

Supporting Information

Theoretical Insights into NH₃ Absorption Mechanisms with Imidazolium-based Protic Ionic Liquids

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Optimized structures

[BIm][Tf₂N]...NH₃ system

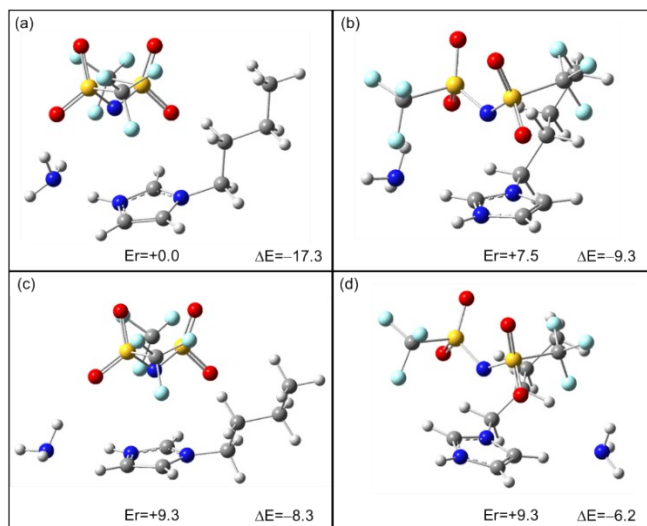


Fig. S1 Optimized conformers of one NH₃ molecule interacting with [BIm][Tf₂N], [BIm][Tf₂N]...NH₃ for short. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer, $\Delta E = E([\text{BIm}][\text{Tf}_2\text{N}] \cdots \text{NH}_3) - E([\text{BIm}][\text{Tf}_2\text{N}]) - E(\text{NH}_3)$). All the energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, paleturquoise).

[BIm][Tf₂N]...2NH₃ system

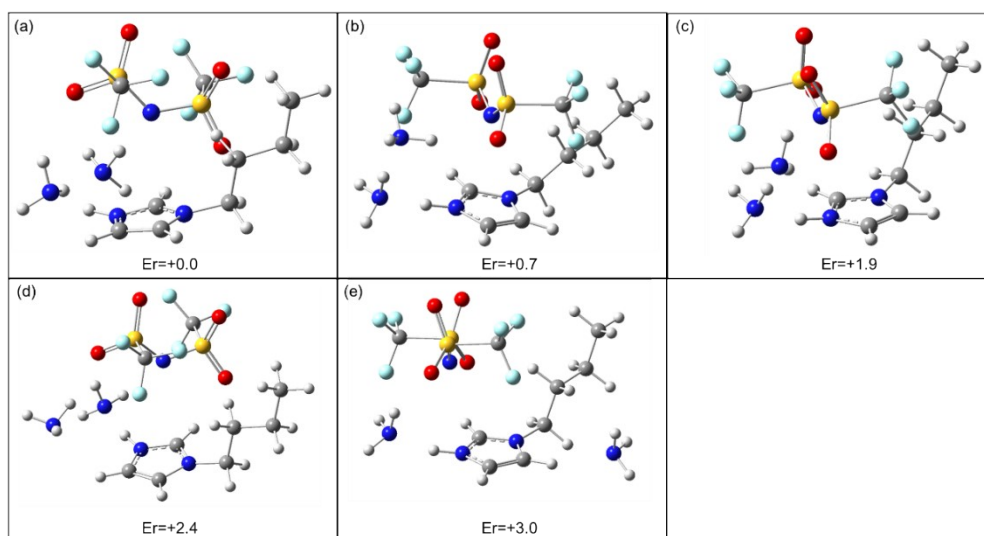


Fig. S2 Optimized conformers of two NH₃ molecules interacting with [BIm][Tf₂N], [BIm][Tf₂N]...2NH₃ for short. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All the energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, paleturquoise).

[BIm][Tf₂N]...3NH₃ system

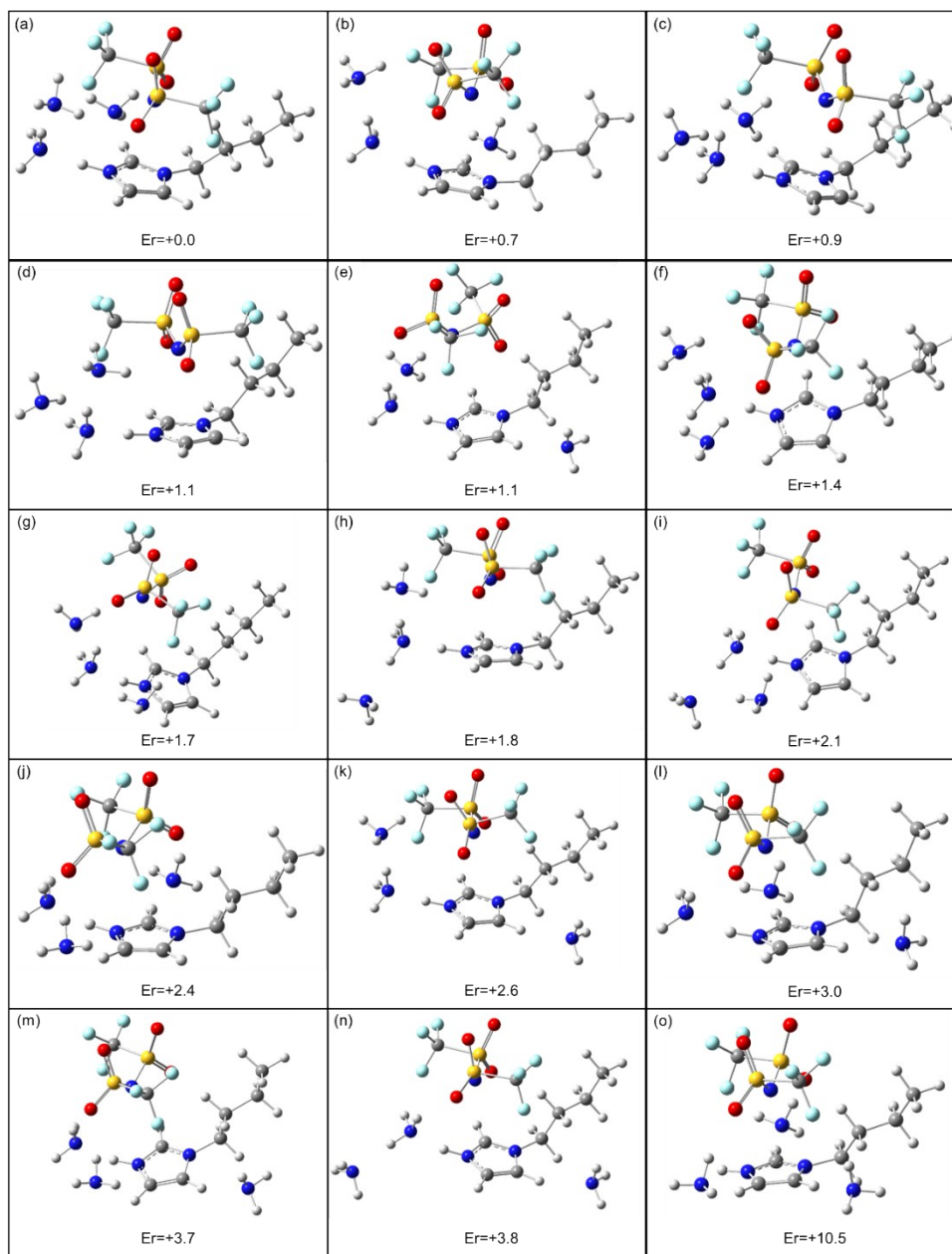


Fig. S3 Optimized conformers of three NH₃ molecules interacting with [BIm][Tf₂N], [BIm][Tf₂N]...3NH₃ for short. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All the energies given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, paleturquoise).

Table S1. The relative energy (E_r), weighting factors (w_i) and the changes of Gibbs energy (ΔG) for the process of $[\text{BIm}][\text{Tf}_2\text{N}] + 3\text{NH}_3 \rightarrow [\text{BIm}][\text{Tf}_2\text{N}] \cdots 3\text{NH}_3$ for different isomers. The energies are given in kcal mol^{-1} .

	a	b	c	d	e	f	g	h
E_r	+0.0	+0.7	+0.9	+1.1	+1.1	+1.4	+1.1	+1.8
w_i	0.432	0.140	0.102	0.074	0.074	0.046	0.074	0.024
ΔG	-0.05	+0.56	+2.87	+1.77	+0.44	+1.28	+1.57	+3.84
	i	j	k	l	m	n	o	
E_r	+2.1	+2.4	+2.6	+3.0	+3.7	+3.8	+10.5	
w_i	0.015	0.009	0.007	0.003	0.001	0.001	0.000	
ΔG	+4.6	+2.24	+1.29	+3.07	+2.11	+3.29	+9.48	

Equation for calculating weighting factors of isomers based on Boltzmann distribution:

$$w_i = \frac{\exp\left(-\frac{E_i - E_{\min}}{RT}\right)}{\sum_i \exp\left(-\frac{E_i - E_{\min}}{RT}\right)} \quad (\text{S5})$$

Where E_i denotes the electronic energy (J mol^{-1}) of isomer i . E_{\min} is the electronic energy (J mol^{-1}) of the isomer with the lowest electronic energy. R stands for the ideal gas constant ($\text{J mol}^{-1} \cdot \text{K}^{-1}$), and T stands for the absolute temperature (K).

[BIm][Tf₂N]...4NH₃ system

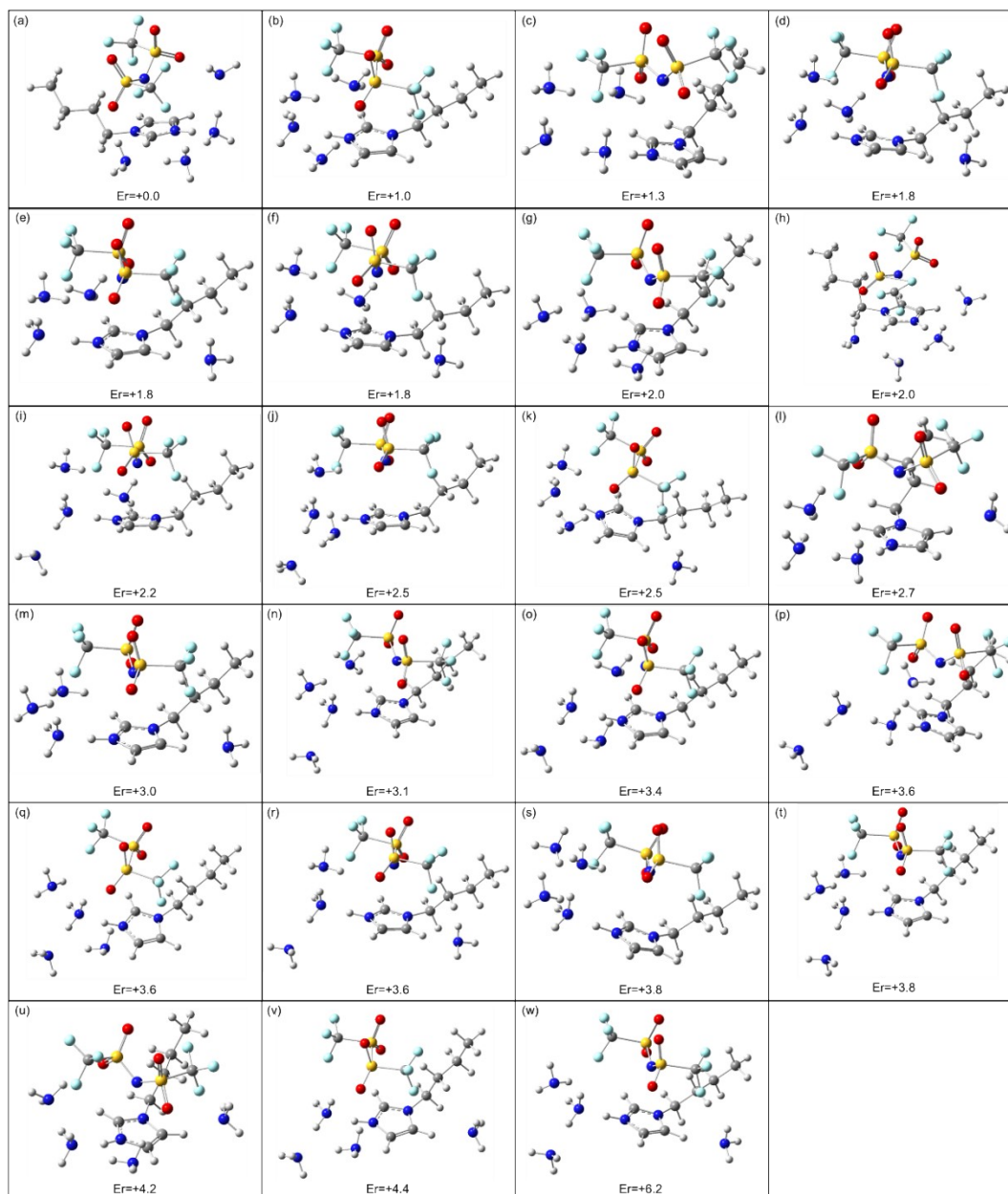


Fig. S4 Optimized conformers of three NH₃ molecules interacting with [BIm][Tf₂N], [BIm][Tf₂N]...4NH₃ for short. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All the energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, pale turquoise).

[Tf₂N]⁻...NH₃ system

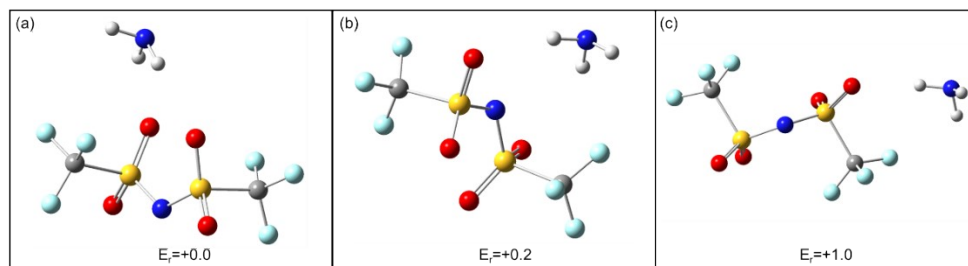


Fig. S5 Optimized conformers of NH₃ interact with [Tf₂N]⁻, [Tf₂N]⁻...NH₃ for short. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All the energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, paleturquoise).

[SCN]⁻...NH₃ system

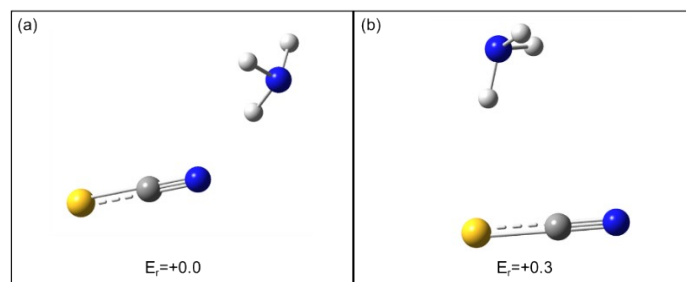


Fig. S6 Optimized conformers of NH₃ interact with [SCN]⁻, [SCN]⁻...NH₃ for short. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All the energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow).

[BIm][Tf₂N]

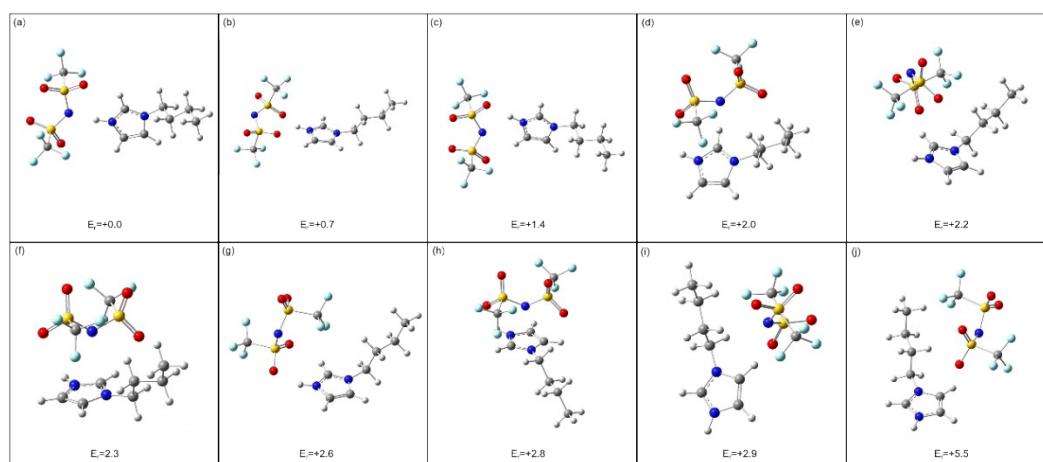


Fig. S7. Optimized conformers of [BIm][Tf₂N]. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, paleturquoise).

[BIm][SCN]

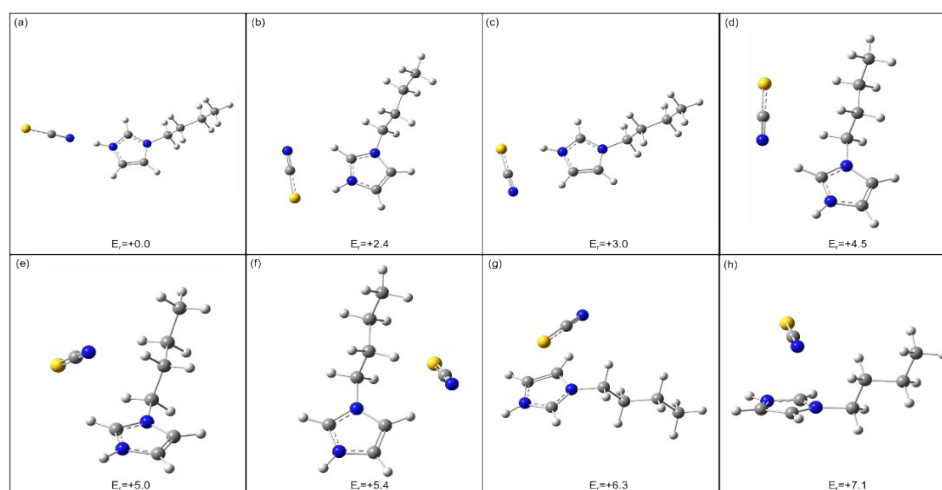


Fig. S8. Optimized conformers of [BIm][SCN]. The calculations were carried at PCM B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All the energies are given in kcal mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; S, yellow).

[BIm][NO₃]

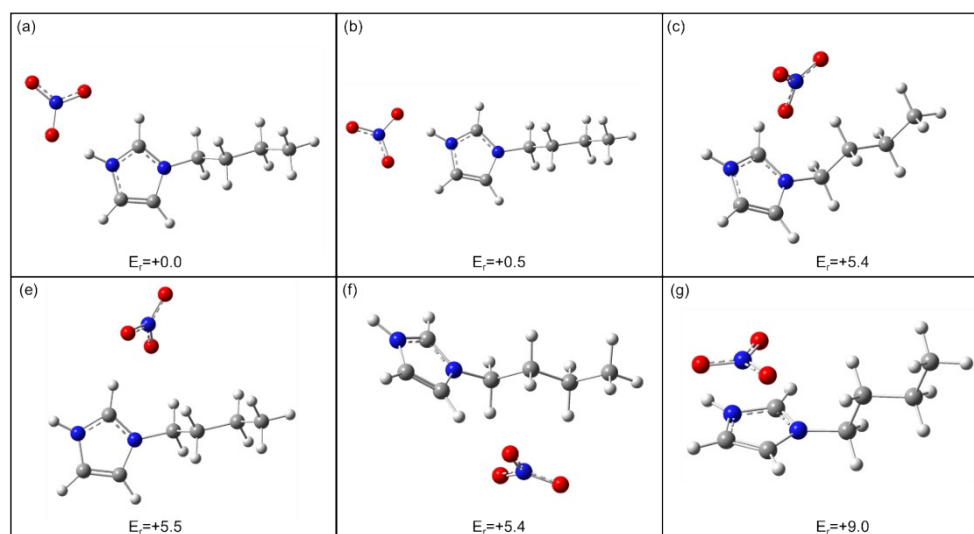


Fig. S9. Optimized conformers of [BIm][NO₃]. The calculations were carried at PCM/B3LYP-D3/6-31+G* level of theory (E_r represents the relative energy with respect to the most stable conformer. All energies are given in kcal·mol⁻¹. Color ligand: N, blue; H, gray; C, dark gray; O, red).

