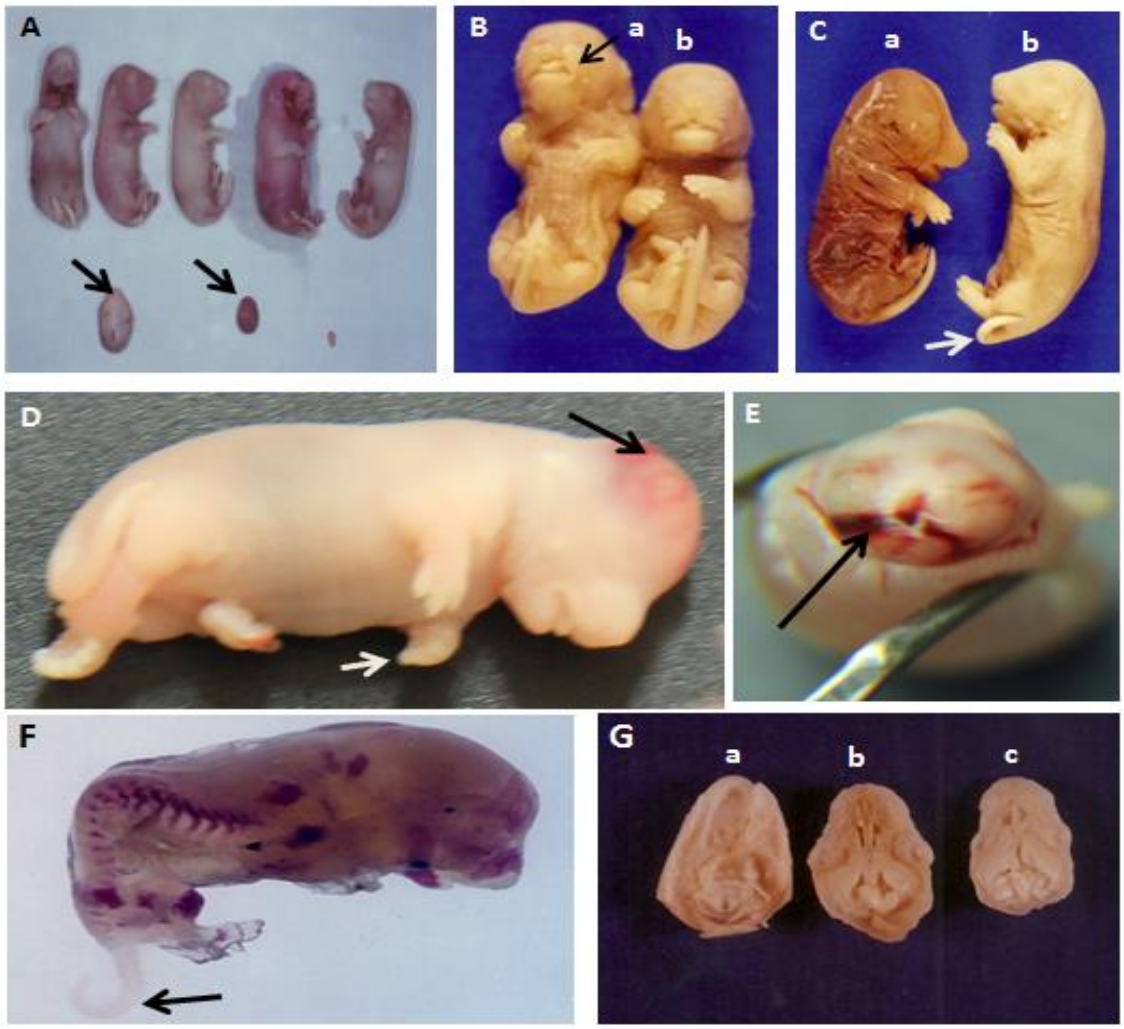
Electronic Supplementary Material (ESI) for RSC Advances.

Suplementary information (S.I.)

