Electronic Supplementary Material (ESI) for RSC Advances.

Evaluation of novel Griess-reagent candidates for nitrite sensing in aqueous media identified via molecular fingerprint searching

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Supporting Information

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Figure S1 Schematic representation of the generation of binary string molecular fingerprint and Tanimoto index based on the structural similarities and differences between two selected molecules, parent and candidate compounds.

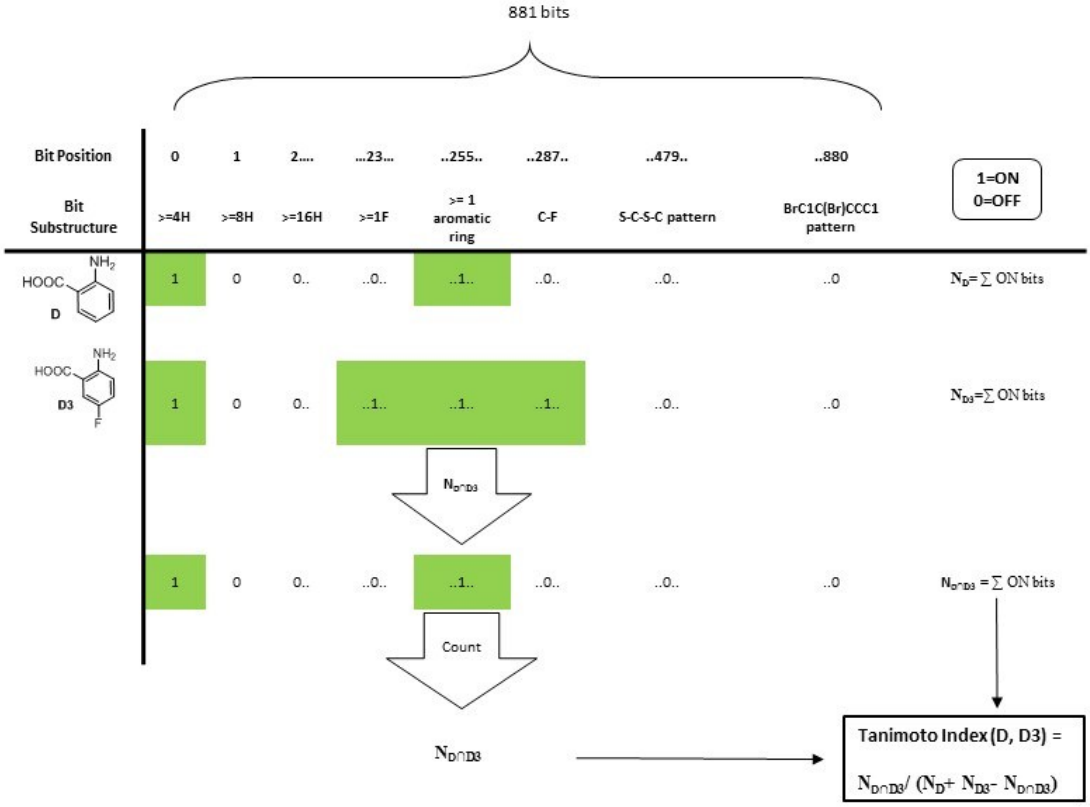

Table S1 Output (new candidate) list generated by molecular fingerprint searching and ranked based on their Tanimoto index for parent compound 2-aminobenzoic acid **D**. Candidates for experimental evaluation were selected (and highlighted in green) if they met all of the selection criteria: 1) Greater than 80% structural similarity which fall within the top 100 rank of the output list; 2) Presence of primary amine substitution (essential for diazotization) on the aromatic ring; 3) Absence of metals; 4) Water solubility in the applied concentration range; 5) Various salt forms of the same core compounds were considered as equivalent; 6) Readily available.

Rank	Tanimoto index	CID	Name	Meets Criteria					
				1	2	3	4	5	6
1	**1.00**	**227**	**2-AMINOBENZOIC ACID**	+	+	+	+	+	+
2	0.99	682386	(2-carboxyphenyl)ammonium	+	+	+	+	-	+
3	0.99	3613879	(2-aminobenzoyl)oxonium	+	+	+	+	-	+
4	0.98	74985	2-aminobenzoic acid;hydrochloride	+	+	+	+	-	+
5	0.97	72911	2-amino-5-iodo-benzoic acid	+	+	+	+	+	-
6	0.97	81962	2-aminobenzoic acid;dihydrochloride	+	+	+	+	-	+
7	0.97	101412	2-amino-5-fluoro-benzoic acid **D3**	+	+	+	+	+	+
8	0.97	349497	2-(hydroxyamino)benzoic acid	+	-	+	+	+	+
9	0.97	2724967	2-amino-4-fluoro-benzoic acid **D2**	+	+	+	+	+	+
10	0.97	21514	2-amino-4-arsoroso-benzoic acid	+	+	-	+	+	-
11	0.96	521142	2-amino-6-fluoro-benzoic acid **D4**	+	+	+	+	+	+
12	0.96	3029235	(2-amino-3-carboxy-phenyl)mercury	+	+	-	+	+	-
13	0.96	23654776	2-aminobenzenecarboperoxoic acid	+	+	+	+	+	-
14	0.96	3734162	2-azaniumylbenzoate	+	-	+	+	+	-
15	0.96	5459842	2-aminobenzoate	+	+	+	+	-	+
16	0.96	55307	2-amino-4-borono-benzoic acid	+	+	+	+	+	-
17	0.96	408313	2-amino-4-dichloroarsanyl-benzoic acid	+	+	-	+	+	-
18	0.96	4669623	2-carboxybenzenediazonium	+	-	+	+	+	+
19	0.96	81510	2-aminobenzoate;cadmium	+	+	-	+	-	-
20	0.96	23663633	potassium;2-aminobenzoate	+	+	+	+	-	+
21	0.96	23663708	lithium;2-aminobenzoate	+	+	-	+	-	-
22	0.96	23674494	sodium;2-aminobenzoate	+	+	+	+	-	+
23	0.95	735965	2-amino-4_5-difluoro-benzoic acid **D5**	+	+	+	+	+	+
24	0.95	282070	2-amino-3-iodo-benzoic acid	+	+	+	+	+	-
25	0.95	586408	2-amino-3-fluoro-benzoic acid **D1**	+	+	+	+	+	+
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Table S2 Parent compounds and candidates ranked by the normalised values of the width of their linear ranges and the gradient within the linear range across all the tested reagents. Data for Figure 3.

Linear Range		Slope	
1.00	**B2** (125-1000μM)	1.00	**A1**
0.27	**A3**	0.93	**A**
0.14	**A2**	0.79	**C**
0.14	**B**	0.79	**C4**
0.14	**B1**	0.77	**B**
0.14	**B3**	0.77	**C3**
0.14	**C**	0.76	**C2**
0.14	**C1**	0.75	**C1**
0.14	**C2**	0.73	**A2**
0.14	**C3**	0.72	**B2** (0-31.25μM)
0.14	**C4**	0.71	**D1**
0.14	**D**	0.70	**D4**
0.14	**D1**	0.67	**B1**
0.14	**D2**	0.67	**D8**
0.14	**D3**	0.63	**D2**
0.14	**D4**	0.56	**D5**
0.14	**D6**	0.39	**D3**
0.14	**D7**	0.32	**D**
0.14	**D8**	0.14	**A3**
0.07	**D5**	0.06	**D7**
0.04	**A**	0.05	**B2** (125-1000μM)
0.04	**A1**	0.02	**D6**
0.04	**B2** (0-31.25μM)	0.01	**B3**