Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Computational development of a phase-sensitive membrane raft probe

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Molecular dynamics simulations – equilibration procedure

Equilibration was performed over six steps as described in section 2.2 of the main text. Restraints were applied with the following force constants (in kcal mol^{-1} $Å^{-2}$) to help keep water molecules from the hydrophobic core.

Selection	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6
Carbon atoms (DPH derivative)	10.0	5.0	2.5	1.0	0.5	0.1
Water	2.5	2.5	1.0	0.5	0.1	0.0
Lipid tails	2.5	2.5	1.0	0.5	0.1	0.0
Lipid heads	2.5	2.5	1.0	0.5	0.1	0.0
Ions	10	0.0	0.0	0.0	0.0	0.0

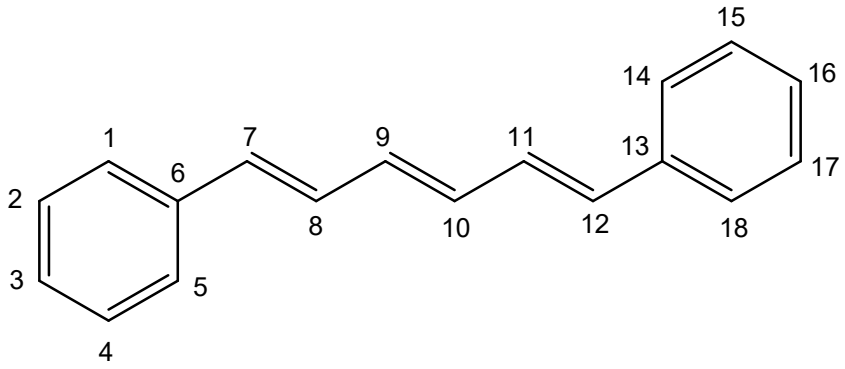

Figure S1. Atom numbering scheme used to identify dihedral angles for 1,6-diphenylhexatriene and derivatives.

	Dihedral angle / °		
	C9-C10-C11-C12	C1-C6-C7-C8	C6-C7-C8-C9
S_0	0.4	37.0	1.4
S_1	0.8	16.1	6.7
MECI	3.3	2.4	42.0
AIMD (S_1)	3.6 ± 2.6	17 ± 6	6.8 ± 4.4
QM/MM (S_1)	31.6 ± 12.3	33.5 ± 10.6	18.1 ± 8.4

Table S1. Selected geometrical parameters for 1,3-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °		
	C8-C9-C10-C11	C1-C6-C7-C8	C6-C7-C8-C9
S_0	0.3	33.0	0.7
S_1	1.2	16.7	0.5
MECI	11.0	48.2	44.0
AIMD (S_1)	5.5 ± 3.9	15.5 ± 5.7	5.2 ± 4.1
QM/MM (S_1)	22.9 ± 10.8	34.1 ± 21.8	22.4 ± 9.5

Table S2. Selected geometrical parameters for 1,4-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °			
	C7-C8-C9-C10	C1-C6-C7-C8	C11-C12-C13-C14	C10-C11-C12-C13
S_0	1.3	31.4	39.6	1.9
S_1	1.9	17.1	15.2	6.2
MECI	1.8	28.8	48.0	36.6
AIMD (S_1)	4.4 ± 3.1	15.5 ± 6	13.6 ± 7.7	5.8 ± 3.9
QM/MM (S_1)	28.7 ± 10.8	46.1 ± 12.1	40.6 ± 13.4	6.8 ± 4.7

Table S3. Selected geometrical parameters for 1,5-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °		
	C8-C9-C10-C11	C6-C7-C8-C9	C1-C6-C7-C8
S_0	1.4	2.6	40.5
S_1	3.8	12.6	18.9
MECI	3.8	37.0	39.8
AIMD (S_1)	7.3 ± 4.8	7.8 ± 5.7	19.2 ± 10.2
QM/MM (S_1)	11.9 ± 9.4	12.2 ± 8.7	52.3 ± 16.6

Table S4. Selected geometrical parameters for 2,3-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °		
	C11-C12-C13-C14	C1-C6-C7-C8	C6-C7-C8-C9
S_0	6.4	33.5	0.7
S_1	0.9	12.3	5.8
MECI	13.0	4.9	45.1
AIMD (S_1)	4 ± 3.3	15.2 ± 4.8	6 ± 3.4
QM/MM (S_1)	28.2 ± 11	61.3 ± 13.8	8.6 ± 5.4

Table S5. Selected geometrical parameters for 2,4-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °			
	C11-C12-C13-C14	C1-C6-C7-C8	C6-C7-C8-C9	C10-C11-C12-C13
S_0	35.5	38.3	2.3	2.3
S_1	12.9	14.9	7.7	7.7
MECI	31.4	46.3	36.2	4.5
AIMD (S_1)	14.4 ± 8.4	15 ± 8.5	9.6 ± 7.1	10.1 ± 6.8
QM/MM (S_1)	30.9 ± 17.5	14.2 ± 8.5	12.5 ± 7.6	9.4 ± 6.5

Table S6. Selected geometrical parameters for 2,5-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °		
	C10-C11-C12-C13	C6-C7-C8-C9	C7-C8-C9-C10
S_0	0.2	0.2	0.1
S_1	0.2	0.2	0.6
MECI	4.6	85.9	61.5
AIMD (S_1)	4.4 ± 3.7	5 ± 3.6	6.9 ± 4.8
QM/MM (S_1)	13.6 ± 9.9	7.7 ± 5.9	23.9 ± 17.1

Table S7. Selected geometrical parameters for 3,4-dimethyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °		
	C14-C13-C12-C11	C1-C6-C7-C8	C8-C9-C10-C11
S_0	0.0	31.3	0.1
S_1	0.2	14.2	0.1
MECI	18.9	29.7	34.5
AIMD (S_1)	9.7 ± 6.9	12.3 ± 8.1	4.5 ± 3.4
QM/MM (S_1)	36.2 ± 26.9	26 ± 8.2	8.3 ± 5.7

Table S8. Selected geometrical parameters for 1-methyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °	
	C1-C6-C7-C8	C6-C7-C8-C9
S_0	38.2	2.1
S_1	14.5	6.5
MECI	47.4	36.9
AIMD (S_1)	30.0 ± 19.5	48.3 ± 27.0
QM/MM (S_1)	19.6 ± 10.2	8.8 ± 6.3

Table S9. Selected geometrical parameters for 2-methyl-1,6-diphenyl-1,3,5-hexatriene.

	Dihedral angle / °	
	C10-C11-C12-C13	C8-C9-C10-C11
S_0	0.0	0.0
S_1	0.1	1.0
MECI	8.7	38.0
AIMD (S_1)	4.9 ± 3.7	4.5 ± 3.2
QM/MM (S_1)	6.9 ± 5.1	27.9 ± 10.6

Table S10. Selected geometrical parameters for 3-methyl-1,6-diphenyl-1,3,5-hexatriene.

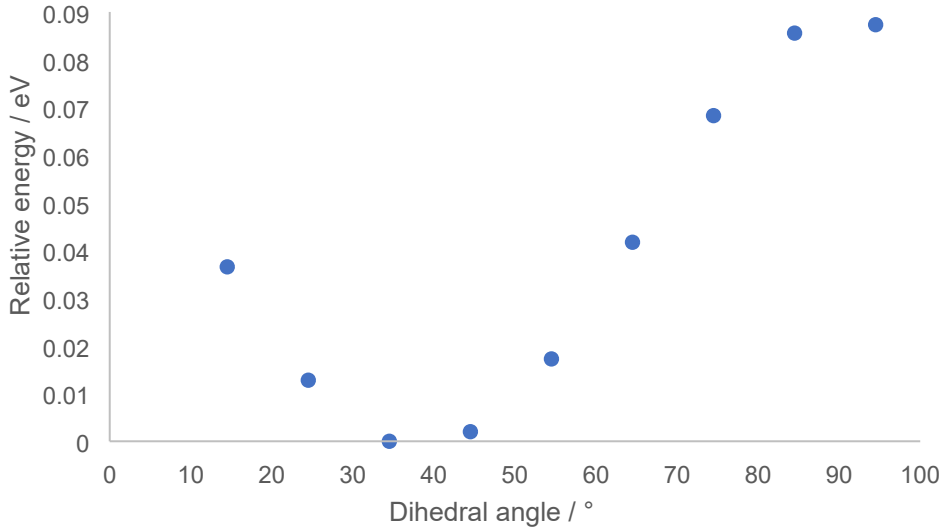

Figure S2. Potential energy scan of the S_0 state of **2Me** as a function of the C1-C6-C7-C8 dihedral angle (see Figure S1 for atom numbering) using BHHLYP/6-31G(d,p).

