

Supplementary Material

Electrochemical reduction, radical anions, and dehalogenation of fluorinated/chlorinated 2,1,3-benzothia/selenadiazoles

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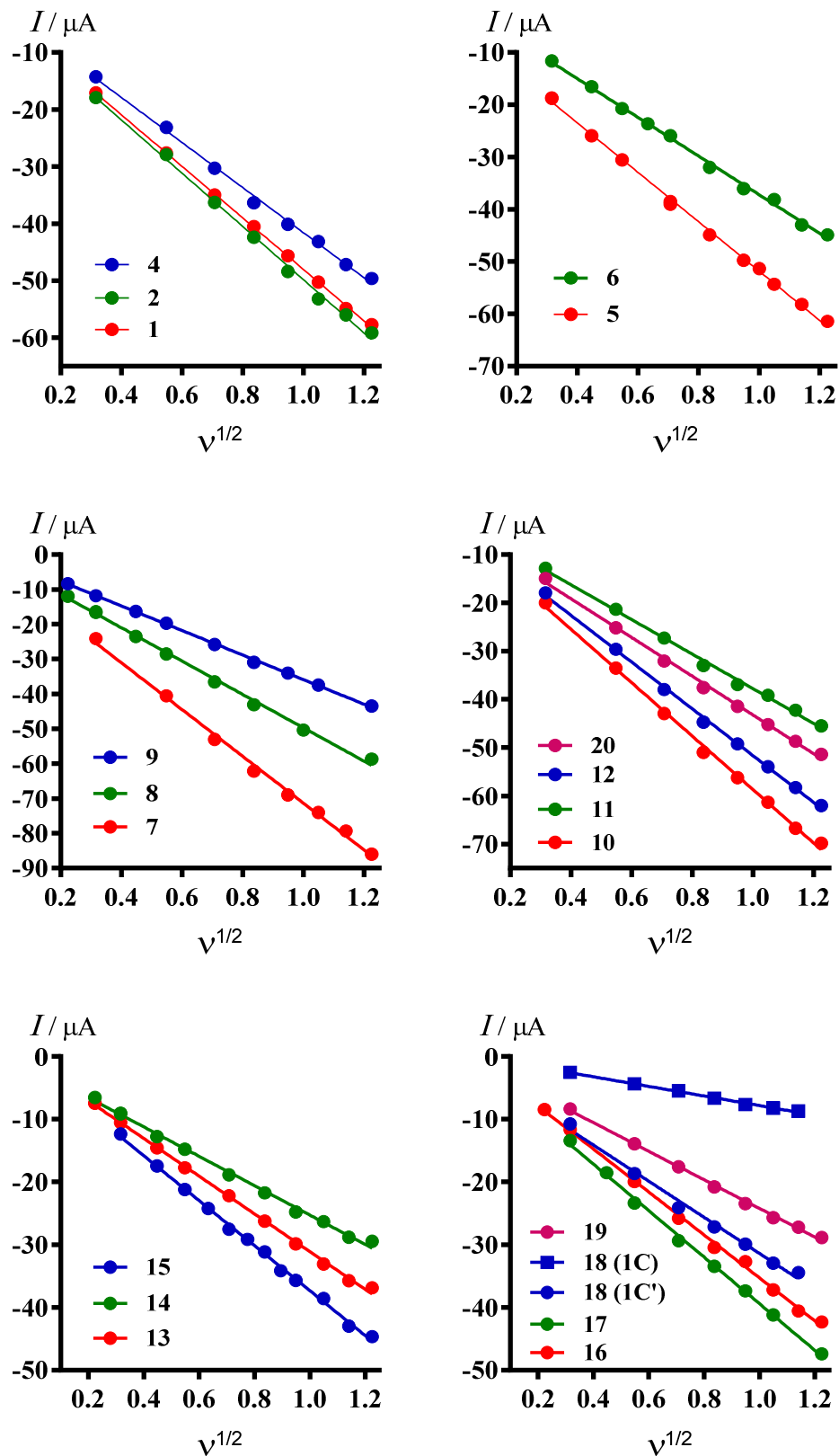
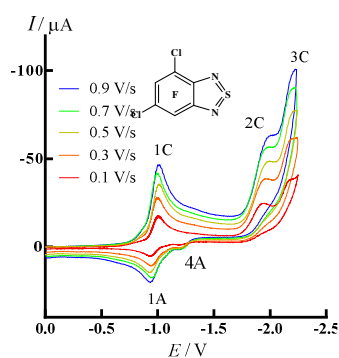
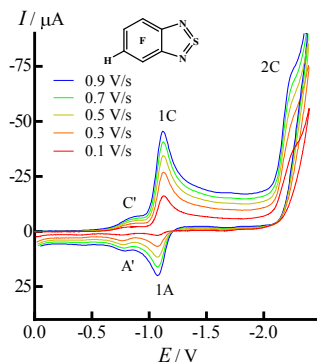
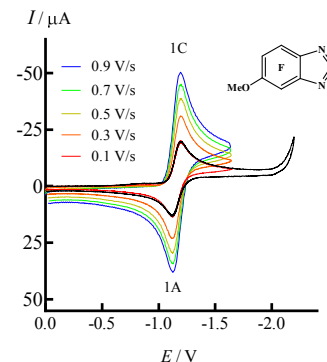


