Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Computational Data

For

Synthesis and Energetic Properties of Homocubane Based High Energy Density Materials

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Table S1. Overall yields for compounds 8-30 Calculated starting from (A) 1,4-dioxaspiro[4.4]nonane. (B) Cyclopentanone

Compound		**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
Overall yield (%)	**A**	38.7 (5)	36.0 (6)	32.8 (7)	28.1 (7)	19.9 (8)	27.1 (6)	25.7 (7)	19.6 (8)	14.9 (9)	21.4 (7)	14.8 (8)
	B	27.1 (6)	25.2 (7)	23.0 (8)	19.7 (8)	13.9 (9)	19.0 (7)	18.0 (8)	13.7 (9)	10.4 (10)	15.0 (8)	10.4 (9)
Compound		**19**	**21a**	**21b**	**24**	**25**	**27**	**28**	**30a**	**30b**	**30c**	
Overall yield (%)	**A**	36.8 (6)	21.3 (7)	20.6 (7)	15.5 (7)	25.7 (7)	25.0 (7)	18.0 (8)	15.7 (7)	14.6 (7)	14.9 (7)	
	B	25.8 (7)	14.9 (8)	14.4 (8)	10.9 (8)	18.0 (8)	17.5 (8)	12.6 (9)	11.0 (8)	10.3 (8)	10.4 (8)	

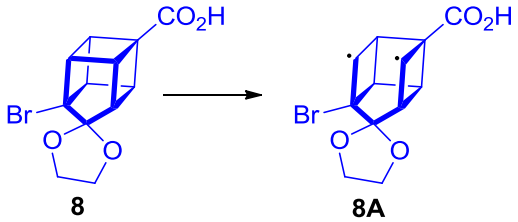
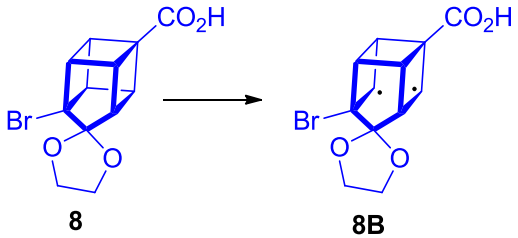
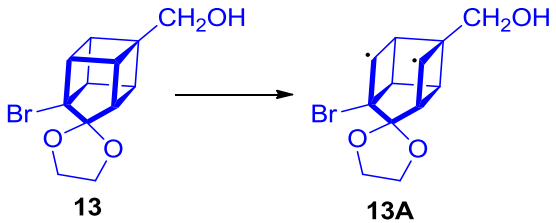
Detonation properties of these homocubanes are reported in Table S1 and compared with that of the well-known explosive RDX. The calculations based on CO_2 as well as CO suggested that, all of these compounds have a negative oxygen balance indicating that they are oxygen deficient compounds. Due to low oxygen contents, these compounds are not good candidates as monopropellants. Compounds **8**, **13**, **18**, **18a** and **19** do not contain nitrogen, whereas compounds **14** and **33** bear, respectively, only 5% and 4.7% nitrogen in the skeleton. Compounds 1**5**, **27** and **31** possess a higher percentage of nitrogen (17.34%, 14.70% and 13.55%, respectively) in their molecule than other homocubanes studied in the present work. Overall percentage of nitrogen and oxygen was also calculated which showed that compounds **15**, **25**, **27**, **28** and **33** are superior in the series, having, respectively, 27.24%, 24.28%, 31.49%, 20.33% and 20.80% of nitrogen and oxygen. This is clearly reflected in their performance as better explosives. Comparison of detonation properties with well-known explosive RDX suggests that compounds **15**, **25**, **28** and **31** are best candidates in the series, however, these compounds are not explosive in nature.

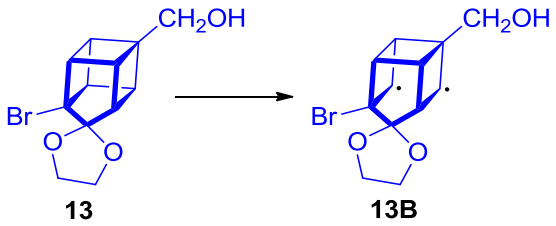
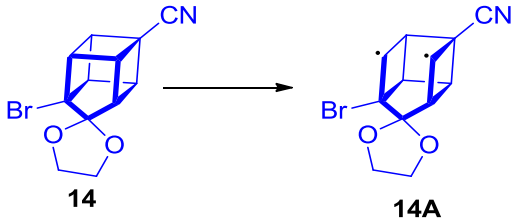
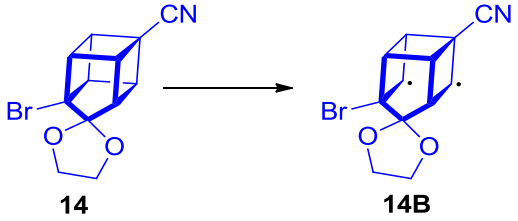
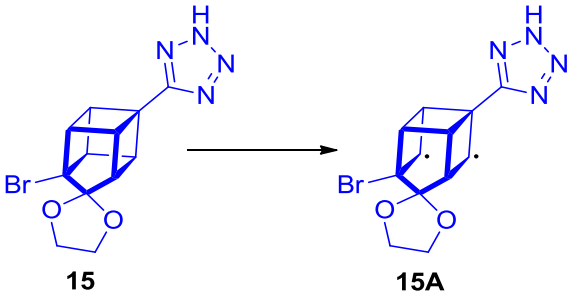
Table S2. Comparison of predicted explosive properties[a-g]

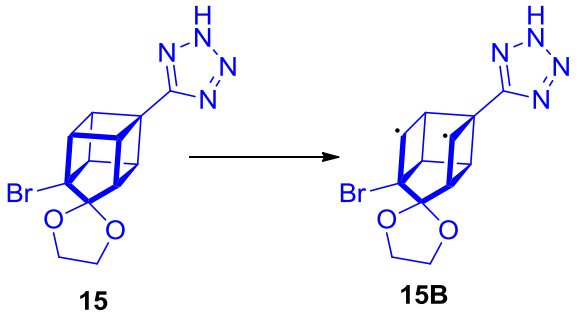
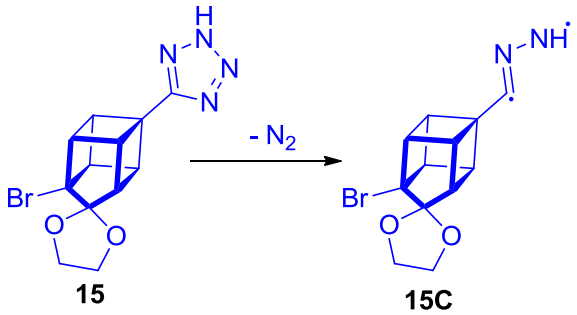
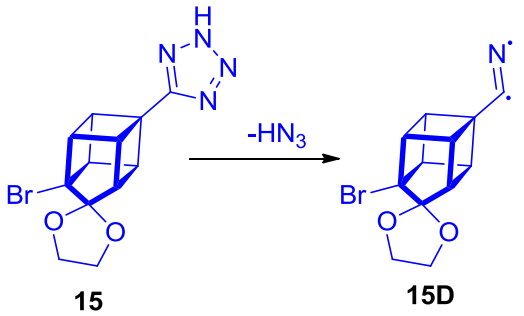
Propellant	OB^{CO2} (%)	OB^{CO} (%)	N (%)[b]	O (%)[c]	N+O (%)[d]	HOF (kJ mol^{-1})	DP[e](GPa)	DV[f] (km s^{-1})
RDX	-21.62	0.0	37.84	43.22	81.06	67.00	35.10	8.93
CB	-307.69	-184.62	-	-	-	601.92 (621.57)[h]	12.70[i]	5.99[i]
CL20	-10.95	10.95	38.36	43.82	82.18	539.33 (550±20)[j]	46.33 (45.60)[k]	9.86 (9.79)[k]
8	-133.82	-69.58	-	21.40	21.40	-107.71	11.90	5.23
13	-151.63	-84.24	-	16.83	16.83	84.14	14.94	5.78
14	-151.48	-82.88	5.00	11.42	16.42	387.66	13.73	5.48
15	-133.79	-74.32	17.34	9.90	27.24	581.25	16.08	5.97
16	-168.46	-92.25	7.02	12.02	19.04	441.14	10.40	4.95
18	-244.21	-143.16	-	16.82	16.82	201.51	10.19	5.09
18a	-166.60	-95.20	-	11.89	11.89	225.45	13.23	5.39
19	-143.18	-76.70	-	20.44	20.44	-86.60	12.66	5.45
21a	-174.38	-96.87	6.78	11.61	18.39	442.54	11.66	5.16
21b	181.78	-99.80	6.23	10.68	16.91	556.43	10.35	4.89
24	-137.30	-73.67	5.86	10.04	15.90	476.10	14.25	5.44
25	-140.17	-79.00	8.95	15.33	24.28	1704.91	25.49	7.48
27	-126.02	-67.21	14.70	16.79	31.49	301.55	10.07	5.12
28	-146.49	-81.38	9.49	10.84	20.33	873.47	26.24	7.05
30a	-195.93	110.31	8.64	6.58	15.22	694.26	7.79	4.38
30b	-165.82	-90.84	7.57	5.76	13.33	680.47	6.10	3.94
30c	-142.92	-78.29	6.52	4.97	11.49	760.33	9.25	4.54
31	-141.98	-80.02	13.55	10.32	23.87	561.73	15.94	5.96
32	-180.62	-102.93	10.19	7.76	17.95	648.48	7.61	4.48
33	-142.33	-77.87	4.70	16.10	20.80	70.91	10.19	4.98

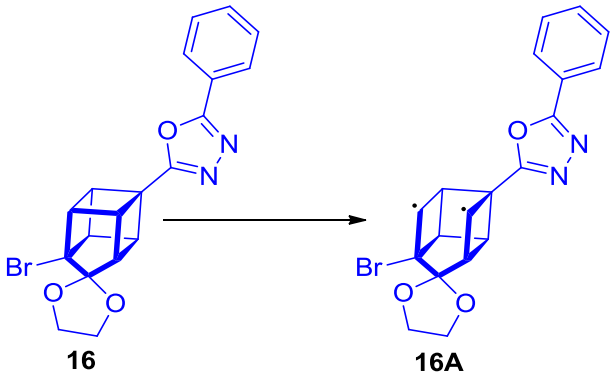
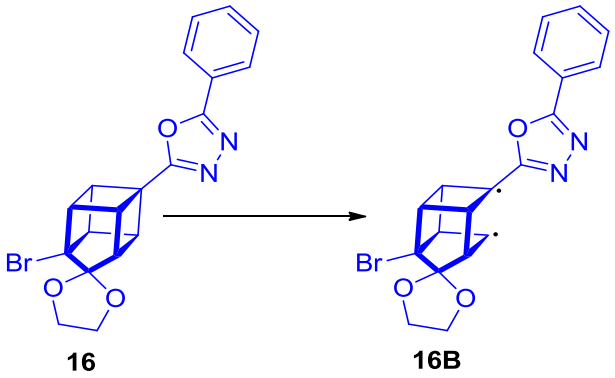
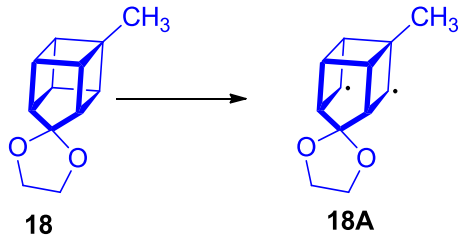
[a]Calculated using Kamlet-Jacobs correlations; literature (experimental or calculated) values in parenthesis. [b]Nitrogen content. [c]Oxygencontent. [d]Nitrogen and oxygen contents. [e]D.P. -detonation pressure. [f]D.V. -detonation velocity. [g]Method: (B3LYP/6-311++g(d,p). [h] Experimental, ref 8, main text). [i] Calculated, ref 26d, main text. [j] Calculated, ref 64, main text. [k] Experimental, B. M. Dobratz and P. C. Crawford, LLNL Explosives Handbook of Properties of Chemical Explosives and Explosive Simulants, UCRL-52997, 1985.

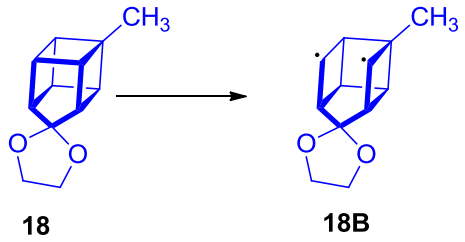
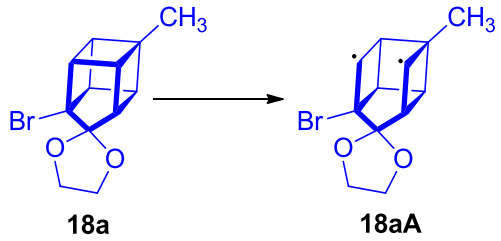
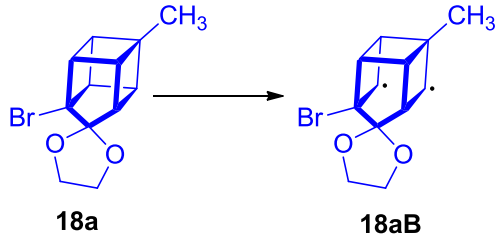
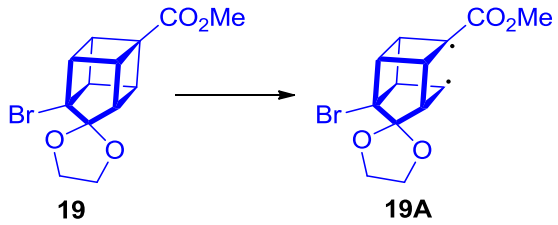
Table S3. Plausible decomposition pathways and corresponding bond dissociation energies[a]

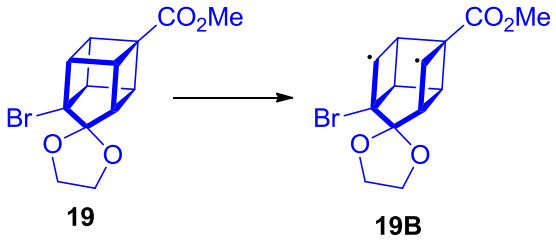
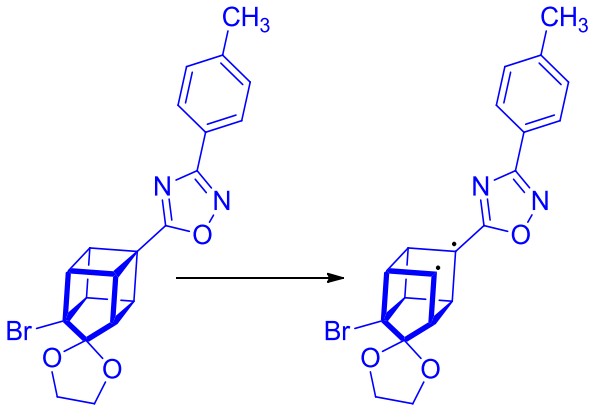
#	Decomposition pathways	LB[b]	LBL (Å)[c]	SLB[d]	SLBL (Å)[e]	BO[f]	HOF[g] kcal/mol	BDE[h] (kcal/mol)
8A	 8 8A	8,13	1.5794	---	---	0.9733	24.31	50.04
8B	 8 8B	---	---	1,4	1.5786	0.9555	24.34	50.08
13A	 13 13A	1,7	1.5805	---	---	0.9633	69.35	49.24

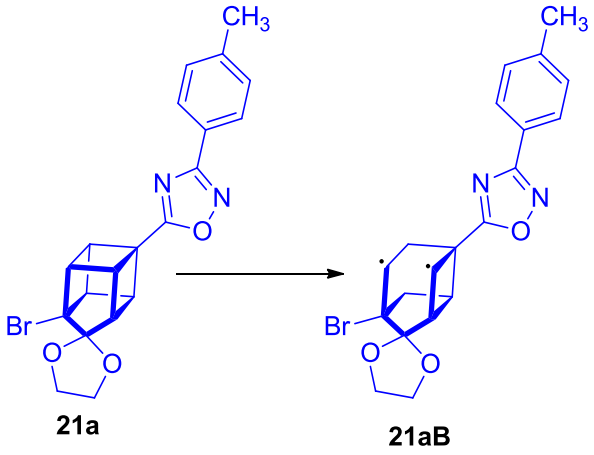
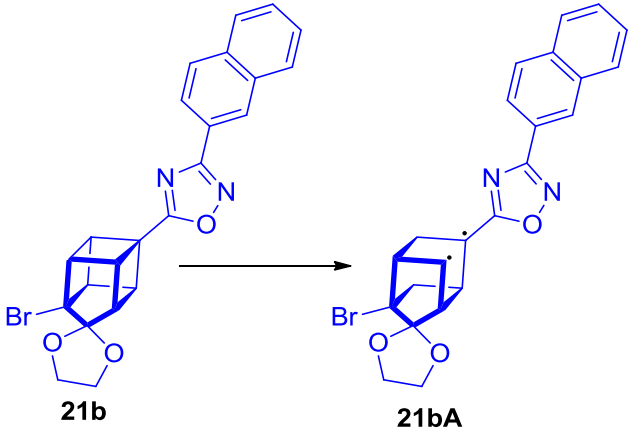
13B		---	---	3,6	1.5791	0.9669	70.05	49.95
14A		8,13	1.5785	---	---	0.9733	143.66	51.03
14B		---	---	1,4	1.5783	0.9528	143.72	51.08
15A		1,4	1.5807	---	---	0.9525	188.96	50.07

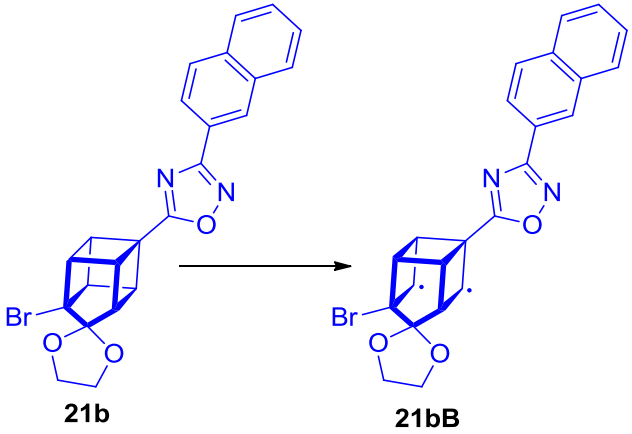
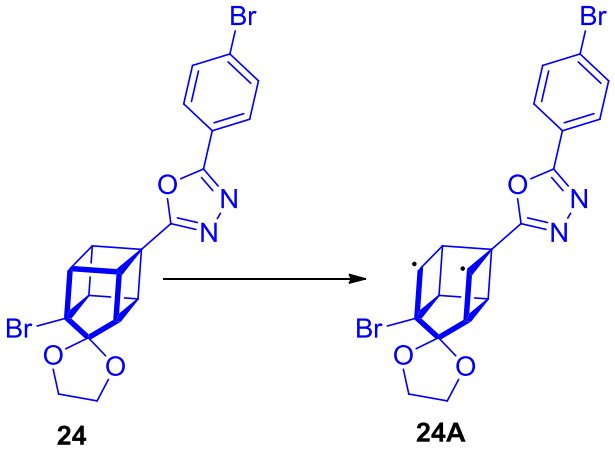
15B		---	---	8,13	1.5779	0.9766	189.20	50.31
15C		---	---	---	---	---	183.43	44.65
15D		---	---	---	---	---	135.21	107.86

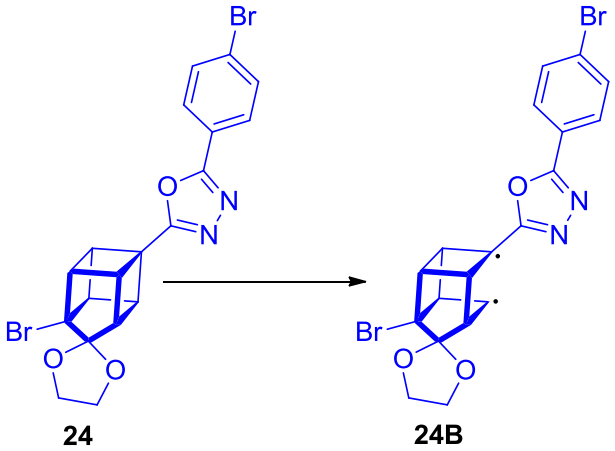
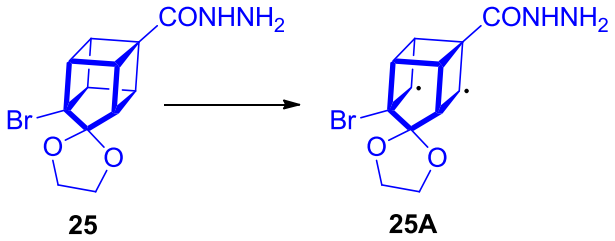
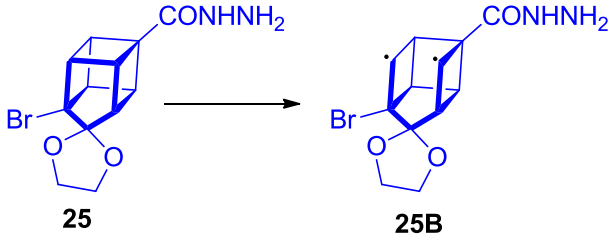
16A		1,7	1.5814	---	---	0.9666	156.01	50.60
16B		---	---	2,3	1.5797	0.9423	134.51	29.10
18A		3,6	1.5802	---	---	0.9759	98.69	50.54

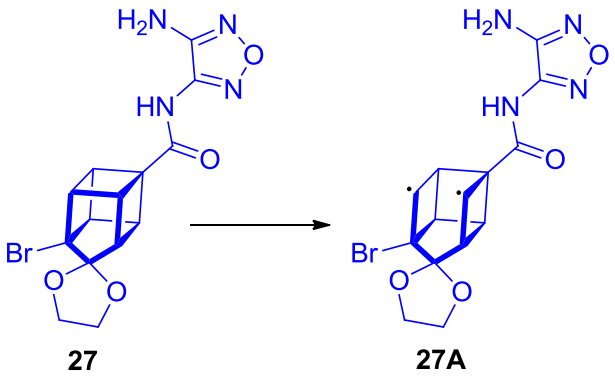
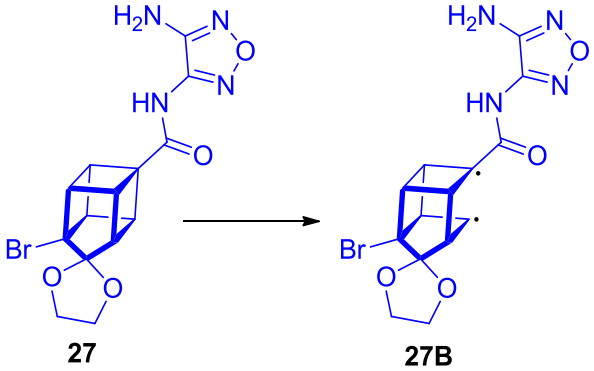
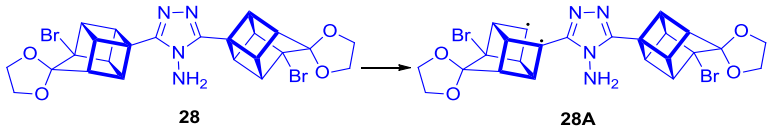
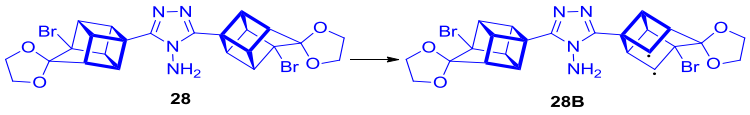
18B		---	---	1,7	1.5799	0.9740	98.67	50.52
18aA		1,7	1.5795	---	---	0.9632	103.47	49.60
18aB		---	---	3,6	1.5791	0.9670	103.56	49.69
19A		2,3	1.5824	---	---	0.9436	-352.47	33.40

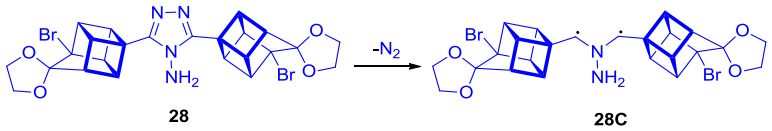
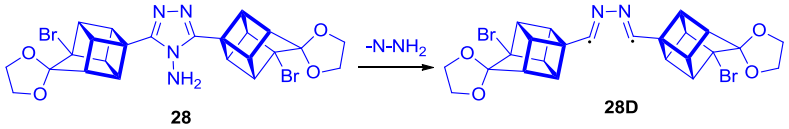
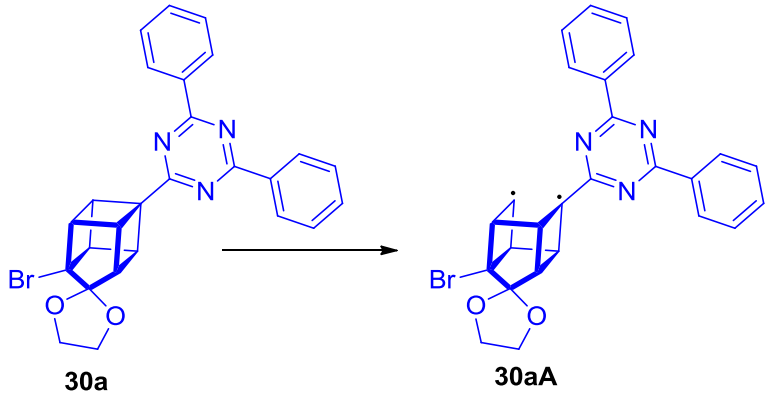
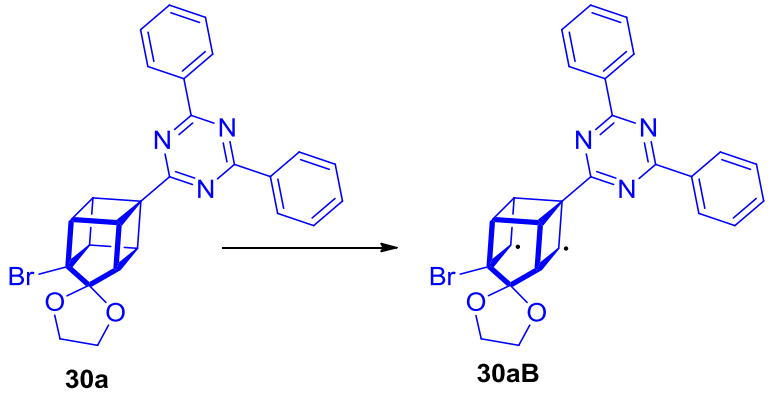
19B	 **19** **19B**	---	---	1,7	1.5817	0.9669	-335.75	50.12
21aA	 **21a** **21aA**	1,2	1.5794	---	---	0.9638	136.09	30.35

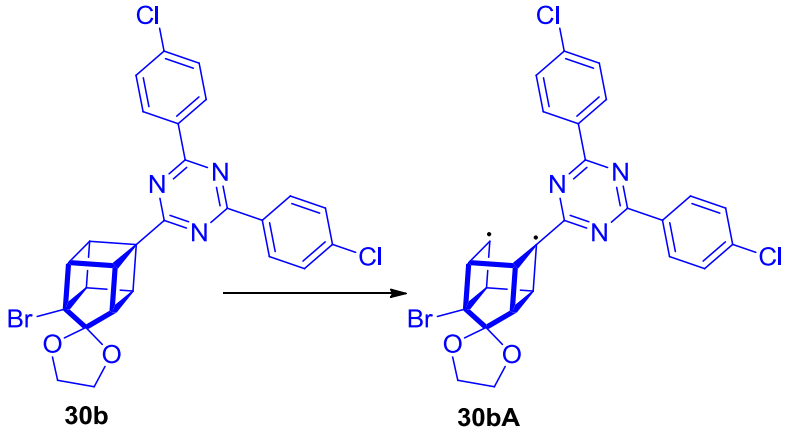
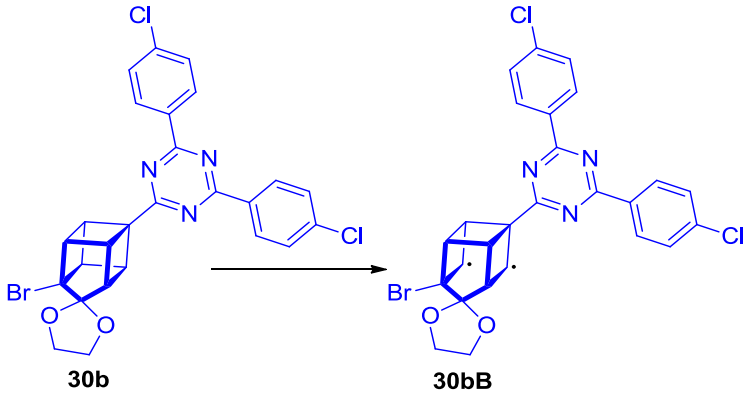
21aB		---	---	1,7	1.5791	0.9662	156.02	50.28
21bA		1,2	1.5799	---	---	0.9638	163.41	30.45

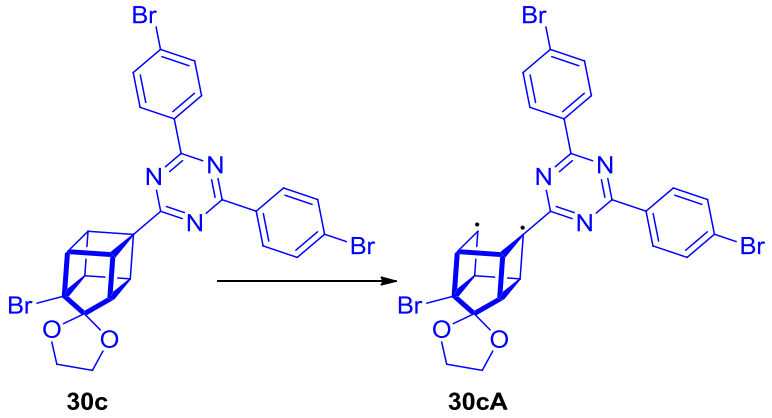
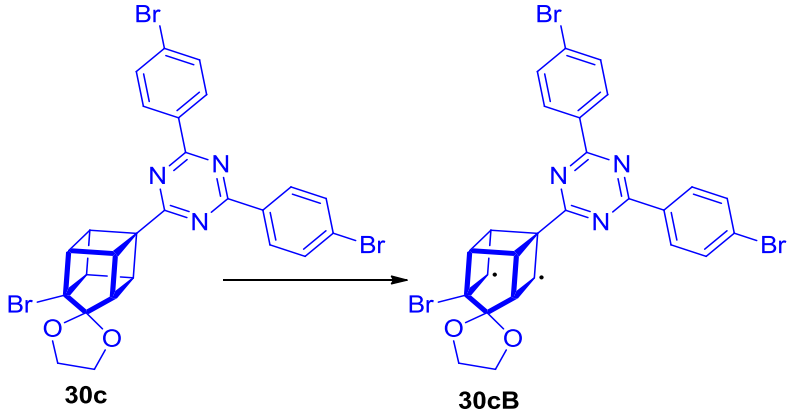
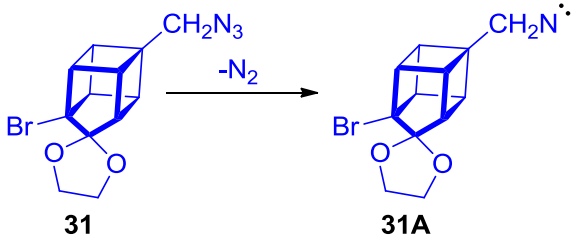
21bB	 **21b** **21bB**	---	---	3,6	1.5789	0.9658	183.30	50.34
24A	 **24** **24A**	1,7	1.5814	---	---	0.9666	164.36	50.60

