Fig.1

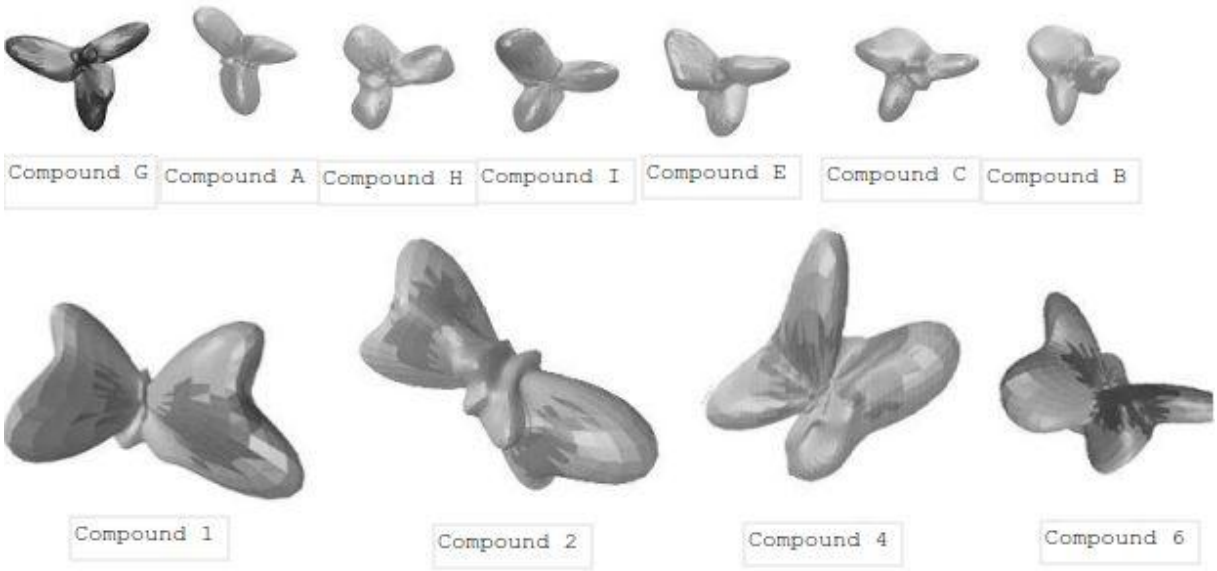

Compound G
Compound A
Compound H
Compound I
Compound E
Compound C
Compound B
Compound 1
Compound 2
Compound 4
Compound 6

Fig. 2

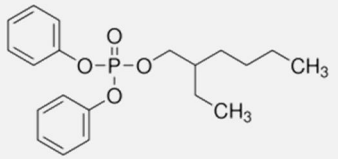
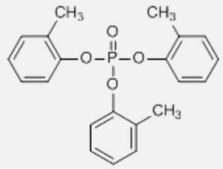
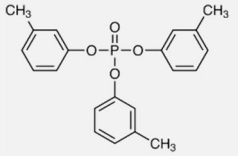
Compound	ECHA's official data	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Spherical harmonic cluster	QSAR neuro-toxicity (%)	QSAR repro-toxicity (%)	Risk level	Chemical structure
Comparative examples								
Compound A	No CMR, no acute toxicity	12.7	0.7	Cluster 1	0.39	1.93	4	
Compound B	Not registrated	15	3.7	Cluster 1	7.35	6.28	5	
Compound C	Not registrated	9.3	2.3	Cluster 1	6.99	3.69	5	

Fig.3

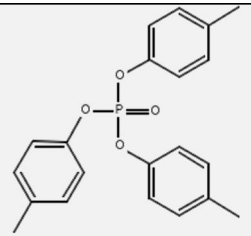
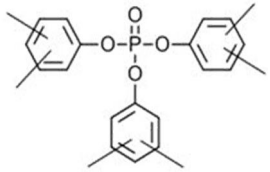
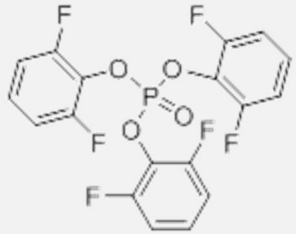
Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound D	Not registrated	9.7	42.7	Cluster 1	8.36	0.74	3	
Compound P	PBT in évaluation* Reprotoxic (Cat 2; H361)	16.9	0.7	Cluster 1	Yes	Yes	4	Mixture of tricrésylphosphate isomers (Durad 125)
Compound E	PBT in évaluation* Reprotoxic (Cat 1b, H360f)	ND	ND	Cluster 1	2.23	1.41	≥2	
Compound F	Not registrated	5.6	8.7	Cluster 1	ND	ND	≥3	