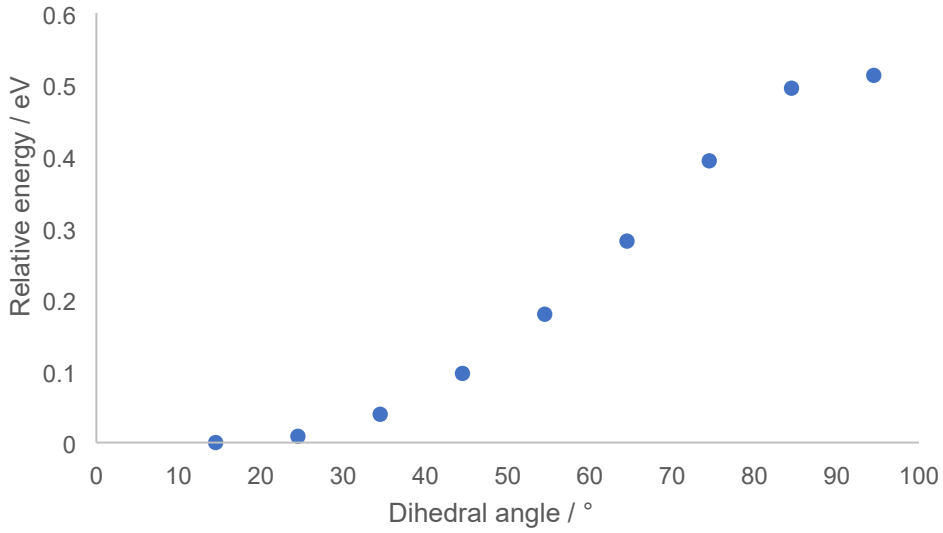

Figure S3. Potential energy scan of the S_1 state of **2Me** as a function of the C1-C6-C7-C8 dihedral angle (see Figure S1 for atom numbering) using BHHLYP/6-31G(d,p).

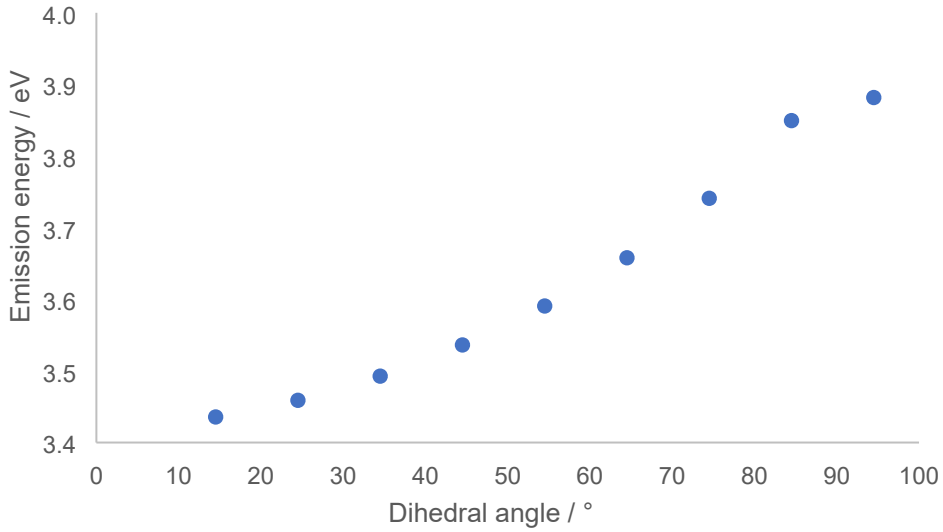

Figure S4. Calculated emission energy of **2Me** as a function of the C1-C6-C7-C8 dihedral angle (see Figure S1 for atom numbering) using BHHLYP/6-31G(d,p).

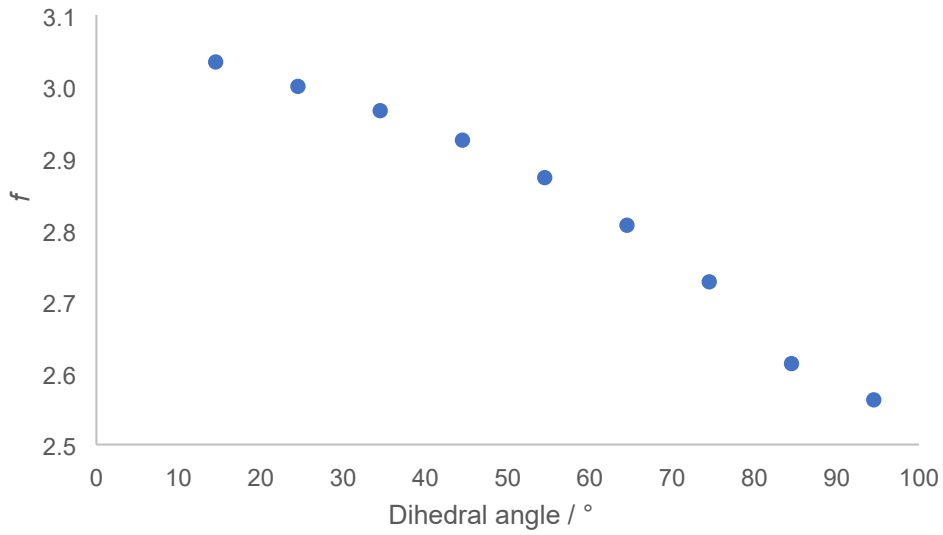

Figure S5. Oscillator strength (*f*) of **2Me** as a function of the C1-C6-C7-C8 dihedral angle (see Figure S1 for atom numbering) taken from the S_1 potential energy scan for the $S_1 \leftarrow S_0$ transition (which approximates emission) using BHHLYP/6-31G(d,p).

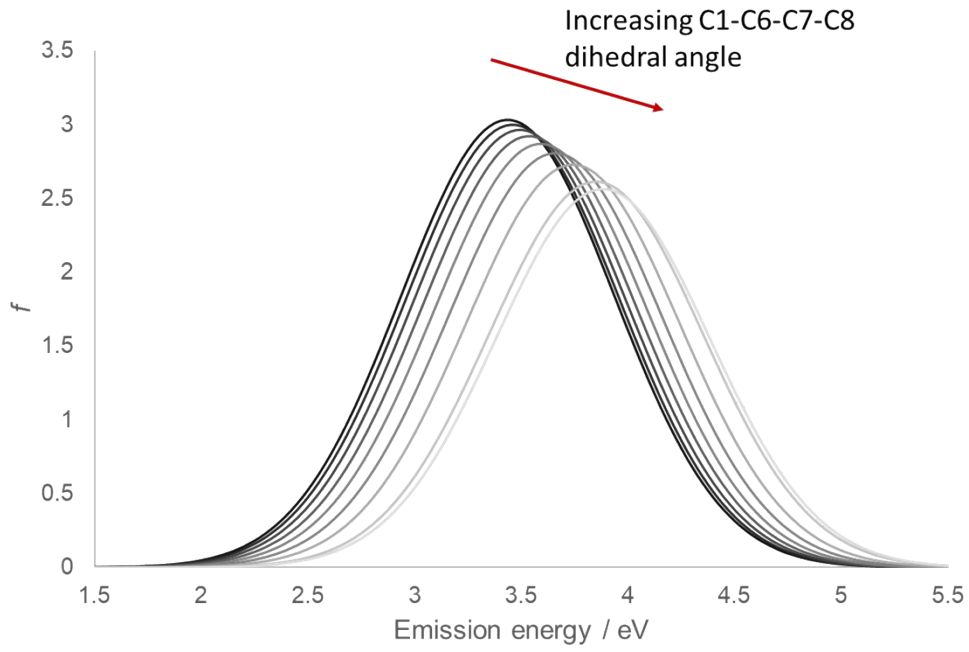

Figure S6. Simulated emission spectra for **2Me** as the C1-C6-C7-C8 dihedral angle increases from ~10° to ~90°. The gaussian function was fitted using a broadening factor of 0.5 eV in the following equation: $f(x) = ae^{-\frac{(x-b)^2}{2c^2}}$, where *a* is the oscillator strength (Figure S5), *b* is the emission energy (Figure S4) and *c* is the broadening factor.

