

Supporting Information

The Mechanism of Guanine Alkylation by Nitrogen Mustards – A Computational Study

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TABLE S1. CARTESIAN COORDINATES (IN Å) FOR MECHLORETHAMINE , PHENYL MUSTARD, MELPHALAN DRUGS, INTERMEDIATES AND THEIR ADDUCTS WITH GUANINE AND ADENINE. 2

TABLE S2. FREQUENCIES (IN CM⁻¹) FOR MECHLORETHAMINE , PHENYL MUSTARD, MELPHALAN DRUGS, INTERMEDIATES AND THEIR ADDUCTS WITH GUANINE AND ADENINE.13

TABLE S3. DETAILED ENERGETICS FOR ALL COMPOUNDS INVESTIGATED.....19

=====				C -2.624728206 -1.526278425 -1.294450603			
1a				C -2.748981092 -2.727930303 -1.987412152			
=====				H -1.758042763 -4.501799790 -2.723307700			
N	-1.244748753	0.237011913	-0.323345353	H	0.453519357	-3.807027168	-1.800347816
C	0.032669359	0.920130422	-0.526282197	H	0.705531310	-1.715835220	-0.595303945
C	1.085395255	0.334705355	0.416505061	H	-3.510381685	-0.916320411	-1.165335062
Cl	2.693977026	1.135858761	0.159528735	H	-3.724500869	-3.006583603	-2.377099031
C	-2.434538509	1.077086021	-0.461901693	=====			
C	-3.490948196	0.640097561	0.554268561	3a			
Cl	-5.004262808	1.626702745	0.374163336	=====			
C	-1.344940105	-0.999802778	-1.095104123	N	-1.077251104	0.188158008	-0.019018540
H	0.387778028	0.856183950	-1.568277851	C	0.190867240	0.822394714	0.304706333
H	-0.082522182	1.981726150	-0.292369694	C	0.686280980	1.703842613	-0.847774064
H	0.804946862	0.497348484	1.457045778	Cl	2.287305272	2.450959758	-0.436350605
H	1.243964590	-0.731296030	0.251778992	C	-2.286436610	0.846890312	0.451609514
H	-2.171605471	2.118399450	-0.258012574	C	-2.751941869	0.273935667	1.795338530
H	-2.859036992	1.045360438	-1.478772753	Cl	-4.254176830	1.117249665	2.360267196
H	-3.785306738	-0.401541427	0.423350112	H	0.062354770	1.439332242	1.198757583
H	-3.130646601	0.783668111	1.572785831	H	0.947687410	0.073481931	0.555205320
H	-0.501257933	-1.658268004	-0.872387701	H	0.826938441	1.126555123	-1.761797545
H	-1.360365090	-0.819100057	-2.184922313	H	-0.005859755	2.523458433	-1.046774960
H	-2.255756336	-1.542393868	-0.828346710	H	-2.084910137	1.915692109	0.568039481
=====				H	-3.087008743	0.764753961	-0.288567979
2a				H	-1.996458633	0.416301456	2.569811103
=====				H	-2.988593978	-0.787606069	1.718817747
N	-1.249902619	0.092863702	-0.064723168	C	-1.237075493	-3.471977334	-2.201653142
C	0.042062647	0.558059165	0.415086485	C	-0.023170261	-2.826454915	-1.937943143
C	0.852374175	1.203603863	-0.714668601	C	0.041304509	-1.627638786	-1.229283480
Cl	2.481733436	1.731111211	-0.116172813	C	-1.128564239	-1.012834922	-0.735963287
C	-2.396172571	0.953868063	0.188184069	C	-2.354478027	-1.662642678	-1.003404349
C	-3.199678277	0.466997512	1.398739225	C	-2.400446663	-2.854925364	-1.717382428
Cl	-4.622867272	1.551079245	1.699298341	C	-1.287771156	-4.789004279	-2.946289911
H	-0.122953304	1.291284004	1.209176934	H	0.903929481	-3.254109359	-2.314547429
H	0.614378120	-0.257044196	0.868282194	H	1.013392214	-1.173974543	-1.078656069
H	1.024727204	0.503933215	-1.532903807	H	-3.290095438	-1.245164661	-0.651180735
H	0.351027081	2.091913221	-1.102116645	H	-3.363429735	-3.323614645	-1.896706063
H	-2.039810298	1.970295754	0.377009293	H	-0.384575146	-4.901460711	-3.557012909
H	-3.045738734	1.018137105	-0.689882997	C	-1.402067477	-6.025880851	-2.021301158
H	-2.593222151	0.477770217	2.305678275	H	-2.147003763	-4.815402437	-3.622682447
H	-3.589296655	-0.539013999	1.240399332	H	-1.302601173	-6.924476009	-2.643822275
C	-1.653350841	-3.566427012	-2.182764132	C	-2.814054185	-6.135360023	-1.396023626

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1b

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C -1.171398744 3.300283647 0.724143257
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C 0.566954200 3.889334545 -1.048220223
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C 1.666856311 1.026229310 -0.521513519
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H -1.153235936 2.923518575 1.741133402
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H 0.942714998 0.457899994 -1.109670909
H 2.323623919 1.578818056 -1.194366697

2b

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3b

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C -1.009665769 -3.403245347 -2.064330161
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1a-TS

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N -1.262046009 0.188600982 -0.728221118
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H -0.177406296 1.913367888 -0.263400814
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H 1.311529320 -0.778821538 -0.103814040
H -3.306149175 0.615286091 -1.521445601
H -2.389177223 2.106796039 -0.958089370
H -1.945180230 1.003583746 1.242163182
H -2.863043074 -0.489652785 0.680900290
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2a-TS

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N -1.184442599 0.187122945 0.250872163
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Cl 2.547951530 1.812472952 -0.021684847
C -2.234615628 1.263671530 0.125369936
C -2.441487665 0.468372599 1.318793447
Cl -5.169058385 0.851917832 1.048625240
H 0.058218653 1.384107394 1.422296996
H 0.732892485 -0.192650994 1.035731679
H 1.043724658 0.585126083 -1.383005057
H 0.385461003 2.168351515 -0.923438292
H -1.829152175 2.266519172 0.227933656
H -2.934075370 1.142105714 -0.692325707
H -2.084614805 0.818568731 2.281034314
H -3.141885709 -0.352404498 1.298054846
C -1.664562924 -3.334740263 -2.096199040
C -0.400940185 -2.965713304 -1.642029387
C -0.231481665 -1.811696855 -0.874469056
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C -2.618648502 -1.389152843 -1.004175223
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H -3.508725275 -0.821552945 -0.736495952
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3a-TS

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G

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N  -0.128462342 -1.340277287  5.312698619
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N  -0.657063683  0.645691996  4.017130596
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O  1.208629224 -2.870059627  1.678600907
H  1.130070019 -3.973936431  3.849663780
H  -0.816401067  1.950765228  2.306698695
H  -1.035695947  1.213451114  4.760349060
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A

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N  -2.297818214 -0.653399855 -0.187461054
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C  -1.168372877  1.519788629 -0.263545843
N  0.123517776  1.991763589 -0.424955668
C  0.841558755  0.904430337 -0.567778754
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H  1.912579067  0.880192669 -0.717806593
H  0.431080190 -1.205048373 -0.590393266
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1cA

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C  -2.797057594  0.927772681  0.495217144
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H  0.372985692  6.043967408  0.041365395
H  1.563874480  4.210522342  1.323292373
H  2.031791589  3.466358743 -0.225744279
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1cA'

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H 2.972405155 4.233751870 -0.872437865
H 3.449041340 3.372067184 -2.345324983
H 2.653999768 5.558564956 -2.923474845
H 1.445335061 4.418516227 -3.529413791
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H 0.677899752 0.975714070 -2.165849514

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1cG

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N -1.726717788 0.439677692 -1.325276148
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H 1.514029759 3.486443544 0.762848295
H 1.409090971 5.255523860 0.847770111
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1b-TSA

