SUPPORTING INFORMATION

for

Molecular Dynamics Simulation Elucidates the Preferential Binding Affinity of Sodium and Tetramethylammonium Ions for Tetrameric Nafion Unit under Aqueous Conditions

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Atom Serial Number	Atom Type	Partial Charge
1	С	1.378066
2	С	-0.647428
3	С	0.875498
4	С	0.238220
5	С	0.654350
6	Ċ	0.567950
7	Č	0 431645
8	Ċ	0 414311
9	Ċ	0 467674
10	Č	0 593316
11	Č	0 484354
12	Č	0 174233
12	C C	0.514580
14	C	-0 154549
14	C	1 150666
15	C C	0.626701
10		0.120701
1/	Г	-0.188134
18	Г Б	-0.208034
19	r F	-0.201048
20	r T	-0.088510
21	F	-0.241007
22	F	-0.255251
23	F	-0.250284
24	F	-0.228394
25	F	-0.244299
26	F	-0.251795
27	F	-0.249718
28	F	-0.246189
29	F	-0.245072
30	F	-0.247093
31	F	-0.249640
32	F	-0.247027
33	F	-0.240924
34	F	-0.245554
35	F	-0.252087
36	F	-0.244259
37	F	-0.249612
38	F	-0.235861
39	F	-0.224827
40	F	-0.246339
41	F	-0.243564
42	F	-0.205165
43	F	-0 115698
44	F	-0 246480
45	F	-0 241871
46	F	-0 264383
47	F	-0 272916
	r C	0.886318
		_0 125358
50	F	-0.123330
50	r F	0.337300
52	Г Г	-0.32/390
52	Г	-0.223299
	C	0.20078
54	L C	-0.306639

55	С	0.502636
56	О	-0.363030
57	О	-0.680195
58	О	-0.597246
59	F	-0.224103
60	F	-0.237333
61	F	-0.078114
62	F	0.113239
63	0	-0.622269
64	S	1.454415
65	Č	1.163358
66	Ċ	0.509542
67	Č	0 579434
68	Č	0.276929
69	Č	0.226031
70		0.458194
70		0.430174
71		0.591311
72		0.250517
73		0.230317
74		0.318002
15		0.747004
/6	C C	-0.055407
//	U C	0.140876
/8		-0.1428/6
79	C C	1.298093
80		0.1/5/41
81	F	-0.270338
82	F	-0.270656
83	F	-0.293075
84	F	-0.253273
85	F	-0.255275
86	F	-0.251069
87	F	-0.248665
88	F	-0.243646
89	F	-0.245834
90	F	-0.245977
91	F	-0.244572
92	F	-0.246153
93	F	-0.244849
94	F	-0.250757
95	F	-0.248492
96	F	-0.248753
97	F	-0.244829
98	F	-0.245876
99	F	-0.245658
100	F	-0.247359
101	F	-0.243202
102	F	-0.254236
103	F	-0.251799
104	F	-0.215788
105	F	-0 229133
106	F	-0 252570
107	F	-0 250647
108	F	-0 172969
100	L F	_0.216605
107	1 '	-0.210003

111F -0.268704 112F -0.245001 113C 0.943717 114O -0.084747 115F -0.251188 117F -0.196343 118C -0.554301 120C 0.036908 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.238798 126F -0.238798 127F -0.238798 128O -0.609787 129S 1.402594 130C 1.25378 131C -0.487423 132C 0.487423 133C 0.140338 134C 0.515593 135C 0.487423 136C 0.57656 136C 0.57656 137C 0.42884 137C 0.42884 138C 0.373033 139C 0.567656 144C 1.251812 145C 0.169988 144C 1.251812 145F -0.195942 150F -0.24773 145F -0.24773 146F -0.24783 156F -0.24703 157F -0.24703 158F -0.24703 159F -0.24703 156F	110	F	-0.242963
112F -0.245001 113C 0.943717 114O -0.084747 115F -0.243272 116F -0.243272 116F -0.243272 117F -0.196343 118C -0.554301 119C 0.036908 120C 0.036908 121O -0.114477 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.241774 126F -0.207552 127F -0.207552 128O -0.609787 129S 1.402594 130C 1.250378 131C -0.487423 132C 0.946712 133C 0.46038 134C 0.515593 135C 0.497556 136C 0.492823 137C 0.492823 138C 0.567656 140C 0.567656 144C 1.251812 145C 0.649950 144C 1.251812 145C 0.23763 146F -0.24773 147F -0.245266 151F -0.24526 152F -0.24773 155F -0.24773 156F -0.24773 157F -0.24526 151F<	111	F	-0.268704
