

# QSPR Modelling of Potentiometric $\text{HCO}_3^-/\text{Cl}^-$ Selectivity for Polymeric Membrane Sensors <sup>†</sup>

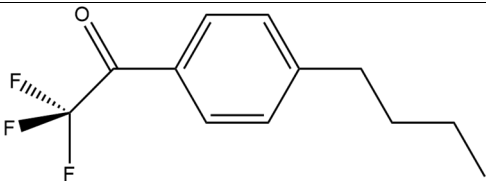
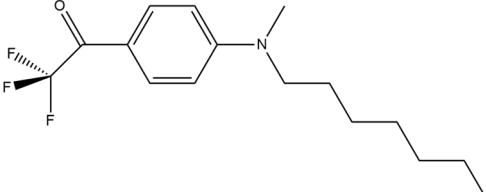
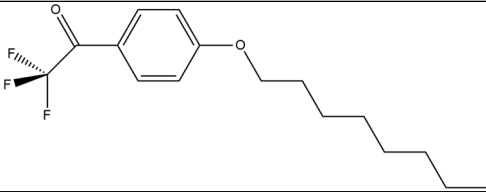
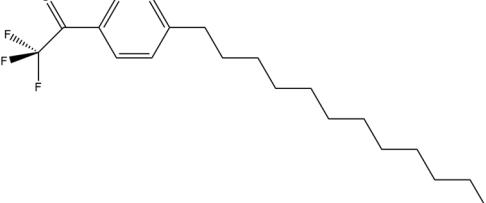
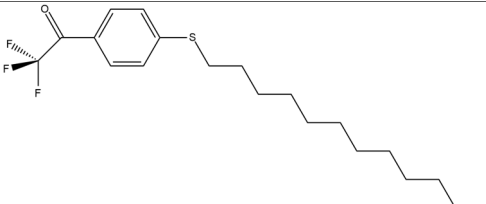
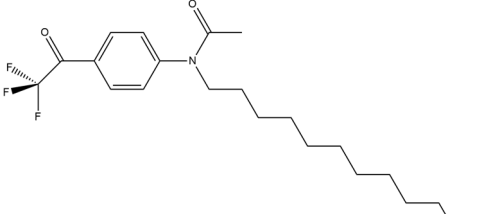
Nadezhda Vladimirova \*, Julia Ashina and Dmitry Kirsanov

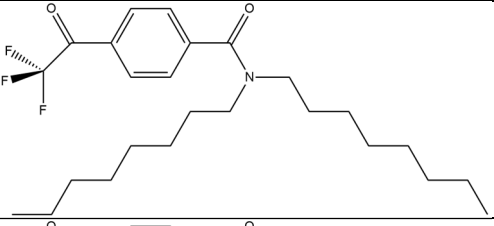
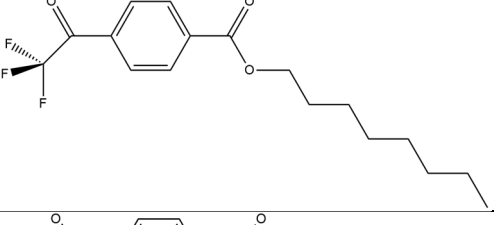
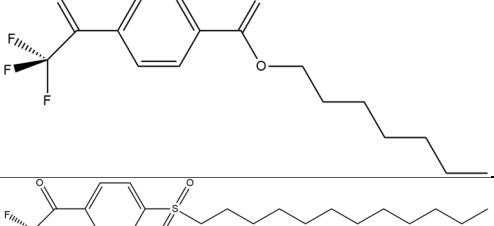
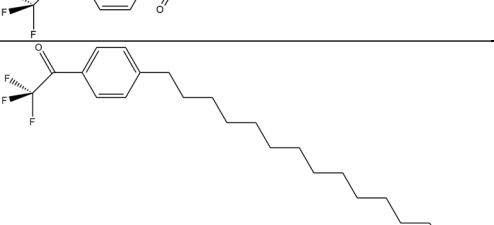
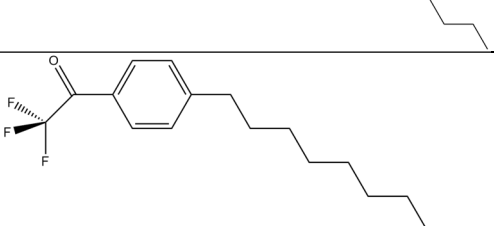
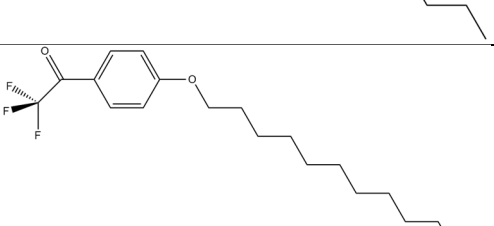
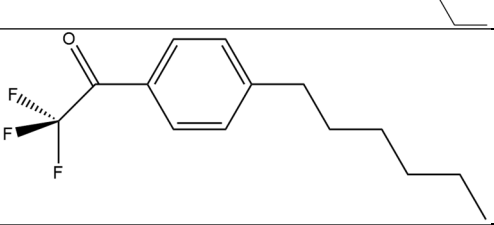
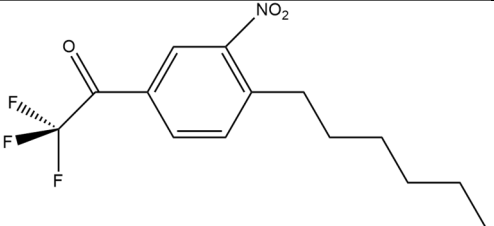

