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All enquiries and manuscripts should be directed to:

Dr Alison Green  
*Australian Journal of Chemistry –  
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CSIRO PUBLISHING  
PO Box 1139 (150 Oxford St)  
Collingwood, Vic. 3066, Australia

Telephone: +61 3 9662 7630  
Fax: +61 3 9662 7611  
E-mail: [publishing.ajc@csiro.au](mailto:publishing.ajc@csiro.au)

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## Accessory Material

**Table S1: Total energies (in atomic units), heats of formation (in kcal/mol) and zero point vibrational energies (in kcal/mol) for the calculated compounds.**

Theory	<b>1</b>	<b>3a</b>	<b>3b</b>	<b>TS1</b>	<b>TS2</b>
Total energies					
HF/STO-3G	-1011.40106	-879.94057	-879.93715	-879.91939	-879.92589
HF/6-31G*	-1024.34498	-891.27107	-891.26195	-891.24275	-891.23898
B3LYP/6-31G*	-1030.67673	-896.72389	-896.71599	-896.69159	-896.68873
Heats of formation					
AM1	-49.98	-47.19	-44.22	-35.68	-38.24
Zero point vibrational energies					
B3LYP/6-31G*	244.78	198.66	198.37	197.51	197.19

**Table S2. Names of compounds 1-6 according to IUPAC.**

Compound	IUPAC names
<b>1</b>	<i>N</i> -(2-{bis[2-(acryloylamino)ethyl]amino}ethyl)acrylamide
<b>2</b>	<i>N</i> -(2-{bis[2-(methacryloylamino)ethyl]amino}ethyl)-2-methylacrylamide
<b>3</b>	<i>N</i> -(2-{acryloyl[2-(acryloylamino)ethyl]amino}ethyl)acrylamide
<b>4</b>	<i>N,N</i> -bis[2-(methacryloylamino)ethyl]-2-methylacrylamide
<b>5</b>	<i>N</i> -{2-[acryloyl(2-{acryloyl[2-(acryloylamino)ethyl]amino}ethyl)amino]ethyl}acrylamide
<b>6</b>	<i>N</i> -[2-(methacryloylamino)ethyl]- <i>N</i> -(2-{methacryloyl[2-(methacryloylamino)ethyl]amino}ethyl)-2-methylacrylamide

B3LYP/6-31G\*-calculated cartesian coordinates of compounds **1**, **3a**, **3b**, **TS1**, and **TS2**.

**1**

6	0	-4.967739	0.240755	-2.505896
6	0	-3.525630	0.553928	-2.259954
7	0	-2.628141	-0.450266	-2.509167
6	0	-1.205907	-0.264198	-2.252480
6	0	-0.835503	-0.464019	-0.772379
7	0	0.556825	-0.091359	-0.513067
6	0	1.236164	-0.960326	0.447408
6	0	1.759487	-2.228641	-0.252595
7	0	2.183898	-3.260122	0.682582
6	0	1.295496	-4.172701	1.178108
6	0	1.823991	-5.158482	2.171336
8	0	-3.182380	1.671883	-1.878292
6	0	-5.435949	-0.667598	-3.365761
8	0	0.113829	-4.199661	0.835276
6	0	2.824810	-4.945511	3.029608
6	0	0.784702	1.337873	-0.318173
6	0	0.232244	1.939979	0.995456
7	0	0.610476	3.338657	1.145577
6	0	1.827573	3.695911	1.652433
6	0	2.122145	5.160807	1.729579
8	0	2.655885	2.867986	2.030461
6	0	1.640962	6.101726	0.912954
1	0	-5.645366	0.889465	-1.956815
1	0	-2.981392	-1.393725	-2.584590
1	0	-0.954564	0.750635	-2.567377
1	0	-0.638672	-0.960080	-2.878666
1	0	-0.969539	-1.518114	-0.505373
1	0	-1.548120	0.108202	-0.158035
1	0	0.583363	-1.265620	1.281276
1	0	2.077116	-0.411896	0.886352
1	0	2.596379	-1.975182	-0.910289
1	0	0.966261	-2.658050	-0.870062
1	0	3.158583	-3.337574	0.930836
1	0	1.252516	-6.082649	2.201261
1	0	-6.502714	-0.806068	-3.517713
1	0	-4.780163	-1.288350	-3.971815
1	0	3.116807	-5.698222	3.756419
1	0	3.373077	-4.006803	3.067549
1	0	0.351419	1.884246	-1.163953
1	0	1.864603	1.519819	-0.339547
1	0	0.633340	1.391312	1.852959
1	0	-0.858994	1.880577	1.027175
1	0	-0.068522	4.056625	0.942281
1	0	2.857822	5.407954	2.490719
1	0	1.943809	7.140845	1.006161
1	0	0.951804	5.875603	0.102339

