

Supplementary information for

Interspecies comparison in COMT-mediated methylation of 3-BTD

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Table S1. Percent Identity Matrix of similarity of amino acid sequences between COMT from different species. (Created by Clustal W)

	Human	Monkey	Pig	Rabbit	Dog	Guinea pig	Rat	Mouse
Human	100	91.85	76.3	75	79.55	75.19	77.65	79.17
Monkey	91.85	100	76.3	76.12	78.44	74.81	76.89	78.03
Pig	76.3	76.3	100	70.9	78.44	70	71.21	72.73
Rabbit	75	76.12	70.9	100	72.28	75.75	76.34	78.63
Dog	79.55	78.44	78.44	72.28	100	75.09	78.71	80.61
Guinea Pig	75.19	74.81	70	75.75	75.09	100	82.2	82.58
Rat	77.65	76.89	71.21	76.34	78.71	82.2	100	90.53
Mouse	79.17	78.03	72.73	78.63	80.61	82.58	90.53	100

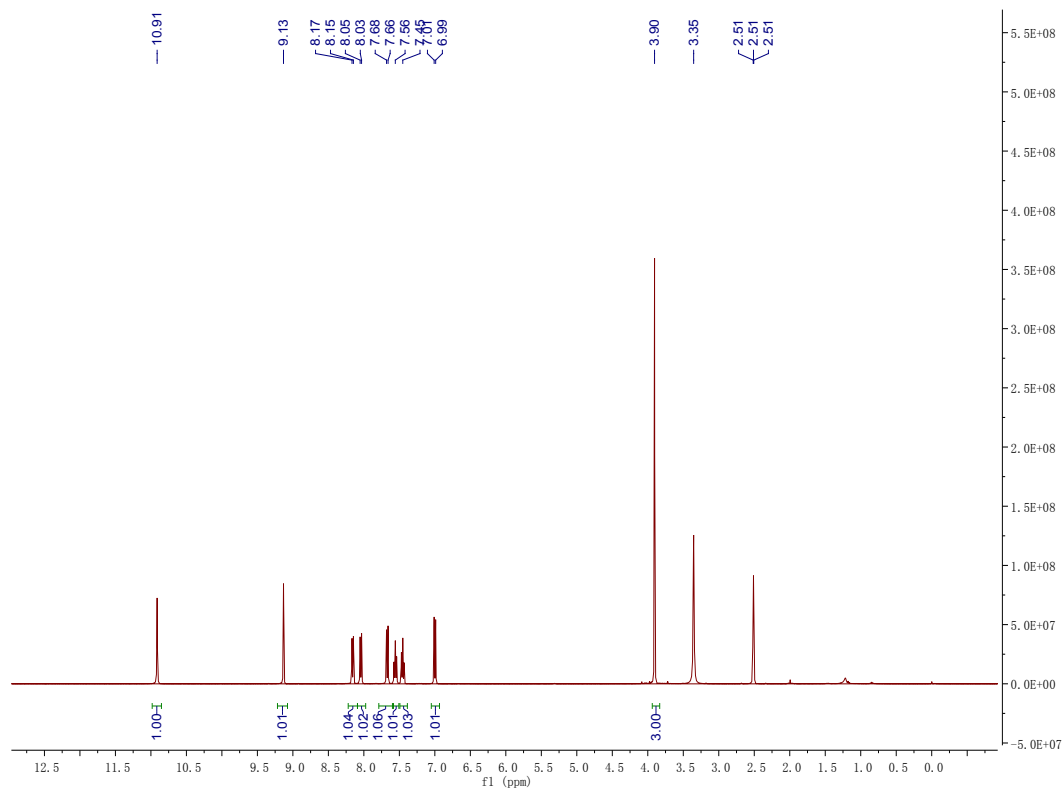


Figure S1. ^1H NMR (400 MHz, DMSO) spectrum of **3-BTMD**.

