

Supporting information for
Sulphur-containing pyrrolidine-fused chlorins as potential candidates for
photodynamic therapy: experimental and theoretical photophysical evaluation

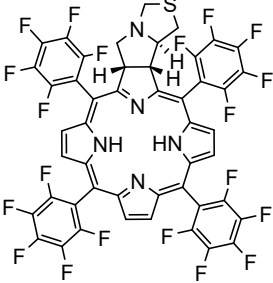
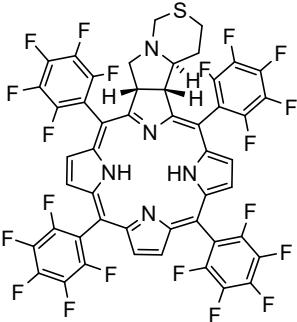
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Giampaolo Barone,* and Ana M. G. Silva*

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Structures

Table S1. Structure, name, molecular formula and molecular weight for the synthesized chlorins

Structure	Name	Molecular Formula	Molecular Weight
	Chlor-SH_ <i>trans</i>	C ₄₈ H ₁₇ F ₂₀ N ₅ S	1075.73
	Chlor-CSH_ <i>trans</i>	C ₄₉ H ₁₉ F ₂₀ N ₅ S	1089.75

NMR Spectra

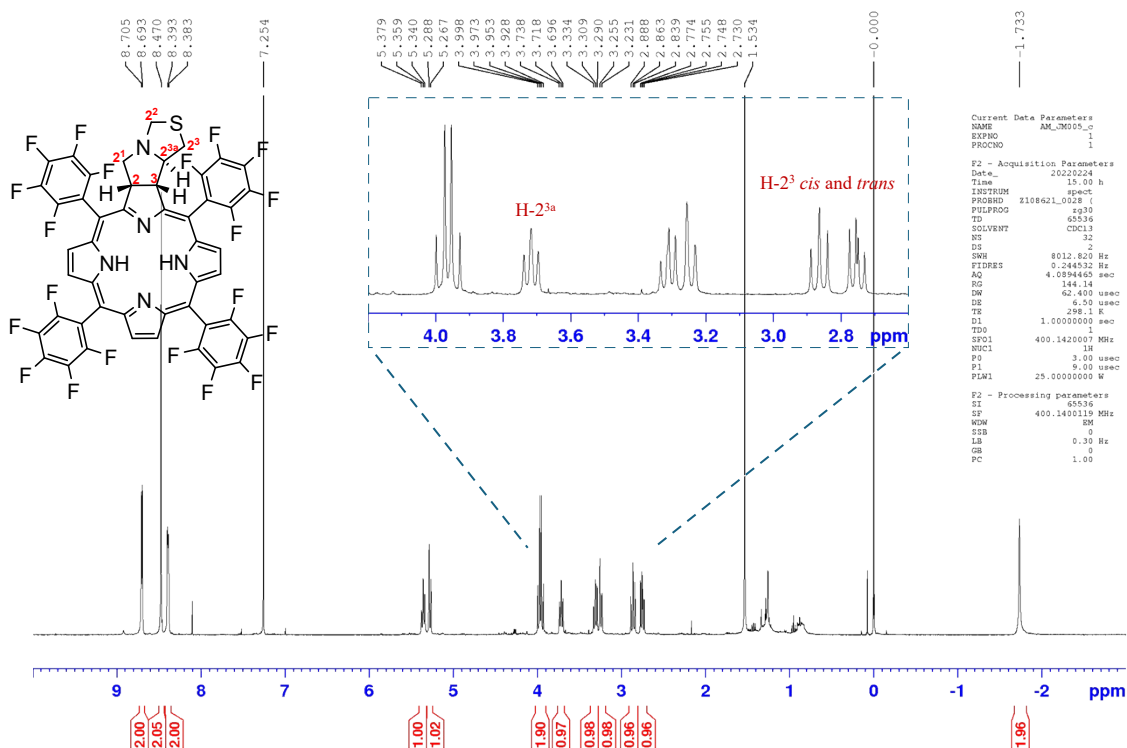


Figure S1. ¹H NMR spectrum (400.14 MHz, CDCl₃) of Chlor-SH_{trans}.

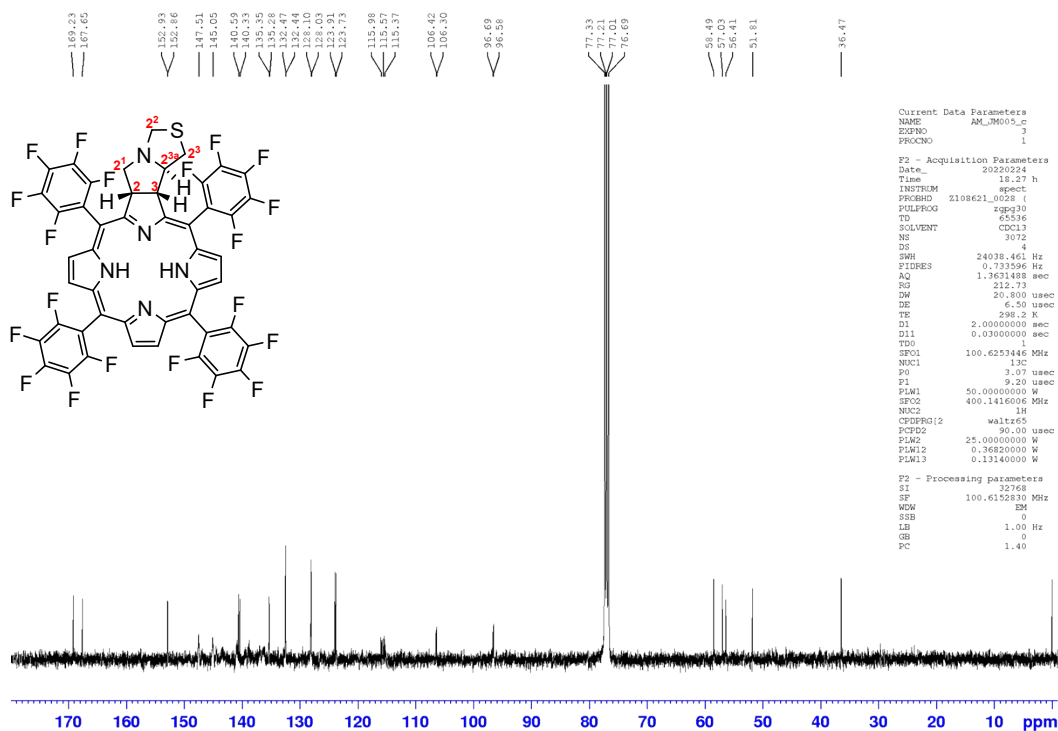


Figure S2. ¹³C NMR spectrum (100.62 MHz, CDCl₃) of Chlor-SH_{trans}.

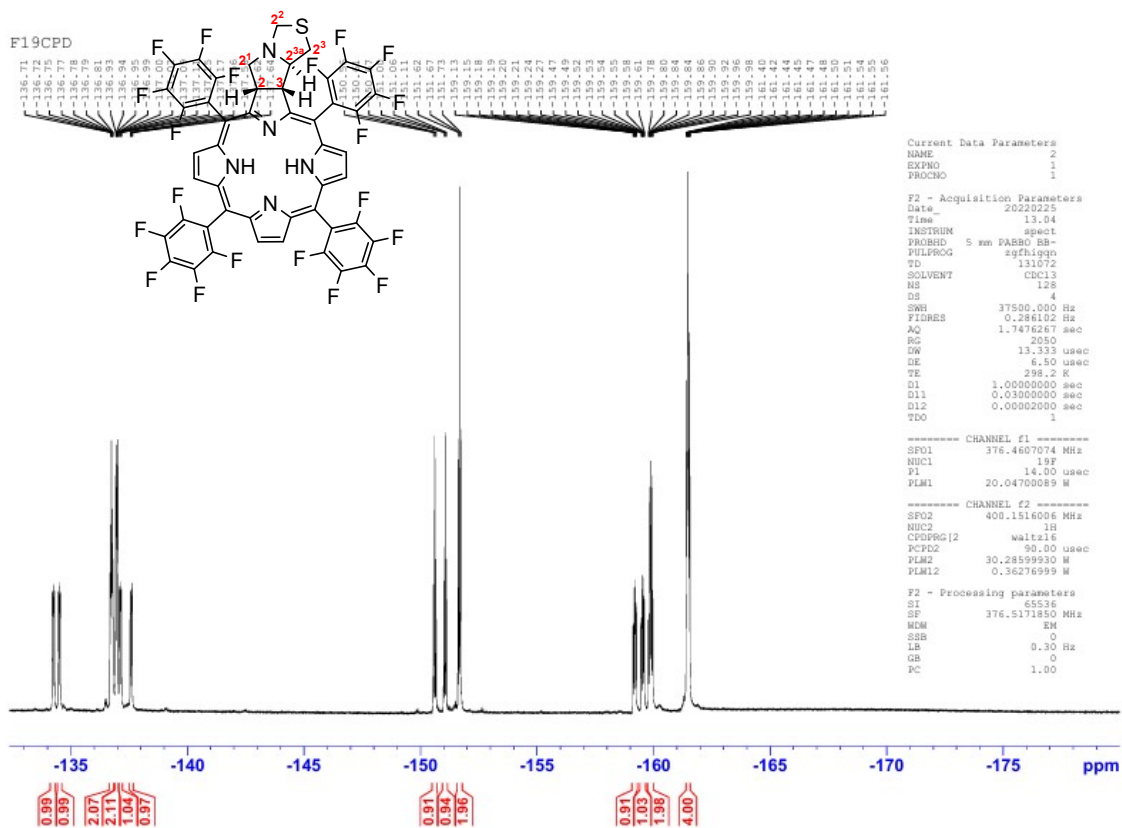


Figure S3. ¹⁹F NMR spectrum (376.52 MHz, CDCl₃) of Chlor-SH_{trans}.

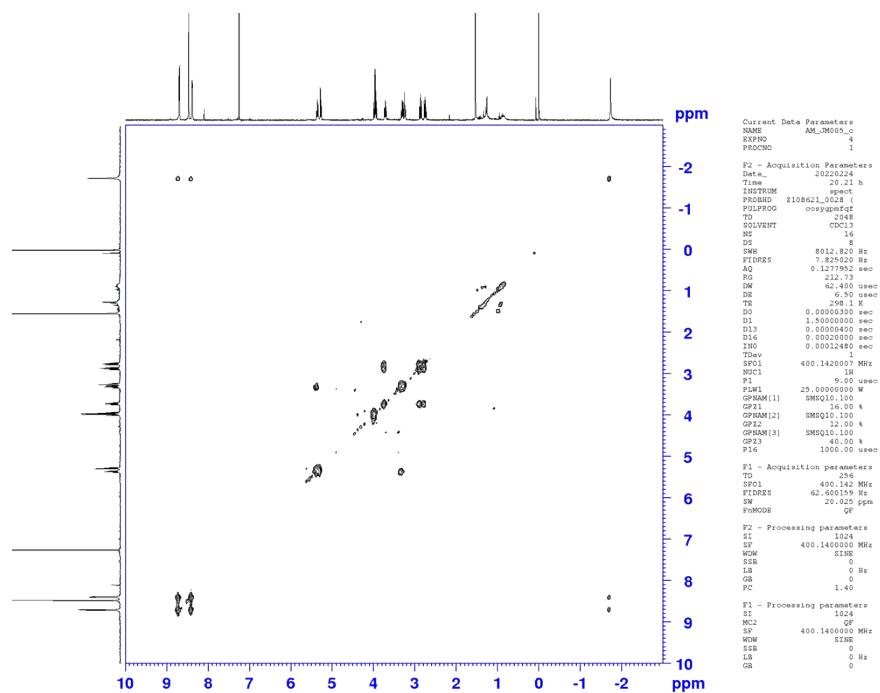


Figure S4. COSY spectrum of Chlor-SH_{trans}.

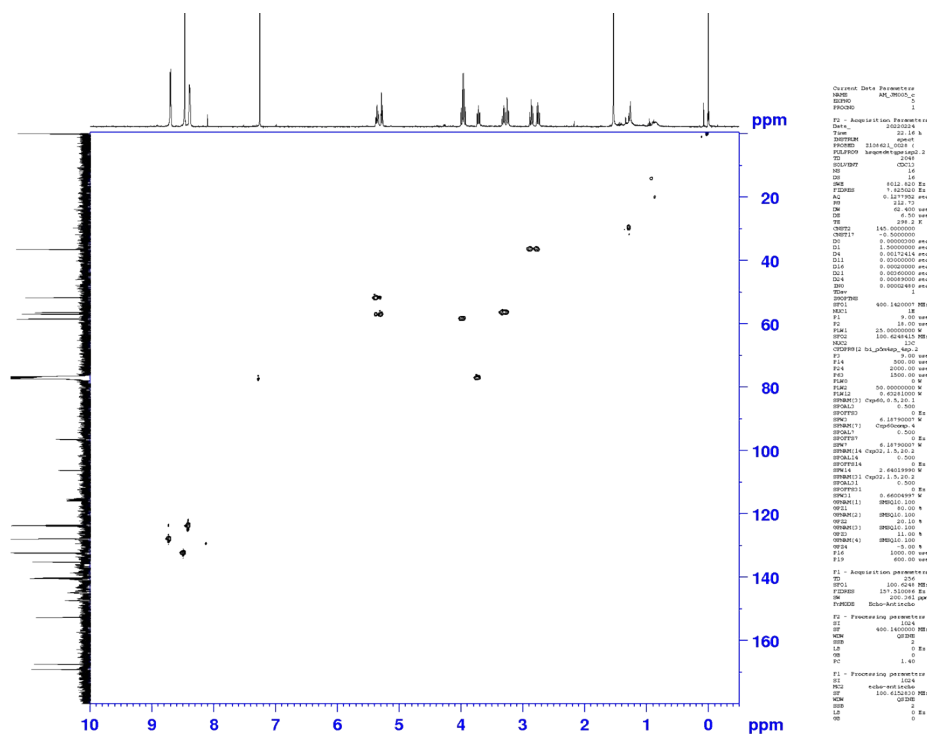


Figure S5. HSQC spectrum of Chlor-SH_{trans}.

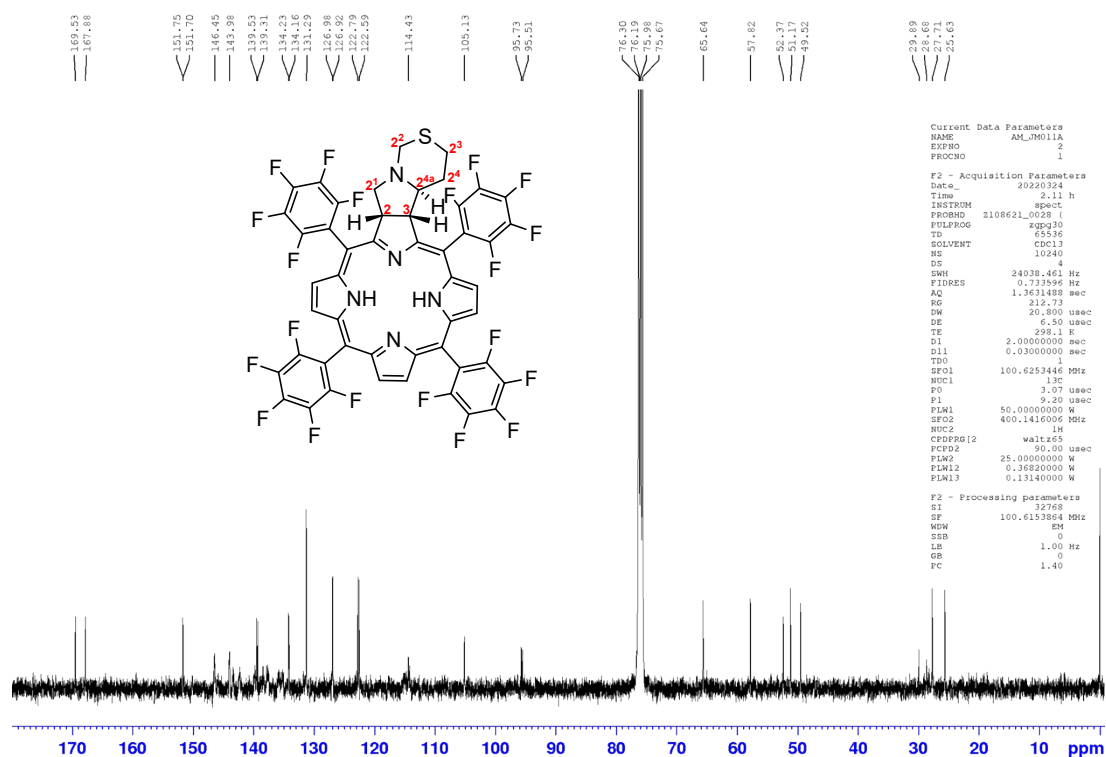


Figure S8. ^{13}C NMR spectrum (100.62 MHz, CDCl_3) of Chlor-CSH_{trans}.

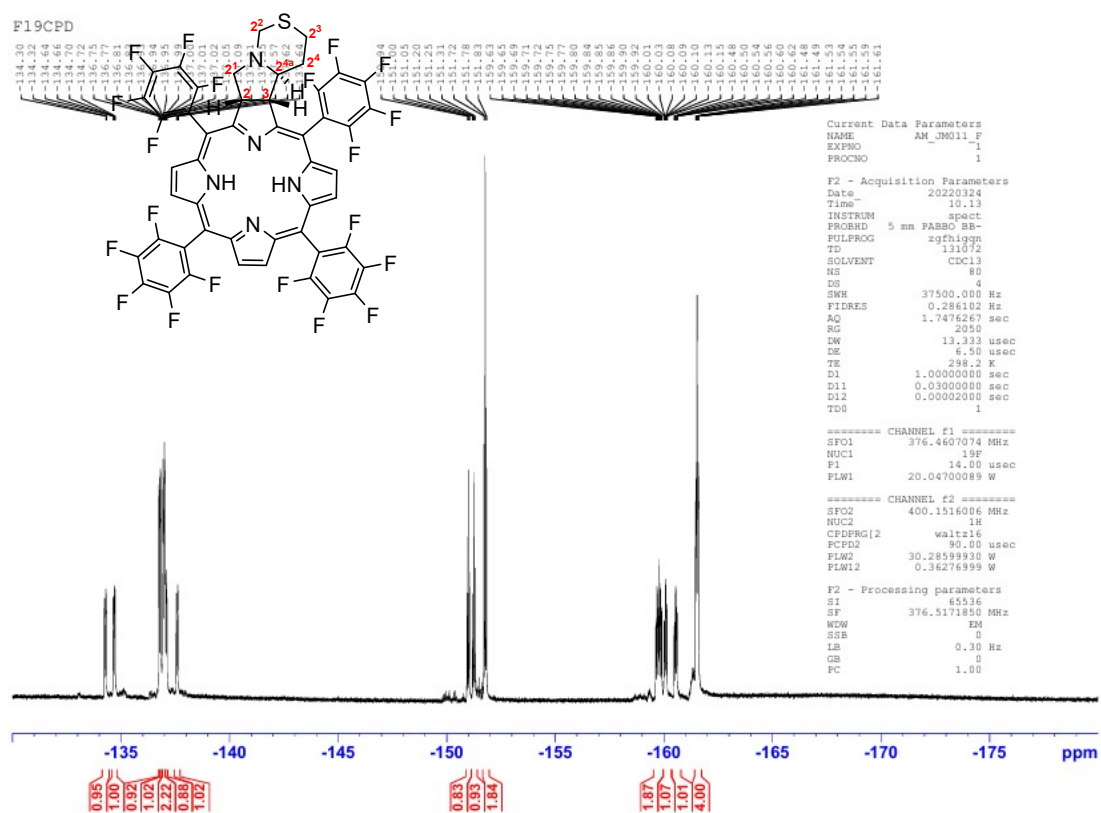


Figure S9. ^{19}F NMR spectrum (376.52 MHz, CDCl_3) of Chlor-CSH_{trans}.