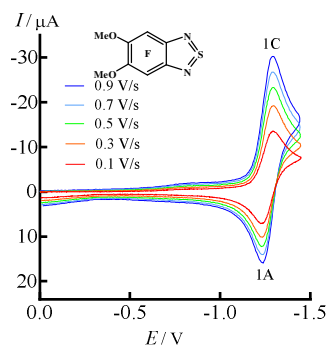
Figure S1. Linear dependences I_p^{1C} vs. $v^{1/2}$ proving diffusion-controlled nature of the first peaks of ECR of 1, 2 and 4-20.

Table S1. Parameters of linear regressions $I_p^{1C} = A \cdot v^{1/2} + B$ for 1, 2 and 4-20^a

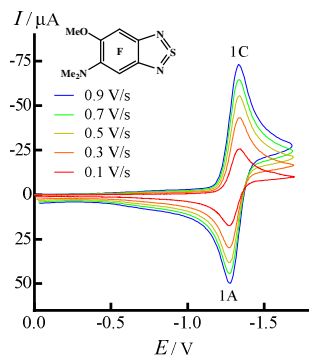
Compound	1	2	4	5	6	7	8
A	-45.15	-46.66	-39.5	-47.28	-37.03	-67.12	-47.83
B	-2.82	-3.174	-2.085	-4.53	-0.178	-4.216	-1.880
r^2	0.999	0.997	0.997	0.998	0.997	0.996	0.997
Compound	9	10	11	12	13	14	15
A	-35.24	-55.36	-35.87	-48.44	-30.08	-23.42	-35.86
B	-0.651	-3.347	-1.937	-3.231	-1.032	-1.860	-1.478
r^2	0.999	0.998	0.997	0.999	0.998	0.996	0.998
Compound	16	17	18 ^b	18 ^c	19	20	
A	-34.26	-37.12	-28.82	-7.65	-22.8	-40.13	
B	-1.044	-2.305	-2.589	-0.167	-1.423	-3.115	
r^2	0.998	0.998	0.992	0.996	0.998	0.998	

^a A in $\mu\text{A}\cdot\text{s}^{1/2}\cdot\text{V}^{-1/2}$, and B in μA ; r is correlation coefficient. ^b Data for peak 1C'. ^c Data for peak 1C.

