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SUPPLEMENTARY MATERIAL

Formation and HERON Reactivity of Cyclic *N,N*-Dialkoxyamides

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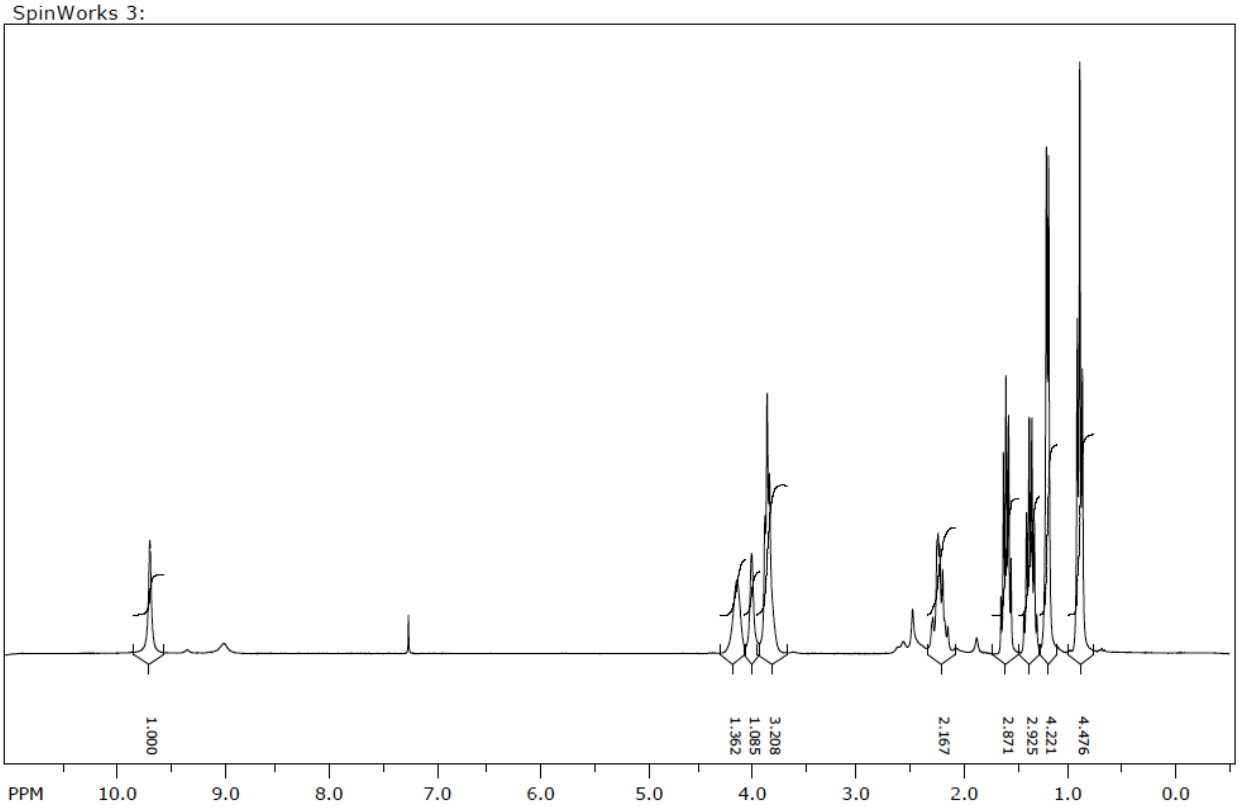
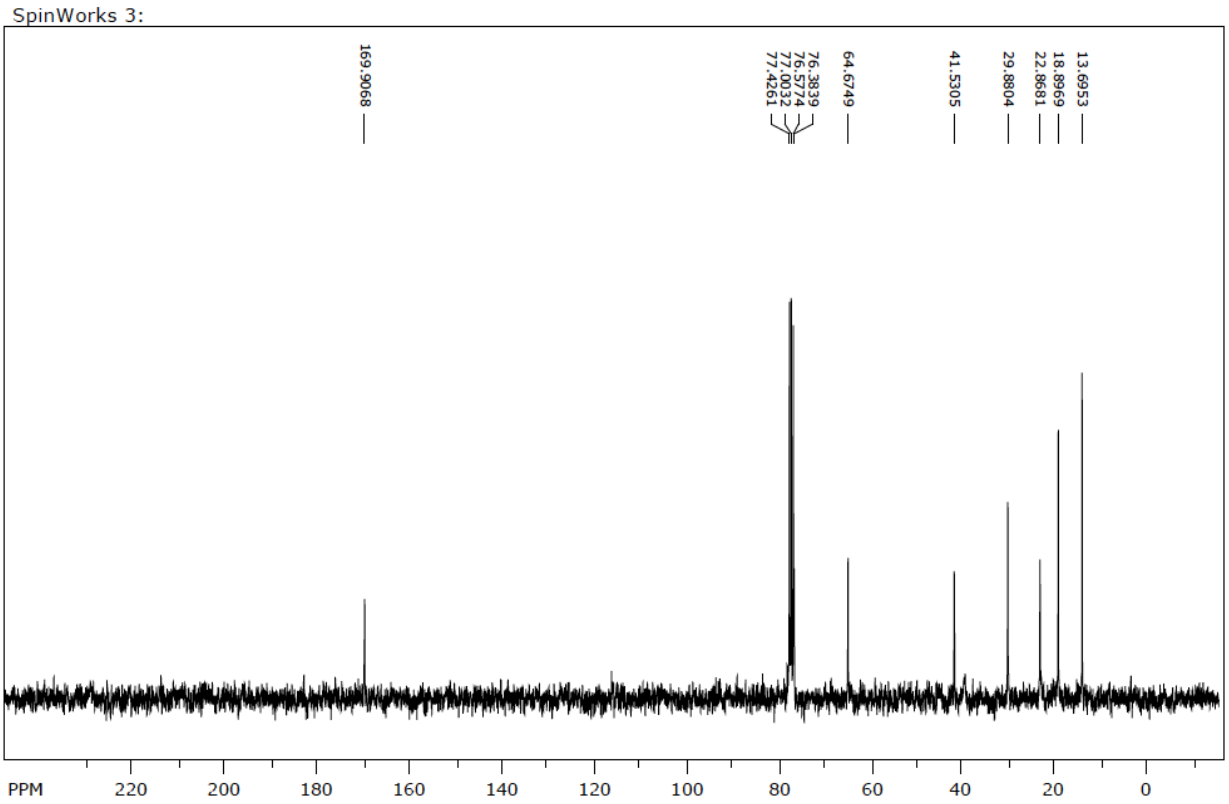
NMR spectra of reactants and products not displayed in Figures 6, 8 and 9 in the text.