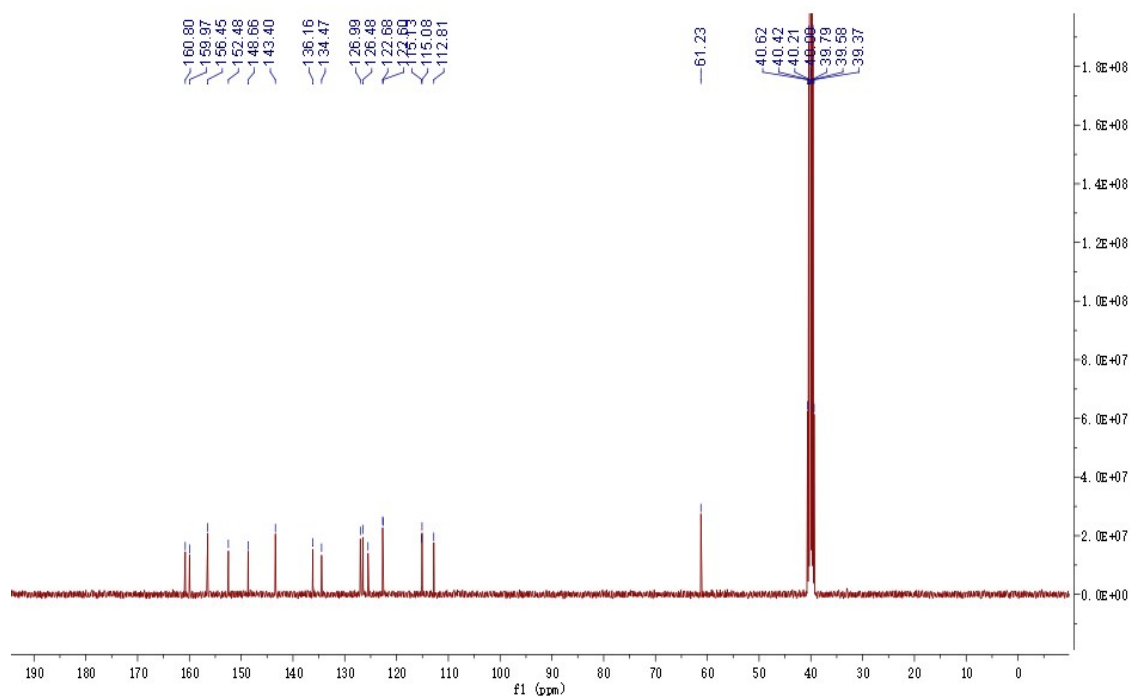


Figure S2. ^{13}C NMR (100 MHz, DMSO) spectrum of **3-BTMD**.

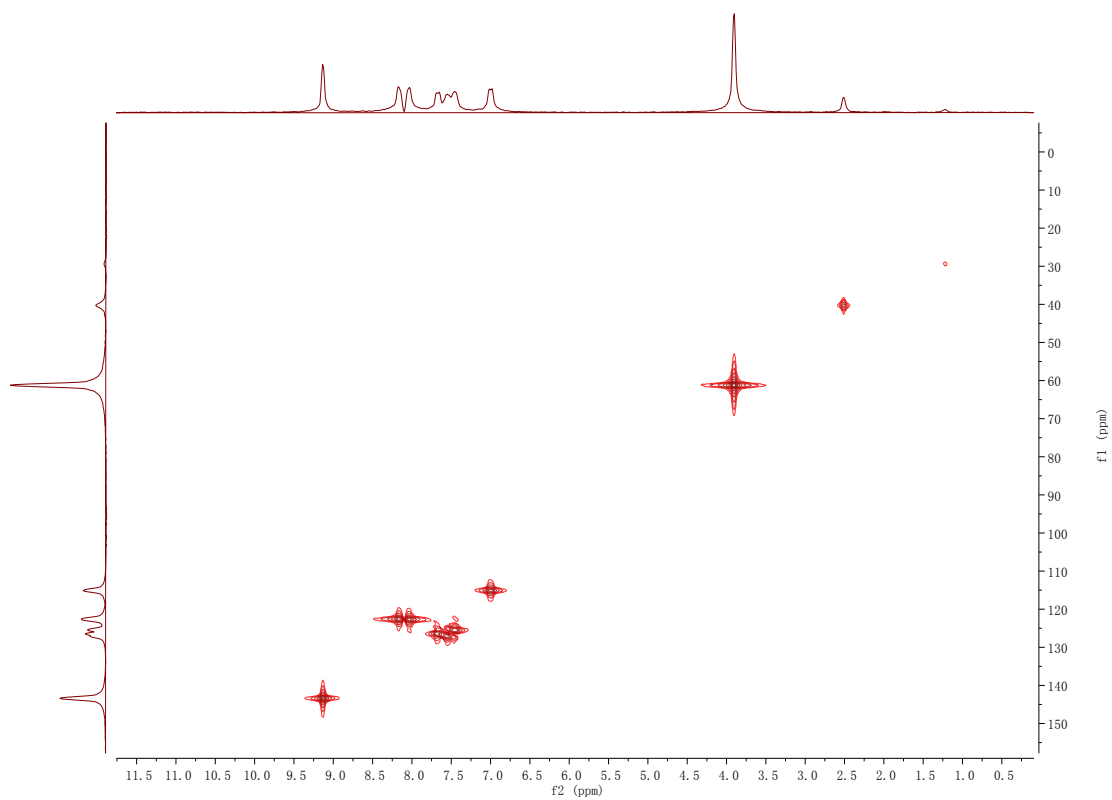


Figure S3. HSQC spectrum of **3-BTMD**.