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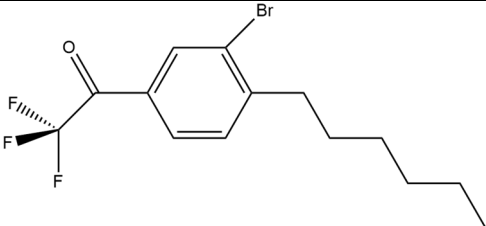
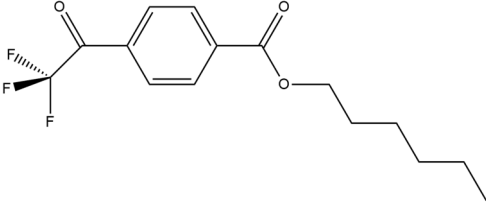
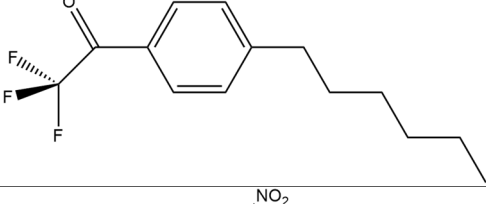
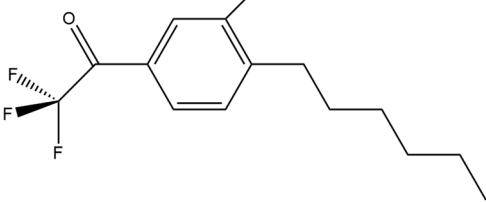
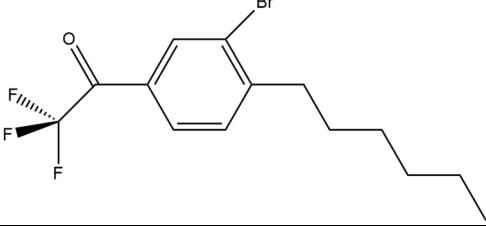
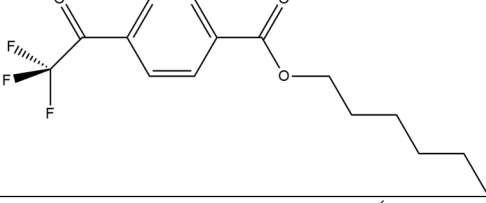
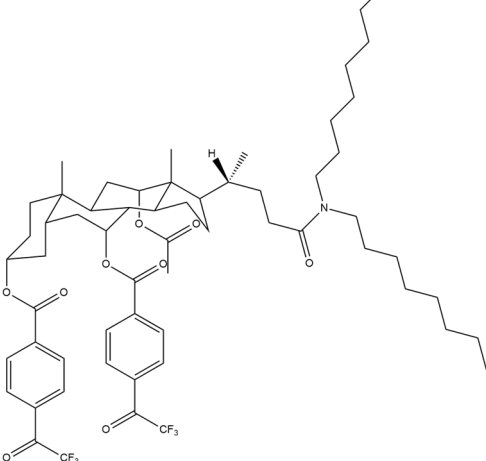
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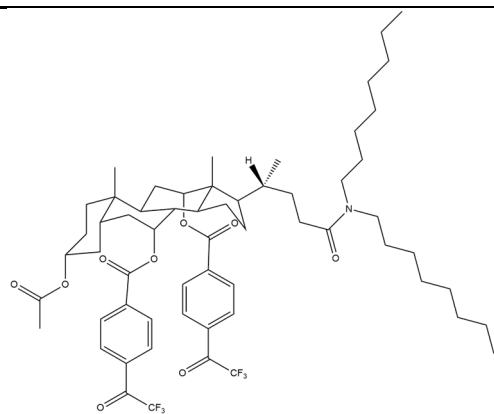
**Table S1.** Structure and selectivity of ionophores of potentiometric sensors.