113C 0.943717 114O -0.084747 115F -0.243272 116F -0.251188 117F 0.05633 118C -0.554301 119C 0.036908 120C 0.843658 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.24774 126F -0.24774 127F -0.23782 128O -0.609787 129S 1.402594 130C 1.25593 132C 0.487423 133C 0.487423 134C 0.51593 135C 0.549556 136C 0.549556 137C 0.462884 138C 0.567656 140C 0.582775 141C 0.233763 143C 0.567656 144C 1.251812 145C 0.51777 146F -0.195942 150F -0.24771 148F -0.195943 154F -0.233783 155F -0.247731 148F -0.195942 159F -0.247731 145C 0.56756 140F -0.247731 145F -0.247731 146F <td>112</td> <td>F</td> <td>-0.245001</td>	112	F	-0.245001
1140 -0.084747 115F -0.243272 116F -0.243272 117F -0.0196343 118C -0.554301 119C 0.036908 120C 0.036908 120C 0.036908 121O -0.111467 122O -0.704170 123O -0.66655 124F -0.228798 125F -0.2207552 128O -0.609787 129S 1.42594 130C 1.250378 131C 0.44743 132C 0.946712 133C 0.140338 134C 0.5593 135C 0.43955 136C 0.449283 137C 0.492823 138C 0.373033 139C 0.567656 140C 0.582775 141C 0.233763 142C 0.649950 143C 0.169988 144C 1.25378 150F -0.24226 151F -0.233743 154F 0.233763 155F 0.233763 156F -0.247140 153F 0.242582 155F 0.242582 155F 0.247531 156F 0.247531 157F 0.247331 158F <td< td=""><td>113</td><td>С</td><td>0.943717</td></td<>	113	С	0.943717
115F -0.243272 116F -0.25132 117F -0.196343 118C -0.554301 119C 0.036908 120C 0.843658 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.244774 126F -0.244774 126F -0.207552 128O -0.609787 129S 1.402594 130C 1.250378 131C -0.487423 132C 0.946712 133C 0.4140338 134C 0.549556 136C 0.42823 137C 0.42823 138C 0.373033 139C 0.567656 140C 0.53775 141C 0.233763 142C 0.649950 143C -0.169988 144C 1.251812 145C 0.516766 140F -0.195942 147F -0.225965 152F -0.247140 153F -0.2470373 156F -0.247033 156F -0.247033 157F -0.247033 158F -0.248031 160F -0.247061 161F -0.247061 162 <td>114</td> <td>0</td> <td>-0.084747</td>	114	0	-0.084747
116F -0.251188 117F -0.196343 118C -0.554301 119C 0.036908 120C 0.843658 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.207195 126F -0.207195 128O -0.6097877 129S 1.402594 130C 1.25378 131C -0.487423 132C 0.4487423 133C 0.57552 138C 0.57552 139S 1.402594 131C -0.487423 132C 0.487423 133C 0.487423 134C 0.515593 135C 0.462884 137C 0.42884 137C 0.42823 138C 0.567656 140C 0.582775 141C 0.252765 142C 0.649950 143C -0.199988 144C 1.251812 145F -0.292787 150F -0.245748 150F -0.245734 154F -0.245734 155F -0.245748 156F -0.247701 161F -0.247701 161F -0.247701 162 <td< td=""><td>115</td><td>F</td><td>-0.243272</td></td<>	115	F	-0.243272
117F -0.196343 118C -0.554301 120C 0.036908 120C 0.83658 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.244774 126F -0.207552 128O -0.609787 129S 1.4025944 130C 1.250378 131C -0.487423 132C 0.946712 133C 0.140338 134C 0.549556 136C 0.4549556 136C 0.373033 139C 0.567565 140C 0.253763 141C 0.253763 142C 0.66988 144C 1.251812 145C 0.516936 144C 1.251812 145F -0.199988 144F -0.199661 145F -0.225065 152F -0.247177 148F -0.225085 151F -0.225085 152F -0.247033 158F -0.247033 159F -0.247033 156F -0.247033 157F -0.247031 160F -0.247061 161F -0.247061 162F -0.247061 163 </td <td>116</td> <td>F</td> <td>-0.251188</td>	116	F	-0.251188
