

Supplementary Material

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

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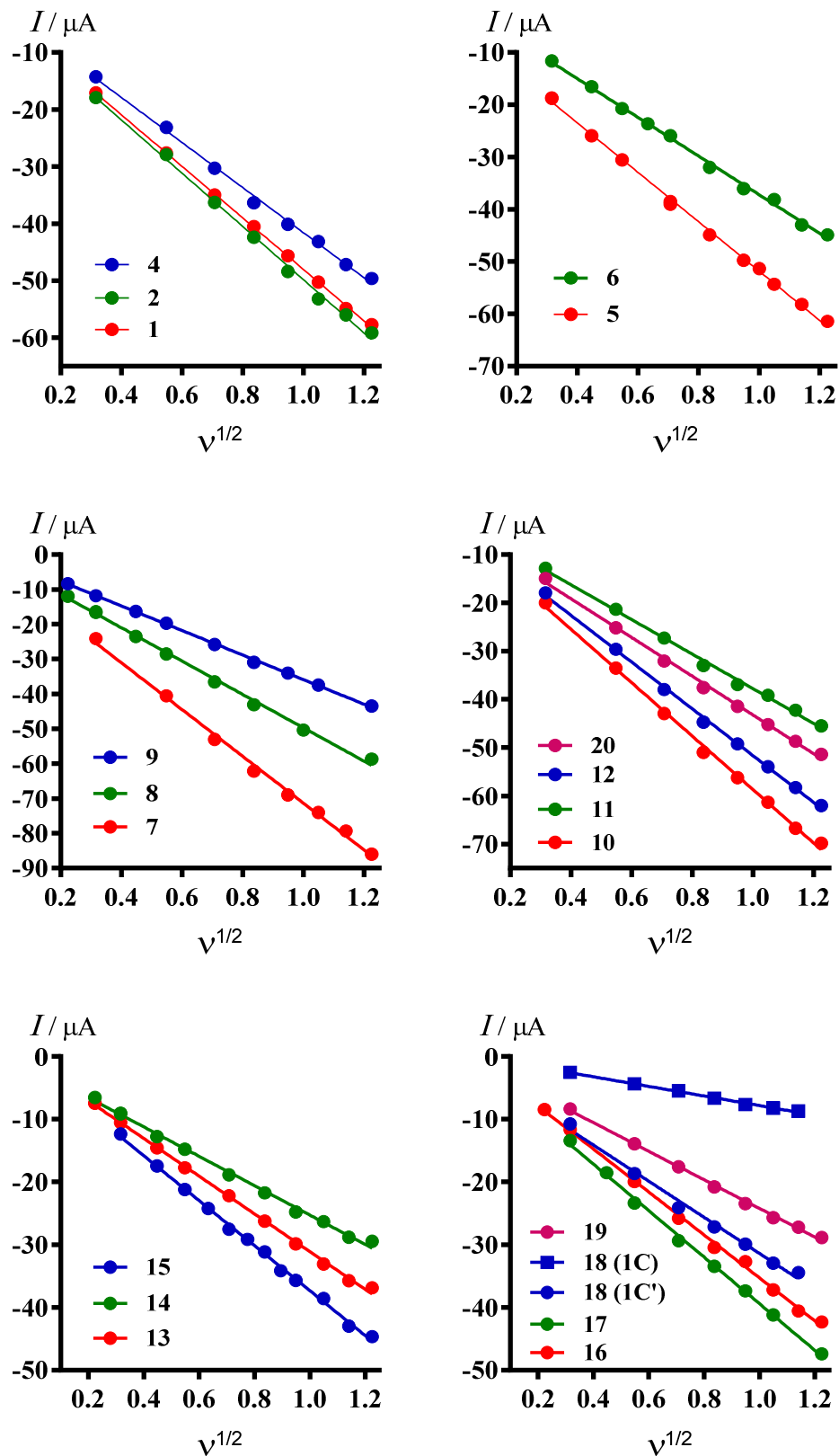
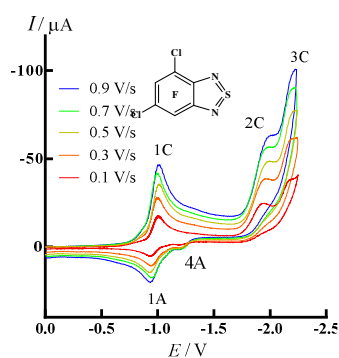
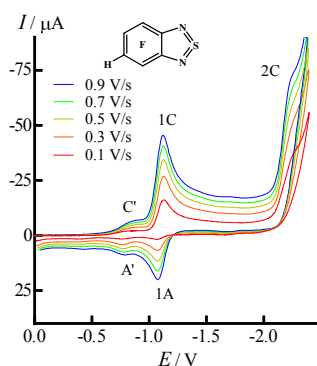
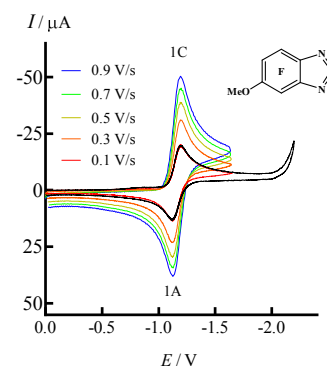


