Supplementary materials
for
Theoretical Investigations of Azole-Fused Tricyclic 1,2,3,4-Tetrazine-2-Oxides

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Summary of surface analysis of compound **A-E**.

Compound A:
Volume: 2074.27920 Bohr^3 (307.37653 Angstrom^3)
Minimal value: -18.32295 kcal/mol
Maximal value: 69.00284 kcal/mol
Overall surface area: 1026.33773 Bohr^2 (287.40388 Angstrom^2)
Positive surface area: 535.51620 Bohr^2 (149.95983 Angstrom^2)
Negative surface area: 490.82153 Bohr^2 (137.44405 Angstrom^2)
Overall average value: 0.01230849 a.u. (7.72370 kcal/mol)
Positive average value: 0.03565103 a.u. (22.37138 kcal/mol)
Negative average value: -0.01315964 a.u. (-8.25781 kcal/mol)
Overall variance (sigma^2_tot): 0.00076323 a.u.^2 (300.53728 (kcal/mol)^2)
Positive variance: 0.00070810 a.u.^2 (278.82900 (kcal/mol)^2)
Negative variance: 0.00005513 a.u.^2 (21.70828 (kcal/mol)^2)
Balance of charges (miu): 0.06701416
Product of sigma^2_tot and miu: 0.00005115 a.u.^2 (20.14025 (kcal/mol)^2)
Internal charge separation (Pi): 0.02618855 a.u. (16.43358 kcal/mol)

Compound B:
Volume: 2065.54638 Bohr^3 (306.08246 Angstrom^3)
Minimal value: -19.74669 kcal/mol Maximal value: 69.58498 kcal/mol
Overall surface area: 1027.33707 Bohr^2 (287.68372 Angstrom^2)
Positive surface area: 551.61405 Bohr^2 (154.46769 Angstrom^2)
Negative surface area: 475.72302 Bohr^2 (133.21603 Angstrom^2)
Overall average value: 0.01320515 a.u. (8.28636 kcal/mol)
Positive average value: 0.03677906 a.u. (23.07923 kcal/mol)
Negative average value: -0.01412946 a.u. (-8.86638 kcal/mol)
Overall variance (sigma^2_tot): 0.00080487 a.u.^2 (316.93132 (kcal/mol)^2)
Positive variance: 0.00074248 a.u.^2 (292.36512 (kcal/mol)^2)

Negative variance: 0.00006239 a.u.^2 (24.56620 (kcal/mol)^2)
Balance of charges (miu): 0.07150447
Product of sigma^2_tot and miu: 0.00005755 a.u.^2 (22.66201 (kcal/mol)^2)
Internal charge separation (Pi): 0.02739873 a.u. (17.19298 kcal/mol)

Compound C:
Volume: 1590.16489 Bohr^3 (235.63818 Angstrom^3)
Minimal value: -20.91166 kcal/mol
Maximal value: 67.72457 kcal/mol
Overall surface area: 808.72951 Bohr^2 (226.46736 Angstrom^2)
Positive surface area: 423.71820 Bohr^2 (118.65320 Angstrom^2)
Negative surface area: 385.01130 Bohr^2 (107.81416 Angstrom^2)
Overall average value: 0.01123245 a.u. (7.04848 kcal/mol)
Positive average value: 0.03539105 a.u. (22.20824 kcal/mol)
Negative average value: -0.01535491 a.u. (-9.63536 kcal/mol)
Overall variance (sigma^2_tot): 0.00077652 a.u.^2 (305.77027 (kcal/mol)^2)
Positive variance: 0.00069260 a.u.^2 (272.72554 (kcal/mol)^2)
Negative variance: 0.00008392 a.u.^2 (33.04473 (kcal/mol)^2)
Balance of charges (miu): 0.09639122
Product of sigma^2_tot and miu: 0.00007485 a.u.^2 (29.47357 (kcal/mol)^2)
Internal charge separation (Pi): 0.02685908 a.u. (16.85434 kcal/mol)

