## **Supporting Information (SI)**

## Enrichment and separation of cationic, neutral, and chiral analytes by micelle to cyclodextrin stacking - micellar electrokinetic chromatography

Alireza Ghiasvand<sup>1,2</sup>, Zikai Feng<sup>1,3</sup>, Joselito P. Quirino<sup>1,\*</sup>

<sup>1</sup>Australian Centre for Research on Separation Science (ACROSS), School of Natural Sciences-Chemistry, University of Tasmania, Private Bag 75, Hobart, Tasmania 7001,

## Australia

<sup>2</sup> Department of Chemistry, Lorestan University, Khoramabad, Iran
<sup>3</sup>School of Medicine-Pharmacy, University of Tasmania, Hobart, Tasmania 7001, Australia

Corresponding author: \*jquirino@utas.edu.au

Additional corresponding author: Prof. Alireza Ghiasvand (a\_ghiasvand@yahoo.com)

## Table of contents:

Figure S1. (page S-2) MCDS-chiral MEKC of chiral analytes dichloroprop (a), mecoprop (b) and chlorpheniramine (c).

Figure S2. (page S-3) MEKC and MCDS-MEKC of small molecules (quaternary ammonium herbicides) after *in-vitro* metabolism in HepG2 cell line media.

Figure S3. (page S-4) %Recovered for the quaternary ammonium herbicides after incubation for up to 6 hours in HepG2 cell line media.

Figure S4. (page S-5) Structures of analytes used.

Table S1. (page S-6) Analytical figures of merit for MCDS-(chiral)-MEKC of cationic, neutral, and chiral analytes.

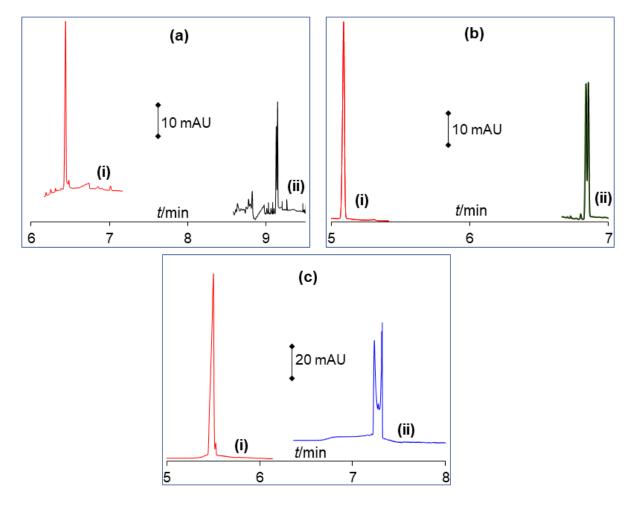


Figure S1. MCDS-chiral MEKC of chiral analytes dichloroprop (a), mecoprop (b) and chlorpheniramine (c). BGS was 50 mM SDS in 50 mM PA. Sample concentration was 4  $\mu$ g/mL of each analyte. Injection was 50 (a and b) and 100 (c) s of sample prepared with 10 mM SDS in 100 mM PA. CD solution was 50 mM  $\gamma$ -CD in 100 mM PA. In (a), the CD solution was injected before the sample for 100 (i) and 250 (ii) s. In (b), the CD solution was injected for 50 (i) and 200 (ii) s. In (c), the CD solution was injected for 25 (i) and 150 (ii) s. In (a-c), the complete stacking by MCDS of the long sample injection is shown in (i) and the optimum chiral separation of the stacked racemate under the experimental conditions used is shown in (ii). Other information in Materials and methods.

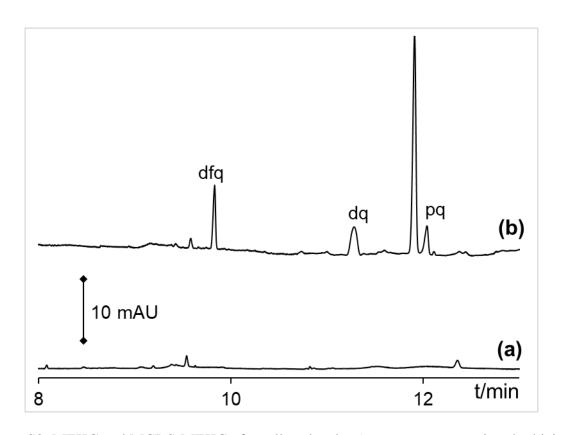


Figure S2. MEKC and MCDS-MEKC of small molecules (quaternary ammonium herbicides) after *in-vitro* metabolism in HepG2 cell line media. Sample was not incubated, or incubation time was t = 0 hr. The concentration of each herbicide difenzoquat (dfq), diquat (dq), and paraquat (pq) in the sample solution was  $0.52 \,\mu\text{g/mL}$ . Injection was typical 5 s injection of sample (a) and MCDS with  $100 \, \text{s}$  CD solution then  $50 \, \text{s}$  of sample (b). MEKC and MCDS conditions are described in Figure 2(a). Sample preparation is described in the Materials and methods and main text.