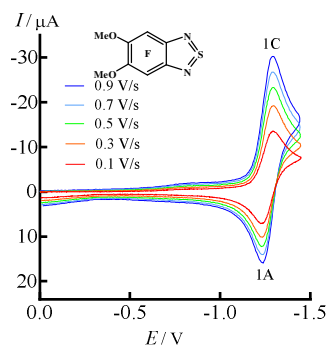
Figure S1. Linear dependences I_p^{1C} vs. $v^{1/2}$ proving diffusion-controlled nature of the first peaks of ECR of 1, 2 and 4-20.

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

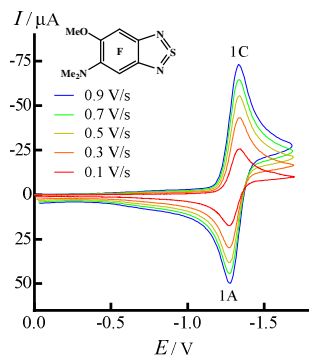
Compound	1	2	4	5	6	7	8
A	-45.15	-46.66	-39.5	-47.28	-37.03	-67.12	-47.83
B	-2.82	-3.174	-2.085	-4.53	-0.178	-4.216	-1.880
r^2	0.999	0.997	0.997	0.998	0.997	0.996	0.997
Compound	9	10	11	12	13	14	15
A	-35.24	-55.36	-35.87	-48.44	-30.08	-23.42	-35.86
B	-0.651	-3.347	-1.937	-3.231	-1.032	-1.860	-1.478
r^2	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.