#	Structure of ionophore	Plasticiser	Log $K(\text{HCO}_3^-/\text{Cl}^-)$	Reference
1		DOS	−2	[1]
2		DOS	1.3	[2]
3		DOS	−1.8	[2]
4		DOS	−3.2	[2]
5		DOS	−3.8	[2]
6		DOS	−4	[2]

7		DOS	-5	[2]
8		DOS	-4	[3]
9		DOS	-5	[2]
10		DOS	-5	[2]
11		DOS	-2.1	[1]
12		DOA	-3.7	[4]
13		DOS	-3	[1]
14		DOS	-2.8	[5]
15		DOS	-3	[5]

16		DOS	-3.2	[5]
17		DOS	-3.2	[5]
18		NPOE	-2.4	[5]
19		NPOE	-2.4	[5]
20		NPOE	-2.8	[5]
21		NPOE	-2.6	[5]
22		DOA	-5.2	[6]

23

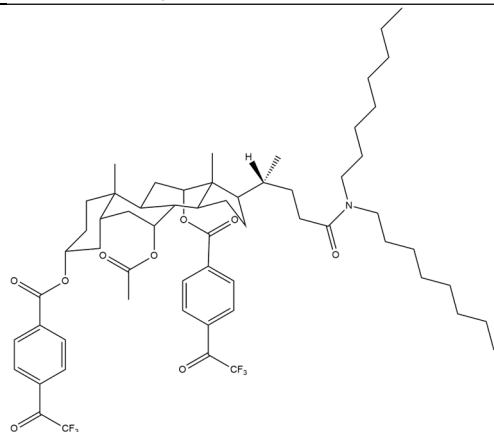


DOA

-4.7

[6]

24

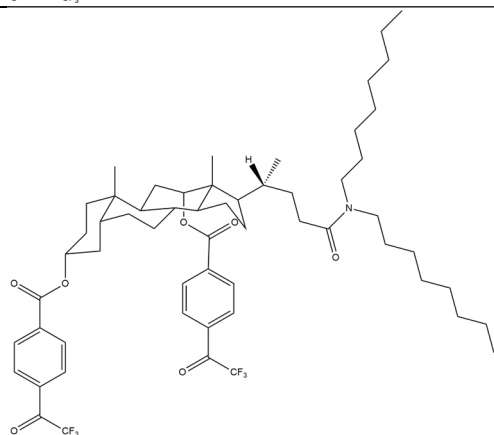


DOA

-5.7

[6]

25

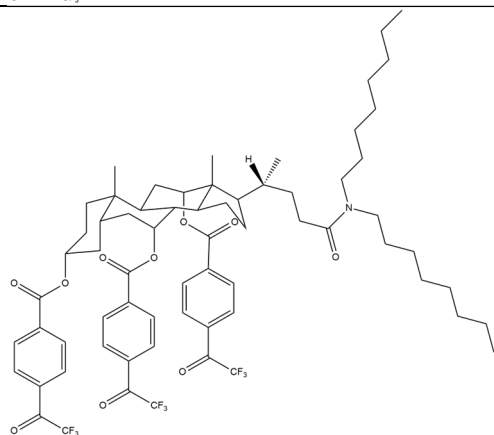


DOA

-3.1

[6]