118C -0.554301 119C 0.036008 120C 0.843658 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.24774 126F -0.207195 127F -0.207195 128O -0.609787 129S 1.402594 130C 1.250378 131C -0.487423 132C 0.946712 133C 0.140338 134C 0.515593 135C 0.482823 138C 0.567656 140C 0.582775 141C 0.233763 142C 0.667656 143C 0.510477 144F -0.195942 147F -0.225965 152F -0.247140 148F -0.19988 144C 1.251812 145C 0.510477 146F -0.199861 149F -0.225965 152F -0.247033 150F -0.247033 154F -0.247033 155F -0.247033 156F -0.247073 157F -0.247073 158F -0.247073 159F -0.247073 156F -0.247701 161 <td>117</td> <td>F</td> <td>-0 196343</td>	117	F	-0 196343
119C 0.036908 120C 0.036908 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.238798 125F -0.244774 126F -0.207195 127F -0.207195 128O -0.609787 129S 1.402594 130C 1.250378 131C -0.487423 132C 0.946712 133C 0.140338 134C 0.549556 136C 0.492823 137C 0.492823 138C 0.373033 139C 0.582775 141C 0.233763 142C 0.669566 143C 0.195942 144F -0.195942 145C 0.51812 146F -0.195942 147F -0.233763 148F -0.195942 147F -0.275177 148F -0.195942 151F -0.235965 152F -0.247140 153F -0.247073 154F -0.247033 156F -0.247033 156F -0.247013 157F -0.247033 158F -0.247033 159F -0.247031 160F -0.243634 163 </td <td>118</td> <td>Ċ</td> <td>-0 554301</td>	118	Ċ	-0 554301
120C 0.843658 121O -0.111467 122O -0.704170 123O -0.640685 124F -0.234774 126F -0.244774 126F -0.207195 127F -0.207195 128O -0.609787 129S 1.402594 130C 1.250378 131C -0.487423 132C 0.487423 133C 0.487423 134C 0.515593 135C 0.449356 136C 0.449323 137C 0.492823 138C 0.557656 140C 0.582775 141C 0.51859 143C 0.510477 144F -0.195942 147F -0.23763 148F -0.195942 147F -0.23765 148F -0.195942 147F -0.23765 151F -0.23787 153F -0.230384 154F -0.247073 155F -0.247701 156F -0.247701 157F -0.247701 161F -0.247701 161F -0.247701 161F -0.247701 161F -0.247701 161F -0.247701 162F -0.247701 <td>119</td> <td>Č</td> <td>0.036908</td>	119	Č	0.036908
1210-0.1114671220-0.7041701230-0.640685124F-0.238798125F-0.244774126F-0.207195127F-0.2071951280-0.609787129S1.402594130C1.250378131C-0.487423132C0.140338133C0.140338134C0.549556136C0.462884137C0.462884138C0.373033139C0.567656140C0.233763141C0.233763142C0.510477143C0.510477144F-0.19961149F-0.275177148F-0.19961149F-0.23378150F-0.244226151F-0.23384154F-0.23384155F-0.24407156F-0.24532157F-0.245732158F-0.245732159F-0.246731160F-0.24634163F-0.243634	120	Č	0.843658
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124F -0.238798 125F -0.244774 126F -0.207195 127F -0.207552 128O -0.609787 129S 1.402594 130C 1.250378 131C -0.487423 132C 0.946712 133C 0.140338 134C 0.515593 135C 0.442844 137C 0.442844 137C 0.442844 137C 0.567656 140C 0.582775 141C 0.233763 142C 0.69950 143C 0.169988 144C 1.251812 145C 0.169988 144F -0.195942 147F -0.275177 148F 0.092878 150F 0.224726 151F 0.224703 153F 0.247140 153F 0.247073 157F 0.247073 158F 0.249733 156F 0.247701 161F 0.24574 163F 0.245748	122	Ő	-0.640685
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132C 0.940712 133C 0.140338 134C 0.515593 135C 0.549556 136C 0.462884 137C 0.492823 138C 0.373033 139C 0.567656 140C 0.582775 141C 0.233763 142C 0.649950 143C -0.169988 144C 1.251812 145C 0.510477 146F -0.195942 147F -0.275177 148F -0.199661 149F -0.22878 150F -0.244226 151F -0.230384 154F -0.247033 155F -0.247073 156F -0.247073 157F -0.247073 158F -0.247732 159F -0.247732 160F -0.247701 161F -0.247634 163F -0.247742	131	C C	-0.48/425