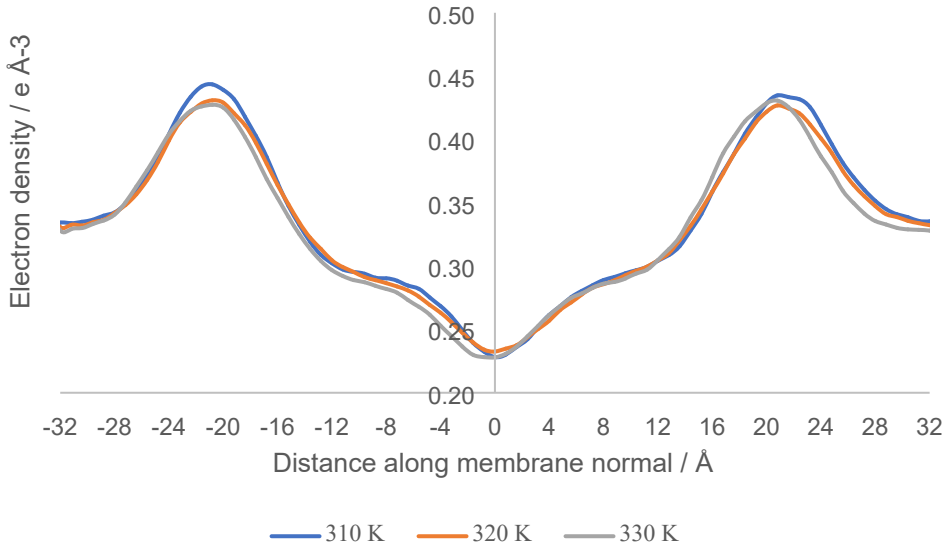

Figure S7. Calculated electron density profile from the non-raft MD simulation.

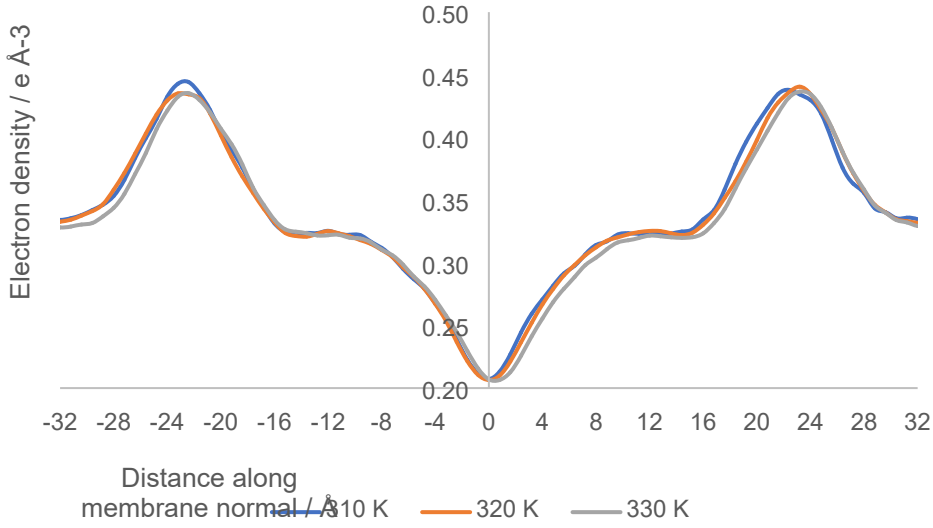

Figure S8. Calculated electron density profile from the raft MD simulation.

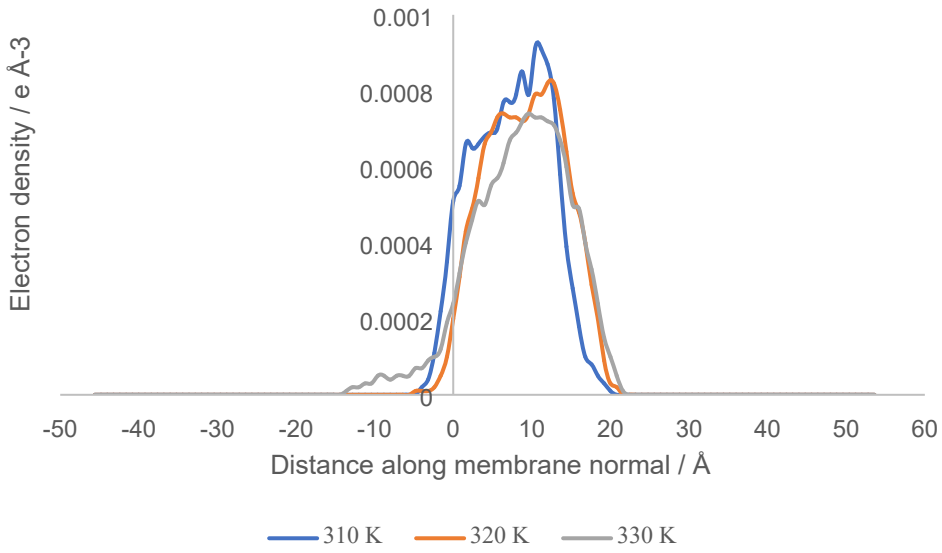

Figure S9. Calculated electron density profile of **2Me** from the non-raft MD simulation

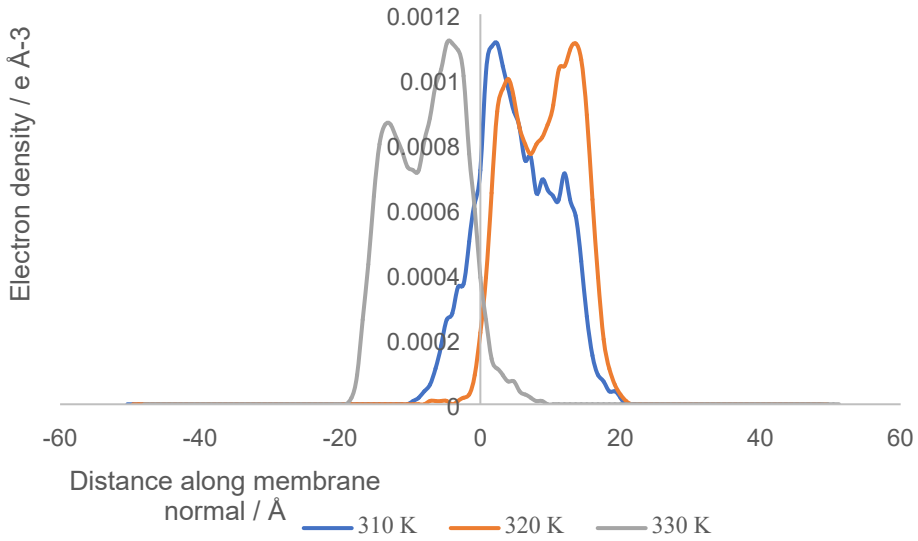

Figure S10. Calculated electron density profile of **2Me** from the raft MD simulation.