S.I. Figures



S.I. Fig. 1. Anomalies and malformations observed among fetuses from dams exposed to various doses of CP –

A- *Litters from a dam treated with CP intermediate dose (15mg/kg/B.wt) arrows showing resorption.*

B- *Pup from CP intermediate dose treated dams showing –* ***a****- cleft lip &* ***b-*** *normal pup from same dam .*

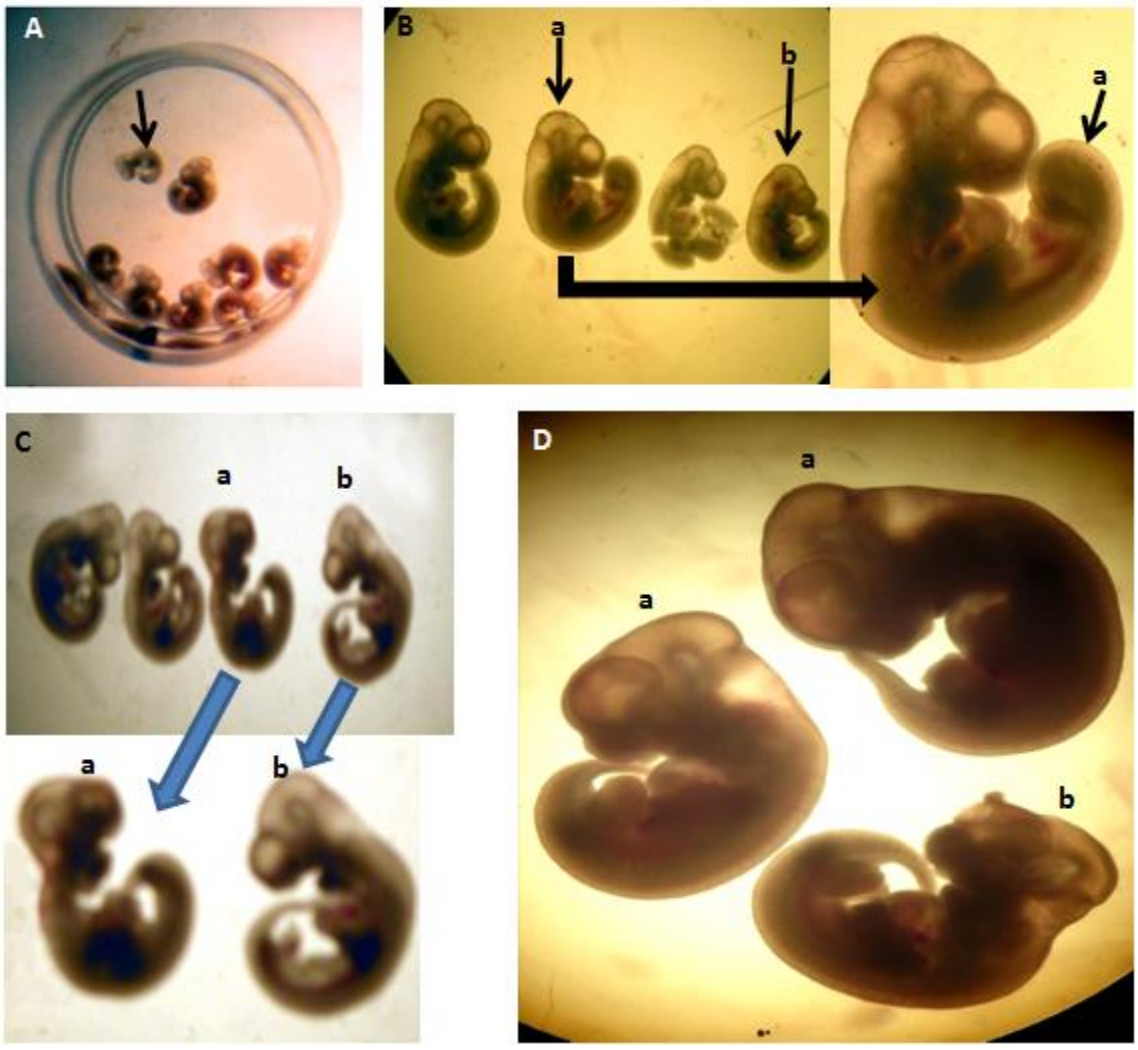
C- *Pups from high dose CP treated dam –* ***a-*** *case of still birth &* ***b-*** *pup from same group showing curling of tail.*