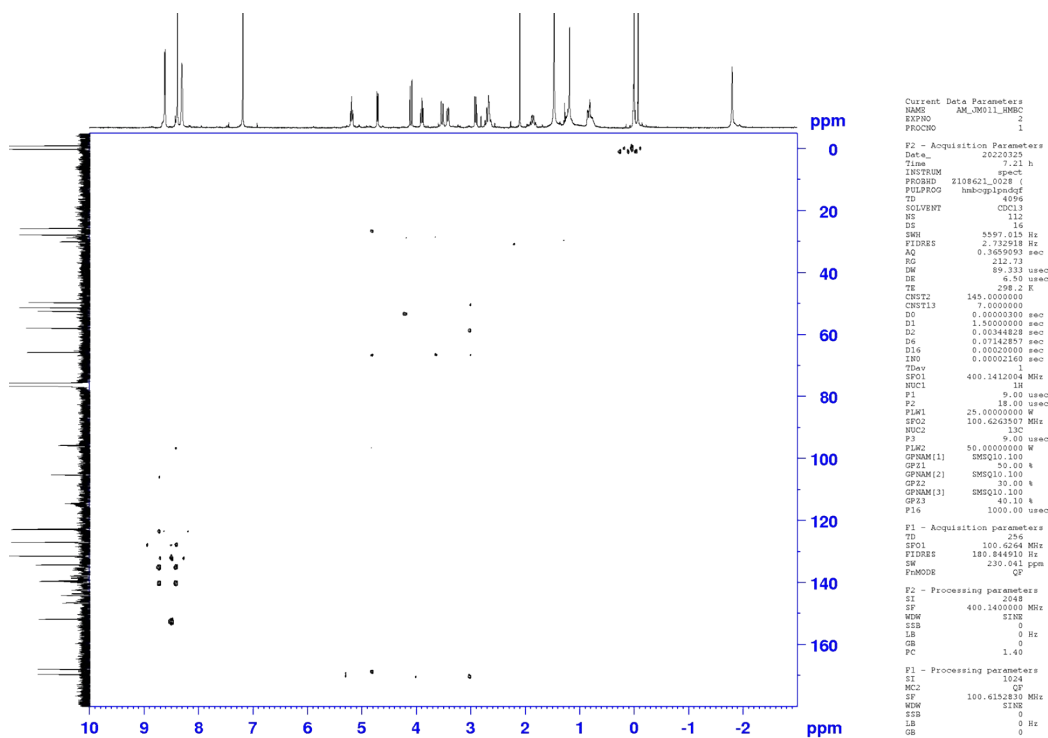


Figure S12. HMBC spectrum of Chlor-CSH_{trans}.

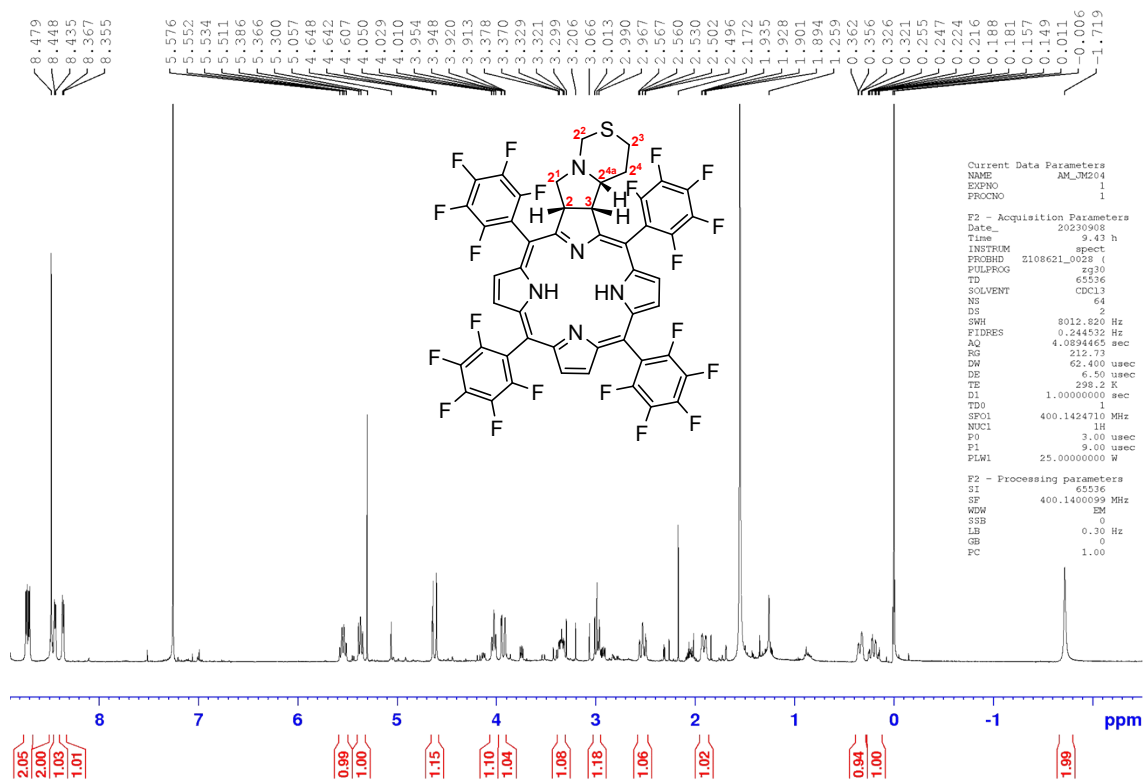


Figure S13. ^1H NMR spectrum (400.14 MHz, CDCl_3) of **Chlor-CSH_{cis}**.

Mass spectrometry

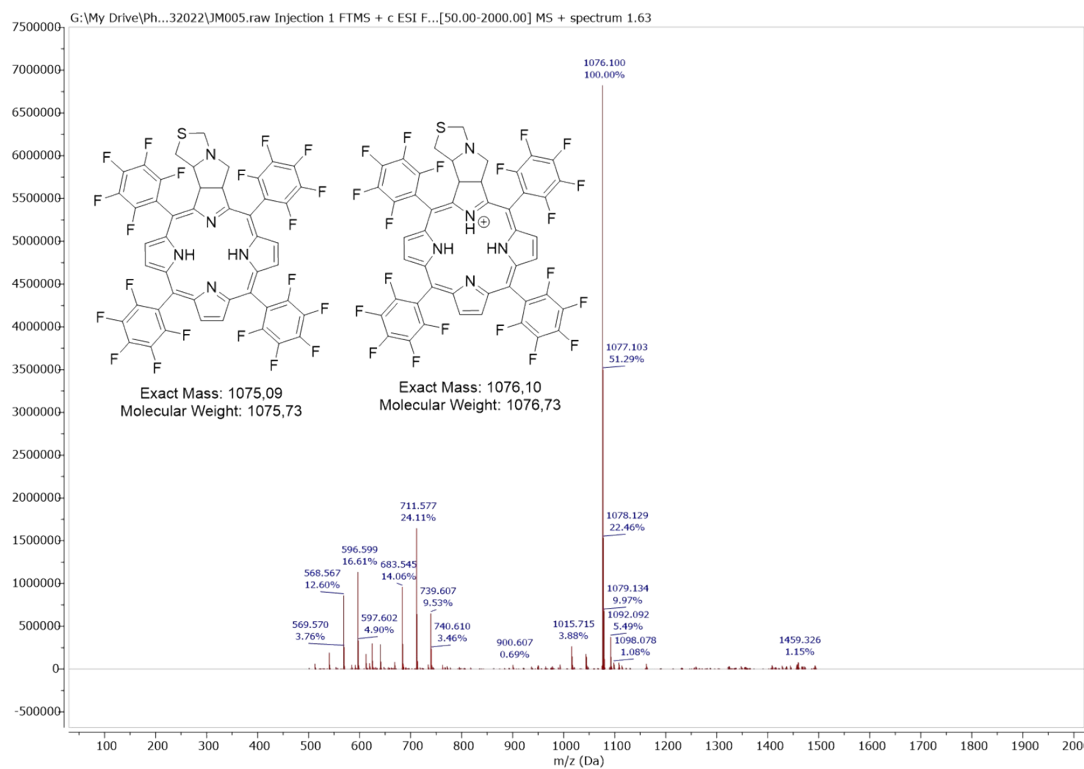


Figure S14. HRMS (ESI) spectrum of **Chlor-SH_{trans}**.

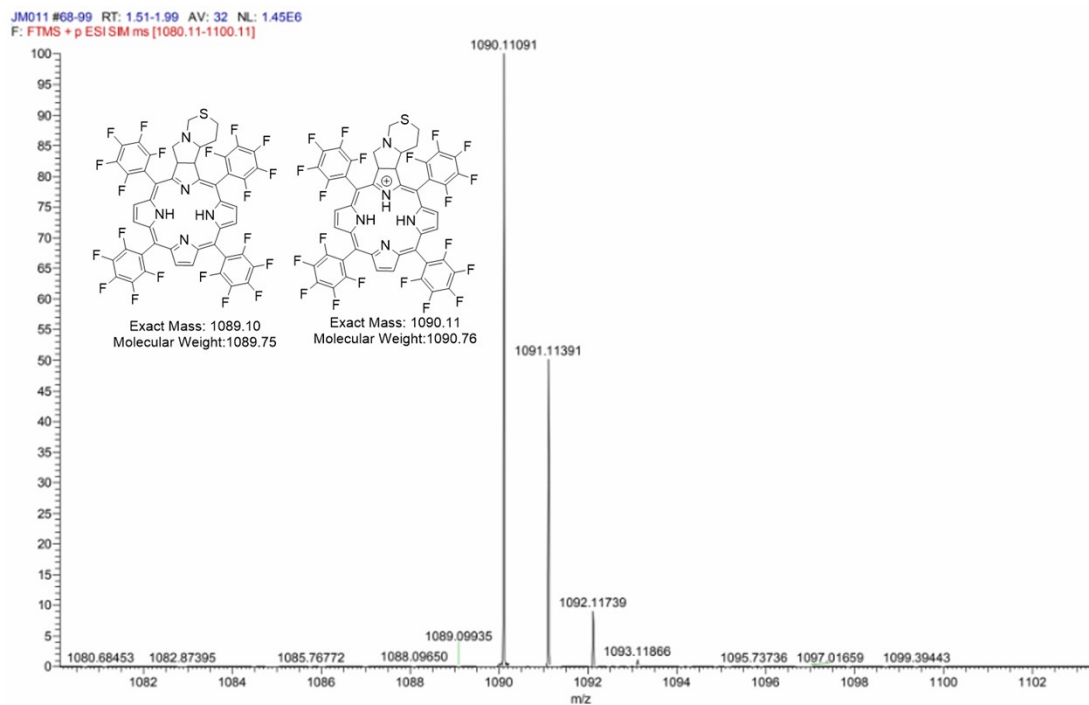


Figure S15. HRMS (ESI) spectrum of **Chlor-CSH_{trans}**.

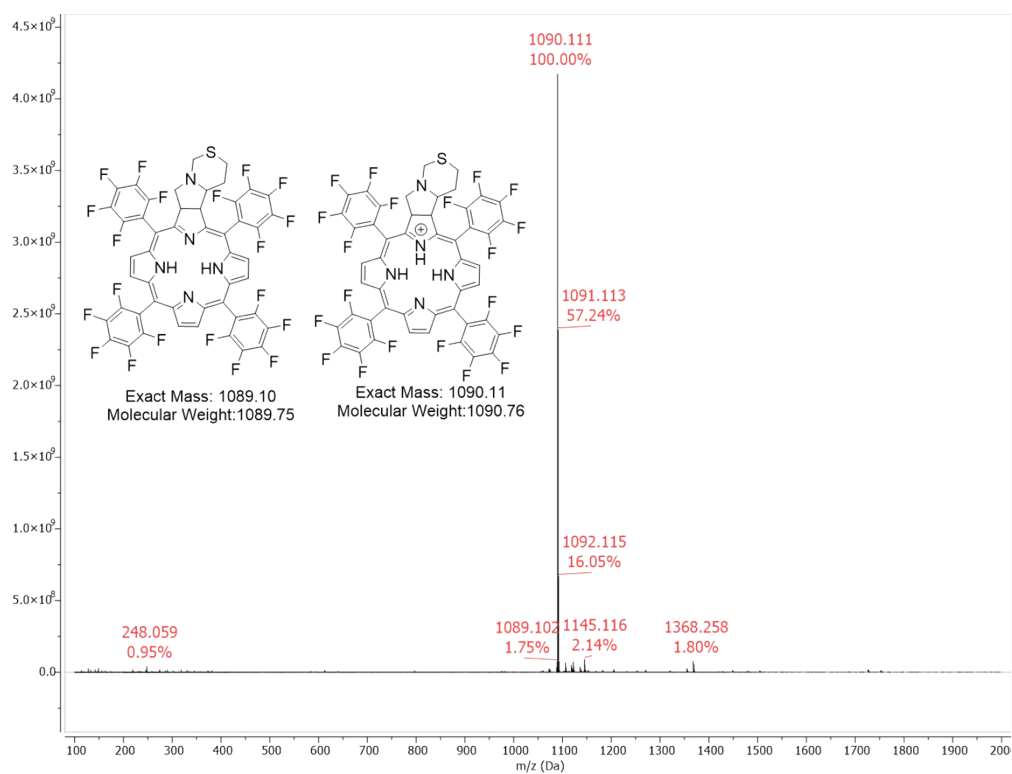


Figure S16. HRMS (ESI) spectrum of **Chlor-CSH_{cis}**.

Computational details

For the DFT calculations with the Gaussian 16 program, we used the following keywords, for geometry optimization in different solvents of energy minimum and of transition state structures, and for the attribution of electronic transitions:

```
# m06l/6-311G(d,p) opt int(grid=ultrafine) scrf(pcm,solvent=ChloroBenzene) freq=noraman
# m06l/6-311G(d,p) opt int(grid=ultrafine) scrf(pcm,solvent=n,n-DiMethylFormamide) freq=noraman
# m06l/6-311G(d,p) opt(qst3,maxstep=3) int(grid=ultrafine) scrf(pcm,solvent=ChloroBenzene)
freq=noraman
# M06l/6-311G(d,p) int(grid=ultrafine) scrf(pcm,solvent=n,n-DiMethylFormamide) tda=(nstates=50,50-50)
```

The functional and basis set were the same of our previous works performed for chlorins.¹⁻³

Convergence criteria were considered below the following cutoff values:

Maximum Force: 0.000450

RMS Force: 0.000300

Maximum Displacement: 0.001800

RMS Displacement: 0.001200

For the SOC calculation using the ORCA program we used the following keywords:

```
! M06L ZORA ZORA-DEF2-SVP SARC/J CPCM(DMF) RI-SOMF(1X) veryTightSCF miniprint
%TDDFT
  NROOTS 10
  TRIPLETS TRUE
  DOSOC TRUE
  TDA TRUE
  PRINTLEVEL 3
END
%method
  Grid 7 # Lebedev 770 points (very large)
end
%pal
  nprocs 24
end
%scf
  maxiter 1000
  ConvForced false
end
```

The Cartesian coordinates of the optimized geometries are the following:

Carbon dioxide

C	0.000000	0.000000	0.000000	C	5.240812	4.618054	-1.368713
O	0.000000	0.000000	1.160271	C	5.476004	5.461127	-0.292133
O	0.000000	0.000000	-1.160271	C	4.723788	5.329947	0.866316

Formaldehyde

C	0.000000	0.000000	-0.514264	F	4.048223	2.856364	-2.328225
O	-0.000000	-0.000000	0.685662	F	5.960112	4.746537	-2.481786
H	0.000000	0.937710	-1.111858	F	6.420157	6.392629	-0.370973
H	-0.000000	-0.937710	-1.111858	F	4.952435	6.137548	1.900094

Water

O	-0.000000	-0.000000	0.129107	F	3.039429	4.248069	2.068506
H	-0.000000	-0.749939	-0.470286	F	4.093561	-2.734944	2.406411
H	0.000000	0.749939	-0.470286	F	6.014846	-4.610354	2.606404

TPFPP

C	3.778047	-4.330266	-0.811168	F	6.470750	-6.318558	0.544784
C	3.517592	-3.437068	0.225934	F	4.990048	-6.139654	-1.724959
C	4.295752	-3.559309	1.375572	F	3.068115	-4.265369	-1.940750
C	5.289533	-4.518672	1.493580	C	1.139874	-2.863436	0.091320
C	5.522412	-5.393738	0.442375	N	0.014896	-2.088094	-0.007335
C	4.763455	-5.301547	-0.715376	C	-1.105127	-2.876055	-0.004040
C	2.458905	-2.401333	0.120779	C	-0.660238	-4.227095	0.101134
C	2.858748	-1.055028	0.069074	C	0.703082	-4.219075	0.164871
C	4.249116	-0.643455	0.053349	C	-2.429476	-2.431222	-0.066835
C	4.240951	0.705849	-0.003128	C	-3.471387	-3.486438	-0.132870
C	2.845523	1.100555	-0.021864	C	-4.375508	-3.693768	0.907244
N	2.020415	0.017619	0.019275	C	-5.353867	-4.674795	0.846344
C	2.430136	2.443001	-0.049905	C	-5.440848	-5.485799	-0.276271
C	3.480330	3.490641	-0.125466	C	-4.553268	-5.308808	-1.327725
C	4.251532	3.651472	-1.274821	C	-3.586787	-4.318218	-1.245296
				F	-4.313860	-2.934942	2.004310
				F	-6.203267	-4.849191	1.856821
				F	-6.372389	-6.430634	-0.344140
				F	-4.639624	-6.084052	-2.406773
				F	-2.750622	-4.170841	-2.276322
				C	-2.845759	-1.088926	-0.071605