Compound D:
Volume: 1594.14943 Bohr^3 (236.22862 Angstrom^3)
Minimal value: -21.14315 kcal/mol
Maximal value: 67.49726 kcal/mol
Overall surface area: 844.72468 Bohr^2 (236.54704 Angstrom^2)
Positive surface area: 437.63743 Bohr^2 (122.55098 Angstrom^2)
Negative surface area: 407.08726 Bohr^2 (113.99606 Angstrom^2)
Overall average value: 0.01167800 a.u. (7.32806 kcal/mol)
Positive average value: 0.03829762 a.u. (24.03214 kcal/mol)
Negative average value: -0.01693931 a.u. (-10.62958 kcal/mol)
Overall variance (sigma^2_tot): 0.00078211 a.u.^2 (307.97013 (kcal/mol)^2)
Positive variance: 0.00070480 a.u.^2 (277.52780 (kcal/mol)^2)
Negative variance: 0.00007731 a.u.^2 (30.44233 (kcal/mol)^2)
Balance of charges (miu): 0.08907732
Product of sigma^2_tot and miu: 0.00006967 a.u.^2 (27.43315 (kcal/mol)^2)
Internal charge separation (Pi): 0.02893838 a.u. (18.15913 kcal/mol)

Compound E:
Volume: 1109.23492 Bohr^3 (164.37169 Angstrom^3)
Minimal value: -21.79792 kcal/mol
Maximal value: 63.85011 kcal/mol
Overall surface area: 602.94419 Bohr^2 (168.84159 Angstrom^2)

Positive surface area: 308.54255 Bohr^2 (86.40073 Angstrom^2)
Negative surface area: 294.40165 Bohr^2 (82.44087 Angstrom^2)
Overall average value: 0.01075678 a.u. (6.74999 kcal/mol)
Positive average value: 0.03441315 a.u. (21.59460 kcal/mol)
Negative average value: -0.01403587 a.u. (-8.80765 kcal/mol)
Overall variance (sigma^2_tot): 0.00076060 a.u.^2 (299.49903 (kcal/mol)^2)
Positive variance: 0.00068736 a.u.^2 (270.66029 (kcal/mol)^2)
Negative variance: 0.00007324 a.u.^2 (28.83873 (kcal/mol)^2)
Balance of charges (miu): 0.08701816
Product of sigma^2_tot and miu: 0.00006619 a.u.^2 (26.06186 (kcal/mol)^2)
Internal charge separation (Pi): 0.02566361 a.u. (16.10417 kcal/mol)

Summary of natural population analysis of **A-E**.

Table S1 Summary of Natural Population Analysis of Compound **A**.

Atom	No.	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
C	1	0.03844	1.99853	3.93489	0.02815	5.96156
C	2	0.29824	1.99878	3.66858	0.0344	5.70176
N	3	-0.20285	1.99932	5.16593	0.0376	7.20285
N	4	-0.00205	1.9992	4.97725	0.0256	7.00205
C	5	0.14488	1.99883	3.83279	0.02349	5.85512
C	6	0.15709	1.99894	3.82214	0.02183	5.84291
N	7	-0.04202	1.99913	5.01054	0.03234	7.04202
N	8	-0.19494	1.99929	5.15895	0.03669	7.19494
C	9	0.30618	1.99878	3.66193	0.03311	5.69382
C	10	0.04704	1.9985	3.92642	0.02803	5.95296
N	11	-0.03583	1.99942	4.99864	0.03777	7.03583
N	12	0.44867	1.99942	4.50966	0.04224	6.55133
O	13	-0.30751	1.99979	6.28487	0.02285	8.30751
N	14	0.48666	1.99943	4.45845	0.05547	6.51334
O	15	-0.33272	1.9998	6.31108	0.02184	8.33272
O	16	-0.30991	1.99979	6.28848	0.02164	8.30991
N	17	0.50622	1.9994	4.4417	0.05267	6.49378
O	18	-0.35162	1.9998	6.32807	0.02376	8.35162
O	19	-0.31271	1.99979	6.29192	0.02099	8.31271
N	20	0.50409	1.9994	4.44427	0.05224	6.49591
O	21	-0.31787	1.99979	6.29714	0.02094	8.31787
O	22	-0.36784	1.9998	6.34387	0.02417	8.36784
N	23	0.48726	1.99943	4.45764	0.05568	6.51274
O	24	-0.31447	1.99979	6.29293	0.02176	8.31447
O	25	-0.33242	1.9998	6.31079	0.02183	8.33242
Total	--	0	49.98395	127.21894	0.79710	178.00000

Table S2 Summary of Natural Population Analysis of Compound **B**.

