

In Vivo Neurochemical Monitoring using Benzoyl Chloride Derivatization and Liquid Chromatography – Mass Spectrometry

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Figure S1	Signal variation of repeated injection with and without internal standard.
Figure S2	Chromatographic traces of analytes detected in rat nucleus accumbens dialysate.
Figure S3	Neurotransmitter level in rat VTA and NAc upon bicuculline infusion.
Table S1	MS/MS conditions of analytes.

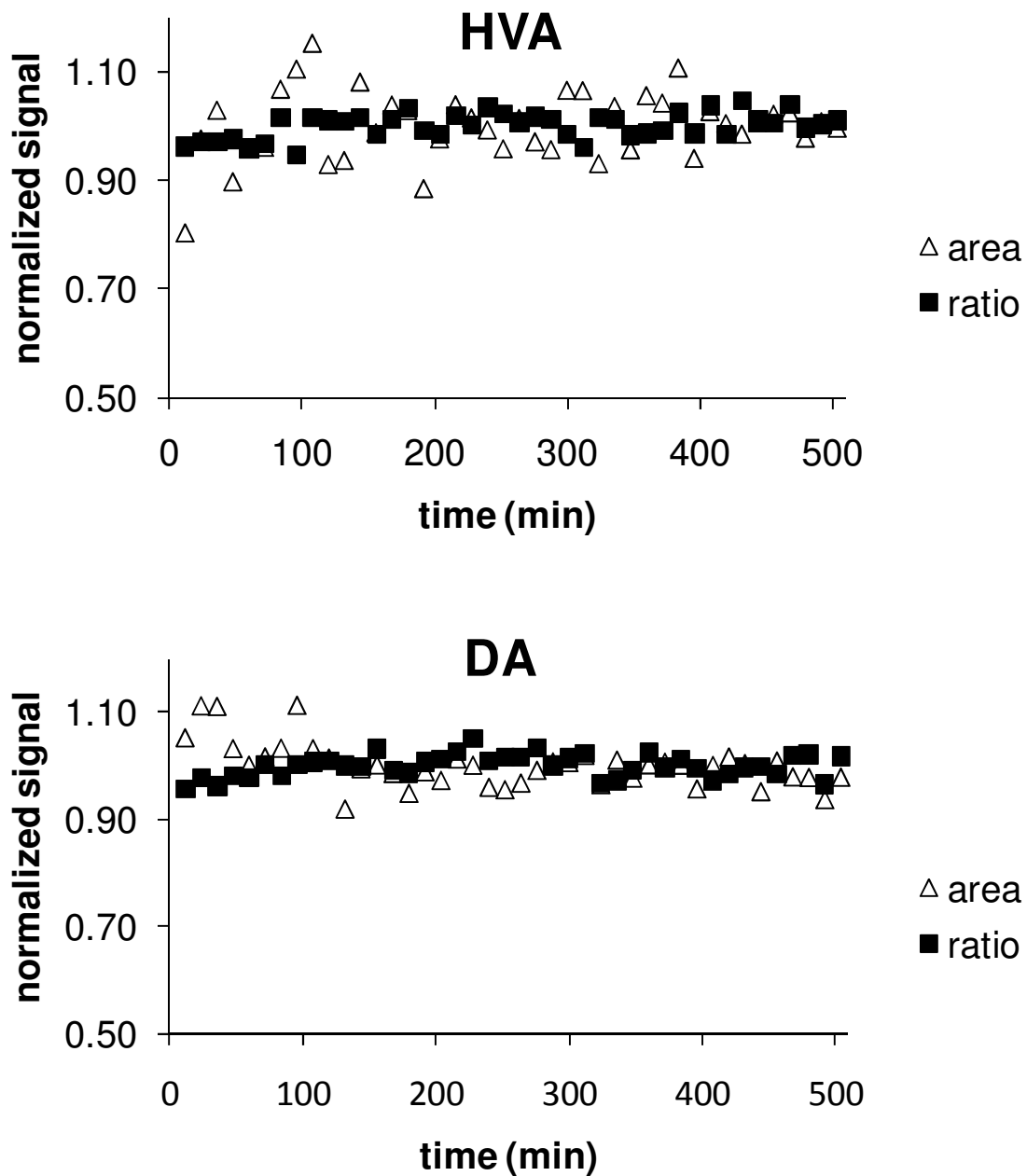
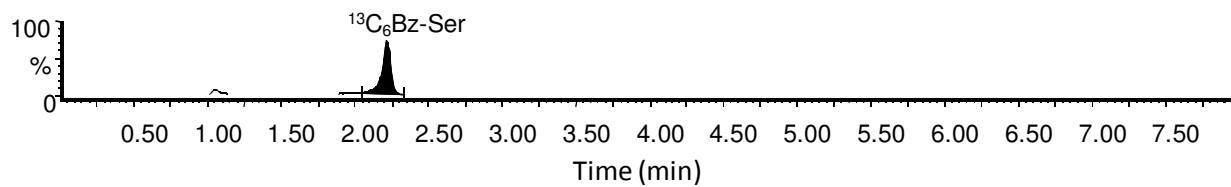
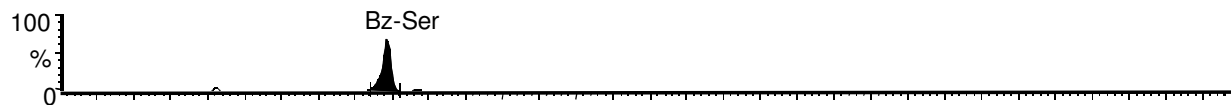
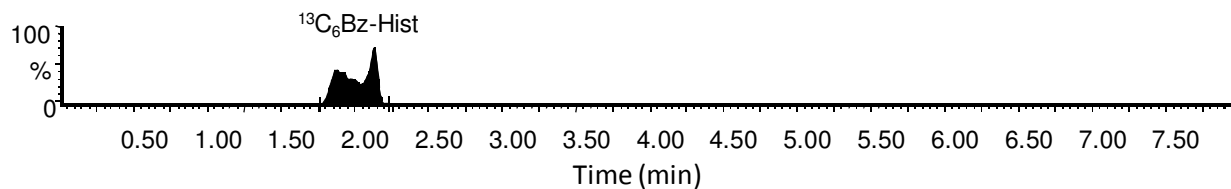
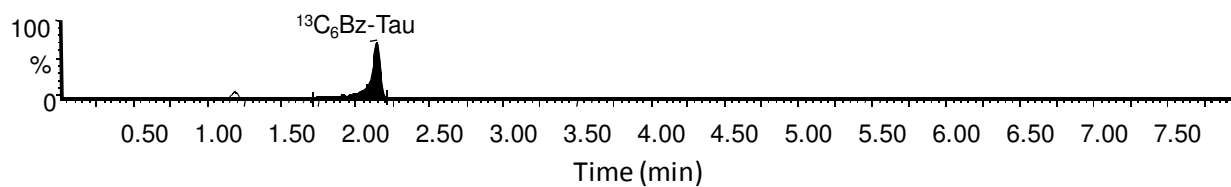