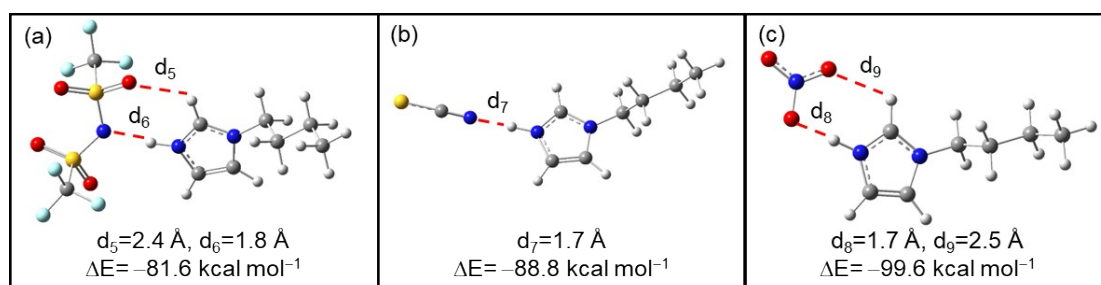


Fig. S10. The most stable structures of ILs, (a) [BIm][Tf₂N], (b) [BIm][SCN], and (c) [BIm][NO₃]. The interaction energies between cation and anions are considerable, the results are comparable with those of other kinds of ILs^{18, 19} (Color ligand: N, blue; H, gray; C, dark gray; S, yellow; O, red; F, pale turquoise).

Cartesian coordinates

NH₃

N	0.000000	0.000000	0.115648
H	0.000000	0.944163	-0.269845
H	-0.817669	-0.472082	-0.269845
H	0.817669	-0.472082	-0.269845

[BIm]⁺

N	-0.966158	-0.174870	0.348132
C	-1.799927	-1.055263	-0.211705
N	-2.926789	-0.410773	-0.534817
C	-2.819122	0.917982	-0.176978
C	-1.581603	1.066934	0.377590
H	-3.733739	-0.844685	-0.969254
C	0.408182	-0.463543	0.804682
C	1.458123	0.078831	-0.168371
C	2.882455	-0.212079	0.322189
C	3.947444	0.324039	-0.641435
H	-3.616728	1.624800	-0.340722
H	-1.092444	1.934620	0.791313
H	-1.600121	-2.103386	-0.371370
H	0.487070	-1.548103	0.909924
H	0.516275	-0.018950	1.797648
H	1.321482	1.161736	-0.285678
H	1.299637	-0.374822	-1.155367
H	3.010649	-1.296174	0.447446
H	3.023932	0.236918	1.315117
H	4.956698	0.108259	-0.272436
H	3.858021	1.411040	-0.761870
H	3.846583	-0.133168	-1.633779

[Tf₂N]⁻

C	0.000000	2.596315	-0.036971
F	1.128351	2.385903	-0.731252
S	-1.013948	1.007169	0.087487
O	-2.092942	1.352016	1.024412
N	0.000000	0.000000	0.849254
S	1.013948	-1.007169	0.087487
O	1.358158	-0.681185	-1.304585
O	-1.358158	0.681185	-1.304585
F	-0.723307	3.539373	-0.665229
F	0.324470	3.047978	1.184374
C	0.000000	-2.596315	-0.036971

F	-1.128351	-2.385903	-0.731252
O	2.092942	-1.352016	1.024412
F	0.723307	-3.539373	-0.665229
F	-0.324470	-3.047978	1.184374

[SCN]⁻

N	0.000000	0.000000	-1.816920
C	0.000000	0.000000	-0.634254
S	0.000000	0.000000	1.032748

[NO₃]⁻

N	-0.000100	-0.000013	0.000066
O	0.732130	1.029512	-0.000019
O	0.525799	-1.148598	-0.000019
O	-1.257841	0.119097	-0.000019

[Blm][Tf₂N]...NH₃

Fig. S1a				Fig. S1b			
N	-2.677401	-0.797396	1.637705	N	-0.620415	2.201023	1.502461
C	-1.377688	-0.993844	1.900943	C	0.655817	1.973633	1.823771
N	-1.087698	-2.276727	1.693167	N	0.665755	1.159484	2.886184
C	-2.225875	-2.930412	1.270782	C	-0.628010	0.841414	3.246672
C	-3.229496	-2.002855	1.233589	C	-1.440731	1.502747	2.375528
H	-0.092065	-2.664009	1.744139	H	1.505725	0.801245	3.323894
C	-3.344667	0.516843	1.645806	C	-1.066901	3.014837	0.356963
C	-3.002488	1.323719	0.390232	C	-1.959513	2.218339	-0.596111
C	-3.676817	2.700128	0.384949	C	-2.284713	3.015622	-1.864129
C	-3.302722	3.515778	-0.858337	C	-3.169626	2.219008	-2.829912
H	-2.228925	-3.983108	1.035339	H	-0.852106	0.174500	4.062684
H	-4.269894	-2.087388	0.961215	H	-2.515127	1.527794	2.296367
H	-0.679743	-0.223163	2.189623	H	1.522417	2.393692	1.308931
H	-3.026818	1.042105	2.550776	H	-0.161210	3.348926	-0.153249
H	-4.418682	0.331228	1.724805	H	-1.586854	3.893659	0.751262
H	-3.304184	0.752583	-0.496835	H	-2.892058	1.938989	-0.089512
H	-1.914297	1.448351	0.338655	H	-1.444338	1.291792	-0.861785
H	-3.383571	3.252202	1.289000	H	-1.346964	3.290494	-2.366674
H	-4.767845	2.576105	0.433636	H	-2.783878	3.956747	-1.593103
H	-3.784484	4.500420	-0.846423	H	-3.390701	2.796878	-3.734943
H	-3.612735	2.999416	-1.775659	H	-4.124182	1.950896	-2.359297
H	-2.217855	3.670249	-0.912671	H	-2.674631	1.288608	-3.135455
C	3.064522	1.012439	1.050511	C	2.883262	-0.669168	-0.527567
F	3.872625	0.555027	0.083894	F	3.023885	-1.940632	-0.128218
S	1.312577	1.242794	0.387691	S	1.121874	-0.347135	-1.128580
O	0.521676	1.572764	1.585784	O	1.096005	1.106541	-1.359925
N	0.917687	-0.260648	-0.047293	N	0.240621	-0.642700	0.189941

S	1.106705	-0.876592	-1.528962	S	-0.401857	-2.080971	0.561911
O	2.032612	-0.180890	-2.432117	O	0.130444	-3.251902	-0.149952
O	1.435309	2.246012	-0.676932	O	0.946698	-1.245473	-2.277429
F	3.538890	2.184419	1.497996	F	3.749581	-0.427691	-1.524659
F	3.066350	0.131059	2.065957	F	3.180920	0.140973	0.503415
C	-0.602226	-0.616316	-2.285593	C	-2.165544	-1.895705	-0.086051
F	-0.882654	0.692097	-2.370574	F	-2.154543	-1.639915	-1.403228
O	1.208818	-2.339220	-1.393437	O	-0.559844	-2.147552	2.020833
F	-0.632802	-1.148270	-3.517372	F	-2.843858	-3.034957	0.128053
F	-1.542432	-1.211520	-1.535019	F	-2.801035	-0.893735	0.541050
N	1.565609	-3.037788	1.619891	N	2.932583	3.218767	0.018994
H	1.920566	-3.921432	1.982921	H	3.890319	2.903167	0.168346
H	2.135835	-2.292464	2.018574	H	2.988501	4.194448	-0.271172
H	1.726428	-3.019931	0.611331	H	2.569794	2.688173	-0.773550

Fig. S1c

N	-1.667913	-0.193706	-2.224610
C	-0.442591	-0.053456	-2.732595
N	-0.180894	1.254042	-2.824960
C	-1.252088	1.981953	-2.345526
C	-2.191401	1.066066	-1.971811
H	0.698719	1.641170	-3.144796
C	-2.316160	-1.479116	-1.904980
C	-2.639938	-1.594513	-0.414521
C	-3.163571	-2.989214	-0.054548
C	-3.479071	-3.113686	1.440560
H	-1.221601	3.063531	-2.270900
H	-3.172509	1.198125	-1.545640
H	0.226507	-0.858096	-2.988195
H	-1.618575	-2.262148	-2.207520
H	-3.218160	-1.559562	-2.519221
H	-3.384066	-0.837976	-0.134788
H	-1.732778	-1.380234	0.156768
H	-2.411608	-3.739485	-0.335525
H	-4.064544	-3.210686	-0.644023
H	-3.846465	-4.116913	1.686059
H	-4.246777	-2.389898	1.742613
H	-2.583982	-2.923717	2.046014
C	3.021807	-1.043293	-0.541633
F	3.706410	-0.145559	0.179930
S	1.306464	-1.330221	0.193766
O	0.650455	-2.195083	-0.800337
N	0.624214	0.129916	0.079885
S	0.698315	1.270276	1.223862

Fig. S1d

N	-1.332635	-2.041312	-1.078228
C	-0.116471	-2.367699	-1.517525
N	0.069950	-1.770756	-2.698910
C	-1.047007	-1.023692	-3.017980
C	-1.936617	-1.195384	-1.997915
H	0.923099	-1.826959	-3.242013
C	-1.917861	-2.470173	0.205586
C	-2.293673	-1.278846	1.086417
C	-2.825311	-1.730599	2.450779
C	-3.208443	-0.538712	3.335969
H	-1.104871	-0.437290	-3.920421
H	-2.926518	-0.779398	-1.828383
H	0.598637	-2.980410	-0.994349
H	-1.169047	-3.093663	0.697846
H	-2.792312	-3.088280	-0.020506
H	-3.050092	-0.671360	0.577100
H	-1.409017	-0.651097	1.220975
H	-2.060107	-2.335073	2.957334
H	-3.698677	-2.383325	2.309830
H	-3.582578	-0.871191	4.311330
H	-3.992212	0.065944	2.861832
H	-2.343090	0.113019	3.509717
C	3.289102	-0.761224	0.211873
F	3.858710	0.349164	-0.276177
S	1.612963	-0.371465	0.988841
O	1.054460	-1.702519	1.277411
N	0.781012	0.238314	-0.252572
S	0.723203	1.806641	-0.643997

O	1.727148	1.107099	2.260292	O	1.755125	2.674556	-0.058335
O	1.550393	-1.856818	1.542856	O	1.914588	0.529901	2.108846
F	3.703600	-2.198984	-0.559428	F	4.101650	-1.297280	1.135738
F	2.912615	-0.588796	-1.802760	F	3.139996	-1.644117	-0.792357
C	-0.938983	1.027039	2.132849	C	-0.883974	2.359962	0.180178
F	-1.034400	-0.229427	2.593680	F	-0.850102	2.103327	1.496581
O	0.550247	2.579330	0.571724	O	0.438185	1.907607	-2.081479
F	-1.005062	1.876379	3.170412	F	-1.047456	3.680630	0.000725
F	-1.975674	1.265948	1.315304	F	-1.936823	1.721488	-0.355030
N	-0.552153	4.968778	-1.294114	N	-4.761643	0.277379	-1.251360
H	-1.277785	5.515940	-0.831558	H	-5.411678	-0.097606	-0.560854
H	0.167532	5.630951	-1.582975	H	-5.324394	0.553836	-2.055796
H	-0.134522	4.371981	-0.579072	H	-4.383685	1.137598	-0.854838

[BIm][Tf₂N]...2NH₃

Fig. S2a				Fig. S2b			
N	2.913745	-0.402450	1.351568	N	1.116601	2.589379	-0.630301
C	2.010131	0.561652	1.582962	C	-0.165125	2.704859	-0.258510
N	2.570921	1.745830	1.341683	N	-0.942045	2.561724	-1.330457
C	3.871835	1.544739	0.932093	C	-0.141830	2.328906	-2.427642
C	4.092716	0.195263	0.936665	C	1.153618	2.347935	-1.993822
H	2.015480	2.678698	1.340527	H	-2.020490	2.547372	-1.313475
C	2.636742	-1.849108	1.387027	C	2.277990	2.635865	0.274059
C	2.296138	-2.385116	-0.006047	C	3.044587	1.312592	0.285932
C	1.854078	-3.851779	0.035710	C	4.194404	1.327313	1.299326
C	1.461023	-4.371702	-1.351912	C	4.949838	-0.006705	1.326894
H	4.525086	2.364663	0.677217	H	-0.553215	2.165396	-3.411212
H	4.967409	-0.386731	0.691557	H	2.082519	2.211649	-2.523989
H	0.987987	0.389201	1.879194	H	-0.501893	2.854442	0.753982
H	1.797723	-1.996131	2.069343	H	1.889593	2.861929	1.269344
H	3.516997	-2.343232	1.807058	H	2.917503	3.465639	-0.043537
H	3.165778	-2.270273	-0.666943	H	3.439658	1.103841	-0.716431
H	1.490995	-1.776098	-0.430570	H	2.344169	0.509262	0.528742
H	0.997868	-3.945721	0.717379	H	3.792730	1.542710	2.299301
H	2.661302	-4.469913	0.453426	H	4.890106	2.143381	1.057897
H	1.145703	-5.420864	-1.307361	H	5.765442	0.013341	2.059146
H	2.302656	-4.302467	-2.053143	H	5.383387	-0.233569	0.344491
H	0.629833	-3.784816	-1.760966	H	4.276523	-0.831199	1.592686
C	-3.129969	-0.895404	0.904743	C	-2.221571	-0.146694	1.914293
F	-3.886756	-0.334339	-0.046614	F	-2.917043	-1.156717	1.368240
S	-1.327315	-1.003493	0.347513	S	-0.367243	-0.395246	1.656216
O	-0.610640	-1.434566	1.558727	O	0.219461	0.852077	2.170930
N	-0.912492	0.543138	0.091085	N	-0.233742	-0.364469	0.047716

S	-1.075419	1.310925	-1.329352	S	-0.327475	-1.663936	-0.907247
O	-2.103646	0.793760	-2.241796	O	-0.893843	-2.885411	-0.317433
O	-1.345146	-1.886445	-0.824860	O	-0.054492	-1.659386	2.335414
F	-3.588517	-2.131937	1.154311	F	-2.493759	-0.094826	3.227029
F	-3.228110	-0.163208	2.024525	F	-2.620324	1.003909	1.345746
C	0.559266	0.959800	-2.212518	C	1.491338	-2.070275	-1.206317
F	0.714971	-0.354258	-2.422149	F	2.119631	-2.275905	-0.038850
O	-1.018081	2.752788	-1.048878	O	-0.812776	-1.225831	-2.225725
F	0.561800	1.591879	-3.396668	F	1.584989	-3.183589	-1.950846
F	1.594427	1.405627	-1.484331	F	2.100784	-1.066630	-1.854252
N	0.961807	3.941045	1.225526	N	-3.683833	2.403052	-1.277316
H	1.291234	4.871036	1.480898	H	-4.174785	2.943565	-1.989382
H	0.158368	3.698117	1.825213	H	-4.090686	2.661024	-0.378436
H	0.597095	3.988124	0.273347	H	-3.892591	1.403125	-1.439397
N	-1.445043	2.634912	2.536817	N	-3.950752	-0.589397	-1.749707
H	-2.338827	3.113498	2.428276	H	-4.609621	-0.991044	-2.415781
H	-1.500859	2.115223	3.412177	H	-4.088093	-1.083829	-0.868887
H	-1.392648	1.943229	1.786508	H	-3.013164	-0.832709	-2.072460
Fig. S2c				Fig. S2d			
N	-2.184822	1.005317	1.769297	N	-2.716207	-0.094385	-1.709471
C	-0.928977	1.394332	2.029927	C	-1.458036	0.258164	-2.008301
N	-0.395482	0.535257	2.898946	N	-1.371378	1.586913	-1.991668
C	-1.318826	-0.446626	3.190121	C	-2.602522	2.114808	-1.665021
C	-2.450116	-0.152374	2.485366	C	-3.452571	1.059245	-1.485045
H	0.633233	0.510814	3.149289	H	-0.448479	2.106540	-2.122873
C	-3.063866	1.616602	0.760717	C	-3.171128	-1.480689	-1.507161
C	-3.121761	0.766638	-0.512089	C	-2.765556	-2.003772	-0.126108
C	-3.951898	1.436609	-1.612208	C	-3.208220	-3.453845	0.097970
C	-4.003489	0.588701	-2.888669	C	-2.768314	-3.981914	1.468633
H	-1.093339	-1.266297	3.853405	H	-2.746424	3.178397	-1.559466
H	-3.401646	-0.656344	2.422011	H	-4.497228	1.020813	-1.218151
H	-0.455810	2.275458	1.600138	H	-0.646383	-0.430373	-2.185560
H	-2.659691	2.610020	0.549951	H	-2.733807	-2.090243	-2.302781
H	-4.054651	1.739655	1.208273	H	-4.256136	-1.486102	-1.637215
H	-3.545057	-0.217619	-0.271931	H	-3.197584	-1.354238	0.646001
H	-2.098536	0.601978	-0.865707	H	-1.675447	-1.934116	-0.030561
H	-3.519934	2.420837	-1.842155	H	-2.785926	-4.088545	-0.693708
H	-4.972402	1.620043	-1.246878	H	-4.301225	-3.523741	0.006097
H	-4.592861	1.081640	-3.670760	H	-3.084889	-5.021397	1.613576
H	-4.457069	-0.391003	-2.691377	H	-3.200673	-3.381308	2.278994
H	-2.994329	0.416262	-3.283505	H	-1.676513	-3.943191	1.570403
N	2.353194	0.234517	3.185284	N	1.158960	2.702794	-2.151520
H	2.852528	0.872844	2.566737	H	1.366973	3.551645	-2.675644

H	2.393979	-0.690624	2.755410	H	1.810075	1.982511	-2.462817
H	2.871418	0.194456	4.061731	H	1.369360	2.878368	-1.168245
N	0.028577	4.053496	0.519170	N	-1.317555	4.545034	0.101357
H	-0.599840	4.833757	0.330277	H	-0.886528	5.419260	0.402077
H	0.099328	3.507592	-0.340247	H	-0.669639	3.801751	0.365024
H	0.949802	4.455859	0.688118	H	-2.146076	4.422374	0.683642
C	2.654119	1.336811	-0.791222	C	3.275761	-1.010927	-0.876516
F	3.576192	0.396380	-0.539078	F	4.013847	-0.341826	0.019850
S	1.042356	0.544071	-1.373447	S	1.529961	-1.291440	-0.215748
O	0.109006	1.677340	-1.472954	O	0.812399	-1.883549	-1.357606
N	0.618748	-0.333462	-0.088450	N	0.988118	0.221159	-0.039713
S	0.999153	-1.890567	0.122152	S	1.065822	1.072888	1.329150
O	2.067974	-2.441247	-0.723230	O	2.031178	0.634210	2.344359
O	1.401263	-0.177715	-2.601159	O	1.702227	-2.091921	1.002606
F	3.122606	2.163940	-1.737914	F	3.858474	-2.192987	-1.125951
F	2.449181	2.045407	0.334527	F	3.233319	-0.301062	-2.016815
C	-0.570678	-2.754071	-0.472384	C	-0.628836	0.754613	2.096117
F	-0.794252	-2.463684	-1.763132	F	-0.798853	-0.555535	2.320805
O	1.037301	-2.156996	1.568294	O	1.021994	2.501270	0.966527
F	-0.425501	-4.083317	-0.345679	F	-0.726696	1.413719	3.260553
F	-1.634022	-2.366730	0.246085	F	-1.600693	1.182538	1.274822

Fig. S2e

N	2.168250	0.863421	1.700722
C	0.904209	1.235157	1.938146
N	0.735405	2.479858	1.495614
C	1.920437	2.919288	0.938057
C	2.828706	1.905603	1.065390
H	-0.220270	2.941177	1.435963
C	2.713691	-0.484119	1.927400
C	2.637519	-1.333894	0.657033
C	3.161219	-2.756247	0.881850
C	3.068343	-3.609295	-0.388744
H	2.015179	3.901229	0.501452
H	3.861505	1.788221	0.754586
H	0.145240	0.603371	2.369948
H	2.135097	-0.937139	2.736504
H	3.745612	-0.365811	2.267533
H	3.212401	-0.842590	-0.138102
H	1.594290	-1.371431	0.324829
H	2.584876	-3.231872	1.687680
H	4.204549	-2.714784	1.226082
H	3.444384	-4.624240	-0.214619
H	3.655848	-3.166541	-1.203231

H	2.029110	-3.687958	-0.731517
N	-1.872000	3.328976	1.088400
H	-2.505378	2.668888	1.538862
H	-1.919889	3.141064	0.085428
H	-2.241029	4.264557	1.252515
N	5.716932	0.701846	0.067244
H	5.867452	-0.240914	0.425695
H	6.599215	1.198844	0.188579
H	5.577163	0.606255	-0.938532
C	0.470995	0.160951	-2.374247
F	0.654325	-1.161325	-2.239951
S	-1.210310	0.660449	-1.678372
O	-1.192049	2.131584	-1.731092
N	-1.073394	0.222767	-0.129577
S	-1.586337	-1.177735	0.488214
O	-1.790365	-2.294108	-0.443562
O	-2.190462	-0.065288	-2.497201
F	0.532850	0.477612	-3.677092
F	1.455893	0.800306	-1.726173
C	-3.314320	-0.725424	1.098433
F	-4.083420	-0.325717	0.075936
O	-0.826831	-1.416378	1.726724
F	-3.883664	-1.790573	1.681720
F	-3.244039	0.271869	1.998581

