Supplementary Information:

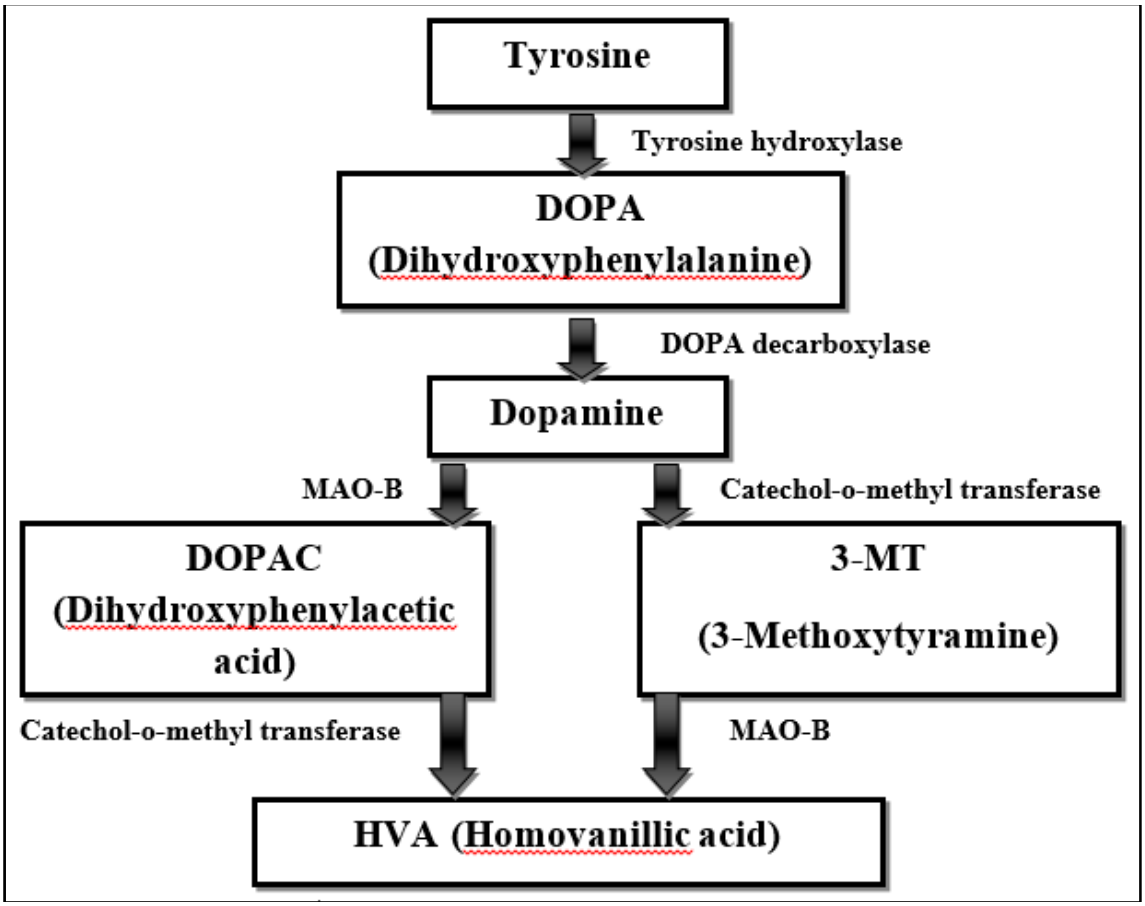

Figure S1: The flowchart indicates the role of MAO-B enzyme in degrading the Dopamine hormone.

Table S1 indicating the PDB entries of MAO-B inhibitors reported in RCSB database.

Name of PDB-ID	NAME OF INHIBITOR	IC-50/Ki VALUE
1OJ9	1PB8	35000 nm (Ki)
1OJA	ISN	3000nm (Ki), 7943nm (IC50)
1OJC	LAZ	
1OJD	LDA	
1OJB	FA8	
2XFU	FA8	
1S2Q	Rasagiline	4.4 nm (IC50)
1S2Y	RSA	127000nm (Ki)
1S3B	RMA	600nm (Ki)
1S3E	RHP	230 nm (IC50), 17000nm (Ki)
2BK3	FARNESOL	2300nm (Ki)
2BYB	DEPRENYL	
2C64	MA0	
2C65	4CR	
2C66	RM2	
2V5Z	SAG	450 nm (Ki), 80 nm (IC50)
2V60	C17	400nm (Ki)
2V61	C18	100 nm (Ki)
2VRL	TOLUENE	
2VRM	PYJ	
2VZ2	MFG	
2XFN	XCG	8300 nm (Ki)
3PO7	ZON	3100 nm (Ki)
4A7A	RGZ	4200 nm (Ki)
4A79	P1B	500 nm (Ki)
4CRT	ASS234	