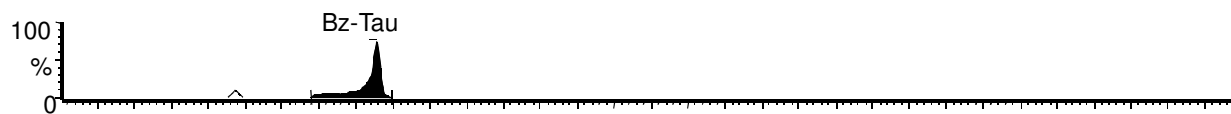
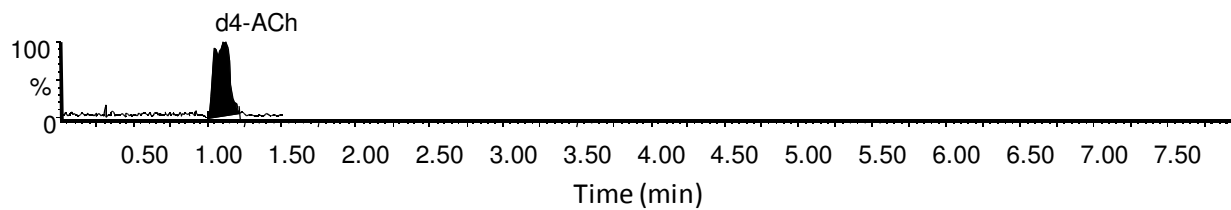
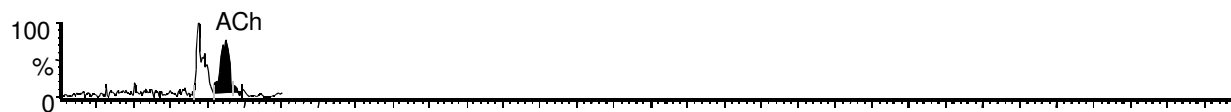
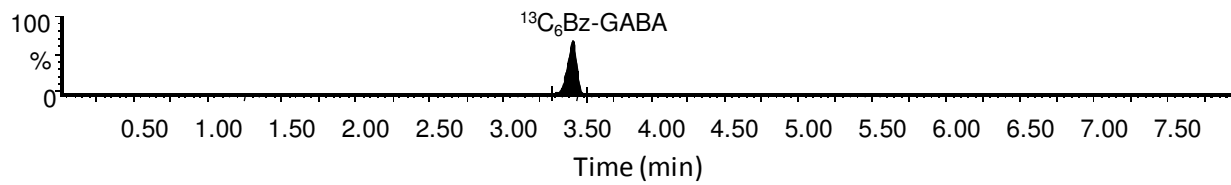
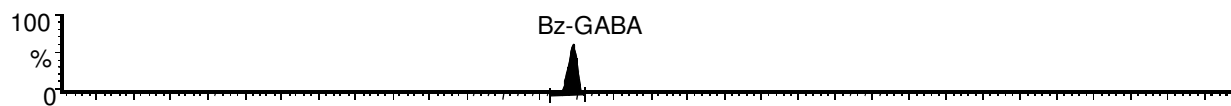
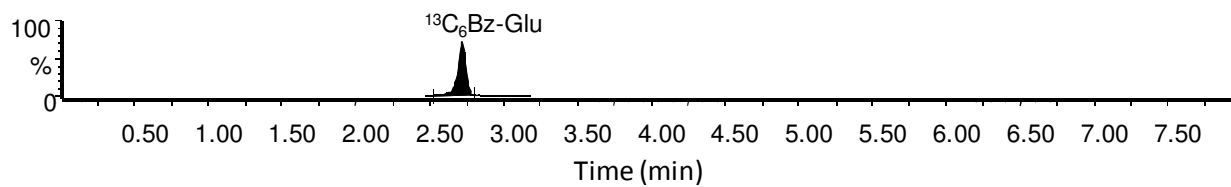
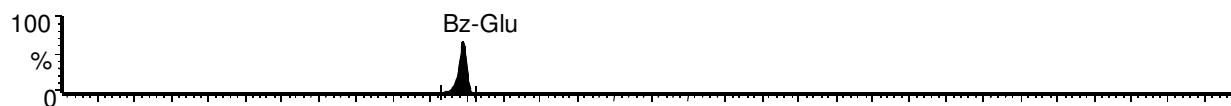
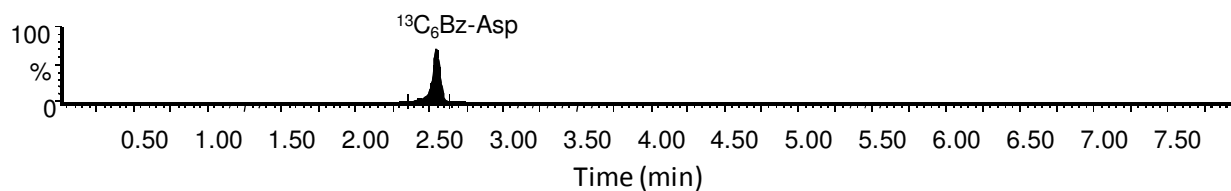
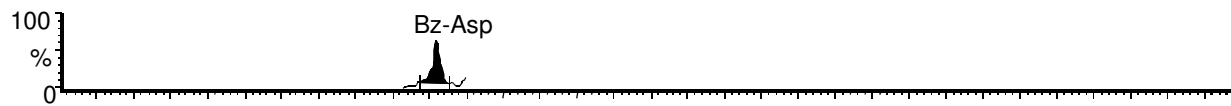