[BIm][Tf₂N]...3NH₃

Fig. S3a				Fig. S3b			
N	-0.883591	1.965464	1.748919	N	1.775950	-1.733679	1.784436
C	0.423446	2.145382	1.510879	C	0.564192	-2.186612	1.432759
N	1.115619	1.376820	2.352959	N	-0.318562	-1.790402	2.350399
C	0.235830	0.670223	3.143536	C	0.335535	-1.049752	3.311244
C	-1.024579	1.040225	2.770565	C	1.655005	-1.011605	2.961693
H	2.181249	1.278552	2.347297	H	-1.378139	-1.933124	2.278707
C	-1.975246	2.599876	0.992390	C	2.993181	-1.859041	0.967665
C	-2.906052	1.568210	0.352842	C	3.294214	-0.562028	0.211069
C	-3.944677	2.226839	-0.561571	C	4.518966	-0.697974	-0.699529
C	-4.875017	1.194518	-1.208927	C	4.812307	0.599974	-1.461538
H	0.571812	-0.037928	3.884087	H	-0.186104	-0.604892	4.143418
H	-1.991212	0.724286	3.128240	H	2.504549	-0.540015	3.430216
H	0.837753	2.813115	0.757665	H	0.378692	-2.791609	0.549933
H	-1.500894	3.215167	0.224657	H	2.823214	-2.686313	0.273977
H	-2.521924	3.260480	1.673406	H	3.815185	-2.135228	1.635139
H	-3.418823	0.993639	1.134856	H	3.454381	0.249701	0.933179

H	-2.299443	0.862468	-0.220735	H	2.414914	-0.292703	-0.382177
H	-3.425995	2.796509	-1.345307	H	4.348589	-1.514005	-1.416251
H	-4.537860	2.952631	0.012924	H	5.396796	-0.984100	-0.102678
H	-5.610496	1.676870	-1.863433	H	5.684754	0.489708	-2.116377
H	-5.423168	0.626204	-0.446520	H	5.013593	1.425849	-0.767274
H	-4.303692	0.478117	-1.812537	H	3.956221	0.888967	-2.084128
C	2.176647	0.263775	-1.760917	C	-1.969066	-1.082028	-1.667117
F	2.771206	-0.938069	-1.693187	F	-3.027152	-0.378659	-1.243410
S	0.299693	0.081725	-1.652915	S	-0.433704	0.014066	-1.756771
O	-0.186788	1.470474	-1.642920	O	0.636379	-0.915975	-2.152844
N	0.096485	-0.517101	-0.169189	N	-0.187479	0.413159	-0.212282
S	0.022238	-2.092714	0.179978	S	-0.771322	1.750327	0.482718
O	0.493720	-3.028520	-0.851012	O	-1.958997	2.353478	-0.147050
O	-0.057890	-0.779365	-2.787994	O	-0.806959	1.092301	-2.682277
F	2.506535	0.843918	-2.925900	F	-2.236562	-1.578689	-2.885877
F	2.636794	1.026781	-0.756204	F	-1.770177	-2.108222	-0.822034
C	-1.840167	-2.385717	0.276685	C	0.614622	3.001809	0.202112
F	-2.420128	-2.060870	-0.888912	F	0.827834	3.190724	-1.107647
O	0.487297	-2.278474	1.563164	O	-0.774899	1.548109	1.935782
F	-2.076307	-3.682764	0.531505	F	0.274632	4.175799	0.759785
F	-2.390899	-1.648813	1.252509	F	1.753406	2.570881	0.766057
N	3.856198	1.005019	2.234558	N	-3.061570	-2.065581	2.075066
H	3.947503	0.013456	1.958107	H	-3.549698	-2.424949	2.895565
H	4.390055	1.141303	3.092627	H	-3.281032	-2.698055	1.305496
H	4.306239	1.568895	1.513738	H	-3.483194	-1.150013	1.844358
N	3.708542	-1.916576	1.383870	N	-4.334122	0.652013	1.393494
H	4.278382	-2.665053	1.776519	H	-5.166158	0.519431	0.819223
H	3.794086	-1.986391	0.370382	H	-3.696394	1.238053	0.854302
H	2.735724	-2.134668	1.604272	H	-4.623940	1.202409	2.201368
N	1.461944	4.010729	-0.899603	N	0.761878	-3.903134	-1.289333
H	2.443208	3.877647	-1.142098	H	-0.059629	-4.397237	-1.636613
H	1.229035	4.972538	-1.144442	H	1.571047	-4.460593	-1.561536
H	0.924570	3.402945	-1.518394	H	0.814344	-3.024468	-1.806329
Fig. S3c				Fig. S3d			
N	0.004187	2.232417	1.416895	N	0.638681	2.743980	-0.733957
C	1.197893	1.627073	1.343484	C	-0.652443	2.437147	-0.539194
N	1.335291	0.822356	2.396496	N	-1.218840	2.156571	-1.710107
C	0.194105	0.892934	3.163655	C	-0.261346	2.268958	-2.695135
C	-0.645264	1.782060	2.555078	C	0.907595	2.637988	-2.088733
H	2.176907	0.167142	2.536944	H	-2.269548	1.818412	-1.826850
C	-0.552094	3.153448	0.412904	C	1.613804	3.063928	0.321803
C	-1.855142	2.624739	-0.189431	C	2.714143	2.006879	0.418853
C	-2.350278	3.510558	-1.337658	C	3.664526	2.274614	1.591136

C	-3.653755	2.982827	-1.948325	C	4.755729	1.203401	1.701174
H	0.067952	0.304685	4.058514	H	-0.484156	2.078779	-3.733652
H	-1.632517	2.123204	2.821747	H	1.888843	2.833532	-2.491550
H	1.925204	1.769750	0.555707	H	-1.133820	2.393071	0.424141
H	0.207608	3.264889	-0.363501	H	1.054152	3.118937	1.257629
H	-0.700194	4.127131	0.891062	H	2.027902	4.054247	0.107315
H	-2.627259	2.564962	0.588283	H	3.283071	1.976905	-0.519464
H	-1.682186	1.608003	-0.551590	H	2.242009	1.028348	0.538368
H	-1.574543	3.560648	-2.114512	H	3.085133	2.306090	2.524460
H	-2.498809	4.537955	-0.975816	H	4.126419	3.265348	1.474610
H	-3.993565	3.620345	-2.772980	H	5.424584	1.403128	2.546513
H	-4.453716	2.947173	-1.197744	H	5.365506	1.167689	0.789289
H	-3.518104	1.966910	-2.340207	H	4.314225	0.209701	1.845940
C	1.942652	-1.370783	-1.463349	C	-2.029647	-0.862653	1.725708
F	1.847488	-2.668987	-1.142198	F	-2.342158	-2.047941	1.178088
S	0.232839	-0.571183	-1.505443	S	-0.173145	-0.540407	1.611079
O	0.523263	0.855285	-1.733672	O	-0.038285	0.845114	2.088213
N	-0.264153	-0.721550	0.019416	N	0.078525	-0.526901	0.016743
S	-1.130292	-1.962273	0.591155	S	0.439529	-1.829045	-0.869518
O	-1.165036	-3.181888	-0.229537	O	0.190602	-3.142400	-0.258283
O	-0.504059	-1.309124	-2.539957	O	0.451669	-1.621118	2.385067
F	2.518806	-1.262832	-2.672179	F	-2.411792	-0.866592	3.012090
F	2.724834	-0.759753	-0.559823	F	-2.706662	0.099283	1.077528
C	-2.888162	-1.277412	0.498786	C	2.318189	-1.711704	-1.010897
F	-3.179309	-0.905831	-0.757813	F	2.876973	-1.701034	0.208923
O	-0.865597	-2.082266	2.030686	O	-0.032926	-1.586954	-2.241906
F	-3.759931	-2.224309	0.882802	F	2.782165	-2.772203	-1.690820
F	-3.027425	-0.213676	1.304259	F	2.675754	-0.594178	-1.660022
N	3.545242	-0.799209	2.522404	N	-3.749729	1.275461	-1.876116
H	4.029630	-0.929512	3.410000	H	-4.306569	1.623026	-2.656724
H	4.187726	-0.314793	1.872352	H	-4.236076	1.531201	-1.003757
H	3.359074	-1.727232	2.143141	H	-3.716001	0.246149	-1.944600
N	5.121855	0.838979	0.502689	N	-4.923371	2.084615	0.877529
H	5.855384	1.469233	0.826278	H	-5.681131	2.758160	0.985724
H	4.429897	1.412107	0.007919	H	-4.131923	2.446133	1.408863
H	5.550676	0.231968	-0.195696	H	-5.220305	1.231445	1.350002
N	3.100226	2.529645	-1.346780	N	-3.274065	-1.757592	-2.046080
H	3.851739	2.497145	-2.036296	H	-3.336477	-2.176369	-1.118755
H	2.816417	3.507834	-1.288482	H	-2.284898	-1.768134	-2.298521
H	2.314930	2.017054	-1.750796	H	-3.751794	-2.392004	-2.685151
Fig. S3e				Fig. S3f			
N	2.590141	0.450280	1.340765	N	-1.180973	2.771613	-0.381383
C	1.455156	1.111822	1.607738	C	0.002218	2.494116	-0.943865

N	1.649758	2.408478	1.370077	N	0.970130	2.756165	-0.067399
C	2.943683	2.587712	0.924158	C	0.398841	3.199265	1.106420
C	3.543173	1.358249	0.903851	C	-0.953897	3.213729	0.913324
H	0.853476	3.135962	1.391057	H	2.012856	2.539232	-0.220485
C	2.761878	-1.010905	1.385593	C	-2.497204	2.504431	-0.983671
C	2.684093	-1.623376	-0.014217	C	-3.192478	1.324319	-0.300873
C	2.789578	-3.151714	0.024260	C	-4.502125	0.942359	-0.998510
C	2.698518	-3.770129	-1.375369	C	-5.176375	-0.260593	-0.328181
H	3.325269	3.562086	0.661063	H	1.007271	3.430566	1.967175
H	4.532493	1.015292	0.618632	H	-1.764959	3.489331	1.568765
H	0.532646	0.652783	1.924049	H	0.132062	2.091078	-1.934655
H	1.972303	-1.408746	2.025380	H	-2.323476	2.291088	-2.041023
H	3.728757	-1.211612	1.854394	H	-3.091219	3.420572	-0.911588
H	3.487818	-1.205513	-0.634096	H	-3.389453	1.573363	0.750320
H	1.734649	-1.333288	-0.478138	H	-2.505827	0.473619	-0.305205
H	1.984576	-3.551730	0.656101	H	-4.293990	0.706395	-2.051594
H	3.737229	-3.443587	0.499259	H	-5.188220	1.801296	-0.998616
H	2.771975	-4.863203	-1.332471	H	-6.107966	-0.530572	-0.839260
H	3.506476	-3.402775	-2.021169	H	-5.417140	-0.043251	0.720299
H	1.744405	-3.513636	-1.851921	H	-4.515741	-1.136663	-0.343960
C	-3.024875	-1.785957	0.823659	C	1.612251	-0.976009	-2.240174
F	-3.897094	-1.482030	-0.145462	F	2.507524	-1.614609	-1.476721
S	-1.267243	-1.307873	0.318065	S	-0.130621	-1.128128	-1.524279
O	-0.481352	-1.523351	1.544027	O	-0.931303	-0.257493	-2.399180
N	-1.353583	0.296833	0.100776	N	-0.027049	-0.383885	-0.093585
S	-1.721079	1.012777	-1.308145	S	0.394404	-1.096732	1.290709
O	-2.530285	0.229293	-2.250923	O	1.266398	-2.278662	1.180791
O	-0.979670	-2.123300	-0.868336	O	-0.397465	-2.572621	-1.508657
F	-3.071983	-3.107626	1.053992	F	1.631393	-1.510732	-3.471051
F	-3.379229	-1.139061	1.944328	F	1.969027	0.317763	-2.329909
C	-0.046891	1.200573	-2.166616	C	-1.239805	-1.752240	1.977368
F	0.519891	0.004637	-2.374146	F	-1.793261	-2.635732	1.137286
O	-2.111213	2.396810	-1.001065	O	0.762073	-0.040640	2.244275
F	-0.229428	1.806374	-3.350816	F	-1.011815	-2.355588	3.155314
F	0.783110	1.948190	-1.424298	F	-2.099958	-0.740842	2.169101
N	-0.560781	4.024102	1.312197	N	3.621765	2.097915	-0.432478
H	-0.539978	5.013440	1.555473	H	4.254940	2.776330	-0.009307
H	-1.227687	3.544381	1.934876	H	3.891585	2.014946	-1.412392
H	-0.948474	3.940519	0.371552	H	3.805830	1.184689	0.013920
N	-2.401474	2.004034	2.656537	N	4.190097	-0.623399	0.902353
H	-3.405265	2.177264	2.610727	H	4.808223	-1.137166	0.274665
H	-2.242234	1.457825	3.502627	H	3.352671	-1.195517	1.011650
H	-2.174587	1.396133	1.866871	H	4.651035	-0.608116	1.811677
N	6.161636	-0.441110	0.023616	N	2.996627	2.110665	2.882954

H	6.067605	-1.388188	0.390123	H	3.061551	2.046578	3.898915
H	7.104701	-0.134123	0.261259	H	3.914327	1.852776	2.522142
H	6.133995	-0.523674	-0.992476	H	2.358559	1.370412	2.587402
Fig. S3g				Fig. S3h			
N	-1.825740	-2.120902	-1.387244	N	-0.123555	2.798777	-0.477754
C	-1.613539	-0.837769	-1.711924	C	0.950958	2.139579	-0.935662
N	-2.750300	-0.161013	-1.549407	N	1.887651	2.115673	0.009008
C	-3.725911	-1.024797	-1.097004	C	1.399879	2.766679	1.121589
C	-3.148394	-2.259614	-0.994673	C	0.137511	3.199326	0.822422
H	-2.819859	0.904726	-1.648210	H	2.859504	1.583694	-0.077211
C	-0.785872	-3.161954	-1.320709	C	-1.387217	2.990054	-1.208225
C	-0.315189	-3.389948	0.118515	C	-2.548701	2.254064	-0.538797
C	0.887297	-4.338270	0.180784	C	-3.841289	2.361715	-1.354969
C	1.391027	-4.535188	1.615019	C	-5.005011	1.619439	-0.687295
H	-4.718563	-0.674197	-0.858741	H	1.980981	2.866912	2.025255
H	-3.549672	-3.210757	-0.681335	H	-0.585552	3.746976	1.406087
H	-0.664699	-0.427340	-2.016541	H	1.017697	1.677852	-1.907094
H	0.042537	-2.822013	-1.944318	H	-1.224806	2.608646	-2.218375
H	-1.200511	-4.073957	-1.758779	H	-1.578456	4.066003	-1.271652
H	-1.144199	-3.789975	0.717743	H	-2.712108	2.659315	0.468229
H	-0.039830	-2.425086	0.558382	H	-2.268101	1.204114	-0.420461
H	1.696087	-3.926460	-0.437903	H	-3.669273	1.948695	-2.358748
H	0.616126	-5.309168	-0.257476	H	-4.106375	3.419757	-1.492079
H	2.253873	-5.211103	1.642854	H	-5.920067	1.693889	-1.286512
H	0.607576	-4.962550	2.253991	H	-5.217764	2.034466	0.306276
H	1.697487	-3.576557	2.051007	H	-4.768721	0.555699	-0.560539
C	3.385786	0.890089	-0.677138	C	1.131702	-1.845484	-1.925907
F	3.629214	1.817259	0.256869	F	1.532158	-2.795948	-1.066981
S	1.881252	-0.155754	-0.211329	S	-0.560367	-1.171005	-1.429003
O	1.644476	-0.976122	-1.410291	O	-0.768387	-0.047278	-2.355890
N	0.667167	0.917793	-0.143558	N	-0.266747	-0.545449	0.030126
S	0.252351	1.751468	1.184334	S	-0.413837	-1.352383	1.422384
O	1.311150	1.972630	2.177801	O	-0.488687	-2.817992	1.339770
O	2.251503	-0.815821	1.046349	O	-1.464513	-2.326296	-1.499509
F	4.457651	0.089807	-0.788102	F	1.066300	-2.375034	-3.156864
F	3.179773	1.503066	-1.852688	F	2.043939	-0.858794	-1.928787
C	-0.984648	0.620535	2.060290	C	-2.122747	-0.815249	2.018658
F	-0.408898	-0.534449	2.415625	F	-3.051666	-1.106630	1.095171
O	-0.569559	2.887501	0.742222	O	0.505640	-0.746417	2.398544
F	-1.437912	1.239290	3.161651	F	-2.423441	-1.463363	3.155409
F	-2.029121	0.351469	1.259439	F	-2.148395	0.504097	2.256577
N	-2.611302	2.588575	-1.720718	N	4.192997	0.750625	-0.177763
H	-3.338738	3.198344	-2.092333	H	5.011453	1.240141	0.214341

H	-1.780748	2.674474	-2.327293	H	4.418343	0.493627	-1.138941
H	-2.324479	2.957423	-0.812847	H	4.050846	-0.124300	0.351581
N	0.164650	2.469642	-2.942728	N	3.447631	-1.737548	1.462980
H	0.654290	3.362010	-3.003761	H	4.052506	-2.160213	2.166262
H	0.529440	1.890207	-3.698232	H	3.147849	-2.490968	0.845108
H	0.461477	2.033696	-2.067379	H	2.609061	-1.412428	1.946113
N	-5.132401	1.457804	0.494478	N	6.590999	2.286574	1.056343
H	-4.436470	1.159327	1.177397	H	7.472145	1.781089	0.968669
H	-5.785150	2.063680	0.990909	H	6.442042	2.439284	2.053446
H	-4.638402	2.048569	-0.173721	H	6.740244	3.205564	0.640664
Fig. S3i				Fig. S3j			
N	-1.018247	2.463845	-1.678059	N	-1.928031	-1.396365	1.730789
C	-0.099061	1.507517	-1.875045	C	-1.299396	-0.321079	2.225939
N	1.071818	1.935930	-1.409560	N	-0.092691	-0.699770	2.648856
C	0.911062	3.199895	-0.881398	C	0.076041	-2.046919	2.403796
C	-0.403461	3.536715	-1.048982	C	-1.081801	-2.490656	1.831067
H	1.953441	1.319655	-1.360962	H	0.667643	-0.028096	2.950200
C	-2.460364	2.306746	-1.929438	C	-3.247787	-1.383445	1.081960
C	-3.146076	1.556539	-0.783359	C	-3.136384	-1.639120	-0.423875
C	-4.645352	1.361855	-1.034256	C	-4.499581	-1.546024	-1.119309
C	-5.322279	0.591882	0.105966	C	-4.396975	-1.798719	-2.628002
H	1.735883	3.708943	-0.403937	H	1.003289	-2.562472	2.618072
H	-0.954286	4.424008	-0.778103	H	-1.374029	-3.468603	1.482368
H	-0.299982	0.534152	-2.294124	H	-1.729389	0.677148	2.263023
H	-2.573910	1.768934	-2.874879	H	-3.685338	-0.401778	1.279715
H	-2.877181	3.308512	-2.060960	H	-3.870782	-2.139597	1.570004
H	-2.989711	2.109003	0.152052	H	-2.701474	-2.633227	-0.594365
H	-2.661564	0.580007	-0.666101	H	-2.447512	-0.902375	-0.851048
H	-4.788046	0.819963	-1.979793	H	-4.928202	-0.549418	-0.942181
H	-5.128094	2.341485	-1.158839	H	-5.194161	-2.269582	-0.669121
H	-6.392182	0.453044	-0.088731	H	-5.378029	-1.722491	-3.111478
H	-5.219159	1.128038	1.057912	H	-3.997270	-2.800147	-2.832810
H	-4.869709	-0.399800	0.231061	H	-3.729033	-1.068776	-3.102446
C	0.606347	-3.208898	-1.029164	N	2.008399	1.082715	3.075681
F	1.334822	-3.630262	0.014827	H	2.566102	1.137417	3.926746
S	-0.701764	-1.972313	-0.461319	H	1.741761	2.034512	2.826012
O	-1.283614	-1.471628	-1.717768	H	2.610461	0.734621	2.327821
N	0.205213	-0.789483	0.155959	N	-2.988077	2.405843	1.961413
S	0.625720	-0.652317	1.707266	H	-4.001139	2.475075	2.052888
O	0.470122	-1.840413	2.556598	H	-2.778337	2.351253	0.964293
O	-1.559105	-2.721300	0.465934	H	-2.605193	3.290801	2.292295
F	0.012896	-4.267486	-1.601206	N	3.068107	-3.397976	1.934966
F	1.429531	-2.639412	-1.925637	H	2.744652	-4.099708	1.269229

