

Appendix A. Conformer selections following Monte Carlo conformational searches.

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C18CA_FE-inc1-inc1.18	61.385590	12.922688	3.791883
C18CA_FE-inc1-inc1.96	68.141037	19.678135	12.817302
C18CA_FE-inc1-inc1.10	59.154327	10.691425	4.109928
C18CA_FE-inc1-inc1.12	60.339859	11.876957	12.594965
C18CA_FE-inc1-inc1.1	48.462902	0.000000	21.726732

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C17CA_FE-inc1-inc1.77	61.617668	18.418526	4.041106
C17CA_FE-inc1-inc1.13	56.402649	13.203506	12.276863
C17CA_FE-inc1-inc1.16	56.701920	13.502777	4.418154
C17CA_FE-inc1-inc1.13	56.402649	13.203506	12.276863
C17CA_FE-inc1-inc1.1	43.199142	0.000000	20.433343

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C16CA_FE-inc1-inc1.239	56.640484	18.699955	4.005531
C16CA_FE-inc1-inc1.287	57.908058	19.967529	11.547385
C16CA_FE-inc1-inc1.52	51.204887	13.264359	4.515499
C16CA_FE-inc1-inc1.17	48.473640	10.533112	11.699133
C16CA_FE-inc1-inc1.1	37.940529	0.000000	19.173940

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C15CA_FE-inc1-inc1.94	45.783642	13.107246	4.088370
C15CA_FE-inc1-inc1.82	45.521961	12.845566	11.004207
C15CA_FE-inc1-inc1.59	43.957329	11.280933	4.567132
C15CA_FE-inc1-inc1.30	42.720318	10.043922	11.347583
C15CA_FE-inc1-inc1.1	32.676395	0.000000	17.878536

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C14CA_FE-inc1-inc1.135	41.605419	14.190153	3.915356
C14CA_FE-inc1-inc1.187	43.647118	16.231852	10.235517
C14CA_FE-inc1-inc1.264	45.433235	18.017969	4.553685
C14CA_FE-inc1-inc1.24	36.875458	9.460192	10.868405
C14CA_FE-inc1-inc1.1	27.415266	0.000000	16.621514

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C13CA_FE-inc1-inc1.47	32.922699	10.774492	3.860612
C13CA_FE-inc1-inc1.153	36.088593	13.940386	9.604895
C13CA_FE-inc1-inc1.67	34.087070	11.938864	4.831830
C13CA_FE-inc1-inc1.18	31.611588	9.463381	9.545906
C13CA_FE-inc1-inc1.1	22.148207	0.000000	15.323190

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C12CA_FE-inc1-inc1.210	30.767138	13.878328	4.595286
C12CA_FE-inc1-inc1.201	30.689775	13.800966	9.330433
C12CA_FE-inc1-inc1.199	30.674608	13.785799	5.350479
C12CA_FE-inc1-inc1.50	26.417366	9.528557	9.245615
C12CA_FE-inc1-inc1.1	16.888809	0.000000	14.070548

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C11CA_FE-inc1-inc1.446	31.389591	19.767228	4.050905
C11CA_FE-inc1-inc1.195	25.264616	13.642253	8.424172
C11CA_FE-inc1-inc1.179	25.064587	13.442224	4.867937
C11CA_FE-inc1-inc1.48	21.183584	9.561221	8.008226
C11CA_FE-inc1-inc1.1	11.622363	0.000000	12.767711

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C10CA_FE-inc1-inc1.443	26.005056	19.643106	4.738711
C10CA_FE-inc1-inc1.362	23.659359	17.297409	8.131298
C10CA_FE-inc1-inc1.128	17.631256	11.269306	5.509898
C10CA_FE-inc1-inc1.18	13.236777	6.874827	8.986162
C10CA_FE-inc1-inc1.1	6.361950	0.000000	11.520947

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C9CA_FE-inc1-inc1.333	20.204557	19.112936	5.128271
C9CA_FE-inc1-inc1.311	19.342356	18.250734	7.677091
C9CA_FE-inc1-inc1.144	13.124329	12.032707	5.514358
C9CA_FE-inc1-inc1.18	7.551607	6.459985	8.392681
C9CA_FE-inc1-inc1.1	1.091622	0.000000	10.213431

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C8CA_FE-inc1-inc1.143	12.163141	16.336082	4.193288
C8CA_FE-inc1-inc1.198	15.229316	19.402256	6.582517
C8CA_FE-inc1-inc1.95	7.835938	12.008879	4.616630
C8CA_FE-inc1-inc1.17	2.311484	6.484425	7.267840
C8CA_FE-inc1-inc1.1	-4.172941	0.000000	8.973913

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C7CA_FE-inc1-inc1.97	10.534484	19.982953	4.203662
C7CA_FE-inc1-inc1.89	8.954543	18.403012	5.939034
C7CA_FE-inc1-inc1.40	0.405733	9.854202	4.979403
C7CA_FE-inc1-inc1.4	-5.826824	3.621645	6.927662
C7CA_FE-inc1-inc1.1	-9.448469	0.000000	7.658304

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C6CA_FE-inc1-inc1.35	2.157592	16.889454	3.708791
C6CA_FE-inc1-inc1.14	-7.763542	6.968320	4.998194
C6CA_FE-inc1-inc1.23	-4.203210	10.528652	4.707257
C6CA_FE-inc1-inc1.3	-11.306248	3.425614	5.567871
C6CA_FE-inc1-inc1.1	-14.731862	0.000000	6.433898

Conformer ID	PE/KJ(mol)-1	Relative PE/KJ(mol)-1	carbonylC-terminalC/Å
C5CA_FE-inc1-inc1.13	-8.536533	11.473686	3.213911
C5CA_FE-inc1-inc1.10	-13.126068	6.884151	3.810262
C5CA_FE-inc1-inc1.10	-13.126068	6.884151	3.810262
C5CA_FE-inc1-inc1.7	-15.568323	4.441896	4.509233
C5CA_FE-inc1-inc1.1	-20.01022	0.000000	5.103157