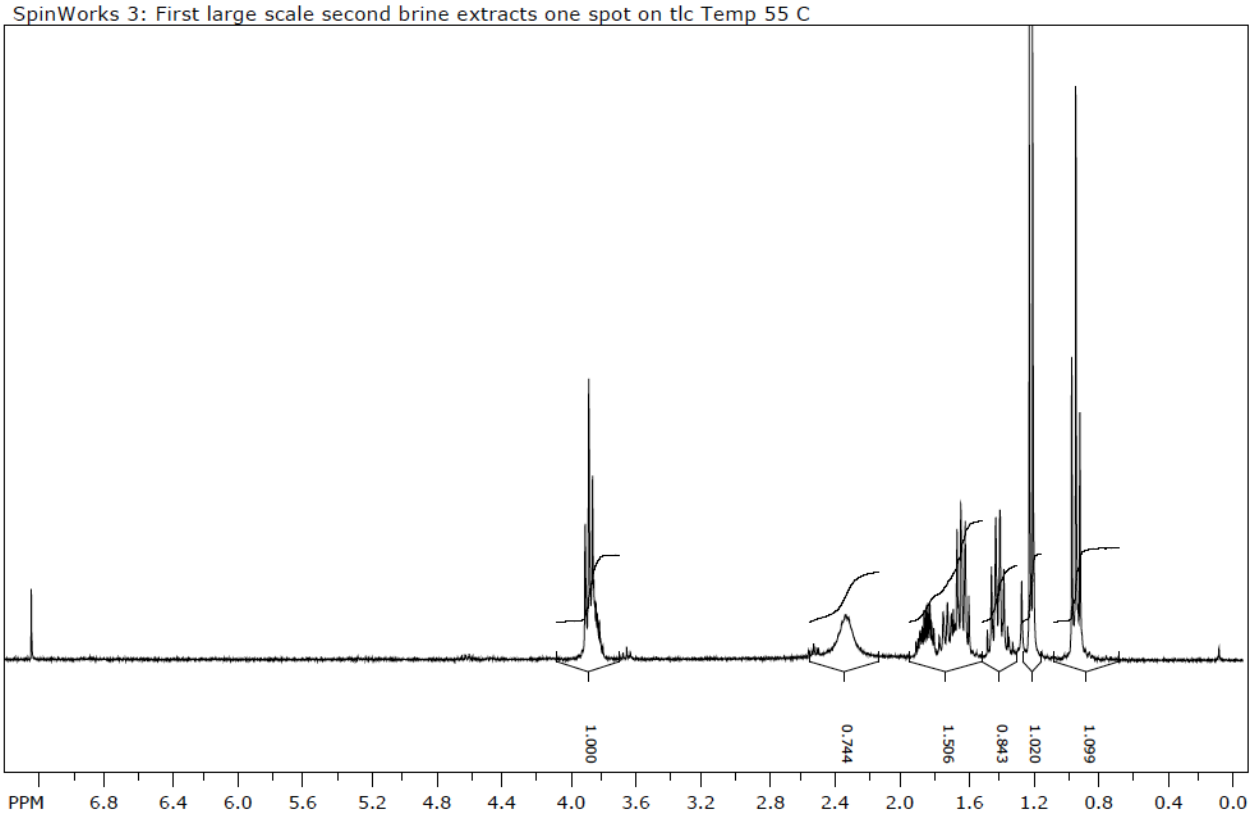
^{1}H NMR for *N*-butoxy-3-hydroxybutanamide **17** in $CDCl_3$



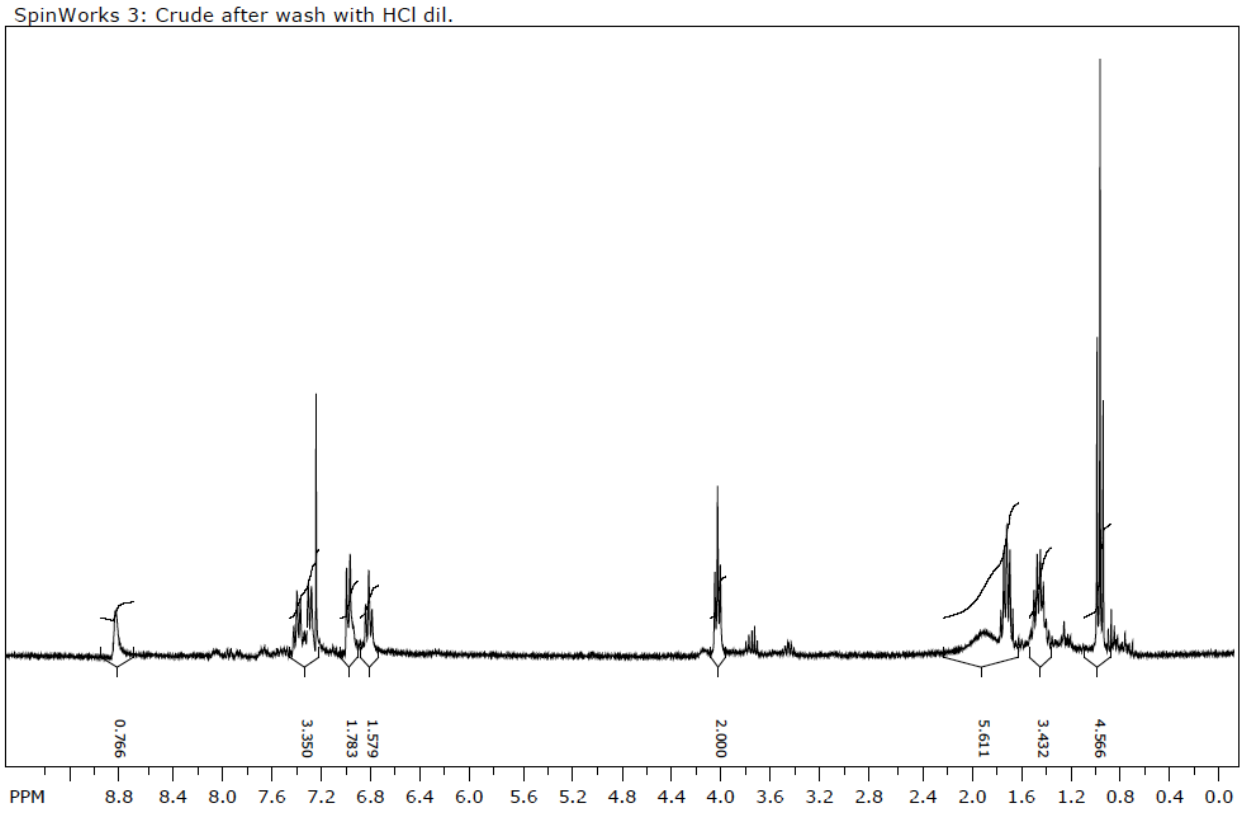
^{13}C NMR for *N*-butoxy-3-hydroxybutanamide **17** in $CDCl_3$



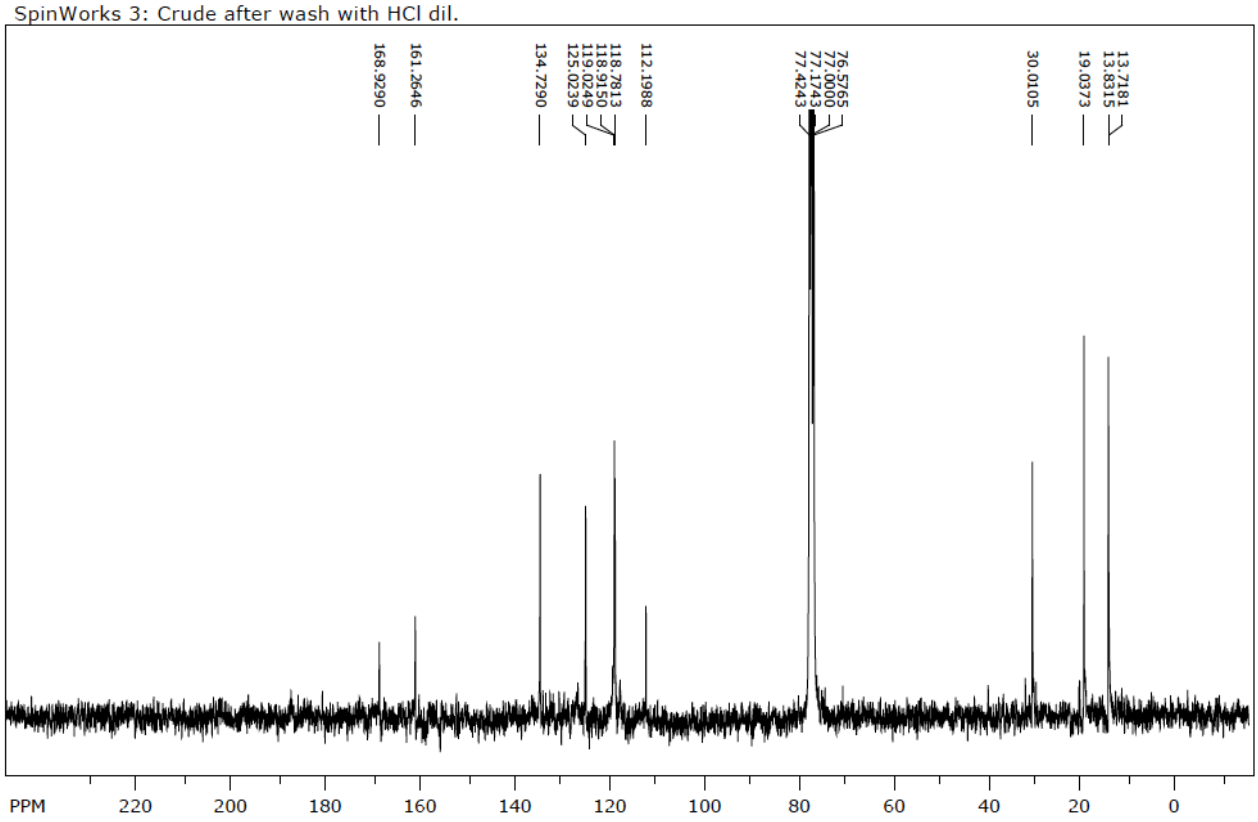
^{1}H NMR for *N*-butoxy-3-hydroxypentanamide **21** in $CDCl_3$