**3a**

6	0	-4.422227	-1.970377	-1.018620
6	0	-5.726693	-1.754855	-0.842823
6	0	-3.416677	-0.944318	-0.609136
8	0	-3.727416	0.131870	-0.096884
7	0	-2.114687	-1.286750	-0.846202
6	0	-1.021604	-0.373651	-0.547738
6	0	-0.746047	-0.281162	0.967011
7	0	0.266578	0.718029	1.296731
6	0	0.007540	2.013936	1.692369
6	0	-1.417357	2.472634	1.723549
6	0	-1.716246	3.649583	2.279624
6	0	1.671192	0.337795	1.153004
6	0	2.339955	0.975388	-0.085306
7	0	3.535138	0.253717	-0.496714
6	0	3.450516	-0.921934	-1.186785
8	0	2.367685	-1.429703	-1.487307
6	0	4.763000	-1.535045	-1.550621
6	0	4.817529	-2.679034	-2.234208
8	0	0.936509	2.767718	1.992982
1	0	-4.061495	-2.895880	-1.465651
1	0	-6.474794	-2.485263	-1.135651
1	0	-6.066027	-0.824678	-0.396079
1	0	-1.904993	-2.174576	-1.278866
1	0	-1.285248	0.622447	-0.920099
1	0	-0.127289	-0.719295	-1.074092
1	0	-0.401731	-1.254215	1.336129
1	0	-1.675397	-0.056076	1.488121
1	0	-2.195564	1.870734	1.263364
1	0	-2.735772	4.023134	2.302320
1	0	-0.936254	4.262953	2.721283
1	0	1.711151	-0.748245	1.049256
1	0	2.216620	0.628605	2.055824
1	0	2.603697	2.012395	0.127212
1	0	1.635605	0.965353	-0.921749
1	0	4.443350	0.621466	-0.253108
1	0	5.673264	-1.021262	-1.244275
1	0	5.761257	-3.139309	-2.510507
1	0	3.898898	-3.176092	-2.532383

**3b**

6	0	-4.417132	-2.552534	0.217932
6	0	-5.716484	-2.531457	-0.003837
6	0	-3.551149	-1.411305	-0.211667
8	0	-3.988386	-0.445355	-0.777636
7	0	-2.239155	-1.554781	0.086771
6	0	-1.233951	-0.576326	-0.275369
6	0	-1.098183	0.514130	0.791147
7	0	0.007046	1.433625	0.531808
6	0	-0.281943	2.732489	0.225804
6	0	0.860946	3.694620	0.082574
6	0	0.632549	4.921124	-0.347742
6	0	1.352554	0.911555	0.711883
6	0	2.093340	0.648235	-0.604687
7	0	3.340747	-0.057289	-0.386559
6	0	3.375373	-1.391745	-0.170588
8	0	2.372396	-2.055251	-0.088293
6	0	4.742161	-1.976546	-0.037208
6	0	4.904533	-3.268661	0.169733
8	0	-1.410344	3.118736	0.073132
1	0	-3.952429	-3.388903	0.712518
1	0	-6.353859	-3.342730	0.297924
1	0	-6.170739	-1.692527	-0.497068
1	0	-1.938130	-2.386207	0.539532
1	0	-1.508075	-0.127265	-1.219544
1	0	-0.300714	-1.108805	-0.403944
1	0	-0.938256	0.049069	1.760002
1	0	-2.008977	1.085302	0.834049
1	0	1.858003	3.394451	0.337976
1	0	1.429826	5.634791	-0.452763
1	0	-0.360963	5.237383	-0.602743
1	0	1.263497	-0.028365	1.235398
1	0	1.945212	1.559355	1.347258
1	0	2.320153	1.576285	-1.113125
1	0	1.468690	0.063659	-1.263828
1	0	4.196293	0.438976	-0.477200
1	0	5.588860	-1.316010	-0.116064
1	0	5.881702	-3.705480	0.265765
1	0	4.054433	-3.920377	0.246244