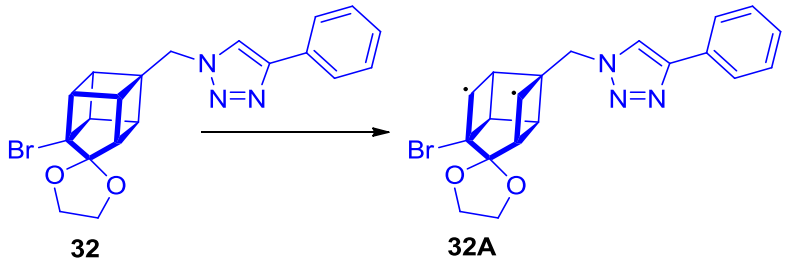
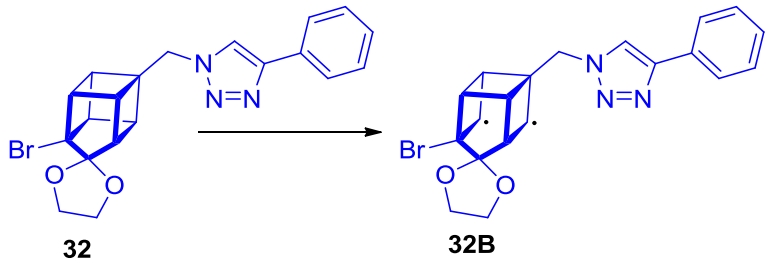
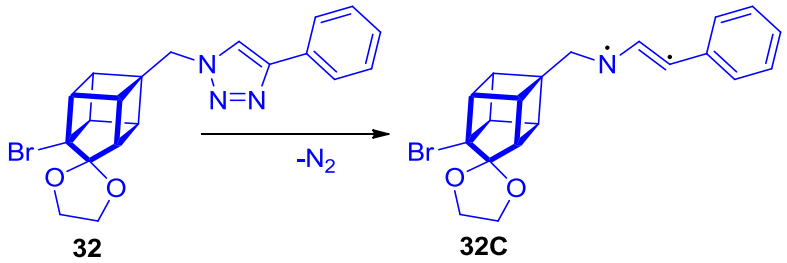
24B		---	---	2,3	1.5800	0.9421	142.88	29.10
25A		3,6	1.5788	---	---	0.9671	456.29	48.91
25B		---	---	1,7	1.5786	0.9621	457.29	50.54

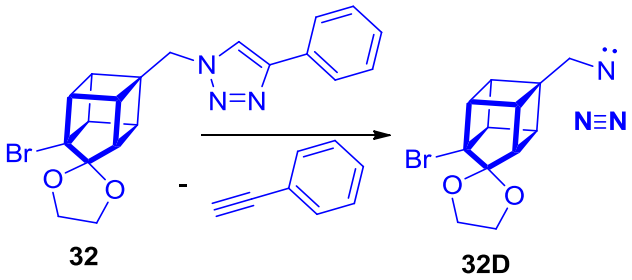
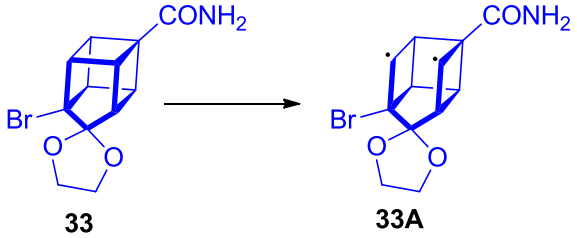
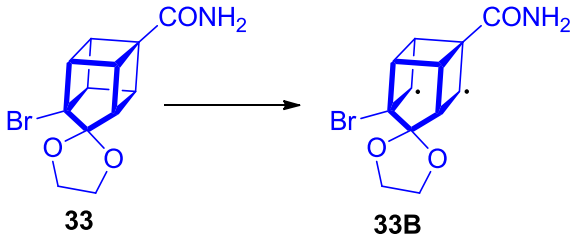
27A		8,13	1.5794	---	---	0.9646	120.97	48.91
27B		---	---	1,2	1.5782	0.9529	114.07	42.01
28A		2,3	1.5823	---	---	0.8783	239.82	31.10
28B		---	---	1,7	1.5793	0.9608	260.11	51.40

28C		---	---	---	---	---	301.92	93.32
28D		---	---	---	---	---	281.15	148.15
30aA		2,8	1.5802	---	---	0.9528	204.51	38.62
30aB		---	---	3,6	1.5790	0.9661	215.58	49.69

30bA		2,8	1.5809	---	---	0.9531	200.96	38.36
30bB		---	---	3,6	1.5789	0.9654	212.32	49.72

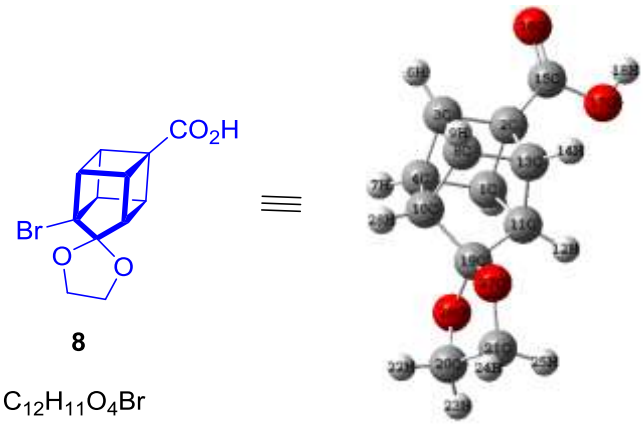
30cA		2,8	1.5809	---	---	0.9531	220.02	38.34
30cB		---	---	3,6	1.5790	0.9654	231.40	49.72
31A[i]		---	---	---	---	---	139.21	5.10

32A		1,7	1.5796	---	---	0.9630	205.20	50.24
32B		---	---	3,6	1.5794	0.9667	205.60	50.65
32C		---	---	---	---	---	190.56	35.72

32D[i]		---	---	---	---	---	140.04	133.94
33A		1,7	1.5789	---	---	0.9630	67.49	50.54
33B		---	---	3,6	1.5783	0.9687	65.84	48.90

[a]Method: B3LYP/6-311++G (d,p); [b]Longest bond (LB), numbering taken from optimized geometry; [c]Longest bond length (LBL); [d]Second longest bond (SLB), numbering taken from optimized geometry; [e]Second longest bond length (SLBL); [f]Bond order (BO). [g]Heat of Formation (HOF); [h]Bond dissociation energy (BDE); [i] Loss of N_2 via N-N bond cleavage to form nitrene is the overwhelmingly preferred pathway.

Table S4. Atomic coordinates for optimized structure of compound **8** obtained using the B3LYP/6-311++G(d,p) level of theory



8

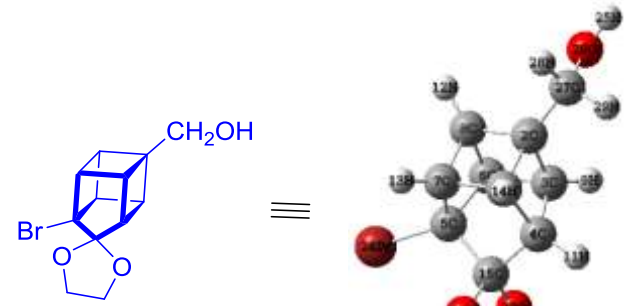
$C_{12}H_{11}O_4Br$

optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.823486	2.314801	0.691627
2	C	0.157983	1.802746	-0.643601
3	C	-1.102676	2.667917	-0.369168
4	C	-0.465321	3.183838	0.967023
5	H	1.199563	1.661489	1.474394
6	H	-2.133603	2.352936	-0.501611
7	H	-0.932519	3.145984	1.946725
8	C	-0.420866	3.895084	-1.066905
9	H	-0.848020	4.481606	-1.875064
10	C	-0.103247	4.541316	0.308085
11	C	1.761145	3.276607	-0.091803
12	H	2.816851	3.023098	-0.155347
13	C	0.869288	3.026047	-1.340243
14	H	1.285621	2.997537	-2.343674
15	C	0.184260	0.404462	-1.131688

16	O	-0.780250	-0.275865	-1.387095
17	O	1.457791	-0.056619	-1.268851
18	H	1.397576	-0.969814	-1.587701
19	C	1.433440	4.693673	0.396139
20	C	2.464504	6.259408	1.732585
21	C	2.889510	6.475259	0.284988
22	H	1.694770	6.972416	2.041638
23	H	3.291269	6.271401	2.443314
24	H	2.834037	7.513518	-0.043010
25	H	3.893842	6.079848	0.092584
26	O	1.928515	4.930151	1.698091
27	O	1.913005	5.724173	-0.443480
28	Br	-1.175198	6.084842	0.830083

Table S5. Atomic coordinates for optimized structure of compound **13** obtained using the B3LYP/6-311++G(d,p) level of theory



13

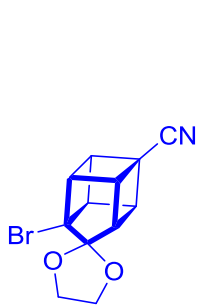
$C_{12}H_{13}O_3Br$

optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.056669	-0.659057	-0.287511

2	C	1.425173	-1.171159	-0.202620
3	C	1.851937	0.338582	-0.175738
4	C	0.425018	0.785997	-0.613933
5	C	0.302644	0.758036	1.668295
6	C	1.766513	0.318227	1.400901
7	C	-0.141752	-0.679854	1.290535
8	C	1.339357	-1.187812	1.359267
9	H	2.747948	0.738515	-0.643604
10	H	2.586548	0.726364	1.984363
11	H	0.288938	1.159720	-1.627142
12	H	1.713305	-1.963538	2.023036
13	H	-0.998414	-1.141283	1.773953
14	H	-0.851496	-1.135828	-0.858563
15	C	-0.114154	1.685578	0.503816
16	C	-1.754003	3.285307	0.238064
17	C	-0.493531	3.936946	0.794343
18	H	-1.873564	3.482420	-0.834110
19	H	-2.666349	3.564344	0.766249
20	H	-0.213973	4.862522	0.290046
21	H	-0.565644	4.105389	1.872898
22	O	-1.513866	1.893497	0.462873
23	O	0.508719	2.954747	0.506529
24	Br	-0.118382	1.367517	3.477311
25	H	3.769582	-3.062466	-1.323771
26	O	3.396197	-2.364572	-0.777306
27	C	2.005602	-2.225978	-1.088273
28	H	1.476685	-3.177059	-0.927026
29	H	1.871137	-1.940461	-2.142570

Table S6. Atomic coordinates for optimized structure of compound **14** obtained using the B3LYP/6-311++G(d,p) level of theory



14

$C_{12}H_{10}NO_2Br$

≡

optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.918422	2.423166	0.883943
2	C	0.309052	1.693212	-0.373930
3	C	-1.012706	2.527871	-0.221470
4	C	-0.417293	3.250881	1.031601
5	H	1.319228	1.904525	1.750192
6	H	-2.022273	2.137057	-0.311655
7	H	-0.894173	3.320338	2.004520
8	C	-0.393113	3.678127	-1.081797
9	H	-0.847109	4.120728	-1.963222
10	C	-0.124654	4.524327	0.192140
11	C	1.808461	3.317468	-0.025929
12	H	2.877037	3.115653	-0.053034
13	C	0.943902	2.852832	-1.232884
14	H	1.368696	2.709615	-2.222371
15	C	0.417847	0.296282	-0.656753
16	N	0.501172	-0.834176	-0.885461

17	C	1.401572	4.769098	0.260514
18	C	2.347452	6.553114	1.366774
19	C	2.771278	6.584538	-0.096657
20	H	1.544993	7.266773	1.573886
21	H	3.168439	6.699844	2.068855
22	H	2.670983	7.563079	-0.566364
23	H	3.792867	6.211527	-0.233697
24	O	1.869824	5.208659	1.517557
25	O	1.832177	5.695979	-0.712989
26	Br	-1.279614	6.063797	0.495121

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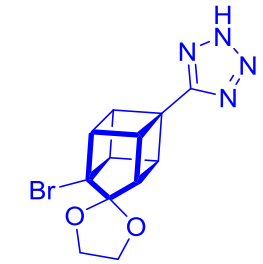
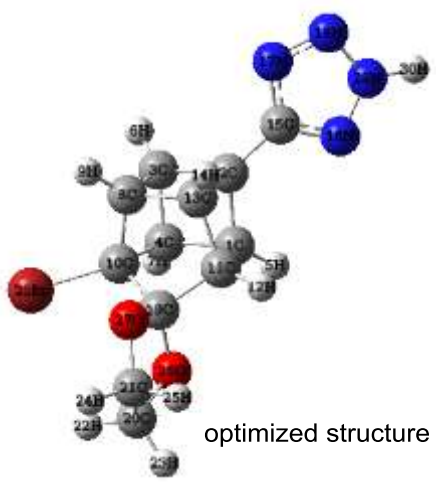
Table S7. Atomic coordinates for optimized structure of compound **15** obtained using the B3LYP/6-311++G(d,p) level of theory



15

$C_{12}H_{11}N_4O_2Br$

≡

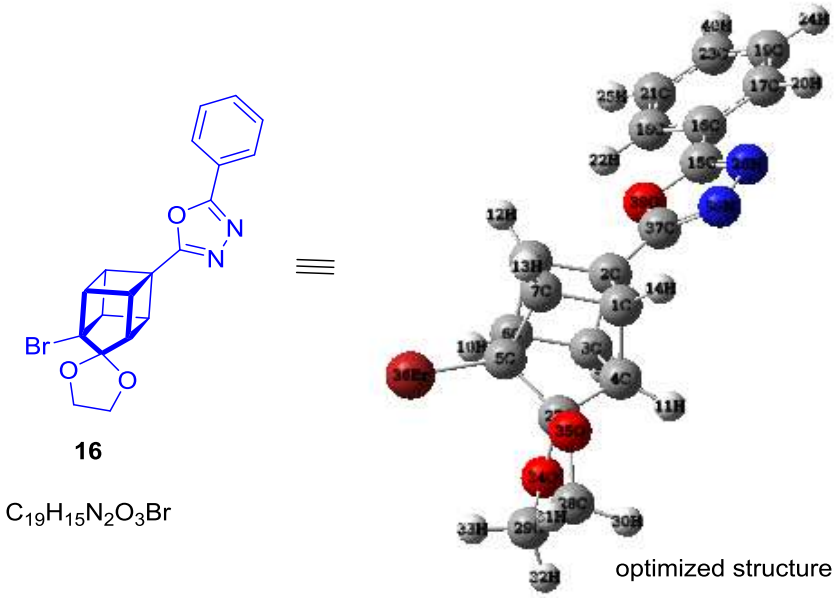


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.587734	1.671793	-0.490938
2	C	0.107423	0.831047	-1.719316
3	C	-0.816962	2.011302	-2.183889

4	C	-0.350095	2.857865	-0.951562
5	H	0.541979	1.332864	0.540256
6	H	-1.838093	1.919290	-2.544587
7	H	-1.003883	3.333547	-0.226327
8	C	0.372424	2.650887	-2.972751
9	H	0.353375	2.942486	-4.018586
10	C	0.587782	3.704551	-1.852904
11	C	1.943661	1.985982	-1.190045
12	H	2.837660	1.489583	-0.818112
13	C	1.310875	1.468120	-2.514397
14	H	1.894644	0.940014	-3.263819
15	C	-0.231745	-0.595379	-1.691915
16	N	-0.164970	-1.369414	-0.610314
17	N	-0.656305	-1.295163	-2.785486
18	N	-0.858877	-2.521530	-2.392902
19	C	2.025854	3.511825	-1.318363
20	C	3.221204	5.192981	-0.295362
21	C	3.994937	4.691276	-1.508530
22	H	2.697390	6.129906	-0.506184
23	H	3.827965	5.298786	0.604426
24	H	4.377194	5.485434	-2.150294
25	H	4.814479	4.022633	-1.219439
26	O	2.281223	4.133643	-0.074786
27	O	2.998224	3.968488	-2.237388
28	Br	0.025300	5.534565	-2.232784
29	N	-0.559540	-2.538439	-1.101926
30	H	-0.631570	-3.375804	-0.541095

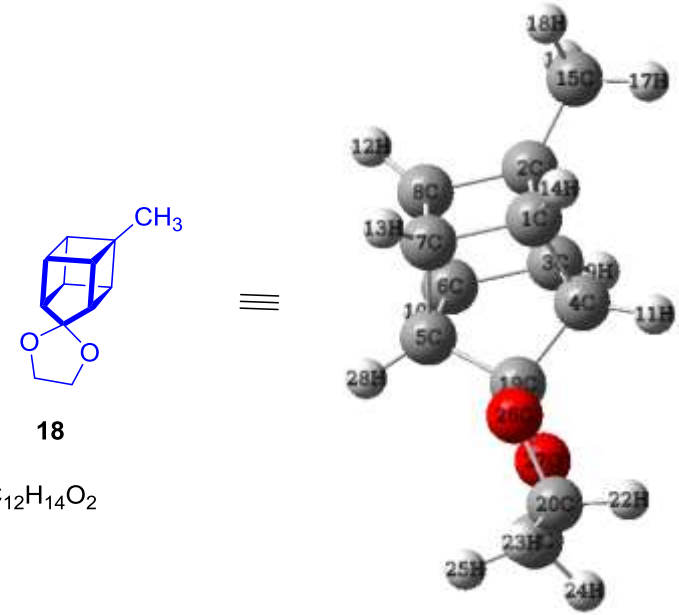
Table S8. Atomic coordinates for optimized structure of compound **16** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.938883	-0.165115	-0.310914
2	C	2.068785	-0.780821	0.575660
3	C	2.307304	0.678779	1.130852
4	C	1.440956	1.278944	-0.014387
5	C	-0.070965	0.879824	1.655535
6	C	1.265508	0.399087	2.281590
7	C	-0.104125	-0.443595	0.844640
8	C	1.037420	-1.046847	1.730594
9	H	3.281482	1.086253	1.388827
10	H	1.522542	0.650691	3.306292
11	H	1.948167	1.818193	-0.811451

12	H	0.965428	-1.949764	2.331659
13	H	-1.045152	-0.931173	0.607844
14	H	0.714484	-0.497184	-1.319970
15	C	4.804145	-2.971245	0.139818
16	C	5.929175	-3.699431	0.715091
17	C	6.736765	-4.484771	-0.120723
18	C	6.213113	-3.626474	2.085132
19	C	7.811619	-5.185236	0.412462
20	H	6.509295	-4.534615	-1.178222
21	C	7.291730	-4.332005	2.610634
22	H	5.590990	-3.020539	2.731980
23	C	8.092495	-5.111866	1.778018
24	H	8.432698	-5.790742	-0.237603
25	H	7.506107	-4.272633	3.671521
26	N	4.400778	-2.946958	-1.092424
27	C	0.276237	2.012637	0.662218
28	C	-0.901017	3.733362	-0.314418
29	C	-0.303553	4.215965	1.001971
30	H	-0.323600	4.085773	-1.177226
31	H	-1.951951	3.992067	-0.445220
32	H	0.196379	5.182508	0.932975
33	H	-1.047320	4.235813	1.803893
34	O	0.692104	3.219330	1.269123
35	O	-0.802947	2.310168	-0.199071
36	Br	-1.549698	1.208601	2.884807
37	C	3.095516	-1.686112	0.073142
38	N	3.287687	-2.112193	-1.134717
39	O	4.022801	-2.191168	0.945035
40	H	8.931715	-5.660594	2.190099

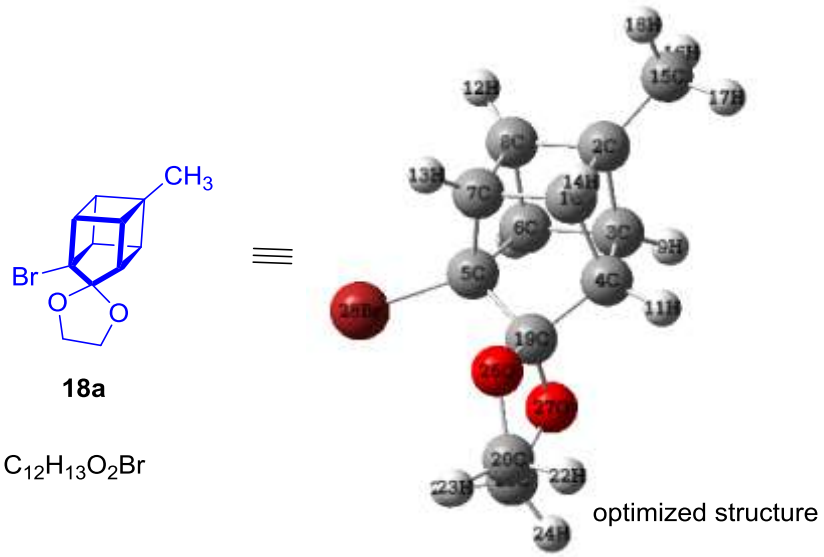
Table S9. Atomic coordinates for optimized structure of compound **18** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.045859	-0.619307	-0.010834
2	C	1.484848	-0.980843	-0.015977
3	C	1.748647	0.563142	-0.158368
4	C	0.253407	0.825921	-0.504257
5	C	0.314653	1.018606	1.791010
6	C	1.790090	0.694372	1.415781
7	C	-0.004041	-0.488734	1.563133
8	C	1.522425	-0.844922	1.543511
9	H	2.552617	1.003935	-0.746318
10	H	2.619269	1.226697	1.877304

11	H	-0.001630	1.088169	-1.529877
12	H	2.022324	-1.515708	2.241898
13	H	-0.760525	-1.001017	2.154014
14	H	-0.827153	-1.224113	-0.469359
15	C	2.126007	-2.057958	-0.844108
16	H	3.211689	-2.076268	-0.697533
17	H	1.936066	-1.901916	-1.912012
18	H	1.736639	-3.046670	-0.576971
19	C	-0.274034	1.763951	0.588202
20	C	-2.079382	3.165282	0.268790
21	C	-0.867737	3.991008	0.681215
22	H	-2.249420	3.215637	-0.814208
23	H	-2.998658	3.426360	0.794899
24	H	-0.716550	4.891976	0.085147
25	H	-0.906663	4.257070	1.745222
26	O	-1.695891	1.847966	0.660709
27	O	0.211459	3.094452	0.421802
28	H	0.112279	1.443876	2.772802

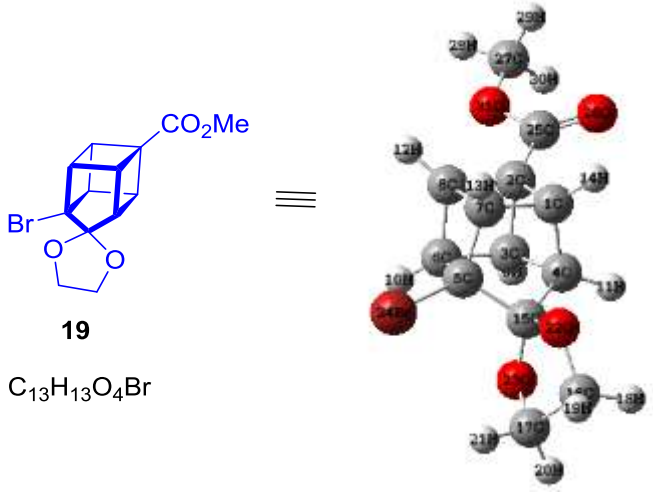
Table S10. Atomic coordinates for optimized structure of compound **18a** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.041731	-0.624814	-0.015383
2	C	1.489009	-0.983917	-0.016762
3	C	1.753796	0.559505	-0.155725
4	C	0.259394	0.821479	-0.508767
5	C	0.314194	1.005025	1.768332
6	C	1.791752	0.686958	1.417816
7	C	-0.004066	-0.499169	1.558635
8	C	1.522381	-0.851251	1.544711
9	H	2.560532	1.005420	-0.734853
10	H	2.602477	1.232150	1.892959
11	H	0.010196	1.079573	-1.536399
12	H	2.018845	-1.519415	2.246238
13	H	-0.765518	-0.993463	2.155511

14	H	-0.824972	-1.227771	-0.471603
15	C	2.133387	-2.059156	-0.844064
16	H	3.218220	-2.076504	-0.693268
17	H	1.947160	-1.902042	-1.912192
18	H	1.743714	-3.047990	-0.579029
19	C	-0.282351	1.771070	0.565416
20	C	-2.090094	3.175950	0.291517
21	C	-0.864217	3.996584	0.675475
22	H	-2.309020	3.250395	-0.780539
23	H	-2.984104	3.421214	0.865823
24	H	-0.717755	4.885978	0.061626
25	H	-0.873742	4.270946	1.734584
26	O	-1.694399	1.843188	0.626128
27	O	0.208687	3.087718	0.402861
28	Br	-0.030129	1.746097	3.544187

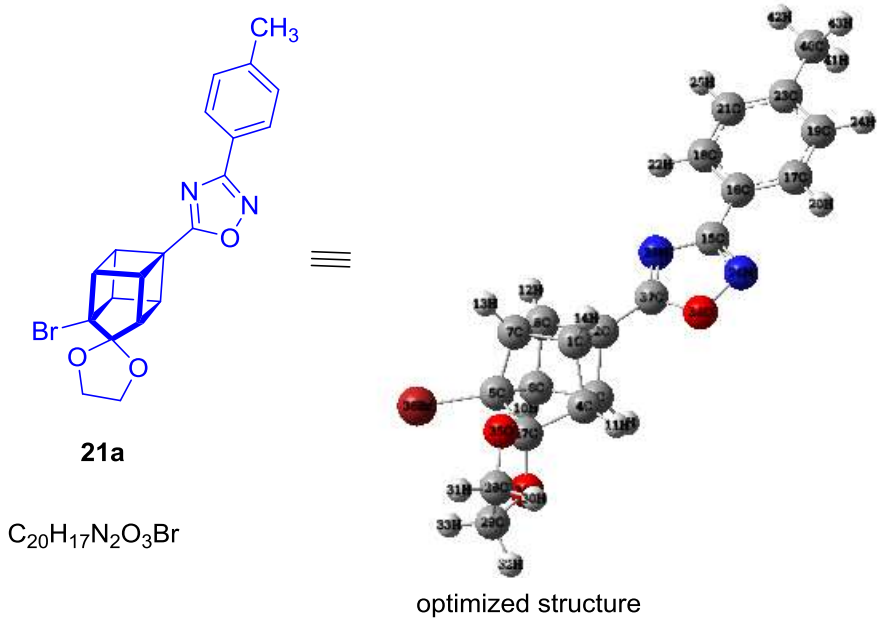
Table S11. Atomic coordinates for optimized structure of compound **19** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.198179	-0.647122	-0.093952
2	C	1.285371	-1.135606	-0.072338
3	C	1.688867	0.391357	-0.170416
4	C	0.229075	0.781490	-0.540627
5	C	0.262968	0.899215	1.743682
6	C	1.715775	0.471185	1.404115
7	C	-0.171523	-0.568224	1.485591
8	C	1.322927	-1.041435	1.486958
9	H	2.543150	0.760404	-0.732128
10	H	2.563272	0.934955	1.900217
11	H	0.023561	1.081003	-1.565892
12	H	1.759172	-1.770410	2.164206
13	H	-0.977709	-1.020948	2.055634
14	H	-1.006710	-1.179463	-0.587199
15	C	-0.249062	1.743789	0.553454
16	C	-1.926367	3.299072	0.281104
17	C	-0.646218	4.005812	0.710245
18	H	-2.112469	3.411588	-0.793497
19	H	-2.810464	3.604896	0.841113
20	H	-0.412490	4.894466	0.123237
21	H	-0.655433	4.252506	1.776025
22	O	-1.649064	1.930873	0.595984
23	O	0.354122	3.016588	0.435203
24	Br	-0.045257	1.614294	3.533676
25	C	1.848292	-2.179140	-0.966502
26	O	1.365311	-2.529847	-2.018753
27	C	3.669656	-3.658243	-1.294304
28	H	4.567318	-3.935093	-0.745804
29	H	3.027193	-4.527069	-1.443714

30	H	3.927842	-3.233653	-2.265525
31	O	3.006174	-2.676670	-0.475457

Table S12. Atomic coordinates for optimized structure of compound **21a** obtained using the B3LYP/6-311++G(d,p) level of theory

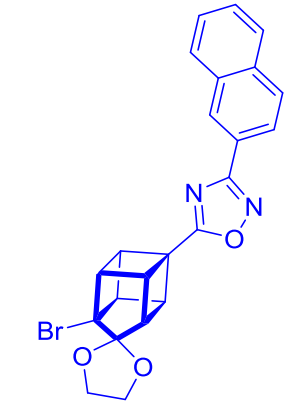


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.186202	-0.221006	0.002163
2	C	2.451638	-0.460645	0.916304
3	C	2.445646	1.099161	1.151929
4	C	1.437793	1.313404	-0.012931
5	C	0.095076	0.999251	1.812846
6	C	1.521433	0.878482	2.412870

7	C	0.263441	-0.442876	1.264194
8	C	1.532389	-0.667140	2.154974
9	H	3.342544	1.704828	1.250958
10	H	1.775565	1.364174	3.350325
11	H	1.807095	1.763510	-0.931723
12	H	1.650674	-1.437601	2.911021
13	H	-0.585165	-1.116652	1.191175
14	H	0.979840	-0.775777	-0.909315
15	C	5.177879	-2.659927	0.376986
16	C	6.039979	-3.813574	0.661201
17	C	7.141767	-4.111300	-0.153508
18	C	5.764683	-4.637766	1.756450
19	C	7.943010	-5.208532	0.129255
20	H	7.360247	-3.480293	-1.006419
21	C	6.575671	-5.735789	2.030102
22	H	4.912804	-4.413664	2.386088
23	C	7.677723	-6.040485	1.226448
24	H	8.790132	-5.427011	-0.513227
25	H	6.345369	-6.366899	2.882318
26	N	5.376763	-1.850839	-0.635418
27	C	0.191457	1.960420	0.605720
28	C	-1.301496	3.241686	-0.587629
29	C	-0.744730	4.065820	0.566974
30	H	-0.824327	3.500992	-1.540035
31	H	-2.385130	3.299196	-0.691672
32	H	-0.418258	5.065689	0.279509
33	H	-1.450039	4.128369	1.400914
34	O	0.414492	3.312785	0.949134
35	O	-0.960626	1.904137	-0.208952
36	Br	-1.364232	1.308890	3.068488
37	C	3.616447	-1.269065	0.561544
38	O	4.336134	-0.914419	-0.520984
39	N	4.081566	-2.327599	1.153504

40	C	8.570933	-7.216369	1.535024
41	H	9.508419	-6.885766	1.995269
42	H	8.090545	-7.911190	2.226729
43	H	8.832289	-7.766410	0.627103