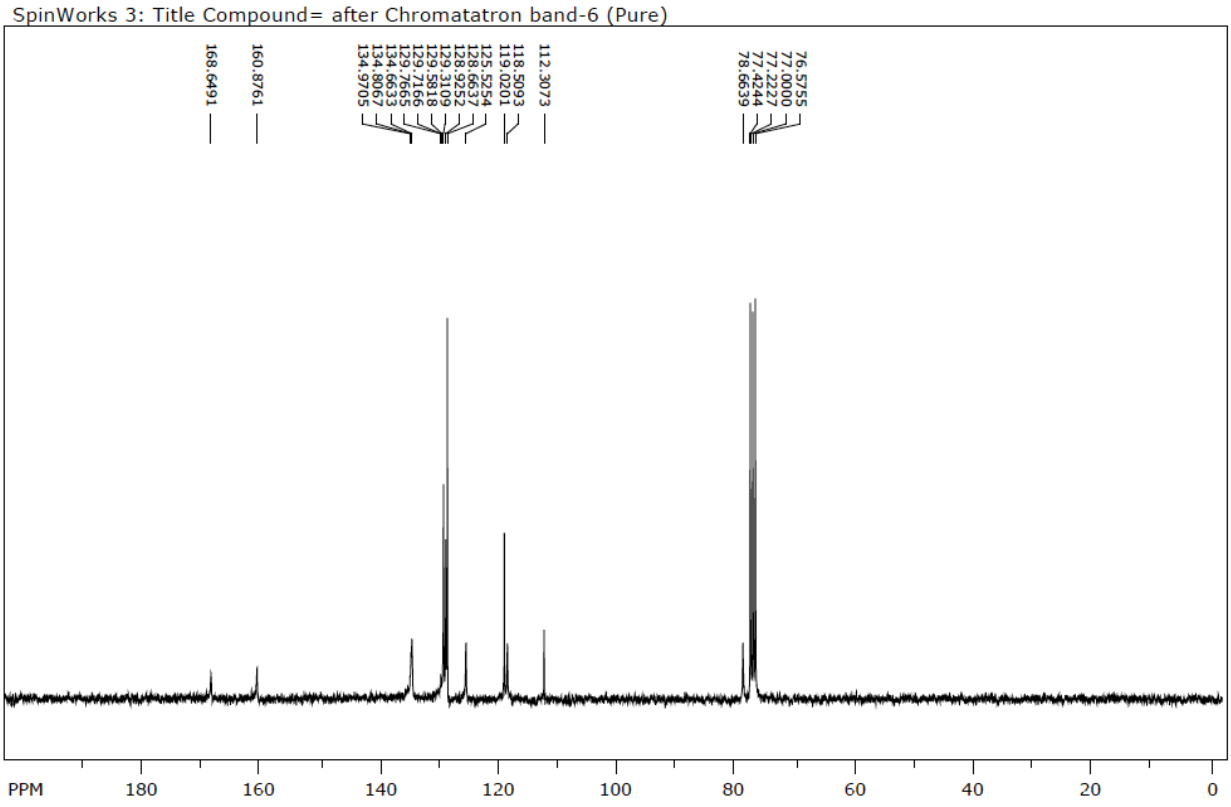
^{1}H NMR of *N*-butoxy-2-hydroxybenzamide **19a**



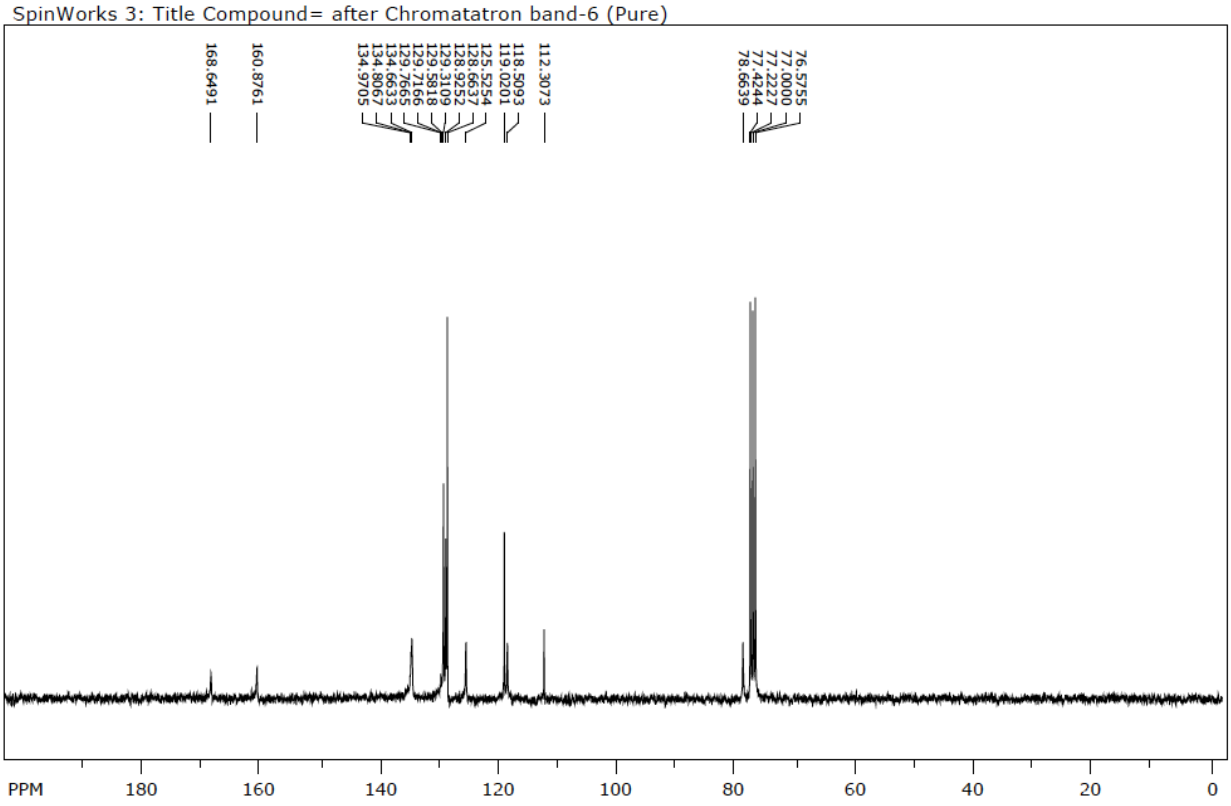
^{13}C NMR of *N*-butoxy-2-hydroxybenzamide **19a**



