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Computational screening of electrochemical properties of biological quinones for use in RFB technology

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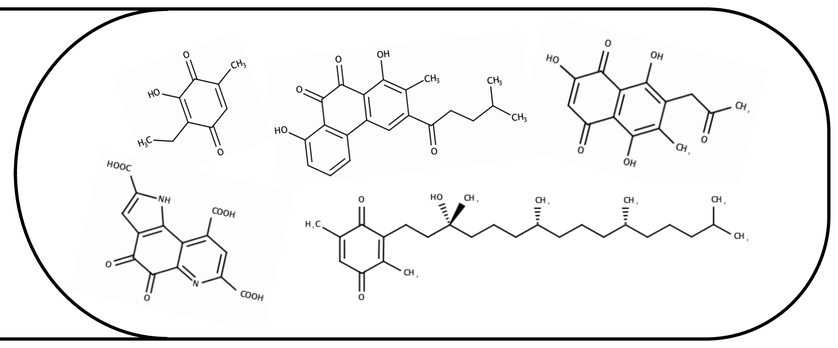
BACKGROUND - Bioqinones as electrontransfer agents in redox flow batteries

Recent quinones has been investigated as organic electrolytes or use in redox flow batteriy technology[1-2]. none has however so far investigated other candidates than synthetical quinones. Quinoes are produced by several sources in the nature, where the compound act as electron transfer agent, antimicrobial agent and oxidant/antioxidant[3-4].

- The aim of this study is to screen and thereby reveal potential quinones produced by biological sources as the best candidates to use in redox flow battery technology.



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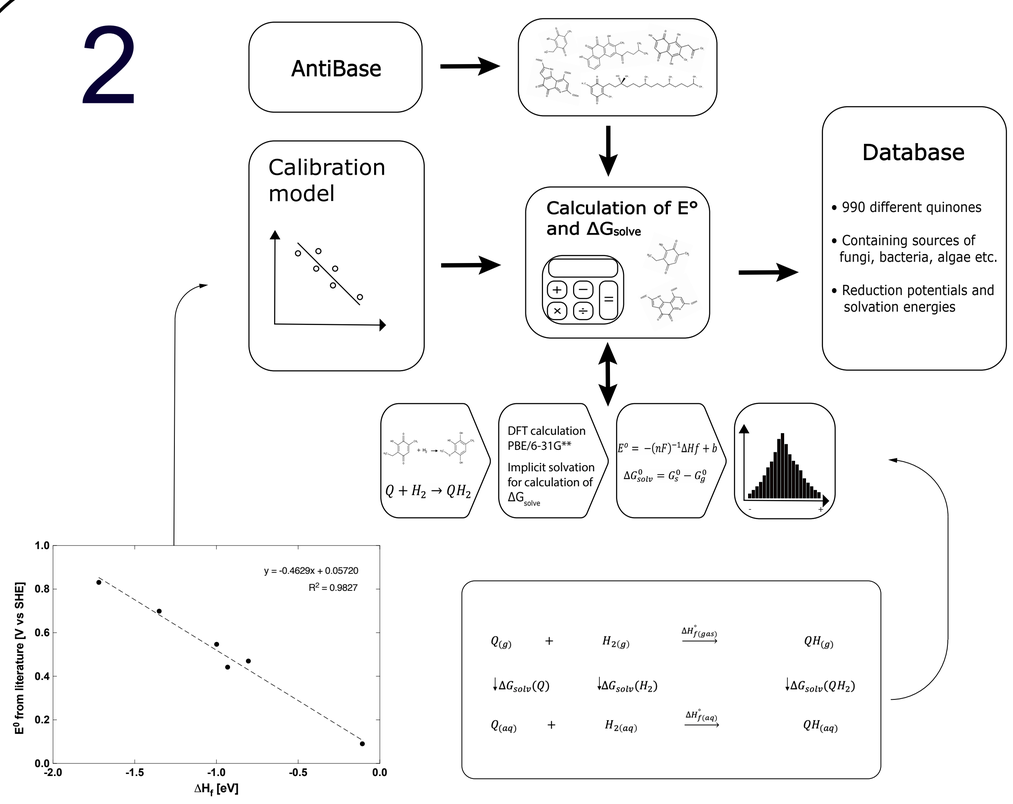

COMPUTATIONAL WORKFLOW

A Database with 990 different quinone structures with origin from various natural sources was compiled. The calibration model was prepared according to previous published[5]. The calibration model was utilized to calculate the reduction potentials based on the simulated energies ΔH_f, using the PBE/6-31G** functional and bassis-set.