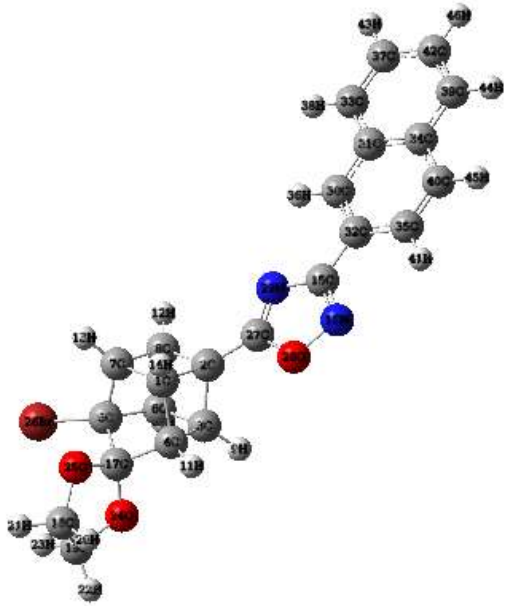
Table S13. Atomic coordinates for optimized structure of compound **21b** obtained using the B3LYP/6-311++G(d,p) level of theory



21b

$C_{23}H_{17}N_2O_3Br$

≡



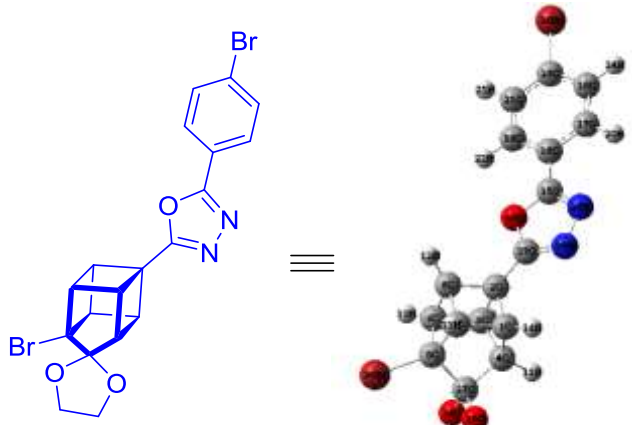
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.078127	-0.003752	-0.282008
2	C	2.186597	-0.009599	0.843739
3	C	2.107817	1.564261	0.781892
4	C	1.294733	1.513849	-0.542607

5	C	-0.315799	1.463411	1.081935
6	C	0.998785	1.526084	1.905044
7	C	-0.029117	-0.043081	0.842231
8	C	1.085367	-0.038247	1.943098
9	H	2.963064	2.223811	0.903026
10	H	1.088958	2.184352	2.764072
11	H	1.795473	1.810125	-1.461644
12	H	1.098234	-0.653527	2.837804
13	H	-0.839792	-0.761707	0.766228
14	H	1.033608	-0.723349	-1.095214
15	C	4.999276	-2.146446	1.121810
16	N	5.356294	-1.493116	0.042437
17	C	-0.049431	2.195571	-0.254355
18	C	-1.372359	3.158964	-1.872783
19	C	-1.028423	4.202630	-0.817177
20	H	-0.760413	3.275949	-2.774882
21	H	-2.427639	3.134326	-2.145196
22	H	-0.694027	5.155194	-1.228952
23	H	-1.855085	4.365525	-0.119463
24	O	0.081968	3.597478	-0.140766
25	O	-1.052915	1.929810	-1.212201
26	Br	-1.964646	1.913444	2.021012
27	C	3.408682	-0.810544	0.823719
28	O	4.298014	-0.594829	-0.166285
29	N	3.781868	-1.746349	1.643471
30	C	5.382396	-3.864620	2.847470
31	C	6.157883	-4.891124	3.441758
32	C	5.821640	-3.205535	1.717830
33	C	5.726075	-5.583305	4.603965
34	C	7.414209	-5.241187	2.854365
35	C	7.071784	-3.556037	1.134689
36	H	4.429812	-3.592621	3.286391
37	C	6.499509	-6.574548	5.159666

38	H	4.772767	-5.315828	5.047545
39	C	8.187968	-6.267912	3.452219
40	C	7.840116	-4.544415	1.690547
41	H	7.404571	-3.030350	0.248534
42	C	7.742142	-6.919670	4.578439
43	H	6.159624	-7.096538	6.046977
44	H	9.140939	-6.532817	3.006100
45	H	8.792543	-4.808339	1.242917
46	H	8.343240	-7.703127	5.026111

Table S14. Atomic coordinates for optimized structure of compound **24** obtained using the B3LYP/6-311++G(d,p) level of theory



24

$C_{19}H_{14}N_2O_3Br_2$

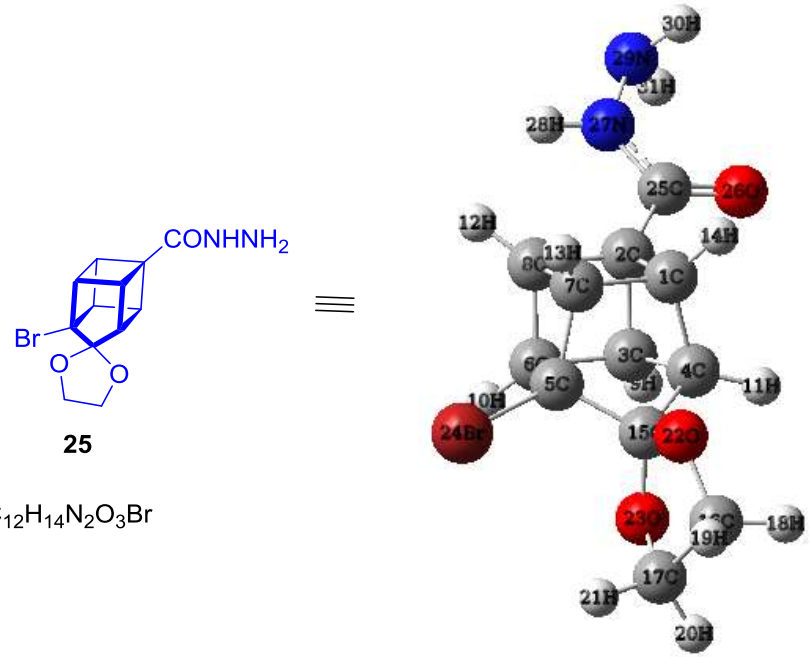
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.938781	-0.166019	-0.308058
2	C	2.073501	-0.777103	0.575687
3	C	2.310034	0.684550	1.127178

4	C	1.437915	1.279896	-0.016128
5	C	-0.066903	0.879770	1.660239
6	C	1.273315	0.404103	2.282225
7	C	-0.099106	-0.445254	0.851908
8	C	1.047203	-1.043547	1.734985
9	H	3.284121	1.095068	1.380649
10	H	1.533464	0.658388	3.305455
11	H	1.940726	1.819043	-0.816018
12	H	0.979824	-1.945533	2.337991
13	H	-1.039425	-0.936227	0.619456
14	H	0.711573	-0.500608	-1.315656
15	C	4.809735	-2.964120	0.136684
16	C	5.933067	-3.694650	0.709266
17	C	6.743234	-4.475481	-0.127366
18	C	6.217273	-3.632115	2.078934
19	C	7.818547	-5.181947	0.395108
20	H	6.521686	-4.522166	-1.186263
21	C	7.292702	-4.338081	2.609029
22	H	5.597581	-3.031695	2.733059
23	C	8.084287	-5.107401	1.761586
24	H	8.443268	-5.784062	-0.251646
25	H	7.510183	-4.289523	3.667972
26	N	4.409670	-2.935639	-1.096248
27	C	0.273490	2.011667	0.663415
28	C	-0.911876	3.727095	-0.312440
29	C	-0.310694	4.214164	1.000606
30	H	-0.338781	4.079041	-1.178259
31	H	-1.964007	3.982504	-0.439765
32	H	0.186793	5.181627	0.927474
33	H	-1.051373	4.234163	1.805325
34	O	0.688400	3.220318	1.266447
35	O	-0.809440	2.304222	-0.194397
36	Br	-1.541510	1.206173	2.894351

37	C	3.101029	-1.680143	0.071720
38	Br	9.564288	-6.081816	2.485304
39	N	3.296427	-2.101783	-1.137441
40	O	4.027581	-2.188517	0.943862

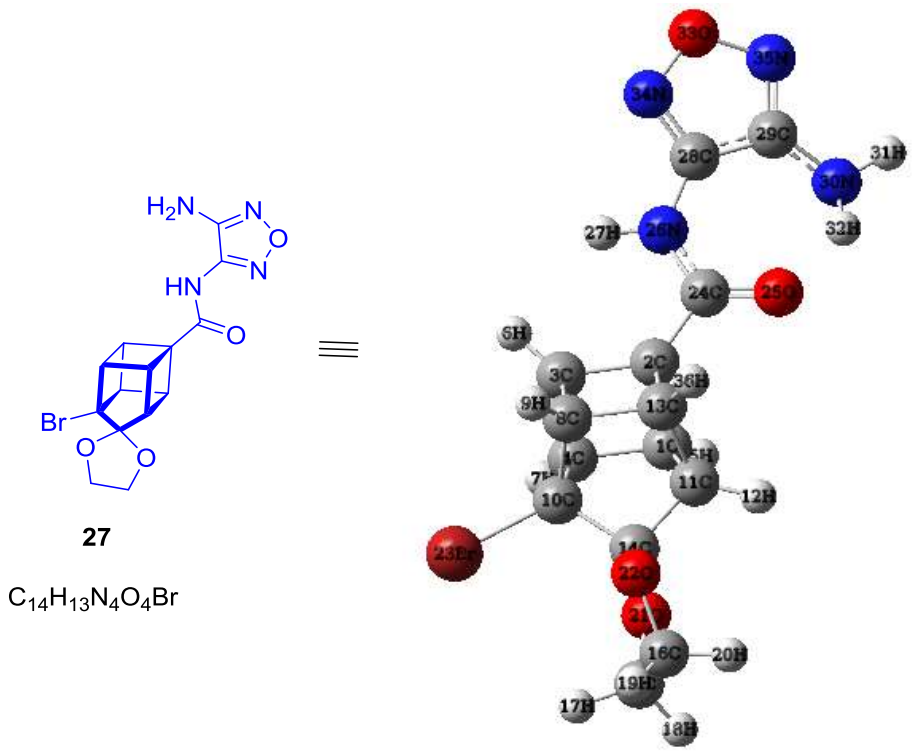
Table S15. Atomic coordinates for optimized structure of compound **25** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.018988	-0.716590	0.002534
2	C	1.549942	-1.058078	-0.116286
3	C	1.774299	0.488678	-0.297228

4	C	0.254904	0.725840	-0.527805
5	C	0.496937	0.932234	1.738220
6	C	1.944346	0.630796	1.265955
7	C	0.186398	-0.578520	1.566172
8	C	1.712085	-0.909235	1.435873
9	H	2.525456	0.919208	-0.954112
10	H	2.787014	1.189586	1.662829
11	H	-0.077048	0.960589	-1.536140
12	H	2.268777	-1.549504	2.118429
13	H	-0.514701	-1.082802	2.225087
14	H	-0.773164	-1.346848	-0.392777
15	C	-0.207793	1.678232	0.581704
16	C	-2.049370	3.045636	0.400520
17	C	-0.817015	3.899110	0.676442
18	H	-2.334781	3.073642	-0.657725
19	H	-2.910557	3.296829	1.020045
20	H	-0.725339	4.766961	0.022563
21	H	-0.764113	4.213085	1.723213
22	O	-1.607601	1.733285	0.761889
23	O	0.254548	2.997626	0.370824
24	Br	0.292588	1.684646	3.526547
25	C	2.078758	-2.072514	-1.076284
26	O	1.829985	-2.031406	-2.274177
27	N	2.858807	-3.052173	-0.527820
28	H	3.081293	-3.055217	0.454148
29	N	3.456150	-4.072768	-1.287461
30	H	2.718039	-4.606228	-1.741329
31	H	3.994505	-3.639637	-2.034695

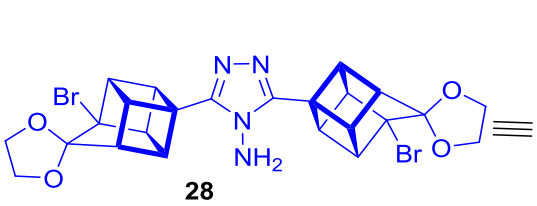
Table S16. Atomic coordinates for optimized structure of compound **27** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.248865	1.243570	-1.542881
2	C	-0.079952	-0.315316	-1.722198
3	C	0.264352	-0.110559	-3.235873
4	C	0.091750	1.437633	-3.070924
5	H	-1.141662	1.709975	-1.134930
6	H	-0.088418	-0.687566	-4.089775

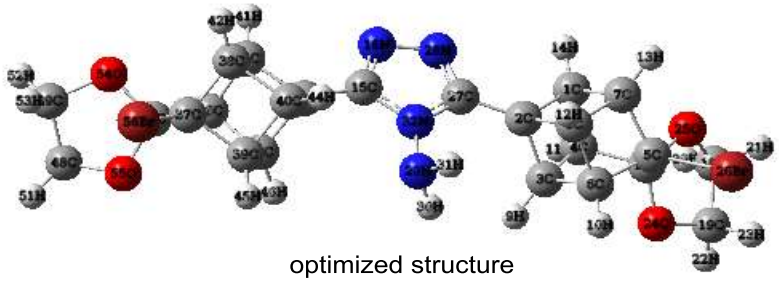
7	H	-0.545576	2.069385	-3.682586
8	C	1.771033	0.102759	-2.864410
9	H	2.607666	-0.440512	-3.293777
10	C	1.631069	1.637094	-3.051797
11	C	1.130831	1.354423	-0.835663
12	H	1.142195	1.537688	0.235900
13	C	1.426864	-0.087682	-1.334774
14	C	1.985423	2.293790	-1.697148
15	C	2.752778	4.456387	-1.483329
16	C	3.773154	3.494134	-0.886100
17	H	3.051160	4.804703	-2.476361
18	H	2.523386	5.309020	-0.843645
19	H	4.799505	3.685859	-1.199344
20	H	3.719260	3.470619	0.208518
21	O	1.576754	3.640090	-1.573711
22	O	3.369759	2.232544	-1.430064
23	Br	2.437167	2.414937	-4.646208
24	C	-0.952587	-1.302549	-1.029609
25	O	-1.015356	-1.363628	0.191906
26	N	-1.688078	-2.115775	-1.862505
27	H	-1.482609	-2.077452	-2.851227
28	C	-2.527852	-3.164590	-1.481244
29	C	-3.364342	-3.341084	-0.318040
30	N	-3.556227	-2.475116	0.725016
31	H	-4.081674	-2.861682	1.496439
32	H	-2.722554	-1.954559	0.980956
33	O	-3.626052	-4.977392	-1.692833
34	N	-2.706188	-4.169695	-2.290201
35	N	-4.013486	-4.468526	-0.463516
36	H	2.008654	-0.788836	-0.742739

Table S17. Atomic coordinates for optimized structure of compound **28** obtained using the B3LYP/6-311++G(d,p) level of theory



28

$C_{24}H_{22}N_4O_4Br_2$



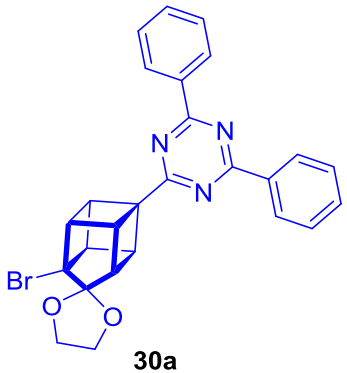
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.253435	0.908238	-0.057763
2	C	0.950918	1.304647	1.423179
3	C	-0.497590	1.699595	0.923531
4	C	-0.026838	1.639267	-0.557770
5	C	-0.749206	-0.490083	-0.134975
6	C	-0.991288	0.229920	1.218898
7	C	0.756370	-0.561832	0.235711
8	C	0.441728	-0.158632	1.714843
9	H	-1.086107	2.537366	1.293200
10	H	-1.915634	0.076061	1.769018
11	H	0.096577	2.577474	-1.094179
12	H	0.666402	-0.767379	2.588642
13	H	1.367968	-1.404507	-0.072327
14	H	2.220266	1.058872	-0.527039
15	C	2.735993	3.289552	3.868761
16	N	3.581631	3.311989	2.865195
17	C	-0.894337	0.576712	-1.244612
18	C	-1.292105	0.546398	-3.509235
19	C	-2.622313	0.624373	-2.769802

20	H	-0.988129	1.522951	-3.904307
21	H	-1.270471	-0.195556	-4.307560
22	H	-3.302394	1.381244	-3.161894
23	H	-3.125286	-0.346426	-2.731895
24	O	-2.218047	1.028409	-1.454520
25	O	-0.390332	0.122579	-2.482236
26	Br	-1.683753	-2.179828	-0.411050
27	C	1.867302	2.128762	2.217140
28	N	3.033869	2.582275	1.826218
29	N	0.523950	2.319635	4.340362
30	H	-0.315704	2.679191	3.896747
31	H	0.415461	1.321424	4.492992
32	N	1.629906	2.551449	3.510969
33	C	2.067862	5.152380	5.729331
34	C	2.914646	3.945035	5.166714
35	C	4.184070	4.782608	5.528883
36	C	3.326907	6.067115	5.728354
37	C	3.351471	5.111238	7.805298
38	C	4.201617	4.122031	6.963885
39	C	2.085576	4.486167	7.159485
40	C	2.924895	3.292974	6.596783
41	H	5.092088	4.785754	4.934033
42	H	5.130526	3.715833	7.353399
43	H	3.395508	6.847973	4.973890
44	H	2.763785	2.243591	6.830768
45	H	1.158867	4.398354	7.718863
46	H	1.118355	5.487273	5.319145
47	C	3.537232	6.512307	7.180249
48	C	3.241861	8.679137	7.897581
49	C	4.666995	8.238012	8.209374
50	H	3.199633	9.316464	7.006098
51	H	2.739900	9.176175	8.728116
52	H	5.427894	8.962959	7.918245

53	H	4.788917	7.971733	9.263601
54	O	4.817208	7.078978	7.380566
55	O	2.576997	7.436510	7.653326
56	Br	3.514439	4.985839	9.747062

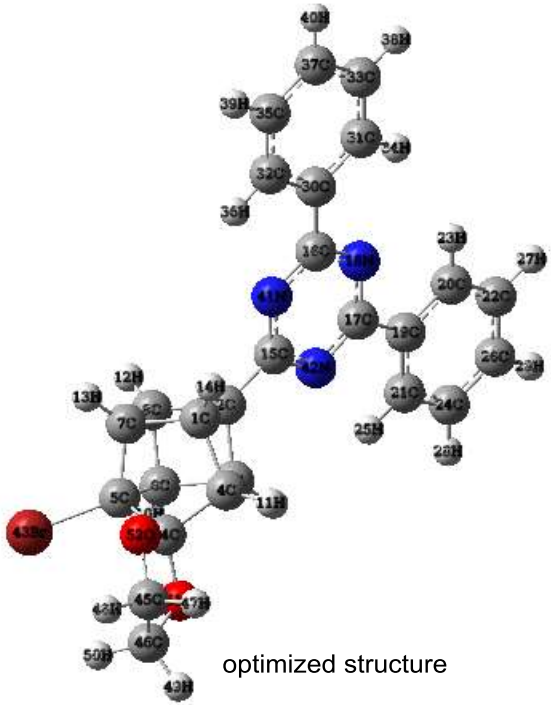
Table S18. Atomic coordinates for optimized structure of compound **30a** obtained using the B3LYP/6-311++G(d,p) level of theory



30a

$C_{26}H_{20}N_3O_2Br$

≡



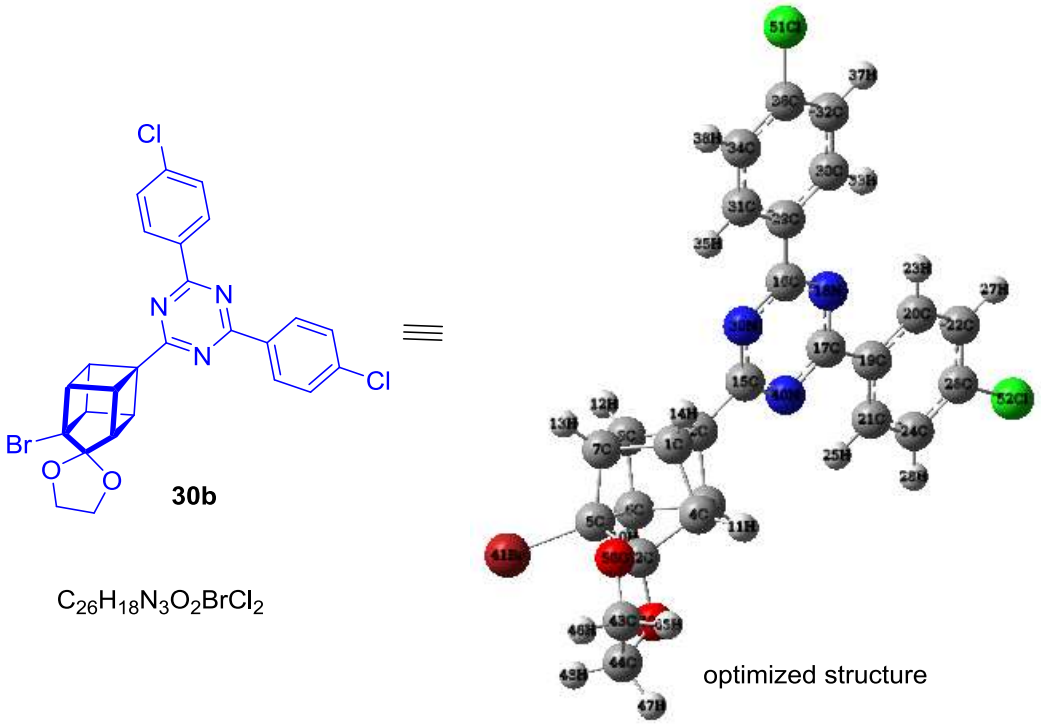
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.124376	-0.804630	-0.118231
2	C	1.397450	-1.080164	-0.367157

3	C	1.581594	0.466270	-0.502625
4	C	0.039657	0.660981	-0.621492
5	C	0.425965	0.816322	1.625909
6	C	1.847153	0.571181	1.050306
7	C	0.145038	-0.698690	1.433853
8	C	1.663470	-0.975554	1.186923
9	H	2.276006	0.941845	-1.189058
10	H	2.699359	1.139885	1.410751
11	H	-0.369225	0.916567	-1.597213
12	H	2.292388	-1.643074	1.770802
13	H	-0.491887	-1.240562	2.126888
14	H	-0.925631	-1.448371	-0.469842
15	C	1.962314	-2.117872	-1.256625
16	C	1.875466	-4.212015	-2.121077
17	C	3.582748	-2.818385	-2.678909
18	N	3.003712	-4.017338	-2.816296
19	C	4.837268	-2.558102	-3.426410
20	C	5.377065	-3.536363	-4.272965
21	C	5.497385	-1.328307	-3.294554
22	C	6.552786	-3.288179	-4.973388
23	H	4.864468	-4.483873	-4.371702
24	C	6.673806	-1.084361	-3.995449
25	H	5.076705	-0.576606	-2.639935
26	C	7.204381	-2.062343	-4.836762
27	H	6.962087	-4.050732	-5.626409
28	H	7.177882	-0.130719	-3.886206
29	H	8.121112	-1.870294	-5.383269
30	C	1.201541	-5.528372	-2.237418
31	C	1.727862	-6.525878	-3.069784
32	C	0.028603	-5.789055	-1.514998
33	C	1.092710	-7.758589	-3.177024
34	H	2.633198	-6.320532	-3.625225
35	C	-0.603044	-7.023472	-1.623888

36	H	-0.373090	-5.015472	-0.874006
37	C	-0.073804	-8.011019	-2.454888
38	H	1.507025	-8.523712	-3.823841
39	H	-1.509061	-7.216305	-1.060496
40	H	-0.567860	-8.972664	-2.539169
41	N	1.315207	-3.287466	-1.327459
42	N	3.095782	-1.833770	-1.907449
43	Br	0.321519	1.517809	3.445798
44	C	-0.376790	1.569516	0.539674
45	C	-2.265497	2.890437	0.562348
46	C	-1.034486	3.763011	0.777693
47	H	-2.642379	2.965988	-0.464603
48	H	-3.075328	3.086048	1.265824
49	H	-1.019847	4.665957	0.166466
50	H	-0.898500	4.022458	1.831777
51	O	0.026028	2.908636	0.331925
52	O	-1.764721	1.573546	0.811266

Table S19. Atomic coordinates for optimized structure of compound **30b** obtained using the B3LYP/6-311++G(d,p) level of theory



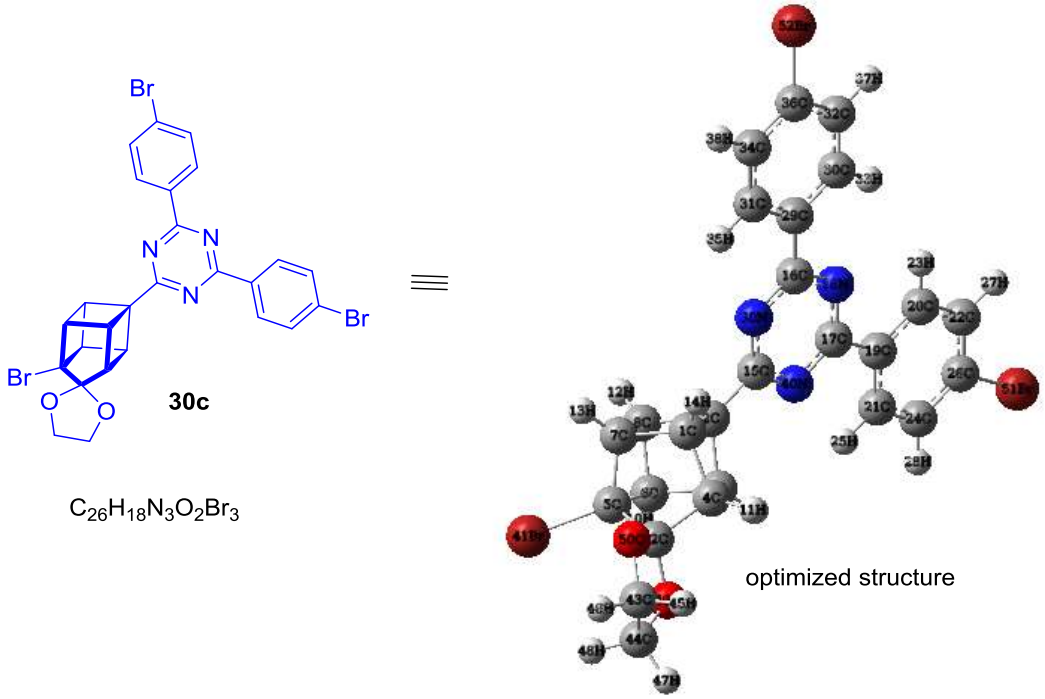
$C_{26}H_{18}N_3O_2BrCl_2$

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.126270	-0.803213	-0.122383
2	C	1.394992	-1.079844	-0.373964
3	C	1.580684	0.466733	-0.506608
4	C	0.038853	0.662924	-0.623318
5	C	0.427984	0.814189	1.624142
6	C	1.848187	0.568569	1.046137
7	C	0.145094	-0.700248	1.429432
8	C	1.662942	-0.977991	1.180727

9	H	2.274429	0.943468	-1.192953
10	H	2.701525	1.135521	1.406565
11	H	-0.370820	0.920654	-1.598113
12	H	2.292045	-1.647408	1.762214
13	H	-0.491442	-1.242654	2.122353
14	H	-0.928950	-1.445080	-0.474237
15	C	1.959111	-2.117192	-1.262647
16	C	1.872559	-4.211295	-2.127919
17	C	3.581980	-2.821465	-2.680709
18	N	3.003130	-4.020292	-2.820502
19	C	4.837507	-2.562314	-3.423840
20	C	5.382465	-3.538858	-4.267994
21	C	5.498251	-1.333458	-3.292619
22	C	6.558946	-3.298564	-4.967256
23	H	4.874371	-4.488211	-4.371048
24	C	6.676034	-1.082200	-3.985871
25	H	5.078637	-0.578601	-2.641077
26	C	7.196346	-2.069230	-4.819169
27	H	6.979344	-4.052858	-5.619858
28	H	7.186949	-0.133447	-3.883690
29	C	1.197005	-5.524980	-2.245339
30	C	1.724639	-6.528104	-3.068973
31	C	0.018074	-5.782241	-1.532641
32	C	1.093306	-7.760720	-3.182094
33	H	2.634645	-6.332095	-3.619925
34	C	-0.621778	-7.011258	-1.637351
35	H	-0.389786	-5.008311	-0.896094
36	C	-0.077218	-7.991228	-2.463541
37	H	1.500900	-8.535479	-3.818630
38	H	-1.531990	-7.210204	-1.086393
39	N	1.311056	-3.286720	-1.336309
40	N	3.095140	-1.836031	-1.911385
41	Br	0.327317	1.510597	3.445377

42	C	-0.375348	1.570145	0.540006
43	C	-2.262309	2.893498	0.569986
44	C	-1.029430	3.763573	0.784590
45	H	-2.642221	2.972687	-0.455475
46	H	-3.069643	3.087767	1.276616
47	H	-1.014765	4.668063	0.175775
48	H	-0.889967	4.019810	1.838925
49	O	0.028806	2.908497	0.333537
50	O	-1.762608	1.574618	0.812832
51	Cl	-0.880758	-9.545810	-2.601883
52	Cl	8.683158	-1.758326	-5.699143

Table S20. Atomic coordinates for optimized structure of compound **30c** obtained using the B3LYP/6-311++G(d,p) level of theory