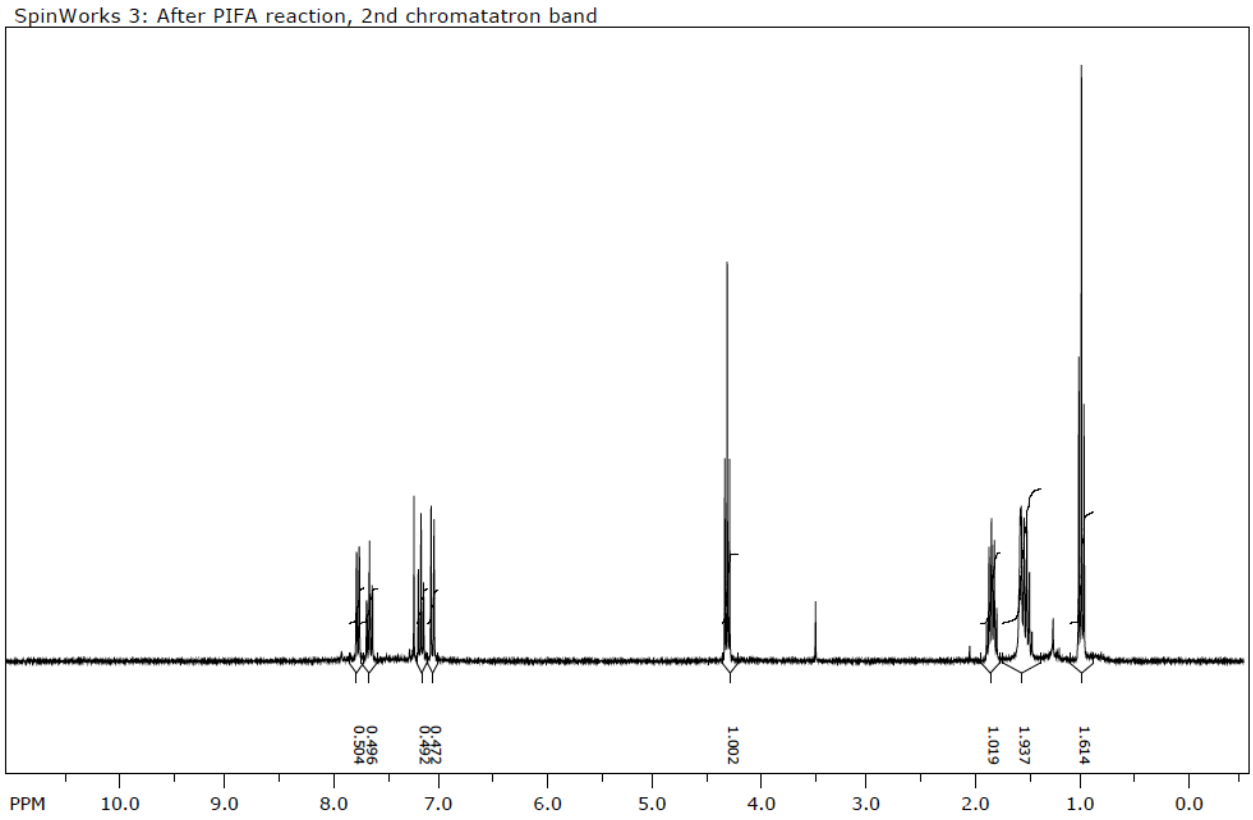
^{1}H NMR of *N*-benzyloxy-2-hydroxybenzamide **19b**



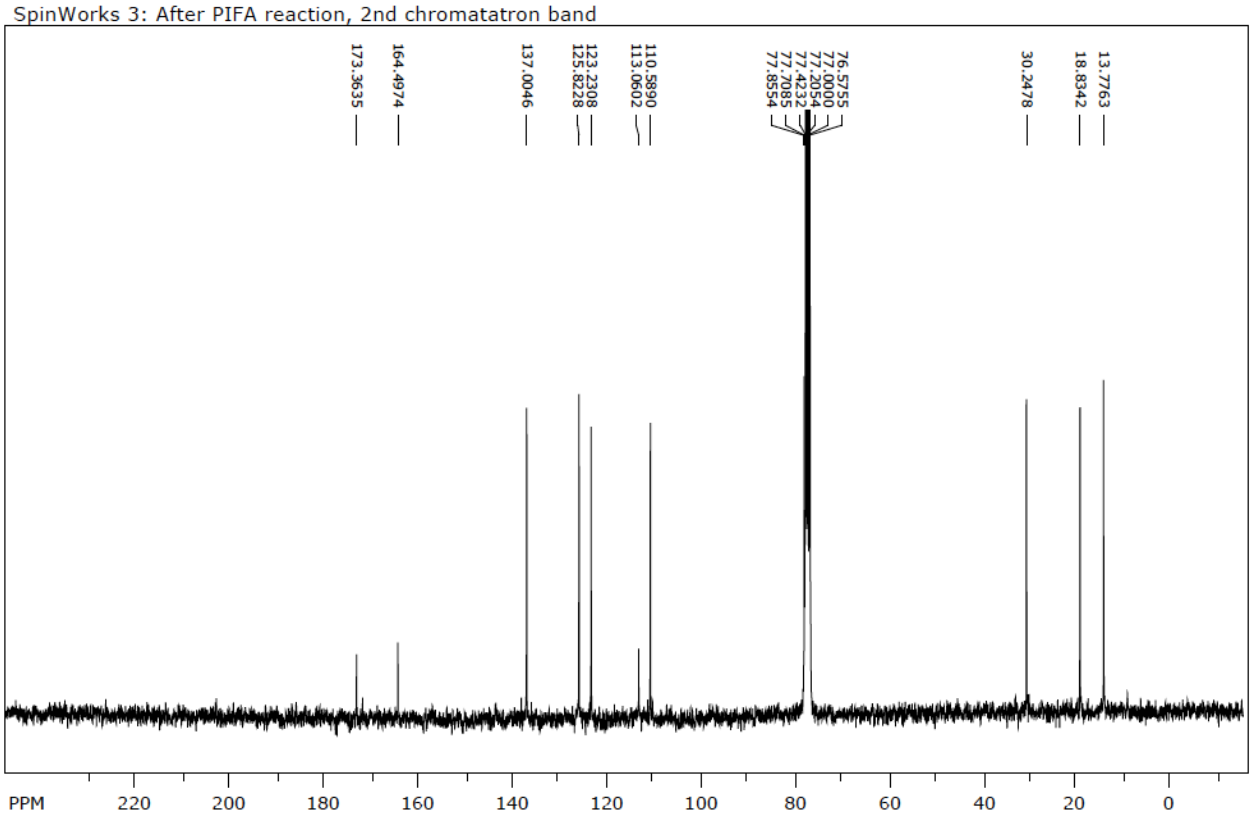
^{13}C NMR of *N*-benzyloxy-2-hydroxybenzamide **19b**