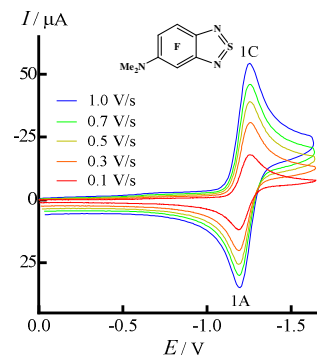
**1****4****5**



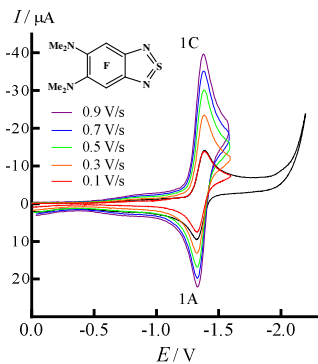
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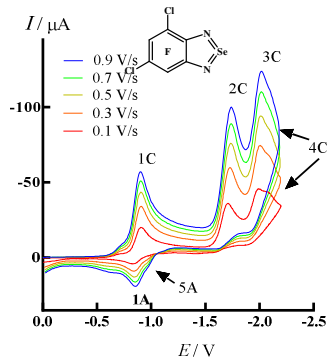
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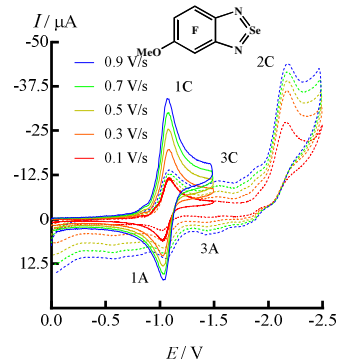
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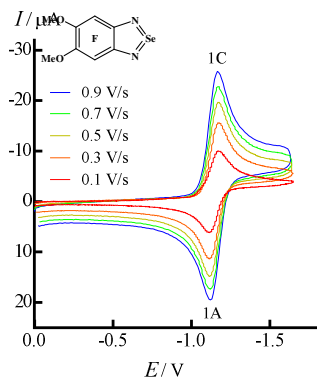
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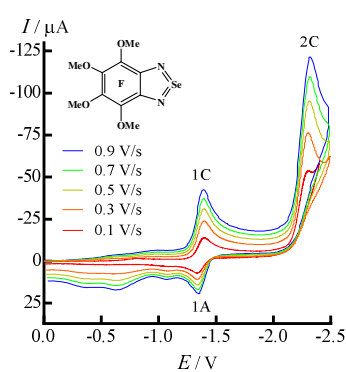
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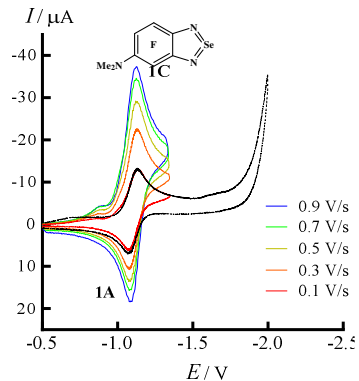
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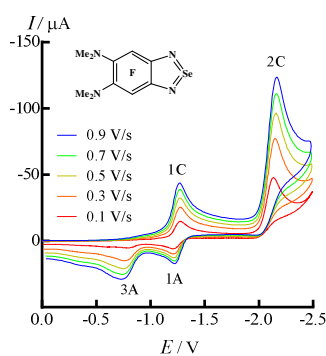
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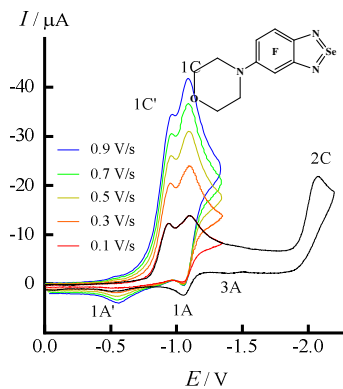
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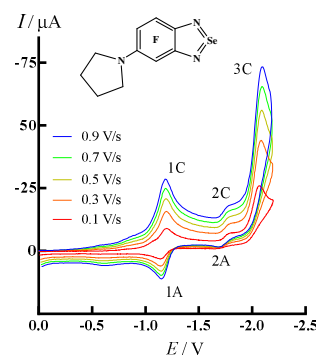
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18