133C 0.14038 134C 0.515593 135C 0.549556 136C 0.402884 137C 0.492823 138C 0.373033 139C 0.567656 140C 0.233763 141C 0.233763 142C 0.649950 143C -0.169988 144C 1.251812 145C 0.510477 146F -0.195942 147F -0.275177 148F -0.199661 149F -0.247176 150F -0.247140 153F -0.230384 154F -0.245982 155F -0.247073 156F -0.247733 156F -0.2477332 159F -0.247701 161F -0.247742	132	U C	0.946/12
134C 0.51593 135 C 0.549556 136 C 0.462884 137 C 0.492823 138 C 0.373033 139 C 0.567656 140 C 0.233763 142 C 0.649950 143 C -0.169988 144 C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.092878 150 F -0.247582 151 F -0.25965 152 F -0.247140 153 F -0.245783 156 F -0.247733 157 F -0.247733 158 F -0.247733 159 F -0.247733 160 F -0.247701 161 F -0.245748 163 F -0.245748	133	C C	0.140338
135C 0.349556 136C 0.462884 137C 0.4492823 138C 0.373033 139C 0.567656 140C 0.582775 141C 0.233763 142C 0.649950 143C -0.169988 144C 1.251812 145C 0.510477 146F -0.195942 147F -0.275177 148F -0.092878 150F -0.244226 151F -0.244226 152F -0.247140 153F -0.230384 154F -0.247073 157F -0.247073 158F -0.247732 160F -0.247701 161F -0.245266 162F -0.245748 163F -0.245748	134	C	0.515593
136C 0.462884 137 C 0.492823 138 C 0.373033 139 C 0.567656 140 C 0.582775 141 C 0.233763 142 C 0.649950 143 C -0.169988 144 C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.199661 149 F -0.092878 150 F -0.244226 151 F -0.245965 152 F -0.247140 153 F -0.247073 156 F -0.247073 157 F -0.247073 158 F -0.247073 159 F -0.247701 161 F -0.247701 161 F -0.245266 162 F -0.245748 164 F 0.245748	135	C	0.549556
137C 0.492823 138 C 0.373033 139 C 0.567656 140 C 0.582775 141 C 0.233763 142 C 0.649950 143 C -0.169988 144 C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.199661 149 F -0.225177 148 F -0.292878 150 F -0.244226 151 F -0.230384 154 F -0.230384 154 F -0.240703 157 F -0.247073 157 F -0.247073 157 F -0.248031 160 F -0.248031 160 F -0.248031 160 F -0.243634 164 F 0.245748	136	C	0.462884
138C 0.373033 139C 0.567656 140C 0.582775 141C 0.233763 142C 0.649950 143C -0.169988 144C 1.251812 145C 0.510477 146F -0.195942 147F -0.275177 148F -0.199661 149F -0.245226 151F -0.245226 151F -0.247140 153F -0.247140 153F -0.247140 154F -0.247073 155F -0.247073 156F -0.247073 157F -0.247033 158F -0.247033 160F -0.247701 161F -0.245266 162F -0.245246 163F -0.245748	137	С	0.492823
139C 0.567656 140C 0.582775 141C 0.233763 142C 0.649950 143C -0.169988 144C 1.251812 145C 0.510477 146F -0.195942 147F -0.275177 148F -0.092878 150F -0.245266 151F -0.245265 152F -0.245282 153F -0.240384 154F -0.240733 155F -0.247073 157F -0.247073 158F -0.247031 160F -0.247701 161F -0.245266 162F -0.245748 164F 0.245742	138	С	0.373033
140C 0.582775 141 C 0.233763 142 C 0.649950 143 C -0.169988 144 C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.092878 150 F -0.244226 151 F -0.245965 152 F -0.247140 153 F -0.230384 154 F -0.247073 156 F -0.247073 157 F -0.247532 159 F -0.247031 160 F -0.247701 161 F -0.245266 164 F -0.245748	139	С	0.567656
