Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Development of a UPLC-MS/MS method for the determination of ten anticancer drugs in hospital and urban wastewaters, and its application for the screening of human metabolites assisted by information-dependant acquisition tool (IDA) in sewage samples

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Table S1. Regression coefficients (r^2) and the slopes of neat standards and matrix match curves using internal standard (Set L_1) and not using I.S. (Set L_2)

Target Compound	Linearity Parameters (n=3)	Set L_1 (using I.S)		Set L_2 (not using I.S)	
		Neat Standard L_1	Matrix Match L_1	Neat Standard L_2	Matrix Match L_2
MTX	r^2	0.9945 ± 0.0055	0.9955 ± 0.0030	0.9978± 0.0017	0.9900 ± 0.0110
	Slope (b)	8.8224 ± 0.8314	8.2345 ± 0.8314	95379.0± 2005.3	62990.0 ± 4436.4
AZA	r^2	0.9989 ± 0.0012	0.9978 ± 0.0023	0.9996± 0.0001	0.9678 ± 0.0401
	Slope (b)	1.1826 ± 0.0712	0.9929 ± 0.1947	35609.5± 918.5	17982 ± 5004.7
CIP	r^2	0.9996 ± 0.0001	0.9999 ± 0.0001	0.9997 ± 0.0021	0.9689 ± 0.0234
	Slope (b)	1.8166 ± 0.0199	2.8516 ± 0.0805	20675.5± 1926.9	160794 ± 1705.5
VIN	r^2	0.9951 ± 0.0057	0.9989 ± 0.0010	0.9900 ± 0.0140	0.9901 ± 0.043
	Slope (b)	3.6510 ± 0.2454	0.9194 ± 0.0187	28918.5 ± 8361.5	5141.1 ± 256.0
IF	r^2	0.9976 ± 0.0003	0.9938 ± 0.0075	0.9993 ± 0.0011	0.9875 ± 0.0082
	Slope (b)	8.2730 ± 0.0395	6.7569 ± 0.1030	44358.0 ± 544.5	44332 ± 581.2
CY	r^2	0.9978 ± 0.0011	0.9981 ± 0.0009	0.9978 ± 0.0011	0.9981 ± 0.0009