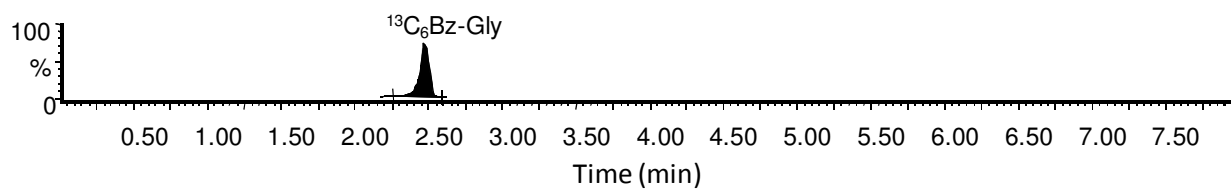
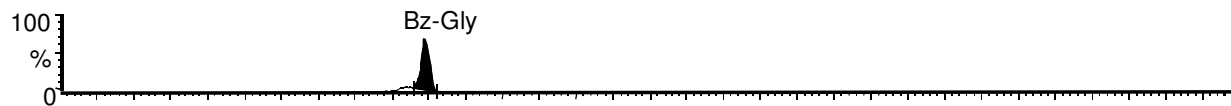
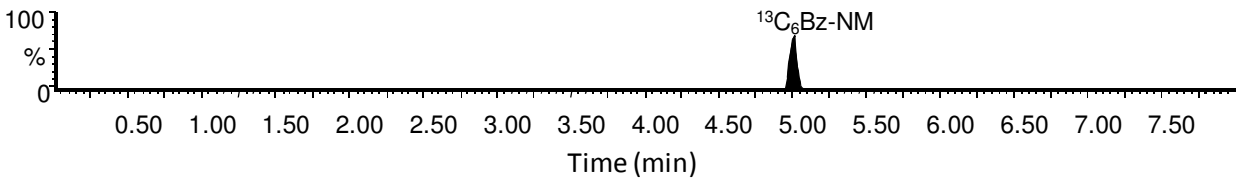
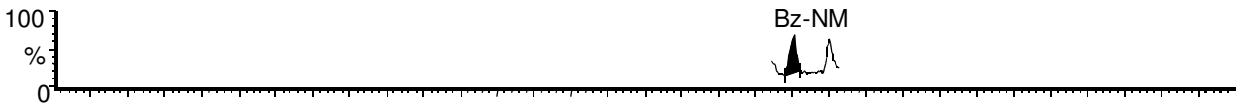
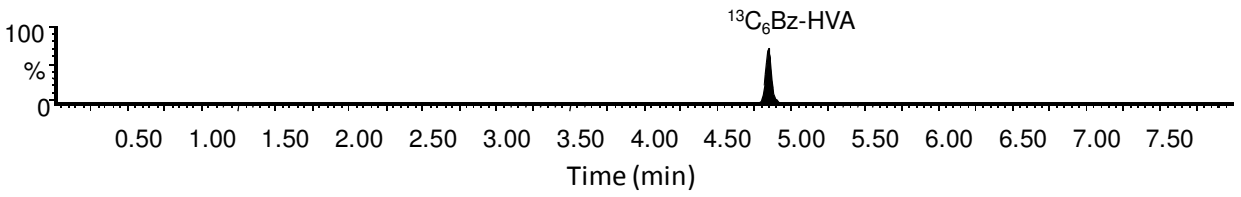
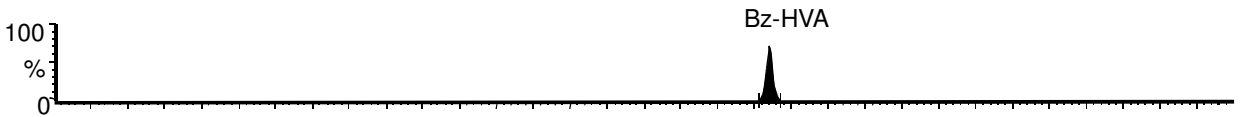
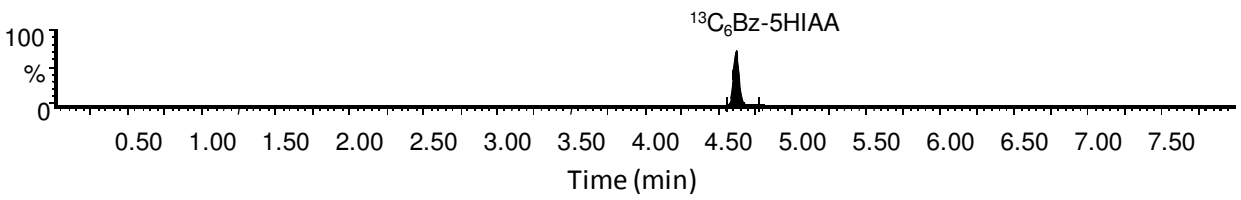
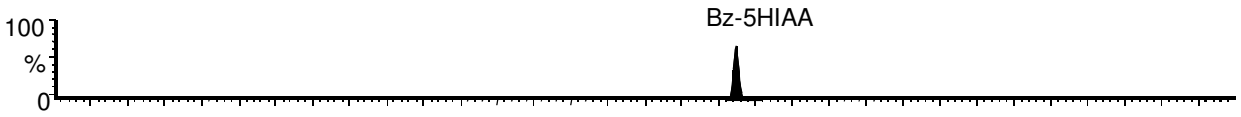