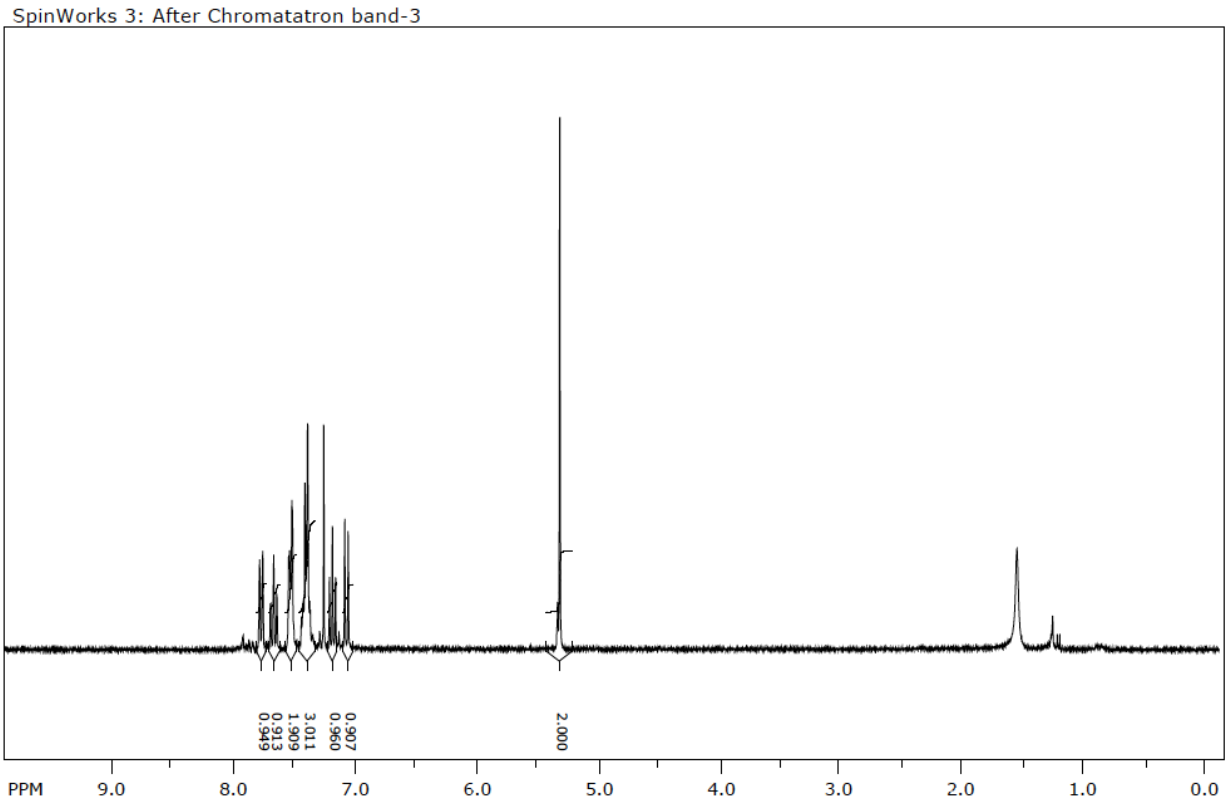
^{1}H NMR of *N*-butoxy-3(*2H*)benzisoxaxolone **22a**



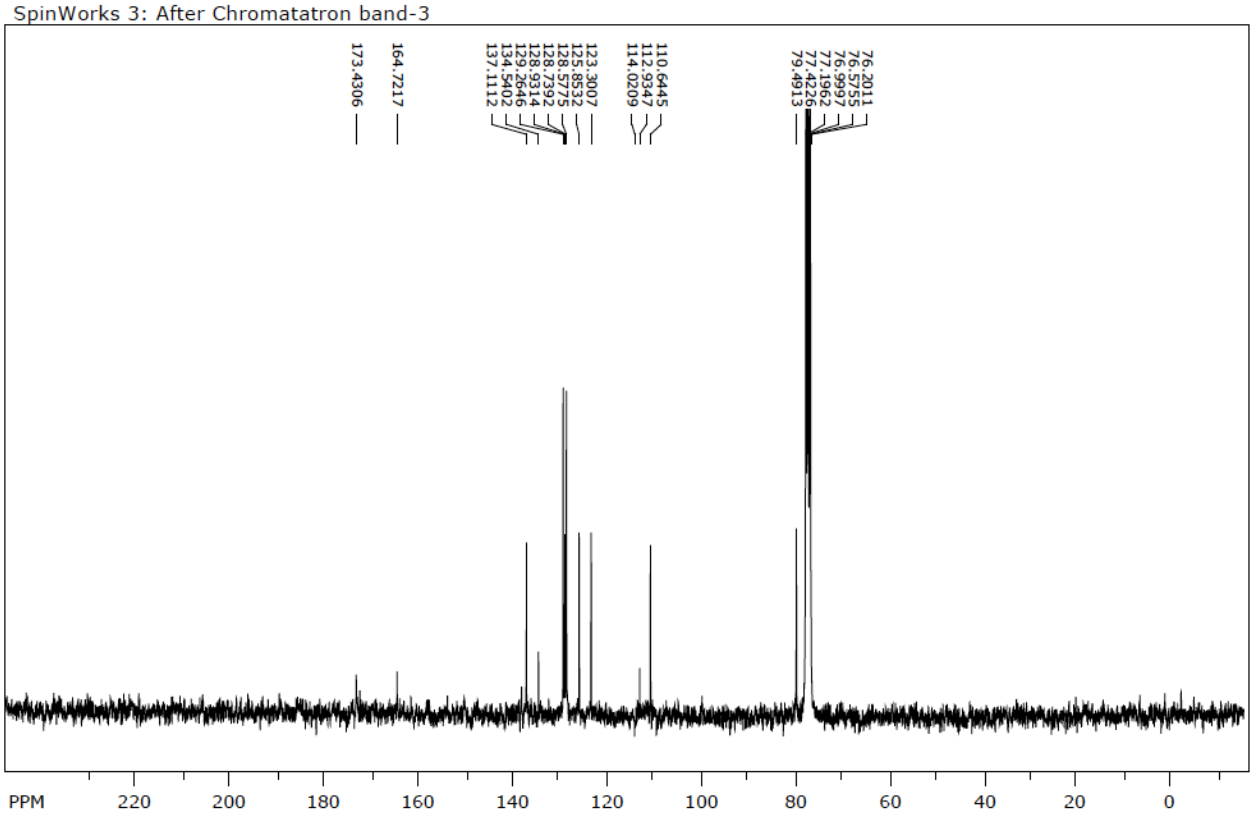
^{13}C NMR of *N*-butoxy-3(*2H*)benzisoxaxolone **22a**



^{1}H NMR of *N*-benzyloxy-3(*2H*)benzisoxaxolone **22b**



^{13}C NMR of *N*-benzyloxy-3(*2H*)benzisoxaxolone **22b**



Supplementary Table 1: B3LYP/6-31G(d) energies of ground state reactants, transition states, singlet and triplet nitrene products and product lactones relating to Schemes 6-10 for HERON reactions of **5**, **6** and **8**.

		GS	**TS**	**Nitrene**		**Lactone/ester**
N,*N*-dimethoxyacetamide **5**:		**5**	**32**	**34(S)**	**34(T)**	**33**
(Scheme 6)	Energies (au)	-438.15048	-438.08231	-169.71811	-169.74628	-268.38848
	ZPE(kJ/mol)	362.87170	354.71780	110.85650	113.52330	236.55250
	Enthalpies(kJ/mol)	390.68040	382.75540	123.31230	125.76440	253.47530
	Entropies(J/K.mol)	396.61510	397.48970	260.07200	259.16400	9.21280
	Enthalpy corr (au)	-438.00165	-437.93650	-169.67113	-169.69837	-268.29192
	Free Energy corr(au)	-438.04670	-437.98165	-169.70067	-169.72781	-268.29297
γ-lactam **6**:		**6**	**35**	**36(S)**	**36(T)**	
(Scheme 7)	Energies (au)	-436.93906	-436.89599	-436.91180	-436.93463	
	ZPE(kJ/mol)	307.50150	301.03940	301.82850	303.71210	
	Enthalpies(kJ/mol)	328.25710	323.23830	324.92300	326.25070	
	Entropies(J/K.mol)	346.71850	355.26860	363.74520	361.48880	
	Enthalpy corr (au)	-436.81401	-436.77285	-436.78802	-436.81035	
	Free Energy corr(au)	-436.85339	-436.81320	-436.82933	-436.85140	
		6	**37**	**34(S)**	**34(T)**	**38**
(Scheme 8)	Energies (au)	-436.93906	-436.86376	-169.71811	-169.74628	-267.15354
	ZPE(kJ/mol)	307.50150	299.97910	110.85650	113.52330	181.42480
	Enthalpies(kJ/mol)	328.25710	322.58580	123.31230	125.76440	194.83760
	Entropies(J/K.mol)	346.71850	359.62590	260.07200	259.16400	283.55120
	Enthalpy corr (au)	-436.81401	-436.74087	-169.67113	-169.69837	-267.07931
	Free Energy corr(au)	-436.85339	-436.78172	-169.70067	-169.72781	-267.11152