Atom	No.	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
C	1	0.28245	1.99871	3.68756	0.03128	5.71755
N	2	-0.38239	1.99925	5.34418	0.03896	7.38239
C	3	0.50248	1.99898	3.46477	0.03377	5.49752
N	4	-0.20611	1.9991	5.18556	0.02145	7.20611
C	5	0.11291	1.99895	3.86682	0.02133	5.88709
C	6	0.14506	1.99879	3.83179	0.02436	5.85494
N	7	-0.25574	1.99905	5.22747	0.02921	7.25574
C	8	0.51418	1.99893	3.45169	0.03519	5.48582
N	9	-0.37411	1.99924	5.33702	0.03785	7.37411
C	10	0.27497	1.99869	3.69572	0.03063	5.72503
N	11	-0.02563	1.99941	4.98983	0.03638	7.02563
N	12	0.45913	1.99942	4.49982	0.04163	6.54087
O	13	-0.32551	1.99979	6.30225	0.02347	8.32551
N	14	0.48966	1.99941	4.45812	0.05281	6.51034
O	15	-0.36947	1.9998	6.34607	0.0236	8.36947
O	16	-0.31006	1.99979	6.28957	0.0207	8.31006
N	17	0.48938	1.99941	4.45828	0.05292	6.51062
O	18	-0.30994	1.99979	6.28927	0.02088	8.30994
O	19	-0.37635	1.9998	6.35287	0.02368	8.37635
N	20	0.47744	1.99943	4.46742	0.05572	6.52256
O	21	-0.32654	1.9998	6.30488	0.02187	8.32654
O	22	-0.30204	1.99979	6.28025	0.02201	8.30204
N	23	0.47074	1.99943	4.47457	0.05526	6.52926
O	24	-0.34369	1.9998	6.32176	0.02212	8.34369
O	25	-0.31082	1.99979	6.28859	0.02244	8.31082
Total	--	0	49.98436	127.21613	0.79951	178.00000

Table S3 Summary of Natural Population Analysis of Compound **C**.

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
C	1	0.24662	1.99874	3.72358	0.03106	5.75338
N	2	-0.18982	1.9994	5.14684	0.04358	7.18982
N	3	-0.00817	1.99955	4.96773	0.04089	7.00817
N	4	-0.02386	1.9992	5	0.02466	7.02386
C	5	0.09983	1.99894	3.88048	0.02075	5.90017
C	6	0.14005	1.99879	3.8365	0.02466	5.85995
N	7	-0.06589	1.99914	5.03393	0.03283	7.06589
N	8	0.00147	1.99953	4.95957	0.03942	6.99853
N	9	-0.17363	1.99941	5.1329	0.04131	7.17363
C	10	0.2432	1.99874	3.72744	0.03063	5.7568

N	11	-0.03352	1.99941	4.99636	0.03775	7.03352
N	12	0.45146	1.99942	4.5073	0.04182	6.54854
O	13	-0.30624	1.99979	6.28343	0.02302	8.30624
N	14	0.48942	1.99942	4.45847	0.05269	6.51058
O	15	-0.35975	1.9998	6.33651	0.02344	8.35975
O	16	-0.31203	1.99979	6.29147	0.02077	8.31203
N	17	0.48809	1.99942	4.45981	0.05268	6.51191
O	18	-0.37328	1.9998	6.34979	0.02369	8.37328
O	19	-0.31393	1.99979	6.29319	0.02095	8.31393
Total	--	0	37.98811	95.38529	0.62660	133.99999

Table S4 Summary of Natural Population Analysis of Compound **D**.