Full Cartesian coordinates for the MECI geometries found.

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H        -3.1116918209    0.1675001111    1.8749379772
H         1.9095767004    1.0134927794    0.2579159845
C        -2.2101452813   -1.6837315068    0.6157571063
H         3.5267568915   -2.6984187550   -0.6839858968
H         1.9762370370   -2.7318940326    0.1388592292
H         3.4562436919   -2.6367851561    1.0624181567
H        -1.9355038984   -2.0521298951   -0.3708164220
H        -3.2609430077   -1.8855357613    0.7698651497
H        -1.6197637430   -2.2362879705    1.3427782050


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2,4Me

C	5.9802848737	0.4643223746	1.4016003194
C	5.7025032782	1.8237982389	1.4456264854
C	4.4624077913	2.3102794000	1.0520338354
C	3.4901411508	1.4374779537	0.6118978975
C	3.7607390745	0.0670838338	0.5562418715
C	5.0099724800	-0.4120321135	0.9627511972
H	5.2072377458	-1.4715914877	0.9227360328
H	6.9449435650	0.0990857976	1.7111303819
H	2.5109371824	1.7602875117	0.3059485320
H	6.4577340721	2.5093483482	1.7940901023
H	4.2620584005	3.3676285827	1.0942388295
C	2.7769306890	-0.8530646638	0.0373231572
C	1.4760751226	-0.5491262519	-0.3139485619
C	0.8462458318	-1.0055051447	-1.5290668231
C	-0.4678690308	-0.9568927179	-1.8388008352
C	-1.3980364409	-0.2595766612	-0.9780143414
C	-2.7347088583	-0.3428351404	-1.0198922806
H	1.5046295583	-1.4051696445	-2.2940920933
C	-0.9797097952	-1.5834673089	-3.1023299462
C	-3.6772343522	0.4239074745	-0.2079782273
C	-3.3086037042	1.5447729779	0.5425421008
C	-5.0178021719	0.0342382500	-0.1713052634
C	-5.9475135425	0.7180709684	0.5917774738
C	-5.5615552111	1.8179539056	1.3397508957
C	-4.2358018186	2.2263906710	1.3073663590
H	-2.2897502448	1.8934117743	0.5133460785
H	-3.9250772318	3.0889772777	1.8752311947
H	-6.9749923964	0.3908892291	0.6015882502
H	-6.2828867647	2.3547043636	1.9339533835
H	-5.3280606763	-0.8234085394	-0.7476456688
H	3.1542071587	-1.8921488742	0.0528123637
H	-3.1902883314	-1.0543500517	-1.6931186974
C	0.9992124105	-1.3858708726	0.9979763974
H	-0.9269584592	0.4129151205	-0.2735923210
H	1.2430962495	-2.4522460288	1.0058624744
H	-0.0745824016	-1.2736346378	0.8994152385
H	1.2956203520	-0.9434192939	1.9423864680
H	-1.5713776409	-0.8783870976	-3.6846852195
H	-1.6243431499	-2.4401447754	-2.9014424615
H	-0.1603527046	-1.9369623310	-3.7216801502

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2,5Me

C	5.9802848737	0.4643223746	1.4016003194
C	5.7025032782	1.8237982389	1.4456264854
C	4.4624077913	2.3102794000	1.0520338354
C	3.4901411508	1.4374779537	0.6118978975
C	3.7607390745	0.0670838338	0.5562418715
C	5.0099724800	-0.4120321135	0.9627511972
H	5.2072377458	-1.4715914877	0.9227360328
H	6.9449435650	0.0990857976	1.7111303819
H	2.5109371824	1.7602875117	0.3059485320
H	6.4577340721	2.5093483482	1.7940901023
H	4.2620584005	3.3676285827	1.0942388295
C	2.7769306890	-0.8530646638	0.0373231572
C	1.4760751226	-0.5491262519	-0.3139485619
C	0.8462458318	-1.0055051447	-1.5290668231
C	-0.4678690308	-0.9568927179	-1.8388008352

C	-1.3980364409	-0.2595766612	-0.9780143414
C	-2.7347088583	-0.3428351404	-1.0198922806
H	1.5046295583	-1.4051696445	-2.2940920933
C	-0.9797097952	-1.5834673089	-3.1023299462
C	-3.6772343522	0.4239074745	-0.2079782273
C	-3.3086037042	1.5447729779	0.5425421008
C	-5.0178021719	0.0342382500	-0.1713052634
C	-5.9475135425	0.7180709684	0.5917774738
C	-5.5615552111	1.8179539056	1.3397508957
C	-4.2358018186	2.2263906710	1.3073663590
H	-2.2897502448	1.8934117743	0.5133460785
H	-3.9250772318	3.0889772777	1.8752311947
H	-6.9749923964	0.3908892291	0.6015882502
H	-6.2828867647	2.3547043636	1.9339533835
H	-5.3280606763	-0.8234085394	-0.7476456688
H	3.1542071587	-1.8921488742	0.0528123637
H	-3.1902883314	-1.0543500517	-1.6931186974
C	0.9992124105	-1.3858708726	0.9979763974
H	-0.9269584592	0.4129151205	-0.2735923210
H	1.2430962495	-2.4522460288	1.0058624744
H	-0.0745824016	-1.2736346378	0.8994152385
H	1.2956203520	-0.9434192939	1.9423864680
H	-1.5713776409	-0.8783870976	-3.6846852195
H	-1.6243431499	-2.4401447754	-2.9014424615
H	-0.1603527046	-1.9369623310	-3.7216801502

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3,4Me

C	5.8994866609	-1.5078888211	0.2410770161
C	6.1740341032	-0.7807565896	1.3934812508
C	5.3652173578	0.2934935261	1.7429288479
C	4.2865156271	0.6378366652	0.9550855783
C	3.9917080327	-0.0866285017	-0.2133252313
C	4.8230981244	-1.1690123978	-0.5511306640
H	4.6102241624	-1.7332977665	-1.4456042597
H	6.5276028265	-2.3398795698	-0.0328358990
H	3.6558212444	1.4738530195	1.2062887102
H	7.0136824439	-1.0493027425	2.0133952707
H	5.5833273101	0.8634600970	2.6315204937
C	2.9174620294	0.2996517479	-1.0718440788
C	1.8711597003	1.2592162497	-0.7740944784
C	0.8692631651	0.3816850288	-0.2893175328
C	-0.4029234684	0.3066666437	-1.0024585059
C	-1.5904333793	0.2570915265	-0.2848031457
C	-2.8588604594	0.3140579806	-0.8206939545
C	0.9971616018	-0.3785891317	0.9987725987
C	-0.4215962475	0.4577615780	-2.4946099145
C	-4.0993446974	0.1710470788	-0.0999624324
C	-4.1746652043	-0.0816867508	1.2779764454
C	-5.3065385386	0.2928261591	-0.8016166788
C	-6.5250308305	0.1761995971	-0.1637121569
C	-6.5769464115	-0.0691321993	1.1992418286
C	-5.3935834424	-0.1972494430	1.9127822311
H	-3.2728637213	-0.1934566772	1.8554421472
H	-5.4239284035	-0.3914664662	2.9728031365
H	-7.4367201578	0.2763220110	-0.7301320163
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H	2.8883876321	-0.2244242426	-2.0237610725

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H        -2.9606003317    0.4756502830   -1.8814497324
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H        -1.5077495168    0.1525092510    0.7843453806
H         2.0181767250   -0.4371823604    1.3469781497
H         0.5854445073   -1.3806774906    0.9169126293
H         0.4336589319    0.1422768564    1.7736049669
H         0.5542881998    0.2592744787   -2.9217222430
H        -0.7139776384    1.4617995248   -2.8068368735
H        -1.1332242160   -0.2325704512   -2.9413986028