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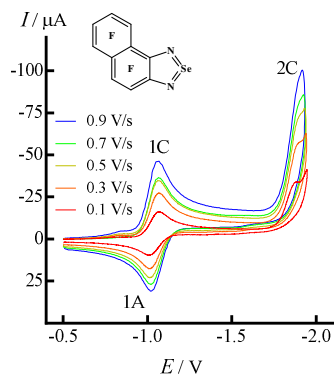
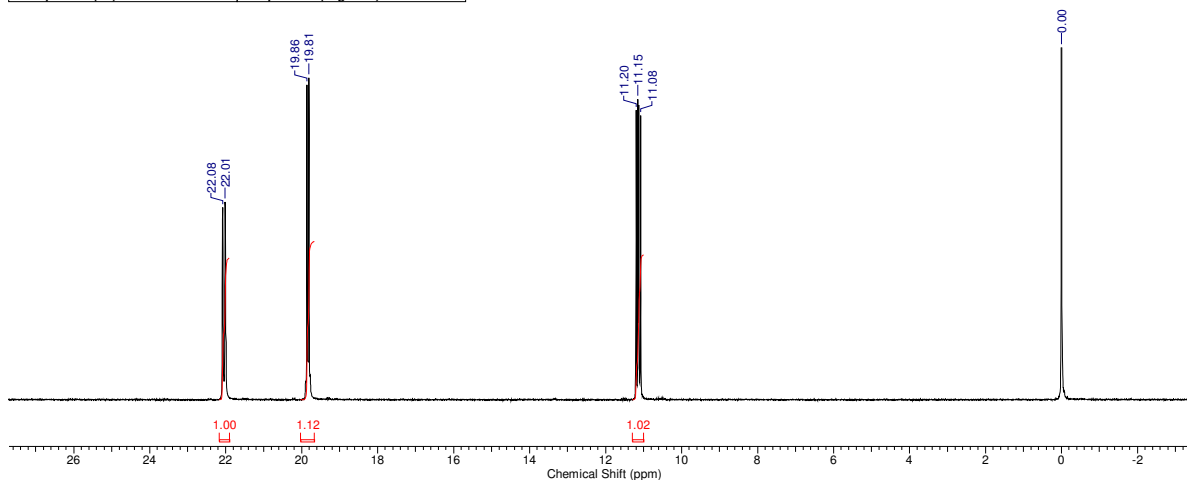
**20**

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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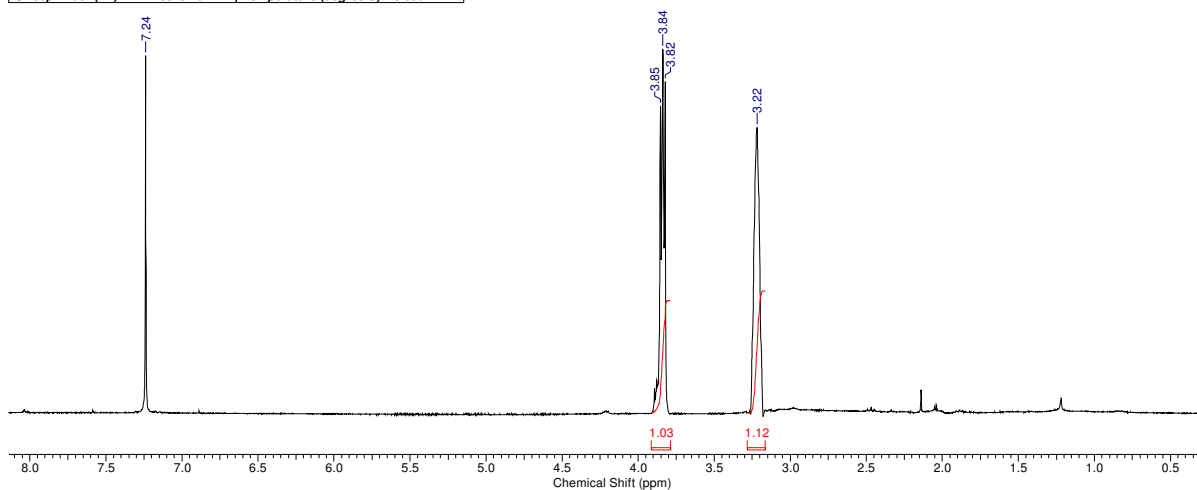
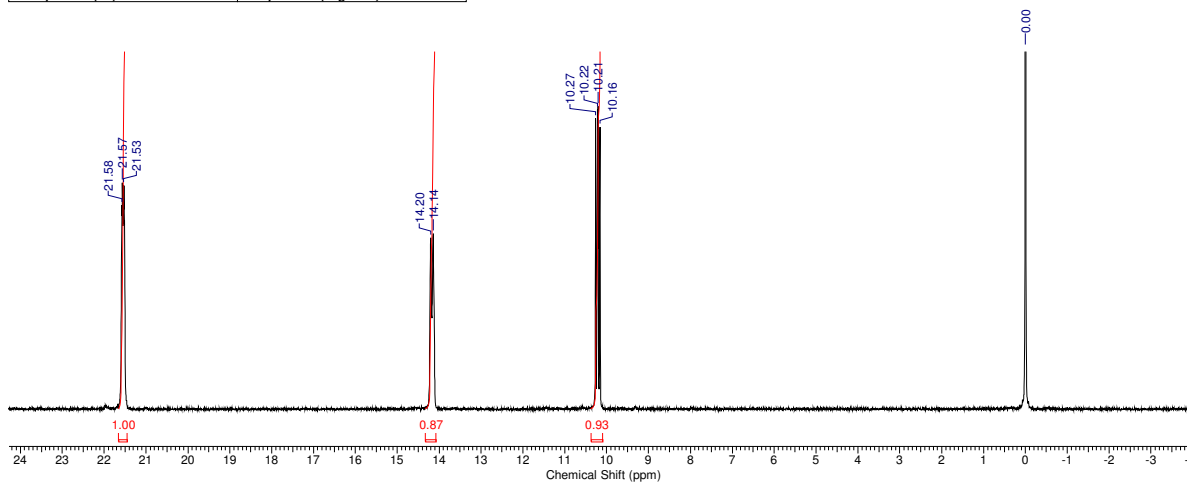


