

Reactivities of Substituted α -Phenyl-*N-tert*-butyl Nitrones

Marie Rosselin,^{†,§} Fanny Choteau,^{†,§} Kamal Zéamari,[‡] Kevin Nash,^{||,#} Amlan Das,^{||,#} Robert Lauricella,[‡] Elisabeth Lojou,^{||} Béatrice Tuccio,[‡] Frederick A. Villamena,^{||,#*} Grégory Durand,^{†,§*}

[†]Avignon Université, Equipe Chimie Bioorganique et Systèmes Amphiphiles, 33 rue Louis Pasteur, F-84000 Avignon, France ;

[§]Institut des Biomolécules Max Mousseron (UMR 5247), 15 avenue Charles Flahault, F-34093 Montpellier Cedex 05, France ;

[‡]Aix-Marseille Université-CNRS, Institut de Chimie Radicalaire (UMR 7273), Equipe Spectrométries Appliquées à la Caractérisation Structurale, avenue Escadrille Normandie-Niemen, F-13397 Marseille Cedex 20, France ;

^{||}Department of Pharmacology and [#]The Davis Heart and Lung Research Institute, College of Medicine, The Ohio State University, Columbus, OH 43210 ;

[¶]CNRS-Aix-Marseille Université, Bioénergétique et Ingénierie des Protéines (UMR 7281), 31 chemin Joseph Aiguier, F-13402 Marseille Cedex 20, France.

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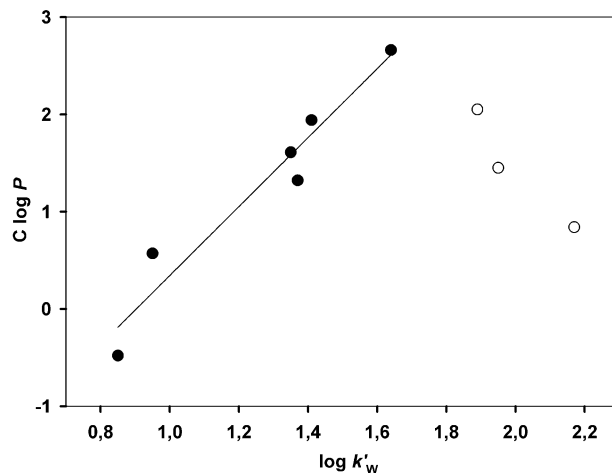


Figure S1. Correlation between $\log k'_w$ and $C \log P$. Hydroxylated compounds **1**, **8** and **9** are marked as (○).

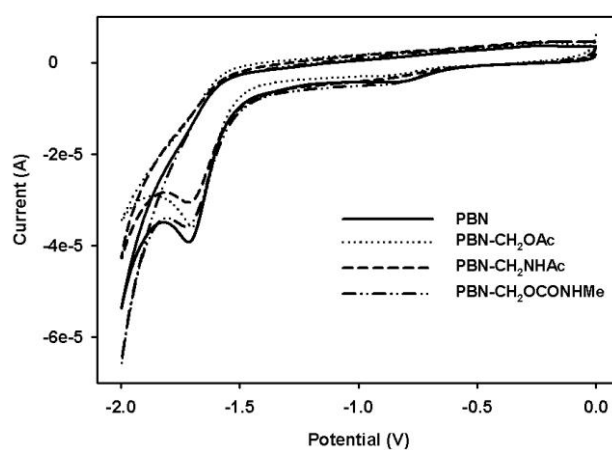


Figure S2. Cyclic voltammograms of PBN and compounds **2**, **6** and **7**, reduction in water containing 50 mM of NaCl with a sweep rate of 0.1 V.s^{-1} .

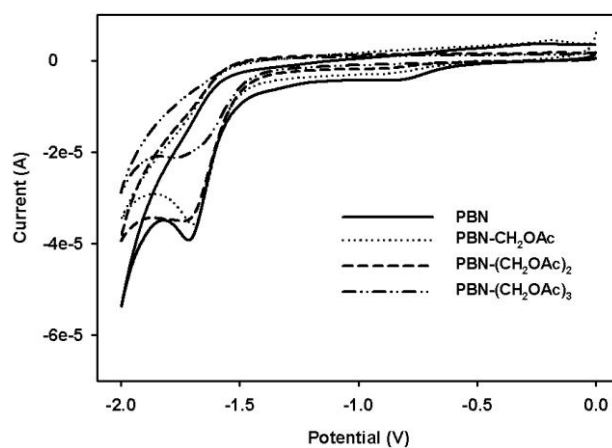


Figure S3. Cyclic voltammograms of PBN and compounds **2**, **10** and **11**, reduction in water containing 50 mM of NaCl with a sweep rate of 0.1 V.s^{-1} .

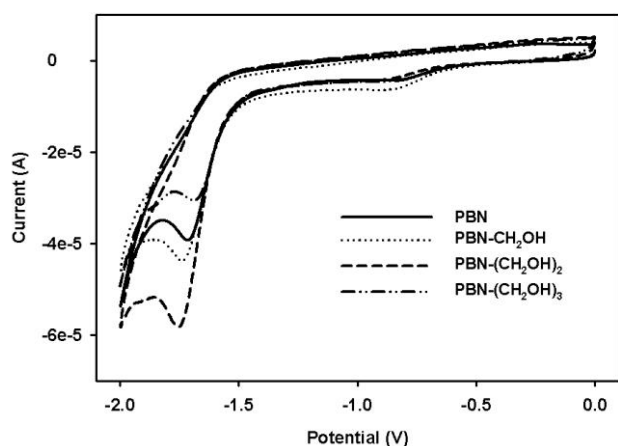


Figure S4. Cyclic voltammograms of PBN and compounds **1**, **8** and **9**, reduction in water containing 50 mM of NaCl with a sweep rate of $0.1 \text{ mV}\cdot\text{s}^{-1}$.

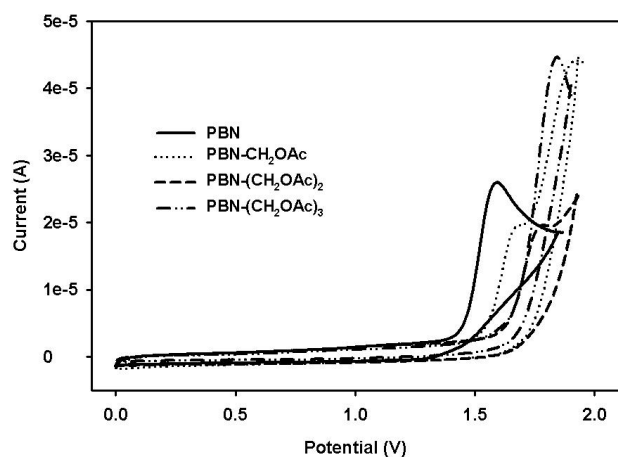


Figure S5. Cyclic voltammograms of PBN and compounds **2**, **10** and **11**, oxidation in acetonitrile containing 50 mM of TBAP with a sweep rate of $0.1 \text{ mV}\cdot\text{s}^{-1}$.

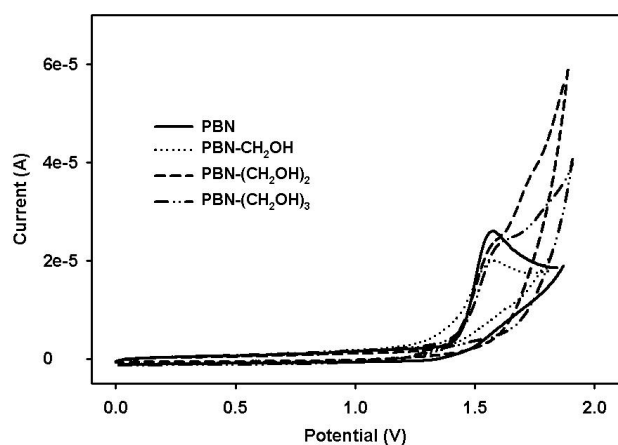


Figure S6. Cyclic voltammograms of PBN and compounds **1**, **8** and **9**, oxidation in acetonitrile containing 50 mM of TBAP with a sweep rate of $0.1 \text{ mV}\cdot\text{s}^{-1}$.

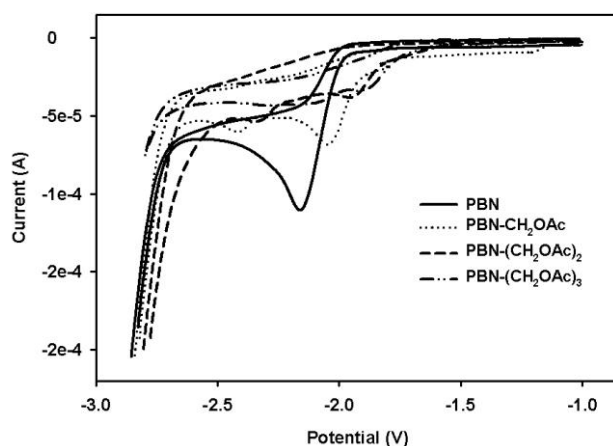


Figure S7. Cyclic voltammograms of PBN and compounds **2**, **10** and **11**, reduction in acetonitrile containing 50 mM of TBAP with a sweep rate of 0.1 V.s⁻¹.

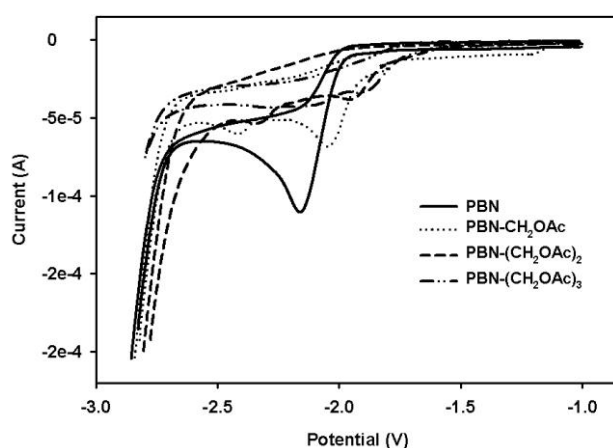


Figure S8. Cyclic voltammograms of PBN and compounds **1**, **8** and **9**, reduction in acetonitrile containing 50 mM of TBAP with a sweep rate of 0.1 V.s⁻¹.

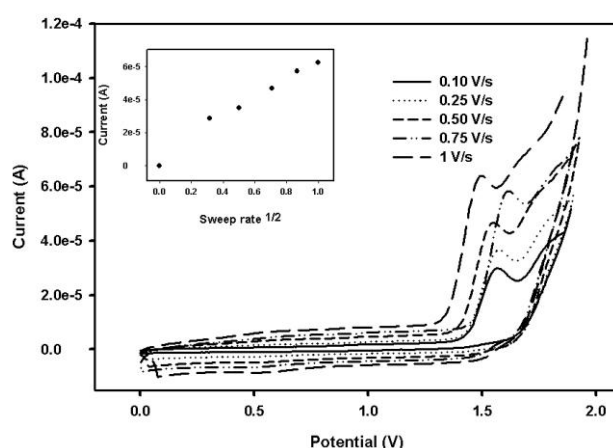


Figure S9. Sweep rate variations on PBN oxidation in acetonitrile containing 50 mM of TBAP at sweep rate ranging from 0.1 V.s⁻¹ to 1 V.s⁻¹ with corresponding linear regression curve.

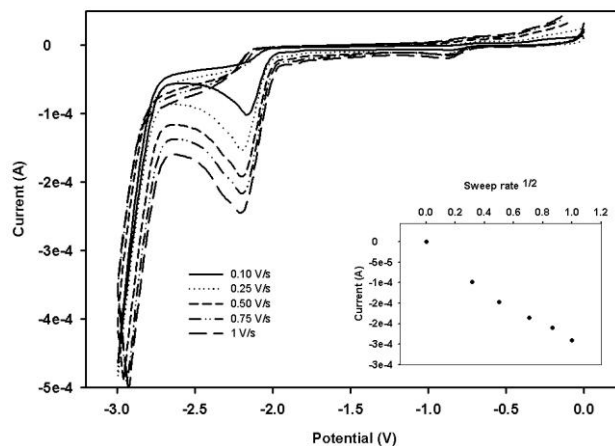


Figure S10. Sweep rate variations on PBN reduction in acetonitrile containing 50 mM of TBAP at sweep rate ranging from 0.1 V.s^{-1} to 1 V.s^{-1} with corresponding linear regression curve.

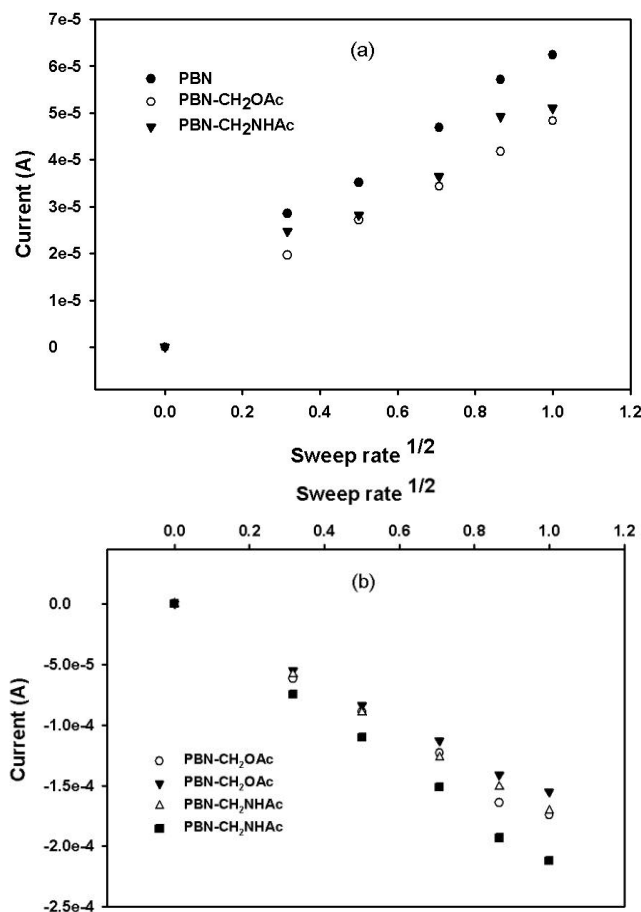


Figure S11. Linear regressions corresponding to sweep rate variations on PBN, PBN- CH_2OAc and PBN- CH_2NHAc oxidation (a) and reduction (b) in acetonitrile containing 50 mM of TBAP at sweep rate ranging from 0.1 V.s^{-1} to 1 V.s^{-1} .

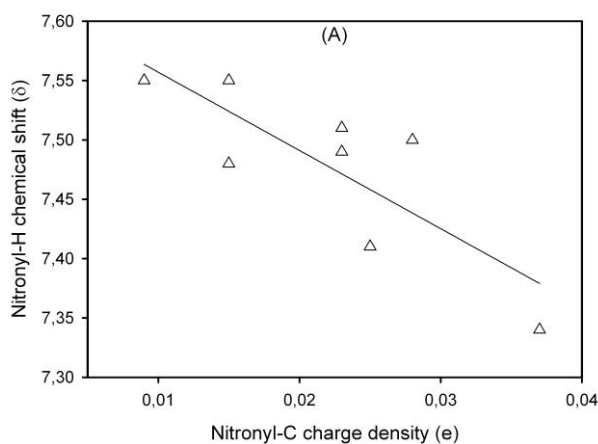


Figure S12. Correlation of the nitronyl-carbon charge densities with the nitronyl-H chemical shifts of nitrones **1**, **2**, **6-8**, **10** and **11** ($R^2 = 0.656$) excluding nitrone **9**.

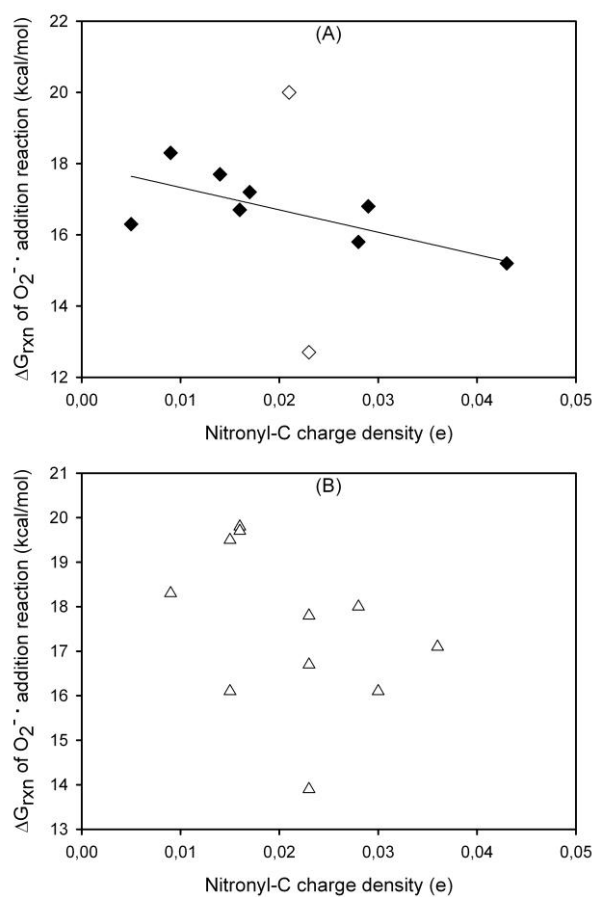


Figure S13. Plots of NPA charge densities of the nitronyl carbon of the monosubstituted nitrones versus their free energies ($\Delta G_{rxn, 298K}$) of $O_2^{\bullet-}$ addition reactions: (A) α -substituted nitrones (\blacklozenge) ($R^2 = 0.473$) excluding $-P(=O)(OMe)_2$ and $-NHC(=O)Me$ derivatives (\diamond). (B) β -substituted nitrones (\triangle) ($R^2 = 0.169$).

Table S1. Natural population analysis (NPA) charge densities of the nitronyl- atoms of PBN derivatives at the PCM/B3LYP/6-31+G**//B3LYP/6-31G* level of theory. In bold are the data for the molecules synthesized.

Nitrones		monosubstitution			disubstitution			trisubstitution		
		C	N	O	C	N	O	C	N	O
PBN	-CH ₃	0.009	0.073	-0.606	n/a	n/a	n/a	n/a	n/a	n/a
α-substitution	-COOH	0.029	0.067	-0.607	0.041	0.059	-0.606	0.050	0.056	-0.590
	-C(=O)OMe	0.005	0.077	-0.577	0.037	0.063	-0.601	0.040	0.061	-0.576
	-C(=O)NH ₂	0.043	0.055	-0.617	0.074	0.037	-0.631	0.068	0.039	-0.613
	-OMe	0.014	0.047	-0.595	0.020	0.030	-0.601	0.023	0.016	-0.595
	-OC(=O)Me	0.028	0.050	-0.596	0.034	0.028	-0.592	0.040	0.012	-0.577
	-OC(=O)NHMe	0.016	0.049	-0.601	0.049	0.017	-0.617	0.049	0.018	-0.584
	-NHC(=O)Me	0.023	0.057	-0.609	0.005	0.055	-0.583	0.004	0.046	-0.564
	-SMe	0.017	0.057	-0.596	0.012	0.048	-0.584	0.014	0.035	-0.567
	-P(=O)(OMe) ₂	0.021	0.048	-0.586	0.031	0.047	-0.575	0.051	0.028	-0.582
β-substitution	-CH ₂ OH	0.015	0.070	-0.608	0.015	0.074	-0.605	0.023	0.062	-0.613
	-CH ₂ OC(=O)Me	0.023	0.065	-0.608	0.025	0.062	-0.605	0.037	0.053	-0.608
	-CH ₂ NHC(=O)Me	0.028	0.063	-0.619	0.035	0.059	-0.620	0.052	0.049	-0.624
	-CH ₂ OC(=O)NHMe	0.023	0.066	-0.608	0.041	0.150	-0.241	0.027	0.056	-0.596
	-CH ₂ C(=O)NH ₂	0.036	0.054	-0.621	0.061	0.042	-0.633	0.038	0.050	-0.609
	-CH ₂ C(=O)OMe	0.023	0.067	-0.610	0.034	0.061	-0.611	0.034	0.063	-0.604
	-CH ₂ OMe	0.016	0.070	-0.607	0.020	0.067	-0.609	0.022	0.066	-0.610
	-CH ₂ P(=O)(OMe) ₂	0.030	0.054	-0.609	0.024	0.055	-0.601	0.008	0.068	-0.566
	-CH ₂ SMe	0.016	0.070	-0.604	0.018	0.071	-0.597	0.022	0.067	-0.594

Table S2. Natural bond orbital (NBO) analysis showing the percent electron localization on the polar σ C-N and N-O (in parentheses); and π C-N bonds at the B3LYP/6-31+G** level of theory.

Nitrones		monosubstitution			disubstitution			trisubstitution			
		C	N	O	C	N	O	C	N	O	
PBN	-CH ₃ σ	37.07	62.93 (50.13)	49.87	n/a	n/a	n/a	n/a	n/a	n/a	
	π	40.32	59.68		n/a	n/a	n/a	n/a	n/a	n/a	
α -substitution	-COOH σ	36.87	63.13 (50.45)	49.55	36.49	63.51 (50.62)	49.38	36.96	63.61 (50.78)	49.22	
	π	39.16	60.84		37.12	62.88		36.19	63.81		
	-C(=O)OMe σ	37.02	62.98 (50.17)	49.83	36.54	63.46 (50.54)	49.46	36.52	63.48 (50.67)	49.33	
	π	39.85	60.15		37.45	62.55		36.98	63.02		
	-C(=O)NH ₂ σ	37.01	62.99 (50.16)	49.84	36.93	63.07 (50.19)	49.81	36.71	63.29 (50.61)	49.39	
	π	38.41	61.59		36.72	63.28		36.21	63.79		
	-OMe σ	37.19	62.81 (50.12)	49.88	36.97	63.03 (50.32)	49.68	37.05	62.95 (50.27)	49.73	
	π	39.91	60.09		38.36	61.64		37.93	62.07		
	-OC(=O)Me σ	36.97	63.03 (50.33)	49.67	36.83	63.17 (50.41)	49.59	36.76	63.24 (50.89)	49.11	
	π	38.96	61.04		37.45	62.55		36.79	63.21		
	-OC(=O)NHMe σ	36.93	63.07 (50.39)	49.61	36.91	63.09 (50.19)	49.81	37.10	62.90 (50.14)	49.86	
	π	39.29	60.71		36.62	63.38		36.92	63.08		
	-NHC(=O)Me σ	37.06	62.94 (50.13)	49.87	37.19	62.18 (49.95)	50.05	37.39	62.61 (49.62)	50.38	
	π	39.13	60.87		40.01	59.99		39.73	60.27		
	-SMe σ	36.93	63.07 (50.24)	49.76	36.77	63.23 (50.39)	49.61	36.79	63.21 (50.26)	49.74	
	π	39.52	60.48		39.08	60.92		38.21	61.79		
	-P(=O)(OMe) ₂ σ	36.90	63.10 (50.38)	49.62	36.59	63.41 (50.44)	49.56	36.38	63.62 (50.49)	49.51	
	π	38.30	61.70		37.84	62.16		36.09	63.91		
	β -substitution	-CH ₂ OH σ	37.01	62.99 (50.22)	49.78	36.99	63.01 (50.22)	49.78	36.76	63.24 (50.33)	49.67
		π	39.88	60.12		40.12	59.88		37.95	62.05	
-CH ₂ OC(=O)Me σ		36.96	63.04 (50.29)	49.71	36.85	63.15 (50.29)	49.71	36.73	63.27 (50.49)	49.51	
π		39.43	60.57		38.38	61.62		37.34	62.66		
-CH ₂ NHC(=O)Me σ		37.06	62.94 (50.08)	49.92	36.98	63.02 (50.16)	49.84	36.96	63.04 (50.16)	49.84	
π		39.41	60.59		38.68	61.32		38.08	61.92		
-CH ₂ OC(=O)NHMe σ		36.96	63.04 (50.29)	49.71	36.86	63.14 (50.39)	49.61	36.82	63.18 (50.46)	49.54	
π		39.46	60.54		38.43	61.57		37.82	62.18		
-CH ₂ C(=O)NH ₂ σ		37.07	62.93 (50.15)	49.85	37.12	62.88 (49.93)	50.07	37.00	63.00 (50.26)	49.74	
π		38.82	61.18		37.68	62.32		38.14	61.86		
-CH ₂ C(=O)OMe σ		36.97	63.03 (50.22)	49.78	36.94	63.06 (50.24)	49.76	36.75	63.25 (50.19)	49.81	
π		39.29	60.71		38.79	61.21		38.70	61.30		
-CH ₂ OMe σ		37.01	62.99 (50.23)	49.77	36.93	63.07 (50.31)	49.69	36.81	63.19 (50.34)	49.66	
π		39.92	60.08		39.54	60.46		38.65	61.35		
-CH ₂ P(=O)(OMe) ₂ σ	36.97	63.03 (50.27)	49.73	37.03	62.97 (50.16)	49.84	37.06	62.94 (49.71)	50.29		

Complete reference (50):

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Revision B.01 ed.; Gaussian, Inc., Wallingford CT, 2004; Pittsburgh PA, 2003.

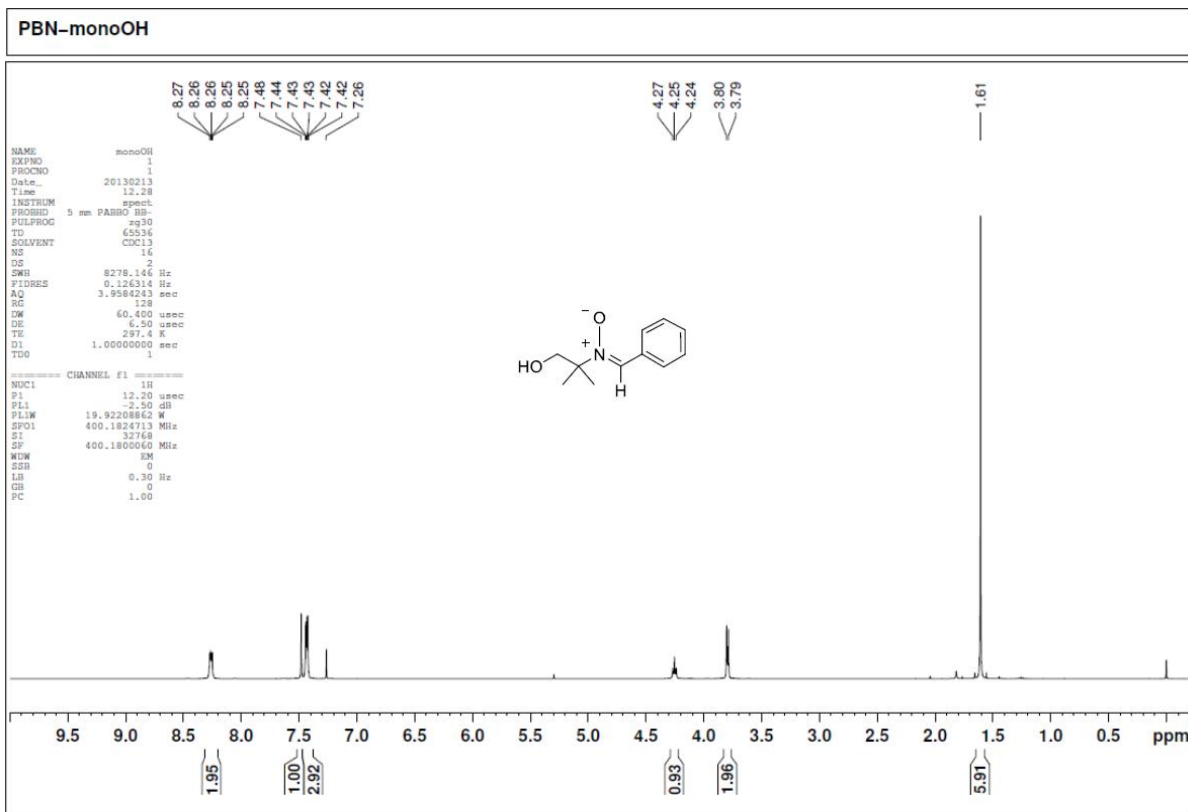


Figure S14. ^1H NMR spectrum of compound **1** in CDCl_3 .

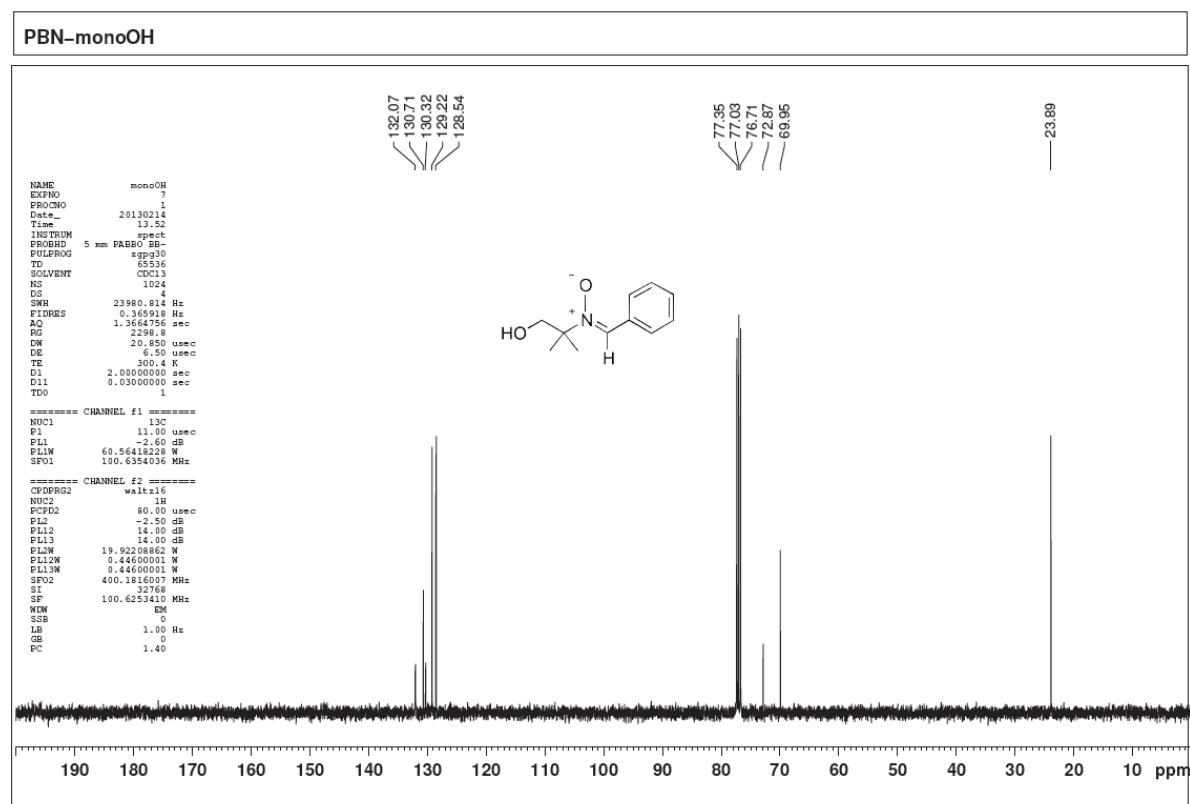


Figure S15. ^{13}C NMR spectrum of compound **1** in CDCl_3 .

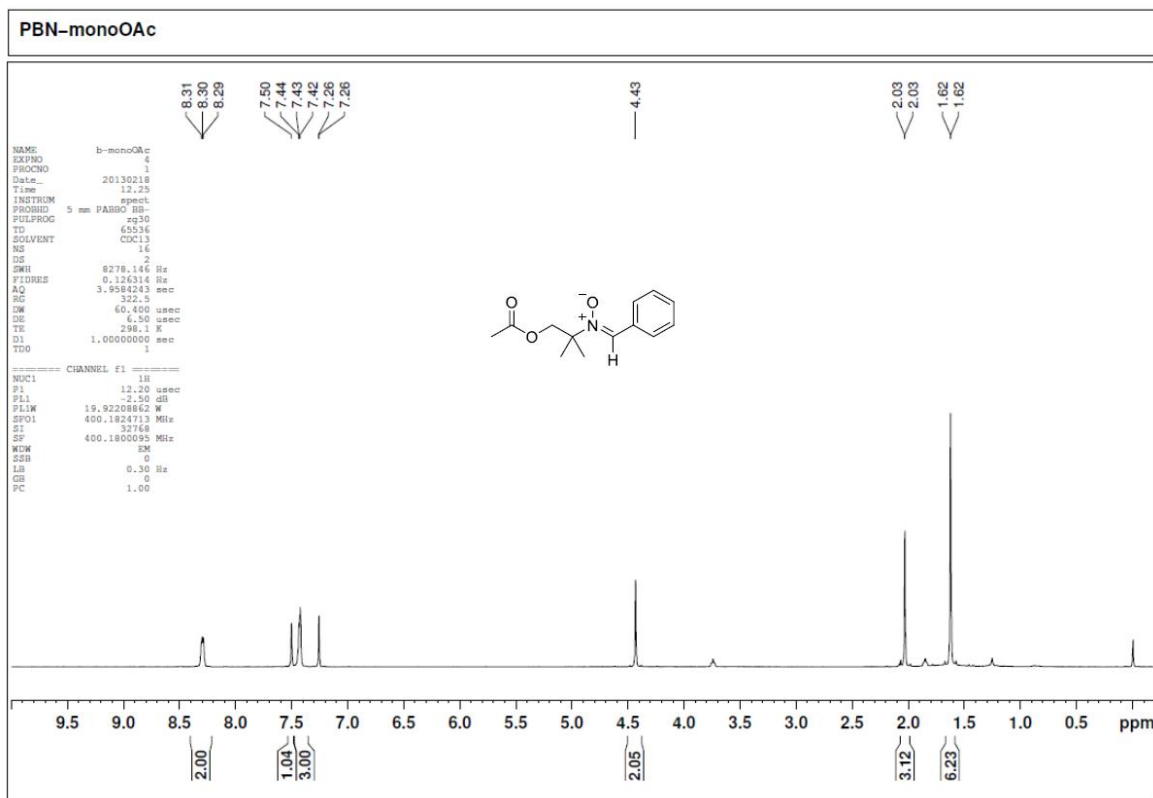


Figure S16. ^1H NMR spectrum of compound **2** in CDCl_3 .

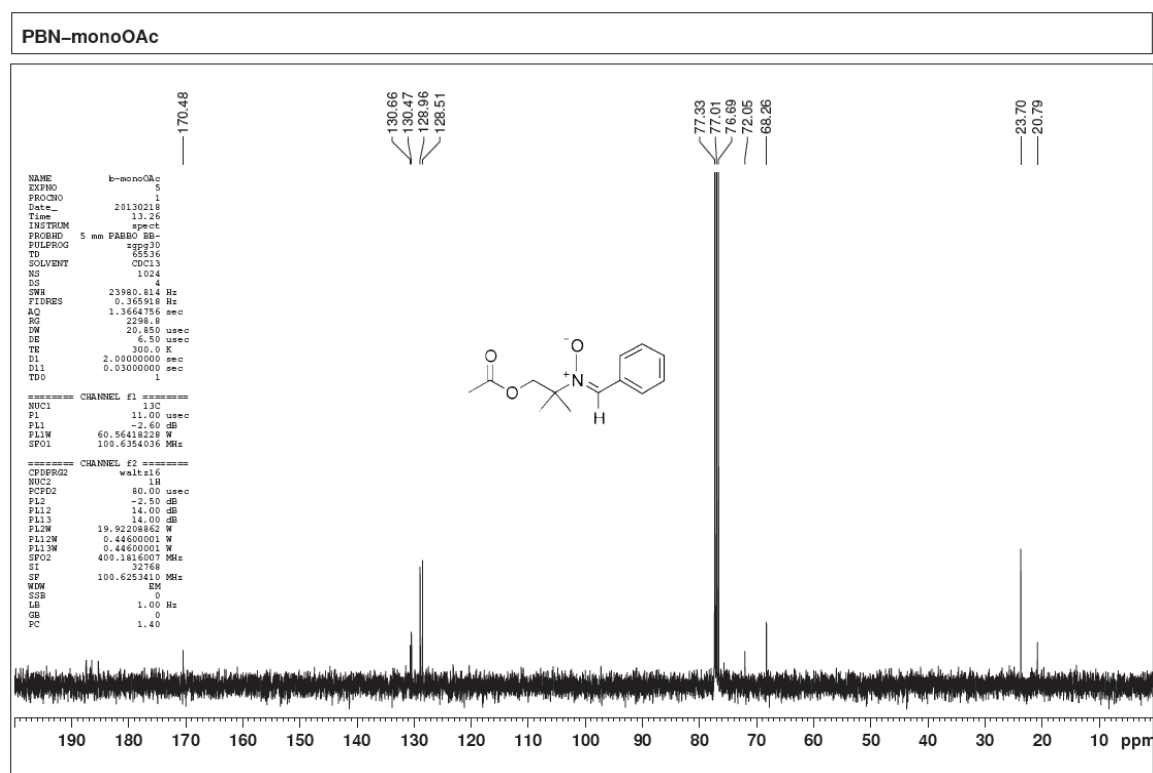


Figure S17. ^{13}C NMR spectrum of compound **2** in CDCl_3

NO₂-C(CH₃)₂-CH₂-OCONH-CH₃

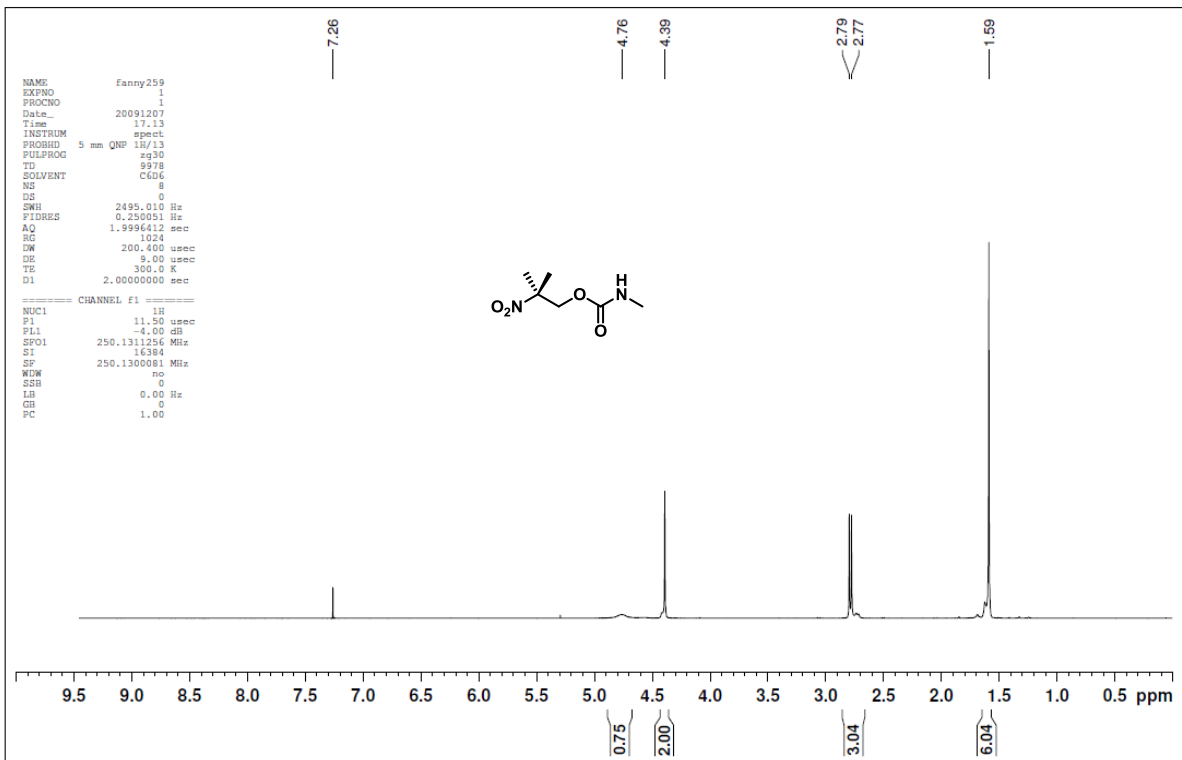


Figure S18. ¹H NMR spectrum of compound 3 in CDCl₃

NO₂-C(CH₃)₂-CH₂-OCONH-CH₃

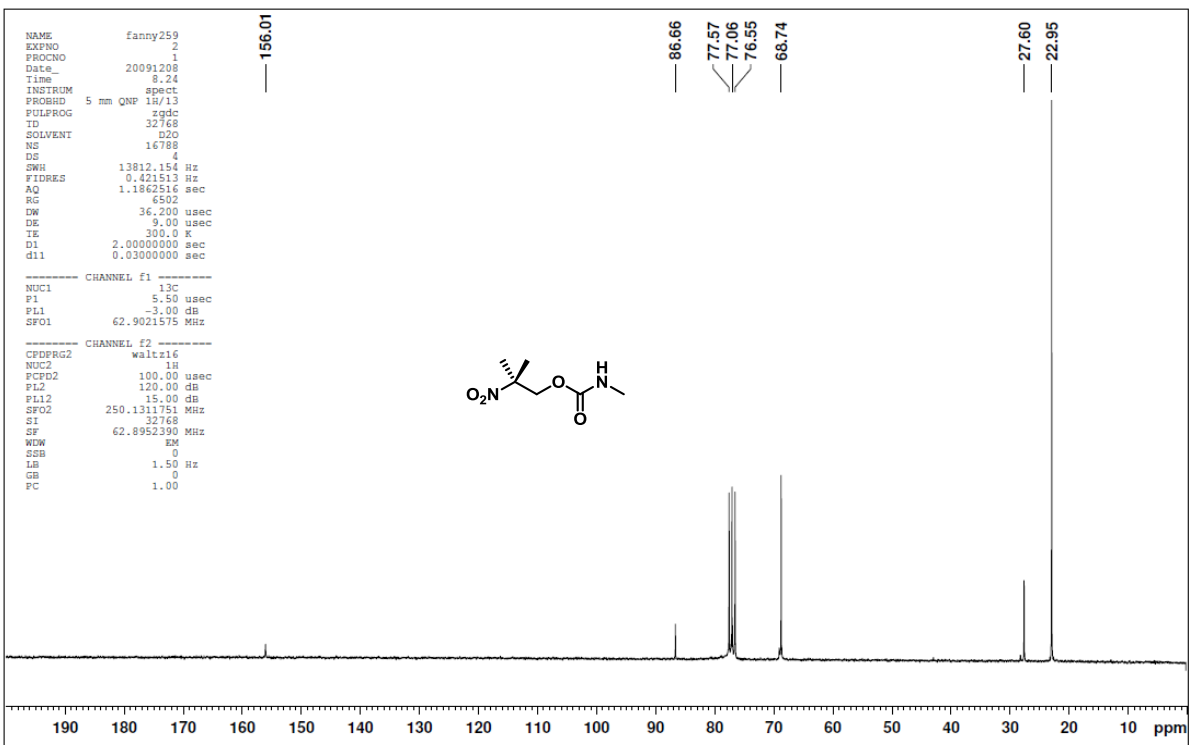


Figure S19. ¹³C NMR spectrum of compound 3 in CDCl₃

NO₂-C(CH₃)₂-CH₂-NHCO-CH₃

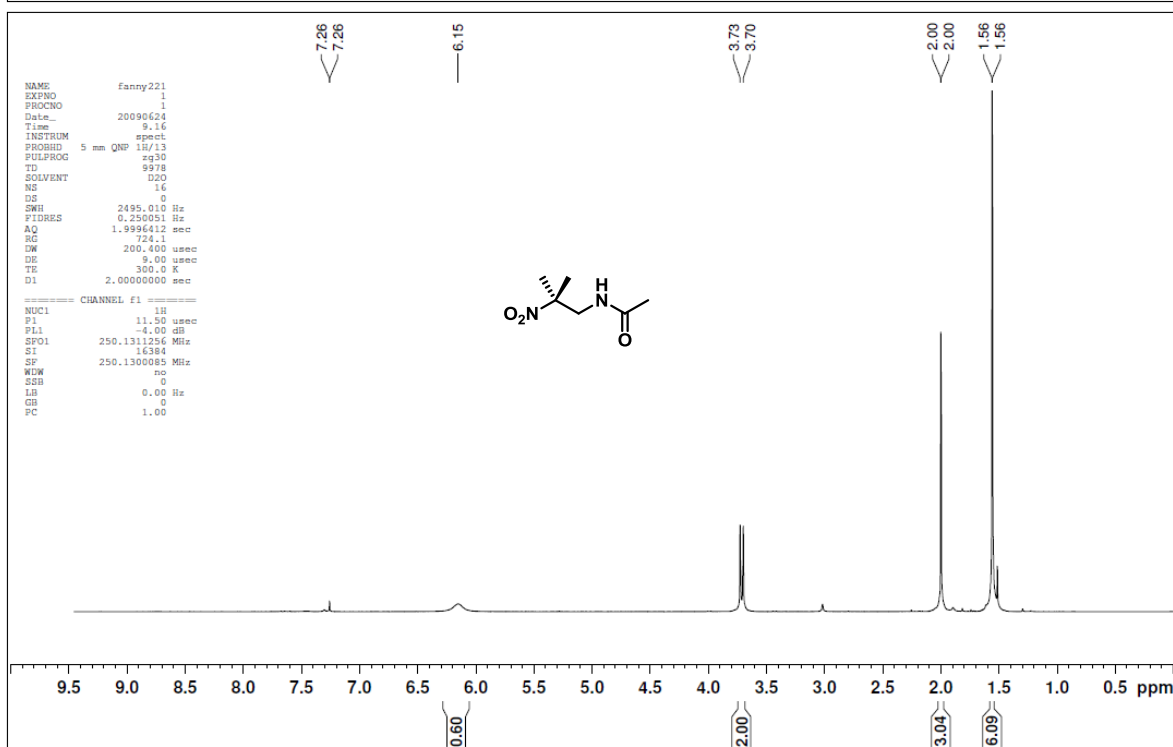


Figure S20. ¹H NMR spectrum of compound **5** in CDCl₃

NO₂-C(CH₃)₂-CH₂-NHCO-CH₃

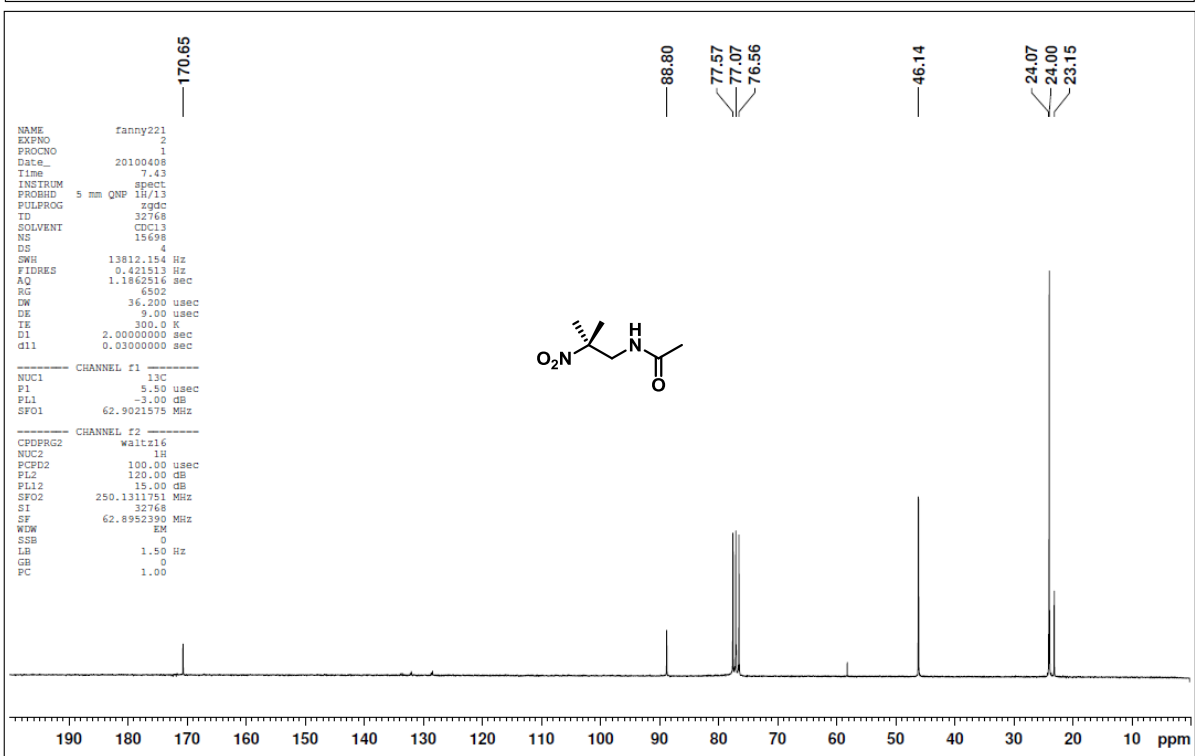


Figure S21. ¹³C NMR spectrum of compound **5** in CDCl₃

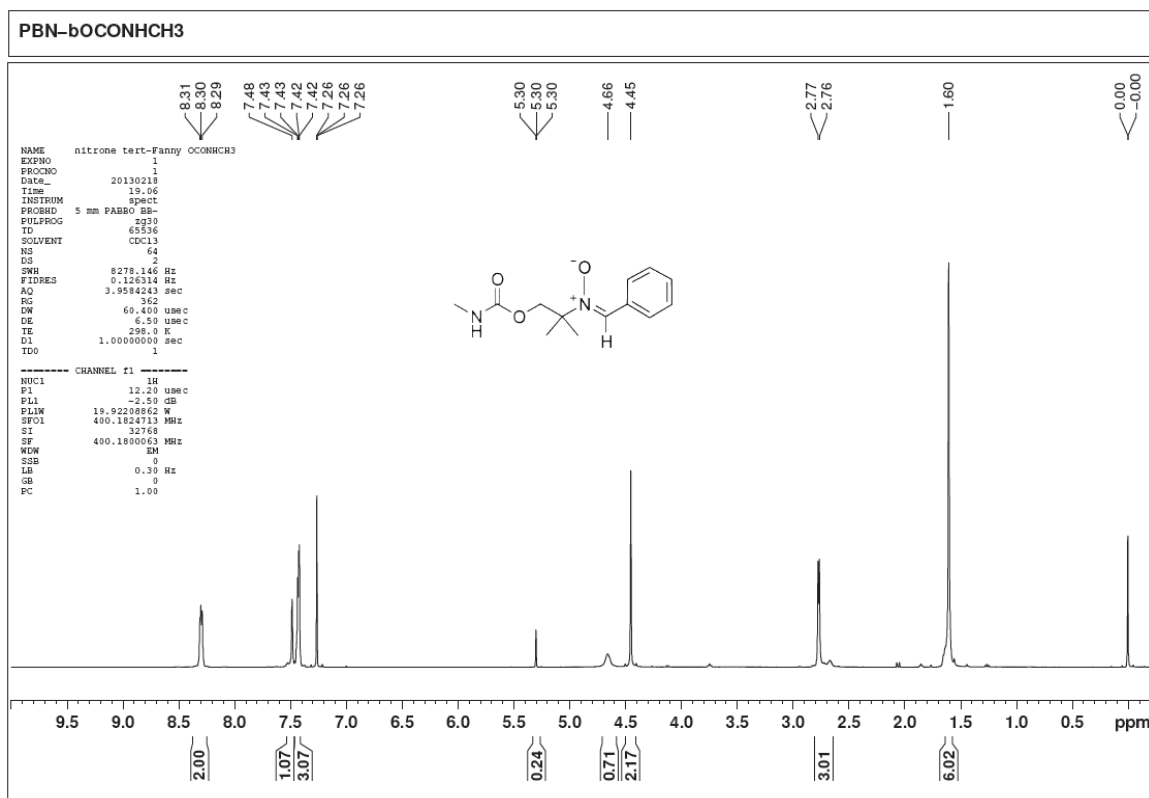


Figure S22. ^1H NMR spectrum of compound **6** in CDCl_3 .

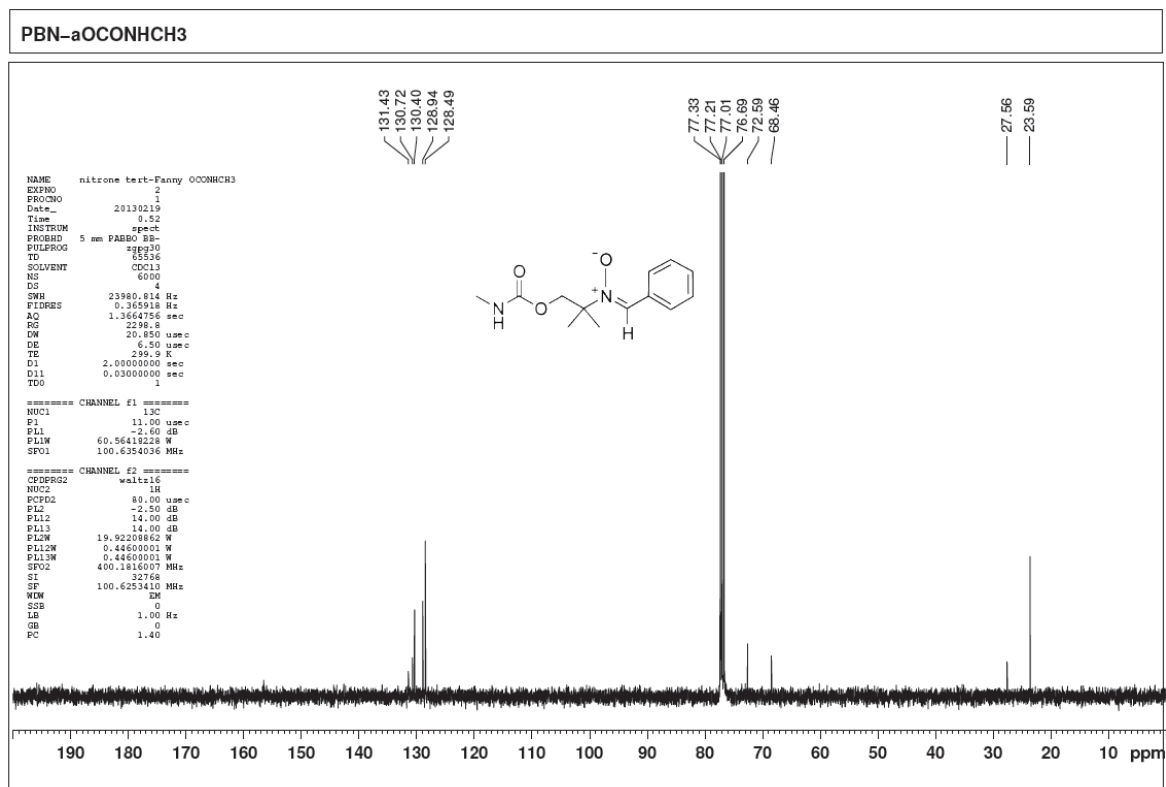


Figure S23. ^{13}C NMR spectrum of compound **6** in CDCl_3 .

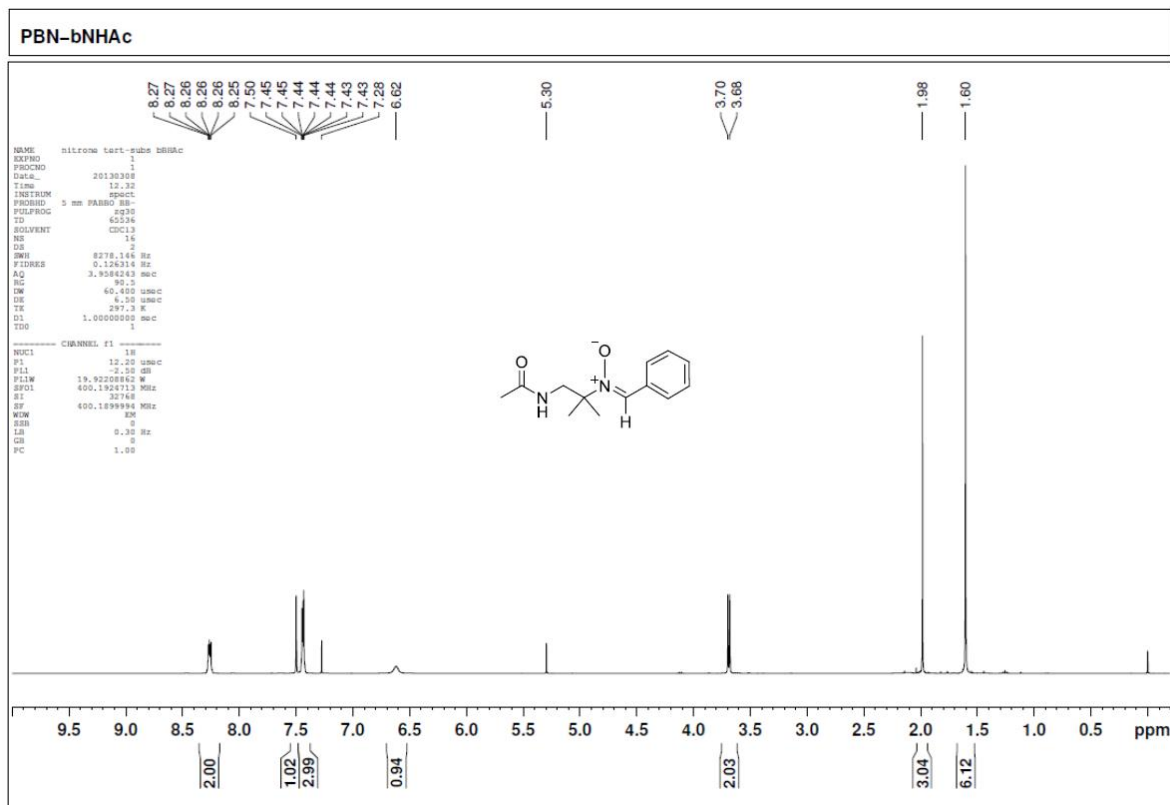


Figure S24. ^1H NMR spectrum of compound 7 in CDCl_3 .