	Slope (b)	11.1880 ± 0.2616	9.4513 ± 0.7414	59997± 1824.3	60093.5 ± 1799.6
ETO	r^2	0.9978 ± 0.0009	0.9912 ± 0.0010	0.9902 ± 0.0033	0.9899 ± 0.0132
	Slope(b)	0.1000 ± 0.0050	0.1942 ± 0.0140	886.6± 73.4	1220.1 ± 103.7
TAM	r^2	0.9988 ± 0.0002	0.9993 ± 0.0005	0.9988 ± 0.0002	0.9993 ± 0.0005
	Slope (b)	1.0769 ± 0.037	0.8986 ± 0.0408	37469.5± 2109.3	166851 ± 7930.9
DOC	r^2	0.9953 ± 0.0022	0.9956 ± 0.0038	0.9953 ± 0.0022	0.9956 ± 0.0038
	Slope (b)	0.4407± 0.0130	0.4965 ± 0.0447	4584.2 ± 340.1	3303.2 ± 258.7
PAC	r^2	0.9987 ± 0.0003	0.9975 ± 0.0001	0.9992± 0.0020	0.9985 ± 0.0015
	Slope (b)	0.3927± 0.0460	0.3197 ± 0.0038	3908± 104.5	2140.2± 8.8

Linearity and Matrix Effects Study
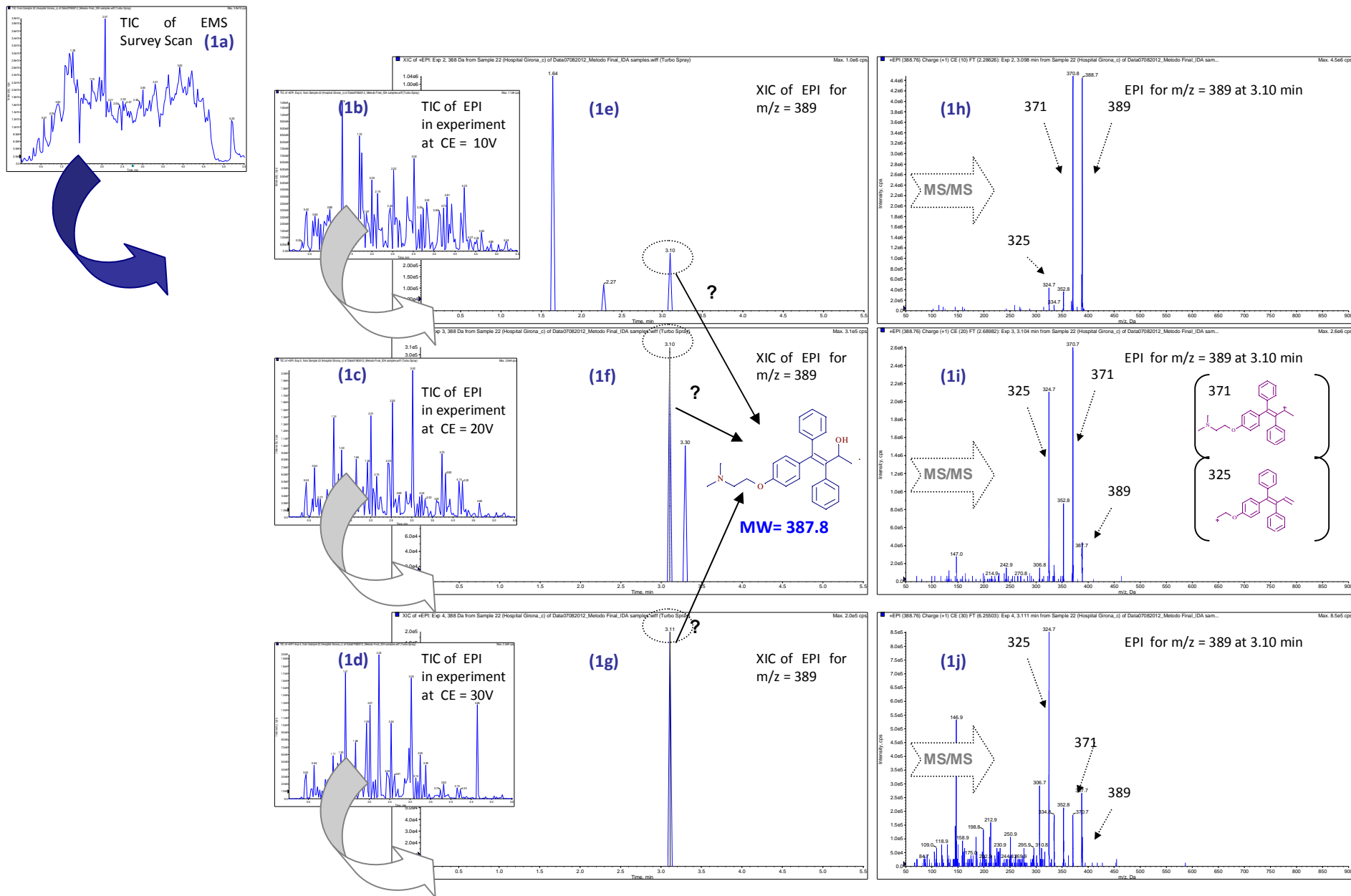