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1b-TSG

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N	0.366409752	2.970545519	0.868381354
C	1.574429826	2.578809426	1.210567711
N	1.778213809	1.257767547	0.903628973
N	-1.165923728	-1.864150023	-1.061766698
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H	-2.674022212	0.174491061	-1.032570819
H	2.331354811	3.192538408	1.677021420
H	2.619572069	0.721248915	1.068559882
H	-0.460525620	-2.584950364	-1.062639010
H	-2.027325946	-2.031432103	-1.555261752
C	-0.756126706	4.740669784	1.042292741
C	-0.845697449	5.340125748	-0.294822849
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C	-1.205755455	7.595831917	0.773309427
C	-1.011859461	8.553022707	-0.403269740
Cl	-2.560500604	9.119906892	-1.139727374
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H	-1.577721779	4.124972627	1.374364490
H	-0.085785684	5.165441326	1.776621917
H	0.055863792	5.806350119	-0.690094329
H	-1.367466822	4.750548832	-1.046037401
H	-1.873670331	8.040165502	1.515982833
H	-0.224544961	7.476251211	1.250208559
H	-0.425801709	8.101027845	-1.206141277
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H	0.165006409	1.483986304	1.010673272
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H	-1.697513907	2.111562003	-0.953891778
H	-2.453338166	0.628166490	-1.520879601
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H	-3.053492335	0.117994696	0.959460820
C	-1.557994358	-3.872992241	-1.434764185
C	-0.486702809	-3.045647764	-1.768046195
C	-0.296377777	-1.823791507	-1.119920957
C	-1.176317578	-1.411037177	-0.105272764
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C	-2.433439641	-3.474453475	-0.422502657
H	-1.699052775	-4.821595044	-1.942081844
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H	-2.890035304	-2.006401077	1.078170040
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H	-5.346200759	-1.740743897	-1.813407414
H	-3.878603223	-1.065835876	-1.214664757
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C	0.286921565	0.369767442	0.441224260	H	0.601957463	2.724704780	-3.942086663
C	0.522825948	-0.237586826	1.828777673	H	0.269648225	3.549756641	-2.405000395
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C	-2.575678496	1.088696028	-1.426920010	H	0.247471021	-0.881707674	-0.221949793
C	-2.137495085	0.464923244	-0.075065980	H	1.511120491	1.293764894	-0.255500522
H	1.184111092	0.254244135	-0.172368287	H	-0.026227677	2.227982896	-0.274574605
H	0.129226751	1.447503111	0.542374668	C	3.350906102	-0.662048393	-4.312410715
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H	-0.333578514	-0.074993477	2.486207284	C	1.008498569	-0.609488026	-3.699301798
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H	-2.926648382	-0.200361715	0.292266760	C	3.634282549	0.251005833	-3.297844709
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C	0.428538146	-2.146981288	-0.993449377	H	2.853875587	1.480599728	-1.728250935
C	-0.810667178	-1.502745665	-0.802285332	H	4.651718189	0.592836295	-3.138377604
C	-1.976783925	-2.178026733	-1.213166094	H	3.303962371	2.164560612	2.117400223
C	-1.895426988	-3.443105185	-1.794911618	H	1.681975497	2.314675588	1.700731087
H	-0.610685711	-5.055771075	-2.438041635	H	3.583292598	-0.466792188	5.551923743
H	1.461782348	-3.877625941	-1.709819313	=====			
H	1.355265713	-1.674563081	-0.691111523	2b-TSG			
H	-2.959606043	-1.744631671	-1.073186756	=====			
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2b-TSA							
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N	-0.179071554	-0.121882547	2.085558257	N	-0.035876023	-0.276185238	1.947566288
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C	2.149422560	0.734297436	2.868320073	C	2.382104571	0.402791043	2.469308030
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C	0.770498362	-0.782230259	4.064321428	C	0.749316186	-0.416851294	4.079905954
C	-1.001442169	-0.920199109	2.746472816	C	-0.985279312	-0.729768089	2.735088216
N	-0.492294345	-1.329588863	3.941957158	N	-0.560448797	-0.832782559	4.035519347
N	2.441980196	1.674892378	1.897763460	N	3.636291417	0.202640339	5.924146032
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C	-0.168949819	2.949537226	-3.204683518	H	3.345156072	-0.108607877	6.837984476
Cl	-1.409805684	3.970555653	-4.013488154	H	4.605337479	0.431442479	5.777407283
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H	-1.201074491	1.061201067	-3.477860197	C	-0.882718267	1.460585432	-2.542175538
H	-1.632499918	1.900410267	-1.987375078	C	-0.635329964	2.830715253	-3.179680915
				Cl	-2.161141746	3.416568278	-3.933896922
				C	0.450148380	1.446225201	-0.435841929
				H	-1.193309314	0.731176454	-3.291052266
				H	-1.697210848	1.537089943	-1.818088254

H	0.124035662	2.784235635	-3.960039461	H	7.891474442	6.890342507	-1.331594252
H	-0.333203988	3.569008625	-2.434287572	H	9.769482460	6.345060837	-2.799336729
H	-1.058675882	-0.167056090	-0.263787759	C	8.001432762	6.247271792	-3.952064543
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H	1.459661786	1.684794269	-0.118023599	O	8.164737508	5.603007572	-5.109721181
H	-0.255516794	2.240559365	-0.200545408	O	7.257733052	7.193569451	-3.816140909
C	3.694639516	-0.365431813	-4.034316304	H	8.787314910	4.865513455	-4.902721935
C	2.460665442	-0.200040006	-4.660524030	H	10.255765126	4.138104692	-2.781907181
C	1.350821937	0.239399205	-3.940103545	H	8.689531595	3.642521763	-2.829852442
C	1.472352491	0.530659536	-2.573707999	C	2.620858345	-0.337216754	2.895954687
C	2.708709279	0.353645223	-1.936226755	C	1.236519837	-0.491364653	2.610954811
C	3.806898752	-0.091045203	-2.672543821	N	0.631916890	-1.581154971	3.106317444
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H	2.350433132	-0.413017457	-5.719139929	N	2.605193718	-2.397090021	4.208398827
H	0.408455124	0.350646181	-4.461836338	C	3.195900016	-1.326676411	3.702789153
H	2.838911607	0.533823035	-0.875512057	N	3.636247836	0.584657685	2.592176999
H	4.757979215	-0.221707857	-2.165901249	C	4.756946544	0.167961648	3.185666058
=====				N	4.528920837	-0.967340467	3.861858470
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N	3.585854597	2.413569536	-0.703027355	H	5.706161430	0.680040278	3.130416055
C	3.644484804	1.270036248	0.168262664	H	5.207023640	-1.484449479	4.409883062
C	3.577631661	1.721016211	1.653864310	H	-0.498479324	0.124187328	1.807245859
C	2.360809030	2.623128117	-1.471193096	H	0.755217567	1.298661442	1.682528119
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Cl	0.904596841	2.331629998	-3.767238203	3cG			
H	4.553471548	0.672210310	0.019101539	=====			
H	2.801167923	0.608304358	-0.047404069	N	0.857759181	-1.202197839	-0.597639089
H	2.664121368	2.284676509	1.851247583	C	1.354466949	-0.267255946	-1.598812549
H	4.415983657	2.382319378	1.881723766	C	2.366750556	-0.917455590	-2.550195120
H	2.091228789	3.682124139	-1.492570545	Cl	2.991755827	0.304943303	-3.725262059
H	1.538554451	2.111887121	-0.961228564	C	1.591263483	-1.277657967	0.639742151
H	3.243682243	2.604838871	-3.467311320	C	0.948018593	-0.363739453	1.718122230
H	2.681013525	1.013619640	-2.909613297	C	-0.210521415	-2.084243026	-0.875354354
C	6.989282496	4.941256256	-1.234131143	C	-0.821975813	-2.110305285	-2.142968602
C	7.076256028	3.743548373	-0.518231263	C	-1.879507325	-2.979166405	-2.407332180
C	5.972322761	2.905187218	-0.342948761	C	-2.376528527	-3.858665961	-1.439495153
C	4.718469322	3.238185096	-0.888041041	C	-1.765966688	-3.821055423	-0.179890942
C	4.630057319	4.441005661	-1.617572489	C	-0.712722282	-2.957077834	0.109144142
C	5.736331466	5.266049502	-1.779941153	C	-3.481912671	-4.844794941	-1.736722039
C	8.190865039	5.842854542	-1.428723683	C	-2.954124098	-6.213362475	-2.220390889
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H	6.116337508	1.982242858	0.209360594	H	1.836065373	0.575732426	-1.091628931
H	3.694576629	4.750885255	-2.067390025	H	3.227654134	-1.312990575	-2.007311681
H	5.630745753	6.184061771	-2.348831689	H	1.913857950	-1.724358454	-3.126680171
H	8.933563455	5.639835614	-0.648934526	H	1.636301051	-2.304595040	1.013299705
C	8.884746420	5.695611448	-2.805940606	H	2.623473241	-0.947638407	0.473752514