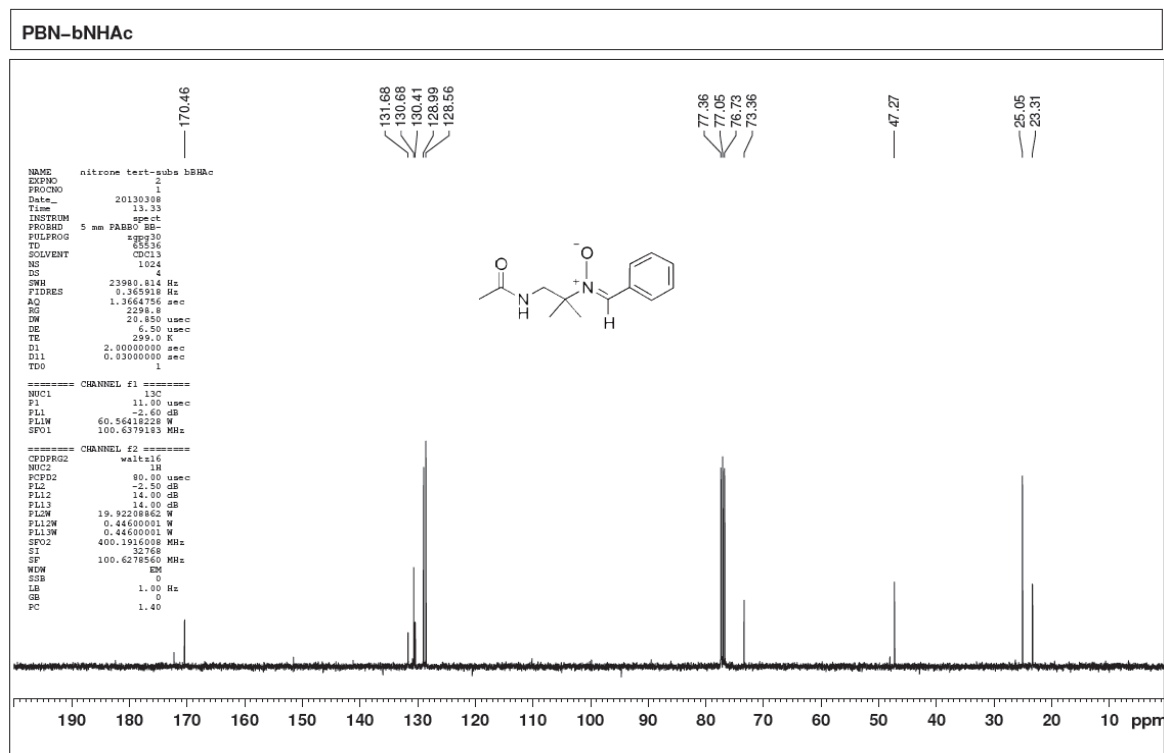


Figure S25. ^{13}C NMR spectrum of compound 7 in CDCl_3

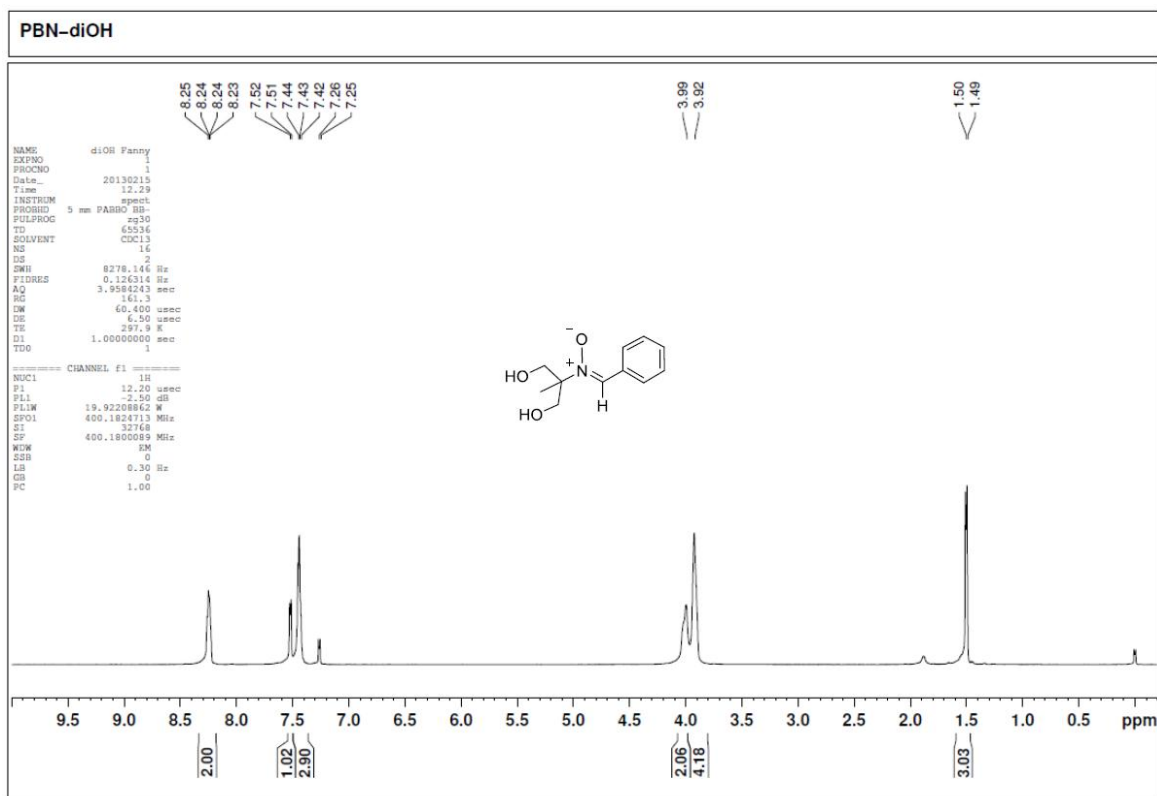


Figure S26. ^1H NMR spectrum of compound **8** in CDCl_3 .

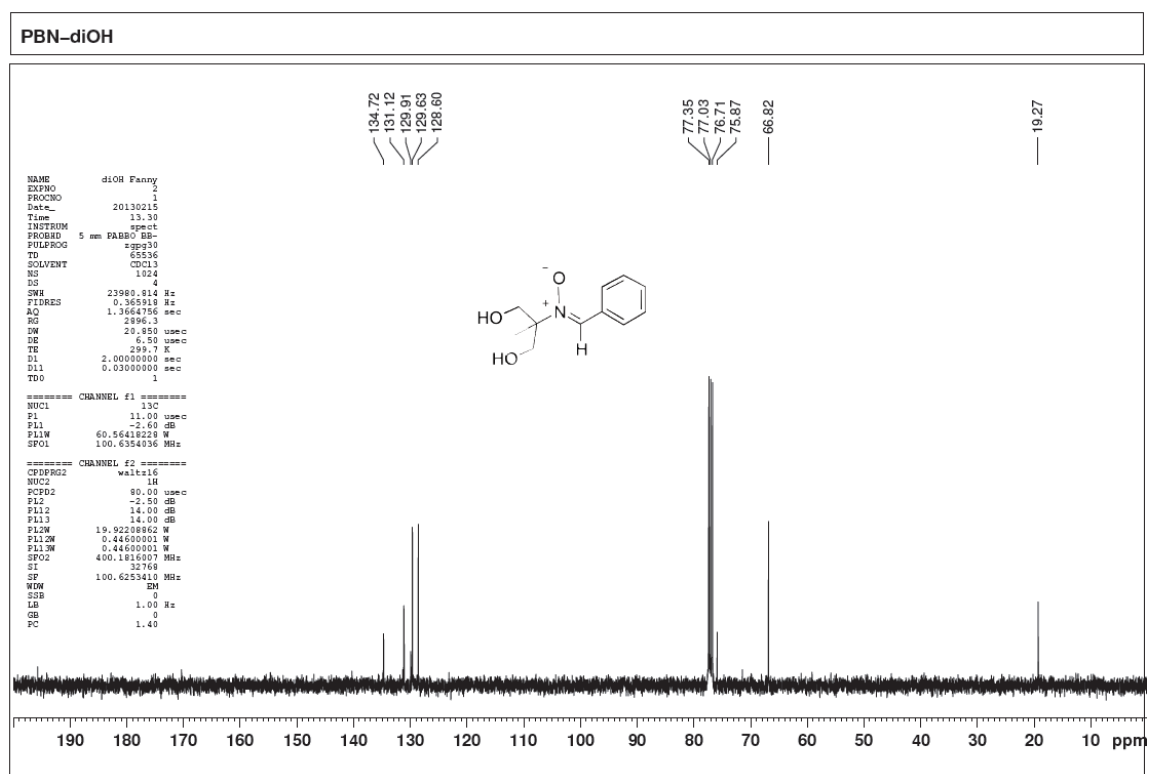


Figure S27. ^{13}C NMR spectrum of compound **8** in CDCl_3 .

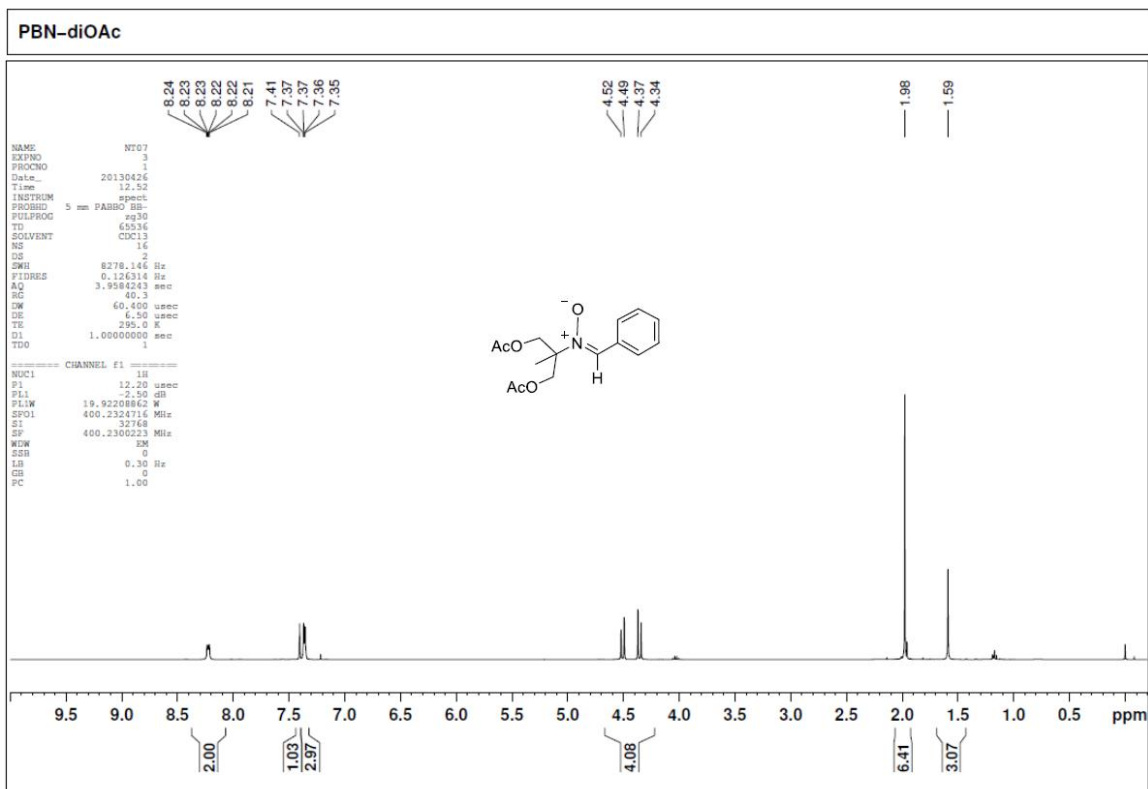


Figure S28. ^1H NMR spectrum of compound **10** in CDCl_3 .

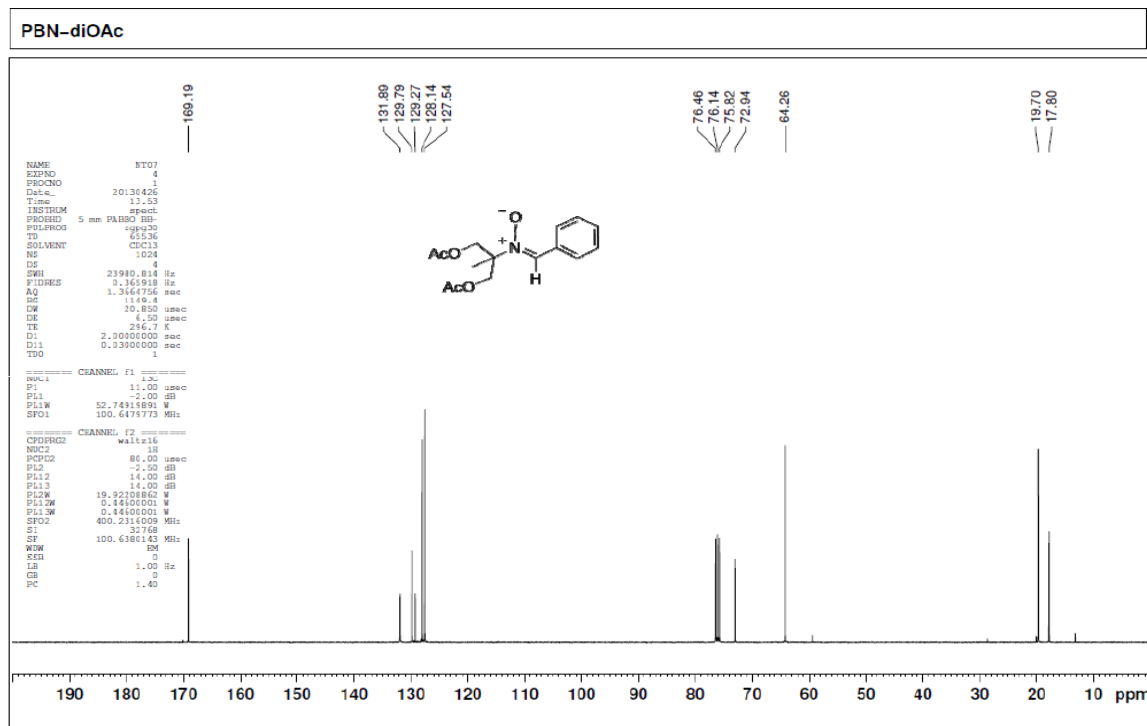


Figure S29. ^{13}C NMR spectrum of compound **10** in CDCl_3 .

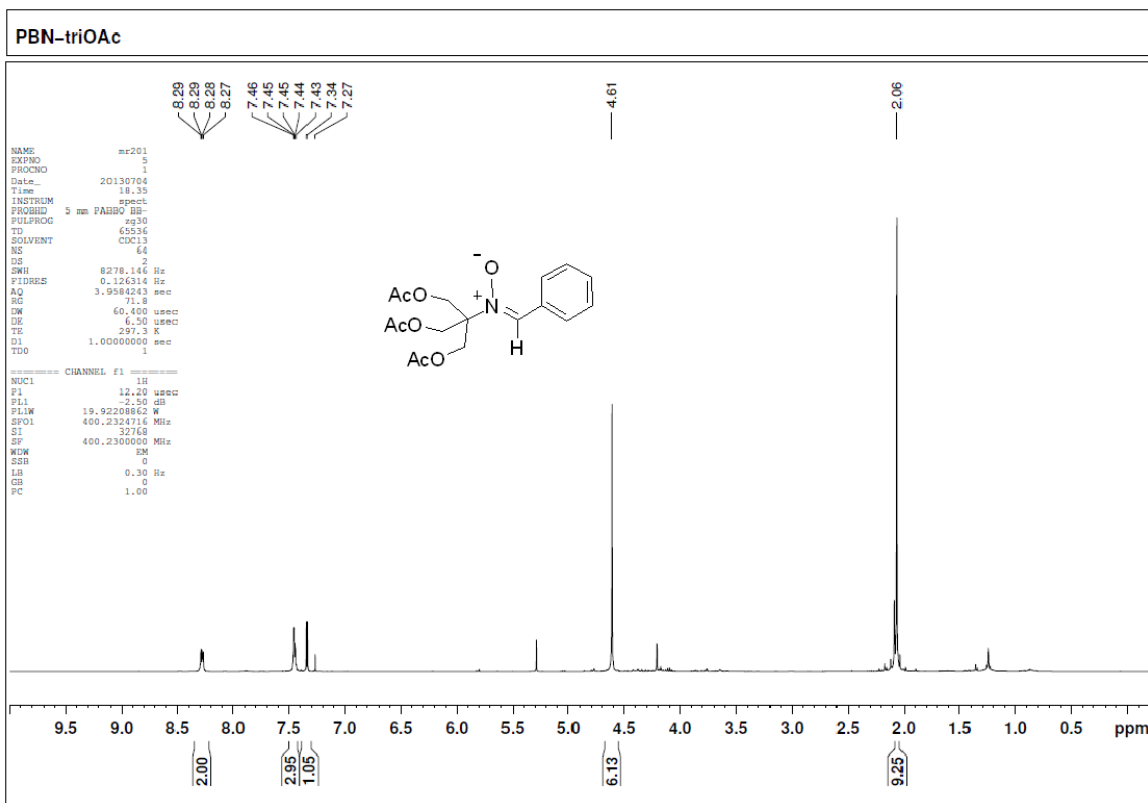


Figure S30. ^1H NMR spectrum of compound **11** in CDCl_3 .

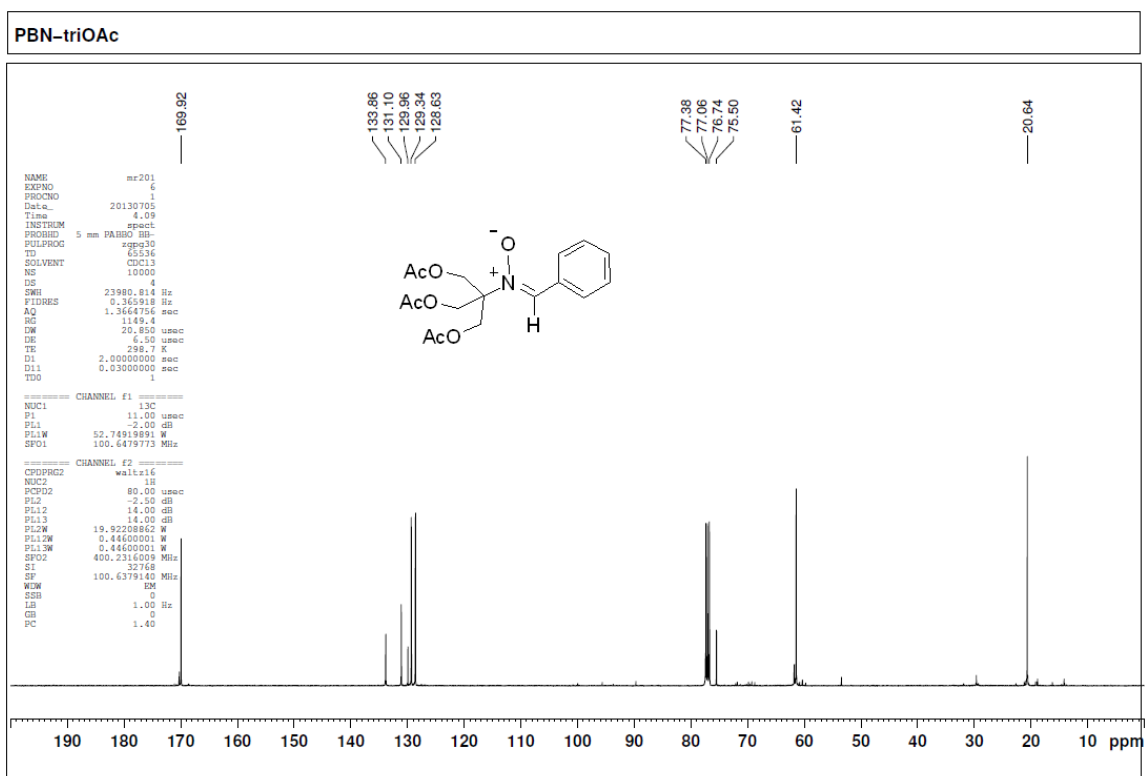


Figure S31. ^{13}C NMR spectrum of compound **11** in CDCl_3 .

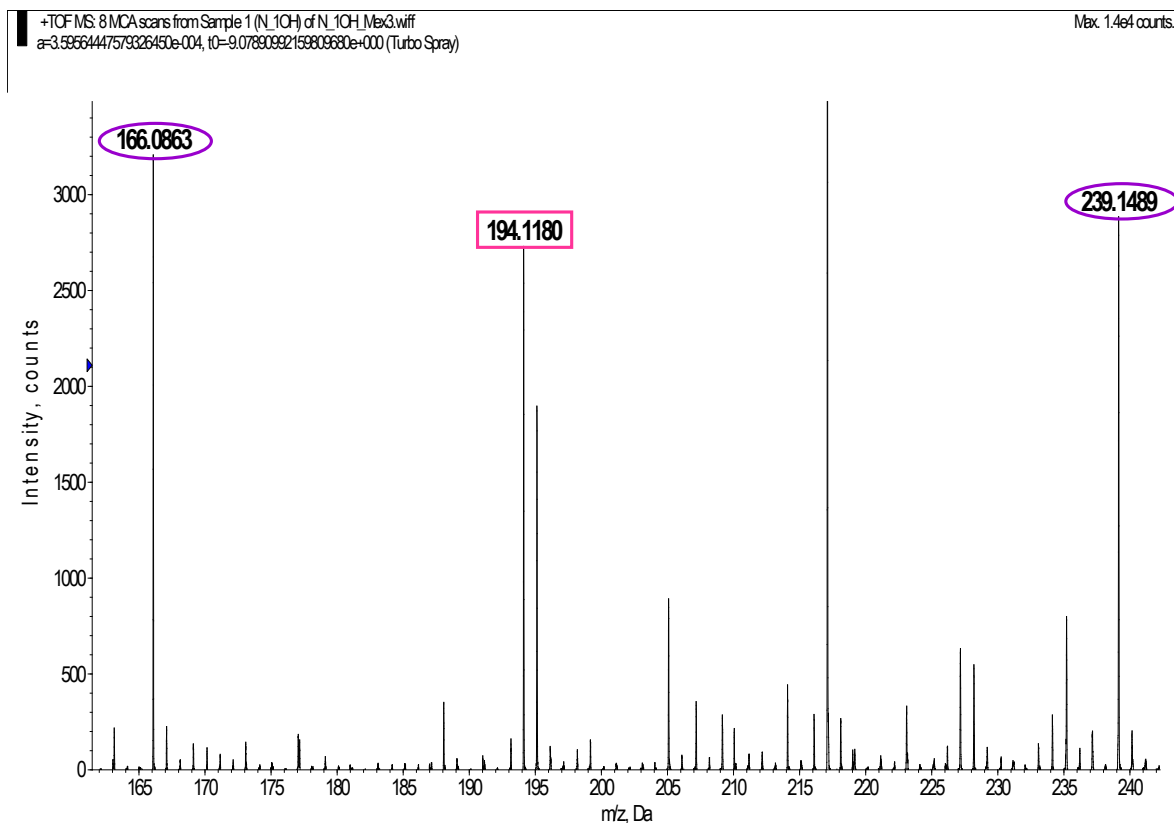


Figure S32. High-resolution mass spectrum of compound 1.

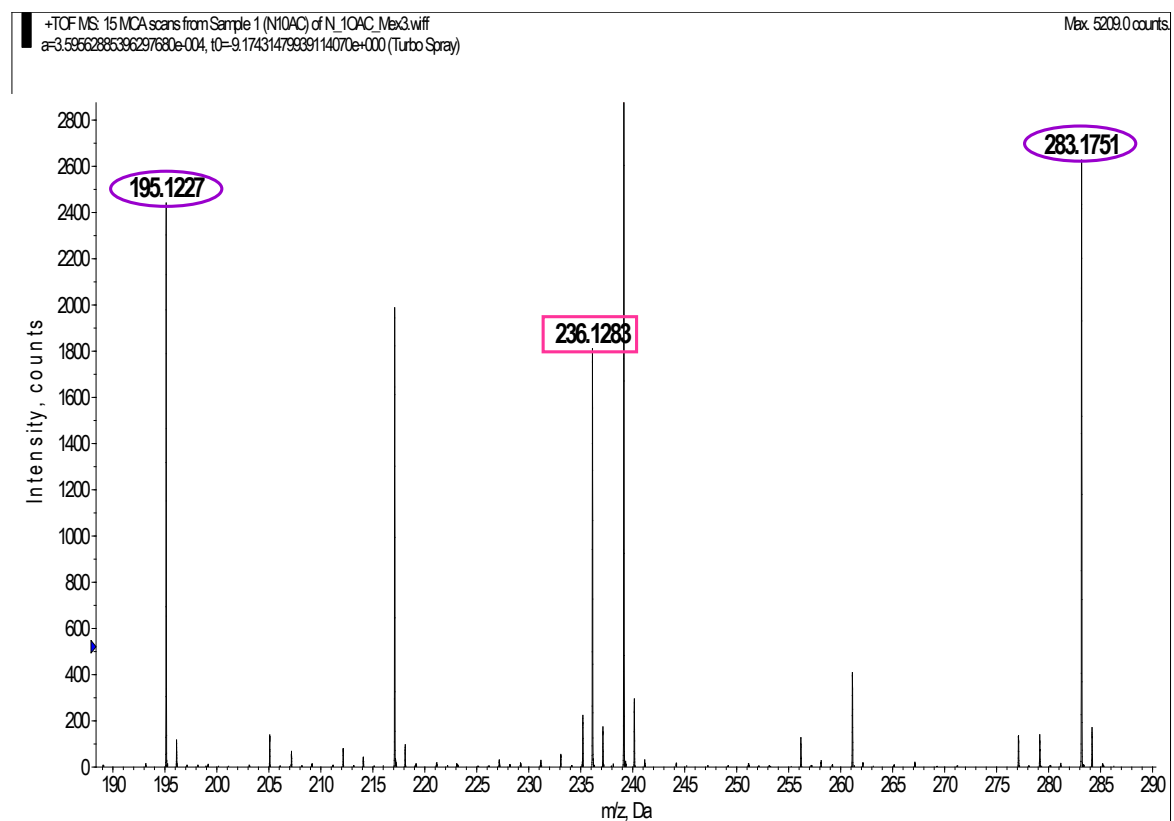


Figure S33. High-resolution mass spectrum of compound 2.

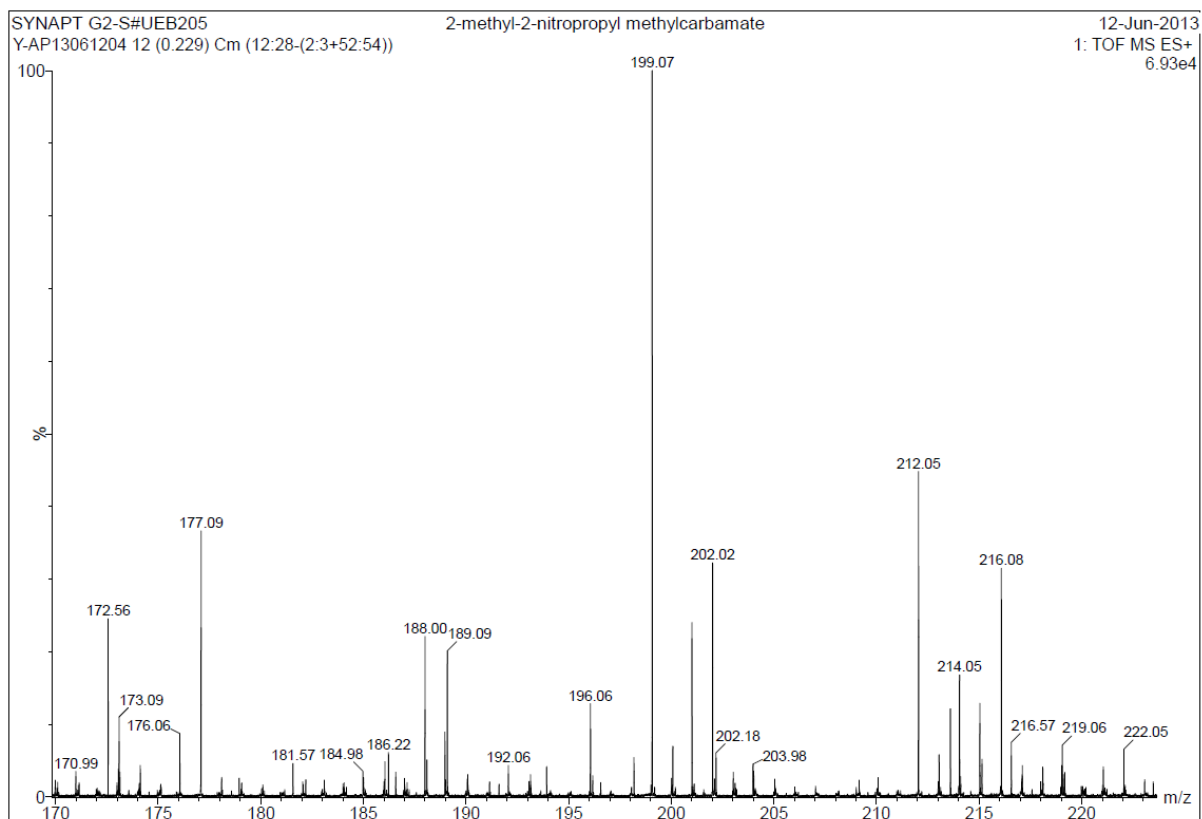


Figure S34. High-resolution mass spectrum of compound **3**.

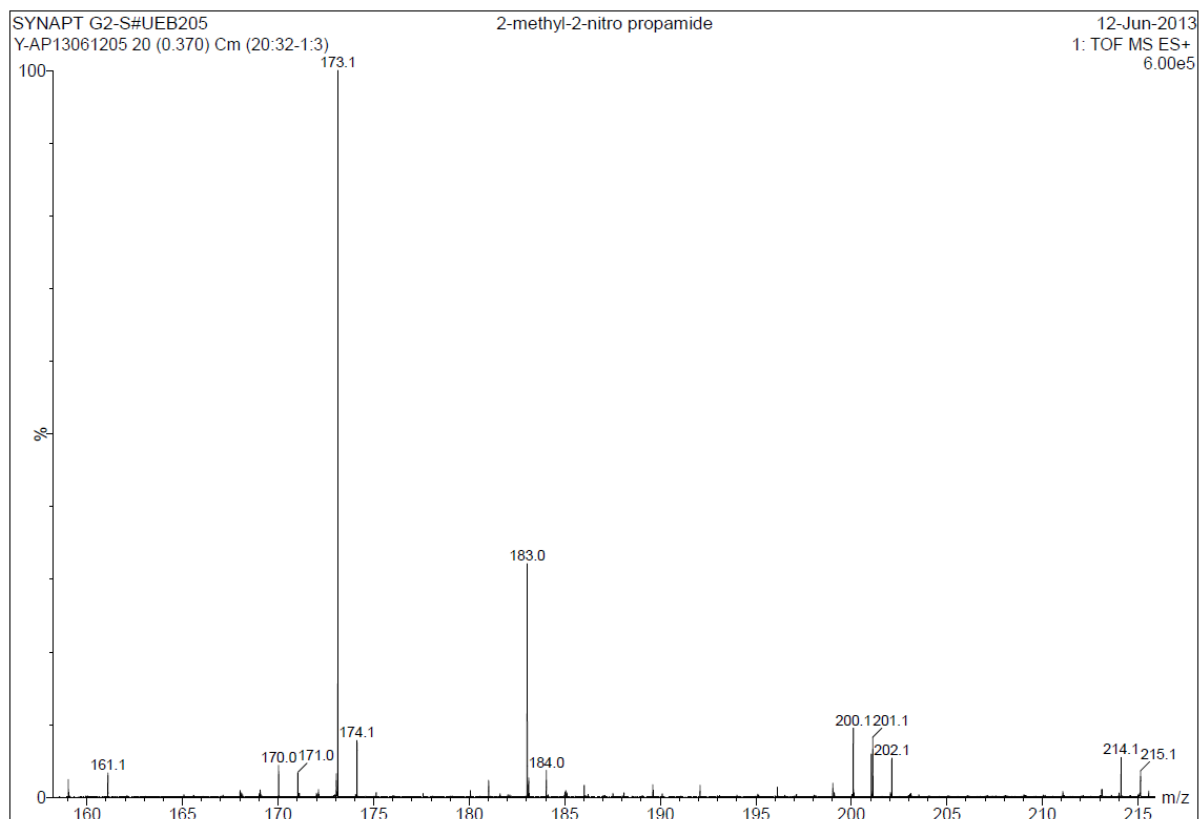


Figure S35. High-resolution mass spectrum of compound **5**.

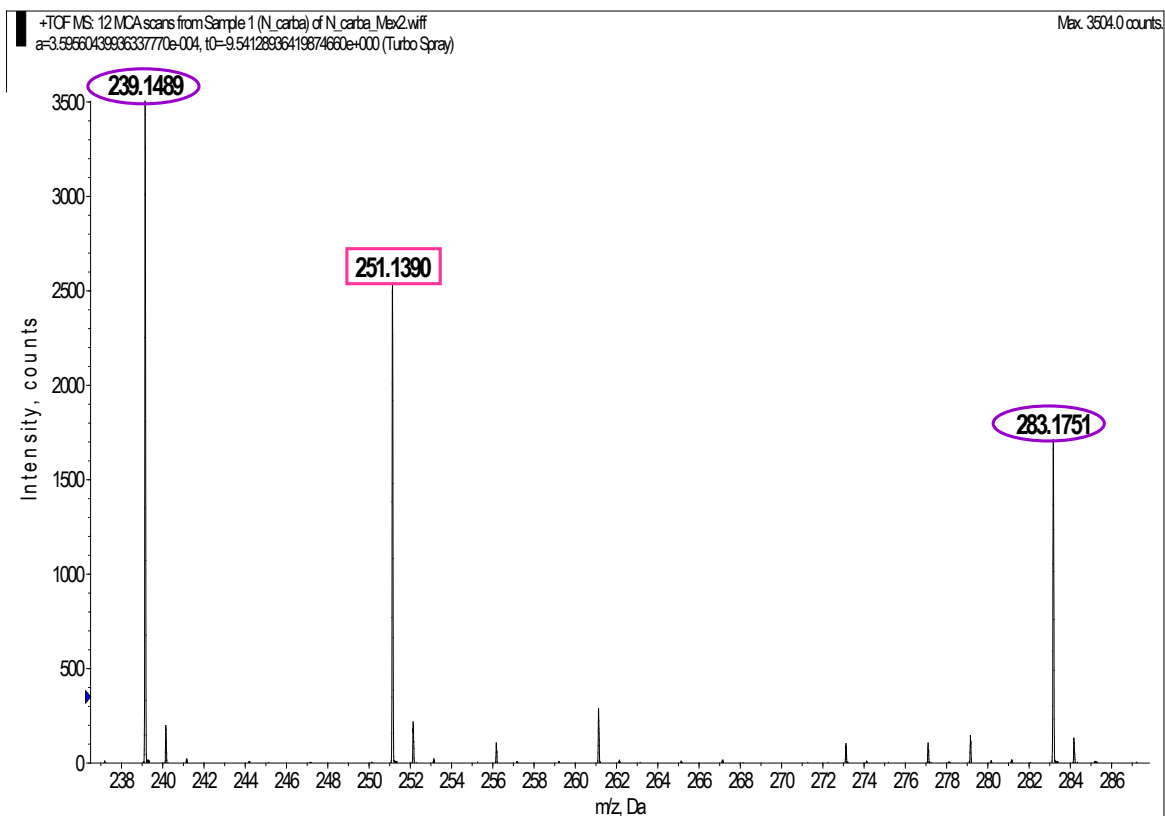


Figure S36. High-resolution mass spectrum of compound 6.

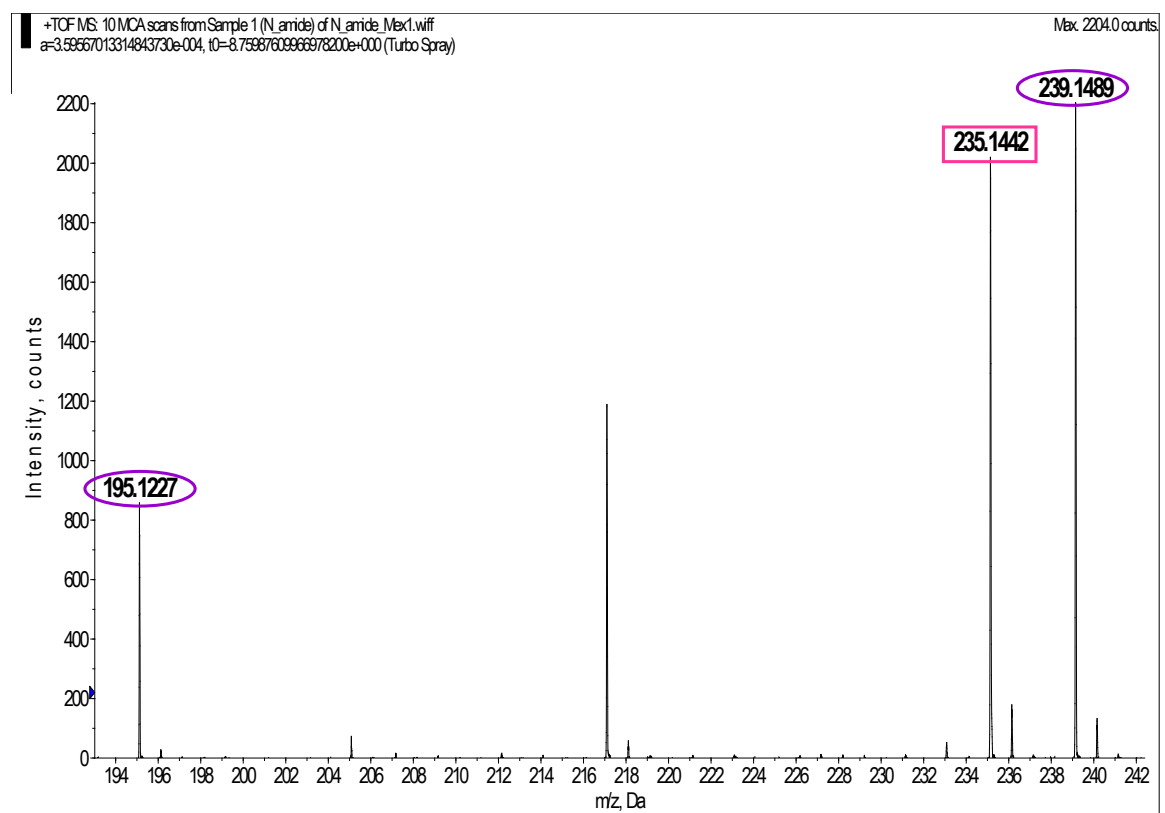


Figure S37. High-resolution mass spectrum of compound 7.

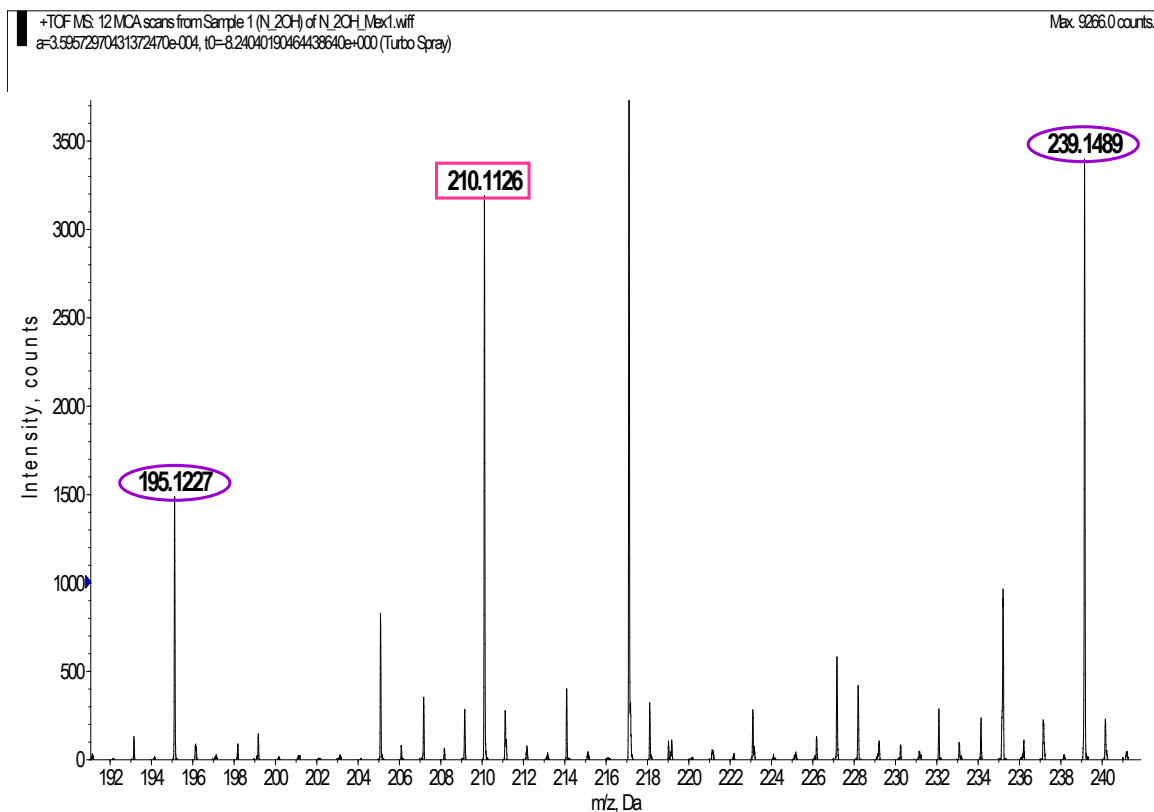


Figure S38. High-resolution mass spectrum of compound **8**.

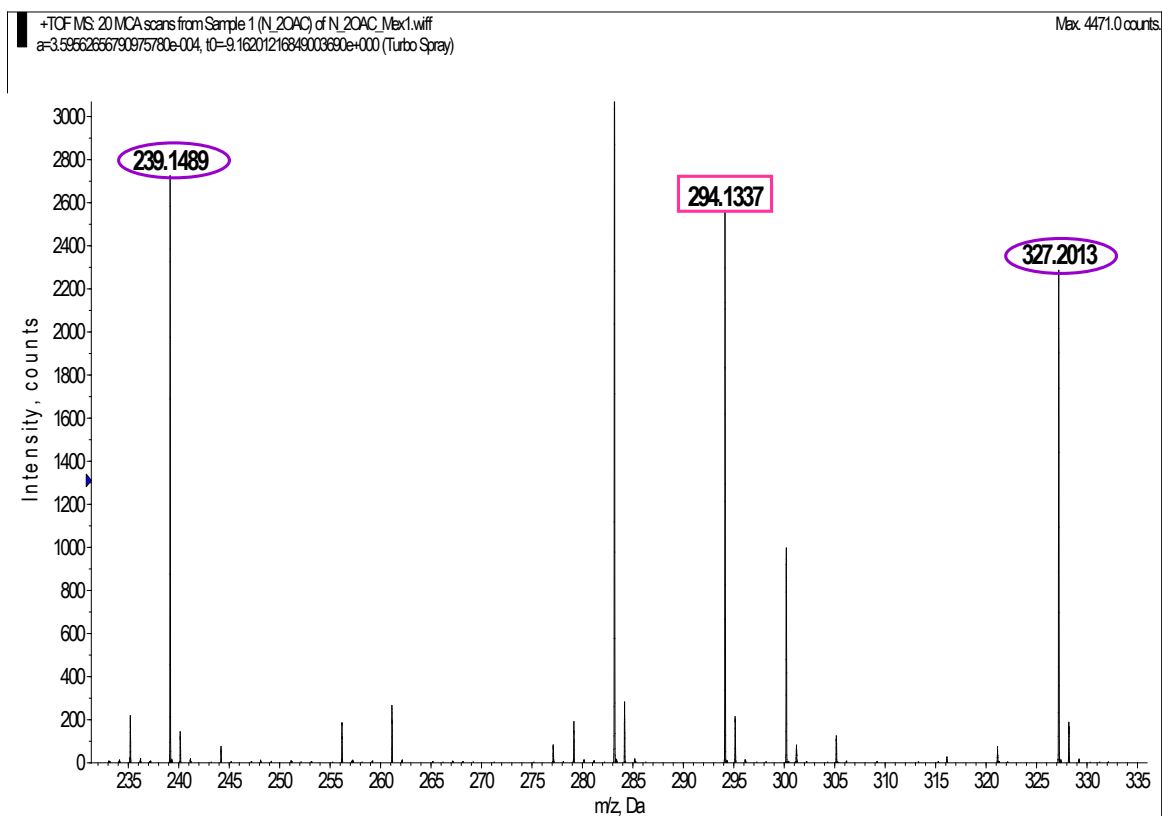


Figure S39. High-resolution mass spectrum of compound **10**.

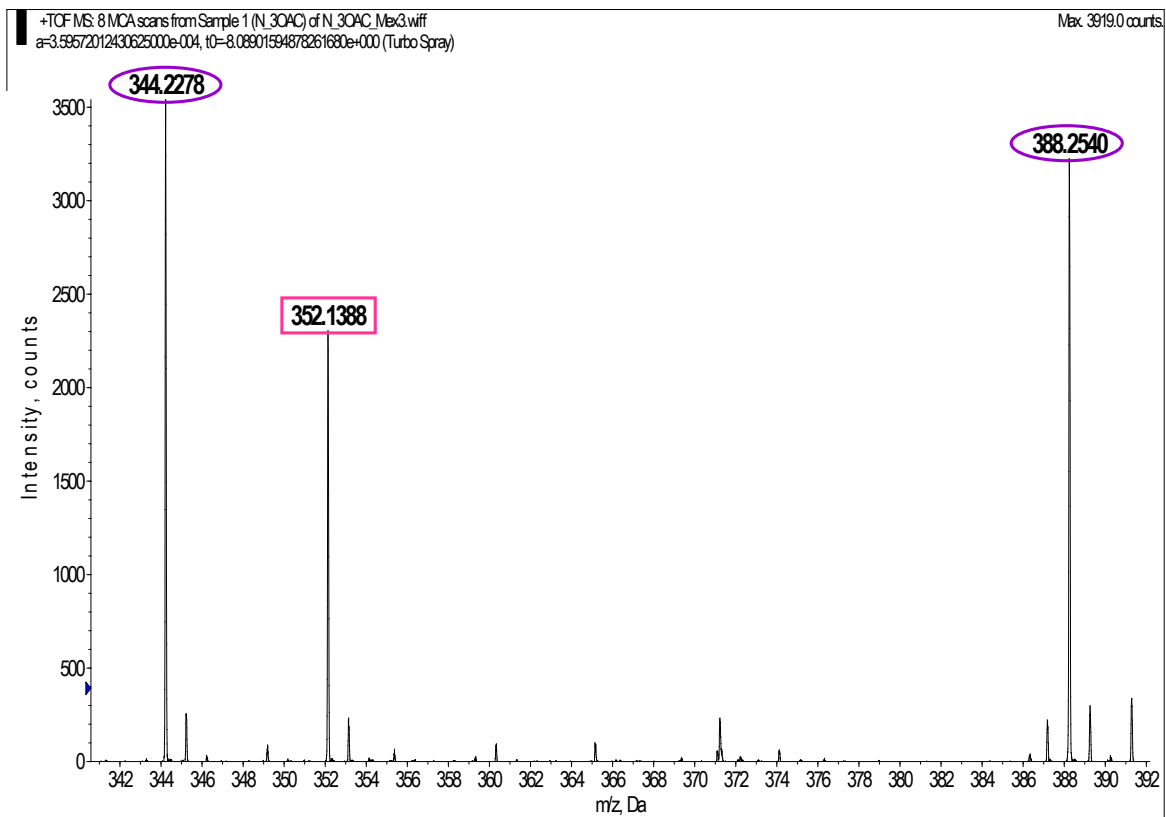


Figure S40. High-resolution mass spectrum of compound **11**.

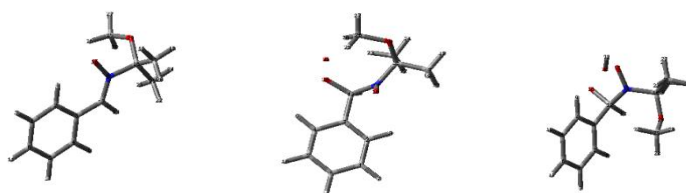
Table S3. Thermodynamic parameters of the nitrones in water at the PCM/B3LYP/6-31+g**//B3LYP/6-31g* level of theory.



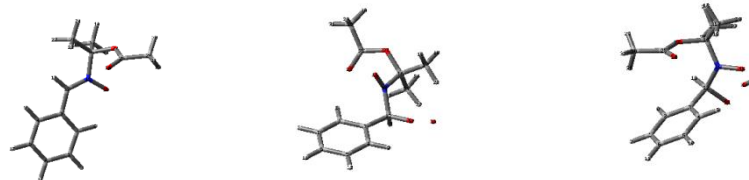
Compound	O2 Radical Anion	OOH Radical
file	o2.log	peroxyIrad.log
E 6-31+g**/PCM	-150.465075	-150.926851
E 6-31g*	-150.2996938	-150.899156
ZPE (raw)	0.002761	0.014031
Therm Corr to H (raw)	0.006082	0.017832
Therm Corr to G (raw)	-0.017041	-0.008160
H (raw)	-150.293612	
G (raw)	-150.316735	
ZPE (scaled)	0.002707	0.013759
Electronic State		2-A"
s2 6-31g*	0.7528	0.754000
Symmetry	C01	CS
N Imag	0	0.000000
Rotational Con. (GHz)	1.63425	608.847080
Rotational Con. (GHz)	0.75785	33.559922
Rotational Con. (GHz)	0.66048	31.806722
H298		
6-31+g* */PCM	-150.459047	-150.909291
6-31g*	-150.293665	-150.881597
G298		
6-31+g* */PCM	-150.482170	-150.935283
6-31g*	-150.316788	-150.907589



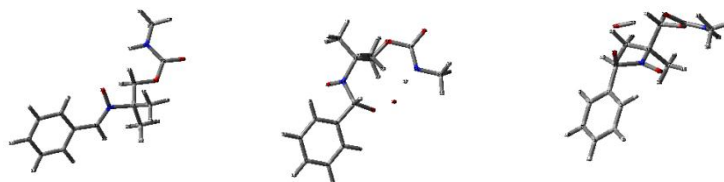
Compound	PBN-mono-OC(O)NHMe	PBN-mono-OC(O)NHMe-O2	PBN-mono-OC(O)NHMe-HO2
file	PBN-alpha-carbamate.log	PBN-alpha-carbamate-O2.log	PBN-alpha-carbamate-O2H.log
E 6-31+g**	-802.102993	-952.560333	-953.045952
E 6-31g*	-802.0482311	-952.4226875	-952.9738242
ZPE (raw)	0.272005	0.275592	0.290109
Therm Corr to H (raw)	0.290165	0.295451	0.311141
Therm Corr to G (raw)	0.225326	0.227129	0.239117
H (raw)			
G (raw)			
ZPE (scaled)	0.266728	0.270246	0.284481
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.718374	0.7408215	0.8196567
Rotational Con. (GHz)	0.2798918	0.2349741	0.2282568
Rotational Con. (GHz)	0.2232464	0.1955388	0.2035903
H298			
6-31+g* *	-801.818105	-952.270228	-952.740439
6-31g*	-801.763343	-952.132583	-952.668311
G298			
6-31+g* *	-801.882944	-952.338550	-952.812463
6-31g*	-801.828182	-952.200905	-952.740335



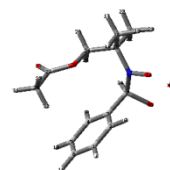
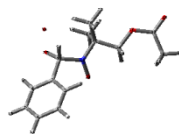
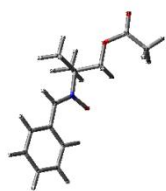
Compound	PBN-mono-OMe	PBN-mono-OMe-O2	PBN-mono-OMe-HO2
file	PBN-alpha-ether.log	PBN-alpha-ether-O2.log	PBN-alpha-ether-O2H.log
E 6-31+g**	-633.368212	-783.824231	-784.322527
E 6-31g*	-633.327056	-783.676431	-784.2680369
ZPE (raw)	0.245009	0.2498	0.263544
Therm Corr to H (raw)	0.259704	0.26646	0.280926
Therm Corr to G (raw)	0.204374	0.206491	0.218806
H (raw)			
G (raw)			
ZPE (scaled)	0.240256	0.244954	0.258431
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7544
Symmetry	C1	C1	C1
N Imag	0.000000	0	0
Rotational Con. (GHz)	1.595910	1.0016998	0.7930845
Rotational Con. (GHz)	0.3488671	0.3495338	0.4100507
Rotational Con. (GHz)	0.3310871	0.2994256	0.3382328
H298			
6-31+g* *	-633.113261	-783.562617	-784.046714
6-31g*	-633.072105	-783.414817	-783.992224
G298			
6-31+g* *	-633.168591	-783.622586	-784.108834
6-31g*	-633.127435	-783.474786	-784.054344



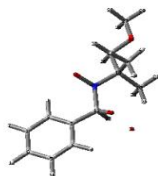
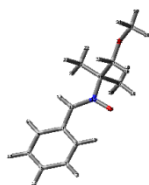
Compound	PBN-mono-OC(O)Me	PBN-mono-OC(O)Me-O2	PBN-mono-OC(O)Me-HO2
file	PBN-alpha-ester.log	PBN-alpha-ester-O2.log	PBN-alpha-ester-O2H.log
E 6-31+g**	-746.730934	-897.189714	-897.681499
E 6-31g*	-746.6864285	-897.0399514	-897.6228738
ZPE (raw)	0.254483	0.259336	0.272601
Therm Corr to H (raw)	0.271066	0.278012	0.29208
Therm Corr to G (raw)	0.210906	0.212774	0.224369
H (raw)			
G (raw)			
ZPE (scaled)	0.249546	0.254305	0.267313
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7544	0.7544
Symmetry	C1	C1	C1
N Imag	0.000000	0	0
Rotational Con. (GHz)	1.0658731	0.6349036	0.551645
Rotational Con. (GHz)	0.2838513	0.3147217	0.394877
Rotational Con. (GHz)	0.2678065	0.2359381	0.2914232
H298			
6-31+g* *	-746.464805	-896.916733	-897.394707
6-31g*	-746.420299	-896.766970	-897.336082
G298			
6-31+g* *	-746.524965	-896.981971	-897.462418
6-31g*	-746.480459	-896.832208	-897.403793



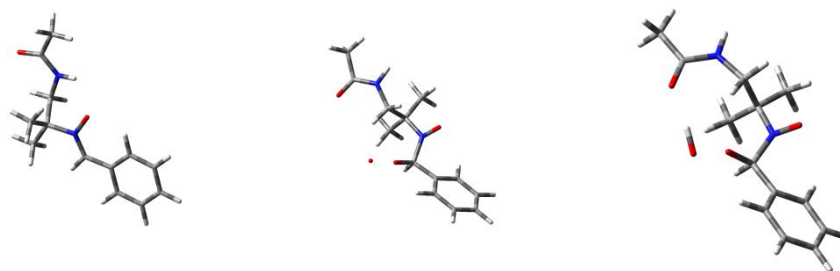
Compound	PBN-mono-CH2-OCONHMe PBN-alpha-methylcarbamate.log	PBN-mono-CH2-OCONHMe-O2 PBN-alpha-methylcarbamate-O2.log	PBN-mono-CH2-OCONHMe-HO2 PBN-alpha-methylcarbamate-O2H.log
file			
E 6-31+g**	-841.41223	-991.87745	-992.368953
E 6-31g*	-841.3495103	-991.7303516	-992.3022749
ZPE (raw)	0.301233	0.306522	0.321083
Therm Corr to H (raw)	0.32068	0.327154	0.342516
Therm Corr to G (raw)	0.252347	0.257583	0.270201
H (raw)			
G (raw)			
ZPE (scaled)	0.295389	0.300575	0.314854
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7544
Symmetry	C1	C1	C1
N Imag	0.000000	0	0
Rotational Con. (GHz)	1.0230754	0.7200958	0.5550306
Rotational Con. (GHz)	0.1559983	0.1889317	0.2175204
Rotational Con. (GHz)	0.146479	0.1606431	0.1942813
H298			
6-31+g* *	-841.097394	-991.556243	-992.032666
6-31g*	-841.034674	-991.409144	-991.965988
G298			
6-31+g* *	-841.165727	-991.625814	-992.104981
6-31g*	-841.103007	-991.478715	-992.038303



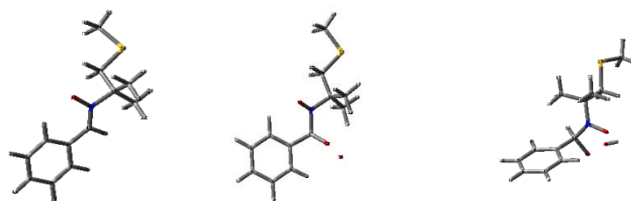
Compound	PBN-mono-CH2OCOME	PBN-mono-CH2OCOME-O2	PBN-mono-CH2OCOME-HO2
file	PBN-alpha-methylester.log	PBN-alpha-methylester-O2.log	PBN-alpha-methylester-O2H.log
E 6-31+g**	-786.042782	-936.499465	-936.99893
E 6-31g*	-785.9899653	-936.3417761	-936.9346061
ZPE (raw)	0.283721	0.288257	0.302086
Therm Corr to H (raw)	0.301636	0.308333	0.322799
Therm Corr to G (raw)	0.237404	0.238544	0.251596
H (raw)			
G (raw)			
ZPE (scaled)	0.278217	0.282665	0.296226
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	1.2708003	0.7413299	0.4543138
Rotational Con. (GHz)	0.1798693	0.1841537	0.3645709
Rotational Con. (GHz)	0.1716097	0.157964	0.2488327
H298			
6-31+g* *	-785.746650	-936.196724	-936.681991
6-31g*	-785.693834	-936.039035	-936.617668
G298			
6-31+g* *	-785.810882	-936.266513	-936.753194
6-31g*	-785.758066	-936.108824	-936.688871



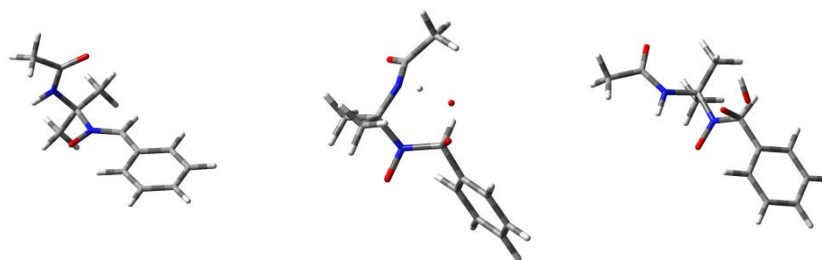
Compound	PBN-mono-CH2OMe PBN-alpha-methylether.log	PBN-mono-CH2OMe-O2 PBN-alpha-methylether-O2.log	PBN-mono-CH2OMe-HO2 PBN-alpha-methylether-O2H.log
file			
E 6-31+g**	-672.68027	-823.131399	-823.629274
E 6-31g*	-672.6390395	-822.9794606	-823.5749547
ZPE (raw)	0.274087	0.278292	0.29262
Therm Corr to H (raw)	0.290152	0.296744	0.311307
Therm Corr to G (raw)	0.231289	0.231805	0.245649
H (raw)			
G (raw)			
ZPE (scaled)	0.268770	0.272893	0.286943
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.755	0.7545
Symmetry	C1	C1	C1
N Imag	0	0.000000	0
Rotational Con. (GHz)	1.5866777	0.9480255	0.731303
Rotational Con. (GHz)	0.2525605	0.2514865	0.3112233
Rotational Con. (GHz)	0.2417921	0.2149952	0.2987838
H298			
6-31+g* *	-672.395435	-822.840054	-823.323644
6-31g*	-672.354205	-822.688115	-823.269324
G298			
6-31+g* *	-672.454298	-822.904993	-823.389302
6-31g*	-672.413068	-822.753054	-823.334982



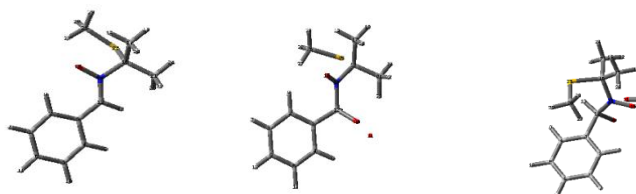
Compound	PBN-mono-CH2NHCOMe	PBN-mono-CH2NHCOMe-O2	PBN-mono-CH2NHCOMe-HO2
file	PBN-CH2NHCOMe-c.out	PBN-CH2NHCOMe-O2c.out	PBN-CH2NHCOMe-HO2c.out
E 6-31+g**/PCM	-766.194579	-916.648137	-917.141629
E 6-31g*	-766.13971	-916.4782989	-917.0713523
ZPE (raw)	0.296666	0.300354	0.315907
Therm Corr to H (raw)	0.314789	0.320942	0.336226
Therm Corr to G (raw)	0.249762	0.249879	0.267266
H (raw)			
G (raw)			
ZPE (scaled)	0.290911	0.294527	0.309778
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7544
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.0982762	1.0022697	0.8434486
Rotational Con. (GHz)	0.2054283	0.178761	0.2053757
Rotational Con. (GHz)		0.165433	0.1782478
H298			
6-31+g* */PCM	-765.885545	-916.333022	-916.811532
6-31g*	-765.830676	-916.163184	-916.741255
G298			
6-31+g* */PCM	-765.950572	-916.404085	-916.880492
6-31g*	-765.895703	-916.234247	-916.810215



