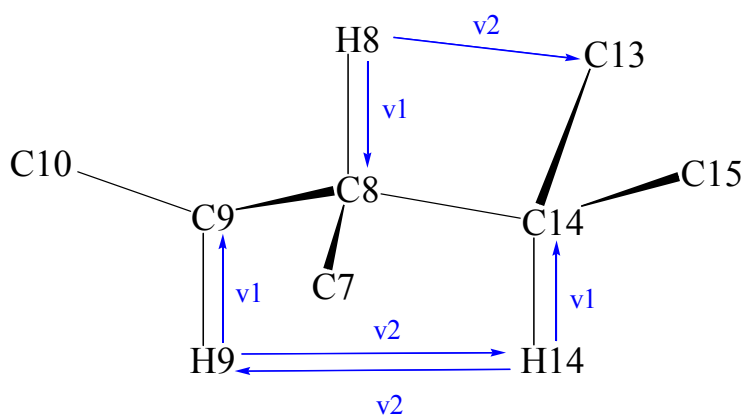
All R₂CH₂ Hydrogens

These include the hydrogens on the following C atoms.
(C6,C7,C11,C12,C15,C16)

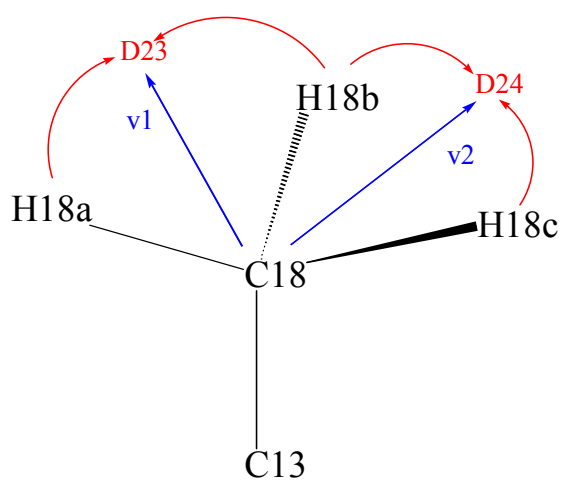
This example is for C6.



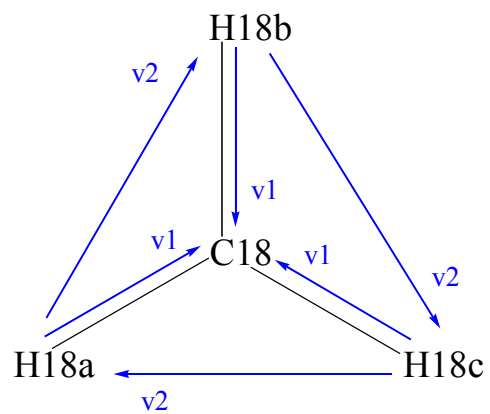
H8, H9, H14 and H17



C18 with Hydrogens



Looking down the 3-fold axis of C18.



Input for XD to describe the local coordinate system for all estrogen hydrocarbon core atoms

ATOM	ATOM0	AX1	ATOM1	ATOM2	AX2	R/L	TP	TBL	KAP	LMX	SITESYM	CHEMCON
C(1)	C(2)	X	C(1)	C(10)	Y	R	2	3	4	4	NO	
C(2)	C(3)	X	C(2)	C(1)	Y	R	2	3	4	4	NO	
C(3)	C(4)	X	C(3)	C(2)	Y	R	2	3	2	4	NO	
C(4)	C(5)	X	C(4)	C(3)	Y	R	2	3	4	4	NO	
C(5)	C(10)	X	C(5)	C(4)	Y	R	2	3	5	4	NO	
C(6)	DUM1	X	C(6)	DUM2	Y	R	2	3	6	4	NO	
C(7)	DUM3	X	C(7)	DUM4	Y	R	2	3	6	4	NO	
C(8)	DUM5	X	C(8)	DUM6	Y	R	2	3	6	4	NO	
C(9)	DUM7	X	C(9)	DUM8	Y	R	2	3	6	4	NO	
C(10)	C(1)	X	C(10)	C(5)	Y	R	2	3	5	4	NO	
C(11)	DUM9	X	C(11)	DUM10	Y	R	2	3	6	4	NO	
C(12)	DUM11	X	C(12)	DUM12	Y	R	2	3	6	4	NO	
C(13)	DUM13	X	C(13)	DUM14	Y	R	2	3	6	4	NO	
C(14)	DUM15	X	C(14)	DUM16	Y	R	2	3	6	4	NO	
C(15)	DUM17	X	C(15)	DUM18	Y	R	2	3	6	4	NO	
C(16)	DUM19	X	C(16)	DUM20	Y	R	2	3	6	4	NO	
C(17)	DUM21	X	C(17)	DUM22	Y	R	2	3	3	4	NO	
C(18)	DUM23	X	C(18)	DUM24	Y	R	2	3	6	4	NO	
C(19)	O(3)	X	C(19)	N(1)	Y	R	2	3	9	4	NO	
H(1)	C(1)	Z	H(1)	C(9)	Y	R	1	4	7	2	NO	
H(2)	C(2)	Z	H(2)	H(1)	Y	R	1	4	7	2	NO	
H(4)	C(4)	Z	H(4)	O(1)	Y	R	1	4	7	2	NO	
H(6A)	C(6)	Z	H(6A)	H(6B)	Y	R	1	4	7	2	NO	
H(6B)	C(6)	Z	H(6B)	H(6A)	Y	R	1	4	7	2	NO	H(6A)
H(7A)	C(7)	Z	H(7A)	H(7B)	Y	R	1	4	7	2	NO	
H(7B)	C(7)	Z	H(7B)	H(7A)	Y	R	1	4	7	2	NO	H(7A)
H(8)	C(8)	Z	H(8)	C(13)	Y	R	1	4	7	2	NO	
H(9)	C(9)	Z	H(9)	H(14)	Y	R	1	4	7	2	NO	
H(11A)	C(11)	Z	H(11A)	H(11B)	Y	R	1	4	7	2	NO	
H(11B)	C(11)	Z	H(11B)	H(11A)	Y	R	1	4	7	2	NO	H(11A)
H(12A)	C(12)	Z	H(12A)	H(12B)	Y	R	1	4	7	2	NO	
H(12B)	C(12)	Z	H(12B)	H(12A)	Y	R	1	4	7	2	NO	H(12A)
H(14)	C(14)	Z	H(14)	H(9)	Y	R	1	4	7	2	NO	
H(15A)	C(15)	Z	H(15A)	H(15B)	Y	R	1	4	7	2	NO	
H(15B)	C(15)	Z	H(15B)	H(15A)	Y	R	1	4	7	2	NO	H(15A)
H(16A)	C(16)	Z	H(16A)	H(16B)	Y	R	1	4	7	2	NO	
H(16B)	C(16)	Z	H(16B)	H(16A)	Y	R	1	4	7	2	NO	H(16A)
H(17)	C(17)	Z	H(17)	O(2)	Y	R	1	4	7	2	NO	
H(18A)	C(18)	Z	H(18A)	H(18B)	Y	R	1	4	7	2	NO	
H(18B)	C(18)	Z	H(18B)	H(18C)	Y	R	1	4	7	2	NO	H(18A)
H(18C)	C(18)	Z	H(18C)	H(18A)	Y	R	1	4	7	2	NO	H(18A)