H	0.828824200	0.650805175	1.332090720	H	2.533069370	0.963242918	1.513737626
H	-0.029957639	-0.745916669	2.011298591	C	-0.815696985	4.907576556	0.702757714
H	-0.482694115	-1.460654460	-2.940751015	C	-0.751932955	5.462707601	-0.650007432
H	-2.331087359	-2.956407672	-3.396130401	N	-1.510552368	6.496711802	0.080537609
H	-2.129318082	-4.476109086	0.608299283	C	-0.791107590	7.745927935	0.442718991
H	-0.306400162	-2.970671053	1.113560722	C	-0.337764781	8.609851607	-0.730721610
H	-4.088137284	-5.029418105	-0.845546310	Cl	-1.703059107	9.256898719	-1.707732990
H	-4.162296439	-4.442468236	-2.498591523	C	-2.960135573	6.521603231	-0.017674109
C	-4.062445220	-7.291675559	-2.154860024	H	-0.097186627	5.218045105	1.447544593
O	-3.952107851	-8.229673676	-3.103091094	H	-1.709243416	4.398046370	1.032882031
O	-4.918122159	-7.303985194	-1.300927723	H	-1.307414067	4.961083181	-1.438154847
N	-2.337721137	-6.242886926	-3.555004254	H	0.219931702	5.798918469	-1.003933442
H	-2.187103439	-6.555117008	-1.512576990	H	-1.446150062	8.316079265	1.102149352
C	1.920383832	-1.240747718	3.922867944	H	0.102585927	7.473659467	1.016786580
C	1.290644987	-2.521950259	4.104901767	H	0.214262857	9.465568841	-0.336112028
N	1.772241522	-3.115558113	5.302151523	H	0.318994749	8.067941434	-1.414181017
C	2.699953752	-2.572024424	6.165848843	C	-3.619946006	6.265504775	-1.219033101
N	3.263724734	-1.385181225	5.968666768	C	-5.016489876	6.301971395	-1.258522404
C	2.838938780	-0.780275233	4.856679380	C	-5.773473516	6.609054594	-0.120927677
N	1.777545685	-0.267295893	2.939825914	C	-5.085481133	6.861413502	1.077609204
C	2.584033759	0.744292301	3.251235480	C	-3.697651609	6.807232401	1.137247947
N	3.236945229	0.465319528	4.402234127	C	-7.284242259	6.690134627	-0.175411011
N	3.042375513	-3.282954265	7.251432280	C	-8.009186591	5.619932734	0.671592715
O	0.472410565	-3.084693112	3.400249637	C	-9.516676965	5.966872979	0.676080608
H	1.365213735	-4.025622273	5.493295639	N	-7.815074806	4.273899050	0.116301577
H	2.694444790	1.651851029	2.677787114	O	-9.947663683	6.922279117	1.274829191
H	3.900844503	1.072355310	4.868019059	O	-10.267735640	5.144741394	-0.064708996
H	2.653862066	-4.187262573	7.467294695	H	-6.896046923	4.169592896	-0.303091672
H	3.719032230	-2.881222023	7.883544653	H	-9.644483384	4.478005831	-0.433725800
H	-1.385773130	-5.891309604	-3.534587939	H	-7.899112319	3.564901109	0.839932142
H	-2.859792607	-5.659420871	-4.205809296	H	-7.618097080	7.664345487	0.196155138
H	-3.194293074	-7.941296923	-3.663235455	H	-7.625373600	6.607572143	-1.213344050
=====				H	-7.673719102	5.711284814	1.713145023
3b-TSA				H	-3.064873987	6.087179289	-2.134524972
=====				H	-5.520781632	6.122387607	-2.203856176
C	-0.344260521	1.699480384	0.344170291	H	-5.643657768	7.105213039	1.977114401
C	-1.555998374	1.234762831	-0.216518736	H	-3.188472528	6.989873695	2.079212619
N	-1.717808339	-0.083130890	-0.382024555	H	-3.332903974	1.593016511	-1.088571696
C	-0.730257142	-0.917683127	-0.019835219	H	-2.415550314	3.012619568	-0.792748213
N	0.460105044	-0.606840118	0.502010857	=====			
C	0.593798532	0.707041694	0.661274108	3b-TSG			
N	0.170376254	2.950212293	0.674821985	=====			
C	1.370690728	2.715236710	1.168858155	C	-0.173840217	1.830340230	0.380421318
N	1.677898282	1.388634419	1.180980099	C	-1.476472356	1.578641879	-0.159881980
H	-0.925163288	-1.974810463	-0.178825830	N	-1.592477381	0.210983786	-0.526514906
N	-2.597091248	2.048603442	-0.565017472	C	-0.607477397	-0.748502574	-0.398788339
H	2.054344376	3.469041279	1.534658335	N	0.591625648	-0.495549572	0.093944113

C 0.745053899 0.787911269 0.466195688
 N 0.378539179 2.997038539 0.873530623
 C 1.598657140 2.680109754 1.247619482
 N 1.869927418 1.353715988 1.019781031
 N -0.910228952 -2.008305699 -0.783144724
 O -2.413334862 2.354435558 -0.322975272
 H -2.503352168 -0.039461704 -0.894453929
 H 2.322403687 3.352051597 1.686116842
 H 2.731904888 0.866770325 1.225680381
 H -0.167256923 -2.689452546 -0.747080787
 H -1.741185180 -2.233071980 -1.305263327
 C -0.815470671 4.841200733 0.892517638
 C -0.848073953 5.300945506 -0.493312178
 N -1.611689871 6.367825276 0.186006910
 C -0.887805876 7.631359161 0.484084782
 C -0.326630474 8.386509264 -0.718264097
 Cl -1.590251607 8.954977800 -1.866203762
 C -3.058480812 6.410625024 0.075817494
 H -0.116654168 5.259207268 1.601461495
 H -1.651926006 4.255251121 1.246499682
 H -1.443374224 4.688119103 -1.163603983
 H 0.080925998 5.637556074 -0.947549287
 H -1.572275936 8.269977985 1.042996602
 H -0.040438655 7.403786463 1.142073287
 H 0.200098411 9.270155479 -0.351539681
 H 0.380869187 7.786680573 -1.293653876
 C -3.709857825 6.074794141 -1.109601690
 C -5.101271954 6.163097262 -1.181068911
 C -5.866187041 6.600028992 -0.092563129
 C -5.190278060 6.921364824 1.096034808
 C -3.805853104 6.818324696 1.187819264
 C -7.370457378 6.740604451 -0.202911088
 C -8.174728867 5.763776761 0.684874344
 C -9.672250441 6.124464591 0.539432815
 N -7.966607940 4.367816304 0.273957377
 O -10.136273325 7.137795888 1.004262874
 O -10.375828985 5.238003771 -0.174990522
 H -7.026601355 4.219083224 -0.082186375
 H -9.730535148 4.533980558 -0.419268897
 H -8.093764420 3.735259348 1.059461568
 H -7.677480284 7.751175401 0.085007457
 H -7.677243303 6.598081980 -1.245231007
 H -7.913031577 5.947586136 1.735270808
 H -3.148225116 5.779195105 -1.988954785
 H -5.595411006 5.918273661 -2.117113287
 H -5.753153998 7.260364279 1.961389281

H -3.307038056 7.058551771 2.122478402

=====

1b'