N	-2.022149	-0.006554	0.009251
C	-2.858429	1.067856	-0.017687
C	-4.245661	0.658554	-0.127547
C	-4.237130	-0.691300	-0.167364
C	-2.459888	2.415487	0.019831
C	-1.140882	2.878275	0.027807
N	-0.012835	2.101121	0.012212
C	1.106249	2.890537	-0.020648
C	0.657186	4.244482	-0.022397
C	-0.706838	4.237145	0.020537
C	-3.525384	3.449576	0.042617
C	-3.747565	4.305365	-1.034109
C	-4.745522	5.268482	-1.014578
C	-5.558028	5.388849	0.103708
C	-5.365255	4.549955	1.191994
C	-4.357407	3.598845	1.150522
F	-2.987756	4.210104	-2.129035
F	-4.196565	2.807387	2.213700
F	-6.143123	4.667565	2.266138
F	-6.519023	6.305896	0.132666
F	-4.933813	6.071047	-2.060378
H	5.108198	-1.298477	0.073553
H	1.356737	-5.072000	0.265408
H	-5.084640	-1.354331	-0.265675
H	-5.101190	1.316026	-0.186641
H	5.092175	1.371139	-0.018848
H	-1.310362	-5.087596	0.142862
H	-1.362544	5.093931	0.042535
H	1.303877	5.107864	-0.054739
H	0.012588	-1.074743	-0.052872
H	-0.007228	1.086780	0.026182

Homocystein

C	1.579315	-0.307358	-0.083489
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C	0.173006	0.227961	-0.325050
C	-0.834362	-0.638031	0.431236
C	-2.262053	-0.313934	0.037409
O	2.470970	0.679227	0.130514
O	1.882379	-1.476254	-0.101420
H	3.334037	0.255409	0.246825
N	-0.047718	1.639237	-0.045553
H	0.004747	0.075587	-1.401687
H	-0.604818	-1.689244	0.237576
H	-0.699960	-0.482988	1.509718
H	0.192544	1.820456	0.926276
H	0.610441	2.193906	-0.583632
S	-3.411033	-1.382707	0.977689
H	-2.406166	-0.481925	-1.033638
H	-2.481231	0.732657	0.251432
H	-4.544825	-0.795138	0.564454

Cystein

C	1.583659	-0.303284	-0.022820
C	0.188021	0.238888	-0.313344
C	-0.847433	-0.642303	0.375035
S	-2.541543	-0.275827	-0.173348
O	2.503031	0.678692	0.018535
O	1.854300	-1.470403	0.124813
H	3.361802	0.255415	0.165466
H	-2.375834	1.058001	-0.092600
N	-0.037470	1.641043	0.002281
H	0.060758	0.123547	-1.399099
H	-0.656384	-1.689535	0.143161
H	-0.773959	-0.529354	1.461591
H	0.244974	1.818047	0.963035
H	0.571015	2.219627	-0.566720

Azomethine Ylide 1 (Chlor-CSH)

C	-2.785999	-0.411590	0.092658
N	-1.568119	-0.007264	-0.285950
C	-0.585425	0.644119	0.341582
H	-3.120718	-0.182506	1.092870
H	-3.439504	-0.812714	-0.663029
H	-1.342930	-0.239595	-1.251302
C	0.742599	0.803948	-0.301592
H	-0.757010	0.901772	1.379478
C	1.748810	-0.262829	0.135104
H	0.637640	0.769230	-1.394603
H	1.159037	1.794075	-0.075417
S	3.374415	0.047373	-0.662725
H	4.003329	-1.026529	-0.160941
H	1.872974	-0.241800	1.220624
H	1.391927	-1.255865	-0.149548

Azomethine Ylide 2 (Chlor-CSH)

C	-0.438842	0.908133	1.052464
C	-1.519688	0.997646	0.023784
N	-2.157552	-0.055111	-0.506130
C	-1.444777	-1.354072	-0.578037
S	-0.633447	-1.820643	0.955118
C	0.421239	-0.336777	0.991863
C	-3.383923	-0.063573	-1.069865
H	-2.175391	-2.123304	-0.816975
H	-0.707447	-1.281342	-1.381836
H	-2.083842	1.922796	-0.034371
H	1.056320	-0.351095	0.100181
H	1.064491	-0.423295	1.868299
H	-0.868858	0.980476	2.066704
H	0.209682	1.787562	0.952168
H	-3.889068	0.890556	-1.151005
H	-3.596742	-0.857189	-1.771811

Cinetic Product (Chlor-CSH)

N	-0.799544	1.953050	-0.296137
C	-0.672286	0.507273	-0.223876
C	-1.998357	-0.201458	-0.001414
O	-1.882775	-1.532438	-0.168393
O	-3.032301	0.343861	0.299682
H	-2.751135	-1.922622	0.008906
H	-0.272567	0.145291	-1.179901
H	-1.332886	2.261486	0.514501
C	0.310390	0.107704	0.884350
H	-0.079926	0.462526	1.847001
C	1.692312	0.685115	0.645099
H	0.356793	-0.983016	0.947643
H	-1.387145	2.192086	-1.089561
S	2.813650	0.246880	2.012218
C	4.323983	1.077626	1.400633
O	4.294698	2.477751	1.432802
H	2.108580	0.299806	-0.293075
H	1.620682	1.772667	0.565877
H	5.118159	0.752719	2.073542
H	4.537909	0.693011	0.396237
H	3.760108	2.777976	0.692348

Thermodynamic product (Chlor-CSH)

N	-0.484963	0.904132	1.031376
C	-1.376569	1.017992	-0.113160
S	-2.437362	-0.448600	-0.288258
C	0.526725	-0.131701	0.865472
C	1.513696	0.195286	-0.253361
O	2.243828	-0.873516	-0.622705
O	1.669176	1.295726	-0.726179
H	2.878231	-0.569317	-1.288904
H	-0.009291	1.796189	1.137485
H	-2.043824	1.867476	0.038502

H	-0.850095	1.166127	-1.068056
H	1.142380	-0.132671	1.775265
C	-1.058990	-1.630481	-0.434505
C	-0.106587	-1.517830	0.742600
H	-0.539766	-1.456823	-1.384905
H	-1.507016	-2.623913	-0.485409
H	-0.647808	-1.724399	1.670006
H	0.685926	-2.264666	0.649040

1,3-DC Chlor-CSH_{trans}

C	-4.903785	-3.862661	0.947581
C	-3.974307	-3.657773	-0.070455
C	-4.014122	-4.540021	-1.148488
C	-4.930678	-5.578309	-1.217179
C	-5.843966	-5.752694	-0.187798
C	-5.832576	-4.891227	0.899780
C	-2.986860	-2.550892	-0.012753
C	-3.471436	-1.231031	-0.097304
N	-2.705305	-0.107779	-0.004481
C	-3.589358	0.923937	-0.106707
C	-4.940803	0.446431	-0.291249
C	-4.866452	-0.905998	-0.286616
C	-3.252963	2.290184	-0.036717
C	-1.965719	2.811674	0.076065
N	-0.793567	2.088584	0.073839
C	0.279498	2.923366	0.199928
C	-0.238114	4.248606	0.296936
C	-1.600480	4.179649	0.218897
C	1.637135	2.556931	0.221933
C	2.155196	1.261284	0.167979
C	3.647727	1.010905	0.115014
C	3.726888	-0.516505	0.105892
C	2.271765	-0.921763	0.193406
N	1.423227	0.127151	0.176619

C	4.390107	-0.918589	-1.234670
N	4.229000	0.290014	-2.044104
C	4.323819	1.464970	-1.186544
C	5.806293	-1.479266	-1.056520
C	1.899258	-2.265058	0.273785
C	2.985671	-3.276063	0.384739
C	3.290868	-4.148046	-0.658769
C	4.300292	-5.094328	-0.561866
C	5.036688	-5.189307	0.610857
C	4.759831	-4.338047	1.671478
C	3.740798	-3.405149	1.548319
F	2.609828	-4.072865	-1.806165
F	4.570517	-5.906325	-1.581431
F	6.004747	-6.092588	0.718034
F	5.461513	-4.432154	2.799022
F	3.499232	-2.600673	2.588684
F	-3.154137	-4.396772	-2.160324
F	-4.944725	-6.402549	-2.263243
F	-6.727781	-6.743579	-0.242960
F	-6.706330	-5.063176	1.890128
F	-4.915154	-3.056151	2.011707
C	-4.362751	3.275577	-0.074387
C	-4.536051	4.143839	-1.150405
C	-5.576182	5.060218	-1.196461
C	-6.479531	5.122826	-0.145355
C	-6.335227	4.272557	0.941653
C	-5.285088	3.367596	0.966223
F	-3.688289	4.105355	-2.181943
F	-5.170377	2.569068	2.030270
F	-7.199366	4.336809	1.953057
F	-7.480607	5.996288	-0.178963
F	-5.717484	5.873448	-2.241786
C	2.603866	3.682534	0.333846
C	2.816304	4.581584	-0.709460

C	3.724775	5.624641	-0.614708
C	4.449819	5.794102	0.556437
C	4.260950	4.920801	1.617548
C	3.341177	3.890288	1.496806
F	2.150367	4.431672	-1.858771
F	3.912136	6.457378	-1.636751
F	5.323875	6.789618	0.661015
F	4.952361	5.085057	2.743949
F	3.183499	3.067304	2.539807
C	0.591518	-2.781109	0.260025
C	0.225759	-4.155454	0.364461
C	-1.135033	-4.240934	0.275723
C	-1.650657	-2.923750	0.120132
N	-0.567760	-2.072971	0.123911
H	-0.640663	-1.065033	0.055780
H	-0.751137	1.078602	0.012502
H	0.921646	-4.969538	0.496786
H	-1.737006	-5.135679	0.325141
H	-5.675661	-1.611666	-0.409898
H	-5.822407	1.058086	-0.420380
H	-2.298928	5.001152	0.269292
H	0.362875	5.136372	0.419852
H	4.141369	1.448520	0.985539
H	4.294250	-0.912376	0.952017
H	3.805571	-1.717854	-1.709522
H	3.805984	2.305639	-1.658304
H	5.355177	1.794868	-0.983209
H	5.725735	-2.353587	-0.397001
H	6.161623	-1.873834	-2.016303
C	6.857696	-0.541967	-0.473160
H	7.650470	-1.120852	0.002406
H	6.427745	0.117741	0.287650
S	7.625695	0.465955	-1.799422
H	8.498073	1.124294	-1.019166

H	4.881208	0.327030	-2.820168
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1,3-DC Chlor-CSH_cis

C	2.183335	1.529683	-0.534572
C	3.684428	1.415915	-0.677860
C	3.906660	-0.093758	-0.580812
C	2.500067	-0.639989	-0.566265
C	2.246044	-2.013700	-0.587223
C	0.991209	-2.645078	-0.535600
C	0.752985	-4.047900	-0.625668
C	-0.593918	-4.256840	-0.531873
C	-1.226652	-2.991546	-0.374096
C	-2.588468	-2.741542	-0.217969
C	-3.186124	-1.473020	-0.082211
C	-4.599370	-1.282435	0.152081
C	-4.790993	0.055994	0.230136
C	-3.491974	0.659790	0.039866
C	-3.276789	2.051693	0.045418
C	-2.045447	2.690939	-0.086901
C	-1.806055	4.092613	-0.145488
C	-0.461295	4.287073	-0.290223
C	0.169784	3.009188	-0.324143
C	1.547700	2.769184	-0.467727
N	1.561080	0.329233	-0.495565
N	-0.226235	-2.044972	-0.391618
N	-2.524445	-0.283224	-0.138750
N	-0.818501	2.075731	-0.199508
C	2.406116	3.981327	-0.549350
C	3.008665	4.372471	-1.741959
C	3.832166	5.485787	-1.822917
C	4.058756	6.251104	-0.687742
C	3.466582	5.895161	0.515979
C	2.652735	4.774049	0.569226
F	2.806786	3.658459	-2.854550

F	4.393196	5.832682	-2.979457
F	4.840082	7.323950	-0.753523
F	3.689542	6.625559	1.606908
F	2.112663	4.444641	1.746454
C	3.425940	-2.919409	-0.621341
C	4.239628	-3.026564	-1.747309
C	5.377603	-3.818250	-1.767630
C	5.722510	-4.547980	-0.638674
C	4.924767	-4.482556	0.494564
C	3.790108	-3.685212	0.486189
F	3.939622	-2.335012	-2.851939
F	6.135239	-3.888920	-2.859734
F	6.810850	-5.309507	-0.645068
F	5.257097	-5.173959	1.582929
F	3.047381	-3.652316	1.598475
C	-3.477988	-3.930064	-0.188509
C	-3.448632	-4.841389	0.865103
C	-4.277834	-5.952493	0.900217
C	-5.171482	-6.171851	-0.137871
C	-5.227365	-5.282661	-1.201471
C	-4.385434	-4.181119	-1.215817
F	-2.605769	-4.656291	1.884482
F	-4.226887	-6.803963	1.922961
F	-5.972157	-7.232204	-0.113744
F	-6.081980	-5.496643	-2.200188
F	-4.461462	-3.347174	-2.255864
C	-4.460575	2.934920	0.198444
C	-5.435020	3.024220	-0.793723
C	-6.545132	3.844976	-0.663567
C	-6.699418	4.609222	0.484234
C	-5.746521	4.545215	1.490479
C	-4.646760	3.714204	1.338395
F	-5.312429	2.307535	-1.913696
F	-7.456947	3.911476	-1.632038

F	-7.757540	5.401790	0.619094
F	-5.896670	5.276164	2.593586
F	-3.751116	3.673069	2.328543
C	4.552437	2.027218	0.436332
N	5.519120	0.962885	0.703300
C	4.755405	-0.290445	0.700611
C	3.934972	-0.534890	1.974399
H	-0.686771	1.071635	-0.213151
H	-0.390444	-1.048408	-0.315743
H	3.992125	1.800456	-1.654698
H	4.473327	-0.468756	-1.434134
H	1.521374	-4.793967	-0.759191
H	-1.111037	-5.203222	-0.576177
H	-5.339723	-2.062521	0.258629
H	-5.718288	0.580700	0.411296
H	-2.573503	4.850118	-0.096734
H	0.056053	5.230135	-0.377834
H	3.925572	2.290249	1.306154
H	5.069343	2.938584	0.123034
H	5.454264	-1.127953	0.571195
H	3.171694	-1.297766	1.799021
H	3.387301	0.375996	2.247492
C	4.818517	-0.981837	3.124741
H	5.322664	-1.918818	2.866214
H	5.586174	-0.235189	3.348484
S	3.796398	-1.245753	4.617280
H	4.798970	-1.605885	5.434226
H	5.996606	1.108547	1.588335

Chlor-CSH_cis (Chlorobenzene)

C	2.269651	1.066979	-0.580218
C	3.733255	0.711740	-0.724664
C	3.716377	-0.807990	-0.541783
C	2.240683	-1.126207	-0.541194

C	1.770874	-2.440842	-0.537762	C	4.740373	-5.553910	-0.479205
C	0.428242	-2.858473	-0.494120	C	3.924766	-5.345185	0.623725
C	-0.035919	-4.203878	-0.574483	C	2.961562	-4.348766	0.580418
C	-1.398841	-4.189305	-0.479427	F	3.470880	-3.058630	-2.746275
C	-1.816211	-2.836758	-0.332205	F	5.353901	-4.978062	-2.676623
C	-3.118563	-2.369701	-0.166543	F	5.666393	-6.505875	-0.452080
C	-3.504487	-1.020887	-0.042784	F	4.071389	-6.100021	1.710325
C	-4.865462	-0.603534	0.205895	F	2.192246	-4.179507	1.662168
C	-4.838881	0.749106	0.269119	C	-4.182249	-3.403125	-0.089331
C	-3.462628	1.134541	0.055478	C	-4.268791	-4.274984	0.994205
C	-3.026719	2.474022	0.039425	C	-5.259459	-5.240951	1.084932
C	-1.710898	2.904468	-0.118252	C	-6.201330	-5.350311	0.072365
C	-1.249495	4.247917	-0.206939	C	-6.144849	-4.496457	-1.019970
C	0.105876	4.219997	-0.377041	C	-5.142293	-3.540739	-1.089688
C	0.522519	2.856420	-0.393300	F	-3.382723	-4.191489	1.990224
C	1.841479	2.394275	-0.546965	F	-5.317528	-6.056612	2.136115
N	1.466218	-0.018335	-0.510398	F	-7.156057	-6.271528	0.148020
N	-0.675018	-2.066042	-0.361167	F	-7.047075	-4.605510	-1.993416
N	-2.661474	0.046797	-0.122880	F	-5.111916	-2.738174	-2.156401
N	-0.601025	2.097301	-0.235092	C	-4.052377	3.536542	0.195025
C	2.881372	3.448558	-0.687962	C	-5.008580	3.773481	-0.790495
C	3.522188	3.678569	-1.902639	C	-5.976702	4.756772	-0.655026
C	4.512341	4.639093	-2.046178	C	-6.001708	5.538498	0.490986
C	4.874192	5.412966	-0.952762	C	-5.061831	5.331098	1.489944
C	4.250531	5.216317	0.271671	C	-4.105157	4.339448	1.332622
C	3.268637	4.244394	0.388198	F	-5.008412	3.043465	-1.908476
F	3.193077	2.951314	-2.975721	F	-6.875766	4.960962	-1.615995
F	5.105429	4.832873	-3.222536	F	-6.923850	6.484883	0.631144
F	5.816052	6.341744	-1.077683	F	-5.088808	6.078231	2.592043
F	4.603995	5.955375	1.321094	F	-3.218659	4.162335	2.315735
F	2.701910	4.062742	1.584359	C	4.704729	1.247239	0.338269
C	2.783387	-3.530139	-0.534784	N	5.446282	0.054760	0.733381
C	3.604572	-3.785222	-1.631227	C	4.472543	-1.044979	0.783077
C	4.581209	-4.769633	-1.612956	C	3.572513	-1.019127	2.024133