37
1Me
H        -4.9407358240    0.2665997742    2.4764487537
C        -5.1738396175    0.2059831313    1.4273837989
C        -6.4142965912   -0.2698544522    1.0433087913
H        -7.1282241180   -0.5648333755    1.7943966700
C        -6.7378967486   -0.3645104575   -0.3000090058
H        -7.7057692822   -0.7313923531   -0.5986099131
C        -5.8144594031    0.0244534522   -1.2580922733
H        -6.0664409190   -0.0249133785   -2.3039513450
C        -4.5695421049    0.4841196430   -0.8767130128
H        -3.8720487204    0.8052916544   -1.6300644858
C        -4.2211963782    0.5720369093    0.4739640602
C        -2.8823066370    1.0290166777    0.8841334038
H         6.1138946050   -1.7807493254    1.2971923440
C         5.9387250836   -0.9820829174    0.5932674913
C         4.6627144777   -0.4708668700    0.4511818117
H         3.8682220264   -0.8694097149    1.0607405772
C         4.3892340346    0.5640806085   -0.4504501009
C         5.4700398157    1.0813450433   -1.1705885852
H         5.2930465906    1.8864196135   -1.8666521093
C         6.7488927209    0.5743556459   -1.0245790732
H         7.5564911550    0.9935211335   -1.6038986157
C         6.9938915494   -0.4682118173   -0.1461038906
H         7.9880303926   -0.8682235648   -0.0324615387
C        -1.8257665832    0.8062258120    0.0643835439
C        -0.4606643204    1.1099910207    0.3381614494
C         0.5446312184    0.9369237716   -0.6075985080
C         1.9008441259    0.5298215475   -0.3220170091
C         3.0563551374    1.1209444829   -0.6559749812
C        -2.7764508928    1.6895412421    2.2253496723
H        -1.9718077641    0.2991875340   -0.8716931013
H        -0.2793268632    1.5884301303    1.3085218509
H         0.5816698759    2.0879159647   -0.5136928599
H         1.9515577454   -0.4524094607    0.1323956965
H         3.0242324133    2.0650308512   -1.1807296601
H        -1.8323462430    2.1941611007    2.3725253426
H        -2.8811514720    0.9526483736    3.0194057282
H        -3.5791268843    2.4100444699    2.3512546843


37
2Me
H         8.7645276421    1.6188889431   -3.9385333266
C         8.1022183559    1.2110832698   -3.1908438340
C         6.7391934303    1.3453810742   -3.3567181574
H         6.3554215475    1.8392195200   -4.2355545419
C         5.8305655543    0.8299570228   -2.4219344938
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C	4.3771077561	0.8687966297	-2.6466819188
C	6.3802791153	0.1846643447	-1.3042237573
H	5.7224186663	-0.2424690009	-0.5624741352
C	7.7485822468	0.0456774802	-1.1479616593
H	8.1268648805	-0.4705098075	-0.2785451698
C	8.6275382106	0.5579145826	-2.0851288383
H	9.6918054862	0.4464188527	-1.9632787717
H	-1.8420548560	-1.9283470905	-0.8888183478
C	-2.4957977321	-1.5440295981	-0.1245642376
C	-3.6769401355	-2.2041363155	0.1464719798
H	-3.9317980166	-3.0925353447	-0.4071658644
C	-4.5342863855	-1.7306513010	1.1311894368
H	-5.4545834408	-2.2503040487	1.3411556470
C	-4.2020491189	-0.5901181368	1.8432036090
H	-4.8616565766	-0.2179493538	2.6093456346
C	-3.0181527988	0.0714190875	1.5722626443
H	-2.7603070680	0.9583384054	2.1290589285
C	-2.1453917874	-0.3919588372	0.5864077725
C	3.5157871439	1.2204979314	-1.5951947418
C	2.2494470713	0.5355713175	-1.5072453178
C	1.2528613121	0.8250743891	-0.6419872377
C	0.0509444777	0.0563288108	-0.5439036858
C	-0.9074378983	0.3356258904	0.3568084082
H	4.2513967397	1.9662923581	-2.9440546143
C	3.7822136934	2.3272781645	-0.6016039174
H	2.1517727877	-0.2805545318	-2.2011924378
H	1.3497067120	1.6607603372	0.0353117635
H	-0.0460665876	-0.7809991998	-1.2162246746
H	-0.7538380630	1.1910114068	1.0000317362
H	4.7409683343	2.7854698838	-0.8009196651
H	3.8096287432	1.9020281362	0.3995409599
H	3.0033320584	3.0861145251	-0.6079337730

37
3Me

H	-6.4725048894	1.9359905685	-2.9986289370
C	-6.7100974118	0.9306409591	-2.6890541259
C	-8.0026930495	0.4582480727	-2.8190321278
H	-8.7694312298	1.0943331494	-3.2278173129
C	-8.3061587478	-0.8327039855	-2.4206086169
H	-9.3119695864	-1.2047094889	-2.5207244224
C	-7.3158215603	-1.6485380319	-1.8888481541
H	-7.5538001591	-2.6503246212	-1.5732370995
C	-6.0253290532	-1.1799856874	-1.7622381862
H	-5.2658539368	-1.8192439946	-1.3471118040
C	-5.7023092983	0.1196937123	-2.1648944425
C	-4.3559045392	0.6564530539	-2.0757138062
H	4.4064728454	-0.8507805972	-4.9195856489
C	4.3241414087	-0.7219287372	-3.8514822107
C	3.0830832156	-0.4914740707	-3.2896752252
H	2.2210887081	-0.4329117229	-3.9339484641
C	2.9279123431	-0.3199090856	-1.9088017619
C	1.6401167765	-0.0847949172	-1.2632449342
C	4.0884030271	-0.3664134455	-1.1305522421
H	4.0036642585	-0.2345162726	-0.0627968106
C	5.3320353823	-0.5925612865	-1.6928397352
H	6.2032161904	-0.6292808179	-1.0576901769
C	5.4615761319	-0.7771728353	-3.0593199977
H	6.4283981147	-0.9556333359	-3.4999914248

C	-3.2552928628	-0.0059158282	-1.6842681494
C	-1.9128427431	0.5282729082	-1.7019059704
C	-0.8819748890	-0.2756868050	-1.1976515381
C	0.4361947721	-0.3138009646	-1.8055536474
H	-4.2617181356	1.6856759025	-2.3862965115
H	1.6911126740	0.2357043861	-0.2321409024
H	-3.2938816720	-1.0288185358	-1.3584742424
C	-1.7148887259	1.9336790488	-2.2031754677
H	-0.7691661822	0.5597809055	-0.4244866272
H	0.4101104504	-0.6935847382	-2.8206379276
H	-2.4457890006	2.6477161450	-1.8349008195
H	-1.8131412356	1.8949639712	-3.2888917822
H	-0.7142579886	2.2737580229	-1.9763049461

Force-fields used for the probe molecules. In each case, the force-fields were initially generated by CGenFF and modified according to the main text. These topologies and parameters should follow the CGenFF topologies and parameters when used in a simulation.