Figure S3. ¹⁹F (above) and ¹H (below) NMR spectra of compound **18**.

18 Apr 2017

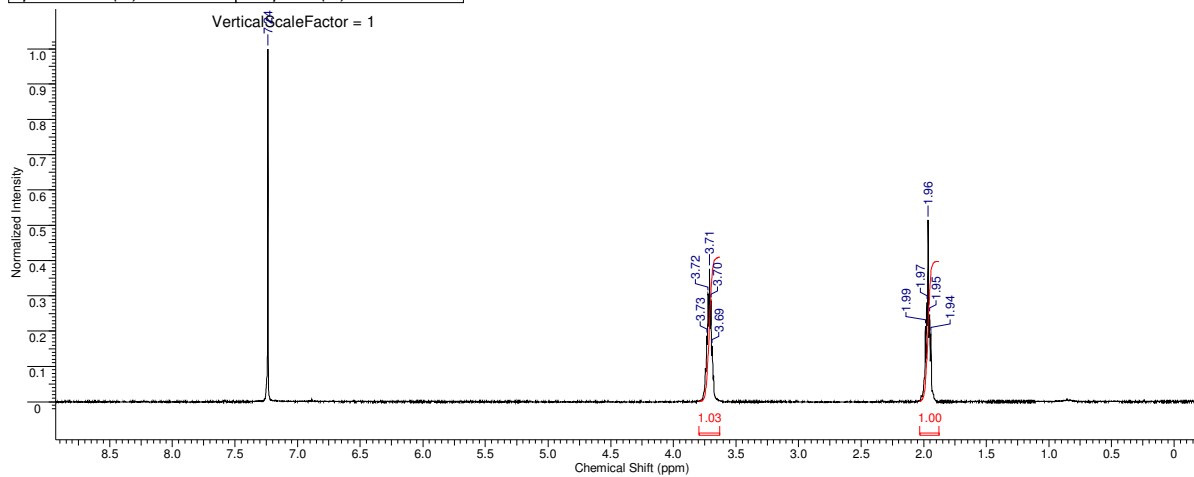
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Original Points Count	65536	Points Count	131072	Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	56497.18	Temperature (degree C)	24.000				



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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Nucleus	1H	Number of Transients	16	Origin	av300	Owner	oper
Points Count	65536	Pulse Sequence	zg	Receiver Gain	574.70	SW(cyclical) (Hz)	6613.76
Spectrum Offset (Hz)	2838.1541	Sweep Width (Hz)	6613.66	Solvent	CHLOROFORM-d		

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