The solvation energies,ΔG_{solv} was also calculated, using an implicit solvation model.

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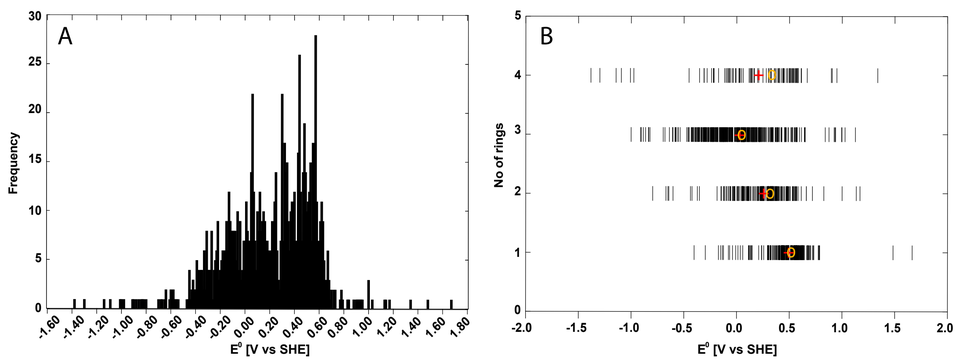
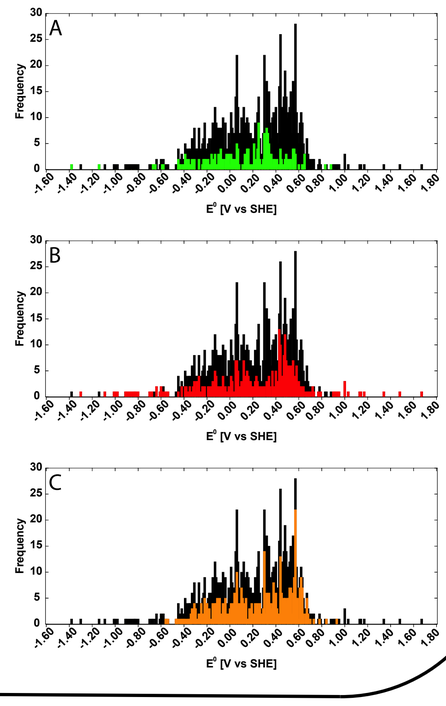


RESULTS - Distribution of bioquinones

The distribution of all the predicted redox potentials (E^0) of the obtained biological quinones is visualized. The predicted values stretch from the most negative value at -1.382V vs SHE to the most positive value at 1.666V vs SHE.

We divided the dataset into three groups: bacteria(green), fungi(red) and others(orange) (plants, algea, animals etc.).
The fungal quinones are more widely distributed compared to the other two groups.Thus, the fungi-produced compounds constitute the most varied group.