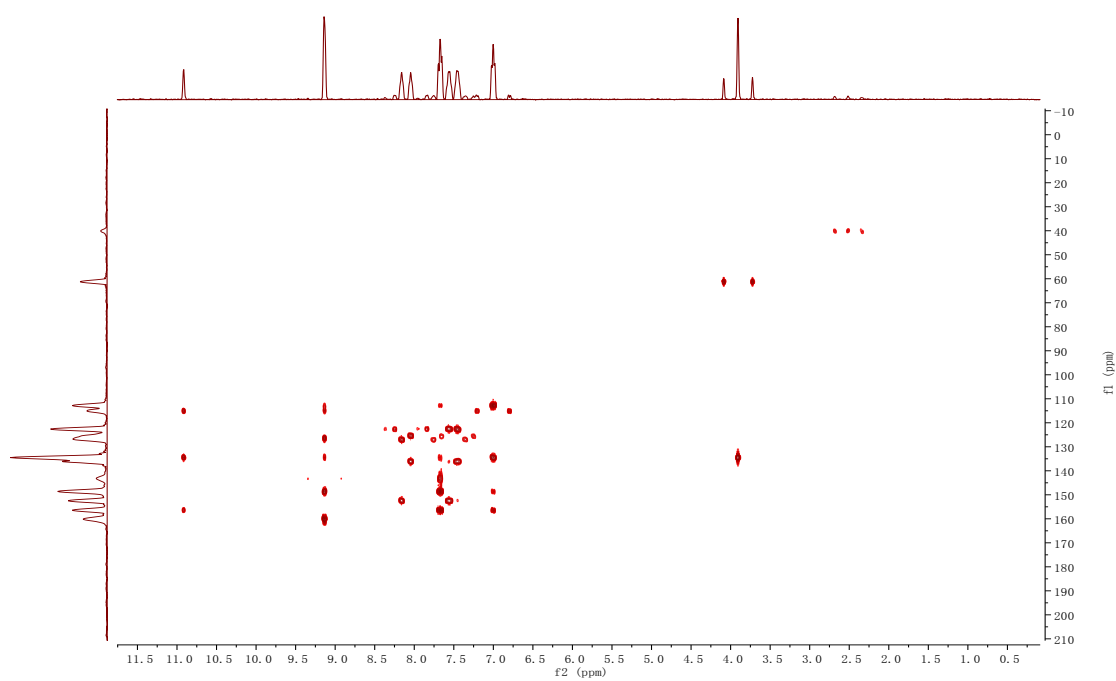


Figure S4. HMBC spectrum of **3-BTMD**.