Fig. S1. Schedule of IDA scans from Hospital C sample: EMS (1a), TIC of each EPI (1b, 1c, 1d), XIC (m/z 389) of each EPI (1e, 1f, 1g) and EPI spectra (1h, 1i, 1j). Fragmentation path suggested for Hydroxy Tamoxifen
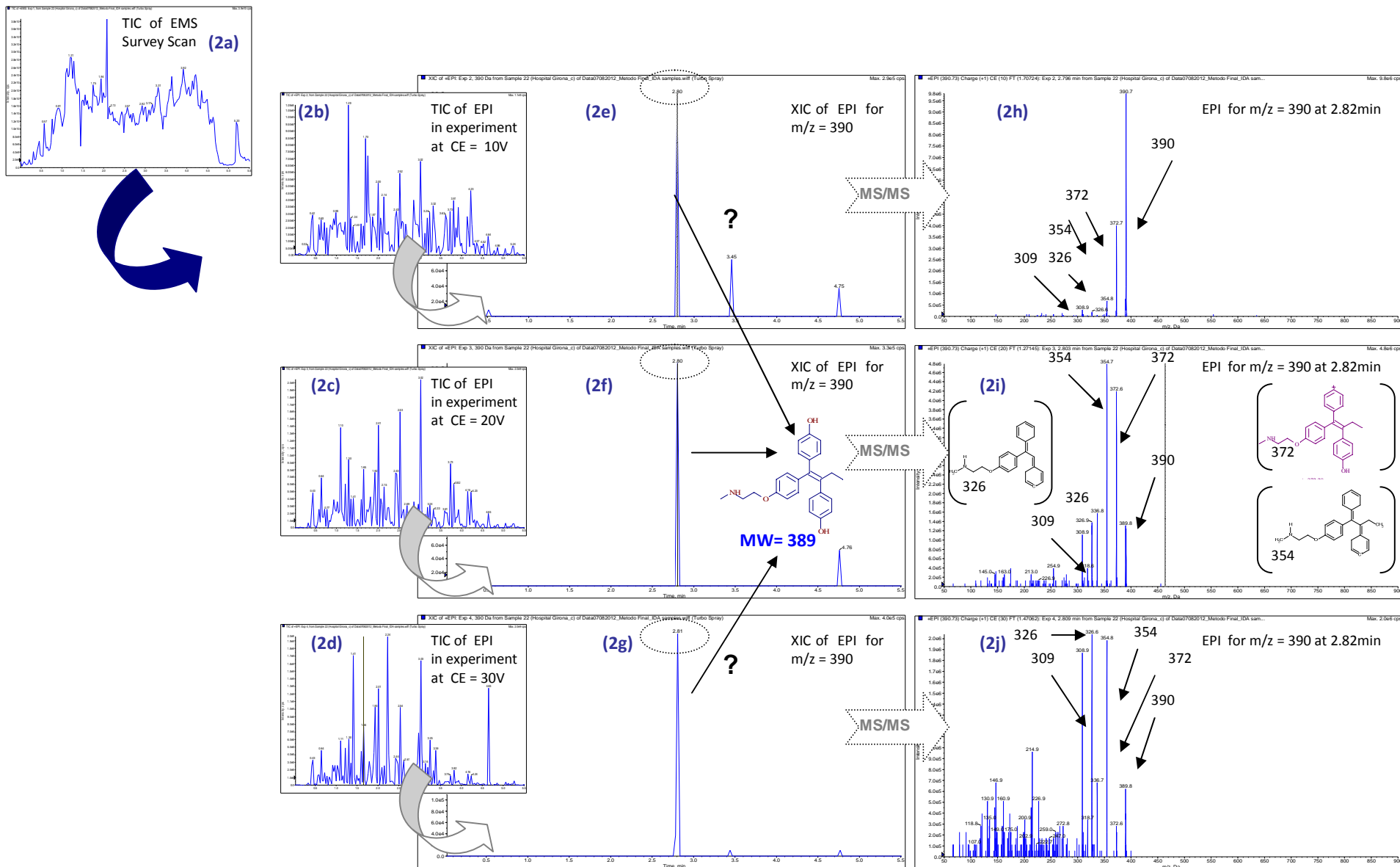
Fig. S2. Schedule of IDA scans from Hospital C sample: EMS (2a), TIC of each EPI (2b, 2c, 2d), XIC (m/z 390) of each EPI (2e, 2f, 2g) and EPI spectra (2h, 2i, 2j). Fragmentation path suggested for 4,4-dihydroxy desmethyltamoxifen (Endoxifen)
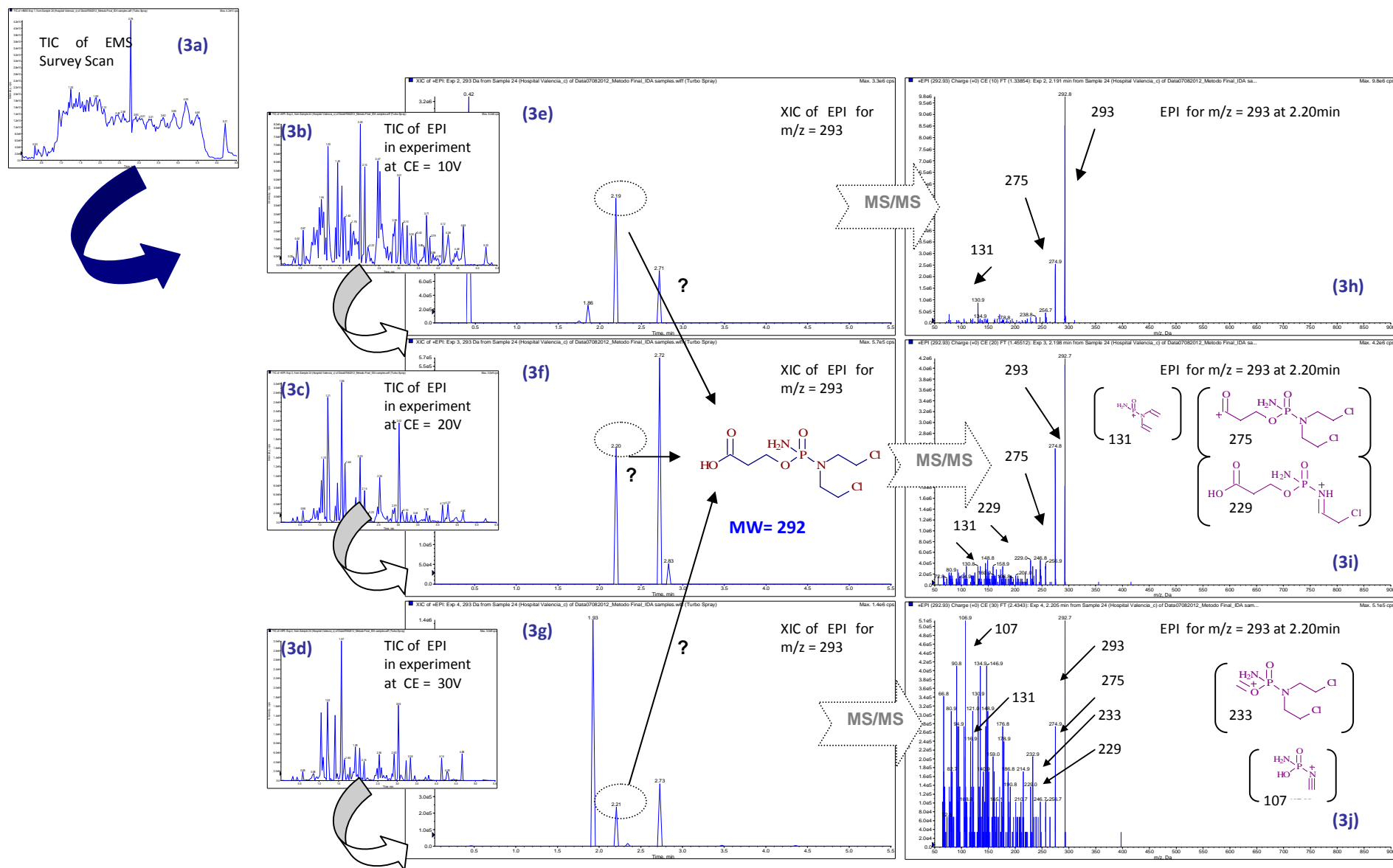
Fig. S3. Schedule of IDA scans from Hospital B sample: EMS (3a), TIC of each EPI (3b, 3c, 3d), XIC (m/z 293) of each EPI (3e, 3f, 3g) and EPI spectra (3h, 3i, 3j). Fragmentation path suggested for Carboxyphosphamide