C	-0.652769	0.576708	2.350594	H	4.025234	-3.652268	2.178213
F	-1.890143	0.083006	2.196161	H	3.115854	-2.516109	1.422882
O	1.894700	0.094064	1.763772	C	1.671953	-1.700976	-1.594496
F	-0.436966	0.807839	3.655171	F	0.880417	-1.429190	-2.642254
F	-0.564214	1.738117	1.685881	S	2.093348	-0.110090	-0.670204
N	3.201023	0.223402	-1.134391	O	2.790187	-0.576064	0.542212
H	4.152867	0.611353	-1.137494	N	0.633145	0.418707	-0.231383
H	3.175531	-0.567771	-1.776506	S	-0.201807	1.552596	-1.020498
H	3.013258	-0.143116	-0.200742	O	0.138688	1.784685	-2.430223
N	6.040360	1.563363	-1.039580	O	2.845397	0.700199	-1.637359
H	6.169703	2.544990	-1.284761	F	2.802482	-2.272863	-2.039363
H	6.498576	1.024206	-1.774767	F	1.040420	-2.565804	-0.787698
H	6.581795	1.403090	-0.190192	C	0.334777	3.125951	-0.124933
N	3.572497	2.821358	0.983813	F	1.657398	3.308678	-0.246001
H	2.959582	2.072326	1.308458	O	-1.617824	1.404254	-0.651845
H	4.080488	3.155140	1.802554	F	-0.301815	4.185400	-0.646686
H	4.262316	2.383239	0.371861	F	0.031942	3.045222	1.183500
Fig. S3k				Fig. S3l			
N	1.718253	2.238137	0.356326	N	1.890359	-1.396000	1.484909
C	0.412981	2.484840	0.522592	C	0.632852	-1.594072	1.903252
N	-0.092239	2.924078	-0.628765	N	0.348504	-0.666584	2.818796
C	0.914799	2.944352	-1.572495	C	1.439835	0.164195	2.975353
C	2.059140	2.515539	-0.959797	C	2.419528	-0.293449	2.142068
H	-1.135133	3.104414	-0.806709	H	-0.624227	-0.474280	3.180657
C	2.615998	1.647110	1.360806	C	2.550132	-2.122130	0.390412
C	2.982205	0.205915	1.001999	C	2.634688	-1.259058	-0.871491
C	3.892202	-0.435782	2.053868	C	3.302829	-1.999536	-2.034210
C	4.249652	-1.882735	1.694122	C	3.378760	-1.132893	-3.296827
H	0.733920	3.253950	-2.589936	H	1.420344	1.008857	3.645449
H	3.076303	2.367990	-1.309762	H	3.424606	0.050999	1.921818
H	-0.134694	2.316908	1.435042	H	-0.023964	-2.387915	1.552728
H	2.094041	1.686808	2.319716	H	1.967519	-3.028995	0.208591
H	3.505677	2.280968	1.425064	H	3.544892	-2.417447	0.737400
H	3.477887	0.193945	0.023550	H	3.195160	-0.345034	-0.640752
H	2.058344	-0.370469	0.901927	H	1.621130	-0.956630	-1.153732
H	3.390569	-0.412460	3.031529	H	2.741241	-2.919001	-2.252354
H	4.811799	0.157977	2.159275	H	4.314592	-2.313655	-1.739615
H	4.894566	-2.336035	2.456134	H	3.851175	-1.674434	-4.124873
H	4.778261	-1.929042	0.733283	H	3.962525	-0.221851	-3.112700
H	3.345467	-2.498306	1.606596	H	2.376205	-0.826668	-3.621150
C	-2.671060	0.103832	1.645422	N	-2.265566	0.132576	3.369447
F	-3.545575	-0.394830	0.763204	H	-2.706266	0.258359	4.279497
S	-0.992832	-0.754896	1.505895	H	-2.918159	-0.390274	2.786333

O	-0.167646	-0.035578	2.489861	H	-2.159514	1.054257	2.942676
N	-0.455876	-0.324415	0.046029	N	-1.060580	-4.033794	0.647825
S	-0.769503	-1.108368	-1.329974	H	-0.662713	-4.946762	0.429871
O	-2.003096	-1.913786	-1.355788	H	-1.093956	-3.502778	-0.222941
O	-1.288744	-2.177973	1.719937	H	-2.026713	-4.196369	0.929285
F	-3.156833	-0.074216	2.884351	N	5.395638	0.368035	0.860738
F	-2.540286	1.424351	1.422975	H	6.174542	0.676062	1.442598
C	0.634470	-2.366865	-1.446697	H	5.246820	1.101423	0.167823
F	0.618121	-3.202012	-0.399267	H	5.725788	-0.448995	0.347450
O	-0.504664	-0.189491	-2.443596	C	0.737940	2.580762	-0.587353
F	0.493811	-3.082160	-2.575159	F	0.803692	2.215002	-1.876669
F	1.819841	-1.739366	-1.480041	S	-0.894073	2.006574	0.168732
N	-2.800135	3.269576	-1.082218	O	-0.750684	2.296850	1.603813
H	-3.023411	3.984568	-1.774920	N	-0.809059	0.404021	-0.025517
H	-3.298047	3.526195	-0.229697	S	-1.466705	-0.399999	-1.259612
H	-3.209004	2.381038	-1.417090	O	-1.750808	0.355224	-2.487196
N	-4.054981	0.650713	-2.111747	O	-1.929224	2.719371	-0.593885
H	-5.000037	0.542475	-1.744676	F	0.818855	3.919680	-0.511835
H	-3.546110	-0.196482	-1.860014	F	1.781072	2.049061	0.064253
H	-4.136315	0.649554	-3.128120	C	-3.164312	-0.861643	-0.572873
N	5.220862	1.710718	-1.461946	F	-3.879225	0.240463	-0.306204
H	5.666743	1.541050	-0.560596	O	-0.771307	-1.691721	-1.375334
H	5.849695	2.320703	-1.983980	F	-3.830009	-1.607489	-1.467689
H	5.214803	0.816308	-1.951913	F	-3.033383	-1.571463	0.563417

Fig. S3m

N	-2.098601	-0.143458	-1.931054
C	-0.873727	0.261229	-2.288828
N	-0.839386	1.592389	-2.256181
C	-2.072570	2.063128	-1.848541
C	-2.872240	0.973614	-1.644239
H	0.060417	2.146442	-2.356156
C	-2.499601	-1.539255	-1.698001
C	-2.428277	-1.888266	-0.209785
C	-2.804606	-3.348100	0.063053
C	-2.710428	-3.694264	1.553704
H	-2.251769	3.117507	-1.705466
H	-3.891835	0.855913	-1.292694
H	-0.046845	-0.392621	-2.512736
H	-1.826812	-2.172683	-2.281198
H	-3.513361	-1.660753	-2.088592
H	-3.094675	-1.217242	0.346736
H	-1.409622	-1.696951	0.143480
H	-2.139025	-4.007849	-0.510906

Fig. S3n

N	-1.667267	1.740073	-1.476811
C	-0.337471	1.663863	-1.618780
N	0.229878	2.613906	-0.879169
C	-0.763653	3.313159	-0.221907
C	-1.961994	2.770659	-0.595347
H	1.291316	2.644137	-0.685332
C	-2.637712	0.786973	-2.035719
C	-3.042461	-0.265927	-1.001593
C	-4.026368	-1.289385	-1.576460
C	-4.417674	-2.353319	-0.544016
H	-0.537518	4.125923	0.450723
H	-2.990664	2.977167	-0.319232
H	0.176712	0.915740	-2.199602
H	-2.167578	0.318961	-2.904298
H	-3.501643	1.361327	-2.380785
H	-3.487319	0.235888	-0.133474
H	-2.137903	-0.774743	-0.651625
H	-3.574783	-1.775483	-2.452634

H	-3.824216	-3.539709	-0.300320	H	-4.927393	-0.771734	-1.935614
H	-2.976362	-4.741897	1.736823	H	-5.118240	-3.081680	-0.969038
H	-3.386807	-3.065403	2.146705	H	-4.896798	-1.895068	0.330682
H	-1.691572	-3.533234	1.927454	H	-3.533941	-2.899948	-0.191811
N	1.652872	2.816964	-2.178015	C	2.683775	-1.816591	-1.198269
H	1.858666	3.735911	-2.567599	F	3.448813	-1.946967	-0.105327
H	2.386983	2.183397	-2.493451	S	0.855990	-1.773004	-0.728058
H	1.733525	2.882012	-1.161848	O	0.177705	-1.456705	-1.996051
N	-1.308602	4.496303	0.238069	N	0.778268	-0.456504	0.199942
H	-1.018050	5.330708	0.747723	S	0.919658	-0.432633	1.807978
H	-0.593410	3.789005	0.411873	O	1.531692	-1.606836	2.445284
H	-2.156880	4.163811	0.696516	O	0.594487	-3.070102	-0.090526
N	-5.656923	-0.116744	-0.254052	F	2.916642	-2.852008	-2.019101
H	-6.574234	0.248389	-0.509784	F	3.029156	-0.680691	-1.831019
H	-5.525226	0.103556	0.733054	C	-0.885762	-0.470484	2.356416
H	-5.726078	-1.132478	-0.313273	F	-1.487731	-1.578896	1.897897
C	-0.487577	0.778034	2.152388	O	1.381682	0.908028	2.200416
F	-0.623012	-0.520565	2.457878	F	-0.949581	-0.465735	3.697592
S	1.185922	1.082391	1.334239	F	-1.543038	0.600856	1.889002
O	1.108035	2.485290	0.887435	N	2.869359	2.350310	-0.230445
N	1.099287	0.145566	0.023934	H	3.542010	3.128875	-0.169799
S	1.699945	-1.350856	-0.084561	H	3.282290	1.621767	-0.812628
O	1.911924	-2.082476	1.170723	H	2.750985	1.944536	0.699244
O	2.178015	0.725860	2.356235	N	4.825567	4.741899	-0.098137
F	-0.576393	1.502537	3.278386	H	5.539258	4.705858	-0.825477
F	-1.484867	1.134539	1.328990	H	5.320389	4.785457	0.792311
C	3.428876	-1.035041	-0.772980	H	4.344390	5.634218	-0.207170
F	4.149580	-0.299338	0.084780	N	-5.183222	2.552609	0.070947
O	1.000563	-2.024797	-1.190264	H	-5.655052	1.930578	-0.585131
F	4.054042	-2.204447	-0.976272	H	-5.785196	3.369323	0.175168
F	3.350139	-0.378839	-1.943068	H	-5.188730	2.075228	0.972177

Fig. S3o

N	-0.828242	1.711240	1.754317
C	0.333683	1.387247	2.327964
N	0.130916	0.271825	3.039962
C	-1.183090	-0.139494	2.912652
C	-1.792071	0.773079	2.101730
H	0.851733	-0.210689	3.561880
C	-1.028829	2.849626	0.840967
C	-1.602517	2.400593	-0.503253
C	-1.696984	3.559808	-1.500594
C	-2.260620	3.104398	-2.851874
H	-1.545248	-1.053024	3.368574

H	-2.808375	0.828783	1.723960
H	1.268182	1.941289	2.233325
H	-0.051189	3.317161	0.706548
H	-1.692175	3.566346	1.336062
H	-2.595630	1.963257	-0.349543
H	-0.959974	1.614372	-0.907882
H	-0.698668	3.995761	-1.646666
H	-2.329569	4.356950	-1.084492
H	-2.319148	3.938406	-3.561091
H	-3.269615	2.687958	-2.736669
H	-1.627516	2.326139	-3.296343
N	-1.977394	-3.291726	3.489086
H	-1.577171	-4.075621	4.004107
H	-1.549498	-3.296515	2.562662
H	-2.964859	-3.508951	3.355956
N	2.973959	3.071938	1.743435
H	3.074357	4.084274	1.809544
H	2.853360	2.844817	0.755979
H	3.866759	2.671021	2.028797
N	-4.786699	0.826466	0.703620
H	-5.519045	0.398386	1.269844
H	-4.588040	0.172944	-0.053401
H	-5.202273	1.651342	0.271398
C	-1.591871	-1.544372	-1.539948
F	-1.247665	-0.787696	-2.592851
S	-0.060583	-2.020751	-0.542598
O	-0.608369	-2.629940	0.677198
N	0.553490	-0.576458	-0.153685
S	1.725446	0.163152	-0.982779
O	1.925309	-0.243277	-2.380167
O	0.729369	-2.858009	-1.456478
F	-2.201754	-2.654884	-1.984837
F	-2.457289	-0.855066	-0.779833
C	3.284260	-0.410637	-0.084210
F	3.419275	-1.740972	-0.173960
O	1.651845	1.599269	-0.670469
F	4.360687	0.173942	-0.634883
F	3.229699	-0.069950	1.214708

[BIm][Tf₂N]...4NH₃

Fig. S4a			Fig. S4b				
N	-0.381762	2.131449	1.689567	N	0.991183	-1.092064	2.360828
C	0.903903	1.792072	1.506534	C	-0.187125	-1.648973	2.046229

N	1.264662	0.931483	2.456079	N	-1.159231	-0.825535	2.440975
C	0.178766	0.692920	3.268951	C	-0.600373	0.298923	3.011219
C	-0.858413	1.446463	2.794984	C	0.754495	0.132742	2.966099
H	2.255628	0.441279	2.497607	H	-2.198480	-0.982112	2.261230
C	-1.164482	3.025156	0.820793	C	2.309042	-1.659870	2.035697
C	-2.403388	2.330554	0.253666	C	3.132863	-0.720710	1.152415
C	-3.118871	3.198982	-0.786698	C	4.432346	-1.377738	0.674985
C	-4.349343	2.495870	-1.371483	C	5.255733	-0.439812	-0.215582
H	0.226836	0.009511	4.102383	H	-1.216326	1.114657	3.364281
H	-1.876282	1.549320	3.135159	H	1.558402	0.772116	3.293445
H	1.539960	2.160184	0.713361	H	-0.315275	-2.612719	1.557592
H	-0.499658	3.331712	0.011016	H	2.120014	-2.603773	1.519476
H	-1.435983	3.913271	1.400786	H	2.827590	-1.879363	2.974889
H	-3.097779	2.083035	1.066861	H	3.366948	0.198693	1.704245
H	-2.092888	1.386741	-0.201375	H	2.524058	-0.433924	0.290999
H	-2.415756	3.442663	-1.595273	H	4.189059	-2.293515	0.118106
H	-3.417412	4.153860	-0.331091	H	5.032646	-1.688105	1.542141
H	-4.848557	3.123650	-2.118856	H	6.176452	-0.924880	-0.560477
H	-5.079224	2.261161	-0.586095	H	5.537573	0.471489	0.327295
H	-4.066235	1.553094	-1.856034	H	4.681000	-0.136883	-1.099862
C	1.894662	-0.672268	-1.843736	C	-1.568338	-1.471363	-1.910813
F	1.981448	-2.012396	-1.834994	F	-2.365841	-0.483115	-2.347459
S	0.101547	-0.122456	-1.629221	S	0.185055	-0.828710	-1.631772
O	0.193073	1.346997	-1.589702	O	0.880224	-1.963865	-1.005920
N	-0.240007	-0.624500	-0.135111	N	-0.047835	0.293216	-0.495498
S	-0.873169	-2.067589	0.224227	S	-0.289828	1.859923	-0.798859
O	-0.826256	-3.095788	-0.825058	O	-0.612724	2.234815	-2.182600
O	-0.626571	-0.747205	-2.741153	O	0.634391	-0.371403	-2.953073
F	2.369160	-0.215671	-3.013989	F	-1.550937	-2.450603	-2.828500
F	2.653420	-0.186309	-0.851144	F	-2.078256	-1.961565	-0.769446
C	-2.707428	-1.659472	0.414146	C	1.425343	2.584494	-0.488666
F	-3.178116	-1.103679	-0.713141	F	2.328580	1.984810	-1.279186
O	-0.443840	-2.427641	1.584370	O	-1.115510	2.416537	0.285608
F	-3.392605	-2.787373	0.660191	F	1.412192	3.898530	-0.762997
F	-2.903868	-0.806322	1.429948	F	1.790885	2.415207	0.789807
N	3.668517	-0.257603	2.367264	N	-3.855910	-1.141296	1.844450
H	4.231055	-0.320909	3.215214	H	-4.511729	-1.077542	2.622834
H	4.198319	0.287157	1.668485	H	-4.059615	-2.013992	1.357573
H	3.519023	-1.212433	2.008074	H	-4.063108	-0.367353	1.193624
N	4.870901	1.559738	0.203166	N	-3.020359	2.549448	2.884771
H	5.645497	2.196074	0.390188	H	-3.650330	1.889953	2.427748
H	4.080044	2.133332	-0.108932	H	-2.387230	2.878233	2.155970
H	5.150761	0.989493	-0.594444	H	-3.588468	3.347324	3.167803
N	2.760424	-3.010627	1.310961	N	-4.103596	1.218611	-0.095756

H	2.823973	-3.070739	0.295389	H	-4.141181	0.798887	-1.024323
H	1.767380	-2.922562	1.531567	H	-3.201493	1.691674	-0.030193
H	3.066413	-3.912198	1.675308	H	-4.819239	1.944507	-0.076509
N	2.516261	3.331775	-1.102518	N	-0.372070	-4.432653	0.418166
H	3.204598	3.586868	-1.811162	H	-1.292413	-4.655456	0.040411
H	2.039465	4.197880	-0.850363	H	0.100831	-5.321903	0.575981
H	1.825179	2.740458	-1.566151	H	0.136828	-3.947720	-0.321315
Fig. S4c				Fig. S4d			
N	-1.272645	2.677234	0.875175	N	0.978193	-2.121122	1.257820
C	0.040628	2.520326	0.658567	C	-0.353730	-2.265388	1.307765
N	0.642727	2.233165	1.810335	N	-0.811969	-1.574148	2.352320
C	-0.312301	2.183677	2.802590	C	0.248924	-0.955883	2.980899
C	-1.517813	2.463609	2.221982	C	1.382431	-1.298881	2.299470
H	1.701153	1.970070	1.909064	H	-1.844593	-1.454159	2.591313
C	-2.287567	2.919046	-0.163495	C	1.852199	-2.688932	0.219511
C	-3.237832	1.728670	-0.310388	C	2.656293	-1.605855	-0.500397
C	-4.198209	1.903369	-1.491306	C	3.479927	-2.176275	-1.659208
C	-5.130935	0.696996	-1.652711	C	4.290258	-1.088321	-2.373827
H	-0.061579	1.954008	3.826441	H	0.110030	-0.319752	3.840836
H	-2.511015	2.530026	2.637259	H	2.422497	-1.022624	2.440373
H	0.515394	2.586113	-0.306528	H	-0.951314	-2.852395	0.614233
H	-1.745073	3.090952	-1.095261	H	1.201212	-3.215728	-0.481911
H	-2.826986	3.834674	0.098630	H	2.513338	-3.421835	0.694031
H	-3.809690	1.595519	0.617455	H	3.321219	-1.109492	0.215705
H	-2.637449	0.825884	-0.449942	H	1.960601	-0.849957	-0.874806
H	-3.614058	2.041527	-2.411684	H	2.807052	-2.665631	-2.377449
H	-4.792887	2.817892	-1.355616	H	4.158037	-2.956292	-1.283817
H	-5.805735	0.826544	-2.507014	H	4.872327	-1.504615	-3.204474
H	-5.746179	0.552345	-0.755389	H	4.989894	-0.601846	-1.681880
H	-4.554288	-0.222707	-1.813673	H	3.629548	-0.311835	-2.779616
C	1.844210	-0.260793	-1.744868	C	-2.737001	-0.058673	-1.325445
F	2.394729	-1.408100	-1.322619	F	-3.232864	1.158726	-1.050443
S	-0.039222	-0.339303	-1.638820	S	-0.876138	0.038628	-1.632576
O	-0.461075	0.990875	-2.106094	O	-0.472360	-1.367730	-1.785958
N	-0.315742	-0.388094	-0.048894	N	-0.322286	0.555570	-0.209172
S	-0.368532	-1.734697	0.839024	S	-0.088402	2.106294	0.176109
O	0.291636	-2.922596	0.274324	O	-0.717958	3.114451	-0.689110
O	-0.412773	-1.523657	-2.423312	O	-0.733634	0.940263	-2.783354
F	2.214346	-0.048405	-3.017862	F	-3.351121	-0.537900	-2.418948
F	2.307993	0.746290	-0.988004	F	-3.003386	-0.873364	-0.291868
C	-2.209922	-2.154757	0.849966	C	1.764684	2.311110	-0.117944
F	-2.660911	-2.331744	-0.400157	F	2.072556	2.013178	-1.389316
O	-0.084563	-1.367675	2.234443	O	-0.230211	2.241784	1.634203