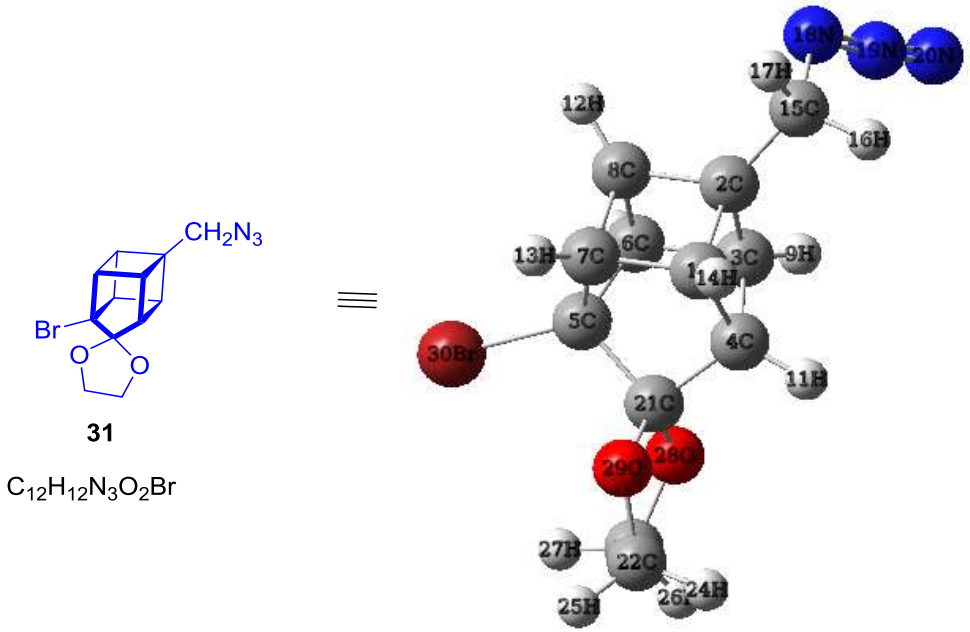


$C_{26}H_{18}N_3O_2Br_3$

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.128117	-0.800761	-0.127029
2	C	1.393566	-1.081039	-0.372970
3	C	1.584128	0.465221	-0.500962
4	C	0.043355	0.666144	-0.623649
5	C	0.423400	0.810639	1.625872
6	C	1.845331	0.562336	1.053238
7	C	0.136986	-0.702459	1.426124
8	C	1.654990	-0.984012	1.183125
9	H	2.282110	0.941739	-1.183131
10	H	2.698828	1.125779	1.418741
11	H	-0.361474	0.927366	-1.599531
12	H	2.279624	-1.656761	1.765580
13	H	-0.503975	-1.244849	2.114958
14	H	-0.931043	-1.439543	-0.483912
15	C	1.958103	-2.117864	-1.261877
16	C	1.872369	-4.212115	-2.126904
17	C	3.580511	-2.821487	-2.680800
18	N	3.002482	-4.020664	-2.820116
19	C	4.835566	-2.561524	-3.425009
20	C	5.383201	-3.539630	-4.265327
21	C	5.492455	-1.330300	-3.298667
22	C	6.559157	-3.298573	-4.966469
23	H	4.878321	-4.491187	-4.364619
24	C	6.669522	-1.077491	-3.993825
25	H	5.071032	-0.574044	-2.649795
26	C	7.192378	-2.066267	-4.823698
27	H	6.977936	-4.057184	-5.614824
28	H	7.173623	-0.125199	-3.892620
29	C	1.197366	-5.526429	-2.244121

30	C	1.723407	-6.527755	-3.070655
31	C	0.020953	-5.785588	-1.528315
32	C	1.092862	-7.761482	-3.183735
33	H	2.631528	-6.330429	-3.624393
34	C	-0.618436	-7.015642	-1.632275
35	H	-0.386072	-5.012961	-0.889515
36	C	-0.075164	-7.993998	-2.461486
37	H	1.502862	-8.531765	-3.823873
38	H	-1.526345	-7.211541	-1.076762
39	N	1.310818	-3.287973	-1.335111
40	N	3.093537	-1.836204	-1.911477
41	Br	0.316885	1.502701	3.448359
42	C	-0.373041	1.571705	0.540178
43	C	-2.255997	2.900708	0.564072
44	C	-1.021581	3.766639	0.786413
45	H	-2.630540	2.982894	-0.463125
46	H	-3.066254	3.096061	1.267033
47	H	-1.001263	4.672298	0.179508
48	H	-0.886514	4.020283	1.841939
49	O	0.036268	2.909291	0.338792
50	O	-1.761382	1.579922	0.807053
51	Br	8.811301	-1.725104	-5.787065
52	Br	-0.949568	-9.690646	-2.611229

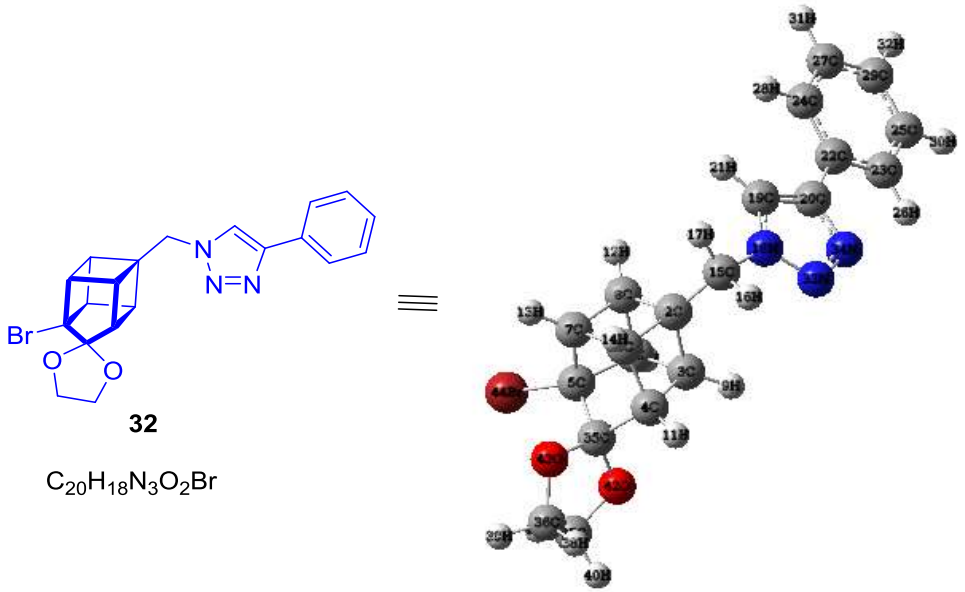
Table S21. Atomic coordinates for optimized structure of compound **31** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.035946	-0.543110	0.059401
2	C	1.489881	-0.902694	0.179216
3	C	1.769779	0.640363	0.059894
4	C	0.307356	0.902813	-0.406280
5	C	0.185360	1.079734	1.870051
6	C	1.684950	0.759350	1.632581
7	C	-0.118146	-0.423625	1.632594
8	C	1.404806	-0.778011	1.736027
9	H	2.617397	1.092857	-0.450090
10	H	2.461079	1.297737	2.168613

11	H	0.137725	1.162918	-1.449375
12	H	1.851296	-1.448923	2.465983
13	H	-0.924692	-0.919125	2.165550
14	H	-0.780129	-1.145072	-0.458672
15	C	2.156518	-1.997236	-0.604321
16	H	2.015087	-1.845327	-1.682143
17	H	1.717853	-2.963304	-0.343721
18	N	3.603994	-2.127525	-0.288078
19	N	4.370703	-1.424346	-0.941347
20	N	5.179439	-0.841336	-1.485959
21	C	-0.317354	1.849368	0.625976
22	C	-2.103925	3.253292	0.230042
23	C	-0.909986	4.071044	0.708762
24	H	-2.248066	3.339019	-0.853468
25	H	-3.036094	3.489890	0.743927
26	H	-0.720528	4.966418	0.116142
27	H	-0.994610	4.333576	1.767253
28	O	0.181561	3.165025	0.503960
29	O	-1.729185	1.915909	0.575360
30	Br	-0.291602	1.813583	3.615708

Table S22. Atomic coordinates for optimized structure of compound **32** obtained using the B3LYP/6-311++G(d,p) level of theory

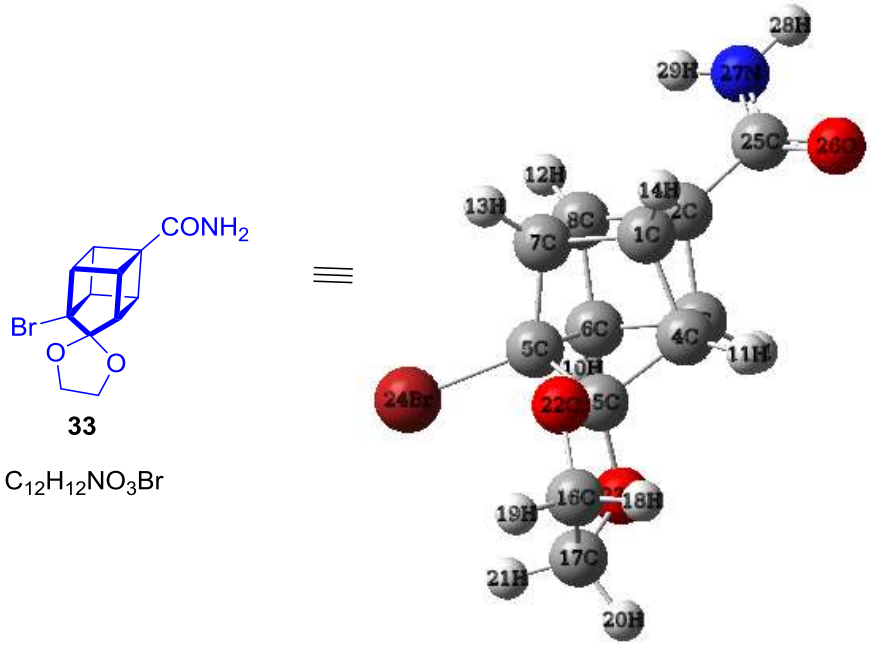


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.083906	-0.542973	-0.140157
2	C	1.414686	-0.996602	-0.015833
3	C	1.784350	0.527959	-0.004985
4	C	0.351704	0.912639	-0.481421
5	C	0.179831	0.917361	1.799419
6	C	1.664688	0.530550	1.569847
7	C	-0.201245	-0.542102	1.435072
8	C	1.295988	-0.991646	1.546543
9	H	2.674996	0.948537	-0.463964
10	H	2.456056	0.978984	2.163085

11	H	0.225784	1.264514	-1.503413
12	H	1.677890	-1.737310	2.241017
13	H	-1.048145	-1.030676	1.908561
14	H	-0.846186	-1.060600	-0.719732
15	C	2.042115	-2.042422	-0.898032
16	H	1.938102	-1.767467	-1.950494
17	H	1.561692	-3.014779	-0.754063
18	N	3.474620	-2.211924	-0.655163
19	C	4.104921	-3.018064	0.233010
20	C	5.449265	-2.728572	0.082034
21	H	3.569865	-3.701645	0.869151
22	C	6.624403	-3.285384	0.763418
23	C	7.887253	-2.706782	0.571267
24	C	6.516135	-4.395125	1.613671
25	C	9.006416	-3.223649	1.216540
26	H	7.976165	-1.851758	-0.086993
27	C	7.636960	-4.908730	2.259162
28	H	5.552822	-4.869110	1.768192
29	C	8.887909	-4.324650	2.064179
30	H	9.975489	-2.763697	1.057632
31	H	7.533893	-5.768471	2.911888
32	H	9.761379	-4.725311	2.565965
33	N	4.369274	-1.453433	-1.321044
34	N	5.552599	-1.762043	-0.880994
35	C	-0.244992	1.810134	0.609827
36	C	-1.933881	3.344904	0.280836
37	C	-0.709803	4.050256	0.852401
38	H	-2.037602	3.518943	-0.796644
39	H	-2.866556	3.598760	0.785366
40	H	-0.450652	4.975501	0.337123
41	H	-0.811096	4.234989	1.925811
42	O	0.332847	3.098379	0.604965
43	O	-1.648762	1.965271	0.534570

44	Br	-0.302399	1.534557	3.587916

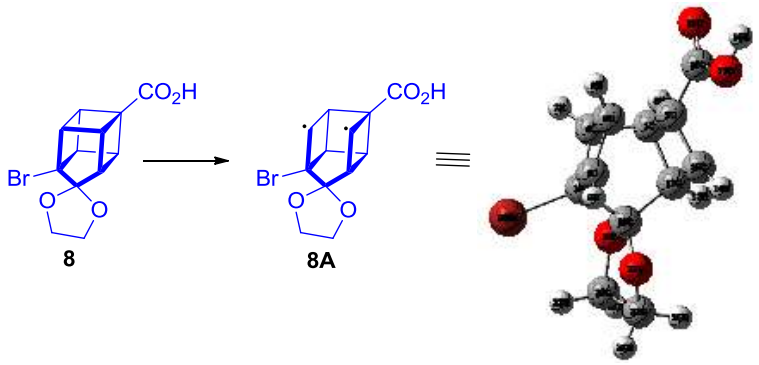
Table S23. Atomic coordinates for optimized structure of compound **33** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.037599	-0.599707	-0.025878
2	C	1.574803	-0.929972	-0.023441
3	C	1.801044	0.621603	-0.162726
4	C	0.303651	0.852635	-0.513332
5	C	0.359612	1.025071	1.767484
6	C	1.842605	0.740661	1.410560

7	C	0.075041	-0.484828	1.548423
8	C	1.609115	-0.803416	1.537352
9	H	2.600210	1.065984	-0.750007
10	H	2.645486	1.299443	1.882819
11	H	0.053746	1.100635	-1.541889
12	H	2.113622	-1.451610	2.252696
13	H	-0.673852	-1.003529	2.140103
14	H	-0.714071	-1.229259	-0.494509
15	C	-0.256076	1.784025	0.569182
16	C	-2.090862	3.139248	0.265252
17	C	-0.892819	3.996830	0.655305
18	H	-2.290628	3.185263	-0.811825
19	H	-3.001419	3.371582	0.818005
20	H	-0.758197	4.879406	0.029256
21	H	-0.926272	4.287744	1.709539
22	O	-1.666778	1.824069	0.636688
23	O	0.208117	3.110673	0.416434
24	Br	0.005576	1.745515	3.546428
25	C	2.193199	-1.923138	-0.955717
26	O	2.017228	-1.862047	-2.163255
27	N	2.963467	-2.889986	-0.373929
28	H	3.405327	-3.577416	-0.964830
29	H	3.103873	-2.934553	0.620810

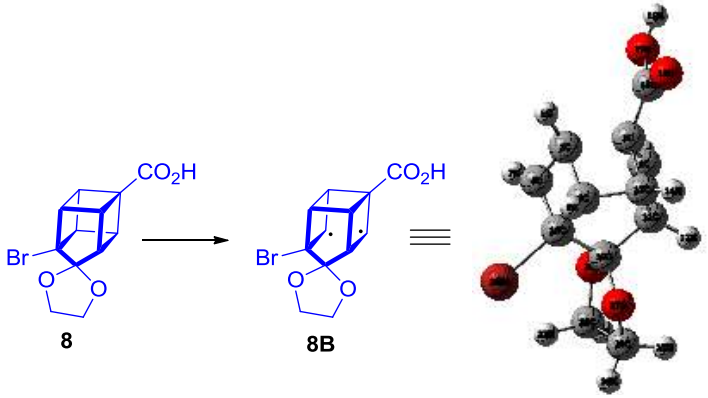
Table S24. Atomic coordinates for optimized structure of biradical **8A** using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.845330	2.226347	0.782196
2	C	0.428337	1.846581	-0.675854
3	C	-0.947172	2.745015	-0.455215
4	C	-0.440810	3.061946	0.992377
5	H	1.137222	1.476252	1.511583
6	H	-1.867989	2.213421	-0.697948
7	H	-1.053583	2.935443	1.879025
8	C	-0.760505	4.176778	-0.796617
9	H	-0.885317	4.760887	-1.698913
10	C	-0.110772	4.503800	0.497050
11	C	1.923359	3.189003	0.173546
12	H	2.958191	3.084273	0.509951
13	C	1.586802	2.632951	-1.183939
14	H	1.916772	2.886299	-2.183026
15	C	0.135080	0.453115	-1.127950
16	O	-0.148581	-0.470266	-0.404240
17	O	0.180153	0.340102	-2.478959

18	H	-0.049578	-0.575931	-2.698101
19	C	1.443502	4.644816	0.476153
20	C	2.525003	6.342897	1.610541
21	C	2.868861	6.420375	0.127962
22	H	1.777151	7.086859	1.896554
23	H	3.391794	6.409053	2.268874
24	H	2.788274	7.422446	-0.293538
25	H	3.862825	6.009479	-0.084152
26	O	1.977961	5.022764	1.729872
27	O	1.857649	5.602790	-0.472134
28	Br	-1.005198	6.030364	1.452938

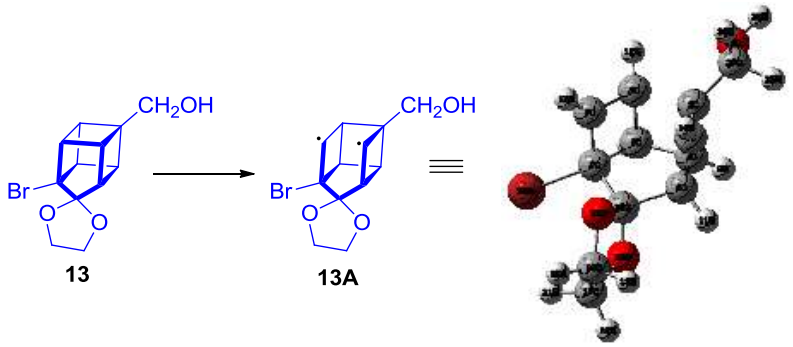
Table S25. Atomic coordinates for optimized structure of biradical **8B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.656149	2.103893	0.250053
2	C	0.506677	1.811052	-0.651766
3	C	-0.897872	2.575565	-0.217920

4	C	-0.736564	3.424901	0.987636
5	H	2.007752	1.640456	1.162562
6	H	-1.797953	1.982832	-0.385113
7	H	-0.846791	3.255666	2.050728
8	C	-0.439669	3.793080	-1.090965
9	H	-1.070609	4.263032	-1.838537
10	C	-0.134390	4.554165	0.236377
11	C	1.942190	3.432661	-0.395992
12	H	2.972127	3.616503	-0.714222
13	C	0.875734	3.078084	-1.488866
14	H	1.169448	3.012216	-2.532521
15	C	0.267375	0.458400	-1.239713
16	O	0.020162	0.234401	-2.399615
17	O	0.317654	-0.516738	-0.297999
18	H	0.125576	-1.356201	-0.743293
19	C	1.416536	4.705696	0.336451
20	C	2.373981	6.124816	1.881410
21	C	2.759887	6.578753	0.477840
22	H	1.577696	6.741266	2.307408
23	H	3.215128	6.072738	2.573340
24	H	2.613294	7.645234	0.304491
25	H	3.791094	6.302607	0.228289
26	O	1.902632	4.788574	1.656883
27	O	1.842793	5.861983	-0.354713
28	Br	-1.095279	6.292223	0.555802

Table S26. Atomic coordinates for optimized structure of biradical **13A** using the B3LYP/6-311++G(d,p) level of theory

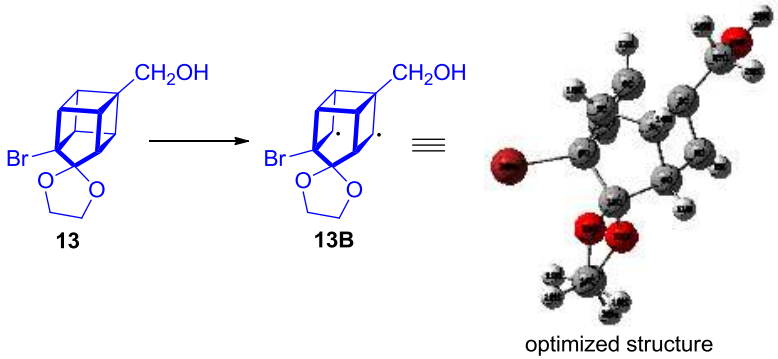


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.104835	-0.413390	-1.015209
2	C	1.293532	-1.076945	-0.399876
3	C	1.935881	0.348682	-0.223793
4	C	0.580594	0.977589	-0.693263
5	C	0.473280	0.795287	1.739306
6	C	1.864843	0.231848	1.317652
7	C	-0.036831	-0.594833	1.809579
8	C	1.199255	-1.184925	1.229857
9	H	2.863255	0.644649	-0.708133
10	H	2.730578	0.445247	1.936428
11	H	0.598719	1.698513	-1.515252
12	H	1.639967	-2.098012	1.630337
13	H	-1.024144	-0.974483	2.039671
14	H	-0.866522	-0.787774	-1.319769
15	C	-0.051072	1.667133	0.558969
16	C	-1.858336	3.073019	0.298640
17	C	-0.683791	3.872420	0.850433

18	H	-1.997678	3.239174	-0.776318
19	H	-2.798480	3.251027	0.821360
20	H	-0.501066	4.808913	0.321946
21	H	-0.785155	4.059862	1.922638
22	O	-1.461948	1.720215	0.544126
23	O	0.425618	3.000089	0.603153
24	Br	0.367240	1.766321	3.505993
25	H	3.589637	-3.302326	-0.859795
26	O	3.162480	-2.569216	-0.407436
27	C	1.946374	-2.249258	-1.088379
28	H	1.256609	-3.106570	-1.076386
29	H	2.145828	-1.987614	-2.136167

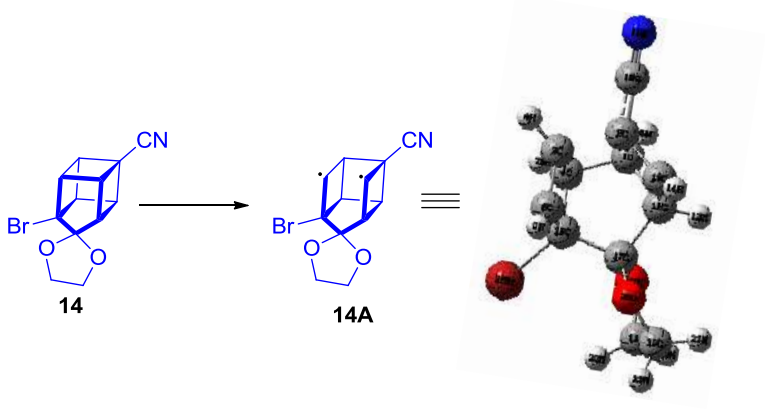
Table S27. Atomic coordinates for optimized structure of biradical **13B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.084959	-0.736298	-0.327203
2	C	1.461483	-1.019621	-0.337549
3	C	1.663407	0.346641	-0.909076
4	C	0.222863	0.745389	-0.732540

5	C	0.152719	0.670387	1.707710
6	C	1.570358	0.297474	1.923897
7	C	-0.125167	-0.784919	1.221134
8	C	1.422816	-1.040841	1.294846
9	H	2.553436	0.925986	-1.121513
10	H	2.417078	0.887648	2.249596
11	H	-0.287221	1.163676	-1.605191
12	H	1.899920	-1.918886	1.733160
13	H	-0.862593	-1.382374	1.748571
14	H	-0.799705	-1.310312	-0.913883
15	C	-0.132042	1.624087	0.506247
16	C	-1.604623	3.391930	0.285422
17	C	-0.276728	3.899382	0.835363
18	H	-1.724325	3.632324	-0.777780
19	H	-2.474516	3.743222	0.841566
20	H	0.094666	4.794668	0.335802
21	H	-0.320299	4.063046	1.915722
22	O	-1.502675	1.976434	0.462527
23	O	0.615649	2.819612	0.529706
24	Br	-0.765424	1.274685	3.403562
25	H	3.904716	-2.966003	-1.123918
26	O	3.489582	-2.209524	-0.698955
27	C	2.084551	-2.243135	-0.961715
28	H	1.630969	-3.148662	-0.532568
29	H	1.889568	-2.241373	-2.042628

Table S28. Atomic coordinates for optimized structure of biradical **14A** using the B3LYP/6-311++G(d,p) level of theory

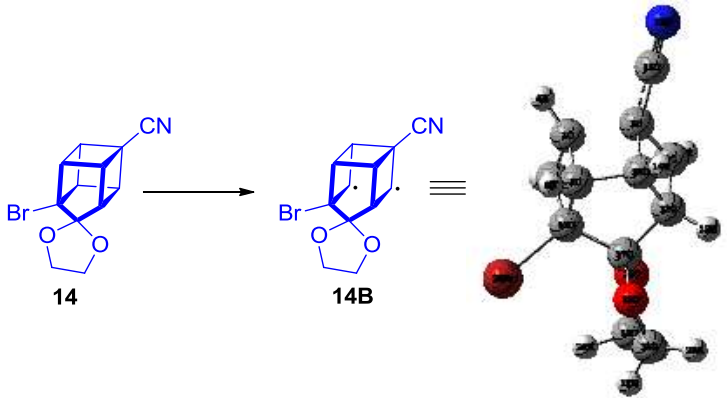


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.850319	2.327939	0.851302
2	C	0.285328	1.822945	-0.539031
3	C	-1.051973	2.746051	-0.256720
4	C	-0.415813	3.179941	1.106898
5	H	1.217528	1.639463	1.606892
6	H	-1.987125	2.197360	-0.369857
7	H	-0.941973	3.127779	2.054529
8	C	-0.905814	4.146233	-0.728328
9	H	-1.126865	4.658232	-1.655454
10	C	-0.139404	4.576450	0.468022
11	C	1.859831	3.228251	0.065353
12	H	2.921618	3.146364	0.310940
13	C	1.406985	2.559516	-1.200335
14	H	1.667526	2.694344	-2.241996
15	C	0.009004	0.445880	-0.860287

16	N	-0.233411	-0.656088	-1.110339
17	C	1.405921	4.708337	0.291404
18	C	2.591075	6.482082	1.179625
19	C	2.793279	6.437614	-0.330240
20	H	1.875890	7.253269	1.476227
21	H	3.516640	6.590273	1.745635
22	H	2.672420	7.402522	-0.822381
23	H	3.762349	6.003412	-0.601492
24	O	2.053753	5.180348	1.455334
25	O	1.729545	5.580768	-0.765239
26	Br	-0.944168	6.175032	1.376428

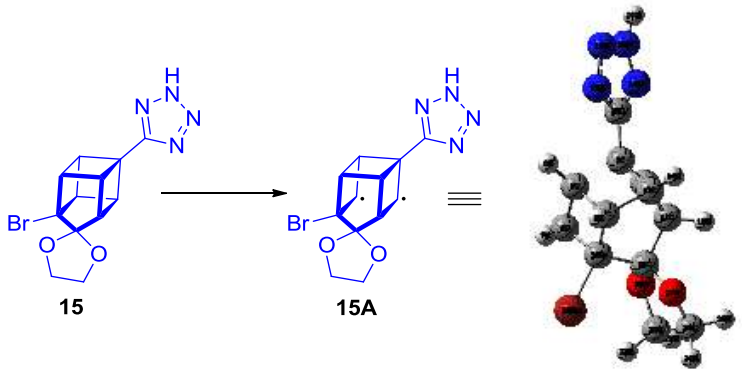
Table S29. Atomic coordinates for optimized structure of biradical **14B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.591821	2.203983	0.742451
2	C	0.536531	1.680680	-0.179923
3	C	-0.892122	2.500189	-0.106346

4	C	-0.876334	3.608450	0.880867
5	H	1.865549	1.937172	1.754714
6	H	-1.765146	1.860622	-0.237147
7	H	-1.126832	3.687595	1.930484
8	C	-0.331219	3.497268	-1.175749
9	H	-0.867152	3.768629	-2.079570
10	C	-0.183400	4.550771	-0.033169
11	C	1.949399	3.359785	-0.147013
12	H	3.009985	3.490550	-0.377700
13	C	1.020476	2.745817	-1.246115
14	H	1.441373	2.450043	-2.202757
15	C	0.406886	0.268594	-0.435476
16	N	0.281580	-0.860565	-0.647413
17	C	1.346261	4.754609	0.212195
18	C	2.101452	6.508889	1.499449
19	C	2.658191	6.652134	0.087270
20	H	1.251794	7.174177	1.673931
21	H	2.847868	6.641938	2.282744
22	H	2.524344	7.646497	-0.339345
23	H	3.714674	6.365731	0.032134
24	O	1.672250	5.138909	1.526192
25	O	1.860004	5.732117	-0.666929
26	Br	-1.165765	6.289734	-0.240889

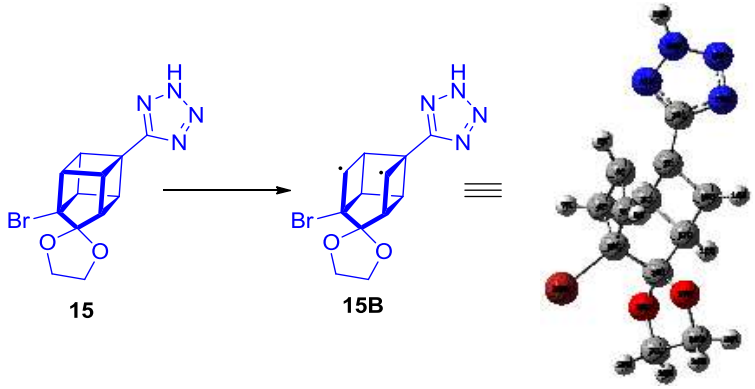
Table S30. Atomic coordinates for optimized structure of biradical **15A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.184597	1.204605	-0.392715
2	C	0.294528	0.793778	-1.516124
3	C	-0.703727	1.986210	-2.050519
4	C	-0.552859	3.258846	-1.299152
5	H	1.078657	1.144924	0.682715
6	H	-1.677398	1.619073	-2.374430
7	H	-1.011431	3.671141	-0.409640
8	C	0.431180	2.467792	-3.014449
9	H	0.280478	2.642784	-4.074806
10	C	0.643874	3.687249	-2.064198
11	C	2.154101	1.935591	-1.277516
12	H	3.212288	1.685864	-1.159042
13	C	1.388202	1.360169	-2.514181
14	H	1.911601	0.721966	-3.221325
15	C	-0.280792	-0.564845	-1.575308
16	N	-0.065963	-1.517432	-0.669823

17	N	-1.095921	-1.001011	-2.579353
18	N	-1.396519	-2.241073	-2.310719
19	C	2.023064	3.488279	-1.359809
20	C	2.992270	5.217165	-0.186327
21	C	3.912436	4.819969	-1.335270
22	H	2.421413	6.121095	-0.414753
23	H	3.504617	5.329879	0.769527
24	H	4.259816	5.664300	-1.931668
25	H	4.772097	4.235474	-0.987000
26	O	2.114971	4.086525	-0.087009
27	O	3.067495	4.009677	-2.157931
28	Br	0.443372	5.529416	-2.855086
29	N	-0.774250	-2.519962	-1.174547
30	H	-0.842911	-3.424311	-0.728862

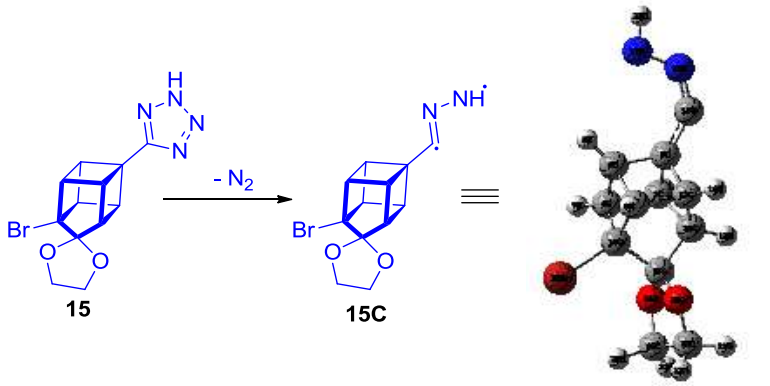
Table S31. Atomic coordinates for optimized structure of biradical **15B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center	Atomic	Coordinates (Angstroms)		
Number	Symbol	X	Y	Z