D- *A case of cranial hematoma with wrist drop from dam treated with high dose CP.*

E- *A foetus from CP-HD treated dam exhibiting excencephaly.*

F- *Alizarin preparation of a pup from CP-HD treated dam showing overall deformity of bones – typical case of scoliosis along with curling of tail.*

G- *Palate Slices of three different pups from dams treated with High dose of CP* ***a-*** *Normal palate and b & c- showing cleft palate.*



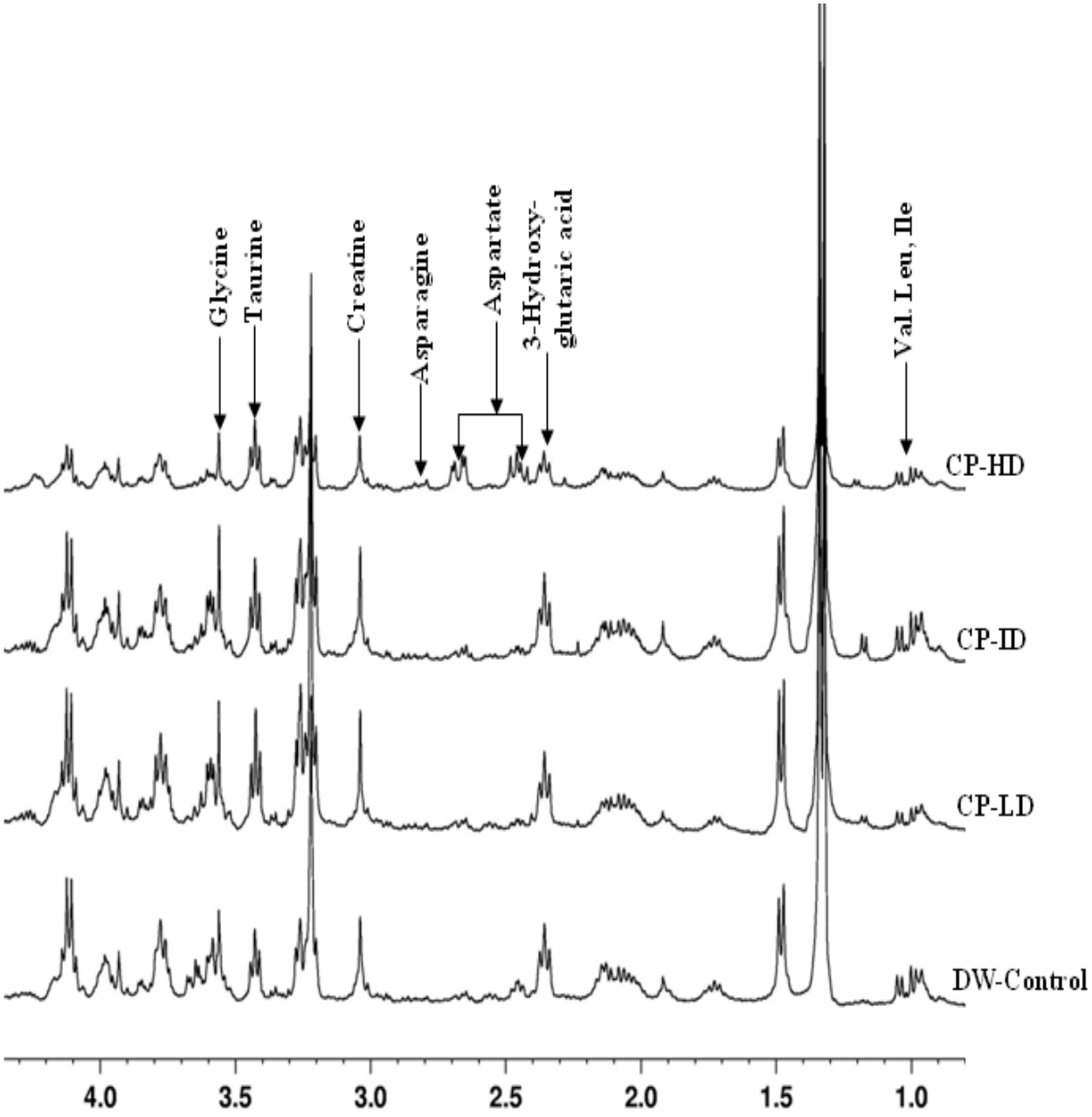
S.I. Fig. 2: Anomalies and malformations observed among embryos from control and various CP treated groups –