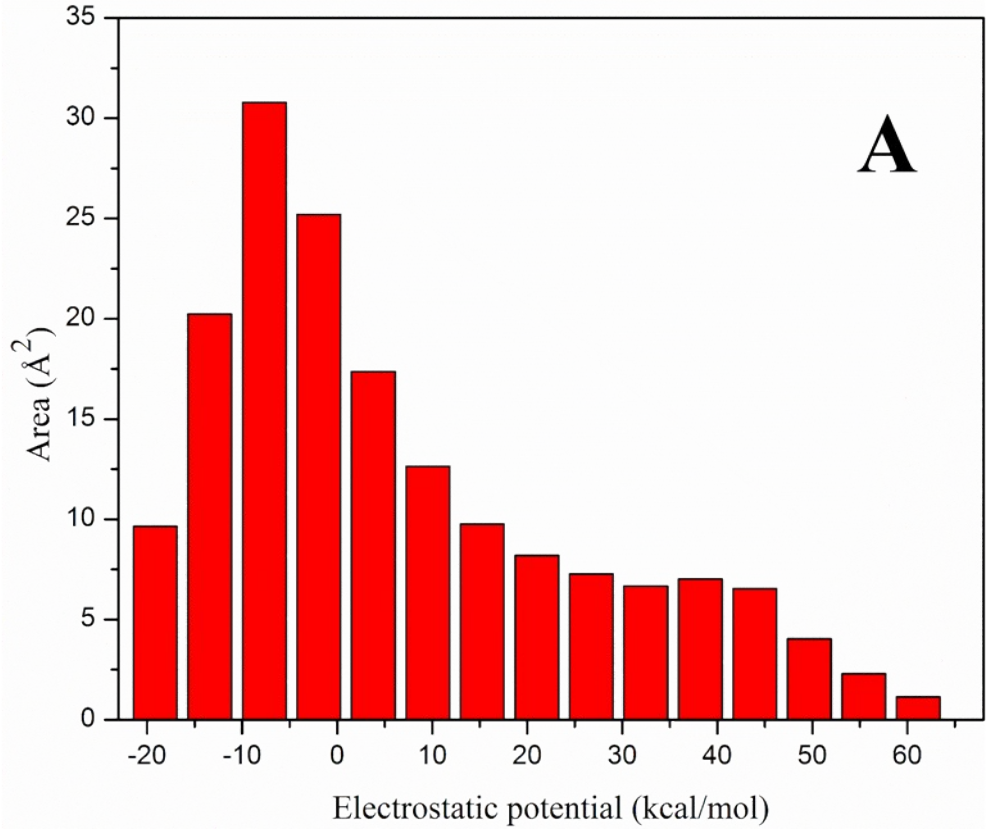
Atom	No.	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
N	1	-0.40933	1.9993	5.37248	0.03755	7.40933
C	2	0.45835	1.99908	3.50529	0.03729	5.54165
N	3	-0.21354	1.99934	5.17603	0.03818	7.21354
N	4	-0.02407	1.99921	4.99853	0.02633	7.02407
C	5	0.31421	1.9991	3.66076	0.02593	5.68579
C	6	0.36744	1.99884	3.60181	0.03192	5.63256
N	7	-0.06832	1.99915	5.03463	0.03454	7.06832
N	8	-0.2087	1.9993	5.17199	0.0374	7.2087
C	9	0.47063	1.99907	3.49442	0.03589	5.52937
N	10	-0.41328	1.9993	5.3746	0.03937	7.41328
N	11	-0.04001	1.99942	5.00282	0.03777	7.04001
N	12	0.44692	1.99943	4.51154	0.04211	6.55308
O	13	-0.31165	1.99979	6.28895	0.02291	8.31165
N	14	0.47294	1.99944	4.47254	0.05508	6.52706
O	15	-0.3218	1.99979	6.29977	0.02223	8.3218
O	16	-0.32883	1.9998	6.30708	0.02196	8.32883
N	17	0.47248	1.99944	4.47309	0.05499	6.52752
O	18	-0.33522	1.9998	6.31329	0.02214	8.33522
O	19	-0.3282	1.99979	6.30611	0.02229	8.3282
Total	--	0	37.98839	95.36573	0.64588	134.00000