δ-lactam **8**:		**8**	**39**	**40(S)**	**40(T)**	
(Scheme 9)	Energies (au)	-476.25462	-476.20262	-476.23015	-476.24950	
	ZPE(kJ/mol)	385.93680	379.58030	373.68960	379.62380	
	Enthalpies(kJ/mol)	408.99560	403.94010	399.55450	404.81580	
	Entropies(J/K.mol)	364.39150	370.95100	386.24300	383.80630	
	Enthalpy corr (au)	-476.09881	-476.04874	-476.07794	-476.09528	
	Free Energy corr(au)	-476.14020	-476.09087	-476.12181	-476.13888	
		8	**41**	**34(S)**	**34(T)**	**42**
(Scheme 10)	Energies (au)	-476.25462	-476.19936	-169.71811	-169.74628	-306.49259
	ZPE(kJ/mol)	385.93680	378.63330	110.85650	113.52330	260.17420
	Enthalpies(kJ/mol)	408.99560	403.18970	123.31230	125.76440	275.49590
	Entropies(J/K.mol)	364.39150	375.42000	260.07200	259.16400	302.48930
	Enthalpy corr (au)	-476.09881	-476.04576	-169.67113	-169.69837	-306.38764
	Free Energy corr(au)	-476.14020	-476.08840	-169.70067	-169.72781	-306.42199

Supplementary Table 2: B3LYP/6-31G(d) energies (au) used in Fig. 5 for deformation of *N*,*N*-dimethoxyacetamide **5**.

	τ° 0	10	20	30	40	50	60	70	80	90
χ°										
0	-438.14513	-438.14529	-438.14344	-438.13966	-438.13424	-438.12775	-438.12055	-438.11321	-438.10688	-438.10320
10	-438.14575	-438.14595	-438.14418	-438.14046	-438.13512	-438.12880	-438.12173	-438.11456	-438.10838	-438.10478
20	-438.14686	-438.14709	-438.14539	-438.14182	-438.13674	-438.13077	-438.12413	-438.11749	-438.11184	-438.10858
30	-438.14830	-438.14854	-438.14693	-438.14359	-438.13891	-438.13352	-438.12762	-438.12186	-438.11712	-438.11448
40	-438.14966	-438.14988	-438.14842	-438.14539	-438.14128	-438.13669	-438.13184	-438.12729	-438.12374	-438.12186
50	-438.15017	-438.15034	-438.14907	-438.14648	-438.14304	-438.13947	-438.13582	-438.13263	-438.13029	-438.12918
60	-438.14836	-438.14852	-438.14744	-438.14531	-438.14263	-438.14010	-438.13758	-438.13547	-438.13402	-438.13351

B3LYP/6-31G(d) optimised Geometries of all structures as XYZ files:

N,*N*-Dimethylacetamide **3**

H	2.755194	0.326591	0.014401
C	1.779074	0.812339	0.000233
H	1.692160	1.459594	0.880257
H	1.712270	1.445637	-0.891670
C	0.728769	-0.294552	-0.003125
O	1.066188	-1.474022	0.006833
N	-0.595856	0.083478	-0.023104
C	-1.080778	1.450835	0.007595
H	-1.601244	1.666425	0.952613
H	-1.793422	1.617913	-0.811633
H	-0.265283	2.163848	-0.103886
C	-1.625976	-0.944090	0.002235
H	-2.234136	-0.861468	0.913711
H	-1.139359	-1.918028	-0.023170
H	-2.291218	-0.839880	-0.865180

N,*N*-dimethoxyacetamide **5**

H	-0.992011	-2.413612	0.214211
C	-1.535167	-1.652034	-0.352055
H	-1.246741	-1.758341	-1.403276
H	-2.611106	-1.804481	-0.252015
C	-1.214037	-0.254974	0.134879
O	-2.044806	0.597196	0.374700
O	1.013224	-0.718830	-0.487468
O	0.558588	1.288732	0.576344
C	0.428122	2.091970	-0.615854
H	0.998436	1.651803	-1.439739
H	0.856670	3.057940	-0.341387
H	-0.623498	2.212318	-0.886654
C	2.150775	-1.202291	0.236570
H	2.698994	-0.371964	0.692525
H	2.775650	-1.697226	-0.510729
H	1.846522	-1.916181	1.010323
N	0.157556	-0.027580	0.398129

N-Methoxy-γ-lactam **6** [**11**(n=1)]

C	0.739378	-0.887855	0.121518
O	0.646652	-2.082067	0.055682
N	-0.379669	-0.028254	0.515323
O	-1.316530	-0.110509	-0.559463
O	0.146590	1.287982	0.570873
C	-2.629022	0.113025	-0.042667
H	-2.874391	-0.623934	0.728885
H	-3.295194	-0.003951	-0.901430
H	-2.722842	1.126195	0.364512
C	1.939195	0.007738	-0.162763
H	2.611892	0.008805	0.703266
H	2.485801	-0.372457	-1.028769
C	1.262932	1.361809	-0.348650
H	0.905497	1.508895	-1.375476
H	1.858324	2.222677	-0.039607

N-Methoxy-3(*2H*)benzisoxalone **7**

H	-2.010331	-2.347932	0.053821
C	-1.977171	-1.262627	0.047874
C	-1.831727	1.586693	0.023446
C	-0.747298	-0.599768	0.006466
C	-3.133863	-0.491687	0.073638
C	-3.052216	0.914438	0.061378

C	-0.683868	0.794177	0.012586
H	-4.107961	-0.970198	0.098884
H	-3.969374	1.496839	0.084308
H	-1.768923	2.669405	0.017002
O	0.588203	1.270130	0.001790
N	1.446654	0.086680	-0.209554
C	0.621476	-1.097894	0.012104
O	1.092675	-2.207917	0.105818
O	2.500263	0.160647	0.668328
C	3.645870	0.733036	0.017660
H	3.915712	0.148948	-0.866743
H	4.440901	0.683733	0.764485
H	3.454814	1.775133	-0.258537

N-Methoxy-δ-lactam **8** [**11**(n=2)]

C	0.252616	-1.127743	0.000308
O	-0.233014	-2.222858	-0.163712
N	-0.546934	0.045728	0.142215
O	0.036561	1.215896	-0.508395
C	1.725686	-0.892121	0.329825
H	1.802719	-0.993210	1.421830
H	2.285118	-1.725672	-0.103073
C	2.281101	0.473276	-0.107046
H	2.489718	0.462887	-1.183021
H	3.224313	0.685450	0.410780
C	1.245628	1.557925	0.167859
H	1.055458	1.679583	1.244239
H	1.535701	2.524665	-0.254778
O	-1.797757	-0.106479	-0.418208
C	-2.763831	0.598173	0.367894
H	-2.793998	0.206986	1.390659
H	-3.717495	0.418143	-0.133038
H	-2.546513	1.671540	0.380381

2-Methoxy-3-tetrahydrofuranone **9**(n=1)

C	-0.747066	1.631171	-0.258914
H	-1.150837	2.570002	0.125180
H	-0.228248	1.827318	-1.205855
C	-1.786460	0.514408	-0.404682
H	-2.185001	0.386836	-1.415186
H	-2.634887	0.653988	0.275892
C	-1.013557	-0.731048	0.033764
O	-1.396546	-1.874250	0.035912
C	0.369178	-0.234442	0.515415
H	0.686857	-0.677207	1.468527
O	0.189216	1.145344	0.728084
O	1.270709	-0.536433	-0.516642
C	2.617015	-0.184826	-0.214414
H	2.722117	0.893249	-0.046775
H	3.218067	-0.483208	-1.076244
H	2.971956	-0.721417	0.677613

2-Methoxy-4,5-dihydro-(2*H*)pyran-3-one **9**(n=2)

C	0.428215	-1.139139	0.060841
O	0.110624	-2.255635	-0.280105
O	-0.150423	1.164573	-0.444626
C	1.863569	-0.725862	0.363196
H	1.954263	-0.648114	1.458219
H	2.532010	-1.526755	0.034589
C	2.211622	0.636072	-0.269679
H	2.304818	0.523127	-1.356430
H	3.175141	1.002573	0.106659
C	1.104746	1.648290	0.021746