A- *Embryos from control group dam treated with distilled water (DW) by i.p route out of which one is having stunted growth indicated by arrow.*

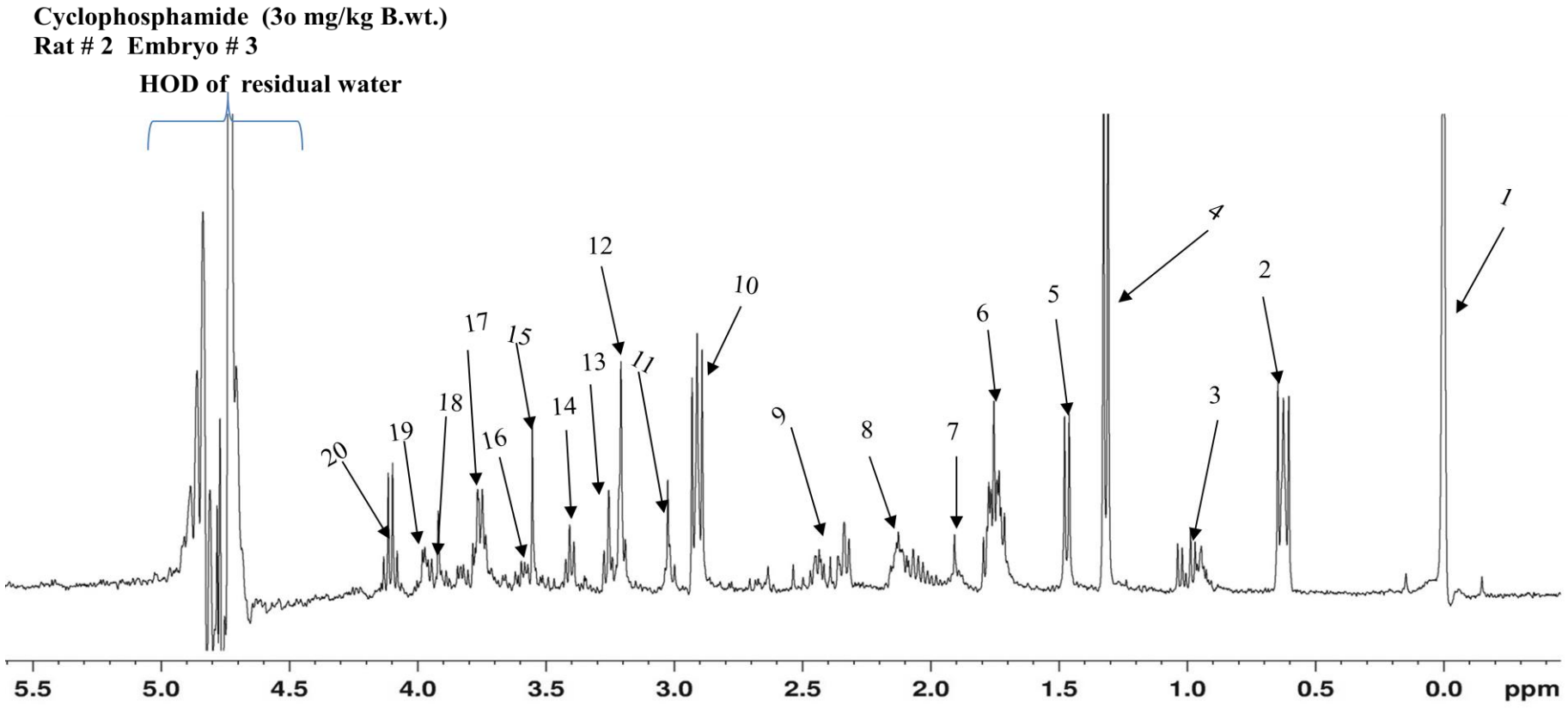
B- *Embryos from dams treated with low dose (5mg/kg-bwt/i,.p) showing* ***a-*** *curling of tail &* ***b-*** *stunted growth.*