1	C	0.596098	1.802535	-0.318005
2	C	0.805263	0.612311	-1.350299
3	C	-0.355854	1.302429	-2.273861
4	C	-0.507355	2.431964	-1.199488
5	H	0.427441	1.625742	0.741149
6	H	-1.147232	0.610879	-2.562823
7	H	-1.460518	2.733668	-0.777115
8	C	0.167918	2.325619	-3.217777
9	H	0.553185	2.294832	-4.228686
10	C	0.220914	3.393090	-2.189618
11	C	1.961455	2.399322	-0.792284
12	H	2.712927	2.635041	-0.034112
13	C	2.177194	1.146606	-1.591611
14	H	2.991924	0.807706	-2.217980
15	C	0.603477	-0.819479	-1.043249
16	N	-0.575163	-1.440426	-1.069125
17	N	1.607460	-1.666484	-0.671384
18	N	1.059450	-2.830802	-0.458476
19	C	1.623930	3.704333	-1.584334
20	C	2.342703	5.869153	-1.206134
21	C	3.313011	5.164902	-2.147057
22	H	1.674856	6.549752	-1.740427
23	H	2.829343	6.391446	-0.381654
24	H	3.585470	5.753045	-3.023591
25	H	4.220600	4.835361	-1.627822
26	O	1.596278	4.774673	-0.658428
27	O	2.556874	4.032218	-2.589211
28	Br	-0.759846	5.063060	-2.742534
29	N	-0.233250	-2.666884	-0.698504
30	H	-0.899265	-3.422474	-0.614883

Table S32. Atomic coordinates for optimized structure of biradical **15C** obtained using the B3LYP/6-311++G(d,p) level of theory

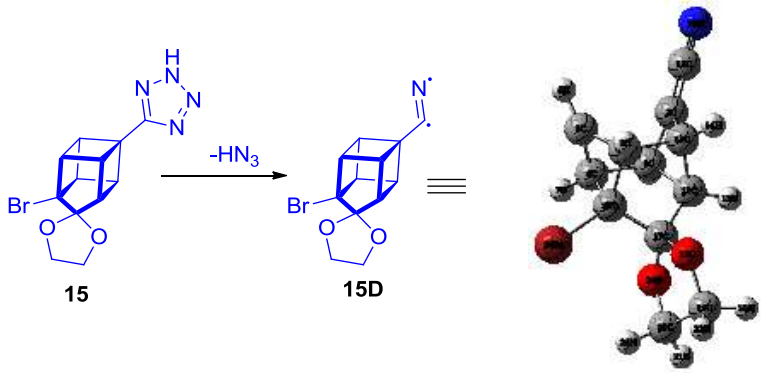


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.974648	1.646774	-0.185763
2	C	0.568054	0.566810	-1.271936
3	C	-0.540081	1.551143	-1.831103
4	C	-0.145932	2.604428	-0.744273
5	H	1.008434	1.437895	0.879920
6	H	-1.549109	1.275873	-2.117472
7	H	-0.833247	3.073803	-0.046496
8	C	0.529315	2.224745	-2.752185
9	H	0.439917	2.358105	-3.826414
10	C	0.624342	3.445509	-1.797535
11	C	2.243806	2.046936	-0.986580
12	H	3.213089	1.739817	-0.600191
13	C	1.650375	1.267289	-2.191351
14	H	2.279887	0.724502	-2.891107
15	C	0.509315	-0.845593	-1.019323
16	N	-0.330855	-1.785519	-1.090670

17	C	2.093304	3.537057	-1.319272
18	C	3.038005	5.506036	-0.594897
19	C	3.839458	4.970885	-1.775774
20	H	2.358998	6.309986	-0.892998
21	H	3.651664	5.828733	0.246509
22	H	4.053965	5.718286	-2.539999
23	H	4.772544	4.494917	-1.452491
24	O	2.293740	4.351622	-0.183497
25	O	2.956062	3.995176	-2.339887
26	Br	-0.217152	5.102212	-2.388875
27	N	-1.593931	-1.614536	-1.506662
28	H	-2.021118	-2.547362	-1.445863

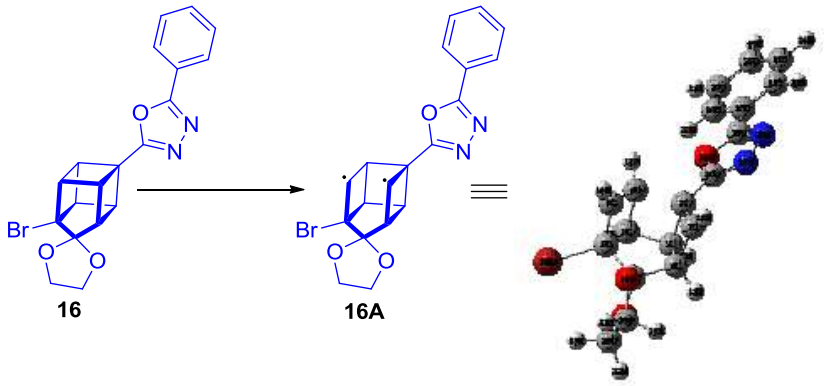
Table S33. Atomic coordinates for optimized structure of biradical **15D** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.622078	1.712341	-0.334350
2	C	0.586520	0.539374	-1.282446
3	C	-0.970958	2.336072	-2.208007

4	C	-0.363952	2.856297	-0.931214
5	H	0.544744	1.575594	0.741316
6	H	-1.829939	1.711494	-2.416724
7	H	-0.944547	3.361436	-0.162410
8	C	0.371265	2.494798	-2.872669
9	H	0.487507	2.655193	-3.942272
10	C	0.619142	3.655615	-1.851430
11	C	1.986359	2.060163	-1.031597
12	H	2.878178	1.604110	-0.606758
13	C	1.365646	1.350042	-2.288199
14	H	1.985384	0.873244	-3.043456
15	C	0.198053	-0.772782	-1.187654
16	N	-0.122490	-1.895793	-1.102626
17	C	2.037925	3.558044	-1.292552
18	C	3.181143	5.348092	-0.405846
19	C	3.981827	4.764119	-1.563743
20	H	2.638132	6.250766	-0.699295
21	H	3.773642	5.541567	0.488464
22	H	4.343864	5.509865	-2.271578
23	H	4.819084	4.150243	-1.212661
24	O	2.259675	4.289301	-0.105951
25	O	3.015657	3.945328	-2.234131
26	Br	0.032833	5.434348	-2.397038

Table S34. Atomic coordinates for optimized structure of biradical **16A** obtained using the B3LYP/6-311++G(d,p) level of theory

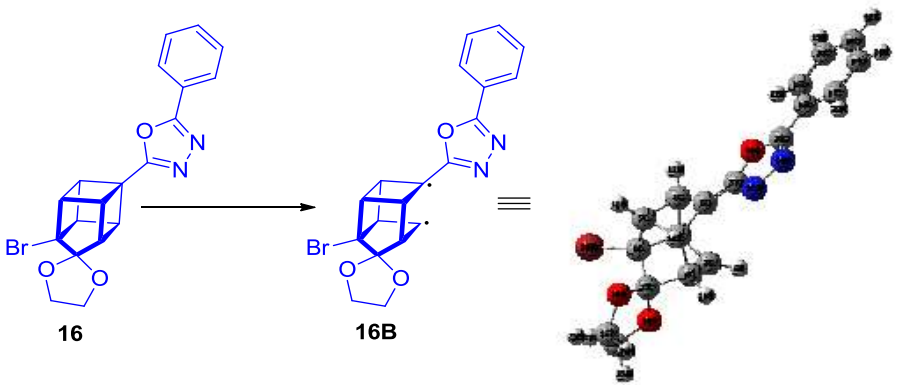


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.483494	0.252437	-0.813695
2	C	2.232304	-0.520911	0.216038
3	C	2.504692	0.847328	0.968337
4	C	1.538767	1.543256	-0.047522
5	C	0.187730	0.850331	1.867101
6	C	1.650757	0.409826	2.182026
7	C	-0.097841	-0.531894	1.409681
8	C	1.317370	-0.967171	1.515784
9	H	3.507407	1.241758	1.111147
10	H	2.024023	0.510257	3.196265
11	H	1.904414	2.420753	-0.587186
12	H	1.586791	-1.941250	1.925259
13	H	-0.993566	-0.970451	0.989794
14	H	0.976492	-0.046539	-1.720873
15	C	4.857229	-2.889670	0.022712
16	C	5.864230	-3.699780	0.697525

17	C	6.679564	-4.552076	-0.061969
18	C	6.028714	-3.639249	2.087602
19	C	7.643694	-5.330367	0.566308
20	H	6.545114	-4.591509	-1.135704
21	C	6.997235	-4.422556	2.708426
22	H	5.401352	-2.981165	2.675763
23	C	7.805710	-5.268927	1.951594
24	H	8.271050	-5.987539	-0.024861
25	H	7.119993	-4.371688	3.784180
26	N	4.592426	-2.816629	-1.244714
27	C	0.263819	1.947851	0.764226
28	C	-1.254928	3.372418	-0.209779
29	C	-0.655168	4.057319	1.013380
30	H	-0.803878	3.730907	-1.142435
31	H	-2.340197	3.450457	-0.273873
32	H	-0.305032	5.072106	0.820646
33	H	-1.342191	4.054132	1.863717
34	O	0.487968	3.239467	1.297696
35	O	-0.920873	1.996533	0.005243
36	Br	-0.961265	1.418506	3.416721
37	C	3.257790	-1.486513	-0.197449
38	N	3.552904	-1.903016	-1.387431
39	O	4.044817	-2.071566	0.757674
40	H	8.559068	-5.878265	2.437713

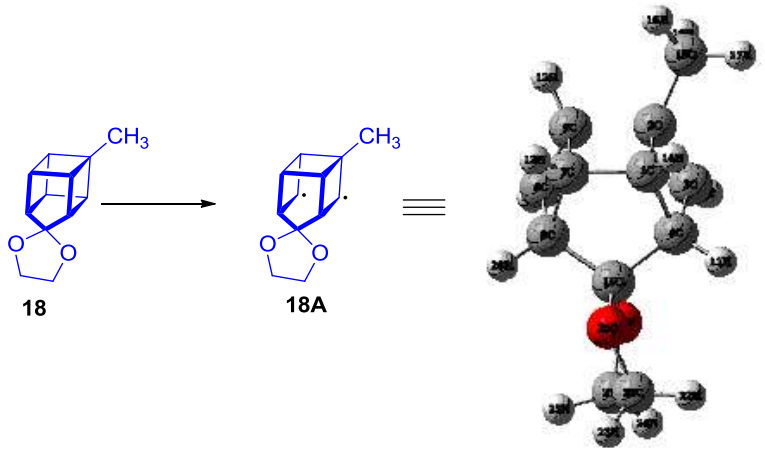
Table S35. Atomic coordinates for optimized structure of biradical **16B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.517274	0.509372	0.037459
2	C	2.364040	-0.632536	0.544751
3	C	2.493688	1.470474	2.086611
4	C	1.872319	1.867400	0.784147
5	C	0.160579	0.985221	2.016584
6	C	1.517632	0.508894	2.673696
7	C	0.349696	-0.089501	0.946650
8	C	1.482489	-0.822031	1.736519
9	H	3.506058	1.650161	2.415992
10	H	1.549880	0.333588	3.745785
11	H	2.399974	2.596043	0.173090
12	H	1.385945	-1.776931	2.248389
13	H	-0.477731	-0.588906	0.451017
14	H	1.353859	0.627642	-1.030815
15	C	4.894774	-2.863448	-0.272392
16	C	5.702927	-4.029499	0.037247

17	C	6.681317	-4.453777	-0.877002
18	C	5.519555	-4.737443	1.234419
19	C	7.459306	-5.568095	-0.591987
20	H	6.815553	-3.901384	-1.798521
21	C	6.304431	-5.852282	1.510532
22	H	4.765955	-4.411578	1.940316
23	C	7.274535	-6.270830	0.600701
24	H	8.212612	-5.891672	-1.301065
25	H	6.158413	-6.395270	2.437258
26	N	4.951627	-2.101560	-1.334410
27	C	0.464727	2.317801	1.288418
28	C	-0.850309	3.940752	0.310180
29	C	-0.591400	4.302287	1.766862
30	H	-0.222248	4.524066	-0.372941
31	H	-1.895278	4.023929	0.010578
32	H	-0.298693	5.340702	1.922702
33	H	-1.442593	4.052017	2.406770
34	O	0.533565	3.473098	2.087806
35	O	-0.480428	2.558595	0.264106
36	Br	-1.447647	0.911915	3.111293
37	C	3.398099	-1.341961	-0.027856
38	N	4.005695	-1.128705	-1.198766
39	O	3.937420	-2.449454	0.602264
40	H	7.884364	-7.140180	0.818679

Table S36. Atomic coordinates for optimized structure of biradical **18A** obtained using the B3LYP/6-311++G(d,p) level of theory

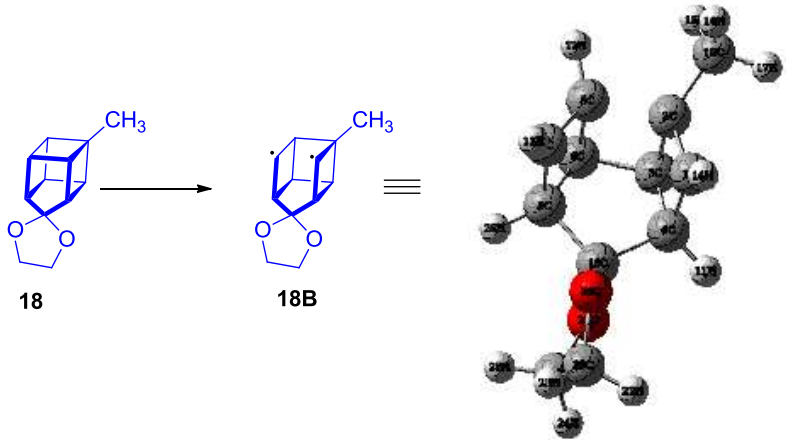


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.072262	-0.688275	-0.016352
2	C	1.492354	-0.815542	-0.153634
3	C	1.488964	0.514402	-0.835575
4	C	0.031637	0.775771	-0.559295
5	C	0.171252	0.911318	1.901630
6	C	1.655084	0.676348	2.026759
7	C	0.024764	-0.605106	1.528357
8	C	1.590417	-0.704616	1.477642
9	H	2.286268	1.173217	-1.162989
10	H	2.475587	1.361814	2.205338
11	H	-0.589964	1.063889	-1.413478
12	H	2.179946	-1.510382	1.922787
13	H	-0.592110	-1.245469	2.155180
14	H	-0.763675	-1.383556	-0.489967
15	C	2.221935	-2.002260	-0.747616

16	H	3.306271	-1.851472	-0.701725
17	H	1.946578	-2.146701	-1.796663
18	H	1.988755	-2.923253	-0.203554
19	C	-0.279917	1.700748	0.647852
20	C	-1.938242	3.249175	0.257431
21	C	-0.664896	3.986220	0.651802
22	H	-2.078541	3.240316	-0.831207
23	H	-2.841822	3.626127	0.737769
24	H	-0.411777	4.820048	-0.004849
25	H	-0.708582	4.336993	1.690030
26	O	-1.685693	1.934529	0.749736
27	O	0.336008	2.977087	0.506187
28	H	-0.353463	1.289591	2.784022

Table S37. Atomic coordinates for optimized structure of biradical **18B** obtained using the B3LYP/6-311++G(d,p) level of theory

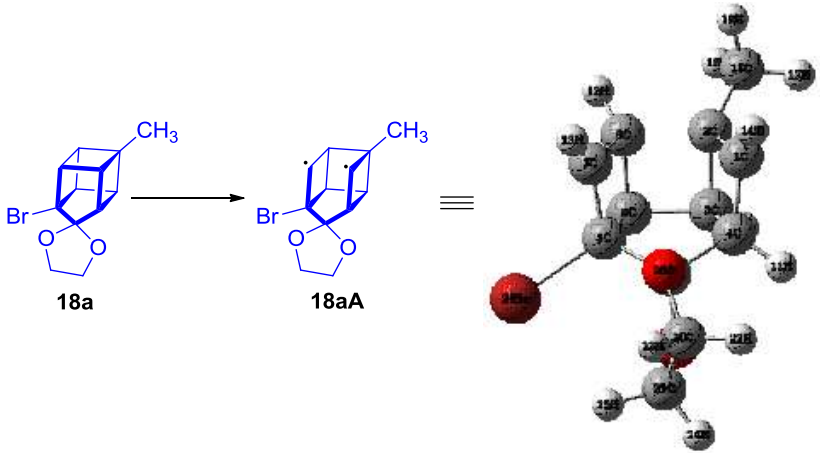


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z

1	C	0.043010	-0.486893	-0.757564
2	C	1.324000	-0.953793	-0.145388
3	C	1.834929	0.535562	-0.214565
4	C	0.403530	0.973535	-0.673084
5	C	0.454718	1.153187	1.788229
6	C	1.865168	0.643318	1.331359
7	C	0.103583	-0.277425	2.106145
8	C	1.340177	-0.827200	1.487732
9	H	2.697696	0.836314	-0.806956
10	H	2.751758	1.014874	1.840726
11	H	0.303564	1.565958	-1.587507
12	H	1.891609	-1.638647	1.969846
13	H	-0.825680	-0.732629	2.428870
14	H	-0.905033	-0.980959	-0.942294
15	C	2.064977	-2.155861	-0.692259
16	H	3.051584	-2.257591	-0.228668
17	H	2.203902	-2.071385	-1.774272
18	H	1.505747	-3.077358	-0.495503
19	C	-0.209266	1.749979	0.518453
20	C	-2.158011	2.997286	0.370482
21	C	-0.999559	3.893845	0.787829
22	H	-2.414480	3.137973	-0.686523
23	H	-3.054029	3.114357	0.982073
24	H	-0.968527	4.855371	0.274315
25	H	-0.987175	4.057568	1.873159
26	O	-1.630860	1.687023	0.587139
27	O	0.131569	3.129634	0.374251
28	H	0.395973	1.874919	2.609593

Table S38. Atomic coordinates for optimized structure of biradical **18aA** obtained using the B3LYP/6-311++G(d,p) level of theory

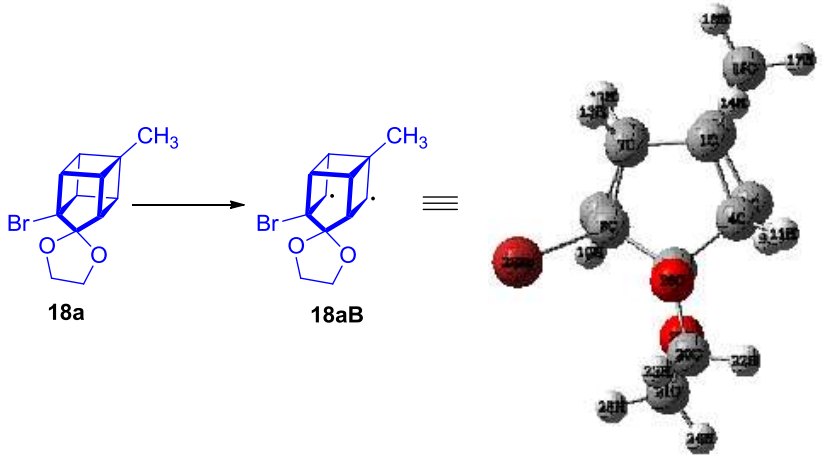


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.036008	-0.461635	-0.737796
2	C	1.325084	-0.946109	-0.156747
3	C	1.831241	0.546276	-0.177011
4	C	0.392047	0.994026	-0.602075
5	C	0.470697	1.078666	1.836366
6	C	1.878695	0.598618	1.369408
7	C	0.103468	-0.334091	2.091640
8	C	1.346298	-0.873633	1.480648
9	H	2.686506	0.874350	-0.764540
10	H	2.755665	0.962044	1.896306
11	H	0.285693	1.617366	-1.494194
12	H	1.885926	-1.700383	1.948293
13	H	-0.825936	-0.773015	2.431158
14	H	-0.906526	-0.955371	-0.948124

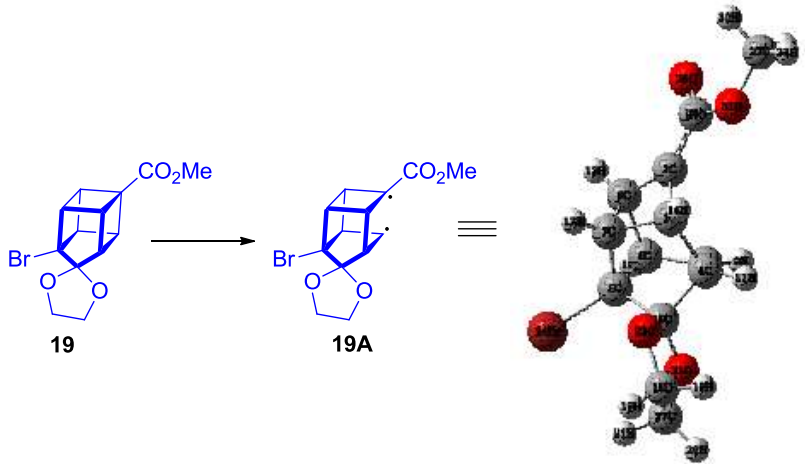
15	C	2.065817	-2.127666	-0.744757
16	H	3.055006	-2.241950	-0.290308
17	H	2.197962	-2.007125	-1.823910
18	H	1.509209	-3.055803	-0.575164
19	C	-0.213723	1.763184	0.615457
20	C	-2.157781	2.968175	0.343971
21	C	-1.029761	3.925727	0.710361
22	H	-2.382203	2.992182	-0.729133
23	H	-3.074108	3.125612	0.913368
24	H	-0.971388	4.804105	0.066312
25	H	-1.077623	4.231982	1.758784
26	O	-1.620365	1.693615	0.709840
27	O	0.138258	3.128454	0.479575
28	Br	0.387481	2.226158	3.495504

Table S39. Atomic coordinates for optimized structure of biradical **18aB** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.055764	-0.695371	-0.048518
2	C	1.509774	-0.835107	-0.163956
3	C	1.525613	0.492049	-0.851985
4	C	0.068245	0.765831	-0.596655
5	C	0.181827	0.907686	1.837639
6	C	1.641854	0.692469	1.972265
7	C	0.020174	-0.605460	1.495803
8	C	1.586517	-0.704244	1.467596
9	H	2.329898	1.134779	-1.192748
10	H	2.442629	1.389802	2.182900
11	H	-0.540460	1.052340	-1.459391
12	H	2.172112	-1.494218	1.943425
13	H	-0.610129	-1.221593	2.129904
14	H	-0.748933	-1.385634	-0.525292
15	C	2.239972	-2.032495	-0.733198
16	H	3.324207	-1.888232	-0.672657
17	H	1.979141	-2.184915	-1.784529
18	H	1.991984	-2.946112	-0.183737
19	C	-0.286823	1.715059	0.588202
20	C	-1.953176	3.292688	0.323418
21	C	-0.654078	3.987906	0.715232
22	H	-2.169997	3.407947	-0.745385
23	H	-2.816709	3.610076	0.909023
24	H	-0.416980	4.856313	0.099566
25	H	-0.641409	4.264988	1.773100
26	O	-1.686418	1.921211	0.628028
27	O	0.328641	2.977570	0.452869
28	Br	-0.670071	1.578425	3.542313

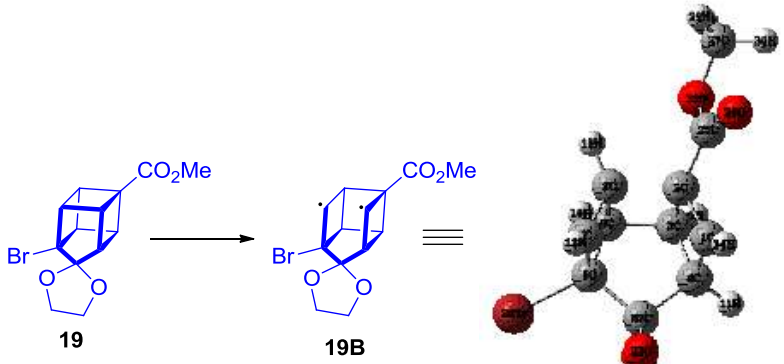
Table S40. Atomic coordinates for optimized structure of biradical **19A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.537337	-0.612917	0.322449
2	C	1.956930	-1.115153	0.342889
3	C	1.787845	1.342007	-0.507830
4	C	0.417537	0.739252	-0.505920
5	C	0.767900	1.430328	1.646383
6	C	2.177830	1.358218	0.930978
7	C	0.818254	-0.088436	1.804539
8	C	2.338225	-0.180643	1.435569
9	H	2.389832	1.628062	-1.356349
10	H	2.961480	2.042505	1.243918
11	H	-0.096609	0.644244	-1.459561
12	H	3.156893	-0.389468	2.119422

13	H	0.351863	-0.617943	2.630162
14	H	-0.282708	-1.305110	0.146867
15	C	-0.280456	1.674912	0.533181
16	C	-2.518715	2.231149	0.524900
17	C	-1.678481	3.499943	0.456969
18	H	-2.933842	1.963563	-0.453699
19	H	-3.317748	2.267117	1.265754
20	H	-2.009110	4.211899	-0.299509
21	H	-1.606315	3.994542	1.429970
22	O	-1.564997	1.248863	0.943040
23	O	-0.397818	2.993670	0.057700
24	Br	0.623394	2.514518	3.256279
25	C	2.656032	-2.209575	-0.272251
26	O	3.818857	-2.507217	-0.050893
27	C	2.484272	-4.010042	-1.802553
28	H	1.717583	-4.431719	-2.449537
29	H	3.342382	-3.679990	-2.390923
30	H	2.818923	-4.750104	-1.073282
31	O	1.862537	-2.895905	-1.144325

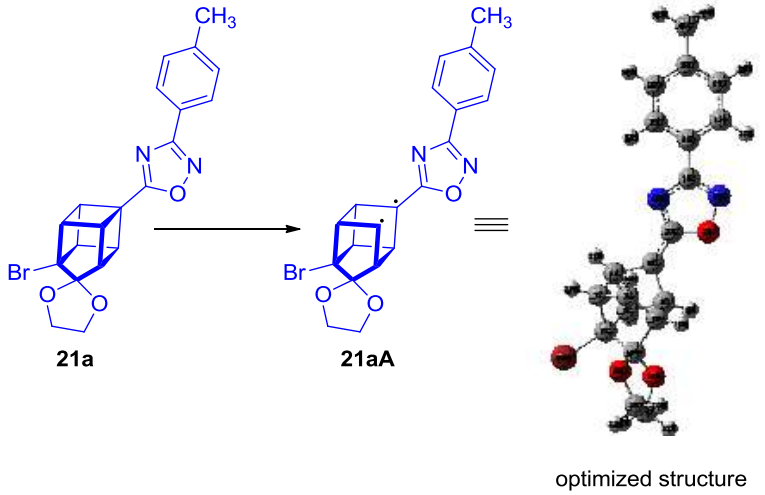
Table S41. Atomic coordinates for optimized structure of biradical **19B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.056900	-0.380328	-0.944999
2	C	1.116370	-1.051750	-0.326641
3	C	1.792034	0.357790	-0.160040
4	C	0.446896	1.004235	-0.638267
5	C	0.346780	0.859712	1.798414
6	C	1.730104	0.270570	1.383248
7	C	-0.183329	-0.523426	1.885512
8	C	1.046815	-1.136637	1.327087
9	H	2.721735	0.619150	-0.657643
10	H	2.600490	0.488321	1.993865
11	H	0.481938	1.713345	-1.469681
12	H	1.465866	-2.054916	1.739401
13	H	-1.174830	-0.891691	2.113985
14	H	-0.999422	-0.754681	-1.321558

15	C	-0.167239	1.723548	0.606267
16	C	-1.948139	3.155654	0.325790
17	C	-0.759483	3.944105	0.862648
18	H	-2.084351	3.302106	-0.752147
19	H	-2.884981	3.359531	0.844547
20	H	-0.559412	4.866734	0.316644
21	H	-0.856863	4.153524	1.931079
22	O	-1.574952	1.800584	0.598459
23	O	0.334751	3.046589	0.632557
24	Br	0.255936	1.844258	3.550708
25	C	1.715797	-2.274878	-0.948391
26	O	1.103174	-3.105545	-1.575395
27	C	3.707608	-3.534980	-1.188508
28	H	4.746757	-3.429985	-0.884747
29	H	3.270310	-4.437786	-0.759809
30	H	3.626925	-3.579527	-2.275274
31	O	3.038720	-2.363055	-0.682776

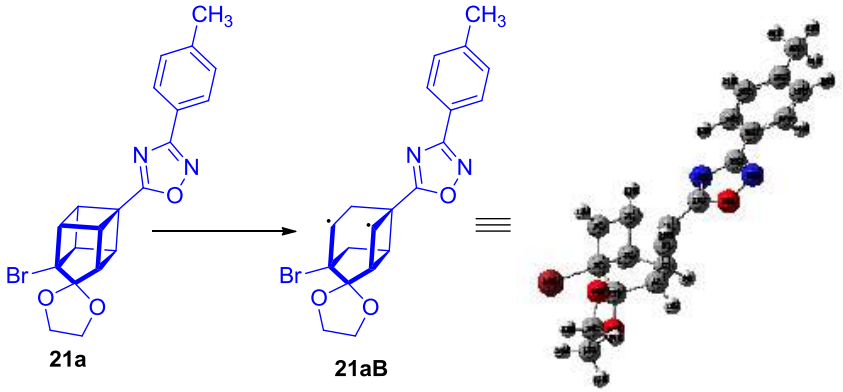
Table S42. Atomic coordinates for optimized structure of biradical **21aA** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.493981	-0.270319	-0.234414
2	C	2.712611	-0.402664	1.127067
3	C	2.284439	1.019659	0.863328
4	C	1.140636	1.080741	-0.239524
5	C	-0.000130	0.971449	1.739440
6	C	1.449355	0.906059	2.219185
7	C	0.159368	-0.506674	1.199567
8	C	1.550759	-0.643868	2.031507
9	H	3.031276	1.803746	0.761698
10	H	1.813986	1.445650	3.088372
11	H	1.457635	1.488780	-1.196604
12	H	1.578234	-1.385764	2.825385
13	H	-0.607188	-1.240261	1.434521
14	H	0.496648	-1.003785	-1.026908
15	C	5.427604	-2.530904	0.677363
16	C	6.218049	-3.758660	0.839390
17	C	7.480131	-3.889144	0.244250
18	C	5.712542	-4.820618	1.596033
19	C	8.213339	-5.057007	0.408915
20	H	7.877940	-3.073346	-0.346889
21	C	6.456085	-5.986028	1.753994
22	H	4.735967	-4.724977	2.053975
23	C	7.718311	-6.125669	1.168226
24	H	9.187705	-5.142852	-0.061490
25	H	6.046922	-6.801559	2.341568
26	N	5.861623	-1.500404	-0.033502
27	C	0.043175	1.905552	0.504075
28	C	-1.409888	3.386121	-0.496225
29	C	-0.619547	4.109940	0.585977

30	H	-1.030563	3.612454	-1.499360
31	H	-2.483848	3.569005	-0.459032
32	H	-0.213827	5.071819	0.271835
33	H	-1.202021	4.230893	1.504180
34	O	0.478840	3.215616	0.807647
35	O	-1.180721	2.008236	-0.180158
36	Br	-1.380014	1.314612	3.066664
37	C	3.864166	-1.127061	0.843861
38	O	4.838806	-0.562008	0.067891
39	N	4.199365	-2.347963	1.238737
40	C	8.536297	-7.377654	1.366425
41	H	9.261047	-7.246399	2.177607
42	H	7.904632	-8.229996	1.625632
43	H	9.099915	-7.632555	0.465493