26

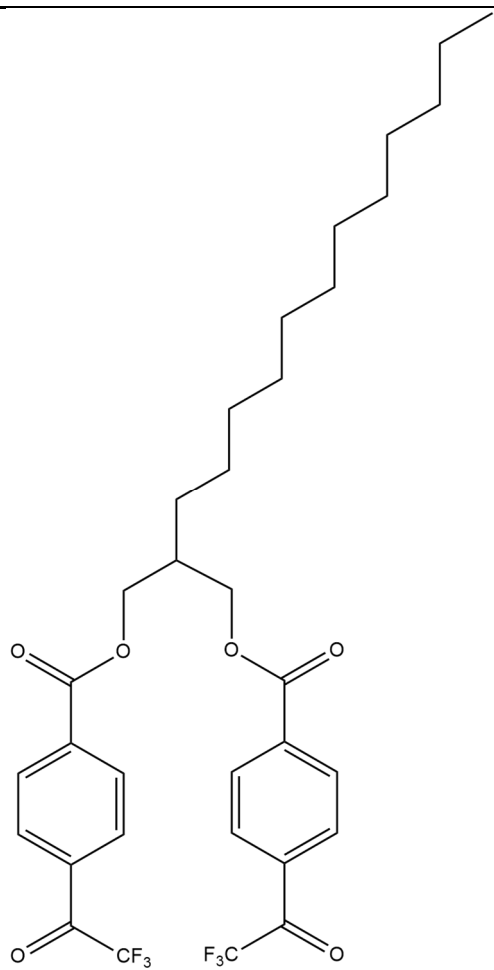


DOA

-5.8

[6]

27

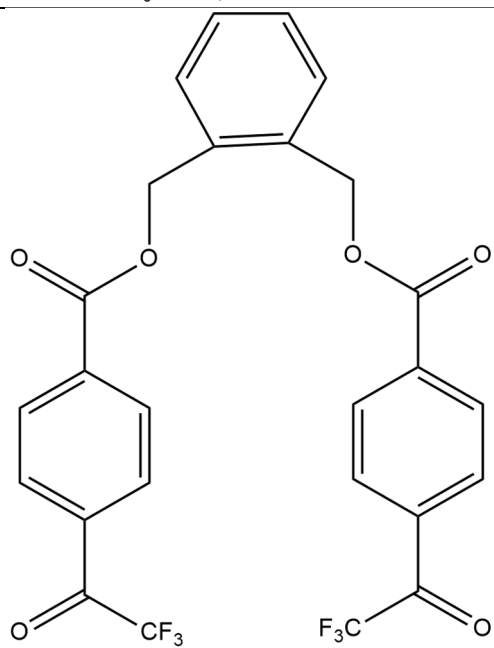


DOA

-4.2

[4]