H	1.050967	1.863107	1.103944
H	1.275183	2.593149	-0.502372
O	-1.823248	-0.389969	-0.219013
C	-2.879391	0.514517	0.083409
H	-2.959306	0.678187	1.169099
H	-3.796968	0.044908	-0.277015
H	-2.737567	1.479111	-0.415593
C	-0.596095	0.000130	0.258143
H	-0.642914	0.249665	1.342079

N-Methoxyisoxazolidine **10** (n=1)

C	-1.696533	-0.308546	-0.652286
H	-1.453563	-0.554195	-1.688686
H	-2.770221	-0.456443	-0.506532
C	-1.243651	1.120824	-0.296910
H	-2.037821	1.737953	0.132598
H	-0.809604	1.642218	-1.156109
C	-0.863620	-1.159357	0.325912
H	-0.515447	-2.109334	-0.080756
H	-1.397492	-1.338242	1.263365
N	0.306555	-0.330871	0.672908
O	-0.244102	0.975190	0.747264
O	1.125645	-0.380189	-0.519689
C	2.414686	0.123436	-0.195226
H	3.002059	0.042119	-1.114209
H	2.880759	-0.469005	0.601357
H	2.362215	1.173573	0.115776

N-Methoxy-3,4,5,6-tetrahydrooxazine **10**(n=2)

N	0.550628	-0.208667	-0.228745
O	0.073139	0.986158	0.492358
C	-1.742165	-1.022273	-0.328286
H	-1.717531	-1.071360	-1.424731
H	-2.424821	-1.808395	0.014975
C	-2.232639	0.364368	0.115928
H	-2.458072	0.352310	1.189896
H	-3.154088	0.638379	-0.413150
C	-1.136041	1.401232	-0.139072
H	-0.966282	1.538316	-1.217445
H	-1.374518	2.371954	0.307621
O	1.792731	-0.471377	0.374113
C	2.800836	0.296809	-0.279125
H	2.839289	0.063709	-1.349752
H	3.739336	0.011615	0.202864
H	2.624349	1.368892	-0.140669
C	-0.331618	-1.305228	0.206229
H	-0.313667	-1.378436	1.302252
H	0.079948	-2.226359	-0.218285

2-Methoxytetrahydrofuran **12**(n=1)

C	-1.685350	0.325904	0.706153
H	-2.758310	0.537200	0.730018
H	-1.285395	0.472582	1.713886
C	-0.916008	1.205005	-0.293758
H	-0.622895	2.177990	0.106852
H	-1.495590	1.360044	-1.210977
C	0.292479	0.325832	-0.603170
H	0.757287	0.499734	-1.584460
O	-0.203782	-0.999158	-0.628131
C	-1.378755	-1.096830	0.200369
H	-2.188844	-1.497626	-0.421560
H	-1.192871	-1.804468	1.016483
O	1.245429	0.529082	0.417341

C	2.412125	-0.263129	0.265502
H	2.181467	-1.334041	0.314599
H	3.084856	0.004147	1.084298
H	2.914225	-0.055749	-0.693014

2-Methoxy-3,4,5,6-tetrahydropyran **12** (n=2)

O	0.150095	-0.993375	-0.347504
C	-1.841533	0.995741	0.260683
H	-1.902447	1.009618	1.359030
H	-2.555854	1.744995	-0.100225
C	-2.214163	-0.404892	-0.248839
H	-2.308207	-0.390650	-1.342531
H	-3.180042	-0.729516	0.159459
C	-1.124021	-1.407887	0.134456
H	-1.090712	-1.528939	1.232256
H	-1.305731	-2.392826	-0.306306
O	1.816904	0.573719	-0.301507
C	2.848392	-0.319536	0.096463
H	2.934613	-0.362309	1.193477
H	3.778519	0.075457	-0.318863
H	2.674673	-1.330719	-0.286464
C	-0.414790	1.364625	-0.176831
H	-0.364161	1.482572	-1.266040
H	-0.088104	2.307503	0.276397
C	0.561513	0.256086	0.203110
H	0.608268	0.143110	1.307590

N,*N*-Dimethylethylamine **13**

H	2.181017	-1.009620	-0.184008
C	2.044653	0.020543	0.161201
H	2.103541	0.026307	1.254891
H	2.880267	0.609093	-0.234035
C	0.717340	0.621358	-0.303382
H	0.656361	0.579054	-1.411396
H	0.702860	1.684800	-0.034289
N	-0.455399	0.006345	0.320425
C	-1.655834	0.791660	0.069782
H	-2.504142	0.351752	0.605982
H	-1.927538	0.851555	-1.003805
H	-1.514121	1.813332	0.439310
C	-0.651490	-1.378270	-0.088139
H	0.213243	-1.986853	0.190467
H	-0.814063	-1.490209	-1.179720
H	-1.526548	-1.789465	0.426823

1,1-Dimethoxypropanone **14**

H	2.514970	1.714988	0.994303
C	1.447588	1.491489	0.945115
H	1.101277	1.075676	1.898158
H	0.873743	2.408389	0.773567
C	1.185483	0.502589	-0.165512
C	-0.246939	-0.043945	-0.294855
O	-1.147666	0.968786	-0.002002
O	-0.393075	-1.093049	0.655891
O	2.052388	0.062016	-0.897312
C	-2.512673	0.610905	-0.197638
H	-2.691450	0.301921	-1.238316
H	-3.100573	1.505515	0.017602
H	-2.811618	-0.198912	0.475754
C	0.064990	-2.360924	0.201284
H	-0.483568	-2.683627	-0.696352
H	-0.125596	-3.066942	1.012961
H	1.137920	-2.350666	-0.028357

H	-0.390473	-0.445262	-1.314297

1-Methoxy-1-propyl methyl ether **15**

H	3.410173	-0.546544	-0.463789
C	2.564362	0.045283	-0.097236
H	2.815206	0.392263	0.913111
H	2.457460	0.925533	-0.738149
C	1.276464	-0.783309	-0.094514
H	1.395165	-1.676203	0.531892
H	1.053518	-1.125093	-1.112028
C	0.076892	-0.001774	0.439816
O	-1.068305	-0.795395	0.691843
C	-1.584246	-1.509133	-0.425777
H	-1.663615	-0.868338	-1.312073
H	-2.581894	-1.851126	-0.137962
H	-0.970432	-2.386531	-0.672067
H	0.311458	0.420143	1.429646
O	-0.185781	1.041318	-0.472669
C	-1.108526	2.007252	0.009049
H	-0.736509	2.487646	0.926984
H	-2.088339	1.562126	0.219769
H	-1.210758	2.763182	-0.773580

N,*N*-dimethoxyacetamide **5**- HERON TS **32**

H	-1.864140	0.103567	-1.625525
C	-1.976370	-0.663720	-0.857593
H	-2.947488	-0.545482	-0.363234
H	-1.960850	-1.647701	-1.332479
C	-0.874218	-0.653603	0.179722
O	-0.661636	-1.536680	0.973016
O	-0.477031	0.757571	0.671787
O	1.616778	-0.576697	-0.148959
C	2.825670	0.238942	-0.073808
H	2.876002	0.885121	-0.952188
H	3.660193	-0.462830	-0.030650
H	2.765606	0.827367	0.845235
C	-1.120025	1.920419	0.154463
H	-0.731370	2.770381	0.723444
H	-2.204748	1.857688	0.296259
H	-0.896664	2.067129	-0.907456
N	0.621175	-0.008718	-0.719552

Methyl acetate **33**

H	-1.890711	-1.164897	0.878911
C	-1.801434	-0.518081	-0.000090
H	-2.597552	0.226976	0.004523
H	-1.893957	-1.156614	-0.884869
C	-0.460575	0.178449	0.000220
O	-0.285146	1.376718	0.000034
O	0.549242	-0.723911	0.000306
C	1.871928	-0.163368	-0.000186
H	2.030148	0.450285	-0.891339
H	2.551512	-1.016272	0.003169
H	2.028277	0.456069	0.887225