141C 0.233763 142 C 0.649950 143 C -0.169988 144 C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.092878 150 F -0.24226 151 F -0.24226 151 F -0.247140 153 F -0.247140 153 F -0.245582 156 F -0.247073 156 F -0.247073 157 F -0.247073 158 F -0.247073 159 F -0.247322 160 F -0.247701 161 F -0.243634 163 F -0.245748 164 F -0.245748	140	С	0.582775
142C 0.649950 143 C -0.169988 144 C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.092878 150 F -0.24226 151 F -0.245265 152 F -0.247140 153 F -0.247140 153 F -0.245582 156 F -0.247073 157 F -0.247073 158 F -0.247033 159 F -0.247031 160 F -0.247701 161 F -0.243634 163 F -0.245748	141	С	0.233763
143C -0.169988 144C1.251812145C 0.510477 146F -0.195942 147F -0.275177 148F -0.092878 150F -0.244226 151F -0.247426 152F -0.247140 153F -0.247140 154F -0.245582 155F -0.247073 156F -0.247073 157F -0.247073 158F -0.247532 159F -0.247701 161F -0.247701 163F -0.243634 164F -0.245748	142	С	0.649950
144C 1.251812 145 C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.199661 149 F -0.092878 150 F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.230384 154 F -0.245582 155 F -0.245783 156 F -0.247073 157 F -0.245934 158 F -0.248031 160 F -0.247701 161 F -0.243634 163 F -0.245748	143	С	-0.169988
145C 0.510477 146 F -0.195942 147 F -0.275177 148 F -0.199661 149 F -0.092878 150 F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.24582 155 F -0.245582 156 F -0.247073 157 F -0.247073 157 F -0.245934 158 F -0.247032 159 F -0.248031 160 F -0.245266 162 F -0.245748 163 F -0.245748	144	С	1.251812
146F -0.195942 147 F -0.275177 148 F -0.199661 149 F -0.092878 150 F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.247140 153 F -0.245582 155 F -0.2450783 156 F -0.247073 157 F -0.247073 158 F -0.247934 158 F -0.248031 160 F -0.247701 161 F -0.245266 162 F -0.243634 163 F -0.245748 164 F -0.245748	145	С	0.510477
147F -0.275177 148 F -0.199661 149 F -0.092878 150 F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.247140 153 F -0.245582 155 F -0.245582 155 F -0.245783 156 F -0.247073 157 F -0.245934 158 F -0.247532 159 F -0.248031 160 F -0.247701 161 F -0.245266 162 F -0.24564 163 F -0.245748	146	F	-0.195942
148F -0.199661 149 F -0.092878 150 F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.230384 154 F -0.245582 155 F -0.245783 156 F -0.247073 157 F -0.245934 158 F -0.245934 158 F -0.247032 159 F -0.247031 160 F -0.247701 161 F -0.245266 162 F -0.245748 164 F -0.245748	147	F	-0.275177
149F -0.092878 150 F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.230384 154 F -0.245582 155 F -0.245783 156 F -0.247073 157 F -0.245934 158 F -0.247532 159 F -0.247532 159 F -0.247701 160 F -0.245266 162 F -0.245748 164 F -0.245748	148	F	-0.199661
150F -0.244226 151 F -0.255965 152 F -0.247140 153 F -0.230384 154 F -0.245582 155 F -0.245783 156 F -0.247073 157 F -0.245934 158 F -0.247532 159 F -0.248031 160 F -0.245266 162 F -0.245266 163 F -0.243634 164 F -0.245748	149	F	-0.092878
151F -0.255965 152 F -0.247140 153 F -0.230384 154 F -0.245582 155 F -0.2450783 156 F -0.247073 157 F -0.245934 158 F -0.247532 159 F -0.248031 160 F -0.245266 162 F -0.243634 163 F -0.245748 164 F -0.245748	150	F	-0.244226