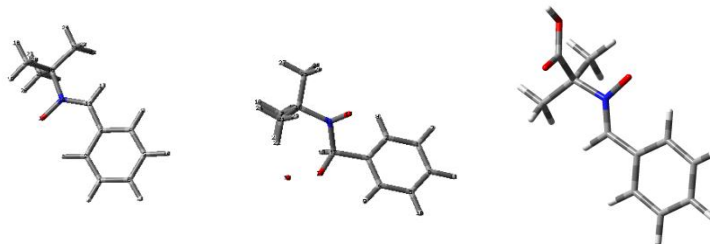
Compound	PBN-mono-CH2SMe PBN-alpha- methylthio.log	PBN-mono-CH2SMe-O2 PBN-alpha-methylthio- O2.log	PBN-mono-CH2SMe-HO2 PBN-alpha-methylthio- O2H.log
file			
E 6-31+g**/PCM	-995.660242	-1146.111629	-1146.609507
E 6-31g*	-995.6197795	-1145.963027	-1146.554755
ZPE (raw)	0.27025	0.274394	0.288535
Therm Corr to H (raw)	0.287027	0.29359	0.30803
Therm Corr to G (raw)	0.225071	0.225735	0.239048
H (raw)			
G (raw)			
ZPE (scaled)	0.265007	0.269071	0.282937
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7549	0.7545
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	1.3928097	0.8696506	0.8142297
Rotational Con. (GHz)	0.2122912	0.2103509	0.221015
Rotational Con. (GHz)	0.2047782	0.1813314	0.2053018
H298			
6-31+g* */PCM	-995.378458	-1145.823362	-1146.307075
6-31g*	-995.337995	-1145.674760	-1146.252323
G298			
6-31+g* */PCM	-995.440414	-1145.891217	-1146.376057
6-31g*	-995.399951	-1145.742615	-1146.321305



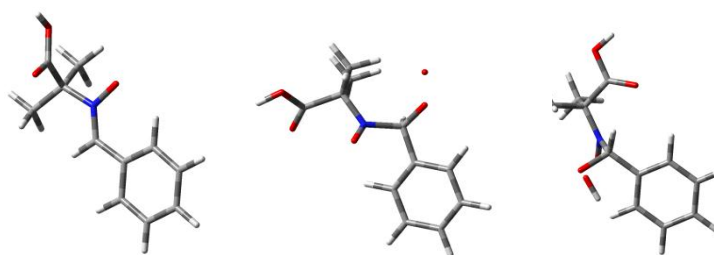
Compound	PBN-mono-NHCOMe	PBN-mono-NHCOMe-O2	PBN-mono-NHCOMe-HO2
file	PBN-NHCOMe-c.out	PBN-NHCOMe-O2c.out	PBN-NHCOMe-HO2c.out
E 6-31+g**/PCM	-726.87404	-877.337384	-877.82096
E 6-31g*	-726.8220775	-877.1935865	-877.7493731
ZPE (raw)	0.267486	0.271346	0.285199
Therm Corr to H (raw)	0.284318	0.290111	0.305159
Therm Corr to G (raw)	0.223054	0.22449	0.235614
H (raw)			
G (raw)			
ZPE (scaled)	0.262297	0.266082	0.279666
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	C1	C1	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.9897488	0.7136828	0.900159
Rotational Con. (GHz)	0.2781133	0.2632657	0.2146572
Rotational Con. (GHz)	0.2672547	0.2545351	0.2087082
H298			
6-31+g* */PCM	-726.594911	-877.052537	-877.521334
6-31g*	-726.542949	-876.908740	-877.449747
G298			
6-31+g* */PCM	-726.656175	-877.118158	-877.590879
6-31g*	-726.604213	-876.974361	-877.519292



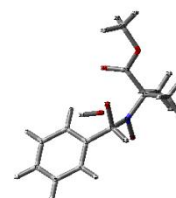
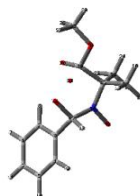
Compound	PBN-mono-SMe	PBN-mono-SMe-O2	PBN-mono-SMe-HO2
file	PBN-alpha-thio.log	PBN-alpha-thio-O2.log	PBN-alpha-thio-O2H.log
E 6-31+g**/PCM	-956.342378	-1106.797004	-1107.295159
E 6-31g*	-956.305779	-1106.649009	-1107.243038
ZPE (raw)	0.241532	0.245455	0.259766
Therm Corr to H (raw)	0.256905	0.263393	0.277894
Therm Corr to G (raw)	0.199587	0.199553	0.213902
H (raw)			
G (raw)			
ZPE (scaled)	0.236846	0.240693	0.254727
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7551	0.7545
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	1.3419568	0.7659551	0.6638948
Rotational Con. (GHz)	0.3051301	0.3275993	0.3914837
Rotational Con. (GHz)	0.2853524	0.2781162	0.3089264
H298			
6-31+g* */PCM	-956.090159	-1106.538373	-1107.022304
6-31g*	-956.053560	-1106.390378	-1106.970183
G298			
6-31+g* */PCM	-956.147477	-1106.602213	-1107.086296
6-31g*	-956.110878	-1106.454218	-1107.034175



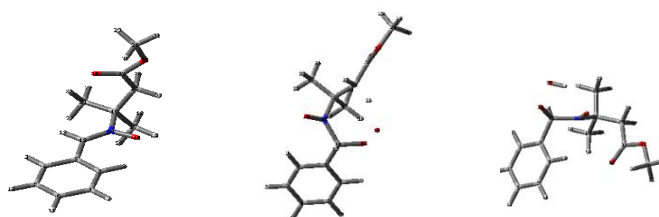
Compound file	PBN PBN.log	PBN-O2 PBN-O2.log	PBN-HO2 PBN-O2H.log
E 6-31+g**/PCM	-558.162931	-708.617074	-709.112085
E 6-31g*	-558.1259776	-708.4689312	-709.0604787
ZPE (raw)	0.240829	0.245281	0.258994
Therm Corr to H (raw)	0.254306	0.260894	0.275292
Therm Corr to G (raw)	0.202102	0.203309	0.214831
H (raw)			
G (raw)			
ZPE (scaled)	0.236157	0.240523	0.253970
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0	0
Rotational Con. (GHz)	2.0324432	1.1569044	0.9379767
Rotational Con. (GHz)	0.400396	0.3896029	0.4185919
Rotational Con. (GHz)	0.3613914	0.3302765	0.3677533
H298			
6-31+g* */PCM	-557.913297	-708.360938	-708.841817
6-31g*	-557.876344	-708.212796	-708.790211
G298			
6-31+g* */PCM	-557.965501	-708.418523	-708.902278
6-31g*	-557.928548	-708.270381	-708.850672



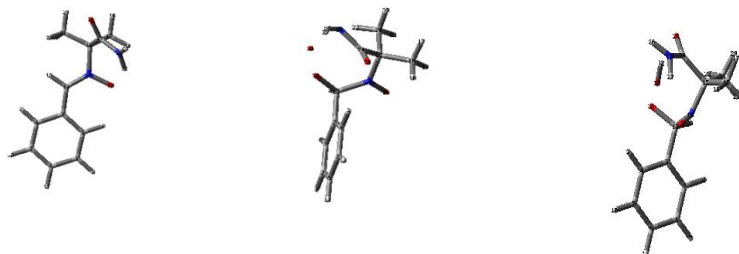
Compound	PBN-COOH	PBN-COOH-O2	PBN-COOH-HO2
file	PBN-alpha-COOH.com.log	PBN-alpha-COOH-O2.com.log	PBN-alpha-COOH-OOH.com.log
E 6-31+g**/PCM	-707.431235	-857.888027	-858.376424
E 6-31g*	-707.369149	-857.7204353	-858.3025633
ZPE (raw)	0.227237	0.231972	0.24507
Therm Corr to H (raw)	0.242184	0.249033	0.263149
Therm Corr to G (raw)	0.185579	0.187132	0.19847
H (raw)			
G (raw)			
ZPE (scaled)	0.222829	0.227472	0.240316
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7545
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.4793173	0.838635	0.8026308
Rotational Con. (GHz)	0.2991951	0.3123442	0.3117894
Rotational Con. (GHz)	0.2842145	0.2548107	0.2852084
H298			
6-31+g* */PCM	-707.193459	-857.643494	-858.118029
6-31g*	-707.131373	-857.475903	-858.044169
G298			
6-31+g* */PCM	-707.250064	-857.705395	-858.182708
6-31g*	-707.187978	-857.537804	-858.108848



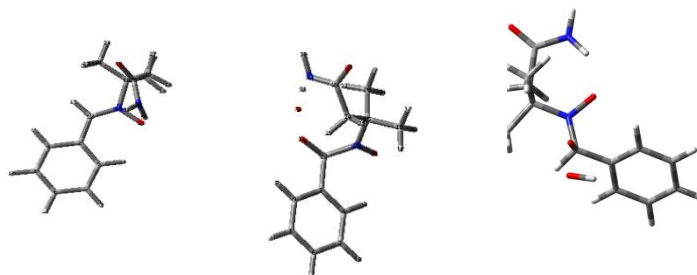
Compound	PBN-mono-COOMe	PBN-mono-COOMe-O2	PBN-mono-COOMe-HO2
file	PBN-alpha-carboxyl.log	PBN-alpha-carboxyl-O2.log	PBN-alpha-carboxyl-O2H.log
E 6-31+g**/PCM	-746.720138	-897.179983	-897.665892
E 6-31g*	-746.6775402	-897.042654	-897.6056095
ZPE (raw)	0.255084	0.260047	0.273071
Therm Corr to H (raw)	0.271960	0.278288	0.292876
Therm Corr to G (raw)	0.210399	0.214107	0.22423
H (raw)			
G (raw)			
ZPE (scaled)	0.250135	0.255002	0.267773
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7544	0.7544
Symmetry	C1	C1	C1
N Imag	0.000000	0	0
Rotational Con. (GHz)	0.9437443	0.8977346	0.7427467
Rotational Con. (GHz)	0.2997874	0.2758941	0.2726384
Rotational Con. (GHz)	0.2671731	0.2531769	0.2606018
H298			
6-31+g* */PCM	-746.453127	-896.906740	-897.378314
6-31g*	-746.410529	-896.769411	-897.318031
G298			
6-31+g* */PCM	-746.514688	-896.970921	-897.446960
6-31g*	-746.472090	-896.833592	-897.386677



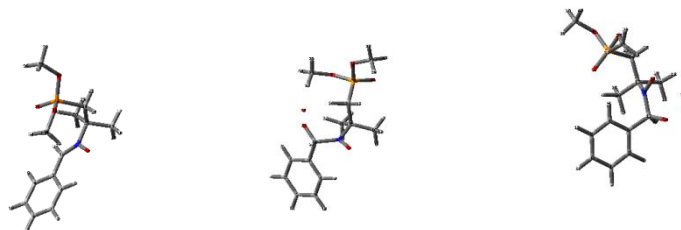
Compound	PBN-mono-CH ₂ COOMe PBN-alpha-methylcarboxy.log	PBN-mono-CH ₂ COOMe-O ₂ PBN-alpha-methylcarboxy-O ₂ .log	PBN-mono-CH ₂ COOMe-HO ₂ PBN-alpha-methylcarboxyl-O ₂ H.log
file			
E 6-31+g**/PCM	-786.043989	-936.498645	-936.991973
E 6-31g*	-785.9963804	-936.3496549	-936.9305986
ZPE (raw)	0.28425	0.287747	0.302515
Therm Corr to H (raw)	0.302144	0.307848	0.323092
Therm Corr to G (raw)	0.237785	0.238745	0.252281
H (raw)			
G (raw)			
ZPE (scaled)	0.278736	0.282165	0.296646
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7548	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0
Rotational Con. (GHz)	0.7223123	0.8821302	0.4875765
Rotational Con. (GHz)	0.266412	0.1894024	0.2878876
Rotational Con. (GHz)	0.2331577	0.1807801	0.2286974
H298			
6-31+g* */PCM	-785.747359	-936.196379	-936.674750
6-31g*	-785.699751	-936.047389	-936.613375
G298			
6-31+g* */PCM	-785.811718	-936.265482	-936.745561
6-31g*	-785.764110	-936.116492	-936.684186



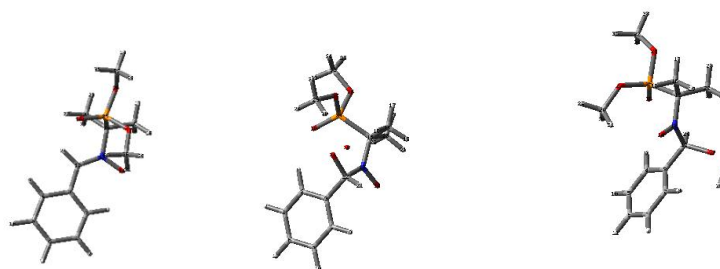
Compound	PBN-mono-CONH2	PBN-mono-CONH2-O2	PBN-mono-CONH2-HO2
file	PBN-alpha-CONH2.log	PBN-alpha-CONH2-O2.log	PBN-alpha-CONH2-HO2.log
E 6-31+g**/PCM	-687.567169	-838.027242	-838.511094
E 6-31g*	-687.5113347	-837.8777783	-838.4453241
ZPE (raw)	0.239944	0.244211	0.258958
Therm Corr to H (raw)	0.255025	0.26105	0.276381
Therm Corr to G (raw)	0.198075	0.200345	0.214241
H (raw)			
G (raw)			
ZPE (scaled)	0.235289	0.239473	0.253934
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.408565	0.8202188	0.9247357
Rotational Con. (GHz)	0.3025985	0.3289981	0.2962875
Rotational Con. (GHz)	0.2851659	0.3245404	0.2842783
H298			
6-31+g* */PCM	-687.316799	-837.770930	-838.239737
6-31g*	-687.260965	-837.621466	-838.173967
G298			
6-31+g* */PCM	-687.373749	-837.831635	-838.301877
6-31g*	-687.317915	-837.682171	-838.236107



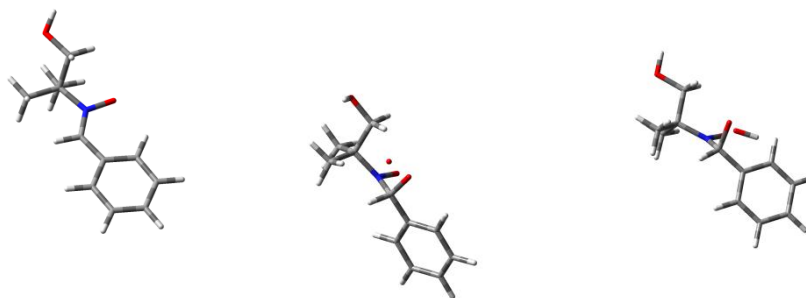
Compound	PBN-mono- CH2CONH2 PBN-alpha- CH2CONH2.log	PBN-mono-CH2CONH2- O2 PBN-alpha-CH2CONH2- O2.log	PBN-mono-CH2CONH2- HO2 PBN-alpha-CH2CONH2- HO2.log
file			
E 6-31+g**/PCM	-726.887839	-877.343451	-877.830381
E 6-31g*	-726.827997	-877.1922673	-877.7522906
ZPE (raw)	0.269338	0.27368	0.286963
Therm Corr to H (raw)	0.285437	0.291722	0.306217
Therm Corr to G (raw)	0.22677	0.227597	0.239157
H (raw)			
G (raw)			
ZPE (scaled)	0.264113	0.268371	0.281396
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.9587036	0.7179466	0.7427507
Rotational Con. (GHz)	0.2975838	0.2719601	0.2427123
Rotational Con. (GHz)	0.2828375	0.2450104	0.212362
H298			
6-31+g* */PCM	-726.607627	-877.057038	-877.529731
6-31g*	-726.547785	-876.905855	-877.451641
G298			
6-31+g* */PCM	-726.666294	-877.121163	-877.596791
6-31g*	-726.606452	-876.969980	-877.518701



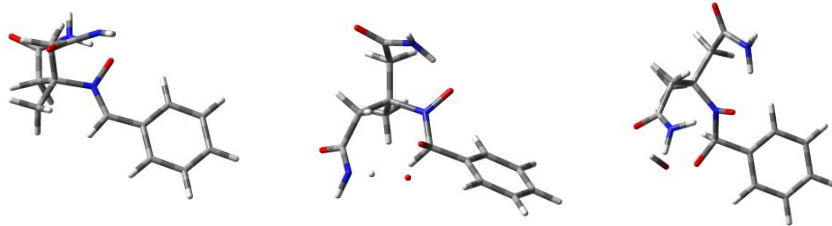
Compound	PBN-mono-CH ₂ PO(OMe) ₂ PBN-alpha-methylphosphoryl.log	PBN-mono-CH ₂ PO(OMe) ₂ -O ₂ PBN-alpha-methylphosphoryl-O ₂ .log	PBN-mono-CH ₂ PO(OMe) ₂ -HO ₂ PBN-alpha-methylphosphoryl-HO ₂ .log
file			
E 6-31+g**/PCM	-1204.480286	-1354.93834	-1355.426832
E 6-31g*	-1204.42836	-1354.790266	-1355.360944
ZPE (raw)	0.323819	0.328325	0.341981
Therm Corr to H (raw)	0.345276	0.351789	0.366286
Therm Corr to G (raw)	0.273809	0.275433	0.287048
H (raw)			
G (raw)			
ZPE (scaled)	0.317537	0.321955	0.335347
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7548	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.5818926	0.6081909	0.4139879
Rotational Con. (GHz)	0.2070483	0.1587611	0.2016113
Rotational Con. (GHz)	0.1836735	0.1475025	0.1726424
H298			
6-31+g* */PCM	-1204.141292	-1354.592921	-1355.067180
6-31g*	-1204.089366	-1354.444846	-1355.001293
G298			
6-31+g* */PCM	-1204.212759	-1354.669277	-1355.146418
6-31g*	-1204.160833	-1354.521202	-1355.080531



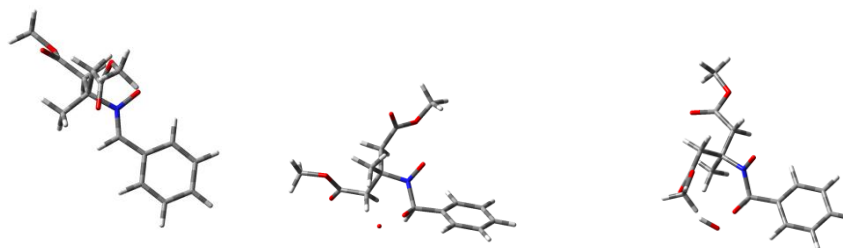
Compound	PBN-mono-PO(OMe) ₂ PBN-alpha-phosphoryl.log	PBN-mono-PO(OMe) ₂ -O ₂ PBN-alpha-phosphoryl-O2.log	PBN-mono-PO(OMe) ₂ -HO ₂ PBN-alpha-phosphoryl-HO2.log
file			
E 6-31+g**/PCM	-1165.154604	-1315.606718	-1316.103942
E 6-31g*	-1165.107118	-1315.461283	-1316.041568
ZPE (raw)	0.294867	0.299846	0.312497
Therm Corr to H (raw)	0.315401	0.322075	0.336239
Therm Corr to G (raw)	0.246006	0.247934	0.258927
H (raw)			
G (raw)			
ZPE (scaled)	0.289147	0.294029	0.306435
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7538	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.8125232	0.5372962	0.5137355
Rotational Con. (GHz)	0.2090801	0.2202036	0.229626
Rotational Con. (GHz)	0.2061113	0.2139904	0.1969613
H298			
6-31+g* */PCM	-1164.844923	-1315.290460	-1315.773765
6-31g*	-1164.797437	-1315.145025	-1315.711391
G298			
6-31+g* */PCM	-1164.914318	-1315.364601	-1315.851077
6-31g*	-1164.866832	-1315.219166	-1315.788703



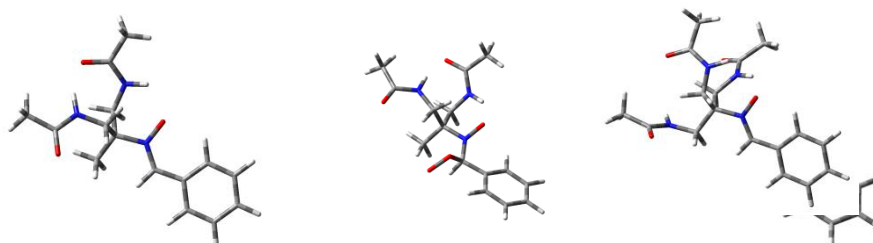
Compound	PBN-mono-CH2OH	PBN-mono-CH2OH-O2	PBN-mono-CH2OH-HO2
file	PBN-alpha-CH2OH.com.log	PBN-alpha-CH2OH-O2.com.log	PBN-alpha-CH2OH-OOH.com.log
E 6-31+g**/PCM	-633.386485	-783.841955	-784.333052
E 6-31g*	-633.3291896	-783.6787818	-784.2598099
ZPE (raw)	0.245535	0.250361	0.26343
Therm Corr to H (raw)	0.260262	0.267221	0.28117
Therm Corr to G (raw)	0.205034	0.206547	0.217995
H (raw)			
G (raw)			
ZPE (scaled)	0.240772	0.245504	0.258319
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.881173	1.1336489	1.060323
Rotational Con. (GHz)	0.3146428	0.3134301	0.2994421
Rotational Con. (GHz)	0.2931836	0.2742802	0.2810294
H298			
6-31+g* */PCM	-633.130986	-783.579591	-784.056993
6-31g*	-633.073691	-783.416418	-783.983750
G298			
6-31+g* */PCM	-633.186214	-783.640265	-784.120168
6-31g*	-633.128919	-783.477092	-784.046925



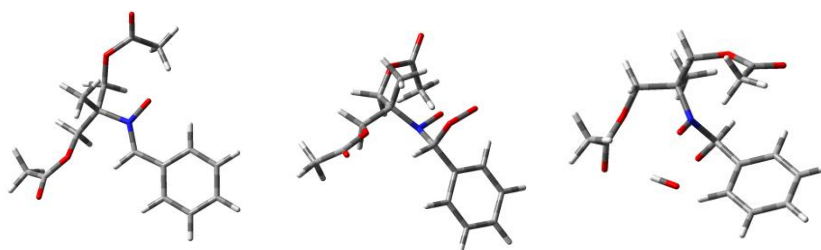
Compound	PBN-di-CH ₂ CONH ₂ PBN-CH ₂ CONH ₂ - 2b.com.log	PBN-di-CH ₂ CONH ₂ -O ₂ PBN-CH ₂ CONH ₂ -2-O ₂ b.out	PBN-di-CH ₂ CONH ₂ -HO ₂ PBN-CH ₂ CONH ₂ -2- OOH.com.log
file			
E 6-31+g**	-895.608688	-1046.068623	-1046.549683
E 6-31g*	-895.5235133	-1045.896431	-1046.455063
ZPE (raw)	0.297269	0.300883	0.315633
Therm Corr to H (raw)	0.316223	0.321845	0.337143
Therm Corr to G (raw)	0.24985	0.251196	0.264689
H (raw)			
G (raw)			
ZPE (scaled)	0.291502	0.295046	0.309510
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7549	0.7543
Symmetry	-	C1	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.5588525	0.4589861	0.4181795
Rotational Con. (GHz)	0.2267132	0.217707	0.2437125
Rotational Con. (GHz)	0.1964316	0.1872048	0.1808318
H298			
6-31+g* *	-895.298232	-1045.752615	-1046.218663
6-31g*	-895.213057	-1045.580423	-1046.124043
G298			
6-31+g* *	-895.364605	-1045.823264	-1046.291117
6-31g*	-895.279430	-1045.651072	-1046.196497



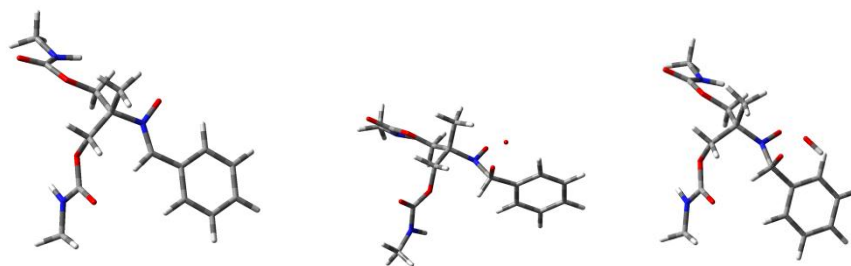
Compound	PBN-di-CH ₂ COOMe	PBN-di-CH ₂ COOMe-O ₂	PBN-di-CH ₂ COOMe-HO ₂
file	PBN-CH ₂ COOMe-2.com.log	PBN-CH ₂ COOMe-2-O ₂ .com.log	PBN-CH ₂ COOMe-2-OOH.com.log
E 6-31+g**	-1013.924528	-1164.376051	-1164.867596
E 6-31g*	-1013.867597	-1164.217074	-1164.80117
ZPE (raw)	0.327684	0.331811	0.346776
Therm Corr to H (raw)	0.349968	0.356154	0.371318
Therm Corr to G (raw)	0.274478	0.276449	0.29057
H (raw)			
G (raw)			
ZPE (scaled)	0.321327	0.325374	0.340049
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7544
Symmetry	-	-	-
N Imag	0.000000	0	#NAME?
Rotational Con. (GHz)	0.3877542	0.3405549	0.3163775
Rotational Con. (GHz)	0.1750447	0.1769674	0.1815871
Rotational Con. (GHz)	0.1356954	0.1340257	0.1296106
H298			
6-31+g* *	-1013.580917	-1164.026334	-1164.503005
6-31g*	-1013.523986	-1163.867358	-1164.436580
G298			
6-31+g* *	-1013.656407	-1164.106039	-1164.583753
6-31g*	-1013.599476	-1163.947063	-1164.517328



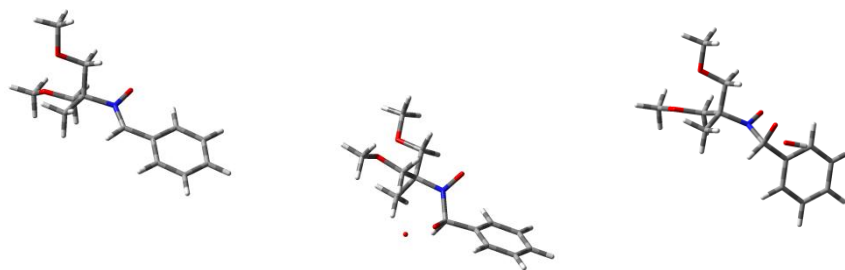
Compound	PBN-di-CH2NHCOMe PBN-CH2NHCOMe- 2.com.log	PBN-di-CH2NHCOMe-O2 PBN-CH2NHCOMe-2- O2.com.log	PBN-di-CH2NHCOMe-HO2 PBN-CH2NHCOMe-2- OOH.com.log
file			
E 6-31+g**	-974.225418	-1124.66851	-1125.16982
E 6-31g*	-974.1569283	-1124.507959	-1125.09215
ZPE (raw)	0.353082	0.356848	0.372446
Therm Corr to H (raw)	0.375503	0.381647	0.397057
Therm Corr to G (raw)	0.300245	0.300378	0.317576
H (raw)			
G (raw)			
ZPE (scaled)	0.346232	0.349925	0.365221
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7567	0.7546
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.4938187	0.4262188	0.3826867
Rotational Con. (GHz)	0.1590578	0.1534529	0.1659876
Rotational Con. (GHz)	0.1297505	0.1216589	0.1280072
H298			
6-31+g* *	-973.856765	-1124.293786	-1124.779988
6-31g*	-973.788275	-1124.133235	-1124.702318
G298			
6-31+g* *	-973.932023	-1124.375055	-1124.859469
6-31g*	-973.863533	-1124.214504	-1124.781799



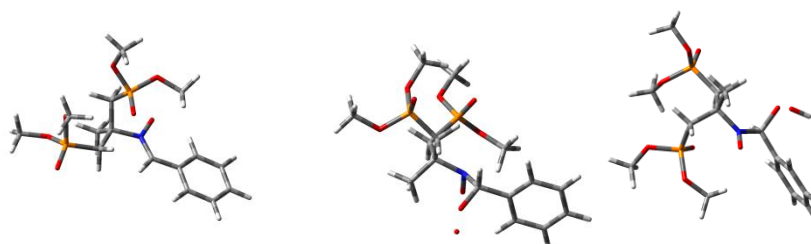
Compound	PBN-di-CH2OCOMe PBN-CH2OCOMe- 2.com.log	PBN-di-CH2OCOMe-O2 PBN-CH2OCOMe-2- O2.com.log	PBN-di-CH2OCOMe-HO2 PBN-CH2OCOMe-2- OOHb.com.log
file			
E 6-31+g**/PCM	-1013.913271	-1164.357442	-1164.86404
E 6-31g*	-1013.844878	-1164.19332	-1164.789871
ZPE (raw)	0.326721	0.331182	0.346435
Therm Corr to H (raw)	0.348848	0.355389	0.370681
Therm Corr to G (raw)	0.27417	0.275547	0.292381
H (raw)			
G (raw)			
ZPE (scaled)	0.320383	0.324757	0.339714
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7571	0.7545
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.2761823	0.2482736	0.3392005
Rotational Con. (GHz)	0.2386522	0.2212898	0.2308601
Rotational Con. (GHz)	0.1366976	0.1388095	0.1680063
H298			
6-31+g* */PCM	-1013.570761	-1164.008478	-1164.500080
6-31g*	-1013.502368	-1163.844356	-1164.425911
G298			
6-31+g* */PCM	-1013.645439	-1164.088320	-1164.578380
6-31g*	-1013.577046	-1163.924198	-1164.504211



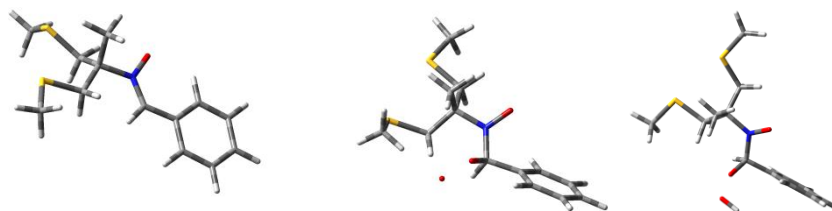
Compound	PBN-di-CH ₂ OCONHMe PBN-CH ₂ OCONHMe- 2.com.log	PBN-di-CH ₂ OCONHMe-O ₂ PBN-CH ₂ OCONHMe-2- O ₂ .com.log	PBN-di-CH ₂ OCONHMe-HO ₂ PBN-CH ₂ OCONHMe-2- OOH.com.log
file			
E 6-31+g**/PCM	-1124.664605	-1275.117868	-1275.611246
E 6-31g*	-1124.585256	-1274.93471	-1275.515814
ZPE (raw)	0.362621	0.366191	0.380703
Therm Corr to H (raw)	0.38765	0.393737	0.408674
Therm Corr to G (raw)	0.30577	0.30473	0.319228
H (raw)			
G (raw)			
ZPE (scaled)	0.355586	0.359087	0.373317
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7547	0.7545
Symmetry	-	-	-
N Imag	0	0	0.000000
Rotational Con. (GHz)	0.336010	0.2585699	0.2907537
Rotational Con. (GHz)	0.1446169	0.1300155	0.1341495
Rotational Con. (GHz)	0.1176766	0.1093048	0.1143833
H298			
6-31+g* */PCM	-1124.283990	-1274.731235	-1275.209958
6-31g*	-1124.204641	-1274.548077	-1275.114525
G298			
6-31+g* */PCM	-1124.365870	-1274.820242	-1275.299404
6-31g*	-1124.286521	-1274.637084	-1275.203971



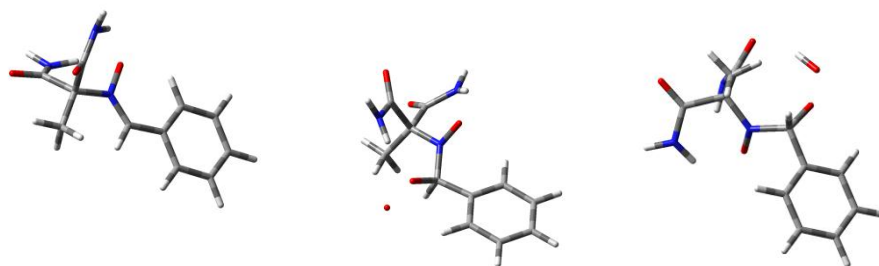
Compound	PBN-di-CH ₂ OMe	PBN-di-CH ₂ OMe-O ₂	PBN-di-CH ₂ OMe-HO ₂
file	PBN-CH ₂ OMe-2.com.log	PBN-CH ₂ OMe-2-O ₂ .com.log	PBN-CH ₂ OMe-2-OOH.com.log
E 6-31+g**/PCM	-787.192622	-937.647622	-938.139038
E 6-31g*	-787.1462878	-937.4937824	-938.076951
ZPE (raw)	0.307167	0.311322	0.325021
Therm Corr to H (raw)	0.325873	0.33232	0.346764
Therm Corr to G (raw)	0.260061	0.26084	0.273089
H (raw)			
G (raw)			
ZPE (scaled)	0.301208	0.305282	0.318716
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7545
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.9270825	0.6616418	0.6426955
Rotational Con. (GHz)	0.205163	0.2148467	0.2038581
Rotational Con. (GHz)	0.1939656	0.1777364	0.1786212
H298			
6-31+g* */PCM	-786.872708	-937.321342	-937.798579
6-31g*	-786.826374	-937.167502	-937.736492
G298			
6-31+g* */PCM	-786.938520	-937.392822	-937.872254
6-31g*	-786.892186	-937.238982	-937.810167



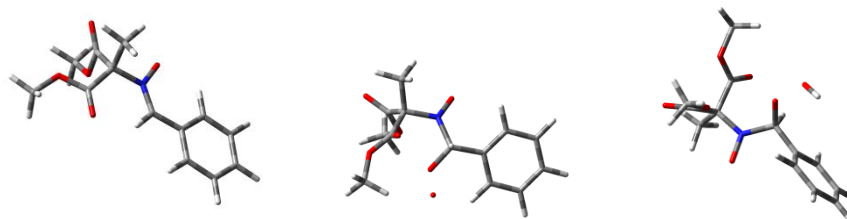
Compound	PBN-di-CH2POOMe2	PBN-di-CH2POOMe2-O2	PBN-di-CH2POOMe2-HO2
file	PBN-CH2POOMe2-2.com.log	PBN-CH2POOMe2-O2.com.log	PBN-CH2POOMe2-OOH.com.log
E 6-31+g**/PCM	-1850.796446	-2001.242029	-2001.743048
E 6-31g*	-1850.725907	-2001.077036	-2001.655316
ZPE (raw)	0.406748	0.410689	0.42457
Therm Corr to H (raw)	0.436391	0.442512	0.4573
Therm Corr to G (raw)	0.345665	0.34682	0.358632
H (raw)			
G (raw)			
ZPE (scaled)	0.398857	0.402722	0.416333
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7564	0.7545
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.2733572	0.2403124	0.2436947
Rotational Con. (GHz)	0.1289011	0.1233458	0.1246421
Rotational Con. (GHz)	0.1048025	0.0996822	0.098627
H298			
6-31+g* */PCM	-1850.367946	-2000.807484	-2001.293985
6-31g*	-1850.297407	-2000.642492	-2001.206252
G298			
6-31+g* */PCM	-1850.458672	-2000.903176	-2001.392653
6-31g*	-1850.388133	-2000.738184	-2001.304920



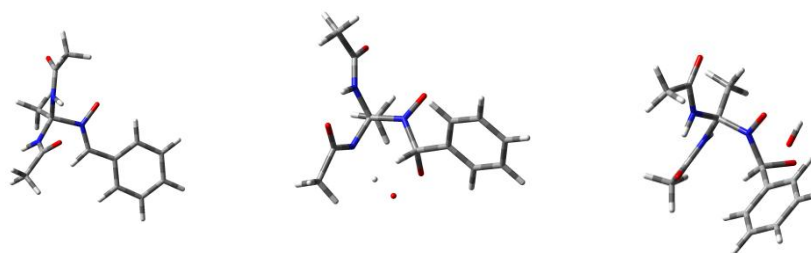
Compound	PBN-di-CH2SMe	PBN-di-CH2SMe-O2	PBN-di-CH2SMe-HO2
file	PBN-CH2SMe-2.com.log	PBN-CH2SMe-2-O2.com.log	PBN-CH2SMe-2-OOH.com.log
E 6-31+g**/PCM	-1433.151196	-1583.606249	-1584.097939
E 6-31g*	-1433.105498	-1583.464857	-1584.03669
ZPE (raw)	0.299351	0.30419	0.317298
Therm Corr to H (raw)	0.319418	0.326135	0.340361
Therm Corr to G (raw)	0.249407	0.252093	0.262612
H (raw)			
G (raw)			
ZPE (scaled)	0.293544	0.298289	0.311142
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7548	0.7545
Symmetry	-	-	-
N Imag	#NAME?	0	0
Rotational Con. (GHz)	0.6103007	0.500021	0.4728437
Rotational Con. (GHz)	0.1827722	0.1843271	0.1727731
Rotational Con. (GHz)	0.152148	0.144671	0.1460972
H298			
6-31+g* */PCM	-1432.837585	-1583.286015	-1583.763734
6-31g*	-1432.791887	-1583.144624	-1583.702485
G298			
6-31+g* */PCM	-1432.907596	-1583.360057	-1583.841483
6-31g*	-1432.861898	-1583.218666	-1583.780234



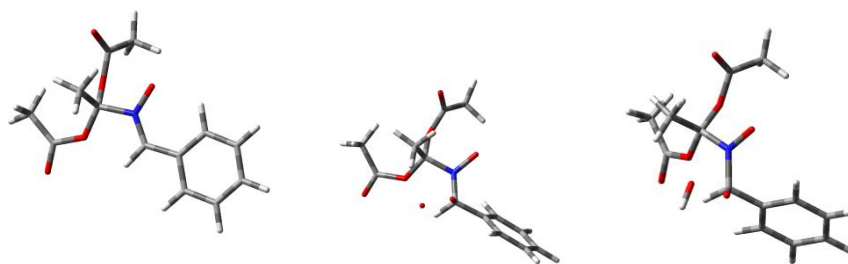
Compound	PBN-di-CONH2	PBN-di-CONH2-O2	PBN-di-CONH2-HO2
file	PBN-CONH2-2.com.log	PBN-CONH2-2-O2b.out	PBN-CONH2-2-OOH.com.log
E 6-31+g**/PCM	-816.967225	-967.427401	-967.910678
E 6-31g*	-816.8917475	-967.2529942	-967.8252959
ZPE (raw)	0.239143	0.243073	0.25773
Therm Corr to H (raw)	0.255588	0.26212	0.276787
Therm Corr to G (raw)	0.195643	0.196165	0.210597
H (raw)			
G (raw)			
ZPE (scaled)	0.234504	0.238357	0.252730
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.755	0.7544
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.9998412	0.6927609	0.6805595
Rotational Con. (GHz)	0.2474605	0.2552142	0.2634044
Rotational Con. (GHz)	0.2412536	0.2170205	0.2192377
H298			
6-31+g* */PCM	-816.716276	-967.169997	-967.638891
6-31g*	-816.640799	-966.995590	-967.553509
G298			
6-31+g* */PCM	-816.776221	-967.235952	-967.705081
6-31g*	-816.700744	-967.061545	-967.619699



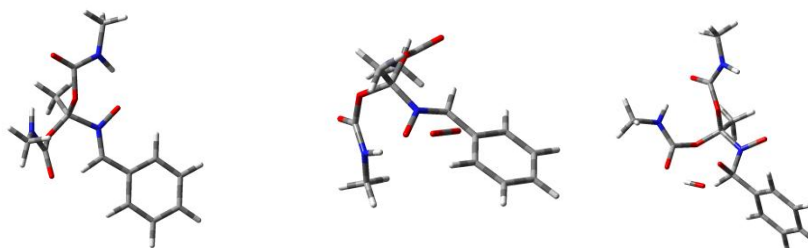
Compound	PBN-di-COOMe	PBN-di-COOMe-O2	PBN-di-COOMe-HO2
file	PBN-COOMe-2.com.log	PBN-COOMe-2-O2.com.log	PBN-COOMe-2-OOH.com.log
E 6-31+g**/PCM	-935.273697	-1085.723619	-1086.221164
E 6-31g*	-935.2270617	-1085.576708	-1086.157529
ZPE (raw)	0.269718	0.274318	0.287619
Therm Corr to H (raw)	0.289686	0.296217	0.310577
Therm Corr to G (raw)	0.220754	0.223428	0.234121
H (raw)			
G (raw)			
ZPE (scaled)	0.264485	0.268996	0.282039
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7547	0.7544
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.6681324	0.5073967	0.5203791
Rotational Con. (GHz)	0.2197261	0.2283274	0.2170866
Rotational Con. (GHz)	0.1914851	0.2059091	0.1964494
H298			
6-31+g* */PCM	-934.989244	-1085.432724	-1085.916167
6-31g*	-934.942608	-1085.285813	-1085.852532
G298			
6-31+g* */PCM	-935.058176	-1085.505513	-1085.992623
6-31g*	-935.011540	-1085.358602	-1085.928988



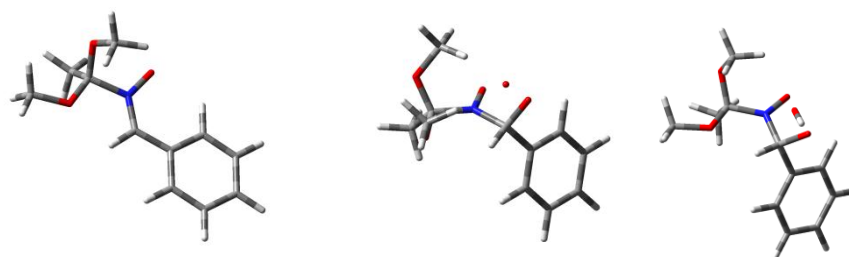
Compound	PBN-di-NHCOMe	PBN-di-NHCOMe-O2	PBN-di-NHCOMe-HO2
file	PBN-NHCOMe-2b.com.log	PBN-NHCOMe-2-O2.com.log	PBN-NHCOMe-2-OOH.com.log
E 6-31+g**/PCM	-895.583199	-1046.047989	-1046.529439
E 6-31g*	-895.5152711	-1045.905594	-1046.448285
ZPE (raw)	0.293686	0.298496	0.311861
Therm Corr to H (raw)	0.313882	0.320624	0.335147
Therm Corr to G (raw)	0.244226	0.245886	0.256984
H (raw)			
G (raw)			
ZPE (scaled)	0.287988	0.292705	0.305811
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7543
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.5486251	0.4347278	0.3768631
Rotational Con. (GHz)	0.2332209	0.2168382	0.2325585
Rotational Con. (GHz)	0.1883868	0.1832114	0.2192871
H298			
6-31+g* */PCM	-895.275015	-1045.733156	-1046.200342
6-31g*	-895.207087	-1045.590761	-1046.119188
G298			
6-31+g* */PCM	-895.344671	-1045.807894	-1046.278505
6-31g*	-895.276743	-1045.665499	-1046.197351



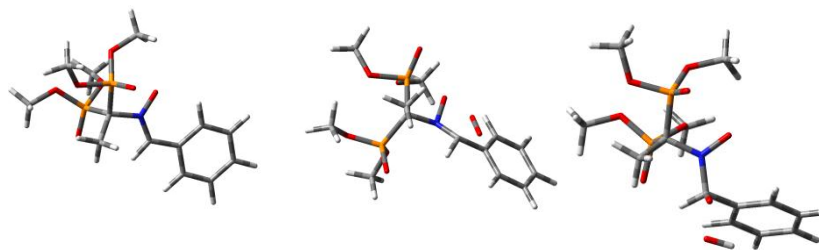
Compound	PBN-di-OCOMe	PBN-di-OCOMe-O2	PBN-di-OCOMe-HO2
file	PBN-OCOMe-2.com.log	PBN-OCOMe-2-O2.com.log	PBN-OCOMe-2-OOH.com.log
E 6-31+g**/PCM	-935.28529	-1085.744111	-1086.236595
E 6-31g*	-935.2346248	-1085.587059	-1086.165281
ZPE (raw)	0.267743	0.272034	0.285313
Therm Corr to H (raw)	0.287488	0.293885	0.308428
Therm Corr to G (raw)	0.218983	0.219931	0.229695
H (raw)			
G (raw)			
ZPE (scaled)	0.262549	0.266757	0.279778
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7542
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.5980483	0.4582455	0.3980708
Rotational Con. (GHz)	0.2238111	0.2081842	0.221057
Rotational Con. (GHz)	0.1778077	0.18249	0.2065701
H298			
6-31+g* */PCM	-935.002996	-1085.455503	-1085.933702
6-31g*	-934.952331	-1085.298452	-1085.862388
G298			
6-31+g* */PCM	-935.071501	-1085.529457	-1086.012435
6-31g*	-935.020836	-1085.372406	-1085.941121



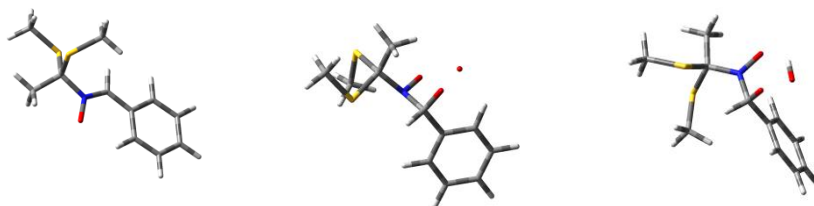
Compound	PBN-di-OCONHMe	PBN-di-OCONHMe-O2	PBN-di-OCONHMe-HO2
file	PBN-OCONHMe-2.com.log	PBN-OCONHMe-2-O2.com.log	PBN-OCONHMe-2-OOH.com.log
E 6-31+g**/PCM	-1046.023898	-1196.475502	-1196.978227
E 6-31g*	-1045.967703	-1196.333811	-1196.90336
ZPE (raw)	0.303736	0.307055	0.322599
Therm Corr to H (raw)	0.325982	0.331969	0.347296
Therm Corr to G (raw)	0.251002	0.25256	0.266084
H (raw)			
G (raw)			
ZPE (scaled)	0.297844	0.301098	0.316341
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7748	0.7543
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.434830	0.3664712	0.4442124
Rotational Con. (GHz)	0.1992356	0.2103622	0.1641014
Rotational Con. (GHz)	0.1497767	0.1925606	0.141354
H298			
6-31+g* */PCM	-1045.703808	-1196.149490	-1196.637189
6-31g*	-1045.647613	-1196.007799	-1196.562322
G298			
6-31+g* */PCM	-1045.778788	-1196.228899	-1196.718401
6-31g*	-1045.722593	-1196.087208	-1196.643534



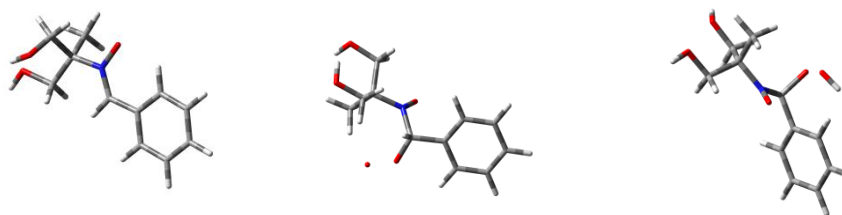
Compound	PBN-di-OMe	PBN-di-OMe-O2	PBN-di-OMe-HO2
file	PBN-OMe-2.com.log	PBN-OMe-2-O2.com.log	PBN-OMe-2-OOH.com.log
E 6-31+g**/PCM	-708.583187	-859.036735	-859.53447
E 6-31g*	-708.5418502	-858.8887596	-859.4724606
ZPE (raw)	0.249635	0.254451	0.267219
Therm Corr to H (raw)	0.265514	0.272274	0.286427
Therm Corr to G (raw)	0.20741	0.209597	0.219107
H (raw)			
G (raw)			
ZPE (scaled)	0.244792	0.249515	0.262035
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7541
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	1.339486	0.8535862	0.7588646
Rotational Con. (GHz)	0.3108924	0.3128262	0.3241001
Rotational Con. (GHz)	0.2864296	0.293851	0.2883744
H298			
6-31+g* */PCM	-708.322516	-858.769397	-859.253227
6-31g*	-708.281179	-858.621422	-859.191218
G298			
6-31+g* */PCM	-708.380620	-858.832074	-859.320547
6-31g*	-708.339283	-858.684099	-859.258538



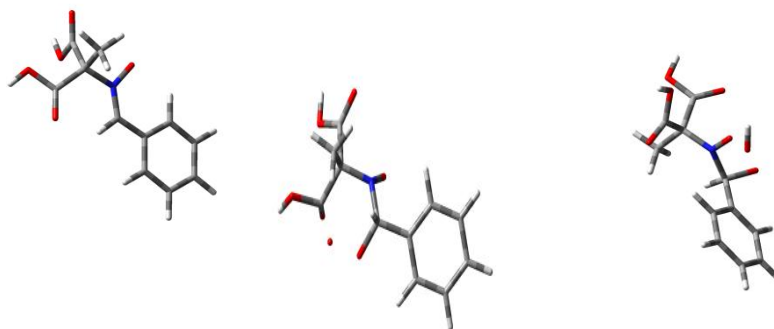
Compound	PBN-di-POOMe2	PBN-di-POOMe2-O2	PBN-di-POOMe2-HO2
file	PBN-POOMe2-2.com.log	PBN-POOMe2-O2b.com.log	PBN-POOMe2-OOH.com.log
E 6-31+g**/PCM	-1772.142353	-1922.577801	-1923.089866
E 6-31g*	-1772.080491	-1922.434641	-1923.012883
ZPE (raw)	0.348356	0.351922	0.366298
Therm Corr to H (raw)	0.37603	0.382056	0.397069
Therm Corr to G (raw)	0.289757	0.287907	0.302943
H (raw)			
G (raw)			
ZPE (scaled)	0.341598	0.345095	0.359192
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.755	0.7544
Symmetry	-	-	-
N Imag	0.000000	0	#NAME?
Rotational Con. (GHz)	0.368157	0.2944433	0.3046197
Rotational Con. (GHz)	0.1560011	0.1463166	0.1486291
Rotational Con. (GHz)	0.1367643	0.1345963	0.1364043
H298			
6-31+g* */PCM	-1771.773081	-1922.202572	-1922.699903
6-31g*	-1771.711219	-1922.059413	-1922.622920
G298			
6-31+g* */PCM	-1771.859354	-1922.296721	-1922.794029
6-31g*	-1771.797492	-1922.153562	-1922.717046



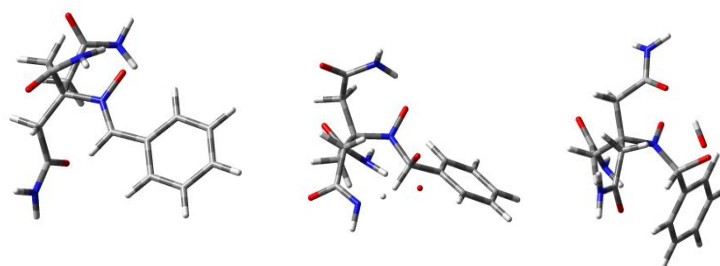
Compound	PBN-di-SMe	PBN-di-SMe-O2	PBN-di-SMe-HO2
file	PBN-SMe-2b.com.log	PBN-SMe-2-O2-b.com.log	PBN-SMe-2-OOHb.com.log
E 6-31+g**/PCM	-1354.519583	-1504.967169	-1505.465619
E 6-31g*	-1354.481285	-1504.828137	-1505.4165
ZPE (raw)	0.241748	0.246084	0.260385
Therm Corr to H (raw)	0.259119	0.265551	0.280373
Therm Corr to G (raw)	0.197009	0.198242	0.211348
H (raw)			
G (raw)			
ZPE (scaled)	0.237058	0.241310	0.255334
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7556	0.7546
Symmetry	-	-	-
N Imag	0.000000	0	0
Rotational Con. (GHz)	0.946050	0.6819104	0.6349068
Rotational Con. (GHz)	0.2550738	0.2436834	0.273674
Rotational Con. (GHz)	0.245413	0.2329895	0.2417374
H298			
6-31+g* */PCM	-1354.265154	-1504.706392	-1505.190297
6-31g*	-1354.226855	-1504.567360	-1505.141179
G298			
6-31+g* */PCM	-1354.327264	-1504.773701	-1505.259322
6-31g*	-1354.288965	-1504.634669	-1505.210204



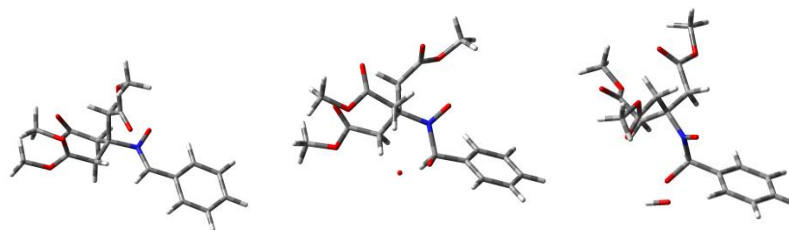
Compound	PBN-di-CH2OH PBN-alpha- 2CH2OH.com.log	PBN-di-CH2OH-O2 PBN-alpha-2CH2OH- O2.com.log	PBN-di-CH2OH-HO2 PBN-alpha-2CH2OH- OOH.com.log
file			
E 6-31+g**/PCM	-708.611121	-859.061083	-859.551853
E 6-31g*	-708.5315278	-858.886611	-859.4527103
ZPE (raw)	0.251127	0.256083	0.267567
Therm Corr to H (raw)	0.266624	0.273512	0.286767
Therm Corr to G (raw)	0.209386	0.211155	0.219872
H (raw)			
G (raw)			
ZPE (scaled)	0.246255	0.251115	0.262376
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.754600	0.7545
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.3489827	0.924519	0.876313
Rotational Con. (GHz)	0.2900041	0.271811	0.2651455
Rotational Con. (GHz)	0.2726558	0.241446	0.2448042
H298			
6-31+g* */PCM	-708.349369	-858.792539	-859.270277
6-31g*	-708.269776	-858.618067	-859.171134
G298			
6-31+g* */PCM	-708.406607	-858.854896	-859.337172
6-31g*	-708.327014	-858.680424	-859.238029



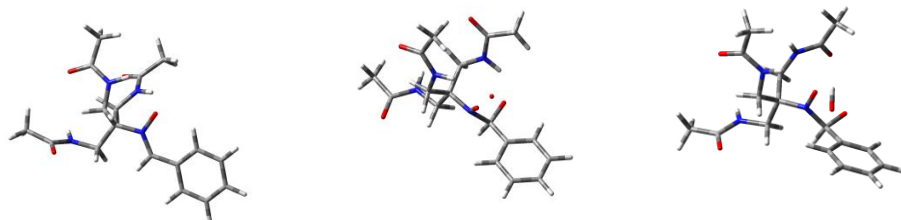
Compound	PBN-di-COOH	PBN-di-COOH-O2	PBN-di-COOH-HO2
file	PBN-alpha-2COOH.com.log	PBN-alpha-2COOH-O2.com.log	PBN-alpha-2COOH-HO2.com.log
E 6-31+g**/PCM	-856.694574	-1007.156529	-1007.643925
E 6-31g*	-856.6111154	-1006.972471	-1007.547501
ZPE (raw)	0.213215	0.218513	0.232354
Therm Corr to H (raw)	0.229731	0.236561	0.251264
Therm Corr to G (raw)	0.168986	0.172601	0.184232
H (raw)			
G (raw)			
ZPE (scaled)	0.209079	0.214274	0.227846
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7543	0.7536
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.0064268	0.7877657	0.68492
Rotational Con. (GHz)	0.2651683	0.2584018	0.26973
Rotational Con. (GHz)	0.2340059	0.2211802	0.21681
H298			
6-31+g* */PCM	-856.468979	-1006.924207	-1007.397169
6-31g*	-856.385521	-1006.740149	-1007.300745
G298			
6-31+g* */PCM	-856.529724	-1006.988167	-1007.464201
6-31g*	-856.446266	-1006.804109	-1007.367777



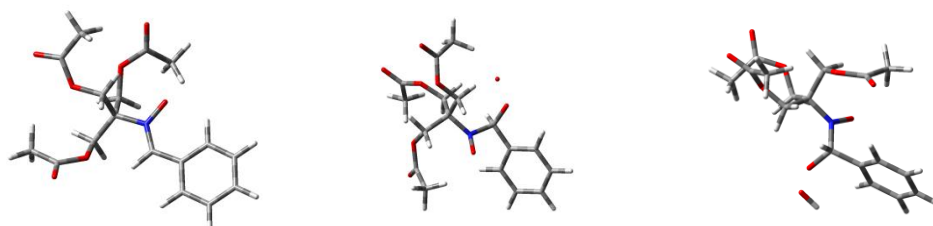
Compound	PBN-tri-CH2CONH2 PBN-CH2CONH2- 3.com.log	PBN-tri-CH2CONH2-O2 PBN-CH2CONH2-3- O2b.com.log	PBN-tri-CH2CONH2-HO2 PBN-CH2CONH2-3- OOH.com.log
file			
E 6-31+g**	-1064.324784	-1214.784888	-1215.276253
E 6-31g*	-1064.214637	-1214.593805	-1215.155638
ZPE (raw)	0.324297	0.328585	0.342739
Therm Corr to H (raw)	0.34665	0.352547	0.367744
Therm Corr to G (raw)	0.272461	0.274518	0.287817
H (raw)			
G (raw)			
ZPE (scaled)	0.318006	0.322210	0.336090
Electronic State	1-A	2-A	2-A
s2 6-31g*	0.000000	0.7548	0.7544
Symmetry	-	-	-
N Imag	0.000000	0.000000	#NAME?
Rotational Con. (GHz)	0.339141	0.3099314	0.2947006
Rotational Con. (GHz)	0.2067062	0.1847968	0.1993875
Rotational Con. (GHz)	0.1894014	0.1655711	0.1917742
H298			
6-31+g* *	-1063.984425	-1214.438716	-1214.915158
6-31g*	-1063.874278	-1214.247633	-1214.794543
G298			
6-31+g* *	-1064.058614	-1214.516745	-1214.995085
6-31g*	-1063.948467	-1214.325662	-1214.874470



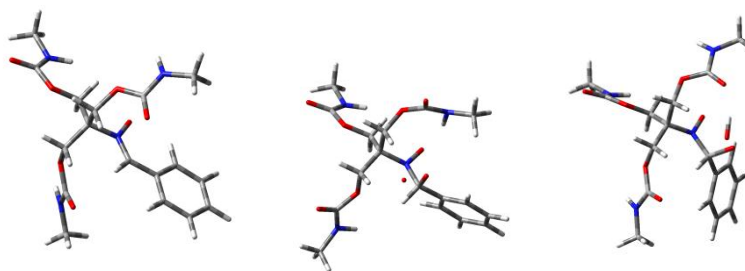
Compound	PBN-tri-CH2COOMe PBN-CH2COOMe- 3.com.log	PBN-tri-CH2COOMe-O2 PBN-CH2COOMe-3- O2.com.log	PBN-tri-CH2COOMe-HO2 PBN-CH2COOMe-3- OOH.com.log
file			
E 6-31+g**	-1241.800941	-1392.254639	-1392.746621
E 6-31g*	-1241.73338	-1392.088369	-1392.656873
ZPE (raw)	0.371309	0.375073	0.388394
Therm Corr to H (raw)	0.397877	0.403755	0.41849
Therm Corr to G (raw)	0.312873	0.313609	0.323138
H (raw)			
G (raw)			
ZPE (scaled)	0.364106	0.367797	0.380859
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7546
Symmetry	-	-	-
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)	0.2919382	0.2575671	0.2299062
Rotational Con. (GHz)	0.1322421	0.1301576	0.1345448
Rotational Con. (GHz)	0.1132622	0.1108923	0.1088917
H298			
6-31+g* *	-1241.410267	-1391.858160	-1392.335666
6-31g*	-1241.342706	-1391.691890	-1392.245918
G298			
6-31+g* *	-1241.495271	-1391.948306	-1392.431018
6-31g*	-1241.427710	-1391.782036	-1392.341270