C- *Embryos from dam treated with high dose (30mg/kg-bwt/i.p) of CP showing* ***a-*** *neural tube defect (NTD) and craniofacial defect both and* ***b-*** *normal embryo*

D- *Embryos from intermediate dose (15 mg/kg-bwt/i.p) treated dam showing* ***a-*** *normal neural tube and* ***b-*** *NTD.*



S.I Fig. 3: *Representative CPMG ^{1}H NMR spectra of DW-control, CP-LD, CP-ID and CP-HD coded embryos showing assignments of metabolites in 0.8 - 4.2 ppm.*



S.I. Fig. 4: *Solution state 1H NMR (400 MHz) spectra of the Rat embryo (cyclophosphamide treated group) highlighting various assignmrnt between (0.0 to 5.5) . The labelled assignments 1,2,6,10. DSS NMR standard; 3. unknown; 4,20. Lactate; 5, 17. alanine; 7. Acetate; 8,9,16. Glutamate; 11,18. Creatine; 12, 15, 19. choline; 13, 14. Taurine*

S.I. Table

S.I. Table 1. Chemical shift assignments of metabolites observed in the HR-MAS ^{1}HNMR spectra of control (distilled water) and Rat embryos treated with Cyclophosphamide obtained by comparing standard NMR spectrum (STD) of individual metabolites taken from Biological Magnetic Resonance Bank (BMRB).

S. No.	Name of metabolites	Chemical Shift (ppm)	Resonances
1	Acetate	1.92 (s)	CH_3
2	Alanine	1.48 (d) 3.78 (q)	β-CH_3 α-CH
3	Asparagine	2.80 (dd) 2.95 (dd) 4.01 (dd)	β-CH β'-CH α-CH
4	Aspartate	2.45(dd) 2.65 (dd) 3.90 (dd)	β-CH β'-CH α-CH
5	Choline	3.21 (s) 3.53 (s) 4.07 (s)	$N(CH_3)_3$ N-CH_2 O-CH_2
6	Creatine	3.03 (s) 3.94 (s)	N-CH_3 N-CH_2
7	Fatty acids (Triacylglycerols (*TAGs*))	0.90/0.96 1.3 1.59	CH_3 -(CH_2)n- $\underline{CH_2}$-CH_2-CO
8	Glycerophosphocholine (GPC)	3.24 (s) 3.7 4.32	$N(CH_3)_3$ N-CH_2 P-CH_2
9	Glutamine	2.13 (m) 2.44 (m) 3.77	β-CH_2 γ-CH_2 α-CH
10	Glutamate	2.02 (m) 2.33 (m) 3.74 (m)	β-CH_2 γ-CH_2 α-CH
11	Glycine	3.56 (s)	α-CH_2
12	3-Hydroxyglutaric acid	2.34 (t)	CH
13	Isoleucine	0.94 (t) 1.01 (d) 1.26 (m) 1.47 (m) 1.98 (m) 3.68 (d)	δ-CH_3 γ-CH_3 γ-CH γ'-CH β-CH α-CH
14	Lactate	1.33 (d) 4.11 (q)	β-CH_3 α-CH
15	Leucine	0.96 (d) 0.97 (d) 1.71 (m)	δ-CH_3 δ'-CH_3 γ-CH/β-CH_2

		3.75	α-CH
16	Lysine	1.47 (m)	γ-CH_2
		1.72 (m)	β-CH_2
		1.9 (m)	δ-CH_2
		3.02	N-CH_2
		3.74	α-CH
17	Phosphocholine	3.22	$N(CH_3)_3$
		3.62	N-CH_2
		4.18	O-CH_2
18	Taurine	3.25 (t)	S-CH_2
		3.41 (t)	N-CH_2
19	Valine	0.99 (d)	γ-CH_3
		1.04 (d)	γ'-CH_3
		3.62 (d)	β-CH
		2.28	α-CH