1,3Me

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RESI AIE            0.000
GROUP             ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.004
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
ATOM H5     HGR61   0.115
ATOM C7     CG2DC1  0.002
ATOM C8     CG2DC1 -0.140
ATOM C9     CG2DC2 -0.006
ATOM C10    CG2DC2 -0.164
ATOM C11    CG2DC1 -0.131
ATOM C12    CG2DC1 -0.150
ATOM C13    CG331  -0.270
ATOM C14    CG331  -0.270
ATOM H6     HGA4    0.150
ATOM H7     HGA4    0.150
ATOM C15    CG2R61 -0.007
ATOM H8     HGA4    0.150
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM C19    CG2R61 -0.115
ATOM C20    CG2R61 -0.115
ATOM H9     HGR61   0.115
ATOM H10    HGR61   0.115
ATOM H11    HGR61   0.115
ATOM H12    HGR61   0.115
ATOM H13    HGR61   0.115
ATOM H14    HGA3    0.090
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
ATOM H19    HGA3    0.090
ATOM H20    HGA4    0.150

BOND H14  C13
BOND H15  C13
BOND H18  C14
BOND H3   C4
BOND H5   C3
BOND C4   C3
BOND C4   C5
BOND C13  C7
BOND C13  H16
BOND C3   C2
BOND C7   C5
BOND C7   C8
BOND C5   C6
```

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BOND H7   C11
BOND C14  C9
BOND C14  H19
BOND C14  H17
BOND H10  C20
BOND H12  C19
BOND C9   C8
BOND C9   C10
BOND C20  C19
BOND C20  C16
BOND C19  C18
BOND C8   H20
BOND H9   C16
BOND C16  C15
BOND C11  C10
BOND C11  C12
BOND C18  H11
BOND C18  C17
BOND C10  H6
BOND C15  C17
BOND C15  C12
BOND C17  H13
BOND C12  H8
BOND C2   H4
BOND C2   C1
BOND C6   C1
BOND C6   H1
BOND C1   H2

END


BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00
CG2R61 CG2DC1 CG331    48.00    113.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.103516        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  8.776453        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    6.016354        2       180
CG331   CG2DC1  CG2R61  CG2R61  1.268181        2       180
CG2R61  CG2DC1  CG331   HGA3    0.074396        3       180
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1,4Me

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RESI AIE           0.000
GROUP            ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.004
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
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ATOM H5     HGR61   0.115
ATOM C7     CG2DC1 -0.001
ATOM C8     CG2DC1 -0.138
ATOM C9     CG2DC2 -0.159
ATOM C10    CG2DC2 -0.011
ATOM C11    CG2DC1 -0.133
ATOM C12    CG2DC1 -0.147
ATOM C13    CG331  -0.270
ATOM H6     HGA4    0.150
ATOM H7     HGA4    0.150
ATOM C14    CG331  -0.270
ATOM H8     HGA4    0.150
ATOM C15    CG2R61 -0.007
ATOM H9     HGA4    0.150
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM C19    CG2R61 -0.115
ATOM C20    CG2R61 -0.115
ATOM H10    HGR61   0.115
ATOM H11    HGR61   0.115
ATOM H12    HGR61   0.115
ATOM H13    HGR61   0.115
ATOM H14    HGR61   0.115
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
ATOM H19    HGA3    0.090
ATOM H20    HGA3    0.090

BOND H3   C4
BOND H5   C3
BOND H15  C13
BOND H20  C14
BOND C4   C3
BOND C4   C5
BOND H11  C20
BOND H10  C16
BOND C3   C2
BOND H16  C13
BOND C20  C16
BOND C20  C19
BOND C16  C15
BOND C13  C7
BOND C13  H17
BOND H7   C9
BOND H8   C11
BOND C7   C5
BOND C7   C8
BOND H13  C19
BOND C19  C18
BOND C5   C6
BOND C9   C8
BOND C9   C10
BOND C8   H6
BOND C11  C10
BOND C11  C12
BOND C15  C12
BOND C15  C17
BOND C10  C14
```

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BOND C2   H4
BOND C2   C1
BOND C12  H9
BOND C14  H18
BOND C14  H19
BOND C18  C17
BOND C18  H12
BOND C17  H14
BOND C6   C1
BOND C6   H1
BOND C1   H2

END
BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00
CG2R61 CG2DC1 CG331    48.00    113.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2R61 CG2DC1 CG331  HGA3       0.3000  3   180.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.074976        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  9.105853        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    5.917803        2       180
CG331   CG2DC1  CG2R61  CG2R61  1.361484        2       180
CG2R61  CG2DC1  CG331   HGA3    0.121966        3       180
```

1,5Me

```
RESI AIE            0.000
GROUP             ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.004
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
ATOM H5     HGR61   0.115
ATOM C7     CG2DC1 -0.001
ATOM C8     CG2DC1 -0.143
ATOM C9     CG2DC2 -0.149
ATOM C10    CG2DC2 -0.154
ATOM C11    CG2DC1  0.010
ATOM C12    CG2DC1 -0.157
ATOM H6     HGA4    0.150
ATOM H7     HGA4    0.150
ATOM C13    CG2R61 -0.002
ATOM C14    CG2R61 -0.115
ATOM C15    CG2R61 -0.115
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM H8     HGR61   0.115
ATOM H9     HGR61   0.115
ATOM H10    HGR61   0.115
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ATOM H11    HGR61   0.115
ATOM H12    HGR61   0.115
ATOM C19    CG331  -0.270
ATOM H13    HGA4    0.150
ATOM H14    HGA4    0.150
ATOM C20    CG331  -0.270
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
ATOM H19    HGA3    0.090
ATOM H20    HGA3    0.090

BOND H9   C18
BOND H8   C14
BOND H5   C3
BOND H3   C4
BOND C18  C14
BOND C18  C17
BOND C14  C13
BOND H19  C20
BOND C3   C4
BOND C3   C2
BOND C4   C5
BOND H15  C19
BOND H4   C2
BOND H16  C19
BOND C2   C1
BOND H11  C17
BOND C17  C16
BOND C5   C7
BOND C5   C6
BOND C13  C12
BOND C13  C15
BOND C7   C8
BOND C7   C19
BOND C8   H14
BOND C8   C9
BOND C12  H13
BOND C12  C11
BOND H6   C9
BOND C9   C10
BOND H7   C10
BOND C19  H17
BOND C10  C11
BOND C11  C20
BOND C20  H20
BOND C20  H18
BOND C1   C6
BOND C1   H2
BOND C6   H1
BOND C16  C15
BOND C16  H10
BOND C15  H12

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00
```

```
CG2R61 CG2DC1 CG331    48.00    113.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.857374        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  5.836502        2       180
CG2R61  CG2DC1  CG2DC1  CG331   0.589424        1       180
CG2R61  CG2DC1  CG2DC1  CG331   7.206005        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    5.077691        2       180
CG331   CG2DC1  CG2R61  CG2R61  1.513733        2       180
CG2R61  CG2DC1  CG331   HGA3    0.214945        3       180
```

2,3Me

```
RESI AIE           0.000
GROUP             ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.002
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
ATOM H5     HGR61   0.115
ATOM C7     CG2DC1 -0.154
ATOM C8     CG2DC1  0.013
ATOM C9     CG2DC2 -0.008
ATOM C10    CG2DC2 -0.161
ATOM C11    CG2DC1 -0.131
ATOM C12    CG2DC1 -0.150
ATOM C13    CG331  -0.270
ATOM C14    CG331  -0.270
ATOM H6     HGA4    0.150
ATOM H7     HGA4    0.150
ATOM C15    CG2R61 -0.007
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM C19    CG2R61 -0.115
ATOM C20    CG2R61 -0.115
ATOM H8     HGR61   0.115
ATOM H9     HGR61   0.115
ATOM H10    HGR61   0.115
ATOM H11    HGR61   0.115
ATOM H12    HGR61   0.115
ATOM H13    HGA4    0.150
ATOM H14    HGA4    0.150
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
ATOM H19    HGA3    0.090
ATOM H20    HGA3    0.090

BOND H3   C4
BOND H5   C3
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BOND H19  C14
BOND C3   C4
BOND C3   C2
BOND C4   C5
BOND H9   C20
BOND H8   C16
BOND C20  C16
BOND C20  C19
BOND H17  C13
BOND C16  C15
BOND H13  C7
BOND C14  H20
BOND C14  C9
BOND C14  H18
BOND H11  C19
BOND H4   C2
BOND C2   C1
BOND H7   C11
BOND C5   C7
BOND C5   C6
BOND C19  C18
BOND C7   C8
BOND C15  C12
BOND C15  C17
BOND C11  C12
BOND C11  C10
BOND C9   C10
BOND C9   C8
BOND C12  H14
BOND C10  H6
BOND C8   C13
BOND C18  C17
BOND C18  H10
BOND C17  H12
BOND C13  H15
BOND C13  H16
BOND C6   C1
BOND C6   H1
BOND C1   H2