C	6.294612	0.180293	1.876522
H	-0.635961	1.085124	-0.238324
H	-0.672399	-1.055848	-0.288511
H	4.074407	0.984151	-1.727929
H	4.245636	-1.313448	-1.349458
H	0.599931	-5.066372	-0.703297
H	-2.064512	-5.038173	-0.517237
H	-5.720105	-1.253231	0.330356
H	-5.667662	1.417127	0.455689
H	-1.882864	5.120688	-0.160538
H	0.765902	5.066112	-0.491370
H	4.162185	1.694581	1.189110
H	5.394673	2.005325	-0.045727
H	5.027360	-1.994184	0.767936
H	2.908583	-1.889375	2.000695
H	2.921855	-0.135844	2.007042
H	6.893387	-0.729828	1.978851
H	6.969511	1.029393	1.754276
S	5.417107	0.445278	3.490328
C	4.366772	-1.036374	3.318809
H	3.707422	-1.051439	4.187711
H	5.002815	-1.928774	3.374860

Chlor-CSH_cis (DMF)

C	2.266333	1.082534	-0.545595
C	3.732987	0.737934	-0.677267
C	3.723764	-0.784037	-0.526761
C	2.250272	-1.111142	-0.514172
C	1.790604	-2.430257	-0.508278
C	0.452553	-2.859363	-0.452510
C	-0.000778	-4.209476	-0.519046
C	-1.363713	-4.205064	-0.422748
C	-1.792341	-2.854142	-0.289567
C	-3.099287	-2.394956	-0.138537

C	-3.496333	-1.047312	-0.032881
C	-4.862131	-0.637880	0.200643
C	-4.846644	0.716113	0.249667
C	-3.472009	1.110112	0.042654
C	-3.045944	2.452735	0.018002
C	-1.732115	2.891996	-0.132053
C	-1.280874	4.238594	-0.228457
C	0.076756	4.220417	-0.382508
C	0.504514	2.860046	-0.381970
C	1.828194	2.406921	-0.518915
N	1.468872	-0.008005	-0.477425
N	-0.656940	-2.074409	-0.322770
N	-2.660815	0.026390	-0.118819
N	-0.614524	2.092677	-0.229601
C	2.861842	3.468162	-0.653610
C	3.506188	3.703868	-1.865060
C	4.490748	4.670254	-2.003053
C	4.842977	5.445228	-0.907595
C	4.214619	5.244044	0.313178
C	3.237959	4.266681	0.423930
F	3.185062	2.976304	-2.940720
F	5.088631	4.868408	-3.176518
F	5.780241	6.379748	-1.027416
F	4.558447	5.984328	1.365697
F	2.663482	4.083186	1.617577
C	2.815392	-3.508344	-0.539078
C	3.605923	-3.736394	-1.663312
C	4.603214	-4.698361	-1.685985
C	4.816115	-5.488009	-0.565300
C	4.030784	-5.308730	0.564123
C	3.044540	-4.334221	0.560702
F	3.422681	-2.999409	-2.764835
F	5.347108	-4.878501	-2.775421
F	5.765292	-6.417598	-0.576734

F	4.229568	-6.069003	1.638825
F	2.306610	-4.190064	1.669250
C	-4.156838	-3.434516	-0.063731
C	-4.247228	-4.302002	1.022513
C	-5.231503	-5.274316	1.108666
C	-6.163157	-5.394904	0.088465
C	-6.103026	-4.545623	-1.006725
C	-5.107205	-3.583375	-1.071438
F	-3.370307	-4.207507	2.026593
F	-5.292868	-6.086217	2.163004
F	-7.111864	-6.323067	0.159795
F	-6.996022	-4.665333	-1.988002
F	-5.074002	-2.783833	-2.141589
C	-4.078681	3.509933	0.161269
C	-5.029673	3.740293	-0.830377
C	-6.000191	4.722113	-0.705060
C	-6.033611	5.508436	0.437264
C	-5.100060	5.306745	1.442788
C	-4.140835	4.316812	1.295193
F	-5.020849	3.004949	-1.946034
F	-6.893586	4.920861	-1.673085
F	-6.958434	6.454069	0.567822
F	-5.135091	6.058628	2.541912
F	-3.259753	4.145232	2.285215
C	4.683990	1.253388	0.416103
N	5.454907	0.063491	0.756632
C	4.505777	-1.052537	0.780612
C	3.613391	-1.076876	2.023716
C	6.336219	0.174826	1.908978
H	-0.639164	1.080318	-0.217615
H	-0.662345	-1.063198	-0.266572
H	4.094246	1.034674	-1.666059
H	4.243985	-1.272118	-1.350908
H	0.641701	-5.068246	-0.639606

H	-2.022011	-5.060110	-0.451316
H	-5.712264	-1.293295	0.326372
H	-5.681854	1.379701	0.423312
H	-1.922472	5.106289	-0.200017
H	0.731166	5.070733	-0.498594
H	4.108020	1.668804	1.263997
H	5.355808	2.045035	0.069143
H	5.068072	-1.994596	0.735231
H	2.942488	-1.936738	2.019264
H	2.984815	-0.180275	2.084082
H	6.933662	-0.742907	1.963976
H	6.983361	1.045367	1.750643
S	5.361714	0.394829	3.382186
C	4.087923	-0.847059	3.441944
H	3.257197	-0.920495	4.112318
H	4.222169	-1.789612	3.930279

Chlor-CSH *trans* (Chlorobenzene)

C	4.805834	-4.002745	-0.949425
C	3.864218	-3.778976	0.053406
C	3.859201	-4.670121	1.124717
C	4.743961	-5.735278	1.200608
C	5.670288	-5.928063	0.186207
C	5.703226	-5.058259	-0.894229
C	2.912779	-2.641726	-0.017733
C	3.437639	-1.338352	0.083873
N	2.712436	-0.190130	-0.028427
C	3.625632	0.811480	0.112859
C	4.953185	0.288730	0.342142
C	4.835420	-1.060427	0.322475
C	3.336755	2.188142	0.039211
C	2.074063	2.752394	-0.132767
N	0.879419	2.069436	-0.189011
C	-0.157786	2.940670	-0.360348

C	0.408282	4.247499	-0.430836	C	6.514624	4.111694	-0.741037
C	1.762257	4.132289	-0.288089	C	5.449082	3.229504	-0.837938
C	-1.525500	2.621305	-0.435493	F	3.704312	3.946357	2.235668
C	-2.089108	1.344706	-0.391376	F	5.374450	2.451932	-1.920911
C	-3.591260	1.147579	-0.373585	F	7.432196	4.175554	-1.704230
C	-3.719136	-0.381547	-0.370736	F	7.634056	5.790491	0.470133
C	-2.277469	-0.834867	-0.394294	F	5.762674	5.668164	2.435627
N	-1.396312	0.186508	-0.364397	C	-2.447587	3.779561	-0.584734
C	-4.452812	-0.729045	0.936124	C	-2.663528	4.689730	0.448135
N	-4.143403	0.431412	1.776885	C	-3.524944	5.768170	0.317242
C	-4.257198	1.608293	0.930602	C	-4.197905	5.962139	-0.880840
C	-4.800813	0.466448	3.043178	C	-4.005238	5.077666	-1.932103
C	-5.945828	-0.973069	0.698701	C	-3.133442	4.010986	-1.774680
C	-1.950616	-2.191175	-0.441873	F	-2.046255	4.517604	1.621869
C	-3.067902	-3.166840	-0.571093	F	-3.716821	6.611330	1.329674
C	-3.439692	-4.002306	0.480667	F	-5.026793	6.991088	-1.020123
C	-4.475890	-4.917051	0.370252	F	-4.647991	5.264813	-3.083037
C	-5.169734	-5.020593	-0.827445	F	-2.970688	3.177367	-2.807969
C	-4.826962	-4.205408	-1.896817	C	-0.662683	-2.752118	-0.381805
C	-3.784477	-3.300707	-1.758105	C	-0.342317	-4.139174	-0.465107
F	-2.800832	-3.916812	1.652020	C	1.012262	-4.270463	-0.342817
F	-4.810839	-5.691383	1.400162	C	1.568794	-2.970548	-0.183037
F	-6.162384	-5.895018	-0.948091	N	0.516244	-2.083236	-0.219236
F	-5.490577	-4.304905	-3.046584	H	0.623875	-1.077982	-0.157958
F	-3.480217	-2.529445	-2.806910	H	0.799103	1.061604	-0.131243
F	2.985845	-4.509458	2.122506	H	-1.062810	-4.929612	-0.608805
F	4.715110	-6.567744	2.239787	H	1.584197	-5.185560	-0.370817
F	6.523864	-6.944550	0.249014	H	5.616510	-1.793020	0.468130
F	6.589251	-5.247504	-1.870272	H	5.849034	0.870257	0.507089
F	4.860523	-3.188125	-2.005852	H	2.489499	4.929882	-0.303360
C	4.470732	3.140236	0.150316	H	-0.155975	5.155325	-0.579104
C	4.605699	3.984497	1.250716	H	-4.060010	1.608606	-1.244699
C	5.660252	4.877182	1.368998	H	-4.268751	-0.760859	-1.235700
C	6.618468	4.939556	0.367736	H	-4.026969	-1.612910	1.429094

H	-3.752633	2.453607	1.406837	C	2.283519	0.820696	-0.398471
H	-5.304444	1.906216	0.749993	N	1.397490	-0.196477	-0.352552
H	-4.532532	1.374317	3.585875	C	4.474083	0.722135	0.908700
H	-6.048901	-1.893005	0.108111	N	4.160435	-0.421847	1.771953
C	-6.730422	-1.104741	1.991836	C	4.257800	-1.613581	0.943287
H	-7.786165	-1.304072	1.802626	C	4.829132	-0.442181	3.032441
H	-6.343702	-1.931605	2.601130	C	5.966783	0.944081	0.650907
S	-6.657172	0.432249	2.972793	C	1.961167	2.178125	-0.454676
H	-4.488246	-0.399930	3.633985	C	3.079532	3.149437	-0.605721
H	-6.369415	-0.164131	0.091136	C	3.464210	3.994566	0.433221
Chlor-CSH_trans (DMF)				C	4.498738	4.907649	0.301966
C	-4.790649	4.016874	-0.896009	C	5.177841	4.999571	-0.904660
C	-3.842028	3.791118	0.099317	C	4.821677	4.175130	-1.962109
C	-3.824957	4.684454	1.168253	C	3.781463	3.271787	-1.802380
C	-4.704868	5.752770	1.249092	F	2.838229	3.920454	1.613149
C	-5.638484	5.947004	0.242108	F	4.845844	5.691704	1.320796
C	-5.683136	5.075572	-0.836147	F	6.169419	5.872695	-1.045484
C	-2.895967	2.649959	0.021594	F	5.471035	4.264272	-3.121248
C	-3.426458	1.348678	0.124965	F	3.462995	2.491329	-2.840760
N	-2.707912	0.196900	-0.000119	F	-2.943602	4.522270	2.159744
C	-3.626641	-0.800937	0.135966	F	-4.664489	6.587234	2.286759
C	-4.949825	-0.272738	0.375910	F	-6.488108	6.966855	0.309966
C	-4.824055	1.076485	0.369576	F	-6.576406	5.265982	-1.805943
C	-3.346649	-2.179013	0.047497	F	-4.856744	3.200068	-1.951405
C	-2.086301	-2.749255	-0.120524	C	-4.491094	-3.121473	0.125749
N	-0.887869	-2.071003	-0.163968	C	-4.655273	-3.987952	1.204155
C	0.146643	-2.946279	-0.332649	C	-5.723209	-4.868660	1.284648
C	-0.424649	-4.250626	-0.411423	C	-6.664629	-4.896734	0.266370
C	-1.779529	-4.129897	-0.280744	C	-6.531574	-4.045962	-0.821297
C	1.515892	-2.632747	-0.404512	C	-5.453757	-3.176453	-0.879952
C	2.085464	-1.358259	-0.372361	F	-3.769790	-3.982851	2.205304
C	3.588051	-1.167613	-0.364320	F	-5.351084	-2.375349	-1.944507
C	3.723162	0.360821	-0.384211	F	-7.433483	-4.075678	-1.801352
				F	-7.692671	-5.736703	0.332778

F	-5.853858	-5.681698	2.331953
C	2.432733	-3.797143	-0.538306
C	2.643533	-4.692077	0.508344
C	3.499199	-5.776473	0.394840
C	4.170126	-5.993224	-0.800048
C	3.981799	-5.124821	-1.865065
C	3.116182	-4.051207	-1.724613
F	2.026115	-4.498191	1.679429
F	3.686507	-6.604863	1.420876
F	4.993583	-7.029180	-0.923192
F	4.622679	-5.334413	-3.013635
F	2.956274	-3.233380	-2.771457
C	0.675994	2.744284	-0.383575
C	0.359799	4.132374	-0.469859
C	-0.992629	4.269676	-0.330464
C	-1.552346	2.972508	-0.158117
N	-0.503592	2.080493	-0.202838
H	-0.613393	1.075835	-0.137424
H	-0.803784	-1.063828	-0.101215
H	1.081145	4.919334	-0.627742
H	-1.561357	5.186912	-0.356697
H	-5.599715	1.812360	0.527672
H	-5.847811	-0.851230	0.540779
H	-2.510137	-4.924169	-0.307477
H	0.136751	-5.160226	-0.560235
H	4.051483	-1.643310	-1.230097
H	4.264462	0.724945	-1.260779
H	4.064307	1.618442	1.392040
H	3.749613	-2.447247	1.435777
H	5.300546	-1.923696	0.759973
H	4.559151	-1.338800	3.592546
H	6.074563	1.851608	0.043097
C	6.766864	1.091915	1.932398
H	7.822649	1.274470	1.727709

H	6.396168	1.934301	2.529749
S	6.686341	-0.425517	2.944364
H	4.531778	0.437319	3.611331
H	6.374172	0.119609	0.053338

Chlor-CSH_trans_triplet

C	-4.901560	3.906060	-0.978540
C	-3.884393	3.762285	-0.034331
C	-3.814373	4.735420	0.963614
C	-4.703175	5.797088	1.021882
C	-5.702136	5.907864	0.066039
C	-5.803939	4.956844	-0.938786
C	-2.927166	2.636606	-0.093350
C	-3.437433	1.323529	0.057599
N	-2.715628	0.189073	-0.070382
C	-3.627127	-0.835494	0.139457
C	-4.940848	-0.302519	0.436798
C	-4.827352	1.040864	0.382407
C	-3.337461	-2.185397	0.064174
C	-2.046444	-2.762895	-0.192932
N	-0.862334	-2.078526	-0.220477
C	0.173506	-2.944415	-0.477888
C	-0.392069	-4.227503	-0.632903
C	-1.761291	-4.113108	-0.452157
C	1.547609	-2.608361	-0.538238
C	2.105371	-1.311151	-0.438251
C	3.602533	-1.125831	-0.329285
C	3.743036	0.401196	-0.293379
C	2.309606	0.872278	-0.377153
N	1.407217	-0.177550	-0.404488
C	4.417923	0.715552	1.051373
N	4.020763	-0.442083	1.862966
C	4.161925	-1.615426	1.015490
C	4.593732	-0.506388	3.169122

C	5.930191	0.902690	0.904104	C	3.218972	-3.889231	-1.898922
C	1.980374	2.199190	-0.437303	F	1.990433	-4.641297	1.405455
C	3.082775	3.193470	-0.513570	F	3.684203	-6.701261	1.035404
C	3.366017	4.057252	0.542942	F	5.094677	-6.908318	-1.275629
C	4.374209	5.005810	0.474273	F	4.793848	-5.042283	-3.226762
C	5.128870	5.116282	-0.685472	F	3.090526	-2.985474	-2.876675
C	4.872459	4.276342	-1.758842	C	0.657642	2.773398	-0.454383
C	3.856366	3.337331	-1.662865	C	0.337896	4.130590	-0.635942
F	2.663944	3.965020	1.677647	C	-1.037960	4.258678	-0.538400
F	4.627504	5.805638	1.508808	C	-1.576115	2.978500	-0.293214
F	6.098342	6.021814	-0.765316	N	-0.512089	2.100126	-0.259463
F	5.593594	4.383617	-2.873494	H	-0.604568	1.099226	-0.139548
F	3.633200	2.547532	-2.719023	H	-0.776541	-1.075352	-0.110202
F	-2.879828	4.653538	1.914829	H	1.052412	4.917366	-0.823050
F	-4.612589	6.703429	1.994260	H	-1.616560	5.164493	-0.638502
F	-6.560588	6.921303	0.114152	H	-5.600046	1.774777	0.562661
F	-6.758839	5.066972	-1.861247	H	-5.822789	-0.881792	0.669533
F	-5.020888	3.015888	-1.968638	H	-2.493702	-4.903563	-0.509328
C	-4.439165	-3.158901	0.234906	H	0.161152	-5.126041	-0.859090
C	-4.447433	-4.060614	1.299139	H	4.128302	-1.580991	-1.169351
C	-5.459626	-4.990513	1.470295	H	4.337226	0.784867	-1.125903
C	-6.504513	-5.038586	0.558504	H	3.996644	1.612110	1.524741
C	-6.525561	-4.160237	-0.514468	H	3.603342	-2.452067	1.446171
C	-5.501262	-3.238025	-0.665406	H	5.209828	-1.940774	0.904732
F	-3.461569	-4.032870	2.200365	H	4.263258	-1.408874	3.685751
F	-5.549040	-2.420000	-1.720403	H	6.105138	1.819530	0.327511
F	-7.523678	-4.213329	-1.394857	C	6.639581	1.001035	2.243062
F	-7.483157	-5.923709	0.714044	H	7.711488	1.160123	2.118161
F	-5.442861	-5.828597	2.505290	H	6.248323	1.839951	2.831714
C	2.478873	-3.746450	-0.726525	S	6.450946	-0.533353	3.213838
C	2.652318	-4.729679	0.247285	H	4.273229	0.366503	3.745458
C	3.527112	-5.790704	0.076883	H	6.358455	0.080377	0.318362
C	4.252897	-5.895804	-1.101195				
C	4.101555	-4.939260	-2.094349				

Azomethine Ylide 1 (Chlor-SH)

C	-2.719993	-0.438764	0.122487
N	-1.518297	-0.029639	-0.274089
C	-0.586461	0.745239	0.304265
H	-3.076475	-0.143543	1.097500
H	-3.328536	-0.982174	-0.579988
H	-1.257334	-0.351867	-1.203976
C	0.734379	0.866874	-0.301640
H	-0.784729	1.062239	1.319967
S	1.926297	-0.509739	0.257456
H	0.692719	0.809078	-1.392427
H	1.216067	1.803448	-0.021854
H	3.027624	-0.038101	-0.353355

Azomethine Ylide 2 (Chlor-SH)