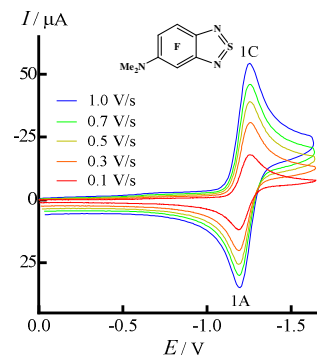
**1****4****5**



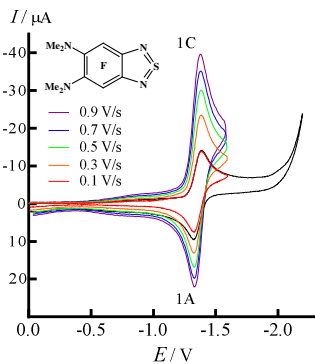
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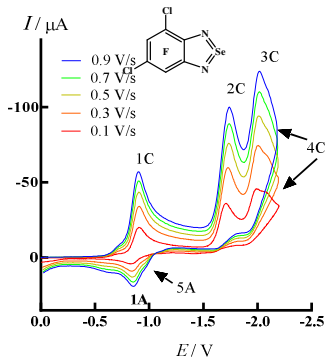
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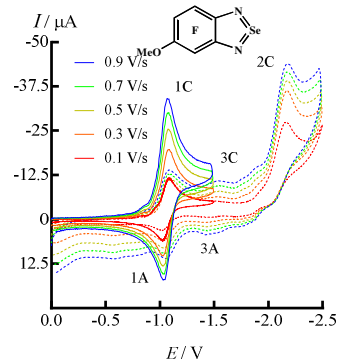
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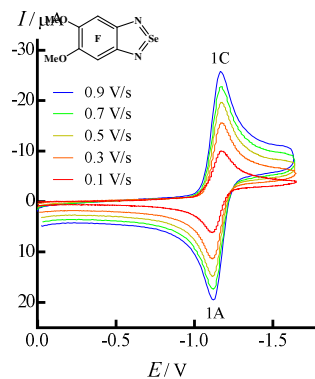
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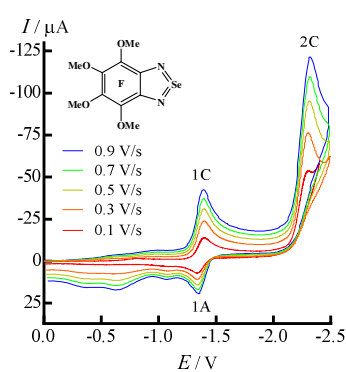
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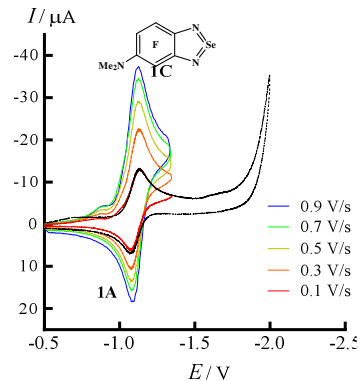
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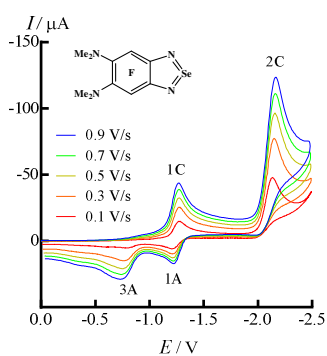
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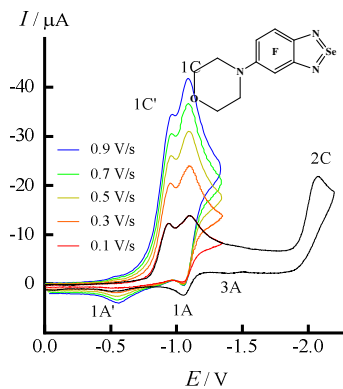
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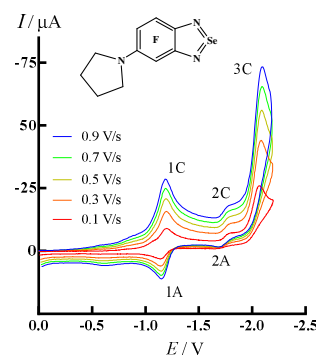
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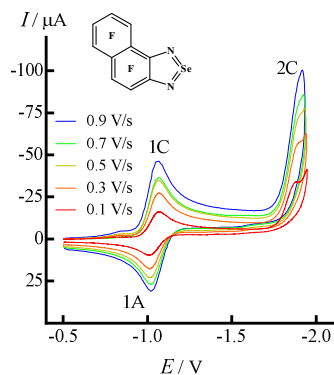
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18