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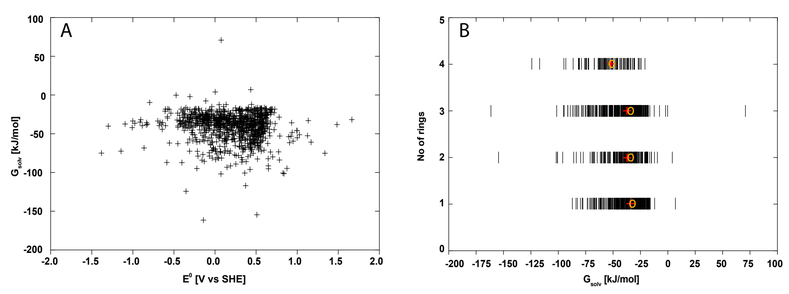
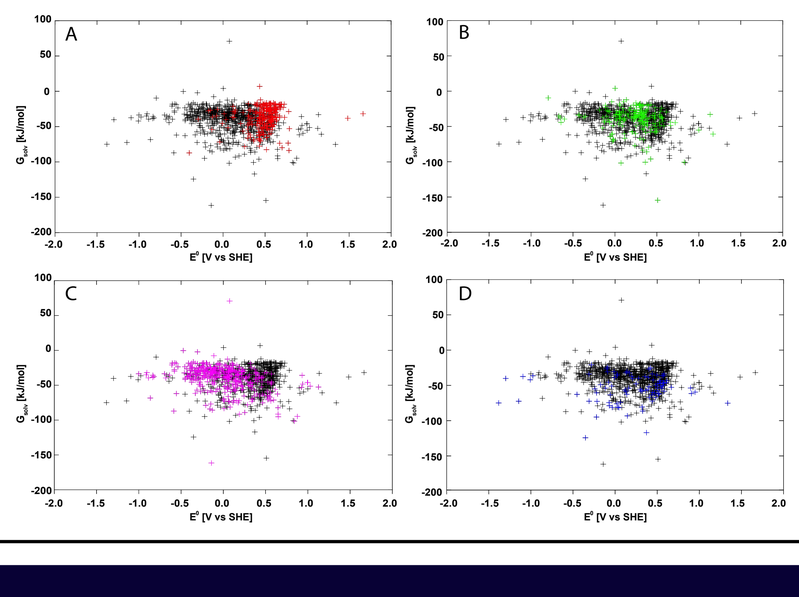


RESULTS - Investigation of solubillity of bioquinones

The distribution of the solubility compared to the redox potentials, with the BQs(red), NQs(green), AQs(purple) and ≥4 ring structures(green) highlighted respectively. The BQs tend to be at the positive side of the distribution, whereas the NQs are more centrally located. The AQs are more distributed towards the negative side compared to the BQs and NQs, which indicates a higher solubility of these compounds



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DISCUSSION AND CONCLUSION

- Top 7 bioquinones of both catholytes and anolytes

The quinones with the lowest and highest calculated redox potentials are listed.
The quinones with the most positive potentials predominantly originated from fungi and are relatively small and simple compounds, whereas the quinones with the most negative potentials are larger and more complex quinone structures.
The compound with the most positive redox potential was phenicin with 1.666V vs SHE, a molecule produced by several Penicillium species.
The compound with the lowest redox potential is Pradimicin M with -1.382V vs SHE and is produced in a mutant of Actinomadura hibisca Bacteria.

Name	E^0 V vs SHE	ΔG_{solv}	Source	Structure
Pradimicin M	-1.382	-74.94	[B] blocked mutant of Actinomadura hibisca p157-2	
Stemphyltoxin I	-1.298	-40.15	[F] Stemphylium botryosum var. lactucum	
Granaticin B	-1.144	-72.42	[B] Streptomyces spiroverticillatus N-9940 (FERM-p 2330)	
Altertoxin I	-1.094	-37.34	[F] Alternaria spp.	
Altertoxin II	-1.008	-41.94	[F] Stemphylium botryosum var. lactucum. Alternaria spp.	
3-O-Methyldihydrofusarubin A	-1.001	-33.43	[F] Fusarium martii	
Stemphyltoxin IV	-0.976	-36.40	[F] Stemphylium botryosum var. lactucum	

Name	E^0 V vs SHE	ΔG_{solv} kJ/mol	Source	Structure
Phenicin	1.666	-31.74	[F] Penicillium spp.	
Tridentoquinone	1.485	-38.10	[F] Suillus tridentinus (Boletales)	
Stemphyperylenol	1.338	-75.20	[F] Stemphylium botryosum var. lactucum	
Citrinin hydrate	1.170	-60.82	[F] Penicillium spp. Aspergillus spp.	
Fusarnaphthoquinone A	1.135	-32.95	[F] Fusarium spp. PSU-F14 and PSU-F135	
5-Hydroxydihydrofusarubin B	1.126	-52.50	[F] endophytic Fusarium sp. BCC14842	
5-Hydroxy-3-methoxydihydrofusarubin D	1.028	-51.20	[F] endophytic Fusarium sp. BCC14842	

[F]-fungi, [B]-bacteria

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