C	-0.525197	1.027147	1.072958
C	-1.492616	1.004152	-0.043350
N	-1.362478	0.002708	-0.915520
C	-0.189996	-0.859952	-0.614304
S	0.924230	0.114483	0.420717
C	-2.149214	-0.398760	-1.922040
H	-0.208608	2.039939	1.336136
H	-0.870485	0.539619	1.996984
H	0.296932	-1.145548	-1.545817
H	-0.560279	-1.753645	-0.106127
H	-2.332211	1.676443	-0.140845
H	-3.064041	0.143607	-2.105935
H	-1.743943	-1.105983	-2.626899

Cinetic Product (Chlor-SH)

N	-1.081627	1.722174	-0.814647
C	-0.761716	0.379659	-0.369012
C	-1.984836	-0.432176	0.027009
O	-1.678815	-1.734782	0.191746
O	-3.093870	0.014649	0.193800

H	-2.489836	-2.189486	0.462828
H	-0.257262	-0.162209	-1.174031
H	-1.773574	2.109641	-0.176211
C	0.205783	0.430255	0.820266
H	-0.172734	1.130285	1.570821
S	1.878171	0.977777	0.365529
H	0.291642	-0.550412	1.294172
C	2.603279	-0.644693	0.053092
O	1.925978	-1.282858	-1.011145
H	2.060263	-2.230107	-0.909844
H	2.554798	-1.245120	0.969723
H	3.658359	-0.451658	-0.179593
H	-1.560610	1.668311	-1.708271

Thermodynamic product (Chlor-SH)

N	-0.526029	1.084781	0.995659
C	-1.339268	1.109439	-0.220119
S	-1.610518	-0.647986	-0.683560
C	-0.487645	-1.243687	0.627301
C	0.388424	-0.041560	0.927207
C	1.493413	0.158978	-0.104373
O	2.180412	-0.972241	-0.333959
O	1.749055	1.216712	-0.626762
H	2.877652	-0.764034	-0.973413
H	0.011553	1.947135	1.036892
H	0.081565	-2.095107	0.258952
H	-1.053629	-1.536282	1.512488
H	-0.853841	1.613872	-1.064497
H	-2.298988	1.591180	-0.021427
H	0.883753	-0.172224	1.898628

1,3 DC Chlor-SH_cis

N	-0.225172	-2.063549	-0.270968
C	0.978923	-2.693388	-0.402139

C	0.708048	-4.090559	-0.485924	C	-3.519829	-4.770336	0.983076
C	-0.643986	-4.266913	-0.400258	C	-4.370292	-5.864922	1.024393
C	-1.247891	-2.985984	-0.256364	C	-5.256238	-6.081952	-0.020785
C	2.248568	-2.091368	-0.446567	C	-5.283081	-5.207078	-1.097365
C	3.407619	-3.023895	-0.474725	C	-4.420166	-4.121896	-1.117575
C	4.231938	-3.141399	-1.591977	F	-2.684620	-4.586705	2.009285
C	5.350440	-3.960350	-1.605014	F	-4.468360	-3.301358	-2.169774
C	5.661122	-4.711120	-0.479828	F	-6.130494	-5.418927	-2.102523
C	4.850577	-4.638114	0.644006	F	-6.077369	-7.126262	0.009048
C	3.738037	-3.810518	0.628942	F	-4.347003	-6.702519	2.059467
F	3.960671	-2.435832	-2.695452	C	-1.951411	2.716420	-0.039909
F	6.119423	-4.040231	-2.688439	N	-0.737019	2.070863	-0.115510
F	6.728227	-5.501848	-0.481853	C	0.276077	2.979213	-0.225195
F	5.145302	-5.356684	1.724279	C	-0.324696	4.272107	-0.215173
F	2.977309	-3.771894	1.729238	C	-1.677098	4.111288	-0.104202
C	-2.605419	-2.704287	-0.117751	C	1.650484	2.706837	-0.342723
C	-3.177840	-1.422072	-0.005522	C	2.536427	3.899913	-0.414424
N	-2.490845	-0.246842	-0.066772	C	3.156949	4.280557	-1.601083
C	-3.442363	0.718066	0.078226	C	4.003572	5.377004	-1.672806
C	-4.756735	0.143483	0.252844	C	4.235901	6.135442	-0.534123
C	-4.590762	-1.199532	0.200536	C	3.626253	5.789624	0.663843
C	-3.199382	2.105540	0.067302	C	2.789446	4.685153	0.707830
C	-4.370998	3.012547	0.162717	F	2.949561	3.572577	-2.716425
C	-5.310019	3.089689	-0.864115	F	4.581383	5.714427	-2.823707
C	-6.412812	3.927014	-0.792614	F	5.039293	7.192185	-0.591047
C	-6.595531	4.722018	0.329809	F	3.854055	6.513790	1.757762
C	-5.677595	4.671856	1.368923	F	2.231203	4.364979	1.879393
C	-4.584384	3.823387	1.275500	C	2.260064	1.453941	-0.399279
F	-5.159726	2.343570	-1.961111	C	3.759450	1.309321	-0.531607
F	-7.290198	3.979479	-1.792993	C	3.949696	-0.205166	-0.441796
F	-7.647126	5.530504	0.409315	C	2.531377	-0.723055	-0.426345
F	-5.854862	5.432369	2.447751	N	1.613001	0.266402	-0.361973
F	-3.722856	3.796075	2.296239	C	4.798663	-0.422377	0.834787
C	-3.519727	-3.873815	-0.083437	N	5.581037	0.814994	0.855040

C	4.632966	1.896747	0.591474
S	5.086899	-1.065697	3.473603
C	3.958628	-0.650858	2.095372
H	-0.364858	-1.062459	-0.207166
H	-0.632705	1.063406	-0.122720
H	1.459119	-4.855564	-0.610026
H	-1.183429	-5.200874	-0.442445
H	-5.348451	-1.962977	0.305621
H	-5.676381	0.689186	0.409028
H	-2.426501	4.887824	-0.081027
H	0.217244	5.201816	-0.296598
H	4.083242	1.691717	-1.503948
H	4.507186	-0.589236	-1.296834
H	3.391006	0.248308	2.350953
H	3.248045	-1.466697	1.963226
H	5.478227	-1.275013	0.706639
H	4.008109	2.165461	1.461554
H	5.166361	2.801501	0.287093
H	4.201986	-0.890012	4.466910
H	6.042248	0.935155	1.753573

1,3-DC Chlor-SH_*trans*

N	-0.160972	-2.067099	0.176049
C	1.083274	-2.608526	0.323441
C	0.910959	-4.020746	0.421779
C	-0.424566	-4.293215	0.324004
C	-1.115510	-3.059482	0.162955
C	2.305659	-1.916610	0.354509
C	3.526417	-2.764562	0.453542
C	3.980795	-3.524092	-0.623081
C	5.138144	-4.285133	-0.558225
C	5.868227	-4.315601	0.621651
C	5.440148	-3.580488	1.718548
C	4.281742	-2.822995	1.622282

F	3.309457	-3.501860	-1.778820
F	5.558699	-4.971937	-1.617045
F	6.976352	-5.043875	0.699820
F	6.139005	-3.611744	2.851463
F	3.906412	-2.111274	2.690408
C	-2.487683	-2.869895	0.013931
C	-3.140112	-1.626015	-0.095414
N	-2.530689	-0.410430	-0.005125
C	-3.541430	0.494132	-0.135115
C	-4.814038	-0.159993	-0.337563
C	-4.562115	-1.490486	-0.312807
C	-3.391740	1.893503	-0.072832
C	-4.622528	2.721319	-0.135688
C	-4.886047	3.565144	-1.212974
C	-6.034699	4.339837	-1.277509
C	-6.959403	4.279654	-0.245139
C	-6.727949	3.449171	0.841930
C	-5.570591	2.687248	0.885456
F	-4.020987	3.643030	-2.227798
F	-6.258942	5.133861	-2.323008
F	-8.064197	5.016407	-0.296852
F	-7.612231	3.395546	1.836338
F	-5.375838	1.905272	1.950042
C	-3.324883	-4.095226	-0.019380
C	-4.219253	-4.387318	1.008803
C	-5.014130	-5.523010	0.993165
C	-4.922501	-6.406740	-0.072488
C	-4.040462	-6.147432	-1.111346
C	-3.258107	-5.002804	-1.074636
F	-4.327571	-3.561280	2.052249
F	-2.424778	-4.780860	-2.094593
F	-3.955638	-6.993548	-2.136354
F	-5.677584	-7.500003	-0.097557
F	-5.856768	-5.775325	1.993144

C	-2.189004	2.585866	0.057222
N	-0.928459	2.031469	0.081168
C	0.017157	3.007464	0.213808
C	-0.679541	4.249205	0.289842
C	-2.017888	3.992092	0.192522
C	1.412754	2.831826	0.258004
C	2.210393	4.084013	0.348815
C	2.282548	4.982663	-0.714005
C	3.020140	6.154104	-0.645370
C	3.714587	6.456081	0.517547
C	3.665409	5.585360	1.596269
C	2.912070	4.424330	1.502579
F	1.647817	4.707294	-1.857421
F	3.076552	6.983260	-1.685698
F	4.427416	7.574817	0.595692
F	4.328516	5.875480	2.714136
F	2.880496	3.611744	2.564985
C	2.100617	1.617561	0.231465
C	3.615917	1.561507	0.213925
C	3.881030	0.053616	0.207206
C	2.491858	-0.534521	0.282600
N	1.518982	0.398131	0.247497
C	4.572611	-0.243336	-1.142842
N	4.192906	0.912335	-1.949393
C	4.268157	2.076506	-1.076651
C	6.072994	-0.462636	-0.944614
S	6.829763	-0.946360	-2.537271
H	-0.376580	-1.079590	0.107273
H	-0.742097	1.037486	0.028197
H	1.713277	-4.729911	0.556947
H	-0.897488	-5.262573	0.368243
H	-5.268063	-2.298516	-0.442216
H	-5.765729	0.328612	-0.490958
H	-2.823697	4.709645	0.223718

H	-0.209556	5.212735	0.413341
H	4.028932	2.057487	1.094561
H	4.500691	-0.272937	1.045520
H	6.554366	0.447036	-0.575092
H	6.235161	-1.255773	-0.207196
H	4.152165	-1.140107	-1.613126
H	3.738087	2.918279	-1.528169
H	5.295111	2.416781	-0.857505
H	8.099275	-0.663701	-2.207984
H	4.785328	1.002906	-2.769523

Chlor-SH_cis (chlorobenzene)

N	-0.525246	-2.070826	-0.312258
C	0.602493	-2.832128	-0.417864
C	0.179010	-4.191024	-0.492925
C	-1.185352	-4.215055	-0.424831
C	-1.644269	-2.873868	-0.299796
C	1.933547	-2.376655	-0.448281
C	2.975706	-3.437594	-0.436496
C	3.806936	-3.675176	-1.529204
C	4.808936	-4.633611	-1.503292
C	4.983730	-5.409371	-0.365968
C	4.158294	-5.218474	0.733105
C	3.170309	-4.246976	0.682527
F	3.657717	-2.956824	-2.647845
F	5.590982	-4.825578	-2.563109
F	5.934130	-6.336547	-0.331934
F	4.320569	-5.964870	1.822724
F	2.393997	-4.089998	1.760817
C	-2.963041	-2.442635	-0.168861
C	-3.389429	-1.104465	-0.064606
N	-2.575340	-0.013744	-0.132351
C	-3.410364	1.051433	0.025517
C	-4.779600	0.628129	0.211522

C	-4.766783	-0.724732	0.152667	C	4.170265	5.344084	0.435732
C	-3.011673	2.402317	0.016864	C	3.211090	4.345955	0.517713
C	-4.066822	3.436894	0.163451	F	3.283911	3.059975	-2.848979
C	-5.014732	3.659123	-0.833330	F	5.154314	4.990350	-3.027132
C	-6.007334	4.618623	-0.703337	F	5.751798	6.512151	-0.857302
C	-6.066426	5.389834	0.448621	F	4.467992	6.089869	1.497548
C	-5.136109	5.195867	1.459123	F	2.608264	4.147391	1.693401
C	-4.154551	4.228163	1.307029	C	2.333695	1.144933	-0.492365
F	-4.981804	2.938256	-1.956797	C	3.811885	0.834304	-0.583406
F	-6.897550	4.810056	-1.675090	C	3.833077	-0.691822	-0.457762
F	-7.012097	6.313452	0.583489	C	2.365172	-1.049685	-0.458862
F	-5.195688	5.932952	2.566606	N	1.561025	0.037071	-0.442717
F	-3.277621	4.063526	2.300728	C	4.604137	-0.954136	0.846800
C	-3.999049	-3.504814	-0.109100	N	5.520200	0.185915	0.903996
C	-4.083242	-4.375759	0.975373	C	4.702819	1.354875	0.554478
C	-5.048497	-5.368520	1.049320	C	6.112788	0.226246	2.201134
C	-5.966432	-5.506616	0.018455	S	4.777134	-0.237522	3.448235
C	-5.911827	-4.654337	-1.075203	C	3.736822	-0.935714	2.127083
C	-4.934809	-3.671516	-1.128026	H	-0.554022	-1.060242	-0.252434
F	-3.219997	-4.265043	1.988532	H	-0.578364	1.080805	-0.214009
F	-4.905686	-2.870620	-2.196060	H	0.841724	-5.036077	-0.599597
F	-6.791095	-4.790896	-2.065982	H	-1.824941	-5.083528	-0.466059
F	-6.896404	-6.453885	0.077966	H	-5.604976	-1.398180	0.261373
F	-5.104892	-6.182943	2.101422	H	-5.630451	1.273290	0.377842
C	-1.705762	2.869171	-0.117871	H	-1.939403	5.079730	-0.162056
N	-0.571974	2.093551	-0.214560	H	0.716313	5.099817	-0.439490
C	0.532869	2.884176	-0.347330	H	4.201402	1.155398	-1.553454
C	0.077976	4.235524	-0.338972	H	4.362479	-1.156931	-1.289880
C	-1.280753	4.225220	-0.196317	H	6.501174	1.217016	2.438281
C	1.867732	2.459683	-0.468025	H	6.914259	-0.509666	2.281384
C	2.882010	3.542591	-0.572268	H	2.848154	-0.309761	1.999584
C	3.557171	3.792957	-1.764276	H	3.403777	-1.936365	2.402556
C	4.526603	4.778638	-1.872363	H	5.184183	-1.883354	0.816018
C	4.830535	5.559345	-0.766080	H	4.095235	1.692492	1.412885

H	5.348596	2.184737	0.256529	F	-6.883170	4.832731	-1.649348
				F	-6.985389	6.333771	0.611770
				F	-5.160772	5.947639	2.586602
Chlor-SH_cis (DMF)				F	-3.247216	4.075096	2.310379
N	-0.530745	-2.069816	-0.318474	C	-4.011565	-3.488739	-0.121910
C	0.593857	-2.836200	-0.423511	C	-4.101483	-4.363393	0.958659
C	0.164373	-4.193083	-0.504553	C	-5.072379	-5.350367	1.028477
C	-1.200423	-4.211158	-0.440378	C	-5.990371	-5.479135	-0.003126
C	-1.653553	-2.868211	-0.310809	C	-5.930333	-4.622986	-1.093084
C	1.927144	-2.386742	-0.447750	C	-4.947791	-3.646100	-1.141426
C	2.963456	-3.453251	-0.426197	F	-3.237887	-4.261056	1.973463
C	3.798156	-3.702830	-1.513265	F	-4.913564	-2.840209	-2.206759
C	4.791780	-4.669207	-1.477148	F	-6.810277	-4.750131	-2.085118
C	4.954749	-5.439878	-0.335014	F	-6.926219	-6.421335	0.052316
C	4.126034	-5.236408	0.758781	F	-5.134045	-6.168608	2.077851
C	3.146406	-4.257859	0.697886	C	-1.689430	2.875102	-0.116674
F	3.659860	-2.988923	-2.636538	N	-0.559102	2.094182	-0.216178
F	5.577766	-4.873446	-2.532244	C	0.548621	2.880268	-0.354526
F	5.897856	-6.374602	-0.291080	C	0.099345	4.233746	-0.347400
F	4.277228	-5.977922	1.853977	C	-1.258984	4.229414	-0.199446
F	2.365604	-4.088715	1.772068	C	1.881363	2.449920	-0.477343
C	-2.970261	-2.431659	-0.177255	C	2.899291	3.528894	-0.586625
C	-3.390522	-1.091810	-0.065817	C	3.568586	3.776934	-1.782152
N	-2.571719	-0.004044	-0.133816	C	4.537899	4.761528	-1.896326
C	-3.401513	1.064592	0.032208	C	4.848818	5.542543	-0.792593
C	-4.771345	0.646548	0.223899	C	4.195036	5.329171	0.412671
C	-4.764846	-0.706784	0.159726	C	3.235349	4.332689	0.500446
C	-2.996748	2.414052	0.023750	F	3.287939	3.043005	-2.864745
C	-4.047224	3.452468	0.175593	F	5.159969	4.971453	-3.054897
C	-4.998884	3.677940	-0.816390	F	5.771124	6.494200	-0.889657
C	-5.988850	4.638796	-0.681272	F	4.499504	6.075389	1.472842
C	-6.041601	5.408543	0.471565	F	2.637627	4.136173	1.680287
C	-5.107388	5.211789	1.477466	C	2.342023	1.133013	-0.499117
C	-4.128372	4.242941	1.319868	C	3.818804	0.816167	-0.588166
F	-4.972534	2.957428	-1.941367				