F	-2.405805	-3.285880	1.546618	F	2.119881	3.582630	0.126883
F	-2.911542	-1.166813	1.425636	F	2.464595	1.505536	0.695167
N	3.247401	1.493376	1.987167	N	-3.503072	-1.107083	2.857799
H	3.705842	1.732712	2.866447	H	-3.591030	-0.093502	2.676828
H	3.808277	1.900867	1.223695	H	-3.862136	-1.290243	3.794446
H	3.294385	0.472302	1.887983	H	-4.119670	-1.590388	2.204951
N	4.853733	2.335520	-0.507798	N	-3.398602	1.872004	2.194438
H	5.717557	2.867106	-0.612790	H	-2.395654	2.063324	2.188069
H	4.263095	2.577612	-1.302593	H	-3.836455	2.595430	2.763710
H	5.090247	1.337400	-0.597831	H	-3.722469	2.017370	1.238852
N	3.074978	-1.702933	1.877468	N	4.539752	-0.274166	2.468378
H	2.768335	-2.316145	1.121559	H	4.407348	0.602281	1.964375
H	2.247880	-1.574206	2.462080	H	5.318119	-0.752761	2.015551
H	3.743096	-2.239203	2.430999	H	4.860550	-0.023683	3.403565
N	5.312750	-0.736766	-0.337548	N	-2.058913	-3.902791	-0.911491
H	5.077215	-1.339751	-1.124746	H	-3.053664	-3.681053	-0.884869
H	4.622522	-0.926847	0.393165	H	-1.981288	-4.849393	-1.281916
H	6.214948	-1.055768	0.014256	H	-1.640136	-3.274637	-1.597746
Fig. S4e				Fig. S4f			
N	0.977335	-2.125013	1.252358	N	0.978179	-2.125040	1.251744
C	-0.354677	-2.268877	1.300864	C	-0.353779	-2.269597	1.299742
N	-0.813446	-1.580301	2.346951	N	-0.813317	-1.580917	2.345424
C	0.247241	-0.964285	2.978118	C	0.246788	-0.964116	2.976804
C	1.381112	-1.305782	2.296554	C	1.381125	-1.305285	2.295857
H	-1.846137	-1.460445	2.585579	H	-1.846132	-1.461810	2.584069
C	1.852000	-2.690662	0.213452	C	1.853678	-2.690429	0.213405
C	2.655265	-1.605976	-0.504949	C	2.655240	-1.605225	-0.506125
C	3.480823	-2.174508	-1.663328	C	3.482094	-2.173646	-1.663637
C	4.290539	-1.085069	-2.376367	C	4.290506	-1.083679	-2.377355
H	0.107971	-0.330353	3.839626	H	0.106808	-0.330073	3.838117
H	2.421211	-1.030515	2.439078	H	2.421054	-1.029463	2.438699
H	-0.951962	-2.854101	0.605539	H	-0.950549	-2.855235	0.604306
H	1.201647	-3.217210	-0.488771	H	1.204193	-3.218871	-0.488212
H	2.513670	-3.423591	0.687184	H	2.516511	-3.421776	0.687949
H	3.318843	-1.109203	0.212119	H	3.317764	-1.106497	0.210539
H	1.958852	-0.850771	-0.879463	H	1.957657	-0.851608	-0.881643
H	2.809348	-2.664255	-2.382611	H	2.811626	-2.665049	-2.382728
H	4.159545	-2.953905	-1.287750	H	4.161814	-2.951695	-1.287066
H	4.874083	-1.500118	-3.206603	H	4.874952	-1.498626	-3.207006
H	4.988768	-0.598117	-1.683333	H	4.987776	-0.595117	-1.684489
H	3.629316	-0.309175	-2.782438	H	3.628328	-0.309087	-2.784353
C	-2.738418	-0.052271	-1.323123	C	-2.739032	-0.051559	-1.322275
F	-3.232227	1.165322	-1.045317	F	-3.232593	1.166000	-1.043952

S	-0.877965	0.043275	-1.632762	S	-0.878789	0.044119	-1.633086
O	-0.475950	-1.363194	-1.789849	O	-0.476686	-1.362250	-1.790752
N	-0.321374	0.556315	-0.209037	N	-0.321378	0.556823	-0.209577
S	-0.084773	2.105666	0.179834	S	-0.084728	2.105992	0.179842
O	-0.712232	3.117000	-0.683146	O	-0.710814	3.117786	-0.683603
O	-0.736666	0.947450	-2.781713	O	-0.738337	0.948559	-2.781922
F	-3.354653	-0.528710	-2.416672	F	-3.355960	-0.527828	-2.415497
F	-3.004562	-0.868460	-0.290677	F	-3.004541	-0.867927	-0.289799
C	1.768600	2.307842	-0.113991	C	1.768971	2.307468	-0.112138
F	2.075812	2.011470	-1.385881	F	2.077183	2.011357	-1.383861
O	-0.226283	2.238104	1.638234	O	-0.227745	2.238239	1.638137
F	2.125894	3.578404	0.132822	F	2.126494	3.577848	0.135332
F	2.467290	1.499861	0.697767	F	2.466657	1.499047	0.700001
N	-3.504470	-1.112004	2.852151	N	-3.504554	-1.115237	2.851457
H	-3.865501	-1.297362	3.787609	H	-3.591651	-0.100973	2.674139
H	-4.120844	-1.592141	2.196775	H	-3.864680	-1.301671	3.787042
H	-3.590157	-0.097685	2.674241	H	-4.120604	-1.595863	2.196137
N	4.539389	-0.283521	2.469371	N	-3.396034	1.867174	2.201512
H	4.859628	-0.034355	3.405104	H	-2.392444	2.054913	2.189739
H	4.407586	0.593652	1.966476	H	-3.827106	2.587530	2.779791
H	5.317940	-0.761702	2.016425	H	-3.726118	2.021546	1.249486
N	-3.393966	1.869971	2.201232	N	-2.069472	-3.895058	-0.919508
H	-3.719190	2.021598	1.247097	H	-3.062622	-3.666961	-0.887784
H	-2.391138	2.061897	2.194938	H	-1.999681	-4.841542	-1.291796
H	-3.831579	2.589095	2.776105	H	-1.649955	-3.268484	-1.606748
N	-2.071292	-3.894812	-0.917926	N	4.539534	-0.284168	2.469039
H	-3.064300	-3.665974	-0.887058	H	4.409104	0.594566	1.968521
H	-2.001945	-4.841786	-1.289048	H	5.313032	-0.765351	2.010649
H	-1.650939	-3.269331	-1.605651	H	4.866450	-0.038370	3.403346

Fig. S4g

N	-0.861621	-1.331793	-2.387942
C	0.421412	-1.499272	-2.036609
N	1.139648	-0.487305	-2.516642
C	0.297601	0.373854	-3.187474
C	-0.961220	-0.153960	-3.111787
H	2.209374	-0.349018	-2.329890
C	-1.975792	-2.214310	-2.007914
C	-2.986402	-1.506803	-1.103577
C	-4.090225	-2.457816	-0.628540
C	-5.088796	-1.759684	0.302205
H	0.668735	1.289423	-3.624752
H	-1.905244	0.198181	-3.496191
H	0.792470	-2.308926	-1.430072

Fig. S4h

N	-0.175582	-1.605763	2.047522
C	-1.353188	-1.158649	1.591195
N	-1.631137	-0.002240	2.194104
C	-0.602449	0.316822	3.053738
C	0.314941	-0.691010	2.966196
H	-2.491980	0.588003	1.978261
C	0.513449	-2.821279	1.584239
C	1.897355	-2.511178	1.010633
C	2.539952	-3.748289	0.373920
C	3.924575	-3.439480	-0.207356
H	-0.608228	1.237072	3.617772
H	1.263077	-0.830642	3.459764
H	-1.970102	-1.657100	0.856078

H	-1.535167	-3.070254	-1.492005	H	-0.124059	-3.266586	0.818005
H	-2.448467	-2.574173	-2.927488	H	0.577861	-3.517675	2.426473
H	-3.433320	-0.659465	-1.639035	H	2.550481	-2.124172	1.803261
H	-2.453227	-1.096348	-0.241954	H	1.794201	-1.720631	0.262829
H	-3.632949	-3.308560	-0.103965	H	1.882842	-4.124644	-0.422546
H	-4.620108	-2.873274	-1.497421	H	2.621037	-4.551446	1.120221
H	-5.868598	-2.452340	0.639961	H	4.368686	-4.328416	-0.670469
H	-5.580411	-0.920091	-0.205767	H	4.610310	-3.088026	0.574151
H	-4.582216	-1.361558	1.190200	H	3.860727	-2.655597	-0.972563
C	1.791710	-0.998409	2.043774	C	-1.719400	0.484752	-2.098883
F	2.180520	0.165200	2.589634	F	-1.664502	1.813425	-2.268020
S	-0.039915	-0.943242	1.588645	S	-0.003363	-0.204658	-1.715988
O	-0.255557	-2.209247	0.871346	O	-0.259780	-1.616294	-1.382498
N	-0.089453	0.247213	0.497883	N	0.380053	0.552352	-0.343583
S	-0.314157	1.806018	0.854330	S	1.213372	1.936008	-0.266437
O	-0.196863	2.196730	2.265966	O	1.267423	2.750297	-1.488962
O	-0.743761	-0.722026	2.858719	O	0.799760	0.098328	-2.907793
F	2.009083	-1.984558	2.928045	F	-2.189126	-0.078416	-3.223936
F	2.535820	-1.227236	0.950574	F	-2.570003	0.212578	-1.096641
C	-2.137938	2.048349	0.435606	C	2.980268	1.317980	-0.015318
F	-2.893757	1.206913	1.156934	F	3.333536	0.492338	-1.012387
O	0.390147	2.614451	-0.155943	O	0.891374	2.593897	1.008092
F	-2.497875	3.309377	0.722871	F	3.823395	2.362650	0.002138
F	-2.360598	1.823338	-0.866828	F	3.087791	0.658026	1.147460
N	3.769356	-0.190444	-1.929319	N	-3.936819	1.358478	1.454877
H	4.394446	0.042666	-2.700714	H	-4.552745	1.769097	2.156500
H	4.102896	-1.070332	-1.508777	H	-4.432609	0.549952	1.038834
H	3.844138	0.557396	-1.224154	H	-3.819575	2.051918	0.716391
N	4.471810	-2.906572	-0.599699	N	-5.105083	-1.164865	0.242588
H	5.176697	-3.546181	-0.965232	H	-5.781589	-1.683540	0.802467
H	3.594452	-3.424931	-0.568793	H	-4.338658	-1.811142	0.024123
H	4.725122	-2.713712	0.368721	H	-5.567270	-0.951152	-0.641184
N	3.570664	2.081375	0.152878	N	-1.478356	3.458758	2.917216
H	3.711694	1.670361	1.075243	H	-2.350824	3.098589	2.531409
H	2.581399	2.325940	0.093808	H	-0.758305	3.287321	2.214044
H	4.090830	2.958185	0.143378	H	-1.588144	4.469844	2.989384
N	2.150635	3.082754	-2.843460	N	-2.828891	-3.209634	-0.713448
H	1.438962	3.122781	-2.113566	H	-3.482570	-3.496542	-1.442556
H	2.464393	4.040206	-3.000322	H	-2.539557	-4.067729	-0.243554
H	2.939423	2.584755	-2.430587	H	-2.005498	-2.841195	-1.191672
Fig. S4i				Fig. S4j			
N	0.243591	2.422711	-1.169990	N	0.181427	-2.558279	-0.915278
C	-0.904849	2.249990	-0.497982	C	-0.799176	-1.842982	-1.483100

N	-1.754496	1.575531	-1.272655	N	-1.803570	-1.724597	-0.617698
C	-1.135249	1.289960	-2.469486	C	-1.462308	-2.365951	0.554217
C	0.120623	1.824202	-2.413350	C	-0.215004	-2.894065	0.369933
H	-2.738713	1.231550	-0.958015	H	-2.712864	-1.161516	-0.780943
C	1.448790	3.075288	-0.635273	C	1.479339	-2.871341	-1.533776
C	2.656520	2.136291	-0.632153	C	2.647593	-2.261950	-0.757429
C	3.874143	2.775758	0.044003	C	3.985678	-2.485969	-1.470306
C	5.085057	1.835415	0.053505	C	5.157245	-1.864547	-0.700792
H	-1.624383	0.724215	-3.246527	H	-2.141370	-2.365780	1.397181
H	0.926298	1.821521	-3.129702	H	0.421003	-3.463986	1.028136
H	-1.099087	2.610202	0.509968	H	-0.756427	-1.412076	-2.469758
H	1.204847	3.389649	0.382057	H	1.445374	-2.472764	-2.550270
H	1.645222	3.971409	-1.233482	H	1.568378	-3.960772	-1.596514
H	2.912878	1.858150	-1.662493	H	2.688999	-2.695724	0.249428
H	2.380440	1.217153	-0.108805	H	2.463130	-1.191108	-0.637806
H	3.612296	3.047506	1.076302	H	3.935667	-2.050003	-2.477983
H	4.134839	3.711758	-0.470315	H	4.158704	-3.563437	-1.603118
H	5.946359	2.300289	0.547562	H	6.107452	-2.029462	-1.222200
H	5.385120	1.569853	-0.968275	H	5.243320	-2.299203	0.303306
H	4.852089	0.904335	0.585322	H	5.018383	-0.782490	-0.584477
C	-1.132102	-0.714345	2.464587	C	-0.654031	2.273390	-1.764867
F	-1.565724	-1.957884	2.203121	F	-1.059020	3.097769	-0.784399
S	0.582173	-0.442334	1.720971	S	0.930424	1.375174	-1.264949
O	0.855067	0.979353	1.984854	O	1.117472	0.382210	-2.333773
N	0.296726	-0.600629	0.141761	N	0.464701	0.584746	0.063040
S	0.434256	-1.984904	-0.678674	S	0.581002	1.167228	1.565099
O	0.486417	-3.225340	0.108880	O	0.869057	2.601675	1.707749
O	1.436092	-1.451173	2.362433	O	1.934026	2.435867	-1.104137
F	-1.079794	-0.546242	3.795622	F	-0.437125	2.995974	-2.874616
F	-2.011107	0.163409	1.955231	F	-1.635289	1.389925	-2.011095
C	2.156188	-1.822538	-1.438223	C	2.130701	0.300612	2.205046
F	3.068375	-1.598960	-0.479666	F	3.175907	0.564843	1.405792
O	-0.472519	-1.925279	-1.835375	O	-0.504145	0.584589	2.370848
F	2.471301	-2.959584	-2.079401	F	2.409211	0.742295	3.442086
F	2.196459	-0.809237	-2.315750	F	1.948139	-1.027009	2.253590
N	-4.163114	0.605962	-0.447887	N	-4.093569	-0.251136	-0.888941
H	-4.967084	0.824685	-1.053581	H	-4.936645	-0.795649	-0.672113
H	-4.398912	0.902205	0.499248	H	-4.242904	0.219792	-1.780430
H	-4.040611	-0.417716	-0.429605	H	-3.983533	0.471685	-0.165362
N	-6.506478	1.252228	-2.401076	N	-6.597113	-2.073066	-0.159164
H	-6.536708	0.533833	-3.124106	H	-7.280676	-1.680855	0.488328
H	-6.389772	2.143572	-2.882158	H	-6.512962	-3.062563	0.074117
H	-7.431332	1.271631	-1.972367	H	-7.027429	-2.036104	-1.083694
N	-3.412940	-2.389935	-0.536676	N	-3.296204	1.728354	1.390636

H	-3.116309	-2.706785	0.385644	H	-3.027513	2.510580	0.793284
H	-2.566561	-2.329442	-1.104285	H	-2.428562	1.375406	1.798484
H	-3.983654	-3.136621	-0.931575	H	-3.840880	2.127323	2.154882
N	-1.261756	3.193245	2.575764	N	-4.198072	-1.485106	2.187009
H	-2.081119	2.792219	3.030838	H	-3.944432	-0.510841	2.015669
H	-1.068899	4.075857	3.048157	H	-4.663337	-1.510767	3.093920
H	-0.481615	2.566877	2.776216	H	-4.904793	-1.716606	1.487012
Fig. S4k				Fig. S4l			
N	-1.247849	1.034375	-2.197863	N	0.241234	2.359665	-0.701134
C	0.039067	0.859742	-2.524952	C	-1.036660	2.005974	-0.896897
N	0.747135	1.874969	-2.033525	N	-1.159559	1.522117	-2.132633
C	-0.103044	2.723640	-1.354148	C	0.074638	1.550405	-2.745564
C	-1.362378	2.201723	-1.456746	C	0.962761	2.079695	-1.851699
H	1.811279	1.957598	-2.080177	H	-2.072347	1.120729	-2.524285
C	-2.344785	0.105653	-2.512616	C	0.795427	2.897723	0.550974
C	-3.010311	-0.437579	-1.247637	C	1.962927	2.056408	1.068569
C	-4.110248	-1.454454	-1.569654	C	2.446887	2.537357	2.440214
C	-4.775289	-1.998402	-0.299614	C	3.618110	1.695397	2.960137
H	0.273733	3.596355	-0.840120	H	0.222072	1.181922	-3.748343
H	-2.316925	2.527459	-1.056253	H	2.031178	2.258580	-1.916086
H	0.431132	0.014317	-3.065550	H	-1.832981	2.098077	-0.171109
H	-1.911659	-0.707251	-3.099828	H	-0.020509	2.904154	1.276442
H	-3.066261	0.638454	-3.140580	H	1.103913	3.932662	0.369356
H	-3.432851	0.394793	-0.673823	H	2.789196	2.095570	0.349277
H	-2.242566	-0.904405	-0.624400	H	1.637791	1.014722	1.133626
H	-3.680750	-2.286104	-2.145636	H	1.613962	2.490094	3.155672
H	-4.869141	-0.986788	-2.213367	H	2.747956	3.593035	2.378562
H	-5.559605	-2.725656	-0.540292	H	3.950881	2.039621	3.946474
H	-5.233434	-1.187577	0.281444	H	4.475397	1.750576	2.276821
H	-4.039400	-2.495088	0.344954	H	3.330472	0.640192	3.049284
C	2.461140	-1.976818	-0.638869	C	-2.459484	-1.436456	0.866855
F	3.177106	-1.744114	0.473100	F	-2.488103	-2.622097	0.241821
S	0.613438	-1.950438	-0.253734	S	-0.688090	-0.974542	1.327837
O	-0.016220	-2.039183	-1.579685	O	-0.816457	0.379520	1.894122
N	0.403067	-0.443816	0.290001	N	0.021596	-0.831887	-0.112101
S	0.487820	-0.008529	1.841129	S	0.801045	-2.029376	-0.870096
O	1.091025	-0.966569	2.777912	O	0.531905	-3.397327	-0.402235
O	0.408843	-3.046982	0.701925	O	-0.231879	-2.059014	2.207589
F	2.804626	-3.176999	-1.130542	F	-3.208900	-1.513512	1.979563
F	2.764245	-1.035702	-1.548098	F	-2.991095	-0.509093	0.055586
C	-1.332081	0.065108	2.334462	C	2.592611	-1.699859	-0.370277
F	-1.914938	-1.126071	2.132133	F	2.713397	-1.689671	0.966270
O	0.925451	1.396319	1.900241	O	0.776140	-1.754787	-2.312341

F	-1.430920	0.381295	3.635288	F	3.384683	-2.662650	-0.869244
F	-1.982349	0.992386	1.615798	F	3.006233	-0.514528	-0.846705
N	3.518705	2.024321	-2.030648	N	-3.599615	0.501412	-2.914645
H	3.918838	2.922837	-2.300593	H	-3.993179	0.773792	-3.814900
H	3.961597	1.317524	-2.617438	H	-4.215655	0.870806	-2.170520
H	3.798565	1.836325	-1.054610	H	-3.633782	-0.516692	-2.869531
N	2.009150	4.213892	0.726064	N	-5.101659	1.677199	-0.539400
H	2.834994	3.756451	0.339869	H	-5.744254	2.457154	-0.676511
H	1.523307	3.496627	1.264638	H	-4.392941	1.987670	0.134301
H	2.347405	4.906185	1.393829	H	-5.636965	0.940593	-0.079972
N	4.030564	1.429558	0.930415	N	4.274310	2.313594	-1.877736
H	4.349040	0.462594	0.987159	H	4.675643	2.422861	-2.808996
H	3.106163	1.454390	1.362210	H	4.433679	1.343431	-1.607289
H	4.650379	1.975182	1.528348	H	4.840893	2.884864	-1.251194
N	-4.247928	2.842428	0.056614	N	-3.071253	2.503067	1.808812
H	-3.987298	2.412579	0.943936	H	-3.875648	2.437310	2.433144
H	-5.132266	2.417417	-0.221351	H	-2.622201	3.393684	2.023509
H	-4.449471	3.821641	0.258287	H	-2.422117	1.768085	2.093713
Fig. S4m				Fig. S4n			
N	0.906780	2.516653	-0.131542	N	-0.047899	1.418647	-2.163370
C	-0.433862	2.511200	-0.132637	C	-1.194040	1.203819	-1.499382
N	-0.867003	2.390376	-1.385243	N	-1.752927	0.083147	-1.951442
C	0.227930	2.297228	-2.218077	C	-0.939002	-0.453640	-2.923534
C	1.348684	2.378717	-1.438458	C	0.132658	0.382470	-3.064885
H	-1.919627	2.295009	-1.665737	H	-2.660611	-0.363712	-1.515026
C	1.760925	2.602520	1.063477	C	0.893163	2.520986	-1.911462
C	2.681890	1.389558	1.199401	C	2.278092	2.011677	-1.507230
C	3.508893	1.442992	2.488141	C	3.203184	3.156554	-1.080236
C	4.436932	0.229802	2.622941	C	4.586626	2.648358	-0.658005
H	0.122340	2.172231	-3.284521	H	-1.176886	-1.380101	-3.422063
H	2.405302	2.327243	-1.680775	H	0.995742	0.329195	-3.708895
H	-1.052602	2.562059	0.748360	H	-1.593239	1.840905	-0.722144
H	1.091102	2.671948	1.922979	H	0.461191	3.120901	-1.107822
H	2.338759	3.530414	0.998360	H	0.944033	3.139493	-2.813482
H	3.350106	1.339509	0.332216	H	2.731654	1.463030	-2.342602
H	2.069377	0.484124	1.188403	H	2.160541	1.303621	-0.682783
H	2.832125	1.486539	3.353002	H	2.740261	3.699291	-0.244307
H	4.103074	2.367891	2.508167	H	3.307456	3.877407	-1.903695
H	5.019084	0.273800	3.550950	H	5.235975	3.474550	-0.345399
H	5.142679	0.180723	1.783718	H	5.082465	2.123742	-1.484726
H	3.860847	-0.703966	2.628861	H	4.504737	1.946322	0.181441
C	-2.552555	-0.841171	1.375634	C	-1.144524	0.000650	2.531082
F	-2.923719	-1.904670	0.644463	F	-1.267115	-1.294929	2.853652