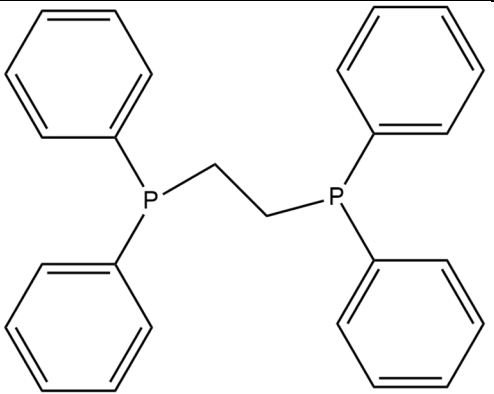
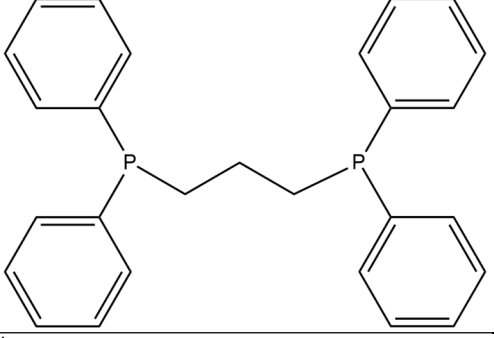
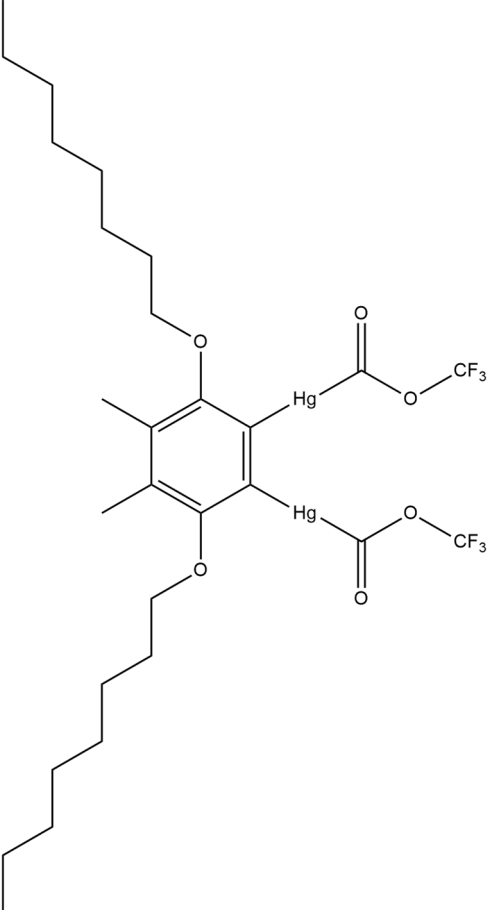
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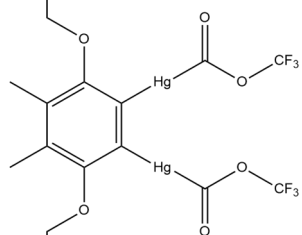
DOA

-2.6

[4]

29		NPOE	1.7	[7]
30		NPOE	1.6	[7]
31		DOS	5.5	[8]

32

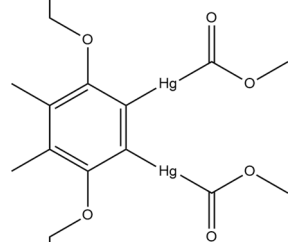


DOS

4.9

[8]

33

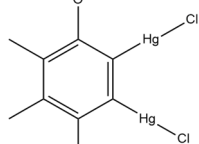


DOS

6.2

[8]

34

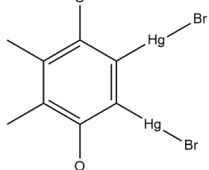


DOS

4.8

[8]

35

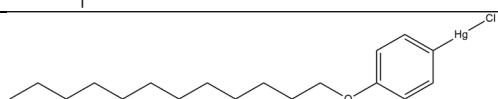


DOS

2.8

[8]