Table S43. Atomic coordinates for optimized structure of biradical **21aB** obtained using the B3LYP/6-311++G(d,p) level of theory

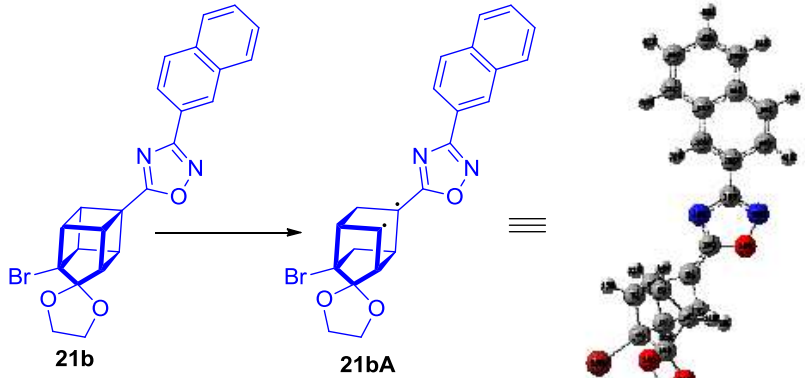


Center	Atomic	Coordinates (Angstroms)		

Number	Symbol	X	Y	Z
1	C	1.573274	0.193979	-0.695283
2	C	2.342461	-0.481269	0.391704
3	C	2.560949	0.956292	1.038226
4	C	1.568029	1.535671	-0.021785
5	C	0.247278	0.920901	1.942344
6	C	1.728641	0.566797	2.281703
7	C	0.022229	-0.501004	1.583450
8	C	1.458944	-0.865991	1.709741
9	H	3.549392	1.394799	1.145922
10	H	2.099211	0.750581	3.285011
11	H	1.894594	2.389342	-0.621243
12	H	1.779438	-1.794602	2.180783
13	H	-0.856831	-1.008434	1.208041
14	H	1.057700	-0.189175	-1.566591
15	C	4.984130	-2.840508	0.071490
16	C	5.906017	-3.885642	0.532400
17	C	6.894723	-4.400950	-0.317494
18	C	5.805469	-4.383385	1.835272
19	C	7.758225	-5.389364	0.134277
20	H	6.977740	-4.024078	-1.329630
21	C	6.677019	-5.374561	2.277097
22	H	5.041280	-3.990741	2.494226
23	C	7.668842	-5.893155	1.439449
24	H	8.515981	-5.779905	-0.537489
25	H	6.582653	-5.751626	3.290234
26	N	5.016140	-2.343510	-1.142360
27	C	0.273500	1.937087	0.760533
28	C	-1.315013	3.207015	-0.312958
29	C	-0.752707	4.009105	0.855004
30	H	-0.882829	3.519803	-1.270690

31	H	-2.402861	3.223700	-0.378945
32	H	-0.455928	5.024195	0.588606
33	H	-1.438307	4.030942	1.706084
34	O	0.431981	3.274553	1.193539
35	O	-0.910125	1.869570	0.000193
36	Br	-0.922709	1.550304	3.451171
37	C	3.436979	-1.421771	0.088979
38	O	3.984183	-1.393594	-1.139574
39	N	4.002496	-2.289764	0.873787
40	C	8.631939	-6.946135	1.928761
41	H	9.581841	-6.494278	2.235145
42	H	8.230722	-7.483848	2.790319
43	H	8.856950	-7.675151	1.146256

Table S44. Atomic coordinates for optimized structure of biradical **21bA** obtained using the B3LYP/6-311++G(d,p) level of theory

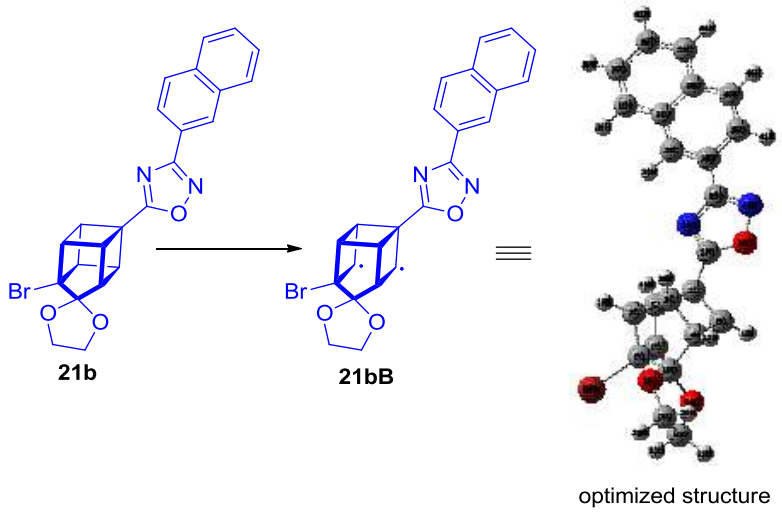


Center	Atomic	Coordinates (Angstroms)		
Number	Symbol	X	Y	Z

1	C	0.338042	-0.183508	-0.432735
2	C	2.440813	0.144012	1.071018
3	C	2.022274	1.420718	0.385806
4	C	0.969557	1.130882	-0.772245
5	C	-0.324651	1.548082	1.066625
6	C	1.082003	1.665514	1.652071
7	C	-0.109049	-0.016508	0.980064
8	C	1.211674	0.128222	1.917019
9	H	2.766244	2.168450	0.121068
10	H	1.370583	2.437697	2.359147
11	H	1.359472	1.262960	-1.778999
12	H	1.183281	-0.359890	2.887766
13	H	-0.885657	-0.677599	1.355266
14	H	0.409936	-1.109908	-0.982817
15	C	5.202398	-1.942030	1.426540
16	N	5.687285	-1.123343	0.505424
17	C	-0.190810	2.097718	-0.375688
18	C	-1.564444	3.188639	-1.866866
19	C	-0.866408	4.215485	-0.984442
20	H	-1.106069	3.124925	-2.860494
21	H	-2.638389	3.346140	-1.966647
22	H	-0.437035	5.053634	-1.533784
23	H	-1.522259	4.585506	-0.190740
24	O	0.210567	3.452626	-0.424650
25	O	-1.358169	1.967759	-1.147362
26	Br	-1.811103	2.207578	2.133265
27	C	3.619001	-0.593662	1.088274
28	O	4.652219	-0.223746	0.270875
29	N	3.929099	-1.654920	1.819812
30	C	5.426164	-3.916533	2.888249
31	C	6.160287	-5.008573	3.413496
32	C	5.987437	-3.062374	1.961573
33	C	5.601801	-5.903513	4.364369

34	C	7.504740	-5.218660	2.972159
35	C	7.324950	-3.273202	1.524224
36	H	4.407251	-3.749743	3.217242
37	C	6.336921	-6.955917	4.855564
38	H	4.581732	-5.742735	4.697151
39	C	8.236272	-6.313038	3.499405
40	C	8.056899	-4.320561	2.018878
41	H	7.753516	-2.595144	0.797034
42	C	7.666777	-7.162375	4.419100
43	H	5.899915	-7.633035	5.580775
44	H	9.256081	-6.471306	3.164346
45	H	9.076774	-4.476507	1.683163
46	H	8.236511	-7.995952	4.814210

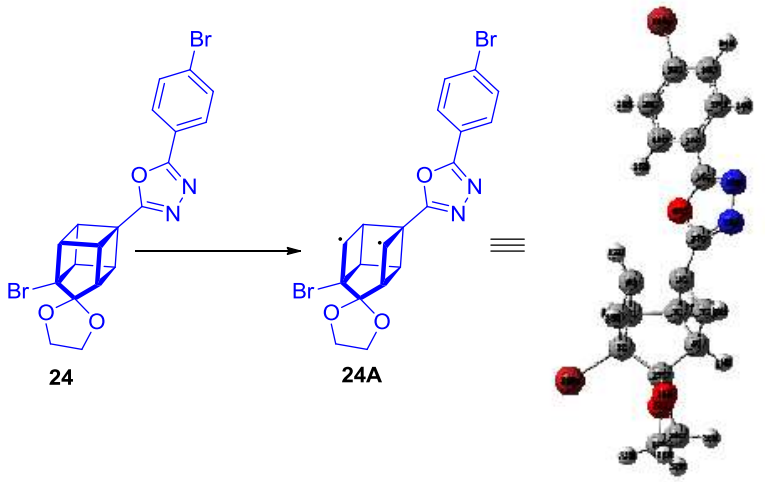
Table S45. Atomic coordinates for optimized structure of biradical **21bB** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.164179	-0.132806	-0.170195
2	C	2.516006	0.291058	0.552784
3	C	2.498284	1.533436	-0.274692
4	C	1.124644	1.285519	-0.827851
5	C	-0.121537	1.427293	1.271543
6	C	1.034426	1.716995	2.155311
7	C	0.377280	-0.047376	1.158771
8	C	1.661519	0.385666	1.943265
9	H	3.161771	2.387245	-0.321150
10	H	1.356105	2.637164	2.625512
11	H	1.013049	1.351652	-1.913616
12	H	2.112136	-0.177853	2.759527
13	H	-0.275724	-0.853831	1.476484
14	H	1.100931	-1.018325	-0.796862
15	C	5.191362	-1.999793	1.034785
16	N	5.674930	-1.350401	0.002317
17	C	-0.066633	2.043941	-0.161819
18	C	-1.714401	2.967478	-1.489874
19	C	-1.089345	4.056586	-0.625357
20	H	-1.356668	3.012881	-2.525134
21	H	-2.804660	2.966293	-1.477528
22	H	-0.826512	4.959663	-1.176860
23	H	-1.718535	4.311211	0.231768
24	O	0.127626	3.439197	-0.181822
25	O	-1.260072	1.762793	-0.864037
26	Br	-1.890678	1.748888	2.173154
27	C	3.712124	-0.567432	0.629847
28	O	4.691903	-0.389976	-0.275447
29	N	3.962112	-1.534715	1.460985

30	C	5.324168	-3.770319	2.744434
31	C	5.983665	-4.853346	3.376855
32	C	5.898047	-3.115439	1.674347
33	C	5.410793	-5.543408	4.477595
34	C	7.264535	-5.265596	2.891919
35	C	7.172842	-3.527059	1.193583
36	H	4.353492	-3.452429	3.106107
37	C	6.072880	-6.591416	5.071551
38	H	4.438768	-5.229428	4.843199
39	C	7.921375	-6.349843	3.527079
40	C	7.831279	-4.570482	1.788851
41	H	7.612164	-3.003768	0.353633
42	C	7.339988	-6.998146	4.591764
43	H	5.625969	-7.111394	5.911304
44	H	8.893322	-6.661824	3.159288
45	H	8.803263	-4.880132	1.419441
46	H	7.852263	-7.826154	5.068749

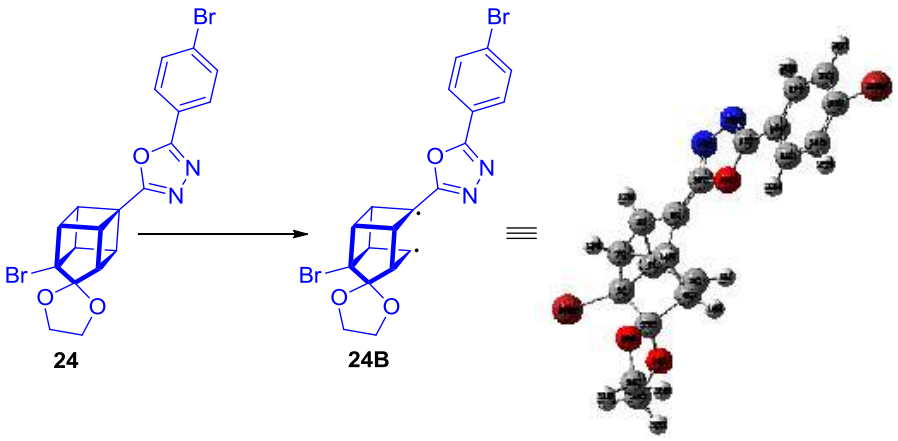
Table S46. Atomic coordinates for optimized structure of biradical **24A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.450518	0.213715	-0.809605
2	C	2.219272	-0.536409	0.222617
3	C	2.509770	0.849015	0.936116
4	C	1.524502	1.522365	-0.076185
5	C	0.211853	0.879285	1.882503
6	C	1.680289	0.442793	2.177343
7	C	-0.085604	-0.512885	1.463928
8	C	1.330647	-0.948986	1.551643
9	H	3.515894	1.244543	1.048839
10	H	2.074671	0.566734	3.180930
11	H	1.880689	2.385545	-0.644429
12	H	1.606068	-1.913702	1.979030

13	H	-0.990837	-0.959946	1.074569
14	H	0.922045	-0.106335	-1.697124
15	C	4.837989	-2.910709	0.029912
16	C	5.860651	-3.703230	0.699471
17	C	6.664648	-4.567861	-0.057140
18	C	6.056171	-3.616935	2.083325
19	C	7.646924	-5.332608	0.558000
20	H	6.511998	-4.632724	-1.127197
21	C	7.038458	-4.380540	2.705869
22	H	5.441340	-2.951496	2.676244
23	C	7.825705	-5.232570	1.936995
24	H	8.267023	-5.999172	-0.027014
25	H	7.188206	-4.312270	3.775390
26	N	4.545648	-2.869646	-1.232614
27	C	0.267356	1.949836	0.751740
28	C	-1.270296	3.353830	-0.222942
29	6	-0.642787	4.066416	0.970115
30	H	-0.840179	3.689758	-1.173657
31	H	-2.356656	3.431628	-0.264402
32	H	-0.295202	5.075487	0.745569
33	H	-1.310827	4.085135	1.835163
34	O	0.505116	3.253036	1.248976
35	O	-0.932439	1.982674	0.016452
36	Br	-0.902268	1.487165	3.441116
37	C	3.234454	-1.513121	-0.189147
38	Br	9.179235	-6.284507	2.787609
39	N	3.503484	-1.959625	-1.374685
40	O	4.043055	-2.075325	0.762912

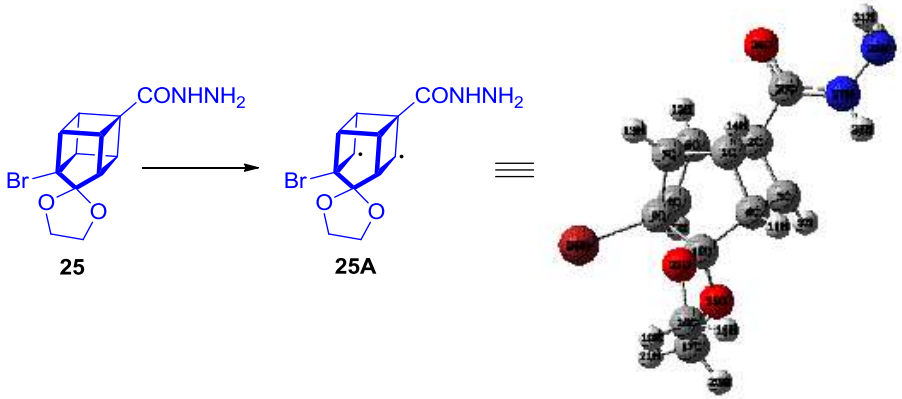
Table S47. Atomic coordinates for optimized structure of biradical **24B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.689199	0.013400	0.392865
2	C	1.601057	-1.279922	1.166240
3	C	1.410222	0.818296	2.706472
4	C	1.915741	1.250690	1.365419
5	C	-0.356381	1.129055	1.135394
6	C	0.038901	0.305252	2.426529
7	C	0.097668	-0.060788	0.290087
8	C	0.168677	-1.033826	1.511591
9	H	1.976397	0.694477	3.617324
10	H	-0.666748	0.248787	3.250797
11	H	2.908404	1.693143	1.316966
12	H	-0.523018	-1.844117	1.726244
13	H	-0.339648	-0.309574	-0.672542
14	H	2.276599	0.064456	-0.521555

15	C	4.175075	-3.606263	1.112280
16	C	5.512363	-4.004905	0.715989
17	C	5.993717	-5.271832	1.083354
18	C	6.334842	-3.147011	-0.028086
19	C	7.270561	-5.672356	0.715575
20	H	5.357608	-5.933832	1.657355
21	C	7.615028	-3.543301	-0.399283
22	H	5.972454	-2.168312	-0.316260
23	C	8.072627	-4.803273	-0.023816
24	H	7.640231	-6.648969	0.999646
25	H	8.248221	-2.879438	-0.973125
26	N	3.301571	-4.295289	1.800409
27	C	0.748152	2.195030	0.934926
28	C	0.990227	4.039968	-0.425920
29	C	0.381133	4.466635	0.903297
30	H	2.058580	4.279454	-0.480522
31	H	0.477897	4.443273	-1.299584
32	H	0.849859	5.346533	1.344437
33	H	-0.699681	4.617764	0.828217
34	O	0.671877	3.342332	1.744705
35	O	0.800859	2.620983	-0.412651
36	Br	-2.200724	1.723514	0.966213
37	C	2.428609	-2.372311	1.314049
38	Br	9.834534	-5.351721	-0.529973
39	N	2.183422	-3.528609	1.937659
40	O	3.700474	-2.379033	0.765509

Table S48. Atomic coordinates for optimized structure of biradical **25A** obtained using the B3LYP/6-311++G(d,p) level of theory

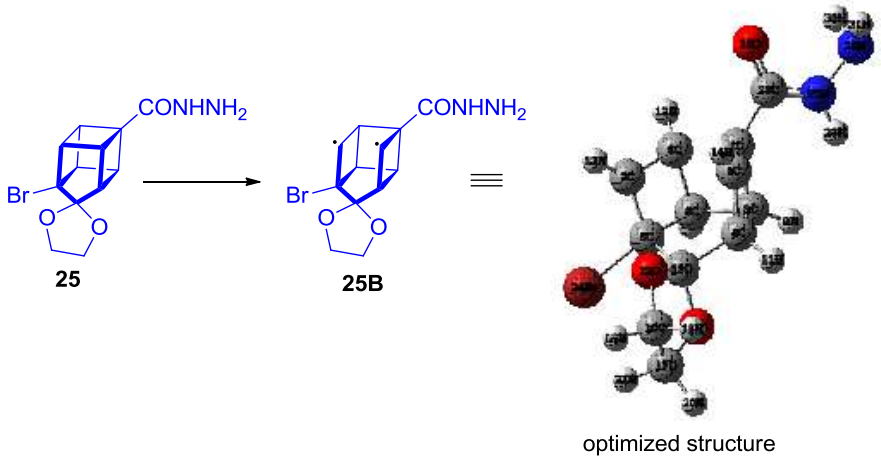


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.008852	-0.839144	-0.067484
2	C	1.545136	-1.089873	0.086650
3	C	1.773786	0.239216	-0.558925
4	C	0.316669	0.612903	-0.549346
5	C	0.023299	0.708271	1.876300
6	C	1.419057	0.367528	2.247480
7	C	-0.194913	-0.781718	1.467252
8	C	1.336141	-1.013758	1.704179
9	H	2.661629	0.856702	-0.646809
10	H	2.222094	0.984168	2.630310
11	H	-0.114771	0.959088	-1.492706
12	H	1.759824	-1.873255	2.222577
13	H	-0.969514	-1.359814	1.960662
14	H	-0.642970	-1.480663	-0.674028
15	C	-0.158039	1.571970	0.586951

16	C	-1.623444	3.296135	0.116095
17	C	-0.352329	3.861786	0.739344
18	H	-1.657746	3.464903	-0.966610
19	H	-2.540734	3.666611	0.574789
20	H	0.052265	4.724437	0.209428
21	H	-0.487620	4.100405	1.797589
22	O	-1.520003	1.895642	0.392354
23	O	0.574033	2.776119	0.589590
24	Br	-1.044281	1.418612	3.429129
25	C	2.207587	-2.369225	-0.368587
26	O	2.061151	-3.434935	0.212925
27	N	2.971039	-2.249866	-1.495348
28	H	2.947007	-1.394744	-2.030614
29	N	3.549413	-3.357124	-2.140290
30	H	4.330951	-3.683768	-1.577000
31	H	2.866474	-4.112144	-2.146700

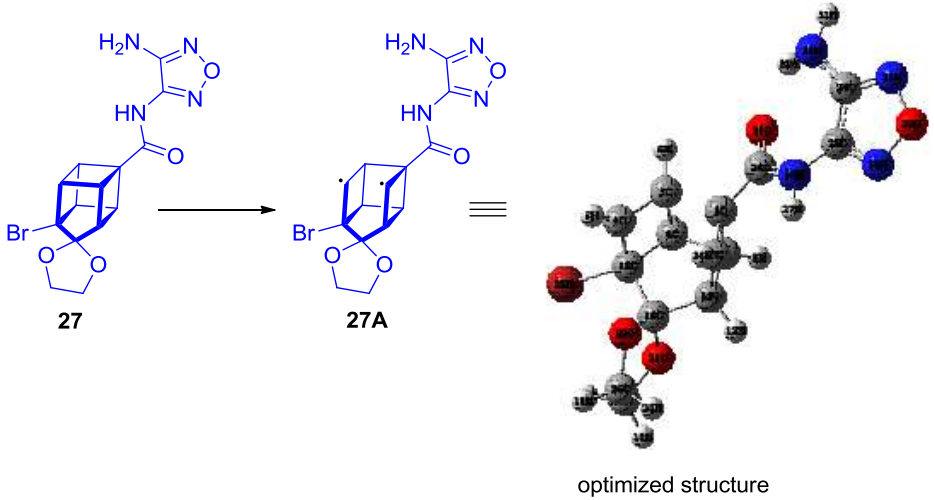
Table S49. Atomic coordinates for optimized structure of biradical **25B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.033481	-0.614195	-0.697800
2	C	1.255468	-1.185053	-0.058612
3	C	1.881808	0.262263	-0.072724
4	C	0.497260	0.809352	-0.560357
5	C	0.484163	0.908136	1.881494
6	C	1.870045	0.320688	1.475762
7	C	0.001720	-0.473372	2.124777
8	C	1.230290	-1.107008	1.578095
9	H	2.781030	0.542584	-0.618619
10	H	2.752543	0.623022	2.030934
11	H	0.473880	1.429577	-1.460340
12	H	1.682231	-1.971485	2.065743
13	H	-0.966490	-0.846116	2.431630
14	H	-0.928321	-1.052924	-0.930826
15	C	-0.094139	1.634643	0.628870
16	C	-1.921372	2.987690	0.267992
17	C	-0.735710	3.856513	0.672030
18	H	-2.101581	3.016813	-0.813026
19	H	-2.843588	3.222769	0.799492
20	H	-0.579829	4.717809	0.021496
21	H	-0.800464	4.180214	1.714083
22	O	-1.501854	1.677328	0.664656
23	O	0.373623	2.964174	0.499564
24	Br	0.420249	2.065950	3.526633
25	C	1.820414	-2.482232	-0.585404
26	O	1.235039	-3.544622	-0.444428
27	N	3.031144	-2.388490	-1.212217
28	H	3.421056	-1.489802	-1.445747
29	N	3.640377	-3.486365	-1.847894

30	H	3.964260	-4.130165	-1.130168
31	H	2.925604	-3.983233	-2.375934

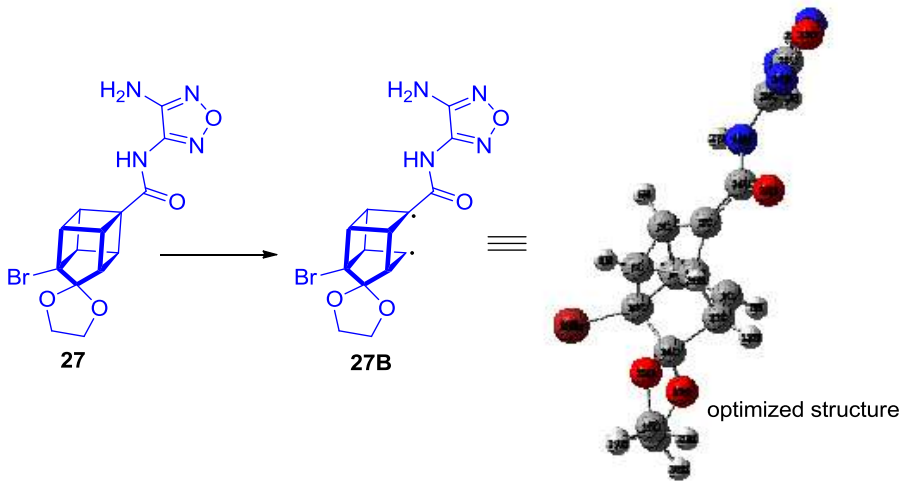
Table S50. Atomic coordinates for optimized structure of biradical **27A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.040833	0.729768	-2.752018
2	C	0.053167	-0.351064	-1.595568
3	C	1.460228	-0.847099	-2.261811
4	C	1.287236	0.241043	-3.373775
5	H	-0.928910	0.843508	-3.368117
6	H	1.481851	-1.921133	-2.443122
7	H	1.363513	0.026566	-4.434627
8	C	2.647371	-0.099199	-1.770521
9	H	3.348067	-0.238701	-0.957660
10	C	2.423031	1.053520	-2.678471

11	C	0.319688	1.825123	-1.695620
12	H	-0.333699	2.697010	-1.609591
13	C	0.204234	0.775754	-0.624890
14	C	1.765901	2.317025	-2.037773
15	C	2.519105	4.450326	-2.505916
16	C	2.619216	4.193362	-1.007160
17	H	3.488450	4.364535	-3.002996
18	H	2.049530	5.400969	-2.759850
19	H	3.576998	4.478912	-0.572335
20	H	1.804521	4.673305	-0.452936
21	O	1.647610	3.396664	-2.940957
22	O	2.500264	2.767196	-0.922864
23	Br	4.036056	1.507823	-3.784321
24	C	-0.963088	-1.452167	-1.445246
25	O	-1.009734	-2.408512	-2.206941
26	N	-1.837908	-1.280019	-0.398660
27	H	-1.791905	-0.395366	0.092623
28	C	-2.946349	-2.073934	-0.099372
29	C	-3.163391	-3.494060	-0.240303
30	N	-2.289705	-4.440592	-0.705926
31	H	-2.698713	-5.355090	-0.837228
32	H	-1.703249	-4.113976	-1.467575
33	O	-4.849596	-2.563942	0.721475
34	N	-3.983289	-1.540477	0.481192
35	N	-4.344387	-3.766400	0.253901
36	H	0.510003	0.791412	0.416282

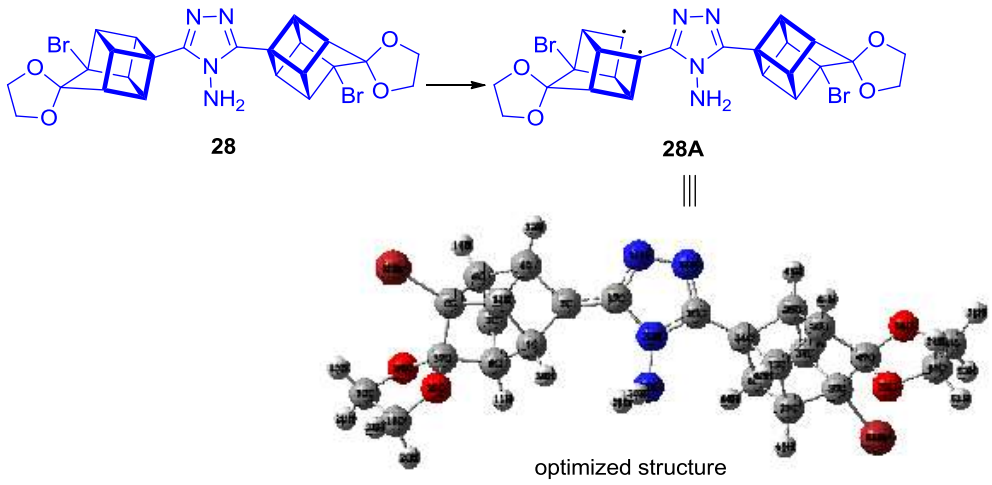
Table S51. Atomic coordinates for optimized structure of biradical **27B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.036774	1.768478	-0.765704
2	C	0.202859	-0.703843	-1.615051
3	C	-0.304611	0.179641	-2.708954
4	C	-0.354184	1.723112	-2.205895
5	H	-0.442947	2.357030	0.002847
6	H	-1.078133	-0.119662	-3.415452
7	H	-1.218093	2.301904	-2.520210
8	C	1.187284	0.468912	-3.081560
9	H	1.715297	0.000169	-3.906467
10	C	1.036330	1.981109	-2.930328
11	C	1.473089	1.342611	-0.773246
12	H	1.997800	1.318737	0.178753
13	C	1.533603	-0.009950	-1.597349
14	C	2.041768	2.366260	-1.816702
15	C	3.183316	4.361788	-1.724026

16	C	4.182806	3.214511	-1.785210
17	H	3.057644	4.845413	-2.696965
18	H	3.407931	5.107650	-0.961617
19	H	4.981335	3.358497	-2.513009
20	H	4.613363	2.993328	-0.802058
21	O	1.973891	3.689341	-1.343151
22	O	3.369227	2.121365	-2.226619
23	Br	1.028057	3.068471	-4.542276
24	C	-0.234349	-1.885321	-0.913478
25	O	0.472567	-2.490575	-0.121626
26	N	-1.553455	-2.280002	-1.207132
27	H	-2.094220	-1.696187	-1.828736
28	C	-2.195098	-3.415789	-0.742612
29	C	-3.616176	-3.519781	-0.540402
30	N	-4.553373	-2.534353	-0.816328
31	H	-5.501141	-2.827259	-0.613605
32	H	-4.349016	-1.642702	-0.380902
33	O	-2.677929	-5.378123	-0.073222
34	N	-1.641222	-4.559156	-0.449529
35	N	-3.894682	-4.723578	-0.134054
36	H	2.434971	-0.589953	-1.416801

Table S52. Atomic coordinates for optimized structure of biradical **28A** obtained using the B3LYP/6-311++G(d,p) level of theory