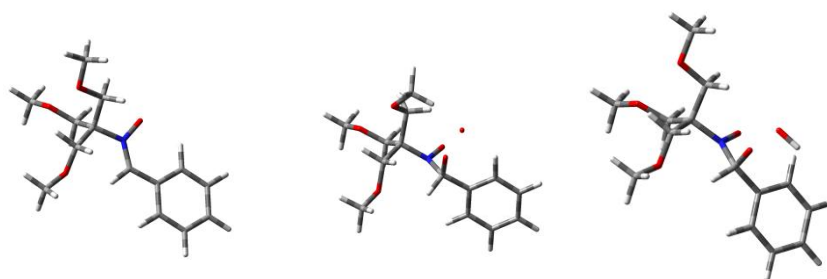
Compound	PBN-tri-CH2NHCOMe PBN-CH2NHCOMe- 3.com.log	PBN-tri-CH2NHCOMe-O2 PBN-CH2NHCOMe-3- O2.com.log	PBN-tri-CH2NHCOMe-HO2 PBN-CH2NHCOMe-3- OOH.com.log
file			
E 6-31+g**	-1182.24663	-1332.706915	-1333.195653
E 6-31g*	-1182.152723	-1332.527535	-1333.095406
ZPE (raw)	0.408242	0.413662	0.427347
Therm Corr to H (raw)	0.435609	0.443031	0.457101
Therm Corr to G (raw)	0.347602	0.351371	0.363326
H (raw)			
G (raw)			
ZPE (scaled)	0.400322	0.405637	0.419056
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.754600	0.754300
Symmetry	-	-	-
N Imag	0	0.000000	0.000000
Rotational Con. (GHz)	0.268081	0.231383	0.208623
Rotational Con. (GHz)	0.1386845	0.134750	0.136669
Rotational Con. (GHz)	0.1102925	0.110900	0.118847
H298			
6-31+g* *	-1181.818941	-1332.271909	-1332.746843
6-31g*	-1181.725034	-1332.092529	-1332.646595
G298			
6-31+g* *	-1181.906948	-1332.363569	-1332.840618
6-31g*	-1181.813041	-1332.184189	-1332.740370



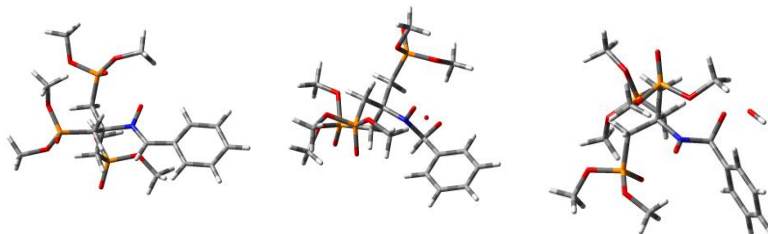
Compound	PBN-tri-CH2OCOME PBN-CH2OCOCH3- 3b.com.log	PBN-tri-CH2OCOME-O2 PBN-CH2OCOME-3- O2b.com.log	PBN-tri-CH2OCOME-HO2 PBN-CH2OCOME-3- OOH.com.log
file			
E 6-31+g**/PCM	-1241.789464	-1392.254591	-1392.733536
E 6-31g*	-1241.715654	-1392.094634	-1392.643461
ZPE (raw)	0.37035	0.375653	0.387989
Therm Corr to H (raw)	0.396479	0.403858	0.417369
Therm Corr to G (raw)	0.312863	0.315576	0.324624
H (raw)			
G (raw)			
ZPE (scaled)	0.363165	0.368365	0.380462
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7544
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.2616267	0.25723	0.2924838
Rotational Con. (GHz)	0.1553378	0.1390775	0.1214266
Rotational Con. (GHz)	0.1085382	0.111247	0.1123227
H298			
6-31+g* */PCM	-1241.400170	-1391.858021	-1392.323694
6-31g*	-1241.326360	-1391.698063	-1392.233619
G298			
6-31+g* */PCM	-1241.483786	-1391.946303	-1392.416439
6-31g*	-1241.409976	-1391.786345	-1392.326364



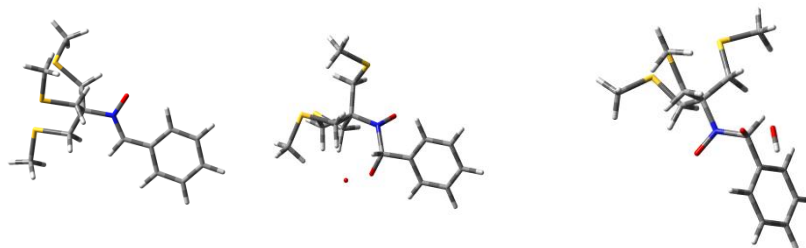
Compound	PBN-tri-CH2OCONHMe-O2 PBN-CH2OCONHMe-3- O2.com.log	PBN-tri-CH2OCONHMe PBN-CH2OCONHMe- 3.com.log	PBN-tri-CH2OCONHMe-HO2 PBN-CH2OCONHMe-3- OOHb.com.log
file			
E 6-31+g**/PCM	-1558.367725	-1407.91669	-1558.869458
E 6-31g*	-1558.1761	-1407.815444	-1558.759114
ZPE (raw)	0.427436	0.422678	0.442566
Therm Corr to H (raw)	0.460381	0.453856	0.475742
Therm Corr to G (raw)	0.358674	0.353693	0.373567
H (raw)			
G (raw)			
ZPE (scaled)	0.419144	0.414478	0.433980
Electronic State	2-A	1-A	2-A
s2 6-31g*	0.7547	0	0.7544
Symmetry	-	-	-
N Imag	0	0	0.000000
Rotational Con. (GHz)	0.1611345	0.188153	0.1556891
Rotational Con. (GHz)	0.1187581	0.1284995	0.1264121
Rotational Con. (GHz)	0.0893827	0.0908211	0.0904877
H298			
6-31+g* */PCM	-1557.915636	-1407.471034	-1558.402302
6-31g*	-1557.724011	-1407.369788	-1558.291958
G298			
6-31+g* */PCM	-1558.017343	-1407.571197	-1558.504477
6-31g*	-1557.825718	-1407.469951	-1558.394133



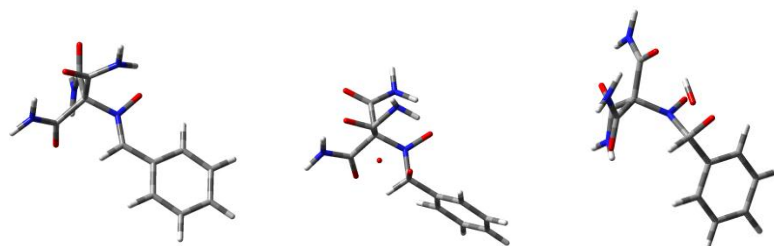
Compound	PBN-tri-CH2OMe PBN-CH2OMe- 3.com.log	PBN-tri-CH2OMe-O2 PBN-CH2OMe-3- O2.com.log	PBN-tri-CH2OMe-HO2 PBN-CH2OMe-3- OOH.com.log
file			
E 6-31+g**/PCM	-901.708178	-1052.15826	-1052.655032
E 6-31g*	-901.6593643	-1052.008405	-1052.590292
ZPE (raw)	0.340497	0.345335	0.358538
Therm Corr to H (raw)	0.361803	0.368566	0.382781
Therm Corr to G (raw)	0.289836	0.292387	0.303451
H (raw)			
G (raw)			
ZPE (scaled)	0.333891	0.338636	0.351582
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7548	0.7546
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.5877978	0.4572142	0.4770708
Rotational Con. (GHz)	0.1928172	0.201493	0.1849479
Rotational Con. (GHz)	0.176976	0.1782263	0.1690251
H298			
6-31+g* */PCM	-901.352981	-1051.796393	-1052.279207
6-31g*	-901.304167	-1051.646538	-1052.214466
G298			
6-31+g* */PCM	-901.424948	-1051.872572	-1052.358537
6-31g*	-901.376134	-1051.722717	-1052.293796



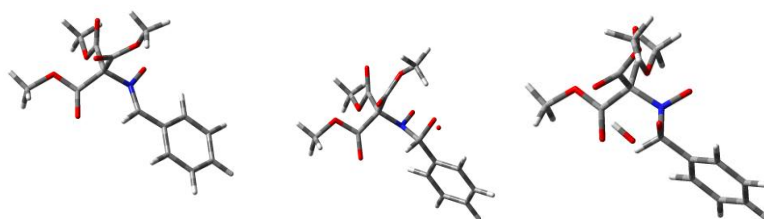
Compound	PBN-tri-CH ₂ POOMe ₂ PBN-CH ₂ POOMe ₂ - 3c.com.log	PBN-tri-CH ₂ POOMe ₂ -O ₂ PBN-CH ₂ POOMe ₂ -3- O2.com.log	PBN-tri-CH ₂ POOMe ₂ -HO ₂ PBN-CH ₂ POOMe ₂ -3- OOH.com.log
file			
E 6-31+g**/PCM	-2497.105572	-2647.565319	-2648.050611
E 6-31g*	-2497.017706	-2647.391982	-2647.949827
ZPE (raw)	0.488747	0.494118	0.506811
Therm Corr to H (raw)	0.526893	0.533882	0.547995
Therm Corr to G (raw)	0.415154	0.419679	0.429014
H (raw)			
G (raw)			
ZPE (scaled)	0.479265	0.484532	0.496979
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7544
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.1423591	0.1230166	0.1248274
Rotational Con. (GHz)	0.0936729	0.1018884	0.0970933
Rotational Con. (GHz)	0.0861287	0.0827501	0.081644
H298			
6-31+g* */PCM	-2496.588161	-2647.041023	-2647.512448
6-31g*	-2496.500294	-2646.867686	-2647.411664
G298			
6-31+g* */PCM	-2496.699900	-2647.155226	-2647.631429
6-31g*	-2496.612033	-2646.981889	-2647.530645



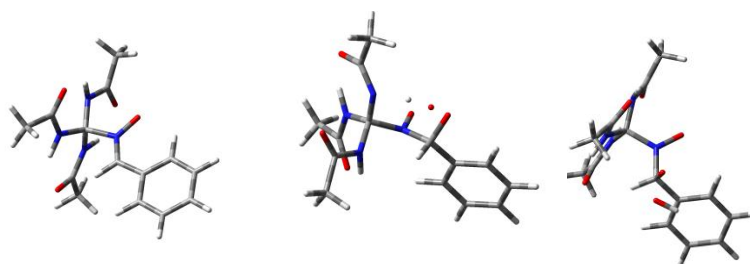
Compound	PBN-tri-CH2SMe PBN-CH2SMe- 3.com.log	PBN-tri-CH2SMe-O2 PBN-CH2SMe-3- O2.com.log	PBN-tri-CH2SMe-HO2 PBN-CH2SMe-3- OOH.com.log
file			
E 6-31+g**/PCM	-1870.638803	-2021.105525	-2021.586192
E 6-31g*	-1870.589507	-2020.964175	-2021.522266
ZPE (raw)	0.328624	0.333597	0.346639
Therm Corr to H (raw)	0.351854	0.359135	0.372788
Therm Corr to G (raw)	0.274677	0.275756	0.288079
H (raw)			
G (raw)			
ZPE (scaled)	0.322249	0.327125	0.339914
Electronic State	1-A	2-A	2-A
s2 6-31g*		0	0.7547
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.4112537	0.3335447	0.3478744
Rotational Con. (GHz)	0.1466717	0.1589735	0.1366444
Rotational Con. (GHz)	0.1340243	0.1373842	0.1338158
H298			
6-31+g* */PCM	-1870.293324	-2020.752862	-2021.220129
6-31g*	-1870.244028	-2020.611512	-2021.156203
G298			
6-31+g* */PCM	-1870.370501	-2020.836241	-2021.304838
6-31g*	-1870.321205	-2020.694891	-2021.240912



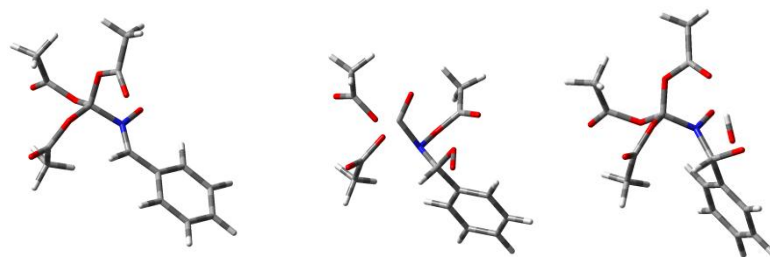
Compound	PBN-tri-CONH2	PBN-tri-CONH2-O2	PBN-tri-CONH2-HO2
file	PBN-CONH2-3.com.log	PBN-TriCONH2-O2.out	PBN-CONH2-3-OOHb.com.log
E 6-31+g**/PCM	-946.364505	-1096.827295	-1097.309626
E 6-31g*	-946.2722994	-1096.646338	-1097.209627
ZPE (raw)	0.236977	0.24289	0.25656
Therm Corr to H (raw)	0.255346	0.262507	0.277183
Therm Corr to G (raw)	0.191126	0.195454	0.206813
H (raw)			
G (raw)			
ZPE (scaled)	0.232380	0.238178	0.251583
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7545
Symmetry	-	C1	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.7070268	0.6217353	0.5176907
Rotational Con. (GHz)	0.2310339	0.2230012	0.232764
Rotational Con. (GHz)	0.2200747	0.2122883	0.2163053
H298			
6-31+g* */PCM	-946.113756	-1096.569500	-1097.037420
6-31g*	-946.021551	-1096.388543	-1096.937421
G298			
6-31+g* */PCM	-946.177976	-1096.636553	-1097.107790
6-31g*	-946.085771	-1096.455596	-1097.007791



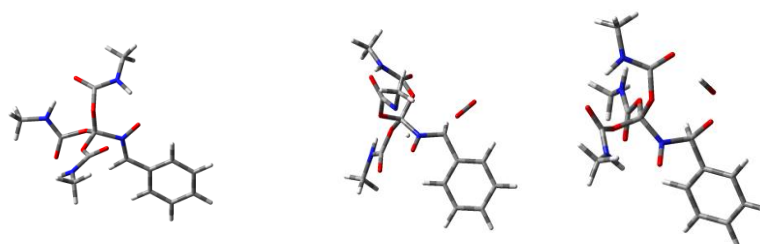
Compound	PBN-tri-COOMe	PBN-tri-COOMe-O2	PBN-tri-COOMe-HO2
file	PBN-COOMe-3.com.log	PBN-COOMe-3-O2.com.log	PBN-COOMe-3-OOH.com.log
E 6-31+g**/PCM	-1123.821814	-1274.278852	-1274.767454
E 6-31g*	-1123.770079	-1274.122424	-1274.707691
ZPE (raw)	0.283755	0.288064	0.302583
Therm Corr to H (raw)	0.307035	0.313383	0.328293
Therm Corr to G (raw)	0.229849	0.232238	0.245462
H (raw)			
G (raw)			
ZPE (scaled)	0.278250	0.282476	0.296713
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7559	0.754400
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.4209902	0.347073	0.340736
Rotational Con. (GHz)	0.1787248	0.1877508	0.186207
Rotational Con. (GHz)	0.1776332	0.1631597	0.165864
H298			
6-31+g* */PCM	-1123.520284	-1273.971057	-1274.445031
6-31g*	-1123.468549	-1273.814630	-1274.385269
G298			
6-31+g* */PCM	-1123.597470	-1274.052202	-1274.527862
6-31g*	-1123.545735	-1273.895775	-1274.468100



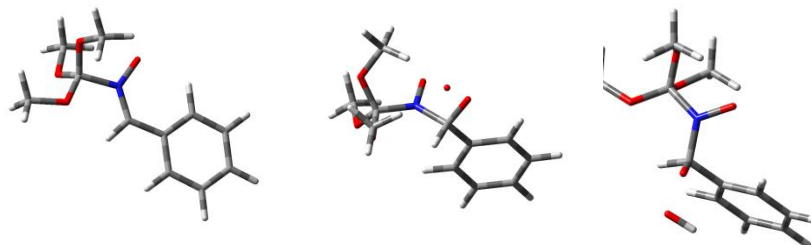
Compound	PBN-tri-NHCOMe PBN-NHCOMe- 3.com.log	PBN-tri-NHCOMe-O2 PBN-NHCOMe-3- O2.com.log	PBN-tri-NHCOMe-HO2 PBN-NHCOMe-3- OOH.com.log
file			
E 6-31+g**/PCM	-1064.288306	-1214.760238	-1215.235847
E 6-31g*	-1064.224148	-1214.609935	-1215.156202
ZPE (raw)	0.320552	0.324818	0.338615
Therm Corr to H (raw)	0.343786	0.350189	0.364813
Therm Corr to G (raw)	0.266471	0.267285	0.280013
H (raw)			
G (raw)			
ZPE (scaled)	0.314333	0.318517	0.332046
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7542	0.7546
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.3434093	0.3306594	0.2978961
Rotational Con. (GHz)	0.1901124	0.1763069	0.1883656
Rotational Con. (GHz)	0.1827485	0.1576798	0.1743604
H298			
6-31+g* */PCM	-1063.950739	-1214.416350	-1214.877603
6-31g*	-1063.886580	-1214.266047	-1214.797958
G298			
6-31+g* */PCM	-1064.028054	-1214.499254	-1214.962403
6-31g*	-1063.963895	-1214.348951	-1214.882758



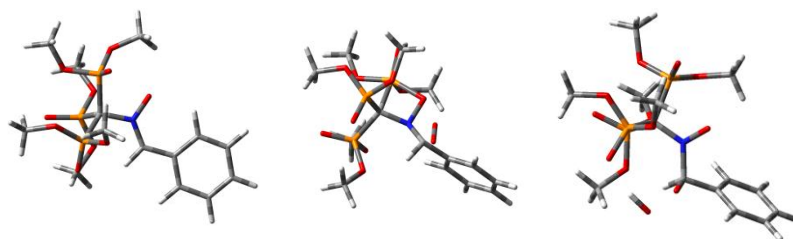
Compound	PBN-tri-OCOMe	PBN-tri-OCOMe-O2	PBN-tri-OCOMe-HO2
file	PBN-OCOMe-3.com.log	PBN-OCOMe-3-O2.com.log	PBN-OCOMe-3-OOH.com.log
E 6-31+g**/PCM	-1123.839554	N/A	-1274.786072
E 6-31g*	-1123.779678		-1274.718803
ZPE (raw)	0.280854		0.299905
Therm Corr to H (raw)	0.303676		0.32517
Therm Corr to G (raw)	0.227462		0.243235
H (raw)			
G (raw)			
ZPE (scaled)	0.275405		0.294087
Electronic State	1-A		2-A
s2 6-31g*	0		0.7539
Symmetry	-		-
N Imag	0.000000		0.000000
Rotational Con. (GHz)	0.4350747		0.3311801
Rotational Con. (GHz)	0.1864728		0.1916365
Rotational Con. (GHz)	0.1694322		0.1665542
H298			
6-31+g* */PCM	-1123.541327		-1274.466720
6-31g*	-1123.481451		-1274.399451
G298			
6-31+g* */PCM	-1123.617541		-1274.548655
6-31g*	-1123.557665		-1274.481386



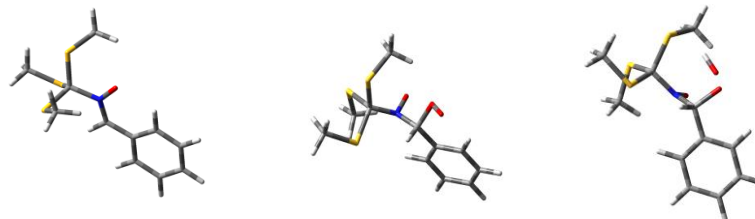
Compound	PBN-tri-OCONHMe PBN-OCONHMe- 3.com.log	PBN-tri-OCONHMe-O2 PBN-OCONHMe-3- O2.com.log	PBN-tri-OCONHMe-HO2 PBN-OCONHMe-3- OOH.com.log
file			
E 6-31+g**/PCM	-1289.960478	-1440.409276	-1440.90837
E 6-31g*	-1289.886852	-1440.252909	-1440.82715
ZPE (raw)	0.334579	0.337828	0.353797
Therm Corr to H (raw)	0.361325	0.366791	0.382922
Therm Corr to G (raw)	0.274405	0.274843	0.290497
H (raw)			
G (raw)			
ZPE (scaled)	0.328088	0.331274	0.346933
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7545	0.7543
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.2626084	0.2411777	0.2503055
Rotational Con. (GHz)	0.1520595	0.1514455	0.1404939
Rotational Con. (GHz)	0.1337627	0.1255845	0.1283657
H298			
6-31+g* */PCM	-1289.605644	-1440.049039	-1440.532312
6-31g*	-1289.532018	-1439.892671	-1440.451092
G298			
6-31+g* */PCM	-1289.692564	-1440.140987	-1440.624737
6-31g*	-1289.618938	-1439.984619	-1440.543517



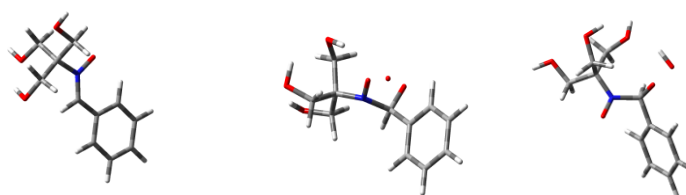
Compound	PBN-tri-OMe	PBN-tri-OMe-O2	PBN-tri-OMe-HO2
file	PBN-OMe-3.com.log	PBN-OMe-3-O2b.com.log	PBN-OMe-3-OOH.com.log
E 6-31+g**/PCM	-783.792744	-934.248473	-934.741688
E 6-31g*	-783.7535674	-934.0985653	-934.6845934
ZPE (raw)	0.254201	0.25916	0.272043
Therm Corr to H (raw)	0.271409	0.278071	0.29234
Therm Corr to G (raw)	0.209551	0.212395	0.221996
H (raw)			
G (raw)			
ZPE (scaled)	0.249270	0.254132	0.266765
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7543	0.7543
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.0904602	0.7011249	0.6892308
Rotational Con. (GHz)	0.2814713	0.3089054	0.2886754
Rotational Con. (GHz)	0.2639659	0.2601099	0.2627712
H298			
6-31+g* */PCM	-783.526266	-933.975430	-934.454626
6-31g*	-783.487090	-933.825522	-934.397531
G298			
6-31+g* */PCM	-783.588124	-934.041106	-934.524970
6-31g*	-783.548948	-933.891198	-934.467875



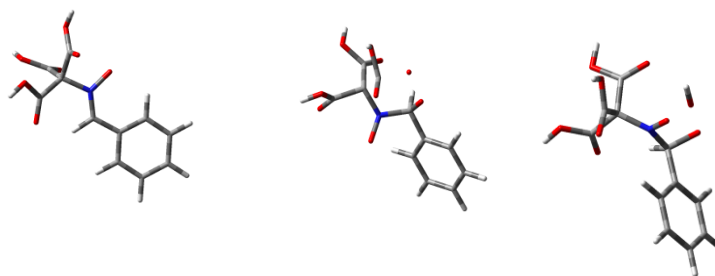
Compound	PBN-tri-POOMe2 PBN-POOMe2- 3.com.log	PBN-tri-POOMe2-O2 PBN-POOMe-3- O2b.com.log	PBN-tri-POOMe2-HO2 PBN-POOMe-3- OOHb.com.log
file			
E 6-31+g**/PCM	-2379.12374	-2529.569597	-2530.069092
E 6-31g*	-2379.056907	-2529.424005	-2529.995128
ZPE (raw)	0.402407	0.407154	0.4213
Therm Corr to H (raw)	0.437065	0.443518	0.458389
Therm Corr to G (raw)	0.335846	0.338718	0.351014
H (raw)			
G (raw)			
ZPE (scaled)	0.394600	0.399255	0.413127
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7544	0.7544
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.2134556	0.1891594	0.1906434
Rotational Con. (GHz)	0.1249908	0.1264207	0.1235934
Rotational Con. (GHz)	0.1214607	0.1165158	0.1147428
H298			
6-31+g* */PCM	-2378.694482	-2529.133978	-2529.618876
6-31g*	-2378.627648	-2528.988386	-2529.544913
G298			
6-31+g* */PCM	-2378.795701	-2529.238778	-2529.726251
6-31g*	-2378.728867	-2529.093186	-2529.652288



Compound	PBN-tri-SMe	PBN-tri-SMe-O2	PBN-tri-SMe-HO2
file	PBN-SMe-3.com.log	PBN-SMe-3-O2-c.com.log	PBN-SMe-3-OOH.com.log
E 6-31+g**/PCM	-1752.692787	-1903.146421	-1903.642013
E 6-31g*	-1752.659135	-1903.006628	-1903.594985
ZPE (raw)	0.241711	0.245793	0.260292
Therm Corr to H (raw)	0.2612	0.267626	0.282317
Therm Corr to G (raw)	0.193847	0.194599	0.208181
H (raw)			
G (raw)			
ZPE (scaled)	0.237022	0.241025	0.255242
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7557	0.7545
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.6722395	0.5002244	0.4975158
Rotational Con. (GHz)	0.2209792	0.2288683	0.2286281
Rotational Con. (GHz)	0.2146102	0.200808	0.2018773
H298			
6-31+g* */PCM	-1752.436276	-1902.883563	-1903.364746
6-31g*	-1752.402624	-1902.743770	-1903.317717
G298			
6-31+g* */PCM	-1752.503629	-1902.956590	-1903.438882
6-31g*	-1752.469977	-1902.816797	-1903.391853



Compound	PBN-tri-CH2OH PBN-alpha- 3CH2OH.com.log	PBN-tri-CH2OH-O2 PBN-alpha-3CH2OH- O2.com.log	PBN-tri-CH2OH-HO2 PBN-alpha-3CH2OH- OOH.com.log
file			
E 6-31+g**/PCM	-783.835028	-934.28536	-934.778065
E 6-31g*	-783.7413479	-934.1068776	-934.6640481
ZPE (raw)	0.256011	0.262246	0.273992
Therm Corr to H (raw)	0.272632	0.280341	0.293548
Therm Corr to G (raw)	0.212953	0.216181	0.225219
H (raw)			
G (raw)			
ZPE (scaled)	0.251044	0.257158	0.268677
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7546	0.7546
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.05713	0.7764751	0.7779518
Rotational Con. (GHz)	0.2780761	0.2442765	0.2577386
Rotational Con. (GHz)	0.2566142	0.2374887	0.2230323
H298			
6-31+g* */PCM	-783.567363	-934.010107	-934.489832
6-31g*	-783.473683	-933.831624	-934.375816
G298			
6-31+g* */PCM	-783.627042	-934.074267	-934.558161
6-31g*	-783.533362	-933.895784	-934.444145



Compound	PBN-tri-COOH PBN-alpha-3COOH.com.log	PBN-tri-COOH-O2 PBN-alpha-3COOH-O2.com.log	PBN-tri-COOH-HO2 PBN-alpha-3COOH-HO2.com.log
file			
E 6-31+g**/PCM	-1005.949879	-1156.421609	-1156.898846
E 6-31g*	-1005.842291	-1156.221144	-1156.781925
ZPE (raw)	0.199009	0.204553	0.217728
Therm Corr to H (raw)	0.217011	0.224085	0.238365
Therm Corr to G (raw)	0.152522	0.1561	0.166717
H (raw)			
G (raw)			
ZPE (scaled)	0.195148	0.200585	0.213504
Electronic State	1-A	2-A	2-A
s2 6-31g*	0	0.7544	0.7541
Symmetry	-	-	-
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.7478393	0.6203126	0.5272232
Rotational Con. (GHz)	0.2261233	0.2206767	0.2378425
Rotational Con. (GHz)	0.2140926	0.2057931	0.2072945
H298			
6-31+g* */PCM	-1005.736729	-1156.201492	-1156.664705
6-31g*	-1005.629141	-1156.001027	-1156.547784
G298			
6-31+g* */PCM	-1005.801218	-1156.269477	-1156.736353
6-31g*	-1005.693630	-1156.069012	-1156.619432

Table S4. Cartesian coordinates.

PBN-alpha-carbamate.log

33

C	4.302955	-0.286573	-0.529872
C	2.969698	-0.677165	-0.420055
C	2.020702	0.202212	0.144116
C	2.458462	1.470457	0.584831
C	3.790548	1.849871	0.470879
C	4.721834	0.970014	-0.088413
H	5.022542	-0.974188	-0.966873
H	2.640900	-1.648762	-0.761365
H	1.737043	2.159821	1.018195
H	4.104012	2.831389	0.816657
H	5.764246	1.263621	-0.179497
C	0.611740	-0.098051	0.312532
H	-0.016603	0.649404	0.773982
N	0.001780	-1.209677	-0.030934
O	0.551400	-2.240032	-0.553834
C	-1.482114	-1.423999	0.274277
C	-2.147808	-2.070069	-0.940173
H	-3.216696	-2.178838	-0.729526
H	-2.016404	-1.461050	-1.832791
H	-1.710424	-3.054006	-1.106269
C	-1.542334	-2.322918	1.509254
H	-0.941300	-3.215613	1.326172
H	-1.147790	-1.794043	2.381866
H	-2.578044	-2.612828	1.708338
C	-2.410397	0.792808	-0.229138
O	-2.048759	0.828408	-1.387039
O	-2.107424	-0.202047	0.681486
N	-3.148396	1.739176	0.410260
H	-3.413723	1.552979	1.366218
C	-3.640592	2.926072	-0.263561
H	-4.734126	2.915944	-0.347269
H	-3.334543	3.833002	0.269799
H	-3.210679	2.940080	-1.265880

PBN-alpha-carboxyl.log

31

C	-3.972849	-0.692545	-0.723843
C	-2.597255	-0.862384	-0.579593
C	-1.843904	0.074903	0.159792
C	-2.518167	1.172022	0.740359
C	-3.890628	1.330896	0.590889
C	-4.626348	0.396670	-0.144201
H	-4.539910	-1.422156	-1.296165
H	-2.088240	-1.704874	-1.026406
H	-1.950601	1.901867	1.313612
H	-4.388228	2.182423	1.047296
H	-5.699769	0.518069	-0.262522
C	-0.411685	0.001573	0.371771
H	0.054006	0.778542	0.966235
N	0.408047	-0.929775	-0.072498
O	0.071465	-1.948824	-0.756377
C	1.897346	-0.851895	0.318878
C	2.026962	-1.367085	1.755780
H	3.081923	-1.424339	2.040624
H	1.521949	-0.707574	2.464488
H	1.589841	-2.368012	1.816862
C	2.694063	-1.716164	-0.662400
H	2.390576	-2.759309	-0.569492
H	2.534398	-1.396553	-1.692427
H	3.759696	-1.628611	-0.424019
C	2.808229	2.407510	-1.230780
H	2.081703	3.073661	-0.758115
H	3.794570	2.588491	-0.796343
H	2.826221	2.561999	-2.309454
C	2.344628	0.617002	0.228639

O 2.595420 1.321666 1.183927
O 2.422263 1.033630 -1.047353

PBN-alpha-CH2CONH2.log

32

C 3.710067 0.479590 -1.119623
C 2.356671 0.164003 -1.014791
C 1.828420 -0.278040 0.217258
C 2.701212 -0.389952 1.322201
C 4.048721 -0.070732 1.207438
C 4.559921 0.367370 -0.017727
H 4.103815 0.816496 -2.074948
H 1.696339 0.243990 -1.866525
H 2.308669 -0.729961 2.277977
H 4.701141 -0.162856 2.071414
H 5.613206 0.617830 -0.110959
C 0.440704 -0.636707 0.450932
H 0.183004 -0.990504 1.437949
N -0.549870 -0.571374 -0.407547
O -0.426448 -0.154218 -1.623783
C -1.977283 -0.984147 -0.042201
C -2.297253 -2.213303 -0.907300
H -3.355578 -2.473899 -0.804130
H -2.081928 -2.000406 -1.956439
H -1.698784 -3.075234 -0.591714
C -2.149777 -1.307922 1.445350
H -1.535501 -2.160399 1.753603
H -1.940488 -0.445855 2.084026
H -3.195105 -1.585134 1.612719
C -2.890714 0.201496 -0.454517
H -2.860538 0.304777 -1.540762
H -3.911603 -0.043094 -0.150329
C -2.518529 1.523401 0.223027
O -2.994693 1.863986 1.299886
N -1.626277 2.281351 -0.480688
H -1.235407 3.081529 -0.000518
H -1.062039 1.824407 -1.192817

PBN-alpha-CH2OH.com.log

29

C 3.590355 -1.270493 -0.069780
C 2.212918 -1.070597 0.003833
C 1.687626 0.239614 -0.001481
C 2.590221 1.323397 -0.082632
C 3.961876 1.112925 -0.155875
C 4.469996 -0.189452 -0.149905
H 3.979323 -2.285499 -0.064192
H 1.528775 -1.904889 0.066011
H 2.201419 2.339543 -0.087948
H 4.635969 1.963173 -0.217706
H 5.542130 -0.357652 -0.207139
C 0.276436 0.572712 0.069671
H 0.013215 1.619414 0.059614
N -0.731233 -0.270911 0.150466
O -0.608417 -1.546590 0.179849
C -2.178012 0.208198 0.232969
C -2.722699 -0.254747 1.591281
H -3.804489 -0.102022 1.616999
H -2.503348 -1.314650 1.736699
H -2.265016 0.315415 2.407128
C -2.335629 1.721361 0.067707
H -1.876276 2.275128 0.892908
H -1.919795 2.077637 -0.881090
H -3.404987 1.946337 0.063343
C -2.897925 -0.520871 -0.923397
O -4.264809 -0.121337 -0.903881
H -4.754896 -0.722917 -1.482812
H -2.782640 -1.599469 -0.782713
H -2.415931 -0.242027 -1.874440

PBN-alpha-CONH2.log

29

C	3.674236	-1.244510	0.088418
C	2.303899	-1.022379	0.209336
C	1.779608	0.273942	0.017188
C	2.673987	1.321803	-0.295737
C	4.038704	1.089261	-0.414761
C	4.545842	-0.199069	-0.222273
H	4.064206	-2.247588	0.239717
H	1.626597	-1.828546	0.451740
H	2.284642	2.326280	-0.446467
H	4.707571	1.910576	-0.656942
H	5.612643	-0.384576	-0.313751
C	0.376609	0.633902	0.114092
H	0.123105	1.669961	-0.050896
N	-0.631525	-0.163591	0.384567
O	-0.498845	-1.429664	0.612167
C	-2.070354	0.347029	0.428521
C	-2.705230	-0.207484	1.717402
H	-3.771209	0.038036	1.721708
H	-2.582109	-1.288373	1.777718
H	-2.237399	0.250447	2.595931
C	-2.167673	1.873386	0.410010
H	-1.626540	2.310015	1.255327
H	-1.806912	2.306062	-0.526770
H	-3.221570	2.144032	0.488668
C	-2.848355	-0.215410	-0.808558
N	-2.573682	-1.496656	-1.142899
H	-3.037697	-1.883150	-1.952796
H	-1.809737	-1.982858	-0.678841
O	-3.688252	0.476987	-1.369399

PBN-alpha-COOH.com.log

28

C	3.607540	-1.375417	0.130823
C	2.247597	-1.077637	0.192982
C	1.808069	0.251102	0.011013
C	2.773636	1.252590	-0.232273
C	4.127466	0.944654	-0.291002
C	4.551383	-0.374932	-0.108875
H	3.932021	-2.403186	0.271187
H	1.513279	-1.849341	0.376426
H	2.448925	2.280921	-0.376320
H	4.852720	1.731692	-0.479374
H	5.609261	-0.619427	-0.154620
C	0.422119	0.678386	0.052440
H	0.216836	1.723747	-0.124804
N	-0.626299	-0.079414	0.284386
O	-0.601677	-1.340156	0.509879
C	-2.034668	0.484398	0.331015
C	-2.534691	0.312410	1.769554
H	-3.588115	0.594796	1.841063
H	-2.420732	-0.724652	2.085672
H	-1.952653	0.957289	2.436774
C	-2.151883	1.941157	-0.134828
H	-1.629126	2.620770	0.545152
H	-1.774242	2.065226	-1.152665
H	-3.209656	2.224764	-0.130727
C	-2.788061	-0.384772	-0.701144
O	-2.507747	-0.408932	-1.876449
O	-3.834334	-1.052290	-0.174915
H	-4.235412	-1.547302	-0.914810

PBN-alpha-ester.log

31

C	3.692550	-1.193138	0.829071
C	2.357093	-0.797859	0.782134

C	1.953877	0.222145	-0.106281
C	2.930635	0.816394	-0.935605
C	4.259458	0.413674	-0.881580
C	4.647625	-0.595587	0.004483
H	3.988430	-1.980161	1.517890
H	1.613556	-1.260777	1.415442
H	2.634263	1.601409	-1.628041
H	4.993257	0.884886	-1.530024
H	5.685884	-0.913490	0.048751
C	0.598039	0.719794	-0.236082
H	0.417540	1.492086	-0.968561
N	-0.453020	0.320725	0.445508
O	-0.458642	-0.597366	1.333530
C	-1.811486	1.008927	0.276871
C	-2.074266	1.775602	1.570714
H	-3.092512	2.174425	1.560329
H	-1.956737	1.096975	2.417217
H	-1.367214	2.605137	1.667718
C	-1.932244	1.894804	-0.961655
H	-1.312492	2.791420	-0.868850
H	-1.674347	1.352058	-1.871447
H	-2.974570	2.220209	-1.033381
C	-2.700249	-1.049728	-0.638936
O	-1.932623	-1.062479	-1.571918
O	-2.798099	-0.029947	0.263623
C	-3.677858	-2.141695	-0.285372
H	-3.325353	-2.648074	0.619923
H	-4.665746	-1.725073	-0.068182
H	-3.736946	-2.857751	-1.105770

PBN-alpha-ether.log

29

C	-3.434398	-1.251101	-0.166653
C	-2.058090	-1.036093	-0.213860
C	-1.538906	0.262205	-0.019268
C	-2.445586	1.318064	0.223822
C	-3.815912	1.092373	0.269577
C	-4.318246	-0.197546	0.073394
H	-3.819031	-2.256197	-0.319346
H	-1.370503	-1.849196	-0.398938
H	-2.061077	2.324488	0.375942
H	-4.493666	1.920882	0.457476
H	-5.389408	-0.377500	0.108168
C	-0.129325	0.606098	-0.049979
H	0.132029	1.640086	0.117657
N	0.877274	-0.214592	-0.271642
O	0.766569	-1.468313	-0.480792
C	2.340937	0.284996	-0.305109
C	2.838781	0.057738	-1.730765
H	3.910947	0.269031	-1.773662
H	2.663576	-0.984578	-2.001347
H	2.315541	0.712352	-2.434701
C	2.492723	1.748094	0.126356
H	2.011795	2.434672	-0.576048
H	2.098747	1.937260	1.128835
H	3.563207	1.972449	0.136022
C	2.667741	-0.780829	1.842769
H	1.701426	-1.296521	1.861991
H	3.424317	-1.422800	2.299368
H	2.605746	0.151927	2.420008
O	3.104321	-0.568962	0.505586

PBN-alpha-ethylester.com.log

34

C	-3.820780	-1.262443	-1.052918
C	-2.546747	-0.708697	-0.942384
C	-2.227034	0.111259	0.161102
C	-3.222249	0.345050	1.135724
C	-4.489083	-0.213320	1.016404

C -4.795147 -1.021465 -0.082505
H -4.052617 -1.892056 -1.908068
H -1.788161 -0.896657 -1.689071
H -2.989304 0.972046 1.993711
H -5.238453 -0.019934 1.779317
H -5.784734 -1.460187 -0.178671
C -0.941549 0.746579 0.377024
H -0.820262 1.336862 1.272713
N 0.111981 0.672924 -0.405995
O 0.186144 0.004157 -1.491761
C 1.377896 1.481494 -0.104587
C 1.475084 2.556688 -1.183875
H 2.431810 3.078959 -1.095414
H 1.406462 2.083918 -2.164973
H 0.661816 3.280068 -1.070415
C 1.446732 2.062765 1.306585
H 0.709837 2.859560 1.443774
H 1.312812 1.292251 2.066391
H 2.439267 2.506463 1.431268
C 2.568632 -0.593762 0.278262
O 1.857439 -0.927385 1.197266
O 2.489080 0.612586 -0.355965
C 3.663667 -1.432333 -0.344898
H 3.334694 -1.663013 -1.366855
H 4.556581 -0.805055 -0.455958
C 3.957304 -2.706367 0.444526
H 4.730140 -3.296327 -0.058619
H 4.306570 -2.473803 1.455564
H 3.058012 -3.321127 0.540191

PBN-alpha-methylcarbamate.log

36

C -4.648548 1.593519 0.553193
C -3.357334 1.070585 0.594766
C -3.029298 -0.062375 -0.180700
C -4.035876 -0.639016 -0.986898
C -5.319919 -0.108977 -1.021582
C -5.632782 1.013417 -0.249138
H -4.886748 2.465573 1.156649
H -2.593111 1.516486 1.215315
H -3.798898 -1.513007 -1.589874
H -6.077570 -0.569823 -1.649626
H -6.635989 1.430403 -0.273504
C -1.724058 -0.696303 -0.220098
H -1.614250 -1.567093 -0.848702
N -0.646434 -0.326612 0.438972
O -0.588008 0.678940 1.234463
C 0.666942 -1.095476 0.329672
C 0.946708 -1.701188 1.711918
H 1.959986 -2.110431 1.733480
H 0.850450 -0.931893 2.481282
H 0.236624 -2.506472 1.927659
C 0.662077 -2.174153 -0.755470
H -0.029401 -2.988613 -0.518145
H 0.411600 -1.766248 -1.740909
H 1.668412 -2.595455 -0.816518
C 1.710547 -0.006267 -0.009701
H 1.718373 0.739340 0.787578
H 1.433776 0.476066 -0.959287
C 4.142371 0.062631 -0.249312
O 5.200471 -0.528959 -0.266357
O 2.977850 -0.652155 -0.131469
N 4.016735 1.423262 -0.317790
H 3.112483 1.839273 -0.478270
C 5.191999 2.250031 -0.547063
H 5.463931 2.303286 -1.609503
H 4.996688 3.260156 -0.176837
H 6.032046 1.820724 0.000332

PBN-alpha-methylcarboxy.log

C	3.802258	0.951008	-1.195305
C	2.525249	0.410688	-1.054698
C	2.129951	-0.157423	0.175507
C	3.055992	-0.158862	1.242049
C	4.326539	0.383602	1.091645
C	4.706898	0.942431	-0.132017
H	4.092068	1.384884	-2.148941
H	1.821028	0.417289	-1.874513
H	2.765290	-0.590844	2.197208
H	5.021052	0.371937	1.927502
H	5.699745	1.367537	-0.253236
C	0.832859	-0.752674	0.439975
H	0.660505	-1.147419	1.429384
N	-0.174337	-0.849956	-0.398718
O	-0.166690	-0.412462	-1.604772
C	-1.483539	-1.538653	-0.014721
C	-1.581623	-2.782526	-0.914854
H	-2.561114	-3.257608	-0.794622
H	-1.444151	-2.500342	-1.960605
H	-0.811435	-3.512287	-0.642625
C	-1.556325	-1.948167	1.461045
H	-0.801958	-2.702944	1.706383
H	-1.455131	-1.089865	2.127221
H	-2.536033	-2.404162	1.641629
C	-2.611380	-0.554753	-0.394574
H	-3.574069	-1.004559	-0.119325
H	-2.620455	-0.408228	-1.475374
C	-3.303765	3.034002	0.108155
H	-3.711492	3.035730	1.122717
H	-2.294836	3.453660	0.129196
H	-3.943784	3.606116	-0.563978
O	-3.280788	1.699810	-0.426716
C	-2.533429	0.812394	0.261578
O	-1.920394	1.098201	1.269026

PBN-alpha-methylether.log

32

C	3.901764	-1.374005	0.028873
C	2.542842	-1.092578	0.158930
C	2.067865	0.217453	-0.066711
C	3.000873	1.216630	-0.423249
C	4.353692	0.925252	-0.550143
C	4.811908	-0.375975	-0.323804
H	4.252028	-2.387687	0.205941
H	1.835800	-1.863110	0.431619
H	2.650661	2.231412	-0.600488
H	5.051784	1.711465	-0.825203
H	5.869150	-0.607632	-0.421896
C	0.680304	0.631082	0.037042
H	0.455792	1.667043	-0.166105
N	-0.347239	-0.126208	0.360690
O	-0.268547	-1.374629	0.639356
C	-1.764395	0.434352	0.447994
C	-2.217847	0.267461	1.904923
H	-3.285208	0.490229	1.979467
H	-2.038699	-0.758232	2.233771
H	-1.666755	0.949813	2.561414
C	-1.876199	1.895069	0.005522
H	-1.329982	2.569594	0.672806
H	-1.525292	2.043055	-1.021678
H	-2.932955	2.171099	0.034214
C	-2.598601	-0.463408	-0.492892
H	-2.514683	-1.506791	-0.167205
H	-2.197223	-0.392166	-1.518768
C	-4.800710	-0.817790	-1.239373
H	-4.801388	-1.866047	-0.902174
H	-5.808079	-0.407016	-1.133152

H -4.514800 -0.796331 -2.303112
O -3.941260 -0.018685 -0.452725

PBN-alpha-methylphosphoryl.log

39

C -4.359861 -0.829013 -1.050664
C -3.126971 -0.185356 -0.958241
C -2.589043 0.132799 0.307710
C -3.328799 -0.217213 1.458954
C -4.554673 -0.863462 1.355739
C -5.077114 -1.173128 0.096501
H -4.763147 -1.064218 -2.032272
H -2.570454 0.086067 -1.844180
H -2.926591 0.020853 2.440980
H -5.103941 -1.126082 2.255829
H -6.035759 -1.678038 0.012253
C -1.329438 0.819344 0.531349
N -0.449540 1.167013 -0.379685
O -0.563377 0.911449 -1.637537
C 0.820717 1.940270 -0.028433
C 0.738882 3.254301 -0.827143
H 1.667141 3.821288 -0.703097
H 0.580109 3.046069 -1.886405
H -0.090328 3.870391 -0.462028
C 0.956986 2.250725 1.466889
H 0.132478 2.878871 1.819748
H 1.024063 1.343896 2.071357
H 1.881472 2.820430 1.610992
C 2.014824 1.108533 -0.555137
H 2.936339 1.666060 -0.360431
H 1.914958 0.988735 -1.636405
H -1.068142 1.056151 1.550926
P 2.258367 -0.567662 0.157533
O 3.875639 -0.607934 0.176527
O 1.956779 -1.639415 -1.018290
C 0.628542 -2.183400 -1.178870
H -0.039539 -1.417113 -1.582241
H 0.724909 -3.009699 -1.885819
H 0.249290 -2.552193 -0.222170
C 4.533577 -1.815564 0.600803
H 4.162176 -2.132018 1.580226
H 4.374274 -2.610927 -0.133089
H 5.596939 -1.579272 0.667524
O 1.563366 -0.853652 1.443843

PBN-alpha-methylthio.log

32

C 4.193370 -1.404218 0.263987
C 2.848162 -1.057318 0.377136
C 2.393622 0.181835 -0.123172
C 3.332197 1.044103 -0.732570
C 4.671152 0.688292 -0.840559
C 5.109267 -0.541672 -0.340960
H 4.528172 -2.361713 0.654651
H 2.136246 -1.722244 0.844991
H 2.997926 2.002872 -1.123409
H 5.374198 1.368708 -1.313660
H 6.155697 -0.823102 -0.423378
C 1.021556 0.653212 -0.063396
H 0.815149 1.625784 -0.482885
N -0.008800 0.018433 0.455194
O 0.051782 -1.141228 0.993616
C -1.419447 0.631191 0.464769
C -1.821232 0.723150 1.944724
H -2.858382 1.055792 2.035631
H -1.715712 -0.252172 2.422673
H -1.177263 1.440296 2.465687
C -1.477861 2.011524 -0.196307

H	-0.847197	2.738366	0.325526
H	-1.192704	1.977986	-1.253009
H	-2.507452	2.378225	-0.150036
C	-2.270156	-0.398318	-0.315517
H	-2.152873	-1.371940	0.163851
H	-1.889716	-0.468766	-1.341648
S	-4.056347	0.039288	-0.373001
C	-4.684332	-1.499495	-1.129491
H	-4.466025	-2.365834	-0.497965
H	-5.768111	-1.389686	-1.219590
H	-4.260859	-1.654102	-2.126567

PBN-alpha-phosphoryl.log

36

C	4.500481	0.003698	1.018231
C	3.155885	0.347487	0.890637
C	2.480498	0.117729	-0.328037
C	3.200305	-0.463719	-1.396238
C	4.539660	-0.805261	-1.256669
C	5.197798	-0.572221	-0.045167
H	5.007684	0.188301	1.961697
H	2.613718	0.797034	1.710311
H	2.692188	-0.649090	-2.339677
H	5.072164	-1.253144	-2.091367
H	6.245594	-0.838022	0.066608
C	1.089867	0.437314	-0.584103
N	0.227891	0.949851	0.271446
O	0.491951	1.217099	1.496711
C	-1.221526	1.208844	-0.174989
C	-1.877144	2.141677	0.848188
H	-2.916541	2.308565	0.555959
H	-1.847696	1.718958	1.850899
H	-1.350670	3.100666	0.865445
C	-1.265883	1.828959	-1.581860
H	-0.606338	2.702311	-1.623052
H	-0.979029	1.127691	-2.368315
H	-2.287843	2.156367	-1.793714
H	0.691504	0.203570	-1.560370
P	-2.034803	-0.466100	-0.203845
O	-3.578840	-0.034843	-0.383169
O	-2.032994	-1.009835	1.316775
C	-0.918232	-1.777340	1.827578
H	-1.295753	-2.318617	2.696983
H	-0.563228	-2.483091	1.072350
H	-0.119531	-1.093718	2.126652
C	-4.575298	-1.065095	-0.539261
H	-4.651628	-1.657507	0.377240
H	-5.519094	-0.551093	-0.727024
H	-4.325347	-1.712659	-1.384281
O	-1.476595	-1.399474	-1.218897

PBN-alpha-thio.log

29

C	3.635728	-1.328548	0.290531
C	2.280958	-1.013247	0.376019
C	1.828271	0.269089	-0.003611
C	2.779996	1.206767	-0.463625
C	4.128543	0.882035	-0.544544
C	4.564140	-0.391493	-0.166548
H	3.968356	-2.320383	0.585673
H	1.560225	-1.736507	0.729621
H	2.447651	2.199091	-0.760943
H	4.841082	1.620298	-0.902675
H	5.618090	-0.648970	-0.228613
C	0.448218	0.713861	0.038990
H	0.242284	1.717619	-0.300471
N	-0.595958	0.014276	0.432057
O	-0.538284	-1.195614	0.852584
C	-2.009281	0.591568	0.374357

C	-2.724773	0.165855	1.658589
H	-3.763446	0.504394	1.621279
H	-2.691667	-0.914242	1.790754
H	-2.233775	0.625945	2.524691
C	-2.034872	2.118944	0.235283
H	-1.453070	2.587278	1.036045
H	-1.656819	2.464118	-0.731420
H	-3.070504	2.457278	0.322757
S	-2.837691	-0.045774	-1.161020
C	-3.019374	-1.842944	-0.869109
H	-2.055329	-2.285153	-0.617952
H	-3.748308	-2.051646	-0.082222
H	-3.389050	-2.253086	-1.813275

PBN-CH2NHCOMe-c.out
35

C	-4.018348	-1.807191	0.152757
C	-2.748633	-1.234417	0.198068
C	-2.588577	0.147545	-0.040093
C	-3.738576	0.917895	-0.322185
C	-5.000071	0.336711	-0.365931
C	-5.145655	-1.032998	-0.127664
H	-4.126189	-2.872472	0.339382
H	-1.874450	-1.830854	0.416170
H	-3.631849	1.984630	-0.507410
H	-5.869966	0.949910	-0.585097
H	-6.130529	-1.491037	-0.160530
C	-1.323384	0.860241	-0.015239
H	-1.355436	1.922753	-0.203014
N	-0.132163	0.355432	0.217589
O	0.080961	-0.892286	0.460280
C	1.134081	1.210839	0.216436
C	2.071615	0.618572	-0.872967
H	2.909574	1.305180	-1.016406
H	1.510748	0.563158	-1.815621
C	0.864514	2.677321	-0.139242
H	0.457328	2.793570	-1.149589
H	0.188912	3.157727	0.575354
C	1.745471	1.104572	1.619259
H	1.826615	0.060157	1.921754
H	1.123566	1.633619	2.349711
N	2.653440	-0.666805	-0.560644
H	1.992923	-1.381232	-0.280027
C	3.992936	-0.814353	-0.325171
O	4.802203	0.098850	-0.457907
C	4.424848	-2.213081	0.089465
H	3.591859	-2.912545	0.208500
H	5.113861	-2.607186	-0.664456
H	4.977516	-2.147099	1.031577
H	1.815464	3.217385	-0.101147
H	2.744467	1.551495	1.618290

PBN.log
28

C	-3.248732	-1.245753	0.000037
C	-1.866895	-1.063361	-0.000075
C	-1.325905	0.240466	-0.000100
C	-2.218029	1.335857	-0.000088
C	-3.594240	1.142909	0.000031
C	-4.117880	-0.153295	0.000101
H	-3.649534	-2.256167	0.000074
H	-1.190964	-1.906606	-0.000181
H	-1.817495	2.347509	-0.000129
H	-4.259872	2.002065	0.000066
H	-5.193587	-0.307851	0.000157
C	0.091582	0.555292	-0.000130
H	0.365370	1.599189	-0.000168
N	1.091127	-0.302389	-0.000121

O 0.953047 -1.574084 -0.000205
C 2.553621 0.156255 0.000084
C 3.184473 -0.445345 -1.265501
H 4.260627 -0.243382 -1.274353
H 3.020843 -1.523966 -1.288714
H 2.744310 -0.004830 -2.167312
C 2.710131 1.680283 -0.001696
H 2.274860 2.141426 -0.894600
H 2.274263 2.143659 0.889765
H 3.779730 1.915013 -0.001643
C 3.183219 -0.442494 1.267619
H 3.019511 -1.521057 1.292920
H 4.259379 -0.240566 1.276936
H 2.742224 0.000068 2.167987

PBN-NHCOMe-c.log
32

C -3.752919 0.946909 -1.036062
C -2.416992 0.558361 -0.956253
C -1.965110 -0.191881 0.150392
C -2.893811 -0.528587 1.159404
C -4.223669 -0.134847 1.070740
C -4.660307 0.606524 -0.031052
H -4.087185 1.524487 -1.894082
H -1.709460 0.821260 -1.730011
H -2.558809 -1.103997 2.019647
H -4.920505 -0.404466 1.859841
H -5.699427 0.916537 -0.103089
C -0.602306 -0.656183 0.335725
H -0.383897 -1.220610 1.229996
N 0.413547 -0.455611 -0.471858
O 0.374775 0.212175 -1.565454
C 1.815295 -1.042149 -0.187992
N 2.753497 0.061484 -0.312827
H 2.931611 0.307024 -1.279358
C 2.775588 1.145318 0.552553
O 2.258569 1.140244 1.658580
C 3.518426 2.353679 0.003711
H 2.855129 2.911573 -0.668774
H 3.797128 3.003513 0.834539
H 4.413267 2.069094 -0.559906
C 1.936846 -1.742782 1.166839
H 1.301748 -2.633281 1.200291
H 2.975313 -2.068377 1.279617
H 1.702442 -1.072445 1.992521
C 2.085911 -2.029722 -1.330497
H 1.395501 -2.875907 -1.265549
H 1.938495 -1.537799 -2.295050
H 3.110872 -2.404912 -1.257902

PBN-alpha-2CH2OH.com.log
30

C -3.893259 -1.060976 0.132735
C -2.503516 -1.010158 0.039904
C -1.846730 0.236212 -0.047598
C -2.632332 1.410252 -0.036480
C -4.017398 1.348274 0.056352
C -4.656471 0.107853 0.141121
H -4.384250 -2.028388 0.199872
H -1.910079 -1.913255 0.034896
H -2.141447 2.379197 -0.101210
H -4.599735 2.265841 0.063205
H -5.739490 0.055188 0.213818
C -0.410220 0.416411 -0.150741
H -0.048591 1.432433 -0.206905
N 0.505640 -0.529257 -0.187685
O 0.251248 -1.781384 -0.140303
C 1.992139 -0.221798 -0.341393
C 2.431493 -0.871642 -1.659873

H 3.483892 -0.640415 -1.844195
H 2.295989 -1.953866 -1.609055
H 1.835891 -0.489516 -2.496493
C 2.283209 1.287264 -0.346667
H 1.894286 1.751521 -1.263651
H 1.814836 1.762264 0.523498
C 2.731039 -0.885547 0.853481
O 2.767790 -0.079214 2.018307
H 3.432791 0.606440 1.840054
H 3.743528 -1.148133 0.522640
H 2.198058 -1.804317 1.102592
O 3.705781 1.426569 -0.268962
H 3.918561 2.365161 -0.382649

PBN-alpha-2COOH.com.log
28

C -4.037309 -1.254908 0.001419
C -2.657726 -1.088368 0.105000
C -2.097215 0.205604 0.042886
C -2.963510 1.308879 -0.123798
C -4.337988 1.131210 -0.225089
C -4.881833 -0.155170 -0.162824
H -4.456002 -2.256665 0.050410
H -2.000000 -1.936517 0.232697
H -2.543526 2.310712 -0.174343
H -4.986235 1.993887 -0.353025
H -5.956362 -0.297295 -0.241826
C -0.681458 0.509692 0.134287
H -0.366121 1.540533 0.072802
N 0.287654 -0.362918 0.287833
O 0.146781 -1.635816 0.404886
C 1.747578 0.010500 0.410870
C 2.152631 -0.146480 1.886382
H 1.665685 0.624463 2.490740
H 1.835996 -1.135509 2.220599
H 3.236300 -0.065029 1.986251
C 2.483001 -1.042919 -0.456144
O 3.333650 -1.794831 -0.056374
O 2.084967 -0.953105 -1.741674
H 2.563953 -1.648566 -2.230124
C 2.152461 1.418507 -0.056780
O 1.473992 2.420123 -0.085437
O 3.464425 1.424523 -0.370865
H 3.690421 2.343963 -0.610551

PBN-CH2CONH2-2b.com.log
36

C 4.087011 -0.829028 -1.214924
C 2.740988 -0.643378 -0.907132
C 2.371027 -0.120940 0.350784
C 3.390962 0.202543 1.273238
C 4.730480 0.014709 0.955944
C 5.084031 -0.502947 -0.293397
H 4.358708 -1.233422 -2.186180
H 1.967190 -0.897410 -1.616887
H 3.120605 0.605289 2.246686
H 5.498574 0.270521 1.680270
H 6.130523 -0.651363 -0.545200
C 1.009653 0.117238 0.796165
H 0.886807 0.501874 1.797642
N -0.098580 -0.077038 0.125432
O -0.113454 -0.518671 -1.099837
C -1.479427 0.185660 0.735879
C -2.119274 -1.187155 1.113705
H -2.851394 -0.998726 1.901974
H -1.335259 -1.824508 1.542015
C -1.380979 1.032160 2.015860
H -0.852749 1.973795 1.849330
H -2.396096 1.286605 2.331159

C -2.319159 0.929589 -0.331894
H -2.432889 0.292860 -1.209547
H -3.308560 1.106737 0.096702
C -1.738301 2.291681 -0.726396
O -2.046649 3.326654 -0.148439
N -0.862930 2.245534 -1.773240
H -0.351861 3.093280 -1.980820
H -0.453030 1.352335 -2.029912
C -2.900271 -1.988681 0.056105
O -4.089395 -2.228806 0.220674
N -2.172698 -2.466891 -0.992070
H -2.700619 -2.906582 -1.734949
H -1.292957 -2.006171 -1.223941
H -0.911994 0.481534 2.838001