=====

N -1.248752756 0.340560872 -0.584880493
 C -0.152465855 0.795718240 -0.072271324
 C 1.149776908 0.079431008 -0.019446364
 C -2.503093624 1.147208672 -0.540490664
 C -3.497703287 0.601979194 0.492566222
 Cl -4.937601357 1.666575998 0.489815811
 C -1.354778021 -0.989044875 -1.221332570
 H -0.220345611 1.793054172 0.359734980
 H 1.880176216 0.676370936 0.526558306
 H 1.049379320 -0.894151992 0.473545809
 H -2.940153681 1.131651029 -1.541580935
 H -2.236898539 2.176954225 -0.297002153
 H -3.068667903 0.612315832 1.496716870
 H -3.833484494 -0.407748554 0.252169879
 H -0.368074202 -1.408865157 -1.399601662
 H -1.882036634 -0.875448418 -2.170332765
 H -1.924056572 -1.657111958 -0.570635067
 H 1.540038811 -0.099002179 -1.029580501

=====

1b'-TS

=====

N 0.205795084 2.997870173 -0.049373028
 C -1.170455348 2.830511566 0.347862656
 C -2.040396345 2.551836537 -0.790179025
 C 0.579284087 3.952542127 -1.108047879
 C 1.245545712 2.139246731 0.526872859
 C 1.485978940 0.848261009 -0.283987945
 Cl 2.820127210 -0.141762652 0.563804605
 H -1.263098571 2.039139371 1.118439932
 H -1.513736302 3.739133435 0.879305784
 H -3.011820041 3.029700728 -0.901664605
 H -1.669107143 1.970500410 -1.631267153
 H 0.805020385 3.469287092 -2.065565313
 H -0.241489833 4.660261105 -1.267471501
 H 1.472211035 4.496086191 -0.784154689
 H 2.175180263 2.715019182 0.568103567
 H 0.951871478 1.875098993 1.549922923
 H 0.605304783 0.206159932 -0.318833625
 H 1.847538424 1.057516034 -1.290548495

=====

4a

=====

N -1.843990920 0.763577807 -0.299385448

C	-0.390448405	0.574116289	-0.395450892
C	0.056758191	-0.788692086	0.139365951
Cl	1.870249192	-0.895236722	0.112127394
C	-2.237589421	2.178191813	-0.273614191
C	-3.476020122	2.358851008	0.603804484
Cl	-3.993896755	4.099236019	0.629752278
C	-2.590293784	-0.000913008	-1.310263542
H	-0.023411694	0.694001857	-1.430587501
H	0.097187091	1.342576565	0.209707358
H	-0.258601928	-0.928070165	1.173615319
H	-0.302713093	-1.621390698	-0.460321061
H	-2.428520940	2.587231483	-1.278956885
H	-1.424703728	2.768480674	0.156429990
H	-3.265531823	2.068829774	1.633394460
H	-4.331395711	1.787645450	0.239710515
H	-3.565994408	0.483464648	-1.436904758
H	-2.095440007	0.059147677	-2.296243078
C	-2.823409642	-1.458734378	-0.952610487
C	-3.181220492	-1.831103925	0.349948338
C	-3.404736909	-3.169129626	0.669905516
C	-3.277974175	-4.157262318	-0.309004272
C	-2.927997169	-3.796453831	-1.610049785
C	-2.701912086	-2.455472824	-1.927073031
H	-3.256283491	-1.064881844	1.115234493
H	-3.673313090	-3.442733468	1.686530563
H	-3.443669064	-5.200572017	-0.056487849
H	-2.819501173	-4.557917006	-2.377110760
H	-2.414214336	-2.181955242	-2.939648215
=====			
4a-TS			
=====			
N	-1.391486004	0.143494035	-0.158890104
C	-0.069308590	0.776390054	-0.406999377
C	1.047263961	0.249260435	0.495962466
Cl	2.551456022	1.192942546	0.155617931
C	-2.629643148	1.102384000	0.009065546
C	-2.125263596	0.458908160	1.193997003
Cl	-4.393409417	1.834241138	2.090831661
C	-1.680654894	-1.158269091	-0.842370846
H	-0.183187672	1.850106643	-0.240835196
H	0.187040074	0.628850706	-1.460226999
H	0.810856925	0.391564919	1.551073047
H	1.278154504	-0.797060132	0.312095399
H	-3.531698293	0.722417256	-0.452249080
H	-2.397456225	2.143113809	-0.177218013
H	-2.664877671	-0.383217938	1.604821285
H	-1.524577964	1.028223294	1.891603804
=====			
C	-0.751773396	-2.290105284	-0.475704522
H	-1.646297540	-0.962449535	-1.919035554
H	-2.713521267	-1.404704186	-0.582295129
C	0.221683448	-2.726025290	-1.383779467
C	1.094562200	-3.761604195	-1.046218573
C	0.999536253	-4.373785094	0.204054946
C	0.022066268	-3.956257962	1.110629016
C	-0.852158570	-2.925227724	0.771080904
H	0.297802627	-2.253774459	-2.360279540
H	1.845455078	-4.089115616	-1.758805308
H	1.678904147	-5.178232374	0.469265810
H	-0.063577534	-4.438293425	2.079764335
H	-1.616825940	-2.616729863	1.478751218
=====			
4b			
=====			
N	-1.844284131	0.515748754	0.195960054
C	-0.820278457	0.350966235	1.274410807
C	-2.251617765	0.252841108	1.616441672
C	-2.078742971	1.904266222	-0.322714638
C	-3.544870774	2.147833931	-0.678551046
Cl	-3.715236715	3.844628711	-1.233440463
C	-1.931454019	-0.590412617	-0.879671456
H	-0.244025570	-0.565482119	1.188223448
H	-0.257115790	1.247687056	1.511793092
H	-2.687147848	-0.725089338	1.781831832
H	-1.433725835	2.041726160	-1.195413324
H	-1.763452490	2.609011987	0.450739484
H	-3.894197827	1.504479046	-1.488080809
H	-4.195408108	2.009691894	0.188578688
H	-0.902537484	-0.745704490	-1.214121057
H	-2.485969972	-0.133504880	-1.700467487
C	-2.595530956	-1.849336351	-0.397964175
C	-1.839702296	-2.963498899	-0.002908541
C	-2.477901562	-4.122240408	0.446834633
C	-3.871386918	-4.172956699	0.508139737
C	-4.632514188	-3.067892009	0.115264845
C	-3.998686640	-1.915424292	-0.336388827
H	-0.754077125	-2.935873766	-0.055106966
H	-1.886818633	-4.984060702	0.741615876
H	-4.367975758	-5.075843921	0.851414715
H	-5.717039954	-3.111414423	0.151175150
H	-4.597906164	-1.061223026	-0.644570574
H	-2.749038662	1.090813760	2.095054835

Table S2. Frequencies (in cm^{-1}) for Mechlorethamine , Phenyl Mustard, Melphalan drugs, intermediates and their adducts with guanine and adenine.