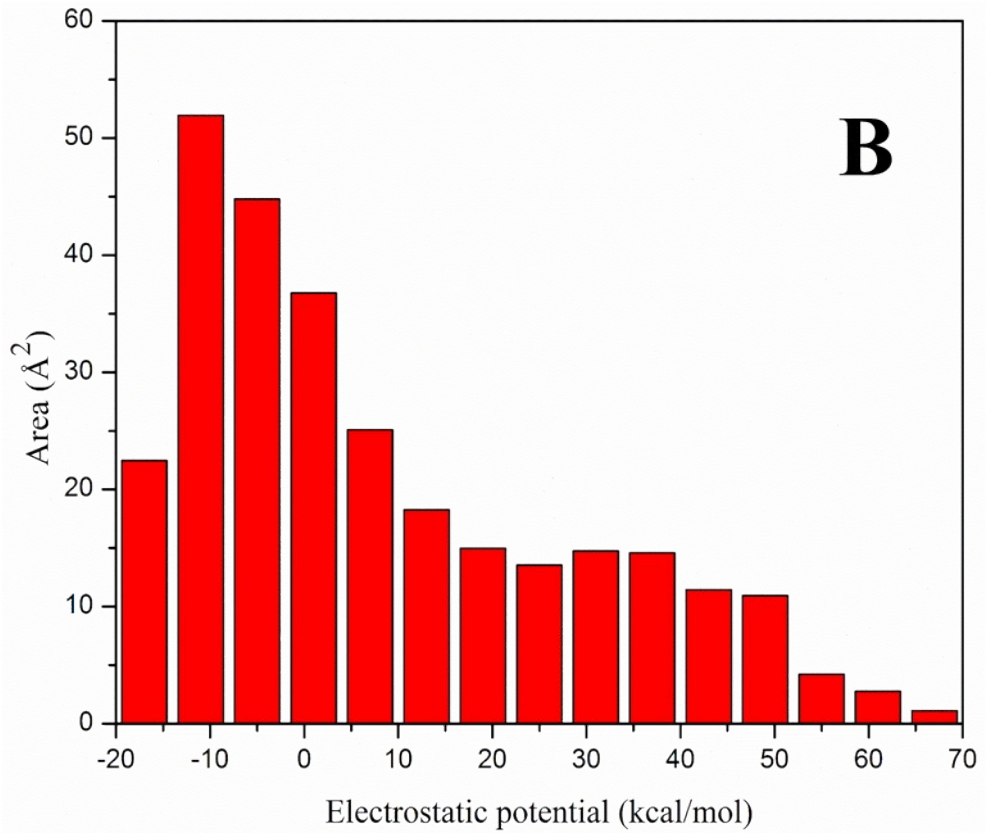
Table S5 Summary of Natural Population Analysis of Compound **E**.

Atom	No.	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
N	1	-0.24324	1.99938	5.20338	0.04048	7.24324
N	2	-0.02998	1.99963	4.98181	0.04853	7.02998
N	3	-0.02525	1.99954	4.98368	0.04204	7.02525
N	4	-0.05047	1.99918	5.02526	0.02603	7.05047

C	5	0.28917	1.99909	3.68405	0.02769	5.71083
C	6	0.32211	1.9991	3.64947	0.02932	5.67789
N	7	-0.08171	1.99912	5.05788	0.02471	7.08171
N	8	-0.01435	1.99952	4.97207	0.04276	7.01435
N	9	-0.01277	1.99963	4.96538	0.04776	7.01277
N	10	-0.24403	1.99937	5.20457	0.04009	7.24403
N	11	-0.03935	1.99942	5.00165	0.03828	7.03935
N	12	0.44751	1.99943	4.50979	0.04327	6.55249
O	13	-0.31763	1.99979	6.29425	0.02359	8.31763
Total	--	0	25.99222	63.53323	0.47455	90.00000

The surface areas in each ESP range.