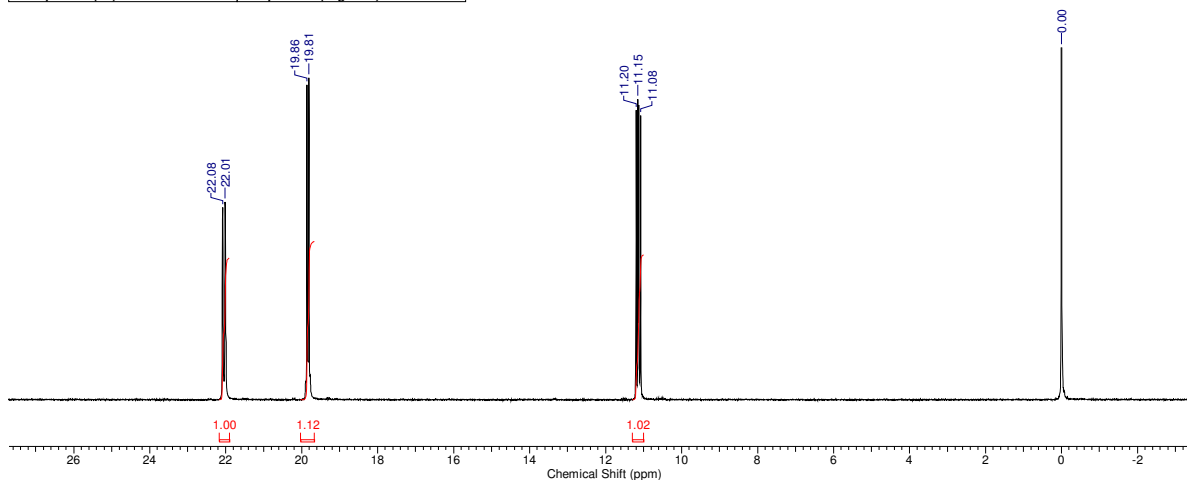
19

**20****Figure S2.** CVs of **1**, **4-10** and **13-20** at different potential sweep rates.

For compound **13**, CVs in the potential sweep range $0 > E > -2.4$ V are indicated by dotted lines; peak 3C is not observed at the cathode branch of the CV in the first cycle of the potential sweep. For compound **16**, no peaks are observed in the anodic branch of the CV in the potential range $-1.4 > E > -2.2$ V. CV of compound **18** reveals an additional irreversible peak 1C' preceding the reversible peak 1C corresponding to the formation of RA **18**; probably, peak 1C' is associated with **18** (specifically) adsorbed at electrode surface.

18 Apr 2017

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Sweep Width (Hz)	56497.18	Temperature (degree C)	23.400	Solvent	CHLOROFORM-D



19 Apr 2017

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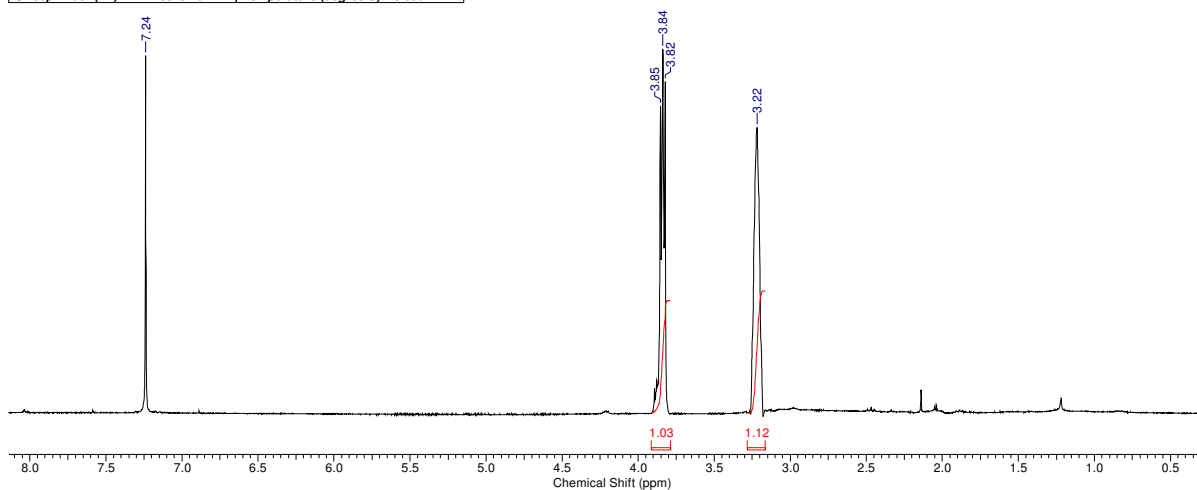
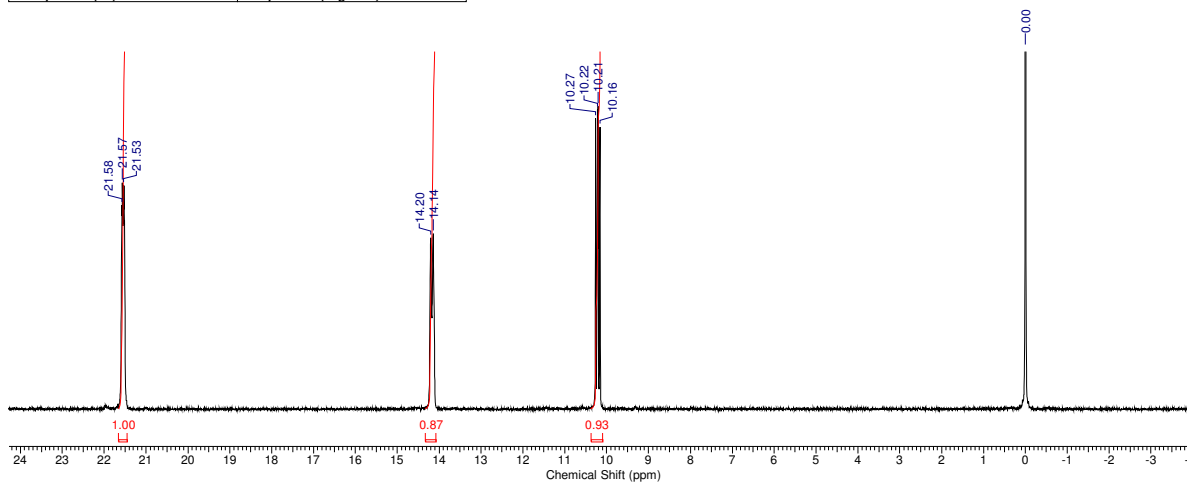