=====	1313.84 1325.08 1360.85 1364.92 1374.31 1396.06
1a	1402.93 1404.65 1425.01 1450.40 1472.05 1491.67
=====	1499.67 1501.35 1509.46 1530.07 1560.78 1611.64
32.72 57.29 68.08 115.44 150.80 192.40	1661.22 1673.25 1861.49 3048.25 3059.45 3068.32
233.33 240.05 316.65 398.26 433.67 495.62	3076.97 3106.35 3108.31 3114.24 3114.62 3119.60
732.55 747.47 777.61 782.92 876.03 1029.20	3166.17 3172.32 3173.89 3202.13 3220.62 3222.44
1041.73 1047.56 1068.17 1073.56 1133.85 1148.68	3406.04 3494.17 3595.77
1168.66 1264.89 1273.40 1297.11 1297.96 1338.57	
1350.50 1392.56 1423.40 1476.59 1495.09 1498.44	=====
1503.88 1512.13 1516.72 1521.20 2961.69 2983.48	1b
2991.38 3092.03 3101.50 3109.86 3111.75 3116.16	=====
3132.66 3177.03 3177.86	79.02 94.26 164.43 211.15 260.93 353.07
=====	379.26 406.69 454.02 702.78 776.74 797.87
2a	798.81 839.74 944.99 980.33 1025.14 1053.51
=====	1072.91 1120.95 1154.81 1165.10 1186.74 1202.92
25.85 44.23 51.14 54.45 115.26 135.38	1225.60 1285.44 1311.48 1321.70 1369.00 1415.72
203.99 219.79 228.24 249.82 287.92 366.42	1466.81 1491.43 1494.57 1507.05 1509.20 1515.02
401.63 429.29 516.41 555.38 566.52 630.09	1533.08 3088.82 3095.12 3103.09 3151.53 3169.98
707.02 726.59 753.98 763.07 766.67 777.98	3172.21 3173.78 3186.35 3191.70 3269.25 3278.08
787.99 822.90 882.15 962.38 984.45 987.81	=====
1001.42 1033.92 1036.58 1038.82 1060.59 1085.00	2b
1121.89 1160.01 1191.87 1210.74 1227.23 1252.72	=====
1288.88 1290.41 1313.15 1323.89 1362.41 1374.66	47.49 64.86 89.35 125.62 161.97 209.03
1397.05 1398.08 1421.00 1496.77 1500.84 1503.17	242.23 305.21 337.47 370.25 418.80 489.28
1510.67 1533.56 1545.94 1631.86 1663.85 3067.58	503.22 564.14 622.51 704.60 709.04 775.32
3074.75 3107.58 3107.64 3111.90 3118.78 3173.27	778.06 790.85 804.08 847.58 859.57 903.16
3173.80 3179.34 3185.67 3207.52 3222.80 3224.85	936.51 961.60 991.59 1015.04 1028.60 1034.11
=====	1048.14 1070.81 1077.52 1115.53 1138.19 1143.47
3a	1177.88 1196.98 1199.30 1205.41 1213.86 1272.47
=====	1287.35 1308.46 1350.96 1359.65 1367.49 1411.85
17.43 25.16 29.03 40.36 49.75 65.99	1486.15 1498.75 1500.64 1510.74 1520.41 1533.16
84.50 90.57 116.47 138.07 166.17 185.72	1642.95 1654.37 3097.59 3105.36 3158.38 3174.27
221.67 224.84 251.51 286.22 306.83 333.68	3175.85 3178.33 3198.24 3201.93 3213.11 3222.67
349.13 364.56 379.10 397.88 432.35 481.67	3230.12 3274.50 3283.21
523.32 529.62 552.17 558.34 607.75 648.73	=====
686.92 729.22 739.02 754.91 770.28 777.24	3b
784.76 792.85 820.67 835.11 857.91 876.70	=====
918.20 934.35 949.86 982.03 987.79 1023.38	17.93 34.87 49.06 65.24 78.03 90.18
1033.36 1034.90 1036.56 1038.43 1078.67 1092.25	101.17 123.68 150.92 179.66 206.66 237.00
1154.49 1165.40 1175.69 1205.19 1222.45 1227.95	289.30 291.25 327.14 337.61 355.86 386.13
1237.28 1249.16 1253.42 1288.33 1290.86 1294.45	402.43 426.03 440.29 495.76 521.04 541.88

551.17 603.19 642.26 657.61 732.26 763.16
771.80 781.86 794.73 803.64 829.62 840.39
849.07 860.47 876.15 886.48 901.49 913.76
954.82 972.81 1007.09 1028.76 1033.08 1037.06
1070.20 1077.98 1100.28 1137.11 1143.30 1147.53
1171.23 1177.68 1197.78 1210.90 1215.41 1217.86
1233.51 1244.64 1272.60 1287.60 1291.83 1306.89
1349.14 1359.52 1364.69 1374.46 1406.29 1412.09
1431.19 1459.35 1486.25 1494.18 1500.08 1510.40
1521.64 1543.81 1635.83 1650.37 1666.26 1857.01
3061.09 3073.31 3097.13 3104.74 3128.15 3158.17
3174.27 3175.24 3177.98 3192.05 3195.32 3205.87
3231.00 3274.35 3282.99 3483.72 3517.18 3610.64

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1a-TS

=====

-249.47 37.22 79.38 87.64 144.78 182.83
188.99 256.80 269.81 327.80 365.90 403.53
508.49 633.50 776.88 789.02 803.28 918.57
960.06 961.59 1045.64 1060.66 1062.48 1073.49
1138.95 1166.67 1203.38 1247.87 1276.11 1304.42
1307.80 1356.61 1410.29 1465.30 1466.46 1497.47
1506.47 1507.09 1517.18 1523.33 3065.47 3078.41
3105.11 3136.00 3146.34 3165.79 3171.03 3202.67
3203.86 3301.82 3315.92

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2a-TS

=====

-354.23 43.81 54.56 63.78 73.41 126.06
161.63 175.02 209.66 245.14 273.02 329.98
370.06 416.04 428.66 481.15 527.17 571.59
626.31 711.74 712.33 754.34 774.03 786.93
794.19 859.59 881.99 909.50 945.31 995.72
1002.08 1008.77 1010.50 1033.78 1051.47 1059.66
1077.96 1120.09 1137.08 1151.37 1197.57 1200.60
1223.05 1240.07 1276.51 1292.62 1299.71 1350.29
1362.37 1388.87 1405.13 1484.14 1498.19 1509.60
1516.34 1532.24 1548.46 1648.09 1655.61 3101.37
3114.58 3147.43 3152.04 3162.83 3181.22 3193.27
3195.60 3206.70 3217.90 3228.80 3267.88 3326.87

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3a-TS

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-358.32 15.79 27.60 36.83 41.17 45.39
53.97 71.61 81.42 120.81 135.35 152.89
186.57 203.09 229.39 245.13 273.38 286.74
316.59 330.21 342.59 378.98 398.16 431.74
462.51 473.30 492.42 537.14 582.65 604.93
620.89 644.07 678.13 737.55 755.41 756.65
775.89 798.23 817.14 830.65 845.28 863.57
881.18 888.26 901.95 919.52 966.43 995.80
1011.56 1018.82 1029.01 1032.38 1059.73 1082.28
1099.87 1124.55 1135.42 1143.59 1175.19 1205.41
1208.22 1210.54 1226.56 1250.71 1262.37 1272.22
1290.23 1299.84 1302.85 1341.12 1352.66 1358.89
1365.56 1379.92 1411.52 1431.65 1464.96 1486.82
1501.86 1509.72 1515.63 1532.06 1558.45 1630.48
1659.28 1664.80 1854.59 3050.14 3084.10 3088.89
3104.25 3117.18 3138.10 3141.22 3162.71 3182.37
3189.00 3192.22 3198.96 3224.21 3264.80 3329.64
3507.98 3601.72 3755.73

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G

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139.94 163.77 203.25 315.31 330.60 334.68
363.22 485.47 525.62 539.43 563.51 602.48
624.91 663.58 668.23 703.08 731.48 780.59
818.96 836.22 946.90 1047.92 1076.00 1077.57
1146.11 1179.99 1312.86 1337.67 1371.03 1394.98
1449.76 1526.18 1568.37 1619.72 1625.68 1673.60
1832.46 3262.81 3582.02 3605.03 3665.32 3700.08

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170.11 211.79 248.92 287.15 315.39 523.15
532.00 560.51 599.09 608.65 617.99 681.51
694.61 721.33 818.27 866.38 896.82 938.55
994.26 1019.76 1087.68 1144.57 1244.10 1264.77
1313.38 1353.06 1370.10 1419.27 1433.20 1500.75
1511.96 1606.42 1630.50 1666.29 3118.39 3203.81
3558.19 3596.51 3699.18

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1cG

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17.11	39.97	57.84	67.95	77.65	118.93
141.35	155.97	168.16	193.87	203.90	211.28
244.74	282.13	298.68	326.48	345.79	369.04
395.76	425.59	444.67	476.13	483.76	514.03
555.67	613.91	627.23	635.39	651.59	661.26
686.52	703.25	729.65	758.87	772.95	783.56
795.30	819.50	846.39	954.45	971.87	1026.07
1029.22	1048.31	1066.02	1073.98	1080.70	1092.99
1137.35	1139.23	1152.44	1167.27	1218.67	1235.98
1254.26	1272.54	1300.41	1318.46	1331.82	1343.19
1370.91	1399.25	1407.57	1416.30	1423.80	1456.73
1474.32	1475.25	1495.54	1501.22	1509.40	1510.16
1518.01	1524.97	1571.07	1590.80	1614.95	1665.70
1692.24	1823.76	2984.41	2994.13	3006.35	3086.78
3091.59	3101.16	3112.98	3115.70	3131.26	3154.29
3168.88	3328.76	3586.41	3617.69	3634.54	3746.69