B
Area (Å^2)
Electrostatic potential (kcal/mol)
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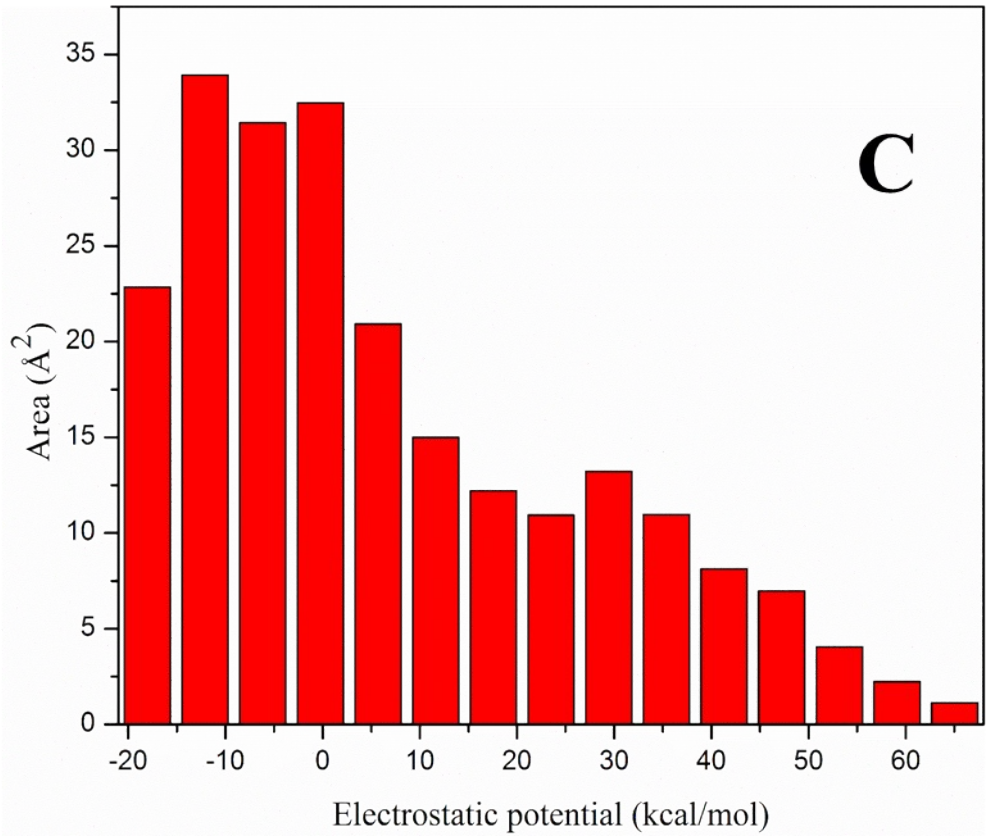
10
20
30
40
50
60
-20
-10
0
10
20
30
40
50
60
70


C
Area (Å^2)
Electrostatic potential (kcal/mol)
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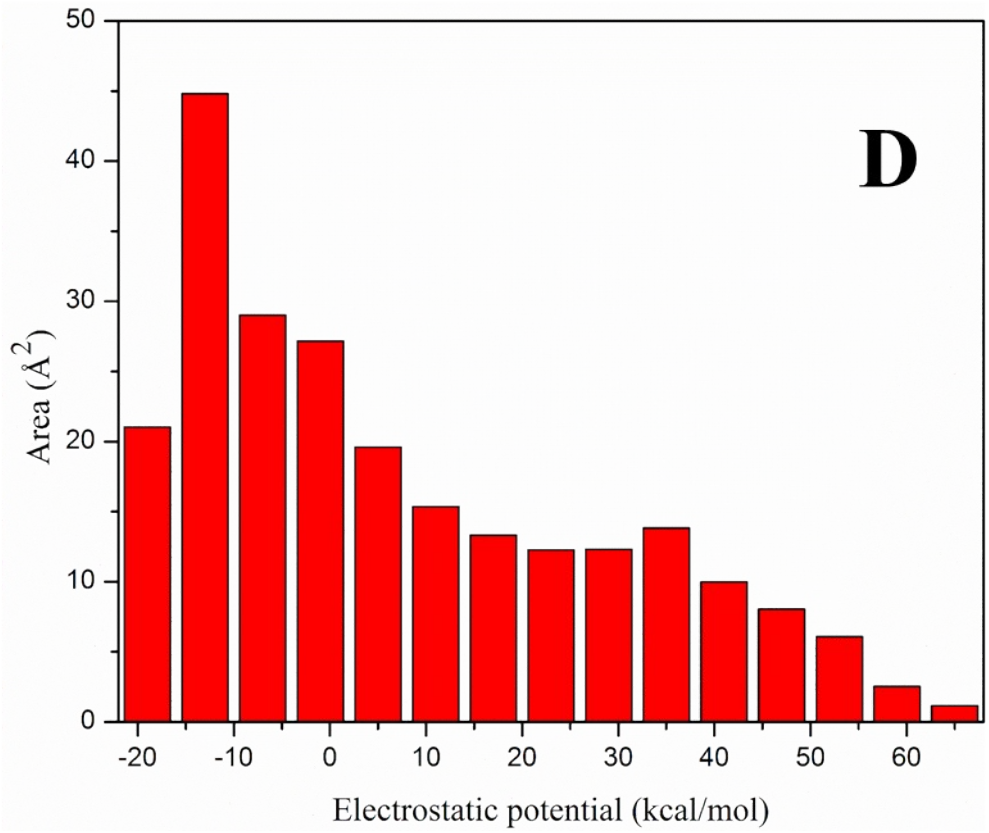
5
10
15
20
25
30
35
-20
-10
0
10
20
30
40
50
60