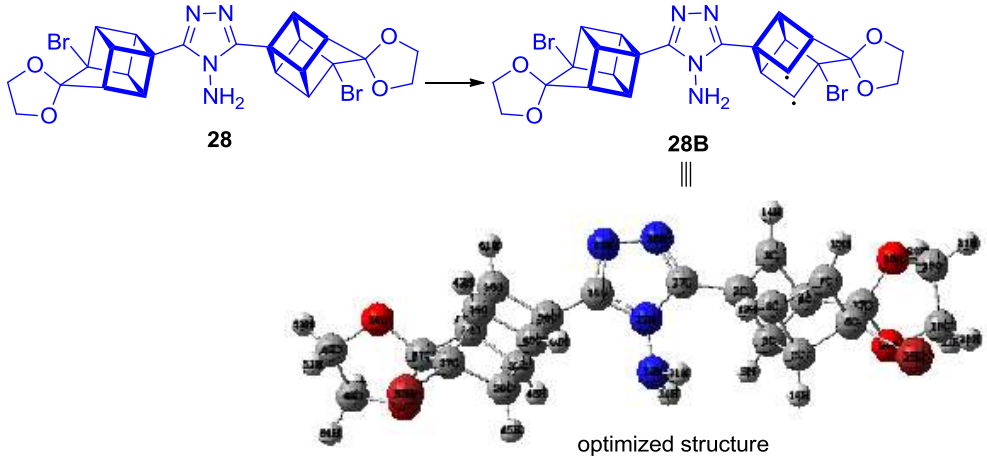


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.300350	1.615899	0.462168
2	C	1.407049	1.216055	1.419196
3	C	-0.595906	-0.474781	1.418408
4	C	-1.026877	0.782787	0.728970
5	C	0.077009	-0.417772	-0.875348
6	C	0.486889	-1.007975	0.542716
7	C	1.055169	0.729295	-0.627381
8	C	1.740506	0.023745	0.582310
9	H	-1.147735	-1.019377	2.169740
10	H	0.729345	-2.063940	0.618233
11	H	-1.848615	1.345730	1.168878
12	H	2.732042	-0.420849	0.582588
13	H	1.581429	1.243940	-1.426521
14	H	0.102340	2.659662	0.224017

15	C	2.575589	2.988790	4.285555
16	N	3.400779	1.958290	4.248830
17	C	-1.325484	0.214957	-0.698255
18	C	-2.899115	1.013363	-2.190554
19	C	-3.163542	-0.458945	-1.901253
20	H	-3.601730	1.666320	-1.660100
21	H	-2.896988	1.261912	-3.252256
22	H	-4.208936	-0.690227	-1.696738
23	H	-2.785459	-1.106089	-2.697647
24	O	-2.420496	-0.667432	-0.692807
25	O	-1.573208	1.201201	-1.682802
26	Br	0.357518	-1.536778	-2.443581
27	C	2.018522	1.730195	2.558163
28	N	3.071507	1.172345	3.185546
29	N	0.665004	3.824066	3.000570
30	H	0.790553	4.234714	2.080380
31	H	-0.234874	3.352913	3.030323
32	N	1.685887	2.899236	3.243940
33	C	2.923224	5.588223	5.000628
34	C	2.595408	4.066786	5.273459
35	C	3.642140	4.141233	6.431791
36	C	4.187635	5.500492	5.903372
37	C	2.528637	6.115384	7.351239
38	C	2.495381	4.565424	7.431927
39	C	1.775435	6.006341	5.998182
40	C	1.453523	4.500194	6.264869
41	H	4.303861	3.322901	6.697808
42	H	2.406723	4.058910	8.388539
43	H	5.163990	5.505181	5.423432
44	H	0.457233	4.070097	6.328803
45	H	1.055965	6.761921	5.696888
46	H	2.954637	6.046539	4.015413
47	C	3.985926	6.520018	7.030691

48	C	5.225975	8.446115	7.268053
49	C	5.353531	7.605727	8.532992
50	H	6.111344	8.352808	6.627852
51	H	5.016830	9.499803	7.454686
52	H	6.378155	7.496466	8.889841
53	H	4.715371	7.981925	9.338236
54	O	4.897695	6.321006	8.092391
55	O	4.084703	7.871154	6.624278
56	Br	1.637645	7.094685	8.786630

Table S53. Atomic coordinates for optimized structure of biradical **28B** obtained using the B3LYP/6-311++G(d,p) level of theory

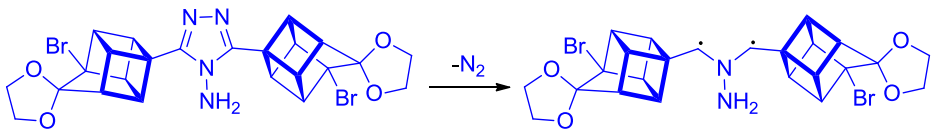


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	1.288625	1.618801	-0.336193
2	C	1.002990	1.634450	1.126162
3	C	-0.502927	1.982524	0.770888
4	C	-0.151662	1.760352	-0.737999

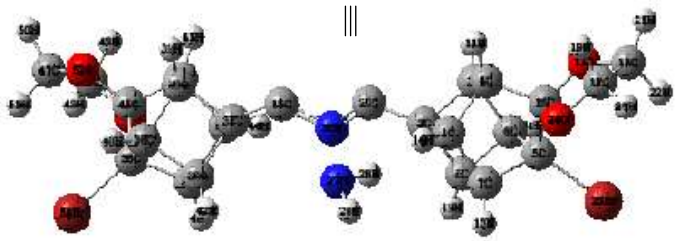
5	C	-0.945810	-0.378863	0.128025
6	C	-1.004673	0.624823	1.320834
7	C	0.356483	-0.868044	0.641583
8	C	0.450885	0.176422	1.689997
9	H	-0.987791	2.912504	1.061329
10	H	-1.847029	0.570032	2.004378
11	H	-0.389929	2.561393	-1.442904
12	H	0.807596	-0.074969	2.691299
13	H	1.045694	-1.602446	0.246503
14	H	2.199648	1.452890	-0.893564
15	C	2.761471	3.392376	3.777364
16	N	3.677999	3.361979	2.838820
17	C	-0.901489	0.462111	-1.182735
18	C	-1.029858	-0.051947	-3.421448
19	C	-2.438047	0.186132	-2.889301
20	H	-0.649029	0.813814	-3.975463
21	H	-0.932949	-0.949625	-4.032039
22	H	-3.034271	0.858820	-3.506776
23	H	-2.978027	-0.749763	-2.724323
24	O	-2.188216	0.838597	-1.636331
25	O	-0.270186	-0.246192	-2.223135
26	Br	-2.355860	-1.813936	0.069506
27	C	1.911318	2.374817	2.024785
28	N	3.140422	2.725766	1.736326
29	N	0.432846	2.667317	4.055550
30	H	-0.322433	3.129395	3.559086
31	H	0.193933	1.690047	4.189839
32	N	1.619664	2.773677	3.316762
33	C	2.110527	5.229912	5.670794
34	C	2.903133	3.986556	5.108828
35	C	4.203526	4.712982	5.584060
36	C	3.428980	6.048481	5.786680
37	C	3.252187	5.012894	7.817710

38	C	4.081974	3.997171	6.987233
39	C	1.988980	4.509752	7.069070
40	C	2.775142	3.280330	6.507518
41	H	5.145811	4.672479	5.046631
42	H	4.952098	3.507318	7.414391
43	H	3.601589	6.851417	5.073075
44	H	2.526112	2.237028	6.685456
45	H	1.024450	4.469458	7.566446
46	H	1.214975	5.648059	5.218435
47	C	3.577328	6.420597	7.266452
48	C	3.389992	8.565193	8.086942
49	C	4.755701	8.000330	8.458900
50	H	3.453463	9.257650	7.239059
51	H	2.869841	9.046782	8.915492
52	H	5.584402	8.681219	8.262037
53	H	4.787260	7.663934	9.499457
54	O	4.877685	6.883970	7.568899
55	O	2.655655	7.393933	7.718245
56	Br	3.279288	4.799886	9.758652

Table S54. Atomic coordinates for optimized structure of biradical **28C** obtained using the B3LYP/6-311++G(d,p) level of theory



28 **28C**



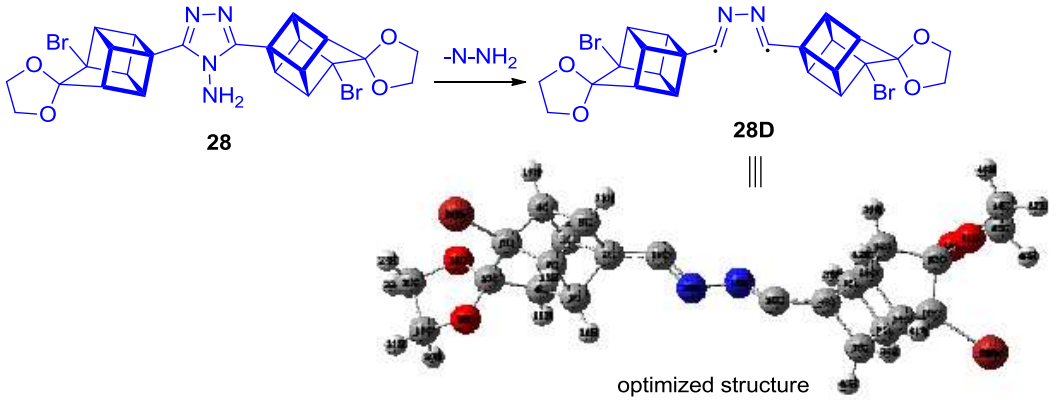
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.942534	0.750184	0.314306
2	C	0.448452	1.784480	1.414695
3	C	-0.593498	2.244600	0.308031
4	C	0.173259	1.491057	-0.811642
5	C	-1.330537	-0.053760	-0.045038
6	C	-1.628542	1.183935	0.841280
7	C	-0.089766	-0.313358	0.849618
8	C	-0.609030	0.698228	1.921850
9	H	-0.911201	3.277130	0.190628
10	H	-2.650780	1.496900	1.035306
11	H	0.744520	2.076715	-1.527546
12	H	-0.877000	0.428776	2.941661
13	H	0.252235	-1.325161	1.049606
14	H	1.984054	0.461000	0.202281
15	C	2.457695	3.856381	3.657984

16	C	-0.811318	0.473839	-1.402766
17	C	-0.642434	-0.402966	-3.525535
18	C	-1.995603	0.281020	-3.369375
19	H	0.064382	0.218065	-4.088566
20	H	-0.696554	-1.395521	-3.973599
21	H	-2.257596	0.937189	-4.200025
22	H	-2.799479	-0.440405	-3.195120
23	O	-1.794240	1.094860	-2.207258
24	O	-0.206645	-0.547561	-2.170599
25	Br	-2.696097	-1.448176	-0.104103
26	C	1.379101	2.748545	1.967674
27	N	0.930262	2.172565	4.397076
28	H	-0.072320	2.297944	4.284073
29	H	1.126220	1.187315	4.239774
30	N	1.572137	2.909161	3.262563
31	C	2.024564	4.916110	6.113682
32	C	2.905978	4.266001	4.949033
33	C	3.907474	5.457484	5.203658
34	C	2.850389	6.228995	6.043581
35	C	3.961641	4.973856	7.596574
36	C	4.676160	4.590306	6.273452
37	C	2.795345	4.039620	7.168915
38	C	3.678282	3.410283	6.045958
39	H	4.473280	5.941744	4.412351
40	H	5.759096	4.522783	6.224726
41	H	2.385142	7.105292	5.596872
42	H	3.940230	2.359129	5.961848
43	H	2.227169	3.478774	7.904736
44	H	0.938486	4.917259	6.121526
45	C	3.461831	6.427910	7.435623
46	C	2.849231	8.100562	8.896446
47	C	4.343933	8.198497	8.615349
48	H	2.279655	8.848593	8.332139

49	H	2.592310	8.164580	9.954152
50	H	4.686216	9.208459	8.387529
51	H	4.939458	7.776776	9.430351
52	O	4.484312	7.404279	7.430787
53	O	2.529909	6.783644	8.437842
54	Br	4.886279	4.537621	9.259472

Table S55. Atomic coordinates for optimized structure of biradical **28D** obtained using the B3LYP/6-311++G(d,p) level of theory

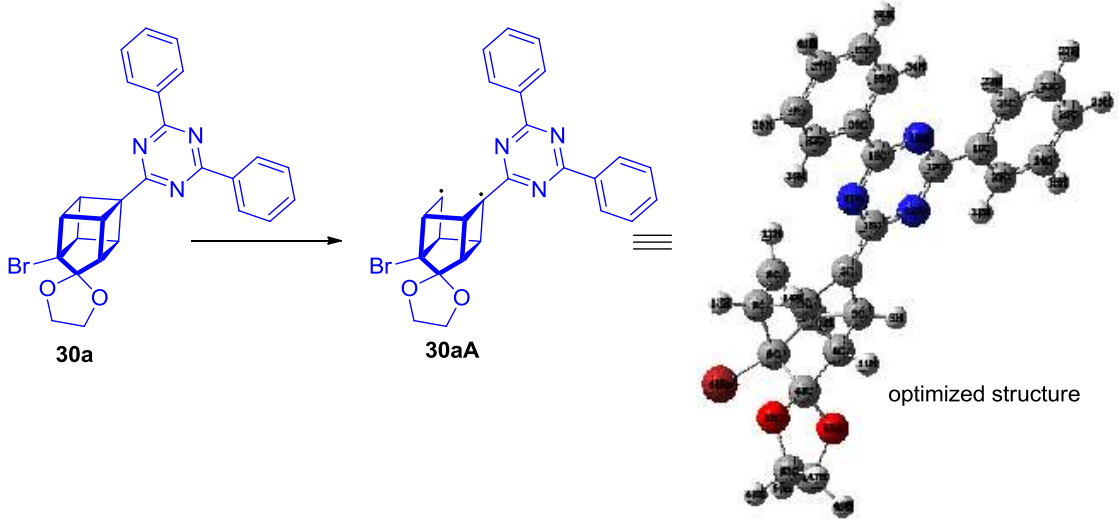


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.047418	0.535800	0.558006
2	C	-0.303570	2.000578	1.057211
3	C	-0.517973	2.360238	-0.465074
4	C	0.178722	1.041024	-0.906467
5	C	-2.025481	0.458407	-0.734633
6	C	-2.039368	1.960581	-0.344669
7	C	-1.475866	0.150870	0.685606

8	C	-1.821242	1.600998	1.161252
9	H	-0.255964	3.319908	-0.902615
10	H	-2.801136	2.629921	-0.733167
11	H	1.176208	1.110986	-1.335341
12	H	-2.487502	1.856745	1.980881
13	H	-1.752280	-0.761121	1.206560
14	H	0.799895	-0.096484	1.020064
15	C	2.415481	3.215421	4.695047
16	N	1.977539	3.489757	3.561551
17	C	-0.856525	0.261163	-1.726695
18	C	-0.312787	-1.315660	-3.312845
19	C	-1.152970	-0.221234	-3.960162
20	H	0.753006	-1.199780	-3.542968
21	H	-0.634185	-2.327334	-3.561309
22	H	-0.750729	0.144533	-4.905413
23	H	-2.193928	-0.530791	-4.091923
24	O	-1.065224	0.839439	-2.999880
25	O	-0.545713	-1.103525	-1.917022
26	Br	-3.735988	-0.344894	-1.219732
27	C	0.424768	2.809678	2.005016
28	N	1.364960	2.522395	2.770078
29	C	2.527363	4.541434	7.017848
30	C	3.133510	4.017454	5.655707
31	C	3.710416	5.484147	5.466394
32	C	2.797022	6.017329	6.604713
33	C	4.707528	5.397871	7.698277
34	C	5.021911	5.040603	6.219567
35	C	3.845221	4.109431	7.769488
36	C	4.443357	3.600203	6.417466
37	H	3.786306	5.986626	4.506552
38	H	5.989412	5.272033	5.783708
39	H	1.944725	6.633919	6.327580
40	H	4.991320	2.672869	6.272477

41	H	3.773350	3.535582	8.688671
42	H	1.565025	4.225145	7.411249
43	C	3.731515	6.597649	7.674104
44	C	3.146741	8.214152	9.210607
45	C	4.344643	8.692367	8.398885
46	H	2.215036	8.685971	8.877138
47	H	3.260582	8.344861	10.287053
48	H	4.255705	9.717625	8.038885
49	H	5.283097	8.566599	8.946609
50	O	4.309050	7.819101	7.262810
51	O	3.118498	6.810574	8.930482
52	Br	6.227449	5.514061	8.917055

Table S56. Atomic coordinates for optimized structure of biradical **30aA** obtained using the B3LYP/6-311++G(d,p) level of theory

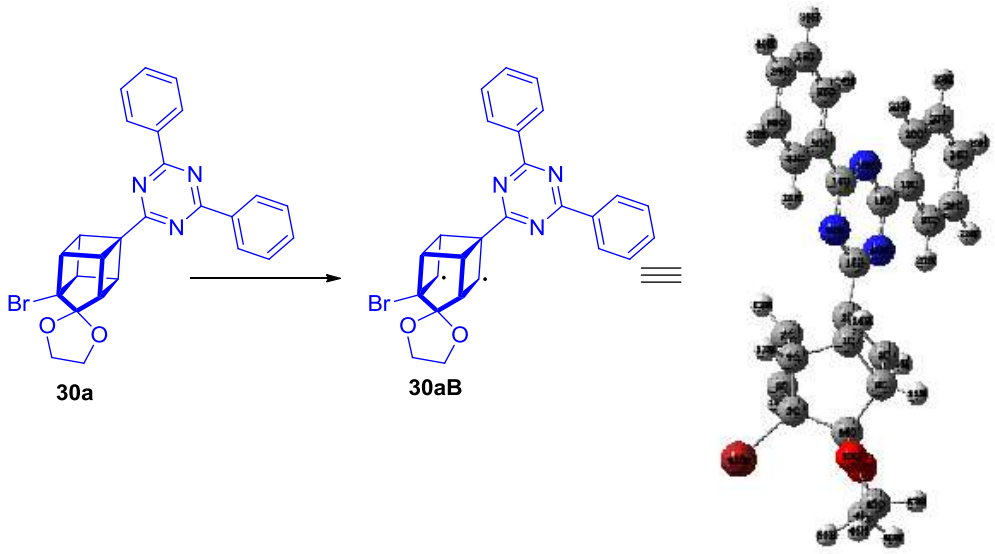


Center	Atomic	Coordinates (Angstroms)		
Number	Symbol	X	Y	Z

1	C	-0.058932	-0.844023	-0.014752
2	C	1.278993	-1.027603	-0.663851
3	C	1.599826	0.415954	-0.427748
4	C	0.045638	0.628807	-0.559688
5	C	0.373609	0.917566	1.652907
6	C	1.830769	0.616809	1.167400
7	C	0.186383	-0.634259	1.577595
8	C	1.667470	-0.722835	1.837853
9	H	2.313062	0.948932	-1.049842
10	H	2.647169	1.298097	1.396773
11	H	-0.337069	0.806491	-1.562632
12	H	2.339854	-1.558868	1.983592
13	H	-0.554663	-1.139097	2.193492
14	H	-0.898730	-1.490946	-0.251452
15	C	1.876275	-2.061900	-1.417153
16	C	1.827308	-4.187000	-2.222888
17	C	3.597052	-2.824082	-2.692150
18	N	3.015104	-4.028057	-2.832742
19	C	4.909103	-2.609471	-3.355377
20	C	5.502274	-3.632801	-4.106704
21	C	5.569725	-1.378737	-3.237571
22	C	6.730691	-3.428381	-4.727439
23	H	4.989252	-4.581047	-4.194903
24	C	6.797723	-1.177678	-3.859142
25	H	5.108315	-0.591783	-2.655777
26	C	7.381913	-2.201152	-4.605782
27	H	7.180732	-4.226709	-5.306873
28	H	7.300783	-0.222112	-3.761661
29	H	8.339235	-2.042891	-5.090047
30	C	1.155381	-5.505792	-2.352063
31	C	1.750177	-6.537416	-3.090584
32	C	-0.081934	-5.734577	-1.734097
33	C	1.119832	-7.772209	-3.208311

34	H	2.705207	-6.356508	-3.565287
35	C	-0.709540	-6.970084	-1.853863
36	H	-0.536576	-4.935423	-1.163617
37	C	-0.111147	-7.992413	-2.590792
38	H	1.588732	-8.563766	-3.782041
39	H	-1.666121	-7.137336	-1.371500
40	H	-0.601540	-8.955268	-2.682758
41	N	1.214115	-3.241389	-1.510292
42	N	3.075553	-1.811911	-1.998168
43	Br	0.203499	1.732611	3.418686
44	C	-0.412558	1.588387	0.528686
45	C	-2.329586	2.858316	0.400250
46	C	-1.127633	3.777940	0.583550
47	H	-2.677848	2.844820	-0.639144
48	H	-3.164333	3.083814	1.064197
49	H	-1.113001	4.626502	-0.101013
50	H	-1.034137	4.128467	1.615366
51	O	-0.029375	2.919057	0.248287
52	O	-1.804809	1.576571	0.763446

Table S57. Atomic coordinates for optimized structure of biradical **30aB** obtained using the B3LYP/6-311++G(d,p) level of theory



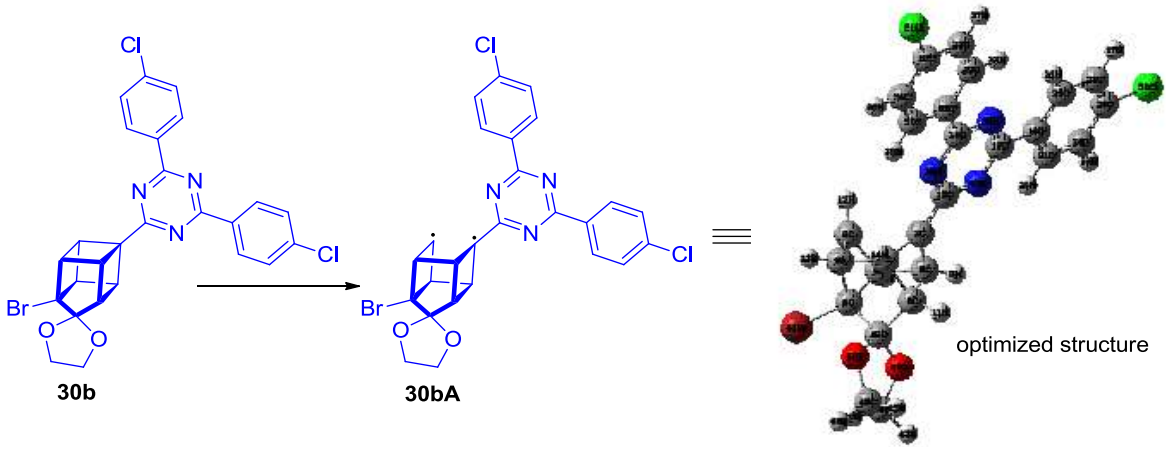
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.302574	-0.689001	-0.535631
2	C	1.244560	-0.898201	-0.713238
3	C	1.360261	0.531191	-1.108060
4	C	-0.074540	0.842112	-0.776892
5	C	0.051050	0.470632	1.632052
6	C	1.492116	0.121612	1.690543
7	C	-0.226704	-0.925280	0.991608
8	C	1.321515	-1.139398	0.932354
9	H	2.204018	1.157440	-1.364216
10	H	2.348420	0.693864	2.023150
11	H	-0.663162	1.337934	-1.554349

12	H	1.840396	-2.056599	1.211141
13	H	-0.905888	-1.609852	1.489668
14	H	-1.028921	-1.227728	-1.137759
15	C	1.883505	-1.997070	-1.487002
16	C	1.909290	-4.168398	-2.134148
17	C	3.567591	-2.759496	-2.794266
18	N	3.044355	-3.991463	-2.822690
19	C	4.831199	-2.518888	-3.532126
20	C	5.459000	-3.561831	-4.227316
21	C	5.412762	-1.243225	-3.541284
22	C	6.644905	-3.332237	-4.916727
23	H	5.006778	-4.544514	-4.217584
24	C	6.598765	-1.017609	-4.232047
25	H	4.923520	-0.442105	-3.003296
26	C	7.218036	-2.060400	-4.921159
27	H	7.123363	-4.145089	-5.451346
28	H	7.041081	-0.027778	-4.233677
29	H	8.142573	-1.882943	-5.459384
30	C	1.295794	-5.518736	-2.131838
31	C	1.901518	-6.575945	-2.824889
32	C	0.102389	-5.753101	-1.434345
33	C	1.324386	-7.841398	-2.819334
34	H	2.822049	-6.390521	-3.362017
35	C	-0.471902	-7.019876	-1.431346
36	H	-0.361107	-4.933878	-0.900795
37	C	0.136896	-8.067157	-2.123023
38	H	1.800322	-8.652936	-3.358168
39	H	-1.394799	-7.191481	-0.888916
40	H	-0.311777	-9.054361	-2.119397
41	N	1.293628	-3.196550	-1.444425
42	N	3.016594	-1.724885	-2.139436
43	Br	-0.732293	0.838189	3.451582
44	C	-0.360181	1.549543	0.582129

45	C	-1.913501	3.256126	0.686927
46	C	-0.566610	3.762964	1.190286
47	H	-2.128017	3.609793	-0.328520
48	H	-2.749225	3.499015	1.344039
49	H	-0.272464	4.724189	0.767727
50	H	-0.527574	3.805774	2.282181
51	O	0.341364	2.767307	0.699296
52	O	-1.741543	1.835862	0.688336

Table S58. Atomic coordinates for optimized structure of biradical **30bA** obtained using the B3LYP/6-311++G(d,p) level of theory

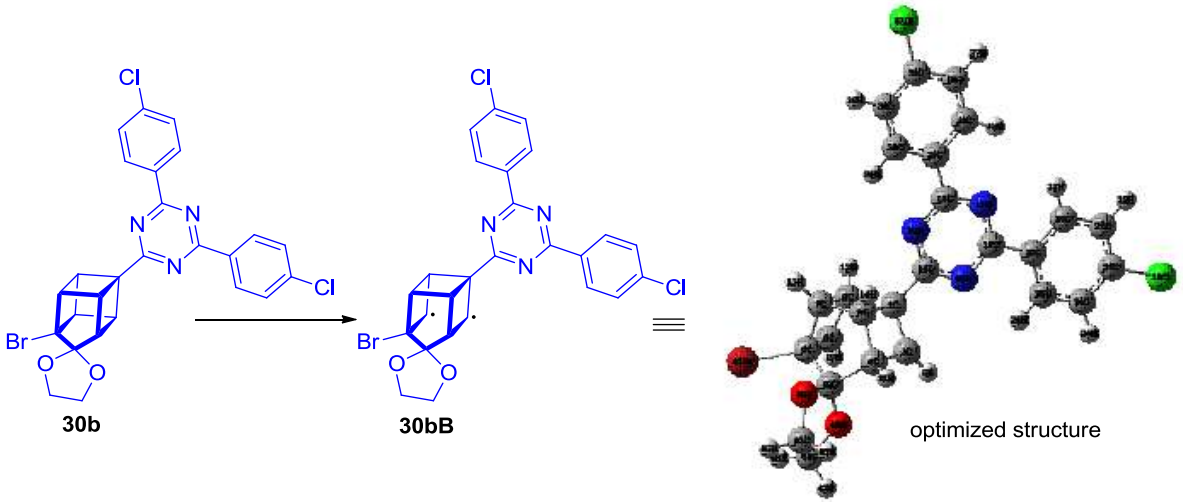


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.009095	-0.869214	0.066417
2	C	1.300402	-1.036167	-0.641759
3	C	1.609927	0.413147	-0.429145
4	C	0.048016	0.600971	-0.492895
5	C	0.471646	0.911008	1.701167
6	C	1.909965	0.629088	1.151856

7	C	0.305444	-0.644082	1.644462
8	C	1.798008	-0.707495	1.838445
9	H	2.285718	0.952084	-1.086863
10	H	2.725347	1.324329	1.338910
11	H	-0.382152	0.765659	-1.478632
12	H	2.490205	-1.530202	1.965870
13	H	-0.399147	-1.155686	2.296439
14	H	-0.848408	-1.530678	-0.127842
15	C	1.876940	-2.062680	-1.420282
16	C	1.817226	-4.184969	-2.232969
17	C	3.554497	-2.805807	-2.762704
18	N	2.979589	-4.015000	-2.887528
19	C	4.838863	-2.577318	-3.470705
20	C	5.412923	-3.587737	-4.252455
21	C	5.497186	-1.344824	-3.366905
22	C	6.615455	-3.377407	-4.917565
23	H	4.906957	-4.540246	-4.333914
24	C	6.699918	-1.122496	-4.026552
25	H	5.055642	-0.563580	-2.762596
26	C	7.249025	-2.143625	-4.797990
27	H	7.058064	-4.158793	-5.521878
28	H	7.208367	-0.170330	-3.945458
29	C	1.150671	-5.506422	-2.344806
30	C	1.721043	-6.530713	-3.110992
31	C	-0.060958	-5.749034	-1.684166
32	C	1.100165	-7.769792	-3.218928
33	H	2.656537	-6.345916	-3.621501
34	C	-0.691454	-6.983344	-1.784474
35	H	-0.502052	-4.959150	-1.090776
36	C	-0.103521	-7.984694	-2.553272
37	H	1.541850	-8.560776	-3.811314
38	H	-1.627241	-7.170385	-1.273555
39	N	1.224192	-3.249621	-1.491687

40	N	3.050466	-1.800226	-2.048031
41	Br	0.370296	1.735074	3.467220
42	C	-0.375836	1.561188	0.609446
43	C	-2.317524	2.798980	0.562808
44	C	-1.123491	3.738747	0.684888
45	H	-2.713820	2.773509	-0.458874
46	H	-3.123701	3.014578	1.264171
47	H	-1.154491	4.583197	-0.004042
48	H	-0.987099	4.096541	1.709297
49	O	-0.028011	2.895130	0.302951
50	O	-1.755133	1.527446	0.907180
51	Cl	-0.895047	-9.547241	-2.684975
52	Cl	8.768737	-1.869646	-5.635230

Table S59. Atomic coordinates for optimized structure of biradical **30bB** obtained using the B3LYP/6-311++G(d,p) level of theory

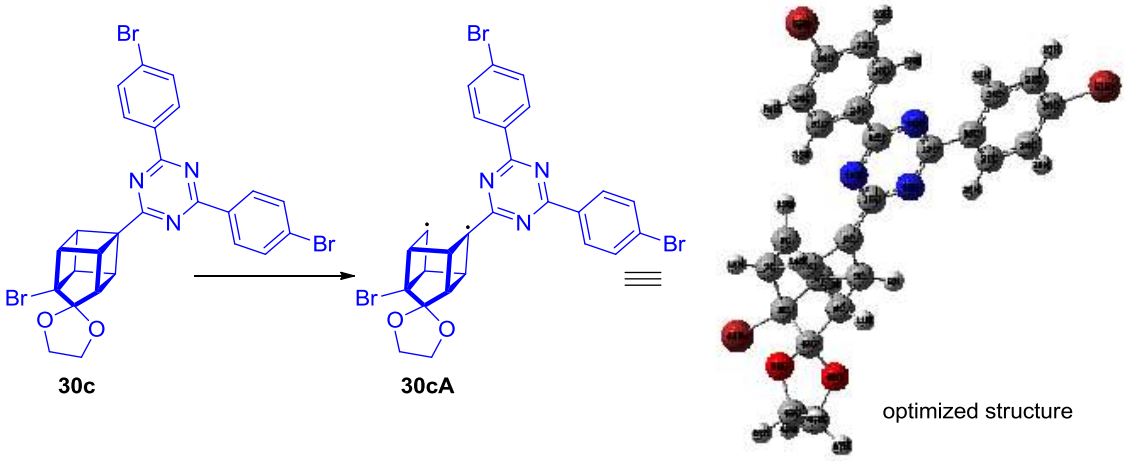


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.303457	-0.689233	-0.536666
2	C	1.243410	-0.899589	-0.715280
3	C	1.360705	0.530060	-1.108645
4	C	-0.073755	0.841671	-0.777120
5	C	0.051875	0.468564	1.632172
6	C	1.492793	0.117437	1.689948
7	C	-0.227529	-0.926582	0.990387
8	C	1.320286	-1.142746	0.931411
9	H	2.205860	1.156996	-1.358522
10	H	2.349897	0.686527	2.025760
11	H	-0.662017	1.338418	-1.554147
12	H	1.838345	-2.060722	1.209269
13	H	-0.907561	-1.610513	1.488169
14	H	-1.030776	-1.226416	-1.139049