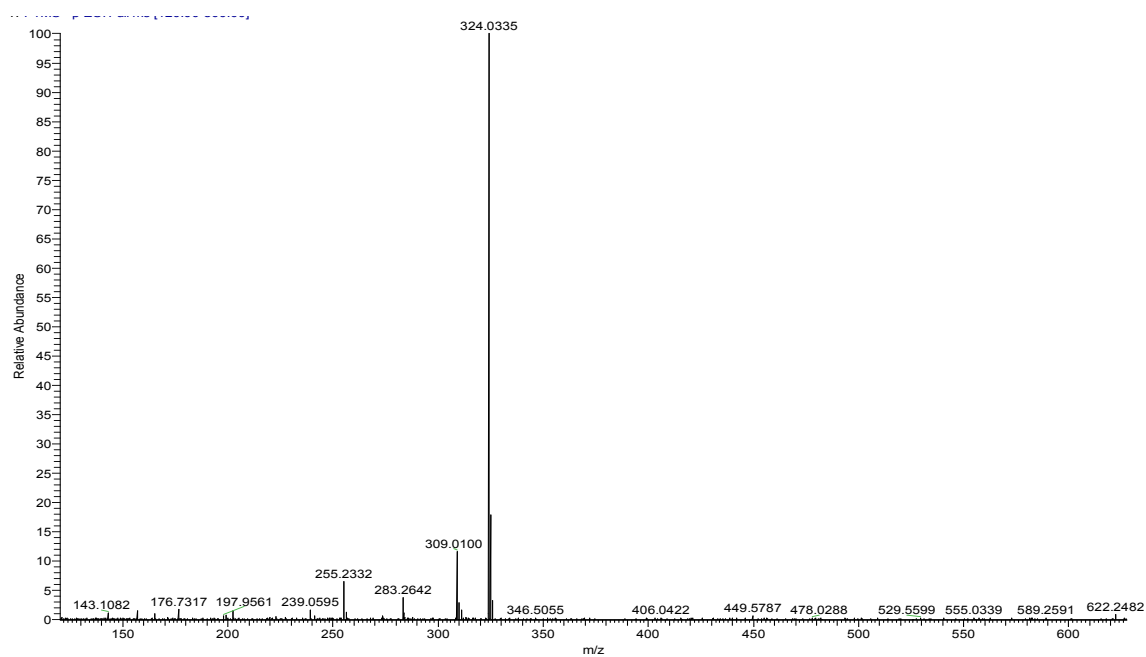
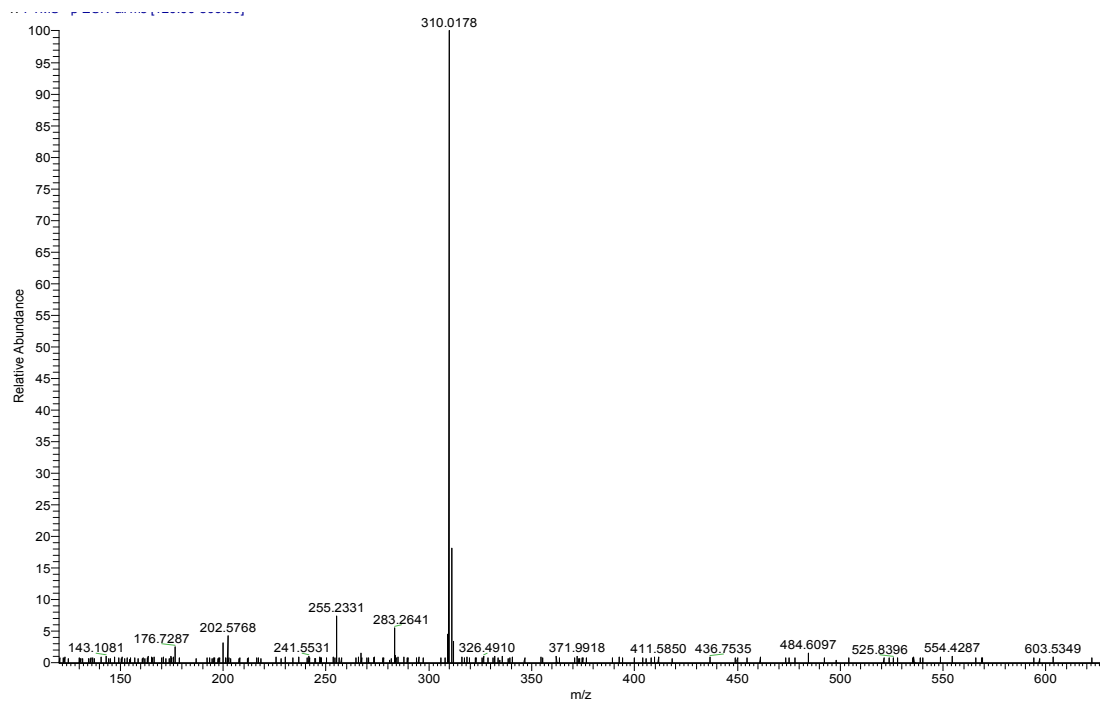


Figure S5. The MS spectrum of 3-BTD and 3-BTMD under positive ion mode.