PBN-CH2COOMe-2.com.log
40

C 4.584951 -1.129689 -1.359862
C 3.238641 -0.868342 -1.111794
C 2.767868 -0.788881 0.216488
C 3.691254 -0.976743 1.268646
C 5.031830 -1.235905 1.010314
C 5.485916 -1.314498 -0.309513
H 4.932947 -1.188010 -2.388001
H 2.538280 -0.721871 -1.921803
H 3.343809 -0.914998 2.297587
H 5.723706 -1.376097 1.836552
H 6.533673 -1.516879 -0.515325
C 1.391868 -0.531433 0.599682
H 1.170478 -0.484081 1.654556
N 0.375527 -0.326141 -0.206948
O 0.449278 -0.310854 -1.489213
C -1.043306 -0.086565 0.321416
C -1.857911 -1.244908 -0.302133
H -1.690014 -1.244533 -1.384525
H -1.463013 -2.201316 0.060395
C -1.146948 -0.118866 1.849687
H -0.851028 -1.094781 2.250168
H -0.546670 0.667523 2.308557
H -2.193319 0.047788 2.118841
C -1.494058 1.265364 -0.271605
H -2.526056 1.451151 0.042102
H -1.493626 1.199803 -1.361618
C -0.199145 4.711929 -0.429351
H -0.429076 5.073340 0.576621
H 0.878423 4.547350 -0.510560
H -0.535634 5.427189 -1.180330
O -0.915762 3.497675 -0.707820
C -0.650715 2.464171 0.118811
O 0.138092 2.536418 1.038730
C -3.351307 -1.232473 -0.045054
O -4.011888 -0.324092 0.418643
O -3.888837 -2.408726 -0.429834
C -5.314964 -2.519210 -0.278831
H -5.568177 -3.517223 -0.636912
H -5.600022 -2.402316 0.769965
H -5.824260 -1.756117 -0.873102

PBN-CH2NHCOMe-2.com.log
42

C -5.041775 1.070485 -0.838527
C -3.689129 0.893322 -0.554154
C -3.252050 -0.282721 0.092534
C -4.214193 -1.258601 0.435773
C -5.560494 -1.072241 0.146961
C -5.981119 0.097156 -0.493129
H -5.364074 1.980693 -1.337393
H -2.959059 1.643453 -0.821836
H -3.892401 -2.170981 0.932987

H -6.282255 -1.837333 0.419541
H -7.033167 0.246261 -0.720753
C -1.876176 -0.584068 0.443680
H -1.688688 -1.527614 0.933175
N -0.817814 0.165543 0.227786
O -0.863258 1.314784 -0.360348
C 0.582630 -0.286966 0.614317
C 1.253109 0.886436 1.384814
H 2.200857 0.524661 1.787367
H 0.607469 1.158245 2.228112
C 0.582133 -1.514052 1.532309
H 0.005308 -1.336648 2.446404
H 0.208101 -2.408089 1.027371
C 1.309101 -0.595325 -0.723535
H 1.211101 0.274506 -1.378079
H 0.823099 -1.449464 -1.201009
N 2.704738 -0.936262 -0.547341
H 3.348871 -0.181960 -0.317095
C 3.150791 -2.226994 -0.629530
O 2.404768 -3.181263 -0.829627
C 4.655082 -2.397306 -0.477754
H 5.076744 -2.692375 -1.444849
H 5.163706 -1.491598 -0.134143
H 4.849022 -3.213199 0.224105
N 1.553979 2.081260 0.620082
H 0.742987 2.529416 0.210775
C 2.796157 2.361360 0.143323
O 3.782192 1.648613 0.362527
C 2.914669 3.639304 -0.668215
H 1.958466 4.145906 -0.826743
H 3.595844 4.321320 -0.149053
H 3.366009 3.404504 -1.636867
H 1.613703 -1.729283 1.820686

PBN-CH2OCOMe-2.com.log

40

C -3.865450 -2.543252 0.146149
C -2.591465 -1.979420 0.179731
C -2.429782 -0.590039 -0.010417
C -3.581724 0.198562 -0.228175
C -4.847297 -0.374247 -0.259600
C -4.994520 -1.751907 -0.073264
H -3.975592 -3.613990 0.296366
H -1.716673 -2.588376 0.357692
H -3.472595 1.271579 -0.368608
H -5.719361 0.252013 -0.426760
H -5.982958 -2.202864 -0.096279
C -1.161004 0.114781 -0.003669
H -1.185162 1.188923 -0.110241
N 0.031149 -0.414063 0.168972
O 0.252699 -1.662271 0.385622
C 1.305698 0.416479 0.168363
C 2.334551 -0.367260 -0.707690
H 3.011388 0.356172 -1.178089
H 1.806508 -0.901022 -1.498575
C 1.150446 1.796273 -0.500744
H 0.737274 1.690455 -1.512960
H 2.153835 2.224484 -0.581014
C 1.770313 0.550740 1.623310
H 1.824616 -0.437991 2.078659
H 1.072958 1.179508 2.181770
O 3.165291 -1.223291 0.060114
O 0.317139 2.658518 0.280190
C 3.181059 -2.591320 -0.060676
O 3.815898 -3.210517 0.754368
C 0.259131 4.012609 0.056755
O -0.527005 4.657844 0.699908
C 1.199312 4.603624 -0.973632
H 2.244179 4.497039 -0.659771
H 1.094278 4.118556 -1.949914

H 0.966423 5.664132 -1.069142
C 2.457036 -3.227046 -1.227338
H 1.380356 -3.056268 -1.139077
H 2.801496 -2.821925 -2.185986
H 2.663960 -4.297170 -1.198749
H 2.767031 1.001453 1.661620

PBN-CH2OCONHMe-2.com.log

44

C -4.519845 -2.367881 -1.011054
C -3.233795 -2.099775 -0.545690
C -2.931637 -0.833538 -0.000999
C -3.953491 0.141092 0.053253
C -5.231494 -0.137434 -0.416451
C -5.521083 -1.396506 -0.950994
H -4.740791 -3.348020 -1.425883
H -2.454570 -2.847451 -0.590722
H -3.726338 1.122060 0.464171
H -6.003289 0.626035 -0.366208
H -6.520077 -1.616906 -1.317969
C -1.638991 -0.431516 0.522786
H -1.571559 0.560879 0.943442
N -0.537483 -1.149125 0.531019
O -0.436389 -2.346107 0.069261
C 0.757225 -0.633989 1.143127
C 0.764446 0.861356 1.479677
H 1.721135 1.074489 1.962365
H -0.043050 1.138425 2.158704
C 0.992959 -1.432269 2.434445
H 0.281533 -1.132980 3.211651
H 0.856301 -2.495643 2.225953
H 2.009283 -1.263531 2.799392
C 1.843442 -0.950295 0.091446
H 1.613104 -0.429280 -0.843690
H 1.855432 -2.029294 -0.080097
C 4.231101 -0.494353 -0.131216
O 5.227850 0.050350 0.292498
O 3.088638 -0.490354 0.624445
N 4.144618 -1.106536 -1.354418
H 3.384334 -1.747268 -1.528392
C 5.349767 -1.272870 -2.154626
H 5.987543 -2.087815 -1.787836
H 5.062870 -1.479880 -3.189101
H 5.925398 -0.346983 -2.118183
O 0.707577 1.676157 0.297310
C -0.245789 2.655584 0.250942
O -1.144146 2.787167 1.068988
N -0.045771 3.430985 -0.841979
H 0.764663 3.226758 -1.408667
C -0.907579 4.547770 -1.180803
H -0.355156 5.494474 -1.161868
H -1.350931 4.415384 -2.174382
H -1.705041 4.589311 -0.438109

PBN-CH2OMe-2.com.log

36

C -4.403161 -0.011797 -1.321827
C -3.029008 -0.007988 -1.088813
C -2.536962 0.002826 0.234237
C -3.468330 0.009559 1.296508
C -4.836434 0.005820 1.052855
C -5.311616 -0.004976 -0.261847
H -4.766718 -0.020287 -2.346161
H -2.322927 -0.013304 -1.907012
H -3.104784 0.017859 2.321918
H -5.533302 0.011208 1.886768
H -6.380880 -0.008091 -0.455929
C -1.132780 0.007680 0.601663
H -0.893894 0.014315 1.654293

N -0.102813 0.003526 -0.218419
O -0.189106 -0.006727 -1.499293
C 1.331047 0.009101 0.288201
C 1.922764 1.327072 -0.260884
H 1.850403 1.324180 -1.356263
H 1.312422 2.168499 0.114051
C 1.456871 -0.042317 1.809757
H 1.000183 0.833358 2.282756
H 1.013000 -0.953062 2.224675
H 2.519905 -0.043313 2.052406
C 1.968370 -1.248528 -0.356137
H 2.077844 -1.092740 -1.436869
H 1.280485 -2.100218 -0.212818
C 3.861796 -2.627760 -0.326156
H 4.070530 -2.465887 -1.395646
H 4.807680 -2.758670 0.205666
H 3.263361 -3.548409 -0.227025
O 3.212066 -1.516674 0.252431
O 3.259296 1.456332 0.168161
C 3.867512 2.633092 -0.319898
H 4.893783 2.643007 0.055819
H 3.887412 2.654405 -1.421141
H 3.346727 3.538314 0.033094

PBN-CH2POOMe2-2.com.log
50

C -5.675255 -0.422843 0.489005
C -4.302952 -0.414327 0.733280
C -3.409432 -0.917703 -0.236837
C -3.942642 -1.423274 -1.443316
C -5.312004 -1.421426 -1.679235
C -6.186797 -0.918997 -0.711348
H -6.351291 -0.036021 1.247086
H -3.904217 -0.034894 1.663452
H -3.266950 -1.816395 -2.199490
H -5.698630 -1.812125 -2.616558
H -7.258227 -0.916495 -0.892838
C -1.965539 -0.982719 -0.091787
N -1.249284 -0.490730 0.894163
O -1.742523 0.160946 1.886510
C 0.279242 -0.693611 1.004208
C 0.455561 -1.574788 2.254709
H 1.512974 -1.668296 2.503557
H -0.087141 -1.128674 3.089948
H 0.056093 -2.578418 2.071283
C 0.840095 -1.377792 -0.261200
H 0.424694 -2.387189 -0.352574
H 0.550475 -0.807083 -1.150388
C 0.888695 0.701568 1.278419
H 1.969294 0.592388 1.398231
H 0.473074 1.086408 2.211604
H -1.417227 -1.476734 -0.877752
P 0.645179 1.995867 0.003767
O 1.967901 2.883710 0.279535
O -0.496508 3.016866 0.521211
C -1.867217 2.893347 0.087241
H -2.367381 2.130870 0.688485
H -2.328110 3.869188 0.253582
H -1.910957 2.636337 -0.974298
C 2.116280 4.147584 -0.390475
H 2.009525 4.026342 -1.473175
H 1.374466 4.861853 -0.022378
H 3.121816 4.502228 -0.157670
O 0.437344 1.510236 -1.393388
P 2.634279 -1.628351 -0.523281
O 2.904780 -2.506868 -1.690236
O 3.342294 -0.171698 -0.599548
O 3.165534 -2.144757 0.914199
C 4.547071 -2.538087 1.034470
H 4.654790 -2.981275 2.025693

H	4.802330	-3.273021	0.266140
H	5.196638	-1.662198	0.945270
C	3.596018	0.442694	-1.884659
H	3.967229	-0.301793	-2.592616
H	2.678036	0.904856	-2.255497
H	4.354487	1.207286	-1.706641

PBN-CH2SMe-2.com.log

36

C	-4.928346	-1.148591	0.179404
C	-3.543416	-1.044077	0.296622
C	-2.888266	0.141474	-0.100303
C	-3.670751	1.200828	-0.611766
C	-5.050927	1.086058	-0.724962
C	-5.688089	-0.093398	-0.328404
H	-5.418065	-2.067884	0.489968
H	-2.953235	-1.859379	0.689604
H	-3.181372	2.121666	-0.922301
H	-5.630975	1.914909	-1.121806
H	-6.767291	-0.186853	-0.415058
C	-1.455903	0.370642	-0.027874
H	-1.098397	1.331623	-0.362802
N	-0.543614	-0.474414	0.405062
O	-0.804891	-1.650398	0.830345
C	0.971492	-0.117498	0.465709
C	1.628655	-1.191664	-0.435643
H	1.065333	-2.116279	-0.296220
H	1.553371	-0.881227	-1.484636
C	1.208174	1.316567	-0.047800
H	0.840450	1.413735	-1.074893
H	0.657484	2.017764	0.588263
C	1.342275	-0.256560	1.949108
H	1.103566	-1.261754	2.297530
H	0.774890	0.468312	2.543582
S	3.395879	-1.538673	-0.051045
S	2.972334	1.865293	-0.029555
C	3.709356	-2.719126	-1.407549
H	4.743833	-3.055975	-1.301673
H	3.045702	-3.586695	-1.338336
H	3.591797	-2.242207	-2.385727
C	2.658745	3.663373	-0.150644
H	2.099730	4.033833	0.714816
H	3.637719	4.149593	-0.171141
H	2.124410	3.918358	-1.071426
H	2.406076	-0.061558	2.098283

PBN-CONH2-2.com.log

30

C	-4.000896	-1.151149	0.537946
C	-2.627859	-0.946322	0.423048
C	-2.138986	0.255632	-0.133019
C	-3.069481	1.228505	-0.562319
C	-4.436882	1.013915	-0.443085
C	-4.908466	-0.180563	0.108891
H	-4.364919	-2.080164	0.968205
H	-1.923016	-1.694284	0.755649
H	-2.706677	2.159309	-0.992111
H	-5.134941	1.775363	-0.779202
H	-5.977234	-0.352118	0.203588
C	-0.739190	0.594199	-0.308966
H	-0.519544	1.556947	-0.744804
N	0.305120	-0.135876	0.001901
O	0.201147	-1.318875	0.547860
C	1.722352	0.360570	-0.218653
C	1.794208	1.671550	-1.002467
H	1.312931	1.571741	-1.980542
H	1.359736	2.502152	-0.442560
H	2.850047	1.889861	-1.156438
C	2.381974	0.589806	1.194894

N 2.358373 -0.491516 2.014902
H 2.667103 -0.338645 2.966192
H 1.666254 -1.211811 1.821619
O 2.900828 1.657805 1.468421
C 2.596828 -0.683139 -0.999619
O 3.731802 -0.356477 -1.309929
N 2.023353 -1.863513 -1.341874
H 2.644079 -2.547945 -1.754076
H 1.206424 -2.171709 -0.820768

PBN-COOMe-2.com.log

34

C -4.493178 -1.071575 0.063719
C -3.117268 -0.945503 0.245604
C -2.485226 0.294329 0.009663
C -3.278077 1.385745 -0.409451
C -4.649550 1.249003 -0.587280
C -5.264489 0.016022 -0.350642
H -4.967117 -2.031974 0.249269
H -2.516206 -1.784063 0.567759
H -2.802773 2.346149 -0.594882
H -5.240159 2.102164 -0.910151
H -6.336879 -0.094176 -0.488434
C -1.065674 0.553556 0.163249
H -0.693278 1.546824 -0.038701
N -0.156788 -0.317291 0.537087
O -0.373733 -1.545845 0.847968
C 1.307407 0.020369 0.719368
C 1.581505 0.111028 2.229741
H 2.656040 0.176590 2.409609
H 1.082149 0.990492 2.647035
H 1.195621 -0.793745 2.701699
C 3.786492 2.362126 -0.712226
H 3.358314 2.615287 -1.684864
H 3.671609 3.211271 -0.034294
H 4.835355 2.084454 -0.810923
C 1.815715 1.312610 0.051903
O 1.188607 2.323763 -0.177369
O 3.135332 1.196548 -0.169016
C 2.055335 -1.195062 0.113322
O 2.828589 -1.896886 0.715123
O 1.754040 -1.311511 -1.190284
C 2.336835 -2.445950 -1.854587
H 1.989912 -3.371143 -1.387871
H 1.995574 -2.385438 -2.888060
H 3.427689 -2.400396 -1.802462

PBN-NHCOMe-2b.com.log

36

C 4.171537 -1.571466 -0.563109
C 2.822492 -1.300614 -0.342076
C 2.425328 -0.030519 0.127505
C 3.422134 0.942062 0.360582
C 4.764827 0.661755 0.136744
C 5.146642 -0.600403 -0.327410
H 4.462616 -2.554351 -0.924489
H 2.064897 -2.050169 -0.524068
H 3.130432 1.926246 0.721351
H 5.514603 1.426062 0.323246
H 6.195589 -0.822869 -0.503923
C 1.053030 0.356702 0.395892
H 0.865172 1.358890 0.754876
N -0.017491 -0.391007 0.249111
O -0.045452 -1.593891 -0.157281
C -1.437004 0.150159 0.700197
N -1.450377 1.603217 0.644820
H -1.543449 2.081324 1.529925
C -1.521146 2.347037 -0.509957
O -1.510029 1.837871 -1.624279

C -1.609105 3.850686 -0.315151
H -1.539957 4.169551 0.729264
H -0.805677 4.323393 -0.887576
H -2.557613 4.203699 -0.732144
N -2.390349 -0.390812 -0.218048
H -2.253696 -0.011078 -1.150657
C -2.993789 -1.639885 -0.143566
O -3.147084 -2.274993 0.884922
C -3.493239 -2.132792 -1.491848
H -2.642445 -2.529984 -2.058176
H -4.217521 -2.932551 -1.331562
H -3.950185 -1.332357 -2.084233
C -1.609459 -0.292615 2.152066
H -0.879113 0.241418 2.770405
H -2.622641 -0.074769 2.498125
H -1.446466 -1.364761 2.232342

PBN-OCOMe-2.com.log

34

C -4.497023 -1.133544 0.062232
C -3.114936 -0.981963 0.151559
C -2.537828 0.299997 0.028244
C -3.387399 1.407345 -0.185982
C -4.764640 1.244405 -0.274496
C -5.325911 -0.029934 -0.150148
H -4.930268 -2.125468 0.159626
H -2.468195 -1.832644 0.315999
H -2.953096 2.399536 -0.283492
H -5.401437 2.109049 -0.440162
H -6.402616 -0.160059 -0.218742
C -1.116792 0.578575 0.108731
H -0.779797 1.599682 0.004529
N -0.162631 -0.303217 0.291517
O -0.298654 -1.571030 0.430838
C 1.312255 0.119820 0.398354
C 1.724739 -0.051269 1.855131
H 1.236878 0.739940 2.432282
H 1.397417 -1.025764 2.213211
H 2.805516 0.014602 1.973393
C 2.343778 -1.984729 -0.334377
O 2.847726 -2.357380 0.690040
O 1.960568 -0.661152 -0.573659
C 2.110635 -2.799795 -1.574495
H 1.029216 -2.922934 -1.694905
H 2.487889 -2.276260 -2.458325
H 2.590455 -3.773863 -1.472599
O 1.360500 1.453626 -0.037755
C 2.491016 2.218874 -0.291784
O 2.298179 3.323976 -0.721083
C 3.858325 1.655779 0.012003
H 4.048611 1.715114 1.089409
H 3.962418 0.615698 -0.297715
H 4.591542 2.280206 -0.500011

PBN-OCONHMe-2.com.log

38

C 4.615812 -1.483295 -0.569026
C 3.271601 -1.290464 -0.258151
C 2.806286 -0.003219 0.084339
C 3.725004 1.068746 0.100803
C 5.063678 0.865184 -0.212735
C 5.514703 -0.414612 -0.548616
H 4.964228 -2.478971 -0.830595
H 2.570199 -2.113001 -0.272998
H 3.372807 2.064643 0.357732
H 5.755823 1.702536 -0.196425
H 6.561061 -0.576442 -0.793656
C 1.434826 0.318684 0.431028
H 1.194382 1.340816 0.690881

N 0.419422 -0.507695 0.448016
O 0.452951 -1.770788 0.169579
C -0.988610 -0.026381 0.832317
C -1.426662 -0.778951 2.080681
H -1.248959 -1.847289 1.967066
H -0.846167 -0.403387 2.926484
H -2.486479 -0.584859 2.264711
C -1.170882 2.355135 0.188238
O -0.253434 3.101946 -0.075873
O -0.986901 1.334614 1.150550
N -2.449376 2.459727 -0.231604
H -3.046816 1.651613 -0.103777
C -2.810013 3.425772 -1.259036
H -2.586541 3.056047 -2.267963
H -3.879355 3.638240 -1.185374
H -2.246261 4.344652 -1.091792
O -1.753421 -0.239019 -0.319790
C -2.775112 -1.208192 -0.374837
O -3.937006 -0.856007 -0.324732
N -2.265123 -2.434095 -0.561937
H -1.244499 -2.488869 -0.510115
C -3.094428 -3.618501 -0.688762
H -4.138353 -3.303615 -0.727992
H -2.848474 -4.160771 -1.607943
H -2.955783 -4.292299 0.165105

PBN-OMe-2.com.log

30

C -3.798167 -1.076376 -0.120248
C -2.408815 -0.988606 -0.185354
C -1.772507 0.262618 -0.034538
C -2.576108 1.404107 0.181314
C -3.960795 1.305232 0.244814
C -4.579700 0.060604 0.094007
H -4.274674 -2.046177 -0.238601
H -1.798810 -1.865495 -0.351831
H -2.098399 2.374208 0.299188
H -4.559103 2.197048 0.411588
H -5.662384 -0.020086 0.143243
C -0.338552 0.474436 -0.084256
H 0.045982 1.475200 0.043226
N 0.578044 -0.450222 -0.271397
O 0.368829 -1.699781 -0.445499
C 2.073705 -0.086040 -0.321091
C 2.554870 -0.312994 -1.748000
H 3.645515 -0.259188 -1.788061
H 2.236707 -1.308714 -2.060050
H 2.123384 0.439000 -2.414535
C 2.324488 -1.074177 1.846793
H 1.374527 -1.616595 1.876431
H 3.092409 -1.650977 2.365759
H 2.217442 -0.093327 2.322809
O 2.780069 -0.953018 0.495511
O 2.153650 1.247461 0.117890
C 3.455648 1.828494 0.078083
H 3.765156 2.052364 -0.950186
H 3.385652 2.761614 0.640977
H 4.195499 1.171596 0.547449

PBN-POOMe2-2.com.log

44

C 5.022406 -1.147686 0.746288
C 3.661855 -0.983142 0.495404
C 3.228221 -0.005112 -0.425460
C 4.199636 0.790599 -1.072230
C 5.553778 0.620285 -0.811308
C 5.971924 -0.352792 0.101163
H 5.343041 -1.906439 1.455313
H 2.923992 -1.596246 0.993158

H 3.878455 1.548897 -1.782547
H 6.284039 1.244607 -1.318896
H 7.030354 -0.489121 0.306378
C 1.845110 0.250225 -0.775498
N 0.785291 -0.348544 -0.277153
O 0.798631 -1.245208 0.642040
C -0.601856 0.027227 -0.728176
C -0.678759 0.246123 -2.252540
H -0.139772 1.145603 -2.555907
H -0.270820 -0.628522 -2.766903
H -1.722083 0.363107 -2.552486
H 1.639914 1.024927 -1.500773
P -1.658698 -1.477832 -0.303488
O -3.049689 -0.885042 -0.903585
O -2.040028 -1.497683 1.257697
C -1.322992 -2.299989 2.216878
H -2.053611 -2.582788 2.978411
H -0.907635 -3.190637 1.741028
H -0.519906 -1.703854 2.650327
C -4.219484 -1.718027 -0.840726
H -4.556047 -1.819323 0.195456
H -4.989307 -1.217976 -1.431716
H -4.011572 -2.705009 -1.264665
O -1.213721 -2.749961 -0.923771
P -1.016993 1.637853 0.136307
O -0.397521 2.796227 -0.563183
O -0.540457 1.323383 1.632927
O -2.614700 1.749079 0.324629
C -3.441643 2.387053 -0.665317
H -2.901225 3.199251 -1.158410
H -3.767892 1.642382 -1.396236
H -4.308779 2.785278 -0.134614
C -0.573239 2.374292 2.618417
H -1.608928 2.608536 2.881357
H -0.045770 1.987426 3.491069
H -0.068000 3.268676 2.243055

PBN-SMe-2b.com.log

30

C -4.231874 0.975055 -0.193710
C -2.839664 1.004647 -0.248784
C -2.101949 -0.190375 -0.104176
C -2.809616 -1.397433 0.093895
C -4.197840 -1.415008 0.147197
C -4.917455 -0.224958 0.003322
H -4.786246 1.903099 -0.306540
H -2.306632 1.932340 -0.400905
H -2.254716 -2.326541 0.204060
H -4.720284 -2.355558 0.299958
H -6.003347 -0.235324 0.044253
C -0.655606 -0.287183 -0.140825
H -0.210320 -1.262059 0.003393
N 0.194328 0.704970 -0.329965
O -0.134221 1.924907 -0.487803
C 1.706950 0.455344 -0.299247
S 2.338953 0.759082 1.412994
C 1.480418 -0.502245 2.412035
H 0.412330 -0.288332 2.495186
H 1.636623 -1.502636 1.999509
H 1.932315 -0.450372 3.406526
S 2.027861 -1.265939 -0.956240
C 3.848228 -1.367613 -0.839650
H 4.094968 -2.421996 -0.990576
H 4.338711 -0.772989 -1.613888
H 4.187787 -1.054568 0.150605
C 2.372576 1.505750 -1.189928
H 1.995357 1.413259 -2.211316
H 2.148479 2.507579 -0.823603
H 3.454401 1.353885 -1.193313

PBN-alpha-3CH2OH.com.log

31

C	3.938198	-1.234266	0.335132
C	2.550390	-1.114497	0.289851
C	1.958903	0.095420	-0.133204
C	2.805871	1.164864	-0.500371
C	4.188685	1.035458	-0.449709
C	4.762637	-0.168619	-0.031062
H	4.379582	-2.172150	0.662690
H	1.907730	-1.935046	0.575986
H	2.362935	2.102781	-0.827240
H	4.820245	1.872146	-0.736470
H	5.843713	-0.273129	0.009457
C	0.531981	0.341252	-0.232518
H	0.199133	1.325007	-0.534254
N	-0.428723	-0.506155	0.065858
O	-0.250589	-1.691392	0.534579
C	-1.893960	-0.139173	-0.112058
C	-2.146848	1.165643	-0.902406
H	-3.234354	1.227011	-1.042361
H	-1.698416	1.070805	-1.898244
C	-2.501510	-1.313026	-0.916746
H	-1.987039	-1.368063	-1.888651
H	-2.306664	-2.242697	-0.375215
C	-2.529660	-0.112344	1.284851
O	-2.071766	1.051506	1.986710
H	-2.482059	1.060898	2.863877
H	-2.230288	-1.024852	1.812646
H	-3.619084	-0.097686	1.164010
O	-3.896124	-1.068476	-1.080691
H	-4.286859	-1.859378	-1.480531
O	-1.634706	2.360223	-0.337497
H	-1.830162	2.318280	0.617932

PBN-alpha-3COOH.com.log

28

C	4.287370	-1.267505	-0.049852
C	2.904586	-1.097705	-0.056093
C	2.355040	0.202334	-0.040325
C	3.233667	1.308220	-0.016759
C	4.611107	1.126719	-0.009784
C	5.144546	-0.165482	-0.026855
H	4.698570	-2.273385	-0.061921
H	2.236973	-1.947609	-0.071407
H	2.821239	2.314320	-0.004076
H	5.269878	1.990651	0.008706
H	6.221580	-0.310391	-0.021435
C	0.938817	0.508056	-0.045895
H	0.628160	1.542169	-0.020316
N	-0.038905	-0.367807	-0.088062
O	0.079183	-1.646110	-0.093306
C	-1.486572	0.037643	-0.017177
C	-2.208732	-1.114445	-0.782239
O	-2.149319	-1.239446	-1.976357
O	-2.926832	-1.891594	0.044068
H	-3.316026	-2.597071	-0.507087
C	-1.873065	0.094106	1.484857
O	-1.152709	-0.210497	2.396434
O	-3.126650	0.571458	1.624348
H	-3.319678	0.569003	2.581442
C	-1.849669	1.402568	-0.647136
O	-1.187677	2.411486	-0.556963
O	-3.045420	1.356983	-1.248231
H	-3.235533	2.261675	-1.563868

PBN-CH2CONH2-3.com.log

40

C -4.060021 -1.769440 -0.349524
C -2.710248 -1.431026 -0.273792
C -2.327162 -0.076697 -0.167032
C -3.338465 0.909318 -0.143493
C -4.681357 0.560940 -0.219230
C -5.048497 -0.784038 -0.321897
H -4.340957 -2.816010 -0.432474
H -1.942311 -2.190673 -0.299614
H -3.057119 1.956985 -0.066590
H -5.442475 1.336016 -0.199500
H -6.097825 -1.059856 -0.381943
C -0.959928 0.403730 -0.075608
H -0.826598 1.471856 -0.000190
N 0.133600 -0.319877 -0.065265
O 0.143045 -1.612851 -0.120160
C 1.528798 0.271812 0.086015
C 2.369176 -0.203323 -1.131884
H 3.328606 0.321336 -1.073176
H 1.873190 0.139042 -2.041588
C 1.537451 1.815048 0.177818
H 1.071654 2.121769 1.120007
H 2.593249 2.099970 0.273264
C 2.085591 -0.295571 1.426332
H 2.306610 -1.353915 1.301613
H 3.025909 0.215722 1.648046
C 1.135635 -0.061024 2.600528
O 1.116906 0.987615 3.239485
N 0.317226 -1.118400 2.876820
H -0.431333 -0.951577 3.537035
H 0.160713 -1.811584 2.151870
C 2.730248 -1.690327 -1.198521
O 3.589030 -2.180018 -0.476549
N 2.129974 -2.396006 -2.213342
H 2.268468 -3.398231 -2.150853
H 1.188715 -2.119516 -2.462944
C 0.981357 2.625862 -0.996822
O 0.965873 2.250961 -2.160339
N 0.483805 3.848266 -0.625525
H 0.253268 4.497377 -1.366405
H 0.641702 4.226170 0.297797

PBN-CH2COOMe-3.com.log

46

C 5.424098 -1.066015 -0.891654
C 4.049771 -0.834944 -0.880126
C 3.371042 -0.676243 0.347029
C 4.117919 -0.756120 1.543279
C 5.488063 -0.986533 1.520549
C 6.149116 -1.143367 0.298845
H 5.933429 -1.185427 -1.844399
H 3.486126 -0.771659 -1.799892
H 3.609408 -0.631967 2.496875
H 6.041729 -1.042673 2.453918
H 7.220712 -1.322906 0.277137
C 1.946118 -0.438274 0.489243
H 1.566376 -0.323701 1.492097
N 1.067397 -0.325335 -0.479972
O 1.349207 -0.413386 -1.728514
C -0.441922 -0.112851 -0.219122
C -1.060576 -1.395516 -0.829908
H -0.632514 -1.511177 -1.832738
H -0.724774 -2.265062 -0.255113
C -0.748437 0.008457 1.293755
H -0.520726 -0.936108 1.795016
H -0.135220 0.810592 1.707923
C -0.835583 1.144013 -1.017080
H -1.921535 1.246189 -1.023925
H -0.514280 1.002634 -2.052903
C -0.181934 4.765134 -0.893050
H -0.473826 5.005466 0.132595

H 0.908033 4.797208 -0.971127
H -0.638035 5.463528 -1.595251
O -0.677579 3.468748 -1.265261
C -0.229470 2.440866 -0.518156
O 0.555654 2.576531 0.398258
C -2.566892 -1.477139 -0.967465
O -3.358405 -0.556389 -0.995380
O -2.932499 -2.766643 -1.120985
C -4.333093 -2.992998 -1.352907
H -4.433237 -4.068793 -1.498082
H -4.921696 -2.666414 -0.491513
H -4.669032 -2.450642 -2.240357
C -2.187697 0.394544 1.596825
O -2.638301 1.513250 1.488854
O -2.899393 -0.664267 2.040712
C -4.288153 -0.392558 2.305377
H -4.789408 -0.096782 1.380722
H -4.699249 -1.326475 2.690296
H -4.387752 0.406023 3.044460

PBN-CH2NHCOMe-3.com.log

49

C -5.329566 0.559368 -1.059935
C -3.954004 0.417503 -0.890618
C -3.449643 -0.572514 -0.020240
C -4.367006 -1.402786 0.661249
C -5.736994 -1.252927 0.484834
C -6.224591 -0.267872 -0.378751
H -5.705164 1.324967 -1.733430
H -3.258419 1.053181 -1.419202
H -3.992690 -2.171278 1.333836
H -6.424789 -1.902530 1.018819
H -7.295339 -0.147938 -0.519263
C -2.043382 -0.818197 0.243505
H -1.809492 -1.614629 0.934718
N -1.013531 -0.184624 -0.265975
O -1.119102 0.788160 -1.120759
C 0.428329 -0.507555 0.094484
C 0.945179 0.584520 1.066840
H 2.039392 0.536579 1.076802
H 0.604410 0.338562 2.083704
C 0.560015 -1.883915 0.815916
H -0.034551 -1.884044 1.735902
H 0.209266 -2.688972 0.165051
C 1.203947 -0.580473 -1.255804
H 0.546604 -1.026124 -2.006892
H 2.058012 -1.240304 -1.123882
N 1.737686 0.664290 -1.755718
H 1.074131 1.337859 -2.109280
C 3.040807 1.019732 -1.543324
O 3.842936 0.287779 -0.967233
C 3.441830 2.387309 -2.070481
H 2.659103 2.877804 -2.657233
H 3.706530 3.028108 -1.223013
H 4.337143 2.276363 -2.688791
N 0.530067 1.937759 0.746269
H -0.183329 2.044645 0.031496
N 1.930479 -2.202631 1.158258
H 2.403247 -1.629530 1.843061
C 2.679322 -3.102522 0.430244
O 2.190683 -3.776410 -0.466691
C 0.921824 2.969420 1.546122
O 1.684449 2.808369 2.494456
C 0.357326 4.335048 1.180815
H -0.290404 4.321056 0.298704
H -0.210029 4.722869 2.032791
H 1.187782 5.025477 1.003476
C 4.150464 -3.139264 0.796980
H 4.583698 -4.075096 0.441155
H 4.650615 -2.300589 0.297010

H 4.316505 -3.042432 1.875437

PBN-CH2OCOCH3-3b.com.log

46

C -5.098522 -1.265289 0.800807
C -3.744004 -1.087668 0.526968
C -3.269777 0.173608 0.106049
C -4.193902 1.234625 -0.022521
C -5.542414 1.046072 0.254009
C -6.001085 -0.208432 0.666642
H -5.451033 -2.240643 1.125435
H -3.041070 -1.901023 0.636747
H -3.840042 2.212721 -0.339809
H -6.236086 1.875763 0.150298
H -7.055030 -0.358668 0.884413
C -1.889820 0.483640 -0.216439
H -1.654198 1.503321 -0.484614
N -0.869021 -0.345084 -0.176071
O -0.934471 -1.580696 0.193088
C 0.539169 0.079316 -0.524316
C 1.133308 -1.023470 -1.456084
H 1.862069 -0.562170 -2.128593
H 0.334988 -1.460683 -2.057111
C 0.642543 1.412771 -1.293067
H 0.013330 1.382293 -2.191176
H 1.680768 1.521072 -1.601981
C 1.293284 0.159331 0.819034
H 1.263921 -0.815477 1.299192
H 0.806200 0.902204 1.458312
O 1.858462 -2.005375 -0.727832
O 0.229143 2.525613 -0.501254
C 1.445128 -3.300472 -0.544673
O 1.989738 -3.929118 0.329740
C 1.019639 3.632725 -0.257887
O 0.550430 4.494841 0.437394
C 2.400851 3.688823 -0.872719
H 3.033238 2.873935 -0.504376
H 2.359624 3.626282 -1.966068
H 2.842377 4.644675 -0.590371
C 0.404228 -3.868340 -1.479504
H -0.562136 -3.394123 -1.284919
H 0.674581 -3.705390 -2.528772
H 0.331010 -4.939148 -1.287545
O 2.621879 0.600724 0.537146
C 3.756385 0.035492 1.074270
O 4.811017 0.499551 0.720068
C 3.602482 -1.099836 2.057789
H 2.941541 -0.829125 2.888385
H 3.191299 -1.990443 1.568387
H 4.593252 -1.331493 2.449714

PBN-CH2OCONHMe-3.com.log

52

C 4.330834 -0.263791 2.237438
C 3.038520 -0.251195 1.716006
C 2.829656 0.064332 0.356033
C 3.952122 0.366225 -0.446293
C 5.236066 0.351143 0.084719
C 5.431778 0.034497 1.432317
H 4.477869 -0.509446 3.286161
H 2.183339 -0.480091 2.335970
H 3.802867 0.616961 -1.493390
H 6.085286 0.586385 -0.551121
H 6.435143 0.021639 1.849849
C 1.537098 0.106557 -0.298991
H 1.520904 0.346898 -1.352478
N 0.363633 -0.101724 0.255645
O 0.175434 -0.393682 1.494099
C -0.897444 -0.041135 -0.595203

C -0.956982 1.246830 -1.435255
H -1.940494 1.299412 -1.908134
H -0.185951 1.273765 -2.206562
C -0.934293 -1.251357 -1.548375
H -0.120729 -1.208522 -2.275340
H -1.895592 -1.262647 -2.068309
C -2.079392 -0.091402 0.394257
H -2.022024 0.752061 1.085488
H -2.040976 -1.028553 0.952197
C -4.508784 0.065444 0.170810
O -5.480727 0.230126 -0.535201
O -3.267903 -0.017099 -0.404172
N -4.550258 -0.017906 1.536802
H -3.746036 -0.363311 2.038328
C -5.836552 -0.060573 2.216172
H -6.293562 -1.058514 2.185242
H -5.699243 0.237926 3.259064
H -6.513539 0.640252 1.726019
O -0.823251 2.397626 -0.597783
C 0.251893 3.216433 -0.846080
O 1.070751 3.033852 -1.729858
N 0.234677 4.252909 0.027752
H -0.472434 4.233788 0.748187
C 1.290913 5.246353 0.075868
H 0.865902 6.254972 0.112279
H 1.944154 5.103463 0.945817
H 1.887502 5.143120 -0.831197
O -0.837847 -2.469418 -0.809520
C 0.313058 -3.202533 -0.984861
O 1.191056 -2.928363 -1.781931
N 0.284196 -4.281278 -0.161877
H -0.451252 -4.304362 0.529635
C 1.417509 -5.178626 -0.032651
H 2.013781 -4.960209 0.862635
H 1.073987 -6.217108 0.013037
H 2.049262 -5.049435 -0.912175

PBN-CH2OMe-3.com.log

40

C 4.623456 -1.346461 0.497528
C 3.238215 -1.210290 0.425661
C 2.669649 -0.002644 -0.034114
C 3.537494 1.046557 -0.411017
C 4.917354 0.901022 -0.333519
C 5.468365 -0.300342 0.122165
H 5.046398 -2.282419 0.853566
H 2.580279 -2.016052 0.718887
H 3.113549 1.983066 -0.766521
H 5.564583 1.723005 -0.627889
H 6.547065 -0.417647 0.183999
C 1.247509 0.258356 -0.159151
H 0.934160 1.236238 -0.495013
N 0.270024 -0.568191 0.148074
O 0.427183 -1.746612 0.636724
C -1.190382 -0.187436 -0.031099
C -1.714312 0.057825 1.397662
H -1.465913 -0.820846 2.009794
H -1.202807 0.935729 1.819491
C -1.429220 1.031248 -0.930669
H -0.951494 0.877990 -1.912433
H -2.510361 1.094373 -1.089046
C -1.835814 -1.438296 -0.693322
H -1.990817 -2.211872 0.067799
H -1.134684 -1.846383 -1.438335
C -3.718838 -2.203866 -1.859331
H -3.971193 -2.943114 -1.083006
H -4.641526 -1.838498 -2.317429
H -3.108966 -2.704862 -2.628820
O -3.055452 -1.084123 -1.313562
O -3.109050 0.268991 1.345193

C -3.660785 0.519752 2.620279
H -4.735509 0.664094 2.482190
H -3.497699 -0.325652 3.307847
H -3.232258 1.425516 3.078843
O -0.952357 2.222165 -0.321709
C -1.368773 3.384245 -1.013164
H -0.968715 4.242216 -0.467062
H -0.984304 3.404191 -2.045075
H -2.466071 3.456879 -1.048935

PBN-CH2POOMe2-3c.com.log

61

C 5.017395 -2.393986 -0.532489
C 3.760607 -1.826149 -0.333403
C 3.229256 -0.933433 -1.288875
C 4.001423 -0.637965 -2.434894
C 5.254298 -1.209392 -2.622957
C 5.769220 -2.092805 -1.669861
H 5.412895 -3.080746 0.211329
H 3.176787 -2.056806 0.545964
H 3.604513 0.045061 -3.182873
H 5.828903 -0.968531 -3.513167
H 6.747841 -2.542293 -1.814716
C 1.937088 -0.281775 -1.189171
N 1.049382 -0.411234 -0.229036
O 1.197981 -1.151495 0.800927
C -0.272321 0.384981 -0.288082
C 0.058787 1.901721 -0.254267
H -0.885035 2.453643 -0.255073
H 0.558488 2.190109 -1.186236
C -0.953513 0.017094 -1.636544
H -0.348030 0.372042 -2.475577
H -0.997666 -1.075891 -1.706806
C -1.116045 -0.015975 0.937793
H -2.062164 0.527516 0.872104
H -0.619451 0.301448 1.853915
H 1.662053 0.392441 -1.989482
P -1.569339 -1.780375 1.153255
O -3.050738 -1.538356 1.778997
O -0.838422 -2.381817 2.463590
C 0.220224 -3.350971 2.381253
H 1.163949 -2.865174 2.635054
H -0.008238 -4.135284 3.108764
H 0.281356 -3.777719 1.378290
C -3.772040 -2.658202 2.310265
H -3.849099 -3.460399 1.568494
H -3.281513 -3.037356 3.211868
H -4.770949 -2.294047 2.559025
O -1.513592 -2.653657 -0.056974
P -2.645035 0.566139 -2.077486
O -2.918396 0.396742 -3.527701
O -3.696670 -0.174191 -1.096779
O -2.714014 2.074318 -1.492131
C -3.902670 2.855070 -1.734065
H -3.686226 3.862241 -1.375022
H -4.129434 2.879078 -2.803413
H -4.746531 2.433466 -1.180507
C -4.298738 -1.426977 -1.498212
H -3.598941 -2.244542 -1.308878
H -5.188042 -1.544977 -0.876588
H -4.577720 -1.390037 -2.553941
P 1.072172 2.695460 1.047888
O 1.324239 4.129545 0.748877
O 0.226174 2.365063 2.384274
O 2.414817 1.822923 1.288454
C 0.721753 2.829187 3.655128
H 0.919125 3.904425 3.618504
H -0.062177 2.620276 4.384490
H 1.633653 2.287499 3.922559
C 3.695280 2.277135 0.809679

H 3.917824 1.795543 -0.146850
H 3.703556 3.363758 0.697594
H 4.436573 1.967592 1.549507

PBN-CH2SMe-3.com.log

40

C -5.258421 -1.389800 -0.058811
C -3.876805 -1.207248 -0.075726
C -3.335410 0.093834 0.002121
C -4.225761 1.186816 0.096002
C -5.601625 0.993688 0.112618
C -6.125692 -0.299975 0.034800
H -5.660197 -2.397842 -0.119230
H -3.203782 -2.049513 -0.147423
H -3.824711 2.196330 0.156972
H -6.266291 1.850217 0.186129
H -7.201188 -0.454844 0.047497
C -1.918569 0.414184 -0.005988
H -1.655694 1.457540 0.068038
N -0.918027 -0.437205 -0.086523
O -1.065783 -1.704653 -0.155336
C 0.588245 0.016208 -0.006842
C 1.221557 -0.656561 -1.249348
H 0.648415 -1.566575 -1.433369
H 1.105514 0.018616 -2.104936
C 0.664825 1.554175 -0.071965
H 0.070804 1.894316 -0.926977
H 0.239344 1.987221 0.840610
C 0.987899 -0.569104 1.373528
H 0.870493 -1.651931 1.316925
H 0.262938 -0.194705 2.104089
S 2.678484 -0.199410 2.002750
C 3.197914 -1.888026 2.476041
H 3.251702 -2.530908 1.593225
H 4.196734 -1.793195 2.911150
H 2.527935 -2.319651 3.225256
S 2.992362 -1.164150 -1.156628
S 2.349907 2.269106 -0.307412
C 3.021762 -2.037981 -2.763830
H 4.030488 -2.441763 -2.885935
H 2.303721 -2.864370 -2.783691
H 2.815791 -1.354323 -3.593969
C 1.813620 4.008404 -0.476543
H 1.317994 4.368076 0.431163
H 2.719528 4.599227 -0.635983
H 1.149644 4.145317 -1.336905

PBN-CONH2-3.com.log

31

C 4.252056 -1.198973 0.262315
C 2.867809 -1.042645 0.262984
C 2.300625 0.210063 -0.056854
C 3.164339 1.283574 -0.369291
C 4.543442 1.115844 -0.367647
C 5.093677 -0.129820 -0.051418
H 4.677000 -2.167712 0.511061
H 2.212037 -1.865434 0.509560
H 2.739384 2.254430 -0.612964
H 5.190156 1.954259 -0.610880
H 6.172008 -0.264127 -0.048603
C 0.880826 0.496671 -0.100836
H 0.583593 1.507061 -0.339886
N -0.098235 -0.339778 0.154028
O 0.059824 -1.584203 0.475480
C -1.546899 0.052037 -0.029149
C -2.035181 -0.499665 -1.412759
N -1.449643 -1.646012 -1.794916
H -1.832995 -2.108233 -2.608095
H -0.878549 -2.158758 -1.125125

O -2.885367 0.081518 -2.087888
C -2.364244 -0.727897 1.080709
O -3.158565 -1.597622 0.773670
N -2.105098 -0.310882 2.338166
H -2.582186 -0.769425 3.100916
H -1.513965 0.494059 2.507937
C -1.756447 1.577156 0.234059
O -1.176907 2.107463 1.183056
N -2.629992 2.207902 -0.562527
H -2.840275 3.175323 -0.357734
H -3.057335 1.694639 -1.336669

PBN-COOMe-3.com.log

37

C -4.689173 -0.348383 1.161679
C -3.305093 -0.261775 1.026368
C -2.723671 -0.221893 -0.259581
C -3.574149 -0.271846 -1.386700
C -4.953086 -0.357711 -1.239546
C -5.517830 -0.396574 0.038891
H -5.124104 -0.378587 2.157280
H -2.659722 -0.224508 1.892684
H -3.137887 -0.244481 -2.382403
H -5.588817 -0.395602 -2.120019
H -6.596043 -0.464258 0.156933
C -1.302979 -0.128859 -0.528445
H -0.967381 -0.123274 -1.555252
N -0.343417 -0.092585 0.371752
O -0.497939 -0.096892 1.643571
C 1.095418 0.098120 -0.046562
C 3.463771 -1.530973 -2.375331
H 3.044357 -2.529987 -2.514581
H 3.282765 -0.928634 -3.268402
H 4.529009 -1.583752 -2.153568
C 1.546761 -0.717775 -1.282653
O 0.839172 -1.105867 -2.182516
O 2.868911 -0.895612 -1.226441
C 1.946622 -0.302844 1.188575
O 2.639846 0.465063 1.807232
C 1.346549 1.591728 -0.372963
O 2.005770 1.953303 -1.321536
O 1.847660 -1.619454 1.400426
O 0.742609 2.388481 0.502649
C 0.960095 3.799625 0.310816
H 0.603119 4.108879 -0.674661
H 0.390083 4.286264 1.101257
H 2.024424 4.028697 0.401762
C 2.533179 -2.103742 2.568922
H 2.116425 -1.635619 3.464003
H 2.359678 -3.179599 2.581395
H 3.601283 -1.882194 2.503415

PBN-NHCOMe-3.com.log

40

C 4.422759 1.641564 -0.067954
C 3.051535 1.398273 -0.020560
C 2.570149 0.071957 -0.001391
C 3.505907 -0.985105 -0.030328
C 4.871645 -0.731064 -0.078420
C 5.337364 0.586858 -0.097322
H 4.779433 2.668195 -0.082346
H 2.341388 2.213526 0.001108
H 3.147686 -2.012140 -0.017526
H 5.574242 -1.559854 -0.101495
H 6.404621 0.788149 -0.134642
C 1.166388 -0.292449 0.046167
H 0.909662 -1.344393 0.048473
N 0.141267 0.528052 0.057252

O 0.176894 1.795048 0.030691
C -1.354406 -0.128597 0.028224
N -1.424937 -1.189902 0.990568
H -1.256790 -2.112914 0.589328
C -1.468526 -0.998900 2.348378
O -1.579713 0.108943 2.868033
C -1.357564 -2.266977 3.172383
H -2.040660 -2.194925 4.021764
H -1.575086 -3.173077 2.599820
H -0.338762 -2.340772 3.570016
N -2.240304 0.942319 0.348924
H -2.158254 1.177471 1.338040
N -1.589727 -0.614043 -1.306107
H -1.916798 0.137711 -1.921288
C -2.547685 1.969781 -0.524312
O -2.516362 1.853479 -1.747623
C -1.302636 -1.853773 -1.796038
O -0.870623 -2.784979 -1.107415
C -2.983272 3.247830 0.155399
H -2.086952 3.775619 0.500614
H -3.514793 3.874018 -0.562301
H -3.619928 3.052090 1.024577
C -1.542703 -2.018967 -3.283221
H -2.173720 -1.233488 -3.707525
H -0.575228 -2.006814 -3.798062
H -1.999449 -2.995919 -3.458528

PBN-OCOMe-3.com.log

37

C 4.623746 0.314585 -1.412938
C 3.241393 0.334233 -1.241376
C 2.675669 -0.136765 -0.036696
C 3.537025 -0.617598 0.974514
C 4.914238 -0.629214 0.792963
C 5.464074 -0.162895 -0.405077
H 5.048284 0.678923 -2.344589
H 2.586872 0.706815 -2.016997
H 3.112065 -0.979853 1.907725
H 5.560106 -1.000670 1.583726
H 6.541036 -0.171273 -0.549689
C 1.256767 -0.176645 0.245977
H 0.936023 -0.530039 1.214533
N 0.297677 0.250371 -0.548730
O 0.426555 0.817574 -1.682044
C -1.163504 0.146822 -0.111186
C -1.102816 2.366873 0.878068
O -0.209222 2.108468 1.635409
O -1.678102 1.443416 0.011129
C -1.778323 3.698643 0.691871
H -1.614203 4.053423 -0.330950
H -2.858703 3.603376 0.840785
H -1.364772 4.412128 1.404906
O -1.787896 -0.482265 -1.174303
C -3.166559 -0.700847 -1.284314
O -3.498659 -1.556170 -2.058155
C -4.121500 0.141883 -0.477895
H -3.878668 0.125758 0.587359
H -4.073946 1.181694 -0.812198
H -5.123981 -0.255088 -0.641045
O -1.349232 -0.506734 1.104810
C -1.293076 -1.901459 1.332750
O -1.521068 -2.240186 2.458636
C -0.971513 -2.842464 0.197834
H -0.732210 -3.808005 0.645788
H -1.835163 -2.960295 -0.463602
H -0.139214 -2.493227 -0.415475

PBN-OCONHMe-3.com.log

43

C 5.107449 -0.909592 -0.329146
C 3.721883 -0.803868 -0.426499
C 3.001564 -0.075997 0.544998
C 3.713669 0.533606 1.601297
C 5.095726 0.419248 1.689669
C 5.799298 -0.304750 0.722487
H 5.652235 -1.470278 -1.084096
H 3.181358 -1.266930 -1.240252
H 3.167691 1.096694 2.354501
H 5.625790 0.893638 2.511005
H 6.880237 -0.395058 0.789014
C 1.564641 0.102039 0.540957
H 1.113636 0.705085 1.319869
N 0.710037 -0.410880 -0.312353
O 0.987497 -1.172139 -1.304522
C -0.781665 -0.020521 -0.094887
C -0.652488 2.036547 -1.375618
O -0.123524 1.537413 -2.338187
O -0.939865 1.360369 -0.181638
N -1.055847 3.319842 -1.217144
H -1.468802 3.573454 -0.331138
C -0.857465 4.324608 -2.245528
H -1.812793 4.765686 -2.551235
H -0.192068 5.122729 -1.896371
H -0.401434 3.833840 -3.106233
O -1.566667 -0.626640 -1.047656
C -2.053935 -1.937633 -0.821237
O -3.158593 -2.103677 -0.329257
N -1.207254 -2.856662 -1.285151
H -0.289428 -2.488208 -1.554418
C -1.472733 -4.281606 -1.201911
H -2.501750 -4.424885 -0.869762
H -1.342140 -4.748296 -2.183672
H -0.795179 -4.764335 -0.488027
O -1.066804 -0.406607 1.199685
C -2.020125 0.360888 1.955862
O -1.628006 1.178324 2.754582
N -3.274223 -0.024314 1.681099
H -3.409995 -0.764764 0.989078
C -4.419057 0.543414 2.372452
H -5.159012 0.902235 1.649164
H -4.894904 -0.200276 3.022547
H -4.075294 1.379110 2.983430

PBN-OMe-3.com.log

31

C -3.932628 -1.149724 0.147727
C -2.546700 -1.005125 0.133639
C -1.971868 0.273142 -0.036044
C -2.832084 1.383057 -0.188974
C -4.212894 1.227451 -0.174106
C -4.770719 -0.043378 -0.004844
H -4.361832 -2.139712 0.279136
H -1.892622 -1.857985 0.250367
H -2.401655 2.373223 -0.320605
H -4.855775 2.095417 -0.294157
H -5.850256 -0.168185 0.007274
C -0.547664 0.543100 -0.063180
H -0.211102 1.560633 -0.197767
N 0.417156 -0.340505 0.063336
O 0.274339 -1.604411 0.225997
C 1.895817 0.099442 -0.079456
C 2.321410 -0.612662 2.164121
H 1.409254 -1.192301 2.327252
H 3.157404 -1.075736 2.691398
H 2.190299 0.416580 2.514478
O 2.678658 -0.640872 0.777067
O 1.919282 1.457775 0.186822
C 3.169115 2.106424 -0.086339
H 3.335608 2.191761 -1.163189

H 3.086697 3.098580 0.361120
H 3.998240 1.559272 0.372841
O 2.310484 -0.112792 -1.372882
C 2.491786 -1.470262 -1.812033
H 1.543349 -2.011388 -1.797150
H 2.870539 -1.386140 -2.832581
H 3.218231 -1.986870 -1.180873

PBN-POOMe2-3.com.log

52

C -5.226961 1.569857 -0.373077
C -3.856494 1.329243 -0.305452
C -3.382097 0.031462 -0.017330
C -4.323502 -0.999637 0.197345
C -5.688181 -0.748322 0.127552
C -6.146409 0.541074 -0.158438
H -5.579607 2.573210 -0.596955
H -3.141690 2.121926 -0.474003
H -3.969280 -2.003904 0.416301
H -6.395438 -1.556086 0.294622
H -7.213226 0.740760 -0.213942
C -1.987357 -0.348401 0.075301
N -0.948835 0.435811 -0.101169
O -1.006591 1.693555 -0.392674
C 0.461918 -0.069891 -0.005646
H -1.749554 -1.378040 0.302296
P 1.494838 1.345595 -0.749449
O 2.914494 0.751964 -0.243255
O 1.509604 2.698427 0.127294
C 0.693591 3.840047 -0.200896
H 1.289880 4.718665 0.057510
H 0.451469 3.848632 -1.265313
H -0.222379 3.804999 0.388766
C 4.127691 1.372433 -0.694640
H 4.201560 2.394394 -0.309593
H 4.946632 0.769595 -0.298493
H 4.166437 1.384683 -1.787792
O 1.357902 1.515591 -2.219078
P 0.949943 -0.467001 1.780788
O 2.218021 -1.229450 1.903781
O -0.350701 -1.172869 2.403156
O 0.886465 0.966377 2.496359
C 2.047905 1.566214 3.107776
H 2.856561 0.838035 3.199170
H 2.361321 2.405919 2.485787
H 1.742311 1.915870 4.096484
C -0.295630 -2.551550 2.847858
H 0.579176 -2.712151 3.481425
H -1.210090 -2.705605 3.423117
H -0.262517 -3.212018 1.980822
P 0.623987 -1.656605 -1.044852
O 0.077268 -2.798369 -0.265238
O -0.176793 -1.330035 -2.380143
O 2.136946 -1.785002 -1.544104
C 0.392051 -1.066096 -3.686311
H 1.088881 -1.861442 -3.959338
H -0.457304 -1.061073 -4.370852
H 0.887118 -0.095428 -3.674439
C 3.121322 -2.559542 -0.813179
H 3.951873 -2.701114 -1.506529
H 3.430761 -2.008811 0.074487
H 2.697416 -3.524383 -0.526619

PBN-SMe-3.com.log

31

C -4.398099 -1.113063 -0.335502
C -3.010728 -1.002672 -0.267883
C -2.413145 0.254830 -0.033757
C -3.253083 1.379329 0.130147

C	-4.635429	1.257074	0.063264
C	-5.215598	0.006758	-0.170929
H	-4.844469	-2.087180	-0.517588
H	-2.376021	-1.868485	-0.392841
H	-2.805665	2.354078	0.310028
H	-5.261864	2.135478	0.192770
H	-6.296524	-0.091869	-0.223963
C	-0.986570	0.497142	0.046915
H	-0.650681	1.505850	0.247419
N	-0.029222	-0.401175	-0.066883
O	-0.211180	-1.652997	-0.221880
C	1.454166	0.064327	0.075973
S	2.601229	-1.253800	-0.449114
C	2.093207	-1.586137	-2.173234
H	1.111804	-2.060310	-2.182542
H	2.086078	-0.662972	-2.758154
H	2.848509	-2.265413	-2.578833
S	1.615469	1.630621	-0.916665
C	3.379474	2.051284	-0.684099
H	3.561016	2.900917	-1.348701
H	3.590142	2.343898	0.345995
H	4.013411	1.211656	-0.975361
S	1.788605	0.445698	1.850359
C	1.441049	-1.165593	2.659244
H	1.310884	-0.938961	3.721063
H	0.522370	-1.600475	2.260704
H	2.268719	-1.863991	2.529088

PBN-alpha-carbamate-O2.log

35

C	4.319737	0.699207	-0.890415
C	2.931449	0.772818	-0.789331
C	2.212567	-0.221950	-0.113180
C	2.908739	-1.290691	0.456753
C	4.300337	-1.364679	0.356180
C	5.011600	-0.371205	-0.316668
H	4.864290	1.482491	-1.413725
H	2.399790	1.613513	-1.224390
H	2.342190	-2.058564	0.971581
H	4.828123	-2.203650	0.805140
H	6.095430	-0.427825	-0.394731
C	0.691906	-0.208373	-0.073506
H	0.284284	-0.464631	-1.050655
N	0.172137	1.126991	0.277221
O	0.855797	1.918549	1.022317
C	-1.309331	1.408091	0.136881
C	-1.940441	1.293081	1.531344
H	-2.998622	1.556439	1.482310
H	-1.840777	0.266612	1.891729
H	-1.410644	1.965577	2.211578
C	-1.468699	2.815724	-0.447188
H	-0.988874	3.565067	0.188860
H	-1.018793	2.850290	-1.445114
H	-2.538507	3.023600	-0.540409
C	-3.018016	-0.220097	-0.535584
O	-4.054498	0.456181	-0.519765
O	-1.768541	0.461110	-0.795492
N	-2.804214	-1.510659	-0.388902
H	-1.314846	-2.012862	-0.084732
C	-4.012978	-2.289966	-0.203535
H	-4.694053	-2.232471	-1.070026
H	-3.742535	-3.344008	-0.057034
H	-4.603828	-1.965002	0.670112
O	0.167255	-1.161776	0.847835
O	-0.324926	-2.306646	0.091451