S	-0.673777	-0.763409	1.536334	S	0.523632	0.323450	1.707222
O	-0.442395	0.516860	2.223064	O	0.429354	1.727431	1.269923
N	-0.201923	-0.584092	0.003331	N	0.449348	-0.597337	0.387774
S	0.115284	-1.800158	-1.011041	S	0.956383	-2.131088	0.304261
O	-0.352210	-3.137810	-0.619142	O	1.191694	-2.823281	1.580253
O	-0.295645	-2.009028	2.217539	O	1.522227	-0.025566	2.726601
F	-3.109326	-0.939144	2.593208	F	-1.244564	0.738471	3.649624
F	-3.013519	0.269376	0.778915	F	-2.147264	0.335700	1.704940
C	1.998022	-1.908359	-0.925124	C	2.676659	-1.927580	-0.447827
F	2.394959	-2.113619	0.339774	F	3.433369	-1.131313	0.323797
O	-0.151102	-1.334839	-2.381617	O	0.185918	-2.814498	-0.742586
F	2.423431	-2.930884	-1.684192	F	3.269398	-3.129513	-0.540743
F	2.560503	-0.776370	-1.375511	F	2.601373	-1.391060	-1.674950
N	-3.491910	2.045147	-1.979480	N	-3.952515	-0.893063	-0.743063
H	-3.883937	2.588970	-2.747920	H	-4.698146	-1.277497	-1.341067
H	-4.050523	2.242657	-1.136544	H	-4.316039	-0.067627	-0.241166
H	-3.595200	1.046210	-2.213500	H	-3.714886	-1.598230	-0.045575
N	-4.903296	2.592339	0.737238	N	-6.122273	-2.041251	-2.655310
H	-5.557442	3.357617	0.898487	H	-5.979117	-3.036523	-2.824469
H	-4.136340	2.718356	1.396929	H	-6.085603	-1.583718	-3.565765
H	-5.381523	1.735457	1.013595	H	-7.078361	-1.938606	-2.316335
N	-3.379823	-0.983167	-2.573813	N	-4.651958	1.747572	0.672499
H	-3.648919	-1.508471	-1.742702	H	-4.812344	1.571704	1.664128
H	-2.369926	-1.098634	-2.670564	H	-5.423103	2.334559	0.355090
H	-3.810289	-1.454801	-3.368430	H	-3.798739	2.312855	0.609261
N	4.565720	1.778247	-2.005746	N	-2.005370	3.594625	0.808292
H	4.450321	0.764985	-1.999984	H	-2.478682	4.065411	1.579970
H	5.311989	1.987358	-1.342871	H	-1.647988	4.335850	0.205076
H	4.923994	2.022748	-2.928820	H	-1.192612	3.124338	1.209418

Fig. S4o

N	-0.304866	0.071401	2.702182
C	0.692633	0.806826	2.192100
N	1.733055	0.003722	1.964924
C	1.397333	-1.286847	2.317594
C	0.115835	-1.247657	2.787501
H	2.619359	0.303795	1.457770
C	-1.656696	0.568710	3.000131
C	-2.711417	-0.111870	2.124600
C	-4.100633	0.506921	2.311526
C	-5.152033	-0.168164	1.422838
H	2.088545	-2.105444	2.175165
H	-0.528801	-2.028536	3.158090
H	0.651556	1.878825	2.013593

Fig. S4p

N	-0.127374	2.700408	0.852746
C	0.999768	1.994837	0.673477
N	1.417885	1.525607	1.846046
C	0.524261	1.925745	2.816196
C	-0.448417	2.663810	2.199688
H	2.313606	0.860616	1.975732
C	-0.924004	3.331614	-0.212102
C	-2.299049	2.677934	-0.355687
C	-3.082709	3.248370	-1.542632
C	-4.456650	2.585428	-1.696269
H	0.648904	1.656994	3.853889
H	-1.323381	3.159461	2.589893
H	1.463899	1.815095	-0.282616

H	-1.639822	1.645048	2.814680	H	-0.352110	3.223701	-1.135660
H	-1.854917	0.405663	4.064446	H	-1.010201	4.397985	0.019686
H	-2.749995	-1.183624	2.358123	H	-2.873290	2.817340	0.569620
H	-2.401752	-0.021268	1.079917	H	-2.156466	1.601748	-0.484788
H	-4.052398	1.578882	2.074015	H	-2.499172	3.102432	-2.462293
H	-4.402077	0.432108	3.366088	H	-3.205881	4.333666	-1.417848
H	-6.139491	0.289180	1.556180	H	-5.002973	2.997275	-2.552921
H	-5.240262	-1.236256	1.659629	H	-5.070088	2.739135	-0.799220
H	-4.879980	-0.082825	0.363213	H	-4.353611	1.503966	-1.848598
C	0.646944	2.269148	-1.803521	C	1.391156	-1.421457	-1.718834
F	1.279691	1.596323	-2.775390	F	1.330842	-2.654830	-1.191836
S	-0.865797	1.308537	-1.209014	S	-0.298808	-0.584366	-1.644788
O	-1.337251	2.079139	-0.047107	O	-0.015754	0.796250	-2.067948
N	-0.206783	-0.055164	-0.654235	N	-0.594287	-0.550634	-0.058344
S	-0.005048	-1.397030	-1.531186	S	-1.343205	-1.720273	0.766690
O	-0.073768	-1.256677	-2.993023	O	-1.485219	-3.022403	0.099950
O	-1.737365	1.209928	-2.387531	O	-1.176073	-1.416653	-2.478414
F	0.266829	3.465931	-2.279287	F	1.798148	-1.516027	-2.994200
F	1.505471	2.464585	-0.788127	F	2.293460	-0.704997	-1.029749
C	-1.541453	-2.395134	-1.073633	C	-3.102695	-1.049946	0.895658
F	-2.650809	-1.695822	-1.359398	F	-3.605998	-0.828660	-0.328278
O	1.105156	-2.163462	-0.948062	O	-0.850921	-1.686232	2.153272
F	-1.559169	-3.541085	-1.773951	F	-3.877492	-1.946016	1.527347
F	-1.544674	-2.690851	0.234226	F	-3.123357	0.099679	1.585763
N	3.951269	0.794062	0.474679	N	3.527091	-0.093669	2.045665
H	4.820472	0.273665	0.657467	H	4.122144	0.045411	2.862396
H	4.159858	1.787109	0.577025	H	4.111523	0.036808	1.202416
H	3.709170	0.648418	-0.505416	H	3.185929	-1.067658	2.064318
N	6.532870	-0.837149	1.118815	N	5.076102	0.411755	-0.549796
H	6.952751	-1.433001	0.405458	H	5.995668	0.871807	-0.518427
H	6.532338	-1.376886	1.984255	H	4.472014	0.977760	-1.145223
H	7.184335	-0.065499	1.264524	H	5.197677	-0.477715	-1.033585
N	0.357019	3.994074	1.717936	N	2.168813	-2.852579	2.055450
H	1.096236	4.444888	1.179944	H	2.156346	-3.258994	1.120676
H	-0.018136	4.701758	2.348551	H	1.209909	-2.565526	2.256819
H	-0.381975	3.757093	1.055656	H	2.395569	-3.609385	2.699635
N	3.808962	-2.823004	0.651952	N	7.880500	1.808313	-0.310504
H	3.064724	-2.556198	0.006772	H	8.358639	1.968338	-1.196637
H	4.290409	-3.617641	0.231721	H	8.505307	1.237108	0.257827
H	4.479382	-2.053696	0.670861	H	7.814511	2.714412	0.152369
Fig. S4q				Fig. S4r			
N	-0.655095	-1.999275	2.194123	N	-0.579285	2.128105	-1.418723
C	0.311406	-1.078328	2.063738	C	0.663327	1.715526	-1.706678

N	1.404339	-1.657562	1.574686	N	1.494819	2.149559	-0.762607
C	1.136527	-2.994690	1.362597	C	0.763501	2.848054	0.174527
C	-0.155399	-3.215924	1.752900	C	-0.542335	2.843055	-0.231645
H	2.293407	-1.084788	1.249381	H	2.557501	1.898910	-0.699218
C	-2.050856	-1.705626	2.554897	C	-1.786073	1.820036	-2.201308
C	-2.942411	-1.641622	1.312055	C	-2.825665	1.059270	-1.377528
C	-4.384499	-1.250713	1.651442	C	-4.037807	0.655618	-2.223755
C	-5.261772	-1.152505	0.397824	C	-5.084453	-0.103829	-1.400051
H	1.871551	-3.647091	0.915828	H	1.224744	3.276750	1.050532
H	-0.757605	-4.111294	1.755076	H	-1.442747	3.253009	0.214459
H	0.185328	-0.030359	2.280094	H	0.928732	1.101448	-2.551487
H	-2.047399	-0.743092	3.071300	H	-1.461384	1.221855	-3.055399
H	-2.387082	-2.475364	3.255309	H	-2.194737	2.764215	-2.576313
H	-2.927308	-2.612536	0.799704	H	-3.151721	1.681884	-0.536654
H	-2.515311	-0.907951	0.620794	H	-2.353058	0.167894	-0.956173
H	-4.383011	-0.284400	2.174806	H	-3.702817	0.028256	-3.061677
H	-4.812107	-1.985152	2.348659	H	-4.494764	1.552232	-2.666766
H	-6.288797	-0.865974	0.652811	H	-5.945500	-0.390140	-2.015455
H	-5.301187	-2.113064	-0.131709	H	-5.453088	0.512213	-0.569699
H	-4.864606	-0.403285	-0.298449	H	-4.656154	-1.018657	-0.971558
C	0.040547	3.320764	0.254474	C	1.765066	-2.293037	-1.237170
F	0.609420	3.606103	-0.926177	F	2.267575	-2.811891	-0.104968
S	-1.088465	1.816047	0.100689	S	-0.042737	-1.804170	-0.997575
O	-1.464359	1.517587	1.492535	O	-0.386566	-1.128643	-2.258197
N	-0.059158	0.666871	-0.377338	N	0.052935	-0.672923	0.150174
S	0.237782	0.264589	-1.911391	S	-0.017874	-0.965810	1.736388
O	-0.110656	1.251168	-2.942787	O	0.145571	-2.362349	2.165830
O	-2.136997	2.217767	-0.845841	O	-0.731650	-3.055944	-0.655442
F	-0.672394	4.381986	0.661502	F	1.860852	-3.210908	-2.211638
F	1.009133	3.080459	1.152344	F	2.498426	-1.221758	-1.580233
C	-0.953442	-1.171817	-2.192376	C	-1.814752	-0.548478	2.140290
F	-2.222259	-0.762030	-2.043762	F	-2.645996	-1.284333	1.387117
O	1.565484	-0.370680	-1.958480	O	0.750803	0.078261	2.432839
F	-0.794471	-1.649510	-3.436798	F	-2.054521	-0.813078	3.434789
F	-0.713794	-2.159106	-1.316694	F	-2.064325	0.750499	1.915115
N	3.406770	-0.132415	0.640659	N	4.108239	1.448427	-0.530252
H	4.315143	-0.584514	0.481129	H	4.734018	2.228195	-0.280959
H	3.552501	0.727003	1.190831	H	4.486185	1.004557	-1.367314
H	3.029041	0.133988	-0.269566	H	4.141634	0.752533	0.230495
N	6.149148	-1.622816	0.130098	N	5.886379	3.866318	0.303448
H	6.518351	-1.608530	-0.820620	H	5.721286	4.069692	1.288922
H	6.344601	-2.552227	0.502217	H	5.675693	4.722230	-0.208987
H	6.724587	-0.974136	0.668145	H	6.888462	3.706694	0.204080
N	3.727787	2.457420	2.306275	N	3.851488	-0.560923	1.799391

H	3.697765	3.239264	1.652670	H	3.758613	-1.518923	1.463788
H	4.586790	2.561516	2.845789	H	2.931320	-0.288619	2.148111
H	2.955884	2.598259	2.957122	H	4.477903	-0.592752	2.602969
N	3.339702	-3.045037	-1.121362	N	-3.408105	3.675590	1.231429
H	2.628804	-2.346767	-1.342980	H	-4.298757	3.733318	0.738020
H	3.658543	-3.423023	-2.013356	H	-3.381255	4.470070	1.870416
H	4.129488	-2.532054	-0.726200	H	-3.453846	2.839076	1.812888
Fig. S4s				Fig. S4t			
N	-1.462816	-2.007726	-1.787752	N	-0.327493	2.694597	-0.770757
C	-0.217522	-2.251343	-1.352005	C	0.815479	2.019997	-0.963544
N	0.658199	-1.803270	-2.247623	N	1.611693	2.196764	0.087353
C	-0.040529	-1.236039	-3.291599	C	0.960079	2.999384	0.998708
C	-1.373086	-1.362002	-3.009979	C	-0.258567	3.316240	0.465552
H	1.766927	-1.833214	-2.107008	H	2.581301	1.713513	0.203315
C	-2.702342	-2.314709	-1.056059	C	-1.480364	2.707141	-1.685914
C	-3.465712	-1.048560	-0.664681	C	-2.710813	2.045378	-1.063891
C	-4.695286	-1.368123	0.192405	C	-3.876885	1.962259	-2.054962
C	-5.457304	-0.101822	0.600301	C	-5.107625	1.286962	-1.438287
H	0.458490	-0.793308	-4.139806	H	1.408479	3.274978	1.940674
H	-2.250455	-1.058576	-3.559290	H	-1.068640	3.918267	0.845672
H	0.020598	-2.707708	-0.404989	H	1.028008	1.406724	-1.823880
H	-2.408268	-2.872040	-0.164660	H	-1.172103	2.168393	-2.583965
H	-3.311735	-2.968595	-1.688143	H	-1.681743	3.748158	-1.958014
H	-3.773640	-0.506693	-1.568544	H	-3.021690	2.604660	-0.171956
H	-2.788181	-0.391542	-0.112737	H	-2.433628	1.041355	-0.731817
H	-4.374620	-1.909899	1.093158	H	-3.555702	1.400470	-2.943149
H	-5.365147	-2.043598	-0.358533	H	-4.141418	2.971690	-2.400573
H	-6.329327	-0.344576	1.218869	H	-5.931960	1.229117	-2.158740
H	-5.811746	0.445770	-0.282413	H	-5.463583	1.843597	-0.561945
H	-4.812234	0.574055	1.175339	H	-4.871239	0.266561	-1.112029
C	1.442860	-0.696805	2.231428	C	1.032570	-2.270929	-1.413725
F	2.201315	0.409300	2.276738	F	1.268896	-3.124807	-0.405069
S	-0.336647	-0.272236	1.766886	S	-0.614143	-1.382978	-1.166041
O	-0.970637	-1.591976	1.618205	O	-0.643495	-0.408617	-2.268450
N	-0.174236	0.353824	0.288031	N	-0.365844	-0.558658	0.199099
S	0.066515	1.921570	-0.024546	S	-0.671401	-1.120099	1.683309
O	0.507343	2.764265	1.096185	O	-0.889782	-2.567246	1.818130
O	-0.805681	0.623826	2.832097	O	-1.622490	-2.450493	-1.136333
F	1.467183	-1.287152	3.436710	F	1.005784	-2.959681	-2.565443
F	1.968932	-1.540703	1.328470	F	2.037037	-1.381657	-1.466280
C	-1.678941	2.521814	-0.420975	C	-2.348590	-0.342265	2.062176
F	-2.504476	2.265635	0.605534	F	-3.248403	-0.704471	1.134888
O	0.775502	2.024146	-1.309410	O	0.246629	-0.453134	2.620463

F	-1.658137	3.846288	-0.639676	F	-2.774646	-0.759701	3.264885
F	-2.151473	1.911860	-1.517855	F	-2.257993	0.995636	2.077639
N	3.291009	-1.870793	-1.786576	N	3.965971	0.919216	0.291598
H	3.887062	-2.079505	-2.587533	H	4.735519	1.460370	0.707166
H	3.467136	-2.587320	-1.066487	H	4.241986	0.634363	-0.657310
H	3.575335	-0.950331	-1.408918	H	3.833739	0.065188	0.850498
N	3.508725	-3.961683	0.492820	N	3.191386	-1.600386	1.983450
H	4.030912	-4.834089	0.417099	H	3.688412	-1.996829	2.780346
H	2.551196	-4.213591	0.735794	H	2.954813	-2.380354	1.371175
H	3.887067	-3.462267	1.296945	H	2.306225	-1.233972	2.336369
N	3.799018	0.922387	-0.664480	N	6.235221	2.636073	1.654484
H	3.756272	0.895853	0.353940	H	7.136937	2.160203	1.654711
H	2.936021	1.373552	-0.970797	H	5.992654	2.798834	2.631395
H	4.576758	1.544274	-0.919196	H	6.390410	3.553145	1.236826
N	6.165015	2.828740	-1.523041	N	4.434823	-0.001800	-2.687412
H	6.103518	3.713016	-1.019282	H	5.242812	0.221675	-3.267703
H	6.091780	3.053772	-2.514806	H	3.610354	0.300054	-3.205620
H	7.108872	2.473241	-1.374009	H	4.383786	-1.018531	-2.635165
Fig. S4u				Fig. S4v			
N	-1.256882	2.466129	0.217168	N	-1.562811	1.474461	-1.812132
C	0.068034	2.649128	0.170570	C	-0.292111	1.117653	-2.038454
N	0.572293	2.416431	1.380941	N	0.510352	2.057867	-1.543910
C	-0.451791	2.056688	2.233232	C	-0.262387	3.044327	-0.961424
C	-1.607949	2.086930	1.505347	C	-1.570516	2.684673	-1.130553
H	1.613276	2.441686	1.571653	H	1.568270	1.930681	-1.450185
C	-2.177271	2.547914	-0.927128	C	-2.743091	0.638112	-2.075109
C	-2.564633	1.159756	-1.440169	C	-3.223861	-0.051549	-0.796272
C	-3.529249	1.232902	-2.628209	C	-4.438811	-0.951501	-1.042946
C	-3.920629	-0.160550	-3.134244	C	-4.901886	-1.652020	0.239966
H	-0.254247	1.793055	3.260571	H	0.197861	3.879104	-0.453374
H	-2.640842	1.862521	1.747190	H	-2.510086	3.131217	-0.823306
H	0.634870	2.920520	-0.703671	H	0.016233	0.193041	-2.497978
H	-1.676921	3.130291	-1.705506	H	-2.458415	-0.097022	-2.832039
H	-3.057999	3.106657	-0.598357	H	-3.518735	1.283471	-2.496356
H	-3.025612	0.595614	-0.622547	H	-3.469950	0.713090	-0.049250
H	-1.653560	0.624660	-1.728866	H	-2.397844	-0.645295	-0.390618
H	-3.064239	1.804893	-3.443537	H	-4.186093	-1.703763	-1.803181
H	-4.432321	1.786944	-2.334089	H	-5.262883	-0.352592	-1.456635
H	-4.610719	-0.096524	-3.983720	H	-5.771190	-2.293201	0.052627
H	-4.411310	-0.741188	-2.342793	H	-5.181815	-0.919193	1.007655
H	-3.035636	-0.722276	-3.458221	H	-4.101893	-2.278846	0.653473
C	2.945161	-0.944728	-1.111252	C	2.066806	-2.708466	-1.011728
F	3.211018	-2.078855	-0.453223	F	2.903441	-2.759452	0.034884