# TS1

6	0	-4.155081	-2.762046	0.338289
6	0	-5.465021	-2.783693	0.089029
6	0	-3.291832	-1.668309	-0.205880
8	0	-3.727027	-0.755476	-0.904928
7	0	-1.969326	-1.764421	0.130507
6	0	-0.981878	-0.796040	-0.324246
6	0	-1.031448	0.499780	0.501702
7	0	-0.034635	1.479246	0.026186
6	0	-0.368700	2.815134	0.483564
6	0	-0.594717	3.794575	-0.613277
6	0	-0.887472	5.074095	-0.356050
6	0	1.358360	1.108011	0.349227
6	0	2.125512	0.681180	-0.915717
7	0	3.404058	0.052758	-0.610737
6	0	3.476167	-1.249416	-0.199056
8	0	2.476140	-1.960517	-0.092104
6	0	4.856030	-1.739695	0.095970
6	0	5.062949	-2.992873	0.503008
8	0	-0.459579	3.102621	1.662262
1	0	-3.686482	-3.538561	0.941890
1	0	-6.111319	-3.567636	0.472191
1	0	-5.912415	-1.999812	-0.515503
1	0	-1.664123	-2.522072	0.723986
1	0	-1.189674	-0.554570	-1.370937
1	0	0.002052	-1.270157	-0.263030
1	0	-0.896760	0.271761	1.571721
1	0	-2.027297	0.935293	0.378233
1	0	-0.516486	3.412398	-1.626431
1	0	-1.058531	5.794219	-1.150910
1	0	-0.964787	5.423449	0.670046
1	0	1.375112	0.280698	1.069117
1	0	1.873255	1.947876	0.830735
1	0	2.307686	1.545144	-1.562359
1	0	1.524506	-0.033806	-1.481442
1	0	4.244826	0.611878	-0.621787
1	0	5.687312	-1.047584	-0.032311
1	0	6.057576	-3.369806	0.720717
1	0	4.221397	-3.669036	0.623153

## TS2

6	0	4.620117	-2.530009	-0.107773
6	0	5.937003	-2.372234	-0.248084
6	0	3.735625	-1.355171	0.165388
8	0	4.160612	-0.207914	0.279879
7	0	2.406095	-1.659291	0.291166
6	0	1.398487	-0.635725	0.534373
6	0	0.991651	0.069054	-0.783432
7	0	-0.000075	1.145659	-0.721875
6	0	0.376794	2.301321	0.052806
6	0	0.643831	3.521430	-0.756523
6	0	1.033333	4.666721	-0.185335
6	0	-1.421369	0.807515	-0.651293
6	0	-1.970247	0.278822	0.696629
7	0	-3.411588	0.078654	0.644604
6	0	-3.962125	-1.052930	0.104784
8	0	-3.271879	-1.968461	-0.339740
6	0	-5.456535	-1.085988	0.112708
6	0	-6.117585	-2.131561	-0.385952
8	0	0.462151	2.286894	1.269778
1	0	4.162295	-3.515510	-0.186097
1	0	6.599670	-3.209845	-0.443878
1	0	6.373813	-1.381198	-0.163871
1	0	2.100853	-2.605577	0.113149
1	0	1.815628	0.094182	1.230378
1	0	0.541507	-1.113873	1.015462
1	0	0.605264	-0.676190	-1.489801
1	0	1.910163	0.479742	-1.219463
1	0	0.519227	3.427375	-1.831171
1	0	1.240066	5.558042	-0.770506
1	0	1.159441	4.726899	0.892227
1	0	-1.624139	0.055982	-1.422252
1	0	-1.992281	1.706277	-0.924937
1	0	-1.735050	0.974244	1.505847
1	0	-1.519381	-0.687172	0.932608
1	0	-4.019810	0.823885	0.952156
1	0	-5.990042	-0.235886	0.536406
1	0	-7.202357	-2.178289	-0.389676
1	0	-5.566831	-2.969862	-0.802966