Figure S3. ¹⁹F (above) and ¹H (below) NMR spectra of compound **18**.

18 Apr 2017

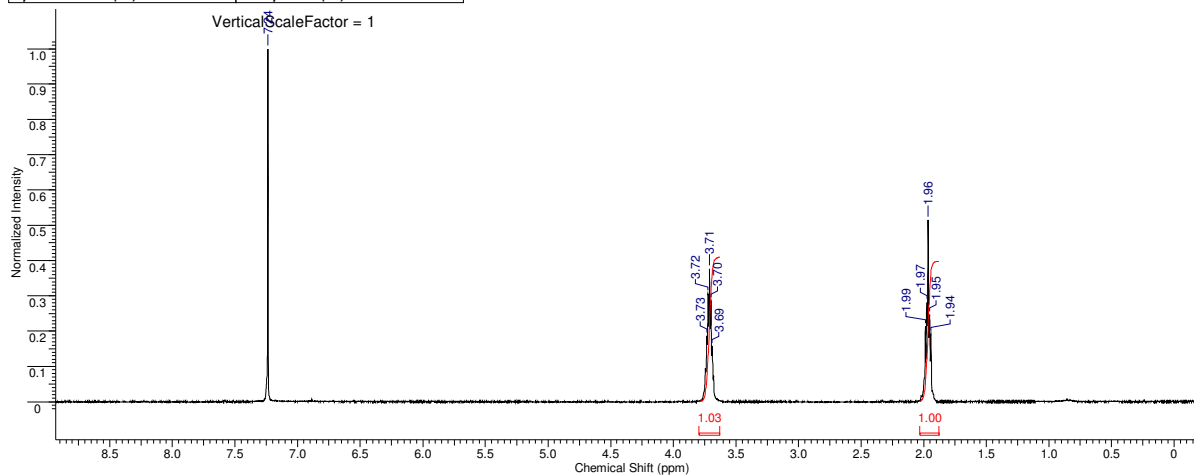
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Sweep Width (Hz)	56497.18	Temperature (degree C)	24.000	Solvent	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	0.00	0.2	1.0000	8	21.52	6077.5	0.0801	1	[10.10 .. 10.38]	0.927	1.84064e+9
2	10.16	2869.7	0.1011	9	21.53	6080.5	0.0801	2	[14.08 .. 14.33]	0.868	1.72338e+9
3	10.21	2882.2	0.1085	10	21.55	6083.5	0.0736	3	[21.46 .. 21.65]	1.000	1.98516e+9
4	10.22	2886.9	0.1072	11	21.56	6087.0	0.0781				
5	10.27	2899.0	0.1042	12	21.57	6090.0	0.0810				
6	14.14	3992.5	0.0628	13	21.58	6092.6	0.0730				
7	14.20	4009.4	0.0613								

19.04.2017 10:51:33

Acquisition Time (sec)	2.4773	Comment	TM - 780; CDCl ₃ C ₆ F ₆	Date	18 Apr 2017 06:17:36
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Spectrum Offset (Hz)	2838.1541	Sweep Width (Hz)	6613.66	Original Points Count	16384
				SW(cyclical) (Hz)	6613.76
				Solvent	CHLOROFORM-d

Figure S4. ¹⁹F (above) and ¹H (below) NMR spectra of compound **19**.