Fig.4

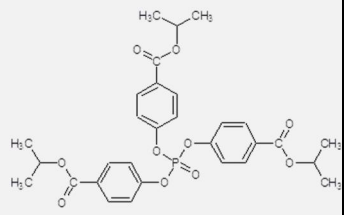
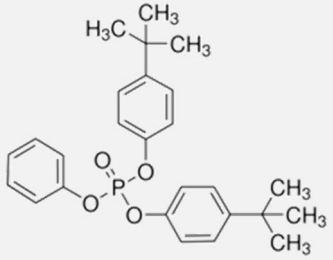
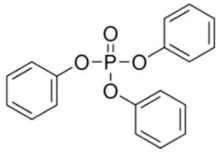
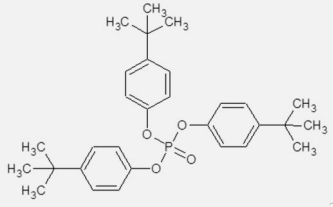
Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound G	Not registrated	15.8	145.5	Cluster 1	0.05	5.56	2	
Compound H	Not registrated	12.1	122.8	Cluster 1	0.02	3.49	3	
Compound I1	No CMR, no acute toxicity	10.8	14.0	Cluster 1	1.01	1.22	4	
Compound I2	Not registrated	8.4	96	Cluster 1	0.32	1.74	3	

Fig.5

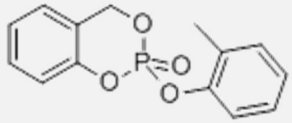
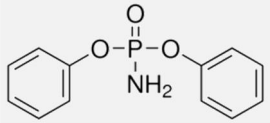
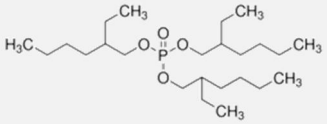
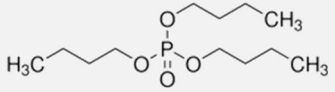
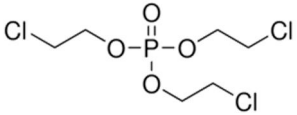
Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound I3	No CMR, no acute toxicity	13.9	34.9	Cluster 1	NA : mixture of neurotoxic compounds	-	≥3	Mixture of derivatives of I1
Compound J	Not registrated	ND	0.7	Cluster 2	5.61	1.67	≥3	
Compound K	Not registrated	9.5	33.9	Cluster 2	1.13	4.4	4	
Compound L	No CMR, no acute toxicity	12.2	121	Cluster 5	0	0.26	2	
Compound M	Carcinogenic Cat 3; R40 (GHS: Cat. 2, H 341)	7.9	21	Cluster 5	9.98	0.23	3	
Compound N	Carcinogenic Reprotoxic	8.2	89.8	Cluster 5	0.59	29.8	4	

Fig.6

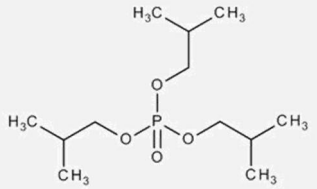
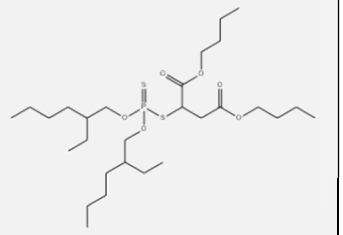
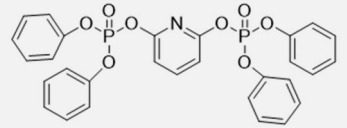
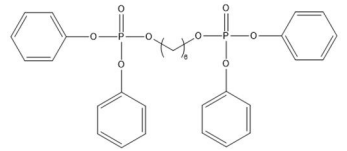
Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound Q	No CMR, no acute toxicity	9.4	12.8	Cluster 5	26.31	1.82	4	
Compound R	No CMR, no acute toxicity	19.3	11.1	ND	ND	ND	≥1	
Compound S	Not registrated	2.9	0.01	Cluster 3	0.32	0.04	3	
Compound U	Not registrated	21.6	1.2	ND	ND	ND	≥1	