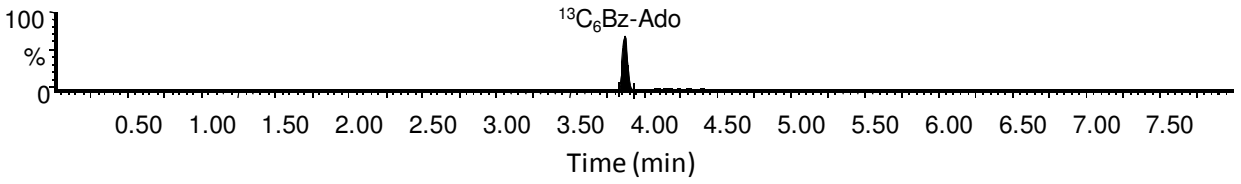
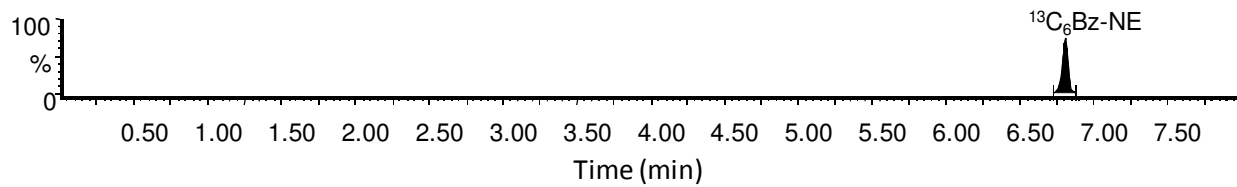
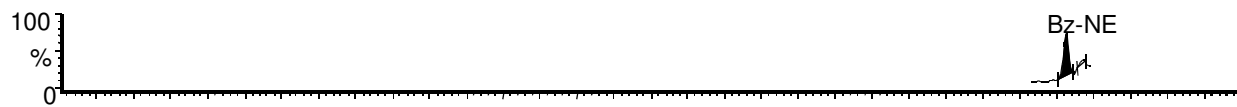
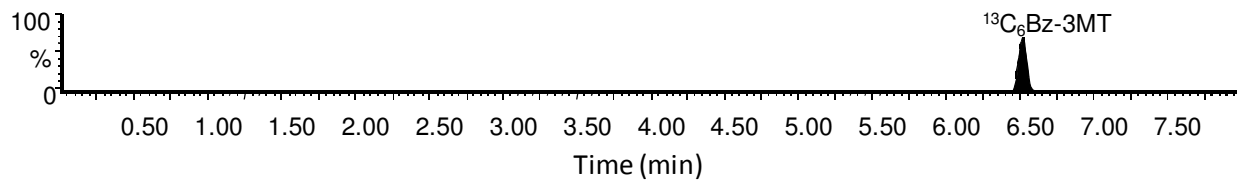
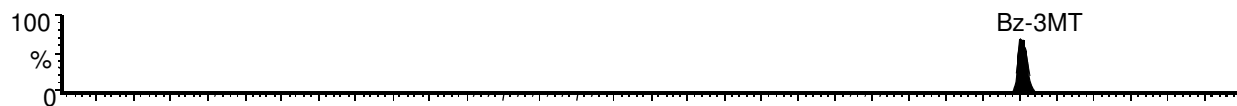
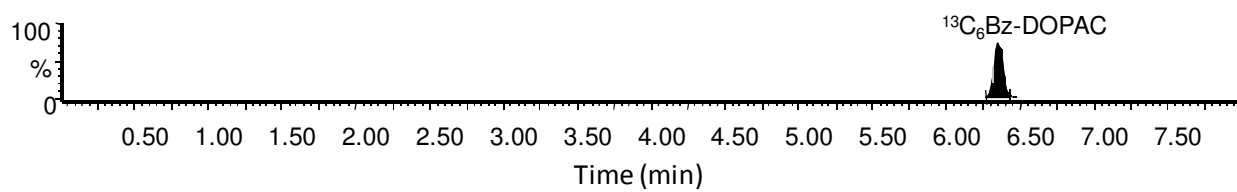
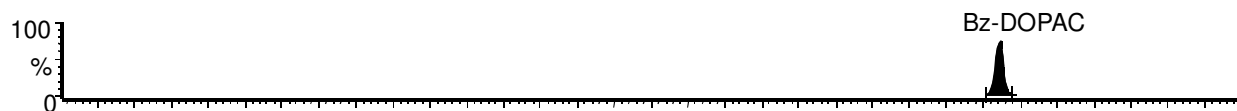
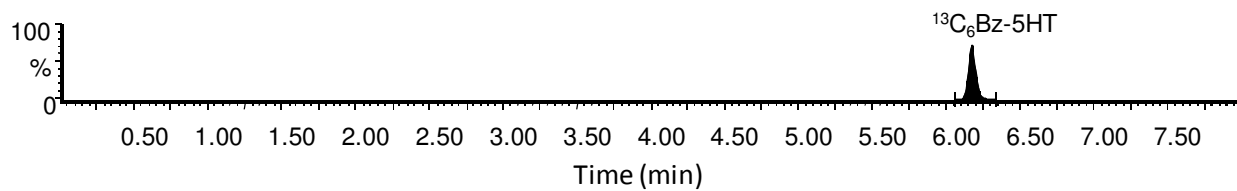
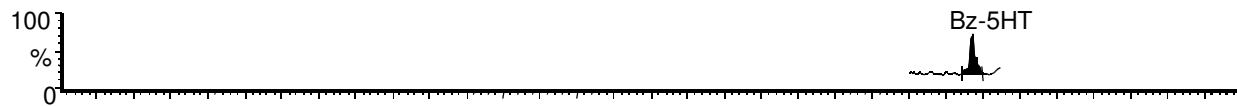


Figure S1. Peak area and peak area ratio of HVA (top) and DA (bottom) in a repeatedly analyzed standard solution. Signals were normalized to their respective averages. RSD was 6% for HVA and 4% for DA using only peak area. It was reduced to 2% for both HVA and DA when peak area ratio to internal standard was used for quantification.