36

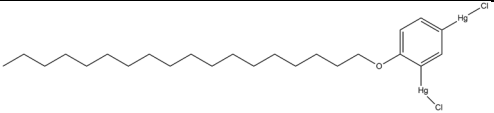
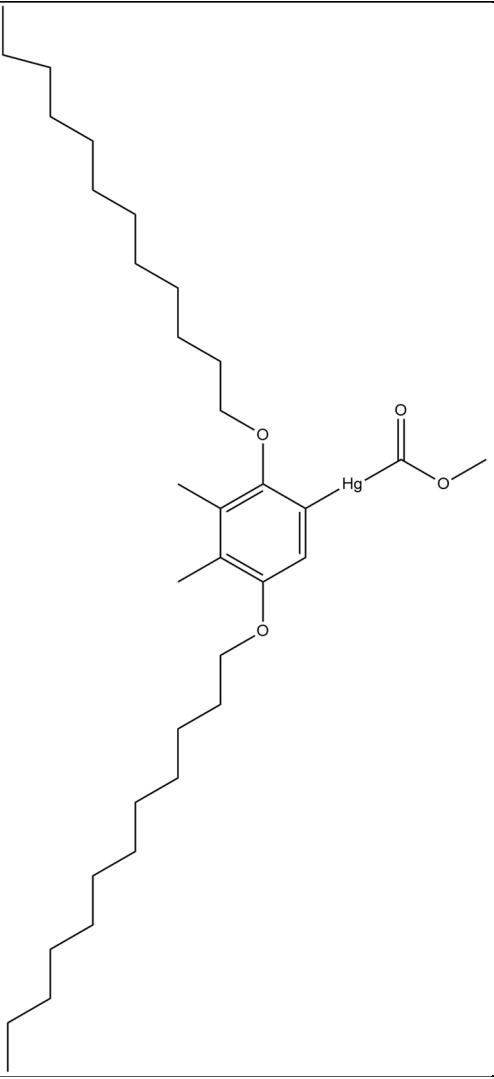
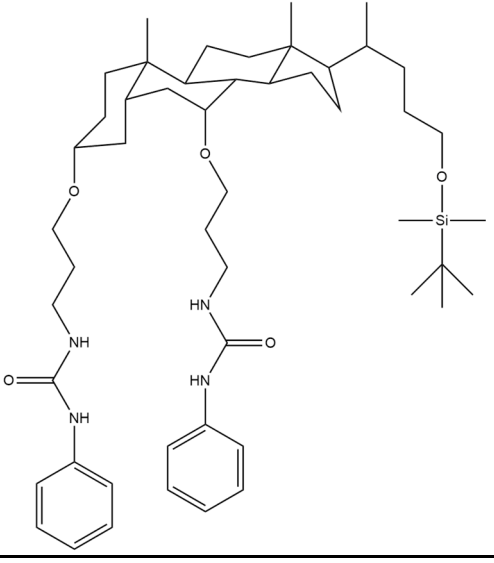


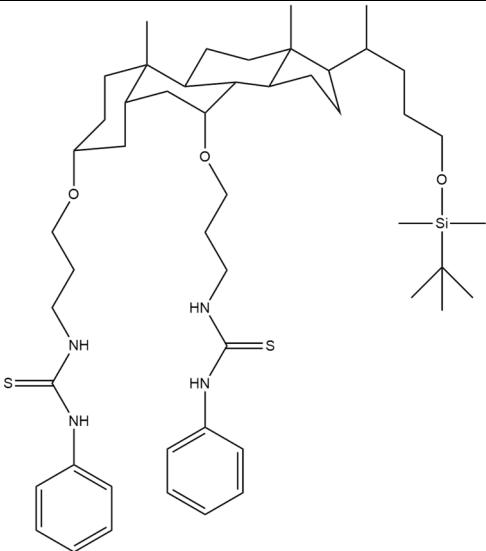
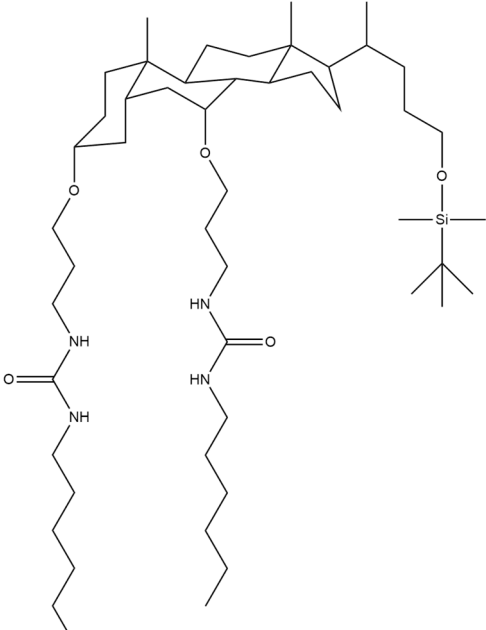
DOS

1.4

[8]



37		DOS	4.5	[8]
38		DOS	0.2	[8]
39		NPOE	2.9	[8]

40		NPOE	1.1	[6]
41		NPOE	1.3	[6]

## References

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