S	1.082029	-0.705248	-1.335948	S	0.337273	-2.202028	-0.450413
O	0.983894	0.633454	-1.944120	O	-0.402939	-2.025332	-1.710212
N	0.518241	-0.587860	0.174091	N	0.601152	-0.733846	0.164680
S	0.109190	-1.868530	1.077592	S	0.943357	-0.421384	1.709833
O	0.682811	-3.164001	0.686204	O	1.376542	-1.548934	2.546050
O	0.651078	-1.867482	-2.124783	O	-0.088638	-3.255775	0.479550
F	3.530767	-0.994823	-2.319324	F	2.020616	-3.917651	-1.591311
F	3.468881	0.085238	-0.425335	F	2.545583	-1.822135	-1.901479
C	-1.743781	-2.066563	0.757337	C	-0.746391	0.067550	2.392163
F	-1.989739	-2.187076	-0.554237	F	-1.614460	-0.945322	2.246575
O	0.173065	-1.461442	2.489346	O	1.721621	0.828236	1.754740
F	-2.181134	-3.171116	1.383809	F	-0.635899	0.359999	3.697835
F	-2.424698	-1.010712	1.229079	F	-1.222750	1.141557	1.747273
N	3.356223	2.547722	1.408824	N	3.160685	1.467237	-1.060823
H	3.821572	3.285932	1.936130	H	3.849422	2.225595	-0.977304
H	3.410439	2.790638	0.407279	H	3.553210	0.746644	-1.665578
H	3.908076	1.699629	1.532714	H	3.039550	1.049666	-0.137204
N	3.207358	2.931829	-1.656629	N	5.135605	3.892709	-0.760580
H	2.933409	3.756337	-2.190691	H	5.610285	3.988366	0.137089
H	2.585845	2.172732	-1.938822	H	4.855631	4.832209	-1.042296
H	4.139692	2.676865	-1.982370	H	5.847645	3.596207	-1.428591
N	1.864385	0.674607	4.082199	N	2.215569	3.989707	1.023503
H	2.543711	1.156843	3.494454	H	3.062049	3.882528	0.462814
H	1.433123	-0.047923	3.503349	H	1.947543	3.051164	1.321781
H	2.397323	0.193547	4.806173	H	2.487552	4.495149	1.866324
N	-4.801954	1.216207	1.462016	N	-4.714604	3.255764	-0.275726
H	-4.655604	0.207067	1.446851	H	-4.773961	2.952587	0.696190
H	-5.297600	1.448141	0.601356	H	-5.353478	2.659350	-0.801179
H	-5.451879	1.401324	2.225900	H	-5.108597	4.195967	-0.307560
Fig. S4w							
N	-0.351810	2.072990	-1.393528				
C	0.916076	1.638576	-1.362453				
N	1.513954	2.120789	-0.275621				
C	0.598320	2.874074	0.427708				
C	-0.577638	2.853291	-0.269694				
H	2.524155	1.850329	0.043881				
C	-1.356207	1.714598	-2.407022				
C	-2.538917	0.963239	-1.794675				
C	-3.545830	0.512468	-2.857905				
C	-4.728472	-0.244145	-2.241349				
H	0.851483	3.348844	1.362762				
H	-1.550680	3.288097	-0.065963				
H	1.358694	0.975359	-2.087569				

H	-0.848163	1.092881	-3.147534
H	-1.684359	2.636978	-2.897202
H	-3.037868	1.607124	-1.061660
H	-2.154493	0.094545	-1.253732
H	-3.038650	-0.132016	-3.589599
H	-3.914501	1.387010	-3.413080
H	-5.439279	-0.568119	-3.010675
H	-5.270338	0.388609	-1.526576
H	-4.383534	-1.135399	-1.702421
C	1.918921	-2.344264	-0.514217
F	2.182993	-2.795463	0.720597
S	0.099925	-1.868088	-0.679478
O	0.024106	-1.272253	-2.022995
N	-0.045347	-0.670927	0.391128
S	-0.455242	-0.863922	1.942051
O	-0.377132	-2.228464	2.485182
O	-0.642950	-3.107956	-0.413473
F	2.217188	-3.308479	-1.400821
F	2.702275	-1.280389	-0.758838
C	-2.303122	-0.473986	1.908703
F	-2.937329	-1.275222	1.038652
O	0.125866	0.241551	2.715535
F	-2.824239	-0.666160	3.131836
F	-2.514099	0.802372	1.549931
N	4.001266	1.338055	0.479840
H	4.608574	2.069720	0.876541
H	4.463795	0.937042	-0.348793
H	3.923725	0.592791	1.172100
N	5.740409	3.611306	1.704735
H	5.494409	3.756168	2.683618
H	5.604180	4.506196	1.235487
H	6.741679	3.420339	1.681946
N	5.063380	0.047994	-2.142510
H	5.240773	-0.935313	-1.939893
H	5.862620	0.384968	-2.678492
H	4.259932	0.071174	-2.769764
N	-3.710263	3.710644	0.441686
H	-4.459081	3.688875	-0.250299
H	-3.866800	4.543508	1.009142
H	-3.861338	2.910438	1.055728

[Tf₂N]⁻...NH₃

Fig. S5a				Fig. S5b			
C	2.656732	-0.102706	-0.365670	C	-2.649003	-0.408925	-0.175580
F	2.241390	0.166201	-1.611743	F	-2.358707	-1.716336	-0.247104
S	1.229426	0.053466	0.861325	S	-1.175403	0.563142	0.496133
O	1.794319	-0.439861	2.125163	O	-1.586711	1.967800	0.343674
N	0.174489	-1.052707	0.326527	N	-0.022493	0.267178	-0.601099
S	-1.023418	-0.741417	-0.716454	S	1.034064	-0.956351	-0.501289
O	-0.857012	0.428666	-1.593690	O	0.677026	-2.077897	0.379748
O	0.823523	1.464542	0.769306	O	-0.965553	0.030561	1.850185
F	3.624135	0.769534	-0.035046	F	-3.703273	-0.244724	0.641343
F	3.169456	-1.342377	-0.339981	F	-2.981824	0.026560	-1.399788
C	-2.461823	-0.283309	0.422306	C	2.515191	-0.144926	0.345083
F	-2.130061	0.741971	1.219704	F	2.164572	0.357524	1.537807
O	-1.440786	-2.017004	-1.314526	O	1.520522	-1.242391	-1.858116
F	-3.523011	0.074358	-0.321355	F	3.483180	-1.057930	0.527475
F	-2.806511	-1.329943	1.187669	F	3.004518	0.851194	-0.412966
N	-1.297298	3.439150	-0.635058	N	0.943783	3.500188	-0.926104
H	-1.458685	2.600841	-1.192813	H	1.338013	2.574818	-1.089330
H	-2.192388	3.684275	-0.212713	H	0.070243	3.327461	-0.428439
H	-0.693819	3.124641	0.124222	H	1.568540	3.969430	-0.271162
Fig. S5c							
C	-2.809942	0.713407	-0.050110				
F	-2.304646	1.560302	-0.959274				
S	-1.623988	-0.725234	0.254255				
O	-2.226583	-1.444831	1.385203				
N	-0.294803	0.025191	0.798854				
S	0.931579	0.493377	-0.145361				
O	0.649721	0.675231	-1.576452				
O	-1.522106	-1.401823	-1.047396				
F	-3.980152	0.236688	-0.508017				
F	-3.036831	1.387888	1.087281				
C	2.096661	-0.992734	-0.077197				
F	1.485504	-2.093716	-0.536937				
O	1.667581	1.547969	0.570894				
F	3.177252	-0.748520	-0.839914				
F	2.502996	-1.218095	1.181374				
N	4.864543	1.898569	0.332477				
H	3.847080	1.863758	0.404253				
H	5.224167	1.916187	1.286364				
H	5.152798	1.006119	-0.067019				

[SCN]⁻...NH₃

Fig. S6a				Fig. S6b			
C	0.615435	-0.295487	-0.008491	C	-1.020837	0.579396	-0.000015
N	-0.503882	-0.677915	-0.020759	N	-1.176909	1.751478	-0.000020
S	2.190702	0.242252	0.008589	S	-0.793731	-1.072447	0.000008
N	-3.593394	0.176735	-0.018701	N	2.789001	0.059333	0.000078
H	-2.612486	-0.117248	-0.018961	H	1.843478	-0.329913	-0.000184
H	-3.778954	0.581884	0.898510	H	2.848663	0.668195	-0.815703
H	-3.671460	0.940518	-0.689804	H	2.847928	0.668817	0.815447

[NO₃]⁻...NH₃

N	-0.901222	0.002501	-0.038818
O	-2.102576	-0.189403	0.293497
O	-0.452454	1.175953	-0.156665
O	-0.139316	-0.985745	-0.254694
N	2.846991	-0.014401	0.023396
H	3.197445	-0.617253	0.767441
H	1.857042	-0.243871	-0.102342
H	2.879891	0.937986	0.385753

[Blm][Tf₂N]

Fig. S7a				Fig. S7b			
N	3.431094	-0.136350	0.989030	N	3.470254	-1.170957	-0.339775
C	2.247781	-0.423209	0.432324	C	2.420398	-0.500501	-0.829677
N	1.309347	0.301462	1.044566	N	1.344348	-0.825650	-0.110802
C	1.895767	1.079395	2.019605	C	1.700544	-1.724658	0.870212
C	3.233997	0.807644	1.985165	C	3.041451	-1.942167	0.729750
H	0.302007	0.262025	0.800968	H	0.404460	-0.453838	-0.280071
C	4.733320	-0.679315	0.562439	C	4.862212	-1.056498	-0.812317
C	5.502564	0.304632	-0.323476	C	5.712529	-0.191629	0.122228
C	6.854911	-0.271270	-0.762876	C	7.160963	-0.082019	-0.371435
C	7.642888	0.704606	-1.644429	C	8.026607	0.777113	0.557464
H	1.320967	1.742840	2.646099	H	0.976552	-2.121232	1.562805
H	4.051785	1.189686	2.575930	H	3.720549	-2.570563	1.284160
H	2.069247	-1.119264	-0.372475	H	2.440530	0.184159	-1.663394
H	4.532580	-1.613844	0.032961	H	4.825656	-0.633876	-1.819406
H	5.294705	-0.920426	1.469192	H	5.261804	-2.071585	-0.887953
H	5.658574	1.242177	0.226184	H	5.696324	-0.624188	1.131205
H	4.892663	0.545184	-1.204242	H	5.263080	0.807524	0.193287
H	6.689886	-1.210497	-1.308991	H	7.169098	0.345785	-1.383618
H	7.448249	-0.526448	0.126266	H	7.594597	-1.088413	-0.453520

H	8.602763	0.272890	-1.950625	H	9.056197	0.843972	0.187409
H	7.849607	1.639817	-1.108868	H	8.059027	0.352977	1.568999
H	7.081178	0.955753	-2.553000	H	7.629137	1.797013	0.634126
C	-2.350685	2.449808	-0.658279	C	-3.236994	-1.988877	-0.418894
F	-2.525095	2.003114	-1.908512	F	-2.527548	-1.866055	-1.550510
S	-2.577517	1.045932	0.584850	S	-2.673555	-0.707057	0.848226
O	-2.199683	1.641382	1.872484	O	-3.624964	-0.841923	1.955304
N	-1.385431	0.019737	0.169738	N	-2.966024	0.694476	0.091057
S	-1.516143	-1.201606	-0.893799	S	-1.871469	1.474597	-0.802638
O	-2.585363	-1.091913	-1.890656	O	-0.736374	0.667343	-1.302110
O	-3.945320	0.560389	0.374289	O	-1.255905	-1.033693	1.087687
F	-3.249481	3.413389	-0.408168	F	-3.046590	-3.220491	0.080170
F	-1.117258	2.966953	-0.550402	F	-4.536466	-1.830657	-0.700747
C	-2.006201	-2.654520	0.208866	C	-1.072245	2.658680	0.432178
F	-3.183544	-2.418801	0.800354	F	-0.464755	1.964204	1.406630
O	-0.147081	-1.527568	-1.322683	O	-2.570816	2.345917	-1.750723
F	-2.104157	-3.764831	-0.537205	F	-0.155977	3.408084	-0.200690
F	-1.074598	-2.847380	1.154704	F	-1.991441	3.463663	0.977912
Fig. S7c				Fig. S7d			
N	-3.602033	0.854724	0.512436	N	-2.688915	-0.666118	-1.411005
C	-2.717503	1.384055	-0.340273	C	-1.949993	0.340591	-1.883022
N	-1.510019	0.893761	-0.049658	N	-2.732527	1.419461	-1.977036
C	-1.611318	0.023236	1.016105	C	-4.008923	1.106535	-1.552810
C	-2.930104	-0.003681	1.368958	C	-3.981370	-0.209825	-1.195255
H	-0.645104	1.143639	-0.543121	H	-2.398490	2.335885	-2.253044
C	-5.057140	1.090086	0.500301	C	-2.178742	-2.005373	-1.056533
C	-5.818754	-0.063408	-0.158345	C	-2.011628	-2.159057	0.456651
C	-7.333014	0.181866	-0.144294	C	-1.526542	-3.563842	0.830435
C	-8.112406	-0.959983	-0.806628	C	-1.264504	-3.697065	2.334773
H	-0.748991	-0.482806	1.419743	H	-4.807915	1.830452	-1.545278
H	-3.444979	-0.544310	2.147518	H	-4.756577	-0.856375	-0.815274
H	-2.942818	2.089699	-1.124794	H	-0.893376	0.301231	-2.091228
H	-5.226688	2.029545	-0.031561	H	-1.218912	-2.127915	-1.562452
H	-5.367539	1.229973	1.539317	H	-2.882094	-2.737732	-1.462447
H	-5.589634	-0.998924	0.368683	H	-2.965640	-1.945957	0.956961
H	-5.465760	-0.181292	-1.191316	H	-1.288802	-1.413106	0.802688
H	-7.553758	1.126968	-0.659744	H	-0.603302	-3.780246	0.279321
H	-7.671179	0.305533	0.893993	H	-2.273278	-4.305964	0.514536
H	-9.191026	-0.766110	-0.784523	H	-0.923319	-4.707385	2.589237
H	-7.930415	-1.911395	-0.291059	H	-2.172834	-3.491485	2.915802
H	-7.813767	-1.084199	-1.855170	H	-0.491310	-2.988883	2.658228
C	1.735761	-2.688512	-0.448936	C	-0.700539	1.668633	1.629905
F	2.211281	-2.399544	-1.667374	F	-0.279076	0.779967	2.539499

S	2.212011	-1.342897	0.788146	S	0.564369	1.853688	0.238022
O	1.498009	-1.724046	2.014889	O	-0.150333	2.652261	-0.771822
N	1.460157	-0.035936	0.196140	N	0.675983	0.348167	-0.341693
S	2.077197	1.005486	-0.866624	S	1.757128	-0.760666	0.133544
O	3.151532	0.538746	-1.748823	O	2.317917	-0.598467	1.481568
O	3.679896	-1.316104	0.778238	O	1.757140	2.415506	0.883738
F	2.247943	-3.862019	-0.047908	F	-0.884855	2.853962	2.230137
F	0.400231	-2.800678	-0.521040	F	-1.878538	1.250241	1.134888
C	2.871046	2.328821	0.221214	C	3.209322	-0.458301	-1.035817
F	3.874218	1.805019	0.936092	F	3.708568	0.773501	-0.864895
O	0.914080	1.702870	-1.461692	O	1.239000	-2.072121	-0.277851
F	3.352449	3.311670	-0.554587	F	4.174636	-1.357112	-0.784871
F	1.960549	2.844197	1.059898	F	2.816802	-0.591964	-2.312424

Fig. S7e

N	-1.736255	2.497912	-0.713393
C	-0.430681	2.454782	-0.986706
N	0.073900	3.675685	-0.774704
C	-0.928838	4.527187	-0.349530
C	-2.070257	3.782458	-0.309564
H	1.047281	3.926021	-0.904585
C	-2.658860	1.346761	-0.764739
C	-3.009281	0.837895	0.635420
C	-4.013081	-0.320180	0.571200
C	-4.317698	-0.898647	1.957409
H	-0.745427	5.565387	-0.123790
H	-3.080053	4.047840	-0.039084
H	0.108975	1.574322	-1.297236
H	-2.162248	0.569601	-1.348625
H	-3.550027	1.675307	-1.307453
H	-3.431146	1.658965	1.230573
H	-2.086744	0.515464	1.130991
H	-3.614620	-1.111568	-0.076446
H	-4.943843	0.029017	0.102425
H	-5.042902	-1.718328	1.893729
H	-4.733986	-0.130971	2.622206
H	-3.406414	-1.290051	2.425878
C	-0.782441	-2.694648	-0.261305
F	-1.253807	-2.006479	0.788634
S	0.647979	-1.761325	-1.068410
O	1.237323	-2.732637	-1.997061
N	1.672312	-1.551329	0.164370
S	1.677749	-0.245818	1.121718
O	0.454595	0.573233	1.128647

Fig. S7f

N	1.681850	-1.858481	1.324271
C	0.441867	-2.230104	1.646055
N	0.131423	-1.669014	2.818638
C	1.188764	-0.897903	3.256800
C	2.168072	-1.020364	2.316226
H	-0.766962	-1.757819	3.278470
C	2.389003	-2.228420	0.082910
C	2.732882	-1.002308	-0.763678
C	3.366371	-1.401007	-2.101129
C	3.702951	-0.177761	-2.962071
H	1.150924	-0.338763	4.177527
H	3.155001	-0.589837	2.266278
H	-0.203120	-2.848808	1.044506
H	1.724280	-2.898503	-0.464922
H	3.287686	-2.783405	0.368491
H	3.419356	-0.348306	-0.211335
H	1.817603	-0.431483	-0.941079
H	2.673491	-2.055901	-2.647229
H	4.276999	-1.988799	-1.918289
H	4.150988	-0.476315	-3.916958
H	4.413096	0.482156	-2.447645
H	2.800625	0.406937	-3.180039
C	-2.965961	-1.002515	-0.536929
F	-3.683816	0.067656	-0.170227
S	-1.229349	-0.491977	-1.074177
O	-0.536437	-1.778235	-1.257721
N	-0.625600	0.183744	0.261702
S	-0.758131	1.749880	0.648203
O	-1.773341	2.527471	-0.076576

O	0.022541	-0.546600	-1.625025	O	-1.432620	0.379062	-2.238881
F	-1.773617	-2.854554	-1.153643	F	-3.590191	-1.617950	-1.553072
F	-0.378169	-3.900779	0.158035	F	-2.897209	-1.852081	0.503550
C	2.965037	0.853455	0.284335	C	0.892781	2.442798	0.047298
F	2.570747	1.151273	-0.969308	F	1.049044	2.212370	-1.265192
O	2.296929	-0.614800	2.399941	O	-0.679809	1.864598	2.110895
F	3.097552	1.999633	0.971464	F	0.926863	3.767725	0.261497
F	4.153438	0.241956	0.226312	F	1.913450	1.874612	0.707988
Fig. S7g				Fig. S7h			
N	2.873738	-2.007181	0.047374	N	2.001183	-0.397223	1.108602
C	1.548554	-1.955969	-0.121621	C	1.473277	0.377750	2.056721
N	0.969388	-2.484812	0.960046	N	0.843470	-0.409358	2.933179
C	1.941044	-2.883700	1.854044	C	0.951336	-1.725558	2.532023
C	3.142761	-2.581386	1.280542	C	1.681915	-1.716574	1.380730
H	-0.047743	-2.534890	1.078219	H	0.310506	-0.068274	3.724203
C	3.874356	-1.452103	-0.883284	C	2.714895	0.077281	-0.089334
C	4.341958	-0.060298	-0.447962	C	4.187362	-0.336282	-0.086876
C	5.374055	0.519819	-1.423241	C	4.907230	0.153415	-1.349882
C	5.840049	1.919605	-1.006388	C	6.384992	-0.253259	-1.373221
H	1.699649	-3.342761	2.799447	H	0.498966	-2.534379	3.082501
H	4.152407	-2.724323	1.632378	H	1.976924	-2.518567	0.724454
H	1.024465	-1.546572	-0.972162	H	1.521852	1.453333	2.096731
H	3.409726	-1.422572	-1.872025	H	2.610372	1.164495	-0.111526
H	4.706231	-2.160342	-0.922695	H	2.180132	-0.332134	-0.950186
H	4.775075	-0.121744	0.559139	H	4.260206	-1.430020	-0.022618
H	3.471315	0.604163	-0.384017	H	4.676366	0.071706	0.807653
H	4.938280	0.561579	-2.431158	H	4.824596	1.247416	-1.414537
H	6.238967	-0.155401	-1.483744	H	4.399011	-0.250792	-2.236362
H	6.576238	2.317814	-1.714159	H	6.878913	0.105549	-2.283637
H	6.304378	1.900407	-0.012265	H	6.493090	-1.344775	-1.339047
H	4.995763	2.619380	-0.968693	H	6.922099	0.163912	-0.511910
C	-3.772902	-0.870379	-0.713975	C	-2.173314	-2.285836	-0.360149
F	-4.076504	0.255448	-1.370881	F	-3.292198	-1.773889	0.173354
S	-1.977414	-0.817649	-0.132893	S	-1.123739	-0.917584	-1.130190
O	-1.847050	-2.038175	0.693908	O	0.134343	-1.591775	-1.484528
N	-1.917592	0.445862	0.862575	N	-0.823040	0.044232	0.133117
S	-1.522342	1.951530	0.393065	S	-1.691958	1.342053	0.539143
O	-1.732224	2.272570	-1.025001	O	-3.086263	1.390731	0.079029
O	-1.172687	-0.745336	-1.364033	O	-1.963248	-0.366852	-2.203478
F	-3.939857	-1.916518	-1.536608	F	-2.512240	-3.174635	-1.308431
F	-4.597048	-1.002298	0.332806	F	-1.490210	-2.924139	0.602442
C	0.354942	1.974121	0.613033	C	-0.822628	2.727650	-0.405920
F	0.939492	1.119697	-0.243918	F	-0.858178	2.498719	-1.725147