PBN-alpha-carboxyl-O2.log

33

C	-3.405909	-1.261526	1.142248
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C	-2.141906	-0.929168	0.658799
C	-2.018550	-0.024954	-0.405058
C	-3.160483	0.535799	-0.974689
C	-4.427855	0.202235	-0.488401
C	-4.551962	-0.698074	0.570248
H	-3.500777	-1.963030	1.968452
H	-1.231720	-1.349606	1.080054
H	-3.056975	1.239981	-1.797065
H	-5.315050	0.646096	-0.935623
H	-5.537567	-0.959970	0.950487
C	-0.624859	0.289397	-0.913610
H	-0.660821	0.917317	-1.821749
N	0.097498	1.094304	0.116953
O	-0.479188	2.211611	0.388756
C	1.575260	0.986898	0.351872
C	2.282812	1.954629	-0.612123
H	3.354153	1.979202	-0.395673
H	2.152871	1.622423	-1.645193
H	1.864569	2.961692	-0.496036
C	1.836227	1.371399	1.811638
H	1.443103	2.369223	2.027612
H	1.363883	0.633758	2.464488
H	2.915972	1.356546	1.995775
C	3.920239	-1.829234	-0.111585
H	3.608241	-2.329988	0.812363
H	3.620481	-2.461974	-0.961119
H	5.011333	-1.707024	-0.127442
C	1.942073	-0.522887	0.136926
O	1.515133	-1.348662	0.978346
O	3.358896	-0.537843	-0.197228
O	-0.039029	-0.953504	-1.174690
O	1.386100	-0.754335	-1.362133

PBN-alpha-CH2CONH2-O2.log

34

C	-3.789790	-1.492506	-0.701010
C	-2.545109	-1.425026	-0.070541
C	-2.003192	-0.190618	0.311041
C	-2.740485	0.975032	0.056587
C	-3.985345	0.904856	-0.569705
C	-4.517182	-0.328748	-0.952782
H	-4.190815	-2.460539	-0.995362
H	-1.975072	-2.324168	0.131987
H	-2.322389	1.931205	0.352656
H	-4.542428	1.820389	-0.759720
H	-5.488147	-0.381245	-1.441536
C	-0.652833	-0.142506	1.038845
N	0.140322	1.074023	0.548079
O	-0.201259	2.168594	1.137392
C	1.476286	1.092499	-0.148972
C	1.524073	2.386659	-0.982837
H	2.491068	2.434991	-1.496158
H	0.730907	2.390456	-1.740153
H	1.400826	3.266863	-0.348632
C	2.552323	1.153229	0.954709
H	2.408935	2.071186	1.534721
H	2.430646	0.288565	1.611988
H	3.554131	1.159801	0.511021
C	1.630017	-0.125665	-1.125713
H	0.783391	-0.799564	-1.005506
H	1.635294	0.248582	-2.153250
C	2.924955	-0.933326	-0.965219
O	3.905849	-0.720216	-1.690569
N	2.876410	-1.887291	-0.007464
H	3.769966	-2.328200	0.179613
H	2.147611	-1.832340	0.783491
H	-0.793761	0.095971	2.102488
O	-0.044073	-1.359196	0.898710
O	1.039535	-1.480728	1.889669

PBN-alpha-CH2OH-O2.com.log

31

C	3.573530	-1.405916	0.377869
C	2.215303	-1.110196	0.485659
C	1.728866	0.160749	0.151166
C	2.633723	1.128060	-0.295491
C	3.994084	0.831534	-0.412845
C	4.471871	-0.435045	-0.074248
H	3.932133	-2.399626	0.640673
H	1.517157	-1.873160	0.817753
H	2.245153	2.109360	-0.543451
H	4.683034	1.596300	-0.767336
H	5.532038	-0.665912	-0.161259
C	0.264734	0.532933	0.367219
N	-0.600538	-0.593233	-0.154769
O	-0.246505	-1.120961	-1.281949
C	-2.067462	-0.649950	0.157611
C	-2.549437	-2.086915	-0.078208
H	-3.642130	-2.110763	-0.012120
H	-2.239208	-2.431957	-1.067075
H	-2.135002	-2.771326	0.673908
C	-2.324938	-0.223624	1.609735
H	-1.764432	-0.854944	2.312196
H	-2.033999	0.828222	1.728298
H	-3.392291	-0.345847	1.830422
C	-2.769385	0.335452	-0.815083
O	-4.192132	0.394585	-0.589170
H	-4.309951	1.083504	0.082060
H	-2.623310	-0.019784	-1.840443
H	-2.313234	1.324522	-0.665493
H	0.064884	0.601882	1.444115
O	-0.015289	1.752544	-0.208357
O	-1.088876	2.426290	0.550831

PBN-alpha-CONH2-O2.log

31

C	-4.056753	-0.502590	0.370308
C	-2.791542	-1.088505	0.461995
C	-1.656369	-0.407014	0.018116
C	-1.797915	0.879924	-0.520181
C	-3.060753	1.463420	-0.615382
C	-4.194705	0.775744	-0.171444
H	-4.932047	-1.044005	0.724205
H	-2.681306	-2.084342	0.885034
H	-0.912239	1.417975	-0.849027
H	-3.161119	2.462400	-1.034877
H	-5.178118	1.236457	-0.243606
C	-0.284121	-1.061895	0.076327
N	0.602033	-0.232880	0.989334
O	0.322801	-0.370398	2.236063
C	1.942586	0.359016	0.647343
C	2.131545	1.589091	1.549593
H	3.135373	2.001481	1.395174
H	1.403011	2.359887	1.291873
H	2.013062	1.301185	2.595951
C	3.014321	-0.703009	0.961374
H	2.969588	-0.941568	2.030479
H	2.808810	-1.604704	0.380243
H	4.014077	-0.327098	0.717464
C	1.973346	0.859286	-0.836557
N	2.599473	0.036163	-1.717799
H	2.469809	0.395787	-2.661540
H	2.246888	-0.999716	-1.605442
O	1.527852	1.980760	-1.114105
H	-0.334164	-2.039938	0.572855
O	0.163549	-1.187695	-1.215522
O	1.287047	-2.139866	-1.249997

PBN-alpha-COOH-O2.com.log

C	-3.262017	-1.818860	0.383536
C	-2.004215	-1.223122	0.467734
C	-1.829385	0.125036	0.126770
C	-2.936782	0.861007	-0.303866
C	-4.196014	0.262468	-0.396473
C	-4.365698	-1.078625	-0.050354
H	-3.380547	-2.867418	0.650562
H	-1.143383	-1.804883	0.783999
H	-2.786120	1.903950	-0.559308
H	-5.047390	0.848994	-0.737468
H	-5.346879	-1.545068	-0.118274
C	-0.487151	0.822076	0.320930
H	-0.303489	0.963893	1.394301
N	0.604169	-0.099623	-0.168787
O	0.411228	-0.749484	-1.269770
C	2.042560	0.165272	0.127669
C	2.584472	1.190634	-0.879552
H	3.661415	1.340288	-0.735783
H	2.408834	0.839299	-1.900004
H	2.038130	2.127798	-0.687111
C	2.234965	0.680938	1.563724
H	1.728042	1.654327	1.618050
H	1.825419	-0.025284	2.293793
H	3.306327	0.806950	1.766001
C	2.691392	-1.226732	0.033772
O	2.398706	-2.183056	0.722002
O	3.712803	-1.303104	-0.862060
H	4.020747	-2.226386	-0.792980
O	-0.474676	2.052600	-0.291704
O	0.446559	2.948089	0.431832

PBN-alpha-ester-O2.log

33

C	-3.004012	-2.083886	0.370806
C	-1.862992	-1.286751	0.454861
C	-1.922758	0.075479	0.130136
C	-3.141387	0.621861	-0.280490
C	-4.282687	-0.179041	-0.372384
C	-4.220430	-1.534190	-0.044957
H	-2.942865	-3.140312	0.626028
H	-0.913072	-1.716614	0.760868
H	-3.171601	1.679069	-0.519394
H	-5.224283	0.259903	-0.697927
H	-5.110108	-2.157923	-0.111912
C	-0.706968	0.974668	0.317653
H	-0.485851	1.070992	1.388297
N	0.490877	0.283308	-0.293697
O	0.344897	-0.287185	-1.440043
C	1.868265	0.749448	0.011661
C	2.244753	1.877694	-0.942211
H	3.293156	2.165779	-0.795268
H	2.098578	1.541431	-1.972622
H	1.568799	2.714431	-0.697688
C	2.041266	1.162097	1.468769
H	1.424821	2.058569	1.614215
H	1.741581	0.360996	2.148180
H	3.098046	1.399156	1.640865
C	2.594251	-1.591618	0.169688
O	1.845591	-1.912436	1.070909
O	2.773514	-0.360643	-0.329629
C	3.477877	-2.576748	-0.575428
H	3.049111	-2.745194	-1.569811
H	4.485520	-2.173165	-0.713752
H	3.516005	-3.522555	-0.031387
O	-0.928097	2.224569	-0.208516
O	-0.082786	3.206722	0.499600

PBN-alpha-ether-O2.log

31

C	3.405276	-1.487216	0.238688
C	2.055768	-1.166867	0.380914
C	1.602706	0.142651	0.172509
C	2.532643	1.123729	-0.183703
C	3.884081	0.803507	-0.336412
C	4.328329	-0.501968	-0.123237
H	3.737349	-2.510808	0.403239
H	1.339581	-1.940921	0.641555
H	2.169585	2.134270	-0.333447
H	4.592509	1.580111	-0.619495
H	5.381569	-0.751779	-0.237544
C	0.149078	0.535880	0.432148
H	-0.044342	0.511903	1.511369
N	-0.745474	-0.517334	-0.187502
O	-0.415746	-0.967399	-1.350852
C	-2.169256	-0.761588	0.217629
C	-2.394767	-2.278776	0.203354
H	-3.454338	-2.490642	0.381698
H	-2.105134	-2.673449	-0.772810
H	-1.798661	-2.766555	0.983014
C	-2.462766	-0.147794	1.590671
H	-1.895075	-0.656839	2.380978
H	-2.193978	0.921406	1.582741
H	-3.531253	-0.280925	1.795622
C	-2.824804	1.058189	-1.254276
H	-2.056001	1.024095	-2.036739
H	-3.774321	1.387092	-1.695200
H	-2.485634	1.753307	-0.468667
O	-3.073944	-0.266120	-0.759318
O	-0.095702	1.811120	-0.024044
O	-1.077268	2.480225	0.855025

PBN-alpha-methylcarbamate-O2.log

38

C	-4.836961	0.583626	0.304302
C	-3.458994	0.728493	0.455961
C	-2.590192	-0.324219	0.138509
C	-3.130100	-1.523725	-0.332690
C	-4.510929	-1.668022	-0.491764
C	-5.370589	-0.617012	-0.172908
H	-5.496760	1.412601	0.552746
H	-3.048226	1.669127	0.810054
H	-2.448226	-2.333064	-0.567892
H	-4.913947	-2.607850	-0.864037
H	-6.446169	-0.729020	-0.294268
C	-1.090881	-0.221231	0.399116
H	-0.906007	-0.273254	1.476198
N	-0.594427	1.121201	-0.068818
O	-1.099720	1.582931	-1.165756
C	0.814226	1.548607	0.223010
C	0.883196	3.077918	0.101760
H	1.931182	3.392653	0.153164
H	0.453725	3.404840	-0.847881
H	0.332995	3.560957	0.918630
C	1.237457	1.116817	1.631756
H	0.564921	1.559185	2.378443
H	1.222735	0.025601	1.720583
H	2.249267	1.485700	1.824609
C	1.690035	0.889250	-0.885222
H	1.556069	1.460725	-1.810326
H	1.349816	-0.127484	-1.063910
C	3.805784	-0.210195	-0.294966
O	5.026078	-0.107189	-0.245819
O	3.086176	0.936360	-0.577697
N	3.112644	-1.356978	-0.117129
H	2.070185	-1.421948	0.137983
C	3.871085	-2.554383	0.182351

H	4.471102	-2.455058	1.098695
H	3.153838	-3.370249	0.311214
H	4.562307	-2.805682	-0.632176
O	-0.406692	-1.280793	-0.194395
O	0.623515	-1.775420	0.739232

PBN-alpha-methylcarboxy-O2.log
36

C	4.444587	1.119202	-0.007778
C	3.168738	0.887808	-0.522674
C	2.505506	-0.321553	-0.268351
C	3.148311	-1.292950	0.508097
C	4.423431	-1.057846	1.027866
C	5.078681	0.147746	0.771379
H	4.945726	2.063008	-0.215118
H	2.668460	1.640618	-1.124463
H	2.630014	-2.226637	0.694636
H	4.906436	-1.821396	1.635004
H	6.073531	0.329711	1.173546
C	1.129126	-0.601091	-0.875317
H	1.204284	-0.728340	-1.964338
N	0.268305	0.656960	-0.770859
O	0.338963	1.452578	-1.781414
C	-0.878029	0.817752	0.189003
C	-0.445923	0.335001	1.585795
H	-1.257506	0.515660	2.293694
H	-0.210964	-0.729258	1.574243
H	0.444116	0.888215	1.910360
C	-1.217891	2.315327	0.252335
H	-0.365038	2.894132	0.627342
H	-1.479136	2.700239	-0.735324
H	-2.062540	2.455110	0.935262
C	-2.053009	0.003713	-0.409889
H	-1.654085	-1.059149	-0.604320
H	-2.262984	0.380868	-1.417172
C	-5.628446	-0.501852	0.192168
H	-5.937633	0.425813	0.686918
H	-6.345698	-0.768328	-0.588465
H	-5.584906	-1.292816	0.948707
O	-4.376387	-0.346680	-0.467061
C	-3.322358	-0.023515	0.359296
O	-3.508982	0.154325	1.553741
O	0.590367	-1.718473	-0.301529
O	-0.507281	-2.195826	-1.159497

PBN-alpha-methylester-O2.log
36

C	-3.666103	-2.242814	0.658497
C	-2.547627	-1.411406	0.693732
C	-2.596665	-0.119049	0.154922
C	-3.790923	0.322755	-0.420850
C	-4.910858	-0.511473	-0.465345
C	-4.855799	-1.796438	0.076026
H	-3.608833	-3.243964	1.082030
H	-1.619323	-1.767055	1.132319
H	-3.818763	1.329080	-0.823285
H	-5.831605	-0.152287	-0.921498
H	-5.729392	-2.444912	0.046427
C	-1.415014	0.836045	0.286045
N	-0.159021	0.104393	-0.137438
O	-0.245099	-0.658363	-1.183605
C	1.195156	0.710667	0.096747
C	1.473333	1.777092	-0.976352
H	2.503570	2.142620	-0.887390
H	1.331957	1.341595	-1.972263
H	0.758414	2.598993	-0.813919
C	1.269490	1.328535	1.497907
H	0.583270	2.183786	1.525414
H	0.997153	0.597089	2.271893

H 2.293676 1.664103 1.691023
C 2.155135 -0.487436 -0.030500
H 2.076930 -0.909062 -1.032375
H 1.889662 -1.257240 0.705755
C 4.565566 -0.840356 0.027794
O 5.681005 -0.438294 0.284473
O 3.506137 -0.034039 0.227103
C 4.310060 -2.235091 -0.522115
H 3.610493 -2.794727 0.107872
H 3.870639 -2.187813 -1.524586
H 5.264640 -2.760593 -0.568840
H -1.274873 1.102726 1.341003
O -1.631118 1.990760 -0.428881
O -0.973297 3.120028 0.243840

PBN-alpha-methylether-O2.log
34

C 3.505392 -2.062382 -0.145933
C 2.213041 -1.527104 -0.135734
C 2.026340 -0.140837 -0.119203
C 3.148324 0.702558 -0.122282
C 4.434405 0.164290 -0.140528
C 4.619495 -1.222223 -0.148784
H 3.639063 -3.143154 -0.144194
H 1.349732 -2.181071 -0.106434
H 2.964644 1.774912 -0.137775
H 5.297811 0.827680 -0.146846
H 5.623871 -1.642800 -0.156714
C 0.683980 0.572621 -0.190336
N -0.471121 -0.258545 0.214159
O -0.333324 -1.084678 1.212895
C -1.845328 0.338584 0.071796
C -2.226827 1.076400 1.368331
H -3.289510 1.342757 1.353660
H -2.032485 0.423601 2.224981
H -1.615345 1.975463 1.464350
C -1.915973 1.290086 -1.130726
H -1.210457 2.125944 -1.012869
H -1.685129 0.759636 -2.064995
H -2.939011 1.673033 -1.212872
C -2.763492 -0.881308 -0.143648
H -2.660593 -1.568486 0.706926
H -2.449570 -1.418523 -1.055435
C -4.998777 -1.534473 -0.438232
H -4.968879 -2.226718 0.421623
H -6.011047 -1.124555 -0.525048
H -4.776537 -2.121265 -1.347540
O -4.117238 -0.456127 -0.277846
H 0.521580 0.871391 -1.229181
O 0.693171 1.754046 0.562794
O 0.789418 2.887348 -0.357727

PBN-alpha-methylphosphoryl-O2.log
41

C -4.792271 1.375256 -0.737729
C -3.522505 1.383521 -0.155439
C -2.974861 0.208913 0.373114
C -3.727428 -0.973147 0.318076
C -4.998028 -0.978610 -0.257905
C -5.536536 0.195680 -0.790725
H -5.200828 2.295611 -1.150857
H -2.935433 2.293444 -0.103041
H -3.302722 -1.883489 0.730485
H -5.569584 -1.904196 -0.292007
H -6.526818 0.190044 -1.241916
C -1.603688 0.229875 1.052040
N -0.841975 -1.040895 0.682980
O -0.978431 -2.023453 1.503634
C 0.293655 -1.074962 -0.301642

C 0.530873 -2.539843 -0.695473
H 1.406064 -2.586301 -1.350554
H 0.703111 -3.155296 0.189779
H -0.338903 -2.945540 -1.226322
C -0.092399 -0.273106 -1.558168
H -1.037685 -0.653430 -1.962344
H -0.207802 0.787276 -1.337943
H 0.682642 -0.401741 -2.320610
C 1.532561 -0.498472 0.443473
H 1.903382 -1.266313 1.135838
H 1.183674 0.366026 1.068539
H -1.708181 0.123795 2.139992
O -0.955077 1.397528 0.751868
O 0.082873 1.636624 1.775614
P 2.941881 0.035446 -0.559216
O 4.110606 0.349989 0.561233
O 2.651674 1.523815 -1.096667
C 2.331804 2.626079 -0.208105
H 2.027479 3.446413 -0.864274
H 1.515514 2.372463 0.491398
H 3.234222 2.917512 0.340924
C 4.903894 -0.733738 1.033416
H 5.736002 -0.300943 1.597088
H 4.328025 -1.387523 1.702799
H 5.293587 -1.328433 0.200175
O 3.402035 -0.873189 -1.649352

PBN-alpha-methylthio-O2.log

34

C 3.668188 -2.202018 -0.128849
C 2.412904 -1.585377 -0.117170
C 2.315114 -0.189920 -0.123283
C 3.488089 0.579828 -0.151669
C 4.737325 -0.039421 -0.171259
C 4.833418 -1.434614 -0.155849
H 3.733077 -3.288833 -0.108920
H 1.509968 -2.182264 -0.068837
H 3.374702 1.661100 -0.184231
H 5.640896 0.567449 -0.196948
H 5.808742 -1.918593 -0.164215
C 1.018521 0.604211 -0.195460
N -0.177027 -0.149051 0.245421
O -0.070287 -0.954005 1.263506
C -1.525808 0.517803 0.102956
C -1.838611 1.282452 1.402703
H -2.859320 1.681779 1.389432
H -1.732795 0.608050 2.257428
H -1.123951 2.101247 1.507215
C -1.541668 1.473131 -1.098993
H -0.768800 2.251460 -0.996232
H -1.375541 0.927318 -2.037582
H -2.527921 1.948035 -1.166993
C -2.485757 -0.680401 -0.106107
H -2.363685 -1.368773 0.733830
H -2.203276 -1.202421 -1.028039
S -4.266504 -0.217289 -0.236017
C -4.964218 -1.901709 -0.343207
H -4.720368 -2.488977 0.548622
H -6.051681 -1.804974 -0.416100
H -4.598015 -2.430422 -1.230195
H 0.859414 0.887037 -1.239251
O 1.111598 1.799979 0.528459
O 1.233291 2.907523 -0.419907

PBN-alpha-phosphoryl-O2.log

38

C 3.437707 -1.844027 -0.902703
C 2.294254 -1.225538 -0.397566
C 2.384383 0.043198 0.191584

C	3.629133	0.675410	0.256565
C	4.774550	0.055598	-0.249167
C	4.682021	-1.209697	-0.829381
H	3.357501	-2.828522	-1.359942
H	1.322100	-1.703861	-0.466159
H	3.697781	1.663764	0.704546
H	5.736393	0.561707	-0.189473
H	5.571290	-1.698215	-1.223818
C	1.157890	0.721408	0.786827
N	0.355020	1.346453	-0.331285
O	0.957319	2.267430	-0.991956
C	-1.147305	1.313862	-0.347945
C	-1.706690	2.084436	0.864753
H	-2.801709	2.029906	0.876943
H	-1.290627	1.664684	1.797504
H	-1.412119	3.137718	0.764152
C	-1.581198	1.972770	-1.671201
H	-1.154398	2.976618	-1.710418
H	-1.218088	1.417698	-2.541582
H	-2.669431	2.026571	-1.715937
H	1.460800	1.544813	1.443095
P	-1.758045	-0.470447	-0.325099
O	-3.131387	-0.251287	-1.215799
O	-2.492066	-0.830012	1.064543
C	-1.902436	-1.642955	2.109475
H	-1.288988	-2.432049	1.665559
H	-1.292353	-0.989687	2.749235
H	-2.751896	-2.088832	2.639330
C	-3.950815	-1.395096	-1.434555
H	-3.366152	-2.221384	-1.855462
H	-4.419085	-1.724471	-0.499491
H	-4.728042	-1.100547	-2.146934
O	-0.877371	-1.526361	-0.907642
O	0.383215	-0.153605	1.511361
O	-0.001762	0.506260	2.790020

PBN-alpha-thio-O2.log

31

C	3.247976	-1.740882	0.344540
C	1.937480	-1.253248	0.410435
C	1.656040	0.062015	0.027848
C	2.704065	0.886948	-0.414019
C	4.005405	0.394563	-0.484831
C	4.284378	-0.923849	-0.105758
H	3.456578	-2.763428	0.655541
H	1.141267	-1.878225	0.798105
H	2.442671	1.902948	-0.706447
H	4.809397	1.040608	-0.833718
H	5.302183	-1.307197	-0.157932
C	0.279044	0.707802	-0.013459
H	-0.039467	0.772742	-1.058430
N	-0.772497	-0.037032	0.696141
O	-0.530525	-0.569605	1.855705
C	-2.177640	0.174531	0.296000
C	-3.103419	-0.387264	1.375491
H	-4.141605	-0.228740	1.067829
H	-2.936566	-1.452247	1.551745
H	-2.919409	0.130885	2.321391
C	-2.501082	1.650744	0.006925
H	-2.541121	2.185854	0.962395
H	-1.736092	2.156958	-0.600927
H	-3.485397	1.722383	-0.474497
S	-2.501948	-0.732340	-1.348828
C	-1.879588	-2.407614	-0.973261
H	-0.850128	-2.357992	-0.609764
H	-2.502226	-2.927911	-0.238613
H	-1.898188	-2.969102	-1.912353
O	0.329675	2.024129	0.472260
O	0.278450	2.916307	-0.687407

PBN-CH2NHCOMe-O2c.out

37

C	4.594037	-1.198652	0.379106
C	3.227774	-0.982273	0.552529
C	2.629375	0.208554	0.120204
C	3.429333	1.178304	-0.490151
C	4.797318	0.960495	-0.673079
C	5.387314	-0.226776	-0.237650
H	5.041256	-2.130543	0.720720
H	2.609981	-1.746757	1.015746
H	2.954708	2.099068	-0.810403
H	5.404419	1.724933	-1.154877
H	6.453770	-0.395325	-0.375558
C	1.158105	0.499081	0.398062
N	0.346092	-0.706711	-0.014747
O	0.678578	-1.267502	-1.134496
C	-1.112101	-0.803752	0.333571
C	-1.501712	-2.280875	0.160550
H	-2.559909	-2.421466	0.406207
H	-0.908352	-2.907603	0.837098
C	-1.356567	-0.345167	1.776689
H	-0.771484	-0.948588	2.484945
H	-1.092035	0.715540	1.858296
C	-1.873485	0.124286	-0.666673
H	-1.395259	0.005639	-1.643912
H	-1.738148	1.164350	-0.328491
N	-3.289478	-0.205826	-0.838821
H	-3.499499	-0.975970	-1.457195
C	-4.345706	0.366323	-0.198510
O	-4.266501	1.262379	0.633097
C	-5.714742	-0.196068	-0.602286
H	-6.325294	0.622038	-0.998475
H	-5.674945	-0.998309	-1.348089
H	-6.218523	-0.572263	0.294187
H	-2.418539	-0.460171	2.020794
H	1.006670	0.627098	1.476768
O	0.750374	1.650764	-0.237410
O	-0.270745	2.327384	0.579397
H	-1.312415	-2.618987	-0.861652

PBN-NHCOMe-O2c.out

34

C	3.673399	0.744442	1.471075
C	2.325805	0.618873	1.138465
C	1.925940	-0.201682	0.074949
C	2.902529	-0.891945	-0.647439
C	4.254774	-0.760385	-0.320040
C	4.646621	0.055969	0.740815
H	3.966216	1.386305	2.299672
H	1.574582	1.167726	1.698190
H	2.580210	-1.531934	-1.460982
H	5.002751	-1.302726	-0.895401
H	5.699049	0.155945	0.999337
C	0.451375	-0.422414	-0.233204
N	-0.254975	0.915320	-0.289543
O	0.402672	1.944030	-0.697145
C	-1.757069	0.947565	-0.542755
N	-2.320400	-0.307887	-0.089943
H	-1.873635	-1.132840	-0.658028
C	-2.801737	-0.607698	1.145496
O	-3.067299	0.177100	2.061997
C	-3.054543	-2.111184	1.307109
H	-4.040059	-2.371889	0.900129
H	-2.298524	-2.692060	0.767293
H	-3.046959	-2.358606	2.371993
C	-1.964855	1.021238	-2.070168
H	-1.651130	0.079678	-2.528043
H	-3.025789	1.191955	-2.288432
H	-1.371865	1.844493	-2.478850

H	-0.008694	-0.982747	0.587516
C	-2.310165	2.204155	0.137734
H	-1.817836	3.079300	-0.294880
H	-3.389155	2.269158	-0.037172
H	-2.145159	2.174764	1.213673
O	0.292520	-1.153268	-1.405333
O	-0.862746	-2.069132	-1.303500

PBN-O2.log

30

C	3.210144	-1.470961	0.484365
C	1.860591	-1.126078	0.544523
C	1.426541	0.147539	0.152868
C	2.375435	1.067252	-0.302607
C	3.727400	0.721270	-0.372801
C	4.152798	-0.547546	0.022941
H	3.527521	-2.465860	0.792271
H	1.127689	-1.852338	0.884338
H	2.026568	2.051576	-0.594036
H	4.451348	1.449323	-0.735053
H	5.206463	-0.816453	-0.026752
C	-0.029032	0.575890	0.318890
H	-0.255123	0.676633	1.388285
N	-0.916644	-0.531088	-0.203857
O	-0.545501	-1.101069	-1.304407
C	-2.401009	-0.520632	0.047684
C	-2.688769	-0.058830	1.483552
H	-3.768286	-0.128577	1.673926
H	-2.176397	-0.694954	2.219052
H	-2.364507	0.984904	1.586209
C	-3.057686	0.452128	-0.951294
H	-2.698171	1.467105	-0.721225
H	-2.782748	0.169414	-1.973769
H	-4.152610	0.409322	-0.856284
C	-2.895177	-1.960426	-0.165636
H	-2.429958	-2.646060	0.555062
H	-3.982572	-2.002739	-0.025870
H	-2.648368	-2.304847	-1.172278
O	-0.252580	1.790989	-0.287995
O	-1.295888	2.528022	0.449679

PBN-alpha-2CH2OH-O2.com.log

32

C	-3.530630	-1.681280	0.662271
C	-2.230411	-1.178010	0.646967
C	-1.965584	0.111835	0.169037
C	-3.031864	0.888324	-0.293233
C	-4.334401	0.383559	-0.286987
C	-4.591366	-0.901604	0.192958
H	-3.716852	-2.685983	1.037493
H	-1.404992	-1.792282	0.997006
H	-2.815560	1.889561	-0.648105
H	-5.152359	1.000425	-0.654866
H	-5.606804	-1.293224	0.203273
C	-0.562486	0.704358	0.245606
H	-0.267496	0.813045	1.297891
N	0.405496	-0.292490	-0.362634
O	0.036847	-0.843191	-1.475558
C	1.888281	-0.168576	-0.169828
C	2.442518	0.886817	-1.142294
H	3.523040	1.022120	-0.997248
H	2.237988	0.590722	-2.178188
H	1.934336	1.839057	-0.898866
C	2.194689	0.236428	1.292505
H	1.809870	1.249374	1.446041
H	1.668259	-0.462388	1.970472
C	2.441327	-1.583130	-0.470498
O	3.880658	-1.659272	-0.391289

H 4.214463 -0.987593 -1.008691
H 2.094575 -1.902732 -1.456990
H 2.073504 -2.299031 0.273133
O 3.592190 0.255190 1.580457
H 3.963534 -0.549371 1.173713
O -0.521627 1.935955 -0.356654
O 0.547630 2.739244 0.255962

PBN-alpha-2COOH-O2.com.log

30

C 3.981634 1.481488 0.161452
C 2.636608 1.177133 0.365958
C 2.172961 -0.134502 0.202727
C 3.077411 -1.132195 -0.173961
C 4.424047 -0.824932 -0.384018
C 4.882462 0.481451 -0.214552
H 4.325996 2.505817 0.287320
H 1.934627 1.959262 0.634945
H 2.712333 -2.144703 -0.304948
H 5.114492 -1.611367 -0.681858
H 5.931172 0.721428 -0.377678
C 0.735497 -0.497018 0.523099
H 0.612682 -0.570974 1.613024
N -0.216514 0.544308 0.071169
O 0.021645 1.127474 -1.056023
C -1.642225 0.267892 0.389096
C -1.887580 0.268554 1.911018
H -1.439761 -0.615982 2.363740
H -1.486675 1.182490 2.361883
H -2.963786 0.221817 2.097273
C -2.419609 1.476973 -0.162317
O -2.249479 2.616285 0.228951
O -3.399206 1.182147 -1.040760
H -3.803644 2.048933 -1.236449
O 0.418967 -1.738397 -0.049015
O -0.891581 -2.088716 0.484645
C -1.995546 -1.123409 -0.301480
O -1.946207 -1.214222 -1.537147
O -3.162271 -1.634083 0.368551
H -3.550751 -2.159402 -0.351174

PBN-CH2CONH2-2-O2b.out

38

C 4.048327 -1.061268 1.339010
C 2.696516 -0.759101 1.161704
C 2.268671 -0.060271 0.027810
C 3.212021 0.344653 -0.925152
C 4.563045 0.044597 -0.742553
C 4.987186 -0.660744 0.386516
H 4.366137 -1.616762 2.219361
H 1.969146 -1.088197 1.897857
H 2.852234 0.926036 -1.769543
H 5.290107 0.365378 -1.486346
H 6.040939 -0.896208 0.524165
C 0.816370 0.353029 -0.188638
N -0.132607 -0.651448 0.321006
O 0.136972 -1.895452 0.106535
C -1.503800 -0.254712 0.816993
C -1.343723 0.157899 2.294138
H -2.286418 0.550089 2.683287
H -0.600943 0.952619 2.404367
C -2.138262 0.875333 -0.059959
H -1.855287 0.701806 -1.099010
H -3.223372 0.757131 0.024659
C -2.429971 -1.502512 0.769251
H -1.889607 -2.353466 1.192413
H -3.296076 -1.282694 1.398016
C -3.002207 -1.878282 -0.602234
O -4.188060 -1.707107 -0.876192

N -2.116119 -2.443799 -1.469499
H -2.412510 -2.525537 -2.432248
H -1.122775 -2.389619 -1.253688
C -1.868776 2.331087 0.351414
O -2.419996 2.801467 1.357440
N -1.070481 3.040041 -0.474591
H -0.880810 3.977515 -0.135084
H -0.332291 2.604122 -1.150629
H 0.627382 1.284191 0.357156
O 0.494819 0.554845 -1.544641
O 0.873862 1.939818 -1.877060
H -1.024557 -0.706770 2.888386

PBN-CH2COOMe-2-O2.com.log

- 42

C -4.415128 0.264843 1.412287
C -3.065976 0.014366 1.167472
C -2.674593 -0.844101 0.131408
C -3.661370 -1.445978 -0.653486
C -5.014066 -1.189441 -0.414642
C -5.397712 -0.335765 0.619792
H -4.701205 0.935390 2.220366
H -2.305466 0.498367 1.773314
H -3.345340 -2.116953 -1.444237
H -5.769794 -1.663450 -1.038142
H -6.451132 -0.138989 0.809521
C -1.210914 -1.212951 -0.078328
N -0.380140 0.060448 -0.075231
O -0.914511 1.115328 -0.593811
C 1.121529 0.001991 -0.196042
C 1.593832 -1.198552 0.660731
H 1.113857 -1.163335 1.644441
H 1.185799 -2.101153 0.109921
C 1.479386 -0.162123 -1.685125
H 1.191318 -1.173571 -1.990965
H 0.936391 0.583574 -2.269476
H 2.551169 -0.018758 -1.840798
C 1.670322 1.320510 0.420319
H 2.760701 1.285354 0.323964
H 1.414403 1.351093 1.483656
C -0.098583 4.532235 0.045756
H 0.676074 5.191968 -0.358469
H -0.786338 4.257118 -0.759453
H -0.640795 5.030433 0.852681
O 0.471205 3.359507 0.625529
C 1.214936 2.608174 -0.233364
O 1.539374 3.004226 -1.333942
C 3.050413 -1.390903 0.941970
O 3.504585 -1.821722 1.988057
O 3.867937 -1.103871 -0.114749
C 5.252736 -1.374248 0.101199
H 5.756904 -1.086400 -0.823688
H 5.642095 -0.794327 0.944214
H 5.415718 -2.436591 0.308365
H -0.865423 -1.814187 0.771013
O -1.040612 -1.950702 -1.228780
O 0.048669 -2.924899 -1.045966

PBN-CH2NHCOMe-2-O2.com.log

44

C -4.785395 1.621041 0.203745
C -3.470778 1.177383 0.363830
C -3.133362 -0.147883 0.065256
C -4.130254 -1.018648 -0.394268
C -5.443396 -0.573085 -0.551325
C -5.776797 0.749997 -0.252974
H -5.033453 2.656694 0.428899
H -2.691740 1.859227 0.680959
H -3.856306 -2.046217 -0.614202

H -6.207296 -1.260873 -0.908772
H -6.799531 1.100493 -0.378787
C -1.752803 -0.735617 0.305398
N -0.698251 0.252627 0.384387
O -0.734215 1.205340 -0.576252
C 0.683545 -0.199562 0.750248
C 1.392337 1.038866 1.369706
H 2.397897 0.776438 1.704291
H 0.808546 1.350358 2.244933
C 0.647919 -1.305067 1.813841
H 0.128503 -0.968598 2.720816
H 0.155106 -2.202912 1.427500
C 1.432093 -0.702918 -0.522924
H 1.139497 -0.047116 -1.349204
H 1.113455 -1.719630 -0.753553
N 2.884861 -0.709920 -0.380353
H 3.353513 0.181568 -0.238357
C 3.655036 -1.831156 -0.393048
O 3.231022 -2.974700 -0.539392
C 5.151958 -1.564211 -0.218891
H 5.676782 -1.886376 -1.125237
H 5.391195 -0.514558 -0.021419
H 5.523494 -2.180607 0.606281
N 1.490876 2.166267 0.450183
H 0.603705 2.254682 -0.078185
C 2.655711 2.571466 -0.096636
O 3.773958 2.130229 0.218234
C 2.529797 3.661728 -1.153232
H 1.492361 3.925198 -1.377320
H 3.060379 4.555654 -0.806702
H 3.024278 3.324871 -2.070109
H 1.674927 -1.572169 2.087146
H -1.775134 -1.304368 1.236788
O -1.441919 -1.704617 -0.713033
O -1.435878 -2.993574 -0.180511

PBN-CH2OCOMe-2-O2.com.log

42

C -3.298892 -3.021864 -0.284675
C -2.216401 -2.280032 0.191175
C -2.217665 -0.879757 0.069987
C -3.320775 -0.259438 -0.529783
C -4.400470 -1.003557 -1.011610
C -4.391448 -2.393362 -0.889081
H -3.288868 -4.105733 -0.183041
H -1.362500 -2.743104 0.662263
H -3.338041 0.826045 -0.618494
H -5.245064 -0.497858 -1.476294
H -5.229039 -2.982146 -1.259470
C -1.091217 -0.007958 0.590872
N 0.176246 -0.292909 -0.097769
O 0.600789 -1.543316 0.165113
C 1.306050 0.680825 0.075145
C 2.435734 0.141611 -0.865298
H 2.999972 0.988548 -1.278600
H 1.972719 -0.400186 -1.689384
C 0.932815 2.042147 -0.549917
H 0.433986 1.860058 -1.510310
H 1.848035 2.620326 -0.723233
C 1.812715 0.812640 1.520091
H 1.799434 -0.184420 1.965672
H 1.148879 1.454539 2.099574
O 3.431623 -0.643392 -0.204327
O 0.073550 2.826176 0.303566
C 3.629238 -1.970181 -0.430594
O 4.486369 -2.529417 0.217981
C -0.387886 4.035492 -0.089793
O -1.060607 4.692353 0.671964
C -0.043386 4.513116 -1.492195
H 1.039761 4.568443 -1.645915

H -0.445500 3.833293 -2.251447
H -0.480033 5.503356 -1.625886
C 2.811652 -2.661182 -1.499269
H 1.748570 -2.571177 -1.240145
H 2.977516 -2.209910 -2.485781
H 3.122894 -3.706561 -1.530696
H 2.834473 1.211536 1.549975
H -1.345784 1.040536 0.419758
O -0.921893 -0.067466 2.008223
O -0.583022 -1.353217 2.421918

PBN-CH2OMe-2-O2.com.log

38

C -4.105151 1.741576 0.121173
C -2.807243 1.282399 0.340827
C -2.482087 -0.067243 0.150963
C -3.485466 -0.946661 -0.264970
C -4.784952 -0.487485 -0.494347
C -5.102532 0.857335 -0.300115
H -4.338712 2.793906 0.273125
H -2.030203 1.975510 0.650890
H -3.222147 -1.990010 -0.397343
H -5.552709 -1.186075 -0.822343
H -6.115651 1.215299 -0.473905
C -1.094942 -0.603814 0.491425
N -0.063076 0.312886 -0.123730
O -0.299707 0.751116 -1.321101
C 1.388987 0.200297 0.231663
C 2.013249 1.536560 -0.236930
H 2.125815 1.537654 -1.329075
H 1.329487 2.361660 0.024943
C 1.567121 -0.003334 1.739857
H 1.103849 0.815404 2.306874
H 1.111347 -0.962572 2.010466
H 2.634917 -0.020636 1.968203
C 1.932345 -1.017866 -0.544180
H 1.689607 -0.888204 -1.611763
H 1.424781 -1.912338 -0.140476
C 3.837561 -2.350947 -0.825365
H 3.670621 -2.498808 -1.908727
H 4.917950 -2.370286 -0.636499
H 3.364356 -3.194697 -0.297484
O 3.352281 -1.112410 -0.378691
O 3.273678 1.750150 0.386654
C 3.905631 2.904148 -0.092205
H 4.860039 3.001374 0.436895
H 4.106916 2.849145 -1.176833
H 3.306411 3.815792 0.089666
H -0.941794 -0.560168 1.576598
O -0.960767 -1.914409 0.088655
O -0.077795 -2.629690 1.026499

PBN-CH2OCONHMe-2-O2.com.log

C -4.416431 -0.968010 -0.097044
C -3.053711 -1.050742 -0.367910
C -2.261624 0.119580 -0.406224
C -2.889169 1.362053 -0.148878
C -4.249852 1.427615 0.134018
C -5.026098 0.265822 0.156143
H -5.011881 -1.879356 -0.082119
H -2.570142 -1.998021 -0.566352
H -2.284672 2.261735 -0.138956
H -4.707719 2.393399 0.338266
H -6.092279 0.320382 0.367349
C -0.843788 0.158740 -0.705531
N -0.077140 -0.879876 -1.026224
O -0.451089 -2.167065 -0.904355
C 1.338031 -0.738100 -1.433763
C 1.589389 -1.561456 -2.692326

H 1.246030 -2.579466 -2.515007
H 1.035451 -1.122855 -3.526423
H 2.659134 -1.545017 -2.914890
C 1.839876 1.713119 -0.973894
O 1.355710 2.765933 -1.347665
O 1.653113 0.592712 -1.793860
N 2.627848 1.560976 0.107335
H 2.919716 0.637340 0.413726
C 2.647196 2.615371 1.113207
H 1.652871 2.756877 1.551001
H 3.346434 2.313807 1.896923
H 2.983487 3.557082 0.668613
O 2.253114 -1.243013 -0.450402
C 2.064175 -1.391255 0.929503
O 2.921242 -0.906798 1.661077
N 1.025437 -2.143589 1.302057
H 0.325801 -2.360433 0.555781
C 0.624969 -2.140483 2.699665
H -0.209060 -2.837863 2.818472
H 1.455251 -2.463647 3.335995
H 0.305686 -1.136727 3.003630
H -0.428872 1.129824 -0.921442
O -0.243860 0.775687 1.471382
O -0.717734 1.922148 1.837755

PBN-CH2POOMe-2-O2.com.log

52

C 5.490950 -0.114113 -0.089437
C 4.236516 -0.597787 -0.465044
C 3.241620 -0.798051 0.507147
C 3.536445 -0.495300 1.842539
C 4.788438 0.000403 2.214814
C 5.773307 0.191002 1.245195
H 6.256441 0.031087 -0.849736
H 3.995438 -0.850882 -1.487058
H 2.773342 -0.645752 2.604474
H 4.991687 0.232936 3.258411
H 6.752760 0.574261 1.526359
C 1.869748 -1.357986 0.178852
N 1.052768 -0.391410 -0.578248
O 1.642322 -0.037434 -1.722801
C -0.416451 -0.720975 -0.804590
C -0.581612 -1.784813 -1.909489
H -1.546878 -1.685366 -2.416084
H 0.239349 -1.655145 -2.618823
H -0.504437 -2.792080 -1.495522
C -1.030984 -1.179716 0.542314
H -0.637004 -2.171104 0.788840
H -0.726482 -0.488841 1.338184
C -1.013882 0.611466 -1.319710
H -2.092559 0.524150 -1.472450
H -0.534856 0.829288 -2.277391
H 1.357907 -1.567401 1.122239
P -0.755737 2.087981 -0.275286
O -1.958998 3.021984 -0.876548
O 0.502124 2.947761 -0.819389
C 1.848281 2.713306 -0.347169
H 2.271870 1.867192 -0.892333
H 2.400020 3.636060 -0.549281
H 1.847207 2.512002 0.727437
C -2.074995 4.361457 -0.396762
H -2.088620 4.387241 0.699022
H -1.245962 4.977416 -0.762129
H -3.020449 4.754986 -0.780770
O -0.792213 1.927389 1.211951
P -2.821663 -1.370212 0.792816
O -3.176609 -2.043350 2.075311
O -3.565148 0.069756 0.604107
O -3.332943 -2.120657 -0.553628
C -4.704879 -2.520148 -0.625677

H -4.805719 -3.128887 -1.527304
H -4.984096 -3.110046 0.253470
H -5.356768 -1.642461 -0.699527
C -3.814945 0.892281 1.760683
H -4.170657 0.278500 2.593105
H -2.901347 1.426464 2.033157
H -4.589187 1.605631 1.465014
O 1.882278 -2.618574 -0.477450
O 2.514847 -2.538384 -1.728867

PBN-CH2SMe-2-O2.com.log

38

C -4.447492 -1.708168 -0.797347
C -3.133370 -1.244590 -0.803501
C -2.797131 -0.038605 -0.173506
C -3.804343 0.694681 0.457199
C -5.121864 0.228346 0.470580
C -5.449991 -0.973525 -0.156451
H -4.690856 -2.648312 -1.288884
H -2.355718 -1.827336 -1.288691
H -3.530567 1.634673 0.923432
H -5.894250 0.811196 0.968957
H -6.476185 -1.336006 -0.150327
C -1.388846 0.542623 -0.261922
H -1.182155 0.805832 -1.304708
N -0.384237 -0.518538 0.143006
O -0.777271 -1.445612 0.951776
C 1.103407 -0.190466 0.214896
C 1.771285 -1.561114 -0.054900
H 1.383951 -2.276042 0.674523
H 1.477051 -1.901570 -1.055414
C 1.435533 0.848497 -0.881465
H 1.487729 0.353221 -1.858101
H 0.655706 1.637057 -0.905710
C 1.386274 0.312419 1.640939
H 1.004980 -0.423260 2.355464
H 0.865857 1.258801 1.799866
S 3.613855 -1.590586 0.041059
S 3.014548 1.784118 -0.700478
C 3.808525 -3.407065 -0.051090
H 4.879518 -3.625518 0.002419
H 3.303689 -3.905397 0.784062
H 3.416837 -3.806880 -0.993316
C 2.422798 3.246799 0.253106
H 1.322610 3.288280 0.183325
H 2.728489 3.172993 1.301772
H 2.864715 4.147129 -0.186142
H 2.458788 0.447493 1.802118
O -1.244845 1.696702 0.491260
O -0.702096 2.777398 -0.362312

PBN-CONH2-2-O2b.out

32

C 3.637410 -1.871105 -0.176744
C 2.326671 -1.407827 -0.033651
C 2.079495 -0.041395 0.130216
C 3.156479 0.855574 0.158289
C 4.463322 0.388237 0.020423
C 4.709070 -0.977187 -0.150963
H 3.819306 -2.935173 -0.315603
H 1.494143 -2.100996 -0.073107
H 2.933252 1.908309 0.311128
H 5.293555 1.091499 0.045796
H 5.728544 -1.341364 -0.263926
C 0.703486 0.554743 0.373087
O -0.269049 -0.798241 -1.310144
C -1.799244 -0.029049 0.330746
C -1.871704 0.840402 1.595968
H -1.472931 0.293710 2.457106

H -1.317557 1.778527 1.473747
H -2.923753 1.046409 1.806249
C -2.580620 0.682084 -0.828504
N -2.006825 1.829196 -1.255133
H -2.423342 2.271038 -2.062159
H -1.040478 2.051291 -0.986274
O -3.651255 0.247847 -1.244492
C -2.525816 -1.386317 0.602604
O -3.337783 -1.508575 1.511776
N -2.168052 -2.404624 -0.220919
H -2.734254 -3.239976 -0.194612
H -1.571214 -2.188095 -1.016137
H 0.569981 0.709789 1.444467
O 0.594778 1.836812 -0.225220
O 0.643125 2.854033 0.810066
N -0.394420 -0.288707 -0.108433

PBN-COOMe-2-O2.com.log

36

C 4.354412 -1.027077 -0.684867
C 3.003046 -0.806933 -0.964927
C 2.264728 0.110398 -0.207426
C 2.903801 0.831356 0.811655
C 4.255233 0.611029 1.082470
C 4.985098 -0.322810 0.342018
H 4.913226 -1.754923 -1.270898
H 2.517601 -1.369114 -1.754366
H 2.318553 1.599116 1.313789
H 4.744324 1.177603 1.873312
H 6.038667 -0.494445 0.557373
C 0.810712 0.472797 -0.482295
H 0.761974 1.142279 -1.353699
N -0.055665 -0.718325 -0.787281
O 0.365422 -1.928792 -0.794067
C -1.537413 -0.556426 -0.823407
C -2.060568 -1.187789 -2.124199
H -3.152505 -1.218665 -2.115309
H -1.715432 -0.587326 -2.968791
H -1.671187 -2.204912 -2.207950
C -2.555945 2.745316 0.526240
H -1.493335 3.029387 0.605094
H -3.064999 3.292113 -0.274447
H -3.092412 2.871650 1.469787
C -1.895140 0.948771 -0.818004
O -1.646060 1.664379 -1.765227
O -2.596709 1.319593 0.263693
C -2.179028 -1.273967 0.381620
O -3.271779 -1.805111 0.344120
O -1.406401 -1.245712 1.474363
C -1.972293 -1.847741 2.638223
H -2.185486 -2.907259 2.463841
H -1.220800 -1.731627 3.420327
H -2.901075 -1.342470 2.920619
O 0.184900 1.113465 0.578794
O 0.537212 2.550343 0.494533

PBN-NHCOMe-2-O2.com.log

38

C -3.663391 -1.701501 1.363462
C -2.445714 -1.117188 1.021236
C -2.391302 -0.096862 0.061400
C -3.576610 0.322680 -0.548020
C -4.796571 -0.269681 -0.210015
C -4.845904 -1.281993 0.747270
H -3.688387 -2.492861 2.109395
H -1.528273 -1.456662 1.490082
H -3.530682 1.115690 -1.285603
H -5.709676 0.066338 -0.697015
H -5.795382 -1.742224 1.012629

C -1.078203 0.610303 -0.236074
N 0.031738 -0.358694 -0.401106
O -0.228969 -1.537096 -0.832291
C 1.481958 0.155888 -0.579654
N 1.536569 1.518834 -0.118806
H 0.364015 2.401905 -0.890792
C 1.778836 1.818836 1.163441
O 2.046865 1.049367 2.126040
C 1.737486 3.324997 1.448828
H 2.653852 3.804554 1.081816
H 0.890391 3.799242 0.941485
H 1.665489 3.489622 2.527496
N 2.332541 -0.740317 0.194668
H 2.352436 -0.431766 1.172421
C 2.993166 -1.870950 -0.165942
O 3.100507 -2.348243 -1.293438
C 3.656039 -2.573815 1.026215
H 3.017370 -3.405698 1.347375
H 4.610584 -2.994370 0.697664
H 3.819596 -1.914288 1.884774
C 1.787089 0.118312 -2.082084
H 1.145535 0.851388 -2.577600
H 2.833938 0.392605 -2.241155
H 1.614462 -0.877318 -2.485989
H -0.821359 1.267508 0.596381
O -1.220527 1.432854 -1.393710
O -0.575518 2.722294 -1.164981

PBN-OCOMe-2-O2.com.log

36

C -3.865939 0.987999 1.595839
C -2.601662 0.565011 1.187370
C -2.453063 -0.255896 0.062258
C -3.593947 -0.643353 -0.646249
C -4.860642 -0.215826 -0.241053
C -5.003137 0.600189 0.881774
H -3.964249 1.626993 2.471395
H -1.716621 0.875597 1.734268
H -3.465385 -1.279586 -1.514937
H -5.738853 -0.523696 -0.805474
H -5.989738 0.932535 1.198982
C -1.091435 -0.805973 -0.343528
H -0.785866 -1.623541 0.315637
N -0.069583 0.275562 -0.175335
O -0.298652 1.432451 -0.736997
C 1.371642 -0.092565 -0.196175
C 1.805604 -0.541024 -1.575997
H 1.248108 -1.472084 -1.805341
H 1.510626 0.235167 -2.283085
H 2.885692 -0.681627 -1.646781
C 2.238264 2.204298 -0.359114
O 2.723245 2.255043 -1.463135
O 2.042525 1.049224 0.365100
C 1.888846 3.401676 0.492486
H 0.801424 3.411250 0.611134
H 2.338793 3.310670 1.486939
H 2.226162 4.318950 0.005583
O 1.475885 -1.094753 0.816239
C 2.619453 -1.641477 1.306044
O 2.524921 -2.402643 2.242304
C 3.957249 -1.311563 0.673124
H 4.083299 -1.902576 -0.240148
H 4.046740 -0.256737 0.411744
H 4.734958 -1.598807 1.383378
O -1.119574 -1.305122 -1.643145
O -0.372776 -2.535501 -1.719944

PBN-OCONHMe-2-O2.com.log

40

C -4.416431 -0.968010 -0.097044
C -3.053711 -1.050742 -0.367910
C -2.261624 0.119580 -0.406224
C -2.889169 1.362053 -0.148878
C -4.249852 1.427615 0.134018
C -5.026098 0.265822 0.156143
H -5.011881 -1.879356 -0.082119
H -2.570142 -1.998021 -0.566352
H -2.284672 2.261735 -0.138956
H -4.707719 2.393399 0.338266
H -6.092279 0.320382 0.367349
C -0.843788 0.158740 -0.705531
N -0.077140 -0.879876 -1.026224
O -0.451089 -2.167065 -0.904355
C 1.338031 -0.738100 -1.433763
C 1.589389 -1.561456 -2.692326
H 1.246030 -2.579466 -2.515007
H 1.035451 -1.122855 -3.526423
H 2.659134 -1.545017 -2.914890
C 1.839876 1.713119 -0.973894
O 1.355710 2.765933 -1.347665
O 1.653113 0.592712 -1.793860
N 2.627848 1.560976 0.107335
H 2.919716 0.637340 0.413726
C 2.647196 2.615371 1.113207
H 1.652871 2.756877 1.551001
H 3.346434 2.313807 1.896923
H 2.983487 3.557082 0.668613
O 2.253114 -1.243013 -0.450402
C 2.064175 -1.391255 0.929503
O 2.921242 -0.906798 1.661077
N 1.025437 -2.143589 1.302057
H 0.325801 -2.360433 0.555781
C 0.624969 -2.140483 2.699665
H -0.209060 -2.837863 2.818472
H 1.455251 -2.463647 3.335995
H 0.305686 -1.136727 3.003630
H -0.428872 1.129824 -0.921442
O -0.243860 0.775687 1.471382
O -0.717734 1.922148 1.837755

PBN-OMe-2-O2.com.log

32

C 3.641909 -1.168552 0.829568
C 2.303957 -0.814054 1.021476
C 1.722796 0.219527 0.279671
C 2.503866 0.894571 -0.668100
C 3.839815 0.545144 -0.858592
C 4.415352 -0.488601 -0.112348
H 4.079229 -1.973483 1.417564
H 1.699301 -1.345149 1.754039
H 2.043595 1.694176 -1.236399
H 4.437241 1.078489 -1.595797
H 5.458183 -0.760575 -0.264825
C 0.271255 0.603500 0.496805
N -0.578107 -0.129573 -0.526571
O -0.265992 -0.006993 -1.765568
C -1.788150 -0.956580 -0.234387
C -1.576628 -2.356578 -0.815676
H -2.510380 -2.919822 -0.728998
H -1.288727 -2.266718 -1.864415
H -0.788119 -2.873864 -0.260685
C -2.985584 0.972996 -1.171821
H -2.609757 1.118905 -2.191797
H -4.048712 1.240723 -1.134490
H -2.398387 1.591407 -0.467480
O -2.937757 -0.432202 -0.843228
O -1.937375 -1.135084 1.155897
C -2.693796 -0.143266 1.870813
H -3.729896 -0.124582 1.510298

H -2.683900 -0.482253 2.912844
H -2.226302 0.850350 1.770976
H -0.077747 0.240272 1.468465
O 0.155080 1.964616 0.391491
O -1.168660 2.358475 0.907940

PBN-POOMe-2-O2b.com.log

46

C -1.708243 -0.391747 -0.785390
N -0.553889 0.115155 -0.213963
O -0.444489 1.521064 -0.012811
C 0.800768 -0.220076 -0.655745
C 0.978928 -0.565103 -2.145929
H 0.464852 -1.495045 -2.408752
H 0.580047 0.249900 -2.753680
H 2.044040 -0.669831 -2.369000
H -1.569273 -1.459643 -0.956338
P 1.445821 1.549676 -0.322328
O 3.040779 0.921371 -0.470336
O 1.741100 1.930263 1.263971
C 0.838096 2.748672 1.993249
H 1.404089 3.150491 2.843118
H 0.465239 3.583100 1.387872
H -0.015066 2.169112 2.357330
C 4.114511 1.835980 -0.475221
H 4.254259 2.298210 0.513246
H 5.029512 1.283140 -0.730874
H 3.955032 2.631817 -1.213800
O 1.427825 2.673975 -1.321005
P 1.327189 -1.656233 0.389647
O 0.665704 -2.925933 -0.045726
O 1.001695 -1.175025 1.897923
O 2.943918 -1.808139 0.522152
C 3.734868 -2.225747 -0.588467
H 3.213119 -2.979798 -1.189107
H 3.988055 -1.355150 -1.200336
H 4.650576 -2.665975 -0.181261
C 1.190026 -2.106553 2.962944
H 2.257805 -2.270162 3.147757
H 0.729066 -1.664437 3.849810
H 0.707045 -3.063619 2.736690
O -1.936099 0.120997 -2.298392
O -2.523831 -0.811577 -3.015480
C -3.012073 -0.105615 -0.086284
C -3.239718 1.058177 0.662712
C -4.048748 -1.041167 -0.218571
C -4.477062 1.266090 1.273406
H -2.432525 1.775380 0.757424
C -5.285923 -0.826861 0.388772
H -3.880982 -1.935096 -0.811925
C -5.504117 0.329076 1.140322
H -4.639545 2.170192 1.856554
H -6.077338 -1.564952 0.276946
H -6.466638 0.497908 1.619134

PBN-SMe-2-O2-b.com.log

32

C 3.701342 -1.718815 0.807157
C 2.416236 -1.186968 0.937127
C 2.094359 0.057290 0.383146
C 3.082563 0.773489 -0.304408
C 4.368378 0.245320 -0.425674
C 4.684529 -1.001192 0.124059
H 3.934374 -2.689111 1.242774
H 1.649849 -1.746454 1.471057
H 2.781797 1.727501 -0.729756
H 5.131262 0.807951 -0.961591
H 5.688419 -1.409998 0.020237
C 0.700141 0.627608 0.606193

H 0.373727 0.369633 1.619960
N -0.245775 -0.007881 -0.350228
O 0.131482 0.173503 -1.596366
C -1.706179 0.239049 -0.135311
S -2.670222 -0.671130 -1.438768
C -1.803462 -2.272757 -1.485585
H -0.798429 -2.121715 -1.883339
H -1.755091 -2.712412 -0.485001
H -2.381696 -2.928518 -2.144723
S -2.084572 -0.493088 1.559754
C -3.826177 0.008578 1.763169
H -4.187355 -0.470199 2.678746
H -3.925598 1.092967 1.866123
H -4.420555 -0.339447 0.912918
C -2.104343 1.715662 -0.269261
H -1.954582 2.238943 0.677389
H -1.416639 2.164808 -0.996809
H -3.146377 1.830110 -0.593174
O 0.604863 2.029526 0.571360
O 0.836118 2.540098 -0.747826

PBN-alpha-3CH2OH-O2.com.log

33

C 3.912386 -1.493561 -0.734896
C 2.633924 -0.996751 -1.000550
C 2.132773 0.104178 -0.298676
C 2.933726 0.704081 0.680938
C 4.211263 0.213201 0.945302
C 4.706234 -0.888899 0.240422
H 4.287735 -2.349834 -1.291932
H 2.015413 -1.469053 -1.761377
H 2.537651 1.560222 1.214513
H 4.824763 0.689098 1.707828
H 5.703290 -1.271292 0.449980
C 0.750227 0.645352 -0.604857
H 0.468462 0.423096 -1.643299
N -0.258105 -0.121311 0.250710
O -0.004816 -0.149009 1.524120
C -1.708852 -0.239582 -0.088248
C -2.463364 0.909122 0.623430
H -3.460847 1.012750 0.188460
H -1.891226 1.830263 0.432005
C -1.975313 -0.169696 -1.603753
H -1.703453 0.828007 -1.962632
H -1.342964 -0.919799 -2.113614
C -2.155418 -1.624350 0.460893
O -3.570364 -1.682079 0.674230
H -3.708694 -1.001233 1.365090
H -1.615540 -1.832628 1.389082
H -1.914610 -2.412711 -0.261483
O -3.353094 -0.411405 -1.897088
H -3.716492 -0.955937 -1.173319
O -2.652767 0.618210 2.021084
H -1.743633 0.416545 2.326997
O 0.717679 1.989371 -0.370398
O -0.486467 2.550302 -0.994610