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1b-TSG

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-431.07	16.31	36.93	47.83	51.09	100.68
105.83	119.88	126.67	162.73	169.88	182.60
204.97	229.19	255.70	302.25	317.04	346.95
349.35	365.94	409.07	429.49	460.90	494.55
527.42	540.19	601.53	627.65	635.59	657.03
665.24	671.30	705.14	730.34	735.36	764.87
784.77	826.13	837.47	901.52	948.06	968.03
1025.53	1031.38	1048.07	1057.07	1076.61	1083.86
1116.16	1125.69	1151.37	1157.18	1166.05	1188.68
1206.22	1230.74	1246.25	1296.95	1325.85	1329.60
1335.30	1359.35	1376.68	1387.36	1406.05	1416.88
1446.19	1449.34	1474.38	1484.39	1487.98	1502.60
1521.35	1524.49	1536.89	1574.10	1614.22	1647.61
1687.99	1790.55	3044.33	3064.49	3079.35	3118.18
3125.03	3142.03	3146.20	3159.76	3203.10	3215.84
3282.99	3343.29	3593.73	3621.09	3643.06	3750.89

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1cA

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15.10	27.35	53.19	55.74	90.35	100.57
125.43	162.39	179.99	202.96	233.75	246.94
278.84	293.96	331.98	352.24	376.65	422.83
470.67	495.29	522.58	536.14	549.25	553.86
576.55	628.64	667.65	669.71	685.63	752.98
761.53	791.46	803.24	812.35	826.20	892.26

940.87	958.89	999.24	1008.62	1026.09	1055.75
1061.42	1074.71	1091.93	1130.38	1139.05	1176.19
1188.99	1202.58	1234.53	1256.13	1278.59	1295.02
1305.19	1317.71	1345.07	1352.21	1376.91	1386.28
1394.44	1414.19	1421.94	1442.63	1474.33	1489.03
1496.08	1504.77	1508.15	1509.30	1517.21	1519.88
1527.19	1593.03	1621.71	1657.11	1690.96	2997.96
3002.66	3028.36	3078.37	3080.57	3092.93	3110.38
3113.03	3136.40	3141.80	3159.64	3213.25	3323.46
3603.73	3627.03	3751.43			

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1cA'

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24.65	46.49	67.75	71.88	96.02	123.39
160.50	186.71	208.99	226.00	250.44	278.52
294.97	326.91	360.84	402.40	431.21	493.90
506.83	523.16	543.87	546.91	574.29	600.12
637.35	666.03	667.02	671.27	692.55	740.25
749.83	765.69	802.65	843.00	892.24	894.47
932.18	956.75	977.61	999.64	1036.44	1052.36
1059.69	1080.85	1104.60	1134.33	1139.65	1157.06
1190.56	1205.18	1244.01	1259.79	1283.39	1296.61
1307.33	1334.85	1351.07	1362.93	1384.66	1398.34
1404.43	1415.48	1434.46	1444.96	1470.00	1485.65
1489.95	1493.97	1496.37	1508.78	1515.04	1519.03
1529.99	1595.64	1616.44	1661.26	1699.83	2967.45
3001.01	3014.42	3091.20	3099.66	3107.46	3113.87
3118.83	3151.89	3155.87	3175.27	3212.47	3299.19
3371.36	3625.81	3650.99			

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1b-TSA

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-435.81	26.18	44.00	47.01	104.95	109.23
136.90	142.58	169.64	195.44	211.40	222.44
254.95	273.13	299.11	314.02	352.90	389.61
418.33	429.46	513.44	526.21	535.53	549.71
594.81	617.46	650.28	664.74	667.62	720.88
731.78	751.71	772.12	826.69	866.40	896.53
908.55	945.95	959.67	996.34	1011.03	1025.89
1050.84	1065.74	1067.27	1092.50	1121.01	1140.29
1149.84	1150.84	1188.49	1232.00	1248.72	1261.15
1266.24	1296.06	1303.65	1310.56	1320.93	1341.49
1354.19	1366.54	1407.59	1417.13	1442.23	1462.44
1468.80	1486.76	1494.15	1503.45	1506.22	1512.95
1523.75	1527.27	1619.56	1634.27	1659.14	2999.54

3029.41 3098.45 3108.54 3112.50 3115.82 3143.61
3158.99 3178.91 3191.12 3213.16 3249.46 3334.32
3527.12 3619.65 3624.29

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2cG

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19.14 25.93 33.42 47.68 50.97 59.71
88.66 114.41 135.61 159.11 191.15 196.76
206.36 221.58 230.67 233.58 286.63 289.61
345.07 364.43 382.74 403.48 412.71 427.30
481.36 486.96 510.05 527.70 562.27 569.38
614.31 630.80 633.49 639.25 652.82 667.90
703.21 711.05 724.56 730.80 755.72 768.47
773.75 776.01 786.57 787.25 815.44 836.77
852.47 903.65 971.93 991.23 999.47 1005.52
1015.75 1027.72 1033.95 1046.25 1066.57 1081.39
1087.18 1115.94 1127.72 1145.69 1154.84 1185.19
1195.37 1215.25 1232.05 1233.12 1262.06 1289.68
1303.39 1322.83 1332.20 1347.16 1364.25 1374.49
1380.92 1392.82 1399.21 1408.80 1421.05 1451.89
1472.99 1493.97 1500.56 1503.63 1511.44 1533.57
1546.87 1574.10 1592.20 1614.45 1637.44 1662.48
1664.45 1694.65 1822.72 3054.81 3076.18 3101.74
3105.27 3107.83 3119.51 3170.46 3171.32 3187.93
3194.35 3214.72 3224.49 3228.07 3304.67 3584.03
3615.69 3631.52 3744.33

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2cA

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16.21 26.90 41.58 48.41 58.17 66.52
80.09 110.69 148.28 194.41 208.24 218.19
240.31 253.17 260.33 277.33 352.83 367.15
385.67 418.72 432.12 453.76 477.12 523.16
538.82 546.64 555.76 565.76 568.27 606.39
629.99 635.77 665.01 689.55 699.27 714.88
748.87 770.50 775.29 788.95 790.85 803.49
807.93 844.75 848.03 894.39 914.78 976.43
981.94 995.53 999.65 1006.22 1010.37 1011.95
1043.97 1054.97 1061.34 1083.85 1116.10 1120.04
1135.73 1168.00 1189.06 1192.96 1210.05 1216.12
1243.57 1273.69 1277.69 1291.33 1307.97 1325.92
1335.08 1350.07 1357.14 1365.87 1375.71 1380.13
1399.79 1411.88 1423.04 1444.24 1489.31 1493.37
1499.19 1506.16 1512.27 1519.19 1528.46 1537.89
1597.37 1622.25 1634.37 1653.63 1656.25 1690.30

3015.47 3069.92 3099.46 3101.72 3115.27 3119.21
3156.23 3179.60 3184.89 3197.24 3201.51 3214.92
3216.10 3222.24 3298.33 3557.23 3625.04 3682.33

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2b-TSG

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-412.37 21.14 24.76 40.77 44.03 47.95
52.63 71.09 100.89 116.04 138.72 149.14
173.21 197.74 200.12 213.86 250.60 286.97
297.86 342.86 348.04 362.97 395.32 419.12
422.74 454.95 479.89 495.95 536.08 549.04
565.32 598.31 625.00 629.12 638.67 657.78
670.37 704.96 706.90 728.66 729.59 770.67
773.89 782.32 784.29 792.68 828.51 837.51
845.98 931.38 937.17 965.05 985.18 1006.83
1011.03 1015.15 1028.91 1042.74 1044.28 1064.44
1082.65 1084.80 1101.80 1118.80 1127.25 1157.80
1163.94 1187.11 1195.91 1199.29 1218.28 1234.94
1252.13 1282.57 1292.95 1305.00 1325.38 1356.03
1358.33 1366.84 1374.85 1382.58 1405.32 1416.25
1443.79 1463.33 1500.59 1507.55 1519.19 1534.50
1538.17 1550.97 1574.82 1613.98 1645.71 1647.15
1654.39 1687.98 1790.90 3097.97 3107.37 3143.25
3152.06 3175.84 3198.55 3206.04 3215.08 3218.33
3223.25 3231.59 3237.42 3279.54 3341.21 3598.12
3625.37 3645.99 3755.39