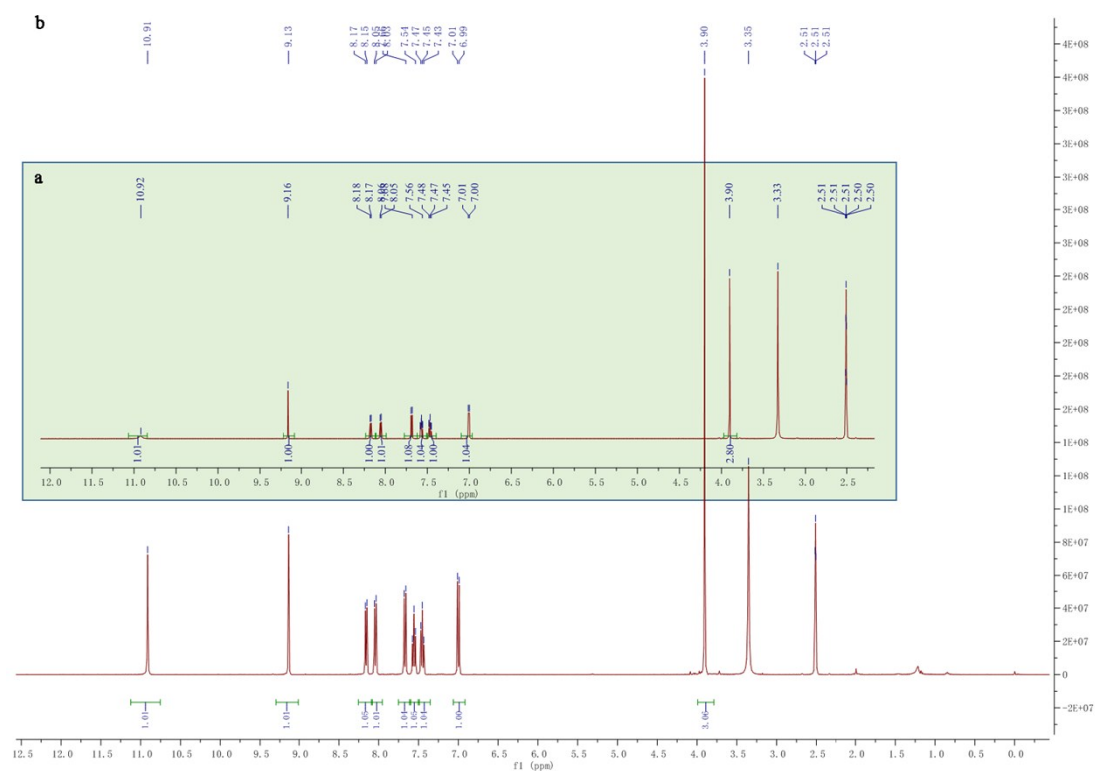


Figure S6. Comparison of ^1H NMR (400 MHz, DMSO) spectrum of bio- (a) and chem- (b) synthesized product of 3-BTD.

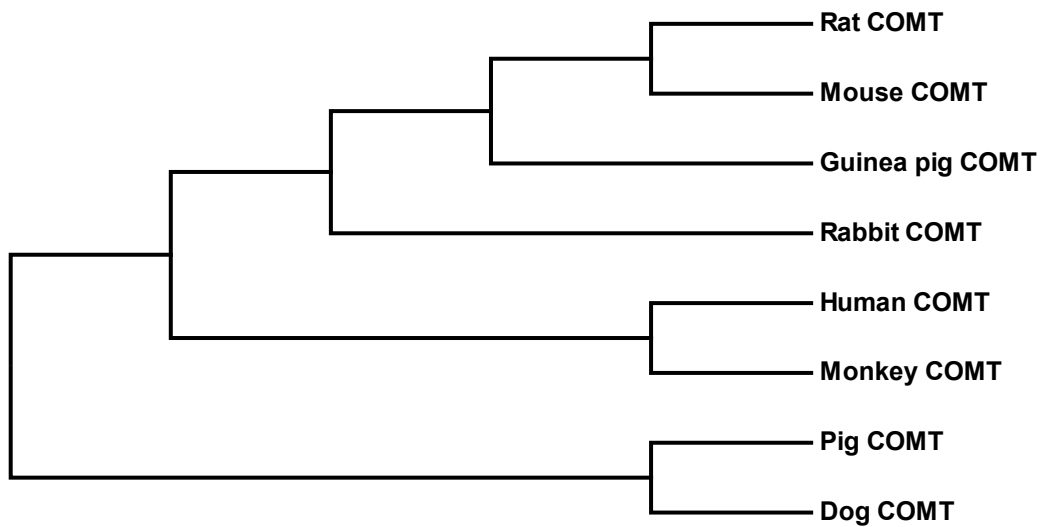


Figure S7. Phylogenetic tree of Catechol-O-methyl transferases (COMT) from different species. (Created by MEGA7.0)

*All amino acid sequences were inquired from website Ensembl (<http://asia.ensembl.org/index.html>) and NCBI (<https://www.ncbi.nlm.nih.gov/protein/>)

Human COMT: NP_000745.1 [Homo sapiens]

Rat COMT: NP_036663.1 [Rattus norvegicus]

Mouse COMT: NP_031770.2 [Mus musculus]

Monkey COMT: EHH65646.1 [Macaca fascicularis]

Pig COMT: NP_001182259.1 [Sus scrofa]

Dog COMT: XP_005636589.1 [Canis familiaris]

Rabbit COMT: G1SQP9 [Oryctolagus cuniculus]

Guinea Pig COMT: H0V363 [Cavia porcellus]