PBN-alpha-3COOH-O2.com.log

30

C -4.164179 -1.528635 0.114452
C -2.813435 -1.222101 0.269122
C -2.372195 0.104709 0.184642
C -3.305482 1.116380 -0.060781
C -4.658769 0.807247 -0.219920
C -5.094196 -0.514688 -0.130954
H -4.491160 -2.564233 0.179133
H -2.090056 -2.012008 0.443063
H -2.960804 2.142067 -0.129434
H -5.372485 1.605047 -0.414748

H -6.148025 -0.755714 -0.254471
C -0.922138 0.448397 0.453102
H -0.702347 0.383474 1.521692
N 0.002977 -0.507574 -0.207716
O -0.306473 -0.923085 -1.389240
C 1.443747 -0.243645 0.022498
C 2.209965 -1.290810 -0.809404
O 2.077061 -2.487105 -0.648317
O 3.103006 -0.787788 -1.679398
H 3.509214 -1.579795 -2.079851
O -0.655449 1.760191 0.011099
O 0.681863 2.062069 0.501231
C 1.687884 1.332591 -0.450368
O 1.549534 1.554048 -1.662865
O 2.899981 1.750697 0.189595
H 3.276058 2.316656 -0.505149
C 1.820250 -0.488220 1.474210
O 1.086463 -0.487903 2.444207
O 3.150252 -0.726737 1.613637
H 3.280145 -0.824907 2.574592

PBN-CH2CONH2-3-O2b.com.log

42

C 4.050529 1.645466 0.346447
C 2.715315 1.228087 0.323328
C 2.397793 -0.132023 0.220402
C 3.440872 -1.071224 0.165925
C 4.769095 -0.649761 0.192866
C 5.082165 0.710716 0.275147
H 4.279293 2.705734 0.435534
H 1.923823 1.959911 0.435178
H 3.155119 -2.120168 0.104727
H 5.567343 -1.388276 0.150413
H 6.120204 1.036916 0.292985
C 0.978961 -0.690526 0.110155
N -0.063388 0.278300 0.486353
O 0.112087 0.931561 1.586594
C -1.440149 0.237749 -0.146042
C -1.347180 0.960273 -1.524882
H -2.294201 0.807892 -2.046493
H -0.583108 0.465245 -2.132235
C -1.952818 -1.233800 -0.331367
H -1.583272 -1.825329 0.507503
H -3.043959 -1.188178 -0.266035
C -2.439478 0.995738 0.772079
H -1.981260 1.923514 1.118426
H -3.305303 1.254773 0.160751
C -2.989477 0.202624 1.963745
O -4.147431 -0.207883 1.986155
N -2.124236 0.022200 3.001819
H -2.400164 -0.642906 3.710952
H -1.136767 0.211963 2.849582
C -1.077624 2.457994 -1.454648
O -1.956715 3.291060 -1.268264
N 0.228052 2.830420 -1.679261
H 0.450375 3.794274 -1.465355
H 0.975774 2.161019 -1.553015
C -1.669277 -1.936416 -1.668378
O -2.295536 -1.608525 -2.686655
N -0.765798 -2.936328 -1.625292
H -0.572981 -3.348066 -2.532267
H -0.010552 -3.048821 -0.849271
H 0.793519 -0.972022 -0.932047
O 0.784847 -1.836775 0.913766
O 1.204167 -3.006814 0.125488

PBN-CH2COOMe-3-O2.com.log

48

C -5.039235 -0.177300 1.088346

C -3.656393 -0.275508 0.943391
C -3.099122 -1.040696 -0.089741
C -3.953893 -1.703113 -0.974649
C -5.340262 -1.598450 -0.835339
C -5.889567 -0.838628 0.197562
H -5.455183 0.423086 1.895054
H -2.999838 0.259029 1.623602
H -3.510879 -2.298718 -1.764781
H -5.991655 -2.117177 -1.536034
H -6.969168 -0.760131 0.309316
C -1.593617 -1.251777 -0.193594
N -0.899600 0.092218 -0.017767
O -1.475737 1.107309 -0.564499
C 0.603950 0.203545 0.090365
C 1.066529 -1.021160 0.907830
H 0.423883 -1.141038 1.787972
H 0.854289 -1.904486 0.238518
C 1.149662 0.176169 -1.372100
H 0.909384 -0.820283 -1.764977
H 0.611010 0.956802 -1.916537
C 0.914130 1.522753 0.847802
H 1.995026 1.675096 0.807199
H 0.610810 1.400161 1.892261
C -1.399843 4.384805 0.725731
H -0.738900 5.220522 0.473926
H -1.976573 4.109561 -0.162437
H -2.070863 4.662856 1.542091
O -0.656745 3.261640 1.196769
C 0.259984 2.778998 0.304153
O 0.548819 3.367894 -0.713346
C 2.478573 -1.063635 1.394444
O 3.428954 -0.381206 1.059018
O 2.613580 -2.055224 2.328185
C 3.939780 -2.243782 2.820679
H 3.873621 -3.059869 3.543511
H 4.625824 -2.510857 2.010566
H 4.314238 -1.336236 3.305519
C 2.625804 0.459057 -1.538005
O 3.176055 1.536546 -1.434436
O 3.304996 -0.668428 -1.888335
C 4.718702 -0.504095 -1.990414
H 5.134217 -0.207458 -1.023184
H 5.108768 -1.478950 -2.292519
H 4.975456 0.255661 -2.735933
H -1.263460 -1.887337 0.636174
O -1.259143 -1.865242 -1.378010
O -0.040016 -2.669394 -1.193308

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51

C -4.687350 -1.002183 -2.037204
C -3.425674 -1.113587 -1.456363
C -3.204408 -0.684378 -0.140910
C -4.272095 -0.146395 0.581592
C -5.536092 -0.026583 -0.002383
C -5.749985 -0.454554 -1.312317
H -4.841500 -1.338678 -3.060300
H -2.599765 -1.525021 -2.029443
H -4.094740 0.164437 1.604986
H -6.356281 0.397724 0.573184
H -6.734715 -0.365870 -1.766435
C -1.857793 -0.899074 0.537807
H -1.683603 -1.972033 0.670502
N -0.755512 -0.373890 -0.354185
O -1.043345 0.647135 -1.098370
C 0.686617 -0.526030 0.020786
C 1.057541 0.406101 1.233589
H 2.098269 0.727866 1.154872
H 0.870854 -0.178522 2.142390
C 0.908054 -2.000126 0.462010

H 0.253952 -2.169963 1.328469
H 0.670035 -2.684774 -0.355683
C 1.536783 -0.240351 -1.237600
H 1.127243 -0.827059 -2.070213
H 2.556976 -0.583520 -1.060166
N 1.637137 1.157710 -1.604473
H 0.754988 1.651214 -1.638751
C 2.824532 1.819107 -1.695193
O 3.919046 1.268832 -1.579194
C 2.699124 3.317339 -1.932926
H 1.815163 3.574761 -2.528227
H 2.614248 3.805992 -0.956193
H 3.598712 3.673377 -2.440628
N 0.227734 1.589762 1.355135
H -0.739975 1.369312 1.582133
N 2.285421 -2.270556 0.852954
H 2.594980 -1.895791 1.737911
C 3.148363 -3.039754 0.131723
O 2.854498 -3.578435 -0.931903
C 0.674439 2.862734 1.369165
O 1.853279 3.196806 1.211013
C -0.407645 3.916614 1.593812
H -1.402474 3.494358 1.764648
H -0.125805 4.535905 2.451797
H -0.448141 4.572180 0.717114
C 4.545906 -3.174029 0.728869
H 4.857997 -4.220114 0.663371
H 5.242723 -2.579764 0.127579
H 4.614939 -2.840481 1.769784
O -1.821592 -0.315514 1.795030
O -1.018066 -1.168303 2.703989

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48

C -5.300304 -1.595032 -0.252552
C -3.923272 -1.824591 -0.298588
C -3.035332 -0.759392 -0.464006
C -3.545843 0.538076 -0.594342
C -4.920217 0.767838 -0.553834
C -5.804588 -0.300268 -0.380764
H -5.980959 -2.433379 -0.119691
H -3.517285 -2.826330 -0.215292
H -2.860450 1.373217 -0.719028
H -5.301114 1.781589 -0.656533
H -6.877496 -0.122964 -0.349104
C -1.539635 -1.010425 -0.583290
H -1.177963 -0.654878 -1.555033
N -0.833542 -0.175280 0.475746
O -1.395650 -0.130476 1.641997
C 0.670110 -0.109250 0.497738
C 1.134352 -1.444882 1.133193
H 0.577844 -1.569765 2.066579
H 0.878295 -2.243316 0.428201
C 1.151587 0.088460 -0.955001
H 0.993853 -0.852379 -1.496070
H 0.571376 0.891962 -1.408519
C 1.094891 1.070801 1.382251
H 2.167998 1.008616 1.559890
H 0.556716 1.028664 2.328040
C -0.162759 3.156879 0.927842
O -0.380448 4.030785 0.114073
O 0.883178 2.325713 0.699703
C -0.965958 2.982832 2.198306
H -1.471939 2.010807 2.203747
H -0.315909 3.025720 3.080066
H -1.697244 3.790652 2.246583
O 2.525361 -1.441843 1.511522
O 2.558194 0.410886 -0.963564
C 3.475134 -2.205437 0.903284
O 4.552799 -2.301685 1.449493

C 3.079652 1.464037 -1.644541
O 4.277002 1.638372 -1.603318
C 3.178861 -2.840468 -0.440596
H 2.168283 -3.243639 -0.555932
H 3.297761 -2.063255 -1.204405
H 3.929850 -3.614248 -0.611406
C 2.146397 2.371380 -2.426043
H 1.556900 1.813822 -3.162193
H 1.453795 2.891866 -1.755772
H 2.766895 3.103341 -2.944754
O -1.240109 -2.350770 -0.465439
O -0.065685 -2.677545 -1.282460

PBN-CH2OCONHMe-3-O2.com.log

54

C 3.328420 2.361640 2.526589
C 2.361054 1.857884 1.659122
C 2.731989 1.157143 0.503652
C 4.090454 0.975601 0.231989
C 5.061604 1.473194 1.105203
C 4.686180 2.168635 2.254509
H 3.023489 2.901610 3.420854
H 1.306459 1.994652 1.880587
H 4.365339 0.448879 -0.674993
H 6.115306 1.320263 0.880929
H 5.441875 2.559769 2.932583
C 1.689597 0.696229 -0.506391
H 1.241349 1.571300 -0.991228
N 0.578253 -0.019337 0.212877
O 0.871628 -0.700064 1.280876
C -0.669608 -0.420143 -0.505837
C -1.166634 0.724806 -1.390571
H -2.128932 0.468703 -1.835784
H -0.415476 0.910158 -2.168015
C -0.421518 -1.640981 -1.435318
H 0.317268 -1.348877 -2.198231
H -1.369725 -1.922556 -1.906553
C -1.672369 -0.775236 0.608190
H -1.767435 0.059348 1.309430
H -1.297774 -1.660886 1.124353
C -4.012089 -1.426300 0.745503
O -5.102219 -1.584643 0.229250
O -2.948108 -1.044470 -0.003616
N -3.788168 -1.580346 2.095296
H -2.836911 -1.675062 2.418293
C -4.834088 -2.148813 2.925707
H -4.921732 -3.239153 2.813794
H -4.624873 -1.915730 3.974386
H -5.788201 -1.702844 2.640164
O -1.329222 1.900666 -0.556510
C -2.053570 2.916023 -1.080293
O -2.637113 2.898547 -2.148843
N -2.058834 3.970887 -0.198029
H -1.379851 3.919062 0.548045
C -2.564205 5.267447 -0.596515
H -3.037717 5.768334 0.255445
H -1.780073 5.925542 -1.000075
H -3.310546 5.106610 -1.376073
O 0.021715 -2.745903 -0.630834
C 1.263862 -3.263242 -0.941391
O 1.521607 -3.818096 -1.991348
N 2.099200 -3.139726 0.131048
H 1.840362 -2.375603 0.755338
C 3.513283 -3.411007 -0.050459
H 4.018122 -2.596160 -0.587022
H 3.987273 -3.545094 0.927679
H 3.625467 -4.327634 -0.633751
O 2.249169 -0.096286 -1.489448
O 1.548741 0.147465 -2.754608

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C	4.205003	-1.848716	-0.098569
C	2.884500	-1.505915	0.199142
C	2.459676	-0.173872	0.138687
C	3.377351	0.822626	-0.215465
C	4.698990	0.478557	-0.503872
C	5.119144	-0.854150	-0.451982
H	4.520144	-2.889902	-0.050405
H	2.171713	-2.280425	0.477369
H	2.988349	1.838955	-0.262139
H	5.409045	1.257748	-0.777264
H	6.150319	-1.115942	-0.684535
C	1.040071	0.180995	0.562425
H	0.797968	-0.410521	1.456096
N	0.071550	-0.281254	-0.484973
O	0.456790	-0.284904	-1.716740
C	-1.395489	-0.061589	-0.278175
C	-2.081520	-1.131977	-1.147831
H	-1.785814	-0.982929	-2.193844
H	-1.751609	-2.131614	-0.830372
C	-1.788126	-0.249200	1.190494
H	-1.294805	0.506302	1.809461
H	-2.872965	-0.111850	1.275810
C	-1.765823	1.379107	-0.765856
H	-2.426755	1.303491	-1.642032
H	-0.819212	1.868856	-1.033121
C	-1.902580	3.440028	0.417260
H	-2.291209	4.131046	-0.354306
H	-2.250259	3.797242	1.395172
H	-0.802762	3.420540	0.371499
O	-2.436404	2.130602	0.245482
O	-3.493890	-1.014787	-1.006233
C	-4.184380	-1.932684	-1.810383
H	-5.255908	-1.772220	-1.648874
H	-3.962842	-1.792413	-2.883008
H	-3.939882	-2.978289	-1.551672
O	-1.428921	-1.566155	1.619707
C	-1.807778	-1.802557	2.950493
H	-1.498481	-2.822016	3.205868
H	-1.323429	-1.099993	3.650021
H	-2.900049	-1.717656	3.090183
O	0.827947	1.494908	0.957799
O	1.009898	2.428644	-0.167929

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63

C	3.789976	-3.327647	-1.032919
C	2.740993	-2.416982	-1.168152
C	3.001226	-1.045697	-1.283424
C	4.325294	-0.599849	-1.264866
C	5.374351	-1.510587	-1.126339
C	5.112195	-2.877343	-1.011106
H	3.573908	-4.390763	-0.947940
H	1.710827	-2.766755	-1.165723
H	4.515280	0.461946	-1.371403
H	6.401180	-1.150734	-1.111232
H	5.931106	-3.586505	-0.908412
C	1.849494	-0.074367	-1.494939
N	1.004172	-0.066419	-0.233539
O	1.636632	-0.039386	0.888560
C	-0.408611	0.449033	-0.187091
C	-0.421358	2.004765	-0.180513
H	-1.455157	2.349706	-0.249021
H	0.107344	2.280228	-1.130378
C	-1.099244	-0.010212	-1.507156
H	-0.641478	0.562541	-2.326465
H	-0.878785	-1.071933	-1.669743
C	-1.067710	-0.129650	1.088648

H -2.122786 0.154415 1.106379
H -0.583290 0.304252 1.963617
P -1.021057 -1.942771 1.314295
O -2.429741 -2.144508 2.113055
O 0.005674 -2.298293 2.522698
C 1.325777 -2.806667 2.247234
H 1.949905 -2.018926 1.821441
H 1.725963 -3.134748 3.210409
H 1.271278 -3.654823 1.559070
C -2.743175 -3.443395 2.618991
H -2.691737 -4.196188 1.824195
H -2.057119 -3.720337 3.426654
H -3.764137 -3.391704 3.005940
O -0.843153 -2.814497 0.111188
P -2.894200 0.072345 -1.771909
O -3.305738 -0.160805 -3.184097
O -3.624187 -0.948133 -0.724074
O -3.347746 1.488375 -1.124153
C -4.705658 1.916825 -1.284658
H -4.755023 2.937487 -0.899981
H -4.991415 1.901513 -2.340948
H -5.379336 1.271310 -0.710590
C -3.894178 -2.299956 -1.134403
H -2.983890 -2.900987 -1.055291
H -4.648456 -2.685137 -0.443037
H -4.280357 -2.318304 -2.157525
P 0.343045 3.073940 1.066048
O -0.257980 4.441377 1.067201
O 0.232425 2.296067 2.496259
O 1.948041 3.067410 0.861470
C 0.900791 2.855988 3.628379
H 0.634744 3.911577 3.756131
H 0.569700 2.288301 4.502292
H 1.985289 2.760814 3.516196
C 2.497756 3.813195 -0.250228
H 2.116177 3.422584 -1.202003
H 2.263111 4.877029 -0.132446
H 3.579019 3.664001 -0.199796
H 1.204260 -0.446807 -2.296496
O 2.319219 1.170949 -1.829475
O 1.264095 1.905749 -2.549929

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42

C -4.854702 1.200109 0.084265
C -3.493861 0.985551 -0.126981
C -2.990259 -0.314586 -0.268584
C -3.874832 -1.393174 -0.194940
C -5.238263 -1.179426 0.024902
C -5.734901 0.116764 0.162980
H -5.229511 2.215959 0.193159
H -2.810673 1.828862 -0.170894
H -3.473962 -2.392718 -0.319851
H -5.913964 -2.030726 0.082779
H -6.797308 0.284578 0.329005
C -1.523820 -0.553778 -0.606624
H -1.316965 -0.151848 -1.604923
N -0.662831 0.232131 0.366970
O -1.095885 0.355932 1.575479
C 0.846864 0.237610 0.222938
C 1.297148 -1.122373 0.833286
H 0.723345 -1.244253 1.756342
H 1.027230 -1.909158 0.119516
C 1.166386 0.365921 -1.277799
H 0.680647 -0.484480 -1.785120
H 0.764628 1.312391 -1.651456
C 1.371179 1.413475 1.070037
H 2.460691 1.447203 1.011857
H 1.086686 1.248579 2.109076
S 0.724428 3.086175 0.627681

C	2.138231	3.777012	-0.308138
H	2.339487	3.213357	-1.223363
H	1.867669	4.802722	-0.578347
H	3.045708	3.803655	0.303748
S	3.081166	-1.292534	1.323349
S	2.948098	0.313222	-1.739214
C	2.853890	-2.621911	2.560350
H	3.842488	-2.878782	2.954022
H	2.216444	-2.292673	3.388527
H	2.413245	-3.514266	2.104022
C	3.125829	-1.446919	-2.255824
H	3.315069	-1.503574	-3.332132
H	3.953022	-1.900553	-1.704726
H	2.198522	-1.976927	-2.016297
O	-1.220740	-1.901167	-0.604369
O	-0.226511	-2.204480	-1.651360

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39

C	3.991538	-2.166049	0.033657
C	2.720168	-1.587136	0.055313
C	2.581115	-0.198614	0.139068
C	3.725265	0.607791	0.206825
C	4.992813	0.025077	0.191522
C	5.131748	-1.363268	0.102980
H	4.090715	-3.247513	-0.042747
H	1.831946	-2.207354	-0.006246
H	3.575929	1.681825	0.290692
H	5.877693	0.656878	0.246773
H	6.121748	-1.816025	0.086668
C	1.232323	0.498421	0.216097
H	0.946525	0.653872	1.260556
N	0.174058	-0.300311	-0.427718
O	0.340466	-0.576064	-1.694911
C	-1.235771	-0.010918	-0.045702
C	-3.286599	-1.045939	2.854355
H	-2.962454	-2.076245	3.029025
H	-2.860235	-0.402118	3.628760
H	-4.375956	-0.980391	2.860556
C	-1.544493	-0.605577	1.344044
O	-0.742335	-1.034445	2.136709
O	-2.880469	-0.597932	1.557786
C	-2.108987	-0.732651	-1.094184
O	-2.862924	-0.222585	-1.884240
C	-1.493090	1.510929	0.055258
O	-1.634098	2.048589	1.137003
O	-1.970087	-2.071175	-0.943001
O	-1.459227	2.133561	-1.118438
C	-1.154522	3.544525	-1.025795
H	-0.225737	3.663652	-0.453023
H	-1.034484	3.871688	-2.060253
H	-1.983931	4.080060	-0.551772
C	-2.641378	-2.857288	-1.928803
H	-2.240405	-2.637394	-2.922572
H	-2.443746	-3.896955	-1.661413
H	-3.717265	-2.656862	-1.924547
O	1.248709	1.758540	-0.420046
O	1.550023	2.773917	0.552358

PBN-NHCOMe-3-O2.com.log

42

C	-4.284043	1.472638	-0.153722
C	-2.970135	1.008768	-0.090242
C	-2.712091	-0.360353	0.063996
C	-3.787171	-1.251549	0.148251
C	-5.101267	-0.784125	0.077633
C	-5.355225	0.579662	-0.071623
H	-4.470139	2.537417	-0.275395
H	-2.139999	1.703834	-0.168787

H -3.580481 -2.310011 0.261276
H -5.927131 -1.489806 0.139305
H -6.378772 0.944642 -0.126076
C -1.287299 -0.868755 0.233594
H -0.984394 -0.822558 1.283491
N -0.340548 -0.016859 -0.516790
O -0.577126 0.161115 -1.761606
C 1.138474 0.063914 -0.054968
N 1.710084 -1.219901 -0.192292
H 0.625138 -2.372409 0.322109
C 2.679687 -1.500817 -1.068274
O 3.296848 -0.727738 -1.851979
C 3.100187 -2.969517 -1.059398
H 3.403264 -3.266740 -2.068171
H 3.966774 -3.091086 -0.397041
H 2.298848 -3.621422 -0.700425
N 1.757321 1.107705 -0.850033
H 2.453646 0.714610 -1.508175
N 1.023913 0.492888 1.348868
H 0.469142 1.346199 1.385168
C 1.352297 2.393380 -0.851184
O 0.508671 2.870608 -0.076507
C 2.028001 0.428906 2.294403
O 3.044765 -0.241415 2.234552
C 2.010501 3.265937 -1.911887
H 1.347451 3.317142 -2.783610
H 2.133779 4.278557 -1.518602
H 2.977293 2.871871 -2.239673
C 1.714017 1.297402 3.519344
H 1.607458 2.351270 3.233268
H 0.774634 0.985258 3.990690
H 2.530841 1.197302 4.236356
O -1.231133 -2.226394 -0.169753
O -0.206817 -2.895408 0.619106

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39

C -3.696012 -0.395024 2.182880
C -2.444790 -0.485014 1.574215
C -2.332060 -0.511928 0.177745
C -3.492654 -0.441279 -0.598023
C -4.744587 -0.348146 0.013465
C -4.853230 -0.327232 1.403954
H -3.764826 -0.372675 3.268085
H -1.544027 -0.518403 2.178509
H -3.414008 -0.451762 -1.678075
H -5.637707 -0.289252 -0.604332
H -5.829833 -0.255011 1.877451
C -0.957064 -0.682867 -0.452067
N 0.040495 0.117034 0.165109
O -0.307213 1.457601 0.516618
C 1.456037 0.197575 -0.427305
C -0.722399 2.344581 -0.453253
O -1.359850 2.070912 -1.435699
O 1.634382 0.969708 -1.367831
C -0.313095 3.734641 -0.023803
H 0.752366 3.847746 -0.252280
H -0.890889 4.478108 -0.576418
H -0.439884 3.868711 1.054134
O 2.239699 0.466631 0.846262
C 3.545624 0.787329 0.830460
O 4.098992 1.027467 1.890798
C 4.296697 0.819348 -0.487191
H 4.159852 -0.113801 -1.040506
H 3.896437 1.608370 -1.126574
H 5.353284 0.985960 -0.265423
O 1.787046 -1.254726 -0.771147
C 2.029410 -2.293457 0.058174
O 2.474733 -3.323165 -0.414392
C 1.744908 -2.183901 1.549181

H 1.563024 -3.195250 1.921884
H 2.620668 -1.772479 2.060564
H 0.909190 -1.520796 1.772409
H -0.628430 -1.720681 -0.370857
O -1.063297 -0.535922 -1.952544
O -1.315665 -1.714228 -2.495182

PBN-OCONHMe-3-O2.com.log

45

C 4.505220 0.975093 -0.624236
C 3.168319 0.607077 -0.466442
C 2.822739 -0.425969 0.415402
C 3.834032 -1.079018 1.131474
C 5.169606 -0.707988 0.968600
C 5.510991 0.321166 0.089936
H 4.759882 1.774457 -1.316561
H 2.388830 1.104964 -1.033269
H 3.573450 -1.878210 1.817198
H 5.943400 -1.226633 1.530604
H 6.552285 0.609324 -0.038884
C 1.357376 -0.764954 0.652880
N 0.497972 -0.359191 -0.370465
O 0.863353 -0.702542 -1.674983
C -0.839163 0.110309 -0.146875
C -0.423772 2.492759 -0.671511
O 0.227731 2.334935 -1.683917
O -0.892973 1.536216 0.172578
N -0.810793 3.714016 -0.170725
H -1.242010 3.701082 0.742547
C -0.267456 4.947241 -0.692649
H -1.048735 5.713063 -0.768878
H 0.552344 5.344733 -0.075251
H 0.122577 4.736224 -1.689903
O -1.675362 -0.066744 -1.207732
C -2.156705 -1.427293 -1.491319
O -3.367367 -1.596800 -1.256305
N -1.230258 -2.203405 -1.969791
H 0.182403 -1.439071 -1.909688
C -1.653362 -3.562658 -2.250824
H -2.207085 -4.011709 -1.412379
H -2.312799 -3.619621 -3.132559
H -0.769480 -4.178948 -2.452605
O -1.283998 -0.482313 1.059252
C -2.377689 0.083990 1.745384
O -2.219238 0.616113 2.828453
N -3.551736 -0.112589 1.121932
H -3.580035 -0.632780 0.229570
C -4.776169 0.365172 1.725235
H -4.736884 1.446886 1.904733
H -5.602674 0.148412 1.043361
H -4.971870 -0.123095 2.689117
H 0.999989 -0.372516 1.604699
O 1.249788 -2.278480 0.848197
O 1.325106 -2.607627 2.124602

PBN-OMe-3-O2b.com.log

33

C -3.419012 1.484916 0.613040
C -2.121264 0.973006 0.614785
C -1.862879 -0.319102 0.138969
C -2.927075 -1.088244 -0.341349
C -4.225880 -0.574237 -0.349118
C -4.478775 0.712624 0.130084
H -3.603208 2.490859 0.985826
H -1.292486 1.578771 0.973921
H -2.713265 -2.087683 -0.702688
H -5.043879 -1.182844 -0.730630
H -5.491361 1.111869 0.126373
C -0.453538 -0.897809 0.211241

N 0.508540 0.109871 -0.378337
O 0.325294 0.465971 -1.598918
C 1.741875 0.619922 0.285336
C 2.901428 -0.810702 -1.332283
H 2.623557 -0.491805 -2.342555
H 3.941395 -1.158030 -1.328243
H 2.218114 -1.609255 -0.985574
O 2.883696 0.338556 -0.452273
O 1.797590 0.188562 1.605995
C 2.495077 -1.039715 1.871507
H 3.546427 -0.953410 1.572000
H 2.440899 -1.156267 2.958906
H 1.997111 -1.876873 1.356393
O 1.655484 2.018127 0.446315
C 1.673720 2.819146 -0.727290
H 0.705740 2.816693 -1.238512
H 1.910589 3.833730 -0.385314
H 2.444351 2.479249 -1.425731
H -0.146551 -0.996695 1.259168
O -0.404914 -2.099611 -0.437690
O 0.862942 -2.767383 -0.080243

PBN-POOMe-3-O2b.com.log

54

C -4.507958 1.656632 0.477919
C -3.266948 1.021018 0.450788
C -3.158386 -0.306669 0.014593
C -4.314707 -0.986976 -0.383207
C -5.556059 -0.347261 -0.354790
C -5.658845 0.976072 0.074119
H -4.574302 2.688437 0.815802
H -2.367863 1.541649 0.764571
H -4.246241 -2.015588 -0.717732
H -6.444598 -0.888756 -0.672239
H -6.626454 1.472965 0.094281
C -1.793873 -0.990276 0.068842
N -0.753456 -0.093283 -0.194398
O -0.738098 0.466396 -1.510286
C 0.666311 -0.159185 0.100982
P 0.980798 1.132107 -1.336576
O 2.397433 1.582884 -0.478790
O 0.401101 2.687198 -1.144269
C -0.707543 3.118640 -1.928566
H -0.709552 4.214138 -1.880056
H -0.600275 2.806836 -2.973916
H -1.649556 2.723483 -1.540094
C 3.321935 2.444107 -1.113841
H 2.919610 3.462157 -1.218682
H 4.222118 2.483561 -0.487312
H 3.585573 2.067598 -2.109026
O 1.480825 0.796568 -2.717581
P 0.954886 0.433693 1.843785
O 2.336765 0.339478 2.391197
O -0.166979 -0.380949 2.697383
O 0.269726 1.898361 1.932864
C 1.078065 3.086468 1.956024
H 2.101033 2.850766 2.258743
H 1.071201 3.534034 0.961765
H 0.621137 3.760606 2.688211
C 0.254574 -1.367793 3.658447
H 0.970870 -0.936344 4.363845
H -0.652842 -1.668211 4.189437
H 0.700445 -2.220104 3.143067
P 1.545536 -1.810234 -0.141480
O 1.428985 -2.650987 1.083403
O 0.916464 -2.529252 -1.418389
O 3.053365 -1.523918 -0.650512
C 1.273049 -2.308709 -2.799241
H 2.251251 -2.760382 -2.994540
H 0.503257 -2.822785 -3.379370

H 1.289344 -1.242259 -3.035095
C 4.102757 -1.165369 0.264755
H 5.029126 -1.207320 -0.314762
H 3.933607 -0.162670 0.656584
H 4.145341 -1.880535 1.091599
H -1.612422 -1.456622 1.038272
O -1.837663 -2.166854 -0.893679
O -2.191693 -3.275094 -0.265018

PBN-SMe-3-O2-c.com.log

33

C 3.715227 -1.869544 -0.009871
C 2.435491 -1.311587 0.021008
C 2.266501 0.071778 0.143700
C 3.399271 0.891528 0.234704
C 4.677501 0.331127 0.206987
C 4.842263 -1.050829 0.085118
H 3.831316 -2.946778 -0.115497
H 1.559387 -1.945964 -0.061964
H 3.243364 1.960643 0.343396
H 5.549953 0.978084 0.280634
H 5.839903 -1.485874 0.061237
C 0.884327 0.707459 0.245372
N -0.117372 -0.092304 -0.445087
O 0.115469 -0.242006 -1.743101
C -1.494247 -0.142228 0.019338
S -2.514766 -1.259891 -1.039006
C -1.441722 -2.730845 -1.196897
H -0.536491 -2.434953 -1.730863
H -1.200952 -3.139784 -0.211038
H -2.008351 -3.473146 -1.769241
S -1.410203 -0.776227 1.782016
C -3.152627 -0.673201 2.325620
H -3.210007 -1.238631 3.261366
H -3.462780 0.358230 2.508811
H -3.805094 -1.134960 1.579561
S -2.475835 1.489808 0.016939
C -1.999826 2.153172 -1.620127
H -2.484000 3.132727 -1.693636
H -0.915545 2.269444 -1.652241
H -2.347178 1.501862 -2.424352
H 0.598725 0.832431 1.292655
O 0.875503 2.021690 -0.332259
O 1.232685 2.956913 0.645095

PBN-TriCONH2-O2.log

33

C -4.549057 0.846588 0.340761
C -3.197454 1.135504 0.136133
C -2.316310 0.124662 -0.251963
C -2.797151 -1.177358 -0.437181
C -4.145017 -1.464404 -0.229854
C -5.026701 -0.451925 0.160123
H -5.229199 1.639923 0.643673
H -2.819221 2.143163 0.270552
H -2.098639 -1.953672 -0.739538
H -4.509367 -2.479185 -0.373821
H -6.079427 -0.675100 0.320411
C -0.855200 0.393570 -0.531420
H -0.594431 0.043248 -1.531176
N 0.012720 -0.344701 0.423769
O -0.386942 -0.287009 1.655492
C 1.456915 -0.304958 0.067262
C 1.907836 1.281938 0.006481
N 1.728919 1.827902 1.337892
H 2.124564 2.765731 1.296180
H 0.736751 1.911000 1.555198
O 3.012235 1.544892 -0.565082
C 2.419427 -1.032111 1.047000

O 3.599784 -1.167882 0.758046
N 1.879436 -1.539000 2.193042
H 2.561412 -1.807507 2.889686
H 0.978779 -1.158359 2.477107
C 1.593964 -1.013967 -1.311495
O 0.778877 -1.864931 -1.684901
N 2.677057 -0.633013 -2.006769
H 2.756168 -0.978456 -2.953029
H 3.136904 0.238258 -1.675572
O -0.560112 1.763940 -0.422919
O 0.806318 1.899415 -0.964422

PBN-alpha-carbamate-O2H.log

36

C -4.095749 -1.061410 -0.743655
C -2.751745 -0.731827 -0.912675
C -2.221822 0.412051 -0.301092
C -3.057327 1.226403 0.470874
C -4.401337 0.888676 0.643781
C -4.924274 -0.254109 0.039003
H -4.495149 -1.950252 -1.224340
H -2.109542 -1.358849 -1.524261
H -2.658577 2.118181 0.941213
H -5.038726 1.523556 1.253327
H -5.970707 -0.513729 0.173701
C -0.767610 0.779535 -0.574025
H -0.661811 1.225097 -1.567166
N 0.133056 -0.392009 -0.647196
O 0.732254 -0.549309 -1.775905
C 0.697644 -1.116073 0.537401
C -0.256283 -1.094622 1.731248
H 0.225305 -1.634136 2.551507
H -0.456751 -0.075317 2.063663
H -1.197952 -1.592288 1.488880
C 1.015284 -2.552053 0.116833
H 0.073137 -3.076623 -0.076638
H 1.636020 -2.579969 -0.774638
H 1.544336 -3.053783 0.929937
C 3.043747 -0.383086 0.304889
O 3.629976 -1.387411 -0.046425
O 1.837105 -0.359654 0.987855
N 3.504180 0.890979 0.202029
H 2.815684 1.619851 0.341375
C 4.746549 1.190214 -0.482849
H 5.239684 2.044062 -0.007058
H 5.395083 0.315703 -0.411301
H 4.589550 1.417395 -1.546143
O -0.371286 1.731386 0.403415
O 0.797203 2.429739 -0.111326
H 0.445273 3.338118 -0.135208

PBN-alpha-carboxyl-O2H.log

34

C 3.221240 -0.833653 -1.596205
C 1.979868 -0.532607 -1.040562
C 1.909905 0.110443 0.203193
C 3.085374 0.435591 0.883752
C 4.329331 0.131474 0.325326
C 4.397269 -0.502767 -0.915021
H 3.273949 -1.325846 -2.563659
H 1.059556 -0.782535 -1.561299
H 3.027839 0.934000 1.848637
H 5.240207 0.391797 0.857631
H 5.363687 -0.738448 -1.352974
C 0.563003 0.376604 0.837947
H 0.677117 0.925459 1.781309
N -0.316139 1.156769 -0.061969
O 0.197616 2.266759 -0.442455
C -1.805102 1.017036 -0.045857

C -2.358137 1.324809 1.356216
H -3.450660 1.302128 1.345720
H -2.010105 0.598050 2.093480
H -2.032263 2.327077 1.654120
C -2.377484 1.997673 -1.086480
H -2.159174 3.026691 -0.796741
H -1.941490 1.811908 -2.070552
H -3.462276 1.860799 -1.141608
C -3.656784 -2.189625 -0.440721
H -3.879946 -2.153341 -1.510132
H -2.869269 -2.926291 -0.264049
H -4.550781 -2.435786 0.132562
C -2.142903 -0.394794 -0.560480
O -1.547393 -0.952327 -1.456702
O -3.241222 -0.896254 0.032353
O -0.133735 -0.846357 1.117827
O 0.461656 -1.396140 2.315225
H 1.157721 -1.959594 1.924708

PBN-alpha-CH2CONH2-HO2.log

35

C 3.865314 -1.067037 1.369971
C 2.715777 -0.275225 1.367668
C 2.040602 -0.011026 0.172732
C 2.533478 -0.537144 -1.028432
C 3.686854 -1.320075 -1.027394
C 4.353086 -1.588773 0.171283
H 4.382481 -1.267315 2.304229
H 2.343441 0.141381 2.300984
H 2.004114 -0.336421 -1.954135
H 4.063165 -1.726870 -1.962094
H 5.251174 -2.200529 0.169297
C 0.811329 0.869026 0.186821
N -0.440154 0.114014 0.049065
O -0.398965 -0.977537 -0.625724
C -1.793186 0.719321 0.328901
C -1.649142 1.904683 1.297263
H -2.642227 2.329802 1.469890
H -1.248617 1.592912 2.268855
H -1.018470 2.695915 0.882477
C -2.395468 1.202997 -1.003414
H -1.813660 2.037582 -1.403272
H -2.395884 0.393999 -1.738076
H -3.430067 1.523684 -0.846306
C -2.678466 -0.373518 1.015451
H -2.030281 -1.045429 1.588383
H -3.344181 0.130124 1.719615
C -3.619977 -1.186767 0.114246
O -4.824529 -0.965340 0.098162
N -3.030000 -2.181908 -0.607746
H -3.606661 -2.641750 -1.299742
H -2.028040 -2.130161 -0.760531
H 0.772521 1.441977 1.114899
O 0.795244 1.802618 -0.912744
O 1.829539 2.785124 -0.643338
H 2.600754 2.358659 -1.065116

PBN-alpha-CH2OH-OOH.com.log

32

C 3.726372 -0.806154 1.080136
C 2.396595 -0.418807 1.253038
C 1.642948 0.034909 0.166565
C 2.237560 0.111040 -1.099873
C 3.568568 -0.267199 -1.270735
C 4.314347 -0.728987 -0.182969
H 4.302580 -1.158607 1.931257
H 1.942166 -0.468185 2.240154
H 1.648656 0.454803 -1.943272
H 4.023110 -0.208564 -2.256074

H 5.351106 -1.024607 -0.320029
C 0.209810 0.468159 0.379362
N -0.764373 -0.490446 -0.141872
O -0.470140 -1.118407 -1.222679
C -2.209306 -0.494912 0.273909
C -2.651515 -1.961946 0.384668
H -3.730704 -2.004719 0.550278
H -2.410382 -2.500132 -0.534838
H -2.143089 -2.455680 1.220078
C -2.419811 0.233994 1.605509
H -1.883101 -0.257754 2.424442
H -2.113263 1.283209 1.551468
H -3.487302 0.212104 1.837370
C -2.986202 0.222098 -0.854034
O -4.372013 0.189430 -0.525326
H -4.852748 0.648242 -1.229803
H -2.781421 -0.299562 -1.798396
H -2.616455 1.253683 -0.938407
H 0.019157 0.621437 1.442749
O -0.093015 1.702607 -0.308884
O 0.637288 2.758570 0.370559
H 1.489140 2.726690 -0.106694

PBN-alpha-CONH2-HO2.log

32

C -3.958991 -0.664203 -0.948448
C -2.605439 -0.427988 -1.194229
C -1.801572 0.163751 -0.216060
C -2.363665 0.524130 1.013486
C -3.716457 0.294740 1.255756
C -4.516464 -0.301773 0.277649
H -4.575713 -1.122690 -1.716627
H -2.173998 -0.704461 -2.153773
H -1.742302 0.988407 1.771275
H -4.147791 0.580290 2.211348
H -5.571145 -0.479306 0.470395
C -0.341170 0.410903 -0.516417
N 0.501278 -0.705033 0.005847
O 0.178980 -1.182408 1.155032
C 1.957196 -0.809785 -0.372523
C 2.416124 -2.252078 -0.094465
H 3.498063 -2.326738 -0.239858
H 2.173702 -2.574547 0.917896
H 1.922966 -2.933510 -0.795303
C 2.174721 -0.482147 -1.852652
H 1.558162 -1.141481 -2.472776
H 1.950683 0.556717 -2.091466
H 3.224141 -0.658005 -2.104498
C 2.707611 0.215162 0.528429
N 2.734748 -0.090471 1.849660
H 3.044733 0.648820 2.468553
H 2.026536 -0.726960 2.201063
O 3.235730 1.229177 0.066039
H -0.177736 0.483244 -1.589878
O 0.074965 1.644563 0.077561
O 0.866240 2.400689 -0.874382
H 1.778833 2.218318 -0.542052

PBN-alpha-COOH-OOH.com.log

31

C 3.236563 -1.781954 -0.390852
C 1.965603 -1.268356 -0.651304
C 1.588675 -0.026120 -0.130824
C 2.492586 0.698623 0.655881
C 3.764968 0.185537 0.909725
C 4.139371 -1.054200 0.386834
H 3.522381 -2.747882 -0.798579
H 1.256375 -1.835266 -1.247775
H 2.187328 1.652440 1.073580

H	4.462205	0.751392	1.521968
H	5.131051	-1.451976	0.585857
C	0.211825	0.528596	-0.430906
H	-0.199930	0.062460	-1.326367
N	-0.728066	0.323300	0.671071
O	-0.344691	0.657794	1.847693
C	-2.184231	0.112750	0.420180
C	-2.883573	-0.105081	1.774172
H	-3.942778	-0.307897	1.600591
H	-2.439362	-0.943767	2.316613
H	-2.779012	0.789136	2.390136
C	-2.792388	1.329403	-0.313716
H	-2.629484	2.225469	0.291381
H	-2.327994	1.493943	-1.289344
H	-3.865866	1.180610	-0.456101
C	-2.352548	-1.163451	-0.420760
O	-1.474400	-1.921112	-0.770098
O	-3.652320	-1.372863	-0.734384
H	-3.676772	-2.202642	-1.248051
O	0.235028	1.958674	-0.627557
O	0.915308	2.191723	-1.887136
H	1.845810	2.222680	-1.590133

PBN-alpha-ester-O2H.log

34

C	-3.470569	0.044746	-0.949329
C	-2.154866	-0.326820	-1.231270
C	-1.296591	-0.716164	-0.197691
C	-1.763137	-0.741810	1.121686
C	-3.076775	-0.370507	1.400918
C	-3.931314	0.024045	0.368049
H	-4.133313	0.345561	-1.756209
H	-1.795729	-0.324283	-2.258105
H	-1.091402	-1.043462	1.918710
H	-3.434147	-0.386183	2.426693
H	-4.954537	0.314842	0.590297
C	0.113641	-1.158828	-0.522677
H	0.404392	-0.830969	-1.526028
N	1.133784	-0.614811	0.426344
O	1.507942	-1.357989	1.402183
C	2.039545	0.493968	0.016676
C	2.760566	1.054743	1.242358
H	3.281312	1.970332	0.945040
H	2.063184	1.279286	2.046322
H	3.496328	0.330627	1.596891
C	3.041878	-0.003195	-1.031750
H	3.612005	-0.838654	-0.617530
H	2.540258	-0.339881	-1.941867
H	3.730769	0.805632	-1.292970
C	0.322381	2.253219	-0.030268
O	0.077206	2.185239	1.148703
O	1.245566	1.480448	-0.685417
C	-0.357063	3.175746	-1.013971
H	0.369211	3.632469	-1.691700
H	-1.062789	2.594335	-1.617877
H	-0.906255	3.942458	-0.466153
O	0.091377	-2.563898	-0.441159
O	1.424881	-3.058785	-0.741659
H	1.802274	-3.003397	0.162499

PBN-alpha-ether-O2H.log

32

C	-3.406791	-0.659419	-0.989929
C	-2.108935	-0.214974	-1.248093
C	-1.346489	0.359540	-0.227169
C	-1.892268	0.495090	1.056312
C	-3.188484	0.051034	1.311722
C	-3.947325	-0.527160	0.289952
H	-3.994182	-1.105934	-1.787651

H -1.686176 -0.314841 -2.244710
H -1.293521 0.945355 1.841968
H -3.609044 0.158229 2.307928
H -4.957916 -0.872200 0.491718
C 0.052964 0.860462 -0.511106
H 0.377493 0.574209 -1.515402
N 1.064781 0.311501 0.445350
O 1.370148 1.021459 1.470187
C 2.037332 -0.743610 -0.011342
C 3.087096 -0.107726 -0.929700
H 3.821488 -0.864867 -1.220505
H 2.626026 0.292745 -1.835591
H 3.597288 0.705956 -0.407516
C 2.689180 -1.364081 1.226653
H 3.307789 -0.625129 1.737123
H 1.944662 -1.724614 1.940564
H 3.319194 -2.200862 0.909277
C 0.490631 -2.606133 -0.146836
H 1.079101 -3.377149 0.365295
H -0.179755 -2.120837 0.571619
H -0.110206 -3.078214 -0.927175
O 1.328969 -1.665482 -0.815905
O -0.021136 2.261231 -0.375255
O 1.303141 2.814180 -0.601222
H 1.653859 2.718400 0.310402

PBN-alpha-methylcarbamate-O2H.log
39

C -3.675214 -1.961297 -0.811265
C -2.461011 -1.497068 -0.307429
C -2.385217 -0.222104 0.268992
C -3.535611 0.570572 0.338762
C -4.748857 0.105661 -0.170892
C -4.819837 -1.162668 -0.747683
H -3.728367 -2.951948 -1.255109
H -1.569220 -2.109015 -0.360664
H -3.485629 1.555733 0.797540
H -5.635591 0.731113 -0.111719
H -5.763524 -1.529655 -1.142789
C -1.083745 0.311379 0.831138
H -1.254343 1.253599 1.351102
N -0.081691 0.563416 -0.237317
O 0.265323 -0.449749 -0.945352
C 0.689148 1.831759 -0.440802
C 0.748455 2.095555 -1.954389
H 1.356276 2.984388 -2.155560
H 1.183468 1.242224 -2.474478
H -0.258947 2.266987 -2.347689
C 0.027360 3.019525 0.274803
H -1.015315 3.134983 -0.038139
H 0.062865 2.925059 1.364574
H 0.556520 3.938772 0.002618
C 2.111890 1.674053 0.148183
H 2.059056 1.418911 1.206848
H 2.649628 2.619927 0.028285
C 3.060148 -0.518661 0.035015
O 2.749945 -0.798057 1.188254
O 2.890390 0.696409 -0.550322
N 3.693076 -1.358778 -0.816708
H 3.756064 -1.052436 -1.777236
C 3.873893 -2.766772 -0.508484
H 4.804434 -3.124761 -0.958446
H 3.935564 -2.874106 0.574912
H 3.038770 -3.377727 -0.874188
O -0.614586 -0.651990 1.751662
O 0.455535 -0.036362 2.520472
H 1.247338 -0.446133 2.094906

PBN-alpha-methylcarboxyl-O2H.log
37

C	4.034583	-1.121635	0.733370
C	3.232606	0.011625	0.602058
C	2.006052	-0.066550	-0.066442
C	1.586748	-1.285458	-0.610289
C	2.389185	-2.417961	-0.475347
C	3.612061	-2.338626	0.194657
H	4.985115	-1.055091	1.255626
H	3.561714	0.962527	1.014941
H	0.629842	-1.346929	-1.116532
H	2.056424	-3.364743	-0.891484
H	4.233371	-3.224113	0.299751
C	1.179507	1.190631	-0.244369
H	1.400366	1.922293	0.542545
N	-0.293429	0.938711	-0.212175
O	-0.922661	0.942035	-1.333468
C	-1.093274	1.114464	1.040679
C	-0.395496	0.424223	2.224601
H	-1.009723	0.552292	3.123004
H	-0.268942	-0.642138	2.033871
H	0.582142	0.868278	2.435672
C	-1.254670	2.627368	1.307098
H	-0.295121	3.095394	1.547792
H	-1.669640	3.128963	0.427646
H	-1.929756	2.791075	2.154490
C	-2.493940	0.518998	0.782336
H	-3.055591	1.150073	0.092136
H	-3.039386	0.521434	1.735222
C	-3.832816	-2.440316	-0.965361
H	-4.808396	-2.440261	-1.452155
H	-3.042854	-2.657497	-1.688963
H	-3.800063	-3.186554	-0.166981
O	-3.670790	-1.116654	-0.429552
C	-2.521530	-0.900359	0.242291
O	-1.676246	-1.754969	0.407860
O	1.547729	1.708828	-1.497416
O	0.826942	2.956078	-1.698528
H	-0.009380	2.573036	-2.044211

PBN-alpha-methylester-O2H.log

37

C	-2.365793	-1.950729	1.318662
C	-1.017387	-1.721331	1.052018
C	-0.611146	-1.367948	-0.241062
C	-1.560351	-1.251659	-1.260239
C	-2.911853	-1.476858	-0.990488
C	-3.315279	-1.828219	0.298690
H	-2.677492	-2.229087	2.321744
H	-0.272673	-1.811909	1.836470
H	-1.245848	-0.986448	-2.266761
H	-3.644835	-1.380510	-1.786452
H	-4.366027	-2.009382	0.509060
C	0.859128	-1.163417	-0.539704
N	1.521158	-0.237411	0.432664
O	2.163693	-0.778061	1.404264
C	1.841136	1.185424	0.083458
C	2.191721	1.926124	1.381255
H	2.394246	2.977234	1.149322
H	1.363726	1.878405	2.091570
H	3.075844	1.489935	1.847691
C	3.042901	1.200128	-0.885170
H	2.815576	0.707335	-1.835857
H	3.347080	2.230738	-1.097473
H	3.887416	0.678132	-0.427168
C	0.638913	1.846937	-0.601971
H	0.331912	1.326461	-1.512843
H	0.909675	2.867831	-0.892987
C	-1.644760	2.315621	-0.200963
O	-1.773338	2.671251	-1.351093
O	-0.463183	1.888735	0.316121

C	-2.734863	2.261353	0.839969
H	-3.631317	2.745720	0.451308
H	-2.955669	1.215102	1.077749
H	-2.410003	2.749773	1.763558
H	1.007494	-0.746790	-1.542353
O	1.437373	-2.442077	-0.453333
O	2.860271	-2.316400	-0.719791
H	3.150053	-2.080834	0.188703

PBN-alpha-methylether-O2H.log

35

C	3.734853	0.571713	-0.691304
C	2.394590	0.263548	-0.917028
C	1.640471	-0.359081	0.085643
C	2.240478	-0.676725	1.307374
C	3.582489	-0.366402	1.532839
C	4.330311	0.258906	0.533951
H	4.316848	1.054462	-1.471738
H	1.923252	0.499783	-1.866314
H	1.657606	-1.170315	2.081418
H	4.042222	-0.613720	2.485824
H	5.375197	0.501530	0.708373
C	0.196505	-0.731514	-0.173919
N	-0.583534	0.402459	-0.781622
O	-0.856314	0.321018	-2.036171
C	-1.434078	1.314629	0.051897
C	-0.696521	1.715743	1.337723
H	-1.320225	2.419473	1.899505
H	-0.499077	0.863889	1.990369
H	0.250498	2.209689	1.100871
C	-1.738061	2.562511	-0.790725
H	-0.806716	3.049731	-1.094568
H	-2.296513	2.309751	-1.693774
H	-2.320776	3.271760	-0.194219
C	-2.757319	0.583539	0.361827
H	-3.149879	0.170969	-0.579691
H	-3.494561	1.306431	0.750016
C	-3.566018	-1.413705	1.335235
H	-3.636201	-1.943229	0.374400
H	-3.308466	-2.130370	2.118865
H	-4.541957	-0.961738	1.570863
O	-2.534754	-0.443582	1.308612
H	-0.330775	-1.021264	0.738375
O	0.249528	-1.807000	-1.077248
O	-1.110727	-2.244763	-1.350943
H	-1.323802	-1.578421	-2.042288

PBN-alpha-methylphosphoryl-HO2.log

42

C	4.437578	-1.757862	-0.492479
C	3.837912	-0.500670	-0.464827
C	2.518536	-0.356392	-0.015504
C	1.802063	-1.478580	0.410203
C	2.404942	-2.737755	0.373907
C	3.719063	-2.880374	-0.072713
H	5.461069	-1.862239	-0.842257
H	4.396239	0.376406	-0.783599
H	0.770409	-1.381717	0.730169
H	1.838839	-3.608559	0.692617
H	4.182599	-3.863136	-0.098862
C	1.942060	1.045241	0.043936
N	0.442557	1.100165	0.067278
O	-0.115613	1.465585	1.167388
C	-0.342677	1.287334	-1.195361
C	-0.118544	2.733216	-1.696956
H	-0.773093	2.938814	-2.550613
H	-0.342615	3.452023	-0.902960
H	0.914093	2.892029	-2.022548

C	0.104222	0.266976	-2.254372
H	1.160680	0.387734	-2.512455
H	-0.056678	-0.755038	-1.905533
H	-0.476695	0.424852	-3.169747
C	-1.845564	1.136064	-0.864575
H	-2.398586	1.203181	-1.806261
H	-2.174665	1.958963	-0.226351
H	2.267918	1.635756	-0.821411
O	2.458640	1.613866	1.218723
O	2.067694	3.014788	1.250456
P	-2.408072	-0.410950	-0.050150
O	-3.750192	-0.659981	-0.924906
O	-3.046513	0.007098	1.378829
C	-2.376068	-0.321228	2.612659
H	-3.113941	-0.172922	3.403724
H	-2.040954	-1.361434	2.602448
H	-1.520646	0.340544	2.762487
C	-4.597746	-1.772085	-0.589188
H	-5.370058	-1.814557	-1.359124
H	-4.025158	-2.704576	-0.586690
H	-5.059812	-1.615243	0.390371
O	-1.452156	-1.552217	0.019147
H	1.174700	2.895799	1.642419

PBN-alpha-methylthio-O2H.log

35

C	4.133367	-0.405346	1.024603
C	2.868716	0.168004	0.907872
C	2.201869	0.145290	-0.323906
C	2.812810	-0.446813	-1.433158
C	4.078689	-1.022654	-1.313347
C	4.739433	-1.002695	-0.084323
H	4.647925	-0.386045	1.981399
H	2.389016	0.633624	1.763190
H	2.299661	-0.455383	-2.391929
H	4.547101	-1.483605	-2.178589
H	5.724866	-1.450910	0.010212
C	0.841300	0.797025	-0.458748
N	-0.099266	0.375364	0.627273
O	-0.219664	1.167560	1.631614
C	-1.167246	-0.665355	0.433631
C	-0.736723	-1.688347	-0.629742
H	-1.442507	-2.523615	-0.630957
H	-0.734588	-1.271989	-1.641687
H	0.258288	-2.085979	-0.408215
C	-1.359495	-1.367205	1.787254
H	-0.444097	-1.898059	2.069245
H	-1.592354	-0.640979	2.567857
H	-2.176751	-2.090395	1.720687
C	-2.432098	0.122939	0.007528
H	-2.213205	0.697416	-0.900015
H	-2.677979	0.830236	0.805992
S	-3.889743	-0.953712	-0.312582
C	-5.100516	0.349635	-0.727434
H	-4.783713	0.919398	-1.606291
H	-6.044347	-0.153165	-0.953469
H	-5.254614	1.029072	0.116311
H	0.372201	0.547804	-1.415468
O	1.076374	2.180607	-0.376388
O	-0.201375	2.863339	-0.491709
H	-0.467471	2.815515	0.452594

PBN-alpha-phosphoryl-HO2.log

39

C	4.247207	-0.734789	0.772391
C	3.209884	0.194061	0.691018
C	2.160800	-0.003479	-0.215759
C	2.156805	-1.137758	-1.035530

C	3.193050	-2.069273	-0.946003
C	4.240229	-1.867838	-0.045010
H	5.058558	-0.577424	1.478150
H	3.200690	1.068984	1.333212
H	1.334836	-1.290362	-1.730025
H	3.185660	-2.947440	-1.586251
H	5.049830	-2.590154	0.019616
C	1.041063	1.006878	-0.336132
N	0.047588	0.901110	0.741099
O	0.433444	0.537098	1.906784
C	-1.411882	1.123294	0.484533
C	-2.111041	1.408186	1.819582
H	-3.180357	1.548033	1.641775
H	-1.970626	0.594804	2.530353
H	-1.699825	2.324355	2.255657
C	-1.629449	2.289664	-0.498015
H	-1.153947	3.192286	-0.104278
H	-1.221631	2.090417	-1.491769
H	-2.702597	2.466847	-0.607496
H	0.526868	0.883106	-1.289512
P	-2.024919	-0.462976	-0.279787
O	-3.593435	-0.133499	-0.459533
O	-2.066992	-1.573448	0.896275
C	-0.942039	-2.448431	1.135287
H	-1.338559	-3.316778	1.664787
H	-0.490534	-2.758815	0.190072
H	-0.203090	-1.933828	1.753866
C	-4.450826	-1.105554	-1.090744
H	-5.418660	-0.619866	-1.223487
H	-4.044147	-1.400298	-2.062252
H	-4.560545	-1.983776	-0.447789
O	-1.273918	-0.876879	-1.499642
O	1.513952	2.364624	-0.228537
O	2.272930	2.636920	-1.435122
H	3.158095	2.318498	-1.171030

PBN-alpha-thio-O2H.log

32

C	3.291568	0.093824	1.274531
C	2.012986	0.589012	1.021459
C	1.437804	0.425084	-0.246015
C	2.153869	-0.227347	-1.253893
C	3.433763	-0.721114	-0.997952
C	4.003642	-0.561416	0.266305
H	3.734818	0.223497	2.258167
H	1.452108	1.102462	1.795865
H	1.707039	-0.353265	-2.236458
H	3.984646	-1.228255	-1.785382
H	5.000779	-0.944856	0.465802
C	0.061793	0.988579	-0.532329
H	-0.288654	0.691229	-1.524145
N	-0.966862	0.533009	0.452369
O	-1.128827	1.252746	1.503714
C	-2.053865	-0.425483	0.079418
C	-2.795550	-0.836677	1.354215
H	-3.297006	0.027464	1.795900
H	-3.540527	-1.595751	1.100881
H	-2.113041	-1.241271	2.105218
C	-3.021175	0.237739	-0.918826
H	-3.418013	1.156917	-0.477409
H	-2.532271	0.498701	-1.861288
H	-3.852395	-0.439688	-1.135619
S	-1.330619	-1.890028	-0.804956
C	-0.353981	-2.711127	0.504349
H	0.335788	-2.009296	0.979446
H	-0.996301	-3.179673	1.253517
H	0.228304	-3.487667	0.001457
O	0.215179	2.388184	-0.441531
O	-1.083236	3.008984	-0.639651

H -1.397388 2.983090 0.288941

PBN-CH₂NHCOMe-HO₂c.log

38

C -4.567821 0.892637 0.315375
C -3.178705 0.901667 0.420751
C -2.439046 -0.251756 0.129149
C -3.109470 -1.412297 -0.265772
C -4.502039 -1.417311 -0.375274
C -5.235168 -0.267713 -0.084877
H -5.129790 1.795202 0.540935
H -2.666306 1.811131 0.718540
H -2.537329 -2.305567 -0.487999
H -5.011257 -2.325200 -0.687868
H -6.318737 -0.272849 -0.169513
C -0.933410 -0.275499 0.342748
N -0.305305 0.976796 -0.138074
O -0.733302 1.448312 -1.258068
C 1.113016 1.323737 0.202322
C 1.241775 2.853477 0.142181
H 2.293869 3.143714 0.249930
H 0.677559 3.324827 0.954034
C 1.481895 0.832748 1.608266
H 0.784488 1.244359 2.346318
H 1.484358 -0.254877 1.692622
C 1.981131 0.661571 -0.922944
H 1.919304 1.283322 -1.820174
H 1.557541 -0.310041 -1.171521
N 3.380137 0.447532 -0.590820
H 4.037612 1.201486 -0.728113
C 3.857549 -0.759645 -0.182996
O 3.135123 -1.743798 -0.002574
C 5.355875 -0.848220 0.039459
H 5.762935 -1.622420 -0.618142
H 5.885217 0.091256 -0.146330
H 5.542022 -1.166001 1.069754
H 2.481776 1.195637 1.863324
H -0.704202 -0.384392 1.402925
O -0.358141 -1.409771 -0.321591
O 0.433284 -2.170374 0.634661
H 0.862411 3.231487 -0.809313
H 1.345487 -2.046677 0.273087