Methoxynitrene **34** Singlet

H	-1.191690	-0.755604	0.901643
C	-1.123956	-0.148430	-0.000000
H	-1.191690	-0.755604	-0.901643
O	0.283625	0.480617	0.000000
H	-1.826885	0.685174	0.000000
N	1.240714	-0.304047	-0.000000

Methoxynitrene **34** Triplet

H	-1.157001	-0.786087	0.898021
C	-1.065084	-0.168683	0.000000
H	-1.157001	-0.786087	-0.898021
O	0.217454	0.509038	-0.000000
H	-1.812113	0.625166	-0.000000
N	1.253855	-0.301885	0.000000

γ-Lactam HERON TS **35**

C	0.295656	0.644047	0.168527
O	1.008070	1.432632	0.765605
N	-0.347953	-0.719077	1.041654
O	0.900023	-0.468050	-0.630279
O	-1.422939	-1.071123	0.529359
C	2.290865	-0.697583	-0.394328
H	2.667724	0.029545	0.329001
H	2.818308	-0.581429	-1.348119
H	2.429248	-1.718920	-0.026510
C	-1.009978	1.063257	-0.569580
H	-1.405202	1.928995	-0.034706
H	-0.737735	1.359214	-1.585615
C	-1.959646	-0.093887	-0.574553
H	-1.933762	-0.726910	-1.461331
H	-2.985519	0.100373	-0.262173

Ring-open nitrene **36** Singlet

C	-0.688860	0.652943	-0.107085
O	-1.429532	1.163021	-0.915097
N	1.366626	-0.889429	-1.221919
O	-1.003728	-0.446470	0.619412
O	2.027409	-0.840001	-0.190932
C	-2.272853	-1.043055	0.303104
H	-3.083317	-0.326970	0.461374
H	-2.372970	-1.894298	0.977233
H	-2.286996	-1.373629	-0.738701
C	0.652309	1.235615	0.311438
H	1.059790	1.755060	-0.559884
H	0.453896	1.998187	1.077516
C	1.646906	0.266421	0.888918
H	1.270834	-0.327063	1.721646
H	2.614180	0.710775	1.128935

Ring-open nitrene **36** Triplet

C	-0.712709	0.652553	-0.173510
O	-1.300844	0.958827	-1.184675
N	1.423654	-1.452840	-0.759977
O	-1.153676	-0.268788	0.710327
O	2.200890	-0.490100	-0.311389
C	-2.362752	-0.953063	0.336304
H	-3.177311	-0.239153	0.191244
H	-2.583280	-1.629081	1.162646
H	-2.206613	-1.514462	-0.588285
C	0.588449	1.283360	0.298556
H	0.979916	1.892544	-0.519372
H	0.351039	1.954564	1.135499
C	1.644624	0.296277	0.787961
H	1.242529	-0.390934	1.535670
H	2.511516	0.822130	1.192463

γ-Lactam TS **37**

C	0.850897	0.700097	0.035179
O	0.630164	1.825235	0.368706
O	0.536021	-0.550293	0.884024

C	1.584535	-1.273582	0.173833
H	1.163816	-2.111792	-0.386465
C	1.988819	-0.049687	-0.660444
H	1.883288	-0.134158	-1.743414
H	2.963059	0.380975	-0.412399
N	-0.662554	-0.275170	-0.685399
O	-1.666159	0.394253	-0.273410
C	-2.829803	-0.409503	0.115003
H	-2.856857	-1.308932	-0.502024
H	-3.702173	0.227949	-0.038902
H	-2.708984	-0.658875	1.171858
H	2.328836	-1.626483	0.893154

β-Propiolactone **38**

C	-0.495713	1.068794	-0.000000
H	-0.525147	1.696800	0.893752
H	-0.525147	1.696800	-0.893752
C	-1.407626	-0.168614	0.000000
H	-2.007417	-0.331379	-0.898415
H	-2.007417	-0.331379	0.898415
O	-0.231842	-1.048131	0.000000
C	0.627890	0.027725	-0.000000
O	1.821570	0.010847	0.000000

δ-Lactam HERON TS **39**

C	0.591746	0.714782	0.327553
O	1.444549	1.203318	1.037903
N	0.071850	-0.929915	0.827601
O	0.994892	-0.341402	-0.720177
O	-1.065977	-1.418510	0.451777
C	2.356393	-0.778876	-0.652179
H	2.832354	-0.374031	0.243765
H	2.866774	-0.407828	-1.548277
H	2.364072	-1.870971	-0.641893
C	-0.599354	1.472176	-0.234076
H	-1.000149	2.066436	0.595018
H	-0.212826	2.179894	-0.977490
C	-1.695557	0.591106	-0.844150
H	-2.561081	1.207503	-1.117187
H	-1.337061	0.106010	-1.757732
C	-2.156558	-0.465994	0.139510
H	-2.480408	-0.032793	1.091800
H	-2.942360	-1.111222	-0.257187

Ring-open nitrene **40** Singlet

C	1.071447	-0.138365	0.053955
O	0.598817	0.958277	-0.158038
N	-2.406831	1.233114	0.846933
O	2.401101	-0.379733	0.087943
O	-2.585879	0.979595	-0.284801
C	3.242374	0.763587	-0.138764
H	3.058718	1.531645	0.617226
H	3.055574	1.189146	-1.128513
H	4.265213	0.392376	-0.068106
C	0.289181	-1.412049	0.315505
H	0.600224	-2.156644	-0.428185
H	0.623010	-1.806459	1.283908
C	-1.232884	-1.216172	0.316692
H	-1.718706	-2.134450	0.664977
H	-1.479056	-0.431257	1.103414
C	-1.847695	-0.706436	-0.910853
H	-1.224893	-0.281460	-1.691891
H	-2.779118	-1.143196	-1.261412

Ring-open nitrene **40** Triplet

C	-1.502973	0.518997	-0.042661
O	-2.370692	0.852600	-0.818710
N	3.017464	-1.342945	0.139976
O	-1.395349	-0.728198	0.468410
O	2.946029	-0.139435	-0.387232
C	-2.397046	-1.664990	0.033463
H	-2.400524	-1.744608	-1.056462
H	-3.387578	-1.347077	0.369793
H	-2.123778	-2.616822	0.489332
C	-0.429472	1.445270	0.507485
H	-0.391143	2.312153	-0.159456
H	-0.792919	1.811281	1.476979
C	0.959102	0.817697	0.708215
H	1.621490	1.557241	1.172788
H	0.887708	-0.035336	1.389653
C	1.586604	0.356923	-0.602245
H	1.008023	-0.440042	-1.079418
H	1.719280	1.180708	-1.308340

δ-Lactam HERON TS **41**

C	0.510331	-0.929572	-0.135079
O	0.091612	-1.977391	-0.548595
O	0.262977	0.354954	-0.969254
C	1.285579	1.314994	-0.683305
H	0.822256	2.302881	-0.604938
H	1.974445	1.312153	-1.538612
C	1.782228	-0.641232	0.651632
H	1.686195	-1.046965	1.661805
H	2.594021	-1.181083	0.149526
C	1.987887	0.875498	0.617597
H	1.507311	1.347478	1.478306
H	3.043342	1.164019	0.620465
N	-0.770590	0.194390	0.666195
O	-1.893734	-0.316862	0.320045
C	-2.954127	0.655862	0.071426
H	-2.827077	1.504109	0.746626
H	-3.894033	0.128972	0.244475
H	-2.870554	0.968792	-0.972211

γ-Butyrolactone **42**

C	-0.026503	1.209954	0.168138
H	0.014800	1.525956	1.218731
H	0.333467	2.041639	-0.440873
C	-1.406841	0.669025	-0.218562
H	-1.575970	0.791079	-1.293881
H	-2.236824	1.144537	0.311196
C	-1.269231	-0.822955	0.128270
H	-1.545018	-1.031364	1.169884
H	-1.840367	-1.486175	-0.525336
O	0.127015	-1.134641	-0.044838
C	0.889458	-0.001603	0.003354
O	2.089061	-0.029385	-0.071027