15	C	1.881573	-1.997564	-1.488773
16	C	1.907007	-4.168039	-2.139740
17	C	3.566446	-2.761250	-2.794766
18	N	3.043256	-3.993213	-2.827017
19	C	4.829442	-2.519977	-3.530400
20	C	5.457521	-3.558091	-4.231220
21	C	5.414738	-1.246628	-3.534618
22	C	6.642933	-3.334988	-4.920901
23	H	5.007716	-4.541810	-4.229584
24	C	6.599898	-1.011660	-4.220948
25	H	4.929964	-0.444560	-2.994146
26	C	7.204447	-2.060561	-4.909220
27	H	7.128348	-4.136871	-5.462101
28	H	7.052014	-0.028220	-4.224402
29	C	1.291463	-5.515766	-2.140884
30	C	1.894950	-6.575208	-2.831166
31	C	0.095096	-5.750176	-1.449687
32	C	1.321241	-7.840721	-2.833921
33	H	2.818275	-6.396783	-3.365644
34	C	-0.488249	-7.011319	-1.445759
35	H	-0.371931	-4.933163	-0.915969
36	C	0.131774	-8.047493	-2.139617
37	H	1.787800	-8.659175	-3.366894
38	H	-1.412336	-7.192143	-0.911953
39	N	1.290978	-3.197489	-1.449819
40	N	3.016633	-1.727113	-2.139681
41	Br	-0.729544	0.834441	3.450782
42	C	-0.357989	1.548875	0.582584
43	C	-1.908497	3.257703	0.689320
44	C	-0.560353	3.762367	1.191442
45	H	-2.123932	3.612029	-0.325595
46	H	-2.743073	3.501045	1.347623
47	H	-0.264872	4.722886	0.768372

48	H	-0.519956	3.805294	2.283217
49	O	0.345789	2.764823	0.699788
50	O	-1.738410	1.836809	0.689461
51	Cl	-0.599083	-9.643342	-2.139251
52	Cl	8.701956	-1.771438	-5.778329

Table S60. Atomic coordinates for optimized structure of biradical **30cA** obtained using the B3LYP/6-311++G(d,p) level of theory

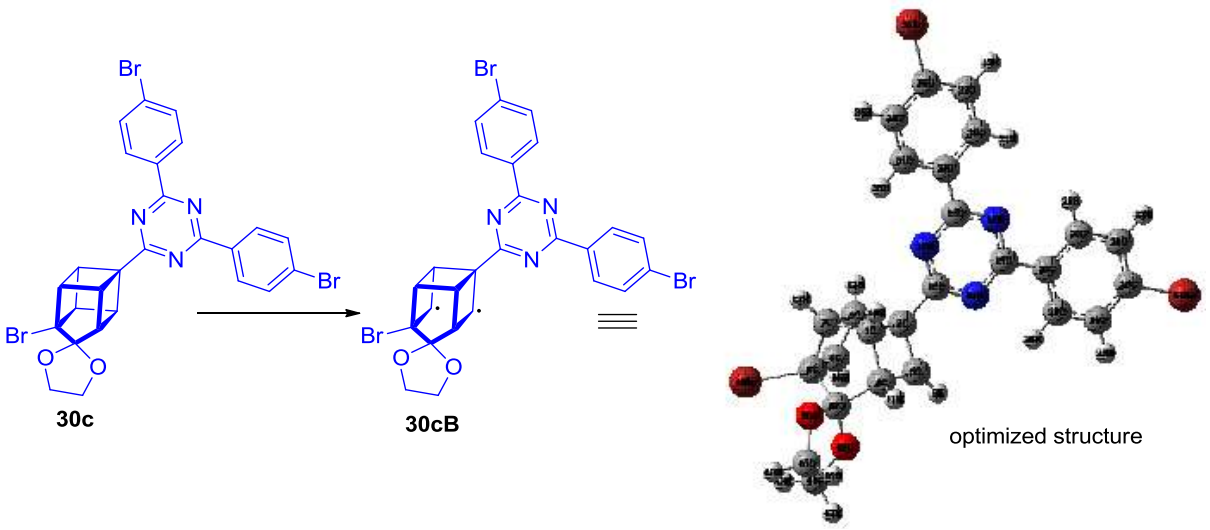


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.009748	-0.868680	0.066086
2	C	1.298923	-1.035518	-0.643584
3	C	1.608738	0.413735	-0.431217
4	C	0.046750	0.601581	-0.493121
5	C	0.473046	0.911335	1.700507
6	C	1.910706	0.629444	1.149459
7	C	0.306715	-0.643749	1.643805

8	C	1.799501	-0.707197	1.836034
9	H	2.283783	0.952697	-1.089675
10	H	2.726348	1.324627	1.335568
11	H	-0.384593	0.766435	-1.478313
12	H	2.491890	-1.529790	1.963119
13	H	-0.397137	-1.155425	2.296518
14	H	-0.849277	-1.530134	-0.127271
15	C	1.874996	-2.061948	-1.422401
16	C	1.815422	-4.184307	-2.234877
17	C	3.552411	-2.805215	-2.764935
18	N	2.977651	-4.014455	-2.889685
19	C	4.837582	-2.577081	-3.472169
20	C	5.414741	-3.589580	-4.248623
21	C	5.493541	-1.343240	-3.371843
22	C	6.619121	-3.380352	-4.912060
23	H	4.910732	-4.543431	-4.327541
24	C	6.697934	-1.121191	-4.029841
25	H	5.049740	-0.560115	-2.771497
26	C	7.250409	-2.144902	-4.795706
27	H	7.060624	-4.166504	-5.510696
28	H	7.200886	-0.166335	-3.948475
29	C	1.148936	-5.506122	-2.346535
30	C	1.717504	-6.528845	-3.115833
31	C	-0.060326	-5.750225	-1.682485
32	C	1.097058	-7.768836	-3.223689
33	H	2.651272	-6.343080	-3.629304
34	C	-0.690800	-6.985324	-1.782019
35	H	-0.500362	-4.961497	-1.086627
36	C	-0.104362	-7.985246	-2.554105
37	H	1.541056	-8.555525	-3.819758
38	H	-1.624538	-7.168938	-1.266471
39	N	1.222535	-3.249172	-1.493443
40	N	3.048324	-1.799525	-2.050711

41	Br	0.373872	1.735092	3.466779
42	C	-0.375719	1.561701	0.609867
43	C	-2.317277	2.799900	0.566501
44	C	-1.122821	3.739338	0.687049
45	H	-2.715306	2.775028	-0.454512
46	H	-3.122209	3.015331	1.269342
47	H	-1.154690	4.584033	-0.001534
48	H	-0.984680	4.096727	1.711359
49	O	-0.028137	2.895583	0.303057
50	O	-1.754630	1.528002	0.909236
51	Br	8.910224	-1.847838	-5.704753
52	Br	-0.966363	-9.690006	-2.696864

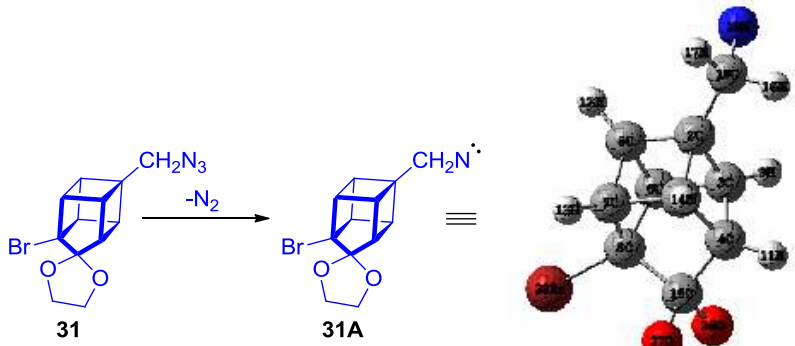
Table S61. Atomic coordinates for optimized structure of biradical **30cB** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.303698	-0.689142	-0.536551
2	C	1.243039	-0.899661	-0.715932
3	C	1.360399	0.530029	-1.109106
4	C	-0.073864	0.841756	-0.776848
5	C	0.052810	0.468248	1.632340
6	C	1.493713	0.116846	1.689402
7	C	-0.227116	-0.926766	0.990441
8	C	1.320633	-1.143180	0.930785
9	H	2.205601	1.156925	-1.358936
10	H	2.351081	0.685643	2.025036
11	H	-0.662383	1.338727	-1.553531
12	H	1.838737	-2.061242	1.208293
13	H	-0.907055	-1.610675	1.488376
14	H	-1.031421	-1.226107	-1.138643
15	C	1.880810	-1.997489	-1.489783
16	C	1.906118	-4.167831	-2.141251
17	C	3.565771	-2.761360	-2.795590
18	N	3.042595	-3.993307	-2.828162
19	C	4.829532	-2.520048	-3.530461
20	C	5.459511	-3.558562	-4.228628
21	C	5.413043	-1.246088	-3.536363
22	C	6.645982	-3.335433	-4.917802
23	H	5.011203	-4.543055	-4.225875
24	C	6.599070	-1.010364	-4.222167
25	H	4.926868	-0.443402	-2.997920
26	C	7.205643	-2.059997	-4.907829
27	H	7.129439	-4.140738	-5.455370
28	H	7.045908	-0.024706	-4.224227
29	C	1.289729	-5.515475	-2.143026

30	C	1.891834	-6.574612	-2.834625
31	C	0.093900	-5.749431	-1.451106
32	C	1.317055	-7.840373	-2.838289
33	H	2.814912	-6.396764	-3.369897
34	C	-0.490936	-7.010541	-1.447585
35	H	-0.372358	-4.932630	-0.916243
36	C	0.127893	-8.046595	-2.143013
37	H	1.786056	-8.655492	-3.373901
38	H	-1.414677	-7.186201	-0.911781
39	N	1.290170	-3.197436	-1.451232
40	N	3.016061	-1.727281	-2.140592
41	Br	-0.727596	0.833855	3.451306
42	C	-0.357386	1.548792	0.583102
43	C	-1.907544	3.257846	0.690896
44	C	-0.559075	3.762203	1.192434
45	H	-2.123454	3.612394	-0.323840
46	H	-2.741751	3.501154	1.349671
47	H	-0.263617	4.722729	0.769373
48	H	-0.518107	3.804942	2.284197
49	O	0.346650	2.764574	0.700143
50	O	-1.737668	1.836909	0.690652
51	Br	8.839320	-1.744138	-5.854750
52	Br	-0.671383	-9.786190	-2.143483

Table S62. Atomic coordinates for optimized structure of biradical **31A** obtained using the B3LYP/6-311++G(d,p) level of theory

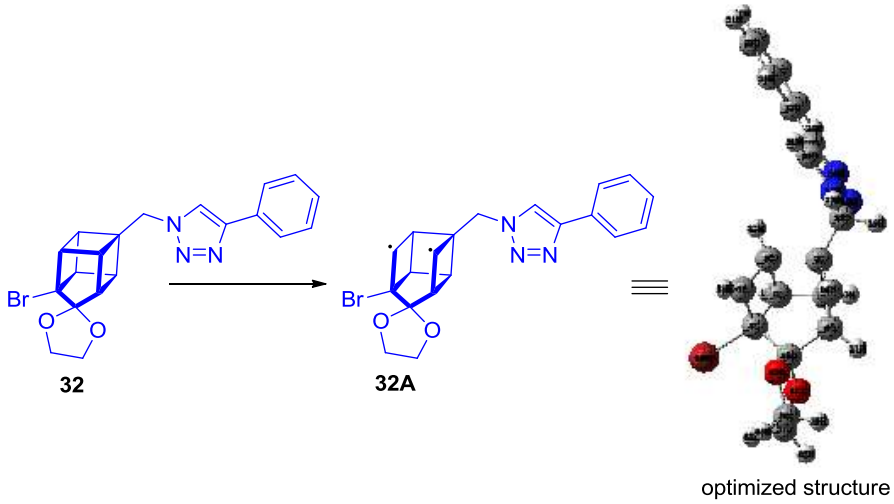


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.054873	-0.559995	0.056703
2	C	1.476318	-0.908485	0.086096
3	C	1.740424	0.630072	-0.071767
4	C	0.249940	0.881586	-0.448476
5	C	0.272131	1.088359	1.828971
6	C	1.755659	0.771936	1.501507
7	C	-0.037909	-0.419395	1.630757
8	C	1.490089	-0.765373	1.643371
9	H	2.556196	1.068141	-0.641883
10	H	2.561325	1.321027	1.979761
11	H	0.013197	1.127825	-1.481842
12	H	1.983160	-1.423459	2.354992
13	H	-0.806485	-0.911603	2.219961
14	H	-0.826495	-1.173570	-0.404548

15	C	2.119714	-2.009183	-0.740838
16	H	1.884705	-1.854524	-1.810435
17	H	1.684392	-2.986203	-0.460439
18	N	3.525917	-2.068013	-0.581639
19	C	-0.311862	1.839108	0.609651
20	C	-2.124201	3.229518	0.297042
21	C	-0.907968	4.061454	0.687289
22	H	-2.331122	3.291186	-0.777991
23	H	-3.026189	3.474347	0.858661
24	H	-0.757879	4.943982	0.064761
25	H	-0.931925	4.348116	1.742726
26	O	0.173933	3.154966	0.439366
27	O	-1.724079	1.901645	0.649515
28	Br	-0.099676	1.844211	3.590493

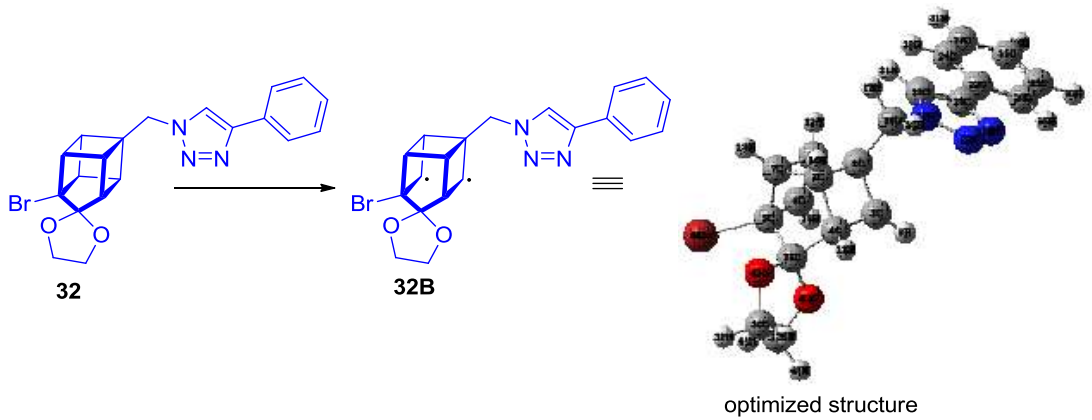
Table S63. Atomic coordinates for optimized structure of biradical **32A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.032706	-0.412702	-0.687428
2	C	1.420747	-0.772293	-0.263507
3	C	1.797638	0.751218	-0.388064
4	C	0.283983	1.068613	-0.632031
5	C	0.662630	1.233065	1.775897
6	C	2.034838	0.853826	1.138876
7	C	0.451828	-0.198009	2.104003
8	C	1.651409	-0.652486	1.349125
9	H	2.550362	1.114246	-1.081618
10	H	2.942721	1.297416	1.534375
11	H	0.011206	1.650915	-1.516194
12	H	2.321630	-1.404302	1.770095
13	H	-0.380615	-0.701579	2.578567
14	H	-0.886724	-0.985890	-0.739766
15	C	2.120066	-1.918770	-0.976090
16	H	2.090573	-1.753652	-2.055448
17	H	1.606981	-2.861106	-0.765730
18	N	3.520162	-2.095161	-0.594331
19	C	4.087733	-3.068834	0.159028
20	C	5.428862	-2.734965	0.218426
21	H	3.516279	-3.883543	0.568977
22	C	6.548583	-3.407972	0.888499
23	C	7.824923	-2.827234	0.877652
24	C	6.372757	-4.632293	1.549089
25	C	8.891796	-3.455616	1.512499
26	H	7.965539	-1.882770	0.367388
27	C	7.441451	-5.257875	2.183852
28	H	5.396959	-5.105497	1.566980
29	C	8.706610	-4.672031	2.168785

30	H	9.872224	-2.992705	1.495261
31	H	7.286420	-6.204569	2.689349
32	H	9.539401	-5.159325	2.663016
33	N	4.449684	-1.201024	-0.986522
34	N	5.593266	-1.581685	-0.499290
35	C	-0.226731	1.821960	0.639190
36	C	-2.284291	2.853420	0.585608
37	C	-1.205978	3.911882	0.786054
38	H	-2.638704	2.821456	-0.451482
39	H	-3.134550	2.954363	1.260342
40	H	-1.300820	4.768646	0.117932
41	H	-1.152182	4.250191	1.824155
42	O	-0.010059	3.204498	0.433141
43	O	-1.598585	1.639736	0.912443
44	Br	0.692139	2.415751	3.404437

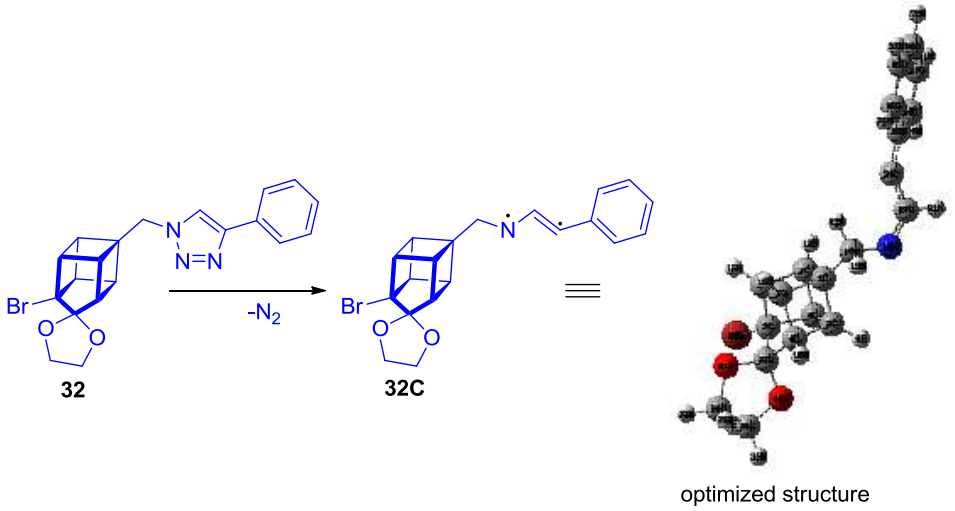
Table S64. Atomic coordinates for optimized structure of biradical **32B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.134348	-0.567491	-0.423821
2	C	1.386408	-0.950428	-0.281575
3	C	1.727396	0.453403	-0.664005
4	C	0.300423	0.924580	-0.615064
5	C	-0.081614	0.589568	1.776146
6	C	1.276331	0.100306	2.115224
7	C	-0.373086	-0.781372	1.092227
8	C	1.135831	-1.149302	1.320554
9	H	2.668364	0.978725	-0.763400
10	H	2.106537	0.592814	2.604492
11	H	-0.070317	1.467992	-1.488876
12	H	1.488167	-2.101971	1.722334
13	H	-1.201450	-1.383165	1.453404
14	H	-0.796057	-1.027358	-1.155153
15	C	2.015422	-2.133515	-1.000765
16	H	1.910281	-2.013523	-2.080410
17	H	1.530396	-3.068988	-0.709414
18	N	3.445819	-2.267237	-0.734963
19	C	4.078764	-2.943883	0.255244
20	C	5.422419	-2.677724	0.064396
21	H	3.546929	-3.543930	0.972743
22	C	6.599120	-3.135473	0.813502
23	C	7.885246	-2.759063	0.400108
24	C	6.469740	-3.949832	1.947668
25	C	9.006727	-3.187024	1.103902
26	H	7.990057	-2.130212	-0.474962
27	C	7.593205	-4.377485	2.648583
28	H	5.486349	-4.252926	2.290430
29	C	8.867855	-3.997773	2.229942

30	H	9.993931	-2.886373	0.770830
31	H	7.472975	-5.006778	3.523416
32	H	9.743230	-4.330271	2.776214
33	N	4.341084	-1.611041	-1.502776
34	N	5.523982	-1.856697	-1.025869
35	C	-0.165567	1.683548	0.667006
36	C	-1.510677	3.544167	0.436277
37	C	-0.246573	3.925426	1.197920
38	H	-1.472944	3.875824	-0.608055
39	H	-2.430483	3.899471	0.901638
40	H	0.232161	4.833370	0.830137
41	H	-0.425608	4.005764	2.273626
42	O	0.626297	2.821177	0.920523
43	O	-1.501891	2.114446	0.501076
44	Br	-1.165958	1.067567	3.405082

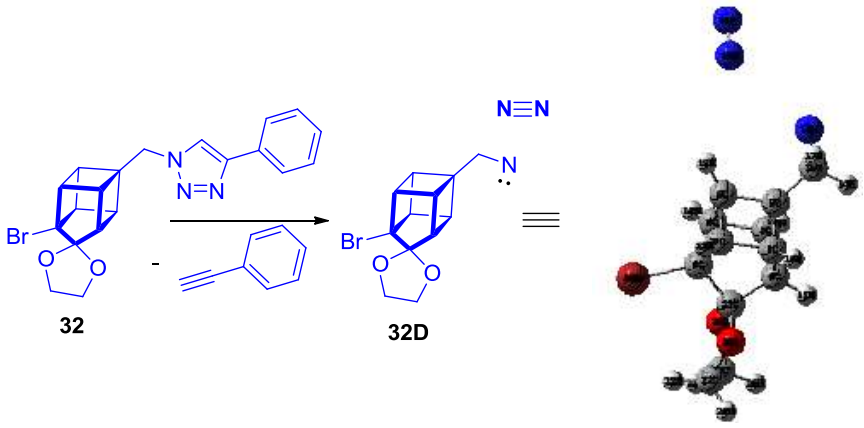
Table S65. Atomic coordinates for optimized structure of biradical **32C** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.772031	-0.430454	-0.095629
2	C	2.216682	-0.122522	0.438264
3	C	1.801272	1.389658	0.431489
4	C	0.535280	1.074756	-0.420559
5	C	-0.200025	0.862839	1.732699
6	C	1.292822	1.244333	1.919331
7	C	0.265564	-0.577538	1.393564
8	C	1.710591	-0.265211	1.913071
9	H	2.469233	2.211563	0.187394
10	H	1.591082	1.980750	2.659814
11	H	0.524818	1.383169	-1.464380
12	H	2.210804	-0.780189	2.730375
13	H	-0.339892	-1.435973	1.671230
14	H	0.522603	-1.212820	-0.810431
15	C	3.483628	-0.683252	-0.149067
16	H	3.522416	-0.418457	-1.216779
17	H	3.478151	-1.784193	-0.091144
18	N	4.652297	-0.097020	0.486174
19	C	5.649144	-0.887933	0.789529
20	C	5.766444	-2.261669	0.594998
21	H	6.521872	-0.392975	1.235074
22	C	6.573728	-3.345720	0.986000
23	C	6.836540	-4.416934	0.092947
24	C	7.122966	-3.417163	2.295791
25	C	7.622836	-5.488559	0.485561
26	H	6.415911	-4.380952	-0.904998
27	C	7.910334	-4.494538	2.671873
28	H	6.915320	-2.620107	2.999993
29	C	8.165407	-5.534563	1.773343

30	H	7.817399	-6.295171	-0.212270
31	H	8.325564	-4.530233	3.672932
32	H	8.778032	-6.375856	2.075781
33	C	-0.673759	1.513399	0.412691
34	C	-2.743409	2.073050	-0.439924
35	C	-2.192653	3.242881	0.367690
36	H	-2.643973	2.242034	-1.518934
37	H	-3.777431	1.820458	-0.202359
38	H	-2.283516	4.207176	-0.133519
39	H	-2.640532	3.296273	1.364480
40	O	-0.800287	2.921052	0.460232
41	O	-1.910674	0.985315	-0.029865
42	Br	-1.365084	1.075373	3.289036

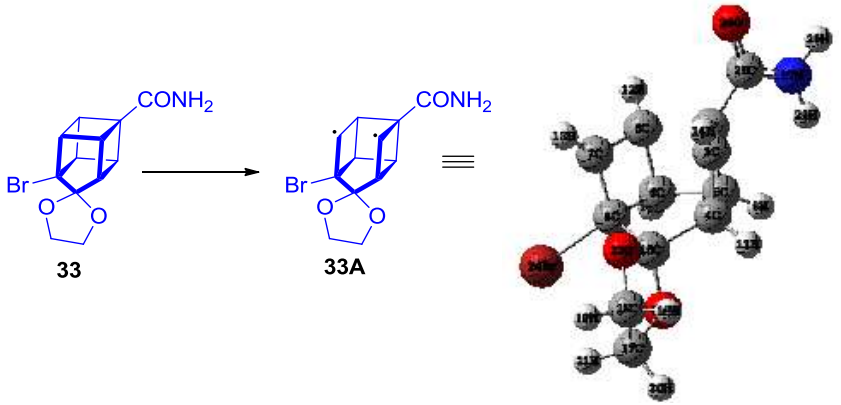
Table S66. Atomic coordinates for optimized structure of biradical **32D** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z

1	C	0.277468	-0.329924	-0.528001
2	C	1.845412	-0.349502	-0.614628
3	C	1.793476	1.191618	-0.322270
4	C	0.260428	1.225947	-0.596628
5	C	0.400219	0.785415	1.642989
6	C	1.891225	0.884677	1.224647
7	C	0.374713	-0.635341	1.018909
8	C	1.938192	-0.650372	0.917234
9	H	2.466808	1.930871	-0.749682
10	H	2.606441	1.430583	1.832845
11	H	-0.091052	1.697581	-1.512329
12	H	2.594736	-1.368964	1.401496
13	H	-0.241553	-1.419982	1.448545
14	H	-0.389888	-0.934314	-1.139510
15	C	2.634645	-1.015872	-1.729363
16	H	2.306580	-0.615456	-2.706674
17	H	2.415037	-2.099368	-1.741722
18	N	4.032851	-0.830730	-1.601081
19	N	4.733768	-3.933545	0.718503
20	N	5.803453	-4.159679	0.787833
21	C	-0.402697	1.710435	0.698610
22	C	-2.432476	2.618451	1.293596
23	C	-1.456917	3.743818	0.968661
24	H	-3.413970	2.737612	0.833709
25	H	-2.539958	2.471184	2.372137
26	H	-1.646844	4.173608	-0.021994
27	H	-1.434732	4.538415	1.715012
28	O	-0.190257	3.078396	0.985252
29	O	-1.797426	1.481656	0.694865
30	Br	0.003233	0.912737	3.550955

Table S67. Atomic coordinates for optimized structure of biradical **33A** obtained using the B3LYP/6-311++G(d,p) level of theory

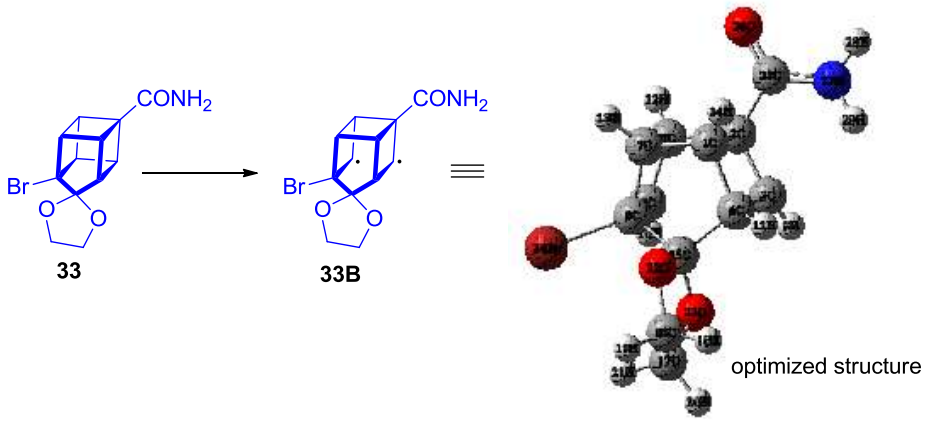


optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.048762	-0.731571	-0.033689
2	C	1.606842	-0.921813	0.169447
3	C	1.802883	0.406103	-0.489139
4	C	0.333395	0.725477	-0.525631
5	C	-0.033321	0.839333	1.889423
6	C	1.362253	0.556289	2.305093
7	C	-0.183562	-0.662735	1.494093
8	C	1.348109	-0.833615	1.776373
9	H	2.669343	1.055571	-0.561365
10	H	2.129828	1.207595	2.703077
11	H	-0.084163	1.044127	-1.484874
12	H	1.789460	-1.670546	2.316443
13	H	-0.949855	-1.263608	1.973062
14	H	-0.541767	-1.404514	-0.650089
15	C	-0.208541	1.680001	0.584067
16	C	-1.725319	3.346043	0.063416

17	C	-0.489446	3.962292	0.709982
18	H	-1.744588	3.510320	-1.020332
19	H	-2.664776	3.683248	0.502657
20	H	-0.104729	4.834668	0.181110
21	H	-0.656978	4.205331	1.762565
22	O	-1.575137	1.951087	0.345696
23	O	0.478940	2.910293	0.590814
24	Br	-1.173755	1.528940	3.400738
25	C	2.325633	-2.185565	-0.255669
26	O	2.231869	-3.228684	0.371155
27	N	3.065243	-2.076549	-1.396604
28	H	3.509673	-2.903235	-1.765216
29	H	3.076053	-1.223357	-1.931603

Table S68. Atomic coordinates for optimized structure of biradical **33B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.125245	-0.473024	-0.731578

2	C	1.313682	-1.026374	-0.020677
3	C	1.895447	0.436307	0.052328
4	C	0.534929	0.958630	-0.523095
5	C	0.338244	0.987513	1.912067
6	C	1.767917	0.451563	1.596331
7	C	-0.118771	-0.413530	2.081736
8	C	1.166148	-0.995812	1.613886
9	H	2.823097	0.756279	-0.420119
10	H	2.596534	0.763979	2.224292
11	H	0.560018	1.602677	-1.406245
12	H	1.607513	-1.860454	2.110843
13	H	-1.096028	-0.822181	2.301838
14	H	-0.798199	-0.933421	-1.058138
15	C	-0.166003	1.733939	0.639461
16	C	-1.996803	3.049250	0.175179
17	C	-0.871135	3.936002	0.694672
18	H	-2.091946	3.104521	-0.915653
19	H	-2.964230	3.245286	0.637657
20	H	-0.690601	4.821258	0.083834
21	H	-1.024885	4.224295	1.737830
22	O	-1.573054	1.739717	0.569583
23	O	0.273047	3.078773	0.582670
24	Br	0.118942	2.094862	3.579182
25	C	1.953186	-2.296526	-0.534905
26	O	1.352165	-3.356610	-0.515856
27	N	3.236754	-2.181091	-0.985206
28	H	3.681650	-2.996824	-1.378216
29	H	3.689487	-1.288078	-1.078700