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2b-TSA

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-357.58 13.97 21.90 33.68 42.90 55.83
61.91 89.47 118.57 124.31 172.34 173.62
200.36 223.02 233.21 247.61 275.02 304.81
322.30 353.58 414.51 419.74 445.64 495.60
525.06 531.09 544.90 555.23 573.02 608.10
617.24 629.09 652.73 665.04 706.81 721.16
737.21 752.61 776.06 777.20 783.06 800.94
830.45 845.08 868.62 896.56 915.14 934.37
947.72 962.31 985.35 986.77 1013.74 1018.04
1028.81 1033.64 1040.91 1054.90 1066.39 1102.66
1115.01 1124.19 1145.49 1163.89 1187.04 1195.23
1213.00 1221.85 1250.73 1267.71 1275.02 1289.37
1305.13 1323.23 1332.67 1349.59 1354.05 1360.52
1368.90 1373.13 1393.42 1421.58 1446.38 1476.77
1495.29 1499.48 1507.97 1515.27 1533.84 1535.70
1537.03 1627.55 1644.47 1645.63 1648.74 1667.81

3093.50 3102.40 3124.60 3152.67 3172.81 3196.73
 3200.75 3207.63 3208.84 3211.32 3216.41 3223.58
 3225.83 3272.51 3332.08 3538.85 3641.06 3647.59

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3cG

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8.43 18.39 22.90 33.22 40.56 46.12
 51.92 57.03 63.46 77.12 87.10 120.13
 136.61 158.93 162.38 177.34 195.72 216.38
 224.80 231.91 239.08 249.39 287.31 308.55
 318.19 342.45 345.40 350.38 374.84 389.65
 403.77 414.50 427.79 435.43 483.46 486.69
 512.70 524.09 536.71 552.24 561.66 613.00
 615.70 633.03 640.08 653.98 654.45 667.06
 696.29 703.65 729.47 730.78 736.29 754.91
 763.86 775.19 781.63 785.46 813.91 822.39
 829.89 842.30 850.46 853.99 880.08 882.34
 922.78 955.80 972.83 991.44 1009.61 1026.43
 1028.69 1032.60 1043.26 1047.56 1081.04 1083.53
 1115.79 1119.70 1126.79 1145.28 1154.62 1169.19
 1186.77 1213.46 1224.61 1229.04 1231.03 1247.79
 1256.61 1263.87 1288.66 1289.82 1306.59 1322.97
 1333.69 1346.56 1358.42 1364.61 1372.24 1374.10
 1392.90 1403.71 1404.87 1415.76 1422.85 1431.89
 1452.17 1471.31 1472.48 1491.10 1499.65 1501.11
 1507.59 1525.84 1562.33 1574.19 1591.93 1614.29
 1620.91 1665.20 1668.03 1673.63 1693.68 1821.71
 1871.54 3039.41 3046.33 3052.15 3065.27 3101.03
 3104.86 3113.71 3117.34 3120.77 3169.35 3176.05
 3179.47 3180.38 3221.86 3223.85 3304.97 3483.00
 3505.36 3584.94 3599.06 3614.81 3630.68 3743.42

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3cA

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-7.54 2.49 24.25 27.47 29.89 42.24
 50.36 55.47 70.33 85.45 100.79 113.46
 141.55 164.30 188.22 198.38 207.23 230.66
 263.60 271.50 284.13 306.84 315.35 330.71
 344.49 354.97 369.12 375.10 380.19 402.68
 428.68 479.38 505.96 523.87 530.23 535.38
 545.71 552.34 557.58 560.98 596.52 611.23
 637.91 651.19 665.85 686.45 687.34 708.18
 730.81 759.48 768.99 773.82 785.27 787.45
 795.15 806.09 808.59 836.56 850.32 858.04
 862.05 892.21 899.15 921.18 941.91 984.42

999.82 1003.19 1008.75 1013.94 1023.25 1036.45
 1038.11 1045.39 1082.72 1096.49 1112.03 1133.68
 1160.55 1174.46 1180.09 1187.68 1205.81 1225.18
 1231.06 1235.94 1249.19 1252.98 1276.91 1286.50
 1291.49 1295.20 1309.72 1323.67 1328.46 1351.18
 1362.24 1367.79 1375.48 1376.88 1392.56 1398.60
 1405.65 1407.54 1420.70 1438.86 1442.12 1470.93
 1487.84 1491.52 1500.87 1503.99 1509.95 1519.36
 1532.84 1556.07 1593.96 1616.82 1620.69 1655.70
 1663.91 1670.92 1689.72 1860.73 3031.12 3052.86
 3062.93 3071.37 3101.06 3105.06 3109.35 3116.98
 3119.25 3158.79 3168.72 3169.09 3195.02 3213.55
 3216.25 3227.84 3297.78 3456.95 3505.17 3593.44
 3601.82 3623.43 3735.70

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3b-TSG

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-405.58 -18.23 12.21 16.75 23.91 31.85
 38.88 39.71 55.08 64.85 79.05 83.19
 110.57 117.95 133.37 138.37 160.86 168.78
 177.70 203.41 228.92 250.37 264.82 272.33
 287.70 323.81 335.13 342.78 345.18 353.31
 364.18 381.90 413.19 422.59 456.86 457.92
 489.46 506.46 527.09 538.03 549.88 584.15
 597.42 623.84 635.62 650.66 652.01 656.38
 658.23 671.21 687.29 704.49 730.13 735.40
 737.04 765.54 784.33 821.68 823.59 832.06
 838.52 842.85 851.45 864.79 880.83 900.48
 950.48 955.06 960.54 966.74 971.99 979.25
 986.10 1025.40 1030.08 1034.65 1056.95 1077.36
 1083.90 1100.38 1113.31 1116.21 1136.46 1154.81
 1160.63 1175.11 1189.73 1202.15 1215.84 1219.24
 1228.68 1231.57 1250.48 1266.11 1283.75 1296.27
 1297.02 1325.35 1331.37 1346.19 1357.10 1357.43
 1361.55 1379.20 1381.50 1391.07 1410.17 1414.72
 1431.17 1446.11 1454.20 1459.74 1485.87 1491.50
 1498.97 1516.02 1534.04 1549.48 1574.30 1614.76
 1631.76 1646.86 1659.70 1668.22 1686.66 1796.87
 1880.08 3037.77 3057.29 3061.57 3098.45 3112.83
 3146.91 3149.73 3162.20 3186.77 3192.63 3201.78
 3216.11 3216.60 3230.82 3279.59 3345.08 3477.76
 3513.14 3594.02 3596.78 3621.81 3646.98 3750.78