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.096978        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  11.415094       2       180
CG2R61  CG2DC1  CG2DC1  CG331   0.193584        1       180
CG2R61  CG2DC1  CG2DC1  CG331   5.531836        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    6.61659 2       180
CG331   CG2DC1  CG2DC2  CG331   0.693951        1       180
CG331   CG2DC1  CG2DC2  CG331   1.317678        2       180
```

2,4Me

```
RESI AIE          0.000
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```
GROUP            ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.002
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
ATOM H5     HGR61   0.115
ATOM C7     CG2DC1 -0.157
ATOM C8     CG2DC1  0.015
ATOM C9     CG2DC2 -0.161
ATOM C10    CG2DC2 -0.008
ATOM C11    CG2DC1 -0.133
ATOM C12    CG2DC1 -0.147
ATOM H6     HGA4    0.150
ATOM C13    CG331  -0.270
ATOM C14    CG2R61 -0.007
ATOM C15    CG2R61 -0.115
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM C19    CG2R61 -0.115
ATOM H7     HGR61   0.115
ATOM H8     HGR61   0.115
ATOM H9     HGR61   0.115
ATOM H10    HGR61   0.115
ATOM H11    HGR61   0.115
ATOM H12    HGA4    0.150
ATOM H13    HGA4    0.150
ATOM C20    CG331  -0.270
ATOM H14    HGA4    0.150
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
ATOM H19    HGA3    0.090
ATOM H20    HGA3    0.090

BOND H3   C4
BOND H5   C3
BOND H20  C13
BOND C4   C3
BOND C4   C5
BOND C3   C2
BOND H12  C7
BOND C7   C5
BOND C7   C8
BOND H18  C13
BOND C5   C6
BOND C2   H4
BOND C2   C1
BOND H10  C18
BOND H8   C19
BOND C18  C19
BOND C18  C17
BOND C19  C15
BOND H9   C17
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BOND C17  C16
BOND C15  H7
BOND C15  C14
BOND H17  C20
BOND C16  C14
BOND C16  H11
BOND C14  C12
BOND H14  C11
BOND C12  C11
BOND C12  H13
BOND C11  C10
BOND C13  C10
BOND C13  H19
BOND H6   C9
BOND C10  C9
BOND C9   C8
BOND C8   C20
BOND C6   C1
BOND C6   H1
BOND C1   H2
BOND C20  H15
BOND C20  H16

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.094644        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  9.162901        2       180
CG2R61  CG2DC1  CG2DC1  CG331   1.244941        1       180
CG2R61  CG2DC1  CG2DC1  CG331   10.107544       2       180
CG2R61  CG2DC1  CG2DC1  HGA4    6.709147        2       180
```

2,5Me

```
RESI AIE           0.000
GROUP             ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.002
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
ATOM H5     HGR61   0.115
ATOM C7     CG2DC1 -0.157
ATOM C8     CG2DC1  0.010
ATOM C9     CG2DC2 -0.151
ATOM C10    CG2DC2 -0.151
ATOM C11    CG2DC1  0.010
ATOM C12    CG2DC1 -0.157
ATOM H6     HGA4    0.150
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ATOM H7     HGA4    0.150
ATOM C13    CG2R61 -0.002
ATOM C14    CG2R61 -0.115
ATOM C15    CG2R61 -0.115
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM H8     HGR61   0.115
ATOM H9     HGR61   0.115
ATOM H10    HGR61   0.115
ATOM H11    HGR61   0.115
ATOM H12    HGR61   0.115
ATOM H13    HGA4    0.150
ATOM H14    HGA4    0.150
ATOM C19    CG331  -0.270
ATOM C20    CG331  -0.270
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
ATOM H19    HGA3    0.090
ATOM H20    HGA3    0.090

BOND H9   C18
BOND H5   C3
BOND H8   C14
BOND H3   C4
BOND C18  C14
BOND C18  C17
BOND C3   C4
BOND C3   C2
BOND C14  C13
BOND C4   C5
BOND H19  C20
BOND H17  C19
BOND H11  C17
BOND H4   C2
BOND C17  C16
BOND C2   C1
BOND C5   C7
BOND C5   C6
BOND C13  C12
BOND C13  C15
BOND C7   H13
BOND C7   C8
BOND C12  H14
BOND C12  C11
BOND H6   C9
BOND C11  C10
BOND C11  C20
BOND C8   C9
BOND C8   C19
BOND C9   C10
BOND H7   C10
BOND C20  H20
BOND C20  H18
BOND C19  H15
BOND C19  H16
BOND C1   C6
BOND C1   H2
BOND C16  C15
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BOND C16  H10
BOND C6   H1
BOND C15  H12

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.04648 1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  12.977052       2       180
CG2R61  CG2DC1  CG2DC1  CG331   0.7836  1       180
CG2R61  CG2DC1  CG2DC1  CG331   7.926638        2       180
```

3,4Me

```
RESI AIE           0.000
GROUP             ! CHARGE
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM C3     CG2R61 -0.115
ATOM C4     CG2R61 -0.115
ATOM C5     CG2R61 -0.007
ATOM C6     CG2R61 -0.115
ATOM H1     HGR61   0.115
ATOM H2     HGR61   0.115
ATOM H3     HGR61   0.115
ATOM H4     HGR61   0.115
ATOM H5     HGR61   0.115
ATOM C7     CG2DC1 -0.147
ATOM C8     CG2DC1 -0.128
ATOM C9     CG2DC2 -0.017
ATOM C10    CG2DC2 -0.017
ATOM C11    CG2DC1 -0.128
ATOM C12    CG2DC1 -0.147
ATOM C13    CG331  -0.271
ATOM C14    CG331  -0.271
ATOM C15    CG2R61 -0.007
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM C19    CG2R61 -0.115
ATOM C20    CG2R61 -0.115
ATOM H6     HGR61   0.115
ATOM H7     HGR61   0.115
ATOM H8     HGR61   0.115
ATOM H9     HGR61   0.115
ATOM H10    HGR61   0.115
ATOM H11    HGA4    0.150
ATOM H12    HGA4    0.150
ATOM H13    HGA4    0.150
ATOM H14    HGA4    0.150
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090
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ATOM H19    HGA3    0.090
ATOM H20    HGA3    0.090

BOND H16  C13
BOND H20  C14
BOND H3   C4
BOND H8   C18
BOND H5   C3
BOND H17  C13
BOND C13  C9
BOND C13  H15
BOND H11  C7
BOND C4   C3
BOND C4   C5
BOND H10  C17
BOND C18  C17
BOND C18  C19
BOND C3   C2
BOND H14  C11
BOND H9   C19
BOND C7   C5
BOND C7   C8
BOND C17  C15
BOND C5   C6
BOND C19  C20
BOND C9   C8
BOND C9   C10
BOND C8   H13
BOND C11  C10
BOND C11  C12
BOND C2   H4
BOND C2   C1
BOND C15  C12
BOND C15  C16
BOND C10  C14
BOND C6   C1
BOND C6   H1
BOND C20  C16
BOND C20  H7
BOND C12  H12
BOND C1   H2
BOND C16  H6
BOND C14  H18
BOND C14  H19

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG331  CG2DC2 CG2DC2 CG331     10.0000  2   180.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.08265 1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  9.758027        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    6.169531        2       180
```

1Me