PBN-NHCOMe-HO₂c.log

35

C -4.019690 0.342666 -1.417524
C -2.723222 0.644412 -1.005253
C -2.195939 0.040210 0.140250
C -2.977037 -0.861369 0.868064
C -4.273113 -1.168502 0.451890
C -4.795742 -0.565565 -0.692758
H -4.425994 0.816498 -2.307020
H -2.116181 1.350892 -1.559976
H -2.573264 -1.325206 1.765770
H -4.874138 -1.869463 1.024711
H -5.806782 -0.797852 -1.016794
O 0.049387 -0.558194 -1.407685
C 1.603127 -0.705494 0.368023
N 2.483329 0.107939 -0.489964
H 2.057821 0.356381 -1.374836
C 3.848305 0.140878 -0.398865
O 4.485491 -0.370180 0.517594
C 4.543347 0.881726 -1.534021
H 5.088341 0.157021 -2.148831
H 3.859522 1.446377 -2.174859
H 5.280452 1.564953 -1.103791
C 1.865753 -2.206031 0.158593
H 1.672049 -2.471763 -0.883445
H 2.907321 -2.424055 0.405644

H 1.211375 -2.803288 0.802452
C 1.764351 -0.308423 1.837017
H 1.118672 -0.914602 2.480314
H 2.803704 -0.485092 2.116504
H 1.542114 0.751931 1.982076
N 0.218893 -0.418231 -0.143656
C -0.790373 0.341816 0.604526
H -0.685903 0.104999 1.665264
O -0.400343 1.711102 0.400818
O -1.207293 2.506964 1.321802
H -0.491208 2.938823 1.822290

PBN-O2H.log

31

C -3.072931 -0.296990 1.343319
C -1.776394 0.153226 1.102682
C -1.298622 0.239301 -0.211323
C -2.128996 -0.120838 -1.276447
C -3.426502 -0.574390 -1.033311
C -3.899069 -0.662979 0.276802
H -3.440825 -0.361785 2.363683
H -1.126193 0.440298 1.923328
H -1.762137 -0.043690 -2.297304
H -4.066184 -0.855313 -1.865478
H -4.909136 -1.015591 0.467595
C 0.097929 0.763942 -0.471749
H 0.399460 0.603706 -1.512279
N 1.121375 0.103631 0.400393
O 1.510611 0.757485 1.436296
C 2.007960 -1.004502 -0.090558
C 1.260160 -1.890542 -1.099849
H 1.888119 -2.755011 -1.339605
H 0.317330 -2.261630 -0.686437
H 1.048940 -1.376121 -2.042483
C 3.251867 -0.360838 -0.733684
H 2.977348 0.277223 -1.580516
H 3.777250 0.254861 0.002365
H 3.937363 -1.136167 -1.093257
C 2.404923 -1.843468 1.134439
H 1.523775 -2.313566 1.584195
H 3.099176 -2.632651 0.827486
H 2.886445 -1.221047 1.890310
O 0.042853 2.139288 -0.189926
O 1.360419 2.700746 -0.436048
H 1.766620 2.479374 0.431151

PBN-alpha-2CH2OH-OOH.com.log

33

C -3.717668 -0.826431 1.465899
C -2.420016 -0.314984 1.412592
C -1.844560 0.032054 0.186844
C -2.586546 -0.123765 -0.991430
C -3.885790 -0.626385 -0.937119
C -4.452596 -0.981285 0.289933
H -4.155046 -1.094378 2.423767
H -1.851704 -0.183716 2.330890
H -2.134514 0.137764 -1.942004
H -4.454999 -0.748363 -1.854705
H -5.465116 -1.374126 0.328428
C -0.443271 0.600510 0.152836
H -0.151012 0.920022 1.155238
N 0.549911 -0.348419 -0.353910
O 0.180752 -1.149630 -1.285748
C 2.037629 -0.195577 -0.142849
C 2.676311 0.280552 -1.454548
H 3.758386 0.333339 -1.331974
H 2.436064 -0.420140 -2.258133
H 2.290175 1.268962 -1.723143
C 2.290926 0.821228 0.988297

H	1.813445	1.775118	0.723564
H	1.835756	0.451325	1.923279
C	2.518133	-1.618901	0.234970
O	3.930556	-1.705933	0.140781
H	4.159129	-2.646651	0.115320
H	2.027889	-2.312971	-0.457886
H	2.167246	-1.849852	1.255222
O	3.690666	0.984657	1.141111
H	3.830103	1.726547	1.748221
O	-0.339189	1.740696	-0.727418
O	-1.089153	2.819901	-0.108221
H	-1.979549	2.656436	-0.475304

PBN-alpha-2COOH-HO2.com.log

31

C	-3.489393	-1.743349	-0.036189
C	-2.226157	-1.157380	0.045833
C	-2.102278	0.234939	0.118078
C	-3.253857	1.031364	0.110372
C	-4.514370	0.440107	0.020602
C	-4.636158	-0.948022	-0.052084
H	-3.574196	-2.825158	-0.093338
H	-1.341368	-1.785588	0.050264
H	-3.158853	2.110124	0.164841
H	-5.401245	1.067966	0.007101
H	-5.618541	-1.407593	-0.121431
C	-0.741992	0.892573	0.299105
H	-0.517331	1.038306	1.358036
N	0.347266	0.074378	-0.276811
O	0.267909	-0.229843	-1.520367
C	1.617314	-0.278538	0.389833
C	1.534152	-0.238170	1.926496
H	1.393744	0.784526	2.285396
H	0.710317	-0.870424	2.264720
H	2.463920	-0.624566	2.349449
C	1.876308	-1.746966	-0.048553
O	1.270175	-2.680162	0.421504
O	2.817016	-1.860601	-0.997103
H	2.863599	-2.806261	-1.237061
O	-0.789538	2.158465	-0.326822
O	0.327855	2.932904	0.179301
C	2.738903	0.667567	-0.089578
O	2.600210	1.629434	-0.812930
O	3.922537	0.327442	0.451546
H	4.580531	0.964942	0.113517
H	1.024418	2.687209	-0.468327

PBN-CH2CONH2-2-OOH.com.log

39

C	3.577013	-2.138996	0.117560
C	2.374628	-1.466432	0.327489
C	2.308063	-0.074383	0.190905
C	3.462308	0.634395	-0.156051
C	4.664498	-0.042428	-0.371636
C	4.726653	-1.428736	-0.235076
H	3.613830	-3.219706	0.224970
H	1.484833	-2.031034	0.589542
H	3.413208	1.712138	-0.259185
H	5.553256	0.519413	-0.646074
H	5.663060	-1.954186	-0.402016
C	1.027853	0.682102	0.521138
N	-0.167666	-0.078724	0.075832
O	-0.124768	-0.507590	-1.138590
C	-1.513303	-0.080068	0.753722
C	-1.942391	-1.554247	1.058542
H	-2.651277	-1.524862	1.888886
H	-1.055191	-2.097348	1.407770
C	-1.442280	0.653781	2.103372
H	-0.793536	0.119819	2.806888

H -1.097258 1.682215 2.004045
H -2.446222 0.677485 2.536325
C -2.533131 0.599946 -0.209421
H -2.751251 -0.071929 -1.040908
H -3.464450 0.766310 0.340122
C -2.040246 1.942782 -0.733323
O -1.955759 2.940096 -0.008446
N -1.709468 1.971088 -2.049509
H -1.221589 2.797520 -2.373494
H -1.475909 1.101504 -2.511161
C -2.660868 -2.394298 -0.011713
O -3.799592 -2.798981 0.183741
N -1.935694 -2.715792 -1.120639
H -2.430041 -3.203063 -1.856487
H -1.123329 -2.155326 -1.362503
H 0.946779 0.849652 1.593935
O 1.059671 1.958985 -0.113302
O 0.660364 2.982951 0.836998
H -0.247222 3.191197 0.503303

PBN-CH2COOMe-2-OOH.com.log

43

C 3.437684 -3.084436 -0.425111
C 2.364732 -2.242254 -0.139954
C 2.585410 -0.896385 0.178005
C 3.894570 -0.407838 0.208638
C 4.968185 -1.252665 -0.080867
C 4.744447 -2.591901 -0.397682
H 3.251784 -4.125604 -0.675260
H 1.351894 -2.630893 -0.178310
H 4.066351 0.633609 0.454959
H 5.980903 -0.858891 -0.058261
H 5.580406 -3.248617 -0.623587
C 1.431916 0.006150 0.594637
N 0.229121 -0.251342 -0.214845
O 0.393009 -0.381750 -1.483322
C -1.185967 -0.007979 0.240724
C -1.962195 -1.255909 -0.251576
H -1.797523 -1.371058 -1.328667
H -1.532626 -2.151411 0.212458
C -1.281763 0.103599 1.767060
H -0.930624 -0.818338 2.245210
H -0.714613 0.947098 2.159526
H -2.330108 0.247223 2.039014
C -1.725342 1.252135 -0.499672
H -2.750017 1.424709 -0.158140
H -1.741048 1.047480 -1.571202
C 0.298989 4.245832 -1.291119
H -0.224427 5.013071 -0.715835
H 1.243802 3.997929 -0.801334
H 0.474582 4.578555 -2.313780
O -0.512295 3.061114 -1.410426
C -0.926649 2.513851 -0.264273
O -0.702580 3.009839 0.832711
C -3.456908 -1.274938 0.006791
O -4.150761 -0.351181 0.382307
O -3.948311 -2.502832 -0.258276
C -5.369154 -2.653966 -0.088546
H -5.583641 -3.690651 -0.348385
H -5.655343 -2.448691 0.946193
H -5.909201 -1.971341 -0.749673
H 1.183360 -0.153681 1.643132
O 1.818664 1.385107 0.471999
O 1.682364 2.034153 1.764679
H 0.883806 2.583519 1.586150

PBN-CH2NHCOMe-2-OOH.com.log

45

C -4.895810 1.220178 0.736514

C -3.586992 0.779520 0.915216
C -3.043380 -0.190676 0.063555
C -3.827424 -0.717092 -0.964654
C -5.138581 -0.269441 -1.145958
C -5.676323 0.697572 -0.298335
H -5.306898 1.973094 1.403788
H -2.981230 1.196541 1.715282
H -3.411086 -1.478423 -1.613692
H -5.739128 -0.684055 -1.951272
H -6.697557 1.041852 -0.438628
C -1.639588 -0.711822 0.320990
N -0.661790 0.412864 0.377973
O -0.891075 1.451211 -0.351185
C 0.762432 0.173781 0.759567
C 1.366808 1.512841 1.273178
H 2.310591 1.283995 1.772028
H 0.682513 1.940449 2.013024
C 0.847903 -0.830117 1.919181
H 0.294869 -0.454415 2.788034
H 0.461347 -1.813574 1.652639
C 1.485498 -0.310843 -0.534426
H 1.577989 0.538573 -1.213582
H 0.866721 -1.049878 -1.034466
N 2.789861 -0.895888 -0.314857
H 3.565709 -0.253690 -0.181654
C 2.958059 -2.240950 -0.272788
O 2.019702 -3.041437 -0.386033
C 4.380057 -2.733535 -0.087800
H 4.660792 -3.335215 -0.958088
H 5.105338 -1.924395 0.036212
H 4.417614 -3.390273 0.786575
N 1.667463 2.523072 0.278047
H 0.869954 2.961371 -0.163364
C 2.897426 2.619106 -0.299990
O 3.841014 1.885274 0.010048
C 3.053851 3.711706 -1.342703
H 2.130331 4.264067 -1.538369
H 3.821050 4.413736 -1.000697
H 3.413580 3.266707 -2.275370
H 1.893361 -0.950669 2.214212
H -1.598309 -1.233560 1.277577
O -1.263375 -1.658996 -0.683354
O -0.797487 -2.880859 -0.042610
H 0.159865 -2.895464 -0.302544

PBN-CH2OCOMe-2-OOHb.com.log

43

C 0.367477 -0.553131 -1.031294
N -0.401561 0.248086 -0.047443
O -0.450832 -0.114768 1.183970
C -1.188940 1.468264 -0.401771
C -2.595705 1.296008 0.212430
H -3.231017 2.138576 -0.078891
H -2.527217 1.252273 1.298673
C -0.510134 2.670226 0.296137
H -0.430921 2.470265 1.366198
H -1.111007 3.574026 0.146209
C -1.285692 1.694290 -1.915793
H -1.684780 0.812434 -2.419178
H -0.315271 1.954869 -2.342737
O -3.177390 0.102862 -0.320821
O 0.763276 2.923657 -0.295026
C -3.550378 -0.947569 0.453572
O -3.672308 -2.026307 -0.087981
C 1.959217 2.648021 0.322132
O 2.959061 2.737145 -0.345569
C 1.953980 2.280554 1.790713
H 1.477714 3.059922 2.396431
H 1.422155 1.339161 1.964356
H 2.992286 2.168747 2.102873

C -3.810942 -0.725411 1.924403
H -2.855768 -0.617270 2.450621
H -4.414045 0.168904 2.109022
H -4.325714 -1.605617 2.310217
H -1.959524 2.537465 -2.103178
H 0.725884 0.143639 -1.791722
O -0.494276 -1.370756 -1.815814
O -1.035170 -2.447346 -1.005950
H -1.994071 -2.230453 -1.016216
C 1.566772 -1.238553 -0.410586
C 2.836597 -0.791199 -0.798844
C 1.465727 -2.288216 0.514981
C 3.990262 -1.382764 -0.281609
H 2.930596 0.035054 -1.499114
C 2.619840 -2.882389 1.021968
H 0.489979 -2.636050 0.823191
C 3.883121 -2.434023 0.627545
H 4.966194 -1.020574 -0.592436
H 2.531274 -3.700363 1.732111
H 4.778091 -2.902136 1.029316

PBN-CH2OCONHMe-2-OOH.com.log
47

C 4.354486 -1.509886 1.851182
C 3.235939 -1.622213 1.024695
C 2.826224 -0.529543 0.242790
C 3.550466 0.668937 0.315985
C 4.664576 0.778037 1.149021
C 5.071894 -0.313607 1.916078
H 4.661426 -2.360883 2.453707
H 2.663737 -2.539961 1.003467
H 3.231705 1.520947 -0.278861
H 5.213602 1.714810 1.195444
H 5.940781 -0.232729 2.564110
C 1.679498 -0.584230 -0.744954
H 1.573104 0.398646 -1.208405
N 0.383771 -0.935665 -0.140489
O 0.361004 -1.759140 0.847066
C -0.909180 -0.757706 -0.878599
C -0.987732 0.605128 -1.584825
H -1.936450 0.645733 -2.122774
H -0.169396 0.751369 -2.290496
C -1.097540 -1.876108 -1.922557
H -0.414946 -1.750893 -2.765723
H -0.885645 -2.843219 -1.457859
H -2.129534 -1.872211 -2.285296
C -2.010578 -0.850904 0.202954
H -1.814487 -0.123578 0.996171
H -2.011880 -1.859669 0.624435
C -4.413873 -0.428119 0.277111
O -5.421498 -0.050622 -0.282183
O -3.256873 -0.566614 -0.440627
N -4.334052 -0.706371 1.617081
H -3.549656 -1.238809 1.962823
C -5.550595 -0.716643 2.416681
H -6.145567 -1.626562 2.263093
H -5.281633 -0.638366 3.473546
H -6.162222 0.141652 2.135266
O -1.016143 1.690281 -0.641154
C 0.000057 2.597522 -0.669389
O 0.998781 2.507690 -1.371591
N -0.265839 3.603043 0.199634
H -1.148887 3.564608 0.687956
C 0.628511 4.726693 0.402628
H 0.141862 5.671951 0.135581
H 0.963303 4.782230 1.444993
H 1.495934 4.582142 -0.242190
O 1.957689 -1.385229 -1.906914
O 2.119201 -2.776469 -1.529861
H 3.087487 -2.817569 -1.413248

PBN-CH2OMe-2-OOH.com.log

39

C	-4.328792	1.435091	0.610713
C	-3.061842	0.967198	0.963304
C	-2.390214	0.054989	0.144163
C	-3.004045	-0.397425	-1.031168
C	-4.273194	0.063340	-1.378733
C	-4.936585	0.981755	-0.560694
H	-4.842097	2.144390	1.254180
H	-2.593392	1.311846	1.882604
H	-2.477083	-1.098472	-1.669377
H	-4.742858	-0.289071	-2.293112
H	-5.925314	1.339923	-0.834813
C	-1.026150	-0.454418	0.552441
N	0.060690	0.123664	-0.238385
O	-0.154826	0.370535	-1.481254
C	1.492338	0.113559	0.206039
C	2.057947	1.486844	-0.239951
H	2.173121	1.502246	-1.332863
H	1.323091	2.266946	0.024068
C	1.624673	-0.057681	1.720488
H	1.139738	0.761246	2.263417
H	1.204735	-1.012421	2.051154
H	2.686689	-0.043826	1.966805
C	2.156240	-1.068263	-0.538752
H	2.022809	-0.920537	-1.621683
H	1.635695	-1.997685	-0.257702
C	4.176343	-2.221451	-0.828436
H	4.139169	-2.138893	-1.926836
H	5.220389	-2.198710	-0.505303
H	3.731802	-3.188171	-0.540777
O	3.524123	-1.138679	-0.200795
O	3.287645	1.734568	0.403630
C	3.872342	2.950859	-0.006370
H	4.810209	3.058091	0.544744
H	4.088773	2.955519	-1.086741
H	3.223147	3.813463	0.218514
H	-0.843794	-0.240400	1.606696
O	-0.897812	-1.880347	0.359193
O	-1.753593	-2.518934	1.343415
H	-2.598325	-2.554662	0.853933

PBN-CH2POOMe-2-OOH.com.log

53

C	5.455663	-0.419758	-0.331003
C	4.136463	-0.822882	-0.539501
C	3.188026	-0.687001	0.487876
C	3.589247	-0.134425	1.711765
C	4.908018	0.274113	1.914710
C	5.846145	0.128372	0.892874
H	6.180135	-0.527134	-1.133975
H	3.832031	-1.216202	-1.500130
H	2.862996	-0.019292	2.512716
H	5.199036	0.702866	2.869708
H	6.874816	0.443560	1.046447
C	1.759652	-1.173312	0.375988
N	1.000751	-0.575357	-0.730269
O	1.627736	-0.152950	-1.767019
C	-0.502177	-0.726100	-0.892442
C	-0.723414	-1.770637	-2.003877
H	-1.781925	-1.837139	-2.259308
H	-0.148963	-1.483335	-2.887765
H	-0.380074	-2.754978	-1.672367
C	-1.121121	-1.178950	0.452511
H	-0.744510	-2.173720	0.708231
H	-0.816607	-0.486573	1.245090
C	-1.022133	0.652594	-1.374975
H	-2.109456	0.621240	-1.473480

H -0.594908 0.865872 -2.357669
H 1.235983 -0.936077 1.303665
P -0.621468 2.078848 -0.296086
O -1.916297 3.005881 -0.580089
O 0.528597 2.956390 -1.022927
C 1.909171 2.881843 -0.612877
H 2.397238 2.047796 -1.121038
H 2.367960 3.827359 -0.909883
H 1.981437 2.754230 0.470025
C -1.950106 4.344224 -0.056218
H -1.796733 4.339122 1.027650
H -1.184280 4.960081 -0.536340
H -2.941359 4.739006 -0.285678
O -0.324931 1.762418 1.134811
P -2.924583 -1.289385 0.714418
O -3.267556 -1.967353 1.991289
O -3.536418 0.209847 0.572401
O -3.487098 -1.966361 -0.641537
C -4.884868 -2.310571 -0.706211
H -5.016834 -2.887551 -1.622901
H -5.169413 -2.913657 0.160318
H -5.494744 -1.402922 -0.746294
C -3.694425 1.029558 1.750945
H -4.119845 0.441517 2.567618
H -2.727327 1.447187 2.044317
H -4.375396 1.835084 1.469959
O 1.640640 -2.609308 0.376820
O 2.255440 -3.153308 -0.817838

PBN-CH2SMe-2-OOH.com.log

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C 4.442211 -0.591843 1.813069
C 3.178157 -0.070539 1.532629
C 2.710602 -0.014289 0.216451
C 3.527032 -0.474105 -0.825215
C 4.793201 -0.986272 -0.545825
C 5.252025 -1.048687 0.772720
H 4.795644 -0.631887 2.839728
H 2.552345 0.297215 2.342916
H 3.159217 -0.437570 -1.845003
H 5.420764 -1.343966 -1.357593
H 6.239074 -1.449603 0.987049
C 1.348037 0.577779 -0.065935
H 1.005850 1.143774 0.801924
N 0.341749 -0.432860 -0.405730
O 0.736206 -1.459413 -1.063935
C -1.159301 -0.152770 -0.428001
C -1.777127 -1.437834 0.180686
H -1.218964 -2.288187 -0.216954
H -1.650783 -1.416775 1.269871
C -1.426473 1.102710 0.431336
H -1.056528 0.937377 1.449878
H -0.885363 1.945919 -0.006638
C -1.551986 0.062238 -1.899442
H -1.294640 -0.824816 -2.482750
H -1.009258 0.921430 -2.304251
S -3.558645 -1.696374 -0.203295
S -3.195677 1.618916 0.538788
C -3.802528 -3.210504 0.787168
H -4.839195 -3.523552 0.638101
H -3.138966 -4.014460 0.453039
H -3.641756 -3.020204 1.853030
C -2.910747 3.380625 0.944086
H -2.361671 3.891496 0.146850
H -3.897465 3.840843 1.044342
H -2.374933 3.494957 1.891631
H -2.623638 0.251617 -1.992637
O 1.365510 1.472455 -1.199968
O 2.115410 2.648993 -0.796028
H 3.021546 2.380401 -1.043212

PBN-CONH2-2-OOH.com.log

33

C -3.755029 -1.660364 -0.383008
C -2.451922 -1.198137 -0.550835
C -2.116811 0.115368 -0.197745
C -3.100678 0.961193 0.318769
C -4.405548 0.492907 0.490880
C -4.736603 -0.815432 0.141605
H -4.004213 -2.680984 -0.660652
H -1.691254 -1.861762 -0.953533
H -2.842701 1.980287 0.581895
H -5.163089 1.157413 0.897464
H -5.752830 -1.176734 0.274070
C -0.713532 0.631881 -0.464414
N 0.303523 -0.334205 0.049837
O 0.068572 -0.827589 1.218946
C 1.739972 -0.224126 -0.358193
C 1.889558 0.172819 -1.831538
H 1.350710 -0.537683 -2.467362
H 1.530724 1.183727 -2.019473
H 2.950047 0.127060 -2.080965
C 2.372704 0.868210 0.567040
N 2.550847 0.496567 1.854316
H 2.797265 1.227347 2.510063
H 2.044954 -0.305591 2.209091
O 2.656793 1.986679 0.142018
C 2.530522 -1.563737 -0.183998
O 3.702451 -1.587093 -0.526461
N 1.857215 -2.649740 0.275162
H 2.411130 -3.480903 0.435481
H 0.985290 -2.529602 0.775358
H -0.542588 0.757446 -1.533186
O -0.521555 1.893749 0.162778
O 0.138730 2.799420 -0.757992
H 1.069723 2.746788 -0.429142

PBN-COOMe-2-OOH.com.log

37

C 4.610053 -0.609544 0.764281
C 3.255087 -0.944717 0.806449
C 2.321986 -0.206478 0.074119
C 2.755383 0.867323 -0.714808
C 4.107751 1.197823 -0.761738
C 5.037167 0.461340 -0.020815
H 5.328748 -1.188539 1.337659
H 2.921360 -1.785572 1.409929
H 2.026454 1.440144 -1.279176
H 4.438570 2.034133 -1.371665
H 6.091542 0.722013 -0.058652
C 0.868701 -0.607617 0.094244
H 0.735906 -1.586481 0.560436
N 0.016370 0.367482 0.789775
O 0.473548 1.510078 1.136750
C -1.448528 0.176226 0.983859
C -1.756657 0.243157 2.490414
H -2.836391 0.236163 2.651889
H -1.301683 -0.614299 2.991315
H -1.344549 1.170204 2.893543
C -3.286885 -2.375156 -1.022792
H -2.453025 -2.882497 -1.513421
H -3.688690 -3.011267 -0.230723
H -4.062028 -2.114896 -1.742923
C -1.892607 -1.208118 0.464791
O -1.465808 -2.249189 0.914731
O -2.836339 -1.118792 -0.477563
C -2.203831 1.312458 0.251179
O -3.196158 1.842327 0.696106
O -1.639546 1.617616 -0.923193

C -2.303689 2.648986 -1.671814
H -2.315200 3.583255 -1.104640
H -1.723860 2.761136 -2.587949
H -3.331405 2.353265 -1.898101
O 0.300764 -0.677580 -1.230706
O 0.790627 -1.905138 -1.833398
H 1.599374 -1.577809 -2.271980

PBN-NHCOMe-2-OOH.com.log

39

C 3.574328 -0.355203 -1.808195
C 2.489588 0.312571 -1.238736
C 2.166013 0.107679 0.106962
C 2.932936 -0.773295 0.880222
C 4.020846 -1.431841 0.308835
C 4.343968 -1.224858 -1.034225
H 3.816862 -0.194070 -2.855075
H 1.878968 0.974191 -1.846457
H 2.671699 -0.939116 1.918398
H 4.615798 -2.111063 0.913435
H 5.191781 -1.741814 -1.476166
C 0.976135 0.828290 0.702095
N -0.184922 -0.062008 0.899177
O -0.018588 -1.112296 1.607516
C -1.608433 0.192296 0.423160
N -1.688034 1.488202 -0.249924
H -2.050833 2.244735 0.312707
C -1.322360 1.761357 -1.540258
O -0.788436 0.930096 -2.272742
C -1.636944 3.167317 -2.020753
H -2.531101 3.132185 -2.653387
H -1.813989 3.878411 -1.208204
H -0.808045 3.520439 -2.638457
N -1.964356 -0.854779 -0.508145
H -1.446329 -0.778192 -1.378213
C -2.590689 -2.057291 -0.240993
O -3.189754 -2.323887 0.787899
C -2.475805 -3.050267 -1.390730
H -1.526013 -3.591943 -1.305645
H -3.291857 -3.770502 -1.313397
H -2.502628 -2.565363 -2.372354
C -2.508279 0.257499 1.660935
H -2.210918 1.131873 2.250454
H -3.555271 0.346036 1.364266
H -2.390140 -0.646433 2.251579
H 0.654951 1.647316 0.062365
O 1.419058 1.347254 1.952706
O 0.316013 2.102816 2.533127
H 0.084065 1.506020 3.268413

PBN-OCOMe-2-OOH.com.log

37

C -3.716673 1.186000 -1.523524
C -2.640057 1.262564 -0.639297
C -2.298842 0.157644 0.147804
C -3.036849 -1.028580 0.045066
C -4.116131 -1.097216 -0.835074
C -4.457858 0.007146 -1.619612
H -3.975213 2.046485 -2.134519
H -2.053043 2.175151 -0.571015
H -2.759312 -1.884713 0.648996
H -4.690691 -2.016542 -0.910256
H -5.298985 -0.052150 -2.305353
C -1.120950 0.262629 1.090145
H -0.780432 1.292585 1.182128
N 0.037013 -0.532174 0.611147
O -0.072913 -1.798472 0.515739
C 1.385812 0.044989 0.322436
C 2.286989 -0.079188 1.545300

H 1.900605 0.593412 2.314614
H 2.259388 -1.102958 1.914255
H 3.321844 0.172444 1.308466
C 2.408507 -1.846044 -0.892866
O 3.045272 -2.326706 0.005981
O 1.823485 -0.587382 -0.868309
C 2.155520 -2.472317 -2.238581
H 1.098139 -2.753442 -2.293358
H 2.350125 -1.759599 -3.045442
H 2.779608 -3.359398 -2.352032
O 1.094939 1.389412 -0.015863
C 1.945294 2.339521 -0.551059
O 1.456405 3.410092 -0.800102
C 3.403211 2.010123 -0.766000
H 3.931588 2.012812 0.193556
H 3.540721 1.032367 -1.228892
H 3.827752 2.792574 -1.396152
O -1.566142 -0.224120 2.342653
O -0.515772 0.064661 3.315347
H -1.021211 0.632681 3.924983

PBN-OCONHMe-2-OOH.com.log

41

C 4.753343 -1.060581 -1.168048
C 3.414068 -0.675222 -1.150711
C 2.893828 -0.003047 -0.041478
C 3.724362 0.282870 1.045283
C 5.063870 -0.107993 1.031417
C 5.579970 -0.780942 -0.076908
H 5.154133 -1.579446 -2.034849
H 2.766608 -0.877982 -1.996822
H 3.323976 0.816962 1.904527
H 5.703824 0.121121 1.879377
H 6.624585 -1.080886 -0.093838
C 1.444689 0.421126 -0.001864
N 0.579173 -0.663338 0.494930
O 0.861598 -1.884738 0.236008
C -0.818639 -0.415889 0.943416
C -1.091869 -1.254661 2.185278
H -0.868864 -2.300492 1.968950
H -0.433265 -0.907596 2.984803
H -2.129576 -1.135959 2.495970
C -1.425285 1.960490 0.451948
O -0.669872 2.841740 0.072076
O -0.972235 0.938029 1.297582
N -2.748457 1.936399 0.256402
H -3.275953 1.139329 0.609226
C -3.399002 2.955162 -0.553222
H -3.008892 2.956410 -1.576818
H -4.469524 2.742652 -0.576930
H -3.238732 3.949143 -0.124366
O -1.601879 -0.798522 -0.193500
C -2.906348 -1.209807 -0.072369
O -3.721274 -0.724971 0.704699
N -3.155016 -2.176120 -0.978841
H -2.364567 -2.504690 -1.516503
C -4.476864 -2.734607 -1.203055
H -5.173034 -2.228712 -0.533323
H -4.795082 -2.578660 -2.239707
H -4.488819 -3.807941 -0.984321
H 1.306024 1.278499 0.659325
O 0.896852 0.743714 -1.285706
O 1.383140 2.066930 -1.630275
H 0.689874 2.600807 -1.177333

PBN-OMe-2-OOH.com.log

33

C -3.711516 0.180723 1.055263
C -2.430672 0.674696 0.812196

C -1.693353 0.194531 -0.279204
C -2.250439 -0.778843 -1.115777
C -3.530906 -1.274803 -0.865868
C -4.263868 -0.793779 0.219801
H -4.280607 0.557075 1.901151
H -1.990192 1.421427 1.462300
H -1.678881 -1.152231 -1.962199
H -3.954386 -2.032815 -1.519415
H -5.262197 -1.176486 0.415131
C -0.299564 0.710913 -0.567186
N 0.664255 0.382456 0.510954
O 0.479504 0.895920 1.666187
C 1.685977 -0.708136 0.429151
C 1.269439 -1.870616 1.327362
H 2.075110 -2.605522 1.397990
H 1.062440 -1.477601 2.324081
H 0.368517 -2.345811 0.929080
C 3.403643 0.966899 0.348711
H 2.810030 1.816769 0.695926
H 4.431526 1.059309 0.705860
H 3.391941 0.941238 -0.745915
O 2.913668 -0.257857 0.906922
O 1.730374 -1.036031 -0.944982
C 2.623289 -2.089365 -1.294936
H 2.230070 -3.068840 -0.994667
H 2.712866 -2.060653 -2.383198
H 3.609178 -1.939606 -0.842489
H 0.099881 0.287372 -1.486419
O -0.425235 2.116905 -0.682081
O 0.848959 2.629004 -1.181661
H 0.534582 3.042330 -2.006052

PBN-POOMe-2-OOH.com.log

47

C 4.753687 -0.782987 1.266171
C 3.615901 -1.150539 0.548282
C 2.919970 -0.191887 -0.198747
C 3.369572 1.132534 -0.220059
C 4.504873 1.498600 0.504929
C 5.199437 0.541182 1.246345
H 5.290371 -1.529391 1.845780
H 3.255100 -2.173895 0.569330
H 2.823492 1.872342 -0.800212
H 4.851097 2.528507 0.482832
H 6.087214 0.824473 1.805770
C 1.700463 -0.572884 -1.007169
N 0.498781 -0.746191 -0.179103
O 0.612644 -1.214100 1.006896
C -0.836894 -0.290293 -0.625837
C -1.056999 -0.595323 -2.125709
H -0.373080 -0.018785 -2.751567
H -0.894905 -1.661065 -2.302498
H -2.079830 -0.341600 -2.410426
H 1.492506 0.195067 -1.753541
P -2.097897 -1.296466 0.345236
O -3.424785 -0.697235 -0.365726
O -2.283419 -0.693201 1.824263
C -1.601867 -1.242506 2.970060
H -2.283895 -1.123616 3.815142
H -1.373716 -2.298701 2.813536
H -0.680162 -0.684087 3.137301
C -4.709260 -1.170333 0.077885
H -4.911681 -0.815353 1.092477
H -5.445889 -0.757158 -0.613357
H -4.747129 -2.263347 0.048267
O -1.906077 -2.763233 0.243404
P -0.861630 1.566203 -0.363667
O 0.025416 2.256285 -1.343632
O -0.463576 1.674934 1.185738
O -2.383143 2.106380 -0.345004

C -3.042219 2.531902 -1.551195
H -2.323614 2.949490 -2.261211
H -3.570502 1.682891 -1.994557
H -3.762967 3.298249 -1.258785
C -0.231032 2.972541 1.767040
H -1.180527 3.500850 1.893604
H 0.227802 2.791923 2.739804
H 0.445640 3.559483 1.139579
O 1.846613 -1.843185 -1.668698
O 2.836967 -1.648691 -2.711363
H 3.657211 -1.862651 -2.226086

PBN-SMe-2-OOH.com.log

33

C -3.346483 -1.245887 1.100336
C -2.115671 -0.601711 0.948756
C -1.840575 0.115567 -0.218480
C -2.809196 0.183927 -1.229750
C -4.035627 -0.456855 -1.074773
C -4.306958 -1.176324 0.092435
H -3.551757 -1.799047 2.012778
H -1.377958 -0.653937 1.741001
H -2.602745 0.759205 -2.127995
H -4.780880 -0.393012 -1.862995
H -5.263600 -1.677345 0.213999
C -0.511939 0.807275 -0.478635
H -0.021184 0.384312 -1.359654
N 0.451523 0.688161 0.638945
O 0.172810 1.344080 1.710621
C 1.740542 -0.034235 0.550027
S 1.501876 -1.890354 0.483801
C 0.785079 -2.240778 -1.160028
H -0.281628 -2.008949 -1.199635
H 1.325257 -1.700911 -1.942507
H 0.918569 -3.315216 -1.313584
S 2.616026 0.688623 -0.936324
C 4.166227 -0.277540 -0.986388
H 4.640553 -0.024107 -1.938466
H 4.840562 -0.004461 -0.171229
H 3.960488 -1.350096 -0.958209
C 2.533545 0.204434 1.836724
H 2.685053 1.274249 1.987254
H 1.994508 -0.192619 2.700808
H 3.501700 -0.295371 1.765519
O -0.638383 2.172556 -0.835226
O -1.488550 2.858372 0.124289
H -0.954707 2.740566 0.941861

PBN-alpha-3CH2OH-OOH.com.log

34

C -3.830515 -1.463455 0.812327
C -2.501205 -1.051005 0.869981
C -2.071050 0.056688 0.130287
C -2.985204 0.753305 -0.660531
C -4.318034 0.339580 -0.717564
C -4.743828 -0.767315 0.016037
H -4.154490 -2.326064 1.388639
H -1.791277 -1.598690 1.486047
H -2.648609 1.617067 -1.222499
H -5.023504 0.886626 -1.337332
H -5.781704 -1.086650 -0.028563
C -0.627601 0.511849 0.241285
H -0.371478 0.699233 1.285677
N 0.293667 -0.507177 -0.283560
O -0.074319 -1.154402 -1.334788
C 1.767428 -0.487672 -0.030298
C 2.162672 0.211463 1.273860
H 3.177660 -0.120936 1.505357
H 1.498673 -0.099523 2.091741

C 2.152547 -1.980583 0.119424
H 1.580000 -2.413721 0.957481
H 1.839859 -2.490505 -0.797282
C 2.466364 0.178797 -1.264661
O 3.765268 0.666972 -0.992490
H 3.636837 1.465118 -0.454748
H 1.805811 0.972510 -1.631598
H 2.565108 -0.568788 -2.054868
O 3.549415 -2.081021 0.344903
H 3.826276 -2.981419 0.122345
O 2.157604 1.651928 1.140802
H 2.599404 2.012489 1.925667
O -0.368231 1.727783 -0.476504
O -0.313757 2.819597 0.476504
H 0.628483 2.726714 0.740568

PBN-alpha-3COOH-HO2.com.log

31

C -3.536855 -1.780279 -0.379391
C -2.305110 -1.123559 -0.357150
C -2.233170 0.215399 0.040179
C -3.404688 0.889173 0.410500
C -4.632534 0.230371 0.382579
C -4.701968 -1.107578 -0.011471
H -3.582051 -2.820223 -0.691316
H -1.407752 -1.655910 -0.653905
H -3.350001 1.931072 0.708814
H -5.535472 0.763578 0.667753
H -5.659404 -1.621388 -0.033182
C -0.911403 0.959939 0.148169
H -0.607249 1.088635 1.186708
N 0.188174 0.225164 -0.542106
O 0.159054 0.193989 -1.823926
C 1.457375 -0.231873 0.050870
C 1.927698 -1.383810 -0.892308
O 1.311633 -2.408535 -1.022042
O 3.088213 -1.096362 -1.499519
H 3.301248 -1.853111 -2.079176
O -1.097476 2.220646 -0.452313
O -0.058195 3.107595 0.037198
C 2.484732 0.934645 0.056728
O 2.396337 1.926090 -0.626530
O 3.490862 0.704314 0.914229
H 4.102000 1.463597 0.845316
C 1.301965 -0.810691 1.478460
O 0.488683 -0.447967 2.292997
O 2.220344 -1.760559 1.711608
H 2.090134 -2.061736 2.631667
H 0.659434 2.925224 -0.604550

PBN-CH2CONH2-3-OOH.com.log

43

C 4.151141 0.801803 0.372979
C 2.827265 1.061055 0.007380
C 2.123832 0.143394 -0.784317
C 2.755762 -1.030672 -1.213990
C 4.080453 -1.278317 -0.855407
C 4.779540 -0.367323 -0.059074
H 4.691195 1.518749 0.985789
H 2.334743 1.973393 0.332610
H 2.206510 -1.739246 -1.822133
H 4.568180 -2.187841 -1.196114
H 5.810895 -0.566780 0.220002
C 0.679716 0.435210 -1.135226
N -0.247843 -0.381670 -0.306940
O -0.073967 -1.652957 -0.335816
C -1.335621 0.123336 0.589134
C -0.781394 0.259377 2.042753
H -1.616200 0.525510 2.700979

H -0.060107 1.077425 2.063942
C -1.932452 1.472293 0.090693
H -1.999784 1.435422 -1.001838
H -2.963415 1.525081 0.455277
C -2.451085 -0.960681 0.577732
H -2.158730 -1.780918 1.233757
H -3.356972 -0.523091 1.016329
C -2.817919 -1.488305 -0.804161
O -2.832350 -0.793124 -1.823460
N -3.231480 -2.781880 -0.825710
H -3.404737 -3.194880 -1.732890
H -3.008696 -3.405614 -0.063379
C -0.167278 -1.023934 2.606745
O -0.852782 -1.929065 3.071727
N 1.197564 -1.059773 2.610478
H 1.617318 -1.956197 2.820821
H 1.732407 -0.442436 2.012168
C -1.234429 2.779045 0.467159
O -0.028287 2.899180 0.668593
N -2.073381 3.852517 0.550741
H -1.648406 4.766360 0.634594
H -3.031864 3.806488 0.237177
H 0.450623 1.482378 -0.955426
O 0.500482 0.115525 -2.502176
O -0.755297 0.700968 -2.936917
H -1.404567 -0.000059 -2.691669

PBN-CH2COOMe-3-OOH.com.log

49

C 4.642188 -2.341757 -0.473208
C 3.414321 -1.932632 0.049967
C 3.150718 -0.576569 0.258359
C 4.130248 0.373703 -0.048953
C 5.357723 -0.034649 -0.565878
C 5.615423 -1.391345 -0.782112
H 4.839592 -3.398899 -0.629250
H 2.660673 -2.675926 0.303432
H 3.922912 1.423542 0.124960
H 6.116182 0.706869 -0.802018
H 6.574850 -1.705772 -1.184516
C 1.810308 -0.155746 0.815403
N 0.910899 0.398561 -0.205371
O 1.419842 1.014824 -1.203591
C -0.575280 0.129014 -0.213860
C -0.711060 -1.276427 -0.862418
H -0.198735 -1.245773 -1.833424
H -0.174614 -2.017324 -0.260890
C -1.096352 0.165705 1.252927
H -0.678176 -0.669306 1.820092
H -0.761521 1.108947 1.686623
C -1.229297 1.204723 -1.099804
H -2.309729 1.044374 -1.101222
H -0.886762 1.096157 -2.130046
C -1.119423 4.873647 -1.379387
H -1.756137 5.163658 -0.539258
H -0.078298 5.095346 -1.130473
H -1.417531 5.400107 -2.286678
O -1.279155 3.477216 -1.675527
C -0.966398 2.635258 -0.668262
O -0.567982 3.010923 0.413283
C -2.106306 -1.820394 -1.121952
O -3.127995 -1.180022 -1.255364
O -2.052006 -3.162295 -1.246537
C -3.294359 -3.806947 -1.578734
H -3.053115 -4.864545 -1.686292
H -4.026130 -3.659838 -0.780178
H -3.698207 -3.405567 -2.511593
C -2.608096 0.120577 1.389489
O -3.357713 1.046226 1.173438
O -3.023075 -1.093400 1.823042

C -4.449782 -1.240221 1.935220
H -4.910855 -1.139910 0.949519
H -4.609652 -2.240544 2.339657
H -4.862227 -0.483082 2.606494
H 1.321562 -1.014430 1.287200
O 1.906603 0.896648 1.784716
O 2.562591 0.300269 2.950708
H 1.973282 0.653231 3.641338

PBN-CH2NHCOMe-3-OOH.com.log

52

C 3.881429 -1.835770 2.145565
C 2.807662 -1.419317 1.360810
C 3.030002 -0.705144 0.177209
C 4.342960 -0.418385 -0.211328
C 5.416361 -0.829258 0.581702
C 5.190513 -1.539255 1.760260
H 3.693667 -2.389527 3.061549
H 1.794046 -1.645523 1.676220
H 4.519931 0.127054 -1.130779
H 6.431037 -0.593880 0.271788
H 6.026969 -1.861279 2.374788
C 1.867257 -0.337845 -0.736880
H 1.606236 -1.190622 -1.365469
N 0.662330 0.031650 0.045880
O 0.850322 0.869217 1.007953
C -0.754595 -0.244433 -0.330785
C -1.378753 0.962141 -1.103588
H -2.464986 0.812594 -1.114318
H -1.020130 0.963458 -2.133515
C -0.817761 -1.497853 -1.255375
H -0.278731 -1.284859 -2.182222
H -0.346396 -2.346460 -0.751870
C -1.545185 -0.550962 0.966069
H -1.026889 -1.348655 1.510561
H -2.530638 -0.925548 0.690133
N -1.785108 0.584426 1.843106
H -0.970439 0.966378 2.304351
C -3.048334 0.922052 2.264703
O -4.063029 0.422227 1.794765
C -3.103348 1.980214 3.357170
H -2.142405 2.470277 3.544522
H -3.849211 2.732217 3.085772
H -3.439966 1.508570 4.286792
N -1.086445 2.273622 -0.563072
H -1.360533 2.434693 0.395281
N -2.168152 -1.914611 -1.591785
H -2.616779 -1.496926 -2.393909
C -2.754885 -3.011195 -1.002239
O -2.213148 -3.626736 -0.093946
C -0.276430 3.178018 -1.168249
O 0.209329 3.012884 -2.294273
C 0.010741 4.437949 -0.376805
H -0.707813 4.616670 0.428777
H 1.012317 4.351732 0.059364
H 0.014402 5.290866 -1.059191
C -4.135025 -3.372576 -1.523544
H -4.204827 -4.459900 -1.605114
H -4.884425 -3.045234 -0.794389
H -4.371939 -2.919716 -2.491559
O 2.289792 0.715192 -1.577540
O 1.467336 0.673413 -2.777411
H 1.038667 1.568158 -2.711016

PBN-CH2OCOMe-3-OOH.com.log

49

C 5.088552 -1.506166 -0.500467
C 3.730634 -1.671325 -0.229170
C 3.001927 -0.629338 0.356336

C 3.637271 0.579443 0.658891
C 4.993467 0.745847 0.375099
C 5.721407 -0.297880 -0.199053
H 5.650606 -2.317621 -0.954558
H 3.227521 -2.600505 -0.479451
H 3.072065 1.397913 1.098479
H 5.480098 1.688433 0.608874
H 6.779172 -0.170279 -0.412433
C 1.535593 -0.801422 0.679847
H 1.257061 -0.147635 1.509947
N 0.665425 -0.510655 -0.465142
O 1.123884 -0.686715 -1.649050
C -0.794280 -0.194073 -0.349854
C -1.566609 -1.355032 -1.047199
H -0.924964 -1.752286 -1.836544
H -1.774222 -2.144986 -0.322626
C -1.194975 -0.057905 1.134561
H -0.910553 -0.960333 1.683301
H -0.707101 0.809058 1.577936
C -1.026887 1.138386 -1.096940
H -2.088077 1.383762 -1.094953
H -0.687461 1.045568 -2.128135
C 0.812828 2.775517 -0.821622
O 1.441482 3.421167 -0.017622
O -0.346299 2.185271 -0.390026
C 1.208700 2.611524 -2.271795
H 1.494062 1.575090 -2.481251
H 0.388497 2.882268 -2.945184
H 2.062445 3.263416 -2.457801
O -2.747634 -0.870868 -1.681987
O -2.618849 0.052341 1.200054
C -4.022403 -1.304520 -1.408973
O -4.923619 -0.777236 -2.008480
C -3.280784 1.046131 1.885335
O -4.480571 0.971549 1.940796
C -4.214027 -2.411370 -0.395732
H -3.628671 -3.303974 -0.641415
H -3.925456 -2.063843 0.600839
H -5.273406 -2.668128 -0.389867
C -2.466615 2.158022 2.512602
H -1.824759 1.775477 3.314625
H -1.826234 2.660039 1.779785
H -3.168187 2.875818 2.937841
O 1.195364 -2.153977 1.042528
O 1.737071 -2.381835 2.369592
H 2.640155 -2.685288 2.150944

PBN-CH2OCONHMe-3-OOHb.com.log
55

C 3.166321 -2.025400 2.879721
C 2.131688 -2.007770 1.944708
C 2.335429 -1.425700 0.686105
C 3.589929 -0.888214 0.371710
C 4.622493 -0.908917 1.310626
C 4.411561 -1.474441 2.568549
H 3.000696 -2.478037 3.853945
H 1.165813 -2.435120 2.182459
H 3.760100 -0.463481 -0.613845
H 5.593288 -0.492363 1.054204
H 5.215160 -1.494082 3.300274
C 1.259559 -1.419991 -0.384108
H 1.613881 -0.883393 -1.262994
N -0.003190 -0.766226 0.069278
O -0.602700 -1.292262 1.078928
C -0.766522 0.279244 -0.670463
C 0.107734 1.083086 -1.643924
H -0.530214 1.817889 -2.142098
H 0.579563 0.454052 -2.400096
C -1.906015 -0.358613 -1.507792
H -1.500012 -1.105288 -2.190035

H -2.415502 0.426859 -2.070324
C -1.350561 1.215971 0.410554
H -0.528013 1.658835 0.980053
H -1.990589 0.627845 1.071528
C -2.642552 3.289301 0.407690
O -3.167932 4.185701 -0.216482
O -2.099800 2.227466 -0.267303
N -2.517162 3.267098 1.771786
H -2.283089 2.400541 2.232368
C -3.175649 4.292675 2.568086
H -4.252919 4.110998 2.677599
H -2.714876 4.323681 3.559091
H -3.040974 5.257402 2.077134
O 1.107735 1.803382 -0.911361
C 2.365812 1.846597 -1.452753
O 2.730544 1.174537 -2.403281
N 3.123022 2.735724 -0.764908
H 2.696670 3.180122 0.035245
C 4.541332 2.909233 -1.017802
H 4.794647 3.973942 -1.038927
H 5.154405 2.412313 -0.255014
H 4.764914 2.470210 -1.990873
O -2.907207 -0.945582 -0.670154
C -2.977829 -2.302507 -0.595767
O -2.309405 -3.083464 -1.263105
N -3.939818 -2.664799 0.282348
H -4.371290 -1.923334 0.814753
C -4.188878 -4.049283 0.641582
H -3.767631 -4.294043 1.624389
H -5.265096 -4.248951 0.653699
H -3.716271 -4.681987 -0.110087
O 1.029889 -2.770760 -0.722078
O 0.323352 -2.787017 -1.994674
H -0.581550 -3.044815 -1.696236

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43

C -4.492577 0.727031 1.179931
C -3.164916 0.890240 0.782801
C -2.548520 -0.076637 -0.028786
C -3.288508 -1.199901 -0.422385
C -4.613927 -1.363222 -0.019196
C -5.220608 -0.396127 0.782405
H -4.957047 1.479600 1.811750
H -2.594716 1.744555 1.121780
H -2.821918 -1.955664 -1.049699
H -5.169160 -2.243524 -0.331602
H -6.253050 -0.518159 1.099254
C -1.144339 0.059555 -0.576051
H -0.877298 -0.846930 -1.123840
N -0.109241 0.255348 0.441313
O -0.395228 0.851250 1.543769
C 1.348427 0.072425 0.153715
C 1.902071 -0.726764 1.357058
H 1.793778 -0.122458 2.268355
H 1.292519 -1.635241 1.476166
C 1.613361 -0.683996 -1.152038
H 1.220187 -0.120749 -2.011101
H 2.700528 -0.758793 -1.257109
C 1.936770 1.500875 0.043360
H 1.850604 1.989827 1.024950
H 1.327028 2.076794 -0.670274
C 3.852661 2.732316 -0.510069
H 3.861304 3.267817 0.452857
H 4.882592 2.594541 -0.849581
H 3.311077 3.351411 -1.243833
O 3.281241 1.447800 -0.386042
O 3.253535 -1.063251 1.126976
C 3.802208 -1.820474 2.182682
H 4.840780 -2.036511 1.918080

H 3.783847 -1.266196 3.135062
H 3.262767 -2.770985 2.327153
O 1.026572 -1.978241 -1.091856
C 1.451561 -2.813323 -2.151641
H 0.954591 -3.778095 -2.020088
H 1.176072 -2.398724 -3.134257
H 2.541420 -2.962611 -2.129749
O -1.043807 1.041276 -1.630532
O -1.331271 2.362702 -1.107308
H -2.291539 2.418371 -1.274248

PBN-CH2POOMe2-3-OOH.com.log

64

C 5.217248 -1.365876 -0.323167
C 4.069295 -0.599573 -0.520129
C 2.937664 -1.173237 -1.114507
C 2.966486 -2.516018 -1.503134
C 4.113470 -3.284720 -1.296380
C 5.241226 -2.708819 -0.709929
H 6.092265 -0.917538 0.139684
H 4.033528 0.436739 -0.201007
H 2.088301 -2.961981 -1.963822
H 4.127513 -4.327378 -1.601564
H 6.137678 -3.303341 -0.555139
C 1.697337 -0.350213 -1.374460
N 0.919485 -0.090909 -0.159326
O 1.534146 -0.059791 0.964437
C -0.487665 0.454613 -0.178555
C -0.456016 2.012493 -0.199214
H -1.486054 2.372842 -0.138379
H -0.082421 2.335759 -1.177436
C -1.176852 -0.042214 -1.480211
H -0.706636 0.426732 -2.350533
H -1.034209 -1.125583 -1.560253
C -1.188598 -0.062156 1.102291
H -2.234264 0.253416 1.084210
H -0.717305 0.382507 1.978955
P -1.199467 -1.877762 1.346777
O -2.592560 -2.013537 2.159375
O -0.141531 -2.244241 2.515171
C 1.104407 -2.910879 2.230444
H 1.875715 -2.166800 2.022840
H 1.358855 -3.483054 3.125583
H 0.993346 -3.582041 1.375379
C -2.941781 -3.276985 2.747301
H -2.945460 -4.068292 1.990638
H -2.240525 -3.532514 3.547035
H -3.945616 -3.157779 3.158780
O -1.052810 -2.721671 0.121526
P -2.970083 0.150085 -1.789703
O -3.324287 -0.139025 -3.202704
O -3.764400 -0.751972 -0.701192
O -3.299210 1.634421 -1.240129
C -4.625181 2.169326 -1.429892
H -4.577760 3.216774 -1.128967
H -4.918121 2.093487 -2.480459
H -5.340321 1.631457 -0.800534
C -4.173282 -2.095946 -1.041659
H -3.319900 -2.772659 -0.950378
H -4.943279 -2.368159 -0.317446
H -4.580367 -2.122804 -2.055106
P 0.471518 3.067808 0.969848
O 0.097463 4.498825 0.810334
O 0.182355 2.403888 2.412641
O 2.061649 2.794402 0.785809
C 0.781926 2.988703 3.583058
H 0.541428 4.054153 3.644761
H 0.359043 2.462136 4.440036
H 1.866305 2.848111 3.558443
C 2.843941 3.673613 -0.043741

H 2.828408 3.312778 -1.076317
H 2.461389 4.695829 0.005227
H 3.865816 3.637976 0.341865
H 1.063549 -0.854606 -2.104141
O 2.010589 0.959986 -1.900267
O 2.470063 0.770276 -3.264194
H 3.419698 0.593091 -3.115643

PBN-CH2SMe-3-OOH.com.log

43

C 5.098940 -1.073343 -0.784309
C 3.805816 -1.132988 -0.265812
C 3.106947 0.048975 0.012846
C 3.718556 1.282958 -0.228760
C 5.009328 1.341880 -0.756106
C 5.701762 0.162308 -1.032989
H 5.635023 -1.993350 -1.001090
H 3.326201 -2.088999 -0.086775
H 3.184512 2.203337 -0.002226
H 5.474829 2.305965 -0.941364
H 6.709094 0.204797 -1.438355
C 1.710645 0.008919 0.595862
H 1.464875 0.974009 1.037328
N 0.691829 -0.340023 -0.404093
O 0.974437 -1.329478 -1.171152
C -0.798324 0.005886 -0.261508
C -1.387694 -1.235380 0.462190
H -1.246627 -2.096621 -0.197960
H -0.777230 -1.401153 1.353341
C -0.888919 1.319439 0.549452
H -0.695801 1.116167 1.608364
H -0.108923 1.992314 0.175473
C -1.259347 0.191521 -1.732893
H -0.795669 -0.595335 -2.329547
H -0.875359 1.150430 -2.093216
S -3.056373 0.189715 -2.097338
C -3.316209 -1.550476 -2.599104
H -3.273883 -2.225794 -1.740912
H -4.321221 -1.596343 -3.028008
H -2.593801 -1.852395 -3.363528
S -3.136570 -1.163794 1.040655
S -2.458249 2.279135 0.414058
C -2.991291 -2.408747 2.375826
H -3.983342 -2.500112 2.826706
H -2.693283 -3.387131 1.985943
H -2.281372 -2.090125 3.145825
C -1.829484 3.823392 1.164468
H -1.006540 4.252156 0.582146
H -2.663256 4.530587 1.166148
H -1.504597 3.665782 2.198128
O 1.579567 -0.995047 1.625461
O 2.356845 -0.533060 2.759485
H 3.231479 -0.914291 2.548887

PBN-CONH2-3-OOHb.com.log

34

C -0.828911 -0.831821 0.332655
H -0.564483 -0.757223 1.385154
N 0.167104 -0.013687 -0.434118
O -0.050633 0.192185 -1.678015
C 1.551955 0.357252 0.001021
C 2.506938 -0.493714 -0.903887
N 3.264593 0.131868 -1.799645
H 3.822511 -0.439105 -2.421198
H 3.187670 1.146869 -1.892548
O 2.529239 -1.728228 -0.755514
C 1.644974 1.927717 -0.203727
O 2.393639 2.462467 -1.019043
N 0.784476 2.627648 0.557423

H 0.837151 3.635801 0.497128
H 0.382342 2.187896 1.379340
C 1.753520 0.048349 1.523175
O 1.049267 0.613024 2.359672
N 2.752666 -0.795297 1.855480
H 2.799963 -1.048974 2.834742
H 3.074463 -1.470199 1.169743
O -0.782681 -2.182809 -0.072494
O 0.370091 -2.793469 0.564480
H 1.085803 -2.585202 -0.083387
C -2.230754 -0.321107 0.095666
C -2.873181 0.382729 1.119424
C -2.899575 -0.552028 -1.112779
C -4.171678 0.860991 0.938858
H -2.357050 0.554277 2.061276
C -4.199124 -0.079220 -1.287453
H -2.400142 -1.095800 -1.905609
C -4.836367 0.629478 -0.265825
H -4.663333 1.406521 1.739778
H -4.715791 -0.262910 -2.225565
H -5.849135 0.997214 -0.408283

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C 4.209245 -1.844399 0.532437
C 2.932275 -1.316023 0.711064
C 2.626757 -0.038096 0.228503
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C 4.884690 0.177803 -0.604158
C 5.188765 -1.097530 -0.127110
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H 5.644048 0.763787 -1.115092
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C 1.234580 0.508169 0.457944
H 0.921868 0.365515 1.490237
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C -1.198603 -0.081729 -0.095417
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H 4.669716 -0.446321 -2.690057
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46

C -4.768227 0.195008 -1.211553
C -3.443179 -0.078293 -0.879644
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C -3.922024 0.419348 1.439734
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H -5.093886 0.102906 -2.244396
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34

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C -1.753227 0.167365 -0.167597

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C	3.243567	0.620520	1.665531
H	3.458550	1.462423	1.000451
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H	4.153426	0.320169	2.188708
O	2.834152	-0.531923	0.915987
O	2.246468	0.582573	-1.031762
C	3.314271	0.161572	-1.890443
H	2.976451	-0.612683	-2.584517
H	3.612868	1.054870	-2.441833
H	4.159875	-0.214355	-1.305816
O	1.605445	-1.544703	-0.670789
C	1.297505	-2.646604	0.193608
H	0.440497	-2.416292	0.834677
H	1.049658	-3.475211	-0.472677
H	2.158171	-2.907222	0.814469
H	-0.044690	0.782860	-1.339800
O	-0.429452	2.213000	0.103047
O	-1.257782	2.915170	-0.857690
H	-2.138176	2.820623	-0.445290

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C	-4.750213	1.631234	0.451619
C	-3.499485	1.026046	0.555821
C	-3.272137	-0.227531	-0.027366
C	-4.307706	-0.871051	-0.705715
C	-5.560180	-0.260913	-0.810049
C	-5.784992	0.988871	-0.234053
H	-4.918953	2.602974	0.908490
H	-2.694646	1.527514	1.088419
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H	-6.360579	-0.767581	-1.342813
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C	-1.918461	-0.894579	0.150152
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C	3.681901	2.503942	-0.493891
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H	4.455819	2.419525	0.270477
H	4.040539	2.097806	-1.442797
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P	0.891033	0.198168	1.834189
O	2.292213	-0.071917	2.241375
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C	0.115120	-1.934297	3.266060

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34

C 3.829736 -1.758178 0.250026
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