C	3.833701	-0.709329	-0.452833	C	-2.809441	-2.636394	-0.023691
C	2.364642	-1.061622	-0.458672	C	-3.335358	-1.332945	-0.119869
N	1.564436	0.028499	-0.448099	N	-2.609952	-0.184569	-0.003189
C	4.596779	-0.965898	0.857628	C	-3.526385	0.817332	-0.121804
N	5.518437	0.169688	0.910880	C	-4.855488	0.295460	-0.342859
C	4.710883	1.341294	0.546677	C	-4.735277	-1.054171	-0.343154
C	6.106168	0.217464	2.208686	C	-3.238945	2.193994	-0.033582
S	4.757262	-0.224215	3.453869	C	-1.972592	2.757694	0.108536
C	3.722172	-0.932173	2.133410	N	-0.777012	2.073212	0.123917
H	-0.554226	-1.059544	-0.252660	C	0.265443	2.943022	0.269326
H	-0.568819	1.081543	-0.212748	C	-0.297273	4.250316	0.361762
H	0.823349	-5.040750	-0.614002	C	-1.655346	4.136515	0.263245
H	-1.843871	-5.076531	-0.487948	C	1.634693	2.623287	0.311458
H	-5.605142	-1.377245	0.271545	C	2.197304	1.345939	0.274950
H	-5.618264	1.294933	0.398247	C	3.699276	1.148537	0.241657
H	-1.914184	5.086654	-0.165979	C	3.827124	-0.381168	0.263092
H	0.740791	5.095156	-0.453457	C	2.385079	-0.835099	0.310545
H	4.209239	1.130104	-1.560170	N	1.504396	0.187137	0.277381
H	4.366097	-1.182467	-1.278430	C	4.537145	-0.731145	-1.051044
H	6.501327	1.206607	2.440290	N	4.220428	0.399600	-1.921662
H	6.898473	-0.526407	2.302064	C	4.355242	1.587125	-1.073656
H	2.836422	-0.304359	1.995864	C	5.079898	0.351583	-3.057376
H	3.385373	-1.929363	2.416491	S	6.785207	-0.196774	-2.454380
H	5.171198	-1.898396	0.837509	C	6.071566	-0.825009	-0.901476
H	4.103403	1.691191	1.400152	C	2.057102	-2.190119	0.380497
H	5.363471	2.163348	0.243200	C	3.171631	-3.166972	0.519099
Chlor-SH_<i>trans</i> (DMF)				C	3.522679	-4.033042	-0.514399
C	-4.698979	-3.998181	0.914162	C	4.549681	-4.955672	-0.391561
C	-3.760890	-3.773712	-0.091371	C	5.258983	-5.031637	0.798490
C	-3.758558	-4.665113	-1.162079	C	4.938313	-4.184493	1.848979
C	-4.642570	-5.730539	-1.235033	C	3.902149	-3.275457	1.699862
C	-5.565373	-5.923719	-0.217937	F	2.868220	-3.972813	-1.679755
C	-5.595262	-5.054152	0.862371	F	4.862284	-5.763107	-1.403272
				F	6.245720	-5.911788	0.930176

F	5.617028	-4.258249	2.992426	H	-0.515400	-1.074103	0.097975
F	3.615961	-2.474897	2.732738	H	-0.700448	1.065611	0.058520
F	-2.887852	-4.503827	-2.163015	H	1.162836	-4.924896	0.584945
F	-4.616483	-6.563178	-2.274567	H	-1.484116	-5.178552	0.349092
F	-6.418869	-6.940769	-0.278055	H	-5.516254	-1.786253	-0.492208
F	-6.478213	-5.243647	1.841704	H	-5.753351	0.878230	-0.492547
F	-4.750513	-3.183095	1.971681	H	-2.381167	4.934318	0.307842
C	-4.381874	3.140121	-0.079668	H	0.271890	5.156986	0.498233
C	-4.568606	4.017669	-1.145430	H	4.178435	1.624279	1.098627
C	-5.638692	4.898174	-1.194680	H	4.389435	-0.749613	1.123401
C	-6.558861	4.915084	-0.156948	H	5.165816	1.322390	-3.545304
C	-6.402454	4.053862	0.919256	H	4.731433	-0.391854	-3.775532
C	-5.323053	3.184985	0.946751	H	6.423164	-0.213277	-0.065387
F	-3.704252	4.023268	-2.164877	H	6.386948	-1.855030	-0.725109
F	-5.197652	2.374103	2.001379	H	4.162526	-1.649025	-1.514532
F	-7.283550	4.073022	1.918226	H	3.863926	2.438413	-1.549249
F	-7.588612	5.754698	-0.193641	H	5.411162	1.858163	-0.907554
F	-5.791670	5.721550	-2.230770	Chlor-SH_<i>trans</i>_triplet			
C	2.557743	3.785648	0.417768	C	-4.815641	3.887831	-1.040052
C	2.742271	4.675547	-0.638198	C	-3.814345	3.746899	-0.078688
C	3.598669	5.761712	-0.550843	C	-3.762730	4.721094	0.919400
C	4.297903	5.985333	0.626469	C	-4.653481	5.781805	0.961179
C	4.137256	5.121398	1.699704	C	-5.635881	5.890357	-0.011963
C	3.270130	4.045753	1.585546	C	-5.719559	4.937897	-1.017167
F	2.097899	4.474294	-1.793264	C	-2.852245	2.624619	-0.119227
F	3.760207	6.584675	-1.585463	C	-3.358277	1.309558	0.028529
F	5.122161	7.023214	0.724736	N	-2.627584	0.178817	-0.077540
F	4.805179	5.337512	2.831419	C	-3.537174	-0.849914	0.121286
F	3.136462	3.232882	2.639959	C	-4.859912	-0.322615	0.388448
C	0.767181	-2.748906	0.333792	C	-4.753084	1.020861	0.327211
C	0.444220	-4.134527	0.431993	C	-3.237853	-2.198209	0.062456
C	-0.910617	-4.264734	0.310661	C	-1.938327	-2.769901	-0.165050
C	-1.465125	-2.965223	0.139647	N	-0.757422	-2.079941	-0.172697
N	-0.410889	-2.079068	0.166587	C	0.287586	-2.942042	-0.405639

C	-0.268958	-4.228896	-0.564862	C	-6.392933	-5.070666	0.518540
C	-1.641612	-4.120281	-0.411317	C	-6.400469	-4.200324	-0.561156
C	1.660695	-2.600138	-0.443521	C	-5.380396	-3.271534	-0.699939
C	2.209778	-1.299182	-0.341016	F	-3.388887	-4.029676	2.209326
C	3.706055	-1.103676	-0.217980	F	-5.414019	-2.461859	-1.761868
C	3.831189	0.424478	-0.167292	F	-7.381517	-4.267450	-1.459545
C	2.397792	0.887086	-0.287484	F	-7.367755	-5.961937	0.662271
N	1.504318	-0.169930	-0.329665	F	-5.362727	-5.837781	2.491187
C	4.456471	0.718098	1.202371	C	2.599503	-3.734184	-0.617875
N	4.085100	-0.448047	2.003281	C	2.762636	-4.717432	0.357774
C	4.275900	-1.599525	1.117597	C	3.642351	-5.776075	0.198433
C	4.868351	-0.449349	3.194187	C	4.384371	-5.878283	-0.969812
S	6.607366	0.123892	2.727598	C	4.243857	-4.921527	-1.964347
C	5.996940	0.815301	1.157714	C	3.355792	-3.874101	-1.780232
C	2.063209	2.211907	-0.357786	F	2.085791	-4.630435	1.507274
C	3.163442	3.210044	-0.400200	F	3.789389	-6.686456	1.158562
C	3.402291	4.080969	0.661511	F	5.231098	-6.888280	-1.133525
C	4.414612	5.026905	0.629866	F	4.951272	-5.022030	-3.087436
C	5.222158	5.124569	-0.494613	F	3.237131	-2.970803	-2.759662
C	5.012251	4.275864	-1.571065	C	0.738068	2.778484	-0.408154
C	3.987810	3.343233	-1.514909	C	0.415262	4.132716	-0.604488
F	2.653353	3.995825	1.766446	C	-0.962858	4.254046	-0.536591
F	4.622877	5.835050	1.667925	C	-1.499325	2.972277	-0.295210
F	6.197656	6.026174	-0.537712	N	-0.431923	2.099756	-0.234916
F	5.784846	4.370201	-2.651914	H	-0.522435	1.099314	-0.109864
F	3.810277	2.545333	-2.574100	H	-0.678511	-1.075808	-0.066317
F	-2.844689	4.641218	1.886668	H	1.129590	4.922058	-0.781225
F	-4.580836	6.689360	1.933883	H	-1.543716	5.156258	-0.654485
F	-6.496049	6.902951	0.020012	H	-5.533420	1.751366	0.487140
F	-6.658324	5.045899	-1.956257	H	-5.743084	-0.905270	0.607594
F	-4.916730	2.995930	-2.030621	H	-2.368842	-4.914700	-0.478553
C	-4.336253	-3.177700	0.219720	H	0.292591	-5.126002	-0.775623
C	-4.357768	-4.071482	1.290431	H	4.237102	-1.544083	-1.062698
C	-5.366068	-5.007653	1.449729	H	4.448662	0.822560	-0.974099

H	4.924725	-1.440282	3.644588	C	-2.943027	-3.671963	-0.405098
H	4.471441	0.262452	3.919174	C	-3.785382	-3.954040	-1.478620
H	6.403913	0.237510	0.322715	C	-4.727639	-4.970728	-1.430480
H	6.322065	1.851165	1.043437	C	-4.836465	-5.750525	-0.287649
H	4.050229	1.618001	1.675199	C	-4.008679	-5.503277	0.797779
H	3.755483	-2.470090	1.523598	C	-3.080726	-4.475756	0.725603
H	5.340178	-1.865655	1.007898	F	-3.706500	-3.226578	-2.596566

Transition State Chlor-SH_*cis* (kinetic studies)

C	-2.440390	-1.251487	-0.441812	F	-5.519645	-5.212277	-2.473990
C	-3.878412	-0.928536	-0.401628	F	-5.732028	-6.731285	-0.232793
C	-3.918283	0.463692	-0.466793	F	-4.117256	-6.245124	1.898848
C	-2.557681	0.911636	-0.496678	F	-2.317587	-4.247308	1.800497
C	-2.189455	2.271591	-0.544368	C	-3.288077	3.261254	-0.681079
C	-0.894764	2.785890	-0.453158	C	-4.008876	3.379677	-1.868475
C	-0.519426	4.164433	-0.494703	C	-5.047368	4.286816	-2.014946
C	0.834882	4.240042	-0.348980	C	-5.389044	5.113538	-0.954090
C	1.342607	2.913012	-0.221257	C	-4.693797	5.022606	0.242542
C	2.674256	2.532012	-0.073948	C	-3.661325	4.104409	0.362461
C	3.154072	1.205964	-0.032003	F	-3.706725	2.600817	-2.909722
C	4.546674	0.871349	0.162209	F	-5.713861	4.375882	-3.164949
C	4.619025	-0.480750	0.120064	F	-6.381486	5.988431	-1.083609
C	3.268625	-0.949409	-0.093205	F	-5.024412	5.810157	1.264988
C	2.930310	-2.312624	-0.190208	F	-3.019342	4.041864	1.536777
C	1.641990	-2.833317	-0.311265	C	3.665863	3.630601	0.039216
C	1.273721	-4.204576	-0.423074	C	4.615999	3.861439	-0.954073
C	-0.089591	-4.274590	-0.483401	C	5.554735	4.876950	-0.854054
C	-0.603921	-2.945983	-0.417988	C	5.554527	5.701445	0.261755
C	-1.953564	-2.566549	-0.441159	C	4.619641	5.502699	1.266918
N	-1.669698	-0.132679	-0.438337	C	3.694240	4.476904	1.146178
N	0.259883	2.068690	-0.288610	F	4.640032	3.092215	-2.045437
N	2.387743	0.089112	-0.172623	F	6.449170	5.072556	-1.821714
N	0.472808	-2.108816	-0.323404	F	6.447500	6.680500	0.366853
				F	4.621973	6.291227	2.340752
				F	2.813645	4.309753	2.136888
				C	4.039399	-3.299462	-0.153342

C	4.962576	-3.389130	-1.193231
C	6.013851	-4.292988	-1.169381
C	6.158401	-5.144934	-0.083838
C	5.254505	-5.084464	0.966850
C	4.214056	-4.168392	0.921708
F	4.849332	-2.587600	-2.255214
F	6.879363	-4.354297	-2.180128
F	7.160459	-6.017846	-0.050979
F	5.396080	-5.899211	2.011433
F	3.366771	-4.131217	1.954202
C	-4.370990	0.834793	2.156744
N	-5.028832	-0.328296	2.041893
C	-4.480999	-1.502718	1.628242
C	-2.947560	0.866990	2.531060
S	-2.702550	0.735798	4.363961
H	0.420221	-1.097365	-0.279415
H	0.318100	1.057060	-0.260658
H	-4.641294	-1.579486	-0.804594
H	-4.788016	1.079684	-0.636370
H	-1.208081	4.984857	-0.628416
H	1.441582	5.133023	-0.345518
H	5.355722	1.570382	0.320125
H	5.498486	-1.097844	0.238218
H	1.970945	-5.027890	-0.460246
H	-0.694255	-5.163706	-0.578940
H	-4.989748	1.702021	2.356680
H	-6.030388	-0.245221	1.916889
H	-5.177278	-2.329869	1.555504
H	-3.492202	-1.737332	2.003873
H	-2.350862	0.096524	2.040881
H	-2.506376	1.828552	2.270874
H	-3.219477	-0.499425	4.477992

Transition State Chlor-SH_ *trans* (kinetic studies)

C	2.483185	0.673792	-0.426925
C	3.804138	0.095330	-0.457233
C	3.625826	-1.282661	-0.341829
C	2.168287	-1.473376	-0.345972
C	1.559175	-2.736916	-0.346008
C	0.182503	-2.993900	-0.279613
C	-0.446300	-4.274783	-0.284101
C	-1.795347	-4.085963	-0.180439
C	-2.043204	-2.684894	-0.122161
C	-3.280306	-2.050946	-0.020008
C	-3.500195	-0.660578	0.017572
C	-4.816205	-0.067129	0.064431
C	-4.625791	1.274592	0.045788
C	-3.196647	1.476931	-0.013703
C	-2.599288	2.752521	-0.093080
C	-1.237659	3.011540	-0.222317
C	-0.608473	4.288106	-0.317061
C	0.735927	4.091281	-0.435783
C	0.985044	2.683922	-0.404742
C	2.233265	2.059906	-0.474340
N	1.511034	-0.284258	-0.314876
N	-0.816144	-2.064661	-0.185953
N	-2.524726	0.292334	-0.027047
N	-0.233472	2.072819	-0.281321
C	3.414846	2.956125	-0.535890
C	4.233539	3.024074	-1.661678
C	5.356703	3.836285	-1.710820
C	5.680985	4.625441	-0.616330
C	4.885749	4.588616	0.519862
C	3.773271	3.760993	0.544494
F	3.949631	2.283495	-2.736291
F	6.117721	3.875109	-2.803129

F	6.750482	5.413421	-0.656925	C	-5.024508	5.394733	1.148989
F	5.197446	5.339780	1.574412	C	-4.180417	4.295391	1.102592
F	3.037456	3.741395	1.664138	F	-3.069374	4.446999	-2.323972
C	2.443903	-3.928518	-0.397273	F	-4.696287	6.589289	-2.248498
C	3.177679	-4.249713	-1.537897	F	-6.001397	7.230923	0.046241
C	4.007635	-5.359470	-1.594562	F	-5.663187	5.712532	2.274075
C	4.114349	-6.192580	-0.489906	F	-4.033632	3.569931	2.214506
C	3.397357	-5.904988	0.662300	C	4.361743	0.615290	1.937074
C	2.577696	-4.787165	0.691908	N	3.692834	-0.502005	2.280596
F	3.098756	-3.471098	-2.620437	C	3.975313	-1.731774	1.787232
F	4.695073	-5.636306	-2.701200	C	5.814313	0.580521	1.674140
F	4.903962	-7.260799	-0.534308	S	6.754100	0.394983	3.271625
F	3.503564	-6.697863	1.727062	H	-0.381990	1.071470	-0.235831
F	1.908913	-4.533222	1.824801	H	-0.679215	-1.060742	-0.163228
C	-4.471222	-2.937505	0.033233	H	4.706367	0.601907	-0.761047
C	-4.883487	-3.672418	-1.075971	H	4.331152	-2.027193	-0.683365
C	-5.998339	-4.496644	-1.041135	H	0.075119	-5.216586	-0.360776
C	-6.736943	-4.597168	0.128789	H	-2.558892	-4.848276	-0.146058
C	-6.354464	-3.877386	1.251545	H	-5.756454	-0.599548	0.089227
C	-5.232831	-3.064136	1.192746	H	-5.380747	2.048012	0.051668
F	-4.197847	-3.594397	-2.219880	H	-1.128203	5.233878	-0.293751
F	-6.367158	-5.185279	-2.120285	H	1.498093	4.848285	-0.540278
F	-7.808530	-5.382334	0.174847	H	3.911698	1.537664	2.284481
F	-7.062086	-3.977122	2.375745	H	2.731959	-0.355374	2.569270
F	-4.890110	-2.387345	2.292054	H	3.300871	-2.519953	2.095596
C	-3.495186	3.936687	-0.056236	H	5.022531	-1.991965	1.700099
C	-3.693732	4.737189	-1.178952	H	6.098756	-0.245034	1.019817
C	-4.528386	5.844534	-1.156783	H	6.121160	1.514919	1.201699
C	-5.197271	6.172826	0.013289	H	7.977558	0.399119	2.71665

Table S2. Relative Gibbs free energy of formation for the three steps of the reaction mechanism of **Chlor-SH** and **Chlor-CSH**, from Pathway 1.

	Chlor-SH		Chlor-CSH	
	ΔG_f (kJ/mol)	Structure	ΔG_f (kJ/mol)	Structure

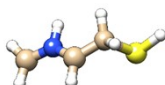
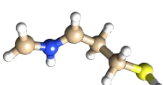
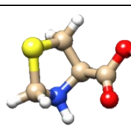
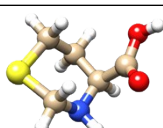
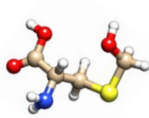
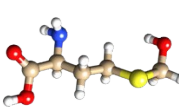
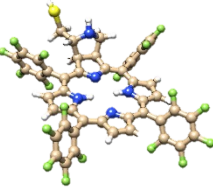
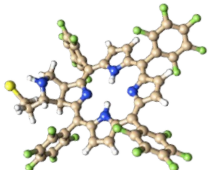
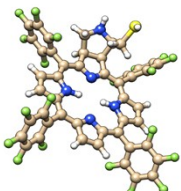
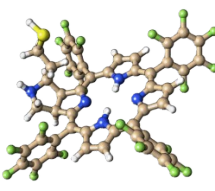
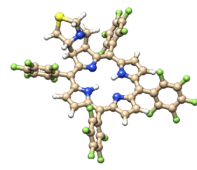
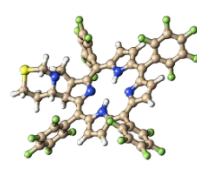
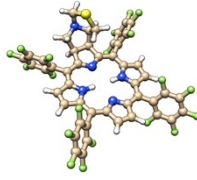
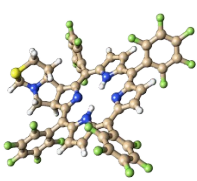
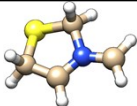
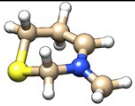
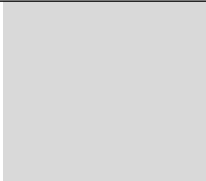
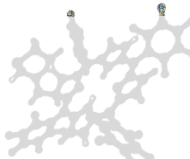
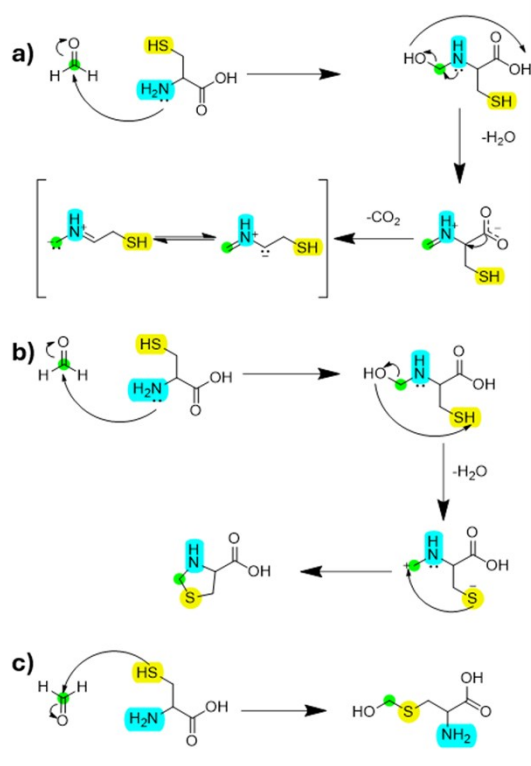
Aminoacid and paraformaldehyde condensation	azomethine ylide 1	7.2		13.6	
	thermodynamic product	-22.3		-28.4	
	cinetic product	18.6		9.9	
1,3-DC	<i>trans</i>	-136.7		-136.7	
	<i>cis</i>	-132.9		-136.8	
2 nd Ring Formation	<i>trans</i>	-51.9		-70.3	
	<i>cis</i>	-50.9		-63.0	

Table S3. Relative Gibbs free energy of formation for the two steps of the reaction mechanism of **Chlor-SH** and **Chlor-CSH**, from Pathway 2.