```
RESI AIE            0.000
GROUP             ! CHARGE
ATOM H1     HGR61   0.115
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM H2     HGR61   0.115
ATOM C3     CG2R61 -0.115
ATOM H3     HGR61   0.115
ATOM C4     CG2R61 -0.115
ATOM H4     HGR61   0.115
ATOM C5     CG2R61 -0.115
ATOM H5     HGR61   0.115
ATOM C6     CG2R61 -0.004
ATOM C7     CG2DC1 -0.001
ATOM H6     HGR61   0.115
ATOM C8     CG2R61 -0.115
ATOM C9     CG2R61 -0.115
ATOM H7     HGR61   0.115
ATOM C10    CG2R61 -0.007
ATOM C11    CG2R61 -0.115
ATOM H8     HGR61   0.115
ATOM C12    CG2R61 -0.115
ATOM H9     HGR61   0.115
ATOM C13    CG2R61 -0.115
ATOM H10    HGR61   0.115
ATOM C14    CG2DC1 -0.143
ATOM C15    CG2DC2 -0.152
ATOM C16    CG2DC2 -0.157
ATOM C17    CG2DC1 -0.136
ATOM C18    CG2DC1 -0.150
ATOM C19    CG331  -0.270
ATOM H11    HGA4    0.150
ATOM H12    HGA4    0.150
ATOM H13    HGA4    0.150
ATOM H14    HGA4    0.150
ATOM H15    HGA4    0.150
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090

BOND H18  C19
BOND H5   C5
BOND H4   C4
BOND H16  C19
BOND C5   C4
BOND C5   C6
BOND H6   C8
BOND C4   C3
BOND H7   C9
BOND C19  C7
BOND C19  H17
BOND H12  C15
BOND C8   C9
BOND C8   C13
BOND C9   C10
BOND H14  C17
BOND C7   C6
BOND C7   C14
```

```
BOND C15  C14
BOND C15  C16
BOND C6   C1
BOND C14  H11
BOND C17  C16
BOND C17  C18
BOND C16  H13
BOND H10  C13
BOND C13  C12
BOND C10  C18
BOND C10  C11
BOND C3   H3
BOND C3   C2
BOND C18  H15
BOND C12  C11
BOND C12  H9
BOND C11  H8
BOND C1   C2
BOND C1   H1
BOND C2   H2

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00
CG2R61 CG2DC1 CG331    48.00    113.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.161071        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  8.51945 2       180
CG2R61  CG2DC1  CG2DC1  HGA4    4.73837 2       180
CG331   CG2DC1  CG2R61  CG2R61  1.590478        2       180
CG2R61  CG2DC1  CG331   HGA3    0.461611        3       60
```

2Me

```
RESI AIE           0.000
GROUP             ! CHARGE
ATOM H1     HGR61   0.115
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM H2     HGR61   0.115
ATOM C3     CG2R61 -0.002
ATOM C4     CG2DC1 -0.157
ATOM C5     CG2R61 -0.115
ATOM H3     HGR61   0.115
ATOM C6     CG2R61 -0.115
ATOM H4     HGR61   0.115
ATOM C7     CG2R61 -0.115
ATOM H5     HGR61   0.115
ATOM H6     HGR61   0.115
ATOM C8     CG2R61 -0.115
ATOM C9     CG2R61 -0.115
ATOM H7     HGR61   0.115
ATOM C10    CG2R61 -0.115
ATOM H8     HGR61   0.115
```

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ATOM C11    CG2R61 -0.115
ATOM H9     HGR61   0.115
ATOM C12    CG2R61 -0.115
ATOM H10    HGR61   0.115
ATOM C13    CG2R61 -0.007
ATOM C14    CG2DC1  0.010
ATOM C15    CG2DC2 -0.154
ATOM C16    CG2DC2 -0.154
ATOM C17    CG2DC1 -0.136
ATOM C18    CG2DC1 -0.150
ATOM H11    HGA4    0.150
ATOM C19    CG331  -0.270
ATOM H12    HGA4    0.150
ATOM H13    HGA4    0.150
ATOM H14    HGA4    0.150
ATOM H15    HGA4    0.150
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090

BOND H17  C19
BOND H1   C1
BOND H2   C2
BOND H18  C19
BOND C1   C2
BOND C1   C7
BOND C2   C3
BOND H10  C12
BOND C19  C14
BOND C19  H16
BOND H9   C11
BOND H13  C16
BOND C12  C11
BOND C12  C13
BOND H15  C18
BOND C11  C10
BOND C16  C15
BOND C16  C17
BOND C14  C15
BOND C14  C4
BOND C18  C17
BOND C18  C13
BOND C15  H12
BOND C17  H14
BOND C13  C8
BOND H5   C7
BOND C7   C6
BOND C4   C3
BOND C4   H11
BOND C3   C5
BOND C10  H8
BOND C10  C9
BOND C8   C9
BOND C8   H6
BOND C9   H7
BOND C6   C5
BOND C6   H4
BOND C5   H3

END
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BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  1.318489        1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  3.914232        2       180
CG2R61  CG2DC1  CG2DC1  CG331   0.126094        1       180
CG2R61  CG2DC1  CG2DC1  CG331   5.227654        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    5.810909        2       180
```

3Me

```
RESI AIE           0.000
GROUP             ! CHARGE
ATOM H1     HGR61   0.115
ATOM C1     CG2R61 -0.115
ATOM C2     CG2R61 -0.115
ATOM H2     HGR61   0.115
ATOM C3     CG2R61 -0.007
ATOM C4     CG2DC1 -0.150
ATOM C5     CG2R61 -0.115
ATOM H3     HGR61   0.115
ATOM C6     CG2R61 -0.115
ATOM H4     HGR61   0.115
ATOM C7     CG2R61 -0.115
ATOM H5     HGR61   0.115
ATOM C8     CG2DC1 -0.131
ATOM C9     CG2DC2 -0.164
ATOM C10    CG2DC2 -0.011
ATOM C11    CG2DC1 -0.133
ATOM C12    CG2DC1 -0.147
ATOM C13    CG2R61 -0.007
ATOM C14    CG2R61 -0.115
ATOM C15    CG2R61 -0.115
ATOM C16    CG2R61 -0.115
ATOM C17    CG2R61 -0.115
ATOM C18    CG2R61 -0.115
ATOM H6     HGA4    0.150
ATOM H7     HGA4    0.150
ATOM H8     HGA4    0.150
ATOM C19    CG331  -0.270
ATOM H9     HGA4    0.150
ATOM H10    HGA4    0.150
ATOM H11    HGR61   0.115
ATOM H12    HGR61   0.115
ATOM H13    HGR61   0.115
ATOM H14    HGR61   0.115
ATOM H15    HGR61   0.115
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090

BOND H18  C19
BOND H12  C15
BOND H13  C16
BOND H4   C6
BOND H3   C5
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BOND C15  C16
BOND C15  C13
BOND C16  C17
BOND C6   C5
BOND C6   C7
BOND C5   C3
BOND H5   C7
BOND C13  C12
BOND C13  C14
BOND C7   C1
BOND C12  H10
BOND C12  C11
BOND C17  H14
BOND C17  C18
BOND H16  C19
BOND H7   C8
BOND C3   C4
BOND C3   C2
BOND C11  C10
BOND C11  H9
BOND C10  C19
BOND C10  C9
BOND C8   C9
BOND C8   C4
BOND C19  H17
BOND H8   C9
BOND C4   H6
BOND C1   C2
BOND C1   H1
BOND C2   H2
BOND C14  C18
BOND C14  H11
BOND C18  H15

END

BONDS

ANGLES
CG2DC1 CG2DC1 CG2R61   29.00    122.00

DIHEDRALS
CG2DC1 CG2DC1 CG2R61 CG2R61     0.7500  2   180.00
CG2DC1 CG2DC1 CG2R61 CG2R61     0.1900  4     0.00
CG2DC2  CG2DC1  CG2DC1  CG2R61  0.08811 1       180
CG2DC2  CG2DC1  CG2DC1  CG2R61  8.721226        2       180
CG2R61  CG2DC1  CG2DC1  HGA4    5.688978        2       180
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