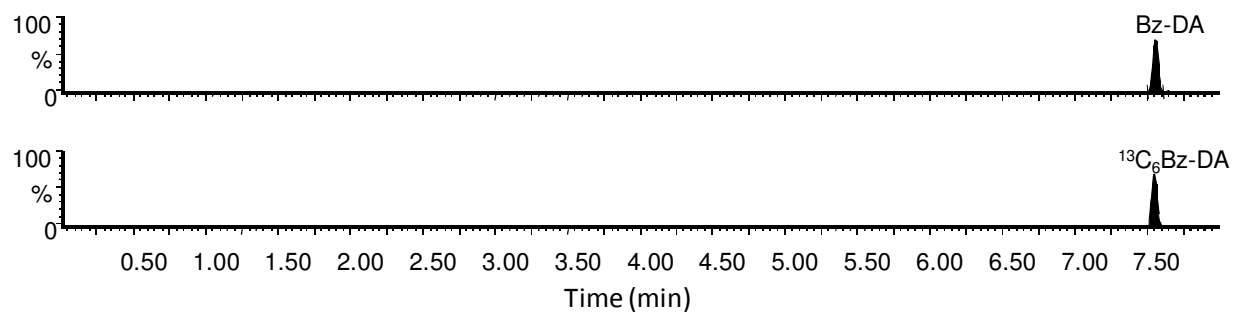


Figure S2. Mass chromatogram traces of neurotransmitters and metabolites detected *in vivo* from rat nucleus accumbens. Probe size was 1.5 mm and dialysis flow rate was 0.6 μ L/min.

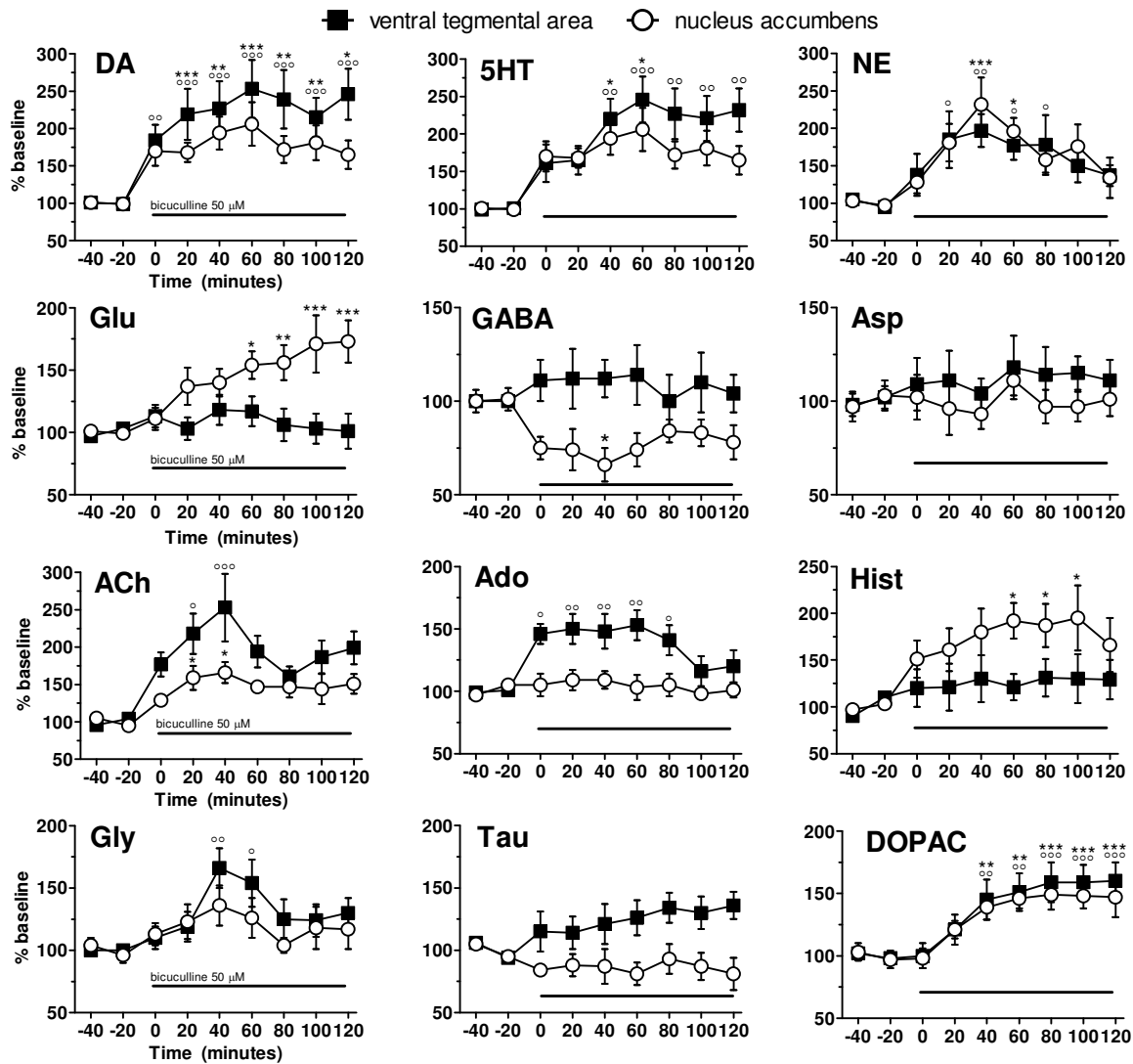


Figure S3 (related to Figure 4). Unilateral dual probe microdialysis of the mesolimbic pathway.

Bicuculline (50 μM) was perfused (black bar) in the VTA while monitoring neurotransmitters locally in VTA (black squares) and distally in the NAc (open circles). Dialysate was collected every 20 min. Error bar is SEM ($n = 8$). Data was expressed as percent of baseline levels. RM ANOVA and a post hoc Tukey test to compare basal levels against post drug levels. * $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$ compared to basal NA levels. ° $p < 0.05$, °° $p < 0.01$, °°° $p < 0.001$ compared to basal VTA levels.

Table S1. MRM conditions of 17 benzoylated neurotransmitters and metabolites and their internal standards.