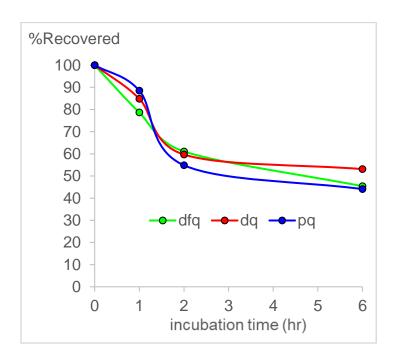


Figure S3. %Recovered for the quaternary ammonium herbicides after incubation for up to 6 hours in HepG2 cell line culture media. The sample preparation and measurement conditions are the same as in Figure S2. Other relevant information in Material and methods.

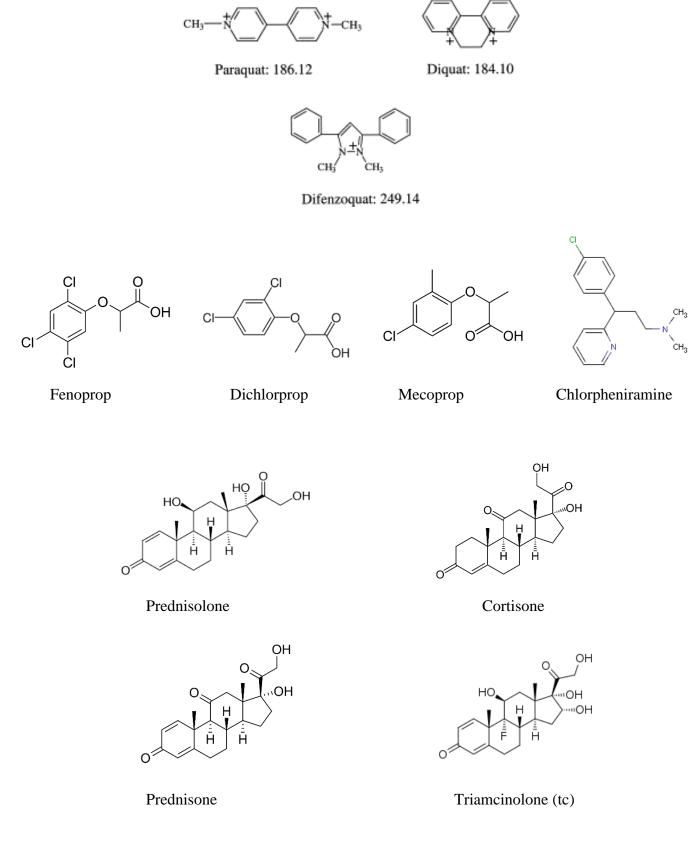


Figure S4. Structures of analytes used.

Table S1. Analytical figures of merit for MCDS-(chiral)-MEKC of cationic, neutral, and chiral analytes.

analyte		LDR (µg/mL)	equation of line	$\mathbb{R}^2$	LOD (ng/mL)	SEF	RSD (%)	
							intra- day	inter- day
cationic <sup>1</sup>	difenzoquat	5×10 <sup>-6</sup> - 10	y = 0.019x + 0.544	0.997	0.001	75	3.9	7.3
	diquat	5×10 <sup>-4</sup> - 10	y = 0.010x - 0.351	0.991	0.01	47	2.3	5.4
	paraquat	5×10 <sup>-4</sup> - 10	y = 0.012x - 0.632	0.994	0.01	120	5.3	8.6
neutral <sup>2</sup>	prednisolone	0.1 - 10	y = 1.860x - 0.087	0.996	30	49	4.7	5.5
	cortisone	0.1 - 10	y = 1.943x - 0.217	0.996	30	16	6.1	7.2
	prednisone	0.5 - 10	y = 1.015x - 0.128	0.993	100	8	4.2	6.3
	triamcinolone	0.05 - 10	y = 1.180x - 0.237	0.995	10	23	9.6	11.7
chiral <sup>3</sup>	chlorpheniramine	0.05 - 40	y = 7.545x + 5.966	0.998	50	94	6.7	9.4
	fenoprop	0.5 - 200	y = 0.788x + 2.884	0.996	200	54	8.5	12.8
	mecoprop	2 - 200	y = 0.936x + 0.596	0.991	500	171	7.4	13.5
	dichlorprop	2 - 200	y = 1.337x + 0.358	0.994	500	146	9.2	14.2

Experimental conditions:

injection regimen (CD solution/sample solution): chlorpheneramine (150 s/ 100 s), fenoprop (100 s/ 50 s), mecoprop (200 s/ 50 s), and dichlorprop (250s / 50s).

<sup>&</sup>lt;sup>1</sup> cationic herbicides, Figure 2(a)(iii).

<sup>&</sup>lt;sup>2</sup> neutral steroids, Figure 2(b)(iii).

<sup>&</sup>lt;sup>3</sup> chiral analytes, Figure 3(b).