O	-2.011241	2.875220	1.423111	O	-1.392854	1.647605	1.947256
F	0.815588	3.209892	0.368442	F	-1.425758	3.898416	-0.150124
F	0.692698	1.624177	1.862185	F	0.465319	2.816445	-0.021431
Fig. S7i				Fig. S7j			
N	3.148781	-0.337884	-0.489995	N	4.106958	0.709743	0.513820
C	4.447378	-0.293636	-0.795760	C	5.401394	0.974677	0.322029
N	4.683027	0.860854	-1.430978	N	6.021550	-0.177101	0.038020
C	3.506887	1.578960	-1.534866	C	5.103918	-1.209416	0.044305
C	2.540170	0.823362	-0.938948	C	3.895715	-0.649517	0.341300
H	5.588264	1.148861	-1.784653	H	7.014709	-0.265954	-0.144359
C	2.465381	-1.413058	0.257056	C	3.050528	1.706338	0.785607
C	2.164489	-0.993148	1.697009	C	2.308513	2.102142	-0.492524
C	1.366932	-2.071783	2.439610	C	1.133805	3.040497	-0.191082
C	1.051731	-1.664038	3.883110	C	0.378032	3.440524	-1.462603
H	3.462782	2.541663	-2.018301	H	5.386625	-2.230957	-0.153292
H	1.483768	0.981626	-0.794076	H	2.911670	-1.076362	0.456250
H	5.178757	-1.054365	-0.572046	H	5.865298	1.946671	0.384405
H	3.113373	-2.292434	0.220572	H	3.531700	2.566808	1.256994
H	1.548348	-1.635131	-0.290359	H	2.367999	1.249920	1.504633
H	1.584250	-0.064406	1.687342	H	1.928775	1.199007	-0.982512
H	3.109616	-0.791547	2.219363	H	3.011738	2.584718	-1.184740
H	1.927148	-3.017919	2.432204	H	1.501126	3.939215	0.324627
H	0.430606	-2.255338	1.898229	H	0.443756	2.538543	0.500229
H	0.477078	-2.443757	4.397168	H	-0.458375	4.109883	-1.230971
H	0.462739	-0.739683	3.900332	H	-0.028436	2.552999	-1.960409
H	1.972422	-1.492474	4.455888	H	1.039840	3.958437	-2.168760
C	-1.085821	2.760771	0.235303	C	-0.118230	-2.642979	-0.325294
F	-1.611566	2.867079	-0.992647	F	-1.072375	-3.032283	-1.181079
S	-1.400408	1.042184	0.954543	S	-0.299660	-0.812312	0.097924
O	-0.682988	1.063686	2.235773	O	0.758991	-0.595223	1.099382
N	-0.567982	0.084522	-0.053901	N	-1.718846	-0.744516	0.863573
S	-1.182081	-0.616489	-1.377009	S	-3.129523	-0.433378	0.124565
O	-2.361034	0.014459	-1.984794	O	-3.186284	-0.676486	-1.324261
O	-2.862260	0.896990	0.950587	O	-0.194212	-0.121409	-1.194315
F	-1.642619	3.688954	1.028443	F	1.084381	-2.842033	-0.897351
F	0.236060	2.998196	0.157415	F	-0.194282	-3.396856	0.781229
C	-1.810795	-2.277726	-0.732977	C	-3.274042	1.441806	0.300372
F	-2.735570	-2.100222	0.219489	F	-2.247992	2.053028	-0.308328
O	-0.040882	-0.982529	-2.230437	O	-4.205255	-0.954454	0.978633
F	-2.356845	-2.968627	-1.746347	F	-4.420866	1.855051	-0.264486
F	-0.796897	-2.995127	-0.221283	F	-3.280071	1.796134	1.594685

[BIm][SCN]

Fig. S8a				Fig. S8b			
N	1.336434	0.682851	0.447418	N	0.721611	0.836370	0.502298
C	0.179849	0.024619	0.606875	C	-0.455801	0.212633	0.376245
N	-0.789469	0.710750	0.000643	N	-1.342920	1.088948	-0.104422
C	-0.248155	1.842748	-0.569054	C	-0.726738	2.307356	-0.296765
C	1.089731	1.827828	-0.292309	C	0.575604	2.149482	0.082051
H	-1.802274	0.426880	-0.023861	H	-2.334688	0.859170	-0.284395
C	2.656827	0.234121	0.923519	C	1.980427	0.209323	0.946014
C	3.510575	-0.344514	-0.208041	C	2.879773	-0.166201	-0.234827
C	4.880524	-0.810226	0.302112	C	4.190801	-0.808453	0.236414
C	5.751130	-1.390492	-0.818156	C	5.099396	-1.198734	-0.935061
H	-0.851039	2.554905	-1.110034	H	-1.257986	3.166758	-0.673761
H	1.876584	2.520183	-0.546823	H	1.399522	2.845597	0.095795
H	0.057332	-0.904715	1.141488	H	-0.667243	-0.818906	0.617781
H	2.480084	-0.511157	1.702994	H	1.709955	-0.671933	1.532817
H	3.144055	1.096557	1.387166	H	2.475309	0.919756	1.613842
H	3.644636	0.415787	-0.988894	H	3.097382	0.733180	-0.825880
H	2.974500	-1.185916	-0.666610	H	2.337177	-0.859455	-0.890853
H	4.738660	-1.565335	1.087888	H	3.963840	-1.699072	0.838892
H	5.400358	0.036240	0.772322	H	4.721250	-0.109666	0.898240
H	6.723777	-1.717735	-0.432927	H	6.029424	-1.655795	-0.577744
H	5.932852	-0.644037	-1.601702	H	5.364984	-0.320530	-1.537080
H	5.265496	-2.256166	-1.286073	H	4.601537	-1.920006	-1.595248
N	-3.449885	-0.048681	-0.055344	N	-2.678780	-2.383298	0.511324
C	-4.583305	-0.384803	-0.069700	C	-3.385960	-1.526370	0.110396
S	-6.167977	-0.854726	-0.089715	S	-4.330303	-0.271091	-0.455225
Fig. S8c				Fig. S8d			
N	-0.934968	0.097143	-0.733208	N	-1.735384	0.154312	0.391712
C	0.003593	-0.848236	-0.602127	C	-1.899857	-1.045528	-0.174369
N	1.162728	-0.251045	-0.317804	N	-3.191993	-1.164717	-0.504648
C	0.973612	1.114559	-0.259938	C	-3.875314	-0.017999	-0.147755
C	-0.348865	1.335153	-0.519542	C	-2.954017	0.815187	0.415641
H	2.068203	-0.730440	-0.164935	H	-3.597389	-1.983536	-0.943353
C	-2.366930	-0.142354	-0.989546	C	-0.444322	0.709528	0.845210
C	-3.205946	-0.009292	0.284151	C	0.189930	1.615276	-0.213241
C	-4.694233	-0.256979	0.006444	C	1.498533	2.235474	0.292608
C	-5.550270	-0.126911	1.271424	C	2.174841	3.108921	-0.769848
H	1.789820	1.787130	-0.046082	H	-4.933878	0.098446	-0.316341
H	-0.918929	2.249151	-0.575500	H	-3.055581	1.804614	0.832779
H	-0.153748	-1.910280	-0.708841	H	-1.106133	-1.774089	-0.328623
H	-2.452867	-1.144657	-1.416341	H	0.205731	-0.137096	1.075252

H	-2.682631	0.575990	-1.751086	H	-0.641467	1.254850	1.772086
H	-3.069015	0.994876	0.706455	H	-0.518606	2.407872	-0.489437
H	-2.838456	-0.725236	1.031030	H	0.382471	1.022360	-1.116994
H	-4.821681	-1.260065	-0.423992	H	2.181149	1.431003	0.595750
H	-5.046071	0.455915	-0.752240	H	1.292446	2.836302	1.189844
H	-6.608935	-0.307078	1.051738	H	3.105036	3.545487	-0.387610
H	-5.462264	0.877483	1.704613	H	1.519947	3.932391	-1.082892
H	-5.236670	-0.849932	2.034917	H	2.422583	2.519235	-1.661430
N	4.415177	1.619282	0.599251	N	0.771900	-2.632007	-0.345966
C	4.364988	0.446651	0.472268	C	1.826126	-2.142372	-0.118293
S	4.242311	-1.209129	0.280862	S	3.296032	-1.445742	0.205847
Fig. S8e				Fig. S8f			
N	-1.296647	0.808603	0.484507	N	1.642316	0.194269	0.390891
C	-1.824959	-0.416558	0.428398	C	2.844433	0.603562	0.802923
N	-3.026091	-0.320587	-0.152724	N	3.770502	-0.083176	0.122989
C	-3.278604	0.996484	-0.484511	C	3.148801	-0.955162	-0.749942
C	-2.185622	1.707769	-0.084382	C	1.805638	-0.779439	-0.583349
H	-3.644794	-1.105100	-0.323027	H	4.771097	0.024387	0.244037
C	0.050490	1.133709	0.994161	C	0.343871	0.718083	0.860656
C	1.046055	1.364977	-0.144759	C	-0.346259	1.566774	-0.209165
C	2.454730	1.643071	0.394789	C	-1.706116	2.080841	0.281156
C	3.472980	1.855037	-0.731298	C	-2.427620	2.913053	-0.784822
H	-4.194641	1.304385	-0.962541	H	3.705241	-1.613820	-1.397246
H	-1.964992	2.761469	-0.147885	H	0.949660	-1.244936	-1.056499
H	-1.347082	-1.319129	0.783114	H	3.036107	1.354180	1.553596
H	0.364021	0.291154	1.614525	H	0.543701	1.299101	1.764615
H	-0.050586	2.018324	1.629124	H	-0.272148	-0.142295	1.135320
H	0.709270	2.208857	-0.761951	H	-0.490457	0.956168	-1.108297
H	1.059867	0.476460	-0.786441	H	0.303986	2.409795	-0.479571
H	2.771272	0.798869	1.022494	H	-1.563898	2.685413	1.188407
H	2.431629	2.528701	1.045589	H	-2.329162	1.223024	0.566254
H	4.473877	2.049246	-0.328398	H	-3.395108	3.274033	-0.416567
H	3.191961	2.708327	-1.361798	H	-2.612447	2.317280	-1.687550
H	3.534270	0.968470	-1.374649	H	-1.830660	3.787055	-1.076025
N	0.348142	-2.021684	-1.869231	N	-1.187971	-1.708275	-1.583824
C	0.685677	-2.263243	-0.762169	C	-1.787067	-1.814578	-0.568642
S	1.122727	-2.567615	0.815788	S	-2.602746	-1.946744	0.872890
Fig. S8g				Fig. S8h			
N	0.037318	-0.795003	-0.082032	N	-0.594170	-1.462992	0.087342
C	0.615751	-1.631967	-0.945147	C	-1.477186	-1.546333	-0.910951
N	1.466110	-2.407449	-0.264305	N	-2.668717	-1.161780	-0.442865
C	1.444566	-2.054056	1.071163	C	-2.549284	-0.799906	0.883206

C	0.541685	-1.038223	1.183985	C	-1.241221	-0.990677	1.216742
H	2.052771	-3.121595	-0.679775	H	-3.515563	-1.108233	-0.996587
C	-0.979464	0.218525	-0.417764	C	0.846853	-1.769433	-0.007342
C	-2.385189	-0.229175	-0.009803	C	1.703826	-0.502786	-0.045145
C	-3.434199	0.838215	-0.347301	C	3.198383	-0.840725	-0.112416
C	-4.850059	0.409024	0.054395	C	4.071272	0.419272	-0.149304
H	2.067705	-2.539132	1.804903	H	-3.386007	-0.440034	1.459631
H	0.239860	-0.448258	2.033651	H	-0.715094	-0.819006	2.141464
H	0.431231	-1.672287	-2.006962	H	-1.267076	-1.873893	-1.916727
H	-0.913570	0.390631	-1.494639	H	0.987315	-2.371722	-0.908358
H	-0.681936	1.137488	0.092563	H	1.095991	-2.393305	0.855884
H	-2.401624	-0.436345	1.068476	H	1.495226	0.106265	0.842145
H	-2.627866	-1.169841	-0.522257	H	1.410270	0.102229	-0.911425
H	-3.404818	1.049327	-1.425445	H	3.397236	-1.453662	-1.003127
H	-3.174202	1.776448	0.161978	H	3.474454	-1.454487	0.756865
H	-5.583610	1.184242	-0.195722	H	5.136217	0.162469	-0.193425
H	-4.912940	0.221509	1.133789	H	3.908168	1.034894	0.743957
H	-5.143924	-0.512611	-0.463841	H	3.835229	1.034801	-1.026366
N	1.325035	2.244920	1.356556	N	-0.037456	2.353876	1.593576
C	1.994907	1.858550	0.461248	C	-0.471370	2.264491	0.497114
S	2.910355	1.288612	-0.805182	S	-1.077600	2.122909	-1.046358

[BIm][NO₃]

Fig. S9a				Fig. S9b			
N	0.916745	0.798666	0.477499	N	-1.067449	0.428011	-0.615934
C	-0.273281	0.187055	0.400571	C	-0.084546	-0.468746	-0.778907
N	-1.154478	1.039288	-0.123398	N	1.044862	0.046282	-0.291769
C	-0.522244	2.233080	-0.396350	C	0.790838	1.306531	0.203049
C	0.783418	2.084585	-0.022186	C	-0.538872	1.549588	0.003533
H	-2.164575	0.808772	-0.277913	H	1.981151	-0.425331	-0.290299
C	2.170749	0.184296	0.946844	C	-2.485101	0.227466	-0.963556
C	3.061998	-0.262696	-0.215240	C	-3.325453	-0.156095	0.257854
C	4.370161	-0.888882	0.284937	C	-4.803017	-0.344766	-0.108884
C	5.270444	-1.351527	-0.866305	C	-5.655751	-0.740560	1.102150
H	-1.045110	3.075452	-0.821030	H	1.574565	1.903822	0.639475
H	1.616391	2.769119	-0.059310	H	-1.148944	2.408104	0.237485
H	-0.495396	-0.821893	0.709320	H	-0.193923	-1.442260	-1.231594
H	1.896489	-0.662091	1.581610	H	-2.523896	-0.550536	-1.730182
H	2.677149	0.923631	1.573422	H	-2.841249	1.158440	-1.412928
H	3.284473	0.601183	-0.855547	H	-3.229325	0.625054	1.023350
H	2.510922	-0.985681	-0.831000	H	-2.924594	-1.081844	0.691249
H	4.138830	-1.742472	0.937365	H	-4.889307	-1.114942	-0.888009
H	4.909281	-0.158763	0.904703	H	-5.191003	0.586278	-0.545197

H	6.198726	-1.795036	-0.487925	H	-6.707164	-0.868715	0.819887
H	5.539751	-0.510604	-1.517942	H	-5.608073	0.027127	1.884791
H	4.764152	-2.104771	-1.482994	H	-5.305997	-1.685245	1.537213
N	-3.919947	-0.831565	-0.081921	N	4.327847	-0.351399	0.241806
O	-3.801594	0.374085	-0.494822	O	3.508088	-1.184183	-0.282062
O	-2.899889	-1.428051	0.354622	O	5.532018	-0.661077	0.357362
O	-5.035366	-1.390663	-0.118755	O	3.895190	0.765170	0.629024
Fig. S9c				Fig. S9d			
N	1.624274	-0.460295	0.358736	N	-1.556206	0.061548	0.368343
C	1.715205	0.735690	-0.233261	C	-1.354057	-1.102576	-0.257601
N	2.987939	0.902768	-0.614288	N	-2.553442	-1.589391	-0.601515
C	3.733875	-0.205862	-0.263285	C	-3.549049	-0.723513	-0.190596
C	2.870196	-1.067007	0.348182	C	-2.917184	0.320879	0.418129
H	3.340169	1.727899	-1.085849	H	-2.695425	-2.468923	-1.084641
C	0.372964	-1.042114	0.886785	C	-0.484958	0.951143	0.857151
C	-0.556259	-1.508837	-0.236865	C	-0.049239	1.960220	-0.209114
C	-1.869292	-2.074367	0.319225	C	1.071135	2.871210	0.308522
C	-2.817115	-2.536427	-0.793326	C	1.533195	3.881376	-0.748041
H	4.789112	-0.280753	-0.471205	H	-4.594832	-0.925415	-0.358133
H	3.029265	-2.044453	0.775516	H	-3.308079	1.212784	0.882107
H	0.886473	1.420366	-0.394486	H	-0.382935	-1.553703	-0.457392
H	-0.108982	-0.272093	1.492617	H	0.345558	0.307430	1.155483
H	0.663499	-1.871208	1.536117	H	-0.873059	1.455099	1.746246
H	-0.043819	-2.268628	-0.841966	H	-0.912141	2.565856	-0.517413
H	-0.772841	-0.658789	-0.896429	H	0.296528	1.414112	-1.096798
H	-2.363960	-1.305288	0.927781	H	1.922496	2.253283	0.625559
H	-1.649908	-2.915765	0.991654	H	0.721903	3.405684	1.203136
H	-3.749063	-2.937056	-0.377768	H	2.334750	4.520865	-0.360415
H	-2.354559	-3.322420	-1.403935	H	0.705520	4.530678	-1.060926
H	-3.075850	-1.702637	-1.457984	H	1.913222	3.368961	-1.640894
N	-1.670689	1.922523	0.093681	N	2.193515	-1.882632	0.051757
O	-1.078627	1.855905	1.208138	O	1.633059	-1.605813	1.149868
O	-0.983771	2.051011	-0.965989	O	1.478903	-2.066638	-0.981315
O	-2.922309	1.851758	0.029638	O	3.443084	-1.973277	-0.023142
Fig. S9e				Fig. S9f			
N	-1.697340	-0.407796	0.334633	N	-0.113059	-1.530228	0.194809
C	-2.921940	-0.938817	0.349366	C	-0.831726	-1.879301	-0.874241
N	-3.754913	-0.071986	-0.239157	N	-2.121297	-1.665726	-0.593497
C	-3.047044	1.043568	-0.644762	C	-2.238394	-1.148111	0.679635
C	-1.747500	0.832862	-0.284326	C	-0.971341	-1.061394	1.175743
H	-4.750595	-0.220409	-0.356993	H	-2.885516	-1.828949	-1.238419
C	-0.472595	-1.040602	0.862810	C	1.359177	-1.542767	0.283155

C	0.480386	-1.453531	-0.261215	C	1.960951	-0.172218	-0.034481
C	1.793197	-2.016975	0.297812	C	3.488947	-0.187603	0.095692
C	2.768794	-2.418688	-0.813940	C	4.109184	1.177675	-0.223959
H	-3.521885	1.874185	-1.141931	H	-3.190063	-0.878928	1.106778
H	-0.853133	1.431401	-0.412558	H	-0.605416	-0.701973	2.123860
H	-3.193359	-1.896441	0.765360	H	-0.439713	-2.266888	-1.801343
H	-0.787793	-1.901086	1.458323	H	1.717741	-2.307595	-0.410650
H	0.002168	-0.308110	1.518799	H	1.611557	-1.865547	1.297056
H	0.695908	-0.579719	-0.888041	H	1.526663	0.578804	0.635855
H	-0.011861	-2.199513	-0.899530	H	1.667060	0.118391	-1.050253
H	1.578166	-2.886721	0.934781	H	3.907711	-0.948827	-0.578089
H	2.261973	-1.260553	0.941030	H	3.766259	-0.488407	1.116071
H	3.700162	-2.819174	-0.396856	H	5.200828	1.149718	-0.126300
H	3.024452	-1.553968	-1.438878	H	3.728406	1.950528	0.455381
H	2.332239	-3.187522	-1.464383	H	3.869765	1.487635	-1.249033
N	1.830101	1.770327	0.120249	N	-1.466894	1.849922	-0.133672
O	1.158682	2.016251	-0.926024	O	-2.712984	1.972931	0.037776
O	3.072791	1.592692	0.046241	O	-1.026415	1.293408	-1.177497
O	1.238382	1.694421	1.234324	O	-0.664016	2.271983	0.744263