D
Area (Å^2)
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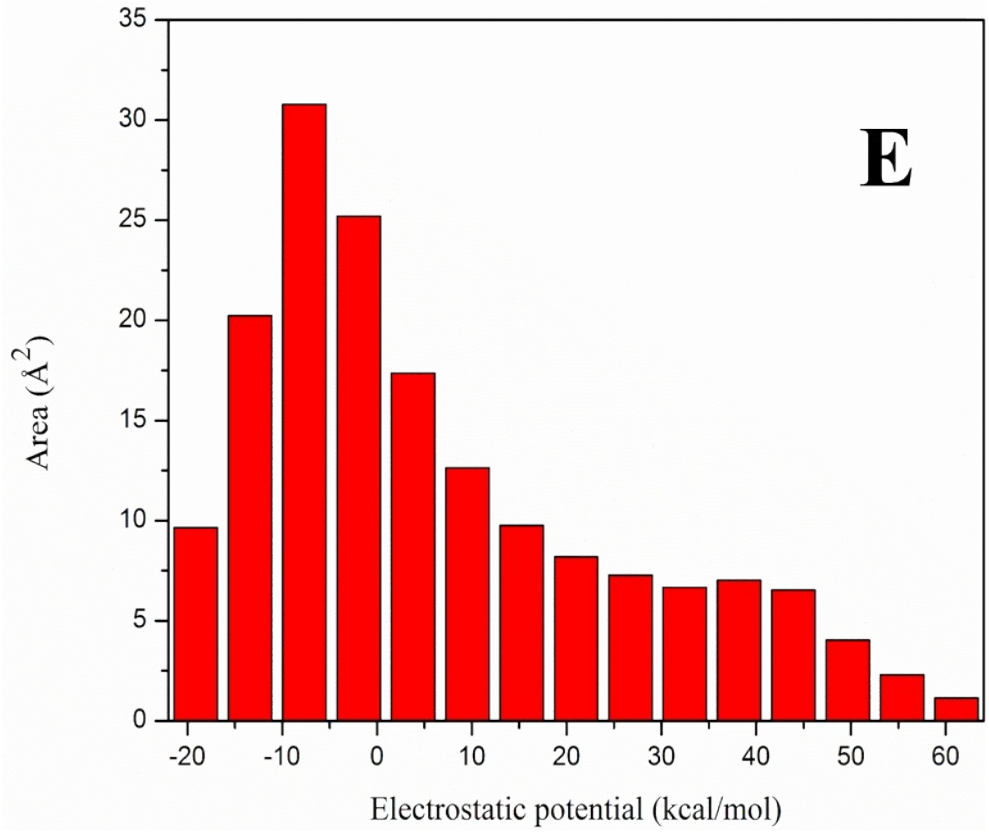
10
20
30
40
50
-20
-10
0
10
20
30
40
50
60
Electrostatic potential (kcal/mol)


E
Area (Å^2)
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5
10
15
20
25
30
35
-20
-10
0
10
20
30
40
50
60
Electrostatic potential (kcal/mol)