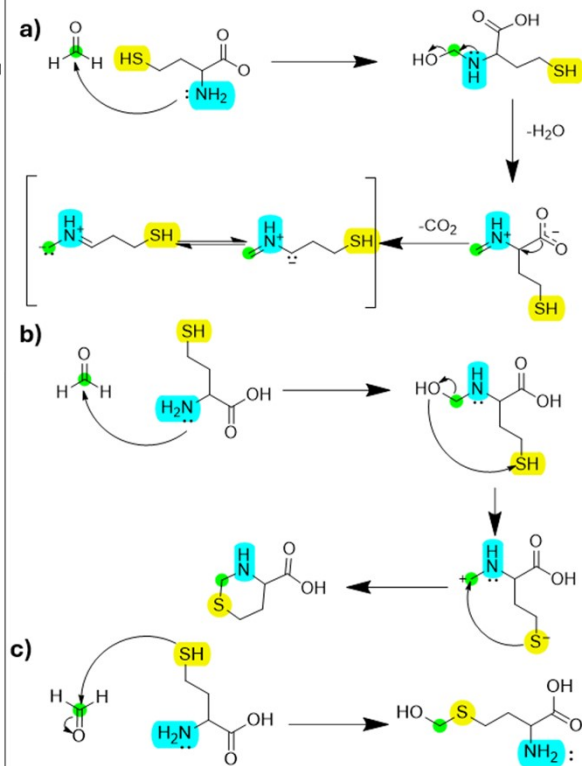
	Chlor-SH		Chlor-CSH	
	ΔG_f (kJ/mol)	Structure	ΔG_f (kJ/mol)	Structure

Azomethine ylide 2		4.8		104.2	
1,3-DC	<i>trans</i>	-163.9		-269.3	
	<i>cis</i>	-159.1		-262.0	

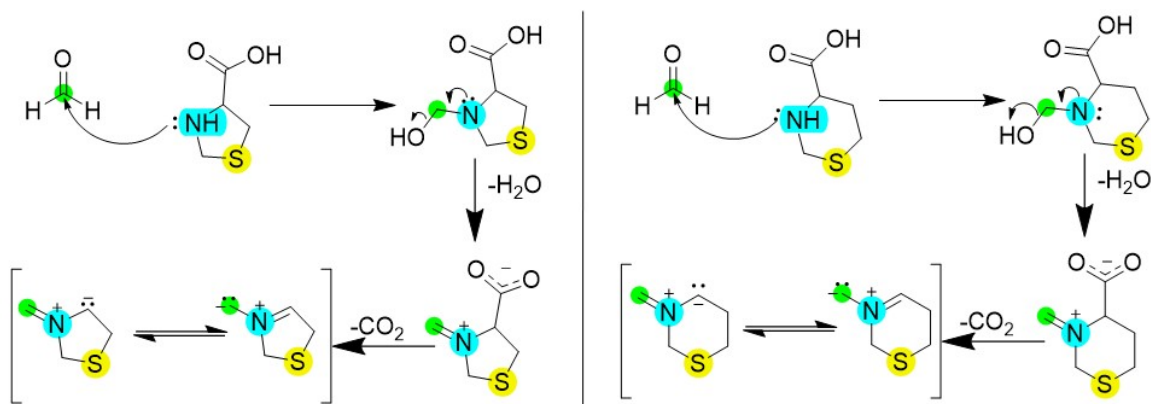
cysteine + paraformaldehyde



homocysteine + paraformaldehyde



Scheme S1. Three possible mechanisms and products for the reaction between cysteine (left) and homocysteine (right) with paraformaldehyde, leading to (a) the azomethine ylide 1, (b) the thermodynamic product and (c) the kinetic product.



Scheme S2. Proposed mechanism for the reaction between L-thiazolidine-4-carboxylic acid (left) or 1,3-thiazinane-4-carboxylic acid (right) with paraformaldehyde, giving rise to azomethine ylide 2.

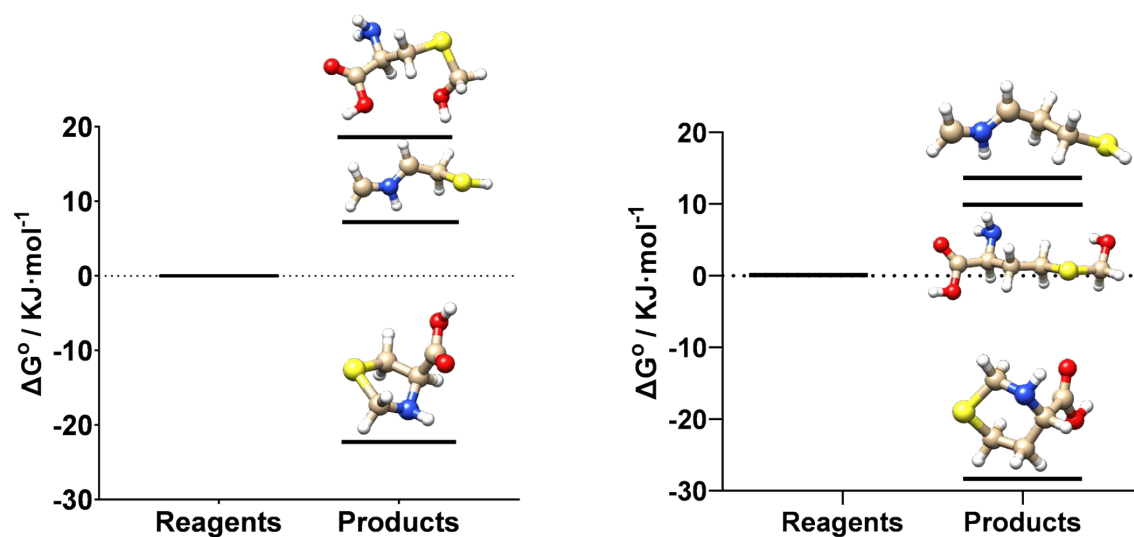


Figure S17. Relative Gibbs free energy variation for the reaction between cysteine (left) and homocysteine (right) and paraformaldehyde.

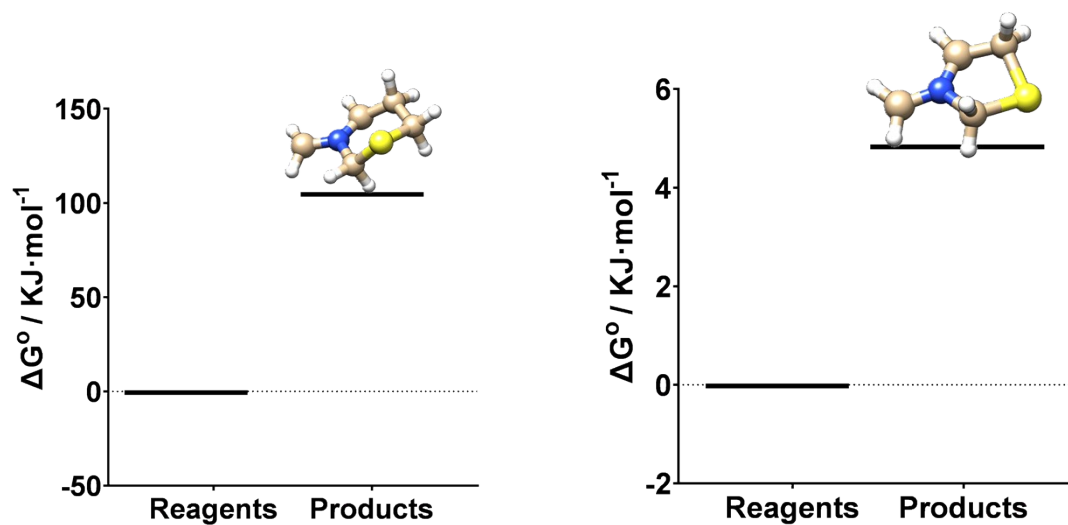


Figure S18. Relative Gibbs free energy variation for the reaction between the L-thiazolidine-4-carboxylic acid (left) or 1,3-thiazinane-4-carboxylic acid (right) and paraformaldehyde.

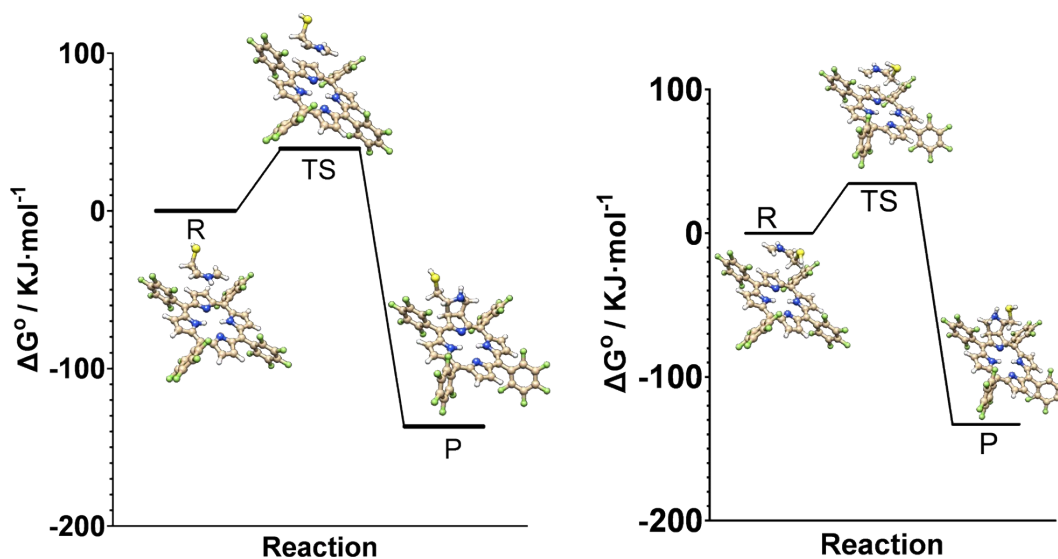


Figure S19. Relative Gibbs free energy variation during the 1,3-dipolar reaction for **Chlor-SH_{trans}** (left side) and **Chlor-SH_{cis}** (right side).

Table S4. Linear regression analysis of theoretical vs. experimental ^1H and ^{13}C NMR chemical shift values for **Chlor-SH**, **Chlor-CSH** and their isomers. The linear fitting is represented in Figures S20 and S21.

	Chlorin	Equation	R ²
^1H NMR	Chlor-SH _{trans}	$Y = 1.136x - 0.7388$	0.9946
	Chlor-SH _{cis}	$Y = 1.181x - 1.111$	0.9873
	Chlor-CSH _{trans}	$Y = 1.135x - 0.5489$	0.9921
	Chlor-CSH _{cis}	$Y = 1.178x - 0.9173$	0.9837
^{13}C NMR	Chlor-SH _{trans}	$Y = 0.9301x + 7.120$	0.9881
	Chlor-SH _{cis}	$Y = 0.9381x + 5.884$	0.9839
	Chlor-CSH _{trans}	$Y = 1.117x + 99.02$	0.9956
	Chlor-CSH _{cis}	$Y = 1.113x + 98.6$	0.9945

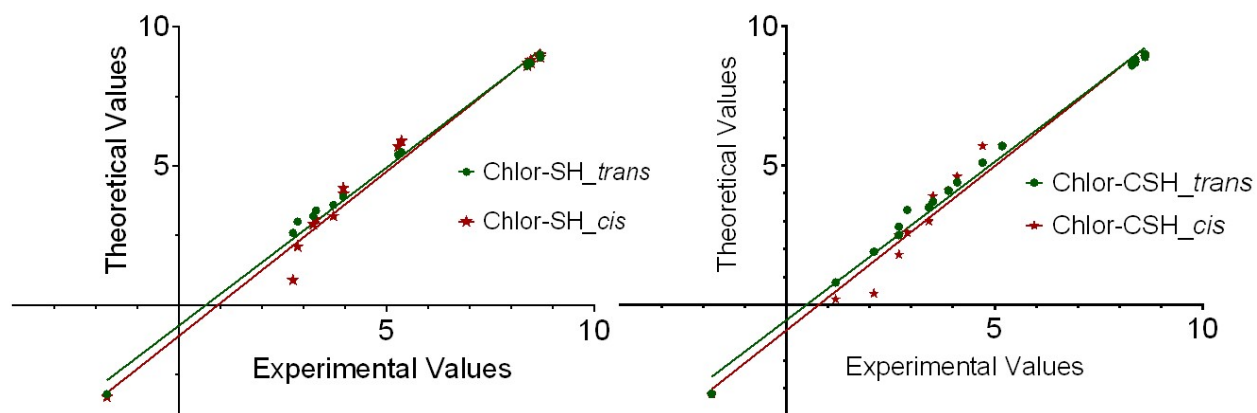


Figure S20. Correlation between experimental and theoretical ^1H NMR chemical shift values for **Chlor-SH_{trans}** and *cis* (left) and **Chlor-CSH_{trans}** and *cis* (right), in CDCl_3 .

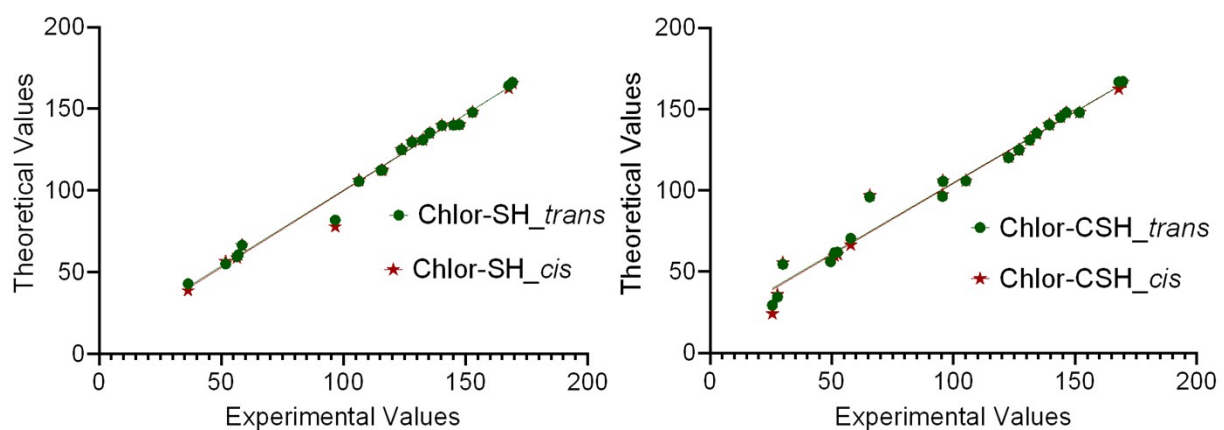


Figure S21. Correlation between experimental and theoretical ^{13}C NMR chemical shift values for **Chlor-SH_{trans}** and *cis* (left) and **Chlor-CSH_{trans}** and *cis* (right), in CDCl_3 .

Synthesis Optimization

Table S5. Summary of studies performed to optimize the reaction conditions

Entry	Compound	Amino acid	Molar ratio amino acid/ paraformaldehyde	Solvent	Heating Method	Temperature (°C)	Time (h)	Yield (%)	Recovered (%)
1	Chlor_SH_trans	Cysteine	5:5	Chlorobenzene	Oil-bath	120	8	7	82
2					MW	135	2	6	81
3		L-thiazolidine-4-carboxylic acid	2:5	Toluene	Oil-bath	80	10	6	70
4			5:5	Chlorobenzene	MW	135	2	9	73
5	Chlor_CSH_trans	Homocysteine	5:5	Toluene	Oil-bath	80	8	10	81
6			5:5	Chlorobenzene	Oil-bath	120	8	22	62
7					MW	135	2	21	62
8			10:10	Chlorobenzene	MW	135	2	8	62
9			10:5	Chlorobenzene	MW	135	2	4	81

UV-Vis and fluorescence spectroscopies

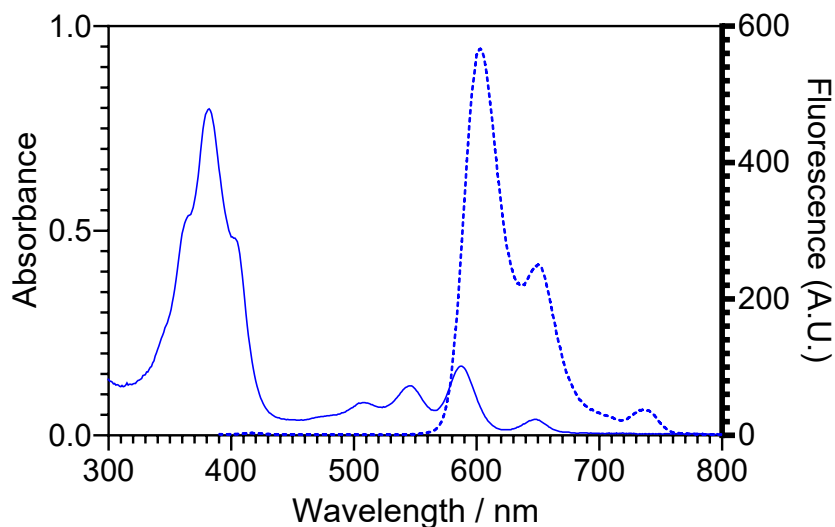


Figure S22. Absorption (full line) and emission (dashed line) spectra of the bisadduct formed during the reaction of **TPFPP** and azomethine ylide generated from paraformaldehyde and homocysteine ($\lambda_{\text{exc}}=370$ nm; slit width=10 nm) in methanol.