analyte	precursor m/z	product m/z	cone voltage (V)	collision energy	dwel time (ms)
ACh	146	87	35	15	150
d ₄ -ACh	150	91	35	15	150
Bz-Gly	180	105	35	10	75
¹³ C ₆ Bz-Gly	186	111	35	10	75
Bz-GABA	208	105	35	20	150
¹³ C ₆ Bz-GABA	214	111	35	20	150
Bz-Ser	210	105	35	20	50
¹³ C ₆ Bz-Ser	216	111	35	20	50
Bz-Hist	216	105	35	20	50
¹³ C ₆ Bz-Hist	222	111	35	20	50
Bz-Tau	230	105	35	10	50
¹³ C ₆ Bz-Tau	236	111	35	10	50
Bz-Asp	238	105	35	10	75
¹³ C ₆ Bz-Asp	244	111	35	10	75
Bz-Glu	252	105	35	20	150
¹³ C ₆ Bz-Glu	258	111	35	20	150
Bz-Ado	372	136	35	30	75
¹³ C ₆ Bz-Ado	378	136	35	30	75
Bz-5HT	385	264	60	20	150
¹³ C ₆ Bz-5HT	397	270	60	20	150
Bz-NE	482	105	60	30	150
¹³ C ₆ Bz-NE	500	111	60	30	150
Bz-DA	466	105	70	30	150
¹³ C ₆ Bz-DA	484	111	70	30	150
Bz-HVA	304	105	35	15	150
¹³ C ₆ Bz-HVA	310	111	35	15	150
Bz-5HIAA	313	146	35	15	150
¹³ C ₆ Bz-5HIAA	319	146	35	15	150
Bz-NM	374	105	60	15	150

¹³ C ₆ Bz-NM	386	111	60	15	150
Bz-3MT	376	105	35	20	150
¹³ C ₆ Bz-3MT	388	111	35	20	150
Bz-DOPAC	394	105	35	20	150
¹³ C ₆ Bz-DOPAC	406	111	35	20	150