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3b-TSA

=====						1529.84	2951.47	2980.37	3036.56	3055.27	3105.27
-421.97	-15.58	8.04	14.25	17.88	26.39	3112.43	3123.15	3134.37	3155.28	3188.49	3272.55
33.60	37.42	55.68	64.63	79.94	83.77	=====					
113.09	119.44	143.95	167.75	171.96	211.39	4a					
227.36	245.90	261.01	266.61	278.90	307.30	=====					
311.91	322.16	340.22	347.51	350.93	381.34	20.15	41.43	44.27	65.39	73.31	84.93
411.80	422.89	455.66	496.88	518.34	526.32	120.34	156.39	216.42	226.13	233.04	278.49
533.71	534.38	549.89	558.42	585.08	609.27	350.72	386.85	418.69	450.16	493.79	504.80
618.99	648.70	651.81	656.54	663.70	687.87	620.88	633.89	714.09	732.66	748.75	756.00
688.83	727.59	734.63	736.25	772.71	815.39	781.17	792.82	830.33	866.02	900.18	925.62
819.69	830.90	836.88	847.39	853.46	863.38	980.04	984.01	1004.31	1016.66	1024.50	1047.33
873.37	896.87	901.89	951.24	951.81	957.89	1052.20	1057.31	1076.49	1108.89	1131.55	1146.41
961.71	969.93	982.17	987.65	988.92	1026.34	1187.17	1203.99	1210.97	1230.08	1245.76	1281.26
1029.25	1035.67	1050.86	1078.98	1101.38	1113.29	1296.37	1308.88	1322.03	1350.03	1361.72	1363.01
1126.47	1134.84	1151.98	1157.23	1176.03	1196.96	1394.01	1408.26	1439.01	1492.44	1495.76	1497.19
1214.67	1216.42	1228.32	1229.78	1247.17	1251.35	1504.33	1511.01	1522.41	1539.50	1643.66	1663.93
1264.63	1278.18	1284.25	1287.48	1295.62	1330.86	2956.90	2963.16	2993.59	3058.86	3101.98	3105.47
1338.08	1345.61	1358.42	1361.55	1365.34	1377.99	3116.07	3124.29	3171.58	3171.67	3181.51	3192.09
1379.58	1390.73	1407.24	1424.81	1430.32	1448.93	3199.95	3202.78	3209.40			
1458.73	1464.22	1484.20	1490.19	1498.28	1516.08	=====					
1520.28	1546.58	1549.07	1622.36	1631.32	1654.38	4a-TS					
1658.05	1666.57	1670.25	1882.18	3036.77	3060.65	=====					
3062.78	3097.21	3113.67	3145.36	3149.37	3162.02	-203.01	29.88	37.67	40.28	65.45	89.15
3189.48	3192.04	3204.18	3207.65	3208.16	3214.91	100.03	147.43	178.34	219.82	244.07	256.11
3217.34	3269.71	3336.83	3500.67	3517.30	3591.63	297.31	325.77	380.55	413.13	417.79	495.55
3597.70	3645.43	3727.78				516.83	591.50	633.98	691.93	719.77	762.19
=====						764.28	792.49	803.92	855.01	864.42	890.77
1b'						937.93	944.74	962.94	983.96	987.99	1014.08
=====						1017.02	1054.16	1056.35	1059.60	1077.04	1080.75
-65.80	26.86	76.40	84.48	149.28	253.37	1119.15	1169.79	1191.92	1198.32	1211.86	1234.84
299.35	316.54	428.09	483.09	595.36	777.49	1256.22	1285.16	1300.20	1313.29	1355.01	1365.66
788.33	808.71	850.52	1010.66	1015.98	1043.49	1377.60	1396.31	1414.55	1466.42	1494.77	1496.21
1066.93	1113.23	1131.49	1148.33	1227.48	1235.28	1500.50	1508.50	1522.70	1540.76	1642.71	1661.61
1302.73	1316.88	1389.13	1399.95	1454.79	1461.21	3069.49	3083.28	3122.97	3123.66	3138.35	3177.51
1476.77	1482.45	1495.79	1501.90	1509.36	1518.35	3186.54	3195.67	3201.86	3203.16	3205.46	3207.51
1731.13	3049.52	3086.94	3097.38	3106.79	3110.81	3215.28	3301.82	3316.44			
3155.09	3166.28	3174.08	3175.62	3190.08	3213.81	=====					
=====						4b					
1b'-TS						=====					
=====						21.05	50.91	75.52	96.00	132.42	162.86
-263.43	85.30	129.86	136.85	182.62	235.95	222.74	258.71	300.81	338.11	371.57	416.13
247.59	335.40	392.45	415.94	542.25	658.24	429.04	452.38	502.51	610.68	632.21	683.30
662.13	783.27	789.39	947.38	999.58	1003.40	718.19	776.90	778.70	792.84	801.05	832.85
1014.41	1071.85	1099.17	1116.63	1169.73	1176.00	849.31	864.21	901.73	947.73	957.80	982.00
1260.99	1269.80	1274.08	1315.09	1331.89	1362.34						
1374.32	1454.44	1467.23	1479.62	1497.34	1502.07						

991.51	1015.62	1028.71	1037.63	1053.79	1075.35	1485.39	1497.77	1500.00	1506.60	1516.15	1528.91
1075.72	1121.28	1140.14	1177.61	1196.75	1198.09	1537.73	1638.69	1656.51	3086.87	3095.78	3100.00
1210.06	1212.75	1228.25	1242.52	1280.99	1302.77	3141.85	3156.04	3160.73	3162.74	3171.16	3173.17
1307.14	1341.43	1367.12	1367.78	1408.89	1411.33	3181.45	3198.90	3208.78	3217.52	3260.96	3276.9

Table S3. Detailed energetics for all compounds investigated.

Compound	E(SCF)	ZPE	S(gas)	ΔG_{solv}	H(gas)	-TS(gas)	G(gas)	G(sol)
	eV	kcal mol ⁻¹	cal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹
1a	-31903.989	100.76	103.65	-4.97	-735605.23	-30.90	-735636.13	-735641.10
2a	-37123.088	134.29	119.39	-5.21	-855924.12	-35.60	-855959.72	-855964.93
3a	-45903.254	190.73	153.02	-15.85	-1058338.31	-45.62	-1058383.93	-1058399.78
1b	-19372.835	100.86	88.59	-60.58	-446636.72	-26.41	-446663.13	-446723.71
2b	-24591.844	133.66	105.56	-52.26	-566954.26	-31.47	-566985.73	-567037.99
3b	-33372.018	189.62	136.20	-60.86	-769369.12	-40.61	-769409.72	-769470.58
1a-TS	-31902.076	99.68	101.52	-39.38	-735562.19	-30.27	-735592.46	-735631.84
2a-TS	-39360.824	207.36	116.08	-32.80	-907453.24	-34.61	-907487.85	-907520.65
3a-TS	-45900.898	188.70	154.48	-45.18	-1058286.01	-46.06	-1058332.07	-1058377.25
1c _A	-32094.404	172.97	135.11	-65.52	-739923.99	-40.28	-739964.27	-740029.79
1c _A '	-32094.663	173.77	128.15	-61.47	-739929.16	-38.21	-739967.37	-740028.84
1c _G	-34143.101	176.15	138.02	-65.89	-787163.76	-41.15	-787204.91	-787270.80
1b-TS _A	-32093.268	170.94	130.63	-60.81	-739899.82	-38.95	-739938.77	-739999.58
1b-TS _G	-34141.904	174.17	140.93	-60.93	-787138.14	-42.02	-787180.15	-787241.08
2c _A	-37313.475	206.43	149.33	-65.31	-860242.30	-44.52	-860286.83	-860352.14
2c _G	-39362.021	209.40	155.97	-70.74	-907478.80	-46.50	-907525.31	-907596.05
2b-TS _A	-37311.987	204.31	152.66	-60.03	-860210.11	-45.52	-860255.63	-860315.66
2b-TS _G	-39360.824	207.36	158.45	-57.93	-907453.24	-47.24	-907500.48	-907558.41
3c _A	-46093.511	262.56	170.61	-79.88	-1062653.80	-50.87	-1062704.67	-1062784.55
3c _G	-48142.105	265.53	183.30	-80.11	-1109891.41	-54.65	-1109946.06	-1110026.17
3b-TS _A	-46092.060	260.140	182.856	-75.55	-1062622.76	-54.52	-1062677.28	-1062752.83
3b-TS _G	-48140.773	262.98	187.86	-72.87	-1109863.25	-56.01	-1109919.25	-1109992.12
Cl-	-12525.338		36.63	-74.70	-288834.29	-10.92	-288845.22	-288919.92
A	-12720.489	70.19	82.25	-17.17	-293264.29	-24.52	-293288.81	-293305.98
G	-14768.532	73.48	88.72	-25.82	-340488.87	-26.45	-340515.32	-340541.14
4a	-38192.995	151.99	127.28	-5.15	-880578.47	37.95	-880616.42	-880621.57
4b	-25661.993	151.84	113.18	-53.56	-591613.72	33.74	-591647.46	-591701.02
4a-TS	-38191.114	150.93	125.30	-38.57	-880536.16	37.36	-880573.52	-880612.09
1b'	-19373.800	98.17	86.71	-59.73	-446661.66	25.85	-446687.51	-446747.24
1b'-TS	-19370.591	96.40	90.50	-63.70	-446589.43	26.98	-446616.41	-446680.11