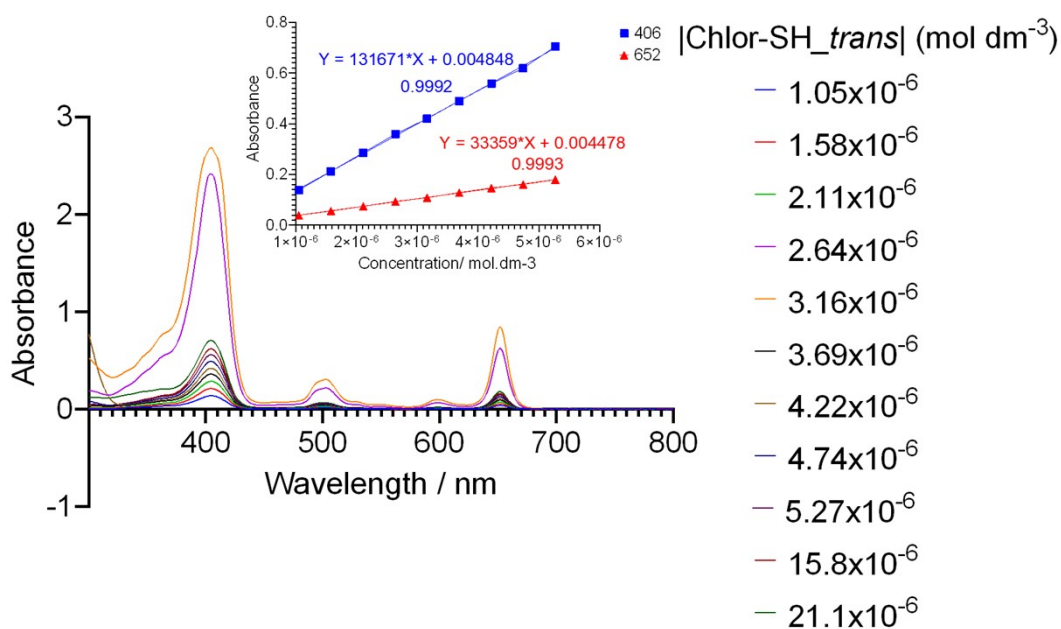


Figure S23. UV-Vis spectra of different concentrations of **Chlor-SH_{trans}** in DMF. The inset shows the absorbance as a function of concentration at 405 and 652 nm, with the corresponding linear regressions (solid lines).

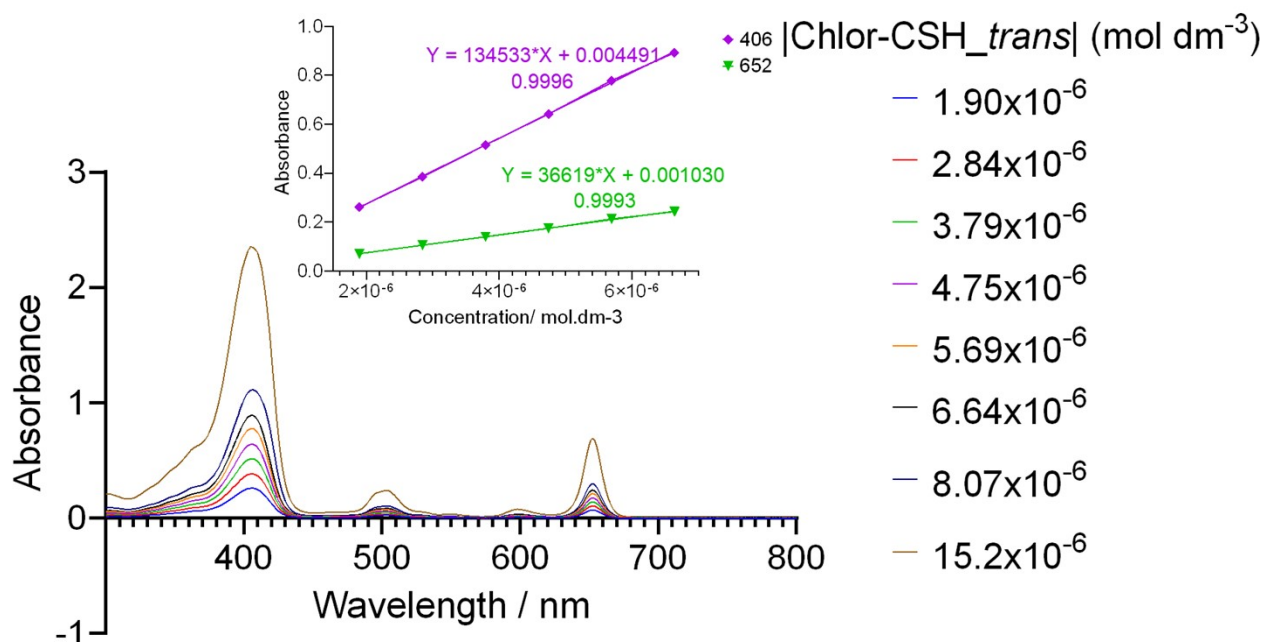


Figure S24. UV-Vis spectra of different concentrations of **Chlor-CSH_{trans}** in DMF. The inset shows the absorbance as a function of concentration at 405 and 652 nm, with the corresponding linear regressions (solid lines).

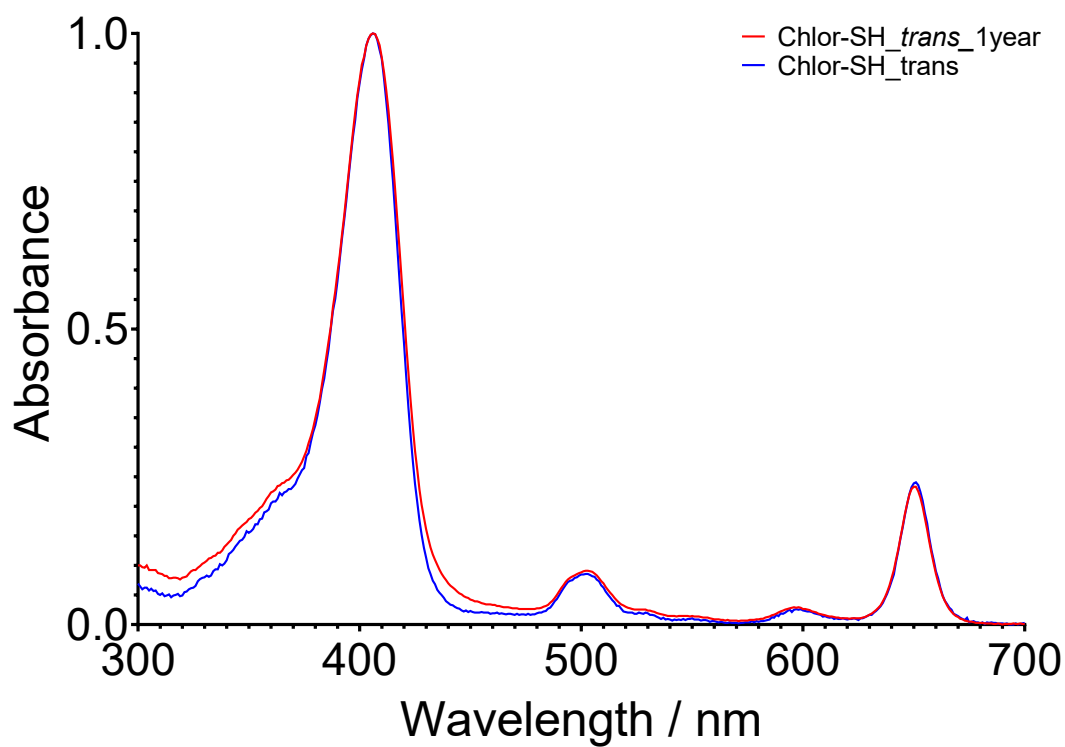


Figure S25. UV-Vis spectra of **Chlor-SH_{trans}** one year apart in DMF.

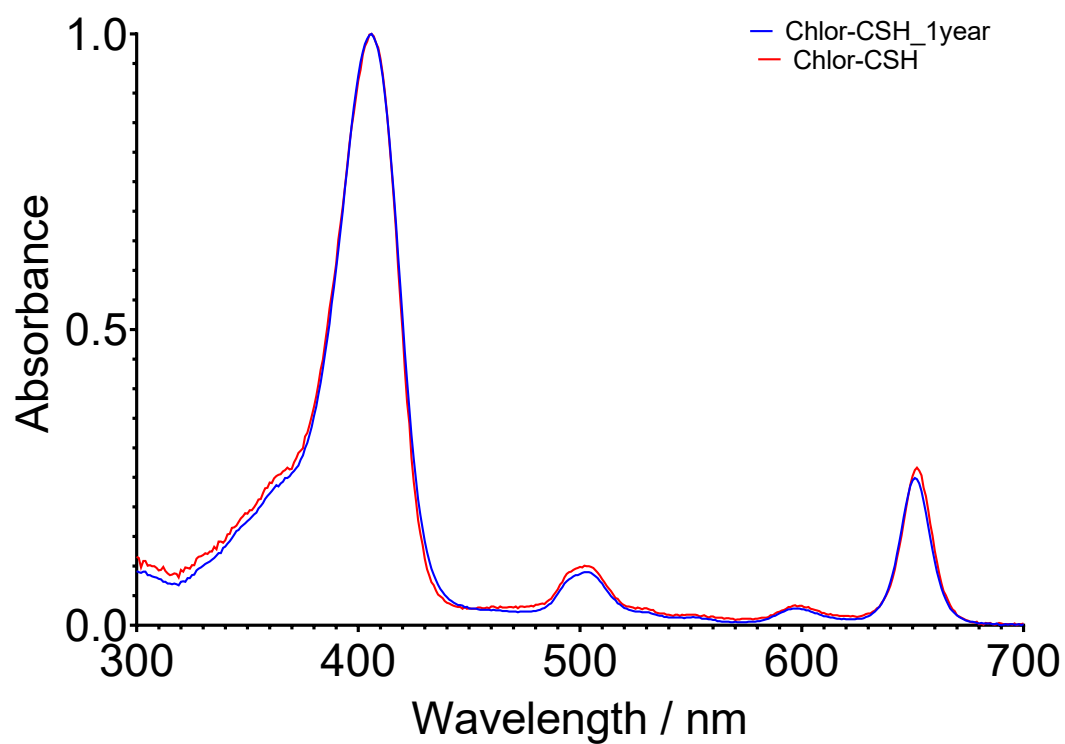


Figure S26. UV-Vis spectra of **Chlor-CSH_{trans}** one year apart in DMF.

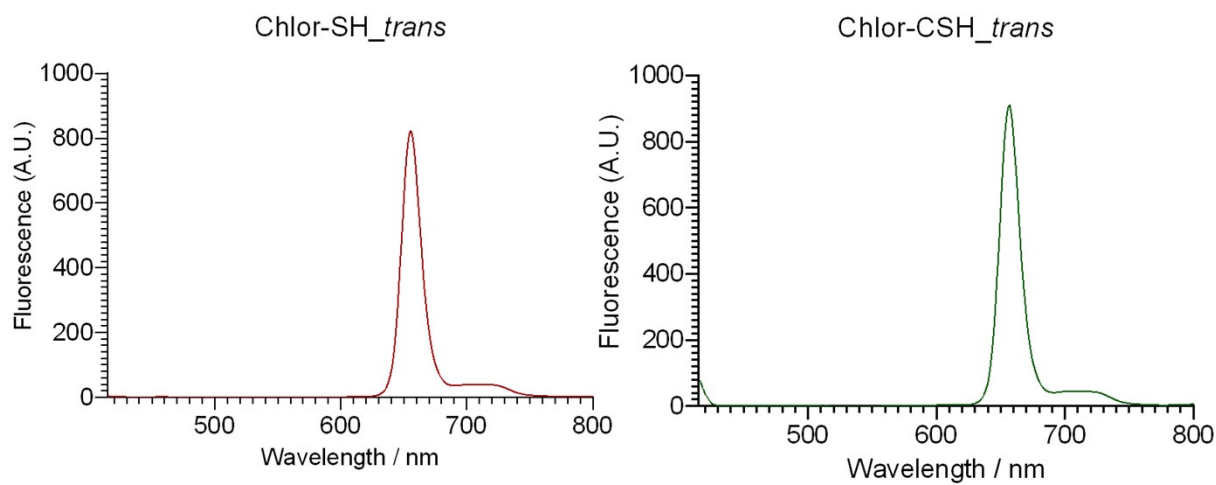


Figure S27. Fluorescence spectra of **Chlor-SH_{trans}** ($\lambda_{\text{exc}} = 405\text{nm}$; slit width = 10 nm) and **Chlor-CSH_{trans}** ($\lambda_{\text{exc}} = 406\text{ nm}$; slit width = 10 nm) in DMF at 25 °C.

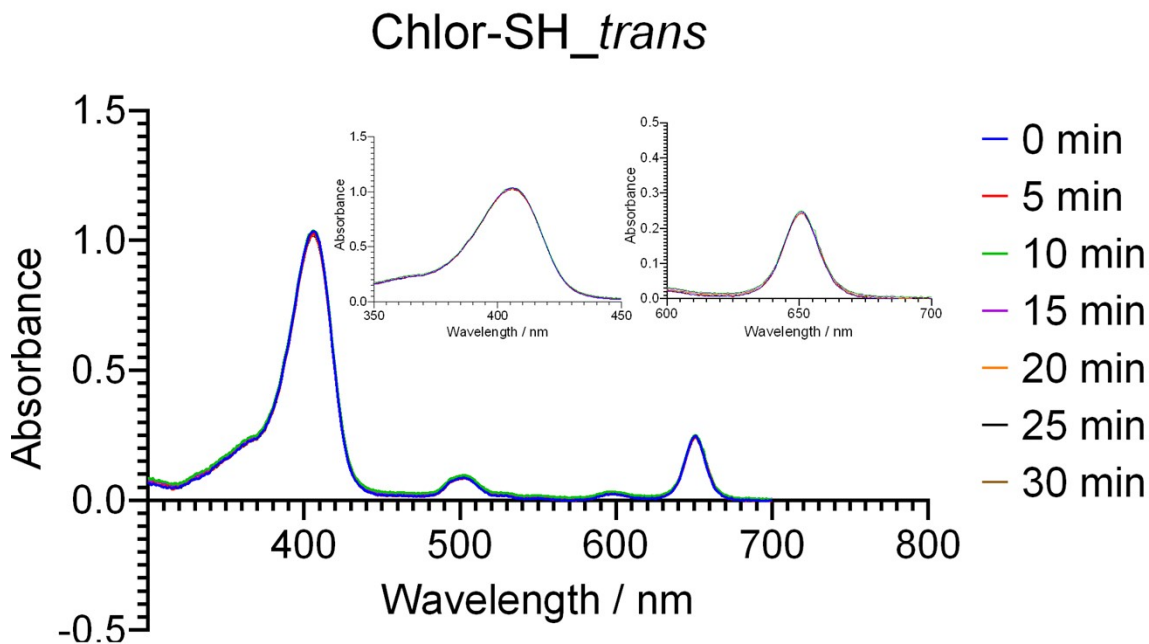


Figure S28. UV-Vis spectra of **Chlor-SH_{trans}** in DMF after 5 min cycles of irradiation under an irradiance of 40 mW/cm².

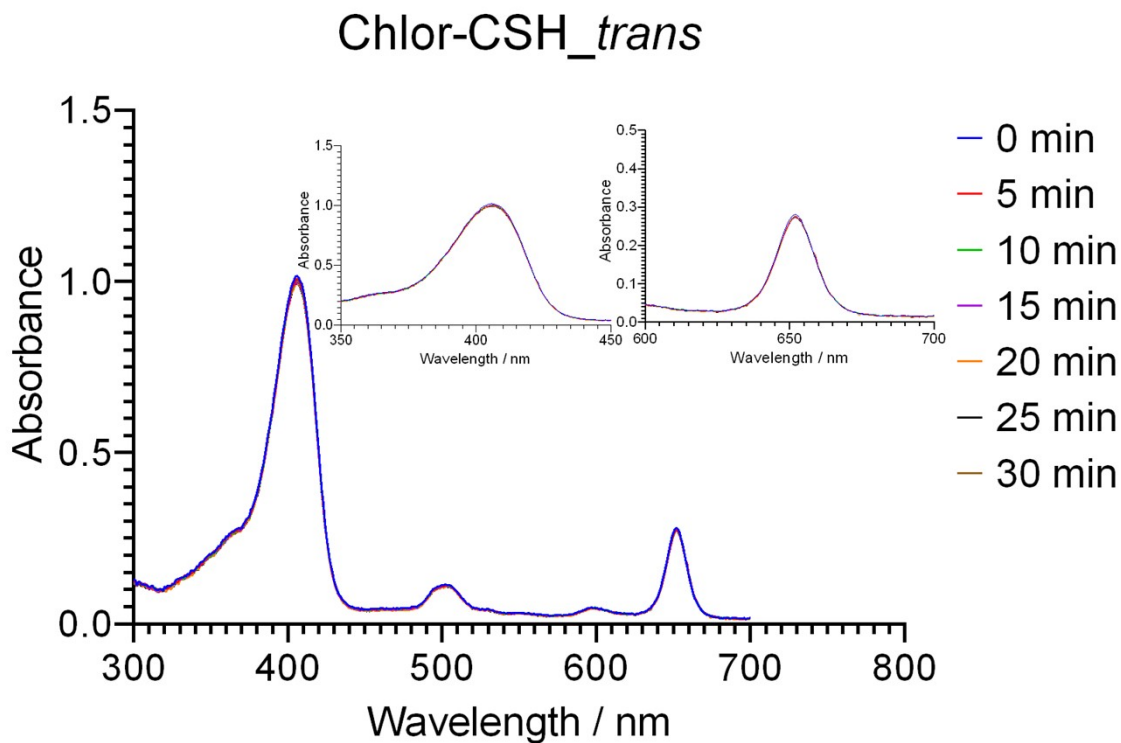


Figure S29. UV-Vis spectra of **Chlor-CSH_{trans}** in DMF after 5 min cycles of irradiation under an irradiance of 40 mW/cm².

References

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