Fig.7

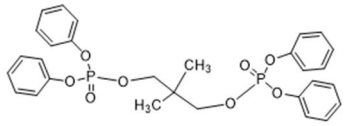
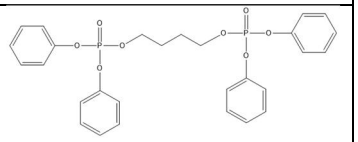
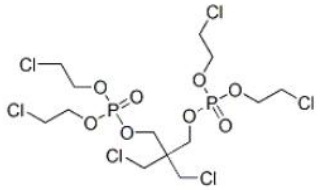
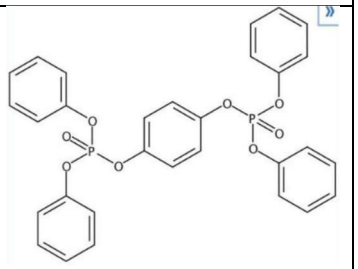
Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound T	Not registrated	17.8	1.8	Cluster 3	0.02	0.1	1	
Compound V	Not registrated	23.8	1.3	ND	ND	ND	≥1	
Compound W	No CMR, no acute toxicity	ND	ND	Cluster 4	91	0.19	≥2	
Compounds according to the invention								
Compound 1	ND	24.1	107	Cluster 3	0.09	0.08	0	

Fig.8

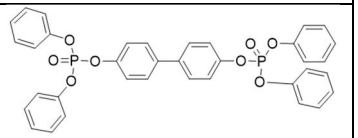
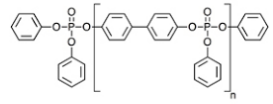
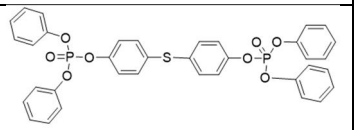
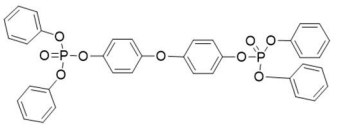
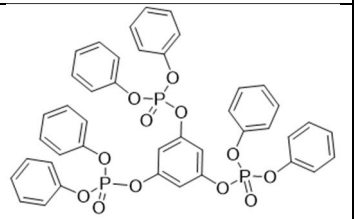
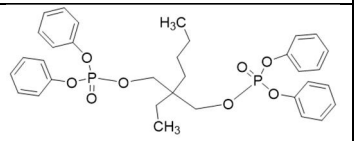
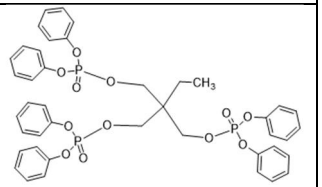
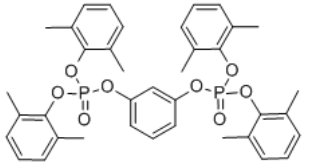
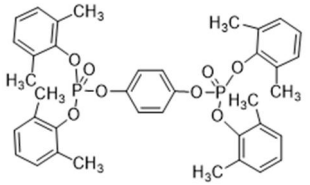
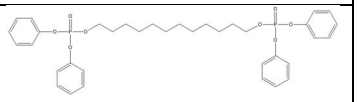
Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound 2	No CMR, no acute toxicity	25 (n=1)	101 (n=1)	Cluster 3	0	0.12	0	
		83 (n=1.5)	159 (n=1.5)					
Compound 3	Not registrated	23.2	113.2	Cluster 3	0	0.04	0	
Compound 4	Not registrated	22.6	78.6	Cluster 3	0	0.09	0	
Compound 5	Not registrated	22.7	82.6	Cluster 3	0.10	0.50	0	

Fig.9

Compound	Données offcielles ECHA	IC_{50} hAChE (mg/L)	IC_{50} eqBuChE (mg/L)	Cluster harmo-niques sphé-riques	QSAR neuro-toxicité (%)	QSAR repro-toxicité (%)	Niveau de risque	Structures chimiques
Compound 6	Not registrated	16.4	58.5	Cluster 3	0	0,52	0	
Compound 7	Not registrated	18.3	120.2	Cluster 3	0	0	0	
Compound 8	No CMR, no acute toxicity	26.3	94.7	Cluster 3	0.08	0.71	0	
Compound 9	Not registrated	30	107	Cluster 3	0.12	0.9	0	
Compound 10	Not registrated	27	97	Cluster 3	0.49	2.04	0	

ND means not determined.
NA: means not applied (in case of mixtures of compounds)
*PBT : Persistent, Bioaccumulative et toxic