152F -0.247140 153 F -0.230384 154 F -0.245582 155 F -0.250783 156 F -0.247073 157 F -0.245934 158 F -0.247532 159 F -0.248031 160 F -0.247701 161 F -0.245266 162 F -0.245634 163 F -0.245748	151	F	-0.255965
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	152	F	-0.247140
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	153	F	-0.230384
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	154	F	-0.245582
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	155	F	-0.250783
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	156	F	-0.247073
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	157	F	-0.245934
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	158	F	-0.247532
$\begin{array}{c ccccc} 160 & F & & -0.247701 \\ 161 & F & & -0.245266 \\ 162 & F & & -0.243634 \\ 163 & F & & -0.245748 \\ 164 & F & & 0.248742 \\ \end{array}$	159	F	-0.248031
161 F -0.245266 162 F -0.243634 163 F -0.245748 164 F 0.248742	160	F	-0.247701
162 F -0.243634 163 F -0.245748	161	F	-0.245266
163 F -0.245748	162	F	-0 243634
164 E 0.240740	163	F	-0 245748
Γ Γ Γ Γ $ \Gamma$ $ \Gamma$ $ \Gamma$	164	F	-0.248742

165	F	-0.241014
166	F	-0.247898
167	F	-0.246035
168	F	-0.233135
169	F	-0.242153
170	F	-0.249000
171	F	-0.245231
172	F	-0 180232
173	F	-0 242548
174	F	-0.257855
175	F	-0.262775
176	F	-0 279946
177	r C	0.703435
178		-0 183999
179	F	-0.280800
180	I F	0.200000
100	r E	-0.298019
101	Г	-0.280440
102	C C	0.226516
183	C C	0.220510
184	U C	0.498131
185	0	-0.318/51
186	0	-0./08955
18/	0	-0.623234
188	F	-0.239508
189	F	-0.245589
190	F	-0.230113
191	F	-0.262875
192	О	-0.636769
193	S	1.412286
194	С	0.087437
195	С	0.220940
196	С	0.657856
197	С	0.172430
198	С	0.704320
199	С	0.338412
200	С	0.349393
201	С	0.749437
202	С	0.346982
203	С	0.383728
204	С	0.982228
205	С	-0.362025
206	С	0.787425
207	С	0.057624
208	С	1.188645
209	С	0.231276
210	F	-0.298088
211	F	-0.304325
212	F	-0 229884
213	F	0 682549
213	F	-0 252988
215	F	-0 229724
215	г Г	_0.102182
210	L F	-0.172102
217	Г F	-0.173330
210	Г Б	-0.247041
219	Г	-0.231102

220	F	-0.241355
221	F	-0.241147
222	F	-0.246585
223	F	-0.251881
224	F	-0.247478
225	F	-0.250444
226	F	-0.252651
227	F	-0.249796
228	F	-0.243731
229	F	-0.244502
230	F	-0.254576
231	F	-0.257171
232	F	-0.211064
233	F	-0.215340
234	F	-0.258057
235	F	-0.252136
236	F	-0.175333
237	F	-0.218798
238	F	-0.252314
239	F	-0.273673
240	F	-0.253406
241	С	0.923318
242	О	-0.076326
243	F	-0.270131
244	F	-0.258869
245	F	-0.199902
246	С	-0.270795
247	С	0.049752
248	С	0.784107
249	О	-0.121046
250	О	-0.683863
251	О	-0.651359
252	F	-0.241072
253	F	-0.245779
254	F	-0.227683
255	F	-0.210843
256	О	-0.599871
257	S	1.383176
258	F	-0.335673
259	F	-0.327052
260	F	-0.304802
261	F	-0.312874
262	F	-0.274670

TABLE S1. Partial charges assigned to the different atoms constituting the 4-mer nafion according to its ground state geometry optimized using the B3LYP model of the Density Functional Theory (DFT) in combination with 6-311++G(d, p) basis set in the Gaussian-09 software. The cumulative sum of the total Mulliken charges listed above comes out to be -4.000.